



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:14 pm BST

PDB ID : 1HBS
Title : REFINED CRYSTAL STRUCTURE OF DEOXYHEMOGLOBIN S. I. RE-
STRAINED LEAST-SQUARES REFINEMENT AT 3.0-ANGSTROMS RES-
OLUTION
Authors : Padlan, E.A.; Love, W.E.
Deposited on : 1982-06-02
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

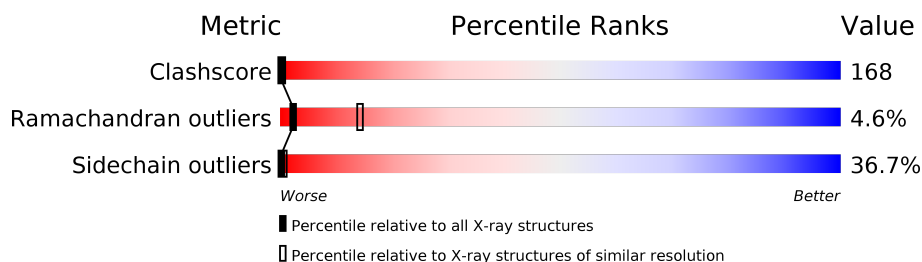
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

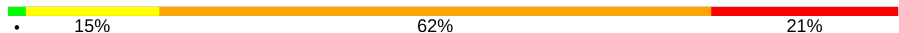







Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	141	
1	C	141	
1	E	141	
1	G	141	
2	B	146	
2	D	146	
2	F	146	
2	H	146	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEM	A	142	-	-	X	-
3	HEM	D	147	-	-	X	-
3	HEM	E	142	-	-	X	-
3	HEM	G	142	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9104 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 HEMOGLOBIN S (DEOXY) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	E	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	G	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called HEMOGLOBIN S (DEOXY) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	D	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	F	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			
2	H	146	Total	C	N	O	S	0	0	0
			1121	724	195	199	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	VAL	GLU	CONFLICT	UNP P68871
D	6	VAL	GLU	CONFLICT	UNP P68871
F	6	VAL	GLU	CONFLICT	UNP P68871
H	6	VAL	GLU	CONFLICT	UNP P68871

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



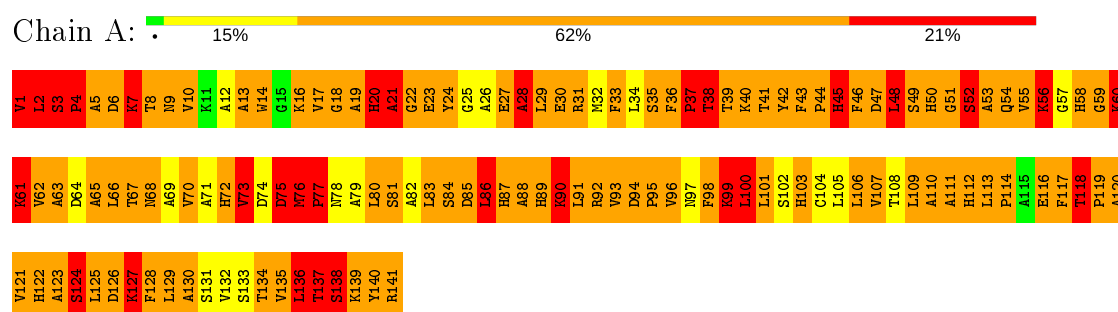
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

3 Residue-property plots

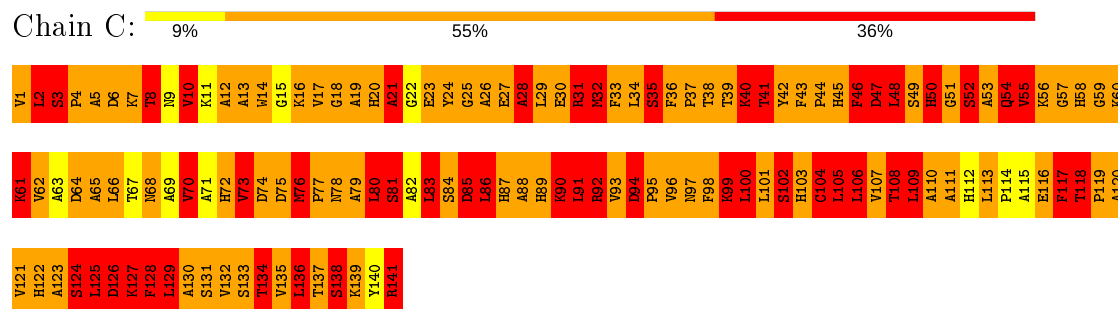
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

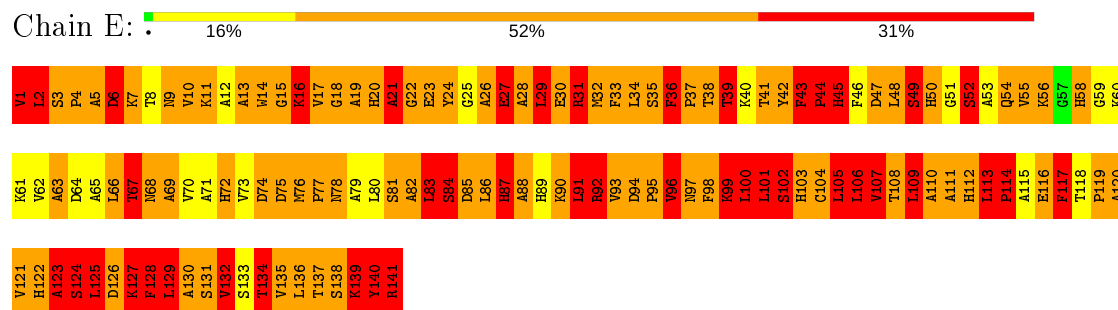
• Molecule 1: HEMOGLOBIN S (DEOXY) (ALPHA CHAIN)



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Chain G:



V121	V61	R61	V1
H122	V62	V62	S2
A123	A63	A63	S3
S124	D64	D64	P4
L125	A65	A65	A5
D126	L66	L66	D6
R127	T67	T67	R7
F128	M68	M68	T8
L129	A69	A69	N9
A130	V70	V70	N9
S131	A71	A71	K11
V132	H72	H72	A12
S133	V73	V73	A13
T134	D74	D74	M14
V135	D75	D75	G15
L136	M76	M76	K16
T137	P77	P77	V17
K138	M78	M78	G18
R139	A79	A79	H19
V140	L80	L80	H20
R141	S81	S81	A21
	A82	A82	G22
	L83	L83	E23
	S84	S84	Y24
	D85	D85	G25
	L86	L86	A26
	H87	H87	E27
	A88	A88	A28
	H89	H89	L29
	K90	K90	E30
	L91	L91	R31
	R92	R92	M32
	V93	V93	F33
	D94	D94	L34
	P95	P95	S35
	V96	V96	F36
	N97	N97	P37
	F98	F98	T38
	K99	K99	T39
	L100	L100	K40
	L101	L101	T41
	S102	S102	Y42
	H103	H103	F43
	C104	C104	P44
	L105	L105	H45
	L106	L106	F46
	V107	V107	D47
	T108	T108	L48
	L109	L109	S49
	A110	A110	H50
	A111	A111	G51
	H112	H112	S52
	L113	L113	A53
	P114	P114	Q54
	A115	A115	V55
	E116	E116	K56
	F117	F117	G57
	T118	T118	H58
	P119	P119	G59
	A120	A120	F60

- Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain B:



E121	F122	G123	H124	I125	J126	K127	L128	M129	N130	O131	P132	Q133	R134	S135	T136	U137	V138	W139	X140	Y141	Z142	A143	B144	C145	D146	E147	F148	G149	H150	I151	J152	K153	L154	M155	N156	O157	P158	Q159	R160	S161	T162	U163	V164	W165	X166	Y167	Z168	A169	B170	C171	D172	E173	F174	G175	H176	I177	J178	K179	L180	M181	N182	O183	P184	Q185	R186	S187	T188	U189	V190	W191	X192	Y193	Z194	A195	B196	C197	D198	E199	F200	G201	H202	I203	J204	K205	L206	M207	N208	O209	P210	Q211	R212	S213	T214	U215	V216	W217	X218	Y219	Z220	A221	B222	C223	D224	E225	F226	G227	H228	I229	J230	K231	L232	M233	N234	O235	P236	Q237	R238	S239	T240	U241	V242	W243	X244	Y245	Z246	A247	B248	C249	D250	E251	F252	G253	H254	I255	J256	K257	L258	M259	N260	O261	P262	Q263	R264	S265	T266	U267	V268	W269	X270	Y271	Z272	A273	B274	C275	D276	E277	F278	G279	H280	I281	J282	K283	L284	M285	N286	O287	P288	Q289	R290	S291	T292	U293	V294	W295	X296	Y297	Z298	A299	B300	C301	D302	E303	F304	G305	H306	I307	J308	K309	L310	M311	N312	O313	P314	Q315	R316	S317	T318	U319	V320	W321	X322	Y323	Z324	A325	B326	C327	D328	E329	F330	G331	H332	I333	J334	K335	L336	M337	N338	O339	P340	Q341	R342	S343	T344	U345	V346	W347	X348	Y349	Z350	A351	B352	C353	D354	E355	F356	G357	H358	I359	J360	K361	L362	M363	N364	O365	P366	Q367	R368	S369	T370	U371	V372	W373	X374	Y375	Z376	A377	B378	C379	D380	E381	F382	G383	H384	I385	J386	K387	L388	M389	N390	O391	P392	Q393	R394	S395	T396	U397	V398	W399	X400	Y401	Z402	A403	B404	C405	D406	E407	F408	G409	H410	I411	J412	K413	L414	M415	N416	O417	P418	Q419	R420	S421	T422	U423	V424	W425	X426	Y427	Z428	A429	B430	C431	D432	E433	F434	G435	H436	I437	J438	K439	L440	M441	N442	O443	P444	Q445	R446	S447	T448	U449	V450	W451	X452	Y453	Z454	A455	B456	C457	D458	E459	F460	G461	H462	I463	J464	K465	L466	M467	N468	O469	P470	Q471	R472	S473	T474	U475	V476	W477	X478	Y479	Z480	A481	B482	C483	D484	E485	F486	G487	H488	I489	J490	K491	L492	M493	N494	O495	P496	Q497	R498	S499	T500	U501	V502	W503	X504	Y505	Z506	A507	B508	C509	D510	E511	F512	G513	H514	I515	J516	K517	L518	M519	N520	O521	P522	Q523	R524	S525	T526	U527	V528	W529	X530	Y531	Z532	A533	B534	C535	D536	E537	F538	G539	H540	I541	J542	K543	L544	M545	N546	O547	P548	Q549	R550	S551	T552	U553	V554	W555	X556	Y557	Z558	A559	B560	C561	D562	E563	F564	G565	H566	I567	J568	K569	L570	M571	N572	O573	P574	Q575	R576	S577	T578	U579	V580	W581	X582	Y583	Z584	A585	B586	C587	D588	E589	F590	G591	H592	I593	J594	K595	L596	M597	N598	O599	P600	Q601	R602	S603	T604	U605	V606	W607	X608	Y609	Z610	A611	B612	C613	D614	E615	F616	G617	H618	I619	J620	K621	L622	M623	N624	O625	P626	Q627	R628	S629	T630	U631	V632	W633	X634	Y635	Z636	A637	B638	C639	D640	E641	F642	G643	H644	I645	J646	K647	L648	M649	N650	O651	P652	Q653	R654	S655	T656	U657	V658	W659	X660	Y661	Z662	A663	B664	C665	D666	E667	F668	G669	H670	I671	J672	K673	L674	M675	N676	O677	P678	Q679	R680	S681	T682	U683	V684	W685	X686	Y687	Z688	A689	B690	C691	D692	E693	F694	G695	H696	I697	J698	K699	L700	M701	N702	O703	P704	Q705	R706	S707	T708	U709	V710	W711	X712	Y713	Z714	A715	B716	C717	D718	E719	F720	G721	H722	I723	J724	K725	L726	M727	N728	O729	P730	Q731	R732	S733	T734	U735	V736	W737	X738	Y739	Z740	A741	B742	C743	D744	E745	F746	G747	H748	I749	J750	K751	L752	M753	N754	O755	P756	Q757	R758	S759	T760	U761	V762	W763	X764	Y765	Z766	A767	B768	C769	D770	E771	F772	G773	H774	I775	J776	K777	L778	M779	N780	O781	P782	Q783	R784	S785	T786	U787	V788	W789	X790	Y791	Z792	A793	B794	C795	D796	E797	F798	G799	H800	I801	J802	K803	L804	M805	N806	O807	P808	Q809	R810	S811	T812	U813	V814	W815	X816	Y817	Z818	A819	B820	C821	D822	E823	F824	G825	H826	I827	J828	K829	L830	M831	N832	O833	P834	Q835	R836	S837	T838	U839	V840	W841	X842	Y843	Z844	A845	B846	C847	D848	E849	F850	G851	H852	I853	J854	K855	L856	M857	N858	O859	P860	Q861	R862	S863	T864	U865	V866	W867	X868	Y869	Z870	A871	B872	C873	D874	E875	F876	G877	H878	I879	J880	K881	L882	M883	N884	O885	P886	Q887	R888	S889	T890	U891	V892	W893	X894	Y895	Z896	A897	B898	C899	D900	E901	F902	G903	H904	I905	J906	K907	L908	M909	N910	O911	P912	Q913	R914	S915	T916	U917	V918	W919	X920	Y921	Z922	A923	B924	C925	D926	E927	F928	G929	H930	I931	J932	K933	L934	M935	N936	O937	P938	Q939	R940	S941	T942	U943	V944	W945	X946	Y947	Z948	A949	B950	C951	D952	E953	F954	G955	H956	I957	J958	K959	L960	M961	N962	O963	P964	Q965	R966	S967	T968	U969	V970	W971	X972	Y973	Z974	A975	B976	C977	D978	E979	F980	G981	H982	I983	J984	K985	L986	M987	N988	O989	P990	Q991	R992	S993	T994	U995	V996	W997	X998	Y999	Z1000
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- Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain D:



E121	K61	V1
F122	A62	H2
T123	H63	L3
P124	G64	T4
P125	K65	P5
V126	A66	V6
Q127	V67	E7
A128	L68	K8
A129	G69	S9
Y130	A70	A10
Q131	F71	V11
K132	S72	T12
V133	D73	A13
V134	G74	L14
A135	L75	A15
G136	A76	G16
V137	H77	K17
A138	L78	V18
M139	D79	M19
A140	N80	V20
L141	L81	D21
A142	K82	E22
H143	G83	V23
K144	T84	G24
Y145	F85	G25
H146	A86	E26
	T87	A27
	L88	L28
	S89	G29
	E90	K30
	L91	L31
	H92	L32
	G93	V33
	D94	V34
	K95	V35
	L96	F36
	H97	K37
	V98	T38
	D99	Q39
	P100	E40
	E101	F41
	M102	F42
	F103	E43
	R104	S44
	L105	F45
	L106	G46
	G107	D47
	M108	L48
	Y109	S49
	L110	T50
	V111	P51
	C112	D52
	V113	A53
	L114	F54
	A115	M55
	H116	G56
	H117	M57
	F118	P58
	G119	K59
		T60

- Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain F:



E121	K61	V1
F122	A62	H2
T123	H63	L3
P124	G64	T4
P125	K65	P5
V126	A66	V6
Q127	V67	E7
A128	L68	K8
A129	G69	S9
Y130	A70	A10
Q131	F71	V11
K132	S72	T12
V133	D73	A13
V134	G74	L14
A135	L75	H15
G136	A76	G16
V137	H77	K17
A138	L78	V18
N139	D79	N19
A140	N80	V20
L141	K81	D21
A142	K82	E22
H143	G83	V23
K144	T84	G24
Y145	F85	G25
H146	A86	E26
	T87	A27
	L88	L28
	S89	G29
	E90	R30
	L91	L31
	H92	L32
	G93	V33
	D94	V34
	K95	V35
	L96	P36
	H97	T37
	V98	T38
	D99	Q39
	P100	R40
	E101	F41
	N102	F42
	F103	E43
	R104	S44
	L105	F45
	L106	G46
	G107	D47
	N108	L48
	V109	S49
	L110	T50
	V111	P51
	G112	D52
	V113	A53
	L114	V54
	A115	M55
	H116	G56
	H117	N57
	F118	P58
	G119	K59
	L120	T60

- Molecule 2: HEMOGLOBIN S (DEOXY) (BETA CHAIN)

Chain H:



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E121	F122	K61	V1
	T123	A62	H2
	P124	H63	L3
	P125	G64	T4
	V126	K65	P5
	Q127	K66	V6
	A128	V67	E7
	A129	L68	K8
	Q131	G69	S9
	K132	A70	A10
V133	F71	V11	
V134	S72	T12	
A135	D73	A13	
G136	G74	L14	
V137	L75	V15	
G138	A76	G16	
A138	H77	K17	
H139	L78	V18	
A140	D79	M19	
L141	M80	V20	
A142	L81	D21	
H143	K82	E22	
K144	G83	V23	
V145	T84	G24	
H146	F85	G25	
	A86	E26	
	T87	A27	
	L88	L28	
	S89	G29	
	E90	R30	
	L91	L31	
	H92	L32	
	C93	V33	
	D94	V34	
	K95	Y35	
	L96	P36	
	H97	W37	
	V98	T38	
	D99	Q39	
	P100	R40	
	E101	F41	
	M102	F42	
	F103	E43	
	R104	S44	
	L105	F45	
	L106	G46	
	G107	D47	
	M108	L48	
	V109	S49	
	L110	T50	
	V111	P51	
	G112	D52	
	V113	A53	
	L114	V54	
	A115	M55	
	H116	G56	
	H117	M57	
	F118	P58	
	G119	K59	
	V120	V60	

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	63.33Å 185.66Å 52.97Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9104	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: HEM

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	4.15	213/1097 (19.4%)	5.92	486/1491 (32.6%)
1	C	4.30	232/1097 (21.1%)	6.41	521/1491 (34.9%)
1	E	3.93	195/1097 (17.8%)	7.24	524/1491 (35.1%)
1	G	4.08	213/1097 (19.4%)	6.34	533/1491 (35.7%)
2	B	4.12	214/1151 (18.6%)	6.08	512/1564 (32.7%)
2	D	4.35	252/1151 (21.9%)	5.80	499/1564 (31.9%)
2	F	4.23	224/1151 (19.5%)	6.33	516/1564 (33.0%)
2	H	3.98	200/1151 (17.4%)	6.16	548/1564 (35.0%)
All	All	4.14	1743/8992 (19.4%)	6.29	4139/12220 (33.9%)

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	1	0
1	C	0	1
2	F	0	2
All	All	1	3

All (1743) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CD-OE2	32.40	1.61	1.25
2	D	26	GLU	CD-OE2	25.33	1.53	1.25
2	B	38	THR	C-O	21.93	1.65	1.23
2	D	90	GLU	CD-OE2	21.93	1.49	1.25
2	D	26	GLU	CD-OE1	-21.33	1.02	1.25
1	G	81	SER	CB-OG	19.33	1.67	1.42
1	E	35	SER	CB-OG	18.77	1.66	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	SER	CB-OG	18.57	1.66	1.42
2	B	101	GLU	CD-OE2	18.18	1.45	1.25
1	E	42	TYR	CE1-CZ	17.94	1.61	1.38
2	D	43	GLU	C-O	17.68	1.56	1.23
2	F	83	GLY	C-O	17.58	1.51	1.23
2	B	41	PHE	C-O	17.58	1.56	1.23
1	E	132	VAL	C-O	17.01	1.55	1.23
2	D	121	GLU	CD-OE2	16.83	1.44	1.25
1	C	15	GLY	C-O	16.67	1.50	1.23
2	F	23	VAL	C-O	16.65	1.54	1.23
1	C	76	MET	C-O	16.42	1.54	1.23
2	D	124	PRO	N-CD	-16.39	1.25	1.47
2	D	49	SER	CA-CB	16.11	1.77	1.52
1	C	23	GLU	CD-OE2	16.09	1.43	1.25
1	G	51	GLY	N-CA	-16.06	1.22	1.46
2	F	90	GLU	CG-CD	15.99	1.75	1.51
1	A	27	GLU	CD-OE2	15.95	1.43	1.25
2	B	129	ALA	C-O	15.88	1.53	1.23
1	G	84	SER	CB-OG	15.86	1.62	1.42
1	G	56	LYS	C-O	15.77	1.53	1.23
2	H	26	GLU	CD-OE2	15.65	1.42	1.25
2	H	30	ARG	CD-NE	15.63	1.73	1.46
2	H	130	TYR	CE2-CZ	15.56	1.58	1.38
1	C	124	SER	CB-OG	15.54	1.62	1.42
1	A	27	GLU	C-O	15.52	1.52	1.23
1	C	141	ARG	CD-NE	15.45	1.72	1.46
2	D	14	LEU	C-O	15.30	1.52	1.23
2	B	35	TYR	CE2-CZ	15.30	1.58	1.38
2	F	37	TRP	NE1-CE2	15.12	1.57	1.37
1	C	39	THR	CB-OG1	14.99	1.73	1.43
1	C	90	LYS	C-O	14.92	1.51	1.23
1	C	95	PRO	N-CA	-14.67	1.22	1.47
2	B	43	GLU	CD-OE1	14.62	1.41	1.25
2	D	118	PHE	C-O	14.59	1.51	1.23
2	D	101	GLU	CG-CD	14.54	1.73	1.51
2	F	15	TRP	CZ3-CH2	14.36	1.63	1.40
1	A	70	VAL	C-O	14.24	1.50	1.23
1	A	35	SER	C-O	14.18	1.50	1.23
1	G	23	GLU	CD-OE1	14.12	1.41	1.25
2	F	64	GLY	N-CA	13.96	1.67	1.46
1	C	37	PRO	C-O	13.93	1.51	1.23
2	F	134	VAL	C-O	13.83	1.49	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	130	TYR	CG-CD1	13.83	1.57	1.39
1	A	78	ASN	C-O	13.78	1.49	1.23
2	H	88	LEU	C-O	13.72	1.49	1.23
2	D	145	TYR	CE2-CZ	13.71	1.56	1.38
2	H	22	GLU	CB-CG	13.67	1.78	1.52
2	H	36	PRO	C-O	13.67	1.50	1.23
1	C	77	PRO	C-O	13.47	1.50	1.23
2	F	9	SER	CA-CB	13.47	1.73	1.52
2	B	26	GLU	CD-OE1	-13.41	1.10	1.25
2	D	130	TYR	CG-CD1	13.39	1.56	1.39
2	F	7	GLU	CD-OE1	-13.28	1.11	1.25
1	G	67	THR	N-CA	13.27	1.72	1.46
1	C	132	VAL	CB-CG1	13.26	1.80	1.52
2	H	83	GLY	N-CA	13.23	1.65	1.46
2	B	93	CYS	C-O	13.16	1.48	1.23
2	D	127	GLN	C-O	13.13	1.48	1.23
2	H	99	ASP	N-CA	13.10	1.72	1.46
1	G	19	ALA	C-O	13.09	1.48	1.23
1	E	15	GLY	N-CA	12.96	1.65	1.46
1	E	42	TYR	CG-CD1	12.94	1.55	1.39
2	H	5	PRO	N-CD	12.90	1.66	1.47
1	E	24	TYR	C-N	12.84	1.56	1.33
2	F	34	VAL	C-O	12.84	1.47	1.23
2	B	12	THR	CB-OG1	12.75	1.68	1.43
1	G	59	GLY	N-CA	-12.72	1.26	1.46
2	F	37	TRP	CZ2-CH2	12.71	1.61	1.37
1	E	31	ARG	NE-CZ	-12.66	1.16	1.33
1	E	23	GLU	CD-OE2	-12.65	1.11	1.25
1	C	102	SER	CB-OG	-12.64	1.25	1.42
1	C	81	SER	CA-CB	12.62	1.71	1.52
1	E	117	PHE	CE1-CZ	12.60	1.61	1.37
1	C	13	ALA	C-O	12.57	1.47	1.23
2	D	100	PRO	C-O	12.46	1.48	1.23
2	B	37	TRP	NE1-CE2	12.43	1.53	1.37
2	B	37	TRP	CD1-NE1	-12.41	1.16	1.38
1	C	75	ASP	CG-OD1	12.38	1.53	1.25
2	F	40	ARG	CD-NE	12.37	1.67	1.46
2	B	95	LYS	CE-NZ	12.36	1.79	1.49
2	H	15	TRP	CZ3-CH2	-12.36	1.20	1.40
1	A	24	TYR	CG-CD1	-12.34	1.23	1.39
2	H	7	GLU	C-O	12.31	1.46	1.23
1	E	141	ARG	CZ-NH2	-12.28	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	82	LYS	CD-CE	12.23	1.81	1.51
2	F	145	TYR	C-N	12.23	1.62	1.34
2	F	125	PRO	N-CD	12.21	1.65	1.47
1	A	125	LEU	C-N	12.18	1.62	1.34
2	H	135	ALA	C-N	-12.18	1.11	1.33
1	A	60	LYS	CE-NZ	12.15	1.79	1.49
1	E	23	GLU	C-O	12.10	1.46	1.23
2	F	69	GLY	CA-C	12.08	1.71	1.51
2	B	38	THR	CB-OG1	12.07	1.67	1.43
1	C	70	VAL	C-O	-12.06	1.00	1.23
2	F	110	LEU	CA-CB	12.06	1.81	1.53
2	B	18	VAL	CB-CG1	12.06	1.78	1.52
2	B	98	VAL	CB-CG2	12.05	1.78	1.52
1	A	122	HIS	CE1-NE2	12.05	1.60	1.32
1	G	31	ARG	CZ-NH1	-12.05	1.17	1.33
1	C	45	HIS	CB-CG	12.04	1.71	1.50
1	C	89	HIS	CB-CG	12.04	1.71	1.50
2	D	131	GLN	C-O	12.02	1.46	1.23
2	B	45	PHE	CG-CD1	11.95	1.56	1.38
2	F	40	ARG	CZ-NH1	11.94	1.48	1.33
2	D	129	ALA	C-N	11.94	1.61	1.34
1	A	141	ARG	CD-NE	11.92	1.66	1.46
2	F	85	PHE	CG-CD1	11.90	1.56	1.38
1	A	37	PRO	CA-CB	11.90	1.77	1.53
2	B	140	ALA	C-O	11.88	1.46	1.23
2	B	89	SER	CB-OG	11.81	1.57	1.42
1	G	23	GLU	C-N	-11.79	1.06	1.34
2	F	36	PRO	N-CA	11.78	1.67	1.47
2	D	77	HIS	CA-CB	11.75	1.79	1.53
1	E	137	THR	CB-OG1	11.71	1.66	1.43
1	C	98	PHE	CB-CG	11.67	1.71	1.51
2	B	7	GLU	CB-CG	11.63	1.74	1.52
2	H	55	MET	C-N	-11.59	1.12	1.33
1	E	14	TRP	C-O	11.59	1.45	1.23
2	B	35	TYR	C-O	-11.56	1.01	1.23
2	F	33	VAL	C-O	11.54	1.45	1.23
2	H	137	VAL	CB-CG2	11.53	1.77	1.52
2	F	83	GLY	N-CA	11.53	1.63	1.46
1	G	119	PRO	N-CA	-11.51	1.27	1.47
1	C	114	PRO	N-CD	11.51	1.64	1.47
1	E	102	SER	CA-CB	-11.51	1.35	1.52
1	E	31	ARG	CZ-NH2	11.49	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	9	SER	CA-CB	11.48	1.70	1.52
2	F	143	HIS	CE1-NE2	11.48	1.59	1.32
1	A	23	GLU	CB-CG	11.47	1.74	1.52
1	G	23	GLU	CD-OE2	11.46	1.38	1.25
1	A	61	LYS	CD-CE	11.45	1.79	1.51
1	G	64	ASP	C-O	-11.44	1.01	1.23
1	G	14	TRP	C-O	-11.42	1.01	1.23
1	G	112	HIS	CA-CB	11.40	1.79	1.53
1	C	139	LYS	C-O	11.38	1.45	1.23
1	C	78	ASN	N-CA	11.32	1.69	1.46
1	G	42	TYR	CB-CG	11.31	1.68	1.51
2	H	46	GLY	N-CA	-11.29	1.29	1.46
1	C	118	THR	N-CA	11.28	1.69	1.46
1	G	69	ALA	C-O	11.28	1.44	1.23
2	H	15	TRP	C-O	11.28	1.44	1.23
1	E	134	THR	C-O	11.27	1.44	1.23
2	F	45	PHE	CG-CD2	11.25	1.55	1.38
1	C	13	ALA	N-CA	11.25	1.68	1.46
1	C	77	PRO	N-CD	11.24	1.63	1.47
1	C	131	SER	CB-OG	11.21	1.56	1.42
2	D	4	THR	CB-OG1	11.21	1.65	1.43
1	G	114	PRO	N-CD	11.21	1.63	1.47
1	C	136	LEU	C-O	-11.20	1.02	1.23
2	F	40	ARG	CG-CD	11.18	1.79	1.51
2	B	9	SER	CB-OG	11.18	1.56	1.42
2	D	11	VAL	N-CA	-11.17	1.24	1.46
1	A	24	TYR	CD1-CE1	-11.15	1.22	1.39
2	D	45	PHE	CE2-CZ	11.15	1.58	1.37
2	H	107	GLY	C-O	11.15	1.41	1.23
2	H	121	GLU	CD-OE2	11.15	1.38	1.25
1	E	69	ALA	N-CA	11.12	1.68	1.46
2	D	142	ALA	CA-CB	11.10	1.75	1.52
1	G	103	HIS	CG-CD2	11.08	1.54	1.35
1	A	69	ALA	CA-CB	-11.08	1.29	1.52
2	D	121	GLU	C-N	11.07	1.59	1.34
1	A	20	HIS	C-O	11.07	1.44	1.23
1	G	117	PHE	CA-CB	11.06	1.78	1.53
2	F	39	GLN	CG-CD	11.06	1.76	1.51
2	B	38	THR	N-CA	11.06	1.68	1.46
2	F	102	ASN	CG-OD1	11.04	1.48	1.24
2	H	112	CYS	CB-SG	-11.04	1.63	1.82
1	C	94	ASP	C-N	11.03	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	119	GLY	CA-C	-11.02	1.34	1.51
2	H	68	LEU	N-CA	10.94	1.68	1.46
1	E	31	ARG	CD-NE	-10.92	1.27	1.46
1	E	36	PHE	CE1-CZ	10.83	1.57	1.37
1	A	121	VAL	N-CA	10.81	1.68	1.46
2	D	130	TYR	CE2-CZ	10.77	1.52	1.38
2	F	83	GLY	CA-C	-10.75	1.34	1.51
1	G	47	ASP	CA-CB	-10.75	1.30	1.53
2	B	71	PHE	CD1-CE1	10.74	1.60	1.39
1	A	70	VAL	C-N	-10.73	1.09	1.34
2	H	103	PHE	N-CA	10.71	1.67	1.46
1	G	67	THR	C-O	10.69	1.43	1.23
1	A	41	THR	N-CA	10.68	1.67	1.46
1	E	42	TYR	CG-CD2	-10.66	1.25	1.39
2	B	74	GLY	CA-C	10.66	1.69	1.51
1	C	45	HIS	CG-CD2	-10.65	1.17	1.35
1	G	30	GLU	C-N	-10.64	1.09	1.34
1	C	71	ALA	C-O	10.63	1.43	1.23
2	H	122	PHE	CE1-CZ	10.63	1.57	1.37
1	E	20	HIS	N-CA	10.63	1.67	1.46
2	D	125	PRO	CA-CB	10.61	1.74	1.53
2	F	92	HIS	CG-ND1	-10.60	1.15	1.38
2	H	84	THR	CB-OG1	10.59	1.64	1.43
2	D	106	LEU	C-N	10.54	1.52	1.33
2	B	103	PHE	CE1-CZ	10.51	1.57	1.37
2	B	45	PHE	C-O	10.48	1.43	1.23
2	F	8	LYS	CB-CG	10.47	1.80	1.52
2	B	130	TYR	C-O	10.47	1.43	1.23
2	H	35	TYR	CG-CD2	10.44	1.52	1.39
1	E	116	GLU	CB-CG	10.43	1.72	1.52
1	G	62	VAL	C-O	10.43	1.43	1.23
1	C	129	LEU	N-CA	10.43	1.67	1.46
2	F	16	GLY	C-O	10.40	1.40	1.23
2	D	43	GLU	N-CA	10.39	1.67	1.46
2	D	48	LEU	C-O	-10.39	1.03	1.23
2	F	36	PRO	C-O	10.35	1.44	1.23
2	F	25	GLY	CA-C	10.34	1.68	1.51
1	G	63	ALA	N-CA	10.33	1.67	1.46
2	H	79	ASP	CG-OD2	10.33	1.49	1.25
1	G	37	PRO	C-N	-10.31	1.10	1.34
2	D	86	ALA	CA-CB	10.31	1.74	1.52
1	C	46	PHE	CG-CD1	10.29	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	ALA	C-N	-10.28	1.10	1.34
2	F	15	TRP	CD1-NE1	-10.25	1.20	1.38
2	H	96	LEU	C-N	-10.25	1.10	1.34
1	A	4	PRO	C-N	10.24	1.57	1.34
2	F	15	TRP	CZ2-CH2	-10.23	1.18	1.37
2	H	127	GLN	CB-CG	10.23	1.80	1.52
2	B	37	TRP	CE2-CZ2	-10.22	1.22	1.39
1	C	64	ASP	CA-CB	10.20	1.76	1.53
2	H	133	VAL	CB-CG1	10.19	1.74	1.52
2	F	93	CYS	CB-SG	10.18	1.99	1.82
2	H	116	HIS	CD2-NE2	10.15	1.63	1.42
1	A	76	MET	CA-CB	10.13	1.76	1.53
2	D	35	TYR	CD1-CE1	10.13	1.54	1.39
2	D	145	TYR	CG-CD1	10.10	1.52	1.39
1	G	141	ARG	C-O	10.09	1.42	1.23
2	F	137	VAL	C-N	-10.07	1.10	1.34
2	D	129	ALA	CA-CB	10.07	1.73	1.52
2	B	101	GLU	CD-OE1	-10.05	1.14	1.25
1	C	95	PRO	CA-CB	10.05	1.73	1.53
1	G	23	GLU	C-O	10.02	1.42	1.23
2	F	133	VAL	N-CA	9.95	1.66	1.46
1	E	95	PRO	C-O	9.94	1.43	1.23
1	C	110	ALA	C-O	9.92	1.42	1.23
1	C	92	ARG	NE-CZ	9.91	1.46	1.33
2	B	104	ARG	CZ-NH1	9.88	1.46	1.33
1	A	95	PRO	C-N	-9.88	1.11	1.34
1	C	121	VAL	CB-CG1	9.87	1.73	1.52
2	F	89	SER	CB-OG	9.83	1.55	1.42
2	F	62	ALA	C-O	9.83	1.42	1.23
1	E	11	LYS	CA-CB	9.81	1.75	1.53
1	G	69	ALA	N-CA	9.80	1.66	1.46
1	C	59	GLY	N-CA	-9.79	1.31	1.46
2	F	5	PRO	N-CD	-9.78	1.34	1.47
1	A	140	TYR	C-O	9.77	1.42	1.23
2	B	37	TRP	CE3-CZ3	9.77	1.55	1.38
2	F	136	GLY	CA-C	9.77	1.67	1.51
2	F	136	GLY	N-CA	-9.76	1.31	1.46
2	F	119	GLY	N-CA	9.76	1.60	1.46
1	A	75	ASP	C-O	9.73	1.41	1.23
1	G	32	MET	CA-CB	9.73	1.75	1.53
1	A	61	LYS	CB-CG	9.72	1.78	1.52
2	D	77	HIS	CG-CD2	9.72	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	138	ALA	C-O	9.71	1.41	1.23
1	A	58	HIS	N-CA	9.70	1.65	1.46
2	H	82	LYS	N-CA	9.70	1.65	1.46
2	D	55	MET	C-O	9.69	1.41	1.23
2	H	56	GLY	C-O	9.68	1.39	1.23
2	F	29	GLY	N-CA	9.67	1.60	1.46
1	G	30	GLU	C-O	9.66	1.41	1.23
1	A	54	GLN	C-N	9.66	1.56	1.34
2	B	102	ASN	CG-OD1	9.64	1.45	1.24
1	G	116	GLU	CD-OE1	-9.63	1.15	1.25
1	G	141	ARG	N-CA	9.64	1.65	1.46
1	A	34	LEU	N-CA	9.62	1.65	1.46
2	H	60	VAL	CB-CG1	9.62	1.73	1.52
2	F	112	CYS	C-N	-9.61	1.11	1.34
1	C	141	ARG	CB-CG	-9.60	1.26	1.52
1	C	116	GLU	CD-OE1	9.59	1.36	1.25
1	C	110	ALA	CA-CB	9.58	1.72	1.52
2	B	130	TYR	CG-CD1	9.58	1.51	1.39
1	E	6	ASP	CB-CG	-9.58	1.31	1.51
1	G	120	ALA	CA-CB	9.57	1.72	1.52
1	A	3	SER	CA-CB	-9.57	1.38	1.52
1	C	10	VAL	C-O	9.55	1.41	1.23
2	D	74	GLY	CA-C	9.54	1.67	1.51
2	F	41	PHE	C-O	9.54	1.41	1.23
2	F	104	ARG	N-CA	9.54	1.65	1.46
1	G	54	GLN	CG-CD	9.52	1.73	1.51
1	E	92	ARG	NE-CZ	9.51	1.45	1.33
1	E	39	THR	C-O	9.51	1.41	1.23
1	E	109	LEU	C-N	-9.50	1.12	1.34
2	D	25	GLY	N-CA	9.49	1.60	1.46
2	H	61	LYS	CE-NZ	9.48	1.72	1.49
1	C	141	ARG	CZ-NH2	9.46	1.45	1.33
2	B	53	ALA	C-O	9.46	1.41	1.23
2	D	65	LYS	CE-NZ	9.44	1.72	1.49
2	B	129	ALA	N-CA	9.43	1.65	1.46
1	E	105	LEU	C-N	-9.43	1.12	1.34
2	D	2	HIS	C-O	9.42	1.41	1.23
1	E	6	ASP	CG-OD1	9.42	1.47	1.25
2	H	12	THR	C-O	9.41	1.41	1.23
1	A	69	ALA	N-CA	9.41	1.65	1.46
1	E	7	LYS	N-CA	9.38	1.65	1.46
2	D	12	THR	CB-OG1	9.37	1.61	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	117	PHE	CG-CD2	9.36	1.52	1.38
2	B	37	TRP	CZ2-CH2	9.36	1.55	1.37
1	C	95	PRO	N-CD	9.36	1.60	1.47
2	F	30	ARG	CZ-NH2	-9.34	1.21	1.33
2	F	36	PRO	N-CD	-9.34	1.34	1.47
1	A	140	TYR	CE1-CZ	9.33	1.50	1.38
2	D	130	TYR	C-O	-9.32	1.05	1.23
2	F	85	PHE	C-O	9.32	1.41	1.23
2	D	44	SER	CA-CB	9.32	1.67	1.52
2	D	101	GLU	CA-CB	-9.32	1.33	1.53
1	A	67	THR	CB-OG1	9.31	1.61	1.43
2	F	1	VAL	N-CA	9.29	1.65	1.46
1	C	96	VAL	CB-CG1	-9.29	1.33	1.52
2	B	90	GLU	C-O	9.29	1.41	1.23
1	C	73	VAL	C-O	9.28	1.41	1.23
2	F	75	LEU	C-O	9.28	1.41	1.23
1	A	21	ALA	CA-CB	9.26	1.72	1.52
1	A	27	GLU	N-CA	9.26	1.64	1.46
1	E	121	VAL	CB-CG2	-9.26	1.33	1.52
1	A	116	GLU	CD-OE2	9.24	1.35	1.25
2	D	8	LYS	C-O	9.24	1.41	1.23
2	B	122	PHE	CE2-CZ	9.24	1.54	1.37
1	G	49	SER	CB-OG	9.24	1.54	1.42
1	E	90	LYS	C-O	9.23	1.40	1.23
2	B	112	CYS	CB-SG	-9.22	1.66	1.82
2	H	118	PHE	N-CA	-9.21	1.27	1.46
1	A	50	HIS	N-CA	9.21	1.64	1.46
1	A	124	SER	C-O	9.20	1.40	1.23
2	B	133	VAL	N-CA	9.20	1.64	1.46
2	B	90	GLU	CG-CD	9.18	1.65	1.51
1	A	138	SER	C-N	-9.18	1.12	1.34
2	F	116	HIS	CG-CD2	9.17	1.51	1.35
2	D	7	GLU	CA-CB	9.16	1.74	1.53
2	H	143	HIS	C-N	-9.16	1.12	1.34
1	A	19	ALA	C-N	9.15	1.55	1.34
1	A	24	TYR	C-O	-9.15	1.05	1.23
1	A	140	TYR	CZ-OH	9.14	1.53	1.37
2	B	80	ASN	CB-CG	9.09	1.72	1.51
1	G	125	LEU	N-CA	9.09	1.64	1.46
1	C	81	SER	CB-OG	9.08	1.54	1.42
1	E	99	LYS	CE-NZ	9.07	1.71	1.49
1	A	24	TYR	CB-CG	9.07	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	138	ALA	C-O	9.05	1.40	1.23
1	E	3	SER	CB-OG	9.05	1.54	1.42
2	F	112	CYS	CB-SG	9.05	1.97	1.82
2	D	34	VAL	N-CA	9.04	1.64	1.46
2	F	22	GLU	CB-CG	9.04	1.69	1.52
2	H	55	MET	C-O	9.04	1.40	1.23
1	C	9	ASN	N-CA	-9.03	1.28	1.46
2	D	108	ASN	C-N	9.03	1.54	1.34
2	H	7	GLU	N-CA	8.99	1.64	1.46
1	G	72	HIS	CG-CD2	8.98	1.51	1.35
1	C	110	ALA	C-N	-8.98	1.13	1.34
2	B	136	GLY	N-CA	-8.97	1.32	1.46
1	C	84	SER	CB-OG	8.97	1.53	1.42
1	A	42	TYR	CG-CD2	8.94	1.50	1.39
1	A	47	ASP	CG-OD1	8.94	1.46	1.25
2	B	133	VAL	C-O	8.93	1.40	1.23
2	F	101	GLU	CD-OE1	8.93	1.35	1.25
2	H	39	GLN	N-CA	8.92	1.64	1.46
1	A	139	LYS	CD-CE	8.90	1.73	1.51
2	H	45	PHE	CE2-CZ	8.90	1.54	1.37
2	D	87	THR	C-N	8.90	1.54	1.34
2	H	73	ASP	C-O	8.89	1.40	1.23
2	D	25	GLY	C-N	8.88	1.54	1.34
2	D	117	HIS	CG-CD2	-8.88	1.20	1.35
2	D	40	ARG	CZ-NH1	8.87	1.44	1.33
1	E	24	TYR	C-O	-8.86	1.06	1.23
2	F	35	TYR	C-O	8.85	1.40	1.23
2	B	16	GLY	C-N	8.84	1.54	1.34
2	H	121	GLU	CB-CG	8.84	1.69	1.52
2	D	85	PHE	CE2-CZ	8.83	1.54	1.37
1	C	30	GLU	N-CA	8.82	1.64	1.46
2	D	107	GLY	N-CA	-8.82	1.32	1.46
1	G	50	HIS	CA-CB	8.82	1.73	1.53
2	H	39	GLN	C-O	8.82	1.40	1.23
1	A	89	HIS	CG-CD2	8.81	1.50	1.35
2	D	91	LEU	N-CA	-8.79	1.28	1.46
1	E	15	GLY	C-N	8.79	1.54	1.34
1	A	61	LYS	CE-NZ	8.79	1.71	1.49
2	B	11	VAL	N-CA	8.78	1.63	1.46
1	C	16	LYS	CG-CD	8.77	1.82	1.52
1	G	7	LYS	C-N	8.77	1.54	1.34
2	D	134	VAL	N-CA	8.77	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	37	PRO	C-O	8.77	1.40	1.23
1	G	50	HIS	C-N	-8.76	1.17	1.33
2	H	104	ARG	C-N	8.75	1.54	1.34
2	H	109	VAL	C-O	8.74	1.40	1.23
2	B	25	GLY	N-CA	8.73	1.59	1.46
2	H	58	PRO	C-O	8.72	1.40	1.23
2	D	104	ARG	NE-CZ	8.71	1.44	1.33
1	A	87	HIS	N-CA	8.69	1.63	1.46
2	H	134	VAL	N-CA	8.69	1.63	1.46
1	G	10	VAL	C-O	8.68	1.39	1.23
2	H	26	GLU	CD-OE1	-8.67	1.16	1.25
1	C	36	PHE	C-N	-8.66	1.17	1.34
2	B	121	GLU	CG-CD	8.66	1.65	1.51
1	E	20	HIS	CG-CD2	-8.65	1.21	1.35
2	D	57	ASN	C-O	8.65	1.39	1.23
1	G	2	LEU	C-O	8.64	1.39	1.23
2	D	65	LYS	C-O	8.64	1.39	1.23
1	A	131	SER	CB-OG	8.63	1.53	1.42
2	D	87	THR	C-O	-8.62	1.06	1.23
1	C	94	ASP	N-CA	8.62	1.63	1.46
2	D	124	PRO	C-N	8.62	1.50	1.34
2	B	8	LYS	CB-CG	8.61	1.75	1.52
1	C	45	HIS	ND1-CE1	8.61	1.56	1.34
1	A	89	HIS	C-N	-8.61	1.14	1.34
2	B	63	HIS	C-N	-8.60	1.17	1.33
2	D	4	THR	N-CA	8.60	1.63	1.46
2	F	68	LEU	CA-CB	8.60	1.73	1.53
2	F	74	GLY	CA-C	8.59	1.65	1.51
2	D	120	LYS	C-O	8.59	1.39	1.23
1	C	38	THR	CA-CB	8.59	1.75	1.53
2	D	120	LYS	N-CA	8.57	1.63	1.46
2	B	56	GLY	C-O	8.57	1.37	1.23
2	D	37	TRP	CZ3-CH2	8.55	1.53	1.40
2	F	37	TRP	N-CA	8.55	1.63	1.46
2	H	41	PHE	CD2-CE2	8.53	1.56	1.39
1	G	53	ALA	CA-CB	8.52	1.70	1.52
2	D	30	ARG	NE-CZ	8.52	1.44	1.33
2	F	23	VAL	N-CA	8.52	1.63	1.46
1	E	45	HIS	C-O	8.51	1.39	1.23
1	E	139	LYS	CD-CE	8.51	1.72	1.51
2	B	104	ARG	N-CA	8.51	1.63	1.46
1	G	127	LYS	C-O	8.50	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	PHE	N-CA	-8.49	1.29	1.46
2	H	40	ARG	CZ-NH2	8.49	1.44	1.33
2	B	8	LYS	C-O	-8.47	1.07	1.23
1	C	119	PRO	N-CA	8.47	1.61	1.47
2	B	125	PRO	C-O	8.46	1.40	1.23
1	A	118	THR	C-N	8.45	1.50	1.34
2	B	30	ARG	CB-CG	8.45	1.75	1.52
1	C	54	GLN	CD-OE1	8.45	1.42	1.24
1	C	9	ASN	CG-OD1	8.44	1.42	1.24
1	E	14	TRP	N-CA	8.43	1.63	1.46
1	G	44	PRO	CA-CB	8.43	1.70	1.53
2	B	2	HIS	N-CA	8.43	1.63	1.46
2	D	61	LYS	N-CA	8.43	1.63	1.46
1	A	19	ALA	N-CA	8.42	1.63	1.46
1	C	13	ALA	CA-C	-8.42	1.31	1.52
2	F	17	LYS	CE-NZ	8.42	1.70	1.49
1	G	76	MET	C-O	8.41	1.39	1.23
2	D	131	GLN	C-N	-8.41	1.14	1.34
2	B	109	VAL	CA-CB	8.40	1.72	1.54
1	C	40	LYS	CG-CD	8.40	1.81	1.52
2	F	143	HIS	C-O	-8.40	1.07	1.23
1	C	83	LEU	C-N	8.39	1.53	1.34
1	G	47	ASP	CA-C	8.39	1.74	1.52
1	E	119	PRO	C-N	-8.38	1.14	1.34
1	E	130	ALA	CA-CB	8.38	1.70	1.52
2	D	89	SER	C-O	8.38	1.39	1.23
2	F	35	TYR	CE2-CZ	8.38	1.49	1.38
2	D	87	THR	CB-OG1	8.38	1.60	1.43
2	H	44	SER	CA-CB	-8.37	1.40	1.52
2	B	37	TRP	CG-CD2	8.37	1.57	1.43
1	C	86	LEU	C-O	-8.37	1.07	1.23
2	D	103	PHE	CE1-CZ	8.37	1.53	1.37
1	A	84	SER	CA-CB	-8.36	1.40	1.52
2	D	15	TRP	C-N	-8.35	1.18	1.33
2	D	117	HIS	C-N	-8.34	1.14	1.34
2	F	13	ALA	C-O	8.34	1.39	1.23
2	F	12	THR	C-N	-8.33	1.14	1.34
2	F	140	ALA	C-O	-8.32	1.07	1.23
2	F	39	GLN	C-O	-8.31	1.07	1.23
2	B	68	LEU	C-N	8.31	1.48	1.33
2	F	37	TRP	CE2-CZ2	-8.31	1.25	1.39
2	F	78	LEU	C-N	-8.31	1.15	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	PHE	CE2-CZ	8.30	1.53	1.37
1	E	112	HIS	CG-CD2	8.30	1.49	1.35
2	H	77	HIS	C-N	8.29	1.53	1.34
1	G	31	ARG	CG-CD	-8.29	1.31	1.51
2	H	145	TYR	CE2-CZ	8.29	1.49	1.38
1	E	3	SER	N-CA	8.28	1.62	1.46
1	C	126	ASP	CG-OD2	8.28	1.44	1.25
2	D	117	HIS	CA-CB	8.28	1.72	1.53
2	F	90	GLU	CD-OE2	-8.28	1.16	1.25
2	D	145	TYR	N-CA	8.28	1.62	1.46
2	D	37	TRP	NE1-CE2	-8.27	1.26	1.37
1	G	40	LYS	C-N	-8.27	1.15	1.34
1	G	62	VAL	CB-CG1	8.27	1.70	1.52
1	E	11	LYS	N-CA	-8.26	1.29	1.46
1	G	58	HIS	CG-CD2	8.26	1.49	1.35
1	C	6	ASP	CA-CB	8.25	1.72	1.53
1	E	116	GLU	CD-OE2	8.24	1.34	1.25
2	F	53	ALA	CA-C	8.23	1.74	1.52
1	E	24	TYR	CG-CD1	-8.23	1.28	1.39
2	F	16	GLY	CA-C	8.22	1.65	1.51
2	F	123	THR	C-O	8.22	1.39	1.23
1	G	129	LEU	CA-CB	8.22	1.72	1.53
2	H	13	ALA	C-O	8.21	1.39	1.23
2	F	97	HIS	CG-ND1	-8.21	1.20	1.38
1	G	63	ALA	C-O	8.21	1.39	1.23
1	E	41	THR	CB-OG1	8.19	1.59	1.43
1	G	14	TRP	NE1-CE2	-8.19	1.26	1.37
1	A	92	ARG	NE-CZ	8.19	1.43	1.33
1	E	7	LYS	CA-CB	-8.16	1.35	1.53
1	G	70	VAL	CB-CG1	8.16	1.70	1.52
1	A	24	TYR	CD2-CE2	-8.16	1.27	1.39
1	C	88	ALA	C-O	8.15	1.38	1.23
1	G	124	SER	CB-OG	8.15	1.52	1.42
2	D	44	SER	CB-OG	8.15	1.52	1.42
2	F	30	ARG	CZ-NH1	8.14	1.43	1.33
1	C	118	THR	C-O	8.14	1.38	1.23
2	F	121	GLU	CA-CB	8.14	1.71	1.53
2	H	6	VAL	C-O	8.14	1.38	1.23
2	H	59	LYS	C-O	8.13	1.38	1.23
2	H	98	VAL	C-O	8.13	1.38	1.23
2	D	104	ARG	CB-CG	8.12	1.74	1.52
1	G	15	GLY	CA-C	8.12	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLY	N-CA	8.12	1.58	1.46
2	B	49	SER	CA-CB	8.12	1.65	1.52
2	F	35	TYR	CZ-OH	-8.12	1.24	1.37
2	D	92	HIS	CD2-NE2	-8.11	1.20	1.38
1	G	125	LEU	CA-CB	-8.10	1.35	1.53
1	E	74	ASP	CG-OD1	8.09	1.44	1.25
2	B	43	GLU	CG-CD	-8.09	1.39	1.51
1	A	59	GLY	C-N	8.08	1.52	1.34
1	G	92	ARG	CZ-NH2	8.07	1.43	1.33
2	D	103	PHE	CB-CG	8.06	1.65	1.51
2	B	126	VAL	N-CA	8.06	1.62	1.46
1	G	20	HIS	CE1-NE2	-8.06	1.14	1.32
1	A	96	VAL	C-O	-8.06	1.08	1.23
2	F	134	VAL	C-N	-8.06	1.15	1.34
2	H	4	THR	C-N	-8.05	1.19	1.34
2	H	15	TRP	C-N	-8.05	1.18	1.33
1	G	116	GLU	C-O	8.04	1.38	1.23
2	H	34	VAL	CB-CG2	8.03	1.69	1.52
1	G	131	SER	CA-CB	8.02	1.65	1.52
2	H	29	GLY	C-N	8.02	1.52	1.34
1	A	103	HIS	CE1-NE2	-8.01	1.14	1.32
2	B	42	PHE	CG-CD2	8.01	1.50	1.38
2	D	48	LEU	C-N	8.00	1.52	1.34
2	D	115	ALA	C-N	8.00	1.52	1.34
2	H	17	LYS	CA-CB	8.00	1.71	1.53
1	E	4	PRO	N-CD	-7.99	1.36	1.47
1	C	60	LYS	CD-CE	7.98	1.71	1.51
1	A	140	TYR	CG-CD2	7.97	1.49	1.39
2	D	14	LEU	N-CA	7.97	1.62	1.46
1	E	108	THR	CB-OG1	7.97	1.59	1.43
1	E	75	ASP	CA-CB	7.96	1.71	1.53
2	H	135	ALA	CA-CB	-7.95	1.35	1.52
1	G	116	GLU	CD-OE2	7.95	1.34	1.25
1	C	81	SER	C-N	-7.94	1.15	1.34
2	H	41	PHE	C-O	7.94	1.38	1.23
1	A	98	PHE	CE2-CZ	7.94	1.52	1.37
2	H	45	PHE	CD2-CE2	-7.94	1.23	1.39
1	E	139	LYS	C-O	7.93	1.38	1.23
2	B	145	TYR	C-O	7.93	1.38	1.23
2	D	118	PHE	CA-CB	7.92	1.71	1.53
2	F	45	PHE	CG-CD1	-7.92	1.26	1.38
2	D	37	TRP	CD2-CE2	7.92	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	76	ALA	N-CA	-7.92	1.30	1.46
2	D	39	GLN	CD-OE1	7.91	1.41	1.24
1	E	36	PHE	CG-CD1	-7.91	1.26	1.38
1	C	58	HIS	C-N	-7.90	1.18	1.33
2	H	70	ALA	C-O	-7.89	1.08	1.23
1	G	60	LYS	CE-NZ	7.88	1.68	1.49
1	A	16	LYS	CA-CB	7.88	1.71	1.53
1	C	92	ARG	CD-NE	7.86	1.59	1.46
1	A	13	ALA	CA-C	7.86	1.73	1.52
1	G	109	LEU	N-CA	-7.85	1.30	1.46
1	A	58	HIS	CG-CD2	7.84	1.49	1.35
2	D	2	HIS	CA-CB	7.84	1.71	1.53
1	G	140	TYR	CA-CB	-7.83	1.36	1.53
2	H	101	GLU	CD-OE1	-7.83	1.17	1.25
2	D	22	GLU	CD-OE2	7.83	1.34	1.25
1	E	58	HIS	CA-CB	7.83	1.71	1.53
1	A	128	PHE	C-N	7.82	1.52	1.34
2	F	95	LYS	CE-NZ	7.82	1.68	1.49
2	D	3	LEU	C-O	-7.81	1.08	1.23
2	B	91	LEU	C-O	7.81	1.38	1.23
2	H	100	PRO	CG-CD	7.81	1.76	1.50
1	A	61	LYS	CA-C	7.80	1.73	1.52
2	H	58	PRO	N-CD	7.80	1.58	1.47
2	D	118	PHE	CG-CD1	7.79	1.50	1.38
2	F	40	ARG	C-O	7.79	1.38	1.23
2	H	71	PHE	C-O	7.78	1.38	1.23
2	H	91	LEU	N-CA	-7.78	1.30	1.46
2	H	15	TRP	CE3-CZ3	7.78	1.51	1.38
1	C	67	THR	C-O	7.77	1.38	1.23
2	H	61	LYS	C-O	7.76	1.38	1.23
1	C	117	PHE	N-CA	-7.76	1.30	1.46
2	F	50	THR	C-O	7.76	1.38	1.23
2	F	123	THR	CA-CB	7.76	1.73	1.53
1	C	48	LEU	CA-CB	7.75	1.71	1.53
1	A	93	VAL	N-CA	7.74	1.61	1.46
1	G	124	SER	N-CA	7.72	1.61	1.46
2	B	19	ASN	CG-OD1	7.72	1.41	1.24
1	A	35	SER	N-CA	7.72	1.61	1.46
1	G	129	LEU	N-CA	-7.72	1.30	1.46
1	G	81	SER	C-N	-7.71	1.16	1.34
1	C	84	SER	CA-CB	7.70	1.64	1.52
2	F	83	GLY	C-N	-7.70	1.16	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	134	THR	CB-OG1	7.70	1.58	1.43
2	B	73	ASP	CA-CB	7.69	1.70	1.53
2	B	127	GLN	CA-CB	7.69	1.70	1.53
1	G	14	TRP	CG-CD1	-7.69	1.25	1.36
2	H	127	GLN	C-O	7.68	1.38	1.23
2	F	1	VAL	C-O	7.68	1.38	1.23
1	E	89	HIS	CG-ND1	7.67	1.55	1.38
2	F	48	LEU	CB-CG	7.67	1.74	1.52
1	E	134	THR	C-N	-7.67	1.16	1.34
2	B	85	PHE	CG-CD1	7.66	1.50	1.38
2	F	108	ASN	C-O	7.64	1.37	1.23
1	C	93	VAL	CB-CG2	7.64	1.68	1.52
2	H	96	LEU	CA-CB	7.64	1.71	1.53
1	E	81	SER	C-O	7.64	1.37	1.23
1	C	71	ALA	N-CA	7.63	1.61	1.46
2	H	130	TYR	CD1-CE1	-7.63	1.27	1.39
1	G	138	SER	CB-OG	7.63	1.52	1.42
2	D	117	HIS	CB-CG	7.63	1.63	1.50
2	H	127	GLN	CD-NE2	7.62	1.51	1.32
2	B	87	THR	C-O	7.62	1.37	1.23
1	C	113	LEU	N-CA	7.62	1.61	1.46
2	B	103	PHE	CA-CB	-7.62	1.37	1.53
1	G	109	LEU	CG-CD1	7.61	1.80	1.51
1	A	2	LEU	C-N	7.61	1.51	1.34
1	A	124	SER	CB-OG	7.61	1.52	1.42
1	E	119	PRO	N-CA	-7.61	1.34	1.47
2	D	127	GLN	C-N	-7.61	1.16	1.34
2	H	117	HIS	N-CA	-7.60	1.31	1.46
2	B	103	PHE	C-O	-7.60	1.08	1.23
2	B	135	ALA	C-O	7.59	1.37	1.23
2	F	48	LEU	C-N	-7.59	1.16	1.34
1	E	117	PHE	C-O	7.59	1.37	1.23
2	F	9	SER	CB-OG	7.58	1.52	1.42
2	D	35	TYR	CA-CB	-7.58	1.37	1.53
2	F	15	TRP	CG-CD1	7.57	1.47	1.36
2	D	52	ASP	C-O	7.57	1.37	1.23
1	A	84	SER	N-CA	7.57	1.61	1.46
1	E	42	TYR	C-O	7.57	1.37	1.23
2	B	107	GLY	CA-C	7.56	1.64	1.51
2	F	50	THR	CB-OG1	7.56	1.58	1.43
2	F	16	GLY	C-N	-7.55	1.16	1.34
2	H	85	PHE	CE2-CZ	7.55	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	45	HIS	CD2-NE2	-7.54	1.21	1.38
2	H	101	GLU	C-N	-7.54	1.16	1.34
2	D	122	PHE	CA-CB	-7.53	1.37	1.53
1	G	94	ASP	CG-OD2	7.53	1.42	1.25
2	H	108	ASN	CB-CG	7.52	1.68	1.51
1	E	50	HIS	CE1-NE2	-7.52	1.15	1.32
2	B	99	ASP	CB-CG	7.51	1.67	1.51
1	E	138	SER	CB-OG	-7.51	1.32	1.42
2	B	77	HIS	CA-CB	-7.50	1.37	1.53
2	D	30	ARG	CB-CG	-7.50	1.32	1.52
1	G	92	ARG	NE-CZ	-7.50	1.23	1.33
2	H	137	VAL	CB-CG1	-7.49	1.37	1.52
1	C	58	HIS	N-CA	-7.49	1.31	1.46
1	C	46	PHE	CE1-CZ	7.48	1.51	1.37
1	C	49	SER	CB-OG	7.48	1.51	1.42
1	G	61	LYS	C-O	7.48	1.37	1.23
1	C	16	LYS	CD-CE	7.47	1.70	1.51
1	A	35	SER	C-N	-7.47	1.16	1.34
2	F	45	PHE	CE1-CZ	7.46	1.51	1.37
1	G	4	PRO	C-O	7.45	1.38	1.23
1	A	141	ARG	CA-CB	7.45	1.70	1.53
2	B	4	THR	CA-CB	7.45	1.72	1.53
2	D	134	VAL	CB-CG2	7.45	1.68	1.52
1	E	56	LYS	N-CA	7.45	1.61	1.46
1	A	89	HIS	CE1-NE2	7.44	1.49	1.32
2	F	97	HIS	CG-CD2	7.43	1.48	1.35
1	G	6	ASP	N-CA	7.43	1.61	1.46
1	G	120	ALA	N-CA	-7.42	1.31	1.46
2	H	107	GLY	N-CA	7.42	1.57	1.46
1	C	18	GLY	CA-C	7.42	1.63	1.51
1	E	41	THR	C-N	-7.41	1.17	1.34
2	D	100	PRO	N-CA	7.41	1.59	1.47
2	B	69	GLY	N-CA	7.41	1.57	1.46
1	A	21	ALA	C-N	7.41	1.46	1.33
2	B	72	SER	CA-CB	-7.40	1.41	1.52
2	D	80	ASN	CG-ND2	7.39	1.51	1.32
1	A	101	LEU	C-O	-7.38	1.09	1.23
2	B	50	THR	N-CA	-7.38	1.31	1.46
2	B	133	VAL	CB-CG2	-7.38	1.37	1.52
2	B	63	HIS	C-O	7.37	1.37	1.23
2	B	7	GLU	C-N	-7.37	1.17	1.34
1	C	45	HIS	CA-CB	7.37	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	PHE	CB-CG	-7.36	1.38	1.51
1	C	32	MET	CG-SD	7.36	2.00	1.81
2	B	18	VAL	CB-CG2	-7.35	1.37	1.52
2	D	98	VAL	N-CA	7.35	1.61	1.46
2	H	32	LEU	CA-CB	7.35	1.70	1.53
1	E	96	VAL	CB-CG1	7.34	1.68	1.52
2	D	100	PRO	CA-C	-7.33	1.38	1.52
1	C	71	ALA	C-N	7.33	1.50	1.34
2	D	121	GLU	CD-OE1	7.33	1.33	1.25
1	A	78	ASN	N-CA	7.33	1.61	1.46
1	C	41	THR	CB-OG1	7.33	1.57	1.43
2	H	103	PHE	CE2-CZ	7.33	1.51	1.37
1	C	39	THR	CA-C	-7.32	1.33	1.52
1	A	100	LEU	C-O	7.32	1.37	1.23
2	D	63	HIS	CA-CB	7.32	1.70	1.53
2	F	129	ALA	N-CA	7.32	1.60	1.46
2	B	15	TRP	CD2-CE2	7.31	1.50	1.41
1	A	42	TYR	CE1-CZ	7.31	1.48	1.38
2	F	34	VAL	C-N	-7.31	1.17	1.34
2	D	15	TRP	N-CA	7.31	1.60	1.46
2	D	120	LYS	CE-NZ	7.30	1.67	1.49
2	F	54	VAL	CB-CG1	7.30	1.68	1.52
1	G	136	LEU	N-CA	-7.30	1.31	1.46
1	A	139	LYS	C-N	7.29	1.50	1.34
1	G	49	SER	N-CA	7.29	1.60	1.46
1	A	64	ASP	C-O	7.29	1.37	1.23
1	E	42	TYR	CB-CG	7.29	1.62	1.51
1	A	76	MET	C-O	7.28	1.37	1.23
2	B	71	PHE	CG-CD1	-7.28	1.27	1.38
2	B	115	ALA	C-O	-7.28	1.09	1.23
1	E	54	GLN	C-O	7.27	1.37	1.23
2	D	59	LYS	CE-NZ	7.26	1.67	1.49
1	A	111	ALA	C-O	7.26	1.37	1.23
2	H	90	GLU	CA-CB	-7.26	1.38	1.53
1	A	136	LEU	C-N	7.26	1.50	1.34
1	A	46	PHE	CG-CD1	7.25	1.49	1.38
1	C	55	VAL	CB-CG2	-7.25	1.37	1.52
1	G	101	LEU	CG-CD1	7.24	1.78	1.51
1	C	14	TRP	CD1-NE1	7.24	1.50	1.38
1	E	43	PHE	CE2-CZ	7.22	1.51	1.37
2	B	86	ALA	CA-CB	7.22	1.67	1.52
2	F	101	GLU	CD-OE2	-7.22	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	PRO	C-O	7.21	1.37	1.23
1	A	101	LEU	CB-CG	7.21	1.73	1.52
1	G	82	ALA	CA-CB	7.21	1.67	1.52
1	G	126	ASP	CG-OD1	-7.20	1.08	1.25
2	D	81	LEU	N-CA	7.20	1.60	1.46
1	E	102	SER	CA-C	7.20	1.71	1.52
1	A	92	ARG	C-O	7.20	1.37	1.23
1	C	47	ASP	C-O	7.20	1.37	1.23
1	G	27	GLU	CG-CD	-7.19	1.41	1.51
2	H	132	LYS	C-N	7.19	1.50	1.34
2	H	2	HIS	CA-CB	7.18	1.69	1.53
2	H	120	LYS	CE-NZ	7.18	1.67	1.49
2	B	8	LYS	N-CA	7.17	1.60	1.46
1	E	137	THR	N-CA	7.17	1.60	1.46
1	E	4	PRO	C-N	-7.17	1.17	1.34
1	E	36	PHE	N-CA	7.17	1.60	1.46
1	G	30	GLU	CD-OE2	7.17	1.33	1.25
1	A	24	TYR	CE2-CZ	7.17	1.47	1.38
1	A	7	LYS	C-O	7.17	1.36	1.23
1	C	72	HIS	CG-CD2	7.16	1.48	1.35
2	D	138	ALA	CA-CB	7.16	1.67	1.52
1	A	62	VAL	CB-CG1	7.16	1.67	1.52
1	A	49	SER	C-O	7.15	1.36	1.23
2	B	35	TYR	CA-C	7.15	1.71	1.52
2	F	17	LYS	CA-CB	7.15	1.69	1.53
1	E	102	SER	C-N	-7.15	1.17	1.34
2	B	21	ASP	N-CA	7.15	1.60	1.46
1	C	119	PRO	CA-C	7.15	1.67	1.52
2	H	94	ASP	N-CA	7.14	1.60	1.46
2	B	37	TRP	CD2-CE3	-7.14	1.29	1.40
1	A	52	SER	N-CA	-7.14	1.32	1.46
1	E	110	ALA	CA-CB	7.14	1.67	1.52
2	B	37	TRP	CA-CB	7.13	1.69	1.53
2	B	40	ARG	CZ-NH1	-7.12	1.23	1.33
1	E	20	HIS	CE1-NE2	-7.12	1.16	1.32
2	F	59	LYS	C-N	7.12	1.50	1.34
2	B	5	PRO	CA-CB	7.11	1.67	1.53
2	B	12	THR	C-O	7.10	1.36	1.23
2	F	49	SER	N-CA	-7.10	1.32	1.46
1	A	31	ARG	CZ-NH1	7.10	1.42	1.33
1	C	35	SER	C-O	7.09	1.36	1.23
2	F	42	PHE	CE1-CZ	7.08	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	TYR	CZ-OH	7.08	1.49	1.37
1	G	90	LYS	C-N	-7.08	1.17	1.34
2	D	53	ALA	CA-CB	7.07	1.67	1.52
2	D	7	GLU	CG-CD	7.07	1.62	1.51
2	D	97	HIS	CA-CB	7.07	1.69	1.53
1	E	117	PHE	N-CA	7.06	1.60	1.46
2	F	53	ALA	N-CA	-7.06	1.32	1.46
2	H	104	ARG	CB-CG	7.06	1.71	1.52
2	D	37	TRP	CB-CG	7.05	1.62	1.50
2	F	18	VAL	C-O	7.04	1.36	1.23
2	D	46	GLY	N-CA	7.04	1.56	1.46
2	F	38	THR	CB-OG1	7.04	1.57	1.43
2	H	103	PHE	CD1-CE1	7.03	1.53	1.39
1	E	121	VAL	C-O	7.03	1.36	1.23
1	E	56	LYS	CE-NZ	7.03	1.66	1.49
2	F	114	LEU	CB-CG	7.02	1.73	1.52
1	A	14	TRP	C-O	-7.02	1.10	1.23
2	H	131	GLN	C-O	-7.01	1.10	1.23
1	A	55	VAL	C-N	-7.01	1.18	1.34
1	A	132	VAL	C-O	7.01	1.36	1.23
1	E	32	MET	C-O	7.01	1.36	1.23
2	F	109	VAL	C-N	7.01	1.50	1.34
1	A	6	ASP	C-N	-7.00	1.18	1.34
1	G	35	SER	C-O	7.00	1.36	1.23
2	F	110	LEU	C-N	7.00	1.50	1.34
1	G	61	LYS	CG-CD	7.00	1.76	1.52
1	A	77	PRO	CA-C	7.00	1.66	1.52
2	B	22	GLU	CB-CG	7.00	1.65	1.52
1	C	56	LYS	N-CA	-7.00	1.32	1.46
1	A	90	LYS	CB-CG	6.99	1.71	1.52
2	F	39	GLN	CA-CB	-6.99	1.38	1.53
1	G	114	PRO	N-CA	-6.99	1.35	1.47
1	E	40	LYS	C-O	6.99	1.36	1.23
2	H	104	ARG	C-O	-6.99	1.10	1.23
2	F	35	TYR	CD2-CE2	-6.99	1.28	1.39
1	G	30	GLU	CD-OE1	-6.99	1.18	1.25
2	D	118	PHE	N-CA	6.98	1.60	1.46
2	D	19	ASN	N-CA	6.98	1.60	1.46
2	D	141	LEU	CG-CD1	6.98	1.77	1.51
2	H	24	GLY	CA-C	6.97	1.63	1.51
2	F	40	ARG	CA-CB	6.97	1.69	1.53
2	F	84	THR	CA-CB	6.97	1.71	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	135	VAL	CA-CB	6.97	1.69	1.54
2	H	60	VAL	C-O	6.96	1.36	1.23
1	A	37	PRO	C-O	6.96	1.37	1.23
1	G	44	PRO	C-O	6.96	1.37	1.23
1	C	91	LEU	CG-CD2	6.96	1.77	1.51
2	D	29	GLY	N-CA	6.96	1.56	1.46
1	E	41	THR	N-CA	-6.95	1.32	1.46
1	C	57	GLY	N-CA	6.95	1.56	1.46
2	F	145	TYR	CA-CB	-6.95	1.38	1.53
1	E	106	LEU	CG-CD1	6.95	1.77	1.51
1	A	106	LEU	N-CA	6.95	1.60	1.46
2	F	17	LYS	N-CA	-6.95	1.32	1.46
2	H	67	VAL	C-O	6.94	1.36	1.23
2	D	17	LYS	CG-CD	-6.94	1.28	1.52
1	C	35	SER	C-N	-6.94	1.18	1.34
1	A	27	GLU	CA-CB	-6.93	1.38	1.53
1	E	40	LYS	N-CA	6.93	1.60	1.46
2	H	131	GLN	CD-OE1	6.92	1.39	1.24
2	H	123	THR	CB-CG2	6.92	1.75	1.52
1	G	18	GLY	N-CA	6.92	1.56	1.46
2	F	146	HIS	CA-CB	6.91	1.69	1.53
2	F	79	ASP	CA-CB	-6.91	1.38	1.53
2	B	47	ASP	CB-CG	-6.91	1.37	1.51
1	A	30	GLU	CD-OE1	6.90	1.33	1.25
1	C	43	PHE	CE2-CZ	6.90	1.50	1.37
2	H	95	LYS	C-N	-6.90	1.18	1.34
1	A	122	HIS	CD2-NE2	-6.90	1.22	1.38
1	C	34	LEU	CB-CG	6.90	1.72	1.52
1	G	126	ASP	CB-CG	6.90	1.66	1.51
2	B	3	LEU	CG-CD2	6.90	1.77	1.51
2	F	115	ALA	C-O	6.89	1.36	1.23
2	B	1	VAL	CB-CG2	6.89	1.67	1.52
2	H	115	ALA	C-N	-6.89	1.18	1.34
1	C	138	SER	CA-CB	6.88	1.63	1.52
2	F	90	GLU	C-O	-6.87	1.10	1.23
2	B	87	THR	CB-OG1	6.87	1.56	1.43
1	G	130	ALA	N-CA	6.87	1.60	1.46
2	D	85	PHE	N-CA	6.87	1.60	1.46
2	B	24	GLY	N-CA	-6.86	1.35	1.46
1	G	103	HIS	CD2-NE2	6.86	1.56	1.42
1	A	129	LEU	C-N	-6.85	1.18	1.34
1	G	121	VAL	CA-CB	6.85	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	97	HIS	C-O	-6.85	1.10	1.23
1	E	33	PHE	CD2-CE2	6.85	1.52	1.39
2	H	52	ASP	CG-OD2	6.84	1.41	1.25
2	D	56	GLY	C-O	6.84	1.34	1.23
1	A	106	LEU	C-O	-6.83	1.10	1.23
2	H	15	TRP	CE2-CZ2	-6.83	1.28	1.39
1	A	22	GLY	N-CA	6.83	1.56	1.46
1	C	100	LEU	N-CA	6.83	1.59	1.46
1	C	62	VAL	C-O	6.82	1.36	1.23
2	D	146	HIS	CG-ND1	-6.82	1.23	1.38
2	B	136	GLY	CA-C	6.82	1.62	1.51
1	C	139	LYS	CE-NZ	6.82	1.66	1.49
1	E	24	TYR	CD2-CE2	6.81	1.49	1.39
1	E	4	PRO	N-CA	6.81	1.58	1.47
1	A	81	SER	CA-CB	-6.81	1.42	1.52
2	H	44	SER	N-CA	6.80	1.59	1.46
2	H	11	VAL	C-N	6.80	1.49	1.34
1	A	127	LYS	CB-CG	-6.79	1.34	1.52
1	G	54	GLN	C-O	6.79	1.36	1.23
1	A	137	THR	CB-OG1	6.79	1.56	1.43
1	A	25	GLY	N-CA	6.79	1.56	1.46
1	A	99	LYS	CB-CG	-6.79	1.34	1.52
2	D	68	LEU	C-O	6.79	1.36	1.23
1	C	90	LYS	CB-CG	6.79	1.70	1.52
1	E	66	LEU	C-O	6.78	1.36	1.23
1	A	34	LEU	C-O	6.78	1.36	1.23
2	D	14	LEU	CG-CD1	6.78	1.76	1.51
2	H	56	GLY	N-CA	-6.77	1.35	1.46
2	H	72	SER	C-O	6.77	1.36	1.23
2	B	104	ARG	CB-CG	6.77	1.70	1.52
2	H	57	ASN	C-N	-6.77	1.21	1.34
2	B	56	GLY	CA-C	-6.76	1.41	1.51
1	A	126	ASP	CA-CB	-6.75	1.39	1.53
2	D	123	THR	C-O	6.75	1.36	1.23
2	F	82	LYS	C-N	-6.75	1.20	1.33
2	F	104	ARG	CZ-NH2	6.75	1.41	1.33
1	G	42	TYR	CA-C	6.75	1.70	1.52
1	G	8	THR	C-O	-6.75	1.10	1.23
2	B	118	PHE	CA-CB	6.75	1.68	1.53
2	F	68	LEU	CB-CG	6.75	1.72	1.52
2	B	133	VAL	CB-CG1	6.75	1.67	1.52
2	B	65	LYS	CB-CG	6.74	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	GLY	C-O	6.74	1.34	1.23
1	C	59	GLY	CA-C	6.74	1.62	1.51
2	B	2	HIS	CG-ND1	6.73	1.53	1.38
1	E	45	HIS	N-CA	-6.73	1.32	1.46
1	G	107	VAL	C-N	-6.72	1.18	1.34
1	A	128	PHE	CG-CD1	6.71	1.48	1.38
2	F	13	ALA	N-CA	6.71	1.59	1.46
2	H	54	VAL	N-CA	6.71	1.59	1.46
1	G	22	GLY	N-CA	6.71	1.56	1.46
2	H	90	GLU	C-N	-6.71	1.18	1.34
1	G	31	ARG	NE-CZ	-6.70	1.24	1.33
1	A	100	LEU	C-N	-6.70	1.18	1.34
2	B	22	GLU	CD-OE2	-6.70	1.18	1.25
2	H	43	GLU	C-O	-6.70	1.10	1.23
1	G	140	TYR	CZ-OH	-6.69	1.26	1.37
2	F	42	PHE	CD2-CE2	6.69	1.52	1.39
1	E	1	VAL	CA-CB	6.69	1.68	1.54
1	G	77	PRO	N-CD	6.69	1.57	1.47
2	D	116	HIS	CA-CB	6.68	1.68	1.53
2	D	31	LEU	C-N	-6.68	1.18	1.34
1	A	79	ALA	C-N	-6.68	1.18	1.34
1	C	4	PRO	N-CD	6.67	1.57	1.47
2	D	85	PHE	CG-CD1	6.67	1.48	1.38
1	E	45	HIS	CA-CB	6.67	1.68	1.53
1	C	104	CYS	CB-SG	-6.67	1.71	1.82
2	H	86	ALA	CA-CB	-6.67	1.38	1.52
2	H	9	SER	C-O	6.67	1.36	1.23
1	E	107	VAL	N-CA	-6.66	1.33	1.46
2	H	65	LYS	N-CA	6.66	1.59	1.46
2	F	24	GLY	N-CA	-6.65	1.36	1.46
2	F	45	PHE	N-CA	6.65	1.59	1.46
2	F	99	ASP	CG-OD1	-6.65	1.10	1.25
2	B	17	LYS	CG-CD	6.65	1.75	1.52
2	D	64	GLY	N-CA	6.64	1.56	1.46
2	D	109	VAL	CA-CB	6.64	1.68	1.54
2	B	64	GLY	N-CA	6.64	1.56	1.46
1	C	64	ASP	CB-CG	6.64	1.65	1.51
1	C	133	SER	N-CA	6.63	1.59	1.46
2	H	135	ALA	C-O	6.63	1.35	1.23
1	E	121	VAL	C-N	-6.63	1.18	1.34
2	B	145	TYR	CZ-OH	6.63	1.49	1.37
1	G	128	PHE	C-O	6.63	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	PHE	CA-CB	6.62	1.68	1.53
2	B	30	ARG	CA-CB	6.61	1.68	1.53
1	C	89	HIS	CD2-NE2	6.61	1.55	1.42
2	F	66	LYS	CD-CE	6.61	1.67	1.51
2	B	122	PHE	C-O	6.59	1.35	1.23
1	E	103	HIS	CA-CB	6.59	1.68	1.53
1	C	90	LYS	C-N	-6.59	1.18	1.34
2	F	57	ASN	N-CA	6.59	1.59	1.46
1	C	25	GLY	CA-C	6.58	1.62	1.51
1	A	42	TYR	CB-CG	-6.58	1.41	1.51
2	B	73	ASP	CG-OD2	6.58	1.40	1.25
2	D	80	ASN	CA-CB	6.58	1.70	1.53
2	B	122	PHE	CG-CD1	6.58	1.48	1.38
1	C	47	ASP	CG-OD1	6.58	1.40	1.25
1	C	133	SER	C-O	6.58	1.35	1.23
2	H	91	LEU	CG-CD1	6.57	1.76	1.51
2	B	44	SER	N-CA	6.57	1.59	1.46
1	G	140	TYR	CG-CD1	6.57	1.47	1.39
2	F	130	TYR	CG-CD2	-6.57	1.30	1.39
2	D	137	VAL	N-CA	6.56	1.59	1.46
1	A	45	HIS	CG-CD2	-6.56	1.24	1.35
1	A	34	LEU	CA-CB	-6.56	1.38	1.53
1	E	36	PHE	CG-CD2	6.56	1.48	1.38
2	H	14	LEU	CG-CD2	6.56	1.76	1.51
2	H	145	TYR	C-O	6.55	1.35	1.23
2	D	121	GLU	CB-CG	-6.55	1.39	1.52
2	H	31	LEU	CA-CB	-6.55	1.38	1.53
2	D	105	LEU	CA-CB	-6.55	1.38	1.53
2	F	41	PHE	CG-CD2	6.55	1.48	1.38
2	B	50	THR	CB-CG2	6.54	1.74	1.52
1	C	124	SER	C-N	-6.54	1.19	1.34
1	C	140	TYR	CE2-CZ	6.54	1.47	1.38
1	G	108	THR	C-O	-6.54	1.10	1.23
1	A	24	TYR	C-N	6.54	1.44	1.33
2	B	144	LYS	N-CA	6.54	1.59	1.46
1	C	89	HIS	CG-ND1	-6.54	1.24	1.38
2	D	90	GLU	CG-CD	-6.54	1.42	1.51
1	C	103	HIS	CE1-NE2	-6.53	1.17	1.32
1	G	57	GLY	CA-C	6.53	1.62	1.51
1	C	30	GLU	C-O	6.53	1.35	1.23
1	E	132	VAL	C-N	-6.53	1.19	1.34
1	E	72	HIS	N-CA	6.53	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	LYS	CA-CB	-6.52	1.39	1.53
1	C	103	HIS	CD2-NE2	6.51	1.55	1.42
2	F	56	GLY	C-O	6.51	1.34	1.23
1	C	1	VAL	CA-CB	6.51	1.68	1.54
2	H	103	PHE	CA-CB	-6.51	1.39	1.53
2	B	59	LYS	CE-NZ	6.50	1.65	1.49
1	C	72	HIS	N-CA	6.50	1.59	1.46
2	F	116	HIS	C-N	-6.50	1.19	1.34
2	B	5	PRO	C-O	-6.50	1.10	1.23
2	H	36	PRO	CA-C	-6.50	1.39	1.52
1	A	12	ALA	N-CA	6.49	1.59	1.46
1	A	105	LEU	C-O	6.49	1.35	1.23
1	A	104	CYS	CB-SG	6.48	1.93	1.82
2	D	122	PHE	CG-CD1	-6.48	1.29	1.38
1	C	69	ALA	N-CA	-6.48	1.33	1.46
2	F	28	LEU	N-CA	-6.48	1.33	1.46
2	B	20	VAL	C-O	6.48	1.35	1.23
1	G	111	ALA	C-O	6.47	1.35	1.23
1	G	137	THR	C-O	6.47	1.35	1.23
2	H	78	LEU	CA-CB	-6.47	1.38	1.53
2	D	17	LYS	CD-CE	6.46	1.67	1.51
2	D	70	ALA	CA-C	6.46	1.69	1.52
2	D	43	GLU	C-N	-6.46	1.19	1.34
1	G	22	GLY	C-O	6.45	1.33	1.23
1	E	54	GLN	C-N	-6.45	1.19	1.34
2	B	145	TYR	CA-CB	6.45	1.68	1.53
2	F	142	ALA	CA-CB	6.44	1.66	1.52
2	D	3	LEU	C-N	-6.44	1.19	1.34
2	F	8	LYS	CA-CB	-6.44	1.39	1.53
2	D	142	ALA	N-CA	-6.43	1.33	1.46
1	C	36	PHE	CA-C	6.43	1.69	1.52
1	A	40	LYS	CA-CB	-6.43	1.39	1.53
2	B	15	TRP	N-CA	6.43	1.59	1.46
1	E	22	GLY	C-N	6.43	1.48	1.34
2	F	9	SER	C-N	6.43	1.48	1.34
1	E	47	ASP	CG-OD1	-6.42	1.10	1.25
1	A	122	HIS	C-O	6.42	1.35	1.23
2	F	99	ASP	N-CA	-6.42	1.33	1.46
1	C	139	LYS	CD-CE	6.39	1.67	1.51
2	D	44	SER	N-CA	-6.39	1.33	1.46
1	C	128	PHE	C-N	-6.39	1.19	1.34
2	H	61	LYS	CB-CG	6.39	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	42	PHE	CE2-CZ	-6.39	1.25	1.37
2	D	52	ASP	CG-OD1	6.38	1.40	1.25
1	C	120	ALA	N-CA	-6.38	1.33	1.46
2	F	124	PRO	N-CD	6.38	1.56	1.47
1	G	114	PRO	CA-C	6.38	1.65	1.52
2	H	97	HIS	CG-ND1	-6.38	1.24	1.38
1	E	16	LYS	CA-CB	6.38	1.68	1.53
2	D	128	ALA	CA-CB	6.38	1.65	1.52
1	C	37	PRO	CA-C	-6.38	1.40	1.52
1	G	132	VAL	C-O	-6.38	1.11	1.23
1	C	105	LEU	C-O	-6.37	1.11	1.23
1	C	134	THR	N-CA	-6.37	1.33	1.46
2	D	108	ASN	CG-OD1	6.37	1.38	1.24
1	A	130	ALA	N-CA	-6.37	1.33	1.46
1	C	22	GLY	CA-C	6.37	1.62	1.51
1	C	132	VAL	CA-CB	-6.37	1.41	1.54
1	A	117	PHE	CA-CB	6.36	1.68	1.53
2	F	71	PHE	CA-CB	6.36	1.68	1.53
1	C	41	THR	C-O	6.36	1.35	1.23
2	D	93	CYS	CB-SG	-6.36	1.71	1.82
2	D	139	ASN	C-O	-6.35	1.11	1.23
1	C	85	ASP	C-O	-6.35	1.11	1.23
2	D	49	SER	CB-OG	6.35	1.50	1.42
2	D	101	GLU	CB-CG	-6.34	1.40	1.52
1	C	64	ASP	CG-OD2	-6.34	1.10	1.25
1	G	23	GLU	CG-CD	-6.34	1.42	1.51
1	C	112	HIS	CB-CG	6.34	1.61	1.50
1	G	133	SER	C-O	6.34	1.35	1.23
2	B	134	VAL	C-O	6.33	1.35	1.23
1	A	125	LEU	N-CA	6.33	1.59	1.46
2	B	135	ALA	CA-C	-6.32	1.36	1.52
2	D	79	ASP	CB-CG	6.32	1.65	1.51
1	C	103	HIS	CG-ND1	6.32	1.52	1.38
1	A	82	ALA	CA-CB	6.31	1.65	1.52
1	A	104	CYS	CA-CB	6.31	1.67	1.53
2	H	82	LYS	CB-CG	6.31	1.69	1.52
1	G	67	THR	C-N	-6.31	1.19	1.34
2	H	37	TRP	CE3-CZ3	6.31	1.49	1.38
2	H	38	THR	CB-CG2	6.31	1.73	1.52
1	E	100	LEU	C-N	6.30	1.48	1.34
2	D	137	VAL	C-O	-6.30	1.11	1.23
1	A	131	SER	C-O	6.30	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	90	GLU	CG-CD	-6.29	1.42	1.51
2	B	130	TYR	CG-CD2	-6.29	1.30	1.39
1	G	98	PHE	N-CA	6.29	1.58	1.46
1	C	116	GLU	C-O	6.29	1.35	1.23
2	D	23	VAL	CA-CB	6.28	1.68	1.54
2	D	72	SER	CB-OG	6.28	1.50	1.42
1	A	90	LYS	CA-C	6.28	1.69	1.52
2	B	82	LYS	CG-CD	6.28	1.73	1.52
1	G	52	SER	C-N	6.27	1.48	1.34
2	B	67	VAL	CB-CG1	6.27	1.66	1.52
1	E	41	THR	CA-C	6.26	1.69	1.52
2	D	77	HIS	C-O	6.26	1.35	1.23
1	C	20	HIS	CB-CG	6.25	1.61	1.50
1	E	63	ALA	CA-CB	6.25	1.65	1.52
2	H	50	THR	C-O	6.25	1.35	1.23
2	B	107	GLY	C-O	6.25	1.33	1.23
2	F	1	VAL	CB-CG2	6.25	1.66	1.52
2	F	7	GLU	CB-CG	6.24	1.64	1.52
1	C	8	THR	N-CA	6.24	1.58	1.46
1	G	56	LYS	N-CA	6.24	1.58	1.46
1	C	46	PHE	CD2-CE2	-6.24	1.26	1.39
1	G	112	HIS	CG-CD2	-6.24	1.25	1.35
2	H	52	ASP	CB-CG	6.23	1.64	1.51
1	C	103	HIS	C-N	-6.23	1.19	1.34
1	C	63	ALA	C-N	-6.23	1.19	1.34
2	D	106	LEU	C-O	6.23	1.35	1.23
1	E	44	PRO	CG-CD	6.23	1.71	1.50
2	F	67	VAL	C-O	6.23	1.35	1.23
1	A	45	HIS	CD2-NE2	-6.22	1.24	1.38
1	C	103	HIS	C-O	6.22	1.35	1.23
2	F	4	THR	C-N	-6.22	1.22	1.34
2	F	33	VAL	N-CA	6.22	1.58	1.46
2	D	45	PHE	CA-CB	6.21	1.67	1.53
1	C	64	ASP	CG-OD1	6.21	1.39	1.25
1	C	17	VAL	CB-CG1	6.21	1.65	1.52
1	A	14	TRP	CZ2-CH2	6.20	1.49	1.37
1	A	65	ALA	C-O	6.20	1.35	1.23
2	D	134	VAL	C-N	-6.20	1.19	1.34
2	B	117	HIS	CG-CD2	6.20	1.46	1.35
1	E	46	PHE	CG-CD2	-6.20	1.29	1.38
1	A	45	HIS	C-N	6.19	1.48	1.34
2	H	1	VAL	CB-CG2	6.19	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	116	GLU	C-O	-6.19	1.11	1.23
1	E	81	SER	CA-CB	6.18	1.62	1.52
1	A	58	HIS	ND1-CE1	6.18	1.50	1.34
2	B	134	VAL	CB-CG1	6.18	1.65	1.52
2	F	140	ALA	CA-CB	-6.18	1.39	1.52
1	E	103	HIS	CB-CG	6.18	1.61	1.50
2	H	124	PRO	C-N	-6.18	1.22	1.34
1	A	57	GLY	C-N	-6.17	1.19	1.34
1	E	45	HIS	CE1-NE2	6.17	1.46	1.32
2	D	133	VAL	N-CA	6.17	1.58	1.46
2	F	45	PHE	CB-CG	-6.17	1.40	1.51
2	D	60	VAL	C-O	6.16	1.35	1.23
2	D	99	ASP	CG-OD2	6.16	1.39	1.25
1	A	132	VAL	CB-CG2	6.16	1.65	1.52
1	G	21	ALA	N-CA	-6.16	1.34	1.46
1	G	133	SER	C-N	6.16	1.48	1.34
2	D	74	GLY	N-CA	6.16	1.55	1.46
1	A	73	VAL	C-O	6.16	1.35	1.23
2	D	97	HIS	CG-CD2	6.16	1.46	1.35
1	A	13	ALA	C-O	6.15	1.35	1.23
1	G	64	ASP	CG-OD2	6.15	1.39	1.25
1	E	12	ALA	CA-CB	6.15	1.65	1.52
1	C	129	LEU	CA-CB	6.14	1.67	1.53
2	B	24	GLY	C-N	-6.14	1.22	1.33
1	C	61	LYS	C-O	-6.14	1.11	1.23
1	G	56	LYS	CD-CE	-6.14	1.35	1.51
1	A	50	HIS	C-O	-6.14	1.11	1.23
1	E	139	LYS	CE-NZ	6.14	1.64	1.49
2	H	92	HIS	N-CA	6.14	1.58	1.46
2	F	17	LYS	C-O	6.13	1.35	1.23
2	H	57	ASN	C-O	6.13	1.35	1.23
1	E	103	HIS	CG-CD2	-6.13	1.25	1.35
2	H	140	ALA	C-O	-6.12	1.11	1.23
2	D	34	VAL	C-O	6.12	1.34	1.23
2	F	22	GLU	CD-OE2	6.12	1.32	1.25
1	G	141	ARG	C-OXT	-6.12	1.11	1.23
1	G	137	THR	CB-OG1	6.12	1.55	1.43
1	A	79	ALA	C-O	6.12	1.34	1.23
1	A	14	TRP	N-CA	6.11	1.58	1.46
2	B	40	ARG	CD-NE	6.11	1.56	1.46
1	E	125	LEU	C-N	6.11	1.48	1.34
1	G	119	PRO	CA-CB	6.11	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	42	PHE	CB-CG	-6.11	1.41	1.51
1	E	23	GLU	CD-OE1	6.11	1.32	1.25
1	G	61	LYS	CE-NZ	-6.11	1.33	1.49
1	G	87	HIS	CD2-NE2	-6.10	1.24	1.38
1	A	116	GLU	CA-CB	6.10	1.67	1.53
2	D	64	GLY	C-O	6.10	1.33	1.23
1	E	132	VAL	N-CA	6.10	1.58	1.46
1	G	19	ALA	C-N	6.10	1.48	1.34
2	B	56	GLY	C-N	6.10	1.48	1.34
1	G	16	LYS	CE-NZ	6.10	1.64	1.49
1	A	30	GLU	N-CA	6.10	1.58	1.46
2	B	63	HIS	CE1-NE2	6.09	1.46	1.32
2	D	119	GLY	C-N	-6.09	1.20	1.34
2	F	47	ASP	CG-OD1	6.09	1.39	1.25
2	H	139	ASN	CA-CB	6.09	1.69	1.53
1	E	28	ALA	C-N	6.08	1.48	1.34
1	A	68	ASN	C-O	6.08	1.34	1.23
1	E	10	VAL	C-O	6.08	1.34	1.23
2	F	4	THR	CA-CB	6.07	1.69	1.53
2	D	116	HIS	CG-CD2	6.07	1.46	1.35
1	G	93	VAL	CB-CG1	-6.07	1.40	1.52
1	G	36	PHE	CG-CD2	6.07	1.47	1.38
1	C	63	ALA	CA-CB	6.07	1.65	1.52
2	D	106	LEU	CA-CB	6.07	1.67	1.53
1	G	45	HIS	C-N	-6.07	1.20	1.34
1	C	16	LYS	C-O	-6.06	1.11	1.23
2	H	101	GLU	CA-CB	-6.06	1.40	1.53
1	E	83	LEU	N-CA	6.05	1.58	1.46
1	G	26	ALA	C-O	6.05	1.34	1.23
2	H	66	LYS	C-O	-6.05	1.11	1.23
1	E	46	PHE	CE1-CZ	6.05	1.48	1.37
2	D	116	HIS	N-CA	-6.05	1.34	1.46
2	D	125	PRO	CA-C	-6.05	1.40	1.52
2	D	72	SER	C-N	-6.05	1.20	1.34
2	F	47	ASP	CG-OD2	6.05	1.39	1.25
2	B	111	VAL	CA-C	6.04	1.68	1.52
1	C	135	VAL	C-N	-6.04	1.20	1.34
1	G	140	TYR	CD1-CE1	6.04	1.48	1.39
2	D	103	PHE	CD1-CE1	6.03	1.51	1.39
2	H	66	LYS	CA-C	6.03	1.68	1.52
2	H	62	ALA	CA-CB	6.03	1.65	1.52
2	D	119	GLY	N-CA	6.02	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	104	CYS	N-CA	-6.02	1.34	1.46
2	F	31	LEU	CG-CD1	6.01	1.74	1.51
1	E	82	ALA	N-CA	-6.01	1.34	1.46
1	E	123	ALA	CA-C	6.01	1.68	1.52
2	D	5	PRO	N-CD	-6.00	1.39	1.47
2	B	85	PHE	CG-CD2	-5.99	1.29	1.38
1	G	71	ALA	N-CA	5.98	1.58	1.46
1	E	46	PHE	CB-CG	5.98	1.61	1.51
1	A	47	ASP	N-CA	5.97	1.58	1.46
1	C	106	LEU	CB-CG	5.97	1.69	1.52
2	H	95	LYS	CE-NZ	5.97	1.64	1.49
1	C	29	LEU	CA-CB	-5.97	1.40	1.53
2	F	77	HIS	CA-CB	5.97	1.67	1.53
2	H	40	ARG	N-CA	5.96	1.58	1.46
1	C	22	GLY	N-CA	-5.96	1.37	1.46
1	G	118	THR	CB-CG2	5.96	1.72	1.52
1	C	37	PRO	C-N	-5.96	1.20	1.34
1	C	76	MET	CG-SD	5.95	1.96	1.81
1	A	124	SER	CA-C	-5.95	1.37	1.52
1	E	89	HIS	C-O	5.95	1.34	1.23
1	G	81	SER	CA-C	5.95	1.68	1.52
1	C	50	HIS	CG-ND1	-5.95	1.25	1.38
1	E	2	LEU	C-O	-5.95	1.12	1.23
1	C	20	HIS	CE1-NE2	-5.94	1.19	1.32
1	G	105	LEU	N-CA	-5.92	1.34	1.46
1	E	128	PHE	C-O	5.92	1.34	1.23
1	E	24	TYR	CD1-CE1	-5.92	1.30	1.39
2	B	4	THR	N-CA	-5.92	1.34	1.46
2	D	1	VAL	C-N	-5.92	1.20	1.34
1	G	98	PHE	CG-CD2	5.92	1.47	1.38
2	B	5	PRO	N-CA	-5.91	1.37	1.47
2	F	93	CYS	C-O	5.91	1.34	1.23
1	C	43	PHE	CA-C	5.91	1.68	1.52
2	F	100	PRO	CA-C	-5.91	1.41	1.52
2	H	118	PHE	CE2-CZ	5.90	1.48	1.37
1	G	134	THR	CA-CB	5.90	1.68	1.53
2	D	59	LYS	CG-CD	5.89	1.72	1.52
2	F	103	PHE	CA-CB	5.89	1.67	1.53
1	A	109	LEU	CA-CB	5.89	1.67	1.53
1	C	9	ASN	C-N	-5.89	1.20	1.34
2	H	145	TYR	C-N	-5.88	1.20	1.34
1	C	76	MET	CA-CB	5.88	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	35	TYR	N-CA	5.88	1.58	1.46
1	C	6	ASP	CG-OD1	5.88	1.38	1.25
1	G	140	TYR	C-N	5.88	1.47	1.34
2	H	6	VAL	CB-CG1	5.88	1.65	1.52
2	H	91	LEU	CA-CB	5.88	1.67	1.53
1	A	85	ASP	CG-OD1	5.88	1.38	1.25
2	F	49	SER	C-O	-5.87	1.12	1.23
2	D	66	LYS	C-N	5.87	1.47	1.34
1	E	118	THR	N-CA	5.87	1.58	1.46
2	D	95	LYS	CG-CD	5.87	1.72	1.52
2	F	53	ALA	CA-CB	5.86	1.64	1.52
1	C	12	ALA	CA-C	5.86	1.68	1.52
1	A	105	LEU	N-CA	-5.85	1.34	1.46
2	B	52	ASP	C-N	-5.85	1.20	1.34
2	B	112	CYS	C-O	5.85	1.34	1.23
1	A	75	ASP	CG-OD2	5.84	1.38	1.25
1	G	14	TRP	CA-CB	5.84	1.66	1.53
1	G	83	LEU	CA-CB	-5.84	1.40	1.53
2	D	92	HIS	CG-ND1	5.84	1.51	1.38
2	D	118	PHE	CA-C	-5.84	1.37	1.52
1	G	30	GLU	CA-CB	-5.84	1.41	1.53
1	A	57	GLY	N-CA	5.83	1.54	1.46
2	F	90	GLU	CA-CB	5.83	1.66	1.53
2	D	110	LEU	C-N	-5.82	1.20	1.34
1	E	8	THR	CB-OG1	-5.82	1.31	1.43
2	B	71	PHE	CB-CG	5.82	1.61	1.51
1	C	40	LYS	CE-NZ	5.82	1.63	1.49
1	C	62	VAL	CA-C	-5.82	1.37	1.52
1	C	141	ARG	C-O	5.82	1.34	1.23
1	C	37	PRO	N-CA	5.81	1.57	1.47
2	D	144	LYS	CE-NZ	5.80	1.63	1.49
2	H	129	ALA	N-CA	-5.80	1.34	1.46
1	C	24	TYR	CE1-CZ	-5.80	1.31	1.38
1	E	88	ALA	C-N	5.80	1.47	1.34
2	D	29	GLY	C-O	-5.79	1.14	1.23
2	B	41	PHE	CD2-CE2	-5.79	1.27	1.39
2	B	109	VAL	CB-CG2	-5.79	1.40	1.52
2	B	114	LEU	CA-CB	5.79	1.67	1.53
2	F	35	TYR	CA-CB	5.79	1.66	1.53
2	B	77	HIS	N-CA	5.79	1.57	1.46
1	C	35	SER	CB-OG	5.79	1.49	1.42
2	D	46	GLY	CA-C	-5.79	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	87	HIS	CG-ND1	5.79	1.51	1.38
1	C	33	PHE	N-CA	-5.79	1.34	1.46
1	C	87	HIS	CA-CB	5.79	1.66	1.53
2	H	42	PHE	CE1-CZ	-5.79	1.26	1.37
2	D	40	ARG	CD-NE	-5.78	1.36	1.46
1	G	121	VAL	N-CA	-5.78	1.34	1.46
1	G	83	LEU	C-N	-5.78	1.20	1.34
1	A	86	LEU	C-N	-5.77	1.20	1.34
1	C	21	ALA	N-CA	-5.76	1.34	1.46
1	G	134	THR	N-CA	-5.76	1.34	1.46
1	E	45	HIS	CG-CD2	-5.75	1.25	1.35
1	E	79	ALA	C-N	5.75	1.47	1.34
1	G	97	ASN	CG-ND2	5.75	1.47	1.32
2	D	76	ALA	CA-CB	5.75	1.64	1.52
1	A	10	VAL	CB-CG2	5.75	1.65	1.52
1	C	15	GLY	N-CA	5.75	1.54	1.46
2	H	11	VAL	N-CA	5.75	1.57	1.46
2	H	42	PHE	C-O	5.75	1.34	1.23
1	G	135	VAL	C-N	5.75	1.47	1.34
2	D	36	PRO	C-O	5.74	1.34	1.23
1	E	4	PRO	C-O	5.74	1.34	1.23
1	A	96	VAL	C-N	5.74	1.47	1.34
2	B	94	ASP	CG-OD2	5.74	1.38	1.25
2	H	115	ALA	CA-CB	5.74	1.64	1.52
2	F	41	PHE	N-CA	5.73	1.57	1.46
2	F	49	SER	CB-OG	5.73	1.49	1.42
1	A	113	LEU	CA-CB	5.73	1.67	1.53
2	B	109	VAL	N-CA	-5.73	1.34	1.46
2	F	71	PHE	CD1-CE1	5.73	1.50	1.39
2	F	100	PRO	CG-CD	5.73	1.69	1.50
1	G	18	GLY	CA-C	5.73	1.61	1.51
1	C	72	HIS	CG-ND1	-5.73	1.26	1.38
1	E	100	LEU	N-CA	5.72	1.57	1.46
1	G	80	LEU	CA-CB	-5.72	1.40	1.53
1	G	128	PHE	N-CA	-5.72	1.34	1.46
2	B	23	VAL	CB-CG2	5.71	1.64	1.52
1	A	124	SER	N-CA	5.71	1.57	1.46
2	D	26	GLU	CB-CG	5.71	1.63	1.52
1	G	47	ASP	CB-CG	5.71	1.63	1.51
2	D	41	PHE	CB-CG	5.71	1.61	1.51
2	D	100	PRO	CA-CB	-5.71	1.42	1.53
1	A	66	LEU	CA-C	5.70	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	42	PHE	C-O	5.70	1.34	1.23
2	F	104	ARG	CD-NE	-5.70	1.36	1.46
2	F	90	GLU	CD-OE1	-5.70	1.19	1.25
2	H	69	GLY	CA-C	5.70	1.60	1.51
2	D	91	LEU	C-O	5.69	1.34	1.23
2	D	97	HIS	C-N	5.69	1.47	1.34
2	D	93	CYS	N-CA	5.69	1.57	1.46
2	H	139	ASN	N-CA	-5.69	1.34	1.46
2	B	122	PHE	CA-CB	-5.68	1.41	1.53
1	E	3	SER	C-N	-5.68	1.23	1.34
1	G	114	PRO	CG-CD	5.68	1.69	1.50
1	G	52	SER	N-CA	-5.68	1.34	1.46
2	H	76	ALA	CA-CB	5.68	1.64	1.52
2	D	145	TYR	CD1-CE1	-5.68	1.30	1.39
1	E	14	TRP	CG-CD1	5.67	1.44	1.36
2	D	51	PRO	N-CD	5.67	1.55	1.47
1	A	19	ALA	C-O	5.67	1.34	1.23
2	F	15	TRP	C-N	5.66	1.43	1.33
1	E	92	ARG	N-CA	5.66	1.57	1.46
2	D	98	VAL	C-O	-5.66	1.12	1.23
2	H	5	PRO	CG-CD	5.66	1.69	1.50
2	B	59	LYS	CB-CG	5.66	1.67	1.52
1	A	116	GLU	CB-CG	5.65	1.62	1.52
1	E	45	HIS	C-N	-5.65	1.21	1.34
2	D	122	PHE	CB-CG	-5.65	1.41	1.51
1	E	38	THR	CA-C	5.65	1.67	1.52
2	H	21	ASP	C-O	5.65	1.34	1.23
1	G	86	LEU	CB-CG	5.64	1.69	1.52
2	F	15	TRP	CD2-CE3	5.64	1.48	1.40
1	E	92	ARG	C-N	5.64	1.47	1.34
1	A	18	GLY	C-O	5.64	1.32	1.23
1	C	140	TYR	CD1-CE1	5.64	1.47	1.39
1	G	26	ALA	N-CA	-5.64	1.35	1.46
1	C	118	THR	CB-CG2	5.64	1.71	1.52
2	B	22	GLU	CG-CD	-5.63	1.43	1.51
2	B	137	VAL	N-CA	5.63	1.57	1.46
1	G	90	LYS	CB-CG	5.63	1.67	1.52
2	B	12	THR	CB-CG2	5.63	1.71	1.52
2	D	37	TRP	CG-CD1	-5.63	1.28	1.36
1	C	95	PRO	C-O	-5.63	1.11	1.23
2	H	61	LYS	C-N	-5.62	1.21	1.34
2	B	36	PRO	CA-CB	5.62	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	95	LYS	C-O	5.62	1.34	1.23
2	B	63	HIS	CD2-NE2	-5.62	1.25	1.38
1	A	103	HIS	C-O	5.62	1.34	1.23
2	F	88	LEU	CG-CD1	5.62	1.72	1.51
1	C	114	PRO	CA-C	5.61	1.64	1.52
1	A	91	LEU	CB-CG	5.61	1.68	1.52
2	D	111	VAL	C-O	-5.61	1.12	1.23
2	F	72	SER	CB-OG	5.61	1.49	1.42
2	F	75	LEU	CA-CB	5.61	1.66	1.53
1	A	127	LYS	CD-CE	5.61	1.65	1.51
1	E	104	CYS	CA-CB	5.60	1.66	1.53
2	F	37	TRP	CB-CG	-5.60	1.40	1.50
1	G	15	GLY	C-O	-5.60	1.14	1.23
1	A	83	LEU	N-CA	5.60	1.57	1.46
1	G	44	PRO	CG-CD	-5.59	1.32	1.50
2	F	95	LYS	C-O	5.59	1.33	1.23
1	E	138	SER	C-O	5.59	1.33	1.23
2	F	38	THR	CA-C	5.59	1.67	1.52
1	G	112	HIS	ND1-CE1	5.59	1.48	1.34
1	G	112	HIS	N-CA	-5.59	1.35	1.46
1	A	45	HIS	CG-ND1	5.58	1.51	1.38
2	D	113	VAL	N-CA	-5.58	1.35	1.46
1	E	118	THR	C-N	5.58	1.44	1.34
2	H	22	GLU	C-N	5.58	1.46	1.34
1	E	134	THR	CA-C	5.58	1.67	1.52
1	C	132	VAL	CB-CG2	-5.58	1.41	1.52
2	D	115	ALA	C-O	-5.58	1.12	1.23
2	B	97	HIS	CB-CG	5.57	1.60	1.50
2	D	75	LEU	N-CA	5.57	1.57	1.46
2	H	59	LYS	CB-CG	5.57	1.67	1.52
1	E	33	PHE	CG-CD1	5.57	1.47	1.38
1	C	33	PHE	CD1-CE1	-5.57	1.28	1.39
1	A	122	HIS	CB-CG	-5.57	1.40	1.50
2	B	23	VAL	CB-CG1	-5.56	1.41	1.52
1	A	30	GLU	CA-CB	-5.56	1.41	1.53
2	B	14	LEU	C-N	-5.56	1.21	1.34
2	F	101	GLU	CB-CG	5.56	1.62	1.52
1	C	74	ASP	CG-OD2	-5.56	1.12	1.25
2	D	66	LYS	CG-CD	5.55	1.71	1.52
1	G	24	TYR	CA-CB	-5.55	1.41	1.53
1	G	85	ASP	CG-OD1	5.55	1.38	1.25
1	G	28	ALA	N-CA	-5.55	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	PHE	CE1-CZ	-5.55	1.26	1.37
1	C	20	HIS	CD2-NE2	5.55	1.53	1.42
2	B	118	PHE	CB-CG	5.54	1.60	1.51
2	D	78	LEU	C-O	5.54	1.33	1.23
1	C	62	VAL	CB-CG1	5.54	1.64	1.52
1	C	86	LEU	CB-CG	5.54	1.68	1.52
1	E	68	ASN	CG-OD1	5.54	1.36	1.24
1	G	78	ASN	CG-ND2	5.54	1.46	1.32
1	A	80	LEU	C-O	5.53	1.33	1.23
2	B	109	VAL	CB-CG1	5.53	1.64	1.52
1	E	18	GLY	C-O	5.53	1.32	1.23
1	E	130	ALA	C-N	5.53	1.46	1.34
1	G	108	THR	C-N	5.53	1.46	1.34
2	B	145	TYR	CE2-CZ	5.53	1.45	1.38
2	B	32	LEU	C-N	5.53	1.46	1.34
1	G	36	PHE	N-CA	-5.53	1.35	1.46
2	H	90	GLU	CB-CG	-5.53	1.41	1.52
2	D	88	LEU	CA-CB	5.52	1.66	1.53
2	F	143	HIS	CA-CB	5.52	1.66	1.53
1	A	86	LEU	CA-C	5.52	1.67	1.52
2	B	21	ASP	CA-CB	-5.52	1.41	1.53
2	D	1	VAL	C-O	5.51	1.33	1.23
2	B	113	VAL	C-N	-5.51	1.21	1.34
2	D	136	GLY	CA-C	5.51	1.60	1.51
1	A	81	SER	N-CA	5.51	1.57	1.46
2	H	38	THR	CA-C	5.51	1.67	1.52
2	D	102	ASN	CG-ND2	5.50	1.46	1.32
2	B	58	PRO	CG-CD	5.50	1.68	1.50
1	C	80	LEU	CB-CG	-5.50	1.36	1.52
2	D	103	PHE	C-O	5.50	1.33	1.23
2	D	18	VAL	CB-CG2	5.49	1.64	1.52
2	F	26	GLU	CB-CG	5.49	1.62	1.52
1	G	70	VAL	N-CA	5.49	1.57	1.46
2	F	57	ASN	C-O	5.48	1.33	1.23
2	D	37	TRP	CE2-CZ2	-5.48	1.30	1.39
2	F	37	TRP	CD2-CE3	-5.48	1.32	1.40
2	H	23	VAL	CA-CB	5.48	1.66	1.54
1	A	85	ASP	C-O	-5.47	1.12	1.23
1	A	91	LEU	C-O	5.47	1.33	1.23
2	D	103	PHE	CG-CD1	-5.47	1.30	1.38
2	D	127	GLN	N-CA	-5.47	1.35	1.46
2	B	33	VAL	CB-CG1	5.47	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	62	ALA	CA-CB	5.47	1.64	1.52
1	A	50	HIS	CA-CB	-5.46	1.42	1.53
2	H	66	LYS	CD-CE	5.46	1.65	1.51
2	B	36	PRO	N-CD	5.46	1.55	1.47
2	D	71	PHE	N-CA	-5.46	1.35	1.46
1	E	2	LEU	CA-CB	-5.46	1.41	1.53
2	F	40	ARG	NE-CZ	5.46	1.40	1.33
1	G	116	GLU	C-N	-5.46	1.21	1.34
1	C	96	VAL	C-O	5.45	1.33	1.23
2	F	141	LEU	CA-CB	-5.45	1.41	1.53
2	D	82	LYS	CB-CG	5.44	1.67	1.52
2	H	136	GLY	N-CA	-5.44	1.37	1.46
2	F	41	PHE	CD1-CE1	5.44	1.50	1.39
2	B	31	LEU	CG-CD2	5.44	1.72	1.51
1	G	40	LYS	CD-CE	5.44	1.64	1.51
2	B	19	ASN	CA-C	5.43	1.67	1.52
1	E	8	THR	C-O	-5.43	1.13	1.23
2	H	27	ALA	C-N	5.43	1.46	1.34
2	F	121	GLU	CD-OE1	-5.42	1.19	1.25
2	F	137	VAL	CB-CG2	-5.42	1.41	1.52
1	G	37	PRO	CA-CB	-5.42	1.42	1.53
2	B	113	VAL	N-CA	5.42	1.57	1.46
2	H	66	LYS	CB-CG	5.42	1.67	1.52
1	A	62	VAL	C-N	-5.42	1.21	1.34
1	C	125	LEU	C-O	5.42	1.33	1.23
2	B	57	ASN	N-CA	5.42	1.57	1.46
1	G	7	LYS	CA-CB	5.42	1.65	1.53
1	A	50	HIS	CG-CD2	5.41	1.45	1.35
1	C	34	LEU	C-N	-5.41	1.21	1.34
1	E	125	LEU	CG-CD2	5.41	1.71	1.51
2	B	84	THR	C-O	-5.41	1.13	1.23
1	E	32	MET	C-N	-5.41	1.21	1.34
1	G	27	GLU	C-O	5.41	1.33	1.23
2	D	90	GLU	CB-CG	5.41	1.62	1.52
1	G	11	LYS	C-O	5.41	1.33	1.23
1	E	26	ALA	C-O	5.40	1.33	1.23
2	F	26	GLU	CG-CD	5.40	1.60	1.51
2	B	124	PRO	C-O	5.40	1.34	1.23
2	D	138	ALA	C-O	-5.40	1.13	1.23
2	B	137	VAL	CB-CG1	5.40	1.64	1.52
1	E	30	GLU	CA-C	5.40	1.67	1.52
2	D	34	VAL	CB-CG1	5.40	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	80	ASN	CA-C	-5.39	1.39	1.52
2	B	90	GLU	C-N	-5.39	1.21	1.34
2	B	26	GLU	CG-CD	5.39	1.60	1.51
1	C	80	LEU	N-CA	5.39	1.57	1.46
1	C	87	HIS	C-N	5.38	1.46	1.34
1	E	97	ASN	C-O	5.38	1.33	1.23
2	D	62	ALA	C-O	5.38	1.33	1.23
2	H	130	TYR	C-N	5.38	1.46	1.34
1	A	33	PHE	CD2-CE2	5.38	1.50	1.39
2	D	80	ASN	C-O	5.38	1.33	1.23
1	C	33	PHE	CE1-CZ	5.37	1.47	1.37
1	G	84	SER	CA-CB	-5.37	1.44	1.52
2	D	38	THR	CB-OG1	5.37	1.53	1.43
2	D	135	ALA	C-O	5.37	1.33	1.23
1	G	78	ASN	C-N	5.37	1.46	1.34
2	B	73	ASP	C-O	5.36	1.33	1.23
2	D	31	LEU	CA-C	5.36	1.66	1.52
1	G	27	GLU	CD-OE1	5.36	1.31	1.25
2	D	104	ARG	CA-CB	5.36	1.65	1.53
1	E	87	HIS	C-N	-5.36	1.21	1.34
2	B	21	ASP	C-N	-5.36	1.21	1.34
2	F	72	SER	C-N	-5.36	1.21	1.34
2	H	41	PHE	CB-CG	-5.36	1.42	1.51
2	F	37	TRP	CE3-CZ3	5.36	1.47	1.38
1	A	43	PHE	CE1-CZ	5.36	1.47	1.37
2	D	136	GLY	N-CA	-5.36	1.38	1.46
2	H	64	GLY	C-O	5.36	1.32	1.23
1	C	36	PHE	N-CA	-5.35	1.35	1.46
1	E	98	PHE	CD2-CE2	5.35	1.50	1.39
1	G	139	LYS	CD-CE	5.35	1.64	1.51
2	D	40	ARG	CZ-NH2	5.35	1.40	1.33
1	G	123	ALA	C-O	-5.34	1.13	1.23
2	D	125	PRO	N-CA	-5.34	1.38	1.47
2	D	1	VAL	CA-CB	5.34	1.66	1.54
1	G	35	SER	CA-CB	5.34	1.60	1.52
2	D	85	PHE	C-N	-5.34	1.21	1.34
1	A	96	VAL	N-CA	5.34	1.57	1.46
2	B	130	TYR	CE2-CZ	5.34	1.45	1.38
1	G	62	VAL	N-CA	5.34	1.57	1.46
2	B	78	LEU	C-N	-5.33	1.21	1.34
1	C	74	ASP	C-N	5.33	1.46	1.34
2	B	50	THR	C-O	-5.33	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	101	GLU	CD-OE1	5.33	1.31	1.25
1	E	56	LYS	CD-CE	5.33	1.64	1.51
2	F	94	ASP	CB-CG	-5.33	1.40	1.51
1	E	113	LEU	CG-CD2	5.33	1.71	1.51
1	A	97	ASN	CG-ND2	5.33	1.46	1.32
1	E	31	ARG	CZ-NH1	5.33	1.40	1.33
1	E	47	ASP	CB-CG	5.33	1.62	1.51
2	F	40	ARG	CB-CG	5.33	1.67	1.52
1	E	140	TYR	CE1-CZ	5.32	1.45	1.38
2	B	11	VAL	CB-CG2	5.32	1.64	1.52
2	B	35	TYR	CG-CD1	5.32	1.46	1.39
1	C	29	LEU	N-CA	-5.32	1.35	1.46
1	E	72	HIS	CG-ND1	5.32	1.50	1.38
1	A	140	TYR	CB-CG	-5.32	1.43	1.51
1	E	46	PHE	CA-CB	5.32	1.65	1.53
1	A	110	ALA	C-O	5.31	1.33	1.23
1	C	50	HIS	CA-C	-5.31	1.39	1.52
1	C	112	HIS	ND1-CE1	5.31	1.48	1.34
1	E	139	LYS	C-N	-5.31	1.21	1.34
1	G	141	ARG	CA-CB	-5.31	1.42	1.53
1	A	62	VAL	C-O	5.31	1.33	1.23
2	D	77	HIS	CG-ND1	-5.31	1.27	1.38
1	E	72	HIS	C-O	-5.31	1.13	1.23
1	G	140	TYR	CG-CD2	5.31	1.46	1.39
2	B	87	THR	CA-CB	5.30	1.67	1.53
1	C	48	LEU	C-O	-5.30	1.13	1.23
2	B	24	GLY	CA-C	-5.30	1.43	1.51
2	H	23	VAL	CB-CG2	-5.30	1.41	1.52
1	C	92	ARG	CG-CD	5.29	1.65	1.51
2	D	33	VAL	CB-CG1	5.29	1.64	1.52
1	G	105	LEU	C-O	5.29	1.33	1.23
1	C	132	VAL	C-O	5.29	1.33	1.23
1	E	122	HIS	C-N	-5.29	1.21	1.34
2	D	93	CYS	CA-CB	-5.29	1.42	1.53
2	F	22	GLU	CA-CB	5.29	1.65	1.53
2	D	22	GLU	C-O	5.28	1.33	1.23
2	H	49	SER	CA-CB	5.28	1.60	1.52
1	C	30	GLU	CG-CD	5.28	1.59	1.51
1	E	6	ASP	N-CA	5.28	1.56	1.46
1	C	82	ALA	N-CA	5.28	1.56	1.46
1	A	95	PRO	C-O	5.27	1.33	1.23
2	H	40	ARG	CD-NE	-5.27	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	108	ASN	CG-OD1	5.27	1.35	1.24
2	H	58	PRO	CA-C	5.27	1.63	1.52
1	A	87	HIS	CG-ND1	-5.27	1.27	1.38
2	B	3	LEU	CA-CB	-5.27	1.41	1.53
1	E	141	ARG	CD-NE	-5.27	1.37	1.46
1	A	43	PHE	CG-CD2	5.26	1.46	1.38
2	B	13	ALA	C-O	5.26	1.33	1.23
2	B	57	ASN	CG-OD1	5.26	1.35	1.24
2	B	59	LYS	N-CA	-5.26	1.35	1.46
1	C	24	TYR	CE2-CZ	5.26	1.45	1.38
2	B	38	THR	C-N	-5.26	1.22	1.34
1	C	55	VAL	C-N	-5.26	1.22	1.34
2	D	37	TRP	CZ2-CH2	-5.26	1.27	1.37
2	H	84	THR	N-CA	5.26	1.56	1.46
1	G	8	THR	CA-CB	5.25	1.67	1.53
1	A	23	GLU	CG-CD	-5.25	1.44	1.51
2	H	2	HIS	CE1-NE2	-5.25	1.20	1.32
1	E	74	ASP	CB-CG	-5.25	1.40	1.51
2	H	43	GLU	CD-OE2	5.25	1.31	1.25
1	G	118	THR	N-CA	5.25	1.56	1.46
2	D	99	ASP	CA-CB	-5.24	1.42	1.53
2	F	37	TRP	CZ3-CH2	-5.24	1.31	1.40
1	E	48	LEU	C-N	5.24	1.46	1.34
2	F	92	HIS	CD2-NE2	-5.24	1.26	1.38
2	D	60	VAL	CB-CG1	-5.24	1.41	1.52
2	B	19	ASN	N-CA	5.24	1.56	1.46
2	D	15	TRP	C-O	5.23	1.33	1.23
2	F	11	VAL	N-CA	5.23	1.56	1.46
1	E	124	SER	N-CA	5.23	1.56	1.46
1	G	61	LYS	N-CA	5.23	1.56	1.46
1	G	91	LEU	N-CA	-5.22	1.35	1.46
1	G	32	MET	N-CA	-5.22	1.35	1.46
2	D	40	ARG	NE-CZ	-5.22	1.26	1.33
2	F	121	GLU	CD-OE2	-5.21	1.20	1.25
2	B	74	GLY	N-CA	-5.21	1.38	1.46
2	H	128	ALA	CA-CB	5.21	1.63	1.52
1	C	5	ALA	N-CA	5.20	1.56	1.46
1	C	136	LEU	C-N	5.20	1.46	1.34
1	E	98	PHE	CG-CD1	5.20	1.46	1.38
2	H	34	VAL	CA-CB	-5.20	1.43	1.54
1	A	21	ALA	N-CA	-5.20	1.35	1.46
2	F	100	PRO	N-CD	5.20	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	50	HIS	CG-CD2	5.20	1.44	1.35
2	F	120	LYS	CE-NZ	5.20	1.62	1.49
1	C	32	MET	CB-CG	5.20	1.68	1.51
1	G	128	PHE	CG-CD2	5.20	1.46	1.38
1	A	36	PHE	CD2-CE2	5.19	1.49	1.39
2	D	36	PRO	N-CD	-5.19	1.40	1.47
1	G	47	ASP	CG-OD1	5.19	1.37	1.25
1	E	132	VAL	CA-CB	-5.19	1.43	1.54
2	F	27	ALA	C-N	-5.19	1.22	1.34
2	H	45	PHE	CD1-CE1	5.19	1.49	1.39
2	D	128	ALA	C-N	-5.19	1.22	1.34
2	B	53	ALA	C-N	-5.19	1.22	1.34
1	C	72	HIS	CA-C	-5.19	1.39	1.52
2	F	73	ASP	C-N	-5.19	1.23	1.33
2	B	61	LYS	CE-NZ	5.18	1.62	1.49
2	F	122	PHE	C-O	5.18	1.33	1.23
2	H	100	PRO	N-CD	-5.18	1.40	1.47
1	G	11	LYS	CE-NZ	5.18	1.62	1.49
2	H	38	THR	C-N	-5.18	1.22	1.34
2	H	57	ASN	CA-CB	-5.18	1.39	1.53
1	C	128	PHE	CD1-CE1	5.18	1.49	1.39
1	G	7	LYS	CE-NZ	5.18	1.61	1.49
1	C	127	LYS	C-O	5.17	1.33	1.23
1	E	51	GLY	N-CA	-5.17	1.38	1.46
2	F	63	HIS	CA-C	5.17	1.66	1.52
2	F	111	VAL	N-CA	-5.17	1.36	1.46
2	D	103	PHE	CG-CD2	-5.17	1.30	1.38
1	C	60	LYS	CE-NZ	5.17	1.61	1.49
1	G	43	PHE	CE2-CZ	5.17	1.47	1.37
1	A	1	VAL	N-CA	5.16	1.56	1.46
1	E	72	HIS	CA-CB	-5.16	1.42	1.53
1	C	60	LYS	N-CA	5.16	1.56	1.46
1	C	116	GLU	N-CA	-5.16	1.36	1.46
2	D	138	ALA	C-N	5.16	1.46	1.34
2	H	54	VAL	CA-C	-5.16	1.39	1.52
1	G	130	ALA	CA-CB	-5.16	1.41	1.52
2	F	125	PRO	C-O	5.16	1.33	1.23
1	A	111	ALA	CA-C	5.15	1.66	1.52
1	A	39	THR	C-N	-5.15	1.22	1.34
2	H	34	VAL	N-CA	5.15	1.56	1.46
1	A	31	ARG	NE-CZ	-5.15	1.26	1.33
2	F	37	TRP	CG-CD1	-5.14	1.29	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	55	MET	N-CA	5.14	1.56	1.46
2	H	73	ASP	CG-OD2	5.14	1.37	1.25
2	H	82	LYS	CD-CE	-5.14	1.38	1.51
2	B	15	TRP	C-N	5.14	1.42	1.33
1	C	47	ASP	N-CA	5.14	1.56	1.46
1	A	52	SER	CB-OG	5.13	1.49	1.42
1	C	49	SER	C-O	5.13	1.33	1.23
2	H	103	PHE	C-O	5.13	1.33	1.23
1	A	104	CYS	N-CA	-5.13	1.36	1.46
2	F	52	ASP	N-CA	-5.13	1.36	1.46
1	A	107	VAL	C-O	5.13	1.33	1.23
2	B	102	ASN	N-CA	5.13	1.56	1.46
1	C	33	PHE	CA-CB	5.13	1.65	1.53
2	H	45	PHE	CG-CD1	-5.13	1.31	1.38
1	A	7	LYS	CE-NZ	5.13	1.61	1.49
2	H	15	TRP	CD2-CE2	5.13	1.47	1.41
1	E	46	PHE	CG-CD1	5.12	1.46	1.38
2	F	12	THR	C-O	5.12	1.33	1.23
2	F	28	LEU	C-O	5.12	1.33	1.23
2	F	146	HIS	ND1-CE1	-5.12	1.22	1.34
1	E	55	VAL	CA-CB	-5.11	1.44	1.54
2	D	146	HIS	CE1-NE2	-5.11	1.20	1.32
2	B	106	LEU	CG-CD2	5.11	1.70	1.51
1	E	36	PHE	CB-CG	-5.11	1.42	1.51
1	E	80	LEU	C-O	5.11	1.33	1.23
1	A	51	GLY	N-CA	5.11	1.53	1.46
1	A	137	THR	CA-CB	5.11	1.66	1.53
2	H	127	GLN	C-N	-5.11	1.22	1.34
1	E	132	VAL	CB-CG2	5.10	1.63	1.52
2	H	65	LYS	CA-CB	-5.10	1.42	1.53
2	B	92	HIS	CB-CG	5.10	1.59	1.50
2	D	134	VAL	CA-CB	-5.10	1.44	1.54
2	B	66	LYS	CA-CB	-5.10	1.42	1.53
2	F	144	LYS	CE-NZ	5.09	1.61	1.49
1	G	8	THR	C-N	-5.09	1.22	1.34
2	F	125	PRO	N-CA	-5.09	1.38	1.47
2	H	122	PHE	CG-CD1	-5.09	1.31	1.38
2	F	38	THR	CB-CG2	5.09	1.69	1.52
1	G	82	ALA	N-CA	-5.09	1.36	1.46
2	F	71	PHE	CD2-CE2	5.08	1.49	1.39
2	B	29	GLY	CA-C	5.08	1.59	1.51
1	C	99	LYS	CA-C	5.08	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	98	PHE	CA-C	5.08	1.66	1.52
1	E	138	SER	N-CA	-5.08	1.36	1.46
1	C	117	PHE	CA-CB	5.08	1.65	1.53
2	D	143	HIS	CA-CB	5.08	1.65	1.53
1	G	45	HIS	CG-ND1	-5.08	1.27	1.38
1	G	48	LEU	N-CA	-5.08	1.36	1.46
2	F	117	HIS	C-O	5.08	1.33	1.23
1	A	112	HIS	C-N	-5.08	1.22	1.34
2	B	5	PRO	N-CD	-5.08	1.40	1.47
2	B	12	THR	N-CA	-5.08	1.36	1.46
1	G	115	ALA	CA-C	-5.08	1.39	1.52
1	C	84	SER	N-CA	-5.07	1.36	1.46
2	B	123	THR	CA-CB	5.07	1.66	1.53
1	C	11	LYS	CB-CG	5.07	1.66	1.52
2	H	26	GLU	CA-CB	-5.07	1.42	1.53
1	G	89	HIS	CA-CB	-5.07	1.42	1.53
1	E	64	ASP	CG-OD1	-5.07	1.13	1.25
1	E	81	SER	CB-OG	5.07	1.48	1.42
1	E	68	ASN	C-O	5.06	1.32	1.23
1	E	96	VAL	CB-CG2	-5.06	1.42	1.52
2	F	98	VAL	CB-CG1	5.06	1.63	1.52
2	D	126	VAL	N-CA	5.06	1.56	1.46
2	D	146	HIS	C-O	5.05	1.32	1.23
2	H	52	ASP	CA-CB	5.05	1.65	1.53
1	C	65	ALA	CA-C	5.05	1.66	1.52
1	C	85	ASP	N-CA	5.05	1.56	1.46
2	B	57	ASN	CG-ND2	5.04	1.45	1.32
2	B	78	LEU	CA-C	-5.04	1.39	1.52
1	C	112	HIS	CG-ND1	-5.04	1.27	1.38
2	F	95	LYS	CA-CB	5.04	1.65	1.53
2	F	106	LEU	CG-CD2	5.04	1.70	1.51
2	B	75	LEU	CA-CB	-5.04	1.42	1.53
2	F	101	GLU	CG-CD	-5.04	1.44	1.51
1	A	4	PRO	N-CD	5.04	1.54	1.47
1	G	122	HIS	CA-CB	-5.04	1.42	1.53
2	F	145	TYR	CE2-CZ	-5.03	1.32	1.38
2	D	122	PHE	C-O	5.03	1.32	1.23
1	C	65	ALA	N-CA	-5.03	1.36	1.46
1	A	3	SER	C-O	-5.03	1.13	1.23
2	H	59	LYS	CA-CB	5.03	1.65	1.53
1	A	77	PRO	CB-CG	5.03	1.75	1.50
2	B	97	HIS	ND1-CE1	5.02	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	12	ALA	N-CA	-5.02	1.36	1.46
1	A	29	LEU	C-O	5.02	1.32	1.23
1	C	124	SER	N-CA	-5.01	1.36	1.46
2	H	17	LYS	C-O	5.01	1.32	1.23
2	D	108	ASN	C-O	5.01	1.32	1.23
2	D	111	VAL	CB-CG2	5.01	1.63	1.52
1	C	14	TRP	CG-CD2	-5.01	1.35	1.43
1	E	70	VAL	C-O	5.01	1.32	1.23
1	G	86	LEU	C-O	-5.01	1.13	1.23
1	G	64	ASP	N-CA	-5.01	1.36	1.46
1	A	32	MET	CG-SD	5.00	1.94	1.81
1	C	4	PRO	CA-CB	-5.00	1.43	1.53
1	E	50	HIS	CG-CD2	-5.00	1.27	1.35
1	A	56	LYS	C-O	-5.00	1.13	1.23

