



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:36 PM UTC

PDB ID : 9GPB / pdb_00009gpb
Title : THE ALLOSTERIC TRANSITION OF GLYCOGEN PHOSPHORYLASE
Authors : Barford, D.; Johnson, L.N.
Deposited on : 1990-12-17
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

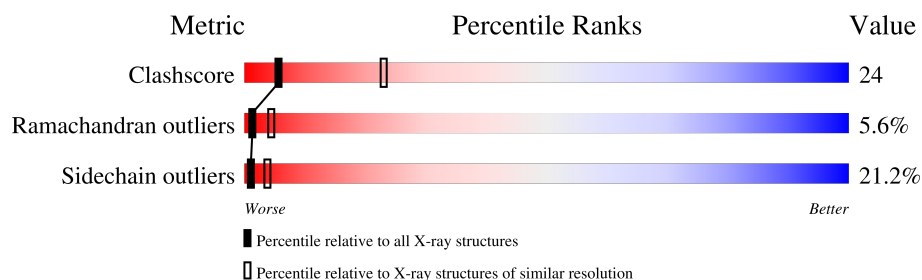
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	
1	B	842	
1	C	842	
1	D	842	

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
2	SO4	C	900	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26873 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	P	S	0	0	0
			6703	4272	1185	1215	1	30			
1	B	823	Total	C	N	O	P	S	0	0	0
			6703	4272	1185	1215	1	30			
1	C	823	Total	C	N	O	P	S	0	0	0
			6703	4271	1185	1216	1	30			
1	D	823	Total	C	N	O	P	S	0	0	0
			6704	4272	1185	1216	1	30			

There are 4 discrepancies between the modelled and reference sequences:

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

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



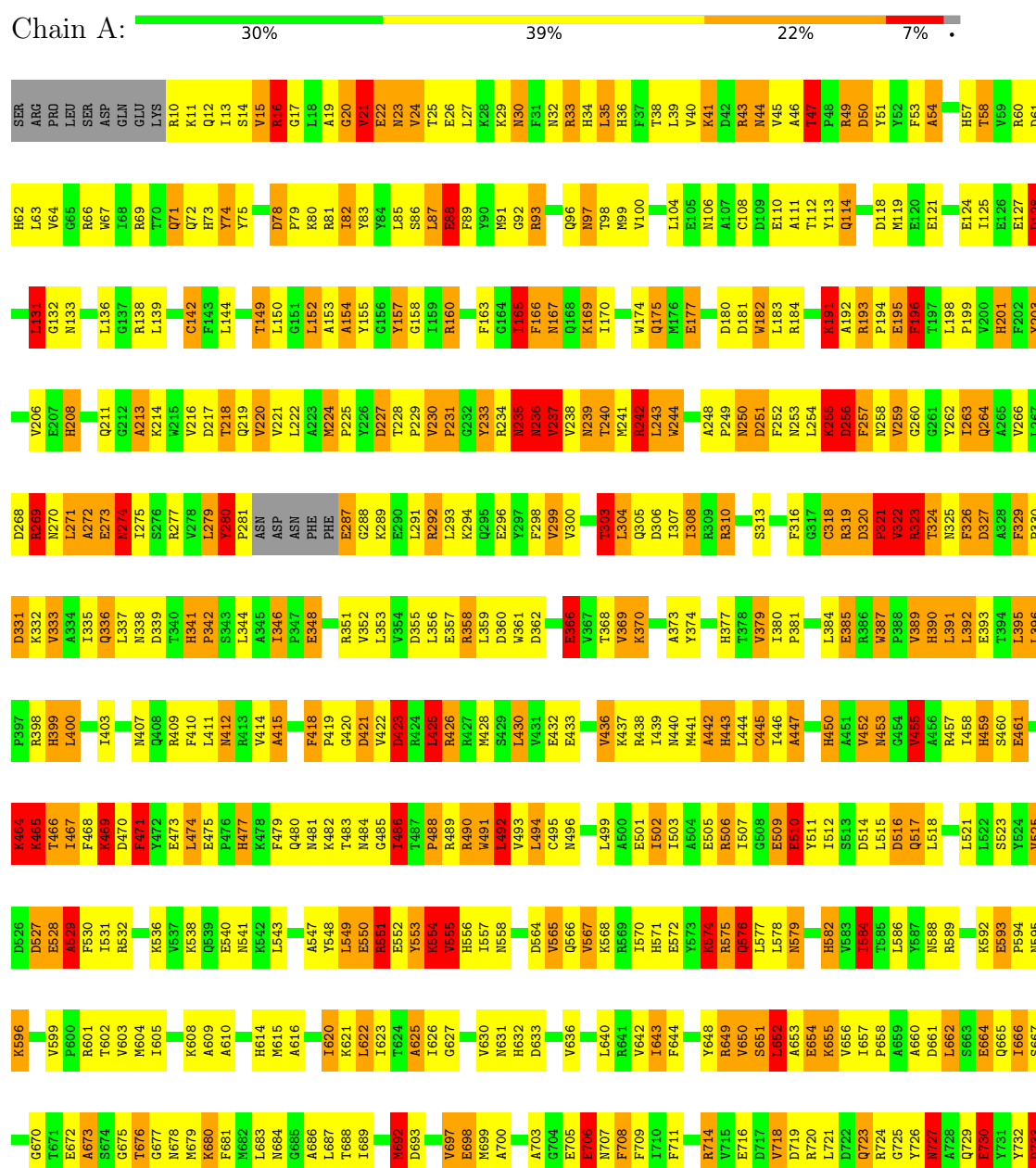
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

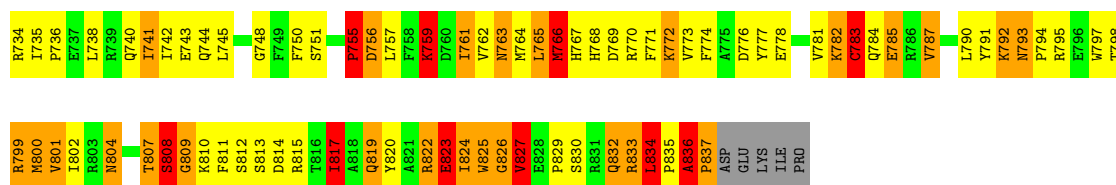
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

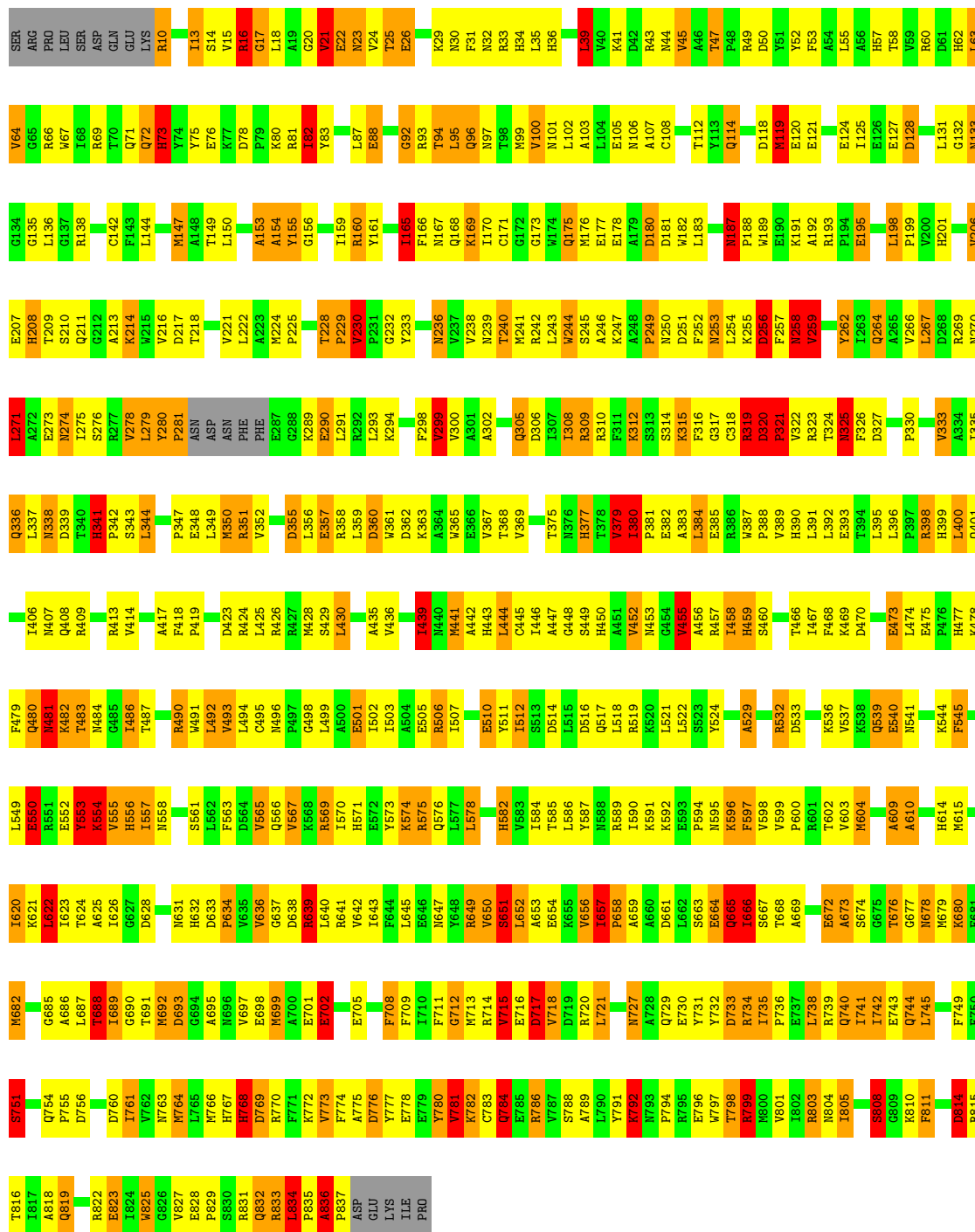
- Molecule 1: Glycogen phosphorylase, muscle form





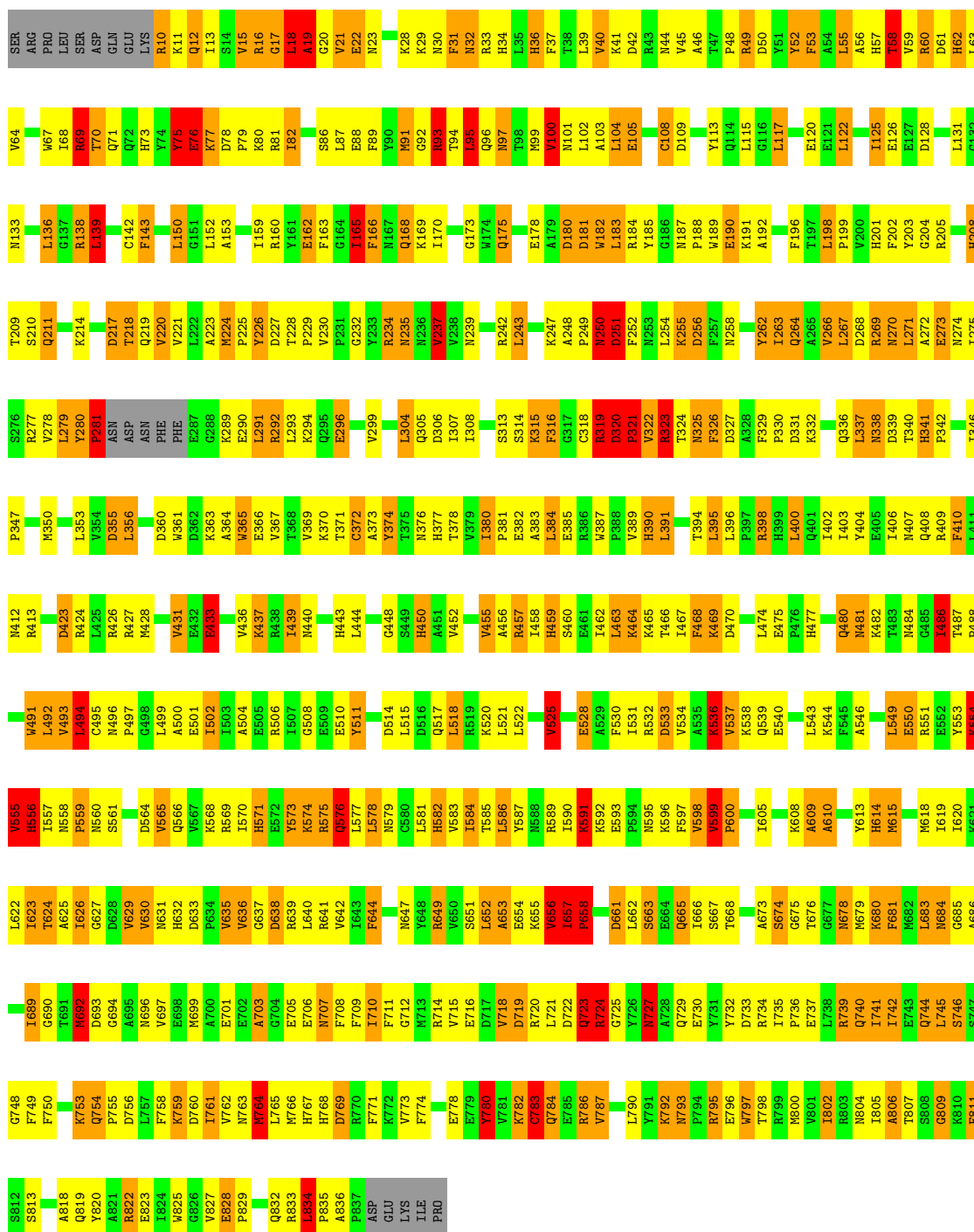
- Molecule 1: Glycogen phosphorylase, muscle form

Chain B: 32% 41% 19% 6%



- Molecule 1: Glycogen phosphorylase, muscle form

Chain C:  32% 39% 22% 5% .



- Molecule 1: Glycogen phosphorylase, muscle form

Chain D:  24% 41% 26% 8%

A836	F774	F711	E646	T585	L521	A456	R386	V322	N258	R193	E124	V64	SER
P837		G712		L586	L522	R457	W387	R323	V259	P194	I125	G65	ARG
ASP	Y777	R713	R649	Y587	S523	T458		T324	G260			R66	PRO
GLU	E778	R714	R650	N588	Y524	H459	R390	N325	G261	L198	D128	W67	LEU
LYS	E779	R715	S651	R589	D525	S460	L391	F326	R262		A129	I68	SER
ILE	E780	E716	L652	I590	D526	E461		D327	I263	V200	G130	R69	ASP
PRD	W781	D717	A653	K591	D527	T462	T394	A328	R264	H201	L131	T70	GLN
	K782	W718	E654	K592	E528	L463	L395	F329	A265	F202	G132	Q71	GLU
	C783	D719	R655	E593	E529	K464	L396	P330	R266	P203	N133	Q72	LYS
	Q784	R720	W656	P594	K465	P397	P397	D331	L267	G204	G134	H73	R10
	Q785	L721	L657	N595	R532	T466	R398	K332	D268	R205	G135	Y74	K11
	R786	D722	P658	K596	D533	L467	H399	V333	R269	V206	L136	Q12	Q12
	W787	Q723	A659	F597			L400	A334	N270	F207	G137	Y75	I13
	S788	R724	K656	V598	K656	D470	Q401	T385	L271	H208	R138	E76	I13
	A789	G725	D661	V599	V537	F471	I402	Q386	A272		L139	K77	S14
	L790	Y726	L662	P600	K638	Y472	I403	E273	R274	A213	F79	D78	V15
	Y791		S663	R601	Q539	E473	Y404	L337		K214	R80	P79	R16
	Q729		E664	T602	E540	L474	E405	D339	W215	F143	R81	R79	G17
	R730		O665	V603	K641	E475	I406	T340	W216	D145	I82	R82	L18
	W731		I666	H604	K542	P476	M407	R341	D217	S146	Y83	Y84	A19
	R795		S667	I605	L543	H477	Q408	P342	T218	M147	Y84	Y84	G20
	E796		T668	G606	K544	R478	R409	S343	Q219	A148	L85	L85	E21
	W797			G607	F545	F479	F410	L344	ASP	T149	S86	S86	N23
	T798		T671	K608			L411		ASN	V220	L87	L87	V24
	R799			A609	L549	T483	N412	E348	PHE	I222	G151	E88	T25
	H800			A610	E550	R484	R413	L349	PHE	A223	L152	F89	E26
	Y801				R551	G485	V414	K350		M224		F90	L27
	T802				E552	T486		R351	G288	R225	Y157	M91	K28
	R803				K614	T487	D421	V352	K289	Y226		G92	K29
	N804				K554	P488	W422	L353	E290	K297	R160	R93	N30
	T805				A616	R489	D423	V354	L291	T228	Y161	T94	F31
	A806				K617	R490	R424	D355	R292	P229	E162	L95	N32
	T807				M618	W491	R426	L356	L293	G232	I165	Q96	R33
	S808				L557	L492	R427	R358	Q295	G231	F166	N97	H34
	G809				P559	V493	M428	L359	E296	R233	M167	M99	H36
	K810				N560	L494	S429	D360	Y287	K234	Q168	V100	F37
	F811				S561	G495	L430	K361	F298	N235	K169	N101	T38
	S812				L562	W496	V431	D362	V299	N236	I170	L102	L39
	S813				F563		E432	K363	V300	V237	C171	A103	V40
	D814				D564	L499		A364		V238	G172	L104	K41
	R815				V565	A500	A435	W365	T303	N239	G173	E105	D42
	T816				Q566	E501	V436	K370	L304	T240	W174	M106	R43
	D766				V567	I502	K437	V367	Q305	M241	Q175	A107	N44
	L757				K568	I503		T368	D306	R242	M176	C108	V45
	F758				R569	A504	R436	V369	I307	L243	E177	D109	A46
	K759				I570	E505	I439	K370	I308	W244	E178	E110	T47
	D760				H571	R506	M440	T371	R309	S245	A179	A111	P48
	I761				E572		M441	C372	R310	A246	D180	T112	R49
	V762				V573	E509	A442	A373	F311	K247	D181	Y113	D50
	N763				K574	E510	H443	Y374	K312	A248	W182	Q114	Y51
	W764				R575	T511	H444	T375	S313	P249	L183	G116	Y52
	L765				Q576	I512	G445	T376	S314	N250	R184	L117	H57
	W766				L577	S513	T446	N376	K315	D251	N187	D118	T58
	H767				L578	D514	A447	H377	F316	P252	P188	M119	V59
	W768				N579	L515	G448	T378	G317	N253	W189	E120	R60
	D769				C580	D516	S449	V379	G318	L254	W189	E120	R60
	R831				L581	Q517	H450	T380	R319	K255	E190	E121	D61
	Q832				L582	L518		P381	D320	H62	K191	L122	H62
	R833				H582	R519	G454	E382	P321	P257	A192	E123	L63
	L834				T584	K520	V455						

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26873	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: SO4, LLP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.26	36/6827 (0.5%)	2.34	427/9236 (4.6%)
1	B	1.27	41/6827 (0.6%)	2.33	384/9236 (4.2%)
1	C	1.28	48/6827 (0.7%)	2.34	396/9237 (4.3%)
1	D	1.26	41/6829 (0.6%)	2.34	426/9240 (4.6%)
All	All	1.27	166/27310 (0.6%)	2.34	1633/36949 (4.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	8
1	C	0	10
1	D	0	6
All	All	0	33

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	VAL	CA-CB	15.48	1.67	1.54
1	C	18	LEU	N-CA	-11.57	1.32	1.46
1	C	565	VAL	CA-CB	9.31	1.66	1.54
1	C	17	GLY	C-N	-8.88	1.21	1.33
1	C	406	ILE	CA-CB	8.77	1.64	1.54
1	B	45	VAL	CA-CB	8.32	1.63	1.54
1	B	450	HIS	CD2-NE2	-8.31	1.28	1.37
1	D	16	ARG	CA-C	-8.13	1.41	1.52
1	D	16	ARG	C-N	-7.76	1.23	1.33
1	D	762	VAL	CA-CB	7.45	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	237	VAL	CA-CB	7.42	1.64	1.54
1	B	582	HIS	CD2-NE2	-7.41	1.29	1.37
1	C	17	GLY	CA-C	-7.33	1.43	1.52
1	A	341	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	565	VAL	CA-CB	7.33	1.67	1.55
1	C	582	HIS	CD2-NE2	-7.29	1.29	1.37
1	D	57	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	259	VAL	CA-CB	7.16	1.64	1.54
1	A	493	VAL	CA-CB	7.16	1.63	1.54
1	D	459	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	333	VAL	CA-CB	7.15	1.64	1.54
1	D	598	VAL	CA-CB	7.13	1.63	1.55
1	A	443	HIS	CD2-NE2	-7.10	1.30	1.37
1	B	623	ILE	CA-CB	7.08	1.61	1.54
1	D	614	HIS	CD2-NE2	-7.08	1.30	1.37
1	C	82	ILE	CA-CB	7.04	1.63	1.54
1	A	582	HIS	CD2-NE2	-6.92	1.30	1.37
1	D	399	HIS	CD2-NE2	-6.91	1.30	1.37
1	D	324	THR	CA-CB	6.90	1.64	1.53
1	A	57	HIS	CD2-NE2	-6.89	1.30	1.37
1	B	399	HIS	CD2-NE2	-6.87	1.30	1.37
1	B	57	HIS	CD2-NE2	-6.86	1.30	1.37
1	B	165	ILE	CA-CB	6.82	1.63	1.54
1	C	450	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	553	TYR	CA-CB	6.70	1.64	1.53
1	C	36	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	341	HIS	CD2-NE2	-6.69	1.30	1.37
1	C	630	VAL	CA-CB	6.65	1.63	1.54
1	C	443	HIS	CD2-NE2	-6.64	1.30	1.37
1	C	73	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.62	1.30	1.37
1	C	199	PRO	CA-CB	-6.60	1.46	1.54
1	D	443	HIS	CD2-NE2	-6.59	1.30	1.37
1	D	377	HIS	CD2-NE2	-6.57	1.30	1.37
1	C	57	HIS	CD2-NE2	-6.55	1.30	1.37
1	C	18	LEU	C-N	-6.54	1.24	1.33
1	C	477	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	571	HIS	CD2-NE2	-6.47	1.30	1.37
1	D	17	GLY	N-CA	-6.46	1.37	1.45
1	D	62	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	299	VAL	CA-CB	6.42	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	VAL	CA-CB	6.41	1.63	1.54
1	A	377	HIS	CG-ND1	-6.40	1.31	1.38
1	D	477	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	459	HIS	CD2-NE2	-6.33	1.30	1.37
1	C	632	HIS	CD2-NE2	-6.33	1.30	1.37
1	B	201	HIS	CD2-NE2	-6.31	1.30	1.37
1	D	620	ILE	CA-CB	6.30	1.61	1.54
1	C	208	HIS	CD2-NE2	-6.28	1.30	1.37
1	C	341	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	377	HIS	CD2-NE2	-6.26	1.30	1.37
1	B	443	HIS	CD2-NE2	-6.25	1.30	1.37
1	D	768	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	73	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	62	HIS	CD2-NE2	-6.20	1.31	1.37
1	D	170	ILE	CA-CB	6.19	1.61	1.53
1	B	377	HIS	CD2-NE2	-6.17	1.31	1.37
1	D	571	HIS	CD2-NE2	-6.14	1.31	1.37
1	C	629	VAL	CA-CB	6.14	1.61	1.54
1	A	614	HIS	CD2-NE2	-6.11	1.31	1.37
1	D	816	THR	CA-CB	-6.09	1.43	1.53
1	B	582	HIS	CG-ND1	-6.09	1.31	1.38
1	B	208	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	477	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	450	HIS	CD2-NE2	-6.08	1.31	1.37
1	D	208	HIS	CD2-NE2	-6.07	1.31	1.37
1	D	556	HIS	CD2-NE2	-6.02	1.31	1.37
1	B	477	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	767	HIS	CD2-NE2	-5.96	1.31	1.37
1	B	62	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	208	HIS	CD2-NE2	-5.90	1.31	1.37
1	C	556	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	244	TRP	CA-CB	-5.89	1.45	1.53
1	C	768	HIS	CD2-NE2	-5.89	1.31	1.37
1	C	165	ILE	CA-CB	5.89	1.62	1.54
1	C	390	HIS	CD2-NE2	-5.88	1.31	1.37
1	C	787	VAL	CA-CB	5.85	1.60	1.54
1	C	767	HIS	CD2-NE2	-5.85	1.31	1.37
1	B	57	HIS	CG-ND1	-5.84	1.31	1.38
1	C	459	HIS	CD2-NE2	-5.83	1.31	1.37
1	C	62	HIS	CD2-NE2	-5.82	1.31	1.37
1	C	819	GLN	CA-CB	-5.78	1.44	1.53
1	A	399	HIS	CD2-NE2	-5.76	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	614	HIS	CD2-NE2	-5.75	1.31	1.37
1	D	626	ILE	CA-CB	5.74	1.60	1.54
1	B	741	ILE	CA-CB	5.73	1.61	1.54
1	A	34	HIS	CD2-NE2	-5.72	1.31	1.37
1	D	582	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	459	HIS	CD2-NE2	-5.70	1.31	1.37
1	D	657	ILE	CA-C	5.68	1.58	1.52
1	C	599	VAL	CA-CB	5.66	1.61	1.54
1	A	455	VAL	CA-C	5.64	1.59	1.52
1	B	768	HIS	CD2-NE2	-5.64	1.31	1.37
1	C	34	HIS	CD2-NE2	-5.62	1.31	1.37
1	C	555	VAL	CA-CB	5.62	1.62	1.54
1	D	767	HIS	CD2-NE2	-5.55	1.31	1.37
1	C	201	HIS	CD2-NE2	-5.55	1.31	1.37
1	D	707	ASN	CA-CB	5.54	1.62	1.53
1	C	571	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	767	HIS	CD2-NE2	-5.53	1.31	1.37
1	B	36	HIS	CD2-NE2	-5.53	1.31	1.37
1	B	571	HIS	CD2-NE2	-5.53	1.31	1.37
1	C	219	GLN	CA-CB	-5.52	1.45	1.53
1	D	341	HIS	CD2-NE2	-5.50	1.31	1.37
1	D	450	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	656	VAL	CA-CB	5.50	1.61	1.54
1	C	19	ALA	N-CA	-5.49	1.39	1.46
1	B	781	VAL	CA-CB	5.48	1.60	1.54
1	A	768	HIS	CD2-NE2	-5.43	1.31	1.37
1	B	556	HIS	CD2-NE2	-5.40	1.31	1.37
1	D	399	HIS	CG-ND1	-5.39	1.32	1.38
1	D	632	HIS	CD2-NE2	-5.39	1.31	1.37
1	C	734	ARG	C-N	5.35	1.39	1.33
1	D	73	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	375	THR	CA-CB	5.33	1.60	1.53
1	B	390	HIS	CD2-NE2	-5.32	1.32	1.37
1	C	464	LYS	CA-C	5.32	1.59	1.52
1	B	614	HIS	CD2-NE2	-5.32	1.32	1.37
1	C	34	HIS	CG-ND1	-5.32	1.32	1.38
1	B	244	TRP	CG-CD2	-5.28	1.34	1.43
1	D	188	PRO	CA-CB	-5.27	1.46	1.53
1	A	390	HIS	CD2-NE2	-5.27	1.32	1.37
1	C	377	HIS	CD2-NE2	-5.27	1.32	1.37
1	B	831	ARG	NE-CZ	5.24	1.38	1.33
1	A	555	VAL	CA-CB	5.24	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	HIS	CD2-NE2	-5.23	1.32	1.37
1	D	390	HIS	CD2-NE2	-5.23	1.32	1.37
1	D	82	ILE	CA-CB	5.23	1.60	1.53
1	A	220	VAL	CA-CB	5.22	1.60	1.53
1	B	632	HIS	CD2-NE2	-5.20	1.32	1.37
1	D	201	HIS	CD2-NE2	-5.18	1.32	1.37
1	D	57	HIS	CG-ND1	-5.18	1.32	1.38
1	A	455	VAL	CA-CB	5.17	1.61	1.54
1	A	54	ALA	CA-CB	-5.17	1.45	1.53
1	D	436	VAL	CA-CB	5.17	1.61	1.54
1	A	557	ILE	CA-CB	-5.17	1.48	1.54
1	D	189	TRP	CG-CD2	-5.16	1.34	1.43
1	D	340	THR	CA-CB	5.16	1.62	1.53
1	A	21	VAL	CA-CB	5.15	1.61	1.54
1	A	698	GLU	CA-CB	-5.13	1.45	1.53
1	A	632	HIS	CD2-NE2	-5.13	1.32	1.37
1	C	62	HIS	CG-ND1	-5.13	1.32	1.38
1	C	57	HIS	CG-ND1	-5.13	1.32	1.38
1	B	567	VAL	CA-CB	5.12	1.60	1.53
1	C	100	VAL	CA-CB	5.12	1.60	1.54
1	B	34	HIS	CG-ND1	-5.09	1.32	1.38
1	B	450	HIS	CG-ND1	-5.07	1.32	1.38
1	C	347	PRO	CA-CB	-5.07	1.46	1.53
1	B	399	HIS	CG-ND1	-5.06	1.32	1.38
1	D	824	ILE	CA-CB	5.05	1.60	1.55
1	B	379	VAL	CA-CB	5.04	1.61	1.54
1	A	36	HIS	CD2-NE2	-5.04	1.32	1.37
1	D	36	HIS	CD2-NE2	-5.04	1.32	1.37
1	C	773	VAL	CA-CB	5.02	1.61	1.54
1	C	710	ILE	CA-CB	5.01	1.59	1.54