All (4139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	31	ARG	NE-CZ-NH1	103.78	172.19	120.30
1	E	31	ARG	NE-CZ-NH2	-80.58	80.01	120.30
1	G	141	ARG	NE-CZ-NH2	-63.78	88.41	120.30
1	E	42	TYR	CB-CG-CD2	60.94	157.56	121.00
2	F	30	ARG	NE-CZ-NH1	-54.59	93.01	120.30
1	E	42	TYR	CB-CG-CD1	-53.38	88.97	121.00
2	H	40	ARG	NE-CZ-NH2	-50.17	95.21	120.30
1	E	33	PHE	CB-CG-CD2	41.52	149.86	120.80
2	D	40	ARG	CD-NE-CZ	39.62	179.07	123.60
2	F	42	PHE	CB-CG-CD2	38.65	147.85	120.80
2	B	40	ARG	CD-NE-CZ	37.76	176.46	123.60
1	C	31	ARG	NE-CZ-NH2	-36.71	101.95	120.30
2	F	40	ARG	NE-CZ-NH1	35.84	138.22	120.30
1	G	126	ASP	CB-CG-OD1	35.55	150.30	118.30
1	C	141	ARG	NE-CZ-NH1	35.40	138.00	120.30
1	C	31	ARG	NE-CZ-NH1	35.00	137.80	120.30
2	F	42	PHE	CB-CG-CD1	-34.94	96.34	120.80
2	F	40	ARG	NE-CZ-NH2	-34.38	103.11	120.30
2	H	104	ARG	NE-CZ-NH1	34.07	137.33	120.30
2	B	47	ASP	CB-CG-OD1	33.98	148.88	118.30
1	A	24	TYR	CB-CG-CD2	-33.58	100.85	121.00
2	B	79	ASP	CB-CG-OD1	33.09	148.08	118.30
2	F	35	TYR	CB-CG-CD1	32.71	140.63	121.00
1	E	33	PHE	CB-CG-CD1	-32.57	98.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	141	ARG	NH1-CZ-NH2	31.44	153.98	119.40
2	B	104	ARG	NE-CZ-NH2	31.40	136.00	120.30
2	F	47	ASP	CB-CG-OD1	31.06	146.26	118.30
2	B	35	TYR	CB-CG-CD2	31.00	139.60	121.00
1	A	128	PHE	CB-CG-CD2	30.07	141.85	120.80
1	A	92	ARG	NE-CZ-NH1	-29.78	105.41	120.30
2	H	79	ASP	CB-CG-OD1	29.26	144.63	118.30
1	A	128	PHE	CB-CG-CD1	-28.43	100.90	120.80
1	C	24	TYR	CB-CG-CD1	28.37	138.02	121.00
2	H	85	PHE	CB-CG-CD2	28.26	140.58	120.80
2	F	90	GLU	OE1-CD-OE2	28.05	156.96	123.30
1	C	64	ASP	CB-CG-OD1	-27.83	93.25	118.30
1	C	36	PHE	CB-CG-CD2	27.81	140.26	120.80
2	B	79	ASP	CB-CG-OD2	-27.59	93.47	118.30
2	F	23	VAL	CA-C-N	27.54	171.29	116.20
1	G	83	LEU	CA-CB-CG	27.21	177.88	115.30
2	D	101	GLU	OE1-CD-OE2	27.11	155.83	123.30
2	F	104	ARG	NE-CZ-NH1	27.03	133.81	120.30
2	F	23	VAL	C-N-CA	26.62	178.20	122.30
1	C	6	ASP	CB-CG-OD1	-26.44	94.50	118.30
2	H	35	TYR	CB-CG-CD2	-26.33	105.20	121.00
2	B	121	GLU	OE1-CD-OE2	26.24	154.79	123.30
1	A	85	ASP	CB-CG-OD2	26.19	141.87	118.30
1	C	46	PHE	CB-CG-CD1	-25.59	102.89	120.80
1	A	24	TYR	CB-CG-CD1	25.43	136.26	121.00
1	A	42	TYR	CG-CD1-CE1	25.29	141.53	121.30
2	F	35	TYR	CB-CG-CD2	-25.14	105.92	121.00
2	B	130	TYR	CB-CG-CD1	-25.10	105.94	121.00
2	B	104	ARG	NE-CZ-NH1	-24.89	107.85	120.30
2	H	104	ARG	NE-CZ-NH2	-24.72	107.94	120.30
2	H	47	ASP	CA-CB-CG	24.71	167.77	113.40
2	D	104	ARG	NE-CZ-NH2	-24.64	107.98	120.30
2	F	135	ALA	C-N-CA	24.59	173.95	122.30
2	B	52	ASP	CB-CG-OD2	-24.50	96.25	118.30
1	G	126	ASP	CB-CG-OD2	-24.43	96.31	118.30
1	G	140	TYR	CB-CG-CD1	-24.21	106.47	121.00
2	D	121	GLU	CA-CB-CG	24.15	166.53	113.40
2	B	30	ARG	NE-CZ-NH1	-24.09	108.25	120.30
1	E	85	ASP	CB-CG-OD2	23.99	139.89	118.30
1	A	122	HIS	CA-CB-CG	23.90	154.23	113.60
1	G	141	ARG	CA-CB-CG	23.65	165.44	113.40
2	D	87	THR	O-C-N	23.47	160.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	79	ASP	CB-CG-OD2	-23.32	97.31	118.30
1	E	31	ARG	CD-NE-CZ	23.26	156.16	123.60
2	F	16	GLY	C-N-CA	23.06	179.36	121.70
1	A	100	LEU	C-N-CA	23.00	179.21	121.70
2	H	40	ARG	NE-CZ-NH1	23.00	131.80	120.30
1	E	46	PHE	CB-CG-CD1	-22.96	104.73	120.80
1	A	98	PHE	CB-CG-CD2	22.82	136.78	120.80
2	H	15	TRP	C-N-CA	22.80	170.18	122.30
2	B	35	TYR	CB-CG-CD1	-22.72	107.37	121.00
1	C	74	ASP	CB-CG-OD1	22.70	138.73	118.30
1	A	31	ARG	CD-NE-CZ	22.65	155.31	123.60
2	H	47	ASP	CB-CG-OD1	22.35	138.41	118.30
1	E	10	VAL	C-N-CA	22.30	177.45	121.70
2	H	55	MET	C-N-CA	22.26	169.05	122.30
2	F	83	GLY	C-N-CA	22.16	177.10	121.70
1	A	31	ARG	NE-CZ-NH2	21.82	131.21	120.30
1	E	116	GLU	CG-CD-OE1	21.64	161.59	118.30
1	C	37	PRO	C-N-CA	21.59	175.69	121.70
1	C	47	ASP	CB-CG-OD1	21.50	137.65	118.30
1	C	31	ARG	CD-NE-CZ	-21.36	93.69	123.60
1	C	92	ARG	NE-CZ-NH2	21.24	130.92	120.30
1	E	109	LEU	C-N-CA	21.22	174.74	121.70
2	D	77	HIS	N-CA-CB	-21.18	72.48	110.60
1	E	138	SER	CA-CB-OG	21.09	168.13	111.20
1	C	46	PHE	CB-CG-CD2	21.07	135.55	120.80
1	G	92	ARG	NE-CZ-NH1	21.07	130.84	120.30
2	H	135	ALA	C-N-CA	21.07	166.54	122.30
2	D	21	ASP	CB-CG-OD1	-20.97	99.43	118.30
1	C	129	LEU	CB-CA-C	20.95	150.01	110.20
1	C	110	ALA	C-N-CA	20.79	173.67	121.70
2	H	73	ASP	CB-CG-OD1	20.72	136.95	118.30
1	A	127	LYS	CA-CB-CG	20.63	158.79	113.40
1	A	30	GLU	OE1-CD-OE2	-20.51	98.68	123.30
1	C	105	LEU	C-N-CA	20.35	172.56	121.70
2	H	89	SER	N-CA-CB	20.28	140.91	110.50
2	B	45	PHE	CB-CG-CD2	20.23	134.96	120.80
2	D	94	ASP	CB-CG-OD2	-20.16	100.15	118.30
1	A	34	LEU	CB-CG-CD2	-20.15	76.75	111.00
1	G	37	PRO	C-N-CA	20.15	172.07	121.70
1	G	134	THR	CA-CB-CG2	20.12	140.57	112.40
1	A	129	LEU	C-N-CA	19.91	171.46	121.70
1	C	30	GLU	OE1-CD-OE2	19.85	147.12	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	ARG	NE-CZ-NH2	19.83	130.21	120.30
1	E	122	HIS	CA-CB-CG	19.81	147.27	113.60
1	G	47	ASP	CB-CG-OD2	-19.75	100.52	118.30
2	F	99	ASP	CB-CG-OD1	-19.63	100.63	118.30
2	D	30	ARG	NE-CZ-NH1	19.63	130.11	120.30
1	E	10	VAL	CA-C-N	19.62	160.37	117.20
2	D	30	ARG	CD-NE-CZ	19.60	151.04	123.60
2	H	73	ASP	CA-C-N	19.54	155.27	116.20
1	A	46	PHE	CB-CG-CD2	19.45	134.42	120.80
1	G	55	VAL	O-C-N	19.41	153.75	122.70
1	G	29	LEU	CA-CB-CG	19.37	159.86	115.30
1	A	36	PHE	CB-CG-CD2	19.34	134.34	120.80
2	H	117	HIS	C-N-CA	19.29	169.94	121.70
2	B	45	PHE	CA-CB-CG	19.21	160.01	113.90
2	F	33	VAL	O-C-N	-19.16	92.04	122.70
1	C	58	HIS	C-N-CA	19.14	162.49	122.30
1	G	23	GLU	C-N-CA	19.11	169.46	121.70
2	F	30	ARG	NH1-CZ-NH2	19.01	140.31	119.40
2	H	140	ALA	C-N-CA	18.95	169.08	121.70
1	C	99	LYS	O-C-N	18.90	152.94	122.70
2	H	30	ARG	CB-CG-CD	18.88	160.69	111.60
2	B	40	ARG	NE-CZ-NH2	-18.80	110.90	120.30
1	G	141	ARG	CA-C-O	-18.79	80.65	120.10
1	C	36	PHE	CB-CG-CD1	-18.76	107.67	120.80
2	F	35	TYR	CG-CD2-CE2	18.75	136.30	121.30
2	B	80	ASN	OD1-CG-ND2	18.72	164.96	121.90
2	H	3	LEU	O-C-N	18.66	152.55	122.70
2	H	11	VAL	O-C-N	18.63	152.51	122.70
2	F	23	VAL	O-C-N	-18.60	91.58	123.20
1	E	141	ARG	NE-CZ-NH1	18.56	129.58	120.30
1	A	62	VAL	N-CA-CB	18.55	152.30	111.50
2	F	141	LEU	CA-CB-CG	18.48	157.81	115.30
2	H	63	HIS	N-CA-CB	18.43	143.77	110.60
1	G	36	PHE	CB-CG-CD1	18.42	133.70	120.80
2	D	30	ARG	NE-CZ-NH2	-18.36	111.12	120.30
1	G	43	PHE	CB-CG-CD1	-18.32	107.98	120.80
1	C	89	HIS	CA-CB-CG	-18.30	82.48	113.60
1	G	85	ASP	CA-CB-CG	18.27	153.60	113.40
1	C	70	VAL	O-C-N	18.21	151.83	122.70
1	G	75	ASP	O-C-N	18.20	151.82	122.70
2	D	113	VAL	O-C-N	18.16	151.76	122.70
1	G	42	TYR	CB-CG-CD1	18.14	131.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	24	TYR	CB-CG-CD1	18.08	131.85	121.00
2	H	38	THR	CA-CB-OG1	18.00	146.81	109.00
1	E	106	LEU	CB-CG-CD1	-17.97	80.45	111.00
2	D	13	ALA	N-CA-CB	17.96	135.25	110.10
1	E	5	ALA	N-CA-CB	17.96	135.24	110.10
1	E	82	ALA	O-C-N	17.94	151.41	122.70
1	G	42	TYR	CB-CG-CD2	-17.91	110.25	121.00
1	C	56	LYS	N-CA-CB	17.90	142.82	110.60
1	A	98	PHE	CB-CG-CD1	-17.74	108.38	120.80
1	G	82	ALA	O-C-N	-17.73	94.33	122.70
1	G	76	MET	CA-CB-CG	17.69	143.38	113.30
1	C	141	ARG	CD-NE-CZ	-17.66	98.87	123.60
2	B	126	VAL	CA-CB-CG2	-17.64	84.45	110.90
1	C	140	TYR	CG-CD1-CE1	17.62	135.40	121.30
1	C	62	VAL	CA-CB-CG2	17.62	137.33	110.90
2	D	79	ASP	CB-CG-OD1	-17.56	102.50	118.30
2	H	130	TYR	CG-CD2-CE2	17.48	135.29	121.30
1	C	126	ASP	O-C-N	-17.47	94.74	122.70
1	C	75	ASP	CA-CB-CG	-17.43	75.06	113.40
1	C	67	THR	CA-CB-CG2	-17.33	88.13	112.40
2	D	108	ASN	CB-CG-OD1	17.24	156.08	121.60
1	A	46	PHE	CB-CG-CD1	-17.21	108.75	120.80
1	C	141	ARG	CA-CB-CG	17.18	151.19	113.40
2	H	131	GLN	N-CA-CB	17.17	141.51	110.60
1	E	72	HIS	C-N-CA	17.15	164.58	121.70
1	G	131	SER	N-CA-CB	17.13	136.20	110.50
2	B	135	ALA	CB-CA-C	17.11	135.77	110.10
1	G	50	HIS	O-C-N	17.07	152.21	123.20
2	B	128	ALA	O-C-N	17.03	149.95	122.70
1	G	36	PHE	CB-CG-CD2	-17.02	108.88	120.80
1	E	72	HIS	CA-CB-CG	16.96	142.43	113.60
2	D	71	PHE	CB-CG-CD2	16.94	132.66	120.80
1	E	90	LYS	CA-C-O	16.93	155.66	120.10
1	C	35	SER	C-N-CA	16.90	163.94	121.70
1	E	90	LYS	O-C-N	-16.89	95.68	122.70
2	B	52	ASP	OD1-CG-OD2	16.83	155.28	123.30
1	A	74	ASP	CB-CG-OD1	-16.78	103.20	118.30
2	B	43	GLU	OE1-CD-OE2	-16.77	103.18	123.30
1	C	60	LYS	CB-CG-CD	16.77	155.20	111.60
1	G	69	ALA	N-CA-CB	-16.75	86.64	110.10
2	B	23	VAL	C-N-CA	16.74	157.46	122.30
1	G	82	ALA	CA-C-N	16.73	154.01	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	85	PHE	CB-CG-CD1	-16.70	109.11	120.80
1	C	71	ALA	CB-CA-C	16.66	135.09	110.10
2	F	118	PHE	O-C-N	16.65	151.51	123.20
1	E	141	ARG	NE-CZ-NH2	-16.59	112.00	120.30
1	A	6	ASP	CB-CG-OD2	-16.58	103.38	118.30
1	C	129	LEU	N-CA-CB	-16.58	77.25	110.40
1	A	41	THR	CA-CB-CG2	-16.57	89.20	112.40
1	C	75	ASP	CB-CG-OD2	16.57	133.21	118.30
1	G	23	GLU	CG-CD-OE1	16.57	151.44	118.30
1	A	129	LEU	CB-CG-CD2	-16.55	82.87	111.00
2	D	77	HIS	CG-ND1-CE1	16.53	131.35	108.20
1	G	27	GLU	CB-CG-CD	16.52	158.81	114.20
1	G	46	PHE	CB-CG-CD1	-16.45	109.28	120.80
2	H	59	LYS	CB-CA-C	16.44	143.29	110.40
1	A	132	VAL	CA-CB-CG1	16.43	135.55	110.90
2	F	130	TYR	CG-CD1-CE1	16.40	134.42	121.30
2	F	79	ASP	CB-CG-OD2	-16.39	103.55	118.30
2	H	127	GLN	C-N-CA	16.39	162.68	121.70
2	H	94	ASP	CB-CG-OD2	-16.39	103.55	118.30
1	C	141	ARG	CG-CD-NE	-16.39	77.39	111.80
2	D	22	GLU	CA-CB-CG	16.38	149.43	113.40
1	A	52	SER	N-CA-CB	16.36	135.03	110.50
2	D	76	ALA	CB-CA-C	-16.32	85.61	110.10
1	E	61	LYS	CA-CB-CG	16.32	149.31	113.40
2	D	10	ALA	C-N-CA	16.28	162.40	121.70
1	E	25	GLY	O-C-N	16.25	148.71	122.70
1	G	37	PRO	O-C-N	-16.21	96.76	122.70
2	F	108	ASN	CA-C-N	16.21	152.86	117.20
1	E	70	VAL	O-C-N	16.20	148.62	122.70
1	E	141	ARG	CA-CB-CG	16.20	149.04	113.40
2	D	86	ALA	N-CA-CB	-16.11	87.54	110.10
2	B	113	VAL	CG1-CB-CG2	16.08	136.63	110.90
1	G	32	MET	C-N-CA	16.07	161.89	121.70
2	F	37	TRP	CG-CD1-NE1	16.04	126.14	110.10
2	F	96	LEU	CB-CA-C	16.01	140.62	110.20
1	E	43	PHE	CB-CG-CD1	16.00	132.00	120.80
2	H	99	ASP	CA-CB-CG	15.99	148.58	113.40
2	H	103	PHE	CB-CA-C	15.99	142.38	110.40
2	B	72	SER	CA-C-O	-15.98	86.54	120.10
2	D	37	TRP	CH2-CZ2-CE2	15.91	133.31	117.40
1	E	23	GLU	OE1-CD-OE2	-15.89	104.23	123.30
2	H	139	ASN	CB-CG-OD1	15.88	153.37	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	50	HIS	CA-C-O	-15.87	86.77	120.10
2	D	7	GLU	OE1-CD-OE2	-15.85	104.28	123.30
2	H	91	LEU	CB-CG-CD2	15.84	137.93	111.00
1	C	110	ALA	CB-CA-C	-15.84	86.34	110.10
2	H	133	VAL	CA-CB-CG1	-15.82	87.17	110.90
1	G	107	VAL	C-N-CA	15.80	161.21	121.70
1	A	70	VAL	C-N-CA	15.80	161.19	121.70
1	A	109	LEU	O-C-N	-15.67	97.63	122.70
2	F	133	VAL	CA-CB-CG1	15.66	134.40	110.90
2	D	101	GLU	CA-CB-CG	15.65	147.84	113.40
1	G	93	VAL	CA-CB-CG1	15.60	134.30	110.90
1	E	24	TYR	CB-CG-CD2	-15.60	111.64	121.00
1	G	115	ALA	CB-CA-C	15.59	133.48	110.10
2	H	75	LEU	C-N-CA	15.58	160.66	121.70
2	D	43	GLU	C-N-CA	15.52	160.51	121.70
1	E	47	ASP	CB-CG-OD2	-15.52	104.33	118.30
1	A	69	ALA	CB-CA-C	15.50	133.36	110.10
1	A	85	ASP	CB-CG-OD1	-15.49	104.36	118.30
1	C	40	LYS	C-N-CA	15.46	160.34	121.70
2	B	9	SER	N-CA-CB	15.43	133.65	110.50
2	B	118	PHE	CB-CG-CD1	-15.43	110.00	120.80
2	H	29	GLY	CA-C-O	15.41	148.35	120.60
1	C	80	LEU	CB-CG-CD2	15.40	137.19	111.00
2	B	126	VAL	CA-CB-CG1	15.33	133.90	110.90
2	F	130	TYR	CB-CG-CD2	15.32	130.19	121.00
1	C	72	HIS	CA-C-N	15.31	150.88	117.20
1	E	106	LEU	C-N-CA	15.30	159.96	121.70
2	B	129	ALA	O-C-N	-15.29	98.24	122.70
1	E	58	HIS	C-N-CA	15.28	154.38	122.30
2	H	12	THR	CA-CB-CG2	15.25	133.75	112.40
1	C	13	ALA	N-CA-CB	-15.24	88.77	110.10
1	A	136	LEU	CB-CA-C	15.23	139.14	110.20
1	G	90	LYS	N-CA-CB	15.23	138.01	110.60
2	B	19	ASN	N-CA-CB	15.23	138.01	110.60
1	C	72	HIS	C-N-CA	15.20	159.71	121.70
2	D	140	ALA	N-CA-CB	15.20	131.37	110.10
1	C	138	SER	CA-C-N	15.16	150.55	117.20
2	B	43	GLU	CA-CB-CG	15.13	146.69	113.40
1	G	43	PHE	CB-CG-CD2	15.13	131.39	120.80
2	D	79	ASP	CB-CG-OD2	15.11	131.90	118.30
1	E	90	LYS	CD-CE-NZ	15.10	146.44	111.70
1	A	75	ASP	CB-CG-OD1	15.08	131.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	125	LEU	CB-CG-CD2	-15.06	85.39	111.00
1	E	24	TYR	CZ-CE2-CD2	-15.06	106.25	119.80
2	H	60	VAL	CA-CB-CG1	-15.05	88.32	110.90
2	H	87	THR	N-CA-CB	15.03	138.86	110.30
1	E	41	THR	N-CA-CB	15.03	138.85	110.30
2	F	82	LYS	O-C-N	15.00	148.71	123.20
2	D	91	LEU	N-CA-CB	15.00	140.39	110.40
1	C	61	LYS	CA-CB-CG	14.96	146.32	113.40
2	B	118	PHE	CB-CG-CD2	14.96	131.27	120.80
2	H	90	GLU	C-N-CA	14.95	159.08	121.70
1	C	28	ALA	C-N-CA	14.94	159.04	121.70
1	G	13	ALA	CB-CA-C	14.92	132.48	110.10
1	G	92	ARG	CD-NE-CZ	14.92	144.49	123.60
2	H	4	THR	CA-CB-CG2	-14.91	91.52	112.40
2	H	118	PHE	CB-CG-CD1	14.88	131.22	120.80
2	F	101	GLU	OE1-CD-OE2	-14.88	105.45	123.30
2	H	68	LEU	CA-CB-CG	14.88	149.52	115.30
2	F	94	ASP	CB-CG-OD2	14.88	131.69	118.30
2	F	97	HIS	C-N-CA	14.87	158.88	121.70
2	F	45	PHE	CB-CG-CD1	14.86	131.20	120.80
1	A	116	GLU	CB-CG-CD	14.85	154.29	114.20
2	F	79	ASP	CA-CB-CG	14.85	146.06	113.40
2	D	99	ASP	N-CA-CB	14.84	137.31	110.60
1	E	15	GLY	CA-C-O	14.83	147.29	120.60
1	C	43	PHE	O-C-N	14.83	149.27	121.10
1	C	67	THR	O-C-N	-14.83	98.98	122.70
1	C	31	ARG	N-CA-CB	14.78	137.20	110.60
2	B	115	ALA	O-C-N	14.76	146.32	122.70
1	E	54	GLN	O-C-N	-14.75	99.10	122.70
1	E	32	MET	CA-CB-CG	-14.72	88.28	113.30
1	C	138	SER	O-C-N	-14.71	99.16	122.70
1	C	94	ASP	CA-C-O	14.71	150.99	120.10
2	H	39	GLN	N-CA-CB	-14.70	84.14	110.60
1	C	8	THR	CA-CB-CG2	14.69	132.96	112.40
1	C	81	SER	CB-CA-C	-14.68	82.21	110.10
2	D	45	PHE	CB-CG-CD2	14.66	131.06	120.80
2	B	47	ASP	OD1-CG-OD2	-14.66	95.45	123.30
1	C	56	LYS	O-C-N	14.66	148.12	123.20
1	G	37	PRO	CA-C-N	14.64	149.41	117.20
1	E	128	PHE	CB-CG-CD2	-14.61	110.57	120.80
1	A	73	VAL	CA-CB-CG1	-14.58	89.02	110.90
2	D	14	LEU	CA-C-O	14.58	150.71	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	104	ARG	NE-CZ-NH2	-14.57	113.01	120.30
2	F	62	ALA	CB-CA-C	14.56	131.95	110.10
1	C	31	ARG	CG-CD-NE	14.56	142.38	111.80
1	E	54	GLN	CB-CA-C	14.55	139.50	110.40
2	B	118	PHE	C-N-CA	14.52	152.79	122.30
1	C	1	VAL	CB-CA-C	-14.51	83.82	111.40
1	A	104	CYS	CA-CB-SG	-14.51	87.89	114.00
1	A	62	VAL	CA-C-O	-14.49	89.66	120.10
1	G	130	ALA	C-N-CA	14.47	157.88	121.70
2	B	115	ALA	N-CA-CB	14.43	130.30	110.10
1	G	35	SER	CA-C-O	14.41	150.37	120.10
2	D	120	LYS	CB-CG-CD	14.40	149.03	111.60
2	F	134	VAL	C-N-CA	14.38	157.66	121.70
1	C	42	TYR	CB-CG-CD1	-14.37	112.38	121.00
1	E	92	ARG	NE-CZ-NH2	14.37	127.48	120.30
2	F	100	PRO	O-C-N	-14.37	99.71	122.70
2	F	132	LYS	O-C-N	14.37	145.69	122.70
2	F	33	VAL	CA-CB-CG2	14.36	132.43	110.90
1	E	98	PHE	CA-C-O	14.35	150.24	120.10
1	G	127	LYS	O-C-N	14.35	145.66	122.70
1	G	23	GLU	OE1-CD-OE2	-14.34	106.09	123.30
2	F	35	TYR	CD1-CE1-CZ	14.31	132.68	119.80
1	G	44	PRO	N-CD-CG	14.28	124.63	103.20
1	G	103	HIS	CG-ND1-CE1	14.28	128.19	108.20
2	B	109	VAL	CA-CB-CG2	14.27	132.31	110.90
1	E	31	ARG	CB-CA-C	14.25	138.90	110.40
1	E	121	VAL	C-N-CA	14.24	157.30	121.70
2	B	39	GLN	CB-CA-C	14.24	138.87	110.40
2	B	144	LYS	CA-CB-CG	14.23	144.72	113.40
2	F	35	TYR	N-CA-CB	14.19	136.14	110.60
2	H	43	GLU	CB-CG-CD	14.17	152.46	114.20
1	C	69	ALA	N-CA-CB	14.16	129.92	110.10
2	F	114	LEU	CA-CB-CG	-14.13	82.79	115.30
1	C	135	VAL	C-N-CA	14.11	156.97	121.70
1	G	112	HIS	CA-CB-CG	-14.11	89.62	113.60
2	F	14	LEU	CB-CA-C	14.09	136.97	110.20
1	E	50	HIS	CA-C-N	14.08	144.36	116.20
2	F	47	ASP	CB-CG-OD2	-14.08	105.63	118.30
2	B	122	PHE	CG-CD2-CE2	14.07	136.28	120.80
2	B	115	ALA	CB-CA-C	-14.07	89.00	110.10
2	H	109	VAL	CA-CB-CG2	14.06	131.98	110.90
1	C	27	GLU	CA-C-O	14.05	149.61	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	127	GLN	CA-CB-CG	-14.03	82.53	113.40
1	C	9	ASN	CB-CG-OD1	-14.02	93.57	121.60
2	H	110	LEU	CA-C-O	14.01	149.52	120.10
1	E	116	GLU	OE1-CD-OE2	-14.01	106.49	123.30
1	C	115	ALA	C-N-CA	13.99	156.67	121.70
1	G	79	ALA	CB-CA-C	13.99	131.08	110.10
1	G	7	LYS	CB-CG-CD	13.98	147.94	111.60
2	D	35	TYR	CB-CG-CD2	-13.97	112.62	121.00
2	B	140	ALA	CA-C-N	13.96	147.90	117.20
2	B	19	ASN	CA-CB-CG	13.94	144.06	113.40
2	H	84	THR	O-C-N	-13.93	100.41	122.70
1	E	97	ASN	OD1-CG-ND2	-13.92	89.89	121.90
1	G	35	SER	O-C-N	-13.91	100.45	122.70
2	B	72	SER	N-CA-CB	13.90	131.36	110.50
2	D	130	TYR	CB-CG-CD2	13.90	129.34	121.00
1	G	91	LEU	C-N-CA	13.89	156.42	121.70
2	B	38	THR	CA-CB-CG2	13.88	131.83	112.40
2	H	142	ALA	CB-CA-C	13.87	130.91	110.10
2	B	1	VAL	CA-CB-CG1	13.87	131.70	110.90
2	H	101	GLU	CG-CD-OE1	13.87	146.03	118.30
1	A	23	GLU	O-C-N	13.86	144.87	122.70
2	D	101	GLU	N-CA-CB	13.86	135.54	110.60
2	B	11	VAL	CG1-CB-CG2	-13.85	88.73	110.90
1	E	125	LEU	CA-CB-CG	13.85	147.15	115.30
2	D	77	HIS	CB-CG-ND1	13.82	157.75	123.20
2	B	16	GLY	CA-C-O	13.80	145.44	120.60
2	B	35	TYR	O-C-N	13.78	147.28	121.10
2	F	51	PRO	C-N-CA	13.78	156.14	121.70
1	A	67	THR	CA-CB-OG1	-13.77	80.08	109.00
2	H	68	LEU	CB-CA-C	13.76	136.34	110.20
2	B	104	ARG	CB-CA-C	13.74	137.89	110.40
1	C	111	ALA	C-N-CA	13.74	156.06	121.70
1	E	51	GLY	CA-C-O	-13.74	95.87	120.60
2	F	105	LEU	CA-CB-CG	13.74	146.89	115.30
2	F	59	LYS	CB-CA-C	13.73	137.86	110.40
2	H	108	ASN	OD1-CG-ND2	13.73	153.48	121.90
1	A	42	TYR	CD1-CE1-CZ	-13.73	107.44	119.80
2	D	34	VAL	CB-CA-C	13.73	137.49	111.40
1	G	50	HIS	CA-CB-CG	-13.73	90.26	113.60
2	D	71	PHE	C-N-CA	13.69	155.94	121.70
1	G	61	LYS	CB-CA-C	13.68	137.77	110.40
2	B	20	VAL	CA-C-N	13.67	147.28	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	VAL	CA-CB-CG2	13.67	131.40	110.90
2	F	60	VAL	CA-CB-CG1	13.67	131.40	110.90
2	D	90	GLU	CG-CD-OE1	13.64	145.58	118.30
2	H	49	SER	N-CA-CB	-13.63	90.05	110.50
2	H	115	ALA	C-N-CA	13.63	155.78	121.70
1	G	109	LEU	CB-CG-CD1	-13.61	87.87	111.00
1	A	21	ALA	N-CA-CB	-13.59	91.08	110.10
1	E	94	ASP	CB-CG-OD1	-13.58	106.08	118.30
1	C	58	HIS	CA-CB-CG	-13.58	90.51	113.60
1	E	106	LEU	CB-CG-CD2	13.55	134.03	111.00
1	G	125	LEU	O-C-N	13.54	144.36	122.70
2	F	67	VAL	CB-CA-C	13.52	137.08	111.40
2	B	110	LEU	CA-C-O	-13.48	91.78	120.10
2	B	114	LEU	O-C-N	13.48	144.27	122.70
1	A	130	ALA	O-C-N	13.48	144.27	122.70
2	D	74	GLY	CA-C-N	13.48	146.85	117.20
1	G	50	HIS	C-N-CA	13.47	150.58	122.30
2	B	3	LEU	CB-CG-CD1	13.45	133.86	111.00
2	B	15	TRP	N-CA-CB	-13.43	86.43	110.60
2	H	130	TYR	CZ-CE2-CD2	-13.43	107.72	119.80
1	A	66	LEU	O-C-N	13.42	144.16	122.70
2	F	39	GLN	CA-CB-CG	13.41	142.91	113.40
2	H	133	VAL	CA-CB-CG2	13.40	131.01	110.90
1	C	141	ARG	NH1-CZ-NH2	-13.40	104.66	119.40
2	F	83	GLY	CA-C-N	13.40	146.68	117.20
2	D	77	HIS	ND1-CG-CD2	-13.39	87.25	106.00
1	C	24	TYR	CB-CG-CD2	-13.39	112.97	121.00
1	C	139	LYS	N-CA-CB	-13.39	86.50	110.60
2	H	6	VAL	CA-CB-CG1	13.38	130.98	110.90
2	B	130	TYR	CG-CD1-CE1	-13.38	110.60	121.30
1	G	63	ALA	CA-C-N	13.38	146.62	117.20
2	F	21	ASP	CB-CG-OD2	-13.37	106.26	118.30
2	B	71	PHE	CB-CG-CD2	-13.37	111.44	120.80
2	F	60	VAL	O-C-N	-13.37	101.31	122.70
2	F	63	HIS	CA-CB-CG	13.37	136.32	113.60
1	C	62	VAL	CG1-CB-CG2	-13.36	89.52	110.90
2	B	62	ALA	N-CA-CB	-13.34	91.42	110.10
1	C	33	PHE	CB-CG-CD1	-13.34	111.46	120.80
2	H	14	LEU	CB-CG-CD1	13.34	133.68	111.00
1	A	28	ALA	CB-CA-C	-13.34	90.09	110.10
2	B	49	SER	C-N-CA	13.34	155.05	121.70
1	E	6	ASP	CB-CG-OD1	13.33	130.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LEU	CB-CA-C	13.33	135.53	110.20
1	A	70	VAL	CA-C-O	-13.33	92.11	120.10
2	D	107	GLY	O-C-N	13.32	144.01	122.70
2	H	98	VAL	CA-C-N	13.32	146.50	117.20
1	A	140	TYR	CA-CB-CG	13.29	138.65	113.40
1	C	121	VAL	CA-CB-CG2	13.28	130.82	110.90
1	C	67	THR	CA-C-O	13.28	147.99	120.10
2	D	47	ASP	CB-CG-OD2	-13.28	106.35	118.30
1	C	50	HIS	CB-CA-C	13.26	136.92	110.40
1	G	40	LYS	C-N-CA	13.25	154.81	121.70
1	E	116	GLU	O-C-N	13.24	143.89	122.70
2	F	109	VAL	CB-CA-C	13.24	136.56	111.40
2	D	47	ASP	CB-CG-OD1	13.24	130.21	118.30
1	E	116	GLU	CG-CD-OE2	-13.22	91.85	118.30
2	D	14	LEU	CB-CA-C	13.19	135.26	110.20
2	D	74	GLY	CA-C-O	-13.19	96.86	120.60
2	F	79	ASP	O-C-N	13.18	143.79	122.70
1	A	42	TYR	CZ-CE2-CD2	13.16	131.65	119.80
1	A	76	MET	CA-CB-CG	-13.16	90.93	113.30
1	C	131	SER	CA-CB-OG	13.16	146.73	111.20
1	G	21	ALA	CA-C-N	-13.14	89.92	116.20
2	F	133	VAL	CA-CB-CG2	-13.14	91.20	110.90
1	C	107	VAL	CA-C-N	13.13	146.09	117.20
1	G	64	ASP	CB-CG-OD1	13.13	130.12	118.30
1	G	114	PRO	O-C-N	13.13	143.71	122.70
2	F	75	LEU	CB-CG-CD1	-13.12	88.70	111.00
1	G	113	LEU	N-CA-CB	-13.11	84.17	110.40
1	A	121	VAL	CA-CB-CG2	-13.10	91.25	110.90
2	H	129	ALA	C-N-CA	13.09	154.43	121.70
2	D	86	ALA	CB-CA-C	13.09	129.73	110.10
1	E	140	TYR	CA-CB-CG	13.08	138.25	113.40
2	F	104	ARG	CD-NE-CZ	13.06	141.88	123.60
2	F	22	GLU	OE1-CD-OE2	-13.06	107.63	123.30
2	D	73	ASP	CB-CG-OD2	-13.03	106.57	118.30
1	C	21	ALA	C-N-CA	13.01	149.62	122.30
2	B	35	TYR	CG-CD2-CE2	13.00	131.70	121.30
2	B	43	GLU	CB-CG-CD	12.99	149.27	114.20
2	B	38	THR	OG1-CB-CG2	-12.98	80.15	110.00
1	G	140	TYR	CG-CD2-CE2	-12.97	110.92	121.30
1	E	82	ALA	CA-C-O	-12.97	92.87	120.10
1	E	110	ALA	N-CA-CB	-12.97	91.95	110.10
1	E	123	ALA	O-C-N	12.96	143.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	GLU	O-C-N	-12.95	101.97	122.70
2	D	71	PHE	CB-CG-CD1	-12.96	111.73	120.80
1	C	30	GLU	CA-C-N	12.94	145.67	117.20
2	F	101	GLU	CG-CD-OE1	12.94	144.18	118.30
2	F	70	ALA	CB-CA-C	12.93	129.50	110.10
2	B	104	ARG	O-C-N	-12.93	102.02	122.70
1	E	2	LEU	CB-CG-CD2	-12.91	89.05	111.00
1	G	69	ALA	CB-CA-C	12.90	129.45	110.10
2	F	109	VAL	CA-C-O	12.88	147.15	120.10
2	F	53	ALA	N-CA-CB	12.87	128.12	110.10
1	C	126	ASP	C-N-CA	12.86	153.86	121.70
2	B	98	VAL	CG1-CB-CG2	-12.86	90.33	110.90
2	B	38	THR	CB-CA-C	12.85	146.29	111.60
2	D	98	VAL	CB-CA-C	12.85	135.81	111.40
1	G	58	HIS	CA-CB-CG	12.84	135.43	113.60
2	F	35	TYR	CZ-CE2-CD2	-12.83	108.25	119.80
2	F	45	PHE	CG-CD1-CE1	12.83	134.91	120.80
1	E	10	VAL	O-C-N	-12.82	102.18	122.70
2	F	54	VAL	CA-CB-CG1	-12.81	91.69	110.90
1	G	94	ASP	N-CA-CB	-12.81	87.55	110.60
2	B	118	PHE	N-CA-C	12.78	145.50	111.00
2	H	39	GLN	CB-CA-C	12.78	135.95	110.40
2	D	22	GLU	OE1-CD-OE2	-12.76	107.99	123.30
2	F	9	SER	CA-C-O	12.75	146.87	120.10
1	E	27	GLU	CA-CB-CG	12.74	141.44	113.40
2	D	47	ASP	O-C-N	12.74	143.09	122.70
2	D	85	PHE	CB-CG-CD1	12.74	129.72	120.80
1	A	109	LEU	C-N-CA	12.73	153.53	121.70
1	A	108	THR	CA-CB-CG2	12.73	130.22	112.40
2	B	139	ASN	OD1-CG-ND2	12.72	151.15	121.90
2	D	112	CYS	CA-C-O	-12.71	93.40	120.10
2	F	136	GLY	O-C-N	12.71	143.04	122.70
1	A	20	HIS	O-C-N	-12.71	102.37	122.70
1	E	33	PHE	O-C-N	-12.71	102.37	122.70
2	D	55	MET	C-N-CA	12.70	148.97	122.30
1	E	41	THR	CA-CB-CG2	12.68	130.15	112.40
1	E	83	LEU	CB-CG-CD2	-12.67	89.45	111.00
1	G	63	ALA	C-N-CA	12.67	153.37	121.70
2	D	120	LYS	CA-C-N	12.67	145.07	117.20
2	H	6	VAL	CG1-CB-CG2	-12.67	90.63	110.90
1	E	30	GLU	O-C-N	12.66	142.96	122.70
2	F	60	VAL	CA-C-O	12.65	146.67	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	ASN	CB-CG-OD1	12.64	146.89	121.60
1	G	129	LEU	CB-CA-C	-12.64	86.19	110.20
2	B	86	ALA	CB-CA-C	-12.64	91.14	110.10
1	G	31	ARG	CG-CD-NE	12.63	138.32	111.80
2	B	44	SER	CA-C-N	-12.62	89.43	117.20
2	B	90	GLU	N-CA-CB	12.61	133.30	110.60
1	G	105	LEU	CA-C-O	12.61	146.57	120.10
1	A	61	LYS	CA-C-N	-12.60	89.48	117.20
2	H	35	TYR	CG-CD1-CE1	-12.60	111.22	121.30
2	F	129	ALA	CB-CA-C	12.59	128.98	110.10
2	H	21	ASP	CB-CG-OD1	-12.59	106.97	118.30
2	D	129	ALA	CA-C-O	12.58	146.52	120.10
1	A	33	PHE	CD1-CE1-CZ	12.58	135.19	120.10
2	B	139	ASN	CB-CG-OD1	-12.58	96.45	121.60
1	C	47	ASP	OD1-CG-OD2	-12.57	99.42	123.30
2	D	12	THR	CA-CB-CG2	12.57	130.00	112.40
1	C	124	SER	C-N-CA	12.57	153.12	121.70
2	B	110	LEU	CB-CG-CD1	-12.56	89.65	111.00
1	E	31	ARG	NH1-CZ-NH2	-12.56	105.59	119.40
2	D	40	ARG	NE-CZ-NH1	12.56	126.58	120.30
2	H	122	PHE	CB-CG-CD2	-12.55	112.01	120.80
1	C	141	ARG	CB-CG-CD	12.54	144.20	111.60
2	D	104	ARG	CA-CB-CG	-12.54	85.81	113.40
1	E	98	PHE	CB-CG-CD1	-12.52	112.04	120.80
1	E	102	SER	CA-C-O	-12.51	93.83	120.10
2	H	102	ASN	O-C-N	12.51	142.71	122.70
1	A	42	TYR	CG-CD2-CE2	-12.50	111.30	121.30
2	B	82	LYS	CB-CA-C	12.50	135.41	110.40
2	F	30	ARG	NE-CZ-NH2	12.50	126.55	120.30
1	C	9	ASN	O-C-N	12.49	142.68	122.70
2	D	130	TYR	N-CA-CB	12.49	133.07	110.60
2	B	44	SER	CB-CA-C	12.48	133.82	110.10
1	C	60	LYS	CD-CE-NZ	-12.48	83.00	111.70
2	B	110	LEU	CB-CG-CD2	12.46	132.19	111.00
2	D	100	PRO	CB-CA-C	12.46	143.14	112.00
2	H	127	GLN	OE1-CD-NE2	-12.45	93.26	121.90
1	A	98	PHE	CZ-CE2-CD2	12.44	135.03	120.10
1	A	141	ARG	N-CA-CB	-12.45	88.20	110.60
2	H	47	ASP	CB-CG-OD2	-12.42	107.13	118.30
1	E	8	THR	CA-CB-CG2	-12.41	95.02	112.40
2	D	45	PHE	CB-CG-CD1	-12.40	112.12	120.80
1	E	5	ALA	CB-CA-C	-12.40	91.50	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	62	ALA	O-C-N	12.39	142.53	122.70
2	F	21	ASP	CB-CG-OD1	-12.39	107.15	118.30
1	G	21	ALA	O-C-N	12.39	144.26	123.20
1	G	31	ARG	CA-CB-CG	12.39	140.66	113.40
2	B	45	PHE	CA-C-N	12.38	140.97	116.20
2	D	134	VAL	C-N-CA	12.38	152.64	121.70
1	A	106	LEU	C-N-CA	12.38	152.64	121.70
2	B	128	ALA	CB-CA-C	-12.37	91.54	110.10
2	H	61	LYS	C-N-CA	12.38	152.64	121.70
2	B	19	ASN	OD1-CG-ND2	-12.37	93.45	121.90
1	C	68	ASN	C-N-CA	12.37	152.63	121.70
2	F	83	GLY	O-C-N	-12.37	102.91	122.70
2	F	118	PHE	CB-CG-CD2	12.36	129.46	120.80
2	D	45	PHE	CA-C-N	12.36	140.91	116.20
1	C	18	GLY	O-C-N	12.32	142.41	122.70
1	E	140	TYR	CB-CA-C	12.31	135.02	110.40
1	C	31	ARG	CB-CA-C	-12.30	85.79	110.40
2	H	40	ARG	NH1-CZ-NH2	12.30	132.94	119.40
2	D	8	LYS	C-N-CA	12.30	152.45	121.70
2	H	138	ALA	C-N-CA	12.30	152.45	121.70
1	C	119	PRO	O-C-N	-12.28	103.06	122.70
2	D	28	LEU	N-CA-CB	12.27	134.93	110.40
2	F	21	ASP	OD1-CG-OD2	12.26	146.58	123.30
2	F	77	HIS	O-C-N	-12.26	103.09	122.70
1	C	64	ASP	CA-CB-CG	-12.25	86.46	113.40
2	F	37	TRP	CD1-NE1-CE2	-12.24	97.98	109.00
2	B	99	ASP	CB-CG-OD1	-12.24	107.28	118.30
1	C	78	ASN	CB-CG-ND2	-12.24	87.32	116.70
2	H	130	TYR	CD1-CE1-CZ	12.24	130.82	119.80
2	H	63	HIS	O-C-N	12.22	143.97	123.20
2	D	118	PHE	O-C-N	-12.21	102.43	123.20
2	D	88	LEU	CA-C-N	12.20	144.04	117.20
2	F	62	ALA	N-CA-CB	-12.20	93.02	110.10
1	A	126	ASP	CB-CA-C	12.19	134.79	110.40
2	H	73	ASP	O-C-N	-12.18	102.50	123.20
2	B	62	ALA	CB-CA-C	-12.18	91.83	110.10
1	G	82	ALA	C-N-CA	12.17	152.13	121.70
1	C	120	ALA	N-CA-CB	12.17	127.14	110.10
1	E	53	ALA	CB-CA-C	12.17	128.36	110.10
1	A	19	ALA	N-CA-CB	-12.16	93.07	110.10
1	G	129	LEU	CA-CB-CG	-12.16	87.34	115.30
2	B	45	PHE	CG-CD2-CE2	12.12	134.14	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	139	ASN	O-C-N	12.12	142.09	122.70
1	E	15	GLY	O-C-N	-12.11	103.32	122.70
1	E	74	ASP	CB-CG-OD2	12.11	129.20	118.30
1	G	54	GLN	OE1-CD-NE2	12.11	149.75	121.90
2	D	131	GLN	CA-C-N	12.10	143.82	117.20
1	G	10	VAL	CA-CB-CG1	-12.10	92.75	110.90
1	E	64	ASP	CB-CG-OD1	12.10	129.19	118.30
2	H	115	ALA	N-CA-CB	12.09	127.03	110.10
1	A	95	PRO	N-CA-CB	12.09	117.81	103.30
2	B	1	VAL	O-C-N	12.09	142.04	122.70
1	C	54	GLN	O-C-N	12.08	142.03	122.70
1	G	131	SER	CA-C-N	12.08	143.77	117.20
1	C	78	ASN	N-CA-CB	-12.07	88.88	110.60
1	G	103	HIS	N-CA-CB	12.07	132.32	110.60
1	E	98	PHE	CD1-CG-CD2	12.06	133.98	118.30
1	A	37	PRO	N-CA-CB	-12.05	88.84	103.30
2	F	37	TRP	CB-CG-CD2	12.05	142.26	126.60
1	E	106	LEU	CB-CA-C	12.04	133.08	110.20
1	G	100	LEU	CB-CG-CD1	-12.04	90.53	111.00
1	E	80	LEU	CA-CB-CG	12.04	142.98	115.30
1	C	11	LYS	CD-CE-NZ	12.01	139.33	111.70
2	B	98	VAL	O-C-N	12.00	141.90	122.70
2	B	101	GLU	CG-CD-OE1	12.00	142.30	118.30
1	C	69	ALA	CB-CA-C	-12.00	92.10	110.10
2	B	41	PHE	CG-CD2-CE2	11.97	133.97	120.80
2	B	138	ALA	CB-CA-C	11.97	128.06	110.10
1	A	27	GLU	CG-CD-OE1	11.97	142.25	118.30
1	C	108	THR	CA-CB-CG2	11.97	129.16	112.40
2	F	61	LYS	N-CA-CB	-11.96	89.07	110.60
1	C	20	HIS	C-N-CA	11.96	151.60	121.70
1	A	9	ASN	CA-CB-CG	11.96	139.71	113.40
2	B	125	PRO	O-C-N	-11.95	103.58	122.70
2	H	12	THR	O-C-N	11.95	141.82	122.70
2	D	25	GLY	CA-C-O	11.94	142.09	120.60
2	H	33	VAL	CA-CB-CG1	11.93	128.80	110.90
1	A	139	LYS	N-CA-CB	-11.93	89.13	110.60
1	G	56	LYS	CA-CB-CG	11.93	139.64	113.40
2	H	123	THR	N-CA-CB	11.92	132.95	110.30
2	B	80	ASN	CB-CG-OD1	-11.91	97.77	121.60
1	E	6	ASP	CA-CB-CG	11.90	139.59	113.40
1	A	101	LEU	O-C-N	11.90	141.74	122.70
2	H	47	ASP	N-CA-CB	11.90	132.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PHE	CB-CG-CD2	-11.89	112.48	120.80
1	G	46	PHE	CB-CG-CD2	11.89	129.12	120.80
1	A	114	PRO	N-CD-CG	11.88	121.02	103.20
2	B	18	VAL	CA-CB-CG2	11.88	128.72	110.90
2	D	6	VAL	CA-CB-CG2	11.88	128.72	110.90
1	G	106	LEU	CB-CG-CD1	11.88	131.20	111.00
1	E	4	PRO	CA-C-O	-11.87	91.71	120.20
2	B	101	GLU	CG-CD-OE2	-11.87	94.56	118.30
2	B	85	PHE	CB-CG-CD2	-11.86	112.50	120.80
1	C	71	ALA	CA-C-O	11.86	145.01	120.10
2	H	19	ASN	CA-CB-CG	11.85	139.48	113.40
1	G	11	LYS	O-C-N	-11.82	103.78	122.70
2	B	30	ARG	CG-CD-NE	11.80	136.59	111.80
2	B	140	ALA	CA-C-O	-11.79	95.33	120.10
2	H	98	VAL	CA-C-O	-11.79	95.33	120.10
2	B	145	TYR	CG-CD1-CE1	11.79	130.73	121.30
2	H	31	LEU	CB-CG-CD1	-11.79	90.97	111.00
1	A	84	SER	CB-CA-C	11.78	132.48	110.10
1	C	64	ASP	OD1-CG-OD2	11.78	145.68	123.30
1	E	122	HIS	C-N-CA	11.77	151.14	121.70
2	F	122	PHE	CB-CG-CD1	11.77	129.04	120.80
1	G	140	TYR	CB-CG-CD2	11.76	128.06	121.00
1	E	49	SER	N-CA-CB	-11.75	92.88	110.50
1	C	116	GLU	C-N-CA	11.74	151.05	121.70
1	C	140	TYR	CZ-CE2-CD2	11.74	130.37	119.80
2	D	75	LEU	CB-CA-C	11.72	132.46	110.20
1	G	14	TRP	CB-CG-CD2	-11.71	111.37	126.60
1	G	75	ASP	CB-CG-OD1	-11.71	107.76	118.30
2	F	34	VAL	C-N-CA	11.71	150.97	121.70
1	E	7	LYS	N-CA-CB	11.70	131.66	110.60
1	A	107	VAL	CB-CA-C	11.69	133.62	111.40
1	C	53	ALA	N-CA-CB	11.69	126.47	110.10
2	B	98	VAL	CA-CB-CG1	11.69	128.43	110.90
2	F	13	ALA	CB-CA-C	11.69	127.63	110.10
1	G	58	HIS	C-N-CA	11.69	146.84	122.30
2	D	120	LYS	O-C-N	-11.68	104.01	122.70
2	D	87	THR	CA-C-N	-11.68	91.50	117.20
1	A	83	LEU	CB-CA-C	11.65	132.34	110.20
1	A	89	HIS	N-CA-CB	11.64	131.56	110.60
1	C	12	ALA	CA-C-O	-11.64	95.65	120.10
1	G	78	ASN	CB-CG-ND2	-11.64	88.76	116.70
1	A	73	VAL	CA-CB-CG2	11.63	128.34	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	GLN	N-CA-CB	-11.62	89.68	110.60
2	F	49	SER	O-C-N	11.62	141.29	122.70
2	D	53	ALA	N-CA-CB	11.62	126.36	110.10
1	A	58	HIS	N-CA-CB	-11.61	89.70	110.60
1	E	104	CYS	CB-CA-C	-11.61	87.19	110.40
1	C	9	ASN	CA-CB-CG	-11.60	87.88	113.40
2	H	79	ASP	N-CA-CB	11.60	131.47	110.60
2	H	47	ASP	O-C-N	11.59	141.25	122.70
1	A	62	VAL	CA-C-N	11.59	142.70	117.20
2	H	101	GLU	C-N-CA	11.59	150.67	121.70
1	A	134	THR	CA-C-O	11.59	144.43	120.10
2	F	82	LYS	N-CA-CB	11.58	131.45	110.60
1	G	141	ARG	CG-CD-NE	11.58	136.12	111.80
1	A	137	THR	CA-CB-CG2	-11.58	96.19	112.40
2	B	52	ASP	N-CA-CB	11.57	131.43	110.60
1	C	5	ALA	CA-C-O	11.57	144.40	120.10
2	D	22	GLU	CG-CD-OE2	11.56	141.42	118.30
2	D	20	VAL	CA-CB-CG2	11.54	128.21	110.90
1	E	98	PHE	O-C-N	-11.54	104.24	122.70
1	G	108	THR	O-C-N	11.54	141.16	122.70
2	F	92	HIS	CG-ND1-CE1	11.54	124.35	108.20
2	B	89	SER	N-CA-CB	11.53	127.80	110.50
1	A	67	THR	OG1-CB-CG2	11.53	136.52	110.00
2	D	12	THR	CA-C-N	11.53	142.56	117.20
1	G	23	GLU	CA-C-N	11.52	142.55	117.20
1	G	32	MET	CA-CB-CG	-11.52	93.72	113.30
1	A	70	VAL	CA-C-N	11.51	142.52	117.20
2	F	52	ASP	CB-CG-OD2	-11.51	107.95	118.30
2	D	87	THR	C-N-CA	-11.50	92.94	121.70
2	H	73	ASP	OD1-CG-OD2	-11.50	101.44	123.30
2	F	55	MET	O-C-N	-11.50	103.65	123.20
2	H	101	GLU	CG-CD-OE2	-11.49	95.32	118.30
2	B	104	ARG	C-N-CA	11.49	150.42	121.70
2	B	101	GLU	O-C-N	11.48	141.07	122.70
2	H	29	GLY	CA-C-N	-11.46	91.98	117.20
1	A	61	LYS	O-C-N	11.46	141.04	122.70
2	B	19	ASN	O-C-N	11.45	141.02	122.70
2	D	14	LEU	O-C-N	-11.45	104.38	122.70
1	G	126	ASP	CA-CB-CG	-11.45	88.22	113.40
1	E	113	LEU	O-C-N	11.44	142.83	121.10
1	C	119	PRO	CA-C-O	11.43	147.62	120.20
1	C	40	LYS	N-CA-CB	-11.42	90.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	SER	C-N-CA	11.41	150.24	121.70
1	E	81	SER	CA-C-O	-11.41	96.14	120.10
1	C	38	THR	CA-CB-CG2	-11.40	96.44	112.40
2	F	90	GLU	N-CA-CB	11.40	131.12	110.60
2	F	133	VAL	N-CA-CB	-11.40	86.42	111.50
1	G	61	LYS	CA-CB-CG	11.40	138.47	113.40
2	H	61	LYS	CA-C-N	11.39	142.27	117.20
2	B	136	GLY	CA-C-N	-11.38	92.16	117.20
2	H	34	VAL	O-C-N	11.38	140.91	122.70
2	H	111	VAL	CB-CA-C	11.37	133.01	111.40
1	G	92	ARG	CG-CD-NE	11.36	135.66	111.80
2	D	42	PHE	CE1-CZ-CE2	11.36	140.45	120.00
1	A	129	LEU	CB-CG-CD1	11.35	130.30	111.00
1	A	136	LEU	O-C-N	-11.34	104.55	122.70
1	G	8	THR	CA-CB-CG2	-11.34	96.52	112.40
1	C	55	VAL	CB-CA-C	-11.33	89.88	111.40
1	E	50	HIS	CA-C-O	-11.32	96.32	120.10
1	C	62	VAL	CA-CB-CG1	-11.32	93.92	110.90
1	A	103	HIS	CA-CB-CG	-11.31	94.38	113.60
2	D	118	PHE	CB-CA-C	11.31	133.01	110.40
1	C	126	ASP	CA-C-O	11.29	143.82	120.10
2	F	134	VAL	CA-CB-CG2	11.29	127.83	110.90
1	C	84	SER	O-C-N	11.29	140.76	122.70
1	E	121	VAL	CA-CB-CG1	-11.29	93.97	110.90
2	B	61	LYS	C-N-CA	11.27	149.88	121.70
2	B	21	ASP	CB-CG-OD2	-11.27	108.16	118.30
2	H	35	TYR	CG-CD2-CE2	-11.26	112.29	121.30
2	F	24	GLY	CA-C-O	-11.26	100.33	120.60
2	F	53	ALA	CB-CA-C	-11.26	93.21	110.10
2	F	116	HIS	CB-CG-ND1	11.26	151.34	123.20
2	H	142	ALA	O-C-N	-11.26	104.69	122.70
1	A	111	ALA	N-CA-CB	11.25	125.85	110.10
2	B	41	PHE	CG-CD1-CE1	11.25	133.17	120.80
1	E	21	ALA	N-CA-CB	-11.25	94.35	110.10
2	H	15	TRP	CZ3-CH2-CZ2	11.25	135.09	121.60
2	F	144	LYS	CA-C-O	-11.24	96.49	120.10
1	G	130	ALA	CB-CA-C	11.23	126.95	110.10
1	C	104	CYS	CA-CB-SG	11.23	134.22	114.00
1	E	104	CYS	CA-CB-SG	-11.23	93.79	114.00
2	D	106	LEU	CB-CA-C	11.23	131.54	110.20
2	D	117	HIS	CB-CG-ND1	-11.23	95.14	123.20
1	E	45	HIS	C-N-CA	11.22	149.75	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	45	PHE	CB-CG-CD2	-11.21	112.95	120.80
2	D	99	ASP	O-C-N	11.19	142.36	121.10
1	G	61	LYS	CD-CE-NZ	11.19	137.43	111.70
2	B	72	SER	CA-CB-OG	11.19	141.40	111.20
1	C	113	LEU	CB-CG-CD1	11.19	130.02	111.00
1	C	94	ASP	O-C-N	-11.18	99.85	121.10
2	B	50	THR	CA-CB-CG2	-11.18	96.75	112.40
2	F	9	SER	C-N-CA	11.17	149.63	121.70
2	F	132	LYS	CA-C-O	-11.17	96.65	120.10
2	H	44	SER	N-CA-CB	11.16	127.24	110.50
2	F	58	PRO	O-C-N	-11.16	104.85	122.70
1	A	105	LEU	O-C-N	11.15	140.54	122.70
1	G	117	PHE	CB-CG-CD2	11.15	128.61	120.80
1	E	125	LEU	CB-CG-CD1	11.14	129.94	111.00
2	H	35	TYR	CB-CG-CD1	11.13	127.68	121.00
1	E	75	ASP	CA-C-O	11.12	143.46	120.10
1	C	81	SER	CA-CB-OG	-11.11	81.20	111.20
2	H	54	VAL	CA-CB-CG2	-11.11	94.23	110.90
2	H	117	HIS	N-CA-CB	11.10	130.58	110.60
1	E	136	LEU	O-C-N	11.09	140.45	122.70
1	A	121	VAL	CA-CB-CG1	11.09	127.53	110.90
2	H	11	VAL	CA-CB-CG1	11.09	127.53	110.90
2	H	60	VAL	CA-CB-CG2	11.08	127.52	110.90
2	B	92	HIS	N-CA-CB	11.07	130.53	110.60
1	E	117	PHE	CB-CG-CD1	11.07	128.55	120.80
2	D	84	THR	CA-CB-OG1	-11.07	85.76	109.00
1	G	111	ALA	CB-CA-C	-11.07	93.50	110.10
1	C	37	PRO	CA-C-N	11.06	141.54	117.20
2	H	127	GLN	O-C-N	-11.06	105.00	122.70
1	C	6	ASP	CB-CG-OD2	11.06	128.26	118.30
2	F	90	GLU	CB-CA-C	-11.05	88.29	110.40
1	E	127	LYS	O-C-N	11.04	140.37	122.70
2	B	72	SER	O-C-N	11.04	140.36	122.70
1	C	115	ALA	N-CA-CB	-11.03	94.65	110.10
2	F	25	GLY	O-C-N	11.03	140.35	122.70
1	C	18	GLY	CA-C-N	-11.03	92.93	117.20
1	C	75	ASP	CB-CG-OD1	-11.03	108.38	118.30
2	B	40	ARG	N-CA-CB	-11.02	90.76	110.60
2	D	128	ALA	C-N-CA	11.02	149.26	121.70
2	F	23	VAL	CA-C-O	-11.02	96.95	120.10
1	E	98	PHE	CG-CD2-CE2	-11.02	108.68	120.80
2	D	112	CYS	CA-CB-SG	-11.01	94.19	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	VAL	CA-CB-CG2	11.01	127.41	110.90
1	C	112	HIS	N-CA-CB	11.00	130.40	110.60
1	E	126	ASP	CB-CG-OD1	11.00	128.20	118.30
2	B	21	ASP	CB-CA-C	10.99	132.38	110.40
2	F	33	VAL	CA-C-O	10.98	143.17	120.10
2	B	144	LYS	CA-C-N	10.98	141.35	117.20
1	E	38	THR	O-C-N	10.98	140.26	122.70
1	E	100	LEU	CB-CA-C	10.97	131.05	110.20
1	C	63	ALA	CB-CA-C	-10.96	93.65	110.10
1	C	133	SER	CA-C-N	10.96	141.31	117.20
2	F	98	VAL	CA-CB-CG1	-10.96	94.46	110.90
1	C	92	ARG	CD-NE-CZ	-10.95	108.26	123.60
1	G	131	SER	CA-C-O	-10.95	97.10	120.10
1	E	41	THR	O-C-N	10.95	140.22	122.70
2	D	90	GLU	C-N-CA	10.94	149.06	121.70
1	A	89	HIS	CA-C-N	10.94	141.27	117.20
2	H	55	MET	CA-C-N	10.94	138.08	116.20
2	B	52	ASP	CB-CG-OD1	-10.94	108.46	118.30
1	G	111	ALA	N-CA-CB	10.94	125.41	110.10
2	F	105	LEU	CA-C-N	10.93	141.25	117.20
1	G	20	HIS	N-CA-CB	10.93	130.27	110.60
1	A	138	SER	O-C-N	-10.92	105.23	122.70
2	B	143	HIS	N-CA-CB	10.92	130.26	110.60
2	F	79	ASP	CA-C-O	-10.92	97.17	120.10
2	F	131	GLN	O-C-N	10.92	140.17	122.70
2	B	90	GLU	CG-CD-OE2	-10.92	96.47	118.30
1	C	1	VAL	N-CA-CB	-10.92	87.48	111.50
1	A	7	LYS	N-CA-CB	-10.91	90.96	110.60
2	F	59	LYS	CB-CG-CD	10.90	139.94	111.60
1	G	87	HIS	CA-CB-CG	-10.90	95.07	113.60
2	D	131	GLN	C-N-CA	10.90	148.94	121.70
1	C	67	THR	CA-CB-OG1	10.89	131.88	109.00
2	D	67	VAL	CA-CB-CG2	10.89	127.24	110.90
1	C	61	LYS	O-C-N	10.89	140.13	122.70
1	A	140	TYR	CA-C-O	10.88	142.96	120.10
2	B	43	GLU	CG-CD-OE2	10.88	140.06	118.30
2	D	41	PHE	CB-CG-CD2	-10.88	113.18	120.80
1	G	19	ALA	O-C-N	-10.88	105.30	122.70
2	B	130	TYR	CD1-CE1-CZ	10.86	129.57	119.80
2	D	104	ARG	NH1-CZ-NH2	10.86	131.34	119.40
2	F	77	HIS	C-N-CA	10.85	148.82	121.70
1	A	94	ASP	CB-CG-OD1	-10.84	108.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	TYR	CA-C-O	-10.84	97.33	120.10
1	C	9	ASN	OD1-CG-ND2	10.84	146.83	121.90
2	H	130	TYR	CB-CG-CD2	10.84	127.50	121.00
2	D	118	PHE	CA-C-N	10.83	137.85	116.20
1	G	47	ASP	CA-CB-CG	-10.82	89.59	113.40
1	C	133	SER	C-N-CA	10.82	148.74	121.70
2	D	14	LEU	N-CA-CB	-10.82	88.76	110.40
1	E	89	HIS	CA-C-N	10.80	140.96	117.20
2	F	91	LEU	CA-C-O	-10.80	97.42	120.10
1	A	92	ARG	CA-C-O	10.79	142.76	120.10
1	E	1	VAL	CB-CA-C	-10.79	90.91	111.40
1	E	10	VAL	CA-C-O	-10.79	97.44	120.10
2	D	141	LEU	CB-CG-CD1	-10.78	92.67	111.00
2	F	130	TYR	CD1-CE1-CZ	-10.78	110.10	119.80
2	F	135	ALA	CA-C-N	10.78	137.76	116.20
2	F	109	VAL	O-C-N	-10.77	105.46	122.70
1	E	130	ALA	CA-C-O	10.77	142.72	120.10
1	A	132	VAL	CG1-CB-CG2	-10.76	93.69	110.90
1	C	34	LEU	CB-CG-CD2	-10.76	92.72	111.00
2	H	20	VAL	CB-CA-C	-10.76	90.97	111.40
1	C	45	HIS	CA-CB-CG	-10.75	95.33	113.60
2	F	108	ASN	CA-C-O	-10.74	97.54	120.10
2	B	2	HIS	CA-C-O	10.74	142.65	120.10
1	C	38	THR	CA-CB-OG1	10.73	131.53	109.00
1	A	3	SER	N-CA-CB	10.73	126.59	110.50
2	D	23	VAL	N-CA-CB	10.73	135.10	111.50
1	A	104	CYS	C-N-CA	10.71	148.47	121.70
2	H	87	THR	CA-CB-CG2	-10.71	97.41	112.40
1	C	63	ALA	CA-C-O	-10.71	97.61	120.10
1	G	14	TRP	CA-CB-CG	-10.71	93.35	113.70
1	G	128	PHE	CB-CG-CD2	10.70	128.29	120.80
1	E	36	PHE	CB-CA-C	10.70	131.80	110.40
1	A	58	HIS	CA-C-O	10.70	142.57	120.10
2	D	45	PHE	CA-CB-CG	-10.70	88.22	113.90
2	F	44	SER	N-CA-CB	10.70	126.55	110.50
1	C	41	THR	CA-CB-OG1	-10.69	86.55	109.00
2	D	93	CYS	N-CA-CB	10.69	129.84	110.60
1	C	30	GLU	CA-C-O	-10.68	97.67	120.10
2	H	62	ALA	CA-C-N	-10.68	93.71	117.20
1	C	44	PRO	CA-C-N	10.67	140.68	117.20
1	A	24	TYR	N-CA-CB	10.67	129.81	110.60
2	F	91	LEU	O-C-N	10.66	139.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	24	GLY	O-C-N	-10.65	105.09	123.20
1	G	124	SER	CB-CA-C	10.65	130.34	110.10
2	H	82	LYS	C-N-CA	-10.65	99.93	122.30
1	E	122	HIS	N-CA-CB	10.64	129.75	110.60
1	A	98	PHE	CB-CA-C	10.64	131.68	110.40
1	E	36	PHE	CG-CD1-CE1	10.64	132.50	120.80
1	G	31	ARG	NE-CZ-NH1	-10.64	114.98	120.30
1	G	55	VAL	C-N-CA	-10.64	95.11	121.70
2	H	136	GLY	O-C-N	10.62	139.69	122.70
2	H	146	HIS	CA-CB-CG	-10.62	95.55	113.60
2	H	39	GLN	OE1-CD-NE2	-10.61	97.49	121.90
2	D	54	VAL	CA-CB-CG1	-10.61	94.99	110.90
2	D	146	HIS	CA-CB-CG	-10.61	95.56	113.60
1	A	26	ALA	O-C-N	10.61	139.67	122.70
1	G	127	LYS	CD-CE-NZ	-10.60	87.31	111.70
1	E	21	ALA	CA-C-N	10.60	137.39	116.20
1	G	85	ASP	CB-CG-OD1	10.59	127.83	118.30
1	C	130	ALA	N-CA-CB	10.59	124.92	110.10
2	D	130	TYR	CG-CD2-CE2	10.59	129.77	121.30
2	F	105	LEU	CB-CA-C	10.59	130.31	110.20
2	F	8	LYS	O-C-N	10.58	139.63	122.70
1	A	64	ASP	CB-CG-OD1	10.58	127.82	118.30
2	B	40	ARG	NE-CZ-NH1	10.58	125.59	120.30
2	D	30	ARG	CA-CB-CG	10.57	136.65	113.40
2	D	94	ASP	OD1-CG-OD2	10.56	143.37	123.30
1	A	77	PRO	O-C-N	10.56	139.60	122.70
1	C	118	THR	CA-CB-CG2	10.56	127.18	112.40
1	A	52	SER	C-N-CA	10.56	148.09	121.70
1	G	29	LEU	CB-CA-C	10.55	130.25	110.20
1	A	30	GLU	CB-CA-C	10.55	131.50	110.40
2	F	69	GLY	O-C-N	10.55	139.58	122.70
1	G	47	ASP	C-N-CA	10.55	148.08	121.70
2	D	84	THR	C-N-CA	10.55	148.07	121.70
2	H	66	LYS	CB-CA-C	-10.55	89.31	110.40
2	F	27	ALA	C-N-CA	10.55	148.06	121.70
2	H	88	LEU	CA-C-O	-10.54	97.97	120.10
2	F	39	GLN	OE1-CD-NE2	10.54	146.13	121.90
1	A	109	LEU	CA-C-O	10.53	142.22	120.10
1	G	121	VAL	CA-C-N	-10.53	94.03	117.20
1	G	62	VAL	CA-C-N	10.52	140.35	117.20
2	D	37	TRP	CB-CG-CD1	10.52	140.67	127.00
2	F	38	THR	CA-CB-CG2	-10.52	97.67	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	55	VAL	CA-C-O	-10.52	98.02	120.10
1	A	101	LEU	N-CA-CB	10.51	131.43	110.40
1	G	53	ALA	C-N-CA	10.51	147.98	121.70
2	F	35	TYR	CG-CD1-CE1	-10.51	112.89	121.30
1	G	140	TYR	CA-CB-CG	10.51	133.36	113.40
2	F	59	LYS	CA-C-N	10.50	140.29	117.20
1	C	41	THR	O-C-N	10.49	139.48	122.70
2	D	31	LEU	C-N-CA	10.48	147.89	121.70
2	B	73	ASP	C-N-CA	10.47	144.28	122.30
1	C	69	ALA	O-C-N	10.47	139.45	122.70
1	A	105	LEU	CA-CB-CG	10.46	139.37	115.30
2	D	89	SER	N-CA-CB	-10.46	94.80	110.50
2	F	33	VAL	C-N-CA	10.46	147.86	121.70
1	E	69	ALA	CB-CA-C	10.46	125.79	110.10
1	G	87	HIS	CB-CA-C	-10.45	89.50	110.40
2	D	20	VAL	N-CA-CB	10.44	134.48	111.50
2	D	113	VAL	CA-C-O	-10.44	98.17	120.10
1	E	14	TRP	CH2-CZ2-CE2	10.44	127.84	117.40
2	H	102	ASN	CB-CG-OD1	-10.44	100.72	121.60
1	A	113	LEU	CA-CB-CG	-10.44	91.29	115.30
2	F	9	SER	O-C-N	-10.44	106.00	122.70
2	D	21	ASP	CB-CG-OD2	10.44	127.69	118.30
1	E	102	SER	O-C-N	10.44	139.40	122.70
1	G	87	HIS	CA-C-O	-10.44	98.19	120.10
2	B	145	TYR	CA-C-N	10.43	140.14	117.20
1	G	26	ALA	N-CA-CB	10.41	124.67	110.10
2	D	14	LEU	CB-CG-CD1	-10.41	93.31	111.00
2	F	43	GLU	CA-C-O	10.41	141.95	120.10
1	C	74	ASP	CA-C-O	10.40	141.94	120.10
1	E	136	LEU	C-N-CA	-10.40	95.70	121.70
2	B	122	PHE	CZ-CE2-CD2	-10.40	107.62	120.10
1	G	125	LEU	CA-C-O	-10.39	98.28	120.10
1	E	118	THR	N-CA-CB	-10.38	90.58	110.30
1	E	33	PHE	CA-C-N	10.38	140.03	117.20
1	C	92	ARG	NH1-CZ-NH2	-10.37	107.99	119.40
1	G	137	THR	CA-CB-OG1	-10.37	87.23	109.00
1	A	132	VAL	CA-C-N	10.36	140.00	117.20
2	H	18	VAL	O-C-N	10.36	139.28	122.70
2	D	49	SER	CB-CA-C	-10.36	90.42	110.10
1	G	67	THR	OG1-CB-CG2	10.35	133.80	110.00
1	A	73	VAL	CB-CA-C	10.35	131.06	111.40
1	G	128	PHE	C-N-CA	10.35	147.56	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	PHE	CB-CG-CD1	-10.34	113.56	120.80
2	H	129	ALA	CB-CA-C	-10.34	94.59	110.10
1	A	27	GLU	CB-CA-C	10.34	131.08	110.40
2	F	118	PHE	CA-C-O	-10.34	98.39	120.10
1	C	117	PHE	CA-C-O	10.33	141.80	120.10
1	E	4	PRO	N-CA-CB	10.33	115.70	103.30
2	H	5	PRO	N-CA-CB	10.33	115.69	103.30
1	G	7	LYS	C-N-CA	-10.32	95.90	121.70
2	F	30	ARG	CG-CD-NE	10.31	133.45	111.80
1	G	11	LYS	CB-CG-CD	10.31	138.41	111.60
1	A	107	VAL	CA-C-O	-10.31	98.45	120.10
1	C	57	GLY	C-N-CA	10.31	147.47	121.70
1	G	140	TYR	CZ-CE2-CD2	10.31	129.08	119.80
2	B	41	PHE	CB-CG-CD1	10.31	128.01	120.80
1	A	33	PHE	CG-CD1-CE1	-10.30	109.47	120.80
2	D	118	PHE	CB-CG-CD1	10.30	128.01	120.80
2	B	110	LEU	O-C-N	10.30	139.18	122.70
2	H	142	ALA	C-N-CA	10.30	147.44	121.70
2	B	95	LYS	C-N-CA	10.28	147.39	121.70
1	E	33	PHE	CG-CD1-CE1	10.28	132.10	120.80
1	G	10	VAL	CG1-CB-CG2	10.28	127.34	110.90
1	E	78	ASN	C-N-CA	10.26	147.35	121.70
1	G	53	ALA	CA-C-O	-10.26	98.55	120.10
1	G	70	VAL	CA-CB-CG2	10.26	126.29	110.90
2	B	90	GLU	OE1-CD-OE2	10.25	135.60	123.30
1	C	103	HIS	CB-CG-ND1	-10.25	97.57	123.20
2	D	10	ALA	O-C-N	-10.25	106.30	122.70
2	H	100	PRO	N-CD-CG	-10.25	87.83	103.20
2	B	112	CYS	CA-CB-SG	-10.24	95.56	114.00
1	C	16	LYS	CB-CG-CD	-10.24	84.97	111.60
1	E	79	ALA	CA-C-N	-10.24	94.68	117.20
1	A	21	ALA	CB-CA-C	-10.23	94.75	110.10
2	D	54	VAL	CA-C-O	10.23	141.59	120.10
2	B	103	PHE	C-N-CA	-10.23	96.12	121.70
2	F	57	ASN	OD1-CG-ND2	-10.23	98.38	121.90
1	G	21	ALA	C-N-CA	-10.22	100.83	122.30
2	D	88	LEU	CB-CG-CD2	10.21	128.37	111.00
1	E	19	ALA	N-CA-CB	10.21	124.40	110.10
2	H	40	ARG	CD-NE-CZ	-10.21	109.30	123.60
1	E	52	SER	CB-CA-C	-10.20	90.71	110.10
2	F	55	MET	CB-CA-C	10.20	130.80	110.40
2	F	118	PHE	CB-CA-C	10.20	130.80	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	LYS	CB-CG-CD	-10.20	85.09	111.60
2	D	49	SER	N-CA-CB	-10.19	95.21	110.50
1	E	124	SER	CA-C-N	10.19	139.62	117.20
1	G	114	PRO	C-N-CA	-10.19	96.23	121.70
2	F	104	ARG	CA-C-O	10.19	141.49	120.10
2	F	59	LYS	CA-CB-CG	10.18	135.81	113.40
1	G	85	ASP	CB-CA-C	10.18	130.77	110.40
2	B	28	LEU	CB-CG-CD2	10.18	128.31	111.00
2	D	25	GLY	O-C-N	-10.18	106.42	122.70
2	F	116	HIS	CB-CG-CD2	-10.18	99.26	130.80
1	G	29	LEU	CB-CG-CD2	10.18	128.30	111.00
2	H	125	PRO	CA-CB-CG	-10.17	84.67	104.00
1	G	82	ALA	N-CA-CB	-10.17	95.86	110.10
2	F	141	LEU	CB-CA-C	10.16	129.51	110.20
1	G	24	TYR	CG-CD1-CE1	-10.16	113.17	121.30
1	C	116	GLU	CA-C-N	10.16	139.55	117.20
1	G	14	TRP	CB-CA-C	-10.15	90.09	110.40
2	F	63	HIS	C-N-CA	-10.15	100.98	122.30
2	F	72	SER	C-N-CA	10.15	147.07	121.70
1	C	128	PHE	CB-CG-CD2	-10.14	113.70	120.80
1	G	116	GLU	C-N-CA	10.14	147.06	121.70
2	B	84	THR	N-CA-CB	-10.14	91.03	110.30
1	E	66	LEU	CB-CG-CD1	10.13	128.23	111.00
1	C	125	LEU	CB-CG-CD2	10.13	128.22	111.00
2	H	87	THR	CA-C-O	-10.13	98.82	120.10
2	D	50	THR	O-C-N	10.13	140.34	121.10
1	A	132	VAL	CA-C-O	-10.12	98.85	120.10
1	A	125	LEU	CB-CA-C	10.12	129.42	110.20
1	E	11	LYS	CA-C-O	10.11	141.33	120.10
2	H	20	VAL	O-C-N	10.11	138.88	122.70
2	D	10	ALA	N-CA-CB	10.10	124.24	110.10
2	B	129	ALA	CA-C-N	10.10	139.41	117.20
2	F	99	ASP	OD1-CG-OD2	10.09	142.48	123.30
1	A	94	ASP	CB-CG-OD2	10.09	127.38	118.30
2	D	133	VAL	O-C-N	10.09	138.84	122.70
1	E	119	PRO	CA-C-O	-10.08	96.00	120.20
2	D	57	ASN	N-CA-CB	-10.08	92.45	110.60
1	G	47	ASP	OD1-CG-OD2	10.08	142.45	123.30
1	E	96	VAL	CA-CB-CG2	10.07	126.00	110.90
2	F	8	LYS	CB-CA-C	10.07	130.53	110.40
2	D	117	HIS	CB-CA-C	-10.06	90.27	110.40
2	B	3	LEU	N-CA-CB	10.06	130.52	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	78	LEU	CB-CA-C	10.05	129.30	110.20
2	B	98	VAL	CA-CB-CG2	-10.05	95.83	110.90
1	A	19	ALA	O-C-N	-10.05	106.62	122.70
2	D	58	PRO	O-C-N	10.05	138.77	122.70
1	A	134	THR	O-C-N	-10.04	106.63	122.70
2	B	113	VAL	CA-C-N	10.04	139.28	117.20
1	C	9	ASN	N-CA-CB	10.03	128.66	110.60
1	G	19	ALA	N-CA-CB	-10.03	96.06	110.10
2	H	44	SER	C-N-CA	10.03	146.78	121.70
2	F	79	ASP	N-CA-CB	10.03	128.65	110.60
1	G	75	ASP	CA-C-O	-10.03	99.04	120.10
2	H	39	GLN	CA-C-O	10.02	141.15	120.10
1	E	113	LEU	CB-CA-C	10.02	129.24	110.20
2	H	133	VAL	O-C-N	10.01	138.72	122.70
1	C	85	ASP	C-N-CA	10.01	146.72	121.70
2	F	90	GLU	CG-CD-OE1	-10.00	98.30	118.30
2	H	103	PHE	CB-CG-CD1	9.99	127.80	120.80
2	B	7	GLU	CA-C-O	9.99	141.08	120.10
1	E	73	VAL	CA-C-O	9.99	141.08	120.10
2	F	31	LEU	CA-C-O	9.98	141.06	120.10
1	E	117	PHE	CB-CG-CD2	-9.98	113.81	120.80
1	E	24	TYR	CA-C-O	9.98	141.05	120.10
2	B	112	CYS	CA-C-O	-9.97	99.15	120.10
2	D	30	ARG	CB-CG-CD	9.97	137.53	111.60
1	G	86	LEU	N-CA-CB	9.97	130.34	110.40
2	B	22	GLU	CG-CD-OE2	-9.97	98.37	118.30
2	H	38	THR	CA-C-O	9.96	141.02	120.10
2	D	98	VAL	N-CA-CB	-9.96	89.59	111.50
1	C	56	LYS	C-N-CA	-9.96	101.39	122.30
2	H	42	PHE	CB-CG-CD2	9.95	127.77	120.80
2	H	84	THR	CA-CB-OG1	-9.95	88.10	109.00
2	H	106	LEU	CB-CA-C	9.95	129.10	110.20
1	E	129	LEU	CB-CG-CD1	9.94	127.90	111.00
1	C	83	LEU	CA-C-O	9.94	140.97	120.10
2	F	17	LYS	N-CA-CB	-9.93	92.72	110.60
2	F	130	TYR	CD1-CG-CD2	-9.93	106.98	117.90
2	F	88	LEU	CA-CB-CG	9.93	138.13	115.30
2	B	131	GLN	OE1-CD-NE2	9.92	144.72	121.90
2	F	134	VAL	CA-C-N	9.92	139.02	117.20
2	H	128	ALA	CB-CA-C	-9.92	95.22	110.10
2	B	65	LYS	CA-C-O	9.91	140.92	120.10
2	F	29	GLY	CA-C-O	9.91	138.43	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	ALA	CA-C-N	9.90	138.99	117.20
1	C	102	SER	CA-CB-OG	9.90	137.94	111.20
2	H	108	ASN	CB-CG-ND2	-9.90	92.93	116.70
2	F	111	VAL	CA-C-O	9.90	140.89	120.10
2	H	130	TYR	CG-CD1-CE1	-9.90	113.38	121.30
1	E	38	THR	N-CA-CB	9.90	129.11	110.30
1	C	86	LEU	CB-CG-CD1	-9.90	94.18	111.00
1	E	98	PHE	CB-CG-CD2	-9.89	113.88	120.80
1	G	64	ASP	CB-CA-C	9.89	130.17	110.40
2	B	34	VAL	CG1-CB-CG2	9.88	126.71	110.90
2	H	30	ARG	CA-C-O	-9.88	99.35	120.10
1	G	129	LEU	O-C-N	9.88	138.50	122.70
1	A	130	ALA	CB-CA-C	-9.88	95.29	110.10
1	E	106	LEU	CA-C-N	9.88	138.93	117.20
1	E	125	LEU	N-CA-CB	9.87	130.15	110.40
2	H	130	TYR	CA-C-O	9.87	140.83	120.10
2	B	133	VAL	CA-C-N	9.87	138.92	117.20
2	D	43	GLU	CB-CA-C	9.87	130.13	110.40
1	A	36	PHE	CZ-CE2-CD2	-9.86	108.26	120.10
2	D	8	LYS	CB-CG-CD	-9.86	85.95	111.60
1	G	54	GLN	CG-CD-OE1	-9.86	101.88	121.60
1	A	14	TRP	CD1-NE1-CE2	9.86	117.87	109.00
2	H	43	GLU	CG-CD-OE1	9.86	138.02	118.30
2	H	124	PRO	CA-N-CD	-9.86	97.70	111.50
2	D	111	VAL	CA-CB-CG2	-9.85	96.12	110.90
2	B	11	VAL	C-N-CA	9.85	146.32	121.70
2	D	39	GLN	CA-C-O	9.84	140.77	120.10
1	E	45	HIS	CA-C-N	9.84	138.85	117.20
2	H	62	ALA	CB-CA-C	-9.84	95.34	110.10
1	G	23	GLU	CA-C-O	-9.84	99.44	120.10
2	D	82	LYS	CA-C-O	9.83	140.75	120.10
1	G	88	ALA	CB-CA-C	9.83	124.85	110.10
2	D	43	GLU	O-C-N	-9.83	106.98	122.70
1	C	16	LYS	CG-CD-CE	-9.82	82.42	111.90
1	E	93	VAL	CA-CB-CG1	-9.82	96.16	110.90
2	H	92	HIS	C-N-CA	9.82	146.25	121.70
1	E	141	ARG	CD-NE-CZ	9.82	137.35	123.60
2	D	84	THR	O-C-N	-9.81	107.00	122.70
2	B	44	SER	CA-C-O	9.81	140.70	120.10
2	B	65	LYS	CB-CA-C	9.81	130.02	110.40
1	E	67	THR	CA-CB-CG2	-9.81	98.66	112.40
1	C	72	HIS	CA-C-O	-9.81	99.50	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	35	TYR	CG-CD1-CE1	-9.81	113.45	121.30
1	G	105	LEU	O-C-N	-9.81	107.00	122.70
2	F	101	GLU	CA-CB-CG	-9.80	91.84	113.40
2	H	96	LEU	C-N-CA	9.80	146.20	121.70
1	E	90	LYS	C-N-CA	9.80	146.19	121.70
2	F	7	GLU	CA-C-N	-9.79	95.65	117.20
2	H	103	PHE	CA-CB-CG	9.79	137.39	113.90
2	B	144	LYS	C-N-CA	9.78	146.16	121.70
2	B	146	HIS	CA-CB-CG	-9.78	96.97	113.60
1	C	76	MET	CA-CB-CG	-9.77	96.69	113.30
1	C	74	ASP	OD1-CG-OD2	-9.76	104.75	123.30
1	E	107	VAL	CA-C-N	-9.76	95.72	117.20
2	H	130	TYR	CA-C-N	-9.76	95.73	117.20
1	C	19	ALA	CB-CA-C	9.76	124.73	110.10
2	D	26	GLU	O-C-N	9.76	138.31	122.70
2	D	123	THR	CA-CB-CG2	9.76	126.06	112.40
2	D	37	TRP	CB-CG-CD2	-9.75	113.92	126.60
2	F	84	THR	CA-CB-CG2	9.75	126.05	112.40
2	B	47	ASP	CA-CB-CG	9.75	134.84	113.40
2	D	18	VAL	CA-CB-CG2	9.74	125.51	110.90
2	F	55	MET	CB-CG-SD	9.74	141.61	112.40
1	C	128	PHE	CB-CG-CD1	9.73	127.61	120.80
1	E	46	PHE	CD1-CG-CD2	9.73	130.95	118.30
2	H	22	GLU	OE1-CD-OE2	9.72	134.97	123.30
1	G	92	ARG	CA-CB-CG	9.72	134.78	113.40
1	A	36	PHE	CB-CG-CD1	-9.72	114.00	120.80
2	H	90	GLU	CA-C-N	9.71	138.56	117.20
2	D	108	ASN	CA-C-O	-9.71	99.72	120.10
2	B	143	HIS	CB-CG-ND1	9.70	147.45	123.20
2	F	104	ARG	CG-CD-NE	9.70	132.17	111.80
2	D	86	ALA	CA-C-O	9.68	140.43	120.10
2	D	54	VAL	CA-C-N	-9.68	95.91	117.20
1	E	109	LEU	CA-C-N	9.68	138.49	117.20
2	H	52	ASP	CB-CG-OD2	-9.67	109.60	118.30
2	D	60	VAL	CB-CA-C	9.66	129.76	111.40
2	D	117	HIS	CA-CB-CG	-9.66	97.17	113.60
1	G	98	PHE	CB-CA-C	9.66	129.73	110.40
1	G	140	TYR	CA-C-N	9.66	138.46	117.20
1	A	64	ASP	CB-CG-OD2	-9.66	109.60	118.30
1	E	12	ALA	O-C-N	9.66	138.16	122.70
1	G	127	LYS	CA-C-O	-9.66	99.81	120.10
2	B	68	LEU	C-N-CA	-9.66	102.02	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	126	VAL	CA-CB-CG2	9.65	125.38	110.90
1	A	33	PHE	CB-CG-CD2	-9.65	114.04	120.80
1	E	43	PHE	CG-CD2-CE2	9.65	131.42	120.80
2	D	89	SER	O-C-N	-9.65	107.27	122.70
1	E	131	SER	CA-C-O	9.64	140.35	120.10
2	B	66	LYS	CD-CE-NZ	-9.64	89.53	111.70
1	E	36	PHE	CB-CG-CD2	9.64	127.55	120.80
2	D	76	ALA	O-C-N	9.63	138.11	122.70
1	A	50	HIS	N-CA-CB	9.63	127.93	110.60
1	C	125	LEU	CB-CA-C	9.62	128.49	110.20
2	H	85	PHE	O-C-N	9.62	138.10	122.70
2	B	118	PHE	N-CA-CB	-9.62	93.29	110.60
2	B	36	PRO	N-CA-CB	9.61	114.83	103.30
2	F	22	GLU	N-CA-CB	9.61	127.90	110.60
2	F	22	GLU	C-N-CA	-9.60	97.69	121.70
1	E	73	VAL	CG1-CB-CG2	-9.60	95.54	110.90
1	A	129	LEU	CA-C-N	9.60	138.31	117.20
2	F	68	LEU	CB-CA-C	-9.59	91.97	110.20
1	E	119	PRO	CA-C-N	9.59	138.29	117.20
2	H	21	ASP	CB-CG-OD2	9.59	126.93	118.30
2	B	63	HIS	CA-CB-CG	-9.59	97.31	113.60
1	E	68	ASN	N-CA-CB	9.58	127.84	110.60
1	A	43	PHE	CG-CD1-CE1	9.57	131.33	120.80
2	H	85	PHE	CG-CD1-CE1	9.57	131.33	120.80
1	C	96	VAL	CA-CB-CG2	-9.57	96.55	110.90
2	H	20	VAL	CA-C-N	-9.57	96.15	117.20
2	D	31	LEU	CA-CB-CG	9.56	137.30	115.30
1	A	38	THR	O-C-N	9.56	138.00	122.70
1	C	89	HIS	CB-CA-C	-9.56	91.27	110.40
1	A	10	VAL	O-C-N	9.56	137.99	122.70
1	A	28	ALA	CA-C-N	-9.56	96.17	117.20
1	G	11	LYS	N-CA-CB	9.56	127.81	110.60
1	A	123	ALA	N-CA-CB	-9.56	96.72	110.10
2	D	96	LEU	CB-CA-C	9.56	128.36	110.20
1	C	108	THR	CA-C-N	-9.55	96.18	117.20
1	G	39	THR	CA-C-O	9.55	140.16	120.10
2	F	42	PHE	O-C-N	9.55	137.98	122.70
2	B	42	PHE	CG-CD2-CE2	-9.55	110.30	120.80
2	B	135	ALA	CA-C-N	9.55	135.30	116.20
2	D	96	LEU	C-N-CA	9.54	145.56	121.70
2	D	131	GLN	CA-C-O	-9.54	100.06	120.10
1	A	122	HIS	CG-ND1-CE1	9.54	121.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5	ALA	N-CA-CB	-9.54	96.75	110.10
2	D	104	ARG	CG-CD-NE	9.54	131.82	111.80
2	F	36	PRO	N-CA-CB	-9.53	91.86	103.30
2	H	88	LEU	CB-CG-CD1	9.53	127.21	111.00
2	B	1	VAL	CB-CA-C	-9.53	93.30	111.40
2	F	5	PRO	N-CD-CG	-9.53	88.91	103.20
2	H	131	GLN	OE1-CD-NE2	-9.53	99.99	121.90
1	A	4	PRO	CA-C-O	9.52	143.06	120.20
1	E	6	ASP	CB-CA-C	9.52	129.45	110.40
1	C	39	THR	CA-CB-OG1	-9.52	89.01	109.00
1	G	140	TYR	O-C-N	-9.52	107.46	122.70
2	F	44	SER	O-C-N	9.52	137.93	122.70
2	B	106	LEU	O-C-N	9.52	139.38	123.20
1	E	98	PHE	CD1-CE1-CZ	-9.51	108.69	120.10
2	D	100	PRO	N-CA-CB	-9.51	91.89	103.30
1	E	70	VAL	C-N-CA	-9.51	97.94	121.70
1	G	64	ASP	CA-C-N	-9.51	96.29	117.20
2	D	128	ALA	O-C-N	-9.50	107.50	122.70
2	F	123	THR	N-CA-CB	-9.50	92.24	110.30
2	F	16	GLY	CA-C-O	-9.50	103.50	120.60
2	F	43	GLU	CG-CD-OE1	9.49	137.29	118.30
2	F	39	GLN	CG-CD-NE2	-9.49	93.92	116.70
1	E	40	LYS	O-C-N	-9.49	107.52	122.70
1	E	87	HIS	CA-C-N	9.48	138.07	117.20
2	H	90	GLU	CA-C-O	-9.48	100.18	120.10
2	B	141	LEU	CB-CG-CD1	9.48	127.11	111.00
1	E	4	PRO	CA-N-CD	-9.48	98.23	111.50
1	E	21	ALA	CB-CA-C	9.48	124.32	110.10
1	C	93	VAL	C-N-CA	-9.47	98.02	121.70
2	H	131	GLN	CB-CG-CD	9.47	136.22	111.60
1	A	56	LYS	CA-C-N	9.46	135.13	116.20
1	A	92	ARG	NE-CZ-NH2	9.46	125.03	120.30
2	B	32	LEU	CB-CA-C	9.46	128.17	110.20
1	G	32	MET	CB-CA-C	-9.46	91.48	110.40
2	D	20	VAL	O-C-N	9.46	137.83	122.70
2	F	113	VAL	CB-CA-C	9.46	129.37	111.40
2	B	113	VAL	CA-CB-CG1	-9.44	96.74	110.90
1	C	116	GLU	OE1-CD-OE2	9.44	134.63	123.30
1	C	140	TYR	O-C-N	-9.44	107.60	122.70
2	H	45	PHE	CB-CG-CD2	-9.43	114.20	120.80
1	E	58	HIS	N-CA-CB	9.42	127.56	110.60
2	D	42	PHE	CD1-CE1-CZ	-9.42	108.80	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ASP	CB-CG-OD2	9.40	126.76	118.30
1	C	35	SER	O-C-N	-9.40	107.65	122.70
2	D	28	LEU	CB-CG-CD2	-9.40	95.02	111.00
2	B	135	ALA	C-N-CA	9.40	142.03	122.30
1	C	26	ALA	CA-C-O	-9.39	100.38	120.10
1	C	125	LEU	CB-CG-CD1	-9.39	95.04	111.00
2	F	95	LYS	C-N-CA	9.39	145.17	121.70
2	H	146	HIS	CG-ND1-CE1	9.39	121.34	108.20
1	A	92	ARG	CA-C-N	-9.38	96.55	117.20
1	C	105	LEU	CB-CG-CD2	9.38	126.94	111.00
2	D	52	ASP	CB-CG-OD1	9.37	126.73	118.30
2	H	121	GLU	CA-CB-CG	-9.37	92.78	113.40
2	D	6	VAL	N-CA-CB	9.37	132.11	111.50
1	G	6	ASP	CB-CG-OD1	9.37	126.73	118.30
2	F	118	PHE	CA-CB-CG	9.36	136.37	113.90
1	A	112	HIS	O-C-N	-9.36	107.72	122.70
2	B	80	ASN	O-C-N	-9.36	107.72	122.70
2	B	31	LEU	CA-C-N	-9.36	96.61	117.20
1	G	32	MET	N-CA-CB	9.36	127.44	110.60
2	H	65	LYS	CA-CB-CG	9.35	133.96	113.40
2	D	90	GLU	CG-CD-OE2	-9.34	99.62	118.30
2	F	8	LYS	CA-C-O	-9.34	100.49	120.10
2	H	129	ALA	CA-C-O	-9.34	100.49	120.10
2	H	3	LEU	CB-CG-CD2	-9.34	95.13	111.00
1	G	20	HIS	CA-CB-CG	-9.33	97.74	113.60
1	E	134	THR	CA-CB-OG1	-9.33	89.41	109.00
1	G	34	LEU	N-CA-CB	9.33	129.06	110.40
1	G	101	LEU	CA-C-O	9.33	139.69	120.10
1	G	132	VAL	CG1-CB-CG2	-9.33	95.98	110.90
1	A	125	LEU	CB-CG-CD2	9.32	126.84	111.00
2	H	47	ASP	CA-C-N	-9.31	96.71	117.20
1	E	105	LEU	C-N-CA	9.31	144.97	121.70
2	D	95	LYS	CD-CE-NZ	9.30	133.10	111.70
2	F	16	GLY	CA-C-N	9.30	137.66	117.20
2	F	111	VAL	CB-CA-C	-9.29	93.75	111.40
1	E	5	ALA	O-C-N	9.29	137.56	122.70
2	D	82	LYS	CA-C-N	-9.28	97.63	116.20
1	C	137	THR	O-C-N	9.28	137.55	122.70
1	E	75	ASP	CB-CG-OD1	-9.28	109.95	118.30
1	A	91	LEU	CA-CB-CG	-9.28	93.97	115.30
1	C	126	ASP	CB-CG-OD1	9.28	126.65	118.30
2	F	42	PHE	CD1-CE1-CZ	-9.28	108.97	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	MET	CG-SD-CE	-9.27	85.36	100.20
1	C	30	GLU	N-CA-CB	9.27	127.28	110.60
1	E	76	MET	CA-CB-CG	9.27	129.06	113.30
1	G	40	LYS	CA-CB-CG	9.27	133.79	113.40
2	H	19	ASN	C-N-CA	9.27	144.87	121.70
2	D	20	VAL	CA-C-O	-9.26	100.66	120.10
2	D	20	VAL	CG1-CB-CG2	-9.25	96.10	110.90
1	G	83	LEU	C-N-CA	9.25	144.82	121.70
1	A	98	PHE	CE1-CZ-CE2	-9.24	103.36	120.00
1	E	55	VAL	CA-CB-CG1	9.24	124.76	110.90
2	D	66	LYS	CB-CG-CD	-9.24	87.58	111.60
1	A	92	ARG	NH1-CZ-NH2	9.23	129.56	119.40
1	C	24	TYR	CG-CD2-CE2	9.23	128.69	121.30
2	D	65	LYS	CB-CA-C	9.23	128.87	110.40
1	G	107	VAL	CG1-CB-CG2	-9.23	96.12	110.90
2	H	146	HIS	N-CA-C	9.22	135.91	111.00
2	F	111	VAL	CA-CB-CG2	-9.22	97.06	110.90
1	C	40	LYS	O-C-N	-9.22	107.95	122.70
2	H	64	GLY	CA-C-O	-9.21	104.02	120.60
2	B	103	PHE	O-C-N	9.21	137.44	122.70
1	E	26	ALA	CB-CA-C	9.21	123.92	110.10
1	C	115	ALA	CB-CA-C	9.21	123.92	110.10
1	E	98	PHE	CE1-CZ-CE2	9.21	136.57	120.00
2	F	80	ASN	CB-CG-OD1	-9.21	103.18	121.60
1	E	53	ALA	O-C-N	9.20	137.43	122.70
1	A	108	THR	CA-CB-OG1	-9.20	89.68	109.00
1	C	89	HIS	O-C-N	9.20	137.41	122.70
1	G	67	THR	O-C-N	-9.20	107.99	122.70
1	C	63	ALA	O-C-N	9.19	137.40	122.70
1	E	85	ASP	CA-C-O	-9.19	100.81	120.10
2	D	114	LEU	N-CA-CB	9.18	128.77	110.40
1	A	41	THR	CA-CB-OG1	-9.18	89.72	109.00
1	A	141	ARG	CA-CB-CG	-9.18	93.20	113.40
2	F	102	ASN	CA-CB-CG	9.18	133.59	113.40
2	B	30	ARG	N-CA-CB	-9.17	94.09	110.60
2	B	3	LEU	CA-C-N	-9.17	97.03	117.20
1	G	76	MET	CB-CA-C	9.17	128.74	110.40
1	C	41	THR	CA-CB-CG2	9.16	125.23	112.40
2	H	98	VAL	N-CA-C	9.16	135.74	111.00
1	C	20	HIS	CB-CG-ND1	-9.16	100.30	123.20
1	C	37	PRO	N-CD-CG	-9.16	89.46	103.20