All (1633) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	GLY	O-C-N	26.32	153.18	122.64
1	B	266	VAL	N-CA-C	-15.28	96.17	110.53
1	A	575	ARG	N-CA-C	15.16	132.75	111.52
1	A	128	ASP	CA-CB-CG	14.59	127.19	112.60
1	D	533	ASP	CA-CB-CG	13.61	126.21	112.60
1	D	256	ASP	CA-CB-CG	13.53	126.13	112.60
1	A	507	ILE	N-CA-C	12.94	124.45	112.29
1	B	259	VAL	N-CA-C	12.63	125.86	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	ASN	CA-CB-CG	12.52	125.12	112.60
1	A	181	ASP	CA-CB-CG	12.32	124.92	112.60
1	B	217	ASP	CA-CB-CG	12.31	124.91	112.60
1	B	257	PHE	CA-CB-CG	-12.18	101.62	113.80
1	C	324	THR	N-CA-C	-12.03	94.94	111.30
1	B	468	PHE	CA-CB-CG	11.96	125.76	113.80
1	A	235	ASN	CA-CB-CG	11.70	124.30	112.60
1	C	17	GLY	CA-C-N	11.60	139.27	121.76
1	C	17	GLY	C-N-CA	11.60	139.27	121.76
1	B	647	ASN	CA-CB-CG	11.56	124.16	112.60
1	C	97	ASN	CB-CG-ND2	11.48	133.63	116.40
1	B	834	LEU	N-CA-C	11.39	128.15	109.58
1	D	558	ASN	CA-CB-CG	11.31	123.91	112.60
1	D	707	ASN	OD1-CG-ND2	-11.27	111.33	122.60
1	C	251	ASP	CA-CB-CG	11.13	123.73	112.60
1	C	32	ASN	CA-CB-CG	-11.03	101.57	112.60
1	B	377	HIS	CA-CB-CG	-11.02	102.78	113.80
1	A	709	PHE	CA-CB-CG	-10.93	102.87	113.80
1	D	808	SER	N-CA-C	10.86	129.28	111.37
1	B	305	GLN	N-CA-C	-10.77	99.62	111.36
1	C	168	GLN	CG-CD-NE2	10.69	132.44	116.40
1	C	771	PHE	CA-CB-CG	-10.68	103.12	113.80
1	C	380	ILE	N-CA-C	-10.58	96.35	107.89
1	A	218	THR	N-CA-C	10.53	124.67	110.35
1	C	281	PRO	N-CA-C	10.53	138.43	112.10
1	B	665	GLN	OE1-CD-NE2	-10.48	112.12	122.60
1	B	481	ASN	OD1-CG-ND2	-10.45	112.15	122.60
1	A	23	ASN	N-CA-C	-10.44	99.70	111.71
1	A	12	GLN	OE1-CD-NE2	-10.41	112.19	122.60
1	B	609	ALA	N-CA-C	10.41	123.60	111.11
1	B	783	CYS	N-CA-C	-10.40	99.34	113.18
1	C	450	HIS	CA-CB-CG	10.37	124.17	113.80
1	D	811	PHE	CA-CB-CG	-10.37	103.43	113.80
1	D	575	ARG	N-CA-C	10.35	126.01	111.52
1	C	17	GLY	N-CA-C	10.34	123.87	112.29
1	C	371	THR	N-CA-C	10.29	122.19	110.97
1	B	341	HIS	CB-CG-CD2	-10.28	117.84	131.20
1	D	555	VAL	N-CA-C	10.21	130.59	109.34
1	A	258	ASN	N-CA-C	-10.16	100.16	111.14
1	D	536	LYS	CA-C-O	-10.13	110.46	120.90
1	A	719	ASP	CA-CB-CG	10.13	122.73	112.60
1	B	477	HIS	CA-CB-CG	10.06	123.86	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASN	O-C-N	10.06	135.00	122.93
1	B	341	HIS	CB-CG-ND1	10.04	137.76	122.70
1	B	435	ALA	N-CA-C	-10.00	93.17	108.67
1	D	793	ASN	N-CA-C	-9.97	88.58	108.71
1	B	749	PHE	CA-CB-CG	9.96	123.76	113.80
1	B	727	ASN	OD1-CG-ND2	-9.95	112.65	122.60
1	B	319	ARG	N-CA-C	9.89	124.64	108.52
1	C	77	LYS	O-C-N	9.87	132.24	122.07
1	B	355	ASP	CA-CB-CG	9.85	122.45	112.60
1	A	595	ASN	CA-CB-CG	9.85	122.44	112.60
1	C	255	LYS	O-C-N	9.84	135.03	122.93
1	C	11	LYS	N-CA-C	9.80	122.98	111.71
1	D	515	LEU	N-CA-C	9.79	125.92	113.88
1	D	676	THR	CA-CB-OG1	-9.75	94.97	109.60
1	B	335	ILE	N-CA-CB	-9.74	102.62	112.06
1	B	733	ASP	CA-CB-CG	9.73	122.33	112.60
1	C	455	VAL	N-CA-CB	-9.64	101.11	112.39
1	B	735	ILE	O-C-N	-9.60	114.73	121.55
1	B	168	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	C	740	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	A	804	ASN	OD1-CG-ND2	-9.57	113.03	122.60
1	C	20	GLY	N-CA-C	-9.54	102.82	115.32
1	A	455	VAL	N-CA-CB	-9.53	95.50	111.23
1	C	305	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	B	274	ASN	CA-CB-CG	9.49	122.09	112.60
1	B	252	PHE	CA-CB-CG	9.47	123.27	113.80
1	C	42	ASP	CA-CB-CG	9.45	122.05	112.60
1	C	390	HIS	CA-CB-CG	9.41	123.21	113.80
1	D	390	HIS	CA-CB-CG	9.36	123.16	113.80
1	B	44	ASN	CA-C-O	-9.36	109.21	119.97
1	A	355	ASP	CA-CB-CG	9.33	121.93	112.60
1	C	323	ARG	N-CA-C	9.30	130.62	110.80
1	D	620	ILE	N-CA-C	-9.30	101.49	110.42
1	A	700	ALA	N-CA-C	-9.28	101.14	111.07
1	B	229	PRO	N-CA-C	9.26	125.30	111.03
1	C	463	LEU	N-CA-C	-9.23	103.12	114.75
1	D	740	GLN	OE1-CD-NE2	-9.22	113.38	122.60
1	B	187	ASN	OD1-CG-ND2	-9.18	113.42	122.60
1	D	250	ASN	OD1-CG-ND2	-9.18	113.42	122.60
1	B	623	ILE	N-CA-CB	9.16	120.24	110.62
1	A	21	VAL	N-CA-C	9.14	128.36	109.34
1	D	394	THR	CA-CB-OG1	-9.11	95.94	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	ASN	OD1-CG-ND2	-9.06	113.54	122.60
1	C	264	GLN	N-CA-C	-9.06	101.40	111.28
1	D	717	ASP	CA-CB-CG	9.05	121.65	112.60
1	B	773	VAL	CA-CB-CG2	-9.00	95.10	110.40
1	C	325	ASN	OD1-CG-ND2	-8.99	113.61	122.60
1	B	455	VAL	N-CA-CB	-8.96	96.44	111.23
1	C	661	ASP	CA-CB-CG	8.95	121.55	112.60
1	D	479	PHE	CA-CB-CG	-8.93	104.87	113.80
1	C	168	GLN	OE1-CD-NE2	-8.92	113.68	122.60
1	B	154	ALA	N-CA-C	8.90	123.75	107.99
1	C	647	ASN	CA-CB-CG	8.89	121.49	112.60
1	A	217	ASP	CA-CB-CG	8.87	121.47	112.60
1	D	73	HIS	CA-CB-CG	8.85	122.65	113.80
1	B	595	ASN	OD1-CG-ND2	-8.84	113.76	122.60
1	D	719	ASP	CA-CB-CG	8.82	121.42	112.60
1	A	61	ASP	CA-CB-CG	8.78	121.38	112.60
1	B	429	SER	N-CA-C	8.76	122.58	110.24
1	D	588	ASN	N-CA-C	8.76	120.90	111.36
1	D	427	ARG	N-CA-C	-8.75	103.02	114.31
1	B	211	GLN	N-CA-C	-8.73	100.11	110.41
1	C	211	GLN	N-CA-C	-8.73	102.17	113.17
1	C	319	ARG	CA-C-O	8.73	132.41	122.37
1	C	18	LEU	N-CA-C	-8.72	92.43	107.61
1	B	447	ALA	O-C-N	8.71	131.49	122.09
1	B	769	ASP	CA-CB-CG	8.70	121.30	112.60
1	B	379	VAL	N-CA-CB	-8.67	96.92	111.23
1	C	355	ASP	N-CA-C	8.67	120.35	111.07
1	C	320	ASP	CA-CB-CG	8.65	121.25	112.60
1	D	319	ARG	N-CA-C	8.61	123.22	110.30
1	D	407	ASN	CA-C-O	-8.58	111.99	121.00
1	B	574	LYS	N-CA-C	-8.55	91.90	107.98
1	C	272	ALA	N-CA-C	-8.55	101.56	112.93
1	A	554	LYS	CA-C-O	-8.52	111.96	121.51
1	B	100	VAL	CA-C-O	-8.52	111.60	121.05
1	C	128	ASP	CA-CB-CG	8.44	121.04	112.60
1	C	760	ASP	CA-CB-CG	8.44	121.04	112.60
1	B	715	VAL	CA-C-O	-8.43	110.24	120.78
1	D	252	PHE	O-C-N	8.43	132.50	123.06
1	A	239	ASN	CA-CB-CG	8.41	121.01	112.60
1	D	16	ARG	O-C-N	8.40	133.76	122.59
1	C	494	LEU	N-CA-C	8.38	121.16	111.11
1	B	816	THR	N-CA-C	-8.37	101.39	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	665	GLN	OE1-CD-NE2	-8.37	114.23	122.60
1	D	561	SER	CA-CB-OG	8.34	127.78	111.10
1	B	553	TYR	CA-CB-CG	8.31	128.86	113.90
1	C	544	LYS	N-CA-C	-8.30	101.77	112.23
1	D	336	GLN	CA-CB-CG	-8.30	97.50	114.10
1	D	317	GLY	O-C-N	8.30	130.35	122.13
1	D	571	HIS	CB-CG-CD2	-8.30	120.41	131.20
1	B	149	THR	N-CA-C	8.28	120.31	111.28
1	B	780	TYR	N-CA-C	-8.28	101.30	111.40
1	A	165	ILE	N-CA-C	-8.26	96.45	109.17
1	B	198	LEU	CA-C-N	8.24	128.27	119.78
1	B	198	LEU	C-N-CA	8.24	128.27	119.78
1	D	631	ASN	CA-CB-CG	8.24	120.84	112.60
1	C	380	ILE	CB-CA-C	8.24	119.18	110.37
1	A	571	HIS	CB-CG-CD2	-8.23	120.51	131.20
1	C	68	ILE	N-CA-C	-8.21	102.33	110.30
1	D	106	ASN	CA-CB-CG	8.21	120.81	112.60
1	A	175	GLN	OE1-CD-NE2	-8.20	114.40	122.60
1	D	42	ASP	CA-CB-CG	8.20	120.80	112.60
1	C	202	PHE	CA-CB-CG	-8.19	105.61	113.80
1	D	496	ASN	OD1-CG-ND2	-8.18	114.42	122.60
1	C	97	ASN	OD1-CG-ND2	-8.18	114.42	122.60
1	A	766	MET	N-CA-C	8.16	120.26	111.36
1	B	554	LYS	N-CA-C	8.16	128.18	110.80
1	C	189	TRP	CG-CD2-CE3	8.16	142.06	133.90
1	D	582	HIS	CA-CB-CG	8.15	121.95	113.80
1	D	224	MET	CA-C-N	8.15	127.91	119.76
1	D	224	MET	C-N-CA	8.15	127.91	119.76
1	A	236	ASN	N-CA-C	8.14	128.15	110.80
1	D	440	ASN	OD1-CG-ND2	-8.14	114.46	122.60
1	A	450	HIS	CB-CG-CD2	-8.13	120.63	131.20
1	D	75	TYR	N-CA-C	-8.13	102.36	111.14
1	D	280	TYR	N-CA-C	8.13	121.53	110.31
1	A	356	LEU	N-CA-C	8.11	119.75	111.07
1	A	475	GLU	CA-C-N	8.11	127.67	119.24
1	A	475	GLU	C-N-CA	8.11	127.67	119.24
1	D	421	ASP	CA-CB-CG	-8.09	104.51	112.60
1	B	571	HIS	CB-CG-CD2	-8.08	120.69	131.20
1	A	716	GLU	CB-CG-CD	8.06	126.31	112.60
1	A	106	ASN	OD1-CG-ND2	-8.06	114.54	122.60
1	B	312	LYS	CG-CD-CE	8.04	129.80	111.30
1	C	723	GLN	N-CA-C	-8.04	93.67	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIS	CB-CG-CD2	-8.04	120.75	131.20
1	A	557	ILE	CB-CG1-CD1	-8.03	96.93	113.80
1	C	270	ASN	N-CA-C	8.02	120.73	111.11
1	C	232	GLY	CA-C-O	-7.98	113.66	120.92
1	A	467	ILE	CB-CA-C	-7.98	101.56	112.02
1	A	196	PHE	CA-CB-CG	7.98	121.78	113.80
1	B	775	ALA	O-C-N	7.96	130.36	122.09
1	A	509	GLU	O-C-N	7.95	131.94	122.96
1	C	320	ASP	N-CA-CB	-7.94	96.23	110.37
1	B	325	ASN	N-CA-C	7.94	121.91	110.24
1	A	193	ARG	CG-CD-NE	-7.92	94.57	112.00
1	D	755	PRO	N-CA-C	7.92	125.30	113.81
1	C	620	ILE	N-CA-C	-7.92	102.62	110.30
1	A	57	HIS	CA-C-O	-7.90	111.17	120.10
1	B	335	ILE	O-C-N	-7.90	113.59	122.36
1	B	567	VAL	CA-C-O	7.90	128.80	120.51
1	C	583	VAL	N-CA-C	-7.88	102.65	110.30
1	D	18	LEU	N-CA-C	7.88	127.58	110.80
1	A	21	VAL	CG1-CB-CG2	-7.86	93.51	110.80
1	D	541	ASN	CA-CB-CG	-7.86	104.74	112.60
1	A	308	ILE	N-CA-CB	-7.84	99.22	110.52
1	A	341	HIS	CA-CB-CG	7.82	121.62	113.80
1	B	236	ASN	CA-CB-CG	-7.80	104.80	112.60
1	D	373	ALA	CA-C-O	-7.80	113.11	121.38
1	B	496	ASN	CA-C-N	7.79	127.51	119.64
1	B	496	ASN	C-N-CA	7.79	127.51	119.64
1	B	678	ASN	CA-CB-CG	7.78	120.38	112.60
1	D	143	PHE	CA-CB-CG	7.76	121.56	113.80
1	D	128	ASP	CA-CB-CG	7.76	120.36	112.60
1	C	404	TYR	O-C-N	-7.75	113.31	122.15
1	B	380	ILE	N-CA-CB	-7.75	100.36	111.21
1	A	574	LYS	CA-C-N	7.74	133.09	122.34
1	A	574	LYS	C-N-CA	7.74	133.09	122.34
1	C	406	ILE	N-CA-C	-7.74	102.80	110.30
1	D	341	HIS	CA-CB-CG	7.73	121.53	113.80
1	D	769	ASP	CA-C-O	7.72	128.57	120.54
1	D	560	ASN	CA-CB-CG	7.71	120.31	112.60
1	B	555	VAL	N-CA-C	7.71	125.37	109.34
1	A	455	VAL	N-CA-C	7.68	125.32	109.34
1	B	447	ALA	N-CA-C	7.68	119.44	111.14
1	C	525	VAL	CB-CA-C	-7.68	101.86	111.70
1	C	706	GLU	CB-CA-C	-7.66	98.07	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	LEU	N-CA-C	-7.65	102.87	111.14
1	C	113	TYR	N-CA-C	-7.65	102.54	111.03
1	C	623	ILE	CB-CA-C	-7.64	101.83	112.14
1	D	796	GLU	N-CA-C	-7.63	103.97	113.20
1	A	614	HIS	CA-C-O	-7.63	112.39	120.55
1	C	404	TYR	CA-C-O	-7.62	112.34	120.42
1	A	250	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	D	60	ARG	CA-CB-CG	-7.61	98.88	114.10
1	A	47	THR	N-CA-CB	-7.61	100.92	109.74
1	D	767	HIS	CB-CG-CD2	-7.60	121.32	131.20
1	B	168	GLN	CG-CD-NE2	7.60	127.80	116.40
1	C	575	ARG	N-CA-C	7.59	126.97	110.80
1	D	47	THR	N-CA-CB	-7.59	99.10	109.88
1	D	373	ALA	O-C-N	-7.59	115.30	123.26
1	B	257	PHE	CA-C-O	7.58	131.35	120.51
1	B	716	GLU	CB-CG-CD	7.58	125.48	112.60
1	D	553	TYR	O-C-N	-7.58	112.51	122.59
1	D	756	ASP	N-CA-C	-7.57	102.63	111.03
1	A	516	ASP	CA-CB-CG	-7.55	105.05	112.60
1	D	707	ASN	CA-CB-CG	7.54	120.14	112.60
1	D	536	LYS	N-CA-C	-7.53	102.67	111.03
1	D	450	HIS	CA-CB-CG	7.53	121.33	113.80
1	B	550	GLU	CB-CG-CD	7.53	125.39	112.60
1	B	825	TRP	CG-CD2-CE3	7.52	141.42	133.90
1	B	264	GLN	N-CA-C	-7.51	103.85	113.16
1	A	650	VAL	N-CA-CB	-7.50	100.33	110.54
1	A	216	VAL	N-CA-C	7.50	119.61	108.96
1	D	239	ASN	CA-CB-CG	7.50	120.10	112.60
1	A	650	VAL	CA-C-O	-7.49	113.16	120.95
1	D	454	GLY	N-CA-C	-7.48	102.50	112.82
1	A	272	ALA	N-CA-C	-7.47	94.88	110.80
1	B	383	ALA	N-CA-C	7.47	121.98	111.30
1	D	60	ARG	N-CA-C	7.47	120.48	111.82
1	D	281	PRO	N-CA-C	7.45	130.74	112.10
1	D	338	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	A	721	LEU	N-CA-C	-7.44	102.86	110.97
1	A	471	PHE	N-CA-C	-7.44	103.16	112.90
1	C	525	VAL	N-CA-CB	7.44	118.43	110.62
1	B	768	HIS	CA-CB-CG	7.43	121.23	113.80
1	B	799	ARG	N-CA-C	-7.43	106.15	114.62
1	A	255	LYS	O-C-N	7.42	132.79	122.77
1	C	44	ASN	CA-CB-CG	7.42	120.02	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	VAL	O-C-N	-7.41	113.31	122.57
1	A	407	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	B	380	ILE	N-CA-C	7.41	124.88	108.88
1	B	661	ASP	CA-CB-CG	7.40	120.00	112.60
1	D	251	ASP	CA-CB-CG	7.40	120.00	112.60
1	B	623	ILE	CB-CA-C	-7.38	102.25	111.70
1	D	218	THR	N-CA-C	7.38	122.05	110.32
1	D	518	LEU	CA-C-N	7.37	131.14	120.38
1	D	518	LEU	C-N-CA	7.37	131.14	120.38
1	B	650	VAL	CG1-CB-CG2	-7.35	94.63	110.80
1	D	459	HIS	CB-CG-CD2	-7.35	121.65	131.20
1	C	696	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	C	316	PHE	N-CA-C	7.32	121.97	112.89
1	D	339	ASP	CA-CB-CG	7.32	119.92	112.60
1	D	181	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	45	VAL	N-CA-CB	-7.30	104.18	112.21
1	C	784	GLN	OE1-CD-NE2	-7.30	115.30	122.60
1	A	450	HIS	CB-CG-ND1	7.29	133.64	122.70
1	D	771	PHE	CA-CB-CG	-7.29	106.51	113.80
1	B	481	ASN	CB-CG-ND2	7.29	127.33	116.40
1	C	730	GLU	CA-CB-CG	7.29	128.67	114.10
1	A	255	LYS	N-CA-C	7.28	119.64	109.15
1	B	510	GLU	CB-CG-CD	7.27	124.96	112.60
1	C	101	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	C	220	VAL	N-CA-C	7.27	118.48	108.89
1	D	496	ASN	CA-CB-CG	-7.27	105.33	112.60
1	C	325	ASN	CA-C-O	7.26	129.18	121.19
1	C	676	THR	CA-CB-OG1	-7.26	98.71	109.60
1	C	28	LYS	N-CA-C	-7.25	103.46	111.36
1	B	784	GLN	CG-CD-NE2	7.24	127.26	116.40
1	C	459	HIS	CB-CG-CD2	-7.24	121.78	131.20
1	D	92	GLY	N-CA-C	7.24	125.48	115.27
1	D	253	ASN	CA-CB-CG	7.24	119.84	112.60
1	B	585	THR	CA-CB-OG1	-7.24	98.75	109.60
1	A	709	PHE	N-CA-C	7.22	122.54	112.72
1	B	228	THR	CA-C-N	7.22	127.63	119.83
1	B	228	THR	C-N-CA	7.22	127.63	119.83
1	D	822	ARG	CA-CB-CG	7.22	128.54	114.10
1	A	47	THR	CA-CB-OG1	-7.22	98.77	109.60
1	A	348	GLU	CB-CG-CD	7.22	124.88	112.60
1	A	555	VAL	N-CA-C	7.22	124.35	109.34
1	D	431	VAL	N-CA-CB	-7.21	102.40	111.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	GLN	CB-CG-CD	7.21	124.85	112.60
1	D	133	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	B	717	ASP	CA-CB-CG	7.20	119.80	112.60
1	B	71	GLN	OE1-CD-NE2	-7.20	115.40	122.60
1	B	325	ASN	CA-C-O	7.20	128.81	120.96
1	A	459	HIS	CA-CB-CG	7.19	120.99	113.80
1	D	133	ASN	CB-CG-ND2	7.18	127.18	116.40
1	B	320	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	718	VAL	CB-CA-C	-7.18	102.60	111.87
1	A	24	VAL	CA-C-O	-7.18	113.56	121.17
1	C	181	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	321	PRO	N-CA-C	7.17	127.25	112.47
1	B	744	GLN	N-CA-C	-7.17	103.46	111.28
1	D	47	THR	CB-CA-C	7.17	119.91	109.09
1	D	592	LYS	CA-CB-CG	7.17	128.43	114.10
1	D	807	THR	N-CA-C	7.17	120.92	111.75
1	C	306	ASP	CA-C-N	7.15	130.14	120.77
1	C	306	ASP	C-N-CA	7.15	130.14	120.77
1	C	591	LYS	N-CA-C	7.14	122.08	113.23
1	C	75	TYR	N-CA-C	-7.13	103.43	111.14
1	D	399	HIS	CA-CB-CG	7.13	120.93	113.80
1	A	718	VAL	CA-C-N	7.12	130.78	120.38
1	A	718	VAL	C-N-CA	7.12	130.78	120.38
1	B	784	GLN	OE1-CD-NE2	-7.12	115.48	122.60
1	C	487	THR	CA-CB-CG2	7.12	122.61	110.50
1	A	633	ASP	CA-C-N	7.11	127.43	119.32
1	A	633	ASP	C-N-CA	7.11	127.43	119.32
1	D	75	TYR	N-CA-CB	7.11	120.38	110.07
1	D	614	HIS	CB-CG-CD2	-7.11	121.96	131.20
1	D	394	THR	CA-CB-CG2	7.11	122.58	110.50
1	C	742	ILE	N-CA-C	-7.10	102.90	110.36
1	C	585	THR	CA-CB-OG1	-7.10	98.95	109.60
1	B	25	THR	O-C-N	7.09	129.64	122.12
1	D	259	VAL	CA-C-O	-7.09	113.33	120.85
1	D	661	ASP	N-CA-C	-7.09	100.71	111.56
1	D	730	GLU	N-CA-C	-7.09	95.70	110.80
1	A	389	VAL	CA-C-O	-7.09	113.90	121.27
1	B	558	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	C	727	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	B	217	ASP	N-CA-C	-7.07	103.95	112.58
1	A	213	ALA	N-CA-C	7.07	118.82	108.86
1	C	769	ASP	CA-CB-CG	7.07	119.67	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	730	GLU	CA-CB-CG	7.07	128.23	114.10
1	D	571	HIS	CB-CG-ND1	7.06	133.29	122.70
1	B	487	THR	CA-CB-OG1	-7.06	99.02	109.60
1	A	672	GLU	N-CA-C	-7.05	99.11	110.32
1	A	201	HIS	CB-CG-CD2	-7.04	122.05	131.20
1	B	424	ARG	N-CA-C	-7.04	104.82	113.41
1	A	771	PHE	N-CA-C	7.04	121.57	112.92
1	C	583	VAL	CA-C-O	-7.03	113.77	121.29
1	D	44	ASN	CA-CB-CG	7.03	119.63	112.60
1	C	469	LYS	N-CA-C	7.03	119.84	111.33
1	D	11	LYS	N-CA-C	-7.03	104.27	112.92
1	A	631	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	B	773	VAL	CA-CB-CG1	7.03	122.35	110.40
1	B	242	ARG	CB-CG-CD	-7.02	95.16	111.30
1	C	166	PHE	N-CA-C	7.02	125.75	110.80
1	C	468	PHE	CA-CB-CG	7.02	120.82	113.80
1	B	258	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	C	486	ILE	N-CA-CB	-7.01	99.67	111.23
1	A	572	GLU	N-CA-C	7.00	118.92	111.28
1	B	718	VAL	O-C-N	7.00	129.43	121.94
1	B	167	ASN	CB-CG-ND2	6.99	126.89	116.40
1	B	341	HIS	O-C-N	-6.99	113.28	121.32
1	B	634	PRO	N-CA-C	6.99	126.86	112.47
1	C	280	TYR	N-CA-C	6.99	121.12	110.50
1	C	761	ILE	N-CA-C	-6.98	104.05	110.82
1	D	326	PHE	CA-CB-CG	-6.98	106.82	113.80
1	C	361	TRP	N-CA-C	-6.98	103.60	111.07
1	C	31	PHE	CA-CB-CG	6.98	120.78	113.80
1	A	626	ILE	N-CA-C	-6.97	103.51	110.62
1	B	823	GLU	N-CA-C	6.97	122.13	112.45
1	C	374	TYR	N-CA-C	6.96	119.86	108.52
1	B	199	PRO	N-CA-C	6.94	122.25	111.21
1	C	218	THR	N-CA-C	6.94	119.93	110.35
1	D	114	GLN	N-CA-C	-6.94	104.07	112.54
1	A	182	TRP	N-CA-C	-6.93	103.50	112.23
1	C	402	ILE	N-CA-C	-6.93	102.58	112.35
1	C	390	HIS	N-CA-CB	6.92	120.30	110.12
1	A	769	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	727	ASN	N-CA-C	-6.92	97.93	109.07
1	C	131	LEU	N-CA-C	-6.92	103.96	112.88
1	B	712	GLY	O-C-N	6.91	130.08	122.68
1	D	121	GLU	CB-CG-CD	6.91	124.35	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	LEU	N-CA-C	-6.91	105.38	113.88
1	B	718	VAL	N-CA-CB	6.90	118.45	110.65
1	A	300	VAL	N-CA-C	6.90	117.05	110.42
1	A	773	VAL	CA-C-O	-6.90	113.39	121.05
1	B	273	GLU	N-CA-C	-6.90	103.69	111.14
1	A	527	ASP	CA-CB-CG	6.90	119.50	112.60
1	C	467	ILE	O-C-N	-6.90	115.15	121.91
1	B	21	VAL	N-CA-C	6.90	123.69	109.34
1	C	325	ASN	O-C-N	6.88	131.34	122.87
1	A	496	ASN	CA-C-N	6.88	126.40	119.24
1	A	496	ASN	C-N-CA	6.88	126.40	119.24
1	D	91	MET	CA-CB-CG	-6.88	100.34	114.10
1	C	635	VAL	N-CA-C	-6.88	106.33	111.90
1	D	684	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	D	754	GLN	CA-C-N	6.88	127.45	119.47
1	D	754	GLN	C-N-CA	6.88	127.45	119.47
1	C	326	PHE	CA-CB-CG	-6.88	106.92	113.80
1	B	665	GLN	N-CA-C	-6.87	101.47	111.30
1	C	408	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	C	795	ARG	N-CA-C	-6.86	103.41	111.03
1	D	322	VAL	N-CA-CB	-6.86	99.91	111.23
1	A	332	LYS	N-CA-C	6.86	120.24	112.97
1	D	78	ASP	CA-CB-CG	6.86	119.46	112.60
1	D	21	VAL	O-C-N	6.85	131.13	122.57
1	A	550	GLU	CB-CG-CD	6.85	124.24	112.60
1	B	341	HIS	CA-CB-CG	6.85	120.65	113.80
1	C	834	LEU	O-C-N	-6.85	116.21	121.14