2	D	43	GLU	N-CA-CB	-9.16	94.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PRO	C-N-CA	9.15	144.58	121.70
2	D	85	PHE	C-N-CA	9.15	144.58	121.70
1	C	66	LEU	CB-CG-CD1	-9.15	95.45	111.00
2	F	145	TYR	CA-CB-CG	9.15	130.78	113.40
1	G	33	PHE	N-CA-CB	9.15	127.06	110.60
1	G	1	VAL	CG1-CB-CG2	9.14	125.53	110.90
1	G	8	THR	OG1-CB-CG2	9.14	131.02	110.00
1	E	128	PHE	CZ-CE2-CD2	-9.13	109.14	120.10
2	H	129	ALA	N-CA-CB	9.13	122.88	110.10
2	D	70	ALA	O-C-N	9.13	137.31	122.70
1	C	107	VAL	O-C-N	-9.12	108.10	122.70
2	F	94	ASP	CA-CB-CG	9.12	133.47	113.40
1	G	139	LYS	CD-CE-NZ	-9.12	90.73	111.70
2	F	97	HIS	CB-CG-ND1	9.12	145.99	123.20
1	C	113	LEU	N-CA-CB	-9.12	92.17	110.40
2	H	1	VAL	CA-CB-CG2	-9.12	97.23	110.90
2	H	61	LYS	CG-CD-CE	9.11	139.22	111.90
2	H	122	PHE	O-C-N	9.10	137.26	122.70
2	B	50	THR	CA-CB-OG1	9.10	128.11	109.00
2	D	121	GLU	CA-C-O	9.10	139.21	120.10
1	G	8	THR	C-N-CA	9.10	144.45	121.70
1	A	43	PHE	CB-CG-CD1	9.10	127.17	120.80
2	D	145	TYR	CB-CG-CD1	-9.09	115.54	121.00
1	E	14	TRP	N-CA-CB	-9.09	94.23	110.60
1	C	133	SER	CA-C-O	-9.09	101.01	120.10
2	B	145	TYR	CD1-CE1-CZ	-9.08	111.63	119.80
1	A	72	HIS	CA-CB-CG	-9.08	98.17	113.60
2	B	109	VAL	CA-CB-CG1	-9.08	97.28	110.90
2	F	81	LEU	CA-CB-CG	9.08	136.18	115.30
2	H	22	GLU	CG-CD-OE2	-9.08	100.15	118.30
1	A	114	PRO	CB-CA-C	9.07	134.67	112.00
1	E	32	MET	CA-C-O	-9.07	101.06	120.10
2	H	19	ASN	N-CA-CB	-9.06	94.29	110.60
2	H	6	VAL	CA-C-O	9.06	139.13	120.10
2	F	105	LEU	O-C-N	-9.05	108.22	122.70
2	H	106	LEU	O-C-N	9.04	138.56	123.20
1	G	53	ALA	CA-C-N	9.03	137.07	117.20
2	D	20	VAL	C-N-CA	9.03	144.27	121.70
2	B	61	LYS	O-C-N	-9.02	108.26	122.70
1	E	102	SER	N-CA-CB	9.02	124.03	110.50
1	G	71	ALA	CB-CA-C	9.02	123.63	110.10
1	G	124	SER	C-N-CA	-9.02	99.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	VAL	O-C-N	-9.02	108.28	122.70
1	E	4	PRO	CA-CB-CG	-9.02	86.87	104.00
2	H	75	LEU	CB-CG-CD1	9.01	126.32	111.00
1	A	125	LEU	N-CA-CB	-9.01	92.39	110.40
2	H	133	VAL	C-N-CA	-9.01	99.18	121.70
1	G	18	GLY	O-C-N	9.00	137.10	122.70
1	C	47	ASP	CA-CB-CG	9.00	133.20	113.40
2	B	12	THR	OG1-CB-CG2	-8.99	89.32	110.00
1	G	116	GLU	N-CA-CB	8.99	126.78	110.60
2	H	45	PHE	C-N-CA	8.99	141.18	122.30
1	A	17	VAL	O-C-N	8.99	138.48	123.20
1	C	64	ASP	C-N-CA	8.98	144.16	121.70
1	E	52	SER	O-C-N	8.98	137.07	122.70
2	B	108	ASN	O-C-N	-8.98	108.33	122.70
1	A	117	PHE	CB-CG-CD1	8.98	127.08	120.80
2	B	19	ASN	CB-CG-ND2	8.97	138.24	116.70
2	D	115	ALA	CA-C-O	8.97	138.94	120.10
1	E	89	HIS	CA-C-O	-8.96	101.28	120.10
2	B	35	TYR	CD1-CE1-CZ	8.96	127.86	119.80
2	B	108	ASN	C-N-CA	8.96	144.09	121.70
2	D	126	VAL	CA-C-O	8.96	138.91	120.10
1	E	117	PHE	CZ-CE2-CD2	8.96	130.85	120.10
1	A	116	GLU	CB-CA-C	8.95	128.30	110.40
1	A	118	THR	CA-CB-OG1	8.95	127.80	109.00
1	A	17	VAL	CG1-CB-CG2	8.95	125.21	110.90
1	C	44	PRO	CA-C-O	-8.94	98.74	120.20
2	H	11	VAL	CA-CB-CG2	-8.94	97.49	110.90
1	C	74	ASP	O-C-N	-8.93	108.41	122.70
2	D	135	ALA	CB-CA-C	8.93	123.50	110.10
2	B	79	ASP	C-N-CA	8.93	144.03	121.70
1	A	54	GLN	CA-CB-CG	-8.93	93.76	113.40
2	B	99	ASP	N-CA-CB	8.93	126.67	110.60
2	H	55	MET	O-C-N	-8.93	108.02	123.20
1	C	120	ALA	CB-CA-C	8.92	123.48	110.10
1	E	73	VAL	N-CA-CB	8.92	131.13	111.50
2	F	8	LYS	CD-CE-NZ	8.92	132.22	111.70
1	A	75	ASP	CA-C-N	8.92	136.82	117.20
2	B	130	TYR	CD1-CG-CD2	8.92	127.71	117.90
1	A	17	VAL	CB-CA-C	-8.91	94.47	111.40
1	E	17	VAL	CA-CB-CG2	-8.91	97.53	110.90
2	H	5	PRO	CA-N-CD	-8.91	99.03	111.50
2	B	55	MET	N-CA-CB	-8.91	94.57	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	84	THR	N-CA-C	8.91	135.05	111.00
1	G	135	VAL	CA-CB-CG2	-8.90	97.55	110.90
1	E	3	SER	N-CA-CB	-8.90	97.15	110.50
1	G	106	LEU	CB-CA-C	8.90	127.10	110.20
2	H	105	LEU	O-C-N	8.90	136.94	122.70
2	D	121	GLU	N-CA-CB	8.89	126.61	110.60
1	E	17	VAL	CG1-CB-CG2	8.89	125.13	110.90
2	F	15	TRP	CE3-CZ3-CH2	-8.88	111.43	121.20
2	B	60	VAL	CA-CB-CG1	-8.88	97.58	110.90
1	G	136	LEU	CA-CB-CG	-8.88	94.87	115.30
2	B	130	TYR	CB-CG-CD2	8.88	126.33	121.00
1	A	31	ARG	NH1-CZ-NH2	-8.88	109.64	119.40
1	C	12	ALA	O-C-N	8.88	136.90	122.70
1	G	85	ASP	OD1-CG-OD2	-8.87	106.44	123.30
1	A	121	VAL	CB-CA-C	8.87	128.25	111.40
2	D	21	ASP	CA-CB-CG	-8.87	93.89	113.40
2	B	10	ALA	CA-C-N	-8.87	97.69	117.20
2	B	67	VAL	CA-C-O	-8.87	101.48	120.10
1	A	101	LEU	C-N-CA	-8.87	99.54	121.70
1	G	134	THR	C-N-CA	8.86	143.86	121.70
1	E	3	SER	CA-C-O	-8.86	101.49	120.10
2	H	3	LEU	CA-C-N	-8.86	97.71	117.20
1	G	7	LYS	N-CA-CB	8.86	126.54	110.60
2	F	100	PRO	CA-C-O	8.85	141.45	120.20
1	E	48	LEU	CB-CA-C	8.85	127.02	110.20
2	D	99	ASP	N-CA-C	-8.85	87.11	111.00
2	H	124	PRO	N-CA-CB	8.85	113.92	103.30
1	A	93	VAL	CA-CB-CG1	8.84	124.16	110.90
1	A	101	LEU	CA-C-O	-8.84	101.53	120.10
2	F	39	GLN	CB-CA-C	8.84	128.09	110.40
1	E	61	LYS	O-C-N	8.84	136.84	122.70
2	F	91	LEU	N-CA-CB	8.84	128.08	110.40
1	E	24	TYR	CG-CD1-CE1	8.84	128.37	121.30
1	G	16	LYS	CG-CD-CE	8.84	138.41	111.90
2	D	133	VAL	CA-CB-CG2	8.83	124.15	110.90
2	F	40	ARG	CD-NE-CZ	8.83	135.97	123.60
1	A	107	VAL	CG1-CB-CG2	-8.83	96.77	110.90
2	B	77	HIS	O-C-N	8.83	136.83	122.70
2	D	93	CYS	CA-CB-SG	8.83	129.90	114.00
1	A	72	HIS	C-N-CA	8.83	143.77	121.70
1	E	36	PHE	CA-C-O	8.83	138.64	120.10
1	C	99	LYS	CA-C-N	-8.83	97.78	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	48	LEU	N-CA-CB	8.83	128.05	110.40
2	D	138	ALA	CA-C-O	8.82	138.63	120.10
1	E	109	LEU	CB-CA-C	8.82	126.96	110.20
1	G	14	TRP	CB-CG-CD1	8.82	138.47	127.00
2	B	45	PHE	CB-CG-CD1	-8.82	114.63	120.80
2	F	59	LYS	O-C-N	-8.81	108.60	122.70
1	G	46	PHE	CG-CD2-CE2	-8.81	111.11	120.80
1	E	93	VAL	CG1-CB-CG2	8.81	125.00	110.90
2	F	137	VAL	CA-CB-CG2	8.81	124.11	110.90
1	G	96	VAL	O-C-N	8.81	136.79	122.70
2	H	127	GLN	CG-CD-NE2	8.81	137.84	116.70
2	H	105	LEU	N-CA-CB	8.80	128.01	110.40
1	A	136	LEU	CA-C-N	8.80	136.56	117.20
2	D	130	TYR	O-C-N	8.80	136.78	122.70
2	B	114	LEU	CA-C-N	-8.79	97.85	117.20
2	D	32	LEU	CB-CA-C	8.79	126.91	110.20
1	E	138	SER	CA-C-O	-8.79	101.63	120.10
2	H	122	PHE	CZ-CE2-CD2	-8.79	109.55	120.10
2	F	17	LYS	CB-CA-C	-8.79	92.82	110.40
1	E	96	VAL	O-C-N	8.79	136.76	122.70
1	C	53	ALA	O-C-N	-8.78	108.65	122.70
2	D	10	ALA	CB-CA-C	-8.78	96.93	110.10
1	G	106	LEU	CB-CG-CD2	-8.77	96.08	111.00
1	A	28	ALA	CA-C-O	8.77	138.51	120.10
2	D	12	THR	CA-CB-OG1	-8.77	90.59	109.00
2	B	45	PHE	CD1-CE1-CZ	8.76	130.62	120.10
2	D	65	LYS	N-CA-CB	-8.76	94.83	110.60
2	F	35	TYR	CA-CB-CG	-8.76	96.75	113.40
2	F	142	ALA	CA-C-O	8.76	138.50	120.10
2	D	105	LEU	CB-CG-CD2	-8.76	96.11	111.00
1	E	49	SER	CB-CA-C	8.76	126.74	110.10
1	C	53	ALA	C-N-CA	8.76	143.59	121.70
2	D	6	VAL	C-N-CA	8.76	143.59	121.70
2	F	94	ASP	OD1-CG-OD2	-8.75	106.67	123.30
1	G	16	LYS	N-CA-C	8.75	134.63	111.00
2	D	114	LEU	CA-CB-CG	-8.75	95.17	115.30
2	D	86	ALA	O-C-N	-8.75	108.71	122.70
2	F	77	HIS	CA-C-N	8.75	136.44	117.20
2	H	80	ASN	CB-CG-OD1	-8.75	104.11	121.60
1	G	94	ASP	CB-CA-C	8.74	127.89	110.40
1	E	39	THR	O-C-N	-8.74	108.71	122.70
1	E	65	ALA	C-N-CA	8.74	143.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	ASP	N-CA-CB	-8.74	94.88	110.60
2	H	105	LEU	CB-CA-C	-8.73	93.61	110.20
1	G	63	ALA	O-C-N	-8.73	108.74	122.70
1	G	112	HIS	CB-CG-ND1	-8.73	101.38	123.20
2	D	33	VAL	CB-CA-C	-8.72	94.82	111.40
1	G	36	PHE	CA-C-O	8.72	138.42	120.10
1	G	104	CYS	CB-CA-C	8.72	127.85	110.40
1	E	137	THR	O-C-N	8.72	136.66	122.70
2	H	109	VAL	CA-C-O	-8.72	101.78	120.10
1	E	73	VAL	CA-CB-CG1	8.72	123.98	110.90
1	C	95	PRO	CA-CB-CG	-8.71	87.44	104.00
1	E	56	LYS	CB-CA-C	8.71	127.83	110.40
1	G	86	LEU	CB-CA-C	-8.71	93.66	110.20
2	B	91	LEU	CA-C-N	8.70	136.34	117.20
2	B	90	GLU	CA-C-O	-8.70	101.83	120.10
1	C	72	HIS	CB-CG-ND1	8.70	144.95	123.20
1	C	25	GLY	C-N-CA	-8.70	99.96	121.70
2	D	127	GLN	C-N-CA	8.69	143.42	121.70
1	C	22	GLY	CA-C-O	8.69	136.23	120.60
2	D	17	LYS	CB-CG-CD	8.69	134.18	111.60
1	A	140	TYR	CA-C-N	-8.68	98.11	117.20
2	H	86	ALA	N-CA-CB	8.68	122.25	110.10
1	E	74	ASP	CB-CA-C	8.67	127.75	110.40
2	F	70	ALA	O-C-N	-8.67	108.82	122.70
2	B	113	VAL	O-C-N	-8.67	108.83	122.70
1	A	1	VAL	CA-CB-CG2	8.67	123.90	110.90
1	G	136	LEU	CB-CG-CD1	-8.67	96.26	111.00
1	G	43	PHE	N-CA-CB	8.66	126.19	110.60
1	A	2	LEU	CB-CG-CD2	-8.66	96.28	111.00
1	A	3	SER	O-C-N	8.66	137.55	121.10
1	C	68	ASN	N-CA-CB	8.65	126.17	110.60
2	F	128	ALA	CB-CA-C	8.65	123.07	110.10
1	E	140	TYR	N-CA-CB	-8.64	95.04	110.60
2	H	12	THR	CA-C-O	-8.64	101.96	120.10
2	B	41	PHE	CD1-CG-CD2	-8.63	107.08	118.30
1	G	73	VAL	CA-CB-CG1	8.62	123.83	110.90
2	D	79	ASP	CA-C-O	8.61	138.19	120.10
2	H	39	GLN	CA-C-N	-8.61	98.25	117.20
2	H	131	GLN	CA-C-N	8.61	136.15	117.20
1	G	2	LEU	O-C-N	-8.61	108.92	122.70
2	B	128	ALA	CA-C-O	-8.60	102.03	120.10
1	E	138	SER	CA-C-N	8.60	136.12	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	11	VAL	CA-C-N	-8.60	98.27	117.20
1	A	50	HIS	CA-CB-CG	8.60	128.22	113.60
2	B	134	VAL	CA-CB-CG2	8.60	123.80	110.90
1	C	96	VAL	CG1-CB-CG2	8.60	124.65	110.90
2	F	45	PHE	N-CA-CB	-8.59	95.13	110.60
2	B	20	VAL	CA-C-O	-8.59	102.07	120.10
2	D	67	VAL	N-CA-CB	8.59	130.39	111.50
1	A	38	THR	CA-C-N	-8.59	98.31	117.20
2	D	80	ASN	CA-CB-CG	-8.59	94.51	113.40
1	E	141	ARG	CG-CD-NE	8.59	129.83	111.80
1	A	58	HIS	CA-CB-CG	-8.58	99.01	113.60
1	E	32	MET	N-CA-CB	8.58	126.05	110.60
1	C	77	PRO	CA-C-N	8.58	136.07	117.20
2	D	101	GLU	CG-CD-OE1	-8.58	101.14	118.30
1	C	56	LYS	CG-CD-CE	8.58	137.63	111.90
2	H	114	LEU	CA-CB-CG	8.58	135.03	115.30
1	C	103	HIS	CB-CG-CD2	8.56	157.35	130.80
1	E	87	HIS	C-N-CA	8.56	143.10	121.70
1	G	32	MET	CA-C-O	8.56	138.08	120.10
2	H	59	LYS	N-CA-C	-8.56	87.89	111.00
2	F	131	GLN	CG-CD-OE1	8.56	138.72	121.60
2	B	65	LYS	N-CA-CB	-8.55	95.20	110.60
2	D	62	ALA	CB-CA-C	8.55	122.93	110.10
2	B	132	LYS	O-C-N	8.55	136.38	122.70
2	B	144	LYS	O-C-N	-8.55	109.03	122.70
1	G	11	LYS	C-N-CA	8.55	143.07	121.70
1	G	131	SER	N-CA-C	-8.54	87.95	111.00
2	H	45	PHE	CG-CD2-CE2	8.53	130.19	120.80
1	A	23	GLU	CG-CD-OE2	-8.53	101.24	118.30
2	D	20	VAL	CB-CA-C	-8.53	95.19	111.40
1	E	114	PRO	CB-CA-C	8.53	133.33	112.00
1	C	77	PRO	C-N-CA	-8.52	100.39	121.70
1	C	54	GLN	CB-CG-CD	8.52	133.75	111.60
1	G	38	THR	CA-CB-OG1	8.52	126.89	109.00
2	H	73	ASP	CA-C-O	-8.52	102.22	120.10
2	H	15	TRP	CE3-CZ3-CH2	-8.51	111.83	121.20
1	A	89	HIS	CA-C-O	-8.51	102.22	120.10
2	F	70	ALA	CA-C-O	8.51	137.97	120.10
2	B	11	VAL	CB-CA-C	8.51	127.56	111.40
1	A	56	LYS	CB-CG-CD	8.51	133.71	111.60
1	E	19	ALA	CA-C-O	-8.50	102.25	120.10
2	F	40	ARG	CA-CB-CG	-8.50	94.70	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	SER	O-C-N	-8.50	109.10	122.70
1	A	100	LEU	CA-C-N	8.50	135.90	117.20
1	C	86	LEU	CA-C-N	8.50	135.90	117.20
1	C	12	ALA	C-N-CA	-8.49	100.47	121.70
1	C	106	LEU	CB-CG-CD2	-8.49	96.56	111.00
2	H	55	MET	CB-CA-C	-8.49	93.42	110.40
2	H	1	VAL	CA-C-O	-8.49	102.28	120.10
1	A	56	LYS	CA-C-O	-8.49	102.28	120.10
2	D	78	LEU	CA-CB-CG	8.48	134.82	115.30
2	D	81	LEU	CB-CG-CD2	-8.48	96.58	111.00
1	G	97	ASN	CA-C-O	8.48	137.91	120.10
1	A	101	LEU	CB-CG-CD2	-8.48	96.58	111.00
2	D	105	LEU	N-CA-CB	8.48	127.36	110.40
1	A	137	THR	OG1-CB-CG2	8.48	129.50	110.00
2	B	89	SER	CB-CA-C	-8.48	93.99	110.10
1	G	114	PRO	CA-N-CD	-8.48	99.63	111.50
2	B	8	LYS	N-CA-CB	-8.47	95.35	110.60
2	D	70	ALA	C-N-CA	8.47	142.88	121.70
2	F	114	LEU	CA-C-N	-8.47	98.56	117.20
2	F	104	ARG	CB-CA-C	8.47	127.34	110.40
2	F	104	ARG	N-CA-CB	-8.47	95.36	110.60
1	C	60	LYS	CA-C-N	-8.46	98.58	117.20
2	F	139	ASN	N-CA-CB	-8.46	95.36	110.60
1	C	141	ARG	NE-CZ-NH2	-8.46	116.07	120.30
2	B	10	ALA	CA-C-O	8.46	137.86	120.10
2	B	139	ASN	CA-CB-CG	-8.46	94.80	113.40
2	D	112	CYS	N-CA-CB	8.46	125.83	110.60
2	F	131	GLN	CA-C-N	-8.46	98.59	117.20
2	B	112	CYS	N-CA-CB	8.46	125.82	110.60
2	B	14	LEU	O-C-N	8.45	136.22	122.70
1	G	6	ASP	CA-CB-CG	8.45	131.98	113.40
2	H	17	LYS	CA-CB-CG	-8.45	94.82	113.40
2	F	80	ASN	C-N-CA	8.44	142.79	121.70
1	G	80	LEU	CA-CB-CG	8.44	134.71	115.30
2	B	73	ASP	CB-CA-C	-8.43	93.53	110.40
1	C	24	TYR	CG-CD1-CE1	8.43	128.05	121.30
1	G	64	ASP	O-C-N	8.43	136.19	122.70
2	B	113	VAL	C-N-CA	8.43	142.76	121.70
2	D	145	TYR	CB-CG-CD2	8.43	126.06	121.00
2	D	57	ASN	OD1-CG-ND2	8.42	141.27	121.90
2	F	45	PHE	CB-CA-C	8.42	127.25	110.40
2	F	104	ARG	O-C-N	-8.42	109.22	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	SER	CA-C-O	8.42	137.78	120.10
2	B	106	LEU	CA-C-O	-8.41	102.43	120.10
2	D	53	ALA	CA-C-N	-8.41	98.69	117.20
2	H	50	THR	CA-CB-CG2	8.41	124.18	112.40
2	B	94	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	C	137	THR	CA-C-O	-8.41	102.44	120.10
1	E	127	LYS	CA-C-O	-8.41	102.44	120.10
2	D	41	PHE	CB-CG-CD1	8.40	126.68	120.80
2	F	139	ASN	O-C-N	-8.39	109.27	122.70
2	B	37	TRP	CB-CA-C	8.39	127.18	110.40
2	B	142	ALA	O-C-N	8.39	136.13	122.70
1	E	40	LYS	C-N-CA	8.39	142.67	121.70
1	A	13	ALA	O-C-N	8.38	136.12	122.70
2	F	122	PHE	CA-C-N	8.38	135.64	117.20
2	D	19	ASN	CB-CA-C	-8.38	93.64	110.40
1	E	74	ASP	CA-CB-CG	8.38	131.84	113.40
2	H	30	ARG	N-CA-CB	8.37	125.67	110.60
2	H	30	ARG	CG-CD-NE	-8.37	94.22	111.80
2	D	52	ASP	CA-C-O	8.37	137.68	120.10
2	H	35	TYR	CD1-CG-CD2	8.37	127.11	117.90
1	E	12	ALA	CB-CA-C	-8.37	97.55	110.10
2	H	121	GLU	OE1-CD-OE2	-8.37	113.26	123.30
2	B	37	TRP	CA-C-O	-8.36	102.54	120.10
1	E	134	THR	N-CA-CB	8.36	126.19	110.30
2	H	80	ASN	CB-CA-C	8.36	127.12	110.40
1	A	72	HIS	O-C-N	-8.36	109.33	122.70
2	B	98	VAL	CB-CA-C	8.36	127.28	111.40
2	B	101	GLU	CB-CG-CD	8.36	136.76	114.20
1	E	44	PRO	N-CD-CG	-8.36	90.66	103.20
2	H	138	ALA	CB-CA-C	8.35	122.62	110.10
1	A	61	LYS	CD-CE-NZ	-8.34	92.51	111.70
1	C	128	PHE	CD1-CE1-CZ	-8.34	110.09	120.10
2	D	136	GLY	C-N-CA	-8.34	100.84	121.70
2	H	35	TYR	N-CA-CB	-8.34	95.59	110.60
2	H	33	VAL	CA-CB-CG2	-8.34	98.40	110.90
1	C	104	CYS	N-CA-CB	8.33	125.59	110.60
2	D	73	ASP	OD1-CG-OD2	8.33	139.12	123.30
1	A	80	LEU	CB-CG-CD1	-8.32	96.85	111.00
2	B	131	GLN	CG-CD-OE1	-8.32	104.96	121.60
2	F	59	LYS	N-CA-C	-8.32	88.53	111.00
1	E	107	VAL	CA-CB-CG1	8.31	123.37	110.90
2	B	11	VAL	O-C-N	-8.31	109.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	45	PHE	CA-C-N	8.31	132.81	116.20
2	F	145	TYR	CB-CA-C	8.30	127.00	110.40
1	C	5	ALA	O-C-N	-8.30	109.42	122.70
2	H	110	LEU	CA-C-N	-8.30	98.94	117.20
2	D	104	ARG	N-CA-CB	-8.30	95.67	110.60
1	E	120	ALA	N-CA-C	8.30	133.41	111.00
2	H	11	VAL	C-N-CA	-8.30	100.95	121.70
1	G	46	PHE	CA-CB-CG	8.29	133.81	113.90
1	A	55	VAL	CB-CA-C	-8.29	95.64	111.40
2	D	11	VAL	CA-C-N	-8.29	98.97	117.20
1	E	5	ALA	C-N-CA	-8.29	100.98	121.70
2	H	8	LYS	CA-CB-CG	8.29	131.63	113.40
2	F	63	HIS	CA-C-N	-8.28	99.63	116.20
2	F	131	GLN	OE1-CD-NE2	-8.28	102.85	121.90
2	B	48	LEU	N-CA-CB	8.28	126.96	110.40
1	G	3	SER	O-C-N	8.28	136.83	121.10
2	D	43	GLU	OE1-CD-OE2	8.28	133.23	123.30
2	D	74	GLY	N-CA-C	-8.28	92.41	113.10
2	H	45	PHE	CA-CB-CG	8.27	133.75	113.90
1	G	101	LEU	CD1-CG-CD2	8.27	135.30	110.50
1	A	122	HIS	CB-CG-ND1	8.26	143.86	123.20
2	D	91	LEU	CA-C-O	-8.26	102.75	120.10
1	A	74	ASP	CB-CG-OD2	8.26	125.73	118.30
1	E	113	LEU	CA-C-O	-8.26	102.76	120.10
2	D	51	PRO	N-CA-CB	8.25	113.20	103.30
2	H	95	LYS	C-N-CA	8.25	142.33	121.70
2	B	24	GLY	CA-C-O	8.25	135.45	120.60
2	D	45	PHE	CA-C-O	-8.25	102.77	120.10
2	D	53	ALA	CB-CA-C	-8.25	97.72	110.10
1	E	39	THR	CA-CB-CG2	-8.25	100.85	112.40
1	G	70	VAL	O-C-N	8.25	135.90	122.70
2	F	47	ASP	O-C-N	-8.25	109.51	122.70
1	E	86	LEU	N-CA-CB	-8.24	93.92	110.40
1	C	16	LYS	CB-CA-C	-8.24	93.92	110.40
2	F	42	PHE	CG-CD1-CE1	8.24	129.86	120.80
1	A	18	GLY	C-N-CA	-8.24	101.11	121.70
2	H	95	LYS	N-CA-CB	8.23	125.42	110.60
2	H	127	GLN	CA-CB-CG	-8.23	95.29	113.40
1	E	51	GLY	CA-C-N	8.23	135.30	117.20
1	E	88	ALA	N-CA-CB	8.23	121.62	110.10
1	E	42	TYR	CG-CD2-CE2	8.22	127.88	121.30
1	A	52	SER	CA-C-O	8.22	137.36	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	SER	C-N-CA	8.22	142.25	121.70
2	H	94	ASP	O-C-N	-8.22	109.55	122.70
2	B	86	ALA	O-C-N	-8.22	109.55	122.70
2	H	44	SER	CB-CA-C	8.21	125.71	110.10
1	G	115	ALA	C-N-CA	8.21	142.23	121.70
1	G	85	ASP	CB-CG-OD2	8.21	125.69	118.30
2	B	104	ARG	CB-CG-CD	-8.21	90.26	111.60
1	C	121	VAL	CA-CB-CG1	-8.21	98.59	110.90
2	D	65	LYS	C-N-CA	-8.20	101.19	121.70
1	G	58	HIS	CB-CG-ND1	8.21	143.71	123.20
1	C	76	MET	O-C-N	-8.20	105.52	121.10
2	B	48	LEU	O-C-N	8.20	135.82	122.70
1	C	72	HIS	O-C-N	-8.20	109.58	122.70
1	A	80	LEU	CB-CA-C	8.20	125.78	110.20
1	C	83	LEU	CA-C-N	-8.20	99.16	117.20
1	C	92	ARG	N-CA-CB	8.20	125.36	110.60
1	E	70	VAL	CG1-CB-CG2	-8.20	97.79	110.90
2	B	42	PHE	CB-CG-CD2	-8.19	115.06	120.80
1	E	14	TRP	CG-CD2-CE3	8.19	141.27	133.90
2	D	110	LEU	C-N-CA	8.19	142.18	121.70
2	F	108	ASN	O-C-N	-8.19	109.59	122.70
1	G	4	PRO	N-CA-C	-8.19	90.81	112.10
2	B	19	ASN	N-CA-C	-8.19	88.90	111.00
2	D	103	PHE	CD1-CE1-CZ	-8.19	110.28	120.10
1	A	30	GLU	CG-CD-OE1	8.18	134.66	118.30
1	C	38	THR	OG1-CB-CG2	8.18	128.82	110.00
2	D	88	LEU	CB-CA-C	8.18	125.74	110.20
1	G	11	LYS	CA-C-N	8.18	135.19	117.20
1	E	16	LYS	N-CA-CB	-8.18	95.89	110.60
1	G	128	PHE	N-CA-CB	8.17	125.31	110.60
2	H	38	THR	CA-CB-CG2	-8.17	100.96	112.40
1	C	17	VAL	CA-C-N	-8.17	99.86	116.20
2	D	105	LEU	CA-C-O	-8.16	102.95	120.10
2	F	6	VAL	CG1-CB-CG2	8.16	123.96	110.90
1	A	109	LEU	CB-CG-CD2	-8.16	97.12	111.00
1	E	24	TYR	N-CA-CB	8.16	125.29	110.60
2	B	41	PHE	CA-CB-CG	8.16	133.49	113.90
2	B	117	HIS	CB-CA-C	8.16	126.72	110.40
2	B	144	LYS	N-CA-CB	-8.16	95.91	110.60
2	F	30	ARG	CB-CG-CD	8.16	132.82	111.60
1	C	88	ALA	CB-CA-C	8.16	122.34	110.10
1	C	106	LEU	CD1-CG-CD2	8.16	134.97	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	92	HIS	O-C-N	8.15	135.75	122.70
2	B	14	LEU	CA-CB-CG	8.15	134.05	115.30
1	A	61	LYS	C-N-CA	-8.15	101.34	121.70
1	C	62	VAL	CB-CA-C	8.15	126.88	111.40
2	H	36	PRO	N-CD-CG	-8.15	90.98	103.20
2	F	88	LEU	CD1-CG-CD2	8.14	134.94	110.50
1	E	60	LYS	N-CA-CB	-8.14	95.94	110.60
1	A	80	LEU	CB-CG-CD2	8.14	124.84	111.00
2	H	110	LEU	CB-CA-C	-8.14	94.73	110.20
2	B	121	GLU	CG-CD-OE1	-8.14	102.02	118.30
1	C	40	LYS	CB-CA-C	8.14	126.68	110.40
2	B	73	ASP	CB-CG-OD1	-8.14	110.98	118.30
2	D	2	HIS	CG-ND1-CE1	8.13	119.59	108.20
1	E	4	PRO	O-C-N	8.13	135.71	122.70
2	B	16	GLY	CA-C-N	-8.13	99.31	117.20
2	H	3	LEU	CB-CG-CD1	8.13	124.82	111.00
1	A	29	LEU	O-C-N	8.13	135.70	122.70
2	H	18	VAL	CA-CB-CG1	-8.13	98.71	110.90
2	B	10	ALA	N-CA-CB	-8.12	98.73	110.10
1	E	70	VAL	CA-C-O	-8.12	103.05	120.10
2	F	48	LEU	C-N-CA	8.12	142.00	121.70
1	C	46	PHE	CA-CB-CG	8.12	133.38	113.90
1	C	30	GLU	CG-CD-OE1	-8.12	102.07	118.30
2	H	37	TRP	CE2-CD2-CG	-8.11	100.81	107.30
1	A	58	HIS	CE1-NE2-CD2	8.11	126.88	106.60
2	D	99	ASP	CA-C-N	-8.11	94.39	117.10
1	A	47	ASP	N-CA-C	-8.10	89.12	111.00
2	D	75	LEU	CB-CG-CD1	-8.10	97.23	111.00
1	G	46	PHE	O-C-N	8.10	135.67	122.70
1	G	126	ASP	C-N-CA	8.10	141.96	121.70
2	B	17	LYS	CA-C-O	-8.10	103.09	120.10
2	F	108	ASN	OD1-CG-ND2	-8.10	103.27	121.90
1	A	128	PHE	C-N-CA	-8.10	101.45	121.70
2	D	114	LEU	CB-CG-CD1	-8.10	97.23	111.00
2	B	80	ASN	CB-CG-ND2	-8.10	97.27	116.70
1	C	27	GLU	CA-C-N	-8.09	99.39	117.20
1	C	77	PRO	N-CA-CB	8.09	113.01	103.30
1	A	81	SER	CB-CA-C	8.09	125.47	110.10
2	F	130	TYR	CG-CD2-CE2	8.09	127.77	121.30
2	B	95	LYS	N-CA-CB	-8.08	96.05	110.60
1	C	24	TYR	CD1-CG-CD2	-8.08	109.01	117.90
1	A	43	PHE	CG-CD2-CE2	8.07	129.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	36	PHE	CD1-CE1-CZ	-8.07	110.42	120.10
1	G	52	SER	CA-C-O	8.07	137.04	120.10
1	G	135	VAL	CB-CA-C	-8.07	96.07	111.40
2	H	40	ARG	CA-CB-CG	8.06	131.14	113.40
1	G	120	ALA	CA-C-N	8.06	134.92	117.20
2	F	101	GLU	CA-C-O	8.05	137.01	120.10
1	G	78	ASN	O-C-N	8.05	135.58	122.70
2	F	47	ASP	OD1-CG-OD2	-8.05	108.01	123.30
2	D	58	PRO	CA-C-N	-8.05	99.50	117.20
1	A	135	VAL	CB-CA-C	8.04	126.68	111.40
2	D	1	VAL	CA-CB-CG2	8.04	122.97	110.90
1	E	111	ALA	N-CA-CB	-8.04	98.84	110.10
1	C	140	TYR	CB-CG-CD1	8.04	125.82	121.00
1	E	87	HIS	O-C-N	-8.04	109.84	122.70
1	G	99	LYS	O-C-N	8.04	135.56	122.70
1	A	125	LEU	CA-C-O	8.04	136.97	120.10
1	C	27	GLU	CA-CB-CG	8.04	131.08	113.40
2	H	1	VAL	CA-CB-CG1	8.04	122.95	110.90
2	H	66	LYS	C-N-CA	8.04	141.79	121.70
1	C	106	LEU	N-CA-C	-8.03	89.32	111.00
2	H	105	LEU	CA-C-O	-8.03	103.25	120.10
1	C	65	ALA	N-CA-CB	-8.02	98.87	110.10
2	B	32	LEU	CB-CG-CD1	8.02	124.64	111.00
2	F	33	VAL	CA-CB-CG1	-8.02	98.87	110.90
1	C	128	PHE	CZ-CE2-CD2	-8.02	110.48	120.10
2	F	45	PHE	CA-CB-CG	8.01	133.13	113.90
1	A	27	GLU	CG-CD-OE2	-8.00	102.30	118.30
2	H	75	LEU	CB-CA-C	8.00	125.40	110.20
2	B	94	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	5	ALA	CA-C-O	7.99	136.88	120.10
1	A	26	ALA	CA-C-O	-7.99	103.32	120.10
1	E	36	PHE	CB-CG-CD1	-7.99	115.21	120.80
2	F	24	GLY	O-C-N	7.99	136.78	123.20
1	C	29	LEU	C-N-CA	-7.99	101.74	121.70
2	D	117	HIS	N-CA-CB	7.98	124.97	110.60
1	A	10	VAL	CB-CA-C	7.98	126.56	111.40
2	H	68	LEU	CB-CG-CD1	7.98	124.56	111.00
2	D	40	ARG	O-C-N	7.97	135.46	122.70
1	C	71	ALA	CA-C-N	-7.97	99.67	117.20
2	H	81	LEU	N-CA-CB	7.97	126.34	110.40
1	C	122	HIS	O-C-N	-7.96	109.96	122.70
2	D	7	GLU	CG-CD-OE1	7.96	134.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	26	GLU	CG-CD-OE1	7.96	134.21	118.30
1	G	132	VAL	CA-CB-CG2	7.95	122.83	110.90
1	A	137	THR	C-N-CA	7.95	141.58	121.70
2	H	91	LEU	CA-C-O	7.95	136.79	120.10
1	C	42	TYR	N-CA-CB	-7.95	96.29	110.60
1	E	42	TYR	CA-C-N	7.95	134.69	117.20
1	E	113	LEU	CA-CB-CG	-7.95	97.02	115.30
1	G	24	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	G	18	GLY	CA-C-N	-7.94	99.72	117.20
2	B	108	ASN	CA-C-O	7.94	136.78	120.10
2	H	63	HIS	CA-C-O	-7.94	103.43	120.10
2	B	50	THR	N-CA-C	7.93	132.43	111.00
1	C	100	LEU	CA-CB-CG	7.93	133.54	115.30
2	F	15	TRP	CH2-CZ2-CE2	7.93	125.33	117.40
1	E	35	SER	N-CA-CB	7.93	122.39	110.50
1	C	103	HIS	C-N-CA	7.93	141.52	121.70
1	E	23	GLU	CB-CA-C	7.92	126.25	110.40
1	G	21	ALA	CB-CA-C	-7.92	98.22	110.10
1	C	15	GLY	C-N-CA	-7.92	101.90	121.70
2	F	139	ASN	CA-C-O	7.92	136.73	120.10
2	D	137	VAL	C-N-CA	7.92	141.49	121.70
2	B	5	PRO	N-CD-CG	7.91	115.07	103.20
1	C	134	THR	N-CA-CB	7.91	125.34	110.30
1	E	126	ASP	OD1-CG-OD2	-7.91	108.27	123.30
1	E	134	THR	CA-CB-CG2	7.91	123.48	112.40
1	G	23	GLU	CG-CD-OE2	-7.91	102.47	118.30
1	E	129	LEU	CA-CB-CG	-7.91	97.11	115.30
1	C	99	LYS	N-CA-CB	7.91	124.83	110.60
2	H	36	PRO	N-CA-CB	-7.91	93.81	103.30
1	E	42	TYR	OH-CZ-CE2	7.91	141.45	120.10
1	C	10	VAL	C-N-CA	7.90	141.45	121.70
2	D	56	GLY	O-C-N	-7.90	110.07	122.70
1	G	106	LEU	C-N-CA	7.89	141.43	121.70
2	B	136	GLY	CA-C-O	7.89	134.80	120.60
2	B	143	HIS	CG-ND1-CE1	7.89	119.24	108.20
2	D	68	LEU	C-N-CA	-7.89	105.74	122.30
1	A	23	GLU	CG-CD-OE1	7.88	134.07	118.30
2	H	88	LEU	CA-C-N	7.88	134.54	117.20
2	D	128	ALA	CA-C-N	7.88	134.54	117.20
2	F	1	VAL	O-C-N	-7.88	110.09	122.70
2	H	119	GLY	CA-C-O	-7.88	106.42	120.60
2	D	88	LEU	O-C-N	-7.87	110.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	121	VAL	CA-CB-CG1	7.87	122.71	110.90
1	E	109	LEU	CA-C-O	-7.87	103.58	120.10
2	H	34	VAL	CA-C-O	-7.87	103.58	120.10
1	A	140	TYR	CB-CG-CD1	7.86	125.72	121.00
1	E	112	HIS	N-CA-CB	-7.86	96.45	110.60
2	D	108	ASN	CB-CA-C	7.86	126.11	110.40
1	G	41	THR	O-C-N	7.86	135.27	122.70
1	E	85	ASP	CB-CG-OD1	-7.86	111.23	118.30
2	B	73	ASP	CA-CB-CG	-7.85	96.12	113.40
2	D	4	THR	OG1-CB-CG2	7.85	128.06	110.00
1	A	43	PHE	CD1-CE1-CZ	-7.85	110.68	120.10
1	C	3	SER	CA-C-O	-7.85	103.61	120.10
2	H	14	LEU	CB-CG-CD2	-7.85	97.65	111.00
1	A	71	ALA	CB-CA-C	-7.85	98.32	110.10
2	F	110	LEU	CB-CG-CD2	7.85	124.34	111.00
1	G	120	ALA	C-N-CA	7.85	141.32	121.70
2	H	43	GLU	N-CA-CB	7.85	124.73	110.60
1	A	87	HIS	CB-CA-C	7.85	126.10	110.40
1	A	140	TYR	CB-CG-CD2	-7.85	116.29	121.00
1	G	89	HIS	CA-CB-CG	7.84	126.94	113.60
1	C	23	GLU	OE1-CD-OE2	7.84	132.71	123.30
2	H	9	SER	CA-CB-OG	-7.84	90.04	111.20
2	H	50	THR	CA-CB-OG1	-7.84	92.54	109.00
2	B	82	LYS	CA-CB-CG	7.83	130.63	113.40
1	E	19	ALA	C-N-CA	-7.83	102.12	121.70
1	A	61	LYS	CA-CB-CG	-7.83	96.17	113.40
2	D	83	GLY	C-N-CA	-7.83	102.13	121.70
1	G	17	VAL	CA-CB-CG2	7.83	122.64	110.90
1	G	54	GLN	CA-C-O	7.83	136.54	120.10
2	H	145	TYR	N-CA-CB	7.83	124.69	110.60
1	C	55	VAL	N-CA-CB	7.82	128.71	111.50
1	C	132	VAL	N-CA-C	-7.82	89.88	111.00
1	E	28	ALA	C-N-CA	-7.82	102.15	121.70
2	F	22	GLU	CG-CD-OE1	7.82	133.94	118.30
2	H	113	VAL	CG1-CB-CG2	-7.82	98.39	110.90
1	E	1	VAL	O-C-N	7.82	135.21	122.70
1	C	120	ALA	N-CA-C	-7.82	89.90	111.00
1	G	133	SER	CA-CB-OG	7.81	132.30	111.20
2	F	146	HIS	CA-C-O	-7.81	103.70	120.10
1	C	101	LEU	O-C-N	7.81	135.20	122.70
2	B	81	LEU	CB-CG-CD2	-7.81	97.73	111.00
1	A	28	ALA	N-CA-CB	7.80	121.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	111	VAL	O-C-N	7.80	135.19	122.70
2	D	95	LYS	CB-CG-CD	-7.80	91.31	111.60
2	H	94	ASP	CA-CB-CG	-7.80	96.23	113.40
2	D	135	ALA	N-CA-CB	-7.80	99.18	110.10
1	E	14	TRP	C-N-CA	-7.79	105.93	122.30
1	A	34	LEU	CA-C-O	-7.79	103.74	120.10
1	G	41	THR	CA-CB-CG2	-7.79	101.49	112.40
1	A	101	LEU	CB-CA-C	-7.79	95.40	110.20
1	C	84	SER	N-CA-CB	7.79	122.18	110.50
1	E	122	HIS	CA-C-O	-7.79	103.75	120.10
2	F	101	GLU	CA-C-N	-7.79	100.07	117.20
1	C	26	ALA	O-C-N	7.78	135.16	122.70
2	H	145	TYR	CB-CG-CD2	7.78	125.67	121.00
1	C	113	LEU	CA-CB-CG	7.78	133.19	115.30
1	E	116	GLU	CA-C-O	-7.78	103.76	120.10
1	C	118	THR	N-CA-CB	-7.78	95.52	110.30
1	C	50	HIS	CB-CG-ND1	7.78	142.64	123.20
1	C	58	HIS	CB-CA-C	7.78	125.95	110.40
1	E	97	ASN	O-C-N	-7.78	110.26	122.70
1	G	55	VAL	N-CA-C	-7.77	90.01	111.00
1	G	114	PRO	CA-C-O	-7.77	101.55	120.20
2	H	86	ALA	CB-CA-C	7.77	121.76	110.10
1	C	60	LYS	CA-CB-CG	7.77	130.49	113.40
1	A	83	LEU	O-C-N	7.76	135.12	122.70
1	C	96	VAL	O-C-N	7.76	135.12	122.70
2	H	13	ALA	CA-C-O	-7.76	103.79	120.10
1	E	33	PHE	CD1-CE1-CZ	-7.76	110.79	120.10
1	E	136	LEU	CA-C-O	-7.76	103.81	120.10
1	E	116	GLU	CA-CB-CG	-7.75	96.35	113.40
2	H	58	PRO	CA-CB-CG	-7.75	89.27	104.00
1	A	43	PHE	CD1-CG-CD2	-7.75	108.23	118.30
1	C	72	HIS	N-CA-CB	-7.75	96.66	110.60
2	D	72	SER	CA-C-O	7.74	136.36	120.10
1	G	68	ASN	O-C-N	7.74	135.09	122.70
2	B	110	LEU	CA-CB-CG	7.74	133.11	115.30
1	C	98	PHE	N-CA-CB	7.74	124.53	110.60
1	C	140	TYR	C-N-CA	7.74	141.05	121.70
2	D	92	HIS	N-CA-CB	7.74	124.53	110.60
1	G	68	ASN	CB-CG-OD1	7.74	137.08	121.60
2	F	66	LYS	CA-C-N	-7.74	100.18	117.20
1	G	117	PHE	CA-CB-CG	-7.74	95.33	113.90
2	F	73	ASP	N-CA-CB	7.73	124.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	LEU	C-N-CA	7.73	141.02	121.70
1	A	47	ASP	CB-CG-OD2	-7.73	111.35	118.30
2	B	28	LEU	CB-CA-C	7.73	124.88	110.20
2	D	101	GLU	CG-CD-OE2	-7.73	102.85	118.30
1	C	94	ASP	CB-CA-C	7.73	125.85	110.40
1	C	95	PRO	CA-C-N	-7.72	100.21	117.20
1	A	58	HIS	CG-CD2-NE2	-7.72	94.53	109.20
2	H	9	SER	CA-C-O	7.71	136.29	120.10
2	D	48	LEU	N-CA-CB	7.71	125.82	110.40
2	F	49	SER	CA-C-N	-7.71	100.24	117.20
2	F	141	LEU	CA-C-N	7.71	134.16	117.20
1	G	75	ASP	OD1-CG-OD2	7.71	137.94	123.30
2	B	111	VAL	N-CA-CB	7.70	128.44	111.50
2	F	7	GLU	O-C-N	7.70	135.02	122.70
2	F	103	PHE	CA-C-N	-7.70	100.27	117.20
1	C	91	LEU	CB-CG-CD2	-7.70	97.92	111.00
1	E	24	TYR	CA-C-N	-7.70	100.81	116.20
1	E	35	SER	CA-CB-OG	-7.69	90.42	111.20
2	F	114	LEU	CB-CG-CD1	-7.69	97.92	111.00
2	D	71	PHE	CG-CD1-CE1	7.69	129.26	120.80
1	E	38	THR	CB-CA-C	-7.69	90.84	111.60
1	E	85	ASP	OD1-CG-OD2	-7.69	108.69	123.30
2	D	97	HIS	C-N-CA	-7.69	102.48	121.70
2	B	35	TYR	CA-C-O	-7.68	103.96	120.10
2	D	89	SER	CA-C-O	7.68	136.24	120.10
2	D	118	PHE	N-CA-CB	-7.68	96.77	110.60
2	B	40	ARG	O-C-N	-7.68	110.41	122.70
2	D	77	HIS	O-C-N	-7.68	110.41	122.70
2	D	129	ALA	CA-C-N	-7.68	100.30	117.20
2	H	45	PHE	CZ-CE2-CD2	-7.68	110.88	120.10
1	G	40	LYS	O-C-N	-7.68	110.42	122.70
1	A	109	LEU	N-CA-CB	-7.67	95.05	110.40
2	D	6	VAL	CG1-CB-CG2	-7.67	98.62	110.90
2	H	38	THR	CA-C-N	-7.67	100.32	117.20
1	C	101	LEU	CB-CG-CD1	7.67	124.04	111.00
1	E	70	VAL	N-CA-C	-7.67	90.29	111.00
1	A	40	LYS	CA-CB-CG	7.67	130.27	113.40
2	B	142	ALA	CA-C-N	-7.67	100.33	117.20
1	E	47	ASP	OD1-CG-OD2	7.67	137.87	123.30
1	G	31	ARG	CA-C-O	-7.67	104.00	120.10
2	H	67	VAL	CA-CB-CG2	7.67	122.40	110.90
2	B	112	CYS	CA-C-N	7.67	134.06	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	GLN	CB-CG-CD	7.67	131.53	111.60
1	G	9	ASN	CA-C-N	-7.66	100.34	117.20
2	D	17	LYS	CG-CD-CE	7.66	134.88	111.90
2	H	33	VAL	CA-C-O	7.66	136.18	120.10
1	E	135	VAL	CB-CA-C	7.66	125.94	111.40
2	H	14	LEU	CB-CA-C	-7.66	95.66	110.20
2	D	26	GLU	CG-CD-OE2	-7.65	102.99	118.30
1	A	97	ASN	CA-CB-CG	7.65	130.23	113.40
1	A	2	LEU	C-N-CA	-7.65	102.57	121.70
2	H	37	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	G	23	GLU	N-CA-C	7.64	131.64	111.00
2	D	101	GLU	N-CA-C	-7.64	90.37	111.00
2	F	63	HIS	O-C-N	7.64	136.19	123.20
2	B	17	LYS	CA-C-N	7.64	134.00	117.20
1	E	67	THR	OG1-CB-CG2	7.64	127.56	110.00
1	E	128	PHE	CG-CD1-CE1	-7.63	112.41	120.80
2	H	122	PHE	CA-C-N	-7.62	100.42	117.20
2	F	45	PHE	CD1-CE1-CZ	-7.62	110.95	120.10
2	D	72	SER	CA-C-N	-7.62	100.44	117.20
2	H	104	ARG	O-C-N	-7.62	110.51	122.70
2	D	59	LYS	CB-CA-C	7.62	125.63	110.40
1	C	61	LYS	CA-C-O	-7.62	104.11	120.10
1	E	14	TRP	CA-C-O	7.62	136.09	120.10
1	G	102	SER	N-CA-C	-7.62	90.44	111.00
1	G	30	GLU	CG-CD-OE1	7.61	133.53	118.30
2	H	93	CYS	N-CA-CB	-7.61	96.89	110.60
1	A	113	LEU	O-C-N	7.61	135.56	121.10
1	C	123	ALA	CB-CA-C	-7.61	98.68	110.10
2	H	33	VAL	O-C-N	-7.61	110.52	122.70
2	B	82	LYS	N-CA-CB	-7.61	96.90	110.60
2	H	104	ARG	CA-C-O	7.61	136.08	120.10
2	H	65	LYS	CD-CE-NZ	7.61	129.20	111.70
2	F	54	VAL	CA-CB-CG2	7.60	122.31	110.90
1	C	65	ALA	CB-CA-C	7.60	121.50	110.10
2	H	30	ARG	CB-CA-C	-7.60	95.19	110.40
1	E	20	HIS	CG-CD2-NE2	-7.60	94.76	109.20
2	D	47	ASP	CA-C-O	-7.60	104.14	120.10
1	E	70	VAL	CA-CB-CG2	7.60	122.30	110.90
2	F	66	LYS	CA-C-O	7.59	136.05	120.10
1	G	33	PHE	O-C-N	7.59	134.84	122.70
1	A	36	PHE	CG-CD2-CE2	7.59	129.15	120.80
2	H	119	GLY	O-C-N	7.59	134.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	VAL	CA-C-O	-7.59	104.17	120.10
2	B	41	PHE	CB-CA-C	7.59	125.57	110.40
2	F	100	PRO	C-N-CA	7.59	140.67	121.70
1	G	134	THR	O-C-N	-7.59	110.56	122.70
2	D	108	ASN	OD1-CG-ND2	-7.58	104.46	121.90
1	A	86	LEU	CA-C-N	-7.58	100.52	117.20
1	C	77	PRO	CB-CA-C	7.58	130.94	112.00
2	D	91	LEU	O-C-N	7.58	134.83	122.70
1	E	56	LYS	O-C-N	-7.58	110.32	123.20
1	E	59	GLY	O-C-N	-7.58	110.58	122.70
2	B	18	VAL	CA-C-O	7.58	136.01	120.10
2	F	110	LEU	CB-CG-CD1	-7.58	98.12	111.00
2	H	121	GLU	CG-CD-OE1	7.57	133.45	118.30
2	B	22	GLU	O-C-N	-7.57	110.59	122.70
1	E	25	GLY	CA-C-O	-7.57	106.98	120.60
2	H	118	PHE	CZ-CE2-CD2	-7.57	111.02	120.10
1	A	38	THR	CA-CB-CG2	-7.56	101.81	112.40
1	G	9	ASN	O-C-N	7.56	134.80	122.70
1	G	40	LYS	N-CA-CB	7.56	124.21	110.60
1	C	130	ALA	CA-C-N	7.56	133.83	117.20
2	B	121	GLU	CG-CD-OE2	-7.55	103.19	118.30
2	B	136	GLY	C-N-CA	-7.55	102.81	121.70
1	G	126	ASP	N-CA-CB	7.55	124.19	110.60
2	H	128	ALA	CA-C-N	-7.55	100.60	117.20
1	C	23	GLU	CA-C-N	7.54	133.80	117.20
1	G	56	LYS	N-CA-CB	-7.54	97.03	110.60
1	E	108	THR	OG1-CB-CG2	7.54	127.34	110.00
2	F	37	TRP	CB-CG-CD1	-7.54	117.20	127.00
1	A	63	ALA	CB-CA-C	7.53	121.40	110.10
1	A	86	LEU	CA-C-O	7.53	135.92	120.10
2	B	20	VAL	O-C-N	-7.53	110.65	122.70
2	F	15	TRP	N-CA-CB	7.53	124.16	110.60
2	F	109	VAL	CA-CB-CG2	7.53	122.19	110.90
2	H	146	HIS	CB-CG-ND1	-7.53	104.38	123.20
1	C	17	VAL	O-C-N	7.52	135.99	123.20
1	G	66	LEU	C-N-CA	-7.52	102.90	121.70
2	D	68	LEU	CB-CA-C	7.52	124.49	110.20
1	E	103	HIS	CG-CD2-NE2	-7.52	94.92	109.20
2	H	112	CYS	N-CA-CB	7.51	124.13	110.60
1	C	114	PRO	C-N-CA	7.51	140.48	121.70
1	C	27	GLU	OE1-CD-OE2	-7.51	114.29	123.30
2	B	22	GLU	CG-CD-OE1	7.51	133.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	LYS	CB-CA-C	7.51	125.42	110.40
2	F	81	LEU	CB-CG-CD2	-7.51	98.24	111.00
2	D	142	ALA	N-CA-CB	-7.50	99.59	110.10
1	E	110	ALA	O-C-N	-7.50	110.69	122.70
2	D	121	GLU	CB-CG-CD	7.50	134.46	114.20
2	B	7	GLU	C-N-CA	7.50	140.45	121.70
2	F	137	VAL	CA-C-O	-7.50	104.36	120.10
1	E	1	VAL	CA-C-N	-7.50	100.71	117.20
2	F	69	GLY	CA-C-O	-7.50	107.11	120.60
2	F	53	ALA	C-N-CA	-7.49	102.97	121.70
2	H	137	VAL	N-CA-CB	7.49	127.98	111.50
2	B	22	GLU	CA-CB-CG	-7.49	96.93	113.40
2	F	129	ALA	N-CA-CB	-7.48	99.63	110.10
1	C	140	TYR	CD1-CG-CD2	-7.48	109.67	117.90
2	F	38	THR	N-CA-CB	7.48	124.50	110.30
2	F	106	LEU	CA-C-O	7.47	135.80	120.10
1	A	44	PRO	N-CA-CB	7.47	112.27	103.30
1	C	42	TYR	O-C-N	7.47	134.66	122.70
1	E	129	LEU	CA-C-O	7.47	135.79	120.10
2	H	93	CYS	CA-CB-SG	-7.47	100.56	114.00
1	E	121	VAL	CA-CB-CG2	7.47	122.10	110.90
2	F	98	VAL	C-N-CA	7.47	140.37	121.70
1	G	120	ALA	O-C-N	-7.47	110.75	122.70
1	A	88	ALA	CB-CA-C	-7.46	98.90	110.10
2	B	143	HIS	CB-CA-C	-7.46	95.47	110.40
2	D	105	LEU	O-C-N	7.46	134.63	122.70
1	C	24	TYR	CZ-CE2-CD2	-7.46	113.09	119.80
2	D	75	LEU	CA-CB-CG	7.46	132.45	115.30
1	E	108	THR	O-C-N	7.45	134.62	122.70
2	B	13	ALA	N-CA-CB	7.45	120.52	110.10
2	B	104	ARG	CD-NE-CZ	-7.44	113.18	123.60
1	C	45	HIS	CB-CA-C	-7.44	95.52	110.40
1	E	79	ALA	CA-C-O	7.44	135.73	120.10
1	A	128	PHE	CA-C-N	-7.44	100.83	117.20
1	E	64	ASP	C-N-CA	-7.44	103.10	121.70
1	A	138	SER	CB-CA-C	7.44	124.23	110.10
2	D	82	LYS	N-CA-CB	7.44	123.98	110.60
2	F	85	PHE	CB-CG-CD1	7.44	126.00	120.80
2	H	6	VAL	C-N-CA	-7.44	103.11	121.70
1	E	45	HIS	CB-CG-ND1	-7.43	104.61	123.20
1	E	109	LEU	CB-CG-CD2	7.43	123.64	111.00
2	D	117	HIS	CB-CG-CD2	7.43	153.84	130.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	VAL	CA-C-N	7.43	133.55	117.20
1	A	138	SER	C-N-CA	7.43	140.28	121.70
1	A	58	HIS	C-N-CA	7.43	137.90	122.30
1	A	50	HIS	CB-CA-C	-7.42	95.56	110.40
1	A	55	VAL	C-N-CA	7.42	140.25	121.70
2	D	108	ASN	O-C-N	7.42	134.57	122.70
2	D	118	PHE	CD1-CG-CD2	-7.42	108.65	118.30
1	A	129	LEU	N-CA-CB	7.41	125.22	110.40
1	C	50	HIS	CB-CG-CD2	-7.41	107.83	130.80
2	F	37	TRP	N-CA-CB	-7.41	97.26	110.60
1	G	86	LEU	CB-CG-CD1	-7.41	98.40	111.00
1	E	126	ASP	CA-C-N	7.41	133.50	117.20
2	F	111	VAL	O-C-N	-7.41	110.85	122.70
1	G	39	THR	CA-C-N	-7.41	100.91	117.20
1	E	1	VAL	N-CA-CB	7.40	127.78	111.50
2	H	17	LYS	CA-C-O	7.40	135.64	120.10
2	D	127	GLN	CG-CD-OE1	7.40	136.40	121.60
1	C	40	LYS	CG-CD-CE	-7.39	89.72	111.90
2	F	89	SER	CB-CA-C	-7.39	96.05	110.10
2	H	50	THR	N-CA-CB	-7.39	96.25	110.30
2	H	18	VAL	CA-C-N	-7.39	100.94	117.20
2	H	116	HIS	ND1-CG-CD2	7.39	119.15	108.80
1	E	38	THR	CA-C-O	-7.38	104.59	120.10
1	C	120	ALA	O-C-N	7.38	134.51	122.70
1	A	7	LYS	C-N-CA	-7.38	103.25	121.70
1	E	1	VAL	CA-CB-CG2	7.38	121.97	110.90
2	F	103	PHE	CA-C-O	7.38	135.59	120.10
2	H	137	VAL	CA-C-O	7.38	135.59	120.10
1	C	139	LYS	CD-CE-NZ	-7.38	94.73	111.70
2	D	66	LYS	N-CA-CB	7.38	123.88	110.60
2	D	110	LEU	CB-CG-CD2	-7.38	98.46	111.00
1	G	63	ALA	CA-C-O	-7.37	104.62	120.10
2	H	108	ASN	C-N-CA	-7.37	103.27	121.70
1	A	17	VAL	CA-C-N	-7.37	101.46	116.20
1	E	88	ALA	CB-CA-C	-7.37	99.05	110.10
2	F	22	GLU	CB-CA-C	-7.36	95.68	110.40
2	F	102	ASN	CA-C-N	7.36	133.40	117.20
1	C	107	VAL	C-N-CA	7.36	140.10	121.70
2	F	47	ASP	C-N-CA	7.36	140.10	121.70
1	C	21	ALA	CB-CA-C	7.36	121.14	110.10
2	H	47	ASP	C-N-CA	7.36	140.09	121.70
2	H	135	ALA	CB-CA-C	7.36	121.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	49	SER	O-C-N	-7.36	110.93	122.70
1	C	56	LYS	CD-CE-NZ	7.36	128.62	111.70
1	E	31	ARG	C-N-CA	7.36	140.09	121.70
1	E	139	LYS	CD-CE-NZ	-7.36	94.78	111.70
1	G	101	LEU	O-C-N	-7.36	110.93	122.70
2	B	38	THR	O-C-N	-7.35	110.94	122.70
1	A	6	ASP	OD1-CG-OD2	7.35	137.26	123.30
2	B	51	PRO	O-C-N	7.35	134.46	122.70
1	G	96	VAL	CA-CB-CG1	7.35	121.92	110.90
2	H	45	PHE	N-CA-C	7.35	130.84	111.00
2	B	114	LEU	N-CA-CB	-7.35	95.71	110.40
2	D	56	GLY	CA-C-O	7.35	133.82	120.60
2	F	65	LYS	CA-CB-CG	7.35	129.56	113.40
2	H	113	VAL	CA-C-O	-7.35	104.67	120.10
1	A	80	LEU	C-N-CA	-7.34	103.34	121.70
2	H	39	GLN	CA-CB-CG	7.34	129.56	113.40
2	D	2	HIS	ND1-CG-CD2	-7.34	95.72	106.00
1	G	78	ASN	OD1-CG-ND2	7.34	138.79	121.90
1	A	132	VAL	N-CA-CB	7.34	127.65	111.50
1	C	95	PRO	N-CA-CB	7.34	112.11	103.30
1	G	27	GLU	CG-CD-OE2	-7.34	103.62	118.30
1	G	33	PHE	CA-C-O	-7.34	104.69	120.10
2	D	100	PRO	CA-C-N	7.34	133.34	117.20
1	C	20	HIS	CB-CG-CD2	7.34	153.54	130.80
1	E	55	VAL	C-N-CA	-7.34	103.36	121.70
2	F	96	LEU	CB-CG-CD1	-7.33	98.53	111.00
1	A	103	HIS	CE1-NE2-CD2	7.33	124.94	106.60
2	D	54	VAL	CA-CB-CG2	7.33	121.90	110.90
1	E	97	ASN	CB-CG-ND2	7.33	134.30	116.70
2	H	145	TYR	CB-CG-CD1	-7.33	116.60	121.00
1	A	137	THR	O-C-N	-7.33	110.97	122.70
2	H	125	PRO	N-CD-CG	-7.33	92.20	103.20
2	D	7	GLU	N-CA-CB	-7.33	97.41	110.60
2	D	73	ASP	CA-CB-CG	-7.33	97.28	113.40
2	D	134	VAL	CA-C-N	7.33	133.32	117.20
2	H	139	ASN	CB-CG-ND2	-7.33	99.11	116.70
1	A	20	HIS	CB-CA-C	7.33	125.05	110.40
1	E	26	ALA	CA-C-N	7.33	133.32	117.20
2	F	113	VAL	O-C-N	-7.33	110.98	122.70
2	F	37	TRP	CD1-CG-CD2	-7.32	100.45	106.30
2	H	109	VAL	CA-CB-CG1	-7.32	99.92	110.90
1	C	27	GLU	O-C-N	-7.32	111.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	125	PRO	N-CA-C	7.32	131.12	112.10
2	H	82	LYS	CA-C-N	-7.32	101.57	116.20
2	H	83	GLY	N-CA-C	-7.32	94.81	113.10
2	H	113	VAL	CA-CB-CG1	7.31	121.87	110.90
1	A	100	LEU	CA-C-O	-7.31	104.75	120.10
1	E	120	ALA	C-N-CA	7.31	139.97	121.70
1	A	72	HIS	N-CA-CB	-7.31	97.45	110.60
1	C	62	VAL	O-C-N	-7.31	111.01	122.70
1	E	89	HIS	CA-CB-CG	7.31	126.02	113.60
2	F	141	LEU	CA-C-O	-7.31	104.75	120.10
2	D	110	LEU	CB-CG-CD1	7.30	123.42	111.00
1	A	117	PHE	N-CA-CB	-7.30	97.46	110.60
2	B	85	PHE	O-C-N	7.30	134.38	122.70
1	C	6	ASP	OD1-CG-OD2	7.30	137.17	123.30
2	D	60	VAL	O-C-N	-7.30	111.02	122.70
1	A	104	CYS	CA-C-O	-7.30	104.77	120.10
2	D	107	GLY	CA-C-O	-7.30	107.46	120.60
2	F	32	LEU	CB-CA-C	7.30	124.06	110.20
1	G	125	LEU	C-N-CA	-7.30	103.46	121.70
1	E	94	ASP	OD1-CG-OD2	7.29	137.16	123.30
2	D	112	CYS	O-C-N	7.29	134.37	122.70
2	H	100	PRO	CA-C-O	7.29	137.70	120.20
2	B	90	GLU	CA-C-N	7.29	133.24	117.20
2	D	37	TRP	CZ3-CH2-CZ2	-7.29	112.86	121.60
2	D	67	VAL	CA-C-O	-7.29	104.79	120.10
2	D	137	VAL	CA-CB-CG1	-7.29	99.97	110.90
1	E	124	SER	O-C-N	-7.29	111.04	122.70
1	G	72	HIS	CB-CG-ND1	7.29	141.42	123.20
1	E	54	GLN	CA-C-N	7.29	133.23	117.20
2	B	90	GLU	CB-CA-C	-7.29	95.83	110.40
1	A	123	ALA	CA-C-O	7.28	135.40	120.10
1	G	14	TRP	CH2-CZ2-CE2	-7.28	110.12	117.40
2	H	17	LYS	CA-C-N	-7.28	101.18	117.20
1	G	102	SER	CB-CA-C	7.28	123.94	110.10
1	A	23	GLU	CA-C-N	-7.28	101.18	117.20
1	C	91	LEU	O-C-N	-7.28	111.05	122.70
2	F	68	LEU	CB-CG-CD2	-7.28	98.62	111.00
2	F	145	TYR	C-N-CA	-7.28	103.50	121.70
2	H	78	LEU	CA-C-N	-7.28	101.18	117.20
1	C	58	HIS	O-C-N	-7.28	110.83	123.20
1	G	48	LEU	CB-CG-CD1	7.28	123.37	111.00
2	H	145	TYR	CA-C-O	-7.28	104.82	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	55	VAL	CG1-CB-CG2	7.27	122.54	110.90
2	H	11	VAL	CB-CA-C	-7.27	97.58	111.40
1	E	84	SER	N-CA-C	-7.27	91.37	111.00
1	G	62	VAL	CA-C-O	-7.27	104.83	120.10
1	C	17	VAL	N-CA-CB	7.27	127.50	111.50
2	B	8	LYS	CB-CG-CD	-7.27	92.71	111.60
2	D	15	TRP	C-N-CA	7.27	137.56	122.30
1	E	85	ASP	O-C-N	7.27	134.33	122.70
2	H	95	LYS	CB-CA-C	-7.27	95.87	110.40
1	A	41	THR	CA-C-O	7.26	135.35	120.10
2	F	30	ARG	CA-C-O	-7.26	104.85	120.10
2	H	133	VAL	CA-C-O	-7.26	104.85	120.10
2	D	30	ARG	CA-C-O	-7.26	104.86	120.10
2	F	82	LYS	CA-C-O	-7.26	104.86	120.10
2	D	98	VAL	C-N-CA	7.25	139.84	121.70
2	B	122	PHE	CG-CD1-CE1	-7.25	112.82	120.80
1	G	121	VAL	CA-CB-CG2	-7.25	100.02	110.90
1	G	139	LYS	CG-CD-CE	-7.25	90.16	111.90
1	C	89	HIS	CG-CD2-NE2	-7.25	95.43	109.20
2	F	119	GLY	C-N-CA	7.24	139.81	121.70
2	H	76	ALA	C-N-CA	7.24	139.81	121.70
2	H	102	ASN	CA-C-O	-7.24	104.89	120.10
2	B	116	HIS	CA-CB-CG	7.24	125.91	113.60
2	D	3	LEU	N-CA-CB	7.24	124.88	110.40
2	F	5	PRO	O-C-N	7.24	134.28	122.70
1	E	132	VAL	CA-CB-CG1	-7.24	100.04	110.90
2	H	61	LYS	O-C-N	-7.24	111.12	122.70
1	C	64	ASP	CB-CA-C	7.24	124.87	110.40
1	C	139	LYS	O-C-N	-7.24	111.12	122.70
2	H	98	VAL	CA-CB-CG2	7.24	121.75	110.90
1	A	130	ALA	CA-C-N	-7.23	101.29	117.20
2	F	57	ASN	CB-CG-ND2	7.23	134.06	116.70
2	B	124	PRO	N-CA-CB	7.23	111.97	103.30
2	H	96	LEU	O-C-N	-7.23	111.13	122.70
2	D	1	VAL	CA-C-O	7.23	135.28	120.10
2	B	80	ASN	CA-C-O	7.22	135.27	120.10
1	A	29	LEU	C-N-CA	-7.22	103.65	121.70
2	F	15	TRP	CD2-CE2-CZ2	-7.22	113.64	122.30
2	H	84	THR	CA-C-O	7.22	135.26	120.10
2	B	3	LEU	CA-C-O	7.22	135.26	120.10
2	H	54	VAL	CG1-CB-CG2	7.22	122.45	110.90
1	G	136	LEU	CA-C-O	-7.22	104.95	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	72	HIS	ND1-CE1-NE2	7.21	125.77	109.90
1	A	66	LEU	CB-CA-C	-7.21	96.50	110.20
2	D	66	LYS	C-N-CA	-7.21	103.67	121.70
1	G	35	SER	N-CA-CB	-7.21	99.69	110.50
1	C	71	ALA	N-CA-CB	-7.21	100.01	110.10
2	F	118	PHE	C-N-CA	-7.21	107.16	122.30
1	A	61	LYS	CB-CG-CD	-7.21	92.86	111.60
2	D	108	ASN	CB-CG-ND2	-7.21	99.40	116.70
1	G	52	SER	C-N-CA	-7.21	103.68	121.70
1	E	101	LEU	CB-CG-CD2	-7.20	98.75	111.00
2	H	52	ASP	CB-CG-OD1	7.20	124.78	118.30
2	H	103	PHE	O-C-N	-7.20	111.17	122.70
1	G	34	LEU	CB-CA-C	-7.20	96.52	110.20
2	B	72	SER	CA-C-N	7.20	133.03	117.20
1	C	16	LYS	C-N-CA	7.20	139.69	121.70
2	D	42	PHE	CB-CG-CD1	-7.20	115.76	120.80
1	G	128	PHE	CG-CD1-CE1	7.20	128.72	120.80
2	B	139	ASN	CA-C-O	-7.19	105.00	120.10
2	H	146	HIS	CB-CG-CD2	7.19	153.10	130.80
1	C	97	ASN	CB-CG-OD1	7.19	135.98	121.60
1	G	36	PHE	CA-CB-CG	7.19	131.15	113.90
1	G	52	SER	N-CA-C	7.19	130.40	111.00
1	G	101	LEU	CB-CG-CD1	-7.19	98.78	111.00
2	H	93	CYS	C-N-CA	-7.19	103.73	121.70
2	B	42	PHE	N-CA-C	7.19	130.40	111.00
1	A	89	HIS	C-N-CA	7.18	139.66	121.70
1	G	30	GLU	C-N-CA	7.18	139.66	121.70
1	E	11	LYS	C-N-CA	7.18	139.65	121.70
2	F	5	PRO	CA-N-CD	7.18	121.75	111.70
1	C	32	MET	C-N-CA	7.18	139.65	121.70
1	C	135	VAL	CA-CB-CG2	-7.18	100.13	110.90
1	G	101	LEU	CB-CA-C	7.18	123.84	110.20
2	H	57	ASN	CB-CG-ND2	7.18	133.93	116.70
1	E	101	LEU	CB-CA-C	-7.18	96.56	110.20
2	B	116	HIS	O-C-N	-7.17	111.23	122.70
1	G	30	GLU	CB-CG-CD	7.17	133.56	114.20
2	H	126	VAL	N-CA-CB	7.17	127.27	111.50
2	H	87	THR	N-CA-C	-7.17	91.64	111.00
1	C	74	ASP	CB-CA-C	7.17	124.73	110.40
2	B	41	PHE	N-CA-CB	-7.16	97.70	110.60
2	B	63	HIS	C-N-CA	7.16	137.34	122.30
1	G	84	SER	CB-CA-C	7.16	123.71	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	PHE	CB-CG-CD2	7.16	125.81	120.80
2	B	32	LEU	CA-C-O	7.16	135.13	120.10
2	H	136	GLY	C-N-CA	7.15	139.59	121.70
1	C	63	ALA	C-N-CA	7.15	139.58	121.70
2	H	87	THR	O-C-N	7.15	134.14	122.70
2	H	53	ALA	O-C-N	7.15	134.14	122.70
1	E	30	GLU	CA-C-N	-7.15	101.47	117.20
2	B	78	LEU	CB-CA-C	7.15	123.78	110.20
2	D	141	LEU	O-C-N	7.14	134.13	122.70
2	F	112	CYS	C-N-CA	7.14	139.56	121.70
1	A	113	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	C	87	HIS	CB-CG-CD2	7.14	152.94	130.80
2	H	82	LYS	CD-CE-NZ	7.14	128.13	111.70
1	C	9	ASN	CA-C-O	-7.14	105.11	120.10
1	C	6	ASP	CA-CB-CG	-7.14	97.70	113.40
1	C	108	THR	CA-CB-OG1	-7.14	94.01	109.00
2	B	6	VAL	CA-CB-CG1	7.13	121.60	110.90
1	E	45	HIS	CA-CB-CG	-7.13	101.49	113.60
1	G	58	HIS	CA-C-N	7.12	130.45	116.20
2	D	34	VAL	CA-CB-CG1	7.12	121.59	110.90
1	G	64	ASP	N-CA-C	-7.12	91.77	111.00
1	G	70	VAL	C-N-CA	-7.12	103.89	121.70
2	D	6	VAL	O-C-N	7.12	134.09	122.70
1	A	44	PRO	O-C-N	-7.12	111.31	122.70
1	G	114	PRO	N-CA-CB	7.12	111.84	103.30
1	G	51	GLY	O-C-N	-7.12	111.32	122.70
1	C	22	GLY	O-C-N	-7.11	111.32	122.70
2	F	43	GLU	CA-C-N	-7.11	101.56	117.20
1	G	114	PRO	N-CD-CG	-7.11	92.54	103.20
1	G	127	LYS	CA-CB-CG	7.11	129.04	113.40
1	G	86	LEU	O-C-N	7.11	134.07	122.70
2	F	41	PHE	CD1-CE1-CZ	-7.11	111.57	120.10
2	H	28	LEU	CA-CB-CG	7.11	131.65	115.30
2	B	25	GLY	O-C-N	7.10	134.07	122.70
1	A	134	THR	CA-CB-CG2	7.10	122.34	112.40
2	H	98	VAL	CA-CB-CG1	-7.10	100.25	110.90
2	D	120	LYS	CB-CA-C	7.10	124.60	110.40
2	D	90	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	A	2	LEU	CA-C-N	-7.10	101.59	117.20
2	B	95	LYS	CG-CD-CE	7.10	133.19	111.90
2	D	130	TYR	C-N-CA	7.10	139.44	121.70
2	B	123	THR	CA-CB-CG2	-7.09	102.47	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	58	HIS	CA-C-O	-7.09	105.20	120.10
2	H	84	THR	CA-CB-CG2	7.09	122.33	112.40
2	F	40	ARG	CG-CD-NE	-7.09	96.90	111.80
1	C	94	ASP	CB-CG-OD2	-7.09	111.92	118.30
2	F	137	VAL	C-N-CA	7.09	139.43	121.70
2	D	42	PHE	CZ-CE2-CD2	-7.09	111.59	120.10
1	E	14	TRP	CB-CA-C	7.09	124.58	110.40
2	H	142	ALA	N-CA-CB	-7.09	100.17	110.10
1	G	127	LYS	N-CA-CB	7.09	123.36	110.60
1	C	37	PRO	O-C-N	-7.08	111.36	122.70
1	E	81	SER	O-C-N	7.08	134.03	122.70
2	H	27	ALA	CB-CA-C	-7.08	99.47	110.10
2	B	38	THR	C-N-CA	7.08	139.41	121.70
2	H	97	HIS	C-N-CA	-7.08	104.00	121.70
2	D	38	THR	CB-CA-C	7.08	130.71	111.60
1	A	29	LEU	CB-CA-C	7.08	123.64	110.20
2	H	111	VAL	CG1-CB-CG2	-7.08	99.58	110.90
1	A	110	ALA	CA-C-O	7.07	134.95	120.10
2	D	122	PHE	CB-CG-CD1	7.07	125.75	120.80
2	B	145	TYR	N-CA-CB	-7.07	97.88	110.60
1	C	126	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	E	97	ASN	CB-CG-OD1	7.07	135.73	121.60
2	D	12	THR	CA-C-O	-7.06	105.27	120.10
2	H	97	HIS	CA-CB-CG	-7.05	101.61	113.60
2	B	41	PHE	CD1-CE1-CZ	-7.05	111.64	120.10
2	B	57	ASN	CA-C-O	7.05	134.91	120.10
2	D	4	THR	O-C-N	7.05	134.49	121.10
2	H	111	VAL	CA-C-O	-7.05	105.29	120.10
2	D	37	TRP	CA-CB-CG	-7.05	100.31	113.70
1	E	16	LYS	CG-CD-CE	7.05	133.04	111.90
2	B	130	TYR	CG-CD2-CE2	-7.04	115.66	121.30
1	A	112	HIS	C-N-CA	7.04	139.31	121.70
2	D	3	LEU	CA-CB-CG	7.04	131.50	115.30
1	E	68	ASN	CB-CG-ND2	7.04	133.60	116.70
1	A	21	ALA	C-N-CA	-7.04	107.52	122.30
2	F	14	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	C	28	ALA	CA-C-O	7.04	134.88	120.10
1	C	90	LYS	CB-CA-C	7.03	124.47	110.40
1	A	37	PRO	CA-N-CD	7.03	121.54	111.70
2	F	86	ALA	N-CA-CB	-7.03	100.26	110.10
1	G	126	ASP	O-C-N	-7.03	111.45	122.70
2	H	101	GLU	CA-C-O	-7.03	105.33	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	GLY	C-N-CA	7.02	139.26	121.70
2	F	137	VAL	N-CA-CB	7.02	126.95	111.50
1	A	62	VAL	CB-CA-C	-7.02	98.06	111.40
1	G	92	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	B	67	VAL	CA-CB-CG2	7.02	121.42	110.90
1	A	48	LEU	CA-C-O	7.02	134.83	120.10
1	A	112	HIS	CB-CA-C	7.01	124.43	110.40
2	B	14	LEU	CA-C-O	-7.01	105.37	120.10
1	A	34	LEU	CA-C-N	7.01	132.63	117.20
1	G	123	ALA	N-CA-CB	7.01	119.92	110.10
2	F	23	VAL	CA-CB-CG2	7.01	121.41	110.90
2	F	70	ALA	C-N-CA	7.01	139.22	121.70
2	B	124	PRO	CA-C-N	7.00	136.71	117.10
2	D	92	HIS	CA-C-N	-7.00	101.79	117.20
2	D	108	ASN	C-N-CA	-7.00	104.19	121.70
1	G	121	VAL	CA-C-O	7.00	134.81	120.10
1	E	99	LYS	N-CA-CB	7.00	123.20	110.60
2	H	12	THR	OG1-CB-CG2	-7.00	93.89	110.00
1	G	48	LEU	CA-CB-CG	-7.00	99.21	115.30
1	C	23	GLU	O-C-N	-6.99	111.51	122.70
1	A	85	ASP	CA-C-N	6.99	132.58	117.20
1	C	79	ALA	CA-C-N	-6.99	101.82	117.20
2	F	127	GLN	CA-C-N	-6.99	101.82	117.20
2	F	17	LYS	O-C-N	6.99	133.88	122.70
2	H	38	THR	OG1-CB-CG2	-6.99	93.93	110.00
1	C	128	PHE	CA-C-O	-6.99	105.43	120.10
1	E	72	HIS	CA-C-O	6.99	134.77	120.10
2	H	110	LEU	O-C-N	-6.99	111.52	122.70
2	H	118	PHE	CG-CD1-CE1	6.99	128.48	120.80
2	B	123	THR	CA-CB-OG1	-6.98	94.34	109.00
2	H	95	LYS	CA-C-O	-6.98	105.44	120.10
2	B	23	VAL	O-C-N	-6.98	111.34	123.20
2	B	59	LYS	CA-CB-CG	-6.98	98.05	113.40
1	C	58	HIS	CA-C-N	6.98	130.16	116.20
1	E	4	PRO	CA-C-N	6.98	132.56	117.20
1	G	60	LYS	CG-CD-CE	6.98	132.83	111.90
2	F	52	ASP	CA-C-O	6.97	134.75	120.10
1	G	140	TYR	CG-CD1-CE1	-6.97	115.72	121.30
1	G	103	HIS	CB-CA-C	-6.97	96.47	110.40
1	A	76	MET	CB-CA-C	-6.96	96.47	110.40
2	B	128	ALA	C-N-CA	-6.96	104.29	121.70
1	G	14	TRP	CA-C-N	-6.96	102.27	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	GLN	C-N-CA	6.96	139.10	121.70
1	G	26	ALA	CA-C-O	-6.96	105.49	120.10
1	E	8	THR	OG1-CB-CG2	6.95	125.99	110.00
2	H	64	GLY	CA-C-N	6.95	132.50	117.20
2	D	23	VAL	CA-CB-CG2	-6.95	100.48	110.90
1	C	131	SER	CA-C-N	-6.95	101.92	117.20
2	F	15	TRP	CB-CA-C	-6.95	96.51	110.40
2	F	31	LEU	CA-C-N	-6.95	101.92	117.20
1	A	141	ARG	CB-CA-C	6.94	124.29	110.40
2	B	120	LYS	O-C-N	6.94	133.81	122.70
1	C	48	LEU	CB-CG-CD1	6.94	122.80	111.00
2	B	82	LYS	O-C-N	-6.94	111.40	123.20
2	B	37	TRP	N-CA-CB	-6.94	98.11	110.60
1	G	14	TRP	CD1-NE1-CE2	6.94	115.24	109.00
1	G	39	THR	N-CA-CB	-6.94	97.12	110.30
1	G	107	VAL	CA-C-N	6.94	132.46	117.20
1	C	27	GLU	CG-CD-OE2	6.93	132.17	118.30
1	E	75	ASP	O-C-N	-6.93	111.61	122.70
1	G	68	ASN	CB-CG-ND2	-6.93	100.06	116.70
1	G	117	PHE	CB-CA-C	-6.93	96.53	110.40
2	B	122	PHE	N-CA-CB	-6.93	98.12	110.60
1	C	14	TRP	O-C-N	6.93	134.98	123.20
1	E	63	ALA	O-C-N	6.93	133.79	122.70
1	E	56	LYS	CD-CE-NZ	-6.93	95.77	111.70
1	C	55	VAL	C-N-CA	6.92	139.01	121.70
2	D	131	GLN	CB-CG-CD	-6.92	93.61	111.60
1	G	88	ALA	CA-C-N	6.92	132.43	117.20
2	B	38	THR	N-CA-CB	-6.92	97.15	110.30
1	A	56	LYS	CB-CA-C	-6.92	96.57	110.40
1	A	141	ARG	CB-CG-CD	-6.92	93.61	111.60
1	C	71	ALA	C-N-CA	-6.92	104.41	121.70
1	C	49	SER	CA-C-N	6.91	132.41	117.20
2	D	22	GLU	CB-CA-C	6.91	124.23	110.40
2	H	113	VAL	CA-CB-CG2	-6.91	100.53	110.90
1	A	117	PHE	CA-CB-CG	-6.91	97.32	113.90
1	C	105	LEU	O-C-N	-6.91	111.65	122.70
2	D	3	LEU	CB-CG-CD1	6.91	122.75	111.00
2	B	137	VAL	CA-CB-CG2	6.91	121.26	110.90
1	E	36	PHE	CA-CB-CG	6.91	130.47	113.90
1	A	24	TYR	CB-CA-C	-6.90	96.59	110.40
2	B	11	VAL	CA-C-O	6.90	134.60	120.10
2	H	31	LEU	CD1-CG-CD2	-6.90	89.79	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	LEU	CA-CB-CG	6.90	131.17	115.30
1	C	8	THR	C-N-CA	6.90	138.94	121.70
1	C	45	HIS	CA-C-N	-6.90	102.03	117.20
2	B	85	PHE	CD1-CE1-CZ	-6.89	111.83	120.10
1	C	33	PHE	CD1-CE1-CZ	6.89	128.37	120.10
2	F	1	VAL	CA-CB-CG1	6.89	121.23	110.90
2	H	34	VAL	CB-CA-C	6.89	124.49	111.40
1	A	65	ALA	O-C-N	6.89	133.72	122.70
1	G	30	GLU	CA-C-N	6.89	132.35	117.20
1	E	43	PHE	CB-CA-C	6.88	124.17	110.40
2	F	20	VAL	CA-CB-CG1	6.88	121.23	110.90
1	E	40	LYS	CA-CB-CG	-6.88	98.26	113.40
1	C	60	LYS	CB-CA-C	6.88	124.16	110.40
1	E	92	ARG	CA-C-N	-6.88	102.06	117.20
1	A	77	PRO	CA-C-N	-6.88	102.07	117.20
2	B	78	LEU	O-C-N	6.88	133.70	122.70
1	C	95	PRO	N-CD-CG	-6.88	92.89	103.20
2	D	59	LYS	CA-CB-CG	6.88	128.53	113.40
1	E	6	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	76	MET	N-CA-CB	-6.88	98.22	110.60
2	H	85	PHE	CA-C-O	-6.88	105.66	120.10
2	H	109	VAL	O-C-N	6.87	133.70	122.70
2	D	127	GLN	CA-CB-CG	-6.87	98.29	113.40
2	F	102	ASN	O-C-N	-6.87	111.71	122.70
2	D	75	LEU	O-C-N	-6.86	111.73	122.70
1	A	135	VAL	CA-CB-CG1	6.86	121.18	110.90
1	E	99	LYS	CB-CG-CD	6.86	129.43	111.60
2	H	10	ALA	O-C-N	6.85	133.67	122.70
1	C	83	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	A	116	GLU	CG-CD-OE1	6.85	132.00	118.30
2	F	12	THR	CA-CB-CG2	6.85	121.99	112.40
2	B	126	VAL	O-C-N	6.85	133.66	122.70
2	F	130	TYR	N-CA-CB	6.85	122.93	110.60
2	H	109	VAL	CB-CA-C	6.85	124.41	111.40
2	B	91	LEU	CA-C-O	-6.84	105.73	120.10
2	F	63	HIS	N-CA-CB	6.84	122.92	110.60
1	A	31	ARG	CA-C-N	-6.84	102.15	117.20
1	G	74	ASP	N-CA-CB	6.84	122.92	110.60
1	E	16	LYS	CA-CB-CG	-6.84	98.35	113.40
1	A	90	LYS	CG-CD-CE	6.84	132.41	111.90
2	H	21	ASP	N-CA-CB	-6.84	98.29	110.60
1	C	1	VAL	CA-CB-CG1	6.84	121.15	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	VAL	CA-C-N	-6.84	102.16	117.20
2	F	15	TRP	CD1-NE1-CE2	6.84	115.15	109.00
2	F	122	PHE	C-N-CA	6.84	138.79	121.70
1	G	19	ALA	CA-C-N	6.84	132.24	117.20
1	E	61	LYS	CB-CA-C	6.83	124.07	110.40
1	G	60	LYS	CA-C-N	-6.83	102.17	117.20
1	C	110	ALA	N-CA-C	6.83	129.44	111.00
1	G	73	VAL	CA-C-N	6.82	132.21	117.20
1	A	10	VAL	CA-CB-CG1	6.82	121.13	110.90
2	D	44	SER	O-C-N	-6.82	111.79	122.70
1	E	44	PRO	O-C-N	6.82	133.61	122.70
1	C	93	VAL	CG1-CB-CG2	-6.82	100.00	110.90
1	C	97	ASN	CA-CB-CG	-6.82	98.40	113.40
1	C	107	VAL	CA-C-O	-6.81	105.79	120.10
2	F	111	VAL	N-CA-CB	6.81	126.49	111.50
1	A	84	SER	C-N-CA	6.81	138.73	121.70
1	E	110	ALA	C-N-CA	6.81	138.72	121.70
1	G	27	GLU	CA-C-O	6.81	134.40	120.10
1	C	129	LEU	CA-C-N	6.81	132.17	117.20
2	F	15	TRP	O-C-N	6.81	134.77	123.20
1	E	14	TRP	O-C-N	-6.80	111.63	123.20
2	F	77	HIS	N-CA-CB	-6.80	98.35	110.60
2	F	90	GLU	CG-CD-OE2	-6.80	104.69	118.30
2	F	122	PHE	CG-CD2-CE2	6.80	128.28	120.80
1	A	138	SER	CA-C-N	6.80	132.16	117.20
2	D	97	HIS	O-C-N	-6.80	111.82	122.70
2	D	103	PHE	CG-CD2-CE2	6.80	128.28	120.80
1	E	74	ASP	CA-C-O	-6.80	105.82	120.10
1	G	89	HIS	CB-CG-ND1	-6.80	106.21	123.20
1	E	20	HIS	CB-CG-ND1	-6.79	106.22	123.20
2	H	6	VAL	CA-C-N	-6.79	102.26	117.20
1	C	98	PHE	CA-CB-CG	-6.79	97.61	113.90
2	B	77	HIS	CB-CA-C	6.79	123.97	110.40
2	D	88	LEU	CA-C-O	-6.78	105.86	120.10
1	G	10	VAL	CA-C-N	6.78	132.11	117.20
1	E	122	HIS	N-CA-C	-6.78	92.71	111.00
1	C	46	PHE	CD1-CE1-CZ	-6.77	111.97	120.10
2	D	132	LYS	C-N-CA	-6.77	104.77	121.70
2	D	139	ASN	CA-C-O	-6.77	105.88	120.10
1	E	104	CYS	CA-C-O	6.77	134.32	120.10
1	G	138	SER	CA-C-N	6.77	132.10	117.20
1	C	32	MET	CG-SD-CE	-6.77	89.37	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	115	ALA	CB-CA-C	-6.77	99.95	110.10
1	A	104	CYS	N-CA-C	6.76	129.27	111.00
1	G	134	THR	CA-CB-OG1	-6.76	94.79	109.00
2	F	43	GLU	CA-CB-CG	6.76	128.28	113.40
1	C	91	LEU	C-N-CA	6.76	138.59	121.70
1	C	32	MET	CA-CB-CG	-6.75	101.82	113.30
2	D	112	CYS	CA-C-N	6.75	132.06	117.20
1	G	26	ALA	CB-CA-C	-6.75	99.97	110.10
2	D	119	GLY	CA-C-O	-6.75	108.44	120.60
1	A	97	ASN	CB-CG-ND2	6.75	132.90	116.70
1	C	128	PHE	CE1-CZ-CE2	6.75	132.15	120.00
1	E	117	PHE	CA-C-O	6.75	134.27	120.10
2	F	20	VAL	CA-C-N	-6.75	102.35	117.20
1	E	47	ASP	N-CA-C	-6.75	92.79	111.00
2	B	91	LEU	CB-CA-C	-6.74	97.39	110.20
1	C	132	VAL	C-N-CA	-6.74	104.85	121.70
2	D	5	PRO	N-CD-CG	6.74	113.31	103.20
1	A	116	GLU	C-N-CA	6.74	138.54	121.70
1	G	30	GLU	N-CA-CB	6.74	122.73	110.60
1	A	14	TRP	NE1-CE2-CD2	-6.74	100.56	107.30
1	G	10	VAL	CA-CB-CG2	6.73	121.00	110.90
2	H	145	TYR	CA-C-N	6.73	132.01	117.20
2	D	89	SER	N-CA-C	6.73	129.17	111.00
1	G	53	ALA	CB-CA-C	6.73	120.20	110.10
1	A	22	GLY	CA-C-N	-6.73	102.40	117.20
2	D	23	VAL	CA-C-O	-6.73	105.97	120.10
1	A	60	LYS	CA-C-O	6.73	134.22	120.10
1	A	85	ASP	CB-CA-C	6.73	123.85	110.40
2	H	94	ASP	OD1-CG-OD2	6.72	136.07	123.30
1	C	70	VAL	CA-C-O	-6.72	105.99	120.10
2	F	108	ASN	CB-CG-OD1	6.72	135.04	121.60
1	C	10	VAL	O-C-N	-6.72	111.95	122.70
2	H	22	GLU	CB-CG-CD	-6.72	96.06	114.20
2	F	52	ASP	OD1-CG-OD2	6.71	136.06	123.30
1	G	33	PHE	CG-CD1-CE1	6.71	128.19	120.80
1	E	35	SER	C-N-CA	-6.71	104.93	121.70
1	C	124	SER	O-C-N	6.71	133.43	122.70
2	D	102	ASN	CB-CG-OD1	6.71	135.01	121.60
2	H	26	GLU	CB-CG-CD	6.71	132.31	114.20
1	G	9	ASN	N-CA-CB	-6.70	98.54	110.60
1	A	72	HIS	CA-C-O	6.70	134.17	120.10
2	B	59	LYS	CD-CE-NZ	-6.70	96.29	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	145	TYR	O-C-N	6.70	133.41	122.70
1	C	86	LEU	CA-CB-CG	-6.70	99.90	115.30
1	A	59	GLY	O-C-N	6.69	133.41	122.70
2	H	6	VAL	CA-CB-CG2	6.69	120.94	110.90
1	E	32	MET	O-C-N	6.69	133.40	122.70
1	G	2	LEU	CB-CG-CD1	6.69	122.37	111.00
2	H	84	THR	N-CA-C	6.69	129.06	111.00
2	H	131	GLN	CG-CD-OE1	6.69	134.97	121.60
1	E	10	VAL	CA-CB-CG2	-6.69	100.87	110.90
2	D	63	HIS	CB-CA-C	-6.68	97.03	110.40
1	G	110	ALA	N-CA-CB	6.68	119.46	110.10
1	G	90	LYS	CG-CD-CE	6.68	131.94	111.90
1	C	132	VAL	O-C-N	6.68	133.38	122.70
1	E	41	THR	CA-C-O	-6.68	106.08	120.10
2	H	84	THR	N-CA-CB	-6.67	97.62	110.30
2	H	118	PHE	CG-CD2-CE2	6.67	128.14	120.80
2	F	5	PRO	CA-C-O	-6.67	104.19	120.20
2	F	78	LEU	O-C-N	6.67	133.37	122.70
2	B	74	GLY	CA-C-O	-6.67	108.60	120.60
2	B	62	ALA	N-CA-C	6.67	129.00	111.00
1	G	14	TRP	CG-CD2-CE3	6.67	139.90	133.90
1	G	140	TYR	CD1-CG-CD2	6.67	125.23	117.90
2	B	49	SER	CB-CA-C	6.66	122.76	110.10
1	G	58	HIS	N-CA-CB	6.66	122.59	110.60
1	E	100	LEU	CB-CG-CD1	6.66	122.32	111.00
2	F	21	ASP	CA-C-N	-6.66	102.55	117.20
2	B	2	HIS	O-C-N	-6.66	112.05	122.70
2	F	47	ASP	CA-CB-CG	-6.66	98.75	113.40
2	F	97	HIS	CA-CB-CG	6.66	124.92	113.60
1	C	42	TYR	CA-C-O	-6.65	106.13	120.10
1	E	14	TRP	CB-CG-CD2	6.65	135.25	126.60
1	E	124	SER	N-CA-C	-6.65	93.04	111.00
2	D	38	THR	CA-CB-CG2	6.65	121.71	112.40
2	F	114	LEU	O-C-N	6.65	133.34	122.70
2	F	115	ALA	N-CA-CB	6.65	119.41	110.10
2	H	116	HIS	O-C-N	6.65	133.34	122.70
2	D	125	PRO	N-CA-CB	-6.64	95.29	102.60
2	F	79	ASP	OD1-CG-OD2	6.64	135.92	123.30
2	D	8	LYS	O-C-N	-6.63	112.09	122.70
1	G	8	THR	N-CA-C	6.63	128.91	111.00
1	C	10	VAL	CB-CA-C	6.63	124.00	111.40
1	A	10	VAL	CA-C-N	-6.63	102.61	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	39	THR	OG1-CB-CG2	6.63	125.25	110.00
1	G	109	LEU	C-N-CA	-6.63	105.12	121.70
2	B	26	GLU	OE1-CD-OE2	6.63	131.25	123.30
2	B	75	LEU	N-CA-CB	6.63	123.65	110.40
2	F	68	LEU	CA-C-N	6.62	129.45	116.20
2	B	49	SER	CA-C-O	6.62	134.00	120.10
2	H	87	THR	CA-CB-OG1	-6.62	95.09	109.00
2	D	51	PRO	N-CD-CG	-6.62	93.27	103.20
1	C	98	PHE	O-C-N	6.62	133.29	122.70
1	E	128	PHE	O-C-N	6.62	133.29	122.70
1	C	29	LEU	N-CA-C	-6.62	93.14	111.00
2	D	104	ARG	CB-CG-CD	-6.62	94.40	111.60
1	E	56	LYS	CA-CB-CG	6.62	127.96	113.40
1	G	22	GLY	O-C-N	-6.62	112.11	122.70
2	D	37	TRP	CG-CD2-CE3	6.61	139.85	133.90
2	D	73	ASP	N-CA-CB	-6.61	98.70	110.60
1	G	93	VAL	CA-CB-CG2	-6.61	100.98	110.90
2	H	15	TRP	CG-CD2-CE3	6.61	139.85	133.90
1	E	21	ALA	CA-C-O	-6.61	106.22	120.10
1	G	119	PRO	C-N-CA	6.61	138.22	121.70
1	A	104	CYS	CB-CA-C	-6.61	97.19	110.40
1	C	100	LEU	CB-CA-C	6.61	122.75	110.20
1	E	119	PRO	CA-CB-CG	-6.61	91.45	104.00
2	B	134	VAL	CA-C-O	6.60	133.97	120.10
2	H	45	PHE	CG-CD1-CE1	-6.60	113.53	120.80
1	A	94	ASP	N-CA-CB	6.60	122.48	110.60
1	A	132	VAL	CA-CB-CG2	-6.60	101.00	110.90
2	F	104	ARG	NH1-CZ-NH2	-6.60	112.14	119.40
1	C	99	LYS	CD-CE-NZ	-6.60	96.52	111.70
2	F	23	VAL	CB-CA-C	6.60	123.94	111.40
1	C	36	PHE	CG-CD1-CE1	6.60	128.06	120.80
1	E	115	ALA	N-CA-C	6.60	128.81	111.00
2	H	1	VAL	N-CA-C	-6.60	93.19	111.00
1	A	103	HIS	CG-ND1-CE1	6.59	117.43	108.20
2	F	15	TRP	NE1-CE2-CZ2	6.59	137.66	130.40
2	D	124	PRO	N-CD-CG	6.59	113.08	103.20
1	E	33	PHE	N-CA-CB	-6.59	98.74	110.60
1	A	13	ALA	CB-CA-C	-6.59	100.22	110.10
2	D	12	THR	O-C-N	-6.59	112.16	122.70
1	E	101	LEU	CA-C-O	-6.59	106.27	120.10
1	A	77	PRO	CA-CB-CG	-6.58	91.49	104.00
1	A	103	HIS	ND1-CE1-NE2	-6.58	95.42	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	ASP	N-CA-CB	6.58	122.44	110.60
2	D	42	PHE	CD1-CG-CD2	6.58	126.86	118.30
2	B	5	PRO	CB-CA-C	-6.58	95.55	112.00
2	D	22	GLU	N-CA-C	-6.58	93.24	111.00
1	A	49	SER	C-N-CA	-6.57	105.28	121.70
1	A	113	LEU	N-CA-CB	-6.57	97.26	110.40
2	B	31	LEU	O-C-N	6.57	133.21	122.70
2	H	6	VAL	CB-CA-C	-6.57	98.92	111.40
2	H	30	ARG	C-N-CA	6.57	138.12	121.70
1	A	136	LEU	N-CA-C	-6.56	93.28	111.00
2	H	130	TYR	N-CA-CB	6.56	122.42	110.60
2	B	23	VAL	CA-C-O	6.56	133.88	120.10
2	F	75	LEU	CA-C-N	-6.56	102.77	117.20
1	C	86	LEU	O-C-N	-6.56	112.21	122.70
1	C	94	ASP	CB-CG-OD1	6.56	124.20	118.30
1	E	14	TRP	CB-CG-CD1	-6.56	118.47	127.00
2	H	66	LYS	CA-C-N	-6.56	102.77	117.20
2	H	133	VAL	CG1-CB-CG2	-6.56	100.41	110.90
1	A	27	GLU	CA-C-O	6.55	133.86	120.10
1	G	49	SER	C-N-CA	6.55	138.09	121.70
2	D	106	LEU	O-C-N	-6.55	112.06	123.20
1	G	76	MET	CG-SD-CE	6.55	110.69	100.20
2	H	17	LYS	CG-CD-CE	-6.55	92.24	111.90
1	A	6	ASP	C-N-CA	6.55	138.08	121.70
1	A	18	GLY	O-C-N	6.55	133.18	122.70
1	A	107	VAL	N-CA-C	-6.55	93.32	111.00
2	B	66	LYS	N-CA-CB	6.55	122.39	110.60
1	E	72	HIS	O-C-N	-6.55	112.22	122.70
1	A	27	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	C	45	HIS	ND1-CG-CD2	6.54	117.95	108.80
2	H	105	LEU	CB-CG-CD2	-6.54	99.88	111.00
2	F	3	LEU	CB-CA-C	-6.54	97.78	110.20
2	F	57	ASN	CA-C-O	-6.53	106.38	120.10
1	G	55	VAL	CA-CB-CG1	-6.53	101.10	110.90
2	F	92	HIS	ND1-CG-CD2	-6.53	96.86	106.00
1	A	34	LEU	CA-CB-CG	6.53	130.31	115.30
2	B	45	PHE	CA-C-O	-6.53	106.39	120.10
1	E	56	LYS	CA-C-O	6.53	133.81	120.10
1	E	86	LEU	CA-C-O	6.53	133.81	120.10
2	B	1	VAL	C-N-CA	-6.52	105.39	121.70
2	B	2	HIS	CB-CA-C	6.52	123.45	110.40
2	D	35	TYR	N-CA-CB	-6.52	98.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	53	ALA	CA-C-N	-6.52	102.85	117.20
1	A	4	PRO	O-C-N	-6.52	112.27	122.70
2	D	58	PRO	CB-CA-C	-6.52	95.70	112.00
1	E	43	PHE	CZ-CE2-CD2	-6.52	112.27	120.10
1	E	123	ALA	CA-C-N	-6.52	102.85	117.20
1	G	108	THR	CA-CB-CG2	-6.52	103.27	112.40
1	A	59	GLY	CA-C-N	-6.52	102.86	117.20
1	C	47	ASP	N-CA-CB	6.52	122.33	110.60
2	B	143	HIS	O-C-N	6.51	133.12	122.70
1	G	92	ARG	NH1-CZ-NH2	-6.51	112.23	119.40
1	G	108	THR	CA-C-N	-6.51	102.88	117.20
2	H	28	LEU	N-CA-C	-6.51	93.42	111.00
1	G	62	VAL	C-N-CA	-6.51	105.42	121.70
2	F	61	LYS	CB-CG-CD	-6.51	94.68	111.60
2	F	70	ALA	N-CA-CB	6.51	119.21	110.10
1	A	29	LEU	CB-CG-CD1	-6.51	99.94	111.00
1	C	68	ASN	CB-CG-ND2	6.50	132.30	116.70
2	B	73	ASP	OD1-CG-OD2	6.50	135.64	123.30
2	B	35	TYR	CZ-CE2-CD2	-6.50	113.95	119.80
2	D	52	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	E	58	HIS	CA-C-O	6.50	133.74	120.10
1	G	20	HIS	CG-ND1-CE1	-6.50	97.26	105.70
1	A	124	SER	CA-CB-OG	-6.49	93.67	111.20
2	B	36	PRO	C-N-CA	-6.49	105.46	121.70
2	D	53	ALA	O-C-N	6.49	133.09	122.70
2	D	81	LEU	CA-C-O	6.49	133.74	120.10
1	G	26	ALA	CA-C-N	6.49	131.49	117.20
1	G	99	LYS	CD-CE-NZ	6.49	126.63	111.70
2	H	105	LEU	C-N-CA	-6.49	105.47	121.70
1	A	103	HIS	CG-CD2-NE2	-6.49	96.87	109.20
2	D	39	GLN	CA-C-N	-6.49	102.92	117.20
1	C	102	SER	C-N-CA	6.49	137.92	121.70
1	E	29	LEU	CB-CG-CD2	-6.49	99.97	111.00
1	E	117	PHE	CB-CA-C	6.49	123.38	110.40
1	A	95	PRO	CA-N-CD	-6.48	102.42	111.50
2	F	66	LYS	CB-CG-CD	6.48	128.46	111.60
1	C	89	HIS	ND1-CG-CD2	6.48	117.88	108.80
2	F	143	HIS	CG-CD2-NE2	6.48	121.52	109.20
1	G	27	GLU	CG-CD-OE1	6.48	131.26	118.30
2	F	140	ALA	CB-CA-C	6.48	119.82	110.10
1	A	26	ALA	C-N-CA	-6.47	105.52	121.70
2	F	95	LYS	CB-CA-C	6.47	123.34	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	36	PHE	CA-C-N	-6.47	98.97	117.10
2	B	107	GLY	CA-C-N	-6.47	102.97	117.20
1	A	7	LYS	CA-C-N	6.47	131.43	117.20
1	E	66	LEU	C-N-CA	6.47	137.87	121.70
1	A	96	VAL	CA-C-O	6.47	133.68	120.10
1	A	84	SER	N-CA-CB	-6.46	100.80	110.50
2	F	90	GLU	N-CA-C	-6.46	93.54	111.00
2	H	93	CYS	CB-CA-C	6.46	123.33	110.40
1	G	132	VAL	O-C-N	6.46	133.04	122.70
1	C	6	ASP	CB-CA-C	-6.46	97.48	110.40
2	B	125	PRO	CA-C-O	6.46	135.70	120.20
1	G	41	THR	CA-C-O	-6.46	106.54	120.10
1	G	84	SER	N-CA-CB	6.46	120.19	110.50
2	B	136	GLY	O-C-N	6.45	133.03	122.70
2	D	45	PHE	CD1-CE1-CZ	6.45	127.84	120.10
1	C	116	GLU	O-C-N	-6.45	112.38	122.70
1	E	121	VAL	CA-C-N	6.45	131.40	117.20
2	H	96	LEU	CA-C-N	6.45	131.39	117.20
2	B	104	ARG	N-CA-CB	-6.45	98.99	110.60
2	B	145	TYR	CG-CD2-CE2	6.45	126.46	121.30
1	A	67	THR	O-C-N	6.45	133.01	122.70
2	H	103	PHE	C-N-CA	6.45	137.81	121.70
1	G	116	GLU	CG-CD-OE2	-6.44	105.41	118.30
2	B	115	ALA	CA-C-O	-6.44	106.57	120.10
2	H	104	ARG	CG-CD-NE	6.44	125.33	111.80
2	B	109	VAL	CG1-CB-CG2	-6.44	100.59	110.90
1	A	7	LYS	CA-C-O	-6.44	106.58	120.10
1	E	80	LEU	CB-CG-CD2	6.44	121.95	111.00
1	A	34	LEU	C-N-CA	-6.44	105.61	121.70
2	B	44	SER	CA-CB-OG	6.43	128.57	111.20
2	D	144	LYS	C-N-CA	-6.43	105.61	121.70
2	F	87	THR	N-CA-CB	6.43	122.53	110.30
1	C	80	LEU	CA-CB-CG	6.43	130.10	115.30
2	F	120	LYS	CA-C-N	6.43	131.35	117.20
1	A	122	HIS	ND1-CE1-NE2	-6.43	95.76	109.90
1	C	87	HIS	CB-CG-ND1	-6.43	107.14	123.20
2	D	65	LYS	CG-CD-CE	6.43	131.18	111.90
2	F	107	GLY	CA-C-O	-6.43	109.03	120.60
2	H	103	PHE	N-CA-CB	-6.43	99.03	110.60
2	H	61	LYS	CA-C-O	-6.42	106.61	120.10
2	H	74	GLY	C-N-CA	6.42	137.76	121.70
2	H	5	PRO	CB-CA-C	-6.42	95.94	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ALA	N-CA-CB	6.42	119.09	110.10
1	C	101	LEU	CA-C-O	-6.42	106.62	120.10
1	C	117	PHE	CA-C-N	-6.42	103.07	117.20
1	C	2	LEU	N-CA-C	-6.42	93.67	111.00
1	E	92	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
2	F	31	LEU	C-N-CA	6.42	137.75	121.70
2	D	103	PHE	O-C-N	-6.42	112.43	122.70
2	H	40	ARG	O-C-N	6.41	132.96	122.70
2	B	28	LEU	N-CA-C	-6.41	93.69	111.00
2	F	4	THR	CA-C-O	-6.41	106.64	120.10
1	G	7	LYS	CA-C-O	6.41	133.56	120.10
1	G	30	GLU	CG-CD-OE2	-6.41	105.48	118.30
1	G	90	LYS	CD-CE-NZ	6.41	126.44	111.70
2	F	135	ALA	O-C-N	-6.41	112.31	123.20
1	C	66	LEU	C-N-CA	-6.41	105.69	121.70
2	B	34	VAL	CA-C-O	6.40	133.55	120.10
2	D	139	ASN	CA-C-N	6.40	131.29	117.20
2	F	77	HIS	CA-CB-CG	-6.40	102.71	113.60
2	B	4	THR	CA-CB-OG1	-6.40	95.55	109.00
1	E	130	ALA	CA-C-N	-6.40	103.11	117.20
1	G	73	VAL	C-N-CA	6.40	137.71	121.70
1	E	44	PRO	CA-CB-CG	-6.40	91.84	104.00
2	D	139	ASN	CB-CG-OD1	-6.40	108.80	121.60
1	A	44	PRO	C-N-CA	6.40	137.70	121.70
2	F	92	HIS	CA-C-O	-6.39	106.67	120.10
2	H	7	GLU	C-N-CA	-6.39	105.71	121.70
2	B	142	ALA	CB-CA-C	-6.39	100.51	110.10
1	E	24	TYR	CG-CD2-CE2	6.39	126.41	121.30
2	H	39	GLN	CG-CD-OE1	6.39	134.39	121.60
2	B	45	PHE	CG-CD1-CE1	-6.39	113.77	120.80
2	B	46	GLY	CA-C-O	-6.39	109.10	120.60
2	D	111	VAL	C-N-CA	6.39	137.67	121.70
1	E	24	TYR	OH-CZ-CE2	-6.39	102.86	120.10
2	F	3	LEU	N-CA-CB	6.38	123.17	110.40
2	H	48	LEU	CB-CG-CD1	6.38	121.85	111.00
2	D	94	ASP	C-N-CA	6.38	137.66	121.70
1	G	46	PHE	CZ-CE2-CD2	6.38	127.76	120.10
2	B	94	ASP	N-CA-C	6.38	128.22	111.00
1	A	52	SER	O-C-N	-6.38	112.50	122.70
2	D	130	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	G	113	LEU	CB-CA-C	6.37	122.31	110.20
1	A	121	VAL	CA-C-O	-6.37	106.72	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	TRP	CD2-CE3-CZ3	6.37	127.08	118.80
2	F	143	HIS	CA-CB-CG	-6.37	102.77	113.60
2	H	53	ALA	CB-CA-C	-6.37	100.55	110.10
1	G	140	TYR	CB-CA-C	6.37	123.13	110.40
1	G	123	ALA	CB-CA-C	6.36	119.65	110.10
1	E	64	ASP	CA-C-O	-6.36	106.74	120.10
1	E	117	PHE	O-C-N	-6.36	112.52	122.70
2	D	120	LYS	C-N-CA	6.36	137.60	121.70
2	B	111	VAL	CB-CA-C	-6.36	99.32	111.40
2	D	22	GLU	CA-C-N	6.36	131.19	117.20
1	A	93	VAL	CA-CB-CG2	-6.36	101.37	110.90
1	A	38	THR	OG1-CB-CG2	6.35	124.61	110.00
2	H	122	PHE	CD1-CG-CD2	6.35	126.56	118.30
2	B	91	LEU	CB-CG-CD1	-6.35	100.21	111.00
1	G	41	THR	N-CA-CB	-6.35	98.23	110.30
1	G	134	THR	N-CA-CB	-6.35	98.24	110.30
1	C	72	HIS	CB-CA-C	6.35	123.10	110.40
1	G	34	LEU	CB-CG-CD1	-6.35	100.21	111.00
1	E	15	GLY	N-CA-C	-6.35	97.23	113.10
2	F	134	VAL	O-C-N	-6.34	112.55	122.70
2	H	112	CYS	CA-C-O	-6.34	106.78	120.10
2	B	129	ALA	C-N-CA	6.34	137.54	121.70
2	B	15	TRP	CA-C-N	6.33	128.87	116.20
2	H	5	PRO	O-C-N	6.33	132.83	122.70
1	A	103	HIS	CA-C-N	-6.33	103.27	117.20
1	E	116	GLU	N-CA-C	-6.33	93.91	111.00
1	C	2	LEU	CB-CG-CD2	-6.32	100.25	111.00
1	C	55	VAL	CA-CB-CG2	6.32	120.38	110.90
1	E	95	PRO	CA-C-N	6.32	131.10	117.20
2	F	90	GLU	C-N-CA	6.32	137.49	121.70
2	F	97	HIS	CG-ND1-CE1	6.32	117.04	108.20
2	H	139	ASN	OD1-CG-ND2	-6.31	107.38	121.90
2	B	54	VAL	CA-CB-CG1	6.31	120.36	110.90
1	C	77	PRO	CA-C-O	-6.31	105.06	120.20
2	H	2	HIS	ND1-CG-CD2	-6.31	97.17	106.00
2	B	124	PRO	CA-C-O	-6.31	105.07	120.20
1	C	16	LYS	N-CA-CB	-6.31	99.25	110.60
1	C	41	THR	C-N-CA	-6.31	105.94	121.70
1	E	107	VAL	O-C-N	6.30	132.79	122.70
1	A	106	LEU	CA-C-O	6.30	133.34	120.10
1	C	130	ALA	O-C-N	-6.30	112.61	122.70
1	A	80	LEU	CA-CB-CG	6.30	129.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	116	HIS	O-C-N	-6.30	112.62	122.70
1	E	138	SER	N-CA-CB	6.30	119.95	110.50
2	B	130	TYR	O-C-N	6.30	132.78	122.70
2	H	96	LEU	CB-CA-C	6.30	122.17	110.20
2	B	3	LEU	CB-CG-CD2	-6.29	100.30	111.00
1	E	11	LYS	O-C-N	-6.29	112.64	122.70
2	H	25	GLY	O-C-N	-6.29	112.64	122.70
2	F	142	ALA	O-C-N	-6.28	112.65	122.70
1	A	53	ALA	CA-C-N	-6.28	103.38	117.20
1	E	64	ASP	OD1-CG-OD2	-6.28	111.36	123.30
2	D	35	TYR	CD1-CG-CD2	6.28	124.81	117.90
2	D	80	ASN	N-CA-CB	6.28	121.90	110.60
1	E	48	LEU	CD1-CG-CD2	-6.28	91.67	110.50
2	F	50	THR	O-C-N	6.28	133.03	121.10
2	H	70	ALA	N-CA-CB	6.28	118.89	110.10
2	F	71	PHE	O-C-N	-6.27	112.66	122.70
1	A	18	GLY	CA-C-N	-6.27	103.40	117.20
1	G	31	ARG	CB-CA-C	6.27	122.94	110.40
1	A	1	VAL	CA-C-O	-6.27	106.93	120.10
1	C	104	CYS	O-C-N	6.27	132.73	122.70
2	D	118	PHE	CA-CB-CG	6.27	128.95	113.90
1	A	101	LEU	CB-CG-CD1	6.27	121.65	111.00
2	F	120	LYS	CA-C-O	-6.27	106.94	120.10
2	H	48	LEU	CB-CA-C	-6.27	98.29	110.20
2	B	85	PHE	CB-CG-CD1	6.27	125.19	120.80
2	D	127	GLN	CB-CA-C	-6.26	97.87	110.40
1	G	38	THR	CB-CA-C	6.26	128.51	111.60
2	H	123	THR	CA-CB-OG1	6.26	122.15	109.00
2	D	50	THR	CA-CB-CG2	6.26	121.17	112.40
2	H	43	GLU	CG-CD-OE2	-6.26	105.78	118.30
1	A	127	LYS	CA-C-N	6.26	130.97	117.20
2	D	4	THR	CA-C-O	-6.26	106.95	120.10
2	H	43	GLU	CA-C-N	-6.26	103.43	117.20
1	E	32	MET	CB-CA-C	-6.25	97.89	110.40
1	E	137	THR	CA-CB-CG2	6.25	121.16	112.40
1	G	49	SER	CB-CA-C	6.25	121.98	110.10
2	F	144	LYS	O-C-N	6.25	132.70	122.70
1	C	40	LYS	CA-C-N	6.25	130.95	117.20
2	B	71	PHE	O-C-N	-6.25	112.70	122.70
2	B	141	LEU	CA-CB-CG	6.25	129.67	115.30
1	C	56	LYS	CA-C-O	-6.25	106.98	120.10
2	H	116	HIS	CG-CD2-NE2	-6.25	97.33	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	36	PRO	CA-C-N	6.24	130.94	117.20
1	G	45	HIS	C-N-CA	-6.24	106.10	121.70
2	F	68	LEU	N-CA-CB	-6.24	97.92	110.40
2	F	133	VAL	O-C-N	6.24	132.68	122.70
2	H	20	VAL	N-CA-CB	6.24	125.23	111.50
2	H	123	THR	OG1-CB-CG2	-6.24	95.65	110.00
2	B	66	LYS	CG-CD-CE	6.24	130.61	111.90
2	H	133	VAL	CB-CA-C	6.24	123.25	111.40
2	H	80	ASN	CA-CB-CG	6.23	127.12	113.40
2	H	118	PHE	CD1-CE1-CZ	-6.23	112.62	120.10
1	A	24	TYR	CA-CB-CG	-6.23	101.56	113.40
1	C	33	PHE	CG-CD1-CE1	-6.23	113.94	120.80
1	C	108	THR	O-C-N	6.23	132.67	122.70
1	A	63	ALA	N-CA-CB	-6.23	101.38	110.10
2	H	66	LYS	O-C-N	6.23	132.67	122.70
2	F	106	LEU	CA-C-N	-6.23	103.74	116.20
1	A	110	ALA	N-CA-CB	-6.23	101.38	110.10
1	E	100	LEU	CA-C-N	6.23	130.90	117.20
1	E	137	THR	CA-C-O	-6.22	107.03	120.10
2	F	23	VAL	CG1-CB-CG2	-6.22	100.94	110.90
2	B	145	TYR	CB-CG-CD2	6.22	124.73	121.00
1	G	45	HIS	CB-CA-C	6.22	122.85	110.40
1	A	33	PHE	CE1-CZ-CE2	-6.22	108.80	120.00
1	A	100	LEU	CB-CG-CD1	6.22	121.57	111.00
2	B	67	VAL	O-C-N	6.22	132.65	122.70
1	C	42	TYR	CE1-CZ-OH	6.22	136.89	120.10
2	H	101	GLU	CA-C-N	6.22	130.88	117.20
2	B	45	PHE	O-C-N	-6.22	112.63	123.20
2	D	11	VAL	O-C-N	6.22	132.65	122.70
2	H	80	ASN	CB-CG-ND2	6.22	131.62	116.70
2	B	120	LYS	CB-CA-C	-6.21	97.97	110.40
1	G	31	ARG	CA-C-N	6.21	130.87	117.20
2	H	76	ALA	CB-CA-C	-6.21	100.78	110.10
2	H	125	PRO	CA-N-CD	-6.21	102.80	111.50
1	A	92	ARG	N-CA-CB	-6.21	99.42	110.60
1	A	93	VAL	O-C-N	6.21	132.64	122.70
2	D	121	GLU	O-C-N	-6.21	112.76	122.70
2	F	13	ALA	C-N-CA	-6.21	106.18	121.70
2	F	66	LYS	N-CA-CB	-6.21	99.43	110.60
1	A	9	ASN	CB-CG-OD1	6.21	134.01	121.60
2	F	35	TYR	CB-CA-C	-6.21	97.98	110.40
1	E	45	HIS	CB-CG-CD2	6.21	150.03	130.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	139	ASN	OD1-CG-ND2	-6.20	107.63	121.90
1	E	65	ALA	CB-CA-C	6.20	119.40	110.10
1	G	67	THR	CB-CA-C	6.20	128.34	111.60
1	C	35	SER	CA-CB-OG	-6.20	94.47	111.20
1	C	87	HIS	CA-CB-CG	-6.20	103.06	113.60
2	D	126	VAL	CA-C-N	-6.20	103.56	117.20
1	G	116	GLU	CG-CD-OE1	6.20	130.70	118.30
1	G	4	PRO	CA-CB-CG	-6.20	92.23	104.00
2	H	68	LEU	N-CA-CB	-6.20	98.01	110.40
2	F	45	PHE	CA-C-O	-6.19	107.10	120.10
1	G	86	LEU	CA-C-O	-6.19	107.10	120.10
1	G	129	LEU	CA-C-N	-6.19	103.58	117.20
1	A	139	LYS	CA-C-N	-6.19	103.58	117.20
2	F	103	PHE	CG-CD2-CE2	6.19	127.61	120.80
2	F	102	ASN	OD1-CG-ND2	-6.19	107.67	121.90
2	B	98	VAL	CA-C-N	-6.18	103.60	117.20
1	A	91	LEU	CB-CG-CD2	-6.18	100.49	111.00
2	F	116	HIS	C-N-CA	6.18	137.15	121.70
2	H	27	ALA	N-CA-CB	-6.18	101.45	110.10
1	E	89	HIS	CB-CG-CD2	6.18	149.95	130.80
2	H	37	TRP	CA-C-O	6.18	133.07	120.10
1	C	10	VAL	N-CA-CB	-6.17	97.93	111.50
2	F	144	LYS	CA-C-N	6.17	130.77	117.20
2	H	43	GLU	CA-C-O	6.17	133.05	120.10
1	C	4	PRO	N-CA-CB	6.16	110.69	103.30
1	G	118	THR	CA-C-N	6.16	134.36	117.10
2	H	67	VAL	CB-CA-C	6.16	123.11	111.40
2	H	88	LEU	CB-CG-CD2	-6.16	100.53	111.00
2	H	49	SER	O-C-N	-6.16	112.84	122.70
1	C	101	LEU	CB-CG-CD2	-6.16	100.53	111.00
1	E	105	LEU	CB-CG-CD1	-6.16	100.53	111.00
1	C	6	ASP	C-N-CA	6.16	137.09	121.70
2	B	23	VAL	CA-CB-CG2	-6.16	101.67	110.90
2	H	85	PHE	CD1-CG-CD2	-6.16	110.30	118.30
1	C	35	SER	CA-C-N	6.15	130.74	117.20
2	F	88	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	E	73	VAL	CA-C-N	-6.15	103.67	117.20
1	E	48	LEU	C-N-CA	-6.14	106.34	121.70
1	G	54	GLN	N-CA-C	6.14	127.58	111.00
1	E	94	ASP	N-CA-CB	-6.14	99.55	110.60
2	B	37	TRP	CA-C-N	6.14	130.70	117.20
2	H	113	VAL	O-C-N	6.13	132.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LYS	N-CA-C	-6.13	94.44	111.00
2	D	38	THR	N-CA-C	-6.13	94.44	111.00
2	D	80	ASN	CB-CA-C	-6.13	98.14	110.40
2	B	45	PHE	CD1-CG-CD2	-6.13	110.33	118.30
1	G	60	LYS	CB-CA-C	-6.13	98.14	110.40
2	H	27	ALA	CA-C-N	-6.13	103.72	117.20
1	A	123	ALA	CA-C-N	-6.12	103.73	117.20
1	C	16	LYS	CA-C-O	-6.12	107.24	120.10
1	E	83	LEU	O-C-N	-6.12	112.90	122.70
1	G	70	VAL	CB-CA-C	6.12	123.03	111.40
1	C	113	LEU	O-C-N	-6.12	109.47	121.10
2	H	131	GLN	N-CA-C	-6.12	94.48	111.00
1	A	101	LEU	N-CA-C	-6.12	94.49	111.00
2	H	137	VAL	CA-C-N	-6.12	103.75	117.20
1	A	97	ASN	OD1-CG-ND2	-6.11	107.84	121.90
1	E	91	LEU	CA-CB-CG	6.11	129.36	115.30
1	G	139	LYS	CA-C-N	-6.11	103.75	117.20
2	D	116	HIS	ND1-CE1-NE2	6.11	123.35	109.90
1	G	79	ALA	O-C-N	6.11	132.48	122.70
1	A	106	LEU	N-CA-CB	-6.11	98.18	110.40
1	E	101	LEU	C-N-CA	6.11	136.98	121.70
1	G	4	PRO	N-CA-CB	6.11	110.63	103.30
2	D	15	TRP	CB-CA-C	-6.10	98.19	110.40
1	A	6	ASP	CA-C-O	6.10	132.91	120.10
2	D	127	GLN	N-CA-CB	6.10	121.59	110.60
1	E	86	LEU	CB-CG-CD2	-6.10	100.63	111.00
2	H	102	ASN	OD1-CG-ND2	6.10	135.94	121.90
1	A	42	TYR	CD1-CG-CD2	-6.10	111.19	117.90
2	D	73	ASP	C-N-CA	-6.10	109.49	122.30
1	G	73	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	G	118	THR	O-C-N	-6.10	109.52	121.10
1	E	103	HIS	CE1-NE2-CD2	6.09	121.83	106.60
2	F	86	ALA	CA-C-N	-6.09	103.79	117.20
1	G	68	ASN	C-N-CA	-6.09	106.47	121.70
2	D	27	ALA	CA-C-O	6.09	132.90	120.10
1	C	111	ALA	N-CA-C	6.09	127.45	111.00
2	H	1	VAL	O-C-N	6.09	132.45	122.70
1	E	131	SER	C-N-CA	-6.09	106.48	121.70
2	F	43	GLU	CG-CD-OE2	-6.09	106.12	118.30
1	C	43	PHE	CA-C-N	-6.09	100.06	117.10
2	D	120	LYS	N-CA-CB	-6.09	99.65	110.60
2	F	36	PRO	CA-CB-CG	6.09	116.36	104.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	PRO	C-N-CA	-6.08	106.49	121.70
2	B	48	LEU	CB-CA-C	-6.08	98.65	110.20
1	E	130	ALA	C-N-CA	6.08	136.91	121.70
1	E	137	THR	C-N-CA	6.08	136.90	121.70
1	A	129	LEU	CA-C-O	-6.08	107.33	120.10
1	C	89	HIS	CA-C-N	-6.08	103.83	117.20
2	F	36	PRO	O-C-N	-6.08	112.97	122.70
2	F	97	HIS	CB-CG-CD2	-6.08	111.96	130.80
1	A	54	GLN	CG-CD-OE1	6.08	133.75	121.60
2	B	28	LEU	N-CA-CB	6.08	122.56	110.40
1	E	100	LEU	N-CA-CB	-6.08	98.25	110.40
1	G	76	MET	N-CA-CB	-6.08	99.66	110.60
2	F	85	PHE	CD1-CE1-CZ	6.08	127.39	120.10
2	F	5	PRO	CA-CB-CG	-6.07	92.46	104.00
2	B	7	GLU	CA-CB-CG	-6.07	100.04	113.40
2	H	32	LEU	CA-C-O	6.07	132.85	120.10
2	B	143	HIS	ND1-CG-CD2	-6.07	97.50	106.00
1	C	139	LYS	CB-CA-C	6.07	122.54	110.40
2	H	41	PHE	CG-CD2-CE2	-6.07	114.12	120.80
1	E	111	ALA	CA-C-O	6.07	132.84	120.10
1	A	12	ALA	CB-CA-C	-6.06	101.00	110.10
1	G	17	VAL	O-C-N	6.06	133.51	123.20
2	F	127	GLN	CG-CD-NE2	6.06	131.25	116.70
1	G	69	ALA	CA-C-N	6.06	130.53	117.20
1	A	37	PRO	O-C-N	-6.06	113.01	122.70
2	F	131	GLN	N-CA-CB	6.06	121.50	110.60
1	G	9	ASN	CB-CG-OD1	-6.06	109.49	121.60
1	G	114	PRO	N-CA-C	-6.06	96.35	112.10
1	A	82	ALA	CB-CA-C	6.05	119.18	110.10
2	D	94	ASP	O-C-N	6.05	132.39	122.70
1	E	43	PHE	CB-CG-CD2	-6.05	116.56	120.80
2	F	63	HIS	CB-CG-ND1	6.05	138.33	123.20
2	H	53	ALA	C-N-CA	-6.05	106.57	121.70
1	E	131	SER	CA-C-N	-6.05	103.89	117.20
2	D	111	VAL	CG1-CB-CG2	6.05	120.58	110.90
1	A	10	VAL	CA-CB-CG2	-6.04	101.83	110.90
1	C	114	PRO	CA-C-N	-6.04	103.90	117.20
1	A	77	PRO	N-CD-CG	-6.04	94.14	103.20
2	D	115	ALA	O-C-N	-6.04	113.03	122.70
2	F	53	ALA	O-C-N	6.04	132.37	122.70
1	A	58	HIS	O-C-N	-6.04	112.93	123.20
1	G	32	MET	CG-SD-CE	-6.04	90.54	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	VAL	CA-CB-CG2	6.04	119.96	110.90
1	C	2	LEU	CD1-CG-CD2	6.04	128.61	110.50
1	G	91	LEU	CA-C-N	6.04	130.49	117.20
2	F	41	PHE	CB-CG-CD1	6.04	125.03	120.80
1	C	29	LEU	CB-CG-CD1	6.03	121.26	111.00
2	F	18	VAL	CA-CB-CG1	6.03	119.95	110.90
1	E	45	HIS	N-CA-CB	6.03	121.46	110.60
2	H	118	PHE	CB-CG-CD2	-6.03	116.58	120.80
2	B	57	ASN	N-CA-CB	6.03	121.45	110.60
2	B	130	TYR	C-N-CA	6.03	136.77	121.70
2	D	37	TRP	NE1-CE2-CZ2	6.03	137.03	130.40
2	H	65	LYS	N-CA-CB	6.03	121.45	110.60
2	H	127	GLN	CA-C-O	6.02	132.74	120.10
1	E	76	MET	CG-SD-CE	6.02	109.83	100.20
1	G	133	SER	CB-CA-C	6.01	121.53	110.10
2	B	22	GLU	N-CA-CB	-6.01	99.78	110.60
2	D	75	LEU	CD1-CG-CD2	6.01	128.53	110.50
2	B	67	VAL	CA-CB-CG1	6.01	119.91	110.90
2	B	108	ASN	CB-CG-OD1	6.01	133.62	121.60
1	C	118	THR	CA-CB-OG1	-6.01	96.38	109.00
1	G	91	LEU	O-C-N	-6.01	113.09	122.70
1	G	108	THR	C-N-CA	6.01	136.72	121.70
1	C	42	TYR	CA-CB-CG	-6.01	101.98	113.40
2	D	57	ASN	CB-CG-ND2	-6.01	102.28	116.70
2	B	87	THR	C-N-CA	6.01	136.72	121.70
2	B	102	ASN	CA-CB-CG	6.00	126.61	113.40
1	E	92	ARG	CA-CB-CG	6.00	126.61	113.40
1	A	141	ARG	CA-C-O	-6.00	107.49	120.10
2	D	60	VAL	N-CA-CB	-6.00	98.29	111.50
1	C	19	ALA	O-C-N	-6.00	113.10	122.70
2	H	87	THR	OG1-CB-CG2	6.00	123.80	110.00
2	F	85	PHE	O-C-N	-6.00	113.10	122.70
1	G	112	HIS	CG-ND1-CE1	-6.00	97.90	105.70
2	H	72	SER	O-C-N	6.00	132.30	122.70
1	E	84	SER	CB-CA-C	6.00	121.49	110.10
1	A	24	TYR	CZ-CE2-CD2	-5.99	114.41	119.80
1	C	109	LEU	N-CA-C	-5.99	94.82	111.00
1	E	18	GLY	CA-C-O	5.99	131.39	120.60
2	H	143	HIS	CA-C-O	5.99	132.68	120.10
1	A	140	TYR	CB-CA-C	5.99	122.38	110.40
1	A	128	PHE	O-C-N	5.99	132.28	122.70
1	E	116	GLU	CB-CA-C	-5.99	98.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	15	TRP	N-CA-C	5.99	127.16	111.00
1	E	104	CYS	CA-C-N	-5.99	104.03	117.20
2	H	45	PHE	O-C-N	-5.98	113.03	123.20
1	A	58	HIS	CB-CG-CD2	-5.98	112.26	130.80
2	D	129	ALA	O-C-N	-5.98	113.13	122.70
2	D	129	ALA	N-CA-C	-5.98	94.85	111.00
1	E	106	LEU	O-C-N	-5.98	113.13	122.70
1	E	108	THR	CA-C-O	-5.98	107.54	120.10
2	F	12	THR	OG1-CB-CG2	5.98	123.76	110.00
2	F	38	THR	CA-CB-OG1	5.98	121.56	109.00
2	D	92	HIS	CA-C-O	5.98	132.65	120.10
1	E	45	HIS	CA-C-O	-5.98	107.55	120.10
1	E	82	ALA	C-N-CA	-5.98	106.76	121.70
1	G	112	HIS	O-C-N	5.98	132.26	122.70
1	A	42	TYR	CB-CG-CD1	5.98	124.59	121.00
2	D	117	HIS	ND1-CE1-NE2	-5.98	96.75	109.90
1	C	9	ASN	CB-CA-C	-5.97	98.45	110.40
1	C	72	HIS	CB-CG-CD2	-5.97	112.28	130.80
1	G	7	LYS	CA-CB-CG	5.97	126.54	113.40
1	G	30	GLU	CB-CA-C	5.97	122.35	110.40
2	D	34	VAL	CA-CB-CG2	-5.97	101.94	110.90
2	F	133	VAL	CA-C-N	-5.97	104.06	117.20
2	D	44	SER	C-N-CA	5.97	136.62	121.70
2	H	94	ASP	C-N-CA	5.97	136.62	121.70
2	D	3	LEU	CD1-CG-CD2	-5.97	92.60	110.50
2	H	121	GLU	CB-CG-CD	-5.97	98.09	114.20
2	F	39	GLN	C-N-CA	5.97	136.61	121.70
2	F	42	PHE	N-CA-CB	5.97	121.34	110.60
1	G	67	THR	CA-C-O	5.97	132.63	120.10
2	H	91	LEU	N-CA-CB	-5.96	98.47	110.40
1	A	16	LYS	CB-CG-CD	5.96	127.09	111.60
2	H	77	HIS	CB-CG-ND1	5.96	138.10	123.20
1	E	117	PHE	CG-CD2-CE2	-5.96	114.25	120.80
1	G	117	PHE	C-N-CA	5.96	136.59	121.70
1	C	85	ASP	CB-CG-OD1	-5.96	112.94	118.30
2	D	70	ALA	CA-C-O	-5.96	107.59	120.10
2	F	136	GLY	CA-C-O	-5.96	109.88	120.60
2	H	126	VAL	N-CA-C	-5.96	94.92	111.00
1	C	122	HIS	CA-CB-CG	5.96	123.72	113.60
1	C	16	LYS	O-C-N	5.95	132.22	122.70
2	H	47	ASP	N-CA-C	-5.95	94.93	111.00
2	F	68	LEU	CA-CB-CG	-5.95	101.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	102	ASN	C-N-CA	5.95	136.57	121.70
2	B	96	LEU	CD1-CG-CD2	5.95	128.34	110.50
2	F	60	VAL	N-CA-C	5.94	127.05	111.00
1	E	47	ASP	N-CA-CB	5.94	121.30	110.60
1	G	104	CYS	CA-C-O	-5.94	107.63	120.10
1	A	13	ALA	C-N-CA	-5.94	106.86	121.70
1	C	14	TRP	CD1-NE1-CE2	-5.94	103.66	109.00
1	E	101	LEU	CA-CB-CG	5.94	128.96	115.30
2	H	100	PRO	O-C-N	-5.94	113.20	122.70
1	C	96	VAL	CA-C-O	-5.93	107.64	120.10
1	C	36	PHE	N-CA-CB	-5.93	99.92	110.60
2	F	60	VAL	CA-CB-CG2	-5.93	102.00	110.90
2	H	82	LYS	CG-CD-CE	5.93	129.70	111.90
2	H	129	ALA	O-C-N	5.93	132.19	122.70
1	A	125	LEU	O-C-N	-5.93	113.22	122.70
2	F	121	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	G	52	SER	CA-C-N	-5.92	104.17	117.20
2	D	85	PHE	CD1-CE1-CZ	5.92	127.21	120.10
2	B	140	ALA	C-N-CA	-5.92	106.89	121.70
1	C	75	ASP	CA-C-N	-5.92	104.18	117.20
2	D	36	PRO	N-CD-CG	5.92	112.07	103.20
2	D	111	VAL	O-C-N	-5.92	113.24	122.70
1	G	47	ASP	O-C-N	5.92	132.16	122.70
1	E	122	HIS	O-C-N	5.91	132.16	122.70
2	H	69	GLY	CA-C-O	5.91	131.25	120.60
1	A	35	SER	N-CA-CB	-5.91	101.63	110.50
2	H	43	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	137	THR	CA-C-O	5.91	132.51	120.10
2	D	99	ASP	CB-CG-OD1	5.91	123.62	118.30
1	E	50	HIS	CA-CB-CG	-5.91	103.56	113.60
2	B	104	ARG	CG-CD-NE	5.91	124.20	111.80
1	C	14	TRP	CB-CG-CD2	-5.91	118.92	126.60
1	C	92	ARG	CG-CD-NE	-5.91	99.40	111.80
2	B	53	ALA	N-CA-C	-5.90	95.06	111.00
1	A	37	PRO	CA-C-N	5.90	130.18	117.20
2	D	19	ASN	OD1-CG-ND2	5.90	135.48	121.90
2	F	14	LEU	N-CA-CB	-5.90	98.60	110.40
2	B	48	LEU	C-N-CA	5.90	136.45	121.70
2	B	69	GLY	N-CA-C	-5.90	98.35	113.10
1	C	19	ALA	N-CA-C	5.90	126.93	111.00
1	C	54	GLN	CA-C-O	-5.90	107.71	120.10
2	D	130	TYR	CZ-CE2-CD2	-5.90	114.49	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	35	SER	C-N-CA	5.90	136.45	121.70
1	G	61	LYS	N-CA-CB	-5.90	99.98	110.60
1	C	77	PRO	CA-N-CD	-5.90	103.24	111.50
1	A	26	ALA	N-CA-CB	-5.89	101.85	110.10
2	B	84	THR	CB-CA-C	5.89	127.51	111.60
1	G	102	SER	CA-C-N	5.89	130.17	117.20
2	H	132	LYS	CA-C-N	-5.89	104.23	117.20
1	A	98	PHE	O-C-N	5.89	132.13	122.70
2	B	11	VAL	CA-CB-CG2	-5.89	102.06	110.90
1	A	2	LEU	CB-CA-C	5.89	121.39	110.20
2	B	31	LEU	CA-CB-CG	5.89	128.85	115.30
1	E	113	LEU	CB-CG-CD1	5.89	121.01	111.00
2	H	134	VAL	O-C-N	-5.89	113.28	122.70
1	G	141	ARG	N-CA-C	-5.89	95.11	111.00
2	H	111	VAL	CA-CB-CG2	5.89	119.73	110.90
2	H	126	VAL	CA-CB-CG2	-5.89	102.07	110.90
2	D	59	LYS	CB-CG-CD	5.88	126.90	111.60
1	G	27	GLU	CA-CB-CG	5.88	126.35	113.40
1	C	32	MET	N-CA-CB	5.88	121.19	110.60
1	E	25	GLY	CA-C-N	-5.88	104.26	117.20
1	G	20	HIS	CA-C-O	-5.88	107.75	120.10
2	H	83	GLY	CA-C-N	5.88	130.14	117.20
1	A	75	ASP	CA-C-O	-5.88	107.75	120.10
1	G	67	THR	CA-CB-OG1	-5.88	96.65	109.00
2	H	73	ASP	CB-CA-C	5.88	122.15	110.40
1	G	24	TYR	CD1-CG-CD2	5.87	124.36	117.90
2	F	44	SER	N-CA-C	-5.87	95.14	111.00
2	H	48	LEU	CB-CG-CD2	-5.87	101.02	111.00
2	B	145	TYR	CB-CA-C	5.87	122.14	110.40
1	G	40	LYS	CA-C-N	5.87	130.11	117.20
1	E	122	HIS	ND1-CG-CD2	-5.87	97.79	106.00
2	B	41	PHE	CB-CG-CD2	5.87	124.91	120.80
1	E	8	THR	N-CA-CB	5.87	121.45	110.30
1	C	46	PHE	CE1-CZ-CE2	5.86	130.56	120.00
1	E	50	HIS	C-N-CA	5.86	134.60	122.30
2	F	75	LEU	CB-CA-C	5.86	121.33	110.20
2	B	12	THR	CA-CB-CG2	5.86	120.60	112.40
2	B	65	LYS	C-N-CA	5.86	136.34	121.70
2	F	98	VAL	CA-C-O	5.86	132.40	120.10
1	C	1	VAL	O-C-N	5.86	132.07	122.70
2	F	34	VAL	CG1-CB-CG2	5.86	120.27	110.90
1	G	77	PRO	C-N-CA	-5.86	107.06	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	HIS	CA-C-N	-5.85	104.49	116.20
2	H	38	THR	CB-CA-C	-5.85	95.79	111.60
1	A	33	PHE	CB-CA-C	-5.85	98.70	110.40
1	G	56	LYS	CB-CA-C	5.85	122.09	110.40
2	D	77	HIS	CA-C-O	5.85	132.38	120.10
1	G	27	GLU	N-CA-CB	5.85	121.12	110.60
1	C	85	ASP	CA-C-O	5.84	132.36	120.10
2	F	129	ALA	N-CA-C	-5.84	95.24	111.00
2	H	66	LYS	CG-CD-CE	-5.84	94.38	111.90
1	A	14	TRP	CH2-CZ2-CE2	-5.83	111.56	117.40
2	H	105	LEU	CB-CG-CD1	5.83	120.92	111.00
1	C	140	TYR	N-CA-CB	5.83	121.10	110.60
1	C	125	LEU	N-CA-CB	-5.83	98.74	110.40
1	E	135	VAL	CG1-CB-CG2	5.83	120.22	110.90
1	G	96	VAL	CA-CB-CG2	-5.83	102.16	110.90
2	H	35	TYR	O-C-N	5.83	132.17	121.10
2	D	95	LYS	N-CA-CB	-5.83	100.11	110.60
2	F	21	ASP	O-C-N	5.83	132.02	122.70
2	F	53	ALA	N-CA-C	-5.83	95.27	111.00
1	G	122	HIS	CB-CA-C	5.83	122.05	110.40
1	A	68	ASN	CB-CG-ND2	-5.82	102.72	116.70
2	B	60	VAL	CA-C-N	-5.82	104.39	117.20
1	E	86	LEU	O-C-N	-5.82	113.38	122.70
1	A	31	ARG	O-C-N	5.82	132.01	122.70
1	G	48	LEU	CB-CG-CD2	5.82	120.89	111.00
1	G	129	LEU	N-CA-C	5.82	126.71	111.00
2	H	141	LEU	N-CA-CB	5.82	122.04	110.40
1	E	19	ALA	CA-C-N	5.82	130.00	117.20
2	F	85	PHE	CA-CB-CG	5.82	127.86	113.90
1	G	129	LEU	C-N-CA	-5.82	107.16	121.70
1	E	126	ASP	CB-CG-OD2	5.81	123.53	118.30
2	F	86	ALA	CB-CA-C	-5.81	101.38	110.10
1	G	141	ARG	CB-CA-C	5.81	122.03	110.40
1	E	106	LEU	CA-C-O	-5.81	107.90	120.10
1	G	129	LEU	N-CA-CB	-5.81	98.79	110.40
1	E	103	HIS	CA-C-O	-5.81	107.91	120.10
2	H	28	LEU	CB-CA-C	5.80	121.23	110.20
2	F	48	LEU	CB-CG-CD2	-5.80	101.14	111.00
2	F	19	ASN	CB-CG-OD1	-5.80	110.00	121.60
1	G	121	VAL	CB-CA-C	-5.80	100.38	111.40
1	A	88	ALA	C-N-CA	5.79	136.19	121.70
1	E	126	ASP	C-N-CA	5.79	136.18	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	PHE	CB-CA-C	-5.79	98.81	110.40
1	C	46	PHE	CB-CA-C	5.79	121.98	110.40
1	G	61	LYS	N-CA-C	-5.79	95.37	111.00
1	G	112	HIS	CB-CA-C	-5.79	98.83	110.40
2	B	132	LYS	CA-C-N	-5.79	104.47	117.20
2	B	79	ASP	CA-C-O	-5.78	107.95	120.10
1	G	87	HIS	CA-C-N	5.78	129.93	117.20
2	H	124	PRO	CA-C-O	-5.78	106.32	120.20
2	D	95	LYS	C-N-CA	-5.78	107.25	121.70
2	B	70	ALA	CA-C-O	5.78	132.24	120.10
2	H	23	VAL	C-N-CA	-5.78	110.16	122.30
1	E	68	ASN	CB-CG-OD1	-5.78	110.05	121.60
1	G	12	ALA	N-CA-CB	-5.78	102.01	110.10
2	D	2	HIS	N-CA-C	-5.78	95.41	111.00
1	G	80	LEU	CB-CA-C	5.78	121.17	110.20
2	H	25	GLY	C-N-CA	5.77	136.13	121.70
2	H	85	PHE	CB-CA-C	-5.77	98.86	110.40
1	C	132	VAL	N-CA-CB	5.77	124.20	111.50
2	F	41	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	G	24	TYR	CA-C-N	-5.77	104.66	116.20
2	B	93	CYS	C-N-CA	-5.77	107.28	121.70
1	G	14	TRP	CD2-CE2-CZ2	5.77	129.22	122.30
2	D	18	VAL	CA-C-O	-5.77	107.99	120.10
2	F	68	LEU	N-CA-C	5.76	126.57	111.00
2	F	25	GLY	C-N-CA	-5.76	107.29	121.70
2	F	113	VAL	C-N-CA	5.76	136.10	121.70
1	G	12	ALA	CA-C-O	5.76	132.19	120.10
1	A	109	LEU	CB-CA-C	5.76	121.14	110.20
2	D	57	ASN	CA-CB-CG	-5.76	100.73	113.40
2	B	19	ASN	CA-C-O	-5.75	108.01	120.10
1	A	33	PHE	C-N-CA	-5.75	107.32	121.70
1	A	84	SER	O-C-N	-5.75	113.49	122.70
2	F	7	GLU	C-N-CA	-5.75	107.32	121.70
1	E	75	ASP	C-N-CA	5.75	136.08	121.70
2	D	110	LEU	CA-CB-CG	-5.75	102.08	115.30
2	D	42	PHE	CG-CD2-CE2	-5.75	114.48	120.80
2	H	146	HIS	CB-CA-C	-5.75	98.91	110.40
2	B	26	GLU	N-CA-C	5.75	126.51	111.00
2	H	37	TRP	CE2-CD2-CE3	5.75	125.59	118.70
2	D	44	SER	CA-CB-OG	-5.74	95.69	111.20
1	E	9	ASN	O-C-N	5.74	131.89	122.70
1	C	59	GLY	C-N-CA	-5.74	107.35	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ASN	N-CA-CB	-5.74	100.27	110.60
2	F	117	HIS	N-CA-C	5.74	126.50	111.00
1	G	67	THR	N-CA-CB	-5.74	99.39	110.30
2	H	99	ASP	N-CA-CB	5.74	120.93	110.60
1	C	116	GLU	CA-C-O	-5.74	108.05	120.10
2	D	22	GLU	CA-C-O	-5.74	108.05	120.10
2	B	17	LYS	CD-CE-NZ	5.74	124.89	111.70
1	C	11	LYS	C-N-CA	5.74	136.04	121.70
1	C	88	ALA	N-CA-CB	-5.74	102.07	110.10
2	F	37	TRP	CB-CA-C	5.74	121.87	110.40
2	H	63	HIS	CG-ND1-CE1	5.73	116.23	108.20
2	H	60	VAL	CA-C-N	5.73	129.81	117.20
2	D	87	THR	CA-C-O	-5.73	108.07	120.10
1	E	48	LEU	N-CA-CB	5.73	121.86	110.40
2	F	127	GLN	N-CA-CB	-5.73	100.29	110.60
2	H	12	THR	C-N-CA	5.73	136.03	121.70
2	H	66	LYS	CD-CE-NZ	-5.73	98.53	111.70
1	C	50	HIS	CA-CB-CG	-5.73	103.87	113.60
2	D	52	ASP	CA-C-N	-5.73	104.60	117.20
2	D	1	VAL	CA-CB-CG1	-5.72	102.31	110.90
1	E	45	HIS	O-C-N	-5.72	113.54	122.70
1	G	127	LYS	CB-CA-C	-5.72	98.95	110.40
1	E	112	HIS	O-C-N	-5.72	113.55	122.70
2	F	68	LEU	CD1-CG-CD2	5.72	127.67	110.50
2	B	60	VAL	C-N-CA	-5.72	107.40	121.70
2	B	135	ALA	CA-C-O	-5.72	108.09	120.10
1	A	78	ASN	CA-C-N	-5.72	104.62	117.20
1	E	50	HIS	N-CA-CB	-5.72	100.31	110.60
1	C	102	SER	N-CA-C	5.71	126.43	111.00
1	E	55	VAL	N-CA-C	-5.71	95.57	111.00
1	G	90	LYS	CA-C-N	5.71	129.77	117.20
1	E	129	LEU	CB-CG-CD2	-5.71	101.29	111.00
2	B	113	VAL	CA-CB-CG2	-5.71	102.34	110.90
1	G	92	ARG	CB-CA-C	5.71	121.82	110.40
1	E	111	ALA	CB-CA-C	5.71	118.66	110.10
2	F	28	LEU	CA-CB-CG	-5.71	102.17	115.30
2	F	98	VAL	O-C-N	-5.71	113.57	122.70
1	A	125	LEU	C-N-CA	-5.70	107.44	121.70
1	G	128	PHE	CB-CA-C	-5.70	98.99	110.40
2	F	127	GLN	CA-C-O	5.70	132.07	120.10
1	A	4	PRO	CA-C-N	-5.70	104.66	117.20
1	A	36	PHE	CE1-CZ-CE2	5.70	130.26	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	ALA	O-C-N	-5.70	113.58	122.70
2	B	37	TRP	CD1-NE1-CE2	5.70	114.13	109.00
2	D	39	GLN	C-N-CA	5.70	135.94	121.70
1	E	45	HIS	CG-CD2-NE2	5.70	120.03	109.20
1	E	81	SER	CA-C-N	5.70	129.73	117.20
1	G	14	TRP	CA-C-O	5.70	132.06	120.10
1	C	140	TYR	CB-CG-CD2	5.69	124.42	121.00
2	D	92	HIS	C-N-CA	-5.69	107.47	121.70
1	C	43	PHE	CB-CA-C	-5.69	99.02	110.40
2	D	35	TYR	O-C-N	5.69	131.91	121.10
2	H	65	LYS	O-C-N	5.69	131.81	122.70
2	H	78	LEU	CB-CG-CD1	-5.69	101.33	111.00
2	B	137	VAL	N-CA-CB	5.69	124.02	111.50
1	E	128	PHE	CD1-CG-CD2	5.69	125.70	118.30
2	F	21	ASP	N-CA-CB	5.69	120.84	110.60
2	F	83	GLY	CA-C-O	-5.69	110.36	120.60
1	G	136	LEU	CD1-CG-CD2	5.69	127.57	110.50
2	D	121	GLU	OE1-CD-OE2	-5.69	116.48	123.30
2	H	44	SER	N-CA-C	-5.69	95.64	111.00
2	H	89	SER	CA-CB-OG	5.68	126.55	111.20
2	H	102	ASN	C-N-CA	-5.68	107.49	121.70
1	A	47	ASP	O-C-N	5.68	131.79	122.70
2	H	35	TYR	CD1-CE1-CZ	5.68	124.91	119.80
1	E	54	GLN	OE1-CD-NE2	5.68	134.96	121.90
1	G	68	ASN	N-CA-C	-5.68	95.66	111.00
1	E	91	LEU	CB-CA-C	5.68	120.99	110.20
1	A	17	VAL	CA-CB-CG2	-5.67	102.39	110.90
1	E	112	HIS	ND1-CG-CD2	-5.67	98.06	106.00
2	H	60	VAL	O-C-N	-5.67	113.62	122.70
1	A	128	PHE	CZ-CE2-CD2	5.67	126.91	120.10
2	H	48	LEU	CA-CB-CG	5.67	128.35	115.30
2	B	82	LYS	CA-C-O	5.67	132.01	120.10
1	C	56	LYS	CA-C-N	-5.67	104.86	116.20
1	E	135	VAL	CA-C-N	-5.67	104.73	117.20
2	F	67	VAL	CA-CB-CG1	5.67	119.40	110.90
1	G	64	ASP	N-CA-CB	5.67	120.80	110.60
2	D	14	LEU	C-N-CA	-5.67	107.53	121.70
1	C	115	ALA	CA-C-N	5.67	129.66	117.20
2	H	57	ASN	CA-CB-CG	5.66	125.86	113.40
1	A	79	ALA	CB-CA-C	5.66	118.59	110.10
2	B	127	GLN	N-CA-C	-5.66	95.71	111.00
1	E	36	PHE	CZ-CE2-CD2	5.66	126.89	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	50	HIS	CB-CA-C	-5.66	99.08	110.40
1	A	24	TYR	C-N-CA	-5.66	110.42	122.30
2	B	118	PHE	CG-CD2-CE2	5.66	127.02	120.80
2	F	49	SER	CB-CA-C	-5.66	99.35	110.10
1	C	69	ALA	CA-C-O	-5.66	108.22	120.10
1	E	77	PRO	C-N-CA	-5.65	107.58	121.70
2	F	71	PHE	CA-C-N	5.65	129.63	117.20
2	H	36	PRO	C-N-CA	5.65	135.83	121.70
2	B	141	LEU	CB-CA-C	5.65	120.93	110.20
1	G	28	ALA	CB-CA-C	-5.65	101.63	110.10
2	B	4	THR	CA-C-O	5.64	131.96	120.10
2	B	15	TRP	C-N-CA	-5.64	110.45	122.30
1	E	103	HIS	ND1-CE1-NE2	-5.64	97.49	109.90
1	A	94	ASP	CB-CA-C	-5.64	99.12	110.40
2	F	96	LEU	CB-CG-CD2	5.64	120.59	111.00
1	G	81	SER	CB-CA-C	-5.64	99.39	110.10
1	G	110	ALA	CA-C-O	-5.64	108.26	120.10
1	C	129	LEU	CB-CG-CD1	-5.64	101.42	111.00
2	D	146	HIS	CA-C-O	5.64	131.94	120.10
1	G	58	HIS	ND1-CG-CD2	-5.63	98.11	106.00
1	C	98	PHE	CZ-CE2-CD2	5.63	126.86	120.10
2	F	13	ALA	CA-C-N	5.63	129.59	117.20
1	G	42	TYR	N-CA-CB	5.63	120.74	110.60
2	D	41	PHE	CA-C-O	-5.63	108.27	120.10
1	G	87	HIS	O-C-N	5.63	131.71	122.70
2	B	59	LYS	CG-CD-CE	5.63	128.79	111.90
2	D	50	THR	N-CA-CB	5.63	120.99	110.30
1	G	62	VAL	CA-CB-CG2	5.62	119.34	110.90
1	G	132	VAL	CA-C-O	-5.62	108.29	120.10
2	H	31	LEU	CB-CA-C	5.62	120.88	110.20
1	A	120	ALA	CA-C-N	-5.62	104.84	117.20
2	H	22	GLU	CA-CB-CG	-5.62	101.04	113.40
2	H	22	GLU	CB-CA-C	5.62	121.64	110.40
2	H	63	HIS	N-CA-C	-5.62	95.83	111.00
2	D	73	ASP	O-C-N	5.61	132.74	123.20
1	A	91	LEU	N-CA-C	5.61	126.15	111.00
2	B	72	SER	C-N-CA	5.61	135.72	121.70
2	F	74	GLY	CA-C-N	-5.61	104.86	117.20
2	F	134	VAL	CA-C-O	-5.61	108.32	120.10
2	B	95	LYS	N-CA-C	5.61	126.14	111.00
2	D	111	VAL	CB-CA-C	5.61	122.06	111.40
2	F	15	TRP	CB-CG-CD2	5.61	133.89	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	PHE	CA-C-O	-5.61	108.33	120.10
2	D	40	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	H	42	PHE	N-CA-C	5.61	126.14	111.00
1	C	116	GLU	CG-CD-OE1	-5.60	107.09	118.30
2	H	22	GLU	C-N-CA	-5.60	107.69	121.70
1	G	64	ASP	C-N-CA	-5.60	107.70	121.70
2	H	53	ALA	N-CA-CB	5.60	117.94	110.10
1	C	119	PRO	N-CA-C	-5.60	97.55	112.10
2	D	76	ALA	N-CA-CB	5.60	117.94	110.10
1	E	7	LYS	CA-C-O	-5.60	108.34	120.10
2	H	30	ARG	CA-C-N	5.60	129.51	117.20
2	B	126	VAL	N-CA-CB	5.59	123.81	111.50
2	H	10	ALA	CB-CA-C	5.59	118.49	110.10
2	H	17	LYS	C-N-CA	5.59	135.69	121.70
2	B	26	GLU	CA-CB-CG	-5.59	101.10	113.40
1	C	59	GLY	CA-C-O	-5.59	110.54	120.60
2	F	43	GLU	OE1-CD-OE2	-5.59	116.59	123.30
2	H	82	LYS	O-C-N	5.59	132.71	123.20
2	H	130	TYR	C-N-CA	-5.59	107.72	121.70
2	H	122	PHE	CD1-CE1-CZ	-5.59	113.39	120.10
2	D	14	LEU	CA-C-N	-5.59	104.91	117.20
1	E	106	LEU	N-CA-C	-5.59	95.92	111.00
2	F	82	LYS	CG-CD-CE	-5.59	95.14	111.90
2	B	130	TYR	OH-CZ-CE2	5.58	135.18	120.10
2	B	26	GLU	C-N-CA	5.58	135.66	121.70
1	A	139	LYS	CA-CB-CG	-5.58	101.12	113.40
2	H	75	LEU	N-CA-CB	5.58	121.56	110.40
2	B	134	VAL	CG1-CB-CG2	-5.58	101.97	110.90
2	H	26	GLU	CA-CB-CG	5.58	125.67	113.40
2	H	87	THR	CB-CA-C	-5.58	96.54	111.60
2	F	106	LEU	CB-CG-CD1	5.58	120.48	111.00
1	E	75	ASP	CA-C-N	-5.58	104.94	117.20
2	F	61	LYS	CG-CD-CE	5.58	128.63	111.90
2	F	65	LYS	CD-CE-NZ	5.57	124.52	111.70
1	A	63	ALA	O-C-N	5.57	131.62	122.70
1	G	37	PRO	N-CD-CG	-5.57	94.84	103.20
1	A	89	HIS	CB-CA-C	-5.57	99.26	110.40
2	H	134	VAL	CA-C-N	5.57	129.45	117.20
2	F	40	ARG	N-CA-CB	-5.57	100.58	110.60
1	G	4	PRO	CA-C-N	5.57	129.45	117.20
2	B	65	LYS	CA-C-N	-5.56	104.96	117.20
2	F	26	GLU	C-N-CA	5.56	135.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	75	LEU	CA-CB-CG	-5.56	102.50	115.30
1	C	32	MET	CA-C-N	-5.56	104.96	117.20
2	D	1	VAL	C-N-CA	5.56	135.61	121.70
1	C	88	ALA	O-C-N	5.56	131.60	122.70
2	B	92	HIS	CB-CG-ND1	-5.56	109.30	123.20
2	F	38	THR	OG1-CB-CG2	-5.56	97.21	110.00
2	B	13	ALA	CB-CA-C	-5.56	101.76	110.10
1	E	30	GLU	CB-CG-CD	5.56	129.21	114.20
2	F	27	ALA	CB-CA-C	5.55	118.43	110.10
2	F	111	VAL	CA-CB-CG1	5.55	119.23	110.90
2	B	66	LYS	N-CA-C	-5.55	96.01	111.00
2	H	146	HIS	ND1-CE1-NE2	-5.55	97.69	109.90
2	F	10	ALA	N-CA-CB	5.55	117.87	110.10
1	G	81	SER	O-C-N	5.55	131.58	122.70
2	H	136	GLY	N-CA-C	-5.55	99.23	113.10
1	A	6	ASP	CA-C-N	-5.54	105.00	117.20
1	E	117	PHE	CG-CD1-CE1	5.54	126.90	120.80
2	B	105	LEU	N-CA-CB	5.54	121.48	110.40
1	E	128	PHE	CA-C-N	-5.54	105.01	117.20
1	A	125	LEU	CD1-CG-CD2	-5.54	93.89	110.50
1	G	109	LEU	CB-CA-C	-5.54	99.67	110.20
2	B	118	PHE	CA-CB-CG	-5.54	100.62	113.90
1	C	94	ASP	C-N-CA	5.54	145.25	122.00
2	F	92	HIS	N-CA-CB	-5.54	100.64	110.60
1	A	74	ASP	CB-CA-C	-5.53	99.33	110.40
1	A	48	LEU	N-CA-CB	-5.53	99.34	110.40
2	D	103	PHE	CA-C-N	5.52	129.35	117.20
1	A	52	SER	CA-CB-OG	-5.52	96.30	111.20
1	C	105	LEU	CB-CG-CD1	-5.52	101.62	111.00
2	D	88	LEU	N-CA-CB	-5.52	99.36	110.40
2	F	91	LEU	CB-CG-CD1	5.52	120.38	111.00
1	E	91	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	G	117	PHE	N-CA-C	5.51	125.88	111.00
2	D	16	GLY	CA-C-O	-5.51	110.68	120.60
1	C	84	SER	CA-CB-OG	-5.51	96.32	111.20
1	G	72	HIS	CA-C-O	-5.51	108.53	120.10
1	E	120	ALA	CA-C-N	-5.51	105.08	117.20
2	F	1	VAL	C-N-CA	5.51	135.47	121.70
2	B	53	ALA	O-C-N	-5.50	113.89	122.70
2	B	99	ASP	O-C-N	5.50	131.55	121.10
2	D	71	PHE	CB-CA-C	5.50	121.40	110.40
1	A	48	LEU	C-N-CA	5.50	135.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	LEU	N-CA-CB	-5.50	99.41	110.40
1	E	24	TYR	CB-CA-C	-5.50	99.41	110.40
2	B	75	LEU	CA-CB-CG	5.50	127.94	115.30
2	B	73	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	C	61	LYS	N-CA-CB	5.49	120.49	110.60
1	C	140	TYR	CD1-CE1-CZ	-5.49	114.86	119.80
2	F	72	SER	CB-CA-C	-5.49	99.66	110.10
1	G	99	LYS	CA-C-O	-5.49	108.56	120.10
1	G	141	ARG	NE-CZ-NH1	-5.49	117.55	120.30
2	D	51	PRO	CA-CB-CG	-5.49	93.56	104.00
2	D	69	GLY	O-C-N	5.49	131.49	122.70
1	E	79	ALA	C-N-CA	-5.49	107.97	121.70
2	B	110	LEU	CD1-CG-CD2	-5.49	94.03	110.50
1	G	14	TRP	N-CA-C	-5.49	96.18	111.00
1	A	106	LEU	CB-CG-CD2	5.49	120.33	111.00
2	D	132	LYS	CA-CB-CG	5.49	125.47	113.40
1	G	44	PRO	C-N-CA	5.49	135.42	121.70
1	C	42	TYR	OH-CZ-CE2	-5.49	105.29	120.10
2	F	55	MET	CA-C-N	5.49	127.17	116.20
1	G	124	SER	CA-CB-OG	-5.49	96.39	111.20
1	C	85	ASP	CB-CA-C	-5.48	99.43	110.40
1	C	37	PRO	CA-CB-CG	-5.48	93.59	104.00
2	H	113	VAL	N-CA-C	-5.48	96.21	111.00
2	F	78	LEU	CA-C-N	-5.48	105.15	117.20
2	B	92	HIS	CA-C-O	5.47	131.59	120.10
1	C	56	LYS	CA-CB-CG	-5.47	101.36	113.40
1	C	128	PHE	CA-C-N	5.47	129.24	117.20
1	A	131	SER	N-CA-CB	5.47	118.71	110.50
2	B	39	GLN	C-N-CA	5.47	135.37	121.70
2	B	75	LEU	CA-C-O	5.47	131.59	120.10
1	E	139	LYS	CG-CD-CE	-5.47	95.49	111.90
2	B	92	HIS	CB-CG-CD2	5.47	147.74	130.80
1	C	37	PRO	CA-C-O	-5.47	107.08	120.20
1	C	87	HIS	CB-CA-C	-5.47	99.47	110.40
2	B	91	LEU	CB-CG-CD2	5.46	120.29	111.00
2	D	91	LEU	CB-CG-CD1	5.46	120.29	111.00
2	D	136	GLY	CA-C-N	-5.46	105.18	117.20
1	E	86	LEU	CB-CG-CD1	5.46	120.29	111.00
1	C	54	GLN	CB-CA-C	-5.46	99.48	110.40
2	D	145	TYR	CD1-CE1-CZ	-5.46	114.89	119.80
1	G	128	PHE	CD1-CE1-CZ	-5.46	113.55	120.10
1	C	122	HIS	CA-C-O	5.46	131.56	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	74	ASP	C-N-CA	-5.46	108.06	121.70
1	G	135	VAL	CA-CB-CG1	5.46	119.08	110.90
2	H	61	LYS	N-CA-CB	-5.46	100.78	110.60
2	D	54	VAL	C-N-CA	5.45	135.33	121.70
2	F	109	VAL	CA-CB-CG1	-5.45	102.72	110.90
1	A	90	LYS	N-CA-CB	5.45	120.41	110.60
2	D	65	LYS	CD-CE-NZ	-5.45	99.16	111.70
1	E	14	TRP	CZ3-CH2-CZ2	-5.45	115.06	121.60
1	E	139	LYS	CA-C-N	-5.45	105.22	117.20
1	E	135	VAL	CA-CB-CG1	-5.45	102.73	110.90
1	G	137	THR	CA-CB-CG2	5.44	120.02	112.40
2	H	23	VAL	CA-C-O	-5.44	108.67	120.10
1	C	39	THR	C-N-CA	5.44	135.31	121.70
2	F	84	THR	OG1-CB-CG2	-5.44	97.48	110.00
2	F	137	VAL	N-CA-C	-5.44	96.31	111.00
1	G	17	VAL	CG1-CB-CG2	-5.44	102.20	110.90
1	A	87	HIS	N-CA-CB	-5.44	100.81	110.60
2	B	68	LEU	CB-CG-CD2	-5.44	101.76	111.00
2	H	35	TYR	CZ-CE2-CD2	5.44	124.69	119.80
2	B	2	HIS	CA-C-N	-5.44	105.24	117.20
1	G	99	LYS	C-N-CA	-5.43	108.12	121.70
1	E	83	LEU	CA-CB-CG	-5.43	102.81	115.30
1	A	83	LEU	CB-CG-CD2	-5.43	101.77	111.00
2	F	132	LYS	CB-CA-C	5.43	121.25	110.40
1	G	85	ASP	N-CA-C	-5.43	96.35	111.00
2	F	77	HIS	CG-CD2-NE2	-5.42	98.89	109.20
1	C	66	LEU	CB-CG-CD2	5.42	120.22	111.00
1	G	31	ARG	N-CA-CB	-5.42	100.84	110.60
2	D	68	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	E	107	VAL	CA-C-O	5.42	131.48	120.10
1	G	96	VAL	CA-C-N	-5.42	105.28	117.20
1	A	43	PHE	CB-CG-CD2	5.42	124.59	120.80
2	F	84	THR	N-CA-CB	5.42	120.59	110.30
2	F	93	CYS	CA-C-N	-5.42	105.28	117.20
1	A	8	THR	CB-CA-C	-5.41	96.99	111.60
1	A	100	LEU	CB-CA-C	5.41	120.48	110.20
2	B	37	TRP	CZ3-CH2-CZ2	-5.41	115.10	121.60
1	C	5	ALA	N-CA-CB	5.41	117.68	110.10
1	G	78	ASN	CB-CG-OD1	5.41	132.42	121.60
2	B	106	LEU	C-N-CA	-5.41	110.94	122.30
1	C	31	ARG	O-C-N	5.41	131.35	122.70
1	G	123	ALA	N-CA-C	-5.41	96.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	135	VAL	O-C-N	-5.41	114.05	122.70
2	H	66	LYS	CA-CB-CG	-5.41	101.50	113.40
1	E	123	ALA	CB-CA-C	-5.41	101.99	110.10
1	E	90	LYS	N-CA-CB	-5.41	100.87	110.60
2	B	100	PRO	C-N-CA	-5.40	108.19	121.70
1	E	3	SER	O-C-N	5.40	131.36	121.10
1	E	101	LEU	N-CA-CB	5.40	121.20	110.40
2	B	32	LEU	CA-C-N	-5.40	105.32	117.20
2	D	87	THR	N-CA-CB	5.40	120.56	110.30
1	A	20	HIS	CA-C-N	5.40	129.08	117.20
2	F	88	LEU	N-CA-CB	5.40	121.20	110.40
1	G	10	VAL	O-C-N	-5.40	114.06	122.70
1	A	101	LEU	CA-CB-CG	5.40	127.71	115.30
2	D	96	LEU	CB-CG-CD1	-5.40	101.83	111.00
2	B	65	LYS	O-C-N	-5.39	114.07	122.70
2	F	42	PHE	N-CA-C	5.39	125.56	111.00
1	G	101	LEU	C-N-CA	5.39	135.18	121.70
1	A	91	LEU	N-CA-CB	-5.39	99.62	110.40
1	C	42	TYR	CD1-CG-CD2	5.39	123.83	117.90
2	F	108	ASN	C-N-CA	5.39	135.17	121.70
2	D	85	PHE	CA-CB-CG	5.39	126.83	113.90
2	F	77	HIS	CE1-NE2-CD2	5.39	120.07	106.60
1	G	139	LYS	CA-C-O	5.39	131.41	120.10
1	A	66	LEU	CA-C-N	-5.38	105.35	117.20
1	E	96	VAL	CG1-CB-CG2	-5.38	102.29	110.90
2	H	125	PRO	C-N-CA	-5.38	108.24	121.70
2	D	42	PHE	CB-CA-C	-5.38	99.64	110.40
1	G	126	ASP	CA-C-N	5.38	129.04	117.20
2	F	43	GLU	C-N-CA	5.38	135.14	121.70
1	G	119	PRO	CA-N-CD	5.38	119.23	111.70
2	H	14	LEU	CD1-CG-CD2	-5.38	94.36	110.50
1	A	42	TYR	CB-CG-CD2	5.37	124.22	121.00
2	B	57	ASN	CA-CB-CG	5.37	125.22	113.40
2	B	110	LEU	CA-C-N	5.37	129.02	117.20
2	B	131	GLN	CB-CA-C	-5.37	99.66	110.40
2	F	12	THR	CA-CB-OG1	-5.37	97.72	109.00
1	A	85	ASP	O-C-N	-5.37	114.11	122.70
2	B	61	LYS	CB-CA-C	5.37	121.14	110.40
2	B	67	VAL	C-N-CA	-5.37	108.28	121.70
2	D	42	PHE	CA-C-N	-5.37	105.39	117.20
1	E	17	VAL	CA-CB-CG1	-5.37	102.85	110.90
1	A	119	PRO	CA-N-CD	5.37	119.21	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	LYS	CA-C-N	-5.37	105.39	117.20
1	G	59	GLY	N-CA-C	5.37	126.51	113.10
2	H	79	ASP	CA-C-N	5.37	129.00	117.20
2	B	41	PHE	CA-C-N	5.36	129.00	117.20
2	D	92	HIS	CG-CD2-NE2	5.36	119.39	109.20
2	H	26	GLU	C-N-CA	5.36	135.11	121.70
1	C	127	LYS	CB-CG-CD	5.36	125.54	111.60
2	H	132	LYS	CA-CB-CG	-5.36	101.60	113.40
2	B	97	HIS	CB-CA-C	5.36	121.12	110.40
2	H	90	GLU	N-CA-C	5.36	125.46	111.00
2	H	96	LEU	CB-CG-CD1	5.36	120.11	111.00
1	A	85	ASP	C-N-CA	5.35	135.09	121.70
2	D	61	LYS	CA-C-N	-5.35	105.42	117.20
2	F	141	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	20	HIS	C-N-CA	5.35	135.08	121.70
2	B	116	HIS	C-N-CA	-5.35	108.32	121.70
2	D	50	THR	CA-CB-OG1	5.35	120.24	109.00
1	E	23	GLU	CG-CD-OE1	5.35	129.00	118.30
2	F	117	HIS	N-CA-CB	-5.35	100.97	110.60
1	C	140	TYR	CE1-CZ-CE2	-5.35	111.24	119.80
2	F	20	VAL	CA-CB-CG2	-5.35	102.88	110.90
1	G	97	ASN	O-C-N	-5.35	114.14	122.70
2	F	2	HIS	CA-C-N	5.35	128.97	117.20
2	H	114	LEU	CB-CG-CD1	5.35	120.09	111.00
1	G	81	SER	C-N-CA	5.35	135.06	121.70
2	B	37	TRP	CE2-CD2-CE3	5.34	125.11	118.70
2	F	47	ASP	CA-C-N	5.34	128.95	117.20
2	H	120	LYS	CA-CB-CG	5.34	125.15	113.40
2	B	61	LYS	CB-CG-CD	5.34	125.48	111.60
1	C	41	THR	CA-C-N	-5.34	105.45	117.20
1	C	135	VAL	CA-CB-CG1	5.34	118.91	110.90
1	E	130	ALA	O-C-N	-5.34	114.16	122.70
2	H	34	VAL	N-CA-CB	-5.34	99.76	111.50
2	D	145	TYR	CB-CA-C	5.34	121.07	110.40
2	F	17	LYS	N-CA-C	5.34	125.41	111.00
1	G	47	ASP	N-CA-C	-5.34	96.59	111.00
2	H	61	LYS	CD-CE-NZ	-5.34	99.42	111.70
2	H	93	CYS	CA-C-O	5.33	131.30	120.10
2	B	132	LYS	N-CA-C	-5.33	96.60	111.00
2	H	130	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	A	60	LYS	CA-CB-CG	5.33	125.13	113.40
1	C	132	VAL	CA-CB-CG1	-5.33	102.90	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	VAL	CA-CB-CG1	-5.33	102.91	110.90
1	A	131	SER	CA-CB-OG	-5.33	96.81	111.20
2	D	85	PHE	CG-CD2-CE2	5.33	126.66	120.80
1	A	116	GLU	CG-CD-OE2	-5.33	107.65	118.30
1	A	1	VAL	O-C-N	5.32	131.22	122.70
2	B	48	LEU	CB-CG-CD1	5.32	120.05	111.00
2	D	106	LEU	CA-CB-CG	-5.32	103.06	115.30
2	D	114	LEU	C-N-CA	-5.32	108.39	121.70
1	E	11	LYS	CA-CB-CG	-5.32	101.69	113.40
1	E	66	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	E	125	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	A	17	VAL	CA-CB-CG1	-5.32	102.92	110.90
2	H	71	PHE	CB-CA-C	5.32	121.03	110.40
1	E	85	ASP	N-CA-CB	5.31	120.17	110.60
2	D	117	HIS	CE1-NE2-CD2	5.31	119.88	106.60
1	E	98	PHE	CA-C-N	-5.31	105.52	117.20
2	B	89	SER	N-CA-C	-5.31	96.67	111.00
2	F	15	TRP	CE2-CD2-CE3	5.31	125.07	118.70
1	G	122	HIS	CA-C-O	-5.31	108.95	120.10
1	C	12	ALA	CB-CA-C	-5.31	102.14	110.10
1	C	23	GLU	N-CA-C	-5.31	96.67	111.00
1	E	87	HIS	N-CA-CB	5.31	120.16	110.60
2	H	13	ALA	CA-C-N	5.31	128.88	117.20
1	C	68	ASN	CB-CA-C	-5.30	99.79	110.40
2	F	69	GLY	C-N-CA	-5.30	108.45	121.70
2	F	72	SER	N-CA-CB	5.30	118.45	110.50
2	B	54	VAL	CA-C-O	-5.30	108.97	120.10
2	B	117	HIS	CA-C-N	5.30	128.86	117.20
1	G	25	GLY	CA-C-O	5.30	130.14	120.60
1	A	40	LYS	CB-CG-CD	-5.30	97.83	111.60
1	C	8	THR	N-CA-CB	5.30	120.36	110.30
1	E	43	PHE	CD1-CG-CD2	-5.30	111.42	118.30
2	B	15	TRP	CB-CG-CD1	5.29	133.88	127.00
2	B	32	LEU	CB-CG-CD2	5.29	120.00	111.00
2	D	49	SER	CA-CB-OG	-5.29	96.91	111.20
1	E	139	LYS	N-CA-CB	-5.29	101.08	110.60
1	G	121	VAL	O-C-N	5.29	131.16	122.70
1	A	30	GLU	C-N-CA	5.29	134.93	121.70
2	H	37	TRP	O-C-N	-5.29	114.24	122.70
2	H	117	HIS	CB-CA-C	-5.29	99.83	110.40
1	E	23	GLU	CA-C-O	5.29	131.20	120.10
1	E	64	ASP	N-CA-CB	5.29	120.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	ASN	N-CA-CB	-5.29	101.09	110.60
2	B	59	LYS	N-CA-CB	5.28	120.11	110.60
2	B	120	LYS	C-N-CA	-5.28	108.50	121.70
1	C	2	LEU	C-N-CA	5.28	134.90	121.70
1	C	105	LEU	CA-C-O	5.28	131.18	120.10
1	E	3	SER	C-N-CD	5.28	139.48	128.40
1	E	56	LYS	CB-CG-CD	-5.28	97.89	111.60
2	F	42	PHE	CB-CA-C	-5.28	99.85	110.40
2	F	118	PHE	CB-CG-CD1	-5.27	117.11	120.80
2	H	136	GLY	CA-C-O	-5.27	111.11	120.60
1	E	26	ALA	CA-C-O	-5.27	109.03	120.10
1	E	89	HIS	CB-CG-ND1	-5.27	110.02	123.20
2	H	11	VAL	N-CA-CB	-5.27	99.90	111.50
1	A	36	PHE	CG-CD1-CE1	5.27	126.60	120.80
1	E	65	ALA	O-C-N	5.27	131.13	122.70
1	E	114	PRO	C-N-CA	5.27	134.88	121.70
2	H	30	ARG	O-C-N	5.27	131.13	122.70
2	B	8	LYS	N-CA-C	-5.27	96.77	111.00
2	F	7	GLU	CB-CG-CD	-5.27	99.97	114.20
1	A	35	SER	N-CA-C	5.27	125.22	111.00
2	D	40	ARG	N-CA-CB	-5.27	101.12	110.60
1	A	75	ASP	C-N-CA	5.27	134.87	121.70
2	D	91	LEU	CB-CG-CD2	-5.27	102.05	111.00
2	F	102	ASN	N-CA-CB	5.26	120.08	110.60
2	H	30	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	108	THR	CA-C-O	5.26	131.15	120.10
2	H	78	LEU	CA-C-O	5.26	131.14	120.10
2	D	85	PHE	CA-C-N	5.25	128.76	117.20
1	E	22	GLY	CA-C-N	-5.25	105.64	117.20
2	F	118	PHE	CG-CD1-CE1	5.25	126.58	120.80
1	A	45	HIS	CA-C-O	-5.25	109.07	120.10
2	F	14	LEU	CD1-CG-CD2	5.25	126.26	110.50
2	F	21	ASP	C-N-CA	-5.25	108.56	121.70
1	G	98	PHE	CG-CD2-CE2	-5.25	115.02	120.80
1	E	80	LEU	C-N-CA	5.25	134.83	121.70
2	B	15	TRP	CB-CG-CD2	-5.25	119.78	126.60
1	C	68	ASN	CB-CG-OD1	-5.25	111.10	121.60
1	A	139	LYS	C-N-CA	5.25	134.82	121.70
2	B	62	ALA	CA-C-O	5.25	131.12	120.10
1	A	6	ASP	CB-CA-C	5.25	120.89	110.40
2	F	116	HIS	O-C-N	-5.25	114.31	122.70
1	A	33	PHE	N-CA-CB	5.24	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	LYS	CD-CE-NZ	5.24	123.76	111.70
2	B	32	LEU	CD1-CG-CD2	-5.24	94.78	110.50
2	F	75	LEU	O-C-N	5.24	131.09	122.70
2	H	38	THR	C-N-CA	5.24	134.80	121.70
2	B	109	VAL	CB-CA-C	-5.24	101.45	111.40
1	C	105	LEU	CB-CA-C	5.24	120.15	110.20
2	H	88	LEU	C-N-CA	5.24	134.79	121.70
1	G	56	LYS	CD-CE-NZ	5.23	123.73	111.70
2	H	98	VAL	N-CA-CB	-5.23	99.99	111.50
1	A	105	LEU	CA-C-N	-5.23	105.69	117.20
1	C	20	HIS	O-C-N	5.23	131.07	122.70
2	H	54	VAL	CB-CA-C	5.23	121.34	111.40
1	A	118	THR	CA-C-O	5.23	131.08	120.10
2	H	92	HIS	N-CA-CB	5.23	120.01	110.60
1	C	20	HIS	CA-C-N	-5.23	105.70	117.20
1	C	103	HIS	ND1-CE1-NE2	5.23	121.40	109.90
1	G	109	LEU	CD1-CG-CD2	-5.23	94.82	110.50
2	D	116	HIS	CA-CB-CG	-5.22	104.72	113.60
1	G	60	LYS	CA-CB-CG	5.22	124.89	113.40
1	A	92	ARG	C-N-CA	-5.22	108.65	121.70
1	A	129	LEU	O-C-N	-5.22	114.35	122.70
2	B	117	HIS	CB-CG-ND1	5.22	136.25	123.20
2	F	1	VAL	CA-C-O	5.22	131.06	120.10
2	H	107	GLY	CA-C-O	-5.22	111.20	120.60
1	G	29	LEU	CA-C-O	5.22	131.06	120.10
1	G	126	ASP	OD1-CG-OD2	-5.22	113.39	123.30
2	H	98	VAL	C-N-CA	-5.22	108.66	121.70
2	B	134	VAL	N-CA-CB	-5.22	100.03	111.50
2	F	100	PRO	CB-CA-C	5.21	125.03	112.00
2	F	126	VAL	CA-C-O	-5.21	109.15	120.10
1	G	3	SER	N-CA-C	-5.21	96.92	111.00
2	D	85	PHE	N-CA-C	5.21	125.07	111.00
2	H	11	VAL	CA-C-O	-5.21	109.15	120.10
2	D	60	VAL	CG1-CB-CG2	5.21	119.24	110.90
2	D	141	LEU	CA-C-O	-5.21	109.16	120.10
2	B	61	LYS	CA-C-N	5.21	128.65	117.20
2	D	51	PRO	CA-N-CD	-5.21	104.21	111.50
2	H	42	PHE	CZ-CE2-CD2	-5.21	113.85	120.10
2	B	59	LYS	N-CA-C	-5.21	96.95	111.00
2	D	109	VAL	CA-CB-CG1	-5.21	103.09	110.90
2	D	23	VAL	CB-CA-C	-5.20	101.51	111.40
1	G	14	TRP	CG-CD1-NE1	-5.20	104.90	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	74	ASP	CA-C-N	-5.20	105.75	117.20
2	B	104	ARG	CA-C-N	5.20	128.65	117.20
1	E	114	PRO	O-C-N	-5.20	114.38	122.70
2	H	49	SER	CB-CA-C	-5.20	100.22	110.10
2	B	93	CYS	CA-C-N	5.20	128.64	117.20
1	E	13	ALA	CB-CA-C	5.20	117.90	110.10
1	E	42	TYR	CE1-CZ-OH	-5.20	106.07	120.10
1	C	99	LYS	CA-C-O	-5.20	109.19	120.10
2	H	19	ASN	CA-C-O	-5.20	109.19	120.10
2	F	29	GLY	CA-C-N	-5.19	105.77	117.20
2	H	43	GLU	C-N-CA	-5.19	108.72	121.70
1	G	83	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	G	86	LEU	C-N-CA	-5.19	108.72	121.70
2	H	30	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	D	87	THR	N-CA-C	-5.18	97.00	111.00
1	C	11	LYS	CB-CG-CD	-5.18	98.13	111.60
2	D	106	LEU	N-CA-CB	-5.18	100.03	110.40
1	C	14	TRP	CA-CB-CG	-5.18	103.86	113.70
1	G	68	ASN	CA-C-N	-5.18	105.80	117.20
2	H	37	TRP	C-N-CA	5.18	134.65	121.70
2	H	84	THR	C-N-CA	5.18	134.65	121.70
2	H	71	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	E	129	LEU	N-CA-CB	-5.18	100.04	110.40
1	G	28	ALA	N-CA-C	-5.18	97.02	111.00
2	B	87	THR	O-C-N	-5.18	114.42	122.70
2	B	106	LEU	N-CA-CB	-5.18	100.05	110.40
2	D	101	GLU	CB-CG-CD	5.18	128.17	114.20
2	F	82	LYS	C-N-CA	-5.17	111.44	122.30
2	F	114	LEU	CD1-CG-CD2	5.17	126.03	110.50
2	B	74	GLY	O-C-N	5.17	130.97	122.70
1	C	60	LYS	CA-C-O	5.17	130.96	120.10
2	B	122	PHE	CD1-CE1-CZ	5.17	126.30	120.10
2	F	33	VAL	N-CA-C	5.17	124.95	111.00
1	A	7	LYS	CB-CG-CD	5.16	125.02	111.60
1	A	126	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	C	115	ALA	O-C-N	-5.16	114.44	122.70
2	H	122	PHE	CE1-CZ-CE2	5.16	129.29	120.00
2	B	68	LEU	CA-C-O	-5.16	109.27	120.10
1	C	51	GLY	CA-C-N	5.16	128.55	117.20
2	F	92	HIS	ND1-CE1-NE2	-5.16	98.55	109.90
2	F	106	LEU	CB-CA-C	-5.16	100.40	110.20
1	G	90	LYS	CA-C-O	-5.16	109.27	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	HIS	C-N-CA	5.16	134.59	121.70
1	C	35	SER	N-CA-C	5.16	124.92	111.00
2	D	109	VAL	CB-CA-C	5.16	121.19	111.40
1	E	92	ARG	O-C-N	5.16	130.95	122.70
1	A	4	PRO	CA-CB-CG	-5.15	94.22	104.00
1	C	125	LEU	CA-C-N	5.15	128.53	117.20
1	G	45	HIS	N-CA-CB	5.15	119.87	110.60
2	B	36	PRO	CA-N-CD	-5.15	104.29	111.50
1	A	72	HIS	CB-CG-ND1	-5.15	110.33	123.20
2	B	137	VAL	CA-CB-CG1	-5.15	103.18	110.90
2	D	26	GLU	CA-C-O	-5.15	109.29	120.10
2	D	114	LEU	N-CA-C	-5.15	97.10	111.00
2	D	143	HIS	O-C-N	-5.14	114.47	122.70
1	E	78	ASN	N-CA-C	5.14	124.89	111.00
1	E	124	SER	CA-C-O	-5.14	109.30	120.10
2	H	15	TRP	O-C-N	-5.14	114.46	123.20
2	B	91	LEU	N-CA-CB	-5.14	100.12	110.40
1	E	34	LEU	CB-CA-C	5.14	119.97	110.20
1	E	74	ASP	OD1-CG-OD2	-5.14	113.53	123.30
1	G	16	LYS	CD-CE-NZ	-5.14	99.88	111.70
2	D	36	PRO	N-CA-C	5.14	125.46	112.10
2	F	124	PRO	O-C-N	-5.14	111.34	121.10
2	H	131	GLN	CA-C-O	-5.14	109.31	120.10
1	A	117	PHE	CB-CA-C	5.14	120.67	110.40
1	A	10	VAL	N-CA-CB	-5.13	100.20	111.50
1	A	36	PHE	CD1-CG-CD2	-5.13	111.63	118.30
2	D	109	VAL	CG1-CB-CG2	5.13	119.11	110.90
2	F	20	VAL	CB-CA-C	-5.13	101.64	111.40
1	G	105	LEU	CB-CG-CD1	5.13	119.73	111.00
2	F	19	ASN	N-CA-C	-5.13	97.14	111.00
1	C	50	HIS	CG-ND1-CE1	5.13	115.38	108.20
1	A	53	ALA	O-C-N	5.13	130.91	122.70
2	H	72	SER	CA-CB-OG	-5.13	97.35	111.20
2	B	42	PHE	N-CA-CB	-5.13	101.37	110.60
2	B	121	GLU	CB-CA-C	-5.13	100.14	110.40
2	F	55	MET	CA-CB-CG	-5.13	104.58	113.30
1	A	33	PHE	CA-CB-CG	-5.13	101.59	113.90
2	H	99	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	3	SER	CA-C-O	-5.12	109.34	120.10
1	A	49	SER	O-C-N	5.12	130.89	122.70
1	C	136	LEU	CB-CA-C	5.12	119.93	110.20
1	E	77	PRO	CB-CA-C	-5.12	99.20	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	G	35	SER	N-CA-C	5.12	124.82	111.00
1	A	2	LEU	O-C-N	5.12	130.88	122.70
2	F	7	GLU	OE1-CD-OE2	-5.12	117.16	123.30
2	H	132	LYS	CD-CE-NZ	-5.12	99.93	111.70
2	D	42	PHE	O-C-N	5.11	130.88	122.70
2	B	84	THR	CA-CB-OG1	-5.11	98.27	109.00
1	E	126	ASP	CA-C-O	-5.11	109.37	120.10
2	F	8	LYS	N-CA-C	-5.11	97.21	111.00
1	A	84	SER	CA-C-N	5.11	128.43	117.20
1	A	69	ALA	O-C-N	5.10	130.87	122.70
2	D	77	HIS	CB-CG-CD2	-5.10	114.98	130.80
2	D	81	LEU	O-C-N	-5.10	114.53	122.70
1	A	119	PRO	CA-C-O	5.10	132.45	120.20
2	H	131	GLN	O-C-N	-5.10	114.54	122.70
2	B	79	ASP	CA-C-N	5.10	128.42	117.20
2	F	87	THR	O-C-N	5.10	130.85	122.70
1	C	114	PRO	N-CA-C	5.10	125.35	112.10
2	F	96	LEU	CA-C-O	-5.10	109.40	120.10
2	H	81	LEU	CA-C-N	5.09	128.41	117.20
2	B	143	HIS	CB-CG-CD2	-5.09	115.01	130.80
1	E	11	LYS	CA-C-N	-5.09	106.00	117.20
1	C	29	LEU	CA-C-N	-5.09	106.00	117.20
2	D	121	GLU	C-N-CA	-5.09	108.97	121.70
1	G	33	PHE	CB-CG-CD2	5.09	124.36	120.80
2	B	95	LYS	O-C-N	5.09	130.84	122.70
2	D	1	VAL	N-CA-CB	5.09	122.70	111.50
2	F	120	LYS	CB-CA-C	5.09	120.58	110.40
1	G	62	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	A	141	ARG	CG-CD-NE	-5.09	101.11	111.80
2	F	69	GLY	N-CA-C	-5.09	100.38	113.10
2	F	88	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	A	94	ASP	O-C-N	5.09	130.77	121.10
2	D	98	VAL	CA-C-N	-5.09	106.01	117.20
1	E	75	ASP	OD1-CG-OD2	5.09	132.97	123.30
2	H	91	LEU	CA-C-N	-5.09	106.01	117.20
2	F	100	PRO	N-CD-CG	-5.08	95.57	103.20
1	A	9	ASN	C-N-CA	5.08	134.41	121.70
1	A	48	LEU	CA-C-N	-5.08	106.02	117.20
2	H	26	GLU	CB-CA-C	-5.08	100.23	110.40
1	A	39	THR	N-CA-CB	5.08	119.95	110.30
1	C	33	PHE	N-CA-CB	5.08	119.75	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	PHE	CB-CA-C	5.08	120.56	110.40
1	C	88	ALA	C-N-CA	-5.08	109.01	121.70
2	D	49	SER	N-CA-C	5.08	124.71	111.00
2	D	138	ALA	CA-C-N	-5.08	106.03	117.20
2	F	10	ALA	CB-CA-C	-5.08	102.48	110.10
1	C	95	PRO	CA-N-CD	-5.08	104.39	111.50
1	G	29	LEU	CB-CG-CD1	-5.08	102.37	111.00
2	B	75	LEU	CB-CG-CD1	5.08	119.63	111.00
1	G	104	CYS	O-C-N	5.08	130.82	122.70
1	G	46	PHE	CD1-CE1-CZ	-5.07	114.01	120.10
1	G	72	HIS	CB-CG-CD2	-5.07	115.07	130.80
1	G	117	PHE	CA-C-O	5.07	130.75	120.10
2	B	14	LEU	N-CA-CB	5.07	120.54	110.40
1	A	54	GLN	N-CA-CB	5.07	119.73	110.60
1	G	103	HIS	CB-CG-ND1	5.07	135.88	123.20
1	A	78	ASN	CB-CA-C	5.07	120.54	110.40
2	F	127	GLN	C-N-CA	-5.07	109.03	121.70
1	C	85	ASP	O-C-N	-5.07	114.59	122.70
2	F	146	HIS	CB-CG-ND1	-5.07	110.53	123.20
2	H	58	PRO	C-N-CA	5.07	134.37	121.70
2	B	45	PHE	CB-CA-C	5.06	120.53	110.40
1	C	30	GLU	C-N-CA	5.06	134.35	121.70
2	F	101	GLU	C-N-CA	5.06	134.36	121.70
2	H	89	SER	CB-CA-C	-5.06	100.48	110.10
1	C	46	PHE	CG-CD2-CE2	5.06	126.36	120.80
1	G	17	VAL	CA-C-N	-5.06	106.08	116.20
2	B	88	LEU	CA-CB-CG	-5.06	103.67	115.30
1	E	108	THR	CA-CB-CG2	-5.06	105.32	112.40
2	D	91	LEU	CA-CB-CG	-5.06	103.67	115.30
1	E	96	VAL	CA-C-O	-5.05	109.48	120.10
2	F	128	ALA	CA-C-O	-5.05	109.49	120.10
1	A	62	VAL	CG1-CB-CG2	-5.05	102.82	110.90
2	B	130	TYR	CB-CA-C	-5.05	100.30	110.40
1	E	14	TRP	CE2-CD2-CE3	-5.05	112.64	118.70
1	C	79	ALA	O-C-N	5.05	130.78	122.70
2	B	77	HIS	CA-C-N	-5.05	106.10	117.20
1	G	139	LYS	CA-CB-CG	5.04	124.50	113.40
1	A	79	ALA	CA-C-O	5.04	130.69	120.10
1	G	113	LEU	C-N-CA	5.04	143.18	122.00
2	D	21	ASP	OD1-CG-OD2	5.04	132.88	123.30
1	G	7	LYS	CB-CA-C	-5.04	100.32	110.40
1	E	67	THR	O-C-N	-5.04	114.64	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	27	ALA	CA-C-N	-5.03	106.13	117.20
1	E	101	LEU	CD1-CG-CD2	5.03	125.60	110.50
1	C	7	LYS	CG-CD-CE	5.03	126.99	111.90
1	E	37	PRO	CA-C-O	5.03	132.27	120.20
1	E	42	TYR	CA-C-O	-5.03	109.54	120.10
1	E	113	LEU	N-CA-C	-5.03	97.43	111.00
1	C	129	LEU	CA-C-O	-5.03	109.55	120.10
1	E	82	ALA	N-CA-CB	5.03	117.14	110.10
1	G	133	SER	N-CA-CB	5.03	118.04	110.50
1	A	100	LEU	CB-CG-CD2	-5.02	102.46	111.00
2	B	31	LEU	CB-CG-CD1	5.02	119.54	111.00
2	D	3	LEU	N-CA-C	-5.02	97.44	111.00
2	F	139	ASN	C-N-CA	5.02	134.26	121.70
1	A	36	PHE	CD1-CE1-CZ	-5.02	114.08	120.10
1	A	85	ASP	OD1-CG-OD2	-5.02	113.77	123.30
2	B	47	ASP	O-C-N	-5.02	114.67	122.70
1	E	42	TYR	CZ-CE2-CD2	5.02	124.32	119.80
2	H	79	ASP	N-CA-C	-5.02	97.45	111.00
2	B	93	CYS	CA-CB-SG	-5.02	104.97	114.00
2	B	122	PHE	C-N-CA	-5.02	109.16	121.70
2	B	132	LYS	C-N-CA	-5.02	109.16	121.70
2	D	42	PHE	N-CA-CB	5.02	119.63	110.60
1	C	5	ALA	CA-C-N	-5.01	106.17	117.20
2	D	31	LEU	CB-CA-C	-5.01	100.67	110.20
2	B	116	HIS	CA-C-N	5.01	128.23	117.20
2	H	49	SER	CA-C-O	5.01	130.62	120.10
1	G	22	GLY	N-CA-C	-5.01	100.57	113.10
2	B	12	THR	C-N-CA	5.01	134.22	121.70
1	E	3	SER	CB-CA-C	5.01	119.61	110.10
2	F	139	ASN	CB-CG-OD1	5.01	131.62	121.60
1	G	103	HIS	O-C-N	5.01	130.71	122.70
2	D	40	ARG	CA-CB-CG	5.01	124.41	113.40
1	G	50	HIS	N-CA-CB	5.01	119.61	110.60
1	A	123	ALA	C-N-CA	5.00	134.21	121.70
1	E	42	TYR	CG-CD1-CE1	5.00	125.30	121.30
2	B	112	CYS	N-CA-C	-5.00	97.49	111.00
2	D	55	MET	CA-CB-CG	5.00	121.81	113.30
2	D	130	TYR	CB-CA-C	-5.00	100.39	110.40
2	D	142	ALA	N-CA-C	5.00	124.51	111.00
2	F	5	PRO	N-CA-CB	-5.00	97.10	102.60
2	F	136	GLY	C-N-CA	5.00	134.20	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	20	HIS	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	141	ARG	Sidechain
2	F	23	VAL	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1048	329	0
1	C	1069	0	1035	398	3
1	E	1069	0	1048	334	0
1	G	1069	0	1044	405	0
2	B	1121	0	1100	378	0
2	D	1121	0	1091	467	3
2	F	1121	0	1094	354	3
2	H	1121	0	1091	438	0
3	A	43	0	30	23	0
3	B	43	0	30	14	0
3	C	43	0	30	15	0
3	D	43	0	30	25	0
3	E	43	0	30	24	0
3	F	43	0	30	16	1
3	G	43	0	30	21	0
3	H	43	0	30	7	0
All	All	9104	0	8791	3010	5