1	D	716	GLU	N-CA-CB	-6.84	100.15	110.07
1	B	305	GLN	CA-C-O	-6.83	113.18	120.42
1	B	651	SER	CA-CB-OG	6.83	124.76	111.10
1	A	673	ALA	N-CA-C	-6.83	104.58	113.12
1	C	325	ASN	CB-CG-ND2	6.83	126.64	116.40
1	B	470	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	444	LEU	N-CA-C	-6.83	103.77	111.14
1	C	487	THR	CA-CB-OG1	-6.82	99.37	109.60
1	C	828	GLU	CA-C-N	6.82	126.86	119.90
1	C	828	GLU	C-N-CA	6.82	126.86	119.90
1	C	250	ASN	N-CA-C	6.82	125.32	110.80
1	C	55	LEU	CA-C-N	6.81	129.71	120.38
1	C	55	LEU	C-N-CA	6.81	129.71	120.38
1	C	268	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	649	ARG	CG-CD-NE	-6.81	97.02	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	410	PHE	N-CA-C	-6.80	103.79	111.14
1	D	341	HIS	O-C-N	-6.79	113.51	121.32
1	D	749	PHE	CA-CB-CG	6.77	120.57	113.80
1	D	160	ARG	CB-CG-CD	-6.77	95.73	111.30
1	B	767	HIS	CB-CG-ND1	6.77	132.85	122.70
1	C	281	PRO	CA-N-CD	-6.77	102.53	112.00
1	D	583	VAL	N-CA-C	-6.77	103.86	113.07
1	A	240	THR	CA-CB-OG1	-6.75	99.47	109.60
1	B	44	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	C	706	GLU	N-CA-CB	6.75	120.05	110.12
1	A	555	VAL	CB-CA-C	-6.75	100.22	111.29
1	B	786	ARG	N-CA-C	-6.75	103.54	111.03
1	C	93	ARG	N-CA-C	6.75	125.18	110.80
1	A	385	GLU	N-CA-C	6.75	120.49	109.76
1	C	97	ASN	CA-CB-CG	6.75	119.35	112.60
1	B	769	ASP	N-CA-C	6.74	120.25	108.52
1	C	806	ALA	N-CA-C	6.74	118.42	111.14
1	B	256	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	785	GLU	N-CA-C	-6.74	103.86	111.07
1	D	754	GLN	OE1-CD-NE2	-6.73	115.87	122.60
1	C	692	MET	N-CA-C	-6.73	98.26	108.96
1	C	235	ASN	CA-CB-CG	6.73	119.33	112.60
1	B	336	GLN	N-CA-C	6.72	119.38	108.63
1	B	357	GLU	O-C-N	-6.72	113.65	122.59
1	D	599	VAL	CA-C-N	6.72	128.49	120.23
1	D	599	VAL	C-N-CA	6.72	128.49	120.23
1	A	452	VAL	N-CA-C	-6.72	98.06	107.80
1	C	745	LEU	CA-C-N	6.72	129.58	120.38
1	C	745	LEU	C-N-CA	6.72	129.58	120.38
1	B	306	ASP	N-CA-C	6.71	119.61	111.82
1	C	189	TRP	CB-CG-CD1	-6.71	116.83	126.90
1	C	657	ILE	N-CA-CB	-6.71	101.81	111.21
1	B	120	GLU	CB-CG-CD	6.71	124.01	112.60
1	D	36	HIS	CA-CB-CG	-6.71	107.09	113.80
1	B	305	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	303	THR	N-CA-C	6.70	118.37	111.14
1	D	676	THR	N-CA-CB	-6.70	100.69	110.40
1	C	319	ARG	N-CA-C	-6.69	96.91	108.56
1	B	727	ASN	CB-CG-ND2	6.68	126.42	116.40
1	D	443	HIS	CA-CB-CG	6.68	120.48	113.80
1	C	77	LYS	CB-CG-CD	6.67	126.65	111.30
1	D	653	ALA	N-CA-C	-6.67	103.94	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	D	760	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	305	GLN	CB-CG-CD	6.66	123.92	112.60
1	C	46	ALA	N-CA-C	6.66	120.02	110.10
1	C	746	SER	N-CA-C	6.65	119.38	111.33
1	A	541	ASN	CA-CB-CG	6.65	119.25	112.60
1	D	166	PHE	N-CA-C	6.65	124.96	110.80
1	B	305	GLN	CA-CB-CG	6.64	127.38	114.10
1	B	62	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	B	792	LYS	CA-CB-CG	6.64	127.38	114.10
1	D	658	PRO	O-C-N	-6.64	113.68	122.64
1	C	539	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	C	61	ASP	N-CA-C	-6.62	103.88	112.23
1	C	30	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	A	510	GLU	N-CA-C	-6.62	96.70	110.80
1	A	577	LEU	N-CA-C	-6.62	104.85	113.12
1	C	433	GLU	N-CA-C	6.62	119.78	109.52
1	A	44	ASN	CA-CB-CG	6.62	119.22	112.60
1	C	477	HIS	CB-CG-CD2	-6.62	122.60	131.20
1	B	390	HIS	CA-CB-CG	6.62	120.42	113.80
1	C	221	VAL	N-CA-C	-6.62	98.95	108.48
1	C	431	VAL	N-CA-C	-6.61	98.67	109.12
1	D	387	TRP	CG-CD2-CE3	6.61	140.51	133.90
1	A	832	GLN	OE1-CD-NE2	-6.61	116.00	122.60
1	D	262	TYR	N-CA-C	6.60	124.86	110.80
1	D	644	PHE	N-CA-C	-6.60	98.48	109.24
1	A	329	PHE	CA-C-O	-6.60	112.81	119.08
1	C	693	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	165	ILE	O-C-N	6.59	128.90	122.97
1	C	228	THR	CA-C-N	6.59	126.35	119.76
1	C	228	THR	C-N-CA	6.59	126.35	119.76
1	A	558	ASN	CA-CB-CG	6.58	119.18	112.60
1	B	702	GLU	N-CA-C	6.58	118.25	111.14
1	C	58	THR	CA-CB-CG2	6.58	121.69	110.50
1	D	676	THR	CA-CB-CG2	6.58	121.69	110.50
1	A	479	PHE	N-CA-C	6.58	124.81	110.80
1	B	392	LEU	N-CA-C	-6.58	104.03	111.07
1	A	257	PHE	CA-C-N	6.57	129.38	120.44
1	A	257	PHE	C-N-CA	6.57	129.38	120.44
1	B	770	ARG	CA-CB-CG	6.57	127.25	114.10
1	C	62	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	B	23	ASN	OD1-CG-ND2	-6.57	116.03	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ALA	N-CA-C	6.56	123.58	113.28
1	C	131	LEU	N-CA-CB	-6.56	100.56	110.73
1	A	227	ASP	N-CA-C	6.56	119.21	108.52
1	B	266	VAL	CB-CA-C	-6.55	103.43	112.02
1	A	14	SER	O-C-N	6.55	130.63	123.10
1	C	31	PHE	N-CA-C	-6.55	104.22	111.82
1	B	661	ASP	N-CA-C	-6.55	103.97	112.68
1	B	620	ILE	O-C-N	-6.54	114.60	122.06
1	D	560	ASN	O-C-N	6.54	129.66	122.20
1	D	659	ALA	CA-C-O	6.54	129.28	121.17
1	B	236	ASN	N-CA-C	6.54	121.20	113.23
1	C	221	VAL	O-C-N	-6.54	116.12	123.18
1	D	182	TRP	CA-CB-CG	6.54	126.02	113.60
1	A	657	ILE	N-CA-CB	-6.53	102.06	111.21
1	B	666	ILE	N-CA-C	6.53	122.93	109.34
1	A	242	ARG	CB-CG-CD	-6.53	96.28	111.30
1	B	487	THR	CA-CB-CG2	6.53	121.60	110.50
1	B	15	VAL	CA-C-O	-6.53	113.59	120.57
1	C	783	CYS	CA-CB-SG	-6.52	99.40	114.40
1	C	481	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	D	240	THR	CA-CB-OG1	-6.52	99.82	109.60
1	D	602	THR	N-CA-C	-6.52	97.78	108.41
1	B	119	MET	CA-C-O	-6.52	113.98	120.82
1	C	407	ASN	CA-CB-CG	-6.51	106.09	112.60
1	C	722	ASP	CA-C-O	6.51	129.82	120.51
1	A	49	ARG	CA-CB-CG	6.50	127.09	114.10
1	A	664	GLU	N-CA-C	6.49	119.40	108.23
1	A	470	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	76	GLU	O-C-N	6.49	129.04	122.03
1	A	756	ASP	CA-CB-CG	6.49	119.09	112.60
1	C	227	ASP	CA-CB-CG	6.49	119.09	112.60
1	C	394	THR	N-CA-C	6.49	121.48	111.56
1	D	395	LEU	N-CA-CB	6.49	119.87	110.20
1	A	596	LYS	N-CA-C	-6.49	99.12	109.76
1	A	157	TYR	N-CA-C	6.48	119.56	108.02
1	B	368	THR	CA-C-O	-6.48	114.01	120.82
1	C	76	GLU	N-CA-C	6.48	118.22	111.03
1	D	493	VAL	N-CA-C	6.48	116.59	110.30
1	C	165	ILE	N-CA-C	-6.48	100.61	109.55
1	B	258	ASN	CA-CB-CG	6.48	119.08	112.60
1	B	34	HIS	CA-CB-CG	-6.47	107.33	113.80
1	D	696	ASN	CA-CB-CG	6.47	119.07	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	THR	CA-CB-OG1	-6.46	99.90	109.60
1	D	426	ARG	CA-C-O	6.46	125.73	119.08
1	A	21	VAL	CA-C-N	6.46	133.88	121.54
1	A	21	VAL	C-N-CA	6.46	133.88	121.54
1	B	481	ASN	CA-CB-CG	6.46	119.06	112.60
1	D	426	ARG	CA-CB-CG	6.46	127.01	114.10
1	B	165	ILE	CA-C-O	6.45	125.96	120.22
1	C	306	ASP	CA-CB-CG	6.45	119.05	112.60
1	D	296	GLU	CA-CB-CG	6.45	127.00	114.10
1	C	712	GLY	O-C-N	6.45	129.50	122.60
1	A	270	ASN	CA-CB-CG	-6.44	106.16	112.60
1	C	34	HIS	N-CA-C	-6.44	104.34	111.36
1	C	60	ARG	N-CA-C	6.44	120.81	113.15
1	D	767	HIS	CB-CG-ND1	6.43	132.35	122.70
1	A	300	VAL	CA-CB-CG2	-6.43	99.47	110.40
1	C	533	ASP	CA-CB-CG	6.43	119.03	112.60
1	D	236	ASN	N-CA-C	6.43	120.90	113.38
1	C	407	ASN	CB-CG-ND2	6.43	126.04	116.40
1	D	264	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	D	539	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	B	26	GLU	N-CA-C	6.42	118.07	111.14
1	A	201	HIS	N-CA-C	6.41	119.72	108.75
1	A	558	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	C	467	ILE	N-CA-CB	-6.41	103.05	110.55
1	A	46	ALA	O-C-N	6.41	130.57	123.01
1	D	167	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	B	814	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	584	ILE	CA-CB-CG2	-6.40	99.62	110.50
1	B	232	GLY	O-C-N	-6.39	117.60	123.42
1	B	664	GLU	N-CA-C	-6.39	99.47	109.25
1	C	638	ASP	CA-C-O	6.39	125.49	118.65
1	C	786	ARG	N-CA-C	-6.39	104.31	111.28
1	B	94	THR	CA-C-O	-6.39	111.68	118.77
1	C	412	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	A	351	ARG	N-CA-C	-6.38	103.95	111.03
1	D	785	GLU	CB-CG-CD	6.37	123.44	112.60
1	A	280	TYR	O-C-N	6.37	126.73	121.44
1	A	465	LYS	CB-CG-CD	6.37	125.95	111.30
1	D	378	THR	CA-C-O	6.37	127.58	120.70
1	D	572	GLU	N-CA-C	6.37	124.36	110.80
1	A	181	ASP	CA-C-O	6.37	128.52	121.39
1	B	290	GLU	N-CA-C	-6.37	104.34	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	807	THR	N-CA-CB	-6.37	100.08	110.14
1	B	379	VAL	CB-CA-C	6.36	121.72	111.29
1	B	761	ILE	N-CA-C	-6.36	104.06	111.00
1	A	300	VAL	N-CA-CB	-6.36	103.11	110.55
1	D	179	ALA	N-CA-C	6.36	124.34	110.80
1	C	390	HIS	CB-CA-C	-6.35	100.25	110.79
1	C	251	ASP	CA-C-O	6.35	129.04	121.17
1	C	684	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	B	571	HIS	CB-CG-ND1	6.34	132.21	122.70
1	A	514	ASP	CA-C-O	6.34	129.57	120.51
1	D	796	GLU	CB-CG-CD	6.34	123.37	112.60
1	B	452	VAL	O-C-N	-6.33	115.47	122.69
1	D	227	ASP	N-CA-C	6.33	119.58	108.56
1	A	47	THR	CA-CB-CG2	6.33	121.26	110.50
1	A	571	HIS	CB-CG-ND1	6.33	132.19	122.70
1	B	114	GLN	CG-CD-NE2	6.32	125.88	116.40
1	B	349	LEU	N-CA-C	-6.32	101.89	110.68
1	A	182	TRP	CG-CD2-CE3	6.32	140.22	133.90
1	C	407	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	582	HIS	CB-CG-CD2	-6.30	123.00	131.20
1	B	101	ASN	CA-CB-CG	6.30	118.90	112.60
1	B	187	ASN	CB-CG-ND2	6.30	125.86	116.40
1	B	699	MET	CG-SD-CE	6.30	114.76	100.90
1	D	374	TYR	N-CA-C	6.30	118.57	107.61
1	A	43	ARG	CA-CB-CG	6.30	126.69	114.10
1	A	287	GLU	CA-CB-CG	6.29	126.68	114.10
1	A	579	ASN	CA-CB-CG	6.29	118.89	112.60
1	D	181	ASP	N-CA-C	-6.29	100.84	109.71
1	A	308	ILE	CB-CA-C	6.28	120.27	112.04
1	D	560	ASN	CA-C-O	-6.28	113.17	120.20
1	C	487	THR	CA-C-N	6.28	126.19	119.28
1	C	487	THR	C-N-CA	6.28	126.19	119.28
1	D	241	MET	N-CA-C	-6.28	100.28	110.20
1	D	305	GLN	OE1-CD-NE2	-6.28	116.32	122.60
1	C	211	GLN	CA-CB-CG	6.27	126.65	114.10
1	C	211	GLN	CB-CG-CD	6.27	123.26	112.60
1	B	479	PHE	CA-CB-CG	-6.27	107.53	113.80
1	A	477	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	A	374	TYR	N-CA-CB	-6.26	99.94	110.83
1	C	825	TRP	CG-CD2-CE3	6.26	140.16	133.90
1	C	322	VAL	CA-C-O	-6.25	115.71	120.96
1	C	749	PHE	CA-CB-CG	6.25	120.05	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	MET	N-CA-C	6.25	119.07	111.82
1	D	431	VAL	CA-CB-CG1	6.25	121.02	110.40
1	D	692	MET	N-CA-C	6.25	118.81	109.25
1	A	651	SER	CA-CB-OG	6.25	123.59	111.10
1	C	689	ILE	N-CA-C	-6.25	99.42	108.17
1	C	143	PHE	CA-CB-CG	6.24	120.04	113.80
1	D	174	TRP	N-CA-C	6.24	118.97	110.35
1	A	812	SER	N-CA-C	-6.24	99.54	109.59
1	C	400	LEU	N-CA-C	-6.24	104.40	111.14
1	B	351	ARG	N-CA-C	-6.24	104.54	111.71
1	A	160	ARG	CB-CG-CD	-6.22	96.99	111.30
1	A	360	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	767	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	B	262	TYR	CA-CB-CG	-6.22	102.71	113.90
1	D	227	ASP	O-C-N	-6.21	115.06	122.46
1	D	579	ASN	CA-CB-CG	6.21	118.81	112.60
1	A	327	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	576	GLN	CB-CG-CD	6.21	123.16	112.60
1	C	802	ILE	O-C-N	6.21	128.00	121.91
1	D	661	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	414	VAL	CA-C-O	-6.21	114.27	120.85
1	C	727	ASN	CA-CB-CG	6.21	118.81	112.60
1	C	740	GLN	CG-CD-NE2	6.21	125.71	116.40
1	C	406	ILE	N-CA-CB	6.21	117.39	110.62
1	C	464	LYS	CA-C-O	6.21	125.61	118.97
1	A	822	ARG	O-C-N	-6.20	115.19	122.32
1	C	93	ARG	CA-C-O	6.20	129.38	120.51
1	A	338	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	B	377	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	D	262	TYR	CA-C-O	6.20	129.37	120.51
1	D	113	TYR	N-CA-C	-6.20	107.56	114.62
1	A	423	ASP	N-CA-C	6.19	117.82	111.14
1	A	541	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	B	450	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	B	823	GLU	CA-C-N	-6.18	116.66	122.66
1	B	823	GLU	C-N-CA	-6.18	116.66	122.66
1	D	109	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	203	TYR	CB-CA-C	-6.18	107.73	115.89
1	D	690	GLY	N-CA-C	6.18	122.26	111.14
1	D	377	HIS	CB-CG-CD2	-6.18	123.17	131.20
1	A	632	HIS	CA-CB-CG	6.17	119.97	113.80
1	D	684	ASN	CB-CG-ND2	6.17	125.65	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIS	CB-CG-ND1	6.16	131.94	122.70
1	D	431	VAL	CA-CB-CG2	-6.16	99.92	110.40
1	C	251	ASP	N-CA-C	-6.16	102.33	111.81
1	A	574	LYS	CB-CG-CD	6.15	125.45	111.30
1	A	834	LEU	N-CA-C	-6.15	101.60	110.40
1	B	575	ARG	N-CA-C	6.15	123.89	110.80
1	D	622	LEU	N-CA-C	-6.14	104.66	111.36
1	C	739	ARG	CA-CB-CG	6.14	126.39	114.10
1	D	198	LEU	O-C-N	-6.14	116.13	121.35
1	D	566	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	A	575	ARG	CB-CA-C	-6.14	103.63	111.86
1	B	64	VAL	CA-CB-CG2	6.14	120.84	110.40
1	D	658	PRO	N-CA-CB	-6.14	96.80	103.25
1	C	308	ILE	CB-CG1-CD1	6.13	126.68	113.80
1	C	727	ASN	CB-CG-ND2	6.13	125.60	116.40
1	D	626	ILE	O-C-N	6.13	128.26	121.94
1	A	655	LYS	CA-CB-CG	6.13	126.36	114.10
1	A	228	THR	CA-C-N	6.13	125.89	119.76
1	A	228	THR	C-N-CA	6.13	125.89	119.76
1	C	653	ALA	N-CA-C	-6.13	104.68	111.36
1	A	459	HIS	CB-CG-CD2	-6.13	123.24	131.20
1	B	257	PHE	O-C-N	6.12	130.73	122.59
1	D	442	ALA	O-C-N	-6.12	115.06	122.22
1	D	458	ILE	CB-CA-C	-6.12	101.25	111.29
1	D	493	VAL	N-CA-CB	-6.12	103.95	110.62
1	C	811	PHE	CA-CB-CG	-6.12	107.69	113.80
1	C	385	GLU	CA-C-O	6.11	128.02	121.05
1	A	549	LEU	CA-C-O	-6.11	112.58	119.79
1	B	73	HIS	CA-CB-CG	6.11	119.91	113.80
1	C	251	ASP	N-CA-CB	-6.11	102.33	111.25
1	B	315	LYS	N-CA-CB	-6.11	104.67	113.65
1	C	95	LEU	CA-C-O	-6.10	111.78	120.51
1	C	211	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	B	740	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	C	338	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	338	ASN	CA-C-O	6.09	127.56	120.98
1	A	469	LYS	N-CA-C	6.09	118.00	111.36
1	A	528	GLU	CB-CG-CD	6.09	122.96	112.60
1	A	303	THR	N-CA-CB	-6.09	101.24	110.07
1	B	240	THR	CA-CB-OG1	-6.09	100.46	109.60
1	C	511	TYR	N-CA-C	6.09	118.72	111.71
1	D	313	SER	CA-CB-OG	6.09	123.28	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	PRO	CA-C-N	-6.09	114.32	122.42
1	A	249	PRO	C-N-CA	-6.09	114.32	122.42
1	A	21	VAL	N-CA-CB	-6.09	101.19	111.23
1	A	369	VAL	N-CA-C	-6.08	106.81	112.83
1	B	180	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	167	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	D	689	ILE	N-CA-C	6.08	116.45	107.15
1	A	390	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	A	493	VAL	CG1-CB-CG2	-6.08	97.43	110.80
1	C	573	TYR	CA-CB-CG	6.08	124.84	113.90
1	A	643	ILE	CA-C-O	-6.08	114.04	120.48
1	B	491	TRP	CG-CD2-CE3	6.08	139.97	133.90
1	B	597	PHE	O-C-N	6.08	130.12	123.13
1	B	540	GLU	N-CA-C	-6.07	104.78	111.82
1	B	649	ARG	CA-C-O	-6.07	114.81	121.31
1	A	244	TRP	CB-CG-CD1	-6.07	117.80	126.90
1	A	552	GLU	O-C-N	6.07	130.91	123.14
1	B	273	GLU	CA-C-O	6.07	126.95	120.70
1	B	622	LEU	N-CA-C	-6.07	104.30	111.03
1	A	244	TRP	N-CA-C	6.06	118.56	108.20
1	D	177	GLU	CA-CB-CG	6.06	126.22	114.10
1	A	257	PHE	CA-C-O	6.06	129.17	120.51
1	D	244	TRP	CE2-CD2-CG	-6.05	99.93	107.20
1	D	785	GLU	N-CA-C	-6.05	104.03	112.45
1	C	258	ASN	CA-CB-CG	6.04	118.64	112.60
1	C	224	MET	CA-C-O	-6.04	112.56	119.32
1	C	766	MET	CG-SD-CE	-6.04	87.62	100.90
1	B	153	ALA	O-C-N	-6.03	114.57	122.59
1	D	526	ASP	O-C-N	6.03	129.05	122.11
1	C	139	LEU	CA-CB-CG	6.03	137.41	116.30
1	C	550	GLU	CB-CG-CD	6.03	122.85	112.60
1	B	206	VAL	N-CA-C	6.03	116.05	106.88
1	B	459	HIS	CB-CG-ND1	6.03	131.75	122.70
1	B	23	ASN	N-CA-C	-6.02	104.79	111.36
1	C	365	TRP	CG-CD2-CE3	6.02	139.92	133.90
1	D	750	PHE	CA-CB-CG	-6.02	107.78	113.80
1	B	233	TYR	N-CA-C	6.01	117.81	109.15
1	D	240	THR	N-CA-C	6.01	118.48	108.20
1	C	187	ASN	CA-C-N	6.01	125.56	119.19
1	C	187	ASN	C-N-CA	6.01	125.56	119.19
1	D	495	CYS	N-CA-C	6.01	117.50	111.07
1	B	473	GLU	N-CA-C	6.01	118.62	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	TRP	CA-C-N	6.01	126.32	119.83
1	C	387	TRP	C-N-CA	6.01	126.32	119.83
1	C	771	PHE	N-CA-C	6.01	121.35	113.30
1	D	387	TRP	CB-CG-CD1	-6.00	117.89	126.90
1	D	792	LYS	CA-CB-CG	6.00	126.11	114.10
1	B	459	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	D	486	ILE	O-C-N	-6.00	115.07	122.57
1	C	459	HIS	CB-CG-ND1	6.00	131.70	122.70
1	A	593	GLU	O-C-N	-6.00	116.00	121.34
1	A	298	PHE	CA-CB-CG	6.00	119.80	113.80
1	A	211	GLN	OE1-CD-NE2	-6.00	116.61	122.60
1	D	193	ARG	CA-C-N	5.99	127.33	119.84
1	D	193	ARG	C-N-CA	5.99	127.33	119.84
1	D	662	LEU	N-CA-C	5.99	118.44	108.20
1	D	666	ILE	N-CA-C	5.98	121.78	109.34
1	A	97	ASN	CB-CG-ND2	5.98	125.37	116.40
1	D	152	LEU	N-CA-C	5.97	118.89	110.23
1	D	63	LEU	N-CA-C	-5.97	103.95	112.13
1	B	449	SER	O-C-N	-5.97	115.63	123.21
1	A	313	SER	N-CA-C	5.96	119.38	111.75
1	C	784	GLN	CG-CD-NE2	5.96	125.34	116.40
1	D	251	ASP	CA-C-O	5.96	126.32	119.35
1	A	258	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	B	39	LEU	N-CA-C	5.95	120.27	112.89
1	D	322	VAL	N-CA-C	5.95	121.72	109.34
1	D	409	ARG	CA-CB-CG	5.95	126.00	114.10
1	B	236	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	A	525	VAL	CG1-CB-CG2	-5.95	97.72	110.80
1	B	338	ASN	N-CA-C	5.95	119.16	107.98
1	B	400	LEU	N-CA-C	-5.94	104.89	111.36
1	D	538	LYS	CA-C-O	-5.94	114.12	120.42
1	A	827	VAL	N-CA-C	5.94	121.69	109.34
1	D	268	ASP	CA-CB-CG	5.94	118.54	112.60
1	C	219	GLN	CB-CG-CD	-5.93	102.51	112.60
1	A	836	ALA	N-CA-C	5.92	122.90	109.81
1	B	181	ASP	CA-CB-CG	5.92	118.52	112.60
1	D	342	PRO	N-CA-C	5.92	124.66	112.47
1	B	676	THR	O-C-N	-5.91	115.46	122.20
1	D	487	THR	CA-C-N	5.91	125.61	119.05
1	D	487	THR	C-N-CA	5.91	125.61	119.05
1	D	491	TRP	CG-CD2-CE3	5.91	139.81	133.90
1	D	832	GLN	CA-CB-CG	5.91	125.92	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	VAL	CA-CB-CG2	-5.91	100.36	110.40
1	D	511	TYR	N-CA-C	5.91	118.20	111.11
1	A	264	GLN	N-CA-C	-5.91	106.42	113.21
1	A	572	GLU	CA-CB-CG	-5.91	102.29	114.10
1	B	749	PHE	CA-C-O	5.90	127.21	120.90
1	C	599	VAL	O-C-N	-5.90	114.38	121.10
1	B	691	THR	CA-CB-OG1	-5.90	100.75	109.60
1	C	684	ASN	CA-CB-CG	5.89	118.50	112.60
1	A	320	ASP	N-CA-CB	-5.89	103.47	110.42
1	A	726	TYR	CA-C-N	-5.89	114.87	123.00
1	A	726	TYR	C-N-CA	-5.89	114.87	123.00
1	B	439	ILE	N-CA-C	-5.89	99.99	108.53
1	C	10	ARG	CB-CG-CD	5.89	124.84	111.30
1	B	325	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	D	32	ASN	CA-CB-CG	-5.88	106.72	112.60
1	D	821	ALA	O-C-N	5.88	128.38	122.08
1	A	237	VAL	CG1-CB-CG2	-5.88	97.86	110.80
1	B	281	PRO	N-CA-C	5.88	126.80	112.10
1	A	169	LYS	CA-CB-CG	5.88	125.86	114.10
1	A	457	ARG	CA-C-O	-5.88	112.11	120.51
1	A	506	ARG	N-CA-C	-5.88	101.93	111.04
1	A	822	ARG	CA-C-O	-5.88	113.45	120.56
1	D	250	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	236	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	D	244	TRP	CG-CD2-CE3	5.88	139.78	133.90
1	D	139	LEU	N-CA-C	-5.87	104.52	111.03
1	D	255	LYS	O-C-N	5.87	130.35	122.96
1	A	792	LYS	O-C-N	5.86	130.12	122.68
1	C	16	ARG	O-C-N	5.86	130.38	122.59
1	B	270	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	C	467	ILE	CA-C-O	-5.85	114.97	121.17
1	C	582	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	B	72	GLN	CA-C-N	5.85	128.12	120.28
1	B	72	GLN	C-N-CA	5.85	128.12	120.28
1	A	507	ILE	O-C-N	5.85	127.35	122.09
1	B	31	PHE	N-CA-C	-5.85	104.99	111.36
1	A	57	HIS	CB-CG-CD2	-5.84	123.60	131.20
1	A	792	LYS	N-CA-C	-5.84	97.70	107.99
1	B	676	THR	N-CA-CB	-5.84	100.91	110.14
1	B	240	THR	CA-CB-CG2	5.84	120.43	110.50
1	D	718	VAL	N-CA-C	-5.84	106.02	111.45
1	C	620	ILE	CA-C-O	-5.84	115.05	121.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	797	TRP	CB-CG-CD1	-5.84	118.14	126.90
1	D	755	PRO	CA-N-CD	-5.83	103.83	112.00
1	A	44	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	529	ALA	N-CA-C	-5.83	98.38	110.80
1	C	217	ASP	N-CA-C	5.83	119.70	112.24
1	C	600	PRO	N-CA-C	5.83	120.36	111.15
1	A	799	ARG	N-CA-C	-5.83	105.66	112.89
1	C	252	PHE	CA-CB-CG	5.83	119.63	113.80
1	C	502	ILE	N-CA-CB	-5.83	103.73	110.55
1	C	18	LEU	O-C-N	5.83	130.93	123.24
1	A	111	ALA	N-CA-C	-5.82	104.57	111.03
1	C	376	ASN	O-C-N	-5.82	115.83	123.16
1	C	666	ILE	N-CA-C	5.82	121.44	109.34
1	A	393	GLU	N-CA-CB	5.82	118.44	110.01
1	D	68	ILE	CB-CA-C	-5.82	104.40	112.02
1	B	480	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	C	663	SER	N-CA-C	-5.82	98.93	108.41
1	B	156	GLY	O-C-N	-5.81	119.13	123.61
1	A	457	ARG	N-CA-C	5.81	123.18	110.80
1	D	646	GLU	CA-CB-CG	5.81	125.73	114.10
1	D	184	ARG	CA-CB-CG	5.81	125.72	114.10
1	B	359	LEU	O-C-N	5.81	130.31	122.59
1	D	77	LYS	N-CA-C	5.81	119.62	112.54
1	B	269	ARG	CB-CG-CD	-5.80	97.95	111.30
1	B	41	LYS	CA-CB-CG	5.80	125.70	114.10
1	D	450	HIS	CB-CG-CD2	-5.80	123.67	131.20
1	D	513	SER	CA-CB-OG	5.79	122.69	111.10
1	A	551	ARG	N-CA-C	5.79	120.48	112.90
1	C	73	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	C	674	SER	CA-C-O	-5.79	115.08	121.33
1	D	240	THR	N-CA-CB	-5.79	100.82	110.37
1	C	180	ASP	CA-C-N	-5.79	114.81	122.85
1	C	180	ASP	C-N-CA	-5.79	114.81	122.85
1	D	767	HIS	CA-CB-CG	5.79	119.59	113.80
1	C	571	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	D	233	TYR	O-C-N	5.78	130.04	122.93
1	C	697	VAL	O-C-N	-5.78	115.89	121.90
1	B	832	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	C	820	TYR	N-CA-C	-5.78	104.67	110.97
1	A	240	THR	CA-CB-CG2	5.78	120.32	110.50
1	D	589	ARG	CA-CB-CG	5.78	125.65	114.10
1	A	177	GLU	O-C-N	-5.77	116.64	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	733	ASP	CB-CA-C	-5.77	101.78	110.90
1	D	477	HIS	N-CA-C	5.77	120.16	113.18
1	A	509	GLU	CA-CB-CG	5.77	125.63	114.10
1	C	78	ASP	N-CA-C	5.77	122.56	109.81
1	B	306	ASP	CA-C-N	5.77	127.94	120.56
1	B	306	ASP	C-N-CA	5.77	127.94	120.56
1	A	62	HIS	N-CA-C	-5.76	105.91	113.12
1	D	774	PHE	CA-CB-CG	5.76	119.56	113.80
1	A	392	LEU	CA-C-O	-5.76	114.44	120.55
1	C	94	THR	N-CA-CB	-5.76	100.76	110.49
1	C	714	ARG	CA-CB-CG	5.76	125.62	114.10
1	D	135	GLY	O-C-N	-5.76	115.21	122.70
1	D	506	ARG	CB-CG-CD	5.76	124.55	111.30
1	D	45	VAL	N-CA-CB	-5.76	104.35	112.12
1	D	100	VAL	CB-CA-C	-5.76	104.48	112.02
1	A	244	TRP	CE2-CD2-CG	-5.76	100.29	107.20
1	B	108	CYS	O-C-N	5.76	128.71	122.15
1	D	240	THR	CA-CB-CG2	5.76	120.29	110.50
1	A	767	HIS	CA-C-O	-5.75	112.08	120.13
1	A	823	GLU	CA-CB-CG	5.75	125.61	114.10
1	B	348	GLU	O-C-N	-5.75	115.49	122.22
1	C	576	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	A	47	THR	CA-C-N	5.75	127.03	119.84
1	A	47	THR	C-N-CA	5.75	127.03	119.84
1	B	266	VAL	N-CA-CB	5.75	117.93	110.57
1	B	776	ASP	N-CA-C	5.75	120.29	113.16
1	D	558	ASN	CB-CG-ND2	5.75	125.02	116.40
1	B	595	ASN	CB-CG-ND2	5.75	125.02	116.40
1	A	183	LEU	O-C-N	5.75	129.30	122.46
1	A	273	GLU	N-CA-C	5.74	123.03	110.80
1	C	341	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	D	144	LEU	CD1-CG-CD2	-5.74	98.16	110.80
1	D	380	ILE	CA-CB-CG2	-5.74	100.74	110.50
1	B	501	GLU	CA-CB-CG	5.74	125.58	114.10
1	D	566	GLN	CG-CD-NE2	5.74	125.01	116.40
1	A	528	GLU	O-C-N	5.73	130.32	122.41
1	D	472	TYR	O-C-N	-5.73	115.51	122.22
1	A	316	PHE	CA-CB-CG	5.73	119.53	113.80
1	B	255	LYS	CA-C-N	5.73	132.49	121.54
1	B	255	LYS	C-N-CA	5.73	132.49	121.54
1	B	501	GLU	N-CA-CB	-5.73	101.76	110.07
1	D	264	GLN	N-CA-C	5.73	123.00	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	733	ASP	N-CA-C	5.73	123.00	110.80
1	C	795	ARG	CB-CG-CD	5.72	124.47	111.30
1	D	232	GLY	N-CA-C	-5.72	104.36	112.37
1	D	291	LEU	CA-C-O	-5.72	114.81	120.82
1	B	745	LEU	CA-C-O	-5.72	114.81	120.70
1	B	740	GLN	CA-CB-CG	5.72	125.54	114.10
1	C	566	GLN	N-CA-C	-5.72	98.02	108.02
1	D	303	THR	CA-CB-OG1	-5.72	101.03	109.60
1	A	834	LEU	CA-C-N	5.71	126.98	119.84
1	A	834	LEU	C-N-CA	5.71	126.98	119.84
1	C	279	LEU	CA-C-O	-5.71	114.54	121.28
1	C	384	LEU	CA-C-O	-5.71	114.54	121.05
1	C	481	ASN	CB-CG-ND2	5.71	124.97	116.40
1	D	88	GLU	CA-CB-CG	-5.71	102.67	114.10
1	D	97	ASN	N-CA-CB	-5.71	100.82	110.41
1	A	88	GLU	O-C-N	-5.71	115.00	122.59
1	B	218	THR	N-CA-C	5.71	118.25	110.55
1	B	825	TRP	CB-CG-CD1	-5.71	118.34	126.90
1	C	273	GLU	N-CA-C	5.70	117.50	111.28
1	D	600	PRO	N-CA-CB	5.70	107.86	103.30
1	A	78	ASP	CA-C-N	5.70	125.68	120.21
1	A	78	ASP	C-N-CA	5.70	125.68	120.21
1	D	96	GLN	CA-C-O	5.70	126.54	120.10
1	C	681	PHE	CA-CB-CG	5.70	119.50	113.80
1	C	626	ILE	N-CA-C	-5.70	105.06	110.42
1	B	545	PHE	N-CA-C	-5.70	104.45	111.40
1	B	665	GLN	N-CA-CB	-5.69	103.00	111.43
1	C	122	LEU	CA-C-N	5.69	127.91	120.28
1	C	122	LEU	C-N-CA	5.69	127.91	120.28
1	D	395	LEU	CB-CA-C	-5.69	100.29	110.70
1	B	271	LEU	CA-CB-CG	5.69	136.21	116.30
1	B	540	GLU	CB-CG-CD	5.69	122.27	112.60
1	D	490	ARG	CG-CD-NE	-5.69	99.48	112.00
1	A	33	ARG	O-C-N	-5.69	116.17	122.09
1	A	274	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	A	459	HIS	CB-CG-ND1	5.69	131.23	122.70
1	C	480	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	D	376	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	D	457	ARG	O-C-N	5.68	127.94	122.03
1	D	592	LYS	CB-CG-CD	-5.68	98.23	111.30
1	A	819	GLN	CB-CG-CD	-5.68	102.95	112.60
1	C	319	ARG	NE-CZ-NH2	-5.68	114.09	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	610	ALA	N-CA-CB	5.67	120.47	110.37
1	A	351	ARG	CA-C-O	-5.67	115.06	120.90
1	A	387	TRP	CG-CD2-CE3	5.67	139.57	133.90
1	A	552	GLU	N-CA-C	-5.67	96.49	107.44
1	C	385	GLU	N-CA-C	5.67	119.16	110.20
1	B	735	ILE	N-CA-CB	-5.67	104.91	111.20
1	C	477	HIS	CB-CG-ND1	5.67	131.20	122.70
1	C	275	ILE	N-CA-C	-5.66	104.11	112.04
1	A	62	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	458	ILE	N-CA-CB	5.66	119.07	110.58
1	D	491	TRP	N-CA-C	5.66	119.88	112.92
1	C	423	ASP	O-C-N	-5.66	114.85	122.43
1	D	274	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	B	764	MET	CA-C-O	-5.65	114.88	120.82
1	C	579	ASN	CB-CG-ND2	5.65	124.88	116.40
1	D	324	THR	CA-CB-CG2	5.65	120.10	110.50
1	A	362	ASP	N-CA-C	-5.65	106.43	113.55
1	B	259	VAL	CA-C-O	5.65	126.47	120.48
1	B	270	ASN	CA-C-N	5.64	132.32	121.54
1	B	270	ASN	C-N-CA	5.64	132.32	121.54
1	D	795	ARG	CB-CG-CD	-5.64	98.32	111.30
1	A	692	MET	N-CA-C	5.64	119.44	110.70
1	B	169	LYS	CA-CB-CG	-5.64	102.82	114.10
1	B	357	GLU	N-CA-C	-5.64	98.79	110.80
1	C	673	ALA	CA-C-N	5.64	131.51	121.75
1	C	673	ALA	C-N-CA	5.64	131.51	121.75
1	D	423	ASP	O-C-N	-5.64	114.93	122.43
1	A	808	SER	CA-C-O	-5.63	112.45	120.51
1	D	57	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	B	96	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	D	450	HIS	CB-CG-ND1	5.63	131.15	122.70
1	B	88	GLU	CB-CA-C	-5.63	100.23	109.80
1	D	740	GLN	CG-CD-NE2	5.63	124.84	116.40
1	D	773	VAL	N-CA-C	-5.63	105.24	110.53
1	A	763	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	B	652	LEU	N-CA-C	-5.62	105.53	112.90
1	B	501	GLU	N-CA-C	5.62	117.21	111.14
1	D	595	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	804	ASN	CB-CG-ND2	5.62	124.83	116.40
1	B	688	THR	CA-C-O	5.62	127.04	120.80
1	B	767	HIS	O-C-N	-5.62	115.12	122.59
1	D	396	LEU	CA-C-N	5.62	126.86	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396	LEU	C-N-CA	5.62	126.86	119.84
1	D	615	MET	N-CA-C	-5.62	105.07	111.14
1	A	622	LEU	O-C-N	5.62	128.55	122.15
1	A	131	LEU	N-CA-C	5.62	121.39	113.02
1	A	308	ILE	CA-CB-CG1	-5.62	100.85	110.40
1	B	486	ILE	N-CA-CB	-5.61	101.54	111.93
1	D	503	ILE	O-C-N	5.61	127.70	121.97
1	D	716	GLU	CA-CB-CG	5.61	125.33	114.10
1	D	758	PHE	CA-CB-CG	-5.61	108.19	113.80
1	B	518	LEU	CA-C-O	5.61	126.28	119.38
1	A	804	ASN	N-CA-C	-5.61	107.08	114.04
1	B	100	VAL	N-CA-CB	5.61	117.75	110.57
1	B	545	PHE	CA-CB-CG	-5.61	108.19	113.80
1	C	615	MET	CG-SD-CE	-5.61	88.56	100.90
1	A	399	HIS	CA-CB-CG	-5.61	108.19	113.80
1	C	614	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	D	617	LYS	N-CA-C	-5.60	107.00	113.88
1	C	440	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	368	THR	CA-CB-OG1	-5.59	101.21	109.60
1	D	374	TYR	O-C-N	-5.59	115.86	123.24
1	A	608	LYS	N-CA-C	-5.59	101.06	109.95
1	B	763	ASN	N-CA-C	5.59	117.45	111.36
1	B	106	ASN	CA-CB-CG	-5.59	107.01	112.60
1	D	108	CYS	N-CA-C	-5.59	106.63	113.50
1	D	635	VAL	N-CA-C	-5.59	97.72	109.34
1	C	325	ASN	N-CA-C	5.58	118.33	110.23
1	D	772	LYS	CA-CB-CG	5.58	125.26	114.10
1	D	16	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	230	VAL	CA-C-N	5.58	125.78	120.31
1	A	230	VAL	C-N-CA	5.58	125.78	120.31
1	A	399	HIS	CB-CG-CD2	-5.57	123.95	131.20
1	C	296	GLU	O-C-N	-5.57	116.21	122.12
1	A	385	GLU	CA-CB-CG	5.57	125.24	114.10
1	A	814	ASP	N-CA-C	-5.57	104.71	112.45
1	B	715	VAL	N-CA-C	5.57	120.93	109.34
1	C	560	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	436	VAL	CA-C-O	5.57	127.74	120.78
1	A	602	THR	CA-C-O	-5.57	114.50	120.46
1	D	739	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	C	577	LEU	N-CA-C	5.57	117.35	111.28
1	C	182	TRP	CG-CD2-CE3	5.56	139.46	133.90
1	D	145	ASP	CA-CB-CG	5.56	118.16	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	412	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	652	LEU	N-CA-C	-5.55	105.23	111.28
1	B	211	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	B	390	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	B	768	HIS	N-CA-C	5.55	118.86	112.97
1	D	326	PHE	N-CA-CB	-5.55	102.42	110.47
1	D	569	ARG	CA-C-O	-5.55	115.09	121.47
1	B	273	GLU	CA-C-N	5.54	129.56	120.63
1	B	273	GLU	C-N-CA	5.54	129.56	120.63
1	D	272	ALA	N-CA-C	-5.54	98.99	110.80
1	D	62	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	B	251	ASP	N-CA-C	-5.54	106.02	112.89
1	B	561	SER	N-CA-C	5.54	117.22	110.41
1	A	433	GLU	N-CA-C	5.54	116.67	108.86
1	B	773	VAL	N-CA-CB	-5.54	104.00	110.64
1	A	323	ARG	N-CA-C	5.54	118.83	111.30
1	B	147	MET	N-CA-C	-5.54	105.15	111.07
1	D	270	ASN	CA-CB-CG	-5.54	107.06	112.60
1	D	406	ILE	N-CA-C	-5.54	104.55	110.36
1	A	620	ILE	O-C-N	5.53	127.49	121.90
1	B	623	ILE	N-CA-C	-5.53	104.48	110.23
1	B	408	GLN	O-C-N	5.53	128.46	122.15
1	A	310	ARG	CA-CB-CG	-5.53	103.05	114.10
1	B	195	GLU	CA-CB-CG	5.52	125.15	114.10
1	B	827	VAL	N-CA-C	5.52	117.14	109.80
1	A	250	ASN	N-CA-C	5.52	117.30	108.41
1	D	558	ASN	N-CA-C	5.52	122.01	109.81
1	D	263	ILE	N-CA-C	5.52	116.15	110.36
1	D	617	LYS	CA-CB-CG	-5.52	103.07	114.10
1	A	219	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	486	ILE	O-C-N	-5.51	117.24	123.03
1	A	523	SER	CA-CB-OG	5.51	122.13	111.10
1	C	549	LEU	CA-C-O	-5.51	112.62	120.51
1	C	767	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	A	393	GLU	CB-CA-C	-5.51	102.23	110.88
1	D	357	GLU	CB-CG-CD	5.51	121.97	112.60
1	A	346	ILE	CA-C-O	-5.51	112.57	119.95
1	A	465	LYS	N-CA-C	5.51	122.53	110.80
1	A	244	TRP	CD1-CG-CD2	5.50	115.11	106.30
1	D	570	ILE	N-CA-C	-5.50	99.67	107.98
1	B	475	GLU	O-C-N	-5.50	116.77	121.23
1	A	264	GLN	OE1-CD-NE2	-5.50	117.10	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	682	MET	N-CA-C	-5.50	105.19	111.07
1	B	348	GLU	N-CA-C	5.50	118.03	111.71
1	D	613	TYR	N-CA-C	-5.50	98.04	107.61
1	C	223	ALA	N-CA-C	-5.50	100.22	108.96
1	D	321	PRO	CA-N-CD	-5.49	104.31	112.00
1	D	581	LEU	CA-C-N	5.49	127.64	120.28
1	D	581	LEU	C-N-CA	5.49	127.64	120.28
1	A	154	ALA	O-C-N	5.49	129.21	123.06
1	A	251	ASP	CA-C-N	5.49	129.14	121.02
1	A	251	ASP	C-N-CA	5.49	129.14	121.02
1	C	109	ASP	N-CA-C	-5.48	105.22	111.14
1	A	25	THR	CA-CB-OG1	-5.48	101.38	109.60
1	B	278	VAL	N-CA-C	5.48	115.58	108.35
1	C	623	ILE	N-CA-CB	5.48	117.99	110.54
1	D	533	ASP	CA-C-O	5.48	127.09	121.07
1	A	114	GLN	CA-CB-CG	5.47	125.04	114.10
1	D	167	ASN	CB-CG-ND2	5.47	124.61	116.40
1	D	35	LEU	CA-C-O	5.47	126.28	120.10
1	A	230	VAL	CA-C-O	-5.47	112.63	119.95
1	D	496	ASN	CA-C-N	5.47	125.16	119.64
1	D	496	ASN	C-N-CA	5.47	125.16	119.64
1	D	825	TRP	CG-CD2-CE3	5.47	139.37	133.90
1	A	58	THR	CA-C-O	5.46	126.21	120.42
1	B	751	SER	CA-C-N	5.46	126.67	119.84
1	B	751	SER	C-N-CA	5.46	126.67	119.84
1	C	82	ILE	CB-CG1-CD1	5.46	125.27	113.80
1	C	372	CYS	CA-C-O	-5.46	115.27	121.72
1	C	802	ILE	N-CA-C	-5.46	105.18	110.42
1	D	27	LEU	CA-CB-CG	5.46	135.41	116.30
1	A	426	ARG	CB-CG-CD	5.46	123.86	111.30
1	A	480	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	665	GLN	CG-CD-NE2	5.46	124.58	116.40
1	C	632	HIS	CB-CG-CD2	-5.46	124.11	131.20
1	B	597	PHE	N-CA-CB	5.45	119.33	110.17
1	D	348	GLU	CB-CG-CD	5.45	121.87	112.60
1	A	625	ALA	N-CA-C	-5.45	99.19	110.80
1	C	181	ASP	N-CA-C	-5.45	97.61	107.75
1	C	811	PHE	N-CA-C	5.45	118.73	112.57
1	C	707	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	654	GLU	CA-C-N	5.45	127.58	120.28
1	A	654	GLU	C-N-CA	5.45	127.58	120.28
1	D	562	LEU	N-CA-C	-5.45	100.92	109.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	GLN	CB-CG-CD	5.44	121.86	112.60
1	B	805	ILE	CB-CA-C	-5.44	104.73	111.70
1	A	770	ARG	CB-CG-CD	5.44	123.82	111.30
1	A	36	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	250	ASN	CA-CB-CG	-5.44	107.16	112.60
1	D	735	ILE	CA-C-N	5.44	125.26	119.28
1	D	735	ILE	C-N-CA	5.44	125.26	119.28
1	A	191	LYS	CG-CD-CE	5.43	123.80	111.30
1	B	16	ARG	N-CA-C	5.43	122.38	110.80
1	C	320	ASP	N-CA-C	-5.43	97.80	109.81
1	A	61	ASP	O-C-N	-5.43	115.27	122.33
1	C	108	CYS	CA-CB-SG	-5.43	101.91	114.40
1	C	477	HIS	CA-CB-CG	5.43	119.23	113.80
1	D	617	LYS	CA-C-N	5.43	128.02	120.63
1	D	617	LYS	C-N-CA	5.43	128.02	120.63
1	D	252	PHE	CA-C-N	5.43	131.91	121.54
1	D	252	PHE	C-N-CA	5.43	131.91	121.54
1	C	793	ASN	CA-C-N	5.42	125.76	119.47
1	C	793	ASN	C-N-CA	5.42	125.76	119.47
1	A	772	LYS	N-CA-C	5.42	119.31	111.56
1	C	804	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	D	407	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	B	657	ILE	N-CA-CB	-5.42	103.62	111.21
1	A	792	LYS	N-CA-CB	5.42	118.42	110.35
1	C	493	VAL	CA-C-O	-5.42	114.01	120.78
1	B	317	GLY	CA-C-O	5.41	125.89	119.50
1	A	676	THR	O-C-N	-5.41	115.89	122.11
1	A	574	LYS	CA-CB-CG	5.41	124.92	114.10
1	B	195	GLU	CB-CA-C	-5.41	102.32	110.92
1	B	333	VAL	CA-C-O	-5.41	115.94	121.67
1	C	202	PHE	N-CA-C	5.41	118.92	110.32
1	D	361	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	A	93	ARG	N-CA-C	5.40	122.31	110.80
1	B	106	ASN	N-CA-C	5.40	118.09	111.82
1	C	62	HIS	O-C-N	5.40	128.31	122.15
1	C	94	THR	CB-CA-C	5.40	121.17	110.42
1	C	491	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	D	121	GLU	CA-CB-CG	5.40	124.90	114.10
1	D	396	LEU	N-CA-C	5.40	121.75	109.81
1	A	420	GLY	N-CA-C	-5.40	107.87	115.32
1	D	27	LEU	N-CA-C	-5.40	106.86	113.50
1	B	206	VAL	CB-CA-C	-5.40	104.42	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	GLN	OE1-CD-NE2	-5.39	117.20	122.60
1	A	492	LEU	CA-C-O	-5.39	112.80	120.51
1	A	655	LYS	N-CA-CB	-5.39	102.19	110.12
1	B	144	LEU	CA-C-O	-5.39	113.77	119.97
1	B	178	GLU	CA-CB-CG	5.39	124.88	114.10
1	D	501	GLU	CA-CB-CG	5.39	124.88	114.10
1	D	80	LYS	N-CA-C	-5.39	101.00	109.25
1	D	187	ASN	CA-C-N	5.39	126.58	119.84
1	D	187	ASN	C-N-CA	5.39	126.58	119.84
1	B	496	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	C	353	LEU	CD1-CG-CD2	-5.39	98.95	110.80
1	B	64	VAL	CA-CB-CG1	-5.38	101.25	110.40
1	D	387	TRP	CA-C-N	5.38	126.57	119.84
1	D	387	TRP	C-N-CA	5.38	126.57	119.84
1	A	348	GLU	CA-C-O	-5.38	115.16	120.70
1	C	819	GLN	CB-CG-CD	-5.38	103.45	112.60
1	A	251	ASP	CA-C-O	5.38	124.87	118.79
1	C	564	ASP	O-C-N	-5.38	116.06	122.63
1	D	80	LYS	CG-CD-CE	5.38	123.68	111.30
1	D	658	PRO	N-CA-C	5.38	123.56	112.47
1	A	326	PHE	CA-C-N	5.38	127.43	120.44
1	A	326	PHE	C-N-CA	5.38	127.43	120.44
1	C	313	SER	N-CA-C	5.38	117.96	111.40
1	D	270	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	425	LEU	N-CA-C	-5.38	105.50	111.36
1	C	692	MET	CA-C-O	-5.38	114.41	120.43
1	D	511	TYR	CA-CB-CG	5.38	123.58	113.90
1	A	180	ASP	CA-C-N	-5.38	114.81	122.77
1	A	180	ASP	C-N-CA	-5.38	114.81	122.77
1	B	245	SER	O-C-N	-5.38	116.95	123.03
1	B	338	ASN	CA-C-N	5.38	131.81	121.54
1	B	338	ASN	C-N-CA	5.38	131.81	121.54
1	C	502	ILE	CB-CG1-CD1	5.38	125.09	113.80
1	A	808	SER	N-CA-C	5.37	122.25	110.80
1	A	650	VAL	CB-CA-C	5.37	119.39	112.14
1	D	75	TYR	CB-CA-C	-5.37	102.41	110.90
1	D	499	LEU	N-CA-C	-5.37	105.46	112.23
1	D	484	ASN	N-CA-C	5.37	122.24	110.80
1	D	463	LEU	N-CA-C	-5.37	106.11	113.30
1	A	633	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	768	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	825	TRP	CB-CG-CD1	-5.36	118.86	126.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	ARG	CA-CB-CG	-5.36	103.38	114.10