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 168.

All (3010) 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:76:MET:CA	1:A:76:MET:CB	1.76	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ARG:CG	2:D:104:ARG:CB	1.74	1.64
2:F:29:GLY:HA3	2:F:55:MET:SD	1.32	1.64
2:H:14:LEU:CG	2:H:14:LEU:CD2	1.76	1.63
1:G:32:MET:CA	1:G:32:MET:CB	1.75	1.62
2:B:3:LEU:CG	2:B:3:LEU:CD2	1.77	1.62
1:G:107:VAL:HG13	2:H:112:CYS:SG	1.36	1.62
2:H:137:VAL:CG2	2:H:137:VAL:CB	1.77	1.62
1:E:43:PHE:CZ	3:E:142:HEM:HBC2	1.28	1.61
1:A:61:LYS:CB	1:A:61:LYS:CG	1.78	1.61
2:B:30:ARG:CG	2:B:30:ARG:CB	1.75	1.61
1:G:101:LEU:CG	1:G:101:LEU:CD1	1.78	1.61
2:D:14:LEU:CD1	2:D:14:LEU:CG	1.76	1.61
2:D:49:SER:CB	2:D:49:SER:CA	1.77	1.61
2:B:18:VAL:CG1	2:B:18:VAL:CB	1.78	1.60
1:G:61:LYS:CG	1:G:61:LYS:CD	1.76	1.60
2:B:98:VAL:CG2	2:B:98:VAL:CB	1.78	1.60
1:G:112:HIS:CA	1:G:112:HIS:CB	1.79	1.60
1:C:38:THR:CB	1:C:38:THR:CA	1.75	1.60
2:H:123:THR:CG2	2:H:123:THR:CB	1.75	1.59
2:D:141:LEU:CG	2:D:141:LEU:CD1	1.77	1.59
2:B:17:LYS:CG	2:B:17:LYS:CD	1.75	1.59
1:C:64:ASP:CB	1:C:64:ASP:CA	1.76	1.58
1:C:132:VAL:CB	1:C:132:VAL:CG1	1.80	1.58
1:C:40:LYS:CG	1:C:40:LYS:CD	1.81	1.58
1:E:106:LEU:CG	1:E:106:LEU:CD1	1.77	1.58
2:H:127:GLN:CG	2:H:127:GLN:CB	1.80	1.58
2:F:8:LYS:CB	2:F:8:LYS:CG	1.80	1.58
2:B:8:LYS:CB	2:B:8:LYS:CG	1.75	1.58
2:F:40:ARG:CD	2:F:40:ARG:CG	1.79	1.57
2:F:110:LEU:CA	2:F:110:LEU:CB	1.81	1.57
2:F:82:LYS:CE	2:F:82:LYS:CD	1.81	1.57
1:E:11:LYS:CB	1:E:11:LYS:CA	1.75	1.57
1:C:118:THR:CA	1:C:118:THR:N	1.68	1.56
1:C:91:LEU:CD2	1:C:91:LEU:CG	1.77	1.56
2:H:22:GLU:CB	2:H:22:GLU:CG	1.78	1.56
1:A:41:THR:N	1:A:41:THR:CA	1.67	1.56
1:G:109:LEU:CD1	1:G:109:LEU:CG	1.80	1.56
1:C:78:ASN:CA	1:C:78:ASN:N	1.69	1.56
1:E:20:HIS:CA	1:E:20:HIS:N	1.67	1.55
2:D:142:ALA:CB	2:D:142:ALA:CA	1.75	1.55
1:G:47:ASP:CA	1:G:47:ASP:C	1.74	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LEU:CD1	1:G:132:VAL:HG11	1.35	1.55
1:A:61:LYS:CE	1:A:61:LYS:CD	1.79	1.54
1:A:121:VAL:N	1:A:121:VAL:CA	1.68	1.54
1:G:117:PHE:CB	1:G:117:PHE:CA	1.78	1.54
2:H:91:LEU:CD1	2:H:91:LEU:CG	1.76	1.54
2:F:48:LEU:CB	2:F:48:LEU:CG	1.74	1.54
3:A:142:HEM:CAD	3:A:142:HEM:CBD	1.80	1.54
2:F:39:GLN:CG	2:F:39:GLN:CD	1.76	1.53
2:H:103:PHE:N	2:H:103:PHE:CA	1.67	1.53
2:F:40:ARG:CD	2:F:40:ARG:NE	1.67	1.53
2:D:77:HIS:CA	2:D:77:HIS:CB	1.79	1.53
2:F:95:LYS:CE	2:F:95:LYS:NZ	1.68	1.53
1:C:16:LYS:CD	1:C:16:LYS:CG	1.82	1.52
2:B:38:THR:CA	2:B:38:THR:N	1.68	1.52
1:C:141:ARG:CD	1:C:141:ARG:NE	1.72	1.52
2:H:30:ARG:CD	2:H:30:ARG:NE	1.73	1.52
2:H:99:ASP:N	2:H:99:ASP:CA	1.72	1.51
2:H:61:LYS:NZ	2:H:61:LYS:CE	1.72	1.51
1:G:60:LYS:CE	1:G:60:LYS:NZ	1.68	1.51
1:C:13:ALA:CA	1:C:13:ALA:N	1.68	1.51
2:D:65:LYS:CE	2:D:65:LYS:NZ	1.72	1.51
2:H:68:LEU:CA	2:H:68:LEU:N	1.68	1.51
2:F:90:GLU:CG	2:F:90:GLU:CD	1.75	1.50
1:A:37:PRO:CA	1:A:37:PRO:CB	1.77	1.50
1:E:69:ALA:N	1:E:69:ALA:CA	1.68	1.50
1:E:99:LYS:CE	1:E:99:LYS:NZ	1.71	1.50
2:F:17:LYS:CE	2:F:17:LYS:NZ	1.70	1.50
2:D:125:PRO:CA	2:D:125:PRO:CB	1.74	1.49
1:A:61:LYS:CE	1:A:61:LYS:NZ	1.71	1.49
1:G:67:THR:N	1:G:67:THR:CA	1.72	1.48
2:D:14:LEU:HD21	2:D:126:VAL:CG1	1.45	1.47
1:A:77:PRO:CG	1:A:77:PRO:CB	1.75	1.45
1:A:60:LYS:NZ	1:A:60:LYS:CE	1.79	1.45
2:D:4:THR:CB	2:D:4:THR:OG1	1.65	1.45
1:G:30:GLU:HG3	1:G:50:HIS:NE2	1.23	1.45
1:E:137:THR:CB	1:E:137:THR:OG1	1.66	1.44
2:H:21:ASP:CG	2:H:65:LYS:HG3	1.38	1.44
2:H:4:THR:CB	2:H:7:GLU:HB2	1.45	1.43
2:H:84:THR:OG1	2:H:84:THR:CB	1.64	1.43
1:G:118:THR:CG2	1:G:120:ALA:HB3	1.47	1.43
2:D:80:ASN:ND2	2:D:83:GLY:CA	1.82	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:SER:CB	1:C:3:SER:OG	1.66	1.42
1:E:35:SER:OG	1:E:35:SER:CB	1.66	1.42
2:D:14:LEU:CD2	2:D:126:VAL:HG11	1.48	1.42
2:H:100:PRO:CG	2:H:100:PRO:CD	1.76	1.41
2:B:95:LYS:CE	2:B:95:LYS:NZ	1.79	1.41
2:B:12:THR:OG1	2:B:12:THR:CB	1.68	1.41
2:B:38:THR:OG1	2:B:38:THR:CB	1.67	1.41
1:G:81:SER:OG	1:G:81:SER:CB	1.67	1.41
1:E:43:PHE:CZ	3:E:142:HEM:CBC	2.03	1.40
1:G:87:HIS:CA	1:G:91:LEU:HD12	1.50	1.39
2:D:3:LEU:CD2	2:D:132:LYS:HB3	1.53	1.38
1:C:64:ASP:OD1	1:C:64:ASP:CA	1.68	1.37
2:H:4:THR:HB	2:H:7:GLU:CB	1.52	1.37
1:C:118:THR:HG22	1:C:121:VAL:N	1.37	1.36
1:A:87:HIS:CG	1:A:136:LEU:HD11	1.60	1.36
2:F:4:THR:HB	2:F:7:GLU:CG	1.52	1.36
2:F:2:HIS:ND1	2:F:132:LYS:NZ	1.73	1.34
1:C:39:THR:OG1	1:C:39:THR:CB	1.73	1.34
2:D:107:GLY:CA	2:D:134:VAL:HG21	1.58	1.34
2:B:38:THR:C	2:B:38:THR:O	1.65	1.33
2:D:32:LEU:HD21	2:D:42:PHE:CE1	1.61	1.33
1:G:66:LEU:HD11	1:G:132:VAL:CG2	1.59	1.32
3:B:147:HEM:CMC	3:B:147:HEM:HBC2	1.43	1.32
1:G:14:TRP:NE1	1:G:67:THR:OG1	1.56	1.32
2:B:45:PHE:CE1	2:B:60:VAL:HG23	1.63	1.32
1:G:95:PRO:HA	1:G:98:PHE:CD2	1.64	1.32
2:H:117:HIS:HD2	2:H:118:PHE:CD1	1.45	1.32
2:F:39:GLN:NE2	2:F:39:GLN:HB3	1.44	1.31
2:B:7:GLU:O	2:B:11:VAL:HG23	1.22	1.31
2:H:26:GLU:O	2:H:30:ARG:HG3	1.20	1.30
2:D:80:ASN:ND2	2:D:83:GLY:HA3	0.99	1.30
2:F:39:GLN:HE21	2:F:39:GLN:CB	1.43	1.29
1:G:87:HIS:HA	1:G:91:LEU:CD1	1.61	1.29
2:F:1:VAL:CG1	2:F:132:LYS:HE2	1.62	1.28
2:F:29:GLY:HA3	2:F:55:MET:CE	1.62	1.28
2:H:20:VAL:CG1	2:H:65:LYS:HB2	1.63	1.28
2:B:50:THR:O	2:B:54:VAL:HG23	1.30	1.27
2:H:117:HIS:HD2	2:H:118:PHE:CE1	1.50	1.27
2:F:28:LEU:O	2:F:32:LEU:HB2	1.34	1.26
1:A:118:THR:OG1	1:A:121:VAL:HG21	1.26	1.26
1:E:106:LEU:CB	1:E:106:LEU:CD1	2.14	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:HIS:N	2:D:77:HIS:CB	1.99	1.26
1:G:79:ALA:O	1:G:82:ALA:HB3	1.30	1.25
2:H:20:VAL:O	2:H:24:GLY:N	1.66	1.25
1:G:107:VAL:CG1	2:H:112:CYS:SG	2.23	1.25
1:C:66:LEU:HD21	1:C:129:LEU:CD2	1.65	1.25
2:F:25:GLY:O	2:F:55:MET:HE3	1.33	1.24
2:F:29:GLY:CA	2:F:55:MET:SD	2.23	1.24
2:D:101:GLU:HA	2:D:104:ARG:NH1	1.50	1.23
2:D:101:GLU:CA	2:D:104:ARG:HH11	1.50	1.23
2:H:3:LEU:CD2	2:H:8:LYS:HE2	1.69	1.23
2:F:80:ASN:HD21	2:F:83:GLY:N	1.38	1.22
1:A:29:LEU:CD2	1:A:101:LEU:HD12	1.67	1.22
1:G:30:GLU:CD	1:G:50:HIS:CD2	2.14	1.21
3:D:147:HEM:CMB	3:D:147:HEM:HBB2	1.56	1.20
2:H:117:HIS:CD2	2:H:118:PHE:CD1	2.29	1.20
1:E:6:ASP:HB3	1:E:124:SER:OG	1.37	1.20
1:G:4:PRO:HG2	1:G:5:ALA:N	1.54	1.20
2:B:98:VAL:CG2	2:B:98:VAL:N	2.03	1.20
1:A:139:LYS:O	1:A:141:ARG:HG3	1.38	1.19
1:C:6:ASP:OD2	1:C:127:LYS:HE2	1.39	1.19
1:C:141:ARG:NE	1:C:141:ARG:CG	2.05	1.19
2:H:31:LEU:CD2	2:H:106:LEU:HB2	1.72	1.19
1:C:107:VAL:O	1:C:110:ALA:HB3	1.40	1.18
2:F:1:VAL:HG12	2:F:132:LYS:CE	1.72	1.18
1:G:114:PRO:HG2	1:G:115:ALA:H	1.06	1.18
2:D:3:LEU:HD22	2:D:132:LYS:HB3	1.19	1.18
2:H:137:VAL:O	2:H:141:LEU:HD23	1.02	1.18
3:B:147:HEM:CMC	3:B:147:HEM:CBC	2.20	1.18
1:G:30:GLU:CG	1:G:50:HIS:NE2	2.06	1.18
2:D:104:ARG:HG2	2:D:104:ARG:N	1.59	1.18
1:E:1:VAL:HG12	1:E:2:LEU:N	1.57	1.17
1:G:84:SER:CA	1:G:136:LEU:HD23	1.75	1.17
2:D:101:GLU:CA	2:D:104:ARG:HD2	1.74	1.17
2:D:107:GLY:HA3	2:D:134:VAL:CG2	1.73	1.17
1:E:102:SER:HB3	1:E:129:LEU:CD2	1.72	1.17
3:B:147:HEM:HMC3	3:B:147:HEM:HBC2	1.21	1.17
2:F:20:VAL:O	2:F:68:LEU:CD1	1.93	1.17
1:G:66:LEU:CD1	1:G:132:VAL:CG1	2.22	1.17
3:A:142:HEM:O2D	3:A:142:HEM:CAD	1.92	1.16
1:A:53:ALA:HA	1:A:56:LYS:HD3	1.24	1.16
2:B:51:PRO:O	2:B:55:MET:HG2	1.02	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:LEU:HD12	2:D:95:LYS:HB2	1.21	1.16
2:H:51:PRO:O	2:H:55:MET:HG2	1.44	1.16
2:D:104:ARG:HG2	2:D:104:ARG:H	1.04	1.16
1:C:66:LEU:HD23	1:C:128:PHE:CZ	1.81	1.16
1:A:127:LYS:HD2	1:C:141:ARG:HD3	1.22	1.16
1:C:40:LYS:CD	1:C:40:LYS:CB	2.23	1.15
1:G:66:LEU:HD11	1:G:132:VAL:CG1	1.74	1.15
1:A:98:PHE:HD1	1:A:133:SER:OG	1.28	1.15
1:E:66:LEU:HD11	3:E:142:HEM:CMB	1.76	1.14
1:C:118:THR:HG23	1:C:120:ALA:HB3	1.26	1.14
1:G:80:LEU:CB	1:G:135:VAL:HG11	1.78	1.14
2:B:68:LEU:HD23	2:B:68:LEU:N	1.62	1.14
2:H:3:LEU:HD21	2:H:8:LYS:HE2	1.24	1.14
1:C:62:VAL:O	1:C:65:ALA:HB3	1.46	1.13
2:D:81:LEU:CD1	2:D:137:VAL:HG23	1.78	1.13
2:H:137:VAL:O	2:H:141:LEU:CD2	1.97	1.13
2:F:25:GLY:O	2:F:55:MET:CE	1.97	1.13
1:A:29:LEU:HD21	1:A:101:LEU:CD1	1.76	1.13
2:H:80:ASN:CG	2:H:83:GLY:HA3	1.69	1.13
1:E:106:LEU:HA	1:E:106:LEU:HD12	1.31	1.13
2:H:117:HIS:CD2	2:H:118:PHE:CE1	2.36	1.13
2:D:82:LYS:HA	2:D:140:ALA:HB1	1.22	1.13
2:D:104:ARG:CG	2:D:104:ARG:H	1.61	1.12
3:E:142:HEM:HBB2	3:E:142:HEM:CMB	1.58	1.12
1:E:66:LEU:HD11	3:E:142:HEM:HMB2	1.16	1.12
2:B:7:GLU:O	2:B:11:VAL:CG2	1.96	1.12
1:G:109:LEU:HA	1:G:109:LEU:HD12	1.28	1.12
1:G:112:HIS:ND1	1:G:112:HIS:HA	1.63	1.12
2:H:20:VAL:HG12	2:H:65:LYS:HB2	1.22	1.12
2:D:10:ALA:O	2:D:14:LEU:HG	1.49	1.12
1:E:76:MET:SD	1:E:135:VAL:HG21	1.88	1.12
1:A:3:SER:CB	1:A:4:PRO:HD2	1.65	1.11
2:B:28:LEU:CD1	2:B:32:LEU:HD22	1.78	1.11
2:H:123:THR:HG22	2:H:124:PRO:HD2	1.18	1.11
2:F:20:VAL:O	2:F:68:LEU:HD13	1.47	1.11
2:B:129:ALA:HA	2:B:132:LYS:HG3	1.31	1.11
1:C:116:GLU:OE1	1:C:116:GLU:HA	1.48	1.11
1:G:112:HIS:CA	1:G:112:HIS:CG	2.32	1.11
2:B:101:GLU:OE1	2:B:104:ARG:NE	1.82	1.11
2:B:129:ALA:O	2:B:133:VAL:HG23	1.51	1.11
1:E:44:PRO:HG2	1:E:45:HIS:H	1.15	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LEU:HD11	2:B:32:LEU:HD22	1.32	1.11
1:G:84:SER:HA	1:G:136:LEU:HD23	1.29	1.11
2:F:29:GLY:CA	2:F:55:MET:CE	2.28	1.10
1:C:118:THR:CG2	1:C:121:VAL:H	1.62	1.10
1:G:14:TRP:CE3	1:G:14:TRP:HA	1.52	1.10
2:F:68:LEU:O	2:F:71:PHE:HB3	1.49	1.10
1:G:79:ALA:O	1:G:82:ALA:CB	1.97	1.10
1:A:127:LYS:CE	1:C:141:ARG:O	2.00	1.10
2:B:4:THR:HG23	2:B:5:PRO:CD	1.80	1.10
2:H:84:THR:N	2:H:84:THR:OG1	1.83	1.10
2:B:19:ASN:O	2:B:23:VAL:HG13	1.50	1.10
2:D:21:ASP:N	2:D:21:ASP:OD1	1.63	1.10
2:F:14:LEU:O	2:F:17:LYS:HB2	1.49	1.10
1:G:49:SER:O	1:G:52:SER:N	1.84	1.10
1:G:87:HIS:CD2	1:G:91:LEU:HD13	1.86	1.10
2:B:51:PRO:O	2:B:55:MET:CG	1.97	1.09
1:C:106:LEU:O	1:C:110:ALA:N	1.84	1.09
1:E:86:LEU:HD11	1:E:90:LYS:HD2	1.28	1.09
2:B:45:PHE:HE1	2:B:60:VAL:CG2	1.64	1.09
1:G:104:CYS:O	1:G:108:THR:OG1	1.69	1.09
2:D:113:VAL:HG12	2:D:114:LEU:HD23	1.10	1.09
1:G:66:LEU:CD1	1:G:132:VAL:HG21	1.81	1.09
1:E:106:LEU:O	1:E:110:ALA:HB2	1.53	1.09
2:F:2:HIS:O	2:F:132:LYS:NZ	1.85	1.09
2:D:131:GLN:HA	2:D:131:GLN:NE2	1.65	1.08
2:F:37:TRP:NE1	1:G:94:ASP:OD1	1.86	1.08
1:C:27:GLU:HG2	1:C:108:THR:HG23	1.17	1.08
1:E:10:VAL:HG13	1:E:125:LEU:HD23	1.33	1.08
1:E:99:LYS:HB3	1:E:100:LEU:HD23	1.09	1.08
1:G:87:HIS:CG	1:G:91:LEU:HD13	1.87	1.08
1:G:112:HIS:ND1	1:G:112:HIS:CA	2.15	1.08
1:E:86:LEU:CD1	1:E:90:LYS:HD2	1.84	1.08
1:A:100:LEU:O	1:A:103:HIS:HB3	1.54	1.08
2:B:96:LEU:HD22	2:B:98:VAL:HG21	1.33	1.08
1:G:121:VAL:O	1:G:125:LEU:N	1.87	1.07
2:F:4:THR:HB	2:F:7:GLU:HG3	1.12	1.07
1:G:118:THR:HG23	1:G:120:ALA:HB3	1.17	1.07
2:D:104:ARG:CG	2:D:104:ARG:CA	2.31	1.07
1:C:31:ARG:HG2	2:D:127:GLN:OE1	1.54	1.07
1:G:118:THR:CG2	1:G:120:ALA:CB	2.32	1.07
2:F:26:GLU:O	2:F:30:ARG:HB2	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:PRO:CA	1:G:98:PHE:HD2	1.67	1.06
1:C:64:ASP:HA	1:C:64:ASP:OD1	1.27	1.06
2:D:45:PHE:N	2:D:45:PHE:HD2	1.37	1.06
2:H:24:GLY:HA2	2:H:68:LEU:HD13	1.12	1.06
1:C:16:LYS:CE	1:C:16:LYS:CG	2.32	1.06
1:C:93:VAL:HG11	3:C:142:HEM:CAC	1.85	1.06
2:D:104:ARG:CG	2:D:104:ARG:N	2.14	1.06
1:G:60:LYS:O	1:G:64:ASP:HB2	1.55	1.06
1:A:127:LYS:HE3	1:C:141:ARG:O	1.54	1.06
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.07	1.06
1:G:109:LEU:CB	1:G:109:LEU:CD1	2.33	1.06
2:D:91:LEU:HD12	2:D:95:LYS:CB	1.83	1.06
2:B:17:LYS:HE2	2:B:17:LYS:HB2	1.34	1.06
1:G:112:HIS:HB3	1:G:113:LEU:HD13	1.34	1.06
1:G:109:LEU:CD1	1:G:109:LEU:CD2	2.33	1.06
2:H:21:ASP:OD1	2:H:65:LYS:HG3	1.53	1.06
3:B:147:HEM:HMC1	3:B:147:HEM:CBC	1.81	1.05
1:G:83:LEU:HD11	3:G:142:HEM:HMA1	1.35	1.05
1:C:40:LYS:CG	1:C:40:LYS:CE	2.33	1.05
1:C:84:SER:CB	1:C:139:LYS:HD2	1.85	1.05
1:E:101:LEU:O	1:E:101:LEU:HD22	1.55	1.05
1:C:16:LYS:CD	1:C:16:LYS:CB	2.35	1.05
2:B:98:VAL:CG2	2:B:98:VAL:CG1	2.33	1.05
2:D:26:GLU:OE1	2:D:30:ARG:NH1	1.89	1.05
1:A:98:PHE:CD1	1:A:133:SER:OG	2.02	1.05
1:E:109:LEU:O	1:E:113:LEU:HD12	1.57	1.05
2:H:20:VAL:HG12	2:H:65:LYS:CB	1.85	1.05
3:D:147:HEM:CMB	3:D:147:HEM:CBB	2.33	1.04
1:A:41:THR:HG23	1:A:41:THR:N	1.70	1.04
2:D:107:GLY:O	2:D:111:VAL:CG2	2.05	1.04
1:E:66:LEU:CD1	3:E:142:HEM:HMB2	1.85	1.04
1:E:14:TRP:HA	1:E:17:VAL:CG2	1.87	1.04
3:A:142:HEM:CAD	3:A:142:HEM:CGD	2.35	1.04
1:E:67:THR:HG22	1:E:68:ASN:N	1.72	1.04
1:G:114:PRO:HG2	1:G:115:ALA:N	1.71	1.04
2:B:106:LEU:HA	2:B:109:VAL:HG23	1.33	1.04
2:B:96:LEU:HD22	2:B:98:VAL:CG2	1.88	1.04
2:H:80:ASN:ND2	2:H:83:GLY:HA3	1.71	1.04
2:D:131:GLN:CA	2:D:131:GLN:HE21	1.53	1.03
2:D:91:LEU:HG	2:D:91:LEU:O	1.58	1.03
1:C:7:LYS:HE2	1:C:74:ASP:OD2	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ASP:OD2	1:G:141:ARG:NH2	1.90	1.03
1:E:102:SER:HB3	1:E:129:LEU:HD22	1.06	1.03
1:G:66:LEU:HD13	1:G:132:VAL:HG11	1.35	1.03
1:A:127:LYS:O	1:A:130:ALA:HB3	1.59	1.03
2:D:101:GLU:O	2:D:104:ARG:CG	2.06	1.03
1:E:66:LEU:CD1	3:E:142:HEM:CMB	2.37	1.03
1:E:1:VAL:HG12	1:E:2:LEU:H	0.87	1.03
1:C:66:LEU:CD2	1:C:129:LEU:CD2	2.37	1.03
1:A:139:LYS:HD2	1:A:139:LYS:N	1.69	1.03
2:H:130:TYR:O	2:H:134:VAL:HG23	1.58	1.03
1:C:107:VAL:HG13	2:D:112:CYS:SG	1.98	1.03
1:E:62:VAL:O	1:E:66:LEU:HD13	1.59	1.03
1:A:110:ALA:HB1	2:B:115:ALA:HB3	1.40	1.02
1:G:14:TRP:CA	1:G:14:TRP:CE3	2.42	1.02
1:A:58:HIS:O	1:A:62:VAL:N	1.93	1.02
1:A:121:VAL:HG23	1:A:121:VAL:N	1.74	1.02
2:H:31:LEU:HD22	2:H:106:LEU:HB2	1.03	1.02
2:H:14:LEU:CD2	2:H:14:LEU:CB	2.37	1.02
2:F:4:THR:CB	2:F:7:GLU:HG3	1.88	1.02
3:A:142:HEM:O2D	3:A:142:HEM:HAD2	1.56	1.02
1:A:76:MET:CA	1:A:76:MET:CG	2.37	1.02
2:B:3:LEU:HD22	2:B:7:GLU:HB3	1.38	1.02
1:E:101:LEU:O	1:E:105:LEU:HD12	1.57	1.02
2:D:131:GLN:CA	2:D:131:GLN:NE2	2.10	1.02
2:D:14:LEU:CD1	2:D:14:LEU:CB	2.36	1.02
2:F:39:GLN:NE2	2:F:39:GLN:CG	2.22	1.02
1:G:83:LEU:HD11	3:G:142:HEM:CMA	1.90	1.02
2:D:82:LYS:HA	2:D:140:ALA:CB	1.90	1.01
1:E:112:HIS:C	1:E:113:LEU:HG	1.74	1.01
2:B:67:VAL:C	2:B:68:LEU:HD23	1.79	1.01
2:F:2:HIS:CG	2:F:132:LYS:HZ1	1.78	1.01
1:A:66:LEU:O	1:A:70:VAL:HG23	1.60	1.01
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.39	1.01
2:D:141:LEU:CB	2:D:141:LEU:CD1	2.37	1.01
1:G:87:HIS:CG	1:G:91:LEU:CD1	2.43	1.01
1:C:16:LYS:HD3	1:C:116:GLU:HG3	1.41	1.01
1:C:27:GLU:HG2	1:C:108:THR:CG2	1.89	1.01
2:F:130:TYR:O	2:F:134:VAL:HG23	1.60	1.01
1:E:132:VAL:O	1:E:136:LEU:HD12	1.60	1.01
3:E:142:HEM:HMB2	3:E:142:HEM:HBB2	1.01	1.01
2:D:76:ALA:HB3	2:D:77:HIS:CG	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:CZ	1:C:141:ARG:CD	2.37	1.01
2:D:113:VAL:HG12	2:D:114:LEU:CD2	1.91	1.00
1:E:43:PHE:HZ	3:E:142:HEM:CBC	1.57	1.00
1:E:33:PHE:CD2	1:E:48:LEU:HD23	1.95	1.00
1:C:7:LYS:NZ	1:C:74:ASP:OD1	1.92	1.00
2:B:59:LYS:CE	2:B:59:LYS:HA	1.72	1.00
2:D:104:ARG:CD	2:D:104:ARG:CB	2.39	1.00
2:D:107:GLY:HA3	2:D:134:VAL:HG21	1.03	1.00
3:D:147:HEM:HBC2	3:D:147:HEM:CMC	1.89	1.00
2:B:3:LEU:CD2	2:B:7:GLU:HB3	1.90	1.00
2:H:81:LEU:O	2:H:85:PHE:CE1	2.13	1.00
2:D:110:LEU:HD23	2:D:110:LEU:C	1.81	1.00
1:C:12:ALA:C	1:C:13:ALA:CA	2.30	1.00
2:D:3:LEU:CD1	2:D:133:VAL:HG23	1.92	1.00
2:F:141:LEU:HD11	3:F:147:HEM:CAB	1.92	1.00
3:D:147:HEM:HMB3	3:D:147:HEM:HBB2	1.42	1.00
2:H:125:PRO:HG2	2:H:126:VAL:N	1.75	0.99
2:B:15:TRP:CE3	2:B:18:VAL:HG21	1.95	0.99
2:F:80:ASN:ND2	2:F:83:GLY:H	1.59	0.99
2:F:7:GLU:O	2:F:11:VAL:HG12	1.63	0.99
1:A:2:LEU:N	1:A:2:LEU:HD23	1.77	0.99
1:E:31:ARG:NH1	2:F:122:PHE:O	1.96	0.99
1:G:66:LEU:HD11	1:G:132:VAL:HG21	1.01	0.99
2:B:50:THR:O	2:B:54:VAL:CG2	2.09	0.99
2:B:98:VAL:O	2:B:145:TYR:OH	1.79	0.99
1:C:107:VAL:HA	1:C:110:ALA:HB2	1.45	0.99
1:A:17:VAL:O	1:A:17:VAL:HG12	1.61	0.99
2:B:8:LYS:CB	2:B:8:LYS:CD	2.40	0.99
2:F:48:LEU:CB	2:F:48:LEU:CD2	2.41	0.99
1:A:3:SER:CB	1:A:4:PRO:CD	2.41	0.99
2:H:93:CYS:HB2	2:H:145:TYR:CE1	1.98	0.99
1:A:118:THR:OG1	1:A:121:VAL:CG2	2.10	0.98
2:B:1:VAL:C	2:B:2:HIS:ND1	2.16	0.98
1:C:40:LYS:CD	1:C:40:LYS:HB3	1.91	0.98
2:D:54:VAL:O	2:D:57:ASN:HB2	1.64	0.98
1:G:117:PHE:CA	1:G:117:PHE:CG	2.46	0.98
2:H:35:TYR:O	2:H:38:THR:HG23	1.63	0.98
2:H:36:PRO:HG2	2:H:37:TRP:CE3	1.96	0.98
1:G:113:LEU:O	1:G:117:PHE:HB2	1.63	0.98
2:D:101:GLU:HA	2:D:104:ARG:HD2	1.46	0.98
2:D:128:ALA:O	2:D:131:GLN:HB2	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:SER:CB	1:E:129:LEU:HD22	1.94	0.98
1:E:99:LYS:HB3	1:E:100:LEU:CD2	1.93	0.98
1:C:118:THR:HG22	1:C:121:VAL:H	0.94	0.98
1:C:107:VAL:O	1:C:110:ALA:CB	2.12	0.98
1:C:77:PRO:C	1:C:78:ASN:CA	2.30	0.98
1:E:1:VAL:CG1	1:E:2:LEU:H	1.74	0.98
1:E:96:VAL:HG21	2:H:101:GLU:CD	1.84	0.98
1:A:83:LEU:HD11	3:A:142:HEM:HMA1	1.46	0.98
1:A:77:PRO:O	1:A:81:SER:HB2	1.64	0.98
1:C:78:ASN:N	1:C:78:ASN:CB	2.27	0.98
3:D:147:HEM:HMB1	3:D:147:HEM:CBB	1.93	0.98
2:F:43:GLU:OE2	1:G:92:ARG:NH1	1.96	0.98
1:G:84:SER:N	1:G:136:LEU:CD2	2.26	0.98
2:H:123:THR:CG2	2:H:124:PRO:HD2	1.92	0.98
1:E:141:ARG:HB3	2:H:36:PRO:HG3	1.42	0.98
1:G:118:THR:HG23	1:G:120:ALA:CB	1.91	0.98
1:A:61:LYS:CB	1:A:61:LYS:CD	2.41	0.97
2:D:45:PHE:N	2:D:45:PHE:CD2	2.08	0.97
1:G:48:LEU:HD23	1:G:48:LEU:N	1.77	0.97
1:G:20:HIS:HB3	1:G:23:GLU:HB2	1.44	0.97
1:A:33:PHE:CD1	1:A:40:LYS:HG2	2.00	0.97
1:A:52:SER:O	1:A:55:VAL:HG22	1.65	0.97
2:D:24:GLY:HA3	2:D:68:LEU:CD2	1.95	0.97
1:G:3:SER:HB2	1:G:4:PRO:HD2	1.47	0.97
2:D:80:ASN:HD21	2:D:83:GLY:CA	1.64	0.97
1:A:87:HIS:CB	1:A:136:LEU:HD11	1.95	0.97
2:D:81:LEU:HD13	2:D:137:VAL:HG23	1.45	0.97
1:G:80:LEU:HB2	1:G:135:VAL:HG11	1.45	0.97
2:H:21:ASP:HA	2:H:65:LYS:HB3	1.44	0.97
2:B:3:LEU:CD2	2:B:3:LEU:CD1	2.43	0.96
2:B:96:LEU:CD2	2:B:98:VAL:HG21	1.94	0.96
2:B:98:VAL:H	2:B:98:VAL:HG23	1.25	0.96
1:C:118:THR:CG2	1:C:120:ALA:HB3	1.94	0.96
1:G:80:LEU:HD11	1:G:132:VAL:HG13	1.47	0.96
2:H:32:LEU:HA	2:H:38:THR:OG1	1.64	0.96
1:A:45:HIS:ND1	1:A:45:HIS:N	2.13	0.96
2:F:141:LEU:HD11	3:F:147:HEM:HAB	1.46	0.96
1:A:139:LYS:CD	1:A:139:LYS:N	2.23	0.96
2:B:98:VAL:CG2	2:B:98:VAL:CA	2.42	0.96
2:H:81:LEU:O	2:H:85:PHE:HE1	1.48	0.96
2:B:28:LEU:HD11	2:B:32:LEU:CD2	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:SER:OG	1:G:136:LEU:HA	1.64	0.96
2:H:26:GLU:O	2:H:30:ARG:CG	2.13	0.96
1:E:104:CYS:O	1:E:108:THR:OG1	1.83	0.96
1:G:118:THR:HG21	1:G:120:ALA:HB3	1.48	0.96
2:B:146:HIS:N	2:B:146:HIS:CD2	2.32	0.95
1:E:128:PHE:O	1:E:131:SER:HB2	1.66	0.95
1:A:118:THR:HG1	1:A:121:VAL:HG21	1.27	0.95
2:B:92:HIS:HA	2:B:96:LEU:CD1	1.95	0.95
2:D:11:VAL:HG12	2:D:12:THR:N	1.79	0.95
2:D:24:GLY:HA3	2:D:68:LEU:HD21	1.46	0.95
2:D:80:ASN:HD22	2:D:83:GLY:HA3	1.23	0.95
2:F:33:VAL:HG21	2:F:51:PRO:HB3	1.45	0.95
2:B:38:THR:OG1	2:B:38:THR:CG2	2.13	0.95
1:C:64:ASP:CG	1:C:64:ASP:CA	2.34	0.95
2:D:44:SER:OG	2:D:45:PHE:HE2	1.50	0.95
2:F:72:SER:O	2:F:75:LEU:HB2	1.66	0.95
1:G:105:LEU:O	1:G:109:LEU:HB2	1.67	0.95
2:B:73:ASP:O	2:B:77:HIS:CE1	2.20	0.95
1:A:61:LYS:CA	1:A:61:LYS:CG	2.44	0.95
2:B:98:VAL:N	2:B:98:VAL:HG23	1.75	0.95
1:A:6:ASP:O	1:A:10:VAL:HG23	1.65	0.95
1:A:53:ALA:CA	1:A:56:LYS:HD3	1.95	0.95
1:G:121:VAL:HA	1:G:124:SER:OG	1.67	0.95
1:G:107:VAL:HG13	2:H:112:CYS:HG	1.20	0.94
2:H:91:LEU:CD1	2:H:91:LEU:CD2	2.45	0.94
1:A:41:THR:H	1:A:41:THR:HG23	1.25	0.94
1:C:118:THR:HB	1:C:121:VAL:HB	1.45	0.94
2:D:47:ASP:OD2	2:D:49:SER:HB3	1.68	0.94
1:G:32:MET:CG	1:G:32:MET:CA	2.45	0.94
2:B:101:GLU:OE1	2:B:104:ARG:NH1	2.00	0.94
2:D:81:LEU:HD11	2:D:137:VAL:HG23	1.46	0.94
2:D:146:HIS:N	2:D:146:HIS:CD2	2.29	0.94
1:E:123:ALA:O	1:E:126:ASP:HB3	1.66	0.94
1:G:32:MET:C	1:G:32:MET:CB	2.35	0.94
1:A:100:LEU:HD23	1:A:100:LEU:N	1.80	0.94
1:A:112:HIS:O	1:A:113:LEU:HD23	1.67	0.94
1:C:66:LEU:HD23	1:C:128:PHE:HZ	1.26	0.94
2:H:102:ASN:C	2:H:103:PHE:CA	2.35	0.94
3:A:142:HEM:CBD	3:A:142:HEM:C3D	2.51	0.94
1:C:123:ALA:O	1:C:127:LYS:HG3	1.68	0.94
1:E:107:VAL:C	1:E:110:ALA:HB3	1.87	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:SER:OG	1:C:139:LYS:HD2	1.68	0.94
1:G:42:TYR:CD1	1:G:93:VAL:HG13	2.03	0.94
1:C:13:ALA:CB	1:C:13:ALA:N	2.31	0.94
2:F:33:VAL:CG2	2:F:51:PRO:HB3	1.97	0.94
2:F:80:ASN:ND2	2:F:80:ASN:O	2.00	0.94
2:F:91:LEU:HD21	2:F:96:LEU:CD1	1.98	0.94
2:H:3:LEU:HD23	2:H:4:THR:N	1.83	0.93
1:G:49:SER:O	1:G:52:SER:OG	1.86	0.93
2:H:78:LEU:HD23	2:H:133:VAL:CG2	1.97	0.93
2:F:94:ASP:OD1	2:F:146:HIS:NE2	2.01	0.93
1:A:86:LEU:HD13	1:A:90:LYS:NZ	1.82	0.93
2:B:114:LEU:O	2:B:118:PHE:HB2	1.68	0.93
1:C:40:LYS:HB3	1:C:40:LYS:HD2	1.50	0.93
2:D:77:HIS:O	2:D:81:LEU:HD23	1.68	0.93
1:G:118:THR:HB	1:G:121:VAL:CG2	1.97	0.93
1:G:46:PHE:HE2	3:G:142:HEM:O1D	1.50	0.93
2:H:24:GLY:HA2	2:H:68:LEU:CD1	1.97	0.93
1:A:4:PRO:HG2	1:A:5:ALA:H	1.34	0.93
2:F:22:GLU:HG2	2:F:23:VAL:N	1.80	0.93
1:G:14:TRP:HE3	1:G:14:TRP:HA	1.23	0.93
2:H:82:LYS:O	2:H:83:GLY:O	1.87	0.93
1:G:118:THR:CB	1:G:121:VAL:HG23	1.98	0.93
2:D:3:LEU:CD2	2:D:132:LYS:CB	2.46	0.93
2:F:39:GLN:NE2	2:F:39:GLN:CB	2.14	0.93
2:H:14:LEU:CD2	2:H:14:LEU:CD1	2.46	0.93
2:D:49:SER:CB	2:D:49:SER:C	2.36	0.93
3:E:142:HEM:CBB	3:E:142:HEM:HMB2	1.97	0.93
1:G:29:LEU:HD21	1:G:58:HIS:NE2	1.83	0.93
2:B:103:PHE:CZ	2:B:141:LEU:HD12	2.03	0.93
2:B:92:HIS:O	2:B:96:LEU:HB3	1.67	0.93
2:F:93:CYS:O	2:F:97:HIS:HA	1.69	0.92
1:G:66:LEU:O	1:G:69:ALA:HB3	1.69	0.92
1:E:19:ALA:C	1:E:20:HIS:CA	2.37	0.92
1:A:112:HIS:O	1:A:113:LEU:CD2	2.17	0.92
2:D:32:LEU:CD2	2:D:42:PHE:CE1	2.51	0.92
1:C:66:LEU:CD2	1:C:129:LEU:HD23	1.99	0.92
1:G:83:LEU:O	1:G:87:HIS:N	2.03	0.92
1:A:41:THR:N	1:A:41:THR:CG2	2.31	0.92
1:C:68:ASN:O	1:C:72:HIS:HD2	1.53	0.92
1:E:44:PRO:HG2	1:E:45:HIS:N	1.80	0.92
1:A:118:THR:HB	1:A:121:VAL:HG23	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:SER:CB	2:D:49:SER:N	2.33	0.92
2:H:39:GLN:O	2:H:42:PHE:N	2.02	0.92
2:H:82:LYS:O	2:H:83:GLY:C	2.06	0.92
2:D:24:GLY:CA	2:D:68:LEU:HD21	2.00	0.92
2:F:1:VAL:CG1	2:F:132:LYS:CE	2.38	0.92
1:A:121:VAL:N	1:A:121:VAL:CG2	2.31	0.92
1:E:96:VAL:CG2	2:H:101:GLU:HG2	2.00	0.92
2:B:30:ARG:O	2:B:34:VAL:HG23	1.68	0.92
1:A:98:PHE:HB3	1:A:133:SER:HB3	1.49	0.91
2:B:51:PRO:HA	2:B:54:VAL:HB	1.48	0.91
2:D:81:LEU:HD13	2:D:137:VAL:CG2	1.99	0.91
3:D:147:HEM:HMB1	3:D:147:HEM:HBB2	1.47	0.91
2:B:21:ASP:OD2	2:B:21:ASP:N	2.01	0.91
2:F:82:LYS:CG	2:F:82:LYS:CE	2.48	0.91
2:B:3:LEU:CB	2:B:3:LEU:CD2	2.49	0.91
2:F:74:GLY:O	2:F:78:LEU:HD13	1.70	0.91
2:H:31:LEU:HD22	2:H:106:LEU:CB	1.98	0.91
1:C:31:ARG:O	1:C:35:SER:OG	1.87	0.91
2:D:11:VAL:HG21	2:D:133:VAL:HG21	1.52	0.91
2:H:33:VAL:HG22	2:H:54:VAL:HG11	1.51	0.91
1:A:47:ASP:OD1	1:A:49:SER:HB3	1.71	0.91
2:F:141:LEU:CD1	3:F:147:HEM:HAB	2.01	0.91
2:H:21:ASP:CG	2:H:65:LYS:CG	2.34	0.91
2:H:3:LEU:HD22	2:H:8:LYS:HE2	1.52	0.91
1:C:84:SER:HB3	1:C:139:LYS:HD2	1.53	0.91
1:C:91:LEU:CD2	1:C:91:LEU:CB	2.49	0.91
2:F:99:ASP:O	2:F:102:ASN:HB2	1.69	0.91
2:H:114:LEU:HD23	2:H:118:PHE:CE1	2.05	0.91
2:B:18:VAL:CG1	2:B:20:VAL:HG23	2.00	0.91
1:E:14:TRP:HA	1:E:17:VAL:HG21	1.52	0.91
1:G:14:TRP:CD1	1:G:67:THR:OG1	2.23	0.91
1:E:109:LEU:O	1:E:113:LEU:CD1	2.19	0.91
2:F:1:VAL:HG11	2:F:132:LYS:CD	1.99	0.91
2:F:91:LEU:HD21	2:F:96:LEU:HD11	1.53	0.91
2:H:127:GLN:CG	2:H:127:GLN:CA	2.49	0.91
2:D:68:LEU:HD13	2:D:68:LEU:N	1.86	0.90
1:E:6:ASP:CB	1:E:124:SER:OG	2.20	0.90
1:E:88:ALA:HA	1:E:140:TYR:CE2	2.05	0.90
1:E:92:ARG:HB3	2:H:37:TRP:HB2	1.50	0.90
2:F:24:GLY:HA3	2:F:68:LEU:HD12	1.51	0.90
1:A:31:ARG:NH1	2:B:122:PHE:O	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:O	1:C:72:HIS:HB2	1.71	0.90
1:G:4:PRO:HG2	1:G:5:ALA:H	1.24	0.90
2:H:103:PHE:CB	2:H:103:PHE:N	2.34	0.90
1:C:47:ASP:O	1:C:52:SER:OG	1.89	0.90
2:F:49:SER:O	2:F:50:THR:HG23	1.70	0.90
2:H:30:ARG:CG	2:H:30:ARG:NE	2.34	0.90
1:C:119:PRO:HA	1:C:122:HIS:HB3	1.53	0.90
2:B:51:PRO:O	2:B:55:MET:N	2.04	0.90
1:G:109:LEU:HD12	1:G:109:LEU:CA	2.00	0.90
2:H:20:VAL:HG11	2:H:65:LYS:HB2	1.51	0.90
2:D:10:ALA:HB1	2:D:126:VAL:HG13	1.53	0.90
1:G:112:HIS:CB	1:G:113:LEU:HD13	2.02	0.90
2:H:20:VAL:HG13	2:H:68:LEU:HD22	1.54	0.90
1:C:107:VAL:CG1	2:D:112:CYS:SG	2.59	0.90
1:A:59:GLY:O	1:A:63:ALA:N	2.05	0.90
1:C:118:THR:CB	1:C:118:THR:N	2.35	0.90
1:C:38:THR:CG2	1:C:38:THR:CA	2.49	0.90
2:F:15:TRP:O	2:F:18:VAL:HG23	1.72	0.89
2:D:113:VAL:CG1	2:D:114:LEU:HD23	2.02	0.89
1:G:118:THR:CG2	1:G:121:VAL:HG23	2.02	0.89
2:H:123:THR:HB	2:H:125:PRO:HD2	1.54	0.89
2:B:106:LEU:HA	2:B:109:VAL:CG2	2.01	0.89
2:B:93:CYS:HB2	2:B:145:TYR:CZ	2.07	0.89
1:C:104:CYS:HA	1:C:107:VAL:CG2	2.02	0.89
2:D:114:LEU:HD23	2:D:114:LEU:N	1.87	0.89
2:H:114:LEU:HD23	2:H:118:PHE:CD1	2.06	0.89
2:H:57:ASN:HB3	2:H:60:VAL:HB	1.54	0.89
2:F:1:VAL:HG11	2:F:132:LYS:HD2	1.54	0.89
2:D:101:GLU:CB	2:D:104:ARG:HD2	2.03	0.89
1:G:87:HIS:CE1	1:G:91:LEU:HD13	2.08	0.89
3:H:147:HEM:CMC	3:H:147:HEM:HBC2	2.01	0.89
1:A:117:PHE:CD2	1:A:117:PHE:O	2.26	0.89
1:A:47:ASP:OD1	1:A:49:SER:CB	2.20	0.89
1:A:134:THR:O	1:A:137:THR:N	2.04	0.89
1:G:20:HIS:O	1:G:23:GLU:N	2.05	0.89
2:H:20:VAL:HB	2:H:21:ASP:OD1	1.71	0.89
2:H:86:ALA:HB1	2:H:144:LYS:CE	2.03	0.89
2:D:146:HIS:HD2	2:D:146:HIS:H	1.10	0.88
2:H:38:THR:O	2:H:41:PHE:CD1	2.26	0.88
2:B:59:LYS:HA	2:B:59:LYS:NZ	1.87	0.88
2:B:65:LYS:O	2:B:69:GLY:N	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:GLY:O	2:D:111:VAL:HG23	1.73	0.88
2:D:32:LEU:HD21	2:D:42:PHE:HE1	1.36	0.88
2:B:58:PRO:HA	2:B:61:LYS:HB2	1.54	0.88
1:C:116:GLU:OE1	1:C:116:GLU:CA	2.19	0.88
1:E:106:LEU:HA	1:E:106:LEU:CD1	2.01	0.88
1:E:43:PHE:CE2	3:E:142:HEM:HBC2	2.08	0.88
1:G:4:PRO:CG	1:G:5:ALA:N	2.37	0.88
2:H:86:ALA:HB1	2:H:144:LYS:HE3	1.55	0.88
2:H:28:LEU:HD21	2:H:63:HIS:CD2	2.09	0.88
2:H:68:LEU:CB	2:H:68:LEU:N	2.36	0.88
2:F:4:THR:HB	2:F:7:GLU:CD	1.93	0.88
2:F:43:GLU:CD	1:G:92:ARG:HH12	1.77	0.88
2:H:93:CYS:HB2	2:H:145:TYR:CD1	2.08	0.88
1:C:64:ASP:OD1	1:C:64:ASP:N	2.07	0.88
2:D:51:PRO:CA	2:D:54:VAL:HG23	2.03	0.88
2:D:142:ALA:CB	2:D:142:ALA:N	2.37	0.87
2:F:135:ALA:O	2:F:138:ALA:HB3	1.74	0.87
1:G:101:LEU:CB	1:G:101:LEU:CD1	2.52	0.87
1:G:29:LEU:HD21	1:G:58:HIS:CD2	2.08	0.87
2:H:38:THR:O	2:H:41:PHE:HD1	1.55	0.87
1:E:38:THR:HG23	1:E:39:THR:N	1.88	0.87
2:D:14:LEU:HD21	2:D:126:VAL:HG13	1.56	0.87
1:E:129:LEU:O	1:E:129:LEU:HD23	1.75	0.87
2:F:39:GLN:HE21	2:F:39:GLN:HB3	0.71	0.87
1:G:109:LEU:CD1	1:G:109:LEU:CA	2.53	0.87
1:G:118:THR:HB	1:G:121:VAL:HG23	1.56	0.87
1:A:110:ALA:HB1	2:B:115:ALA:CB	2.04	0.87
3:E:142:HEM:CBB	3:E:142:HEM:CMB	2.51	0.87
1:C:118:THR:O	1:C:122:HIS:N	2.08	0.86
1:C:7:LYS:CE	1:C:74:ASP:OD1	2.23	0.86
1:E:99:LYS:CB	1:E:100:LEU:HD23	2.02	0.86
2:H:20:VAL:HG13	2:H:68:LEU:CD2	2.05	0.86
1:A:87:HIS:CB	1:A:136:LEU:CD1	2.54	0.86
1:C:45:HIS:ND1	1:C:45:HIS:N	2.16	0.86
1:G:61:LYS:CG	1:G:61:LYS:CE	2.54	0.86
1:A:76:MET:CB	1:A:76:MET:N	2.37	0.86
1:C:132:VAL:CA	1:C:132:VAL:CG1	2.52	0.86
1:C:24:TYR:CD2	1:C:24:TYR:N	2.38	0.86
2:D:110:LEU:O	2:D:110:LEU:CG	2.24	0.86
1:G:84:SER:N	1:G:136:LEU:HD23	1.89	0.86
2:B:101:GLU:CD	2:B:104:ARG:HE	1.79	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:TYR:N	1:C:24:TYR:HD2	1.72	0.86
2:F:31:LEU:HD13	2:F:109:VAL:CG2	2.04	0.86
2:F:20:VAL:C	2:F:68:LEU:HD13	1.96	0.86
1:E:106:LEU:CD2	1:E:106:LEU:CD1	2.54	0.86
1:A:20:HIS:H	1:A:20:HIS:CD2	1.93	0.86
1:A:51:GLY:O	1:A:56:LYS:CE	2.23	0.86
1:A:61:LYS:CE	1:A:61:LYS:CG	2.53	0.86
2:B:141:LEU:HD21	3:B:147:HEM:HBB2	1.56	0.86
1:C:130:ALA:HA	1:C:133:SER:OG	1.74	0.86
1:E:2:LEU:HA	1:E:127:LYS:NZ	1.91	0.86
1:G:103:HIS:O	1:G:107:VAL:CG2	2.24	0.86
3:H:147:HEM:HMC1	3:H:147:HEM:CBC	2.05	0.86
2:H:98:VAL:HG13	2:H:102:ASN:OD1	1.74	0.86
2:F:14:LEU:O	2:F:17:LYS:CB	2.21	0.86
1:G:87:HIS:ND1	1:G:91:LEU:CD1	2.38	0.86
1:G:31:ARG:NH1	2:H:122:PHE:O	2.09	0.86
2:H:9:SER:O	2:H:13:ALA:HB3	1.75	0.86
1:C:141:ARG:NE	1:C:141:ARG:HG2	1.89	0.86
2:D:51:PRO:O	2:D:55:MET:HB2	1.74	0.86
1:G:118:THR:O	1:G:119:PRO:C	2.07	0.86
2:H:34:VAL:C	2:H:36:PRO:HD2	1.96	0.86
2:H:82:LYS:H	2:H:82:LYS:HD3	1.39	0.85
2:F:4:THR:CB	2:F:7:GLU:CG	2.47	0.85
1:A:87:HIS:CG	1:A:136:LEU:CD1	2.54	0.85
1:C:110:ALA:HB1	2:D:115:ALA:HB1	1.58	0.85
2:D:11:VAL:HG21	2:D:133:VAL:CG2	2.06	0.85
2:F:26:GLU:HA	2:F:55:MET:HE2	1.55	0.85
1:C:16:LYS:HE2	1:C:16:LYS:CG	2.06	0.85
1:C:68:ASN:O	1:C:72:HIS:CD2	2.29	0.85
2:D:14:LEU:CD1	2:D:14:LEU:CD2	2.55	0.85
2:D:64:GLY:O	2:D:68:LEU:HD22	1.76	0.85
1:A:118:THR:HB	1:A:121:VAL:CG2	2.06	0.85
1:C:16:LYS:CD	1:C:16:LYS:HB2	2.05	0.85
2:F:31:LEU:HD13	2:F:109:VAL:HG21	1.56	0.85
1:G:32:MET:SD	1:G:101:LEU:HB2	2.17	0.85
1:A:118:THR:HG22	1:A:119:PRO:HD2	1.55	0.85
2:D:76:ALA:HB3	2:D:77:HIS:ND1	1.91	0.85
1:A:100:LEU:N	1:A:100:LEU:CD2	2.39	0.85
1:C:118:THR:CB	1:C:121:VAL:HB	2.07	0.85
2:D:15:TRP:CD1	2:D:130:TYR:OH	2.28	0.85
1:A:4:PRO:HG2	1:A:5:ALA:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:HG23	1:C:120:ALA:CB	2.07	0.85
1:G:103:HIS:O	1:G:107:VAL:HG22	1.77	0.85
1:C:3:SER:O	1:C:6:ASP:HB2	1.77	0.85
2:F:98:VAL:O	2:F:145:TYR:OH	1.94	0.85
2:F:63:HIS:HE1	3:F:147:HEM:ND	1.75	0.84
1:G:27:GLU:O	1:G:31:ARG:HB2	1.76	0.84
1:A:20:HIS:CD2	1:A:20:HIS:N	2.40	0.84
1:A:51:GLY:O	1:A:56:LYS:HE2	1.76	0.84
2:D:107:GLY:CA	2:D:134:VAL:CG2	2.42	0.84
2:D:33:VAL:HG22	2:D:54:VAL:HG21	1.58	0.84
1:G:30:GLU:HG3	1:G:50:HIS:CD2	2.12	0.84
1:E:6:ASP:HA	1:E:124:SER:OG	1.75	0.84
2:H:22:GLU:CB	2:H:22:GLU:CD	2.45	0.84
2:H:78:LEU:HB3	2:H:81:LEU:HD21	1.57	0.84
2:D:101:GLU:HA	2:D:104:ARG:HH11	0.71	0.84
1:C:58:HIS:O	1:C:62:VAL:N	2.11	0.84
1:C:117:PHE:C	1:C:118:THR:CA	2.45	0.84
2:H:82:LYS:CD	2:H:82:LYS:H	1.90	0.84
1:A:76:MET:C	1:A:76:MET:CB	2.45	0.84
2:B:59:LYS:O	2:B:62:ALA:HB3	1.77	0.84
1:E:52:SER:HB2	1:E:54:GLN:H	1.43	0.84
2:F:127:GLN:O	2:F:131:GLN:N	2.11	0.84
1:G:66:LEU:C	1:G:67:THR:CA	2.45	0.84
1:G:93:VAL:HG11	3:G:142:HEM:CAC	2.08	0.84
1:A:87:HIS:O	1:A:91:LEU:HB2	1.77	0.84
2:F:50:THR:O	2:F:53:ALA:HB3	1.77	0.84
1:C:17:VAL:CG1	1:C:21:ALA:HA	2.07	0.84
1:A:127:LYS:HE2	1:C:141:ARG:O	1.78	0.83
2:B:42:PHE:O	2:B:45:PHE:HB2	1.79	0.83
1:C:7:LYS:CE	1:C:74:ASP:OD2	2.26	0.83
2:B:17:LYS:HE2	2:B:17:LYS:CB	2.08	0.83
2:F:58:PRO:O	2:F:62:ALA:HB3	1.77	0.83
2:F:80:ASN:HD21	2:F:83:GLY:H	0.90	0.83
2:H:109:VAL:HG13	2:H:109:VAL:O	1.77	0.83
2:H:21:ASP:N	2:H:21:ASP:OD1	2.06	0.83
1:C:132:VAL:CG2	1:C:132:VAL:CG1	2.56	0.83
1:E:13:ALA:O	1:E:16:LYS:HB2	1.78	0.83
2:F:30:ARG:H	2:F:55:MET:HE1	1.42	0.83
2:B:110:LEU:HD12	2:B:110:LEU:O	1.79	0.83
2:F:90:GLU:CG	2:F:90:GLU:OE1	2.26	0.83
1:A:36:PHE:CE1	1:A:100:LEU:HD13	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:VAL:HG11	3:C:142:HEM:HAC	1.61	0.83
2:B:92:HIS:HA	2:B:96:LEU:HD12	1.58	0.83
2:H:86:ALA:HB1	2:H:144:LYS:NZ	1.94	0.83
2:D:63:HIS:O	2:D:67:VAL:N	2.11	0.83
2:H:68:LEU:O	2:H:72:SER:OG	1.96	0.83
2:B:38:THR:CB	2:B:38:THR:N	2.40	0.82
1:C:16:LYS:HZ2	1:C:116:GLU:HG3	1.42	0.82
1:G:87:HIS:CE1	1:G:91:LEU:CD1	2.61	0.82
1:A:88:ALA:HB2	1:A:139:LYS:CB	2.09	0.82
1:E:122:HIS:CE1	2:F:30:ARG:HD3	2.14	0.82
2:H:22:GLU:CA	2:H:22:GLU:CG	2.56	0.82
2:B:17:LYS:CG	2:B:17:LYS:CE	2.57	0.82
2:B:107:GLY:HA3	2:B:134:VAL:HG22	1.61	0.82
1:E:11:LYS:CG	1:E:11:LYS:CA	2.57	0.82
2:H:4:THR:HG22	2:H:7:GLU:H	1.44	0.82
2:D:44:SER:C	2:D:45:PHE:HD2	1.82	0.82
2:D:44:SER:OG	2:D:45:PHE:CE2	2.26	0.82
2:F:11:VAL:HG23	2:F:130:TYR:CE1	2.13	0.82
1:E:122:HIS:ND1	2:F:30:ARG:NE	2.28	0.82
1:G:109:LEU:HA	1:G:109:LEU:CD1	2.06	0.82
1:G:112:HIS:O	1:G:113:LEU:HD12	1.80	0.82
1:C:37:PRO:O	1:C:40:LYS:HB2	1.80	0.82
2:D:91:LEU:CG	2:D:91:LEU:O	2.27	0.82
2:F:8:LYS:CB	2:F:8:LYS:CD	2.57	0.82
2:H:98:VAL:C	2:H:99:ASP:CA	2.46	0.82
1:E:66:LEU:CD1	3:E:142:HEM:HMB1	2.10	0.82
2:H:146:HIS:CD2	2:H:146:HIS:H	1.95	0.82
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.09	0.82
2:H:9:SER:O	2:H:13:ALA:CB	2.28	0.82
1:C:27:GLU:CG	1:C:108:THR:HG23	2.06	0.82
2:D:47:ASP:OD2	2:D:49:SER:CB	2.27	0.82
2:F:80:ASN:ND2	2:F:83:GLY:N	2.21	0.82
1:A:76:MET:CA	1:A:76:MET:HG2	2.08	0.82
2:D:44:SER:HB3	2:D:45:PHE:CD2	2.14	0.82
2:F:4:THR:HG22	2:F:6:VAL:H	1.44	0.82
1:G:29:LEU:HB2	1:G:101:LEU:HD11	1.62	0.82
2:H:93:CYS:CB	2:H:145:TYR:CE1	2.62	0.82
1:E:27:GLU:O	1:E:31:ARG:HB2	1.80	0.81
1:G:88:ALA:HB2	1:G:140:TYR:CD2	2.15	0.81
1:A:38:THR:O	1:A:41:THR:HG23	1.79	0.81
2:B:107:GLY:CA	2:B:134:VAL:HG21	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:GLY:HA2	2:B:134:VAL:HG21	1.61	0.81
2:B:28:LEU:HD12	2:B:32:LEU:HD22	1.60	0.81
2:D:68:LEU:H	2:D:68:LEU:HD22	1.44	0.81
2:D:75:LEU:N	2:D:75:LEU:HD13	1.95	0.81
1:A:38:THR:O	1:A:41:THR:CG2	2.28	0.81
2:B:59:LYS:CE	2:B:59:LYS:CA	2.57	0.81
2:D:72:SER:HA	2:D:75:LEU:HD22	1.62	0.81
2:D:80:ASN:CG	2:D:83:GLY:HA3	2.01	0.81
1:A:87:HIS:ND1	1:A:136:LEU:HD11	1.95	0.81
1:A:1:VAL:C	1:A:2:LEU:HD23	2.00	0.81
2:B:146:HIS:HD2	2:B:146:HIS:N	1.75	0.81
1:C:88:ALA:C	1:C:89:HIS:ND1	2.34	0.81
2:D:65:LYS:CD	2:D:65:LYS:NZ	2.43	0.81
1:E:88:ALA:HB2	1:E:140:TYR:CD2	2.15	0.81
1:A:65:ALA:HB1	1:A:80:LEU:CD2	2.10	0.81
1:C:27:GLU:CG	1:C:108:THR:CG2	2.57	0.81
1:C:47:ASP:O	1:C:52:SER:CB	2.28	0.81
1:G:80:LEU:CG	1:G:135:VAL:HG11	2.10	0.81
1:G:66:LEU:HD21	1:G:132:VAL:HG21	1.61	0.81
2:H:31:LEU:HD23	2:H:106:LEU:CD2	2.11	0.81
2:H:117:HIS:CD2	2:H:118:PHE:CZ	2.68	0.81
2:H:21:ASP:OD1	2:H:65:LYS:CG	2.27	0.81
2:H:26:GLU:OE1	2:H:30:ARG:NH1	2.13	0.81
2:B:14:LEU:HD11	2:B:114:LEU:HD13	1.60	0.81
2:B:72:SER:HA	2:B:75:LEU:CD1	2.10	0.81
2:D:48:LEU:HD21	2:D:60:VAL:HG21	1.62	0.81
2:D:87:THR:CG2	2:D:88:LEU:N	2.44	0.81
1:E:43:PHE:HZ	3:E:142:HEM:HBC2	1.00	0.81
1:G:87:HIS:N	1:G:91:LEU:HD12	1.94	0.81
1:A:6:ASP:O	1:A:10:VAL:CG2	2.29	0.81
1:C:16:LYS:CD	1:C:116:GLU:HG3	2.10	0.81
2:D:141:LEU:CD2	2:D:141:LEU:CD1	2.57	0.81
2:D:24:GLY:CA	2:D:68:LEU:CD2	2.57	0.81
2:D:81:LEU:HA	2:D:84:THR:HG22	1.61	0.81
1:A:98:PHE:HE1	3:A:142:HEM:CAB	1.92	0.81
2:B:96:LEU:O	2:B:97:HIS:HB2	1.80	0.81
1:C:113:LEU:HD22	1:C:116:GLU:CB	2.10	0.81
1:C:66:LEU:HD21	1:C:129:LEU:HD21	1.61	0.81
1:C:7:LYS:HE2	1:C:74:ASP:OD1	1.81	0.81
2:H:84:THR:CA	2:H:84:THR:OG1	2.28	0.81
1:C:10:VAL:HG23	1:C:125:LEU:HD23	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ARG:NH1	2:D:127:GLN:OE1	2.14	0.81
2:D:72:SER:CA	2:D:75:LEU:HD22	2.11	0.81
2:F:2:HIS:CE1	2:F:132:LYS:HZ1	1.96	0.81
1:G:6:ASP:OD1	1:G:127:LYS:CE	2.29	0.81
1:G:110:ALA:HB3	2:H:115:ALA:HB3	1.61	0.81
2:H:66:LYS:HB3	2:H:67:VAL:HG23	1.63	0.81
1:A:40:LYS:C	1:A:41:THR:CA	2.49	0.81
1:C:16:LYS:O	1:C:16:LYS:CG	2.27	0.81
1:E:106:LEU:CD1	1:E:106:LEU:HB2	2.10	0.81
1:E:93:VAL:HG11	3:E:142:HEM:HAC	1.63	0.81
1:E:35:SER:OG	1:E:35:SER:CA	2.29	0.81
1:G:112:HIS:C	1:G:112:HIS:CB	2.49	0.81
1:E:15:GLY:O	1:E:16:LYS:C	2.14	0.80
2:F:29:GLY:N	2:F:55:MET:CE	2.44	0.80
1:G:117:PHE:CB	1:G:117:PHE:C	2.49	0.80
2:H:46:GLY:O	2:H:48:LEU:HD23	1.81	0.80
1:A:127:LYS:CD	1:C:141:ARG:HD3	2.09	0.80
1:C:16:LYS:HG3	1:C:16:LYS:O	1.80	0.80
2:D:102:ASN:HB3	3:D:147:HEM:HMC1	1.61	0.80
2:D:87:THR:HG23	2:D:88:LEU:N	1.97	0.80
3:H:147:HEM:CMC	3:H:147:HEM:CBC	2.55	0.80
1:C:43:PHE:HD2	1:C:46:PHE:CG	1.99	0.80
1:E:120:ALA:O	1:E:123:ALA:HB3	1.82	0.80
2:F:1:VAL:CG1	2:F:132:LYS:CD	2.57	0.80
2:H:135:ALA:O	2:H:138:ALA:HB3	1.81	0.80
2:B:92:HIS:CA	2:B:96:LEU:HD13	2.12	0.80
2:H:117:HIS:CD2	2:H:118:PHE:CG	2.69	0.80
2:H:80:ASN:O	2:H:84:THR:OG1	1.98	0.80
1:A:30:GLU:OE1	1:A:50:HIS:ND1	2.15	0.80
1:A:98:PHE:CE1	3:A:142:HEM:HAB	2.17	0.80
2:B:21:ASP:HB3	2:B:65:LYS:HB2	1.64	0.80
2:B:35:TYR:HB3	2:B:37:TRP:CZ2	2.17	0.80
2:D:110:LEU:O	2:D:110:LEU:CD2	2.29	0.80
2:D:146:HIS:HD2	2:D:146:HIS:N	1.69	0.80
2:F:63:HIS:HE1	3:F:147:HEM:C1D	2.00	0.80
2:B:92:HIS:HA	2:B:96:LEU:HD13	1.63	0.80
2:D:121:GLU:O	2:D:123:THR:N	2.15	0.80
1:G:17:VAL:HG13	1:G:24:TYR:CD1	2.16	0.80
1:A:10:VAL:HG13	1:A:125:LEU:HD23	1.64	0.80
2:B:4:THR:CG2	2:B:5:PRO:CD	2.59	0.80
1:A:88:ALA:HB2	1:A:139:LYS:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:SER:HB2	1:E:54:GLN:HB3	1.64	0.80
3:G:142:HEM:HMB1	3:G:142:HEM:HBB2	1.63	0.80
2:D:71:PHE:O	2:D:75:LEU:HD13	1.82	0.80
1:G:62:VAL:O	1:G:65:ALA:HB3	1.82	0.80
1:E:32:MET:HG2	1:E:39:THR:HG21	1.63	0.80
2:F:63:HIS:HE1	3:F:147:HEM:C4D	1.99	0.80
2:F:90:GLU:CD	2:F:90:GLU:CB	2.50	0.79
2:H:91:LEU:CD1	2:H:91:LEU:CB	2.58	0.79
2:H:98:VAL:O	2:H:98:VAL:HG12	1.81	0.79
1:C:55:VAL:O	1:C:55:VAL:HG13	1.82	0.79
2:D:14:LEU:HD11	2:D:130:TYR:HE2	1.47	0.79
2:D:127:GLN:O	2:D:131:GLN:HG2	1.82	0.79
2:F:1:VAL:CB	2:F:132:LYS:HG3	2.13	0.79
2:B:111:VAL:CG1	2:B:111:VAL:O	2.28	0.79
1:G:29:LEU:HD13	1:G:33:PHE:CE2	2.17	0.79
2:D:42:PHE:O	2:D:45:PHE:HB2	1.80	0.79
1:E:4:PRO:HA	1:E:7:LYS:HD2	1.63	0.79
2:B:131:GLN:O	2:B:135:ALA:CB	2.31	0.79
2:D:77:HIS:CB	2:D:77:HIS:H	1.96	0.79
1:G:17:VAL:O	1:G:19:ALA:N	2.16	0.79
1:G:30:GLU:CG	1:G:50:HIS:HE2	1.82	0.79
2:H:30:ARG:CZ	2:H:30:ARG:CD	2.61	0.79
2:B:107:GLY:CA	2:B:134:VAL:CG2	2.60	0.79
2:B:92:HIS:O	2:B:97:HIS:N	2.16	0.79
1:E:141:ARG:CG	2:H:37:TRP:HZ3	1.95	0.79
1:G:20:HIS:HB3	1:G:23:GLU:CB	2.12	0.79
2:H:92:HIS:CD2	2:H:103:PHE:CZ	2.71	0.79
2:D:14:LEU:HD21	2:D:126:VAL:HG11	0.81	0.79
2:H:73:ASP:O	2:H:76:ALA:CB	2.30	0.79
1:G:67:THR:N	1:G:67:THR:CB	2.46	0.79
2:H:117:HIS:HD2	2:H:118:PHE:CZ	2.00	0.79
2:H:34:VAL:O	2:H:36:PRO:HD2	1.83	0.79
2:H:4:THR:CG2	2:H:7:GLU:HB2	2.13	0.79
1:A:80:LEU:O	1:A:84:SER:N	2.16	0.79
1:C:118:THR:C	1:C:118:THR:N	2.35	0.79
1:C:141:ARG:HG3	1:C:141:ARG:NE	1.98	0.78
1:G:76:MET:CE	1:G:131:SER:HB2	2.13	0.78
1:A:98:PHE:HB3	1:A:133:SER:CB	2.13	0.78
1:C:78:ASN:CG	1:C:78:ASN:N	2.36	0.78
2:D:80:ASN:HD21	2:D:83:GLY:HA2	1.47	0.78
1:G:109:LEU:CD1	1:G:109:LEU:HD22	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:GLU:O	2:D:104:ARG:HG2	1.83	0.78
2:D:107:GLY:HA2	2:D:134:VAL:HG21	1.63	0.78
2:D:73:ASP:O	2:D:76:ALA:CB	2.31	0.78
2:F:20:VAL:O	2:F:68:LEU:HD12	1.81	0.78
2:B:4:THR:CG2	2:B:5:PRO:N	2.45	0.78
2:D:113:VAL:O	2:D:116:HIS:HB3	1.83	0.78
1:E:68:ASN:OD1	1:E:72:HIS:NE2	2.16	0.78
2:H:137:VAL:C	2:H:141:LEU:HD23	2.02	0.78
2:D:11:VAL:CG1	2:D:12:THR:N	2.45	0.78
2:D:14:LEU:C	2:D:14:LEU:HD12	2.04	0.78
2:F:49:SER:C	2:F:50:THR:HG23	2.03	0.78
1:A:118:THR:CB	1:A:121:VAL:CG2	2.62	0.78
1:A:110:ALA:O	2:B:116:HIS:HA	1.84	0.78
1:C:55:VAL:O	1:C:55:VAL:CG1	2.24	0.78
1:E:121:VAL:O	1:E:121:VAL:CG1	2.32	0.78
2:F:49:SER:O	2:F:50:THR:CG2	2.31	0.78
1:E:141:ARG:HG2	2:H:37:TRP:HZ3	1.47	0.78
1:E:107:VAL:O	1:E:110:ALA:HB3	1.84	0.78
2:H:80:ASN:OD1	2:H:83:GLY:HA3	1.84	0.78
2:H:92:HIS:CD2	2:H:98:VAL:HG21	2.19	0.78
1:G:80:LEU:CB	1:G:135:VAL:CG1	2.59	0.78
2:H:67:VAL:C	2:H:68:LEU:CA	2.53	0.78
1:A:61:LYS:HA	1:A:61:LYS:CG	2.14	0.77
2:B:18:VAL:CG1	2:B:18:VAL:CG2	2.60	0.77
2:D:58:PRO:O	2:D:62:ALA:CB	2.32	0.77
1:C:16:LYS:HD3	1:C:116:GLU:CG	2.14	0.77
1:C:39:THR:CA	1:C:39:THR:OG1	2.32	0.77
1:G:118:THR:HG22	1:G:121:VAL:HG23	1.64	0.77
2:H:92:HIS:O	2:H:96:LEU:HB2	1.85	0.77
2:H:21:ASP:CA	2:H:65:LYS:HB3	2.14	0.77
2:H:24:GLY:CA	2:H:68:LEU:HD13	2.06	0.77
1:G:84:SER:CA	1:G:136:LEU:CD2	2.59	0.77
2:B:68:LEU:N	2:B:68:LEU:CD2	2.46	0.77
2:D:51:PRO:C	2:D:54:VAL:HG23	2.05	0.77
1:E:52:SER:CB	1:E:54:GLN:HB3	2.14	0.77
1:A:111:ALA:HB1	2:B:119:GLY:HA2	1.65	0.77
1:C:40:LYS:CG	1:C:40:LYS:HE2	2.15	0.77
1:G:75:ASP:C	1:G:77:PRO:HD2	2.05	0.77
2:H:137:VAL:CG1	2:H:137:VAL:CG2	2.61	0.77
1:G:3:SER:HB2	1:G:4:PRO:CD	2.15	0.77
2:H:39:GLN:O	2:H:41:PHE:N	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:O	2:B:61:LYS:N	2.16	0.77
2:F:14:LEU:HD21	2:F:118:PHE:CD2	2.19	0.77
1:G:30:GLU:CG	1:G:50:HIS:CD2	2.58	0.77
2:H:23:VAL:HG23	2:H:68:LEU:HD21	1.66	0.77
2:B:92:HIS:CG	2:B:96:LEU:CD1	2.68	0.76
1:E:16:LYS:HE2	1:E:116:GLU:OE2	1.84	0.76
1:E:39:THR:HG1	1:E:43:PHE:HE1	1.33	0.76
2:D:141:LEU:HB3	2:D:141:LEU:CD1	2.13	0.76
2:F:54:VAL:HG12	2:F:54:VAL:O	1.84	0.76
1:G:112:HIS:HB3	1:G:113:LEU:CD1	2.13	0.76
2:H:20:VAL:CG1	2:H:65:LYS:CB	2.51	0.76
2:B:15:TRP:CH2	2:B:71:PHE:CE2	2.74	0.76
2:D:112:CYS:O	2:D:115:ALA:HB3	1.85	0.76
1:E:88:ALA:HA	1:E:140:TYR:CD2	2.20	0.76
1:E:96:VAL:HG23	2:H:101:GLU:HG2	1.67	0.76
2:H:123:THR:CG2	2:H:123:THR:OG1	2.33	0.76
2:B:92:HIS:CG	2:B:96:LEU:HD13	2.19	0.76
2:D:91:LEU:CD1	2:D:95:LYS:CB	2.62	0.76
1:E:69:ALA:N	1:E:69:ALA:CB	2.48	0.76
2:H:84:THR:HG1	2:H:84:THR:H	1.33	0.76
2:B:73:ASP:O	2:B:77:HIS:HE1	1.68	0.76
2:B:8:LYS:HD3	2:B:8:LYS:HB3	1.67	0.76
2:D:26:GLU:CD	2:D:30:ARG:HH11	1.86	0.76
1:E:13:ALA:O	1:E:17:VAL:HG23	1.86	0.76
2:F:1:VAL:HG12	2:F:132:LYS:HE2	0.83	0.76
2:H:35:TYR:O	2:H:38:THR:CG2	2.32	0.76
1:C:110:ALA:CB	2:D:115:ALA:HB1	2.15	0.76
2:D:44:SER:CB	2:D:45:PHE:CD2	2.69	0.76
2:H:93:CYS:CB	2:H:145:TYR:CD1	2.69	0.76
1:G:121:VAL:CA	1:G:124:SER:OG	2.34	0.76
1:G:28:ALA:HA	1:G:108:THR:HG21	1.68	0.76
2:F:6:VAL:O	2:F:9:SER:HB3	1.84	0.76
1:A:37:PRO:CB	1:A:37:PRO:C	2.53	0.76
1:E:27:GLU:CD	1:E:112:HIS:HE2	1.90	0.76
2:F:114:LEU:HD23	2:F:114:LEU:C	2.04	0.76
2:F:8:LYS:CA	2:F:8:LYS:CG	2.62	0.76
2:F:90:GLU:CG	2:F:90:GLU:OE2	2.34	0.76
1:G:114:PRO:CG	1:G:115:ALA:N	2.46	0.76
1:G:76:MET:HE2	1:G:131:SER:HB2	1.67	0.76
2:H:26:GLU:CD	2:H:30:ARG:HH11	1.87	0.76
2:B:14:LEU:CD1	2:B:114:LEU:HD13	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:PRO:O	2:F:116:HIS:NE2	2.18	0.76
2:H:137:VAL:CA	2:H:137:VAL:CG2	2.63	0.76
2:F:91:LEU:CD2	2:F:96:LEU:CD1	2.63	0.75
1:G:6:ASP:OD1	1:G:127:LYS:HE3	1.84	0.75
2:B:101:GLU:OE1	2:B:104:ARG:CZ	2.34	0.75
2:D:15:TRP:O	2:D:18:VAL:HG23	1.85	0.75
1:C:119:PRO:HB3	2:D:30:ARG:HG3	1.67	0.75
1:E:106:LEU:CA	1:E:106:LEU:CD1	2.64	0.75
2:F:124:PRO:N	2:F:125:PRO:CD	2.49	0.75
2:H:4:THR:HB	2:H:7:GLU:HB2	0.78	0.75
1:E:141:ARG:HG2	2:H:37:TRP:CZ3	2.21	0.75
1:G:66:LEU:HD12	1:G:132:VAL:HG11	1.63	0.75
2:H:31:LEU:HD23	2:H:106:LEU:HD23	1.67	0.75
2:D:113:VAL:HG12	2:D:114:LEU:N	2.00	0.75
2:F:40:ARG:CB	2:F:40:ARG:CD	2.63	0.75
1:A:127:LYS:HD2	1:C:141:ARG:CD	2.12	0.75
1:C:64:ASP:CB	1:C:64:ASP:N	2.48	0.75
1:G:66:LEU:HD11	1:G:132:VAL:HG11	1.16	0.75
1:A:87:HIS:HB3	1:A:136:LEU:CD1	2.17	0.75
2:D:51:PRO:HA	2:D:54:VAL:HG23	1.65	0.75
2:F:81:LEU:HD22	2:F:85:PHE:HE1	1.51	0.75
2:H:32:LEU:HD12	2:H:38:THR:OG1	1.87	0.75
2:B:15:TRP:HE1	2:B:72:SER:HB3	1.52	0.75
2:B:17:LYS:CB	2:B:17:LYS:CD	2.65	0.75
2:B:4:THR:HG22	2:B:6:VAL:H	1.49	0.75
2:B:51:PRO:CA	2:B:54:VAL:HB	2.16	0.75
1:C:17:VAL:HG11	1:C:21:ALA:HA	1.69	0.75
1:G:130:ALA:O	1:G:134:THR:N	2.20	0.75
2:H:85:PHE:N	2:H:85:PHE:CD1	2.53	0.75
2:H:87:THR:HG22	2:H:88:LEU:N	1.91	0.75
1:A:65:ALA:HB1	1:A:80:LEU:HD21	1.67	0.75
2:B:131:GLN:O	2:B:135:ALA:HB3	1.87	0.75
1:C:77:PRO:O	1:C:78:ASN:CA	2.34	0.75
3:D:147:HEM:CBC	3:D:147:HEM:CMC	2.64	0.75
1:E:39:THR:O	1:E:43:PHE:CE1	2.39	0.75
1:E:45:HIS:N	1:E:45:HIS:ND1	2.22	0.75
1:G:84:SER:N	1:G:136:LEU:HD21	2.02	0.75
2:H:11:VAL:HG23	2:H:12:THR:N	2.01	0.75
2:D:3:LEU:HD23	2:D:132:LYS:HB3	1.68	0.75
2:D:14:LEU:O	2:D:15:TRP:C	2.23	0.75
1:E:10:VAL:O	1:E:10:VAL:HG12	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LEU:HD11	1:G:132:VAL:CB	2.17	0.75
2:H:109:VAL:O	2:H:109:VAL:CG1	2.34	0.75
1:A:139:LYS:C	1:A:141:ARG:HG3	2.08	0.74
2:D:90:GLU:O	2:D:94:ASP:N	2.19	0.74
2:F:101:GLU:O	2:F:104:ARG:HB2	1.86	0.74
2:B:59:LYS:HE3	2:B:62:ALA:CB	2.16	0.74
1:C:119:PRO:O	1:C:120:ALA:C	2.17	0.74
2:D:146:HIS:H	2:D:146:HIS:CD2	1.93	0.74
1:E:129:LEU:HD23	1:E:129:LEU:C	2.05	0.74
2:F:2:HIS:CE1	2:F:132:LYS:NZ	2.54	0.74
2:F:45:PHE:O	2:F:57:ASN:ND2	2.20	0.74
1:G:43:PHE:N	1:G:43:PHE:CD1	2.55	0.74
1:G:60:LYS:NZ	1:G:60:LYS:CD	2.50	0.74
2:H:93:CYS:HB2	2:H:145:TYR:CZ	2.22	0.74
2:B:18:VAL:HG11	2:B:20:VAL:HG23	1.69	0.74
1:C:113:LEU:HB3	1:C:116:GLU:HB2	1.67	0.74
1:C:16:LYS:HZ2	1:C:113:LEU:HD23	1.51	0.74
1:C:36:PHE:HZ	1:C:103:HIS:CE1	2.04	0.74
2:D:26:GLU:O	2:D:30:ARG:N	2.20	0.74
2:F:29:GLY:CA	2:F:55:MET:HE1	2.17	0.74
1:G:30:GLU:HG3	1:G:50:HIS:HE2	0.87	0.74
2:B:92:HIS:CB	2:B:96:LEU:HD13	2.17	0.74
1:C:6:ASP:OD2	1:C:127:LYS:CE	2.29	0.74
1:E:96:VAL:CG2	2:H:101:GLU:CG	2.65	0.74
2:H:21:ASP:CB	2:H:65:LYS:HG3	2.18	0.74
1:A:98:PHE:HE1	3:A:142:HEM:HAB	1.51	0.74
2:D:101:GLU:CB	2:D:104:ARG:HH11	2.01	0.74
1:G:118:THR:HB	1:G:121:VAL:HG21	1.69	0.74
1:G:84:SER:HG	1:G:136:LEU:HA	1.52	0.74
1:G:49:SER:C	1:G:52:SER:HG	1.89	0.74
2:B:88:LEU:HD21	2:H:6:VAL:HG13	1.67	0.74
2:D:58:PRO:O	2:D:62:ALA:HB2	1.85	0.74
1:G:42:TYR:CE1	1:G:93:VAL:HG13	2.23	0.74
2:B:107:GLY:HA3	2:B:134:VAL:CG2	2.17	0.74
2:D:44:SER:CB	2:D:45:PHE:CE2	2.70	0.74
1:G:47:ASP:C	1:G:48:LEU:HD23	2.08	0.74
2:D:28:LEU:O	2:D:28:LEU:HD12	1.88	0.74
2:F:26:GLU:O	2:F:55:MET:HE1	1.88	0.74
1:C:66:LEU:HD21	1:C:129:LEU:HD22	1.64	0.74
1:C:7:LYS:HE2	1:C:74:ASP:CG	2.08	0.74
2:D:128:ALA:C	2:D:131:GLN:HB2	2.08	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:HIS:N	2:D:77:HIS:HB2	1.99	0.74
1:E:88:ALA:HB2	1:E:140:TYR:HD2	1.53	0.74
1:E:14:TRP:HA	1:E:17:VAL:CB	2.17	0.74
1:E:106:LEU:CA	1:E:106:LEU:HD12	2.15	0.73
1:E:67:THR:CG2	1:E:68:ASN:N	2.42	0.73
1:G:80:LEU:HB3	1:G:135:VAL:HG11	1.66	0.73
1:G:83:LEU:C	1:G:136:LEU:CD2	2.55	0.73
2:D:124:PRO:N	2:D:125:PRO:HD2	2.03	0.73
2:D:3:LEU:HD22	2:D:132:LYS:CB	2.11	0.73
1:G:30:GLU:CD	1:G:50:HIS:NE2	2.36	0.73
1:G:36:PHE:N	1:G:37:PRO:HD3	2.01	0.73
1:C:107:VAL:CA	1:C:110:ALA:HB2	2.17	0.73
2:D:101:GLU:O	2:D:104:ARG:HD2	1.88	0.73
1:E:43:PHE:CE1	3:E:142:HEM:CBC	2.69	0.73
1:G:118:THR:HG22	1:G:121:VAL:N	2.04	0.73
2:H:4:THR:CG2	2:H:7:GLU:H	2.01	0.73
2:F:29:GLY:H	2:F:55:MET:HE3	1.52	0.73
1:G:87:HIS:NE2	1:G:91:LEU:HD13	2.03	0.73
2:B:146:HIS:H	2:B:146:HIS:HD2	1.34	0.73
2:F:14:LEU:HA	2:F:17:LYS:HG3	1.69	0.73
1:C:84:SER:OG	1:C:139:LYS:CD	2.37	0.73
1:C:70:VAL:HA	1:C:73:VAL:HG23	1.70	0.73
2:F:29:GLY:N	2:F:55:MET:HE3	2.04	0.73
1:A:120:ALA:C	1:A:121:VAL:CA	2.55	0.73
1:A:93:VAL:HG21	3:A:142:HEM:CAC	2.19	0.73
1:A:80:LEU:O	1:A:84:SER:HB2	1.89	0.73
1:E:14:TRP:HA	1:E:17:VAL:HB	1.69	0.73
1:E:68:ASN:C	1:E:69:ALA:CA	2.54	0.73
2:H:89:SER:HB3	2:H:144:LYS:HB2	1.69	0.73
3:H:147:HEM:HMC3	3:H:147:HEM:HBC2	1.69	0.73
2:H:61:LYS:NZ	2:H:61:LYS:CD	2.51	0.73
1:A:29:LEU:HD21	1:A:101:LEU:HD12	0.82	0.73
1:C:36:PHE:N	1:C:37:PRO:CD	2.50	0.73
2:D:99:ASP:OD2	2:D:100:PRO:HD2	1.88	0.73
1:E:121:VAL:O	1:E:121:VAL:HG13	1.89	0.73
1:G:76:MET:N	1:G:77:PRO:CD	2.51	0.73
1:C:37:PRO:O	1:C:40:LYS:CB	2.37	0.72
2:H:26:GLU:OE1	2:H:30:ARG:HD2	1.88	0.72
2:H:51:PRO:O	2:H:55:MET:CG	2.32	0.72
1:A:116:GLU:O	1:A:121:VAL:HG11	1.89	0.72
2:B:93:CYS:HB2	2:B:145:TYR:CE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LEU:O	1:C:113:LEU:HD12	1.89	0.72
2:H:3:LEU:HD23	2:H:4:THR:H	1.53	0.72
2:B:3:LEU:HB3	2:B:3:LEU:CD2	2.20	0.72
2:B:45:PHE:HE1	2:B:60:VAL:HG23	0.71	0.72
1:E:14:TRP:CA	1:E:17:VAL:CG2	2.66	0.72
2:B:60:VAL:O	2:B:61:LYS:C	2.23	0.72
1:G:80:LEU:HG	1:G:135:VAL:HG11	1.71	0.72
2:H:6:VAL:O	2:H:7:GLU:C	2.23	0.72
2:D:110:LEU:CD2	2:D:110:LEU:C	2.48	0.72
2:D:11:VAL:HG12	2:D:12:THR:H	1.53	0.72
2:D:94:ASP:OD1	2:D:146:HIS:CE1	2.43	0.72
1:E:82:ALA:HA	1:E:85:ASP:HB2	1.71	0.72
1:G:31:ARG:HH21	1:G:31:ARG:HG3	1.55	0.72
2:B:18:VAL:CA	2:B:18:VAL:CG1	2.66	0.72
1:E:117:PHE:O	1:E:117:PHE:CD2	2.42	0.72
1:E:125:LEU:O	1:E:129:LEU:HB2	1.89	0.72
1:E:39:THR:O	1:E:43:PHE:CD1	2.42	0.72
1:E:32:MET:HG3	1:E:32:MET:O	1.89	0.72
2:F:48:LEU:CB	2:F:48:LEU:CD1	2.67	0.72
2:H:49:SER:O	2:H:50:THR:HG23	1.89	0.72
2:B:105:LEU:O	2:B:109:VAL:HG23	1.90	0.72
3:C:142:HEM:CMC	3:C:142:HEM:HBC2	2.17	0.72
2:D:44:SER:HG	2:D:45:PHE:HE2	0.74	0.72
1:E:76:MET:N	1:E:77:PRO:HD2	2.04	0.72
1:E:141:ARG:CB	2:H:36:PRO:HG3	2.18	0.72
1:E:128:PHE:O	1:E:132:VAL:N	2.22	0.72
2:D:15:TRP:CE3	2:D:18:VAL:HB	2.24	0.72
2:D:85:PHE:HB3	2:D:88:LEU:HB3	1.72	0.72
2:F:124:PRO:CD	2:F:125:PRO:HD3	2.19	0.72
2:F:67:VAL:HG22	3:F:147:HEM:NB	2.05	0.72
1:G:61:LYS:CB	1:G:61:LYS:CD	2.65	0.72
2:B:59:LYS:HE3	2:B:59:LYS:O	1.88	0.71
2:D:21:ASP:HA	2:D:65:LYS:HG2	1.72	0.71
2:D:37:TRP:O	2:D:40:ARG:HB2	1.90	0.71
2:H:7:GLU:O	2:H:10:ALA:HB3	1.90	0.71
1:A:61:LYS:NZ	1:A:61:LYS:CD	2.53	0.71
1:C:31:ARG:CG	2:D:127:GLN:OE1	2.35	0.71
2:D:81:LEU:CD1	2:D:137:VAL:CG2	2.60	0.71
1:E:33:PHE:CD2	1:E:48:LEU:CD2	2.72	0.71
2:H:138:ALA:O	2:H:141:LEU:HB2	1.90	0.71
1:A:8:THR:O	1:A:8:THR:CG2	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:VAL:HA	1:C:76:MET:HG3	1.73	0.71
2:D:125:PRO:CB	2:D:125:PRO:C	2.56	0.71
2:D:67:VAL:C	2:D:68:LEU:HD13	2.11	0.71
2:F:110:LEU:O	2:F:110:LEU:HD12	1.89	0.71
2:F:99:ASP:O	2:F:102:ASN:CB	2.38	0.71
2:B:4:THR:HG23	2:B:5:PRO:N	2.04	0.71
2:F:114:LEU:HD23	2:F:114:LEU:O	1.91	0.71
1:G:80:LEU:HB3	1:G:135:VAL:CG1	2.20	0.71
2:H:139:ASN:N	2:H:139:ASN:HD22	1.79	0.71
2:B:18:VAL:CG1	2:B:18:VAL:C	2.59	0.71
2:B:4:THR:O	2:B:8:LYS:HB2	1.91	0.71
2:B:98:VAL:HG22	2:B:98:VAL:N	2.03	0.71
2:D:63:HIS:CE1	3:D:147:HEM:C4D	2.78	0.71
2:F:28:LEU:O	2:F:32:LEU:CB	2.27	0.71
2:H:102:ASN:HB3	3:H:147:HEM:HMC1	1.71	0.71
2:H:20:VAL:O	2:H:24:GLY:CA	2.38	0.71
2:H:68:LEU:HB2	2:H:68:LEU:N	2.05	0.71
2:B:3:LEU:CD1	2:B:133:VAL:HG22	2.20	0.71
2:H:78:LEU:HB3	2:H:81:LEU:CD2	2.19	0.71
1:A:6:ASP:OD1	1:A:124:SER:HA	1.89	0.71
1:A:83:LEU:HD11	3:A:142:HEM:CMA	2.19	0.71
1:E:10:VAL:O	1:E:10:VAL:CG1	2.38	0.71
1:G:4:PRO:O	1:G:5:ALA:C	2.27	0.71
2:H:33:VAL:CG2	2:H:54:VAL:HG11	2.19	0.71
2:B:12:THR:CG2	2:B:12:THR:OG1	2.38	0.71
1:C:99:LYS:HE2	1:C:100:LEU:CD2	2.20	0.71
2:D:20:VAL:O	2:D:20:VAL:CG1	2.37	0.71
2:F:80:ASN:O	2:F:84:THR:OG1	2.05	0.71
2:H:36:PRO:HG2	2:H:37:TRP:CZ3	2.25	0.71
2:B:98:VAL:CG2	2:B:98:VAL:HG13	2.18	0.71
2:D:41:PHE:CZ	2:D:98:VAL:HG13	2.26	0.71
1:A:92:ARG:HG2	2:D:37:TRP:HA	1.73	0.70
2:B:52:ASP:O	2:B:53:ALA:C	2.28	0.70
2:D:110:LEU:O	2:D:110:LEU:HG	1.88	0.70
2:D:73:ASP:O	2:D:76:ALA:HB3	1.91	0.70
1:E:20:HIS:CB	1:E:20:HIS:N	2.51	0.70
3:G:142:HEM:HBB2	3:G:142:HEM:CMB	2.19	0.70
1:A:134:THR:C	1:A:137:THR:H	1.94	0.70
2:B:3:LEU:HD11	2:B:133:VAL:HG22	1.73	0.70
1:C:57:GLY:O	1:C:61:LYS:HB2	1.91	0.70
1:E:78:ASN:O	1:E:81:SER:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:THR:O	2:H:88:LEU:C	2.29	0.70
1:C:31:ARG:HG2	2:D:127:GLN:CD	2.12	0.70
1:G:60:LYS:O	1:G:64:ASP:CB	2.35	0.70
2:B:45:PHE:CE1	2:B:60:VAL:CG2	2.52	0.70
2:D:14:LEU:HD22	2:D:126:VAL:HG11	1.69	0.70
1:E:66:LEU:HD12	3:E:142:HEM:CMB	2.20	0.70
1:E:62:VAL:O	1:E:66:LEU:CD1	2.38	0.70
2:F:20:VAL:CG2	2:F:21:ASP:N	2.54	0.70
2:B:8:LYS:CB	2:B:8:LYS:HD3	2.20	0.70
2:B:96:LEU:CG	2:B:98:VAL:HG21	2.20	0.70
3:D:147:HEM:HMC1	3:D:147:HEM:HBC2	1.69	0.70
1:G:47:ASP:N	1:G:47:ASP:C	2.44	0.70
2:H:54:VAL:HG12	2:H:55:MET:SD	2.32	0.70
2:B:37:TRP:C	2:B:38:THR:CA	2.57	0.70
1:C:7:LYS:CE	1:C:74:ASP:CG	2.58	0.70
2:D:17:LYS:HD3	2:D:17:LYS:H	1.56	0.70
2:B:111:VAL:HG13	2:B:122:PHE:CZ	2.26	0.70
2:B:62:ALA:O	2:B:65:LYS:HG2	1.91	0.70
2:D:124:PRO:O	2:D:127:GLN:HB3	1.91	0.70
1:E:88:ALA:CB	1:E:140:TYR:CD2	2.75	0.70
1:E:4:PRO:HG2	1:E:5:ALA:N	2.05	0.70
1:C:104:CYS:HA	1:C:107:VAL:HG22	1.72	0.70
1:C:10:VAL:HG23	1:C:125:LEU:CD2	2.22	0.70
1:C:25:GLY:O	1:C:28:ALA:HB3	1.91	0.70
2:D:123:THR:HB	2:D:125:PRO:HD2	1.72	0.70
1:E:107:VAL:C	1:E:110:ALA:CB	2.60	0.70
2:F:30:ARG:N	2:F:55:MET:HE1	2.07	0.70
1:G:51:GLY:O	1:G:52:SER:C	2.30	0.70
1:G:87:HIS:HA	1:G:91:LEU:HD12	0.76	0.70
1:A:113:LEU:O	1:A:117:PHE:HB3	1.92	0.69
2:B:15:TRP:HA	2:B:18:VAL:HB	1.72	0.69
2:D:94:ASP:OD1	2:D:146:HIS:NE2	2.25	0.69
2:H:73:ASP:O	2:H:76:ALA:HB2	1.92	0.69
2:H:92:HIS:CD2	2:H:103:PHE:HZ	2.10	0.69
2:B:106:LEU:CA	2:B:109:VAL:HG23	2.18	0.69
1:G:110:ALA:HB3	2:H:115:ALA:CB	2.21	0.69
1:C:38:THR:CG2	1:C:38:THR:N	2.55	0.69
2:B:33:VAL:HG21	2:B:51:PRO:HB3	1.74	0.69
1:C:113:LEU:HD22	1:C:116:GLU:HB3	1.73	0.69
2:F:2:HIS:ND1	2:F:132:LYS:CE	2.53	0.69
2:B:93:CYS:HB2	2:B:145:TYR:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:HB	1:C:118:THR:N	2.05	0.69
1:C:60:LYS:O	1:C:64:ASP:HB2	1.92	0.69
2:D:42:PHE:CD1	2:D:42:PHE:N	2.58	0.69
1:A:127:LYS:HE3	1:C:141:ARG:HB2	1.75	0.69
2:B:1:VAL:O	2:B:2:HIS:ND1	2.24	0.69
1:E:29:LEU:CD2	1:E:101:LEU:HG	2.22	0.69
1:E:97:ASN:OD1	2:H:99:ASP:OD1	2.10	0.69
1:G:2:LEU:HA	1:G:6:ASP:OD2	1.93	0.69
1:A:138:SER:C	1:A:139:LYS:HD2	2.13	0.69
1:A:77:PRO:O	1:A:81:SER:CB	2.40	0.69
2:B:107:GLY:HA2	2:B:134:VAL:CG2	2.20	0.69
1:C:110:ALA:HB1	2:D:115:ALA:CB	2.21	0.69
2:D:3:LEU:HD11	2:D:133:VAL:HG23	1.72	0.69
3:D:147:HEM:CBC	3:D:147:HEM:HMC1	2.22	0.69
1:A:65:ALA:O	1:A:80:LEU:HD21	1.93	0.69
2:B:92:HIS:CD2	2:B:103:PHE:HE1	2.11	0.69
1:G:48:LEU:N	1:G:48:LEU:CD2	2.46	0.69
1:C:118:THR:CG2	1:C:121:VAL:N	2.28	0.69
2:D:101:GLU:OE1	2:D:104:ARG:CZ	2.41	0.69
2:H:93:CYS:HA	2:H:145:TYR:CE1	2.28	0.69
2:B:99:ASP:OD2	2:B:100:PRO:HD2	1.93	0.69
1:C:106:LEU:N	1:C:109:LEU:HB2	2.08	0.69
2:F:63:HIS:CE1	3:F:147:HEM:C4D	2.80	0.69
1:A:83:LEU:HD23	1:A:136:LEU:CD2	2.23	0.68
2:B:4:THR:HG22	2:B:6:VAL:N	2.07	0.68
2:D:73:ASP:OD1	2:D:73:ASP:N	2.24	0.68
2:D:92:HIS:HA	2:D:96:LEU:HB2	1.74	0.68
2:H:93:CYS:SG	2:H:145:TYR:CD1	2.86	0.68
1:E:86:LEU:HD12	1:E:90:LYS:HD2	1.74	0.68
2:F:4:THR:CG2	2:F:6:VAL:HG12	2.23	0.68
2:H:37:TRP:O	2:H:40:ARG:HB2	1.93	0.68
2:B:50:THR:OG1	2:B:53:ALA:HB2	1.93	0.68
1:C:89:HIS:ND1	1:C:89:HIS:N	2.24	0.68
1:E:30:GLU:OE2	1:E:50:HIS:ND1	2.27	0.68
1:G:1:VAL:HG13	1:G:2:LEU:N	2.06	0.68
2:B:19:ASN:O	2:B:23:VAL:CG1	2.37	0.68
2:B:58:PRO:O	2:B:62:ALA:HB2	1.93	0.68
2:F:25:GLY:O	2:F:55:MET:HE2	1.91	0.68
2:H:2:HIS:O	2:H:132:LYS:HD3	1.94	0.68
2:H:92:HIS:HA	2:H:96:LEU:HB2	1.76	0.68
1:A:98:PHE:CE1	3:A:142:HEM:CAB	2.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:PRO:HD3	2:F:145:TYR:CE1	2.27	0.68
1:G:47:ASP:CG	1:G:47:ASP:C	2.53	0.68
1:C:31:ARG:CG	1:C:31:ARG:HH11	2.05	0.68
1:A:47:ASP:OD1	1:A:49:SER:HB2	1.91	0.68
2:B:87:THR:O	2:B:91:LEU:N	2.27	0.68
2:D:51:PRO:O	2:D:54:VAL:HG23	1.93	0.68
2:F:94:ASP:CG	2:F:146:HIS:HE2	1.97	0.68
2:F:80:ASN:ND2	2:F:80:ASN:C	2.47	0.68
2:B:59:LYS:HA	2:B:59:LYS:HZ2	1.58	0.68
2:D:69:GLY:O	2:D:72:SER:HB2	1.93	0.68
1:E:96:VAL:HG21	2:H:101:GLU:CG	2.22	0.68
2:F:1:VAL:HB	2:F:132:LYS:HG3	1.74	0.68
2:H:88:LEU:O	2:H:91:LEU:HB3	1.94	0.68
1:A:41:THR:N	1:A:41:THR:CB	2.56	0.68
1:A:111:ALA:CB	2:B:119:GLY:HA2	2.23	0.68
2:B:15:TRP:CH2	2:B:71:PHE:HE2	2.11	0.68
1:C:13:ALA:N	1:C:14:TRP:N	2.41	0.68
2:H:84:THR:HB	2:H:85:PHE:CE1	2.28	0.68
1:A:9:ASN:ND2	1:A:124:SER:OG	2.26	0.67
1:A:14:TRP:HE1	1:A:67:THR:HG1	1.26	0.67
1:C:66:LEU:HD21	1:C:129:LEU:HD23	1.59	0.67
1:G:31:ARG:CG	2:H:127:GLN:OE1	2.43	0.67
1:A:3:SER:OG	1:A:4:PRO:CD	2.42	0.67
1:C:91:LEU:CD2	1:C:91:LEU:CD1	2.67	0.67
2:D:101:GLU:HA	2:D:104:ARG:CZ	2.23	0.67
3:D:147:HEM:HMC3	3:D:147:HEM:HBC2	1.77	0.67
2:D:77:HIS:HB2	2:D:77:HIS:H	1.54	0.67
1:G:47:ASP:CA	1:G:48:LEU:N	2.56	0.67
1:G:46:PHE:C	1:G:48:LEU:HD21	2.15	0.67
1:A:38:THR:OG1	1:A:39:THR:N	2.26	0.67
2:B:15:TRP:CZ3	2:B:18:VAL:HG21	2.29	0.67
2:D:101:GLU:O	2:D:104:ARG:CD	2.41	0.67
2:H:20:VAL:CG1	2:H:68:LEU:HD22	2.25	0.67
2:B:28:LEU:CD1	2:B:32:LEU:CD2	2.60	0.67
1:C:102:SER:HA	1:C:129:LEU:HD11	1.74	0.67
2:D:3:LEU:HD12	2:D:133:VAL:HG23	1.73	0.67
1:E:122:HIS:HE1	2:F:30:ARG:HD3	1.60	0.67
1:G:27:GLU:OE1	1:G:31:ARG:NE	2.28	0.67
1:G:80:LEU:HB2	1:G:135:VAL:CG1	2.22	0.67
2:B:4:THR:CG2	2:B:6:VAL:H	2.07	0.67
2:D:97:HIS:C	2:D:98:VAL:CG2	2.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:GLU:CD	2:D:104:ARG:HD3	2.15	0.67
1:G:30:GLU:OE2	1:G:50:HIS:CE1	2.47	0.67
2:H:20:VAL:HG13	2:H:68:LEU:HB3	1.75	0.67
2:H:93:CYS:CA	2:H:145:TYR:CE1	2.77	0.67
2:D:77:HIS:N	2:D:77:HIS:CG	2.62	0.67
1:G:11:LYS:HG3	1:G:70:VAL:HG23	1.77	0.67
1:G:14:TRP:O	1:G:15:GLY:C	2.34	0.67
1:G:30:GLU:OE1	1:G:50:HIS:CD2	2.47	0.67
2:H:20:VAL:O	2:H:68:LEU:HD22	1.93	0.67
1:G:6:ASP:OD1	1:G:127:LYS:HE2	1.95	0.66
2:H:47:ASP:HB3	2:H:49:SER:OG	1.95	0.66
1:C:129:LEU:O	1:C:133:SER:N	2.27	0.66
1:C:13:ALA:C	1:C:13:ALA:N	2.44	0.66
1:C:66:LEU:HD23	1:C:128:PHE:CE2	2.30	0.66
2:D:58:PRO:HA	2:D:61:LYS:HG2	1.75	0.66
1:E:28:ALA:O	1:E:29:LEU:C	2.32	0.66
2:F:41:PHE:CD1	3:F:147:HEM:HBC1	2.29	0.66
2:H:87:THR:O	2:H:88:LEU:O	2.14	0.66
2:B:111:VAL:HG13	2:B:111:VAL:O	1.95	0.66
2:B:138:ALA:O	2:B:139:ASN:C	2.30	0.66
2:D:39:GLN:O	2:D:41:PHE:N	2.28	0.66
1:E:105:LEU:O	1:E:109:LEU:HB2	1.94	0.66
1:E:20:HIS:N	1:E:21:ALA:N	2.43	0.66
1:E:29:LEU:HD21	1:E:101:LEU:CD1	2.24	0.66
1:E:44:PRO:CG	1:E:45:HIS:N	2.57	0.66
2:F:4:THR:HG22	2:F:6:VAL:HG12	1.75	0.66
2:F:69:GLY:O	2:F:70:ALA:C	2.31	0.66
1:G:97:ASN:O	1:G:98:PHE:C	2.33	0.66
2:H:34:VAL:C	2:H:36:PRO:CD	2.64	0.66
1:A:118:THR:CB	1:A:121:VAL:HG21	2.25	0.66
2:D:78:LEU:HD11	2:D:133:VAL:HG22	1.77	0.66
1:E:33:PHE:CE2	1:E:48:LEU:CD2	2.77	0.66
2:F:4:THR:HB	2:F:7:GLU:OE2	1.94	0.66
2:F:63:HIS:CE1	3:F:147:HEM:C1D	2.84	0.66
1:G:66:LEU:CD2	1:G:132:VAL:HG21	2.25	0.66
1:G:31:ARG:HG2	2:H:127:GLN:OE1	1.95	0.66
1:G:47:ASP:O	1:G:52:SER:HB3	1.95	0.66
1:A:125:LEU:O	1:A:126:ASP:C	2.34	0.66
1:E:88:ALA:CA	1:E:140:TYR:CD2	2.78	0.66
1:E:22:GLY:O	1:E:26:ALA:N	2.27	0.66
1:E:66:LEU:HD12	3:E:142:HEM:HMB1	1.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:LEU:CD2	2:H:133:VAL:CG2	2.72	0.66
1:A:121:VAL:CB	1:A:121:VAL:N	2.56	0.66
1:A:20:HIS:H	1:A:20:HIS:HD2	1.39	0.66
2:B:41:PHE:CG	3:B:147:HEM:HAC	2.30	0.66
2:D:33:VAL:HG12	2:D:34:VAL:CG2	2.25	0.66
2:F:124:PRO:HD2	2:F:125:PRO:HD3	1.75	0.66
2:F:73:ASP:OD1	2:F:73:ASP:N	2.24	0.66
1:G:6:ASP:O	1:G:10:VAL:HG23	1.96	0.66
2:B:96:LEU:HD22	2:B:98:VAL:HG22	1.75	0.66
2:D:14:LEU:CD2	2:D:126:VAL:CG1	2.33	0.66
2:D:3:LEU:HD21	2:D:132:LYS:HB3	1.66	0.66
2:D:51:PRO:HA	2:D:54:VAL:CG2	2.25	0.66
2:H:33:VAL:CG1	2:H:51:PRO:HB3	2.25	0.66
1:A:127:LYS:O	1:A:130:ALA:CB	2.41	0.66
1:E:15:GLY:O	1:E:17:VAL:N	2.29	0.66
2:F:77:HIS:HB2	2:F:84:THR:HG21	1.78	0.66
2:H:22:GLU:CB	2:H:22:GLU:OE2	2.44	0.66
2:B:23:VAL:HG23	2:B:24:GLY:N	2.10	0.66
2:H:78:LEU:HD23	2:H:133:VAL:HG23	1.78	0.66
1:A:31:ARG:O	1:A:35:SER:N	2.25	0.65
1:A:126:ASP:OD2	1:C:141:ARG:NH1	2.30	0.65
1:C:7:LYS:HE3	1:C:73:VAL:HG12	1.77	0.65
2:D:14:LEU:HD11	2:D:130:TYR:CE2	2.31	0.65
2:D:72:SER:HB3	2:D:73:ASP:OD1	1.96	0.65
1:E:78:ASN:O	1:E:81:SER:CB	2.43	0.65
1:G:80:LEU:O	1:G:82:ALA:N	2.28	0.65
2:H:42:PHE:N	2:H:42:PHE:CD1	2.62	0.65
1:E:141:ARG:O	1:E:141:ARG:HD2	1.95	0.65
2:F:40:ARG:NE	2:F:40:ARG:CG	2.59	0.65
2:B:30:ARG:CD	2:B:30:ARG:CB	2.71	0.65
1:C:43:PHE:CD2	1:C:46:PHE:CG	2.82	0.65
2:D:49:SER:OG	2:D:53:ALA:HB2	1.96	0.65
1:G:33:PHE:CZ	1:G:43:PHE:CE1	2.84	0.65
2:H:8:LYS:HG2	2:H:78:LEU:HD11	1.77	0.65
2:B:96:LEU:O	2:B:97:HIS:CB	2.40	0.65
1:C:68:ASN:OD1	1:C:72:HIS:CD2	2.49	0.65
2:D:101:GLU:C	2:D:104:ARG:HD2	2.15	0.65
2:D:42:PHE:HB3	2:D:45:PHE:CG	2.31	0.65
2:D:80:ASN:ND2	2:D:83:GLY:HA2	1.98	0.65
1:G:106:LEU:O	1:G:110:ALA:N	2.30	0.65
2:H:81:LEU:C	2:H:85:PHE:HE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:HG2	1:C:100:LEU:HD23	1.77	0.65
1:C:119:PRO:O	1:C:120:ALA:O	2.14	0.65
1:C:83:LEU:HD21	3:C:142:HEM:CMA	2.26	0.65
1:G:111:ALA:HB1	2:H:119:GLY:C	2.16	0.65
1:G:4:PRO:CG	1:G:5:ALA:H	2.03	0.65
1:G:79:ALA:O	1:G:80:LEU:C	2.35	0.65
2:D:71:PHE:O	2:D:75:LEU:CD1	2.45	0.65
1:E:105:LEU:O	1:E:109:LEU:N	2.26	0.65
2:F:63:HIS:CE1	3:F:147:HEM:ND	2.63	0.65
1:G:118:THR:HG22	1:G:120:ALA:C	2.17	0.65
2:D:110:LEU:O	2:D:110:LEU:HD23	1.91	0.65
2:F:3:LEU:HB3	2:F:8:LYS:HB2	1.78	0.65
2:B:41:PHE:CE2	2:B:98:VAL:HG12	2.31	0.65
2:B:59:LYS:CE	2:B:62:ALA:CB	2.75	0.65
1:C:136:LEU:N	1:C:136:LEU:HD23	2.11	0.65
2:F:19:ASN:O	2:F:23:VAL:N	2.26	0.65
2:H:17:LYS:HB3	2:H:118:PHE:CE2	2.32	0.65
1:A:137:THR:O	1:A:140:TYR:HB2	1.96	0.65
1:A:92:ARG:CB	2:D:37:TRP:HB2	2.27	0.65
1:E:14:TRP:CA	1:E:17:VAL:HG21	2.26	0.65
2:B:3:LEU:HD23	2:B:7:GLU:HB3	1.74	0.65
1:C:38:THR:N	1:C:38:THR:HG22	2.12	0.65
2:D:87:THR:CG2	2:D:88:LEU:H	2.10	0.65
2:D:91:LEU:CD1	2:D:95:LYS:HB3	2.27	0.65
1:E:93:VAL:HG11	3:E:142:HEM:CAC	2.27	0.64
2:F:70:ALA:O	2:F:73:ASP:CG	2.35	0.64
1:E:127:LYS:HG2	1:G:141:ARG:HD3	1.79	0.64
1:G:11:LYS:O	1:G:15:GLY:CA	2.45	0.64
1:G:77:PRO:O	1:G:81:SER:HB2	1.97	0.64
2:B:4:THR:CB	2:B:5:PRO:HD2	2.24	0.64
2:B:72:SER:O	2:B:75:LEU:HD12	1.97	0.64
1:E:127:LYS:HG2	1:G:141:ARG:CD	2.27	0.64
2:D:26:GLU:OE1	2:D:30:ARG:CZ	2.45	0.64
2:D:67:VAL:HG12	3:D:147:HEM:C4A	2.31	0.64
1:E:36:PHE:C	1:E:38:THR:N	2.50	0.64
1:E:75:ASP:OD2	1:E:78:ASN:OD1	2.15	0.64
1:C:66:LEU:CD2	1:C:129:LEU:HD21	2.20	0.64
1:E:101:LEU:O	1:E:101:LEU:CD2	2.40	0.64
2:H:31:LEU:CD2	2:H:106:LEU:CD2	2.75	0.64
1:A:134:THR:O	1:A:135:VAL:C	2.34	0.64
1:C:128:PHE:CE2	1:C:129:LEU:HD23	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:PHE:CD2	2:D:88:LEU:HD13	2.32	0.64
2:D:41:PHE:CE2	2:D:98:VAL:HG13	2.32	0.64
1:G:106:LEU:O	1:G:109:LEU:HB3	1.98	0.64
2:D:101:GLU:HA	2:D:104:ARG:CD	2.26	0.64
2:F:95:LYS:NZ	2:F:95:LYS:CD	2.57	0.64
1:A:92:ARG:HB3	2:D:37:TRP:HB2	1.80	0.64
1:C:43:PHE:HD2	1:C:46:PHE:CD2	2.15	0.64
1:E:141:ARG:HG2	2:H:36:PRO:HG3	1.79	0.64
1:A:16:LYS:HG3	1:A:116:GLU:OE2	1.97	0.64
2:B:113:VAL:HG12	2:B:114:LEU:N	2.07	0.64
1:C:38:THR:CB	1:C:38:THR:HA	2.13	0.64
2:B:38:THR:OG1	2:B:38:THR:CA	2.45	0.64
1:E:20:HIS:N	1:E:21:ALA:H	1.96	0.64
2:F:4:THR:CB	2:F:7:GLU:OE2	2.46	0.64
1:A:27:GLU:O	1:A:28:ALA:C	2.37	0.64
1:A:86:LEU:HD13	1:A:90:LYS:HZ1	1.59	0.64
2:B:131:GLN:NE2	2:B:131:GLN:HA	2.13	0.64
2:B:103:PHE:CE1	2:B:141:LEU:HD12	2.32	0.64
2:H:30:ARG:HG2	2:H:30:ARG:NE	2.12	0.64
2:H:92:HIS:HD2	2:H:98:VAL:HB	1.63	0.64
1:A:58:HIS:O	1:A:62:VAL:CA	2.46	0.63
2:B:128:ALA:O	2:B:131:GLN:HB2	1.98	0.63
2:D:80:ASN:HD22	2:D:83:GLY:CA	1.90	0.63
1:E:29:LEU:HD21	1:E:101:LEU:HG	1.81	0.63
1:E:47:ASP:OD1	1:E:49:SER:HB3	1.97	0.63
2:F:68:LEU:O	2:F:71:PHE:CB	2.37	0.63
1:G:75:ASP:C	1:G:77:PRO:CD	2.67	0.63
1:A:109:LEU:O	1:A:113:LEU:HB2	1.99	0.63
1:A:122:HIS:O	1:A:126:ASP:N	2.18	0.63
1:C:13:ALA:N	1:C:14:TRP:H	1.95	0.63
2:B:50:THR:O	2:B:54:VAL:CB	2.46	0.63
1:C:86:LEU:HD21	3:C:142:HEM:HBA2	1.81	0.63
2:D:24:GLY:HA2	2:D:68:LEU:HD21	1.81	0.63
1:E:106:LEU:HD13	1:E:106:LEU:HB2	1.79	0.63
1:E:39:THR:O	1:E:39:THR:OG1	2.16	0.63
1:E:95:PRO:HG3	1:E:137:THR:CG2	2.28	0.63
2:F:106:LEU:O	2:F:110:LEU:HB3	1.98	0.63
2:F:29:GLY:CA	2:F:55:MET:HE3	2.27	0.63
2:B:63:HIS:O	2:B:67:VAL:HG23	1.98	0.63
2:D:44:SER:HB3	2:D:45:PHE:CE2	2.31	0.63
2:F:81:LEU:HD13	2:F:137:VAL:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:SER:OG	2:D:49:SER:CA	2.45	0.63
2:D:84:THR:O	2:D:84:THR:OG1	2.14	0.63
1:E:6:ASP:HB3	1:E:124:SER:HG	1.59	0.63
1:G:27:GLU:O	1:G:31:ARG:CB	2.45	0.63
1:G:80:LEU:O	1:G:81:SER:C	2.36	0.63
1:G:83:LEU:HD23	1:G:136:LEU:HD11	1.79	0.63
1:G:87:HIS:CA	1:G:91:LEU:CD1	2.42	0.63
1:A:33:PHE:CD1	1:A:40:LYS:CG	2.80	0.63
1:A:88:ALA:HB2	1:A:139:LYS:HB3	1.79	0.63
1:C:30:GLU:OE2	1:C:50:HIS:HB2	1.98	0.63
1:E:36:PHE:O	1:E:37:PRO:C	2.34	0.63
1:G:87:HIS:ND1	1:G:91:LEU:HD13	2.10	0.63
2:H:73:ASP:O	2:H:76:ALA:HB3	1.96	0.63
1:C:78:ASN:CG	1:C:78:ASN:H	2.02	0.63
2:F:72:SER:O	2:F:75:LEU:CB	2.45	0.63
2:F:43:GLU:CD	1:G:92:ARG:NH1	2.46	0.63
1:A:33:PHE:CG	1:A:40:LYS:HG2	2.34	0.63
1:A:86:LEU:HD13	1:A:90:LYS:HZ2	1.64	0.63
2:D:63:HIS:HE1	3:D:147:HEM:C4D	2.16	0.63
2:D:5:PRO:HA	2:D:8:LYS:HB3	1.81	0.63
1:E:2:LEU:HD21	1:E:131:SER:OG	1.99	0.63
1:E:35:SER:CB	1:E:35:SER:HG	2.10	0.63
2:F:100:PRO:O	2:F:101:GLU:C	2.37	0.63
2:F:49:SER:C	2:F:50:THR:CG2	2.65	0.63
2:F:74:GLY:C	2:F:75:LEU:HD22	2.19	0.63
2:H:3:LEU:HD21	2:H:8:LYS:CE	2.15	0.63
2:B:131:GLN:NE2	2:B:131:GLN:CA	2.60	0.63
2:B:17:LYS:HB2	2:B:17:LYS:CE	2.21	0.63
1:E:102:SER:HB3	1:E:129:LEU:HD21	1.78	0.63
2:H:92:HIS:CD2	2:H:98:VAL:CG2	2.82	0.63
1:C:36:PHE:N	1:C:37:PRO:HD2	2.12	0.62
2:D:82:LYS:O	2:D:86:ALA:HB2	1.99	0.62
1:E:105:LEU:HD22	1:E:129:LEU:HD11	1.80	0.62
2:F:6:VAL:HA	2:F:9:SER:HB2	1.81	0.62
2:F:71:PHE:O	2:F:72:SER:C	2.38	0.62
1:G:21:ALA:O	1:G:22:GLY:C	2.36	0.62
1:G:87:HIS:CE1	1:G:91:LEU:HD11	2.34	0.62
2:H:78:LEU:HA	2:H:81:LEU:HD23	1.81	0.62
2:B:131:GLN:O	2:B:135:ALA:HB2	1.99	0.62
1:E:29:LEU:HD21	1:E:101:LEU:HD11	1.79	0.62
1:E:36:PHE:O	1:E:39:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:VAL:O	2:F:145:TYR:CZ	2.52	0.62
2:F:93:CYS:O	2:F:97:HIS:CA	2.47	0.62
2:B:50:THR:HB	2:B:53:ALA:H	1.65	0.62
1:E:93:VAL:CG1	3:E:142:HEM:HAC	2.29	0.62
1:E:47:ASP:N	1:E:54:GLN:OE1	2.32	0.62
2:H:63:HIS:O	2:H:66:LYS:HB2	1.99	0.62
1:A:3:SER:O	1:A:7:LYS:HB2	1.99	0.62
2:B:38:THR:OG1	2:B:38:THR:HG23	1.97	0.62
3:D:147:HEM:HHA	3:D:147:HEM:HBA2	1.81	0.62
1:E:127:LYS:HA	1:E:130:ALA:HB3	1.82	0.62
1:G:91:LEU:HD22	3:G:142:HEM:C1D	2.34	0.62
2:B:30:ARG:CA	2:B:30:ARG:CG	2.77	0.62
2:D:64:GLY:O	2:D:68:LEU:N	2.30	0.62
2:F:29:GLY:H	2:F:55:MET:CE	2.08	0.62
2:F:81:LEU:O	2:F:85:PHE:HB2	1.98	0.62
1:G:94:ASP:C	1:G:96:VAL:H	2.03	0.62
2:H:88:LEU:O	2:H:90:GLU:N	2.31	0.62
1:C:99:LYS:CG	1:C:99:LYS:O	2.48	0.62
2:D:110:LEU:HD23	2:D:111:VAL:N	2.15	0.62
2:F:24:GLY:HA3	2:F:68:LEU:CD1	2.26	0.62
2:H:92:HIS:C	2:H:96:LEU:HB2	2.19	0.62
2:B:72:SER:HA	2:B:75:LEU:HD12	1.79	0.62
2:B:92:HIS:HD2	2:B:103:PHE:HE1	1.48	0.62
1:C:117:PHE:O	1:C:118:THR:CA	2.47	0.62
2:F:70:ALA:O	2:F:73:ASP:OD1	2.18	0.62
2:H:39:GLN:O	2:H:40:ARG:C	2.38	0.62
1:A:139:LYS:O	1:A:141:ARG:CG	2.31	0.62
1:C:46:PHE:HD1	1:C:48:LEU:HD23	1.65	0.62
2:D:3:LEU:HD21	2:D:132:LYS:C	2.19	0.62
2:F:118:PHE:O	2:F:121:GLU:HB2	2.00	0.62
2:F:58:PRO:O	2:F:59:LYS:C	2.32	0.62