1	D	58	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	395	LEU	CA-C-N	-5.36	116.83	123.21
1	A	395	LEU	C-N-CA	-5.36	116.83	123.21
1	D	560	ASN	N-CA-C	5.36	118.61	111.75
1	A	655	LYS	N-CA-C	5.36	117.12	111.28
1	B	97	ASN	CB-CG-ND2	5.36	124.43	116.40
1	A	26	GLU	CA-CB-CG	-5.35	103.40	114.10
1	A	771	PHE	CA-CB-CG	-5.35	108.45	113.80
1	C	763	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	D	151	GLY	CA-C-N	5.35	128.31	120.71
1	D	151	GLY	C-N-CA	5.35	128.31	120.71
1	D	191	LYS	CA-CB-CG	-5.35	103.40	114.10
1	A	541	ASN	CB-CG-ND2	5.35	124.42	116.40
1	A	811	PHE	N-CA-CB	-5.35	103.05	111.39
1	D	678	ASN	CA-CB-CG	5.34	117.94	112.60
1	C	718	VAL	CA-C-O	-5.34	115.19	120.85
1	A	74	TYR	CA-CB-CG	5.34	123.51	113.90
1	D	61	ASP	N-CA-C	-5.34	105.62	111.82
1	D	828	GLU	CA-C-N	5.34	126.52	119.84
1	D	828	GLU	C-N-CA	5.34	126.52	119.84
1	A	331	ASP	N-CA-C	-5.34	104.35	112.04
1	C	408	GLN	CG-CD-NE2	5.34	124.41	116.40
1	A	771	PHE	N-CA-CB	-5.34	102.77	110.56
1	B	393	GLU	CB-CG-CD	-5.34	103.53	112.60
1	A	714	ARG	N-CA-C	-5.33	101.65	109.81
1	B	541	ASN	CB-CA-C	-5.33	101.78	110.85
1	B	693	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	837	PRO	N-CA-CB	-5.33	97.13	103.00
1	B	610	ALA	CA-C-N	5.33	126.50	119.84
1	B	610	ALA	C-N-CA	5.33	126.50	119.84
1	C	367	VAL	CA-C-O	-5.33	115.13	121.05
1	C	450	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	B	178	GLU	O-C-N	-5.33	116.45	122.68
1	C	536	LYS	O-C-N	5.32	127.55	122.07
1	D	436	VAL	CA-C-O	5.32	127.43	120.78
1	A	259	VAL	CA-C-N	5.32	131.83	121.41
1	A	259	VAL	C-N-CA	5.32	131.83	121.41
1	A	667	SER	CA-C-O	-5.32	115.93	121.99
1	B	541	ASN	N-CA-CB	5.32	118.03	110.16
1	C	208	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	342	PRO	CA-N-CD	-5.32	104.56	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ASN	N-CA-C	-5.31	105.66	111.82
1	C	19	ALA	O-C-N	5.31	129.66	122.59
1	D	227	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	462	ILE	CA-CB-CG2	-5.31	101.47	110.50
1	C	78	ASP	CA-CB-CG	-5.31	107.29	112.60
1	A	61	ASP	CA-C-O	5.31	125.88	119.61
1	A	579	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	312	LYS	CB-CG-CD	5.31	123.51	111.30
1	B	667	SER	CA-C-O	-5.31	115.36	121.47
1	C	750	PHE	CA-CB-CG	-5.31	108.49	113.80
1	D	607	GLY	N-CA-C	-5.31	101.90	110.18
1	C	724	ARG	N-CA-C	5.31	119.24	112.34
1	D	26	GLU	CA-CB-CG	-5.31	103.48	114.10
1	D	291	LEU	CB-CA-C	-5.31	102.55	110.88
1	A	827	VAL	CB-CA-C	-5.30	102.59	111.29
1	B	529	ALA	O-C-N	5.30	127.82	122.09
1	D	459	HIS	CB-CG-ND1	5.30	130.65	122.70
1	B	221	VAL	N-CA-C	-5.30	100.85	108.48
1	C	69	ARG	N-CA-C	5.30	116.74	111.07
1	C	278	VAL	CA-C-N	5.30	131.65	122.64
1	C	278	VAL	C-N-CA	5.30	131.65	122.64
1	C	356	LEU	CA-C-O	-5.30	114.88	120.71
1	B	558	ASN	CB-CG-ND2	5.30	124.35	116.40
1	B	769	ASP	O-C-N	-5.30	115.38	122.38
1	C	491	TRP	CE2-CD2-CG	-5.30	100.84	107.20
1	C	676	THR	CA-CB-CG2	5.30	119.51	110.50
1	A	412	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	B	610	ALA	CB-CA-C	-5.30	99.73	110.17
1	B	831	ARG	CA-CB-CG	5.30	124.70	114.10
1	A	50	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	167	ASN	CB-CG-ND2	5.30	124.35	116.40
1	A	759	LYS	CB-CG-CD	5.29	123.48	111.30
1	A	687	LEU	N-CA-C	-5.29	101.07	109.96
1	C	318	CYS	CA-CB-SG	-5.29	102.22	114.40
1	C	629	VAL	CA-C-O	-5.29	115.17	121.05
1	B	582	HIS	N-CA-CB	-5.29	102.39	110.33
1	D	241	MET	N-CA-CB	5.29	118.05	110.06
1	D	291	LEU	N-CA-CB	5.29	117.68	110.01
1	D	603	VAL	O-C-N	-5.29	117.16	123.03
1	A	191	LYS	N-CA-C	-5.29	100.11	108.73
1	B	604	MET	CG-SD-CE	-5.29	89.27	100.90
1	A	706	GLU	CB-CA-C	-5.29	102.01	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	LEU	N-CA-C	-5.29	105.69	111.82
1	C	636	VAL	N-CA-C	-5.29	105.24	111.00
1	D	52	TYR	N-CA-C	-5.28	105.43	111.14
1	C	210	SER	CA-CB-OG	5.28	121.66	111.10
1	A	676	THR	OG1-CB-CG2	-5.28	98.75	109.30
1	A	761	ILE	CB-CA-C	-5.28	104.94	112.22
1	B	811	PHE	CA-CB-CG	-5.28	108.52	113.80
1	C	12	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	C	568	LYS	N-CA-C	-5.28	101.42	109.65
1	D	16	ARG	CB-CA-C	-5.28	99.92	110.42
1	A	38	THR	N-CA-C	5.27	118.50	111.75
1	D	165	ILE	N-CA-C	-5.27	100.73	108.85
1	A	203	TYR	CB-CA-C	-5.27	110.52	116.63
1	B	585	THR	CA-CB-CG2	5.27	119.46	110.50
1	C	539	GLN	CG-CD-NE2	5.27	124.31	116.40
1	B	539	GLN	CA-CB-CG	5.27	124.64	114.10
1	C	227	ASP	N-CA-C	5.27	118.14	109.76
1	C	754	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	C	555	VAL	CA-C-O	-5.27	114.19	120.78
1	A	98	THR	O-C-N	-5.27	115.38	122.23
1	D	246	ALA	O-C-N	-5.27	117.22	123.22
1	A	387	TRP	CE2-CD2-CG	-5.26	100.88	107.20
1	A	817	ILE	CA-C-O	-5.26	115.27	120.85
1	D	763	ASN	CA-CB-CG	5.26	117.86	112.60
1	D	805	ILE	N-CA-C	5.26	115.88	110.36
1	B	804	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	447	ALA	CA-C-O	-5.26	115.29	121.07
1	B	663	SER	CA-CB-OG	5.26	121.61	111.10
1	C	720	ARG	CA-CB-CG	5.26	124.61	114.10
1	D	244	TRP	CD1-CG-CD2	5.26	114.71	106.30
1	C	117	LEU	CD1-CG-CD2	-5.25	99.24	110.80
1	B	387	TRP	N-CA-C	-5.25	102.89	110.40
1	C	390	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	A	236	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	614	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	C	198	LEU	O-C-N	-5.25	117.46	121.55
1	D	148	ALA	N-CA-C	-5.25	105.64	111.36
1	D	201	HIS	O-C-N	-5.25	116.82	123.01
1	D	305	GLN	N-CA-C	-5.25	105.23	111.69
1	A	244	TRP	CG-CD1-NE1	-5.25	103.38	110.20
1	A	801	VAL	CA-CB-CG2	-5.25	101.48	110.40
1	A	727	ASN	OD1-CG-ND2	-5.25	117.36	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	ARG	CA-C-O	5.25	126.16	120.55
1	C	528	GLU	CA-CB-CG	5.25	124.59	114.10
1	D	834	LEU	N-CA-C	-5.25	103.17	109.83
1	A	467	ILE	N-CA-CB	5.24	117.28	110.57
1	B	399	HIS	CB-CG-CD2	-5.24	124.38	131.20
1	D	529	ALA	N-CA-C	-5.24	104.49	112.04
1	B	633	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	780	TYR	CB-CG-CD2	-5.24	112.94	120.80
1	A	201	HIS	CA-CB-CG	5.23	119.03	113.80
1	B	686	ALA	CA-C-O	5.23	126.35	120.70
1	A	341	HIS	O-C-N	-5.23	115.31	121.32
1	A	767	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	D	37	PHE	N-CA-C	5.23	118.76	112.38
1	D	545	PHE	N-CA-C	-5.23	105.64	112.23
1	A	274	ASN	CA-C-N	5.23	127.85	120.42
1	A	274	ASN	C-N-CA	5.23	127.85	120.42
1	A	366	GLU	N-CA-C	-5.23	105.75	111.82
1	B	267	LEU	CA-C-O	-5.23	114.19	120.10
1	A	477	HIS	CA-CB-CG	-5.23	108.57	113.80
1	B	455	VAL	N-CA-C	5.23	120.21	109.34
1	B	823	GLU	CA-CB-CG	-5.23	103.64	114.10
1	C	470	ASP	CA-C-O	5.23	125.96	120.42
1	B	365	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	C	627	GLY	O-C-N	-5.23	116.81	122.19
1	A	684	ASN	N-CA-C	5.22	119.75	113.17
1	A	20	GLY	CA-C-O	5.22	129.66	120.57
1	A	72	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	437	LYS	N-CA-CB	-5.22	102.35	110.29
1	B	734	ARG	O-C-N	-5.22	116.19	122.15
1	B	198	LEU	O-C-N	-5.22	118.17	121.88
1	D	656	VAL	N-CA-CB	5.22	119.84	111.23
1	C	408	GLN	CB-CG-CD	5.22	121.47	112.60
1	D	348	GLU	CA-C-O	-5.22	114.97	120.55
1	C	764	MET	N-CA-C	-5.22	105.28	110.97
1	D	166	PHE	CA-C-O	5.22	127.97	120.51
1	A	114	GLN	N-CA-C	-5.22	106.42	112.89
1	B	398	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	708	PHE	CA-CB-CG	-5.21	108.59	113.80
1	D	174	TRP	CG-CD2-CE3	5.21	139.12	133.90
1	C	690	GLY	O-C-N	5.21	129.48	122.70
1	D	239	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	D	545	PHE	CA-CB-CG	-5.21	108.59	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ASP	N-CA-C	5.21	117.59	108.52
1	B	833	ARG	N-CA-C	5.21	117.57	109.60
1	D	387	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	A	258	ASN	CA-CB-CG	5.21	117.81	112.60
1	C	656	VAL	N-CA-CB	-5.21	102.64	111.23
1	D	729	GLN	N-CA-C	-5.21	102.68	110.23
1	C	658	PRO	N-CA-C	5.20	123.19	112.47
1	A	47	THR	CB-CA-C	5.20	117.64	109.37
1	B	447	ALA	CB-CA-C	-5.20	102.68	110.90
1	C	589	ARG	CB-CG-CD	5.20	123.26	111.30
1	D	689	ILE	O-C-N	-5.20	116.54	122.62
1	A	736	PRO	CA-C-N	5.20	127.51	120.44
1	A	736	PRO	C-N-CA	5.20	127.51	120.44
1	B	82	ILE	CB-CA-C	5.20	118.32	110.63
1	B	124	GLU	CB-CG-CD	5.20	121.44	112.60
1	B	270	ASN	O-C-N	5.20	129.85	122.68
1	D	501	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	44	ASN	CB-CA-C	-5.20	102.17	110.79
1	A	493	VAL	CA-CB-CG2	5.20	119.23	110.40
1	B	639	ARG	CB-CG-CD	5.20	123.25	111.30
1	D	716	GLU	CB-CA-C	5.19	119.11	110.90
1	A	595	ASN	N-CA-C	-5.19	104.39	111.56
1	B	321	PRO	CA-N-CD	-5.19	104.73	112.00
1	B	780	TYR	CB-CG-CD2	-5.19	113.02	120.80
1	D	306	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	624	THR	N-CA-CB	-5.19	103.91	110.45
1	D	378	THR	N-CA-C	5.19	117.85	109.40
1	D	394	THR	N-CA-CB	-5.19	102.45	110.13
1	A	320	ASP	O-C-N	-5.19	116.28	120.38
1	A	321	PRO	CA-N-CD	-5.19	104.74	112.00
1	A	490	ARG	NE-CZ-NH2	-5.18	114.53	119.20
1	B	344	LEU	CD1-CG-CD2	-5.18	99.40	110.80
1	C	365	TRP	CB-CG-CD1	-5.18	119.13	126.90
1	B	13	ILE	O-C-N	5.18	129.04	122.57
1	B	818	ALA	O-C-N	5.18	127.61	122.12
1	D	183	LEU	N-CA-CB	-5.18	102.48	110.46
1	A	184	ARG	N-CA-C	-5.18	99.77	110.80
1	D	250	ASN	CA-C-N	5.18	131.08	122.54
1	D	250	ASN	C-N-CA	5.18	131.08	122.54
1	D	802	ILE	CB-CA-C	-5.18	105.42	111.94
1	B	597	PHE	CB-CA-C	-5.17	101.58	110.22
1	C	714	ARG	NE-CZ-NH2	-5.17	114.54	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	VAL	N-CA-C	5.17	115.89	110.62
1	C	314	SER	CA-C-O	5.17	126.56	120.98
1	D	174	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	466	THR	N-CA-C	5.17	119.04	111.34
1	D	188	PRO	O-C-N	5.17	129.62	122.64
1	A	415	ALA	N-CA-C	-5.17	107.53	113.88
1	D	564	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	595	ASN	CA-CB-CG	-5.17	107.44	112.60
1	B	651	SER	N-CA-C	5.17	117.58	111.33
1	C	20	GLY	O-C-N	5.17	129.96	122.68
1	D	633	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	730	GLU	N-CA-C	-5.16	99.80	110.80
1	C	16	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	C	615	MET	N-CA-C	-5.16	105.72	112.23
1	A	491	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	B	804	ASN	CB-CG-ND2	5.16	124.14	116.40
1	C	340	THR	CA-CB-OG1	-5.16	101.86	109.60
1	C	681	PHE	CB-CA-C	-5.16	100.29	110.10
1	B	491	TRP	CB-CG-CD1	-5.16	119.16	126.90
1	B	784	GLN	N-CA-C	5.16	119.20	113.01
1	B	88	GLU	CA-CB-CG	5.16	124.42	114.10
1	D	822	ARG	CB-CG-CD	5.16	123.16	111.30
1	B	36	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	D	219	GLN	N-CA-C	-5.16	102.12	110.32
1	D	374	TYR	CA-CB-CG	5.16	123.18	113.90
1	B	36	HIS	CB-CG-ND1	5.15	130.43	122.70
1	D	203	TYR	CA-C-O	-5.15	113.14	120.51
1	C	629	VAL	CA-CB-CG1	5.15	119.16	110.40
1	D	90	TYR	N-CA-CB	-5.15	102.82	110.60
1	D	105	GLU	CA-CB-CG	-5.15	103.80	114.10
1	C	91	MET	O-C-N	5.15	128.03	122.11
1	C	409	ARG	CB-CG-CD	-5.15	99.46	111.30
1	C	754	GLN	CA-C-N	5.15	126.28	119.84
1	C	754	GLN	C-N-CA	5.15	126.28	119.84
1	D	83	TYR	O-C-N	-5.15	117.35	123.22
1	A	235	ASN	CB-CG-ND2	5.14	124.12	116.40
1	B	589	ARG	CB-CG-CD	5.14	123.13	111.30
1	C	88	GLU	CA-C-O	5.14	126.61	120.28
1	A	336	GLN	CG-CD-NE2	5.14	124.11	116.40
1	A	725	GLY	O-C-N	-5.14	117.91	123.00
1	B	578	LEU	CA-C-O	5.14	126.40	120.90
1	A	300	VAL	CA-CB-CG1	5.14	119.14	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	475	GLU	CA-C-N	5.14	124.64	119.19
1	C	475	GLU	C-N-CA	5.14	124.64	119.19
1	D	665	GLN	CB-CG-CD	5.14	121.34	112.60
1	C	701	GLU	N-CA-C	-5.14	105.13	111.40
1	A	23	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	B	187	ASN	CA-CB-CG	5.14	117.74	112.60
1	C	597	PHE	N-CA-CB	5.14	117.82	110.06
1	C	656	VAL	CB-CA-C	5.14	119.72	111.29
1	A	180	ASP	N-CA-CB	-5.13	104.60	110.35
1	B	377	HIS	N-CA-C	5.13	119.82	113.50
1	C	315	LYS	N-CA-C	5.13	121.74	110.80
1	D	106	ASN	CB-CG-ND2	5.13	124.10	116.40
1	A	127	GLU	CB-CG-CD	5.13	121.33	112.60
1	B	133	ASN	CA-CB-CG	5.13	117.73	112.60
1	D	533	ASP	CA-C-N	5.13	127.71	120.42
1	D	533	ASP	C-N-CA	5.13	127.71	120.42
1	A	369	VAL	N-CA-CB	-5.13	103.46	112.08
1	C	558	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	D	106	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	D	503	ILE	CA-C-O	5.13	125.01	120.34
1	A	469	LYS	CA-C-O	-5.13	114.98	120.42
1	D	565	VAL	N-CA-C	5.13	116.04	108.45
1	A	464	LYS	N-CA-C	-5.13	99.88	110.80
1	A	555	VAL	CA-C-N	5.13	131.33	121.54
1	A	555	VAL	C-N-CA	5.13	131.33	121.54
1	B	309	ARG	CA-C-O	-5.12	115.62	121.00
1	D	98	THR	N-CA-C	-5.12	105.15	111.40
1	B	805	ILE	N-CA-CB	5.12	116.00	110.62
1	A	219	GLN	N-CA-C	-5.12	101.62	109.76
1	B	777	TYR	CA-C-O	-5.12	115.43	120.70
1	A	235	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	778	GLU	CA-CB-CG	5.12	124.33	114.10
1	B	764	MET	N-CA-C	-5.12	105.60	111.07
1	D	781	VAL	CA-C-O	-5.12	115.43	120.85
1	C	255	LYS	CA-C-N	5.11	131.31	121.54
1	C	255	LYS	C-N-CA	5.11	131.31	121.54
1	D	824	ILE	CB-CA-C	-5.11	106.58	111.44
1	C	278	VAL	N-CA-CB	-5.11	102.91	112.36
1	D	573	TYR	N-CA-C	5.11	119.23	113.15
1	C	652	LEU	N-CA-C	-5.11	107.05	113.28
1	D	412	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	306	ASP	CA-C-O	5.11	125.18	119.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ALA	N-CA-C	-5.11	105.41	111.69
1	C	371	THR	O-C-N	-5.10	116.72	122.03
1	D	113	TYR	CA-C-O	5.10	124.97	118.54
1	D	724	ARG	CA-CB-CG	5.10	124.30	114.10
1	D	595	ASN	CB-CG-ND2	5.10	124.04	116.40
1	A	820	TYR	CA-C-N	5.09	129.28	121.19
1	A	820	TYR	C-N-CA	5.09	129.28	121.19
1	D	390	HIS	N-CA-C	-5.09	106.33	112.54
1	A	782	LYS	N-CA-C	-5.09	98.00	108.53
1	C	773	VAL	CG1-CB-CG2	-5.09	99.61	110.80
1	D	223	ALA	CA-C-O	-5.09	115.34	120.84
1	B	201	HIS	CB-CG-CD2	-5.09	124.59	131.20
1	B	160	ARG	CB-CG-CD	-5.08	99.61	111.30
1	D	244	TRP	N-CA-C	5.08	118.01	110.48
1	C	644	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	686	ALA	N-CA-C	-5.08	101.42	109.96
1	B	47	THR	CA-CB-OG1	-5.08	101.98	109.60
1	C	744	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	D	629	VAL	CA-C-O	-5.08	115.10	120.64
1	A	491	TRP	CG-CD1-NE1	-5.08	103.60	110.20
1	C	703	ALA	N-CA-C	5.08	117.55	111.71
1	D	44	ASN	N-CA-CB	5.08	118.36	110.44
1	C	556	HIS	CA-CB-CG	5.08	118.88	113.80
1	A	262	TYR	N-CA-C	5.07	116.92	107.99
1	B	458	ILE	CA-CB-CG1	-5.07	101.77	110.40
1	D	110	GLU	CA-C-O	-5.07	115.67	121.00
1	D	599	VAL	N-CA-CB	-5.07	104.11	111.21
1	B	565	VAL	O-C-N	5.07	128.54	123.07
1	A	550	GLU	N-CA-C	-5.07	107.09	113.28
1	B	97	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	B	350	MET	CA-CB-CG	5.07	124.23	114.10
1	A	182	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	B	609	ALA	CB-CA-C	-5.07	102.70	110.81
1	B	673	ALA	N-CA-C	5.07	116.88	111.36
1	D	657	ILE	O-C-N	-5.07	115.33	121.10
1	A	450	HIS	CA-CB-CG	5.06	118.86	113.80
1	C	578	LEU	N-CA-C	-5.06	105.76	111.28
1	B	244	TRP	N-CA-C	5.06	117.49	109.24
1	B	247	LYS	CA-CB-CG	5.06	124.23	114.10
1	C	610	ALA	CB-CA-C	-5.06	100.19	110.17
1	D	47	THR	CA-C-N	5.06	126.17	119.84
1	D	47	THR	C-N-CA	5.06	126.17	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	390	HIS	CA-C-N	5.06	127.32	120.44
1	C	390	HIS	C-N-CA	5.06	127.32	120.44
1	A	124	GLU	CB-CG-CD	5.06	121.20	112.60
1	B	455	VAL	CB-CA-C	5.06	119.59	111.29
1	D	20	GLY	O-C-N	5.06	129.27	122.70
1	D	789	ALA	CA-C-O	-5.06	115.19	120.55
1	A	256	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	294	LYS	N-CA-C	-5.05	105.68	111.14
1	A	198	LEU	CA-C-N	5.05	126.16	119.84
1	A	198	LEU	C-N-CA	5.05	126.16	119.84
1	C	443	HIS	N-CA-C	-5.05	105.87	112.23
1	C	589	ARG	N-CA-C	-5.05	105.66	111.07
1	A	584	ILE	CA-CB-CG1	5.05	118.98	110.40
1	C	663	SER	CA-CB-OG	5.05	121.19	111.10
1	A	152	LEU	N-CA-C	5.04	121.54	110.80
1	C	44	ASN	CB-CG-ND2	5.04	123.97	116.40
1	C	796	GLU	CB-CG-CD	5.04	121.17	112.60
1	D	411	LEU	O-C-N	-5.04	116.32	122.22
1	B	17	GLY	O-C-N	5.04	129.25	122.70
1	D	435	ALA	O-C-N	5.04	128.46	122.46
1	D	466	THR	N-CA-C	5.04	119.17	112.72
1	A	41	LYS	N-CA-C	-5.04	101.79	108.74
1	C	455	VAL	CB-CA-C	5.04	117.98	112.19
1	C	595	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	79	PRO	CA-C-O	-5.03	115.21	122.31
1	A	681	PHE	CA-CB-CG	5.03	118.83	113.80
1	D	499	LEU	O-C-N	-5.03	115.59	122.33
1	B	175	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	C	705	GLU	CA-C-N	5.03	127.02	120.28
1	C	705	GLU	C-N-CA	5.03	127.02	120.28
1	D	248	ALA	CA-C-O	-5.03	115.00	120.69
1	D	396	LEU	O-C-N	-5.03	115.53	121.32
1	A	410	PHE	CA-C-O	-5.03	115.52	120.70
1	B	362	ASP	CA-C-O	5.03	125.75	120.42
1	B	418	PHE	O-C-N	-5.03	116.84	121.37
1	C	361	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	D	555	VAL	CA-C-N	5.03	131.14	121.54
1	D	555	VAL	C-N-CA	5.03	131.14	121.54
1	D	264	GLN	CG-CD-NE2	5.03	123.94	116.40
1	A	260	GLY	N-CA-C	-5.02	101.28	113.18
1	A	268	ASP	N-CA-C	-5.02	105.70	111.07
1	B	610	ALA	N-CA-CB	5.02	119.31	110.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	142	CYS	CA-C-N	5.02	127.26	120.38
1	A	142	CYS	C-N-CA	5.02	127.26	120.38
1	C	294	LYS	CA-C-N	5.02	127.42	120.29
1	C	294	LYS	C-N-CA	5.02	127.42	120.29
1	B	595	ASN	N-CA-C	5.02	118.24	112.57
1	C	576	GLN	CG-CD-NE2	5.02	123.93	116.40
1	C	102	LEU	N-CA-CB	-5.01	103.73	110.95
1	C	320	ASP	CB-CA-C	5.01	120.05	110.17
1	C	599	VAL	CA-C-O	-5.01	113.23	119.95
1	A	412	ASN	CA-CB-CG	5.01	117.61	112.60
1	B	735	ILE	CA-C-O	5.01	121.93	119.12
1	B	825	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	C	105	GLU	N-CA-C	-5.01	104.91	111.02
1	C	719	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	71	GLN	CB-CG-CD	5.01	121.12	112.60
1	A	745	LEU	N-CA-C	-5.01	105.47	111.03
1	B	267	LEU	N-CA-C	5.01	117.47	111.71
1	C	780	TYR	N-CA-C	-5.01	105.90	111.36
1	C	101	ASN	CB-CG-ND2	5.01	123.91	116.40
1	D	787	VAL	CG1-CB-CG2	-5.01	99.79	110.80
1	B	147	MET	O-C-N	5.00	127.22	122.07
1	A	666	ILE	N-CA-C	5.00	119.75	109.34
1	C	208	HIS	CA-CB-CG	-5.00	108.80	113.80
1	D	193	ARG	CA-C-O	-5.00	116.19	121.29
1	D	490	ARG	O-C-N	5.00	127.50	122.09
1	D	707	ASN	CB-CG-ND2	5.00	123.91	116.40
1	A	684	ASN	CA-C-O	5.00	125.20	119.35
1	D	81	ARG	N-CA-C	-5.00	101.16	109.46

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	242	ARG	Sidechain
1	A	256	ASP	Mainchain
1	A	280	TYR	Peptide
1	A	418	PHE	Peptide
1	A	51	TYR	Sidechain
1	A	733	ASP	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	836	ALA	Peptide
1	B	280	TYR	Peptide
1	B	320	ASP	Peptide
1	B	341	HIS	Peptide
1	B	380	ILE	Peptide
1	B	657	ILE	Peptide
1	B	751	SER	Peptide
1	B	834	LEU	Peptide
1	B	836	ALA	Peptide
1	C	18	LEU	Mainchain
1	C	226	TYR	Sidechain
1	C	320	ASP	Peptide
1	C	52	TYR	Sidechain
1	C	613	TYR	Sidechain
1	C	657	ILE	Peptide
1	C	69	ARG	Sidechain
1	C	75	TYR	Sidechain
1	C	780	TYR	Sidechain
1	C	836	ALA	Peptide
1	D	19	ALA	Mainchain
1	D	320	ASP	Peptide
1	D	52	TYR	Sidechain
1	D	558	ASN	Peptide
1	D	657	ILE	Peptide
1	D	836	ALA	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	6703	0	6658	316	0
1	B	6703	0	6659	296	0
1	C	6703	0	6653	297	0
1	D	6704	0	6659	397	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	4	0
2	D	15	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26873	0	26629	1259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1259) 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:C:37:PHE:CE2	1:D:18:LEU:HB3	1.46	1.51
1:C:37:PHE:HE2	1:D:18:LEU:CB	1.32	1.42
1:C:37:PHE:CE2	1:D:18:LEU:CB	2.06	1.32
1:C:15:VAL:O	1:C:17:GLY:N	1.79	1.14
2:C:900:SO4:O3	1:D:43:ARG:NH2	1.79	1.13
1:D:16:ARG:HG3	1:D:17:GLY:N	1.64	1.07
1:C:707:ASN:HA	1:C:800:MET:SD	1.97	1.03
1:C:37:PHE:CE2	1:D:18:LEU:HB2	1.95	1.02
1:D:19:ALA:HB3	1:D:62:HIS:NE2	1.77	1.00
1:D:16:ARG:CG	1:D:17:GLY:N	2.14	0.99
1:C:165:ILE:HB	1:C:279:LEU:HD13	1.43	0.99
1:D:16:ARG:HG3	1:D:17:GLY:CA	1.95	0.97
1:A:32:ASN:HD21	1:B:13:ILE:HA	1.26	0.96
1:D:19:ALA:CB	1:D:62:HIS:NE2	2.31	0.93
1:C:33:ARG:HG2	1:D:18:LEU:HG	1.52	0.92
1:D:165:ILE:HD11	1:D:281:PRO:HA	1.53	0.91
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.53	0.90
1:A:550:GLU:HA	1:A:554:LYS:HA	1.53	0.90
1:C:37:PHE:CZ	1:D:18:LEU:HB2	2.07	0.90
1:C:289:LYS:CB	1:C:289:LYS:CD	2.50	0.90
1:A:21:VAL:HA	1:A:24:VAL:HB	1.53	0.89
1:D:80:LYS:HE3	1:D:334:ALA:HB2	1.55	0.88
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.56	0.86
1:D:18:LEU:O	1:D:19:ALA:HB2	1.75	0.86
1:D:766:MET:HE3	1:D:774:PHE:HE2	1.40	0.86
1:D:171:CYS:HB2	1:D:176:MET:SD	2.15	0.86
1:D:707:ASN:HA	1:D:800:MET:SD	2.16	0.85
1:B:713:MET:SD	1:B:718:VAL:HA	2.16	0.85
1:C:15:VAL:HG23	1:C:69:ARG:HH21	1.41	0.85
1:C:21:VAL:O	1:C:23:ASN:N	2.09	0.84
1:B:21:VAL:HA	1:B:24:VAL:HB	1.58	0.83
1:D:455:VAL:HG13	1:D:484:ASN:ND2	1.93	0.83
1:D:83:TYR:HE1	1:D:333:VAL:HG13	1.44	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.60	0.83
1:B:569:ARG:O	1:B:569:ARG:HG2	1.79	0.82
1:D:605:ILE:HG21	1:D:623:ILE:HD13	1.62	0.81
1:C:165:ILE:HD11	1:C:281:PRO:HA	1.61	0.81
1:B:171:CYS:SG	1:B:176:MET:SD	2.78	0.81
1:B:81:ARG:HG2	1:B:155:TYR:HE1	1.45	0.80
1:A:299:VAL:O	1:A:303:THR:HB	1.81	0.80
1:C:550:GLU:HA	1:C:554:LYS:HA	1.64	0.80
1:D:463:LEU:HD23	1:D:467:ILE:HD12	1.65	0.79
1:C:15:VAL:C	1:C:17:GLY:H	1.87	0.79
1:C:18:LEU:HG	1:D:33:ARG:HD3	1.65	0.79
1:C:173:GLY:HA2	1:C:624:THR:HG21	1.64	0.78
1:A:322:VAL:HG13	1:A:325:ASN:HB2	1.65	0.78
1:B:732:TYR:HE1	1:B:742:ILE:HG21	1.47	0.78
1:C:95:LEU:HD22	1:C:99:MET:HE2	1.65	0.78
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.65	0.78
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.65	0.78
1:C:18:LEU:HB3	1:D:37:PHE:HE2	1.47	0.78
1:B:87:LEU:HD11	1:B:299:VAL:HG11	1.64	0.77
1:C:456:ALA:HB2	1:C:674:SER:HB2	1.66	0.77
1:C:33:ARG:CG	1:D:18:LEU:HG	2.14	0.77
1:C:37:PHE:CZ	1:D:18:LEU:CB	2.68	0.77
1:D:18:LEU:O	1:D:19:ALA:CB	2.31	0.76
1:A:511:TYR:HB2	1:A:518:LEU:HD12	1.66	0.76
1:C:15:VAL:CG2	1:C:69:ARG:HH21	1.97	0.76
1:C:96:GLN:O	1:C:100:VAL:HG13	1.85	0.76
1:A:136:LEU:HD11	1:A:339:ASP:HB2	1.68	0.76
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.67	0.76
1:C:18:LEU:HB3	1:D:37:PHE:CE2	2.22	0.75
1:C:522:LEU:HD13	1:C:806:ALA:HB3	1.67	0.75
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.68	0.74
1:B:198:LEU:HD11	1:B:302:ALA:HA	1.68	0.74
1:B:545:PHE:HE2	1:B:604:MET:HE1	1.51	0.74
1:C:742:ILE:HD11	1:C:774:PHE:HZ	1.52	0.74
1:A:259:VAL:HG21	1:A:263:ILE:HG22	1.68	0.74
1:C:764:MET:SD	1:C:769:ASP:HA	2.27	0.74
1:D:550:GLU:HA	1:D:554:LYS:HA	1.69	0.74
1:A:486:ILE:HD13	1:A:679:MET:HB2	1.70	0.73
1:B:133:ASN:OD1	1:B:165:ILE:HG21	1.88	0.73
1:A:815:ARG:HD2	1:A:819:GLN:OE1	1.88	0.73
1:B:578:LEU:HD23	1:B:666:ILE:HD13	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:ASN:HB3	1:B:699:MET:SD	2.29	0.72
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.23	0.72
1:A:195:GLU:HB2	1:A:196:PHE:HD1	1.54	0.72
1:B:343:SER:HB3	1:B:445:CYS:SG	2.30	0.72
2:C:900:SO4:O3	1:D:43:ARG:CZ	2.37	0.72
1:C:689:ILE:HA	1:C:709:PHE:HB2	1.72	0.72
1:C:326:PHE:HA	1:C:329:PHE:HB2	1.70	0.72
1:C:15:VAL:HG23	1:C:69:ARG:NH2	2.05	0.71
1:C:224:MET:SD	1:C:247:LYS:HD3	2.30	0.71
1:C:495:CYS:HB2	1:C:658:PRO:HG2	1.73	0.71
1:A:509:GLU:HG3	1:A:512:ILE:HB	1.72	0.71
1:B:336:GLN:NE2	1:B:825:TRP:HE1	1.88	0.71
1:B:766:MET:HE3	1:B:774:PHE:HE2	1.52	0.71
1:A:784:GLN:HA	1:A:787:VAL:HB	1.71	0.71
1:A:822:ARG:HA	1:A:826:GLY:O	1.91	0.70
1:A:322:VAL:O	1:A:325:ASN:HB2	1.90	0.70
1:D:21:VAL:C	1:D:23:ASN:H	1.98	0.70
1:D:804:ASN:O	1:D:807:THR:HB	1.91	0.70
1:A:326:PHE:HA	1:A:329:PHE:HB2	1.73	0.70
1:C:423:ASP:HA	1:C:426:ARG:HG2	1.74	0.69
1:C:576:GLN:H	1:C:576:GLN:HE21	1.39	0.69
1:C:53:PHE:CE2	1:C:188:PRO:HG3	2.27	0.69
1:C:783:CYS:SG	1:C:786:ARG:NH2	2.65	0.69
1:C:784:GLN:O	1:C:787:VAL:HB	1.92	0.69
1:B:482:LYS:HD2	1:B:819:GLN:HB3	1.75	0.69
1:A:81:ARG:HG2	1:A:155:TYR:HE2	1.57	0.69
1:B:81:ARG:HG2	1:B:155:TYR:CE1	2.27	0.69
1:D:783:CYS:HA	1:D:786:ARG:HE	1.58	0.69
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.75	0.69
1:D:363:LYS:O	1:D:366:GLU:HB3	1.93	0.68
1:D:491:TRP:C	1:D:495:CYS:SG	2.77	0.68
1:A:348:GLU:O	1:A:352:VAL:HG23	1.94	0.68
1:D:231:PRO:HA	1:D:238:VAL:HG22	1.73	0.68
1:A:194:PRO:HA	1:A:224:MET:SD	2.34	0.68
1:A:292:ARG:HB3	1:A:387:TRP:HH2	1.59	0.68
1:A:588:ASN:HD21	1:A:744:GLN:HE22	1.41	0.68
1:D:748:GLY:HA3	1:D:755:PRO:HG3	1.75	0.68
1:A:732:TYR:HA	1:A:738:LEU:HD23	1.76	0.68
1:C:175:GLN:OE1	1:C:609:ALA:HB3	1.94	0.68
1:D:573:TYR:HD2	1:D:671:THR:HB	1.58	0.68
1:D:173:GLY:HA2	1:D:624:THR:HG21	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:VAL:HG13	1:D:484:ASN:HD22	1.59	0.67
1:C:665:GLN:HG2	1:C:678:ASN:HD22	1.57	0.67
1:D:49:ARG:HA	1:D:125:ILE:HG21	1.76	0.67
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.77	0.67
1:C:37:PHE:HE2	1:D:18:LEU:HB3	0.53	0.67
1:D:350:MET:SD	1:D:365:TRP:HE3	2.18	0.67
1:D:692:MET:HB3	1:D:714:ARG:HD2	1.75	0.67
1:C:741:ILE:HG22	1:C:744:GLN:HG3	1.76	0.67
1:B:529:ALA:HA	1:B:532:ARG:NH1	2.09	0.67
1:D:160:ARG:NH2	1:D:183:LEU:HD21	2.09	0.67
1:D:604:MET:HA	1:D:643:ILE:O	1.95	0.67
1:C:711:PHE:CE1	1:C:780:TYR:HB2	2.30	0.67
1:D:652:LEU:O	1:D:656:VAL:HG23	1.95	0.67
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.77	0.66
1:B:271:LEU:HA	1:B:274:ASN:HB3	1.76	0.66
1:D:562:LEU:HD13	1:D:601:ARG:NH1	2.11	0.66
1:C:15:VAL:C	1:C:17:GLY:N	2.46	0.66
1:D:19:ALA:HB1	1:D:62:HIS:NE2	2.10	0.66
1:D:68:ILE:HG22	1:D:72:GLN:HE21	1.59	0.66
1:D:21:VAL:O	1:D:23:ASN:N	2.25	0.66
1:B:230:VAL:HG22	1:B:239:ASN:HB2	1.78	0.65
1:B:258:ASN:OD1	1:B:259:VAL:HG22	1.96	0.65
1:A:439:ILE:HG22	1:A:441:MET:SD	2.36	0.65
1:B:96:GLN:HA	1:B:99:MET:HE2	1.77	0.65
1:D:16:ARG:CG	1:D:17:GLY:CA	2.67	0.65
1:C:15:VAL:O	1:C:17:GLY:CA	2.45	0.65
1:D:741:ILE:HA	1:D:744:GLN:HG2	1.79	0.65
1:A:32:ASN:ND2	1:B:13:ILE:HA	2.05	0.65
1:A:138:ARG:NH1	1:A:142:CYS:SG	2.69	0.65
1:B:481:ASN:HD22	1:B:482:LYS:N	1.94	0.65
1:B:388:PRO:HD2	1:B:391:LEU:HD13	1.78	0.65
1:D:796:GLU:HA	1:D:799:ARG:HG3	1.79	0.65
1:A:336:GLN:HG3	1:A:825:TRP:HE1	1.60	0.65
1:B:557:ILE:HG13	1:B:602:THR:HG21	1.79	0.65
1:A:174:TRP:CH2	1:D:435:ALA:HB2	2.33	0.64
1:D:139:LEU:HD21	1:D:484:ASN:ND2	2.12	0.64
1:D:265:ALA:O	1:D:268:ASP:HB3	1.96	0.64
1:B:336:GLN:HE21	1:B:825:TRP:HE1	1.44	0.64
1:D:818:ALA:O	1:D:822:ARG:HG2	1.96	0.64
1:B:389:VAL:HG12	1:B:439:ILE:HD12	1.79	0.64
1:C:536:LYS:HZ2	1:C:540:GLU:CD	2.04	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:TYR:HA	1:B:276:SER:O	1.98	0.64
1:D:721:LEU:HD23	1:D:772:LYS:HE2	1.80	0.64
1:A:22:GLU:H	1:A:24:VAL:HB	1.63	0.64
1:B:536:LYS:O	1:B:540:GLU:HG2	1.98	0.64
1:C:546:ALA:HB1	1:C:557:ILE:HG21	1.78	0.64
1:B:492:LEU:HD21	1:B:499:LEU:HD23	1.79	0.64
1:A:488:PRO:HB3	1:A:515:LEU:HD13	1.80	0.64
1:B:320:ASP:HA	1:B:324:THR:HA	1.79	0.64
1:B:395:LEU:O	1:B:396:LEU:HD12	1.98	0.63
1:D:151:GLY:HA3	1:D:830:SER:HB3	1.81	0.63
1:D:254:LEU:HA	1:D:259:VAL:HG22	1.79	0.63
1:A:110:GLU:O	1:A:114:GLN:HG3	1.99	0.63
1:C:304:LEU:HD12	1:C:307:ILE:HD12	1.80	0.63
1:D:550:GLU:HG2	1:D:555:VAL:HG23	1.80	0.63
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.62	0.63
1:D:574:LYS:HA	1:D:667:SER:OG	1.98	0.63
2:C:900:SO4:S	1:D:43:ARG:NH2	2.69	0.63
1:D:414:VAL:HG11	1:D:428:MET:HG3	1.81	0.63
1:A:165:ILE:HG12	1:A:279:LEU:HB3	1.78	0.63
1:D:89:PHE:O	1:D:131:LEU:HB2	1.98	0.63
1:A:455:VAL:O	1:A:483:THR:HA	1.98	0.63
1:A:74:TYR:OH	1:A:153:ALA:HA	1.99	0.62
1:B:423:ASP:HA	1:B:426:ARG:HG2	1.80	0.62
1:D:206:VAL:HA	1:D:214:LYS:O	1.98	0.62
1:B:506:ARG:HB2	1:B:507:ILE:HG23	1.80	0.62
1:D:170:ILE:HG12	1:D:646:GLU:HB3	1.80	0.62
1:A:307:ILE:HG21	1:A:335:ILE:HD11	1.79	0.62
1:C:521:LEU:HD21	1:C:530:PHE:HZ	1.64	0.62
1:D:16:ARG:HG3	1:D:17:GLY:HA2	1.80	0.62
1:A:834:LEU:HG	1:A:835:PRO:HD2	1.81	0.62
1:C:403:ILE:HG21	1:C:439:ILE:HD13	1.80	0.62
1:A:348:GLU:HA	1:A:399:HIS:HE1	1.64	0.62
1:B:533:ASP:O	1:B:537:VAL:HG23	2.00	0.62
1:D:403:ILE:HG21	1:D:439:ILE:HD12	1.81	0.62
1:D:593:GLU:O	1:D:596:LYS:HB2	1.99	0.62
1:D:143:PHE:CG	1:D:817:ILE:HD11	2.35	0.62
1:D:165:ILE:HD11	1:D:281:PRO:CA	2.29	0.62
1:B:575:ARG:HD2	1:B:668:THR:OG1	1.98	0.61
1:D:338:ASN:OD1	1:D:377:HIS:HE1	1.82	0.61
1:D:565:VAL:HG12	1:D:604:MET:HB2	1.80	0.61
1:A:703:ALA:HB1	1:A:804:ASN:HD22	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:HA	1:C:63:LEU:HB2	1.83	0.61
1:A:21:VAL:HA	1:A:24:VAL:CB	2.27	0.61
1:A:149:THR:HG21	1:A:489:ARG:NH2	2.16	0.61
1:A:825:TRP:O	1:A:827:VAL:HG22	2.00	0.61
1:B:503:ILE:O	1:B:507:ILE:HG12	2.00	0.61
1:B:293:LEU:HD23	1:B:395:LEU:HD23	1.82	0.61
1:C:703:ALA:HA	1:C:807:THR:HG21	1.83	0.61
1:B:208:HIS:HA	1:B:213:ALA:HA	1.83	0.61
1:B:600:PRO:HA	1:B:639:ARG:O	2.00	0.61
1:A:157:TYR:HE1	1:A:242:ARG:HD3	1.65	0.61
1:D:252:PHE:HB2	1:D:269:ARG:NH2	2.16	0.61
1:D:322:VAL:O	1:D:325:ASN:HB2	2.01	0.61
1:A:409:ARG:O	1:A:412:ASN:HB2	2.01	0.61
1:A:426:ARG:CZ	1:D:755:PRO:HD2	2.30	0.61
1:D:235:ASN:HB2	1:D:833:ARG:HA	1.82	0.61
1:D:515:LEU:HG	1:D:518:LEU:HD12	1.82	0.61
1:A:357:GLU:O	1:A:358:ARG:HB2	2.00	0.60
1:A:381:PRO:HA	1:A:384:LEU:HD13	1.83	0.60
1:B:791:TYR:HA	1:B:797:TRP:CD1	2.36	0.60
1:D:793:ASN:HD21	1:D:796:GLU:HB3	1.66	0.60
1:A:601:ARG:HH12	1:A:787:VAL:HG12	1.67	0.60
1:D:99:MET:SD	1:D:119:MET:SD	3.00	0.60
1:D:373:ALA:HA	1:D:449:SER:HB3	1.83	0.60
1:B:511:TYR:HA	1:B:514:ASP:O	2.02	0.60
1:B:766:MET:HA	1:B:766:MET:HE2	1.84	0.60
1:C:424:ARG:HA	1:C:427:ARG:NH2	2.16	0.60
1:D:175:GLN:HE21	1:D:617:LYS:HE2	1.66	0.60
1:D:351:ARG:O	1:D:355:ASP:HB2	2.00	0.60
1:C:598:VAL:HG12	1:C:639:ARG:HH21	1.67	0.60
1:D:330:PRO:HG3	1:D:367:VAL:HG13	1.83	0.60
1:A:653:ALA:HA	1:A:656:VAL:HG12	1.83	0.60
1:B:267:LEU:HD22	1:D:262:TYR:HE2	1.66	0.60
1:B:590:ILE:HG21	1:B:636:VAL:HG23	1.83	0.60
1:B:741:ILE:HA	1:B:744:GLN:HE21	1.66	0.60
1:C:675:GLY:HA3	1:C:678:ASN:OD1	2.01	0.60
1:D:19:ALA:HB1	1:D:62:HIS:CE1	2.37	0.60
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.67	0.60
1:A:432:GLU:HB3	1:A:438:ARG:HG3	1.83	0.59
1:B:495:CYS:HB3	1:B:654:GLU:HB2	1.83	0.59
1:C:322:VAL:O	1:C:325:ASN:HB2	2.02	0.59
1:D:22:GLU:OE1	1:D:22:GLU:HA	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASN:ND2	1:B:189:TRP:H	2.01	0.59
1:B:267:LEU:HD22	1:D:262:TYR:CE2	2.37	0.59
1:B:669:ALA:HA	1:B:693:ASP:HB2	1.84	0.59
1:C:792:LYS:NZ	1:C:792:LYS:HB3	2.17	0.59
1:C:330:PRO:HG2	1:C:370:LYS:HE3	1.83	0.59
1:C:337:LEU:HG	1:C:342:PRO:HB2	1.83	0.59
1:D:269:ARG:O	1:D:273:GLU:HB3	2.03	0.59
1:A:547:ALA:O	1:A:551:ARG:HB2	2.03	0.59
1:B:173:GLY:HA2	1:B:624:THR:HG21	1.84	0.59
1:C:173:GLY:HA2	1:C:624:THR:CG2	2.32	0.59
1:B:128:ASP:OD1	1:B:651:SER:HB3	2.02	0.59
1:B:678:ASN:ND2	1:B:695:ALA:HB3	2.17	0.59
1:C:692:MET:HG2	1:C:710:ILE:HD12	1.85	0.59
1:D:521:LEU:HA	1:D:524:TYR:CD1	2.37	0.59
1:D:729:GLN:HG3	1:D:732:TYR:HB3	1.84	0.59
1:A:414:VAL:HG12	1:A:425:LEU:HD22	1.85	0.59
1:D:573:TYR:CD2	1:D:671:THR:HB	2.37	0.59
1:A:403:ILE:HG21	1:A:439:ILE:HD13	1.83	0.59
1:A:502:ILE:HD12	1:A:530:PHE:HE1	1.68	0.59
1:B:67:TRP:HA	1:B:238:VAL:HB	1.85	0.59
1:C:32:ASN:OD1	1:D:13:ILE:HG22	2.03	0.59
1:D:792:LYS:NZ	1:D:792:LYS:HB3	2.18	0.59
1:A:195:GLU:HB2	1:A:196:PHE:CD1	2.37	0.59
1:B:222:LEU:HG	1:B:249:PRO:HG3	1.85	0.59
1:B:236:ASN:HD22	1:B:836:ALA:HB3	1.68	0.58
1:B:459:HIS:CD2	1:B:673:ALA:HB1	2.38	0.58
1:D:90:TYR:HD2	1:D:138:ARG:HB2	1.68	0.58
1:D:615:MET:HE3	1:D:615:MET:HA	1.83	0.58
1:A:609:ALA:HB2	1:A:620:ILE:HD11	1.83	0.58
1:B:88:GLU:HB3	1:B:132:GLY:HA2	1.85	0.58
1:D:150:LEU:HD12	1:D:829:PRO:HB3	1.85	0.58
1:A:231:PRO:HA	1:A:238:VAL:HA	1.85	0.58
1:B:161:TYR:CE2	1:B:279:LEU:HG	2.39	0.58
1:C:192:ALA:HB2	1:C:226:TYR:CE2	2.38	0.58
1:B:319:ARG:HG2	1:B:321:PRO:HD2	1.85	0.58
1:D:790:LEU:HD12	1:D:793:ASN:HD22	1.68	0.58
1:D:252:PHE:HB2	1:D:269:ARG:HH21	1.68	0.58
1:D:790:LEU:HG	1:D:797:TRP:CD1	2.39	0.58
1:A:251:ASP:HB3	1:A:255:LYS:HB2	1.84	0.58
1:C:237:VAL:HG12	1:C:834:LEU:HD23	1.85	0.58
1:C:360:ASP:HB2	1:C:363:LYS:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:PHE:HD2	1:D:269:ARG:HE	1.48	0.58
1:B:10:ARG:HD2	1:B:13:ILE:HD12	1.86	0.58
1:B:738:LEU:HD12	1:B:741:ILE:HD11	1.86	0.58
1:C:584:ILE:HA	1:C:587:TYR:HB3	1.85	0.58
1:C:661:ASP:HB3	1:C:797:TRP:CH2	2.39	0.58
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.86	0.58
1:C:615:MET:HE1	1:C:761:ILE:HG23	1.84	0.58
1:A:35:LEU:HD12	1:A:54:ALA:HB2	1.85	0.58
1:B:330:PRO:HD3	1:B:367:VAL:HG13	1.85	0.58
1:B:361:TRP:HH2	1:B:406:ILE:HA	1.68	0.58
1:D:119:MET:O	1:D:123:GLU:HG3	2.03	0.58
1:D:399:HIS:O	1:D:403:ILE:HG13	2.04	0.58
1:D:491:TRP:HA	1:D:495:CYS:SG	2.44	0.58
1:D:689:ILE:HD12	1:D:784:GLN:HE21	1.68	0.57
1:C:488:PRO:HG3	1:C:515:LEU:HD22	1.85	0.57
1:C:748:GLY:HA3	1:C:755:PRO:HA	1.87	0.57
1:D:165:ILE:HB	1:D:279:LEU:HD13	1.86	0.57
1:B:87:LEU:CD1	1:B:299:VAL:HG11	2.34	0.57
1:C:323:ARG:HB2	1:C:325:ASN:CG	2.29	0.57
1:A:30:ASN:HB3	1:A:58:THR:HG23	1.85	0.57
1:A:670:GLY:H	1:A:693:ASP:CG	2.13	0.57
1:C:582:HIS:HB2	1:C:780:TYR:HE2	1.70	0.57
1:A:203:TYR:HA	1:A:395:LEU:HA	1.87	0.57
1:B:379:VAL:HG22	1:B:380:ILE:H	1.69	0.57
1:C:790:LEU:HG	1:C:797:TRP:HD1	1.68	0.57
1:D:360:ASP:HB2	1:D:363:LYS:HB3	1.86	0.57
1:C:501:GLU:HB3	1:C:502:ILE:HD12	1.86	0.57
1:C:518:LEU:HD12	1:C:805:ILE:HG22	1.86	0.57
1:D:320:ASP:HB3	1:D:321:PRO:O	2.05	0.57
1:D:170:ILE:HA	1:D:174:TRP:O	2.05	0.57
1:D:578:LEU:HA	1:D:581:LEU:HD12	1.87	0.57
1:A:39:LEU:HD21	1:A:53:PHE:HB2	1.87	0.57
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.87	0.57
1:B:138:ARG:NH1	1:B:142:CYS:SG	2.75	0.57
1:B:615:MET:CE	1:B:761:ILE:HG12	2.35	0.57
1:D:589:ARG:HA	1:D:592:LYS:HD3	1.86	0.57