1:A:114:PRO:O	2:B:116:HIS:CD2	2.53	0.62
2:B:17:LYS:CB	2:B:17:LYS:CE	2.77	0.62
2:B:15:TRP:HA	2:B:18:VAL:H	1.64	0.62
1:C:38:THR:CB	1:C:38:THR:N	2.59	0.62
1:C:44:PRO:HG2	1:C:45:HIS:ND1	2.15	0.62
2:D:58:PRO:O	2:D:62:ALA:N	2.33	0.62
2:D:91:LEU:O	2:D:91:LEU:CD1	2.48	0.62
1:E:38:THR:CG2	1:E:39:THR:N	2.61	0.62
1:E:72:HIS:O	1:E:75:ASP:N	2.32	0.62
1:A:39:THR:O	1:A:40:LYS:C	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:TRP:C	2:B:17:LYS:N	2.52	0.61
2:D:101:GLU:O	2:D:104:ARG:HG3	1.99	0.61
2:D:72:SER:CB	2:D:73:ASP:OD1	2.48	0.61
1:G:30:GLU:CD	1:G:50:HIS:CG	2.72	0.61
1:C:40:LYS:HG3	1:C:40:LYS:HE2	1.80	0.61
1:G:101:LEU:CD1	1:G:101:LEU:HB2	2.29	0.61
2:B:95:LYS:CD	2:B:95:LYS:NZ	2.59	0.61
1:E:13:ALA:O	1:E:17:VAL:CG2	2.49	0.61
1:G:112:HIS:CB	1:G:112:HIS:N	2.59	0.61
1:C:123:ALA:HB2	2:D:34:VAL:HG22	1.82	0.61
1:C:99:LYS:HE2	1:C:100:LEU:HD21	1.82	0.61
2:D:14:LEU:CA	2:D:14:LEU:CD1	2.78	0.61
2:D:33:VAL:CG2	2:D:54:VAL:HG21	2.29	0.61
1:E:35:SER:HA	2:F:128:ALA:HB2	1.81	0.61
1:E:35:SER:HA	2:F:128:ALA:CB	2.30	0.61
2:F:30:ARG:HH11	2:F:30:ARG:HG3	1.57	0.61
2:F:50:THR:O	2:F:54:VAL:N	2.33	0.61
2:F:63:HIS:O	2:F:67:VAL:HB	2.01	0.61
2:H:133:VAL:O	2:H:133:VAL:HG13	2.00	0.61
2:B:72:SER:CA	2:B:75:LEU:HD12	2.30	0.61
2:B:85:PHE:HA	2:B:88:LEU:HD13	1.82	0.61
1:C:32:MET:SD	1:C:101:LEU:HD23	2.40	0.61
2:D:3:LEU:HD11	2:D:133:VAL:CG2	2.30	0.61
1:E:132:VAL:O	1:E:136:LEU:CD1	2.44	0.61
2:F:99:ASP:OD1	1:G:42:TYR:OH	2.18	0.61
1:G:20:HIS:O	1:G:23:GLU:CB	2.48	0.61
2:B:59:LYS:HE3	2:B:59:LYS:CA	2.30	0.61
1:C:42:TYR:CD1	1:C:93:VAL:HG22	2.35	0.61
1:E:39:THR:OG1	1:E:43:PHE:CE1	2.54	0.61
2:F:29:GLY:N	2:F:55:MET:HE1	2.15	0.61
1:A:36:PHE:CG	1:A:100:LEU:HD12	2.36	0.61
2:F:37:TRP:O	2:F:40:ARG:HB2	2.01	0.61
1:G:47:ASP:O	1:G:52:SER:CB	2.48	0.61
2:H:134:VAL:O	2:H:138:ALA:HB2	2.00	0.61
2:H:82:LYS:HD3	2:H:82:LYS:N	2.11	0.61
1:A:110:ALA:CB	2:B:115:ALA:CB	2.78	0.61
1:C:118:THR:HB	1:C:121:VAL:CG2	2.31	0.61
1:E:31:ARG:CG	2:F:124:PRO:HG3	2.30	0.61
1:E:31:ARG:HD3	2:F:127:GLN:OE1	2.00	0.61
2:F:31:LEU:HD13	2:F:109:VAL:HG22	1.83	0.61
1:G:94:ASP:O	1:G:96:VAL:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:HE	1:C:141:ARG:CG	2.13	0.61
2:F:91:LEU:CD2	2:F:96:LEU:HD12	2.30	0.61
1:G:88:ALA:HB2	1:G:140:TYR:HD2	1.60	0.61
1:G:30:GLU:OE2	1:G:50:HIS:CG	2.53	0.61
2:H:109:VAL:O	2:H:113:VAL:HG23	2.01	0.61
2:B:8:LYS:CA	2:B:8:LYS:CG	2.75	0.61
1:E:95:PRO:HB3	1:E:137:THR:HG21	1.83	0.61
1:G:118:THR:HG22	1:G:120:ALA:CA	2.30	0.61
2:H:92:HIS:CD2	2:H:103:PHE:CE1	2.89	0.61
1:A:42:TYR:CE1	1:A:93:VAL:HG22	2.36	0.60
1:G:116:GLU:O	1:G:121:VAL:HG21	2.00	0.60
1:A:17:VAL:HG13	1:A:24:TYR:CE1	2.36	0.60
2:F:33:VAL:HG22	2:F:51:PRO:HB3	1.80	0.60
2:F:4:THR:OG1	2:F:7:GLU:OE2	2.20	0.60
1:A:28:ALA:O	1:A:31:ARG:HB2	2.01	0.60
1:A:42:TYR:HB2	3:A:142:HEM:HBC1	1.84	0.60
2:D:54:VAL:O	2:D:57:ASN:CB	2.42	0.60
1:G:83:LEU:CD1	3:G:142:HEM:CMA	2.73	0.60
2:D:7:GLU:O	2:D:10:ALA:N	2.33	0.60
2:D:7:GLU:OE1	2:D:7:GLU:HA	2.01	0.60
1:E:32:MET:CG	1:E:32:MET:O	2.46	0.60
1:E:66:LEU:HD11	3:E:142:HEM:HBB2	1.83	0.60
1:E:98:PHE:CE1	3:E:142:HEM:CHC	2.84	0.60
1:G:101:LEU:CD1	1:G:101:LEU:HG	2.16	0.60
1:G:109:LEU:HD23	1:G:125:LEU:CD1	2.32	0.60
1:G:6:ASP:CG	1:G:127:LYS:HE3	2.20	0.60
1:A:53:ALA:N	1:A:56:LYS:HD3	2.17	0.60
1:C:36:PHE:HZ	1:C:103:HIS:HE1	1.49	0.60
1:C:55:VAL:HG12	1:C:56:LYS:N	2.05	0.60
2:D:131:GLN:C	2:D:131:GLN:HE21	2.04	0.60
1:E:44:PRO:HG2	1:E:45:HIS:ND1	2.16	0.60
2:H:84:THR:HG1	2:H:84:THR:CB	2.08	0.60
1:A:51:GLY:O	1:A:56:LYS:NZ	2.35	0.60
1:C:7:LYS:O	1:C:10:VAL:HG12	2.01	0.60
2:D:64:GLY:O	2:D:68:LEU:CD2	2.47	0.60
1:E:6:ASP:CB	1:E:124:SER:HG	2.12	0.60
2:F:136:GLY:O	2:F:140:ALA:HB2	2.00	0.60
1:G:29:LEU:HB2	1:G:101:LEU:CD1	2.31	0.60
1:G:3:SER:OG	1:G:5:ALA:HB3	2.02	0.60
2:H:80:ASN:ND2	2:H:83:GLY:CA	2.57	0.60
1:A:83:LEU:HD23	1:A:136:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:O	2:B:54:VAL:N	2.34	0.60
2:D:42:PHE:CB	2:D:45:PHE:CG	2.84	0.60
1:G:66:LEU:CG	1:G:132:VAL:HG21	2.32	0.60
1:G:47:ASP:OD1	1:G:49:SER:OG	2.20	0.60
1:G:93:VAL:O	1:G:140:TYR:OH	2.18	0.60
1:C:3:SER:HG	1:C:3:SER:CB	2.09	0.60
2:D:100:PRO:HB2	2:D:103:PHE:CE2	2.36	0.60
1:E:52:SER:HB2	1:E:54:GLN:CB	2.31	0.60
2:F:14:LEU:HD21	2:F:118:PHE:CG	2.37	0.60
2:H:99:ASP:C	2:H:101:GLU:H	2.05	0.60
2:H:122:PHE:CE1	2:H:126:VAL:HG13	2.37	0.60
1:C:16:LYS:NZ	1:C:113:LEU:HD23	2.16	0.60
2:D:93:CYS:HB2	2:D:145:TYR:CE1	2.36	0.60
1:E:141:ARG:HG2	2:H:36:PRO:CG	2.31	0.60
1:E:20:HIS:C	1:E:20:HIS:N	2.49	0.60
1:G:27:GLU:O	1:G:31:ARG:N	2.35	0.60
2:H:87:THR:O	2:H:90:GLU:N	2.32	0.60
1:A:106:LEU:HD13	1:A:129:LEU:HD12	1.84	0.60
1:A:36:PHE:CD1	1:A:100:LEU:CD1	2.85	0.60
2:F:28:LEU:HD23	2:F:60:VAL:HG13	1.84	0.60
2:F:8:LYS:HA	2:F:8:LYS:CG	2.32	0.60
1:C:42:TYR:CE1	1:C:93:VAL:HG22	2.37	0.59
2:D:128:ALA:HA	2:D:131:GLN:CG	2.31	0.59
2:D:23:VAL:O	2:D:23:VAL:CG1	2.49	0.59
1:E:86:LEU:O	1:E:87:HIS:O	2.19	0.59
1:E:103:HIS:HE1	2:F:131:GLN:OE1	1.85	0.59
2:F:33:VAL:HG21	2:F:51:PRO:CB	2.28	0.59
1:G:30:GLU:HG3	1:G:50:HIS:CE1	2.23	0.59
2:D:15:TRP:CE2	2:D:75:LEU:CD2	2.86	0.59
1:E:95:PRO:HG3	1:E:137:THR:HG21	1.84	0.59
1:G:76:MET:CE	1:G:131:SER:CB	2.80	0.59
1:G:46:PHE:CE2	3:G:142:HEM:O1D	2.43	0.59
2:H:98:VAL:CG1	2:H:102:ASN:OD1	2.47	0.59
2:H:8:LYS:HA	2:H:11:VAL:HG21	1.84	0.59
2:B:73:ASP:O	2:B:77:HIS:ND1	2.35	0.59
2:B:92:HIS:CD2	2:B:103:PHE:CE1	2.89	0.59
1:C:70:VAL:HA	1:C:73:VAL:CG2	2.31	0.59
2:D:10:ALA:CB	2:D:126:VAL:HG13	2.31	0.59
1:E:127:LYS:O	1:E:130:ALA:HB3	2.02	0.59
1:E:52:SER:C	1:E:54:GLN:N	2.56	0.59
2:F:4:THR:CG2	2:F:6:VAL:CG1	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:122:PHE:CD1	2:H:126:VAL:CG1	2.85	0.59
2:H:31:LEU:CD2	2:H:106:LEU:HD23	2.31	0.59
2:H:33:VAL:HG11	2:H:51:PRO:HB3	1.82	0.59
2:B:15:TRP:CE3	2:B:18:VAL:CG2	2.80	0.59
1:G:33:PHE:HZ	1:G:43:PHE:CZ	2.20	0.59
2:H:78:LEU:HD23	2:H:133:VAL:HG22	1.82	0.59
2:D:113:VAL:CG1	2:D:114:LEU:N	2.64	0.59
2:D:3:LEU:CD1	2:D:133:VAL:CG2	2.76	0.59
1:A:29:LEU:CG	1:A:101:LEU:HD12	2.32	0.59
1:A:4:PRO:O	1:A:7:LYS:HB3	2.03	0.59
2:B:59:LYS:O	2:B:62:ALA:CB	2.50	0.59
2:B:67:VAL:O	2:B:70:ALA:HB3	2.03	0.59
1:C:70:VAL:CA	1:C:73:VAL:HG23	2.31	0.59
1:E:29:LEU:CD2	1:E:101:LEU:HD11	2.32	0.59
3:G:142:HEM:HHD	3:G:142:HEM:HBC2	1.85	0.59
2:H:124:PRO:O	2:H:127:GLN:CB	2.50	0.59
1:A:87:HIS:HB3	1:A:136:LEU:HD13	1.85	0.59
1:C:43:PHE:CD2	1:C:46:PHE:CD2	2.91	0.59
1:E:100:LEU:N	1:E:100:LEU:HD23	2.17	0.59
1:E:101:LEU:HD23	1:E:104:CYS:SG	2.43	0.59
1:E:2:LEU:HA	1:E:127:LYS:HZ3	1.66	0.59
2:F:1:VAL:CG1	2:F:132:LYS:HG3	2.33	0.59
2:H:123:THR:CB	2:H:125:PRO:HD2	2.31	0.59
2:H:47:ASP:OD2	2:H:49:SER:OG	2.15	0.59
1:A:113:LEU:N	1:A:114:PRO:HD3	2.18	0.59
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.67	0.59
1:E:42:TYR:HB2	1:E:43:PHE:CE1	2.38	0.59
1:C:16:LYS:NZ	1:C:116:GLU:HG3	2.14	0.59
2:F:43:GLU:OE1	1:G:92:ARG:NH1	2.35	0.59
2:H:123:THR:CG2	2:H:123:THR:CA	2.75	0.59
2:H:25:GLY:O	2:H:29:GLY:N	2.35	0.59
1:E:141:ARG:CG	2:H:36:PRO:HG3	2.31	0.59
2:H:92:HIS:CA	2:H:96:LEU:HB2	2.32	0.59
2:B:38:THR:CB	2:B:38:THR:HG1	2.10	0.59
2:D:127:GLN:O	2:D:127:GLN:HG2	2.02	0.59
2:D:40:ARG:HG2	2:D:41:PHE:CE1	2.38	0.59
2:D:64:GLY:O	2:D:65:LYS:C	2.38	0.59
1:E:7:LYS:HE2	1:E:74:ASP:OD1	2.03	0.59
2:H:31:LEU:HD23	2:H:106:LEU:HD22	1.83	0.59
2:H:39:GLN:C	2:H:41:PHE:N	2.57	0.59
2:H:71:PHE:CE2	2:H:75:LEU:CD1	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASN:N	1:C:79:ALA:N	2.50	0.58
2:D:33:VAL:O	2:D:33:VAL:HG12	2.02	0.58
1:G:17:VAL:CG1	1:G:24:TYR:CD1	2.85	0.58
1:A:10:VAL:CG1	1:A:128:PHE:HB2	2.32	0.58
2:B:15:TRP:O	2:B:16:GLY:C	2.40	0.58
2:B:59:LYS:NZ	2:B:59:LYS:CA	2.65	0.58
1:C:48:LEU:HA	1:C:52:SER:HG	1.68	0.58
1:G:32:MET:CA	1:G:32:MET:HG2	2.32	0.58
1:G:87:HIS:ND1	1:G:91:LEU:HD11	2.18	0.58
1:A:20:HIS:O	1:A:23:GLU:N	2.30	0.58
1:A:72:HIS:O	1:A:75:ASP:N	2.28	0.58
1:A:88:ALA:CB	1:A:139:LYS:HB3	2.33	0.58
1:C:36:PHE:HE1	1:C:104:CYS:SG	2.26	0.58
1:E:36:PHE:O	1:E:38:THR:N	2.35	0.58
2:F:48:LEU:CG	2:F:48:LEU:CA	2.75	0.58
1:A:42:TYR:CD1	1:A:93:VAL:HG22	2.38	0.58
3:D:147:HEM:CBA	3:D:147:HEM:HHA	2.34	0.58
2:D:93:CYS:HB2	2:D:145:TYR:CD1	2.37	0.58
1:G:76:MET:HE1	1:G:131:SER:CB	2.33	0.58
1:G:42:TYR:CE1	1:G:93:VAL:CG1	2.86	0.58
2:H:124:PRO:O	2:H:127:GLN:HB3	2.04	0.58
2:H:20:VAL:HG12	2:H:65:LYS:HA	1.83	0.58
2:H:78:LEU:CB	2:H:81:LEU:HD21	2.32	0.58
1:A:43:PHE:HA	1:A:45:HIS:CE1	2.39	0.58
1:C:24:TYR:O	1:C:28:ALA:HB2	2.04	0.58
2:D:15:TRP:CE2	2:D:75:LEU:HD23	2.39	0.58
1:G:32:MET:CB	1:G:33:PHE:N	2.67	0.58
1:G:64:ASP:O	1:G:65:ALA:C	2.42	0.58
2:B:111:VAL:HG12	2:B:111:VAL:O	1.97	0.58
2:B:23:VAL:CG2	2:B:24:GLY:N	2.67	0.58
1:E:29:LEU:HD11	1:E:58:HIS:HD2	1.69	0.58
1:G:11:LYS:O	1:G:15:GLY:N	2.37	0.58
1:C:36:PHE:HE1	1:C:104:CYS:HG	1.52	0.58
2:D:91:LEU:O	2:D:95:LYS:HB2	2.03	0.58
1:E:88:ALA:CA	1:E:140:TYR:CE2	2.82	0.58
1:G:59:GLY:O	1:G:63:ALA:N	2.33	0.58
2:H:17:LYS:CB	2:H:118:PHE:CE2	2.86	0.58
2:H:82:LYS:CD	2:H:82:LYS:N	2.64	0.58
2:B:39:GLN:HG3	2:B:48:LEU:HD12	1.84	0.58
2:B:4:THR:HG23	2:B:5:PRO:CG	2.34	0.58
2:B:92:HIS:ND1	2:B:96:LEU:CD1	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLU:CD	1:C:108:THR:HG22	2.24	0.58
1:E:2:LEU:HD23	1:E:2:LEU:N	2.19	0.58
1:E:27:GLU:O	1:E:31:ARG:N	2.37	0.58
1:G:118:THR:HG22	1:G:121:VAL:H	1.67	0.58
2:H:35:TYR:HE2	2:H:109:VAL:HG23	1.69	0.58
2:H:81:LEU:O	2:H:85:PHE:CD1	2.57	0.58
2:B:59:LYS:CE	2:B:62:ALA:HB2	2.34	0.58
1:C:118:THR:HG22	1:C:121:VAL:CA	2.30	0.58
2:D:128:ALA:HA	2:D:131:GLN:HB2	1.85	0.58
2:D:128:ALA:CA	2:D:131:GLN:HB2	2.34	0.58
2:D:34:VAL:C	2:D:36:PRO:HD3	2.23	0.58
2:D:91:LEU:O	2:D:91:LEU:HD12	2.04	0.58
1:E:2:LEU:C	1:E:3:SER:O	2.41	0.58
1:E:43:PHE:CD1	1:E:43:PHE:N	2.71	0.58
2:F:20:VAL:CA	2:F:68:LEU:HD13	2.34	0.58
1:G:81:SER:HG	1:G:81:SER:CB	2.10	0.58
2:H:123:THR:O	2:H:126:VAL:N	2.37	0.58
2:B:136:GLY:O	2:B:140:ALA:CB	2.51	0.58
1:C:118:THR:O	1:C:118:THR:N	2.36	0.58
1:C:125:LEU:O	1:C:126:ASP:C	2.42	0.58
1:C:130:ALA:HA	1:C:133:SER:HG	1.68	0.58
2:D:24:GLY:CA	2:D:68:LEU:HD23	2.33	0.58
2:F:34:VAL:O	1:G:141:ARG:HG2	2.04	0.58
2:H:4:THR:HG22	2:H:5:PRO:N	2.19	0.58
2:H:67:VAL:HG13	3:H:147:HEM:C1B	2.39	0.58
1:C:20:HIS:O	1:C:23:GLU:CB	2.52	0.57
2:H:123:THR:HG22	2:H:124:PRO:CD	2.12	0.57
1:A:83:LEU:CD1	3:A:142:HEM:HMA1	2.26	0.57
1:E:126:ASP:OD2	1:G:141:ARG:CZ	2.52	0.57
2:F:124:PRO:CD	2:F:125:PRO:CD	2.82	0.57
2:F:39:GLN:HG3	2:F:48:LEU:HD13	1.85	0.57
1:A:122:HIS:O	1:A:123:ALA:C	2.41	0.57
1:A:114:PRO:O	2:B:116:HIS:NE2	2.37	0.57
2:B:71:PHE:CE1	2:B:137:VAL:HG21	2.39	0.57
2:B:38:THR:C	2:B:38:THR:N	2.50	0.57
2:D:42:PHE:HB3	2:D:45:PHE:CD2	2.39	0.57
2:F:4:THR:HG22	2:F:6:VAL:CG1	2.34	0.57
1:G:61:LYS:O	3:G:142:HEM:HMA3	2.04	0.57
1:C:105:LEU:O	1:C:109:LEU:HB2	2.04	0.57
2:D:103:PHE:CE1	2:D:141:LEU:HD12	2.38	0.57
1:E:86:LEU:O	1:E:87:HIS:C	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:VAL:HG13	1:G:125:LEU:CD2	2.34	0.57
1:G:128:PHE:O	1:G:128:PHE:CD1	2.57	0.57
1:G:66:LEU:CD1	1:G:132:VAL:CG2	2.54	0.57
2:D:81:LEU:O	2:D:82:LYS:C	2.42	0.57
1:E:29:LEU:CD1	1:E:58:HIS:HD2	2.17	0.57
1:E:86:LEU:HD11	1:E:90:LYS:CD	2.20	0.57
2:F:17:LYS:NZ	2:F:121:GLU:OE1	2.36	0.57
2:F:26:GLU:O	2:F:30:ARG:CB	2.41	0.57
2:F:58:PRO:O	2:F:62:ALA:CB	2.50	0.57
1:C:40:LYS:HG3	1:C:40:LYS:CE	2.31	0.57
2:F:124:PRO:CB	2:F:125:PRO:HD3	2.34	0.57
2:F:1:VAL:CG2	2:F:132:LYS:O	2.53	0.57
1:G:98:PHE:HE2	1:G:140:TYR:HH	1.52	0.57
2:B:42:PHE:O	2:B:45:PHE:CB	2.51	0.57
2:D:10:ALA:HB1	2:D:126:VAL:CG1	2.32	0.57
1:G:118:THR:CG2	1:G:120:ALA:CA	2.83	0.57
1:G:29:LEU:CD1	1:G:33:PHE:CE2	2.86	0.57
1:C:17:VAL:O	1:C:19:ALA:N	2.37	0.57
2:D:97:HIS:C	2:D:98:VAL:HG22	2.24	0.57
1:E:123:ALA:O	1:E:126:ASP:CB	2.48	0.57
1:G:91:LEU:CD2	3:G:142:HEM:C3D	2.88	0.57
1:A:98:PHE:CZ	3:A:142:HEM:CHC	2.87	0.57
2:B:33:VAL:HG23	2:B:54:VAL:HG11	1.87	0.57
2:B:60:VAL:HG12	2:B:61:LYS:N	2.15	0.57
1:C:118:THR:CG2	1:C:120:ALA:CB	2.75	0.57
1:C:134:THR:O	1:C:135:VAL:C	2.41	0.57
1:E:44:PRO:CG	1:E:45:HIS:H	2.01	0.57
1:G:103:HIS:O	1:G:107:VAL:HG23	2.04	0.57
1:G:107:VAL:CG1	2:H:112:CYS:CB	2.82	0.57
1:G:129:LEU:N	1:G:129:LEU:HD23	2.10	0.57
1:A:36:PHE:CZ	1:A:100:LEU:HD13	2.40	0.57
1:C:104:CYS:CA	1:C:107:VAL:CG2	2.81	0.57
1:E:11:LYS:C	1:E:11:LYS:CB	2.70	0.57
2:F:1:VAL:HB	2:F:132:LYS:CG	2.35	0.57
2:H:28:LEU:O	2:H:29:GLY:C	2.43	0.57
2:H:55:MET:SD	2:H:55:MET:N	2.78	0.57
2:H:68:LEU:N	2:H:68:LEU:C	2.53	0.57
2:H:69:GLY:HA2	2:H:72:SER:OG	2.05	0.57
1:A:20:HIS:O	1:A:21:ALA:C	2.44	0.56
1:A:40:LYS:O	1:A:41:THR:CA	2.52	0.56
1:A:46:PHE:CD1	1:A:54:GLN:HG2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:HB1	2:B:119:GLY:CA	2.32	0.56
1:E:102:SER:HA	1:E:105:LEU:HD13	1.87	0.56
1:G:112:HIS:C	1:G:113:LEU:HD12	2.25	0.56
1:G:33:PHE:HZ	1:G:43:PHE:CE1	2.22	0.56
2:H:114:LEU:HD23	2:H:118:PHE:HD1	1.66	0.56
2:F:81:LEU:HD13	2:F:137:VAL:CA	2.35	0.56
2:F:82:LYS:NZ	2:F:82:LYS:CD	2.60	0.56
2:H:123:THR:O	2:H:127:GLN:N	2.37	0.56
2:H:78:LEU:CD2	2:H:133:VAL:HG23	2.34	0.56
2:H:20:VAL:HG12	2:H:65:LYS:HB3	1.85	0.56
2:H:35:TYR:N	2:H:36:PRO:CD	2.68	0.56
1:A:118:THR:N	1:A:121:VAL:HB	2.21	0.56
1:C:107:VAL:HG12	2:D:112:CYS:SG	2.43	0.56
1:C:102:SER:OG	1:C:129:LEU:CD1	2.53	0.56
1:C:47:ASP:O	1:C:52:SER:HB3	2.05	0.56
2:D:112:CYS:O	2:D:115:ALA:N	2.38	0.56
2:F:94:ASP:OD1	2:F:146:HIS:CD2	2.58	0.56
2:F:24:GLY:N	2:F:68:LEU:HD11	2.20	0.56
2:H:130:TYR:O	2:H:134:VAL:CG2	2.45	0.56
2:H:68:LEU:N	2:H:69:GLY:N	2.53	0.56
2:D:58:PRO:HA	2:D:61:LYS:CG	2.35	0.56
2:F:24:GLY:CA	2:F:68:LEU:HD12	2.31	0.56
1:G:2:LEU:HB3	1:G:6:ASP:HB2	1.86	0.56
1:A:36:PHE:CD1	1:A:100:LEU:HD13	2.39	0.56
2:F:81:LEU:HD22	2:F:85:PHE:CE1	2.37	0.56
1:A:121:VAL:C	1:A:121:VAL:N	2.56	0.56
2:B:131:GLN:HE21	2:B:131:GLN:CA	2.18	0.56
2:D:25:GLY:CA	2:D:61:LYS:HA	2.35	0.56
1:E:137:THR:OG1	1:E:137:THR:CG2	2.50	0.56
1:E:29:LEU:O	1:E:32:MET:HB3	2.06	0.56
1:G:17:VAL:O	1:G:20:HIS:N	2.38	0.56
2:B:88:LEU:HD22	2:H:6:VAL:HG22	1.87	0.56
1:A:38:THR:O	1:A:41:THR:CB	2.53	0.56
2:D:85:PHE:CB	2:D:88:LEU:HB3	2.35	0.56
2:F:1:VAL:HG11	2:F:132:LYS:CG	2.35	0.56
1:G:67:THR:O	1:G:68:ASN:C	2.44	0.56
2:H:15:TRP:O	2:H:15:TRP:CD1	2.58	0.56
2:B:1:VAL:C	2:B:2:HIS:CG	2.79	0.56
1:C:130:ALA:CA	1:C:133:SER:OG	2.49	0.56
1:G:35:SER:C	1:G:37:PRO:HD3	2.26	0.56
1:G:84:SER:OG	1:G:136:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:O	1:A:129:LEU:C	2.43	0.56
1:A:62:VAL:HG13	1:A:62:VAL:O	2.05	0.56
1:A:3:SER:O	1:A:7:LYS:HG2	2.06	0.56
2:B:41:PHE:CZ	2:B:102:ASN:OD1	2.58	0.56
2:F:89:SER:OG	2:F:141:LEU:O	2.19	0.56
1:C:93:VAL:CG1	3:C:142:HEM:CAC	2.74	0.56
1:C:36:PHE:O	1:C:39:THR:HG23	2.06	0.56
1:C:50:HIS:CD2	1:C:50:HIS:C	2.77	0.56
2:D:101:GLU:N	2:D:104:ARG:HH11	2.01	0.56
2:F:3:LEU:HD13	2:F:8:LYS:CA	2.35	0.56
1:G:109:LEU:HD23	1:G:125:LEU:HD13	1.88	0.56
2:H:88:LEU:CD2	2:H:91:LEU:HD23	2.35	0.56
1:A:52:SER:C	1:A:56:LYS:HD2	2.25	0.56
1:A:59:GLY:O	1:A:62:VAL:C	2.44	0.56
2:D:114:LEU:O	2:D:115:ALA:C	2.41	0.56
2:D:33:VAL:HG12	2:D:34:VAL:HG22	1.87	0.56
2:D:4:THR:CB	2:D:4:THR:HG1	2.09	0.56
2:D:4:THR:CA	2:D:4:THR:OG1	2.49	0.56
2:D:64:GLY:O	2:D:67:VAL:N	2.38	0.56
2:F:17:LYS:HB3	2:F:118:PHE:CZ	2.40	0.56
1:G:80:LEU:HD11	1:G:132:VAL:CG1	2.31	0.56
1:G:31:ARG:HG3	2:H:127:GLN:OE1	2.06	0.56
2:H:8:LYS:HG2	2:H:78:LEU:CD1	2.36	0.56
2:H:80:ASN:OD1	2:H:83:GLY:CA	2.53	0.56
2:B:115:ALA:HA	2:B:122:PHE:CD2	2.42	0.55
2:B:146:HIS:H	2:B:146:HIS:CD2	2.13	0.55
2:B:21:ASP:OD1	2:B:65:LYS:HE3	2.06	0.55
2:D:14:LEU:CA	2:D:14:LEU:HD12	2.36	0.55
2:F:110:LEU:C	2:F:110:LEU:CB	2.67	0.55
2:F:41:PHE:CE1	3:F:147:HEM:HBC1	2.40	0.55
2:F:1:VAL:HG11	2:F:132:LYS:HG3	1.87	0.55
2:H:98:VAL:O	2:H:99:ASP:CA	2.53	0.55
2:B:3:LEU:HD21	2:B:129:ALA:HB1	1.88	0.55
1:C:101:LEU:HD13	1:C:105:LEU:HD12	1.88	0.55
2:D:136:GLY:O	2:D:140:ALA:N	2.40	0.55
1:E:17:VAL:HG13	1:E:24:TYR:CE1	2.40	0.55
1:G:67:THR:C	1:G:69:ALA:N	2.54	0.55
1:C:106:LEU:O	1:C:110:ALA:CA	2.54	0.55
1:C:129:LEU:O	1:C:133:SER:OG	2.21	0.55
1:C:97:ASN:O	1:C:98:PHE:C	2.38	0.55
2:D:112:CYS:O	2:D:115:ALA:CB	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:LEU:HD11	2:D:32:LEU:CD1	2.36	0.55
2:D:57:ASN:HB3	2:D:60:VAL:HB	1.88	0.55
1:G:118:THR:HG22	1:G:120:ALA:CB	2.30	0.55
2:B:103:PHE:CE2	2:B:141:LEU:HD12	2.39	0.55
2:B:50:THR:OG1	2:B:53:ALA:CB	2.54	0.55
1:C:42:TYR:CE1	1:C:93:VAL:HG13	2.41	0.55
2:F:31:LEU:CD1	2:F:109:VAL:HG21	2.34	0.55
1:E:31:ARG:HG3	2:F:124:PRO:HG3	1.89	0.55
2:F:20:VAL:CG2	2:F:21:ASP:OD1	2.55	0.55
1:G:30:GLU:OE2	1:G:50:HIS:CD2	2.58	0.55
2:H:135:ALA:C	2:H:138:ALA:HB3	2.27	0.55
2:B:101:GLU:O	2:B:104:ARG:N	2.40	0.55
2:B:92:HIS:CA	2:B:96:LEU:CD1	2.73	0.55
2:F:50:THR:O	2:F:53:ALA:CB	2.52	0.55
1:G:20:HIS:O	1:G:23:GLU:HB2	2.07	0.55
1:A:2:LEU:N	1:A:2:LEU:CD2	2.59	0.55
1:A:8:THR:HG22	1:A:8:THR:O	2.06	0.55
1:C:119:PRO:CD	1:C:120:ALA:H	2.19	0.55
2:D:124:PRO:CD	2:D:125:PRO:HD2	2.36	0.55
1:A:87:HIS:CB	1:A:136:LEU:HD13	2.35	0.55
1:A:88:ALA:CB	1:A:139:LYS:CB	2.84	0.55
1:A:84:SER:HA	1:A:136:LEU:HD22	1.87	0.55
2:B:32:LEU:O	2:B:39:GLN:NE2	2.40	0.55
2:B:41:PHE:CD2	2:B:98:VAL:HG12	2.41	0.55
1:C:75:ASP:O	1:C:78:ASN:N	2.39	0.55
1:C:42:TYR:CZ	1:C:93:VAL:HG13	2.42	0.55
2:D:77:HIS:HB3	2:D:84:THR:HG21	1.89	0.55
1:G:28:ALA:CA	1:G:108:THR:HG21	2.37	0.55
2:H:15:TRP:CG	2:H:15:TRP:O	2.59	0.55
1:A:31:ARG:HD3	2:B:124:PRO:HA	1.89	0.55
2:B:103:PHE:CE1	2:B:141:LEU:CD1	2.89	0.55
1:C:26:ALA:HB1	1:C:55:VAL:CG1	2.37	0.55
2:F:89:SER:O	2:F:90:GLU:C	2.44	0.55
2:F:91:LEU:HD23	2:F:96:LEU:HD12	1.88	0.55
1:G:79:ALA:O	1:G:82:ALA:HB2	1.99	0.55
1:A:83:LEU:O	1:A:136:LEU:HD21	2.06	0.55
3:B:147:HEM:HBA2	3:B:147:HEM:HHA	1.89	0.55
2:B:7:GLU:O	2:B:11:VAL:N	2.36	0.55
2:D:17:LYS:H	2:D:17:LYS:CD	2.16	0.55
1:G:94:ASP:C	1:G:96:VAL:N	2.60	0.55
2:H:26:GLU:O	2:H:30:ARG:CD	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:TRP:HH2	1:C:141:ARG:HH21	1.55	0.54
1:C:70:VAL:HG23	1:C:128:PHE:CE1	2.41	0.54
1:E:134:THR:C	1:E:137:THR:H	2.10	0.54
1:E:14:TRP:HE1	1:E:67:THR:HG1	1.54	0.54
2:F:12:THR:O	2:F:16:GLY:N	2.39	0.54
1:G:121:VAL:C	1:G:124:SER:OG	2.46	0.54
1:A:98:PHE:CE1	3:A:142:HEM:HHC	2.42	0.54
2:B:88:LEU:CD2	2:H:6:VAL:HG22	2.37	0.54
2:D:21:ASP:CG	2:D:65:LYS:HG2	2.28	0.54
1:E:17:VAL:O	1:E:20:HIS:N	2.26	0.54
1:C:32:MET:O	1:C:36:PHE:HB2	2.08	0.54
2:D:44:SER:CB	2:D:45:PHE:HD2	2.19	0.54
2:D:68:LEU:N	2:D:68:LEU:CD1	2.54	0.54
2:F:42:PHE:O	2:F:48:LEU:HD11	2.07	0.54
2:H:8:LYS:HA	2:H:11:VAL:CG2	2.37	0.54
1:A:137:THR:HG22	1:A:138:SER:N	2.21	0.54
1:C:58:HIS:O	1:C:61:LYS:HB3	2.06	0.54
1:E:106:LEU:HD22	1:E:106:LEU:CD1	2.38	0.54
2:H:99:ASP:C	2:H:101:GLU:N	2.60	0.54
1:C:118:THR:HB	1:C:121:VAL:CB	2.28	0.54
1:E:36:PHE:O	1:E:39:THR:CG2	2.55	0.54
2:H:92:HIS:CG	2:H:103:PHE:HZ	2.25	0.54
1:A:76:MET:O	1:A:77:PRO:C	2.45	0.54
1:C:62:VAL:O	1:C:65:ALA:CB	2.38	0.54
2:D:31:LEU:HD13	2:D:106:LEU:HB2	1.90	0.54
1:C:111:ALA:HB2	2:D:115:ALA:O	2.08	0.54
2:B:96:LEU:CD2	2:B:98:VAL:CG2	2.69	0.54
1:E:13:ALA:O	1:E:16:LYS:CB	2.54	0.54
1:E:36:PHE:C	1:E:38:THR:H	2.11	0.54
2:F:11:VAL:HA	2:F:130:TYR:CE2	2.42	0.54
1:G:126:ASP:O	1:G:129:LEU:HB2	2.07	0.54
2:F:37:TRP:CE2	1:G:94:ASP:OD1	2.61	0.54
2:H:88:LEU:HD22	2:H:91:LEU:HD23	1.90	0.54
2:H:93:CYS:HB2	2:H:145:TYR:CG	2.43	0.54
1:C:118:THR:N	1:C:121:VAL:HB	2.23	0.54
1:C:78:ASN:N	1:C:78:ASN:C	2.56	0.54
1:E:83:LEU:O	1:E:87:HIS:ND1	2.34	0.54
1:E:98:PHE:CE1	3:E:142:HEM:HHC	2.43	0.54
1:G:117:PHE:O	1:G:117:PHE:CD2	2.61	0.54
1:G:95:PRO:HA	1:G:98:PHE:HD2	0.71	0.54
2:H:4:THR:CB	2:H:7:GLU:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:THR:O	1:C:137:THR:CG2	2.54	0.54
2:D:68:LEU:N	2:D:68:LEU:HD22	2.18	0.54
2:D:85:PHE:HD2	2:D:88:LEU:HD13	1.72	0.54
2:H:85:PHE:CE2	2:H:137:VAL:HG13	2.43	0.54
2:H:66:LYS:O	2:H:66:LYS:HG3	2.08	0.54
1:A:111:ALA:HB2	2:B:115:ALA:O	2.08	0.54
1:C:48:LEU:HA	1:C:52:SER:OG	2.08	0.54
2:F:100:PRO:HD3	2:F:145:TYR:CZ	2.43	0.54
1:G:111:ALA:CB	2:H:119:GLY:O	2.56	0.54
1:A:38:THR:O	1:A:41:THR:OG1	2.19	0.53
1:C:3:SER:CA	1:C:3:SER:OG	2.54	0.53
2:D:72:SER:HA	2:D:75:LEU:CD2	2.37	0.53
1:E:104:CYS:O	1:E:107:VAL:HB	2.08	0.53
2:F:124:PRO:N	2:F:125:PRO:HD2	2.23	0.53
1:G:29:LEU:CD1	1:G:33:PHE:HE2	2.20	0.53
1:G:35:SER:O	1:G:36:PHE:CD2	2.62	0.53
2:H:11:VAL:HG23	2:H:12:THR:H	1.73	0.53
2:H:66:LYS:HB3	2:H:67:VAL:CG2	2.35	0.53
2:H:99:ASP:N	2:H:99:ASP:HA	2.07	0.53
1:A:118:THR:H	1:A:121:VAL:HB	1.74	0.53
1:A:86:LEU:HD13	1:A:90:LYS:CE	2.38	0.53
2:B:38:THR:N	2:B:39:GLN:N	2.55	0.53
2:B:92:HIS:O	2:B:98:VAL:HG23	2.09	0.53
2:D:39:GLN:O	2:D:42:PHE:N	2.38	0.53
2:H:48:LEU:HD23	2:H:48:LEU:N	2.23	0.53
1:C:101:LEU:CD1	1:C:105:LEU:HD12	2.38	0.53
2:D:107:GLY:O	2:D:111:VAL:HG21	2.04	0.53
1:E:140:TYR:O	1:E:141:ARG:HB3	2.07	0.53
1:G:83:LEU:HB3	1:G:136:LEU:HD21	1.91	0.53
1:E:96:VAL:CG2	2:H:101:GLU:CD	2.69	0.53
1:E:96:VAL:HG21	2:H:101:GLU:HG2	1.81	0.53
2:H:112:CYS:O	2:H:115:ALA:HB3	2.08	0.53
1:A:53:ALA:HA	1:A:56:LYS:CD	2.17	0.53
2:D:93:CYS:SG	2:D:146:HIS:NE2	2.80	0.53
1:E:107:VAL:CA	1:E:110:ALA:CB	2.86	0.53
2:F:89:SER:HB2	2:F:144:LYS:HG2	1.89	0.53
1:A:31:ARG:HH11	2:B:127:GLN:HB2	1.74	0.53
1:C:93:VAL:O	1:C:94:ASP:C	2.41	0.53
2:D:117:HIS:N	2:D:117:HIS:ND1	2.51	0.53
2:D:42:PHE:HB3	2:D:45:PHE:CD1	2.43	0.53
2:D:72:SER:O	2:D:75:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:VAL:HG13	1:E:125:LEU:CD2	2.22	0.53
1:E:127:LYS:HA	1:E:130:ALA:CB	2.38	0.53
1:E:9:ASN:HB2	1:E:124:SER:OG	2.07	0.53
2:F:37:TRP:CZ2	2:F:105:LEU:HD11	2.43	0.53
2:F:77:HIS:O	2:F:80:ASN:N	2.34	0.53
2:F:7:GLU:HB3	2:F:129:ALA:HB1	1.89	0.53
1:G:75:ASP:CA	1:G:77:PRO:HD2	2.39	0.53
1:A:53:ALA:N	1:A:56:LYS:CD	2.71	0.53
2:B:12:THR:CB	2:B:12:THR:HG1	2.12	0.53
2:B:41:PHE:CD1	3:B:147:HEM:CAC	2.92	0.53
1:E:132:VAL:C	1:E:136:LEU:HD12	2.29	0.53
1:E:33:PHE:CE2	1:E:48:LEU:HD21	2.44	0.53
2:F:124:PRO:HD2	2:F:125:PRO:CD	2.38	0.53
1:G:91:LEU:CD2	3:G:142:HEM:C2D	2.91	0.53
2:B:27:ALA:O	2:B:109:VAL:HG11	2.09	0.53
1:C:95:PRO:HA	1:C:98:PHE:CD2	2.43	0.53
2:D:101:GLU:CB	2:D:104:ARG:CD	2.83	0.53
2:D:35:TYR:CE2	2:D:105:LEU:HD22	2.44	0.53
2:D:15:TRP:NE1	2:D:75:LEU:CD2	2.72	0.53
1:G:112:HIS:C	1:G:113:LEU:CD1	2.77	0.53
1:G:87:HIS:CG	1:G:91:LEU:HD12	2.30	0.53
1:G:91:LEU:HD21	3:G:142:HEM:C4D	2.43	0.53
1:A:42:TYR:CE1	1:A:93:VAL:HA	2.44	0.53
1:A:76:MET:CB	1:A:77:PRO:HD3	2.39	0.53
2:D:49:SER:OG	2:D:50:THR:N	2.42	0.53
1:E:106:LEU:O	1:E:110:ALA:CB	2.43	0.53
2:F:20:VAL:HG22	2:F:21:ASP:OD1	2.08	0.53
1:G:117:PHE:CB	1:G:117:PHE:N	2.60	0.53
1:G:2:LEU:CA	1:G:6:ASP:OD2	2.56	0.53
1:G:93:VAL:O	1:G:98:PHE:HE2	1.92	0.53
2:B:35:TYR:HB3	2:B:37:TRP:CH2	2.43	0.53
2:B:15:TRP:NE1	2:B:72:SER:HB3	2.21	0.53
1:C:51:GLY:O	1:C:52:SER:C	2.47	0.53
2:D:4:THR:O	2:D:7:GLU:HB2	2.09	0.53
2:F:90:GLU:OE1	2:F:90:GLU:CB	2.57	0.53
2:H:117:HIS:HB3	2:H:118:PHE:CD1	2.44	0.53
1:E:141:ARG:HG3	2:H:37:TRP:HZ3	1.72	0.53
2:H:76:ALA:HB1	2:H:77:HIS:ND1	2.24	0.53
1:A:76:MET:HA	1:A:76:MET:HG2	1.88	0.53
2:B:35:TYR:C	2:B:37:TRP:H	2.13	0.53
2:D:63:HIS:CE1	2:D:67:VAL:HG13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:C	1:E:110:ALA:HB2	2.27	0.53
2:F:29:GLY:C	2:F:55:MET:SD	2.86	0.53
1:A:98:PHE:CE1	3:A:142:HEM:CHC	2.91	0.52
2:D:20:VAL:O	2:D:20:VAL:HG12	2.07	0.52
2:D:3:LEU:HA	2:D:132:LYS:HD2	1.90	0.52
2:D:51:PRO:O	2:D:55:MET:CB	2.53	0.52
2:F:11:VAL:HG23	2:F:130:TYR:CZ	2.44	0.52
3:G:142:HEM:HHD	3:G:142:HEM:CBC	2.39	0.52
2:H:3:LEU:CD1	2:H:78:LEU:O	2.57	0.52
2:H:48:LEU:N	2:H:48:LEU:CD2	2.73	0.52
1:C:39:THR:O	1:C:42:TYR:HB2	2.08	0.52
2:D:63:HIS:NE2	3:D:147:HEM:C1D	2.76	0.52
2:D:45:PHE:HB2	2:D:48:LEU:HD11	1.89	0.52
2:F:24:GLY:CA	2:F:68:LEU:CD1	2.88	0.52
1:G:117:PHE:CD1	1:G:117:PHE:CA	2.93	0.52
2:H:32:LEU:H	2:H:32:LEU:HD13	1.74	0.52
2:H:3:LEU:HD22	2:H:8:LYS:CE	2.33	0.52
2:H:92:HIS:HD2	2:H:98:VAL:CG2	2.22	0.52
3:A:142:HEM:CMB	3:A:142:HEM:HBB2	2.40	0.52
1:A:17:VAL:O	1:A:19:ALA:N	2.42	0.52
1:A:3:SER:OG	1:A:4:PRO:N	2.37	0.52
2:B:48:LEU:N	2:B:48:LEU:HD23	2.24	0.52
1:C:101:LEU:HD13	1:C:101:LEU:O	2.09	0.52
1:C:118:THR:H	1:C:118:THR:HB	1.74	0.52
1:C:83:LEU:HD21	3:C:142:HEM:C3A	2.45	0.52
2:D:33:VAL:HG12	2:D:34:VAL:HG23	1.90	0.52
2:D:87:THR:HG22	2:D:88:LEU:H	1.73	0.52
1:E:78:ASN:HA	1:E:81:SER:OG	2.10	0.52
2:F:98:VAL:HG13	2:F:102:ASN:OD1	2.09	0.52
1:C:102:SER:CB	1:C:129:LEU:CD1	2.88	0.52
2:D:85:PHE:O	2:D:89:SER:N	2.42	0.52
1:E:68:ASN:O	1:E:72:HIS:HD2	1.92	0.52
1:G:42:TYR:HB2	3:G:142:HEM:HBC1	1.90	0.52
2:H:22:GLU:C	2:H:22:GLU:CG	2.77	0.52
2:D:31:LEU:HB3	2:D:32:LEU:HD12	1.91	0.52
1:E:38:THR:HG23	1:E:39:THR:H	1.68	0.52
2:H:103:PHE:C	2:H:103:PHE:N	2.56	0.52
1:A:17:VAL:CG1	1:A:17:VAL:O	2.43	0.52
1:E:129:LEU:CD2	1:E:129:LEU:C	2.78	0.52
1:G:39:THR:O	1:G:43:PHE:HE1	1.92	0.52
1:G:47:ASP:OD1	1:G:47:ASP:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:VAL:HA	1:G:76:MET:HG3	1.90	0.52
1:G:103:HIS:NE2	2:H:108:ASN:HB3	2.25	0.52
1:A:4:PRO:CG	1:A:5:ALA:N	2.68	0.52
1:A:62:VAL:O	1:A:62:VAL:HG22	2.10	0.52
2:B:50:THR:HG22	2:B:51:PRO:CD	2.40	0.52
1:C:37:PRO:O	1:C:40:LYS:CG	2.58	0.52
2:D:101:GLU:CA	2:D:104:ARG:NH1	2.34	0.52
2:D:49:SER:CB	2:D:49:SER:H	2.19	0.52
1:E:86:LEU:HD12	1:E:90:LYS:HB2	1.92	0.52
1:G:117:PHE:CG	1:G:117:PHE:C	2.83	0.52
2:B:20:VAL:C	2:B:22:GLU:H	2.12	0.52
1:C:32:MET:SD	1:C:101:LEU:CD2	2.98	0.52
1:C:119:PRO:HG3	2:D:30:ARG:CZ	2.40	0.52
2:D:131:GLN:O	2:D:131:GLN:NE2	2.43	0.52
1:G:43:PHE:HD1	1:G:43:PHE:N	2.08	0.52
1:A:99:LYS:C	1:A:100:LEU:HD23	2.29	0.52
1:C:118:THR:HG22	1:C:120:ALA:C	2.22	0.52
1:C:137:THR:O	1:C:137:THR:HG22	2.10	0.52
1:C:31:ARG:NH1	1:C:31:ARG:CG	2.68	0.52
1:C:37:PRO:O	1:C:40:LYS:HE2	2.10	0.52
1:C:46:PHE:HD1	1:C:48:LEU:CD2	2.22	0.52
1:C:90:LYS:HG2	1:C:91:LEU:CG	2.40	0.52
1:E:55:VAL:O	1:E:56:LYS:C	2.43	0.52
2:F:89:SER:CB	2:F:144:LYS:HG2	2.40	0.52
1:A:31:ARG:HD2	2:B:127:GLN:OE1	2.10	0.52
1:C:1:VAL:O	1:C:1:VAL:HG12	2.10	0.52
1:C:37:PRO:HG2	1:C:38:THR:HG22	1.91	0.52
1:C:58:HIS:O	1:C:61:LYS:CB	2.58	0.52
2:D:123:THR:HB	2:D:125:PRO:CD	2.37	0.52
2:D:15:TRP:O	2:D:18:VAL:N	2.40	0.52
2:D:88:LEU:HD21	3:D:147:HEM:HMA1	1.91	0.52
1:E:112:HIS:O	1:E:113:LEU:HG	2.06	0.52
2:F:35:TYR:CD1	2:F:37:TRP:CH2	2.98	0.52
2:H:117:HIS:CD2	2:H:118:PHE:CD2	2.97	0.52
2:B:50:THR:C	2:B:54:VAL:HG23	2.18	0.51
2:B:75:LEU:HA	2:B:78:LEU:HD22	1.92	0.51
2:D:128:ALA:HA	2:D:131:GLN:CB	2.39	0.51
1:E:1:VAL:O	1:E:127:LYS:NZ	2.39	0.51
2:F:26:GLU:HA	2:F:55:MET:CE	2.34	0.51
1:G:101:LEU:O	1:G:105:LEU:HB2	2.11	0.51
1:G:32:MET:C	1:G:32:MET:HB3	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:LEU:HA	2:H:117:HIS:HB2	1.92	0.51
2:H:125:PRO:CG	2:H:126:VAL:N	2.57	0.51
2:H:20:VAL:CG1	2:H:65:LYS:HA	2.39	0.51
2:B:1:VAL:CA	2:B:2:HIS:ND1	2.74	0.51
2:D:142:ALA:CB	2:D:142:ALA:C	2.68	0.51
1:E:120:ALA:O	1:E:123:ALA:CB	2.57	0.51
1:E:122:HIS:CE1	2:F:30:ARG:CD	2.92	0.51
1:E:30:GLU:OE2	1:E:50:HIS:CE1	2.64	0.51
2:H:123:THR:CB	2:H:124:PRO:HD2	2.40	0.51
1:A:126:ASP:O	1:A:129:LEU:N	2.43	0.51
1:A:36:PHE:CD1	1:A:100:LEU:HD12	2.45	0.51
2:B:124:PRO:O	2:B:127:GLN:HB3	2.10	0.51
2:B:28:LEU:HD11	2:B:32:LEU:HD21	1.89	0.51
1:C:20:HIS:O	1:C:23:GLU:HB3	2.10	0.51
1:E:15:GLY:C	1:E:17:VAL:N	2.62	0.51
2:F:91:LEU:HD23	2:F:91:LEU:C	2.31	0.51
1:G:20:HIS:O	1:G:23:GLU:CA	2.58	0.51
1:G:11:LYS:HA	1:G:70:VAL:HG21	1.92	0.51
2:H:86:ALA:CB	2:H:144:LYS:HE3	2.35	0.51
1:A:134:THR:O	1:A:138:SER:OG	2.25	0.51
2:B:136:GLY:O	2:B:140:ALA:HB2	2.10	0.51
2:D:50:THR:HB	2:D:51:PRO:CD	2.40	0.51
1:G:123:ALA:HB2	2:H:34:VAL:HG22	1.93	0.51
1:G:131:SER:O	1:G:134:THR:HB	2.10	0.51
1:G:46:PHE:C	1:G:48:LEU:CD2	2.78	0.51
2:H:65:LYS:O	2:H:69:GLY:N	2.43	0.51
1:A:10:VAL:HG11	1:A:128:PHE:HB2	1.91	0.51
1:A:30:GLU:OE1	1:A:50:HIS:CE1	2.62	0.51
1:C:70:VAL:O	1:C:73:VAL:HG23	2.11	0.51
2:D:24:GLY:HA3	2:D:68:LEU:HD23	1.88	0.51
1:E:128:PHE:C	1:E:131:SER:HB2	2.31	0.51
2:H:99:ASP:O	2:H:102:ASN:OD1	2.28	0.51
2:H:67:VAL:C	2:H:69:GLY:N	2.64	0.51
2:H:79:ASP:C	2:H:79:ASP:OD2	2.49	0.51
2:B:45:PHE:CZ	2:B:60:VAL:HA	2.45	0.51
2:D:101:GLU:CG	2:D:104:ARG:CD	2.88	0.51
1:E:35:SER:CA	2:F:128:ALA:HB2	2.41	0.51
2:F:109:VAL:HA	2:F:112:CYS:HB2	1.92	0.51
1:A:112:HIS:C	1:A:113:LEU:HD23	2.29	0.51
2:D:101:GLU:CG	2:D:104:ARG:HD3	2.41	0.51
2:D:25:GLY:HA2	2:D:61:LYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:PHE:CE1	3:E:142:HEM:HBC1	2.45	0.51
1:E:19:ALA:O	1:E:20:HIS:CA	2.58	0.51
2:F:47:ASP:C	2:F:47:ASP:OD2	2.41	0.51
3:G:142:HEM:CHD	3:G:142:HEM:HBC2	2.40	0.51
2:B:37:TRP:HB2	1:C:92:ARG:HB3	1.92	0.51
1:C:81:SER:O	1:C:84:SER:HB3	2.11	0.51
1:C:90:LYS:CG	1:C:91:LEU:CD2	2.89	0.51
1:E:84:SER:HB3	1:E:136:LEU:HA	1.92	0.51
2:F:11:VAL:HA	2:F:130:TYR:CZ	2.46	0.51
1:E:31:ARG:HG2	2:F:124:PRO:HG3	1.92	0.51
2:H:127:GLN:CG	2:H:127:GLN:HA	2.38	0.51
2:H:60:VAL:O	2:H:60:VAL:HG13	2.11	0.51
2:H:21:ASP:OD2	2:H:65:LYS:HG3	2.03	0.51
2:B:91:LEU:HG	2:B:91:LEU:O	2.10	0.51
1:G:105:LEU:O	1:G:106:LEU:C	2.48	0.51
2:H:45:PHE:CD1	2:H:60:VAL:HG23	2.46	0.51
2:H:45:PHE:HD1	2:H:60:VAL:HG23	1.76	0.51
1:A:121:VAL:O	1:A:125:LEU:HB2	2.10	0.51
1:C:87:HIS:O	1:C:92:ARG:HA	2.12	0.51
2:F:77:HIS:CB	2:F:84:THR:HG21	2.41	0.51
2:H:123:THR:CG2	2:H:123:THR:HA	2.40	0.51
1:A:13:ALA:O	1:A:17:VAL:HG23	2.11	0.50
2:B:17:LYS:O	2:B:18:VAL:C	2.49	0.50
1:C:64:ASP:CG	1:C:64:ASP:HA	2.16	0.50
2:D:24:GLY:HA2	2:D:68:LEU:CD2	2.37	0.50
2:D:77:HIS:CA	2:D:77:HIS:CG	2.84	0.50
2:F:101:GLU:OE1	2:F:101:GLU:HA	1.92	0.50
1:G:36:PHE:O	1:G:39:THR:HG23	2.11	0.50
1:G:107:VAL:HG12	2:H:112:CYS:CB	2.41	0.50
1:A:8:THR:HG23	1:A:8:THR:O	2.10	0.50
2:B:41:PHE:CD1	3:B:147:HEM:HAC	2.46	0.50
2:B:74:GLY:C	2:B:76:ALA:H	2.14	0.50
2:D:113:VAL:CG1	2:D:114:LEU:CD2	2.77	0.50
2:D:11:VAL:CG1	2:D:12:THR:H	2.16	0.50
2:D:146:HIS:CD2	2:D:146:HIS:C	2.73	0.50
2:D:15:TRP:O	2:D:16:GLY:C	2.49	0.50
1:E:33:PHE:CE2	1:E:48:LEU:HD23	2.41	0.50
2:F:123:THR:OG1	2:F:126:VAL:HB	2.11	0.50
1:A:2:LEU:CD1	1:A:128:PHE:HA	2.41	0.50
1:A:66:LEU:O	1:A:70:VAL:CG2	2.48	0.50
1:A:86:LEU:HA	1:A:90:LYS:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:TRP:HZ3	1:C:141:ARG:HG3	1.76	0.50
1:C:97:ASN:HA	1:C:100:LEU:HB2	1.93	0.50
2:F:22:GLU:HG2	2:F:23:VAL:CA	2.38	0.50
2:H:30:ARG:HD3	2:H:113:VAL:HG13	1.92	0.50
1:G:110:ALA:CB	2:H:115:ALA:HB3	2.37	0.50
2:D:15:TRP:NE1	2:D:75:LEU:HD23	2.27	0.50
1:E:101:LEU:O	1:E:105:LEU:CD1	2.46	0.50
1:E:88:ALA:N	1:E:140:TYR:CE2	2.79	0.50
2:F:31:LEU:CD1	2:F:35:TYR:CE2	2.95	0.50
1:G:24:TYR:O	1:G:28:ALA:HB2	2.12	0.50
2:H:36:PRO:O	2:H:39:GLN:HB2	2.10	0.50
1:C:66:LEU:HD23	1:C:129:LEU:HD23	1.86	0.50
2:D:9:SER:O	2:D:13:ALA:N	2.42	0.50
2:D:15:TRP:CZ2	2:D:75:LEU:HD21	2.46	0.50
2:F:48:LEU:CD2	2:F:48:LEU:HB3	2.38	0.50
1:G:12:ALA:O	1:G:15:GLY:HA3	2.10	0.50
2:H:122:PHE:CE1	2:H:126:VAL:CG1	2.95	0.50
1:A:3:SER:OG	1:A:4:PRO:HD2	2.05	0.50
1:C:10:VAL:CG2	1:C:125:LEU:CD2	2.89	0.50
1:C:31:ARG:HG3	2:D:124:PRO:HA	1.94	0.50
1:E:137:THR:CB	1:E:137:THR:HG1	2.10	0.50
2:F:118:PHE:O	2:F:121:GLU:N	2.45	0.50
2:F:81:LEU:HD13	2:F:137:VAL:N	2.27	0.50
1:G:28:ALA:O	1:G:31:ARG:HB3	2.11	0.50
1:G:114:PRO:O	2:H:116:HIS:NE2	2.45	0.50
2:H:32:LEU:HD13	2:H:32:LEU:N	2.26	0.50
2:H:92:HIS:CG	2:H:103:PHE:CZ	3.00	0.50
1:A:7:LYS:HD2	1:A:73:VAL:HG22	1.94	0.50
1:A:111:ALA:HB1	2:B:119:GLY:C	2.32	0.50
1:C:119:PRO:HD2	1:C:120:ALA:H	1.76	0.50
2:D:35:TYR:N	2:D:36:PRO:HD3	2.26	0.50
2:D:15:TRP:CE2	2:D:75:LEU:HD21	2.47	0.50
2:F:146:HIS:C	1:G:40:LYS:NZ	2.65	0.50
2:F:20:VAL:HG23	2:F:21:ASP:N	2.19	0.50
2:H:11:VAL:CG2	2:H:12:THR:N	2.73	0.50
1:C:104:CYS:HA	1:C:107:VAL:HG23	1.89	0.50
2:H:8:LYS:O	2:H:11:VAL:HG23	2.12	0.50
1:A:17:VAL:O	1:A:20:HIS:N	2.45	0.50
2:D:39:GLN:O	2:D:40:ARG:C	2.51	0.50
1:E:102:SER:CB	1:E:129:LEU:CD2	2.66	0.50
2:F:72:SER:O	2:F:75:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:ALA:C	1:G:15:GLY:HA3	2.32	0.50
1:G:14:TRP:CA	1:G:14:TRP:HE3	2.05	0.50
1:G:46:PHE:O	1:G:48:LEU:HD21	2.12	0.50
2:H:124:PRO:HA	2:H:127:GLN:HB2	1.93	0.50
2:H:68:LEU:N	2:H:69:GLY:H	2.10	0.50
1:A:43:PHE:N	1:A:44:PRO:HD3	2.27	0.49
1:C:78:ASN:N	1:C:79:ALA:H	2.10	0.49
1:E:122:HIS:HE2	2:F:109:VAL:HG12	1.77	0.49
2:F:37:TRP:HE1	1:G:94:ASP:CG	2.06	0.49
1:G:17:VAL:HG13	1:G:24:TYR:CE1	2.46	0.49
1:G:98:PHE:O	1:G:102:SER:HB3	2.12	0.49
2:H:25:GLY:HA3	2:H:61:LYS:HG2	1.94	0.49
1:A:112:HIS:C	1:A:113:LEU:CG	2.79	0.49
1:A:86:LEU:O	1:A:87:HIS:C	2.47	0.49
1:C:33:PHE:CD1	1:C:40:LYS:HG2	2.47	0.49
1:G:32:MET:CG	1:G:32:MET:HA	2.41	0.49
1:A:43:PHE:HA	1:A:45:HIS:HE1	1.75	0.49
1:A:4:PRO:HA	1:A:7:LYS:CG	2.43	0.49
2:B:15:TRP:CH2	2:B:71:PHE:CD2	3.01	0.49
1:C:83:LEU:HA	1:C:86:LEU:HB3	1.93	0.49
1:G:101:LEU:O	1:G:105:LEU:N	2.40	0.49
1:G:3:SER:CB	1:G:4:PRO:HD2	2.32	0.49
1:G:76:MET:N	1:G:77:PRO:HD2	2.20	0.49
2:H:102:ASN:O	2:H:106:LEU:N	2.43	0.49
1:A:112:HIS:C	1:A:114:PRO:HD3	2.33	0.49
1:A:112:HIS:C	1:A:113:LEU:HG	2.31	0.49
2:B:58:PRO:HG2	2:B:59:LYS:N	2.27	0.49
2:D:123:THR:O	2:D:124:PRO:C	2.49	0.49
1:E:112:HIS:O	1:E:114:PRO:HD3	2.13	0.49
1:E:2:LEU:CA	1:E:127:LYS:HZ3	2.25	0.49
2:H:80:ASN:HD21	2:H:83:GLY:HA3	1.69	0.49
1:A:121:VAL:HG23	1:A:121:VAL:H	1.70	0.49
1:A:85:ASP:O	1:A:89:HIS:CD2	2.65	0.49
1:A:95:PRO:HB3	1:A:137:THR:OG1	2.12	0.49
1:A:94:ASP:OD2	1:A:96:VAL:CG2	2.60	0.49
2:B:20:VAL:HG21	2:B:72:SER:OG	2.13	0.49
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.13	0.49
2:D:32:LEU:HD21	2:D:42:PHE:CD1	2.39	0.49
2:D:3:LEU:HD23	2:D:132:LYS:CG	2.43	0.49
2:D:42:PHE:CB	2:D:45:PHE:CD1	2.95	0.49
2:D:47:ASP:OD2	2:D:49:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:LEU:CD1	2:H:32:LEU:N	2.75	0.49
1:A:16:LYS:HG3	1:A:116:GLU:CD	2.33	0.49
1:C:46:PHE:HB3	1:C:48:LEU:HD21	1.95	0.49
2:D:77:HIS:C	2:D:77:HIS:CB	2.72	0.49
1:E:2:LEU:HA	1:E:127:LYS:HZ2	1.76	0.49
2:F:124:PRO:N	2:F:125:PRO:HD3	2.26	0.49
1:G:114:PRO:HA	2:H:116:HIS:CD2	2.48	0.49
2:H:17:LYS:HB3	2:H:118:PHE:HE2	1.74	0.49
2:H:19:ASN:OD1	2:H:22:GLU:OE2	2.30	0.49
2:H:38:THR:C	2:H:40:ARG:N	2.60	0.49
2:H:47:ASP:O	2:H:53:ALA:HB1	2.13	0.49
1:A:87:HIS:CD2	1:A:136:LEU:HD11	2.34	0.49
1:A:55:VAL:HG23	1:A:56:LYS:N	2.28	0.49
2:B:102:ASN:HA	2:B:105:LEU:HD12	1.93	0.49
2:B:51:PRO:C	2:B:54:VAL:HB	2.33	0.49
2:B:58:PRO:HG2	2:B:59:LYS:H	1.77	0.49
1:C:105:LEU:O	1:C:109:LEU:N	2.46	0.49
1:C:83:LEU:C	1:C:86:LEU:HB3	2.32	0.49
2:D:103:PHE:CD1	2:D:141:LEU:HD12	2.48	0.49
2:F:1:VAL:CG1	2:F:132:LYS:CG	2.90	0.49
1:G:83:LEU:HD11	3:G:142:HEM:HMA2	1.88	0.49
2:B:98:VAL:O	2:B:145:TYR:CZ	2.65	0.49
1:E:121:VAL:O	1:E:121:VAL:HG12	2.04	0.49
2:F:124:PRO:HB2	2:F:125:PRO:HD3	1.95	0.49
2:H:4:THR:HB	2:H:7:GLU:HB3	1.73	0.49
2:H:79:ASP:OD2	2:H:80:ASN:N	2.46	0.49
2:H:92:HIS:O	2:H:96:LEU:CB	2.58	0.49
2:B:14:LEU:CD1	2:B:114:LEU:CD1	2.88	0.49
2:B:41:PHE:HZ	2:B:102:ASN:OD1	1.96	0.49
3:C:142:HEM:CMC	3:C:142:HEM:CBC	2.89	0.49
2:D:81:LEU:HD13	2:D:137:VAL:HG22	1.88	0.49
2:F:7:GLU:HB3	2:F:129:ALA:CB	2.43	0.49
2:B:92:HIS:CG	2:B:96:LEU:HD11	2.48	0.49
1:C:16:LYS:HG3	1:C:16:LYS:HE2	1.90	0.49
2:D:77:HIS:CB	2:D:84:THR:HG21	2.42	0.49
2:D:85:PHE:CA	2:D:88:LEU:HB3	2.43	0.49
2:F:31:LEU:HD11	2:F:35:TYR:CE2	2.48	0.49
2:H:134:VAL:O	2:H:134:VAL:HG12	2.12	0.49
2:H:61:LYS:NZ	2:H:61:LYS:HD3	2.28	0.49
1:C:124:SER:C	1:C:127:LYS:HB2	2.34	0.48
2:F:2:HIS:CG	2:F:2:HIS:O	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:LYS:HE2	2:B:17:LYS:CG	2.37	0.48
1:E:87:HIS:HA	1:E:91:LEU:HD12	1.95	0.48
2:H:46:GLY:O	2:H:48:LEU:CD2	2.58	0.48
1:A:92:ARG:HG2	2:D:37:TRP:CB	2.43	0.48
2:B:111:VAL:HG13	2:B:122:PHE:HZ	1.75	0.48
1:C:102:SER:OG	1:C:129:LEU:HD13	2.14	0.48
2:D:107:GLY:HA2	2:D:134:VAL:CG2	2.33	0.48
2:F:60:VAL:O	2:F:61:LYS:C	2.52	0.48
2:F:90:GLU:HB3	2:F:90:GLU:OE1	2.13	0.48
1:G:75:ASP:OD1	1:G:77:PRO:HD2	2.13	0.48
2:H:2:HIS:O	2:H:132:LYS:CD	2.61	0.48
1:A:141:ARG:HB3	1:A:141:ARG:CZ	2.44	0.48
2:B:118:PHE:O	2:B:121:GLU:HB2	2.13	0.48
2:B:103:PHE:HB2	2:B:138:ALA:HB1	1.94	0.48
2:B:15:TRP:CZ3	2:B:71:PHE:HE2	2.31	0.48
2:B:52:ASP:C	2:B:54:VAL:N	2.53	0.48
1:C:90:LYS:HG2	1:C:91:LEU:HG	1.94	0.48
1:C:31:ARG:CD	2:D:127:GLN:OE1	2.61	0.48
2:F:20:VAL:HG22	2:F:21:ASP:N	2.29	0.48
1:G:62:VAL:O	1:G:65:ALA:CB	2.58	0.48
1:G:61:LYS:O	1:G:65:ALA:HB2	2.14	0.48
2:H:114:LEU:CD2	2:H:118:PHE:CE1	2.87	0.48
2:B:18:VAL:HG12	2:B:18:VAL:C	2.33	0.48
2:B:38:THR:HB	2:B:41:PHE:HE1	1.77	0.48
1:C:88:ALA:O	1:C:92:ARG:HG2	2.13	0.48
2:D:124:PRO:HD2	2:D:125:PRO:HD2	1.95	0.48
2:D:49:SER:HG	2:D:53:ALA:HB2	1.78	0.48
1:E:139:LYS:HG2	1:E:139:LYS:HZ3	1.37	0.48
1:G:104:CYS:HA	1:G:107:VAL:HG23	1.96	0.48
1:G:90:LYS:O	1:G:91:LEU:C	2.50	0.48
2:H:101:GLU:O	2:H:104:ARG:HB2	2.13	0.48
2:B:89:SER:O	2:B:90:GLU:C	2.52	0.48
2:D:50:THR:HB	2:D:51:PRO:HD2	1.95	0.48
1:E:141:ARG:CG	2:H:37:TRP:CZ3	2.85	0.48
2:F:107:GLY:HA2	2:F:134:VAL:CG1	2.43	0.48
1:E:141:ARG:O	1:G:127:LYS:HD2	2.14	0.48
2:H:14:LEU:CD2	2:H:14:LEU:HD13	2.42	0.48
1:A:14:TRP:CH2	1:A:66:LEU:HD22	2.49	0.48
1:A:4:PRO:C	1:A:7:LYS:CB	2.82	0.48
2:B:119:GLY:C	2:B:121:GLU:H	2.16	0.48
2:B:130:TYR:O	2:B:134:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:SER:HA	2:B:75:LEU:HD11	1.95	0.48
2:D:42:PHE:HB2	2:D:45:PHE:CG	2.48	0.48
1:E:14:TRP:C	1:E:17:VAL:HB	2.34	0.48
1:E:69:ALA:C	1:E:71:ALA:N	2.61	0.48
2:F:35:TYR:O	2:F:37:TRP:N	2.47	0.48
2:H:42:PHE:O	2:H:45:PHE:HB2	2.14	0.48
2:H:67:VAL:C	2:H:69:GLY:H	2.16	0.48
1:A:62:VAL:O	1:A:62:VAL:CG1	2.59	0.48
2:F:2:HIS:CG	2:F:132:LYS:NZ	2.59	0.48
2:F:1:VAL:HG21	2:F:132:LYS:O	2.14	0.48
1:G:128:PHE:C	1:G:128:PHE:CD1	2.85	0.48
1:G:91:LEU:CD2	3:G:142:HEM:C4D	2.97	0.48
1:A:100:LEU:O	1:A:103:HIS:CB	2.44	0.48
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.19	0.48
1:C:121:VAL:O	1:C:125:LEU:HB2	2.14	0.48
1:C:37:PRO:O	1:C:40:LYS:HG3	2.14	0.48
1:E:6:ASP:HA	1:E:124:SER:HG	1.75	0.48
2:F:63:HIS:HA	2:F:66:LYS:HB2	1.96	0.48
2:B:47:ASP:C	2:B:48:LEU:HD23	2.34	0.48
1:C:43:PHE:HB3	1:C:46:PHE:HB2	1.96	0.48
2:F:67:VAL:HG22	3:F:147:HEM:C1B	2.49	0.48
2:H:60:VAL:HG12	2:H:61:LYS:N	2.16	0.48
1:A:42:TYR:C	1:A:44:PRO:HD3	2.34	0.47
1:C:27:GLU:CG	1:C:108:THR:HG22	2.39	0.47
1:C:94:ASP:HA	1:C:95:PRO:HD2	1.29	0.47
1:E:75:ASP:C	1:E:77:PRO:HD2	2.35	0.47
2:F:111:VAL:O	2:F:111:VAL:HG12	2.14	0.47
2:F:118:PHE:HB3	2:F:121:GLU:CB	2.44	0.47
2:H:77:HIS:C	2:H:79:ASP:H	2.17	0.47
1:A:135:VAL:O	1:A:136:LEU:C	2.51	0.47
1:C:46:PHE:HB3	1:C:48:LEU:CD2	2.44	0.47
1:C:86:LEU:HD21	3:C:142:HEM:CBA	2.44	0.47
2:D:21:ASP:CA	2:D:65:LYS:HG2	2.41	0.47
2:F:118:PHE:HB3	2:F:121:GLU:HB3	1.95	0.47
1:G:66:LEU:HD12	1:G:132:VAL:CG1	2.28	0.47
1:G:75:ASP:CG	1:G:77:PRO:HD2	2.35	0.47
2:H:141:LEU:N	2:H:141:LEU:HD22	2.27	0.47
2:H:20:VAL:C	2:H:24:GLY:H	2.02	0.47
2:H:36:PRO:O	2:H:39:GLN:CG	2.62	0.47
1:A:127:LYS:HE3	1:C:141:ARG:CB	2.43	0.47
1:A:42:TYR:CB	3:A:142:HEM:HBC1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:CYS:HB2	2:B:145:TYR:CD2	2.49	0.47
2:B:41:PHE:CD2	2:B:98:VAL:CG1	2.97	0.47
2:D:63:HIS:HE1	3:D:147:HEM:CHA	2.27	0.47
1:G:121:VAL:O	1:G:124:SER:N	2.46	0.47
2:H:11:VAL:HG22	2:H:11:VAL:H	0.95	0.47
2:H:31:LEU:CD2	2:H:106:LEU:CB	2.67	0.47
2:H:92:HIS:NE2	2:H:98:VAL:HG21	2.29	0.47
2:B:93:CYS:HB2	2:B:145:TYR:CD1	2.49	0.47
1:C:70:VAL:C	1:C:72:HIS:N	2.65	0.47
2:D:33:VAL:C	2:D:34:VAL:HG23	2.33	0.47
1:E:128:PHE:O	1:E:131:SER:CB	2.52	0.47
1:E:98:PHE:O	1:E:99:LYS:C	2.51	0.47
2:F:11:VAL:O	2:F:12:THR:C	2.52	0.47
2:H:93:CYS:HB2	2:H:145:TYR:CE2	2.50	0.47
1:A:112:HIS:C	1:A:113:LEU:CD2	2.83	0.47
3:C:142:HEM:HMC1	3:C:142:HEM:HBC2	1.96	0.47
1:C:43:PHE:CE2	1:C:46:PHE:CZ	3.02	0.47
2:D:124:PRO:N	2:D:125:PRO:CD	2.75	0.47
2:D:78:LEU:HD11	2:D:133:VAL:CG2	2.44	0.47
1:E:101:LEU:HD22	1:E:104:CYS:HB2	1.96	0.47
2:F:1:VAL:HG23	2:F:132:LYS:O	2.15	0.47
2:F:80:ASN:O	2:F:84:THR:CB	2.62	0.47
1:G:17:VAL:CG1	1:G:24:TYR:HD1	2.27	0.47
2:B:4:THR:OG1	2:B:5:PRO:HD2	2.15	0.47
2:B:77:HIS:HB2	2:B:84:THR:HG21	1.96	0.47
1:C:93:VAL:CG1	3:C:142:HEM:HAC	2.38	0.47
2:H:15:TRP:CE3	2:H:130:TYR:OH	2.67	0.47
2:H:72:SER:O	2:H:75:LEU:HB2	2.14	0.47
2:H:82:LYS:H	2:H:82:LYS:HD2	1.77	0.47
2:H:81:LEU:CA	2:H:85:PHE:HE1	2.27	0.47
1:A:38:THR:C	1:A:41:THR:H	2.17	0.47
2:B:4:THR:CB	2:B:7:GLU:HB2	2.45	0.47
2:D:137:VAL:HG12	2:D:138:ALA:N	2.29	0.47
2:D:50:THR:CB	2:D:51:PRO:HD2	2.43	0.47
2:D:21:ASP:OD2	2:D:65:LYS:HE3	2.15	0.47
2:F:107:GLY:CA	2:F:134:VAL:HG11	2.45	0.47
2:F:24:GLY:N	2:F:68:LEU:CD1	2.78	0.47
2:F:3:LEU:HD22	2:F:7:GLU:HB2	1.96	0.47
1:G:125:LEU:O	1:G:126:ASP:C	2.52	0.47
2:H:102:ASN:C	2:H:103:PHE:C	2.73	0.47
2:H:93:CYS:O	2:H:94:ASP:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:HIS:O	1:A:107:VAL:HB	2.14	0.47
1:C:128:PHE:CD2	1:C:129:LEU:HB2	2.49	0.47
1:C:29:LEU:HD11	1:C:62:VAL:HG21	1.97	0.47
1:C:90:LYS:HG3	1:C:91:LEU:CD2	2.45	0.47
2:F:4:THR:HG21	2:F:6:VAL:CG1	2.45	0.47
1:G:31:ARG:CG	1:G:31:ARG:HH21	2.21	0.47
3:A:142:HEM:HMB1	3:A:142:HEM:HBB2	1.95	0.47
1:C:97:ASN:O	1:C:101:LEU:N	2.44	0.47
2:D:110:LEU:O	2:D:114:LEU:HG	2.15	0.47
1:E:49:SER:O	1:E:50:HIS:C	2.52	0.47
2:F:114:LEU:CD2	2:F:114:LEU:C	2.75	0.47
3:A:142:HEM:HHA	3:A:142:HEM:HAA1	1.45	0.47
2:B:7:GLU:O	2:B:11:VAL:CB	2.62	0.47
2:H:41:PHE:N	2:H:41:PHE:CD1	2.82	0.47
2:H:81:LEU:HB3	2:H:85:PHE:CE1	2.50	0.47
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.43	0.47
2:B:38:THR:O	2:B:39:GLN:N	2.37	0.47
1:C:17:VAL:CG1	1:C:21:ALA:CA	2.87	0.47
2:D:101:GLU:CD	2:D:104:ARG:CD	2.83	0.47
2:D:65:LYS:HD2	2:D:65:LYS:NZ	2.27	0.47
1:E:42:TYR:OH	1:E:94:ASP:HB2	2.15	0.47
2:F:80:ASN:HD21	2:F:83:GLY:CA	2.23	0.47
2:F:96:LEU:HD22	3:F:147:HEM:CAD	2.45	0.47
1:G:116:GLU:O	1:G:121:VAL:HG11	2.14	0.47
1:G:127:LYS:HZ2	1:G:127:LYS:HG2	1.37	0.47
1:G:24:TYR:N	1:G:24:TYR:CD2	2.79	0.47
1:G:6:ASP:OD2	1:G:127:LYS:HE3	2.15	0.47
1:A:83:LEU:HD23	1:A:136:LEU:HD23	1.95	0.46
1:A:107:VAL:HG23	2:B:112:CYS:SG	2.55	0.46
2:B:32:LEU:O	2:B:36:PRO:HA	2.15	0.46
2:D:136:GLY:HA2	2:D:139:ASN:HB3	1.96	0.46
2:D:51:PRO:CA	2:D:54:VAL:CG2	2.84	0.46
1:G:38:THR:O	1:G:41:THR:OG1	2.25	0.46
1:G:111:ALA:HB2	2:H:119:GLY:O	2.15	0.46
1:A:42:TYR:OH	1:A:94:ASP:HB2	2.15	0.46
2:B:133:VAL:O	2:B:137:VAL:HG23	2.14	0.46
2:B:21:ASP:CB	2:B:65:LYS:HB2	2.42	0.46
1:C:55:VAL:HG12	1:C:56:LYS:HA	1.96	0.46
1:E:104:CYS:O	1:E:108:THR:N	2.49	0.46
1:G:17:VAL:C	1:G:19:ALA:N	2.69	0.46
1:A:27:GLU:O	1:A:30:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:CH2	1:A:66:LEU:CD2	2.98	0.46
2:B:132:LYS:O	2:B:135:ALA:HB3	2.16	0.46
2:B:3:LEU:CD2	2:B:3:LEU:HD13	2.43	0.46
2:B:41:PHE:CE2	2:B:98:VAL:CG1	2.99	0.46
1:C:46:PHE:CD1	1:C:48:LEU:CD2	2.98	0.46
1:C:43:PHE:HE2	1:C:46:PHE:CZ	2.33	0.46
1:C:4:PRO:CD	1:C:5:ALA:N	2.77	0.46
1:C:90:LYS:HG2	1:C:91:LEU:CD2	2.46	0.46
2:D:75:LEU:N	2:D:75:LEU:CD1	2.74	0.46
1:G:20:HIS:N	1:G:20:HIS:CD2	2.83	0.46
2:D:44:SER:OG	2:D:45:PHE:CD2	2.69	0.46
1:G:114:PRO:O	1:G:115:ALA:HB2	2.15	0.46
2:H:114:LEU:HD23	2:H:118:PHE:HE1	1.74	0.46
2:H:96:LEU:HD23	2:H:96:LEU:N	2.23	0.46
1:A:98:PHE:CD1	1:A:133:SER:CB	2.98	0.46
2:B:67:VAL:HG12	2:B:68:LEU:CD2	2.45	0.46
1:E:52:SER:C	1:E:54:GLN:H	2.19	0.46
2:F:3:LEU:HD13	2:F:8:LYS:HA	1.98	0.46
2:B:35:TYR:C	2:B:37:TRP:N	2.68	0.46
1:C:10:VAL:O	1:C:14:TRP:HB2	2.16	0.46
1:C:39:THR:HG1	1:C:39:THR:CB	2.16	0.46
2:D:66:LYS:HG2	2:D:66:LYS:O	2.16	0.46
1:G:36:PHE:N	1:G:37:PRO:CD	2.69	0.46
1:G:83:LEU:C	1:G:136:LEU:HD21	2.32	0.46
2:H:135:ALA:HA	2:H:138:ALA:HB3	1.97	0.46
1:C:107:VAL:HA	1:C:110:ALA:CB	2.32	0.46
1:C:26:ALA:HB1	1:C:55:VAL:HG11	1.98	0.46
1:C:43:PHE:HE2	1:C:46:PHE:CE2	2.34	0.46
1:C:4:PRO:CD	1:C:5:ALA:H	2.26	0.46
2:D:106:LEU:O	2:D:110:LEU:N	2.48	0.46
2:D:2:HIS:O	2:D:132:LYS:HD2	2.15	0.46
2:D:33:VAL:O	2:D:33:VAL:CG1	2.62	0.46
2:D:11:VAL:HG11	2:D:78:LEU:HD21	1.97	0.46
1:E:132:VAL:CG1	1:E:133:SER:N	2.73	0.46
2:F:110:LEU:CA	2:F:110:LEU:CG	2.82	0.46
1:G:114:PRO:O	2:H:116:HIS:CD2	2.69	0.46
1:G:13:ALA:C	1:G:15:GLY:N	2.60	0.46
2:B:143:HIS:O	2:B:143:HIS:CD2	2.68	0.46
1:C:32:MET:SD	1:C:101:LEU:HA	2.56	0.46
2:H:133:VAL:HG12	2:H:134:VAL:N	2.25	0.46
1:A:106:LEU:HD13	1:A:129:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASN:OD1	1:A:72:HIS:CD2	2.69	0.46
2:B:133:VAL:C	2:B:135:ALA:H	2.17	0.46
1:C:118:THR:O	1:C:121:VAL:CA	2.64	0.46
1:C:4:PRO:O	1:C:5:ALA:C	2.53	0.46
1:C:83:LEU:HD23	1:C:87:HIS:HE1	1.80	0.46
1:C:87:HIS:ND1	1:C:87:HIS:N	2.64	0.46
2:F:14:LEU:CD2	2:F:118:PHE:CD2	2.97	0.46
3:G:142:HEM:HMB1	3:G:142:HEM:CBB	2.41	0.46
2:H:69:GLY:O	2:H:70:ALA:C	2.54	0.46
1:A:134:THR:O	1:A:135:VAL:O	2.34	0.46
2:D:122:PHE:CE2	2:D:127:GLN:HG3	2.51	0.46
1:E:14:TRP:O	1:E:17:VAL:HB	2.15	0.46
2:F:50:THR:HA	2:F:51:PRO:HD3	1.78	0.46
2:F:3:LEU:HD13	2:F:8:LYS:HB2	1.98	0.46
1:G:118:THR:O	1:G:120:ALA:N	2.49	0.46
2:B:3:LEU:HD23	2:B:7:GLU:CB	2.45	0.45
2:B:74:GLY:C	2:B:76:ALA:N	2.69	0.45
1:C:102:SER:CA	1:C:129:LEU:CD1	2.94	0.45
1:C:104:CYS:CA	1:C:107:VAL:HG22	2.44	0.45
1:C:43:PHE:CE2	1:C:46:PHE:CE2	3.04	0.45
2:D:49:SER:OG	2:D:49:SER:C	2.54	0.45
1:A:42:TYR:OH	2:D:99:ASP:OD1	2.33	0.45
1:E:39:THR:O	1:E:43:PHE:HE1	1.92	0.45
1:E:86:LEU:HD12	1:E:90:LYS:CB	2.46	0.45
1:G:66:LEU:O	1:G:67:THR:CA	2.63	0.45
1:A:107:VAL:O	1:A:110:ALA:HB3	2.16	0.45
1:A:43:PHE:N	1:A:44:PRO:CD	2.79	0.45
2:B:123:THR:HB	2:B:124:PRO:HD2	1.98	0.45
2:B:43:GLU:C	2:B:45:PHE:N	2.49	0.45
1:C:88:ALA:O	1:C:92:ARG:CG	2.65	0.45
1:E:17:VAL:HG23	1:E:17:VAL:H	1.41	0.45
1:E:68:ASN:O	1:E:69:ALA:CA	2.64	0.45
1:G:95:PRO:CA	1:G:98:PHE:CD2	2.59	0.45
1:C:102:SER:CA	1:C:129:LEU:HD11	2.43	0.45
1:C:141:ARG:NH1	1:C:141:ARG:CD	2.77	0.45
2:D:135:ALA:O	2:D:139:ASN:CB	2.63	0.45
2:D:8:LYS:O	2:D:8:LYS:HG3	2.15	0.45
1:E:1:VAL:CG1	1:E:2:LEU:N	2.31	0.45
2:B:28:LEU:O	2:B:29:GLY:C	2.54	0.45
1:C:16:LYS:CD	1:C:116:GLU:CG	2.85	0.45
1:C:135:VAL:HG12	1:C:136:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ASP:OD1	1:C:124:SER:OG	2.34	0.45
2:D:66:LYS:CG	2:D:66:LYS:O	2.62	0.45
1:E:127:LYS:HE2	1:E:127:LYS:HB3	1.48	0.45
1:G:47:ASP:OD1	1:G:48:LEU:N	2.49	0.45
2:B:96:LEU:CG	2:B:98:VAL:CG2	2.92	0.45
2:D:135:ALA:O	2:D:139:ASN:HB2	2.17	0.45
2:F:75:LEU:N	2:F:75:LEU:HD22	2.32	0.45
1:G:106:LEU:HD12	1:G:125:LEU:HB2	1.99	0.45
2:H:141:LEU:HD13	2:H:141:LEU:HA	1.55	0.45
2:B:59:LYS:CE	2:B:62:ALA:HB1	2.47	0.45
2:D:93:CYS:HG	2:D:146:HIS:CD2	2.34	0.45
2:D:72:SER:HB2	2:D:73:ASP:OD1	2.16	0.45
2:F:35:TYR:CE2	2:F:105:LEU:HD22	2.51	0.45
2:F:58:PRO:HA	2:F:61:LYS:HD3	1.98	0.45
2:H:76:ALA:CB	2:H:77:HIS:ND1	2.80	0.45
1:A:133:SER:O	1:A:137:THR:N	2.50	0.45
1:A:4:PRO:C	1:A:7:LYS:HB3	2.37	0.45
2:B:88:LEU:N	2:B:88:LEU:HD12	2.31	0.45
1:C:113:LEU:HD22	1:C:116:GLU:HB2	1.93	0.45
2:D:13:ALA:C	2:D:15:TRP:N	2.69	0.45
2:D:32:LEU:CD2	2:D:42:PHE:CD1	2.98	0.45
2:F:101:GLU:O	2:F:104:ARG:CB	2.62	0.45
2:F:7:GLU:HA	2:F:10:ALA:HB3	1.98	0.45
1:G:16:LYS:HE3	1:G:116:GLU:OE2	2.16	0.45
1:G:80:LEU:O	1:G:82:ALA:C	2.55	0.45
2:H:107:GLY:HA3	2:H:134:VAL:HG11	1.97	0.45
2:H:17:LYS:CB	2:H:118:PHE:HE2	2.26	0.45
1:A:100:LEU:HD22	1:A:100:LEU:HA	1.44	0.45
1:A:117:PHE:CD2	2:B:116:HIS:CD2	3.04	0.45
2:D:63:HIS:NE2	3:D:147:HEM:ND	2.64	0.45
1:E:78:ASN:O	1:E:81:SER:OG	2.34	0.45
2:F:35:TYR:O	2:F:36:PRO:C	2.54	0.45
2:H:126:VAL:O	2:H:127:GLN:C	2.53	0.45
2:H:3:LEU:HD13	2:H:78:LEU:O	2.17	0.45
1:A:98:PHE:CZ	1:A:136:LEU:HD12	2.52	0.45
1:C:124:SER:O	1:C:127:LYS:HB2	2.17	0.45
1:C:131:SER:O	1:C:132:VAL:C	2.54	0.45
2:D:25:GLY:HA3	2:D:61:LYS:HA	1.97	0.45
1:E:35:SER:CB	2:F:131:GLN:HG3	2.47	0.45
2:F:6:VAL:HA	2:F:9:SER:CB	2.47	0.45
1:C:79:ALA:C	1:C:81:SER:H	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:HE2	1:C:100:LEU:HD23	1.98	0.45
2:D:105:LEU:HA	2:D:105:LEU:HD23	1.87	0.45
2:D:106:LEU:O	2:D:109:VAL:N	2.50	0.45
2:D:16:GLY:C	2:D:18:VAL:H	2.21	0.45
2:D:21:ASP:CB	2:D:65:LYS:HG2	2.47	0.45
2:D:21:ASP:OD2	2:D:65:LYS:CE	2.65	0.45
2:D:93:CYS:HB2	2:D:145:TYR:CZ	2.52	0.45
2:F:107:GLY:CA	2:F:134:VAL:CG1	2.95	0.45
1:G:76:MET:HE1	1:G:131:SER:HB3	1.99	0.45
2:H:84:THR:HB	2:H:85:PHE:CD1	2.52	0.45
1:A:94:ASP:OD2	1:A:96:VAL:HG23	2.17	0.44
2:B:38:THR:O	2:B:41:PHE:HD1	2.00	0.44
2:B:67:VAL:HG12	2:B:68:LEU:HD21	1.98	0.44
1:E:43:PHE:N	1:E:44:PRO:CD	2.77	0.44
1:G:34:LEU:HD22	2:H:125:PRO:HA	1.99	0.44
2:H:133:VAL:O	2:H:137:VAL:HG23	2.17	0.44
2:H:17:LYS:HB2	2:H:118:PHE:CZ	2.51	0.44
2:H:24:GLY:O	2:H:27:ALA:HB3	2.17	0.44
2:B:101:GLU:O	2:B:104:ARG:CA	2.65	0.44
1:C:101:LEU:CD1	1:C:105:LEU:CD1	2.95	0.44
1:C:4:PRO:HA	1:C:7:LYS:HG3	1.98	0.44
2:D:121:GLU:C	2:D:123:THR:N	2.70	0.44
2:D:17:LYS:CD	2:D:17:LYS:N	2.80	0.44
2:D:74:GLY:HA2	2:D:84:THR:HG21	2.00	0.44
2:F:75:LEU:HD13	2:F:78:LEU:HD22	1.99	0.44
2:H:134:VAL:O	2:H:138:ALA:CB	2.64	0.44
2:H:20:VAL:HG13	2:H:68:LEU:HD23	1.93	0.44
2:B:7:GLU:OE1	2:B:132:LYS:HD2	2.16	0.44
1:C:118:THR:CB	1:C:121:VAL:H	2.30	0.44
1:C:86:LEU:CD2	3:C:142:HEM:CBA	2.95	0.44
1:E:11:LYS:CG	1:E:11:LYS:HA	2.46	0.44
1:E:68:ASN:OD1	1:E:72:HIS:CD2	2.69	0.44
2:B:58:PRO:HA	2:B:61:LYS:CB	2.36	0.44
1:C:66:LEU:CD2	1:C:128:PHE:CZ	2.76	0.44
2:D:27:ALA:O	2:D:28:LEU:C	2.55	0.44
1:E:132:VAL:HG13	1:E:136:LEU:HD12	2.00	0.44
1:E:95:PRO:CG	1:E:137:THR:HG21	2.48	0.44
1:E:68:ASN:O	1:E:72:HIS:CD2	2.69	0.44
2:F:114:LEU:HD23	2:F:114:LEU:HA	1.39	0.44
1:G:47:ASP:CB	1:G:47:ASP:C	2.64	0.44
1:A:86:LEU:O	1:A:91:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:PRO:HA	1:C:98:PHE:HD2	1.82	0.44
2:D:101:GLU:OE1	2:D:104:ARG:NH1	2.50	0.44
2:H:6:VAL:C	2:H:8:LYS:N	2.68	0.44
2:B:96:LEU:HD21	3:B:147:HEM:C1D	2.53	0.44
2:D:15:TRP:O	2:D:18:VAL:CG2	2.61	0.44
1:E:23:GLU:O	1:E:27:GLU:N	2.44	0.44
1:E:2:LEU:N	1:E:2:LEU:CD2	2.79	0.44
2:H:137:VAL:HG12	2:H:141:LEU:HD21	2.00	0.44
1:A:121:VAL:O	1:A:124:SER:HB2	2.18	0.44
1:E:21:ALA:O	1:E:63:ALA:CB	2.66	0.44
1:G:121:VAL:C	1:G:124:SER:H	2.21	0.44
1:G:80:LEU:HB3	1:G:135:VAL:HG12	1.99	0.44
2:H:14:LEU:CD1	2:H:122:PHE:HE1	2.31	0.44
2:H:32:LEU:HA	2:H:38:THR:HG1	1.76	0.44
2:B:15:TRP:HE1	2:B:72:SER:CB	2.27	0.44
1:C:118:THR:H	1:C:121:VAL:HB	1.83	0.44
1:C:6:ASP:HA	1:C:124:SER:OG	2.17	0.44
1:C:59:GLY:C	1:C:62:VAL:H	2.20	0.44
1:C:75:ASP:O	1:C:76:MET:C	2.55	0.44
1:C:81:SER:O	1:C:84:SER:CB	2.66	0.44
1:C:83:LEU:O	1:C:86:LEU:HB3	2.17	0.44
1:E:117:PHE:HD2	1:E:117:PHE:O	1.99	0.44
2:F:127:GLN:O	2:F:130:TYR:CA	2.65	0.44
2:F:126:VAL:O	2:F:130:TYR:HD2	2.00	0.44
2:F:131:GLN:O	2:F:135:ALA:HB2	2.18	0.44
2:F:26:GLU:O	2:F:55:MET:CE	2.62	0.44
1:G:4:PRO:HA	1:G:7:LYS:HG3	1.99	0.44
2:H:27:ALA:HB3	2:H:28:LEU:H	1.39	0.44
2:H:54:VAL:CG1	2:H:55:MET:SD	3.04	0.44
2:H:86:ALA:HB1	2:H:144:LYS:HZ1	1.77	0.44
1:A:38:THR:C	1:A:41:THR:HG23	2.36	0.44
2:B:113:VAL:HG13	2:B:113:VAL:O	2.16	0.44
1:A:122:HIS:ND1	2:B:30:ARG:HG2	2.33	0.44
2:B:59:LYS:HZ2	2:B:59:LYS:CA	2.25	0.44
2:B:4:THR:HG21	2:B:6:VAL:HG22	1.99	0.44
2:B:80:ASN:OD1	2:B:83:GLY:HA3	2.18	0.44
2:B:37:TRP:HZ3	1:C:141:ARG:HE	1.64	0.44
2:D:108:ASN:HA	2:D:111:VAL:CG2	2.47	0.44
2:D:25:GLY:O	2:D:29:GLY:HA3	2.17	0.44
2:D:68:LEU:CD2	2:D:68:LEU:H	2.15	0.44
2:D:82:LYS:O	2:D:83:GLY:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:TRP:CA	1:E:17:VAL:HG23	2.48	0.44
2:F:33:VAL:CG2	2:F:51:PRO:CB	2.85	0.44
1:G:4:PRO:O	1:G:6:ASP:N	2.50	0.44
1:G:11:LYS:CG	1:G:70:VAL:HG23	2.47	0.44
1:A:81:SER:HA	1:A:84:SER:HB3	2.00	0.43
2:B:126:VAL:O	2:B:130:TYR:HD2	2.00	0.43
1:C:103:HIS:O	1:C:107:VAL:HG22	2.17	0.43
1:C:49:SER:O	1:C:50:HIS:C	2.55	0.43
2:D:137:VAL:O	2:D:141:LEU:N	2.47	0.43
1:G:29:LEU:O	1:G:30:GLU:C	2.52	0.43
1:A:46:PHE:HA	1:A:54:GLN:OE1	2.18	0.43
2:B:60:VAL:O	2:B:61:LYS:O	2.37	0.43
2:D:14:LEU:CD1	2:D:130:TYR:HE2	2.25	0.43
2:D:20:VAL:O	2:D:20:VAL:HG13	2.18	0.43
1:E:42:TYR:C	1:E:43:PHE:CD1	2.91	0.43
2:F:128:ALA:O	2:F:132:LYS:HB2	2.18	0.43
2:F:35:TYR:HB3	2:F:37:TRP:CZ3	2.53	0.43
1:G:94:ASP:HA	1:G:95:PRO:HD2	1.91	0.43
2:B:35:TYR:HB3	2:B:37:TRP:CE2	2.49	0.43
1:C:7:LYS:NZ	1:C:74:ASP:CG	2.68	0.43
1:C:86:LEU:HA	1:C:86:LEU:HD12	1.36	0.43
2:D:40:ARG:HG2	2:D:41:PHE:CZ	2.52	0.43
2:D:67:VAL:CG1	3:D:147:HEM:NA	2.81	0.43
2:D:7:GLU:O	2:D:8:LYS:C	2.56	0.43
1:E:84:SER:HB2	1:E:139:LYS:HD2	2.00	0.43
1:G:1:VAL:HG13	1:G:2:LEU:O	2.18	0.43
2:H:45:PHE:CE1	2:H:60:VAL:HA	2.53	0.43
1:A:86:LEU:CD1	1:A:90:LYS:HZ2	2.27	0.43
2:B:106:LEU:O	2:B:109:VAL:HB	2.19	0.43
2:B:8:LYS:HA	2:B:11:VAL:HB	1.99	0.43
1:C:132:VAL:CG1	1:C:132:VAL:C	2.87	0.43
1:C:50:HIS:CD2	1:C:50:HIS:O	2.70	0.43
1:C:83:LEU:HD21	3:C:142:HEM:HMA2	1.98	0.43
2:D:11:VAL:HG11	2:D:133:VAL:HG21	2.00	0.43
1:E:6:ASP:O	1:E:10:VAL:HG23	2.18	0.43
2:F:129:ALA:O	2:F:132:LYS:HB3	2.18	0.43
3:F:147:HEM:HAA1	3:F:147:HEM:HHA	1.57	0.43
2:H:107:GLY:CA	2:H:134:VAL:HG11	2.47	0.43
2:H:117:HIS:CD2	2:H:118:PHE:CE2	3.05	0.43
2:H:92:HIS:HA	2:H:96:LEU:CB	2.47	0.43
1:A:135:VAL:HA	1:A:138:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:C	1:C:19:ALA:N	2.71	0.43
3:D:147:HEM:CBA	3:D:147:HEM:CHA	2.95	0.43
2:D:67:VAL:HG12	3:D:147:HEM:NA	2.33	0.43
2:F:121:GLU:O	2:F:123:THR:HG23	2.19	0.43
2:H:28:LEU:HD21	2:H:63:HIS:HD2	1.76	0.43
1:A:118:THR:HG22	1:A:119:PRO:CD	2.38	0.43
2:B:59:LYS:HE3	2:B:62:ALA:HB2	1.93	0.43
2:B:75:LEU:CA	2:B:78:LEU:HD22	2.48	0.43
1:C:104:CYS:CA	1:C:107:VAL:HG23	2.46	0.43
2:D:39:GLN:C	2:D:41:PHE:N	2.69	0.43
1:E:16:LYS:HD3	1:E:116:GLU:OE1	2.18	0.43
1:E:129:LEU:O	1:E:132:VAL:HG12	2.18	0.43
2:F:14:LEU:HD22	2:F:14:LEU:HA	1.80	0.43
2:B:59:LYS:HE3	2:B:59:LYS:C	2.39	0.43
2:D:33:VAL:CG1	2:D:34:VAL:HG23	2.48	0.43
1:E:35:SER:HB3	2:F:131:GLN:HG3	2.00	0.43
2:F:3:LEU:HD23	2:F:3:LEU:HA	1.33	0.43
2:H:45:PHE:HZ	2:H:63:HIS:HB2	1.83	0.43
2:H:20:VAL:CG1	2:H:68:LEU:HB3	2.47	0.43
1:A:91:LEU:HG	1:A:91:LEU:H	1.39	0.43
2:D:44:SER:C	2:D:45:PHE:CD2	2.72	0.43
1:G:109:LEU:HD22	1:G:109:LEU:HD13	1.96	0.43
2:H:133:VAL:HG13	2:H:137:VAL:HG23	2.00	0.43
1:A:140:TYR:C	1:A:141:ARG:HG2	2.39	0.43
2:B:28:LEU:HD12	2:B:28:LEU:O	2.18	0.43
2:D:85:PHE:CE1	2:D:137:VAL:HG22	2.54	0.43
2:D:49:SER:OG	2:D:49:SER:N	2.52	0.43
1:E:39:THR:O	1:E:43:PHE:HD1	1.99	0.43
2:F:41:PHE:CZ	2:F:102:ASN:OD1	2.72	0.43
2:F:98:VAL:O	2:F:145:TYR:CE1	2.72	0.43
1:C:103:HIS:O	1:C:106:LEU:HB3	2.17	0.43
1:E:52:SER:OG	1:E:54:GLN:HB3	2.18	0.43
1:E:92:ARG:HB3	2:H:37:TRP:CB	2.33	0.43
2:F:131:GLN:O	2:F:135:ALA:CB	2.67	0.43
2:F:35:TYR:HB3	2:F:37:TRP:CE3	2.53	0.43
2:H:88:LEU:HD23	2:H:88:LEU:HA	1.67	0.43
2:B:3:LEU:HD11	2:B:133:VAL:CG2	2.44	0.42
2:B:95:LYS:HD2	2:B:95:LYS:NZ	2.34	0.42
1:C:109:LEU:HA	1:C:109:LEU:HD13	1.98	0.42
1:C:117:PHE:O	2:D:30:ARG:NH2	2.52	0.42
1:C:118:THR:CG2	1:C:120:ALA:CA	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:HIS:O	1:E:76:MET:N	2.52	0.42
1:G:2:LEU:HB3	1:G:6:ASP:CB	2.49	0.42
2:H:67:VAL:HG13	3:H:147:HEM:C2B	2.54	0.42
1:A:76:MET:N	1:A:77:PRO:CD	2.83	0.42
2:B:127:GLN:O	2:B:128:ALA:C	2.58	0.42
2:D:28:LEU:C	2:D:28:LEU:HD12	2.36	0.42
2:D:37:TRP:O	2:D:40:ARG:CB	2.64	0.42
2:D:81:LEU:C	2:D:83:GLY:N	2.67	0.42
2:F:127:GLN:O	2:F:130:TYR:C	2.55	0.42
2:F:15:TRP:CE3	2:F:15:TRP:HA	2.53	0.42
1:G:32:MET:HG3	1:G:101:LEU:HD12	2.01	0.42
1:G:117:PHE:O	1:G:117:PHE:CG	2.72	0.42
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.41	0.42
2:B:81:LEU:HA	2:B:81:LEU:HD13	1.40	0.42
1:C:43:PHE:N	1:C:44:PRO:CD	2.82	0.42
1:C:84:SER:HB3	1:C:139:LYS:CD	2.37	0.42
1:C:91:LEU:O	1:C:92:ARG:C	2.57	0.42
2:D:113:VAL:O	2:D:116:HIS:CB	2.63	0.42
2:F:31:LEU:CD1	2:F:35:TYR:HE2	2.32	0.42
2:H:21:ASP:CA	2:H:65:LYS:CB	2.94	0.42
2:B:102:ASN:C	2:B:104:ARG:N	2.68	0.42
1:C:14:TRP:HA	1:C:14:TRP:CE3	2.54	0.42
1:C:94:ASP:C	1:C:94:ASP:OD2	2.58	0.42
2:D:108:ASN:C	2:D:110:LEU:N	2.73	0.42
2:D:7:GLU:OE1	2:D:7:GLU:CA	2.68	0.42
1:G:104:CYS:C	1:G:108:THR:OG1	2.51	0.42
1:A:40:LYS:O	1:A:41:THR:C	2.58	0.42
2:B:33:VAL:HG21	2:B:51:PRO:CB	2.46	0.42
2:B:96:LEU:CD1	2:B:98:VAL:HG21	2.49	0.42
3:C:142:HEM:HMC1	3:C:142:HEM:CBC	2.49	0.42
2:F:17:LYS:NZ	2:F:17:LYS:CD	2.72	0.42
2:F:24:GLY:C	2:F:26:GLU:N	2.71	0.42
2:F:42:PHE:CD1	2:F:42:PHE:N	2.87	0.42
2:H:14:LEU:CD2	2:H:14:LEU:CA	2.96	0.42
2:H:20:VAL:HG12	2:H:65:LYS:CA	2.40	0.42
2:H:32:LEU:HD12	2:H:32:LEU:HA	1.85	0.42
2:B:88:LEU:O	2:B:92:HIS:N	2.53	0.42
1:C:2:LEU:HA	1:C:6:ASP:OD2	2.19	0.42
1:C:88:ALA:O	1:C:89:HIS:ND1	2.52	0.42
2:D:82:LYS:CA	2:D:140:ALA:CB	2.80	0.42
2:D:23:VAL:HG13	2:D:113:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:GLY:HA2	2:D:77:HIS:HB2	2.00	0.42
2:F:115:ALA:O	2:F:116:HIS:C	2.56	0.42
2:F:1:VAL:HG21	2:F:132:LYS:HA	2.02	0.42
1:G:113:LEU:HG	1:G:116:GLU:HG3	2.01	0.42
1:G:110:ALA:HB1	2:H:116:HIS:HB2	2.00	0.42
2:H:36:PRO:CG	2:H:37:TRP:CZ3	2.98	0.42
2:H:90:GLU:O	2:H:94:ASP:HB2	2.18	0.42
1:A:42:TYR:CG	3:A:142:HEM:HBC1	2.54	0.42
1:A:7:LYS:CD	1:A:73:VAL:HG22	2.50	0.42
2:B:99:ASP:O	2:B:102:ASN:OD1	2.38	0.42
1:C:80:LEU:O	1:C:81:SER:C	2.57	0.42
1:E:139:LYS:HZ2	1:E:139:LYS:CB	2.29	0.42
1:E:27:GLU:OE1	1:E:112:HIS:NE2	2.52	0.42
1:E:35:SER:OG	1:E:35:SER:N	2.53	0.42
2:F:26:GLU:OE2	2:F:117:HIS:HE1	2.01	0.42
2:F:114:LEU:HD21	2:F:118:PHE:HE1	1.84	0.42
2:H:76:ALA:HB1	2:H:77:HIS:CE1	2.54	0.42
1:A:20:HIS:O	1:A:24:TYR:N	2.48	0.42
1:A:41:THR:O	1:A:44:PRO:HD3	2.20	0.42
1:C:38:THR:O	1:C:41:THR:OG1	2.10	0.42
1:C:84:SER:HA	1:C:136:LEU:HD22	2.01	0.42
1:A:136:LEU:HD22	1:A:136:LEU:HA	1.97	0.42
1:A:22:GLY:HA3	1:A:60:LYS:HA	2.00	0.42
2:B:119:GLY:C	2:B:121:GLU:N	2.73	0.42
2:B:125:PRO:HA	2:B:128:ALA:HB2	2.01	0.42
2:B:28:LEU:O	2:B:32:LEU:HB2	2.20	0.42
2:B:5:PRO:HB2	2:B:6:VAL:HG13	2.00	0.42
2:B:96:LEU:HD21	3:B:147:HEM:CHD	2.49	0.42
2:D:15:TRP:C	2:D:18:VAL:HG23	2.39	0.42
1:E:76:MET:SD	1:E:135:VAL:CG2	2.82	0.42
2:F:114:LEU:CD2	2:F:114:LEU:O	2.65	0.42
2:F:26:GLU:OE1	2:F:30:ARG:NH1	2.52	0.42
1:G:100:LEU:C	1:G:103:HIS:H	2.23	0.42
1:G:93:VAL:CG1	3:G:142:HEM:CAC	2.90	0.42
1:G:47:ASP:CA	1:G:47:ASP:O	2.48	0.42
1:G:8:THR:HG22	1:G:8:THR:O	2.20	0.42
2:H:25:GLY:O	2:H:29:GLY:CA	2.68	0.42
1:A:65:ALA:HB1	1:A:80:LEU:HD23	1.98	0.42
2:B:30:ARG:HB3	2:B:109:VAL:CG1	2.50	0.42
2:D:73:ASP:O	2:D:76:ALA:N	2.49	0.42
2:F:3:LEU:CD1	2:F:8:LYS:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:GLU:CD	1:G:50:HIS:CE1	2.94	0.42
1:A:42:TYR:CD1	1:A:93:VAL:CG2	3.03	0.41
2:B:30:ARG:HD2	2:B:30:ARG:CB	2.48	0.41
1:C:20:HIS:HB3	1:C:24:TYR:CZ	2.55	0.41
2:D:3:LEU:HD23	2:D:132:LYS:CB	2.39	0.41
2:D:51:PRO:O	2:D:55:MET:HG2	2.20	0.41
2:D:77:HIS:O	2:D:81:LEU:CD2	2.55	0.41
1:E:100:LEU:CD2	1:E:100:LEU:N	2.81	0.41
2:F:3:LEU:HD13	2:F:8:LYS:CB	2.50	0.41
2:H:26:GLU:OE1	2:H:30:ARG:CD	2.64	0.41
2:B:80:ASN:CG	2:B:80:ASN:O	2.58	0.41
1:C:8:THR:O	1:C:12:ALA:CB	2.68	0.41
2:F:31:LEU:HD12	2:F:31:LEU:HA	1.58	0.41
2:F:29:GLY:O	2:F:33:VAL:N	2.53	0.41
1:G:32:MET:HE3	1:G:39:THR:HB	2.02	0.41
2:H:99:ASP:O	2:H:101:GLU:N	2.53	0.41
1:A:4:PRO:C	1:A:7:LYS:HB2	2.41	0.41
2:F:31:LEU:HD22	2:F:106:LEU:HA	2.01	0.41
1:G:105:LEU:O	1:G:109:LEU:CB	2.52	0.41
2:H:63:HIS:O	2:H:66:LYS:CB	2.68	0.41
2:D:123:THR:C	2:D:125:PRO:HD2	2.40	0.41
1:E:101:LEU:O	1:E:104:CYS:HB2	2.20	0.41
1:G:43:PHE:CB	1:G:46:PHE:HB2	2.50	0.41
1:A:10:VAL:HG13	1:A:128:PHE:HB2	2.01	0.41
1:A:14:TRP:O	1:A:17:VAL:HG23	2.21	0.41
1:A:24:TYR:HA	1:A:24:TYR:HD2	0.98	0.41
1:A:40:LYS:HE3	1:A:40:LYS:HB2	1.62	0.41
2:B:97:HIS:C	2:B:98:VAL:HG22	2.40	0.41
2:D:98:VAL:O	2:D:100:PRO:HB3	2.19	0.41
2:D:74:GLY:C	2:D:76:ALA:H	2.23	0.41
1:E:137:THR:O	1:E:137:THR:CG2	2.69	0.41
1:A:17:VAL:HG13	1:A:24:TYR:CD1	2.55	0.41
1:A:28:ALA:HB3	1:A:29:LEU:H	1.07	0.41
1:A:42:TYR:HB2	3:A:142:HEM:CBC	2.49	0.41
1:C:12:ALA:O	1:C:13:ALA:CA	2.64	0.41
2:F:136:GLY:O	2:F:140:ALA:CB	2.66	0.41
2:F:42:PHE:HZ	3:F:147:HEM:HBC2	1.84	0.41
1:G:7:LYS:O	1:G:11:LYS:HD2	2.21	0.41
2:H:112:CYS:O	2:H:115:ALA:CB	2.68	0.41
1:A:33:PHE:HB3	1:A:40:LYS:CG	2.50	0.41
2:B:50:THR:HG22	2:B:51:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:CA	1:C:109:LEU:HB2	2.49	0.41
1:C:39:THR:O	1:C:42:TYR:HD2	2.03	0.41
2:D:102:ASN:HB3	3:D:147:HEM:CMC	2.40	0.41
2:D:85:PHE:HA	2:D:88:LEU:CB	2.51	0.41
2:F:32:LEU:HA	2:F:32:LEU:HD12	1.27	0.41
1:G:104:CYS:SG	2:H:127:GLN:NE2	2.94	0.41
1:G:30:GLU:OE2	1:G:50:HIS:ND1	2.52	0.41
2:H:17:LYS:CB	2:H:118:PHE:CZ	3.04	0.41
1:A:76:MET:HB2	1:A:77:PRO:HD3	2.03	0.41
2:B:111:VAL:HG13	2:B:122:PHE:CE2	2.55	0.41
2:B:18:VAL:HG12	2:B:20:VAL:HG23	1.93	0.41
2:B:1:VAL:N	2:B:2:HIS:ND1	2.68	0.41
2:D:42:PHE:O	2:D:45:PHE:CB	2.62	0.41
2:D:50:THR:HG22	2:D:51:PRO:HD2	2.02	0.41
2:D:77:HIS:HB3	2:D:84:THR:CG2	2.51	0.41
1:E:42:TYR:HE2	2:H:99:ASP:OD1	2.04	0.41
1:G:2:LEU:HD13	1:G:10:VAL:HG21	2.03	0.41
1:G:27:GLU:O	1:G:28:ALA:C	2.59	0.41
2:H:18:VAL:CG1	2:H:19:ASN:N	2.82	0.41
2:H:27:ALA:O	2:H:31:LEU:N	2.54	0.41
1:A:113:LEU:N	1:A:114:PRO:CD	2.83	0.41
1:A:118:THR:CG2	1:A:119:PRO:HD2	2.40	0.41
2:B:113:VAL:O	2:B:117:HIS:N	2.47	0.41
1:A:35:SER:OG	2:B:131:GLN:HG3	2.21	0.41
1:C:118:THR:CG2	1:C:121:VAL:HG23	2.51	0.41
2:D:68:LEU:HA	2:D:71:PHE:HB3	2.03	0.41
1:E:29:LEU:CD2	1:E:101:LEU:CD1	2.94	0.41
2:F:123:THR:CB	2:F:125:PRO:HD2	2.51	0.41
2:H:22:GLU:HB3	2:H:22:GLU:OE2	2.19	0.41
2:B:141:LEU:CD2	3:B:147:HEM:HBB2	2.40	0.41
2:B:62:ALA:HB3	2:B:63:HIS:H	1.23	0.41
2:B:8:LYS:CA	2:B:11:VAL:HB	2.51	0.41
1:C:102:SER:OG	1:C:129:LEU:HD12	2.21	0.41
1:E:117:PHE:C	1:E:117:PHE:CD2	2.94	0.41
1:E:72:HIS:C	1:E:74:ASP:H	2.20	0.41
2:F:69:GLY:O	2:F:70:ALA:O	2.38	0.41
2:D:129:ALA:O	2:D:130:TYR:C	2.58	0.41
1:C:119:PRO:CB	2:D:30:ARG:HG3	2.46	0.41
2:F:17:LYS:HB3	2:F:118:PHE:HZ	1.84	0.41
2:H:68:LEU:HA	2:H:71:PHE:HB3	2.03	0.41
2:B:123:THR:CB	2:B:124:PRO:CD	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:147:HEM:HAD1	3:B:147:HEM:HHA	1.68	0.40
1:C:134:THR:O	1:C:138:SER:N	2.54	0.40
2:D:104:ARG:C	2:D:104:ARG:CG	2.88	0.40
2:D:103:PHE:HB3	2:D:138:ALA:HA	2.03	0.40
2:D:63:HIS:CE1	3:D:147:HEM:ND	2.88	0.40
2:F:63:HIS:CA	2:F:66:LYS:HB2	2.50	0.40
2:B:93:CYS:CB	2:B:145:TYR:CE2	3.01	0.40
2:B:141:LEU:CD2	3:B:147:HEM:HMB3	2.50	0.40
2:B:68:LEU:HA	2:B:71:PHE:HB3	2.02	0.40
1:C:107:VAL:C	1:C:110:ALA:CB	2.87	0.40
1:C:124:SER:O	1:C:127:LYS:CB	2.69	0.40
1:C:128:PHE:CE2	1:C:129:LEU:HB2	2.56	0.40
1:C:59:GLY:C	1:C:61:LYS:N	2.66	0.40
2:D:101:GLU:N	2:D:104:ARG:NH1	2.64	0.40
2:H:123:THR:HB	2:H:125:PRO:CD	2.38	0.40
1:A:134:THR:O	1:A:137:THR:CA	2.69	0.40
1:C:106:LEU:HD21	1:C:126:ASP:HB2	2.02	0.40
1:C:105:LEU:C	1:C:109:LEU:HB2	2.42	0.40
1:C:40:LYS:CB	1:C:40:LYS:HD2	2.17	0.40
1:C:83:LEU:HA	1:C:86:LEU:CB	2.51	0.40
1:C:86:LEU:CD2	3:C:142:HEM:HBA1	2.51	0.40
2:D:35:TYR:CD2	2:D:105:LEU:HD22	2.56	0.40
1:E:76:MET:N	1:E:77:PRO:CD	2.76	0.40
1:E:96:VAL:O	1:E:100:LEU:CD2	2.69	0.40
1:E:35:SER:HB3	2:F:128:ALA:HB2	2.03	0.40
2:F:91:LEU:CG	2:F:91:LEU:O	2.69	0.40
1:G:49:SER:N	1:G:52:SER:OG	2.54	0.40
1:G:60:LYS:HD2	1:G:60:LYS:NZ	2.35	0.40
2:H:4:THR:HB	2:H:7:GLU:CG	2.41	0.40
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.86	0.40
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.56	0.40
2:B:130:TYR:O	2:B:134:VAL:N	2.51	0.40
2:D:142:ALA:CB	2:D:142:ALA:H	2.28	0.40
1:E:101:LEU:CD2	1:E:104:CYS:SG	3.09	0.40
2:F:3:LEU:CD1	2:F:8:LYS:HB2	2.51	0.40
1:G:52:SER:O	1:G:53:ALA:C	2.58	0.40
1:A:106:LEU:O	1:A:109:LEU:HB2	2.21	0.40
1:A:29:LEU:O	1:A:30:GLU:C	2.60	0.40
1:A:39:THR:C	1:A:41:THR:N	2.67	0.40
1:A:86:LEU:CD1	1:A:90:LYS:NZ	2.70	0.40
2:B:137:VAL:O	2:B:140:ALA:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ALA:CB	2:D:115:ALA:CB	2.90	0.40
2:D:50:THR:O	2:D:53:ALA:N	2.53	0.40
2:D:60:VAL:O	2:D:61:LYS:C	2.60	0.40
2:D:65:LYS:O	2:D:66:LYS:C	2.59	0.40
2:D:91:LEU:O	2:D:96:LEU:N	2.54	0.40
2:D:9:SER:O	2:D:10:ALA:C	2.60	0.40
1:E:111:ALA:HB2	2:F:115:ALA:HB1	2.02	0.40
1:E:29:LEU:HD11	1:E:58:HIS:CD2	2.52	0.40
2:F:54:VAL:CG1	2:F:54:VAL:O	2.60	0.40
2:F:91:LEU:O	2:F:91:LEU:HG	2.21	0.40
1:G:31:ARG:HD3	1:G:108:THR:HG23	2.04	0.40
1:G:84:SER:CB	1:G:136:LEU:HD23	2.43	0.40
1:G:17:VAL:HG12	1:G:21:ALA:N	2.36	0.40
2:H:124:PRO:HG2	2:H:125:PRO:CD	2.52	0.40
2:H:4:THR:CG2	2:H:7:GLU:N	2.78	0.40
2:B:88:LEU:CD2	2:H:6:VAL:HG13	2.44	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ALA:CB	2:F:43:GLU:O[1_454]	1.28	0.92
2:D:6:VAL:CG2	2:F:73:ASP:OD2[1_455]	1.92	0.28
1:C:54:GLN:OE1	2:F:46:GLY:CA[1_454]	1.94	0.26
1:C:85:ASP:OD2	2:D:83:GLY:O[1_554]	2.00	0.20
2:D:9:SER:OG	3:F:147:HEM:O2A[1_455]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	6 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	139/141 (99%)	116 (84%)	13 (9%)	10 (7%)	1	5
1	E	139/141 (99%)	113 (81%)	20 (14%)	6 (4%)	2	15
1	G	139/141 (99%)	105 (76%)	24 (17%)	10 (7%)	1	5
2	B	144/146 (99%)	120 (83%)	23 (16%)	1 (1%)	22	60
2	D	144/146 (99%)	120 (83%)	17 (12%)	7 (5%)	2	13
2	F	144/146 (99%)	123 (85%)	14 (10%)	7 (5%)	2	13
2	H	144/146 (99%)	114 (79%)	22 (15%)	8 (6%)	2	10
All	All	1132/1148 (99%)	932 (82%)	148 (13%)	52 (5%)	2	14