1:B:799:ARG:O	1:B:803:ARG:HD3	2.04	0.57
1:D:486:ILE:HG13	1:D:491:TRP:CD1	2.40	0.57
1:B:82:ILE:HD12	1:B:147:MET:SD	2.45	0.56
1:C:511:TYR:HA	1:C:514:ASP:O	2.05	0.56
1:D:380:ILE:HG22	1:D:382:GLU:HG3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:LEU:O	1:D:525:VAL:HG23	2.04	0.56
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.86	0.56
1:B:192:ALA:HB1	1:B:224:MET:HE1	1.86	0.56
1:C:481:ASN:O	1:C:482:LYS:HG2	2.04	0.56
1:C:758:PHE:HB3	1:C:761:ILE:HD12	1.87	0.56
1:D:311:PHE:O	1:D:316:PHE:HB2	2.05	0.56
1:A:133:ASN:OD1	1:A:165:ILE:HG21	2.04	0.56
1:D:511:TYR:HA	1:D:514:ASP:O	2.04	0.56
1:D:655:LYS:HA	1:D:658:PRO:HG2	1.87	0.56
1:C:455:VAL:HG22	1:C:484:ASN:OD1	2.05	0.56
1:B:766:MET:HE3	1:B:774:PHE:CE2	2.37	0.56
1:C:570:ILE:HB	1:C:609:ALA:HA	1.88	0.56
1:D:569:ARG:NH2	1:D:608:LYS:HB2	2.20	0.56
1:A:199:PRO:HA	1:A:222:LEU:HD23	1.87	0.56
1:A:741:ILE:HA	1:A:744:GLN:NE2	2.21	0.56
1:B:308:ILE:HD13	1:B:352:VAL:HG11	1.86	0.56
1:D:657:ILE:HG21	1:D:680:LLP:O	2.05	0.56
1:D:515:LEU:CD2	1:D:812:SER:HB2	2.35	0.56
1:B:442:ALA:O	1:B:446:ILE:HG13	2.05	0.56
1:C:325:ASN:HB3	1:C:327:ASP:HB2	1.88	0.56
1:A:548:TYR:HD2	1:A:549:LEU:HD12	1.70	0.56
1:B:584:ILE:HG22	1:B:741:ILE:HG22	1.87	0.56
1:D:262:TYR:HB3	1:D:264:GLN:NE2	2.21	0.56
1:D:529:ALA:HA	1:D:532:ARG:NE	2.21	0.56
1:D:766:MET:HE3	1:D:774:PHE:CE2	2.30	0.56
1:A:191:LYS:HD2	1:A:192:ALA:O	2.06	0.55
1:A:366:GLU:O	1:A:370:LYS:HB2	2.05	0.55
1:C:721:LEU:HD12	1:C:724:ARG:NE	2.21	0.55
1:D:331:ASP:HB2	1:D:332:LYS:HE2	1.86	0.55
1:C:19:ALA:HB1	1:C:21:VAL:HG22	1.89	0.55
1:B:649:ARG:HG2	1:B:649:ARG:HH11	1.71	0.55
1:C:492:LEU:HG	1:C:683:LEU:CD2	2.31	0.55
1:D:175:GLN:NE2	1:D:617:LYS:HE2	2.21	0.55
1:D:614:HIS:O	1:D:618:MET:HB2	2.06	0.55
1:B:569:ARG:CD	1:B:574:LYS:HE3	2.36	0.55
1:D:352:VAL:HA	1:D:356:LEU:HD12	1.87	0.55
1:D:603:VAL:HB	1:D:642:VAL:HG13	1.89	0.55
1:D:60:ARG:HG3	1:D:189:TRP:CZ3	2.41	0.55
1:B:169:LYS:O	1:B:176:MET:HB2	2.07	0.55
1:C:322:VAL:HG13	1:C:325:ASN:HB2	1.88	0.55
1:D:261:GLY:O	1:D:262:TYR:HB2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ARG:HG3	1:D:18:LEU:CD1	2.37	0.55
1:C:52:TYR:HE1	1:C:95:LEU:HD12	1.72	0.55
1:D:64:VAL:HG12	1:D:67:TRP:HE3	1.72	0.55
1:D:64:VAL:HG12	1:D:67:TRP:CE3	2.42	0.55
1:D:428:MET:SD	1:D:470:ASP:HB3	2.47	0.55
1:B:22:GLU:O	1:B:25:THR:HB	2.07	0.54
1:B:764:MET:HE2	1:B:769:ASP:HA	1.89	0.54
1:C:13:ILE:O	1:D:43:ARG:HG2	2.07	0.54
1:D:813:SER:O	1:D:817:ILE:HG12	2.06	0.54
1:A:13:ILE:HG23	1:B:32:ASN:OD1	2.07	0.54
1:B:338:ASN:OD1	1:B:377:HIS:HE1	1.90	0.54
1:C:822:ARG:HD2	1:C:828:GLU:OE2	2.07	0.54
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.42	0.54
1:A:33:ARG:HH12	1:B:18:LEU:HD22	1.71	0.54
1:B:256:ASP:HB3	1:B:258:ASN:ND2	2.23	0.54
1:D:549:LEU:HD23	1:D:557:ILE:CD1	2.37	0.54
1:B:506:ARG:HB3	1:B:524:TYR:CZ	2.43	0.54
1:D:369:VAL:HA	1:D:448:GLY:O	2.08	0.54
1:D:526:ASP:HA	1:D:799:ARG:NH1	2.23	0.54
1:A:280:TYR:HE2	1:A:291:LEU:HD22	1.72	0.54
1:A:395:LEU:HG	1:A:396:LEU:HD22	1.88	0.54
1:A:609:ALA:HB1	1:A:616:ALA:HB1	1.90	0.54
1:A:734:ARG:HG3	1:A:735:ILE:HG13	1.90	0.54
1:D:21:VAL:HG12	1:D:22:GLU:N	2.23	0.54
1:A:203:TYR:OH	1:A:294:LYS:NZ	2.41	0.54
1:A:490:ARG:O	1:A:495:CYS:HB3	2.07	0.54
1:A:509:GLU:HA	1:A:511:TYR:CD1	2.43	0.54
1:A:766:MET:HE3	1:A:774:PHE:HE2	1.72	0.54
1:B:666:ILE:HG22	1:B:690:GLY:HA2	1.89	0.54
1:B:755:PRO:HD2	1:C:426:ARG:CZ	2.38	0.54
1:B:801:VAL:O	1:B:805:ILE:HG13	2.08	0.54
1:C:136:LEU:HD22	1:C:338:ASN:HD21	1.73	0.54
1:D:499:LEU:HB2	1:D:537:VAL:HG11	1.90	0.54
1:B:159:ILE:HG13	1:B:299:VAL:HB	1.90	0.54
1:B:666:ILE:HG22	1:B:711:PHE:HE1	1.73	0.54
1:C:678:ASN:HB2	1:C:699:MET:SD	2.48	0.54
1:A:49:ARG:HA	1:A:125:ILE:HG21	1.88	0.54
1:A:221:VAL:HG13	1:A:272:ALA:HB1	1.89	0.54
1:C:182:TRP:H	1:C:182:TRP:CD1	2.26	0.54
1:B:30:ASN:HA	1:B:33:ARG:HB2	1.89	0.53
1:B:764:MET:HA	1:B:768:HIS:ND1	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:692:MET:HG2	1:D:697:VAL:HG22	1.89	0.53
1:A:67:TRP:CZ3	1:A:229:PRO:HD3	2.43	0.53
1:A:269:ARG:HH11	1:A:269:ARG:HG2	1.73	0.53
1:A:446:ILE:HG23	1:A:452:VAL:HG21	1.90	0.53
1:A:515:LEU:HD21	1:A:683:LEU:HD21	1.91	0.53
1:B:503:ILE:HG12	1:B:521:LEU:HD21	1.89	0.53
1:C:366:GLU:O	1:C:370:LYS:HG3	2.08	0.53
1:D:67:TRP:O	1:D:71:GLN:HB2	2.07	0.53
1:D:91:MET:HE1	1:D:241:MET:SD	2.48	0.53
1:A:15:VAL:HB	1:A:69:ARG:HH21	1.73	0.53
1:A:550:GLU:HG3	1:A:554:LYS:HB2	1.91	0.53
1:B:361:TRP:CH2	1:B:406:ILE:HA	2.43	0.53
1:D:30:ASN:HB3	1:D:58:THR:HG23	1.90	0.53
1:A:322:VAL:HG13	1:A:325:ASN:CB	2.38	0.53
1:B:47:THR:HB	1:B:50:ASP:OD2	2.08	0.53
1:C:49:ARG:O	1:C:53:PHE:HB2	2.08	0.53
1:D:224:MET:HE2	1:D:226:TYR:CE1	2.44	0.53
1:B:63:LEU:HD22	1:B:238:VAL:HG21	1.91	0.53
1:C:457:ARG:HA	1:C:481:ASN:OD1	2.09	0.53
1:D:157:TYR:CE2	1:D:242:ARG:HG2	2.44	0.53
1:B:170:ILE:HD13	1:B:175:GLN:HA	1.89	0.53
1:C:491:TRP:C	1:C:495:CYS:SG	2.92	0.53
1:C:522:LEU:HD13	1:C:806:ALA:CB	2.38	0.53
1:D:527:ASP:OD2	1:D:529:ALA:HB3	2.09	0.53
1:A:652:LEU:HA	1:A:655:LYS:HE2	1.91	0.53
1:C:21:VAL:HG12	1:C:22:GLU:N	2.24	0.53
1:D:309:ARG:NH2	2:D:902:SO4:O1	2.42	0.53
1:D:615:MET:SD	1:D:764:MET:HG3	2.49	0.53
1:A:666:ILE:HG22	1:A:711:PHE:CZ	2.44	0.53
1:C:556:HIS:HE1	1:C:638:ASP:HB3	1.74	0.53
1:A:574:LYS:NZ	2:A:901:SO4:O2	2.37	0.52
1:B:75:TYR:O	1:B:315:LYS:HD3	2.09	0.52
1:D:407:ASN:OD1	1:D:430:LEU:HB2	2.09	0.52
1:C:251:ASP:OD2	1:C:255:LYS:HD2	2.09	0.52
1:D:102:LEU:HB3	1:D:104:LEU:HD22	1.90	0.52
1:D:677:GLY:O	1:D:681:PHE:HD2	1.91	0.52
1:B:688:THR:HB	1:B:708:PHE:CE2	2.44	0.52
1:C:293:LEU:HD23	1:C:395:LEU:HD11	1.91	0.52
1:D:28:LYS:HE3	1:D:114:GLN:HB3	1.91	0.52
1:D:781:VAL:O	1:D:785:GLU:HG3	2.09	0.52
1:B:455:VAL:HG12	1:B:459:HIS:HD2	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:GLU:HG2	1:B:810:LYS:HZ3	1.74	0.52
1:A:60:ARG:O	1:A:64:VAL:HG22	2.09	0.52
1:B:312:LYS:HD2	1:B:326:PHE:HZ	1.73	0.52
1:B:407:ASN:HB2	1:B:430:LEU:HG	1.91	0.52
1:D:709:PHE:CD2	1:D:787:VAL:HG23	2.44	0.52
1:A:83:TYR:OH	1:A:310:ARG:HD2	2.10	0.52
1:B:64:VAL:HG12	1:B:67:TRP:HE3	1.75	0.52
1:C:605:ILE:O	1:C:644:PHE:HA	2.09	0.52
1:D:250:ASN:HA	1:D:269:ARG:NH2	2.24	0.52
1:D:555:VAL:HG11	1:D:643:ILE:HG12	1.91	0.52
1:A:582:HIS:HD2	1:A:781:VAL:HG12	1.75	0.52
1:D:41:LYS:HE2	1:D:50:ASP:OD2	2.10	0.52
1:D:70:THR:OG1	1:D:237:VAL:HA	2.10	0.52
1:D:558:ASN:HB2	1:D:561:SER:OG	2.10	0.52
1:A:89:PHE:O	1:A:131:LEU:HB3	2.09	0.52
1:B:550:GLU:HG2	1:B:555:VAL:HG23	1.91	0.52
1:B:573:TYR:CE1	1:B:574:LYS:HG3	2.44	0.52
1:C:521:LEU:HD21	1:C:530:PHE:CZ	2.45	0.52
1:D:171:CYS:CB	1:D:176:MET:SD	2.95	0.52
1:D:537:VAL:O	1:D:541:ASN:HB2	2.10	0.52
1:A:568:LYS:NZ	1:A:680:LLP:OP2	2.43	0.52
1:C:21:VAL:C	1:C:23:ASN:N	2.68	0.52
1:A:85:LEU:HD21	1:A:303:THR:CG2	2.35	0.51
1:B:653:ALA:O	1:B:657:ILE:HG13	2.09	0.51
1:A:677:GLY:HA2	1:A:680:LLP:HE2	1.92	0.51
1:C:481:ASN:ND2	1:C:482:LYS:H	2.08	0.51
1:D:492:LEU:HD21	1:D:499:LEU:HD22	1.90	0.51
1:D:777:TYR:O	1:D:780:TYR:HB3	2.10	0.51
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.92	0.51
1:B:486:ILE:HG12	1:B:680:LLP:HG3	1.92	0.51
1:C:652:LEU:HD23	1:C:656:VAL:HB	1.92	0.51
1:D:536:LYS:HA	1:D:539:GLN:CD	2.35	0.51
1:D:735:ILE:HD13	1:D:778:GLU:HG3	1.93	0.51
1:D:737:GLU:O	1:D:740:GLN:HB3	2.10	0.51
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.93	0.51
1:A:759:LYS:NZ	1:A:763:ASN:OD1	2.43	0.51
1:A:808:SER:O	1:A:810:LYS:N	2.43	0.51
1:D:80:LYS:HE2	1:D:825:TRP:O	2.10	0.51
1:D:169:LYS:HB3	1:D:176:MET:HB2	1.93	0.51
1:D:404:TYR:CE1	1:D:431:VAL:HG21	2.46	0.51
1:A:711:PHE:HB3	1:A:783:CYS:SG	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LYS:O	1:A:538:LYS:HG3	2.10	0.51
1:B:271:LEU:CA	1:B:274:ASN:HB3	2.40	0.51
1:D:790:LEU:HG	1:D:797:TRP:HD1	1.76	0.51
1:A:96:GLN:O	1:A:100:VAL:HG13	2.10	0.51
1:A:662:LEU:HD11	1:A:784:GLN:HE22	1.76	0.51
1:B:455:VAL:HG12	1:B:459:HIS:CD2	2.46	0.51
1:C:543:LEU:HD13	1:C:559:PRO:HG3	1.93	0.51
1:A:692:MET:SD	1:A:697:VAL:HG23	2.50	0.51
1:B:155:TYR:N	1:B:155:TYR:CD1	2.79	0.51
1:B:590:ILE:HG12	1:B:598:VAL:HG11	1.93	0.51
1:C:350:MET:HE2	1:C:365:TRP:CE3	2.46	0.51
1:C:653:ALA:HA	1:C:656:VAL:HG12	1.93	0.51
1:C:778:GLU:O	1:C:782:LYS:HD2	2.10	0.51
1:D:160:ARG:CZ	1:D:183:LEU:HD21	2.41	0.51
1:D:754:GLN:O	1:D:757:LEU:HB2	2.10	0.51
1:A:40:VAL:HG21	1:B:191:LYS:HG3	1.92	0.51
1:A:271:LEU:HA	1:A:274:ASN:ND2	2.25	0.51
1:A:428:MET:HE1	1:A:474:LEU:HD21	1.93	0.51
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.25	0.51
1:D:459:HIS:HA	1:D:462:ILE:HG13	1.92	0.51
1:D:721:LEU:HG	1:D:726:TYR:HB2	1.92	0.51
1:B:182:TRP:H	1:B:182:TRP:CD1	2.28	0.50
1:D:66:ARG:CZ	1:D:837:PRO:HB3	2.41	0.50
1:D:138:ARG:HH11	1:D:650:VAL:HG11	1.76	0.50
1:A:80:LYS:HG3	1:A:331:ASP:O	2.11	0.50
1:A:795:ARG:O	1:A:799:ARG:HG3	2.11	0.50
1:A:799:ARG:HA	1:A:802:ILE:HD12	1.93	0.50
1:B:133:ASN:ND2	1:B:279:LEU:HD13	2.27	0.50
1:B:381:PRO:HG3	1:B:467:ILE:HG13	1.93	0.50
1:B:734:ARG:O	1:B:736:PRO:HD3	2.11	0.50
1:C:262:TYR:HB3	1:C:264:GLN:HE21	1.74	0.50
1:C:582:HIS:CE1	1:C:586:LEU:HD22	2.46	0.50
1:D:97:ASN:HD22	1:D:494:LEU:HD11	1.76	0.50
1:A:421:ASP:HB3	1:A:425:LEU:HD23	1.93	0.50
1:C:600:PRO:HB3	1:C:639:ARG:HA	1.93	0.50
1:C:732:TYR:HE2	1:C:742:ILE:HG21	1.76	0.50
1:D:28:LYS:CE	1:D:114:GLN:HB3	2.41	0.50
1:D:88:GLU:HG2	1:D:132:GLY:HA2	1.94	0.50
1:D:526:ASP:HA	1:D:799:ARG:HH11	1.75	0.50
1:B:319:ARG:O	1:B:324:THR:HG23	2.11	0.50
1:C:97:ASN:HA	1:C:494:LEU:HD11	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:VAL:O	1:C:269:ARG:HB2	2.11	0.50
1:C:818:ALA:O	1:C:822:ARG:HB2	2.11	0.50
1:D:111:ALA:O	1:D:115:LEU:HB2	2.11	0.50
1:D:689:ILE:HG21	1:D:784:GLN:NE2	2.26	0.50
1:D:738:LEU:HA	1:D:741:ILE:HG12	1.93	0.50
1:A:235:ASN:O	1:A:237:VAL:HG12	2.12	0.50
1:B:82:ILE:HG23	1:B:154:ALA:HB2	1.94	0.50
1:C:70:THR:HG21	1:C:237:VAL:HB	1.92	0.50
1:C:614:HIS:O	1:C:618:MET:HB2	2.11	0.50
1:B:481:ASN:HD22	1:B:482:LYS:H	1.60	0.50
1:C:80:LYS:HE2	1:C:331:ASP:O	2.11	0.50
1:C:159:ILE:HG13	1:C:299:VAL:CG2	2.42	0.50
1:D:19:ALA:CB	1:D:62:HIS:CE1	2.95	0.50
1:D:165:ILE:CD1	1:D:281:PRO:HA	2.35	0.50
1:B:493:VAL:HG21	1:B:512:ILE:HD12	1.93	0.50
1:B:549:LEU:HB3	1:B:555:VAL:HG21	1.94	0.50
1:B:819:GLN:O	1:B:823:GLU:HB2	2.11	0.50
1:C:52:TYR:CE1	1:C:95:LEU:HD12	2.46	0.50
1:C:100:VAL:O	1:C:234:ARG:NH1	2.44	0.50
1:D:515:LEU:HD22	1:D:812:SER:HB2	1.94	0.50
1:A:251:ASP:HB3	1:A:255:LYS:CB	2.42	0.50
1:B:49:ARG:HA	1:B:125:ILE:HG21	1.93	0.50
1:B:206:VAL:CG1	1:B:213:ALA:HB1	2.42	0.50
1:C:497:PRO:HA	1:C:500:ALA:HB3	1.94	0.50
1:D:63:LEU:HD22	1:D:238:VAL:HG11	1.93	0.50
1:D:521:LEU:HA	1:D:524:TYR:HD1	1.75	0.50
1:A:11:LYS:HA	1:B:43:ARG:NE	2.26	0.50
1:A:208:HIS:CE1	1:A:213:ALA:HB2	2.47	0.50
1:B:262:TYR:HE1	1:C:263:ILE:HG13	1.77	0.50
1:C:280:TYR:OH	1:C:291:LEU:HD13	2.12	0.50
1:C:289:LYS:CD	1:C:289:LYS:HA	2.42	0.50
1:D:63:LEU:HD21	1:D:231:PRO:HB3	1.92	0.50
1:D:424:ARG:HG2	1:D:427:ARG:NH2	2.27	0.50
1:A:666:ILE:HG22	1:A:711:PHE:HZ	1.77	0.49
1:B:456:ALA:HB2	1:B:674:SER:HB2	1.92	0.49
1:B:715:VAL:HA	1:B:718:VAL:HG23	1.94	0.49
1:C:496:ASN:HD22	1:C:658:PRO:HG3	1.77	0.49
1:D:712:GLY:H	1:D:779:GLU:HG2	1.76	0.49
1:A:395:LEU:O	1:A:396:LEU:HD13	2.13	0.49
1:B:566:GLN:HB2	1:B:664:GLU:HB2	1.93	0.49
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:ASP:HA	1:C:739:ARG:CZ	2.42	0.49
1:A:248:ALA:HB3	1:A:269:ARG:NH1	2.26	0.49
1:A:742:ILE:HD11	1:A:774:PHE:CE1	2.47	0.49
1:B:150:LEU:HD21	1:B:814:ASP:HB3	1.94	0.49
1:B:385:GLU:O	1:B:441:MET:HB2	2.12	0.49
1:C:21:VAL:C	1:C:23:ASN:H	2.14	0.49
1:C:162:GLU:OE1	1:C:277:ARG:NH1	2.46	0.49
1:D:80:LYS:NZ	1:D:330:PRO:O	2.45	0.49
1:C:267:LEU:HD22	1:C:271:LEU:HD11	1.93	0.49
1:C:480:GLN:HE22	1:C:823:GLU:HB3	1.77	0.49
1:C:619:ILE:O	1:C:622:LEU:HB2	2.12	0.49
1:D:98:THR:O	1:D:102:LEU:HB2	2.12	0.49
1:A:830:SER:OG	1:A:832:GLN:HB3	2.12	0.49
1:B:688:THR:O	1:B:709:PHE:HB2	2.13	0.49
1:C:104:LEU:HB3	1:C:108:CYS:SG	2.53	0.49
1:C:649:ARG:HG3	1:C:651:SER:HB3	1.95	0.49
1:C:93:ARG:HD3	1:C:126:GLU:HG2	1.95	0.49
1:D:60:ARG:HG3	1:D:189:TRP:CE3	2.47	0.49
1:A:16:ARG:HG3	1:A:17:GLY:H	1.78	0.49
1:A:166:PHE:HD2	1:A:167:ASN:O	1.96	0.49
1:A:623:ILE:HG21	1:A:644:PHE:HD1	1.78	0.49
1:B:732:TYR:O	1:B:739:ARG:NH1	2.46	0.49
1:A:165:ILE:HD11	1:A:281:PRO:HG3	1.93	0.49
1:A:330:PRO:HG3	1:A:370:LYS:HZ2	1.78	0.49
1:B:66:ARG:HG2	1:B:236:ASN:ND2	2.28	0.49
1:B:99:MET:HE1	1:B:119:MET:SD	2.52	0.49
1:B:159:ILE:HD11	1:B:299:VAL:HG12	1.95	0.49
1:B:481:ASN:O	1:B:482:LYS:HD3	2.12	0.49
1:B:575:ARG:CZ	1:B:578:LEU:HD22	2.43	0.49
1:C:80:LYS:HD2	1:C:827:VAL:HG13	1.94	0.49
1:C:459:HIS:O	1:C:463:LEU:HG	2.13	0.49
1:D:70:THR:O	1:D:73:HIS:HB3	2.12	0.49
1:D:709:PHE:CE2	1:D:787:VAL:HG23	2.48	0.49
1:B:64:VAL:HG12	1:B:67:TRP:CE3	2.48	0.49
1:B:417:ALA:C	1:B:419:PRO:HD3	2.38	0.49
1:C:576:GLN:HE21	1:C:576:GLN:N	2.07	0.49
1:D:14:SER:HB2	2:D:900:SO4:O2	2.13	0.49
1:D:341:HIS:HB2	1:D:342:PRO:HD3	1.95	0.49
1:D:783:CYS:HA	1:D:786:ARG:NE	2.27	0.49
1:A:82:ILE:O	1:A:154:ALA:HA	2.12	0.49
1:C:652:LEU:O	1:C:656:VAL:HB	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:ILE:O	1:D:765:LEU:HD22	2.13	0.49
1:B:699:MET:HE3	1:B:708:PHE:HZ	1.78	0.48
1:C:55:LEU:O	1:C:58:THR:HB	2.13	0.48
1:D:208:HIS:HA	1:D:213:ALA:HA	1.95	0.48
1:D:410:PHE:O	1:D:413:ARG:HB3	2.13	0.48
1:A:389:VAL:HG23	1:A:390:HIS:N	2.27	0.48
1:A:729:GLN:HB2	1:A:766:MET:HE2	1.94	0.48
1:B:486:ILE:HD12	1:B:486:ILE:HA	1.59	0.48
1:D:161:TYR:CE2	1:D:279:LEU:HG	2.48	0.48
1:A:250:ASN:HB2	1:A:269:ARG:HH22	1.77	0.48
1:A:777:TYR:O	1:A:781:VAL:HG22	2.13	0.48
1:B:815:ARG:O	1:B:819:GLN:HB2	2.13	0.48
1:D:83:TYR:CE1	1:D:333:VAL:HG13	2.35	0.48
1:A:264:GLN:NE2	1:C:267:LEU:HD13	2.28	0.48
1:A:575:ARG:NH2	1:A:776:ASP:HB2	2.28	0.48
1:B:573:TYR:HE1	1:B:672:GLU:HG3	1.77	0.48
1:C:510:GLU:HB3	1:C:517:GLN:OE1	2.13	0.48
1:D:231:PRO:CA	1:D:238:VAL:HG22	2.43	0.48
1:D:316:PHE:HB3	1:D:324:THR:OG1	2.13	0.48
1:B:52:TYR:HE1	1:B:95:LEU:HD12	1.79	0.48
1:B:78:ASP:HB2	1:B:315:LYS:HG2	1.96	0.48
1:B:466:THR:OG1	1:B:467:ILE:HD12	2.13	0.48
1:B:678:ASN:HD22	1:B:695:ALA:HB3	1.76	0.48
1:C:33:ARG:CG	1:D:18:LEU:CG	2.89	0.48
1:C:55:LEU:HD22	1:C:122:LEU:HD12	1.96	0.48
1:C:571:HIS:ND1	1:C:573:TYR:HD2	2.12	0.48
1:D:90:TYR:CD2	1:D:138:ARG:HB2	2.48	0.48
1:D:801:VAL:O	1:D:805:ILE:HG13	2.14	0.48
1:A:248:ALA:HB3	1:A:269:ARG:HH11	1.79	0.48
1:B:66:ARG:O	1:B:69:ARG:HB2	2.13	0.48
1:B:133:ASN:ND2	1:B:281:PRO:HA	2.28	0.48
1:B:369:VAL:HA	1:B:448:GLY:O	2.14	0.48
1:D:241:MET:HB3	1:D:243:LEU:HD13	1.96	0.48
1:D:322:VAL:HG22	1:D:325:ASN:HB2	1.95	0.48
1:D:471:PHE:O	1:D:474:LEU:HD12	2.13	0.48
1:A:157:TYR:HE1	1:A:242:ARG:CD	2.26	0.48
1:A:158:GLY:O	1:A:243:LEU:HA	2.13	0.48
1:C:224:MET:HB2	1:C:247:LYS:HE2	1.95	0.48
1:D:173:GLY:HA2	1:D:624:THR:CG2	2.42	0.48
1:D:662:LEU:HD11	1:D:787:VAL:HG11	1.95	0.48
1:A:163:PHE:CE1	1:A:277:ARG:NH1	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:GLU:O	1:B:702:GLU:HB2	2.14	0.48
1:D:677:GLY:H	1:D:680:LLP:P	2.37	0.48
1:A:19:ALA:HA	1:A:21:VAL:HG22	1.96	0.48
1:A:510:GLU:HB3	1:A:517:GLN:NE2	2.29	0.48
1:C:761:ILE:O	1:C:765:LEU:HB2	2.14	0.48
1:D:23:ASN:O	1:D:27:LEU:HG	2.13	0.48
1:D:264:GLN:O	1:D:267:LEU:HB2	2.13	0.48
1:D:484:ASN:O	1:D:679:MET:HE1	2.14	0.48
1:D:657:ILE:HG23	1:D:681:PHE:CD1	2.49	0.48
1:D:810:LYS:HA	1:D:815:ARG:NE	2.29	0.48
1:A:337:LEU:HD23	1:A:445:CYS:SG	2.54	0.47
1:A:418:PHE:HE2	1:A:474:LEU:HB3	1.79	0.47