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	C	73	VAL
2	D	11	VAL
2	D	40	ARG
2	D	54	VAL
2	F	24	GLY
2	F	80	ASN
1	G	18	GLY
1	G	81	SER
1	G	82	ALA
2	H	15	TRP
2	H	88	LEU
2	H	89	SER
1	C	18	GLY
1	C	81	SER
2	D	17	LYS
1	E	18	GLY
1	E	21	ALA
2	F	67	VAL
2	F	73	ASP
1	G	28	ALA
1	G	50	HIS
2	H	40	ARG
2	H	117	HIS
1	A	28	ALA
1	C	21	ALA
1	C	106	LEU
2	D	8	LYS

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Mol	Chain	Res	Type
1	E	123	ALA
2	F	40	ARG
1	G	52	SER
2	H	97	HIS
1	C	28	ALA
1	C	32	MET
1	E	87	HIS
1	E	106	LEU
2	F	36	PRO
2	H	119	GLY
1	A	21	ALA
1	C	86	LEU
1	C	92	ARG
1	E	114	PRO
1	G	95	PRO
1	C	52	SER
2	D	16	GLY
2	F	2	HIS
1	G	73	VAL
2	H	115	ALA
2	D	36	PRO
1	G	15	GLY
2	B	36	PRO
1	G	114	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	113/113 (100%)	84 (74%)	29 (26%)	0	3
1	C	113/113 (100%)	66 (58%)	47 (42%)	0	0
1	E	113/113 (100%)	69 (61%)	44 (39%)	0	0
1	G	113/113 (100%)	67 (59%)	46 (41%)	0	0
2	B	118/118 (100%)	73 (62%)	45 (38%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	118/118 (100%)	82 (70%)	36 (30%)	0	1
2	F	118/118 (100%)	81 (69%)	37 (31%)	0	1
2	H	118/118 (100%)	63 (53%)	55 (47%)	0	0
All	All	924/924 (100%)	585 (63%)	339 (37%)	0	1

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	2	LEU
1	A	3	SER
1	A	4	PRO
1	A	7	LYS
1	A	20	HIS
1	A	37	PRO
1	A	38	THR
1	A	45	HIS
1	A	48	LEU
1	A	52	SER
1	A	56	LYS
1	A	60	LYS
1	A	61	LYS
1	A	73	VAL
1	A	75	ASP
1	A	76	MET
1	A	77	PRO
1	A	86	LEU
1	A	90	LYS
1	A	99	LYS
1	A	100	LEU
1	A	102	SER
1	A	118	THR
1	A	124	SER
1	A	127	LYS
1	A	136	LEU
1	A	137	THR
1	A	138	SER
2	B	2	HIS
2	B	8	LYS
2	B	11	VAL
2	B	14	LEU

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Mol	Chain	Res	Type
2	B	18	VAL
2	B	21	ASP
2	B	26	GLU
2	B	28	LEU
2	B	30	ARG
2	B	35	TYR
2	B	44	SER
2	B	48	LEU
2	B	49	SER
2	B	58	PRO
2	B	59	LYS
2	B	60	VAL
2	B	61	LYS
2	B	65	LYS
2	B	66	LYS
2	B	72	SER
2	B	73	ASP
2	B	75	LEU
2	B	78	LEU
2	B	79	ASP
2	B	80	ASN
2	B	81	LEU
2	B	82	LYS
2	B	88	LEU
2	B	89	SER
2	B	91	LEU
2	B	92	HIS
2	B	95	LYS
2	B	96	LEU
2	B	98	VAL
2	B	101	GLU
2	B	104	ARG
2	B	114	LEU
2	B	116	HIS
2	B	120	LYS
2	B	121	GLU
2	B	131	GLN
2	B	139	ASN
2	B	144	LYS
2	B	145	TYR
2	B	146	HIS
1	C	2	LEU

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Mol	Chain	Res	Type
1	C	3	SER
1	C	8	THR
1	C	10	VAL
1	C	31	ARG
1	C	32	MET
1	C	34	LEU
1	C	35	SER
1	C	40	LYS
1	C	41	THR
1	C	46	PHE
1	C	47	ASP
1	C	48	LEU
1	C	50	HIS
1	C	52	SER
1	C	54	GLN
1	C	55	VAL
1	C	61	LYS
1	C	70	VAL
1	C	76	MET
1	C	80	LEU
1	C	83	LEU
1	C	85	ASP
1	C	90	LYS
1	C	91	LEU
1	C	92	ARG
1	C	94	ASP
1	C	96	VAL
1	C	99	LYS
1	C	100	LEU
1	C	102	SER
1	C	104	CYS
1	C	105	LEU
1	C	106	LEU
1	C	108	THR
1	C	109	LEU
1	C	117	PHE
1	C	118	THR
1	C	124	SER
1	C	125	LEU
1	C	126	ASP
1	C	127	LYS
1	C	128	PHE

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Mol	Chain	Res	Type
1	C	129	LEU
1	C	134	THR
1	C	136	LEU
1	C	138	SER
2	D	4	THR
2	D	7	GLU
2	D	8	LYS
2	D	9	SER
2	D	11	VAL
2	D	12	THR
2	D	14	LEU
2	D	15	TRP
2	D	17	LYS
2	D	22	GLU
2	D	26	GLU
2	D	30	ARG
2	D	40	ARG
2	D	42	PHE
2	D	45	PHE
2	D	54	VAL
2	D	65	LYS
2	D	66	LYS
2	D	68	LEU
2	D	72	SER
2	D	73	ASP
2	D	75	LEU
2	D	81	LEU
2	D	85	PHE
2	D	90	GLU
2	D	93	CYS
2	D	100	PRO
2	D	104	ARG
2	D	106	LEU
2	D	109	VAL
2	D	117	HIS
2	D	123	THR
2	D	125	PRO
2	D	141	LEU
2	D	143	HIS
2	D	146	HIS
1	E	1	VAL
1	E	2	LEU

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Mol	Chain	Res	Type
1	E	6	ASP
1	E	16	LYS
1	E	27	GLU
1	E	29	LEU
1	E	31	ARG
1	E	34	LEU
1	E	36	PHE
1	E	39	THR
1	E	41	THR
1	E	43	PHE
1	E	44	PRO
1	E	45	HIS
1	E	49	SER
1	E	52	SER
1	E	67	THR
1	E	83	LEU
1	E	84	SER
1	E	91	LEU
1	E	92	ARG
1	E	96	VAL
1	E	99	LYS
1	E	100	LEU
1	E	101	LEU
1	E	102	SER
1	E	105	LEU
1	E	107	VAL
1	E	109	LEU
1	E	113	LEU
1	E	114	PRO
1	E	117	PHE
1	E	119	PRO
1	E	124	SER
1	E	125	LEU
1	E	127	LYS
1	E	128	PHE
1	E	129	LEU
1	E	132	VAL
1	E	134	THR
1	E	138	SER
1	E	139	LYS
1	E	140	TYR
1	E	141	ARG

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Mol	Chain	Res	Type
2	F	1	VAL
2	F	3	LEU
2	F	5	PRO
2	F	6	VAL
2	F	7	GLU
2	F	12	THR
2	F	15	TRP
2	F	18	VAL
2	F	22	GLU
2	F	23	VAL
2	F	30	ARG
2	F	38	THR
2	F	39	GLN
2	F	41	PHE
2	F	42	PHE
2	F	44	SER
2	F	48	LEU
2	F	55	MET
2	F	59	LYS
2	F	65	LYS
2	F	66	LYS
2	F	67	VAL
2	F	73	ASP
2	F	78	LEU
2	F	79	ASP
2	F	80	ASN
2	F	89	SER
2	F	95	LYS
2	F	96	LEU
2	F	97	HIS
2	F	112	CYS
2	F	114	LEU
2	F	120	LYS
2	F	121	GLU
2	F	132	LYS
2	F	144	LYS
2	F	146	HIS
1	G	1	VAL
1	G	4	PRO
1	G	8	THR
1	G	11	LYS
1	G	16	LYS

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Mol	Chain	Res	Type
1	G	23	GLU
1	G	27	GLU
1	G	29	LEU
1	G	31	ARG
1	G	32	MET
1	G	35	SER
1	G	38	THR
1	G	41	THR
1	G	43	PHE
1	G	48	LEU
1	G	49	SER
1	G	52	SER
1	G	60	LYS
1	G	66	LEU
1	G	67	THR
1	G	70	VAL
1	G	73	VAL
1	G	76	MET
1	G	80	LEU
1	G	84	SER
1	G	85	ASP
1	G	91	LEU
1	G	93	VAL
1	G	95	PRO
1	G	96	VAL
1	G	97	ASN
1	G	101	LEU
1	G	102	SER
1	G	105	LEU
1	G	106	LEU
1	G	107	VAL
1	G	108	THR
1	G	118	THR
1	G	124	SER
1	G	126	ASP
1	G	127	LYS
1	G	131	SER
1	G	134	THR
1	G	136	LEU
1	G	139	LYS
1	G	141	ARG
2	H	2	HIS

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Mol	Chain	Res	Type
2	H	3	LEU
2	H	8	LYS
2	H	11	VAL
2	H	14	LEU
2	H	17	LYS
2	H	21	ASP
2	H	22	GLU
2	H	26	GLU
2	H	28	LEU
2	H	32	LEU
2	H	33	VAL
2	H	38	THR
2	H	39	GLN
2	H	42	PHE
2	H	43	GLU
2	H	44	SER
2	H	48	LEU
2	H	49	SER
2	H	50	THR
2	H	54	VAL
2	H	58	PRO
2	H	59	LYS
2	H	65	LYS
2	H	66	LYS
2	H	68	LEU
2	H	72	SER
2	H	75	LEU
2	H	78	LEU
2	H	80	ASN
2	H	82	LYS
2	H	84	THR
2	H	85	PHE
2	H	87	THR
2	H	89	SER
2	H	92	HIS
2	H	96	LEU
2	H	101	GLU
2	H	104	ARG
2	H	106	LEU
2	H	109	VAL
2	H	110	LEU
2	H	112	CYS

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Mol	Chain	Res	Type
2	H	113	VAL
2	H	114	LEU
2	H	120	LYS
2	H	121	GLU
2	H	122	PHE
2	H	123	THR
2	H	125	PRO
2	H	126	VAL
2	H	130	TYR
2	H	131	GLN
2	H	139	ASN
2	H	146	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	20	HIS
1	A	78	ASN
1	A	89	HIS
1	A	112	HIS
2	B	39	GLN
2	B	77	HIS
2	B	102	ASN
2	B	139	ASN
2	B	143	HIS
1	C	50	HIS
1	C	58	HIS
1	C	72	HIS
1	C	97	ASN
1	C	122	HIS
2	D	63	HIS
2	D	80	ASN
2	D	131	GLN
1	E	58	HIS
1	E	78	ASN
1	E	97	ASN
1	E	103	HIS
2	F	39	GLN
2	F	63	HIS
2	F	80	ASN
2	F	131	GLN

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Mol	Chain	Res	Type
2	F	143	HIS
1	G	68	ASN
1	G	72	HIS
1	G	97	ASN
2	H	19	ASN
2	H	39	GLN
2	H	63	HIS
2	H	92	HIS
2	H	117	HIS
2	H	139	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
3	HEM	H	147	-	27,50,50	3.47	14 (51%)	17,82,82	5.44	11 (64%)
3	HEM	E	142	1	27,50,50	3.83	17 (62%)	17,82,82	5.97	14 (82%)
3	HEM	F	147	2	27,50,50	3.78	15 (55%)	17,82,82	4.56	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	D	147	2	27,50,50	2.60	9 (33%)	17,82,82	4.18	11 (64%)
3	HEM	B	147	2	27,50,50	4.95	19 (70%)	17,82,82	3.37	10 (58%)
3	HEM	C	142	1	27,50,50	2.99	15 (55%)	17,82,82	5.51	13 (76%)
3	HEM	A	142	1	27,50,50	3.16	13 (48%)	17,82,82	6.43	13 (76%)
3	HEM	G	142	-	27,50,50	3.81	12 (44%)	17,82,82	5.05	13 (76%)

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	HEM	H	147	-	-	4/6/54/54	-
3	HEM	E	142	1	-	0/6/54/54	-
3	HEM	F	147	2	-	1/6/54/54	-
3	HEM	D	147	2	-	2/6/54/54	-
3	HEM	B	147	2	-	2/6/54/54	-
3	HEM	C	142	1	-	0/6/54/54	-
3	HEM	A	142	1	-	0/6/54/54	-
3	HEM	G	142	-	-	0/6/54/54	-

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C3C-C2C	-15.51	1.18	1.40
3	G	142	HEM	C3C-C2C	14.14	1.60	1.40
3	E	142	HEM	CAD-C3D	9.74	1.69	1.52
3	B	147	HEM	CAA-C2A	9.35	1.65	1.52
3	A	142	HEM	C3C-C2C	-9.21	1.27	1.40
3	B	147	HEM	CAD-C3D	9.20	1.68	1.52
3	D	147	HEM	C4D-C3D	8.66	1.62	1.42
3	E	142	HEM	CMC-C2C	8.64	1.72	1.51
3	H	147	HEM	C1A-NA	8.37	1.53	1.36
3	E	142	HEM	C3C-C2C	-8.32	1.28	1.40
3	F	147	HEM	C3C-C2C	-8.10	1.29	1.40
3	F	147	HEM	C3B-C2B	-8.04	1.29	1.40
3	F	147	HEM	CMA-C3A	6.92	1.66	1.51
3	G	142	HEM	C3B-CAB	6.52	1.61	1.47
3	H	147	HEM	C3B-CAB	6.51	1.61	1.47
3	C	142	HEM	CMD-C2D	6.30	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C3C-C2C	-6.29	1.31	1.40
3	F	147	HEM	C4A-NA	6.25	1.49	1.36
3	A	142	HEM	C1D-ND	6.06	1.48	1.36
3	B	147	HEM	CMC-C2C	5.77	1.65	1.51
3	E	142	HEM	CMD-C2D	5.65	1.63	1.51
3	F	147	HEM	CAA-C2A	-5.61	1.43	1.52
3	B	147	HEM	C1D-ND	5.49	1.47	1.36
3	F	147	HEM	C1A-NA	-5.41	1.25	1.36
3	C	142	HEM	C1D-ND	-5.36	1.25	1.36
3	C	142	HEM	C3B-C2B	-5.34	1.33	1.40
3	H	147	HEM	C3C-C2C	5.32	1.47	1.40
3	G	142	HEM	C4D-C3D	5.24	1.54	1.42
3	C	142	HEM	C3C-CAC	5.18	1.58	1.47
3	D	147	HEM	C3B-C2B	-5.10	1.33	1.40
3	B	147	HEM	C1A-NA	5.06	1.46	1.36
3	H	147	HEM	C4A-NA	-5.05	1.25	1.36
3	A	142	HEM	CMC-C2C	4.88	1.63	1.51
3	H	147	HEM	C1A-CHA	-4.83	1.27	1.41
3	G	142	HEM	C4A-NA	4.79	1.46	1.36
3	B	147	HEM	CMA-C3A	4.77	1.61	1.51
3	H	147	HEM	CMD-C2D	4.73	1.61	1.51
3	H	147	HEM	CMC-C2C	4.66	1.62	1.51
3	B	147	HEM	C3C-CAC	4.59	1.57	1.47
3	A	142	HEM	C3B-CAB	4.58	1.57	1.47
3	F	147	HEM	C1C-C2C	4.52	1.52	1.42
3	A	142	HEM	C3B-C2B	-4.36	1.34	1.40
3	G	142	HEM	CBC-CAC	4.30	1.57	1.29
3	E	142	HEM	C1B-C2B	4.16	1.52	1.42
3	H	147	HEM	C3B-C2B	-4.05	1.34	1.40
3	B	147	HEM	C3B-CAB	3.94	1.56	1.47
3	H	147	HEM	C4B-CHC	-3.88	1.30	1.41
3	A	142	HEM	C1C-C2C	-3.81	1.33	1.42
3	A	142	HEM	CBD-CAD	3.76	1.80	1.53
3	E	142	HEM	C4B-NB	3.72	1.43	1.36
3	C	142	HEM	C1B-C2B	3.68	1.50	1.42
3	G	142	HEM	CMA-C3A	-3.66	1.44	1.51
3	B	147	HEM	C3D-C2D	-3.65	1.26	1.37
3	B	147	HEM	C1A-CHA	-3.56	1.31	1.41
3	D	147	HEM	C3C-CAC	3.55	1.55	1.47
3	B	147	HEM	CBC-CAC	3.52	1.52	1.29
3	E	142	HEM	C3B-C2B	-3.51	1.35	1.40
3	H	147	HEM	C4D-C3D	3.48	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	147	HEM	C3B-CAB	3.48	1.55	1.47
3	G	142	HEM	CMC-C2C	-3.45	1.43	1.51
3	D	147	HEM	CBB-CAB	3.38	1.51	1.29
3	F	147	HEM	C4B-CHC	3.37	1.50	1.41
3	F	147	HEM	C2A-C3A	3.37	1.47	1.37
3	C	142	HEM	CMA-C3A	3.37	1.58	1.51
3	D	147	HEM	C3C-C2C	-3.36	1.35	1.40
3	E	142	HEM	C3D-C2D	-3.30	1.27	1.37
3	D	147	HEM	C3B-CAB	3.25	1.54	1.47
3	B	147	HEM	C4A-CHB	-3.23	1.32	1.41
3	E	142	HEM	C3C-CAC	3.11	1.54	1.47
3	B	147	HEM	C1D-CHD	-3.08	1.32	1.41
3	G	142	HEM	CMD-C2D	-3.07	1.45	1.51
3	G	142	HEM	C4B-NB	2.95	1.42	1.36
3	A	142	HEM	CMB-C2B	2.94	1.58	1.51
3	H	147	HEM	C4A-CHB	2.92	1.49	1.41
3	G	142	HEM	C1D-CHD	-2.92	1.32	1.41
3	F	147	HEM	CBB-CAB	2.91	1.48	1.29
3	F	147	HEM	C1A-CHA	-2.91	1.32	1.41
3	H	147	HEM	CAA-C2A	-2.90	1.47	1.52
3	B	147	HEM	C4B-CHC	-2.89	1.33	1.41
3	F	147	HEM	C1B-C2B	2.82	1.48	1.42
3	A	142	HEM	C3D-C2D	-2.81	1.29	1.37
3	E	142	HEM	CAA-C2A	2.80	1.56	1.52
3	C	142	HEM	CMC-C2C	2.75	1.58	1.51
3	C	142	HEM	CAA-C2A	2.71	1.56	1.52
3	B	147	HEM	C2A-C3A	-2.67	1.29	1.37
3	E	142	HEM	CMA-C3A	2.64	1.57	1.51
3	F	147	HEM	CBD-CAD	2.63	1.72	1.53
3	A	142	HEM	C2A-C3A	-2.62	1.29	1.37
3	H	147	HEM	CBC-CAC	2.53	1.46	1.29
3	A	142	HEM	CMD-C2D	-2.51	1.46	1.51
3	E	142	HEM	CBD-CAD	2.50	1.71	1.53
3	C	142	HEM	CBD-CAD	2.46	1.70	1.53
3	E	142	HEM	CMB-C2B	2.46	1.57	1.51
3	E	142	HEM	C1D-CHD	-2.44	1.34	1.41
3	A	142	HEM	C1D-CHD	-2.39	1.34	1.41
3	F	147	HEM	C4A-CHB	2.38	1.47	1.41
3	C	142	HEM	C1A-CHA	2.32	1.47	1.41
3	G	142	HEM	C1A-NA	-2.32	1.31	1.36
3	B	147	HEM	CMB-C2B	2.30	1.57	1.51
3	D	147	HEM	C3D-C2D	-2.29	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	147	HEM	CMA-C3A	2.26	1.56	1.51
3	E	142	HEM	CBB-CAB	2.20	1.43	1.29
3	D	147	HEM	C4B-CHC	-2.18	1.34	1.41
3	B	147	HEM	C3B-C2B	2.18	1.43	1.40
3	B	147	HEM	C1C-C2C	-2.17	1.37	1.42
3	G	142	HEM	CBA-CAA	2.08	1.68	1.53
3	C	142	HEM	C1C-C2C	-2.08	1.37	1.42
3	E	142	HEM	C4B-CHC	-2.05	1.35	1.41
3	H	147	HEM	C1D-ND	-2.05	1.31	1.36
3	E	142	HEM	C3B-CAB	2.04	1.52	1.47
3	C	142	HEM	C4A-CHB	2.03	1.46	1.41
3	A	142	HEM	C1A-NA	-2.02	1.32	1.36
3	C	142	HEM	CAD-C3D	-2.02	1.48	1.52
3	C	142	HEM	C4B-NB	2.00	1.40	1.36

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CAD-CBD-CGD	-15.44	86.77	112.67
3	C	142	HEM	CMA-C3A-C4A	14.45	150.68	128.46
3	E	142	HEM	CAA-CBA-CGA	14.18	136.45	112.67
3	A	142	HEM	CBA-CAA-C2A	14.00	138.31	112.49
3	H	147	HEM	CAA-CBA-CGA	-12.37	91.92	112.67
3	D	147	HEM	CAD-CBD-CGD	12.10	132.97	112.67
3	H	147	HEM	CBA-CAA-C2A	10.29	131.47	112.49
3	C	142	HEM	CMA-C3A-C2A	-10.19	105.72	124.94
3	G	142	HEM	C4A-C3A-C2A	-9.26	100.56	107.00
3	F	147	HEM	CAA-CBA-CGA	9.20	128.10	112.67
3	G	142	HEM	CAD-CBD-CGD	9.14	128.00	112.67
3	E	142	HEM	CAD-CBD-CGD	-8.87	97.78	112.67
3	B	147	HEM	CAD-CBD-CGD	8.60	127.10	112.67
3	A	142	HEM	CBD-CAD-C3D	-8.54	96.74	112.48
3	F	147	HEM	CAD-CBD-CGD	-8.20	98.91	112.67
3	H	147	HEM	CBD-CAD-C3D	8.15	127.50	112.48
3	E	142	HEM	CMB-C2B-C3B	7.98	139.60	124.68
3	E	142	HEM	CBA-CAA-C2A	7.22	125.80	112.49
3	G	142	HEM	CMD-C2D-C1D	-7.16	117.47	128.46
3	E	142	HEM	CMD-C2D-C1D	-6.93	117.82	128.46
3	G	142	HEM	C4C-C3C-C2C	-6.90	102.08	106.90
3	A	142	HEM	CMA-C3A-C4A	-6.89	117.87	128.46
3	H	147	HEM	CAD-CBD-CGD	6.74	123.98	112.67
3	G	142	HEM	CMD-C2D-C3D	6.67	137.51	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	142	HEM	CMA-C3A-C4A	-6.50	118.48	128.46
3	A	142	HEM	CMA-C3A-C2A	6.47	137.13	124.94
3	C	142	HEM	C1D-C2D-C3D	-6.39	102.55	107.00
3	F	147	HEM	CMA-C3A-C2A	-6.25	113.16	124.94
3	G	142	HEM	CBD-CAD-C3D	5.65	122.89	112.48
3	C	142	HEM	CMB-C2B-C3B	5.48	134.94	124.68
3	B	147	HEM	CMA-C3A-C4A	-5.46	120.07	128.46
3	F	147	HEM	CMA-C3A-C4A	5.44	136.82	128.46
3	H	147	HEM	CMD-C2D-C1D	5.38	136.73	128.46
3	F	147	HEM	CAA-C2A-C3A	5.30	142.48	127.25
3	F	147	HEM	CBD-CAD-C3D	5.23	122.12	112.48
3	H	147	HEM	CMD-C2D-C3D	-5.14	115.25	124.94
3	D	147	HEM	C4C-C3C-C2C	5.14	110.48	106.90
3	C	142	HEM	CAA-C2A-C3A	5.12	141.96	127.25
3	D	147	HEM	CMD-C2D-C1D	-5.12	120.60	128.46
3	C	142	HEM	C4A-C3A-C2A	-5.00	103.52	107.00
3	G	142	HEM	CMA-C3A-C4A	4.98	136.11	128.46
3	E	142	HEM	CMC-C2C-C3C	-4.90	115.51	124.68
3	F	147	HEM	C4C-C3C-C2C	-4.83	103.53	106.90
3	A	142	HEM	CAA-C2A-C3A	4.81	141.08	127.25
3	G	142	HEM	CAA-CBA-CGA	4.78	120.70	112.67
3	E	142	HEM	CMA-C3A-C2A	4.72	133.84	124.94
3	F	147	HEM	CBA-CAA-C2A	4.70	121.15	112.49
3	B	147	HEM	CBD-CAD-C3D	-4.68	103.85	112.48
3	H	147	HEM	CMA-C3A-C4A	-4.47	121.60	128.46
3	H	147	HEM	C4C-C3C-C2C	-4.37	103.84	106.90
3	F	147	HEM	C4A-C3A-C2A	4.31	110.00	107.00
3	D	147	HEM	CBD-CAD-C3D	4.28	120.36	112.48
3	C	142	HEM	CBA-CAA-C2A	4.24	120.31	112.49
3	A	142	HEM	C4C-C3C-C2C	-4.14	104.00	106.90
3	D	147	HEM	CMC-C2C-C3C	4.12	132.38	124.68
3	D	147	HEM	C4A-C3A-C2A	-4.07	104.16	107.00
3	E	142	HEM	CMD-C2D-C3D	4.00	132.48	124.94
3	C	142	HEM	C4C-C3C-C2C	3.99	109.69	106.90
3	B	147	HEM	CMA-C3A-C2A	3.90	132.30	124.94
3	A	142	HEM	CMB-C2B-C3B	3.89	131.96	124.68
3	E	142	HEM	C1D-C2D-C3D	3.89	109.70	107.00
3	C	142	HEM	CAD-C3D-C2D	-3.82	116.26	127.25
3	E	142	HEM	C4C-C3C-C2C	3.76	109.52	106.90
3	D	147	HEM	CMD-C2D-C3D	3.64	131.80	124.94
3	E	142	HEM	C3B-C4B-NB	-3.38	104.84	109.21
3	A	142	HEM	CMD-C2D-C3D	3.36	131.28	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	C3C-C4C-NC	-3.30	104.71	110.94
3	F	147	HEM	CMC-C2C-C3C	3.22	130.70	124.68
3	A	142	HEM	CMD-C2D-C1D	-3.18	123.57	128.46
3	D	147	HEM	CMB-C2B-C3B	3.02	130.33	124.68
3	C	142	HEM	C3C-C4C-NC	-2.98	105.31	110.94
3	E	142	HEM	C3C-C4C-NC	-2.96	105.36	110.94
3	D	147	HEM	C3B-C4B-NB	-2.95	105.40	109.21
3	H	147	HEM	CMC-C2C-C3C	-2.95	119.16	124.68
3	H	147	HEM	CMA-C3A-C2A	2.91	130.42	124.94
3	G	142	HEM	CBA-CAA-C2A	-2.89	107.15	112.49
3	G	142	HEM	C3B-C4B-NB	2.88	112.94	109.21
3	A	142	HEM	C4A-C3A-C2A	-2.88	104.99	107.00
3	H	147	HEM	CAA-C2A-C3A	-2.86	119.03	127.25
3	G	142	HEM	C1D-C2D-C3D	-2.84	105.02	107.00
3	C	142	HEM	CAA-CBA-CGA	2.79	117.35	112.67
3	C	142	HEM	CMC-C2C-C3C	2.72	129.76	124.68
3	B	147	HEM	C3B-C4B-NB	2.68	112.67	109.21
3	A	142	HEM	C1D-C2D-C3D	-2.67	105.14	107.00
3	B	147	HEM	CMD-C2D-C1D	-2.66	124.38	128.46
3	G	142	HEM	CMC-C2C-C3C	-2.60	119.82	124.68
3	D	147	HEM	CMA-C3A-C4A	2.59	132.44	128.46
3	B	147	HEM	CAA-CBA-CGA	2.48	116.84	112.67
3	G	142	HEM	CMB-C2B-C3B	2.47	129.30	124.68
3	B	147	HEM	C4C-C3C-C2C	-2.35	105.26	106.90
3	E	142	HEM	CAD-C3D-C2D	2.28	133.79	127.25
3	B	147	HEM	CMC-C2C-C3C	-2.25	120.47	124.68
3	D	147	HEM	CAA-C2A-C3A	2.23	133.65	127.25
3	C	142	HEM	CAD-CBD-CGD	-2.22	108.95	112.67
3	A	142	HEM	CMC-C2C-C3C	2.15	128.69	124.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	147	HEM	C2A-CAA-CBA-CGA
3	H	147	HEM	C2D-C3D-CAD-CBD
3	H	147	HEM	C4D-C3D-CAD-CBD
3	H	147	HEM	C3D-CAD-CBD-CGD
3	D	147	HEM	C3A-C2A-CAA-CBA
3	B	147	HEM	C1A-C2A-CAA-CBA
3	B	147	HEM	C3A-C2A-CAA-CBA
3	F	147	HEM	C2A-CAA-CBA-CGA

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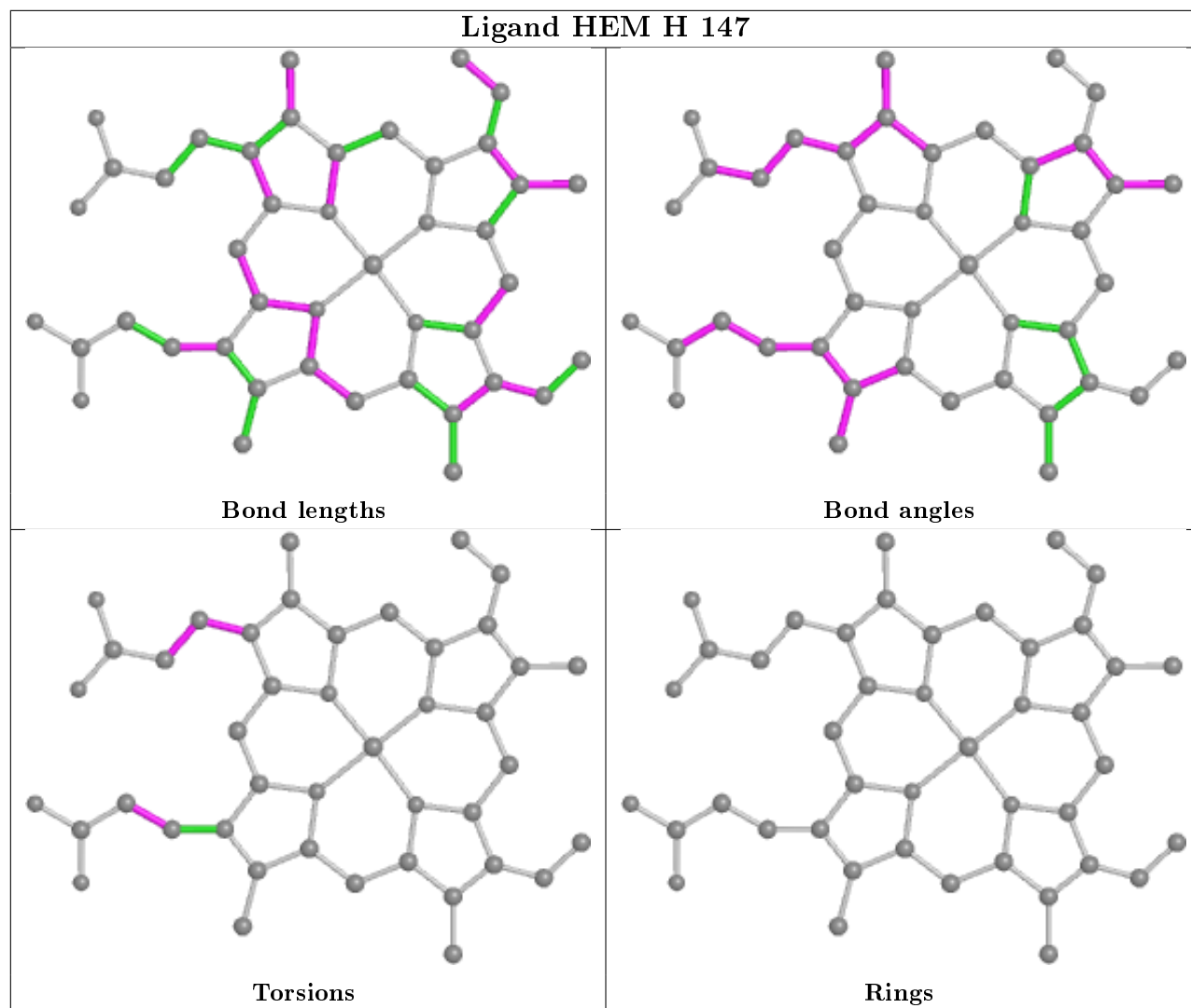
Mol	Chain	Res	Type	Atoms
3	D	147	HEM	C1A-C2A-CAA-CBA

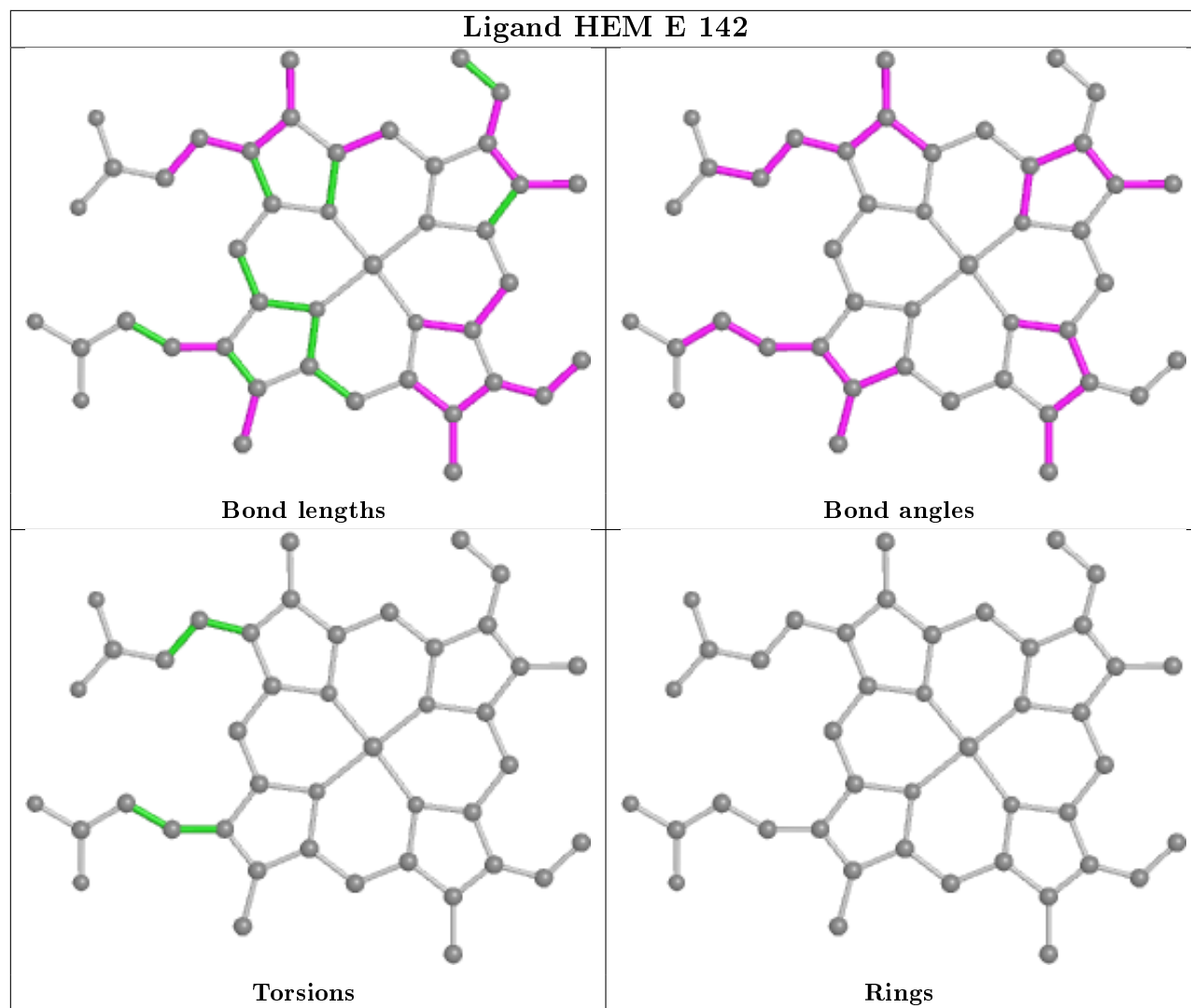
There are no ring outliers.

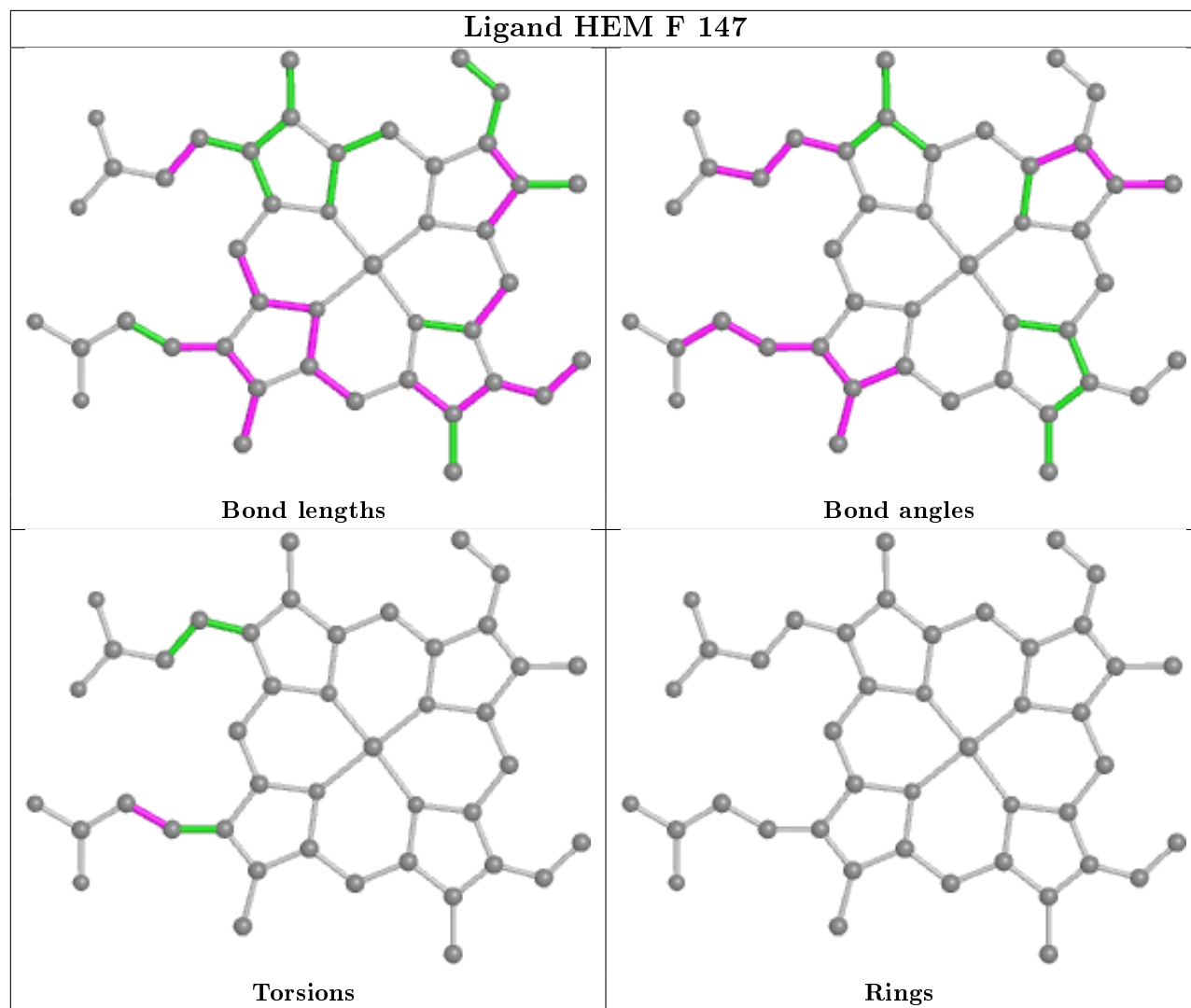
8 monomers are involved in 146 short contacts:

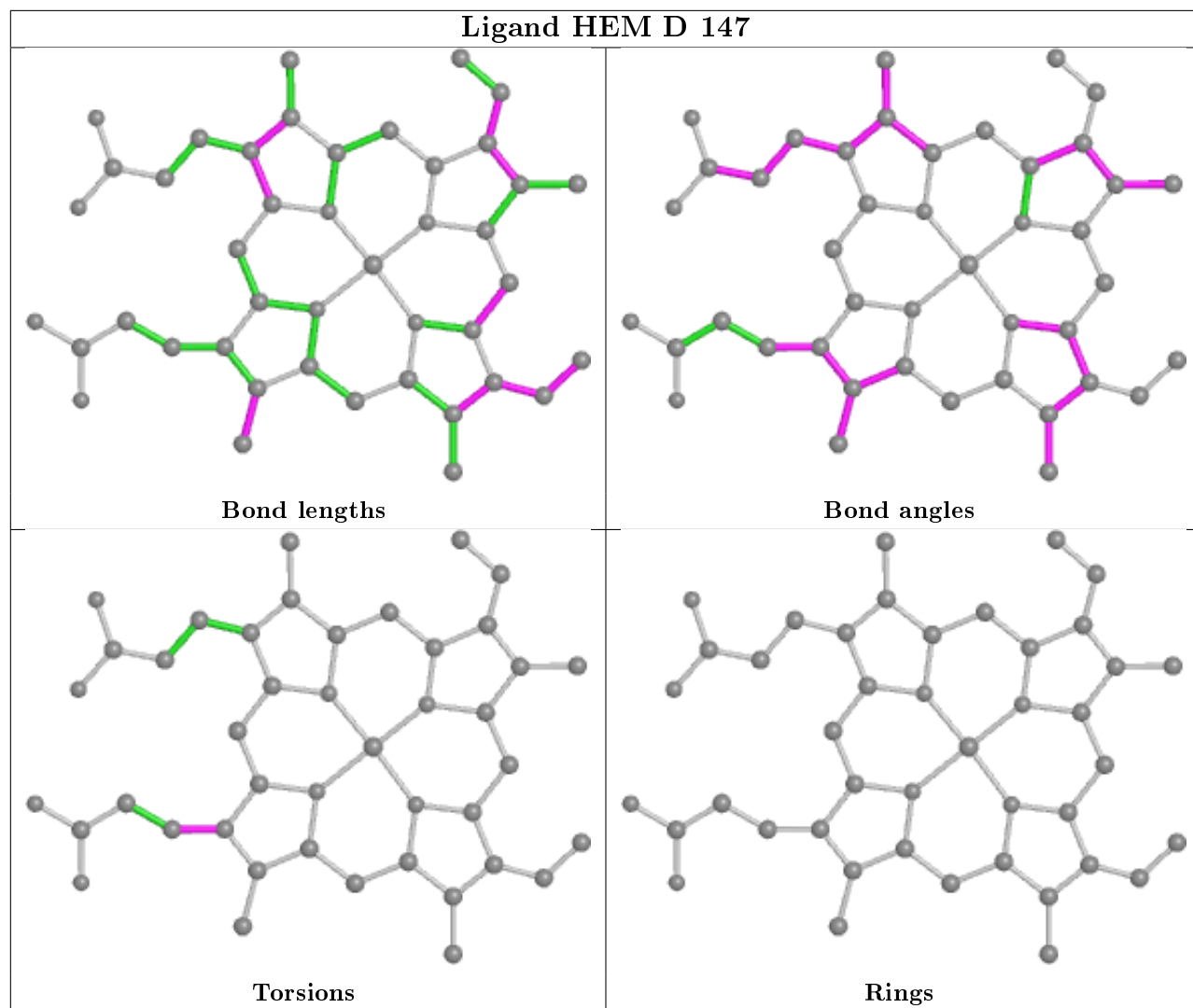
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	147	HEM	7	0
3	E	142	HEM	24	0
3	F	147	HEM	16	1
3	D	147	HEM	25	0
3	B	147	HEM	14	0
3	C	142	HEM	15	0
3	A	142	HEM	23	0
3	G	142	HEM	21	0

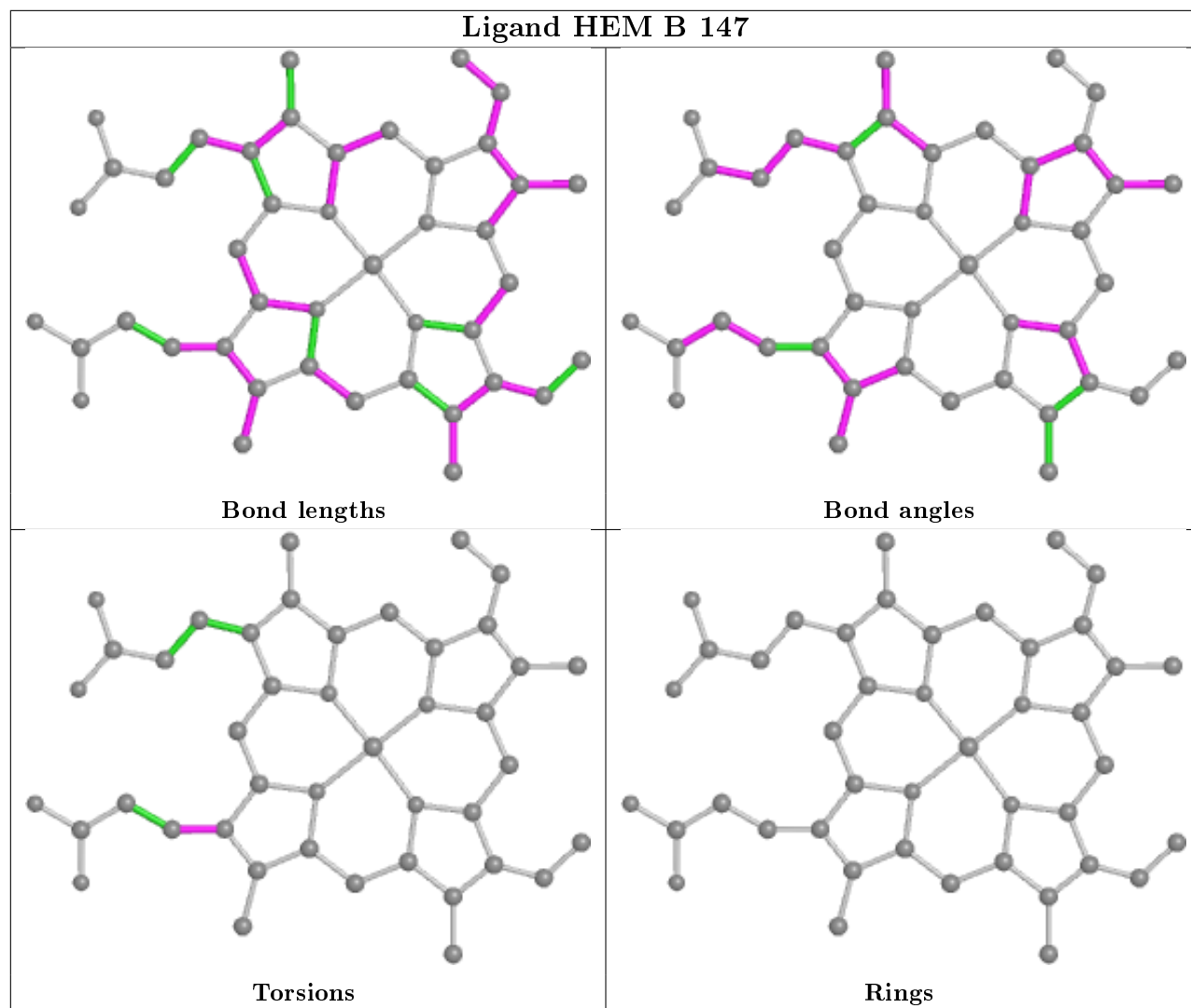
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

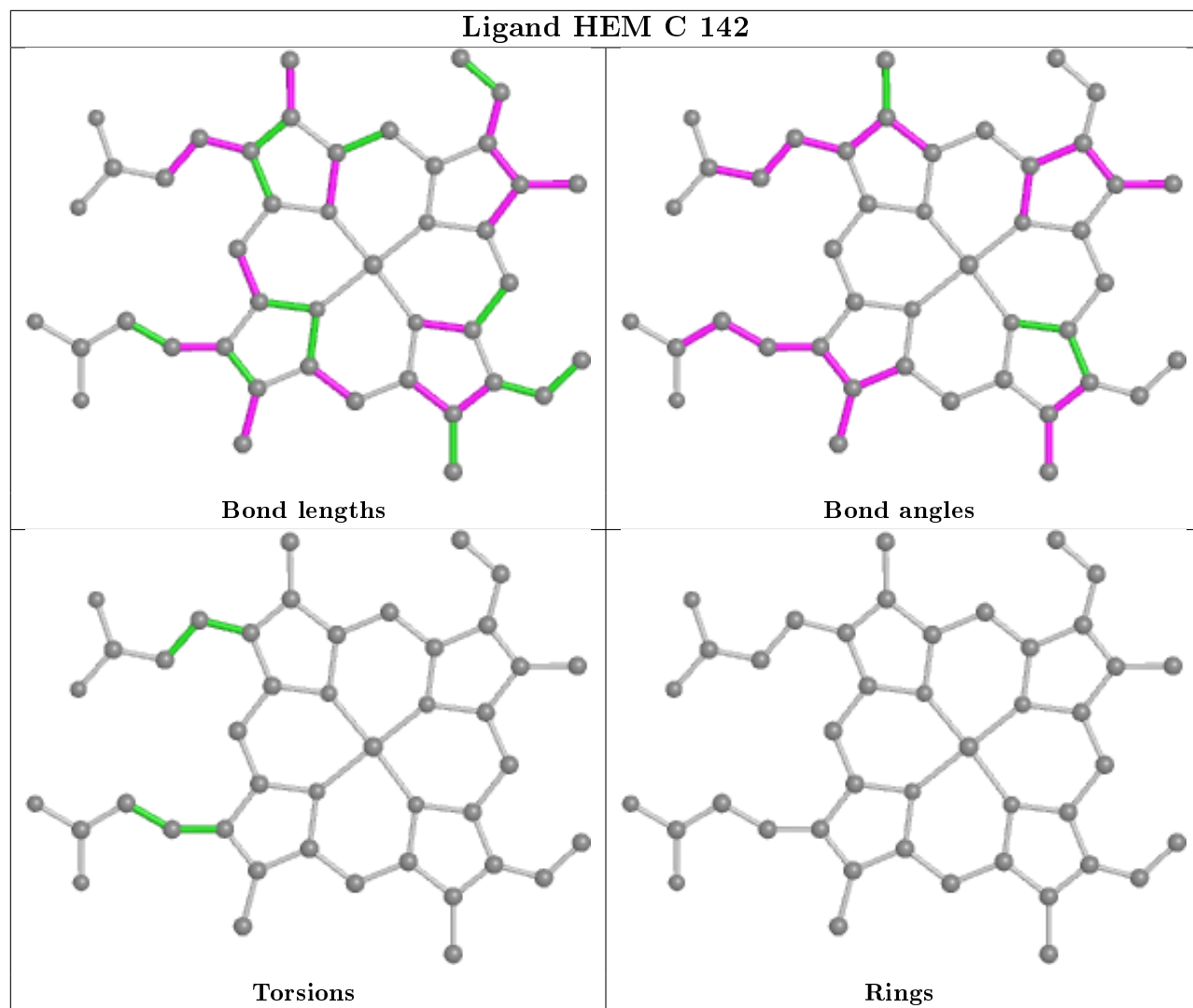


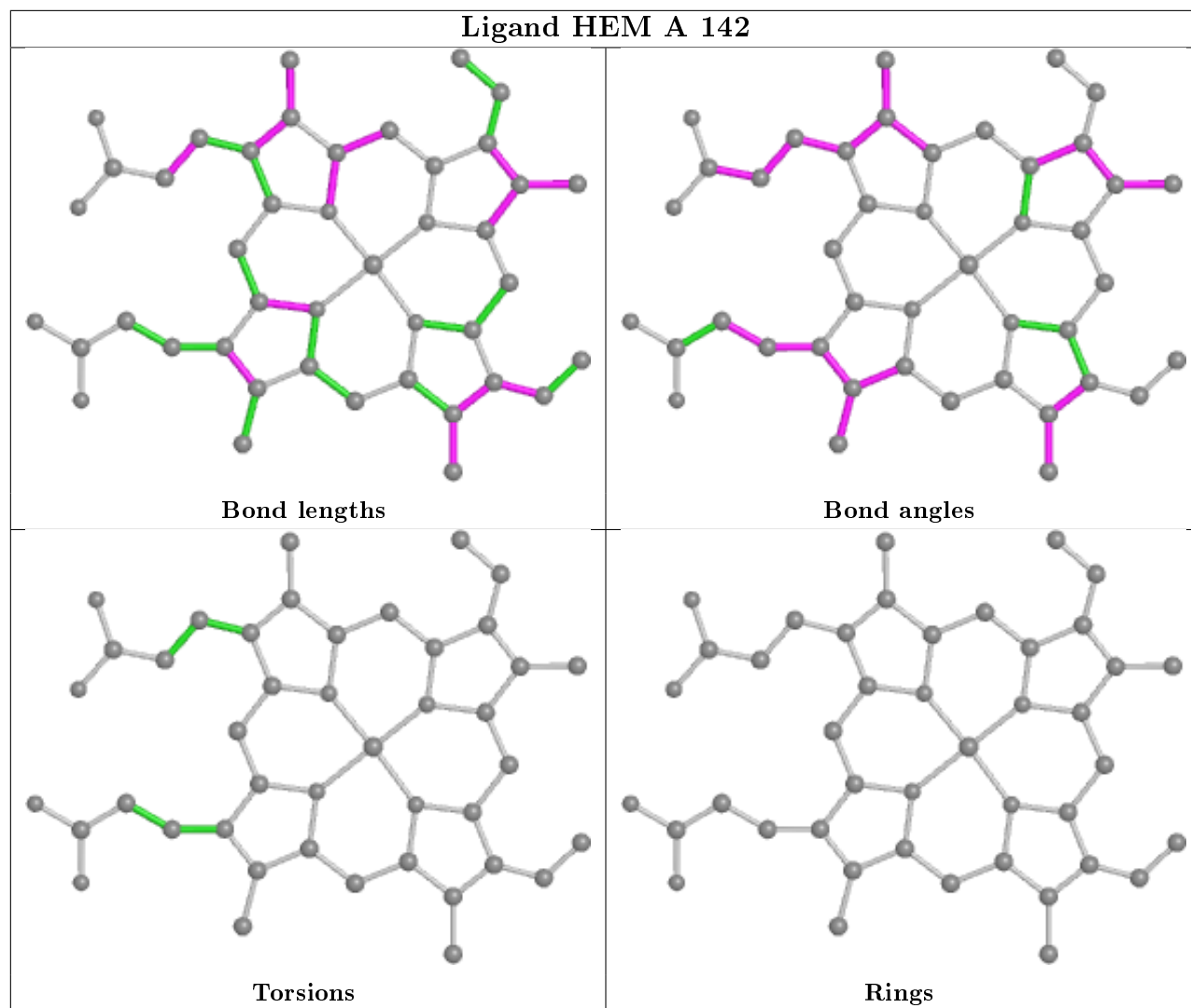


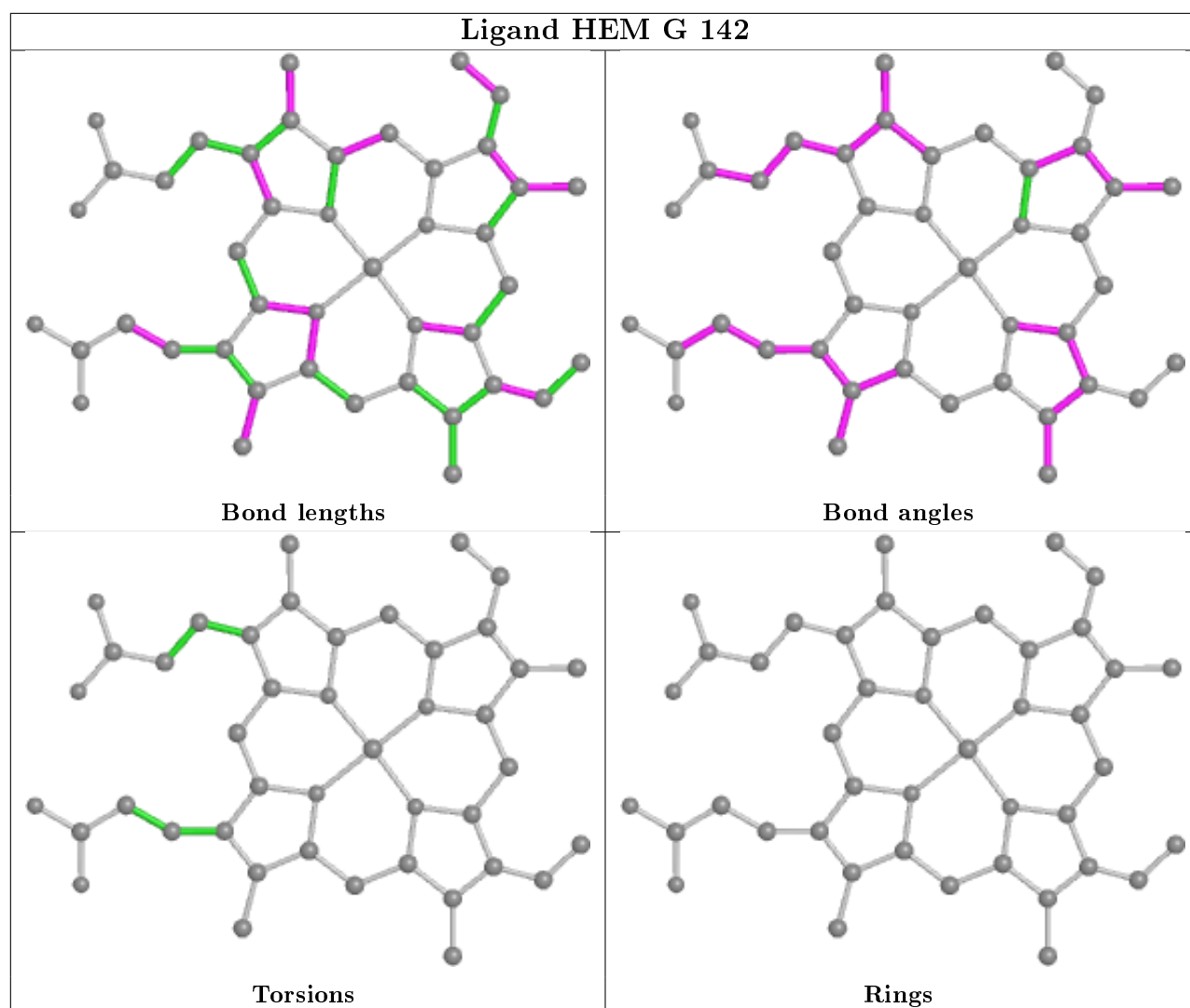












5.7 Other polymers [i](#)

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
2	D	12
1	C	12
1	A	12
1	G	11
2	F	11
1	E	10

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Mol	Chain	Number of breaks
2	H	10
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	125:LEU	C	126:ASP	N	1.62
1	F	145:TYR	C	146:HIS	N	1.62
1	D	129:ALA	C	130:TYR	N	1.61
1	C	37:PRO	C	38:THR	N	1.20
1	C	135:VAL	C	136:LEU	N	1.20
1	D	1:VAL	C	2:HIS	N	1.20
1	D	72:SER	C	73:ASP	N	1.20
1	D	119:GLY	C	120:LYS	N	1.20
1	G	45:HIS	C	46:PHE	N	1.20
1	A	57:GLY	C	58:HIS	N	1.19
1	C	63:ALA	C	64:ASP	N	1.19
1	C	103:HIS	C	104:CYS	N	1.19
1	C	124:SER	C	125:LEU	N	1.19
1	C	128:PHE	C	129:LEU	N	1.19
1	D	3:LEU	C	4:THR	N	1.19
1	D	43:GLU	C	44:SER	N	1.19
1	D	134:VAL	C	135:ALA	N	1.19
1	E	54:GLN	C	55:VAL	N	1.19
1	E	132:VAL	C	133:SER	N	1.19
1	F	116:HIS	C	117:HIS	N	1.19
1	G	67:THR	C	68:ASN	N	1.19
1	A	79:ALA	C	80:LEU	N	1.18
1	A	100:LEU	C	101:LEU	N	1.18
1	A	129:LEU	C	130:ALA	N	1.18
1	C	35:SER	C	36:PHE	N	1.18
1	C	58:HIS	C	59:GLY	N	1.18
1	C	90:LYS	C	91:LEU	N	1.18
1	D	15:TRP	C	16:GLY	N	1.18
1	D	31:LEU	C	32:LEU	N	1.18
1	E	121:VAL	C	122:HIS	N	1.18
1	G	107:VAL	C	108:THR	N	1.18
1	H	4:THR	C	5:PRO	N	1.18
1	H	15:TRP	C	16:GLY	N	1.18
1	H	90:GLU	C	91:LEU	N	1.18
1	H	95:LYS	C	96:LEU	N	1.18
1	H	115:ALA	C	116:HIS	N	1.18
1	A	6:ASP	C	7:LYS	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	55:VAL	C	56:LYS	N	1.17
1	B	7:GLU	C	8:LYS	N	1.17
1	B	63:HIS	C	64:GLY	N	1.17
1	C	36:PHE	C	37:PRO	N	1.17
1	E	4:PRO	C	5:ALA	N	1.17
1	E	41:THR	C	42:TYR	N	1.17
1	E	102:SER	C	103:HIS	N	1.17
1	F	34:VAL	C	35:TYR	N	1.17
1	G	50:HIS	C	51:GLY	N	1.17
1	G	90:LYS	C	91:LEU	N	1.17
1	A	35:SER	C	36:PHE	N	1.16
1	D	127:GLN	C	128:ALA	N	1.16
1	E	134:THR	C	135:VAL	N	1.16
1	F	16:GLY	C	17:LYS	N	1.16
1	F	48:LEU	C	49:SER	N	1.16
1	F	83:GLY	C	84:THR	N	1.16
1	G	81:SER	C	82:ALA	N	1.16
1	H	101:GLU	C	102:ASN	N	1.16
1	C	81:SER	C	82:ALA	N	1.15
1	F	134:VAL	C	135:ALA	N	1.15
1	G	40:LYS	C	41:THR	N	1.15
1	A	89:HIS	C	90:LYS	N	1.14
1	D	117:HIS	C	118:PHE	N	1.14
1	D	131:GLN	C	132:LYS	N	1.14
1	E	119:PRO	C	120:ALA	N	1.14
1	F	12:THR	C	13:ALA	N	1.14
1	F	78:LEU	C	79:ASP	N	1.14
1	C	110:ALA	C	111:ALA	N	1.13
1	H	143:HIS	C	144:LYS	N	1.13
1	A	138:SER	C	139:LYS	N	1.12
1	E	105:LEU	C	106:LEU	N	1.12
1	E	109:LEU	C	110:ALA	N	1.12
1	F	112:CYS	C	113:VAL	N	1.12
1	H	55:MET	C	56:GLY	N	1.12
1	A	95:PRO	C	96:VAL	N	1.11
1	H	135:ALA	C	136:GLY	N	1.11
1	F	137:VAL	C	138:ALA	N	1.10
1	G	37:PRO	C	38:THR	N	1.10
1	G	63:ALA	C	64:ASP	N	1.10
1	H	96:LEU	C	97:HIS	N	1.10
1	A	70:VAL	C	71:ALA	N	1.09
1	G	30:GLU	C	31:ARG	N	1.09

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	23:GLU	C	24:TYR	N	1.06

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.