1:A:555:VAL:HG11	1:A:643:ILE:HD11	1.95	0.47
1:B:669:ALA:O	1:B:718:VAL:HG21	2.14	0.47
1:D:689:ILE:HG23	1:D:689:ILE:O	2.14	0.47
1:A:21:VAL:HG13	1:A:110:GLU:HG2	1.96	0.47
1:B:455:VAL:HG22	1:B:484:ASN:OD1	2.14	0.47
1:B:740:GLN:O	1:B:744:GLN:HG3	2.14	0.47
1:C:350:MET:SD	1:C:364:ALA:HB1	2.55	0.47
1:A:250:ASN:ND2	1:A:252:PHE:HB2	2.28	0.47
1:A:490:ARG:HG2	1:A:491:TRP:CE2	2.50	0.47
1:B:781:VAL:HA	1:B:784:GLN:HB2	1.95	0.47
1:C:163:PHE:O	1:C:180:ASP:HB3	2.14	0.47
1:C:741:ILE:HA	1:C:744:GLN:HG2	1.96	0.47
1:D:87:LEU:HD11	1:D:299:VAL:HG11	1.96	0.47
1:D:621:LYS:NZ	1:D:624:THR:O	2.44	0.47
1:D:759:LYS:O	1:D:759:LYS:HD3	2.14	0.47
1:A:525:VAL:O	1:A:531:ILE:HD11	2.14	0.47
1:A:678:ASN:HB3	1:A:699:MET:HE1	1.95	0.47
1:B:727:ASN:HD21	1:C:725:GLY:HA3	1.78	0.47
1:B:208:HIS:CE1	1:B:213:ALA:HB2	2.49	0.47
1:C:152:LEU:HD22	1:C:827:VAL:CG2	2.45	0.47
1:D:293:LEU:HD22	1:D:391:LEU:HD23	1.97	0.47
1:D:329:PHE:HB3	1:D:330:PRO:HD3	1.95	0.47
1:B:639:ARG:HG3	1:B:639:ARG:HH11	1.79	0.47
1:C:316:PHE:CE1	1:C:319:ARG:HB3	2.50	0.47
1:A:23:ASN:O	1:A:27:LEU:HG	2.15	0.47
1:A:538:LYS:NZ	1:A:660:ALA:O	2.47	0.47
1:C:41:LYS:HE3	1:C:50:ASP:OD2	2.15	0.47
1:C:191:LYS:HG3	1:D:40:VAL:HG21	1.96	0.47
1:C:262:TYR:CD2	1:C:264:GLN:HB3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ARG:NH2	1:C:322:VAL:H	2.13	0.47
1:C:573:TYR:CZ	1:C:574:LYS:HE3	2.49	0.47
1:C:753:LYS:H	1:C:753:LYS:HD2	1.78	0.47
1:D:262:TYR:HB3	1:D:264:GLN:CD	2.40	0.47
1:D:528:GLU:HG3	1:D:795:ARG:NH1	2.30	0.47
1:D:675:GLY:HA3	1:D:678:ASN:HD21	1.79	0.47
1:A:423:ASP:HA	1:A:426:ARG:HG2	1.97	0.47
1:A:707:ASN:HA	1:A:800:MET:SD	2.55	0.47
1:B:30:ASN:HB2	1:B:58:THR:HG23	1.97	0.47
1:B:312:LYS:HD2	1:B:326:PHE:CZ	2.50	0.47
1:B:322:VAL:HG13	1:B:325:ASN:HB2	1.96	0.47
1:B:688:THR:HG22	1:B:689:ILE:O	2.14	0.47
1:D:551:ARG:HD2	1:D:552:GLU:OE1	2.15	0.47
1:A:320:ASP:HA	1:A:324:THR:HA	1.96	0.47
1:A:336:GLN:HA	1:A:373:ALA:O	2.14	0.47
1:A:471:PHE:N	1:A:471:PHE:CD1	2.83	0.47
1:A:486:ILE:HD13	1:A:679:MET:SD	2.55	0.47
1:A:588:ASN:ND2	1:A:744:GLN:HE22	2.10	0.47
1:C:15:VAL:O	1:C:17:GLY:HA2	2.14	0.47
1:C:181:ASP:O	1:C:184:ARG:NH2	2.48	0.47
1:C:458:ILE:O	1:C:462:ILE:HG12	2.15	0.47
1:D:742:ILE:HD11	1:D:774:PHE:HZ	1.80	0.47
1:A:81:ARG:HG2	1:A:155:TYR:CE2	2.45	0.47
1:A:99:MET:SD	1:A:108:CYS:CB	3.03	0.47
1:A:698:GLU:HB3	1:A:810:LYS:HZ3	1.79	0.47
1:A:724:ARG:O	1:A:724:ARG:HG2	2.15	0.47
1:B:712:GLY:O	1:B:714:ARG:HG3	2.14	0.47
1:C:431:VAL:HG13	1:C:437:LYS:HD3	1.97	0.47
1:A:83:TYR:HD1	1:A:155:TYR:HB2	1.80	0.46
1:A:455:VAL:HA	1:A:482:LYS:O	2.15	0.46
1:A:609:ALA:CB	1:A:620:ILE:HD11	2.45	0.46
1:B:39:LEU:HD21	1:B:53:PHE:HB2	1.97	0.46
1:C:86:SER:HB3	1:C:89:PHE:CE1	2.50	0.46
1:C:515:LEU:HG	1:C:809:GLY:HA2	1.95	0.46
1:D:515:LEU:HG	1:D:515:LEU:O	2.15	0.46
1:D:566:GLN:HB2	1:D:664:GLU:O	2.15	0.46
1:A:550:GLU:CA	1:A:554:LYS:HA	2.37	0.46
1:A:698:GLU:HB3	1:A:810:LYS:NZ	2.30	0.46
1:B:711:PHE:CD2	1:B:780:TYR:HA	2.49	0.46
1:C:75:TYR:O	1:C:315:LYS:NZ	2.42	0.46
1:C:196:PHE:HB2	1:C:225:PRO:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:584:ILE:HG13	1:C:741:ILE:HD12	1.96	0.46
1:D:485:GLY:HA2	1:D:679:MET:SD	2.55	0.46
1:D:525:VAL:HA	1:D:802:ILE:HD12	1.96	0.46
1:D:781:VAL:HG23	1:D:782:LYS:HD3	1.96	0.46
1:A:525:VAL:O	1:A:799:ARG:HD2	2.16	0.46
1:B:604:MET:HE2	1:B:645:LEU:HD21	1.96	0.46
1:C:511:TYR:CD2	1:C:518:LEU:HD21	2.50	0.46
1:D:632:HIS:O	1:D:634:PRO:HD3	2.15	0.46
1:D:662:LEU:HD22	1:D:689:ILE:HG22	1.97	0.46
1:A:414:VAL:HG13	1:A:428:MET:SD	2.55	0.46
1:B:175:GLN:OE1	1:B:609:ALA:HB3	2.16	0.46
1:B:587:TYR:CE1	1:B:591:LYS:HD2	2.50	0.46
1:C:168:GLN:OE1	1:C:608:LYS:HA	2.15	0.46
1:D:21:VAL:C	1:D:23:ASN:N	2.64	0.46
1:D:424:ARG:HG2	1:D:427:ARG:HH22	1.81	0.46
1:D:622:LEU:HG	1:D:758:PHE:CD1	2.51	0.46
1:D:711:PHE:CE2	1:D:780:TYR:HB2	2.51	0.46
1:D:783:CYS:HB2	1:D:786:ARG:HH21	1.81	0.46
1:A:293:LEU:O	1:A:293:LEU:HG	2.15	0.46
1:A:421:ASP:O	1:A:425:LEU:HD23	2.15	0.46
1:A:630:VAL:HG21	1:A:642:VAL:CG2	2.38	0.46
1:B:92:GLY:O	1:B:490:ARG:NH2	2.48	0.46
1:B:641:ARG:HG2	1:B:641:ARG:HH11	1.80	0.46
1:B:687:LEU:HD13	1:B:709:PHE:HE2	1.80	0.46
1:A:85:LEU:CD2	1:A:303:THR:HG21	2.37	0.46
1:B:327:ASP:CG	1:B:363:LYS:HZ3	2.24	0.46
1:B:26:GLU:OE2	1:B:29:LYS:NZ	2.48	0.46
1:B:665:GLN:HE21	1:B:678:ASN:HA	1.80	0.46
1:C:150:LEU:HD13	1:C:829:PRO:HB3	1.98	0.46
1:D:68:ILE:O	1:D:72:GLN:HG3	2.16	0.46
1:D:601:ARG:HH12	1:D:787:VAL:HG12	1.81	0.46
1:B:516:ASP:O	1:B:519:ARG:HG3	2.16	0.46
1:B:569:ARG:HD3	1:B:574:LYS:HE3	1.97	0.46
1:C:77:LYS:HG2	1:C:79:PRO:HD3	1.98	0.46
1:C:289:LYS:CD	1:C:289:LYS:CA	2.94	0.46
1:C:380:ILE:HA	1:C:381:PRO:HD3	1.70	0.46
1:D:479:PHE:CD1	1:D:479:PHE:N	2.83	0.46
1:A:99:MET:HE1	1:A:119:MET:SD	2.56	0.46
1:A:422:VAL:O	1:A:426:ARG:HG2	2.16	0.46
1:A:616:ALA:O	1:A:620:ILE:HG13	2.16	0.46
1:A:797:TRP:CZ3	1:A:801:VAL:HG21	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:756:ASP:O	1:C:759:LYS:HB2	2.16	0.46
1:C:798:THR:O	1:C:802:ILE:HG12	2.16	0.46
1:D:27:LEU:HD11	1:D:107:ALA:O	2.16	0.46
1:D:461:GLU:HB3	1:D:465:LYS:HD2	1.97	0.46
1:A:118:ASP:HB3	1:A:121:GLU:HB2	1.97	0.46
1:A:366:GLU:HA	1:A:369:VAL:HG12	1.98	0.46
1:A:511:TYR:HB2	1:A:518:LEU:CD1	2.40	0.46
1:A:592:LYS:NZ	1:A:593:GLU:OE2	2.49	0.46
1:B:14:SER:OG	1:B:16:ARG:HG3	2.16	0.46
1:B:480:GLN:NE2	1:B:482:LYS:HE3	2.31	0.46
1:C:665:GLN:HE21	1:C:678:ASN:ND2	2.14	0.46
1:D:110:GLU:HG2	1:D:114:GLN:HE21	1.80	0.46
1:D:203:TYR:CE1	1:D:395:LEU:HD22	2.51	0.46
1:D:486:ILE:HD11	1:D:680:LLP:HE3	1.98	0.46
1:D:712:GLY:HA2	1:D:779:GLU:HG2	1.97	0.46
1:A:99:MET:SD	1:A:108:CYS:SG	3.14	0.45
1:A:485:GLY:C	1:A:486:ILE:HD12	2.40	0.45
1:A:509:GLU:HA	1:A:511:TYR:HD1	1.80	0.45
1:B:118:ASP:HB3	1:B:121:GLU:HB2	1.98	0.45
1:B:322:VAL:HG23	1:B:323:ARG:HH21	1.81	0.45
1:B:498:GLY:O	1:B:501:GLU:HB3	2.16	0.45
1:C:75:TYR:HD2	1:C:76:GLU:OE1	1.99	0.45
1:C:322:VAL:HG13	1:C:325:ASN:HD22	1.81	0.45
1:C:528:GLU:HA	1:C:531:ILE:HB	1.98	0.45
1:C:637:GLY:O	1:C:641:ARG:NH2	2.49	0.45
1:A:481:ASN:C	1:A:482:LYS:HG2	2.40	0.45
1:A:489:ARG:NH1	1:A:512:ILE:O	2.49	0.45
1:A:532:ARG:O	1:A:536:LYS:HB2	2.16	0.45
1:B:100:VAL:HG21	1:B:494:LEU:HD13	1.99	0.45
1:B:582:HIS:O	1:B:586:LEU:HD13	2.16	0.45
1:C:323:ARG:HE	1:C:323:ARG:HA	1.80	0.45
1:C:413:ARG:CZ	1:C:413:ARG:HB3	2.46	0.45
1:D:638:ASP:HA	1:D:641:ARG:NH2	2.32	0.45
1:A:47:THR:HB	1:A:50:ASP:OD2	2.17	0.45
1:B:573:TYR:OH	1:B:574:LYS:HE2	2.15	0.45
1:B:575:ARG:HH22	1:B:776:ASP:CB	2.28	0.45
1:C:138:ARG:NH1	1:C:142:CYS:SG	2.87	0.45
1:C:341:HIS:HB2	1:C:342:PRO:HD3	1.97	0.45
1:D:516:ASP:O	1:D:519:ARG:HG2	2.16	0.45
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.51	0.45
1:A:729:GLN:HA	1:A:732:TYR:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:VAL:O	1:C:450:HIS:HB3	2.16	0.45
1:D:33:ARG:HD2	1:D:37:PHE:CD2	2.52	0.45
1:D:733:ASP:O	1:D:739:ARG:NH2	2.49	0.45
1:A:323:ARG:HG2	1:A:325:ASN:HD22	1.82	0.45
1:C:428:MET:HE2	1:C:428:MET:HB3	1.82	0.45
1:D:379:VAL:HG11	1:D:671:THR:O	2.15	0.45
1:D:381:PRO:HB3	1:D:467:ILE:HG23	1.98	0.45
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.80	0.45
1:A:442:ALA:HB1	1:A:468:PHE:HZ	1.82	0.45
1:B:550:GLU:HG2	1:B:556:HIS:H	1.81	0.45
1:B:677:GLY:HA2	1:B:680:LLP:HD3	1.98	0.45
1:C:455:VAL:H	1:C:459:HIS:CD2	2.34	0.45
1:C:486:ILE:HG12	1:C:680:LLP:HG2	1.99	0.45
1:A:791:TYR:HD1	1:A:797:TRP:CD1	2.35	0.45
1:A:807:THR:HG22	1:A:808:SER:N	2.31	0.45
1:C:18:LEU:CB	1:D:37:PHE:HE2	2.23	0.45
1:D:214:LYS:HB3	1:D:216:VAL:HG13	1.99	0.45
1:D:568:LYS:HE2	1:D:665:GLN:NE2	2.32	0.45
1:A:160:ARG:HB2	1:A:243:LEU:HB2	1.99	0.45
1:A:230:VAL:HG23	1:A:239:ASN:HB2	1.98	0.45
1:A:235:ASN:HB2	1:A:833:ARG:HA	1.99	0.45
1:A:336:GLN:HG3	1:A:825:TRP:NE1	2.31	0.45
1:A:348:GLU:HA	1:A:399:HIS:CE1	2.48	0.45
1:B:290:GLU:O	1:B:294:LYS:HB2	2.16	0.45
1:B:506:ARG:HB3	1:B:524:TYR:CE2	2.52	0.45
1:B:563:PHE:HD2	1:B:659:ALA:O	1.99	0.45
1:C:37:PHE:CE2	1:D:18:LEU:CG	2.96	0.45
1:C:37:PHE:HD1	1:D:64:VAL:HG23	1.82	0.45
1:C:190:GLU:HG3	1:C:226:TYR:HD2	1.81	0.45
1:C:191:LYS:HG3	1:D:40:VAL:CG2	2.46	0.45
1:D:329:PHE:HE2	1:D:371:THR:HG21	1.81	0.45
1:D:810:LYS:HA	1:D:815:ARG:HD3	1.98	0.45
1:A:174:TRP:CE2	1:A:621:LYS:HD3	2.52	0.45
1:A:499:LEU:HD12	1:A:502:ILE:HD11	1.99	0.45
1:A:706:GLU:H	1:A:706:GLU:CD	2.24	0.45
1:C:658:PRO:HD3	1:C:684:ASN:CG	2.42	0.45
1:D:735:ILE:HA	1:D:736:PRO:HD3	1.73	0.45
1:A:494:LEU:HD23	1:A:494:LEU:H	1.82	0.45
1:A:793:ASN:N	1:A:794:PRO:HD3	2.32	0.45
1:B:469:LYS:HE2	1:B:473:GLU:OE2	2.17	0.45
1:D:47:THR:O	1:D:50:ASP:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HD13	1:D:82:ILE:O	2.17	0.45
1:D:587:TYR:CD1	1:D:630:VAL:HG12	2.52	0.45
1:D:699:MET:HB3	1:D:708:PHE:CZ	2.52	0.45
1:D:729:GLN:O	1:D:730:GLU:HB3	2.16	0.45
1:A:22:GLU:C	1:A:24:VAL:N	2.72	0.44
1:A:391:LEU:O	1:A:395:LEU:HD23	2.17	0.44
1:B:452:VAL:HG23	1:B:478:LYS:HD2	1.99	0.44
1:B:457:ARG:HA	1:B:481:ASN:OD1	2.17	0.44
1:B:529:ALA:O	1:B:532:ARG:HB3	2.16	0.44
1:B:545:PHE:CE2	1:B:604:MET:HE1	2.42	0.44
1:B:636:VAL:O	1:B:639:ARG:HG3	2.16	0.44
1:C:13:ILE:HD11	1:D:31:PHE:HE1	1.82	0.44
1:D:699:MET:HB3	1:D:708:PHE:HZ	1.81	0.44
1:D:784:GLN:HA	1:D:787:VAL:HB	1.99	0.44
1:A:233:TYR:CZ	1:A:234:ARG:HD2	2.52	0.44
1:A:411:LEU:HD22	1:A:425:LEU:HD13	1.99	0.44
1:A:443:HIS:HA	1:A:446:ILE:HD12	1.99	0.44
1:A:527:ASP:OD2	1:A:529:ALA:HB3	2.16	0.44
1:B:22:GLU:HA	1:B:25:THR:HB	1.99	0.44
1:B:532:ARG:HB3	1:B:532:ARG:HH11	1.82	0.44
1:C:63:LEU:HD13	1:C:229:PRO:HG2	2.00	0.44
1:C:170:ILE:HD13	1:C:175:GLN:HA	1.98	0.44
1:C:398:ARG:HH11	1:C:398:ARG:HD3	1.57	0.44
1:D:256:ASP:OD2	1:D:258:ASN:HB3	2.18	0.44
1:D:630:VAL:HG23	1:D:631:ASN:H	1.81	0.44
1:D:679:MET:HB3	1:D:811:PHE:HB3	1.98	0.44
1:A:33:ARG:NH1	1:B:18:LEU:HB2	2.33	0.44
1:A:182:TRP:H	1:A:182:TRP:CD1	2.36	0.44
1:A:446:ILE:HD11	1:A:468:PHE:CZ	2.52	0.44
1:B:721:LEU:HD12	1:B:772:LYS:HD3	1.99	0.44
1:C:266:VAL:HG22	1:C:269:ARG:HG3	1.99	0.44
1:C:410:PHE:O	1:C:413:ARG:HB2	2.16	0.44
1:D:492:LEU:HG	1:D:683:LEU:HD22	1.99	0.44
1:D:633:ASP:OD2	1:D:635:VAL:HB	2.17	0.44
1:D:741:ILE:O	1:D:745:LEU:HB2	2.17	0.44
1:B:52:TYR:CE1	1:B:95:LEU:HD12	2.52	0.44
1:B:575:ARG:NH2	1:B:578:LEU:HD22	2.33	0.44
1:B:596:LYS:HD3	1:B:597:PHE:O	2.18	0.44
1:C:162:GLU:O	1:C:183:LEU:HD11	2.17	0.44
1:C:293:LEU:HD22	1:C:391:LEU:HD22	2.00	0.44
1:D:94:THR:O	1:D:95:LEU:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:593:GLU:HB2	1:D:596:LYS:HG3	1.99	0.44
1:B:727:ASN:O	1:B:730:GLU:HB3	2.18	0.44
1:B:822:ARG:NH2	1:B:829:PRO:HD2	2.33	0.44
1:C:248:ALA:HB1	1:C:250:ASN:HD22	1.82	0.44
1:D:75:TYR:HD2	1:D:76:GLU:OE2	2.00	0.44
1:D:675:GLY:HA3	1:D:678:ASN:ND2	2.32	0.44
1:D:742:ILE:HD11	1:D:774:PHE:CZ	2.53	0.44
1:B:83:TYR:HA	1:B:155:TYR:O	2.18	0.44
1:B:246:ALA:HB2	1:B:298:PHE:CZ	2.51	0.44
1:C:150:LEU:CD1	1:C:829:PRO:HB3	2.47	0.44
1:C:378:THR:O	1:C:459:HIS:CE1	2.71	0.44
1:D:138:ARG:NH1	1:D:650:VAL:HG11	2.32	0.44
1:D:398:ARG:HD2	1:D:398:ARG:HA	1.86	0.44
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.98	0.44
1:B:357:GLU:O	1:B:358:ARG:NH1	2.50	0.44
1:B:599:VAL:HG21	1:B:788:SER:HB3	1.99	0.44
1:B:713:MET:HE3	1:B:713:MET:HB3	1.93	0.44
1:B:733:ASP:HA	1:B:739:ARG:HH12	1.82	0.44
1:C:56:ALA:O	1:C:60:ARG:HG2	2.18	0.44
1:C:423:ASP:OD1	1:C:426:ARG:HD3	2.17	0.44
1:C:581:LEU:HD22	1:C:741:ILE:HG13	1.99	0.44
1:C:592:LYS:HZ2	1:C:593:GLU:CD	2.26	0.44
1:D:171:CYS:SG	1:D:176:MET:SD	3.16	0.44
1:D:602:THR:HA	1:D:641:ARG:O	2.17	0.44
1:D:822:ARG:NH1	1:D:828:GLU:OE1	2.50	0.44
1:A:80:LYS:HD2	1:A:827:VAL:HG13	2.00	0.44
1:A:460:SER:OG	1:A:481:ASN:HB2	2.18	0.44
1:A:486:ILE:CD1	1:A:679:MET:SD	3.06	0.44
1:B:377:HIS:CD2	1:B:455:VAL:HG21	2.53	0.44
1:B:603:VAL:HG23	1:B:642:VAL:HG13	2.00	0.44
1:B:786:ARG:O	1:B:789:ALA:HB3	2.17	0.44
1:C:587:TYR:OH	1:C:591:LYS:NZ	2.48	0.44
1:D:24:VAL:O	1:D:28:LYS:HB2	2.17	0.44
1:D:70:THR:CG2	1:D:237:VAL:HG23	2.47	0.44
1:D:139:LEU:HD11	1:D:484:ASN:HB3	1.99	0.44
1:D:720:ARG:O	1:D:723:GLN:HB2	2.18	0.44
1:A:41:LYS:HE3	1:B:193:ARG:NH1	2.33	0.44
1:A:430:LEU:CD1	1:A:444:LEU:HD23	2.48	0.44
1:A:567:VAL:HB	1:A:648:TYR:CZ	2.53	0.44
1:A:579:ASN:HB2	1:A:666:ILE:HD11	2.00	0.44
1:B:80:LYS:HE3	1:B:333:VAL:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LYS:HE2	1:D:193:ARG:NH1	2.33	0.44
1:C:69:ARG:NH2	2:C:900:SO4:O2	2.50	0.44
1:C:320:ASP:H	1:C:321:PRO:HD2	1.83	0.44
1:C:758:PHE:O	1:C:762:VAL:HG23	2.18	0.44
1:D:295:GLN:O	1:D:298:PHE:HB3	2.18	0.44
1:A:330:PRO:HG3	1:A:370:LYS:NZ	2.33	0.43
1:A:464:LYS:O	1:A:466:THR:N	2.51	0.43
1:A:599:VAL:HG11	1:A:791:TYR:HD2	1.83	0.43
1:B:165:ILE:HD11	1:B:281:PRO:HG3	1.98	0.43
1:D:206:VAL:HG23	1:D:397:PRO:HB2	1.99	0.43
1:D:460:SER:O	1:D:464:LYS:HG3	2.17	0.43
1:D:605:ILE:HG21	1:D:623:ILE:CD1	2.42	0.43
1:A:206:VAL:CG1	1:A:398:ARG:HD2	2.48	0.43
1:A:762:VAL:O	1:A:765:LEU:HB2	2.19	0.43
1:B:127:GLU:OE2	1:B:182:TRP:HA	2.18	0.43
1:B:631:ASN:HA	1:B:641:ARG:NH1	2.34	0.43
1:B:665:GLN:NE2	1:B:678:ASN:HA	2.32	0.43
1:B:731:TYR:HB3	1:B:735:ILE:HD12	2.00	0.43
1:C:230:VAL:HG23	1:C:239:ASN:HB2	1.99	0.43
1:C:575:ARG:NE	1:C:668:THR:OG1	2.51	0.43
1:D:95:LEU:O	1:D:99:MET:HG3	2.18	0.43
1:D:354:VAL:O	1:D:358:ARG:HA	2.18	0.43
1:A:163:PHE:HE1	1:A:277:ARG:NH1	2.16	0.43
1:A:575:ARG:NH2	1:A:578:LEU:HD22	2.33	0.43
1:A:604:MET:HA	1:A:643:ILE:O	2.19	0.43
1:B:666:ILE:HG22	1:B:711:PHE:CE1	2.51	0.43
1:C:522:LEU:O	1:C:525:VAL:HG22	2.18	0.43
1:D:682:MET:HE2	1:D:811:PHE:HD2	1.83	0.43
1:B:207:GLU:OE1	1:B:214:LYS:NZ	2.52	0.43
1:B:380:ILE:HA	1:B:381:PRO:HD3	1.57	0.43
1:B:689:ILE:HD13	1:B:689:ILE:HG21	1.81	0.43
1:C:554:LYS:HD3	1:C:555:VAL:N	2.33	0.43
1:C:681:PHE:HB3	1:C:686:ALA:HB3	2.00	0.43
1:A:13:ILE:HB	1:B:43:ARG:HB3	2.00	0.43
1:A:27:LEU:HA	1:A:30:ASN:HB2	2.00	0.43
1:B:310:ARG:NH2	2:B:902:SO4:O1	2.51	0.43
1:B:455:VAL:H	1:B:459:HIS:CD2	2.36	0.43
1:C:13:ILE:HA	1:D:32:ASN:OD1	2.18	0.43
1:C:346:ILE:HD13	1:C:448:GLY:HA3	2.00	0.43
1:C:715:VAL:O	1:C:718:VAL:HB	2.18	0.43
1:D:542:LYS:NZ	1:D:791:TYR:OH	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:GLU:O	1:D:702:GLU:HG2	2.18	0.43
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.84	0.43
1:A:576:GLN:H	1:A:576:GLN:HG2	1.57	0.43
1:A:724:ARG:HH22	1:A:727:ASN:H	1.64	0.43
1:C:32:ASN:OD1	1:C:36:HIS:HE1	2.02	0.43
1:D:486:ILE:HG12	1:D:680:LLP:HG3	2.01	0.43
1:D:489:ARG:H	1:D:489:ARG:HD3	1.83	0.43
1:A:415:ALA:HB2	1:A:425:LEU:HD11	2.01	0.43
1:A:486:ILE:HD11	1:A:676:THR:O	2.18	0.43
1:B:60:ARG:NH1	1:B:188:PRO:O	2.50	0.43
1:B:88:GLU:HG2	1:B:279:LEU:HD21	2.00	0.43
1:B:761:ILE:HG21	1:B:761:ILE:HD13	1.86	0.43
1:B:789:ALA:O	1:B:792:LYS:NZ	2.52	0.43
1:C:534:VAL:O	1:C:537:VAL:HB	2.19	0.43
1:D:326:PHE:HD1	1:D:329:PHE:CD1	2.36	0.43
1:D:472:TYR:O	1:D:476:PRO:HA	2.19	0.43
1:D:520:LYS:O	1:D:522:LEU:N	2.52	0.43
1:C:290:GLU:HA	1:C:391:LEU:HD21	2.01	0.43
1:D:69:ARG:O	1:D:72:GLN:HB2	2.19	0.43
1:D:406:ILE:O	1:D:409:ARG:HB2	2.19	0.43
1:D:591:LYS:NZ	1:D:633:ASP:OD2	2.52	0.43
1:A:231:PRO:HB3	1:A:238:VAL:HG22	2.01	0.43
1:C:33:ARG:HG3	1:D:18:LEU:HD11	2.01	0.43
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.91	0.43
1:C:582:HIS:HB2	1:C:780:TYR:CE2	2.51	0.43
1:C:657:ILE:HD13	1:C:680:LLP:HB3	2.01	0.43
1:D:458:ILE:O	1:D:461:GLU:HB2	2.19	0.43
1:D:568:LYS:O	1:D:607:GLY:HA3	2.19	0.43
1:D:582:HIS:HA	1:D:585:THR:OG1	2.18	0.43
1:A:47:THR:O	1:A:50:ASP:HB2	2.19	0.43
1:A:724:ARG:HG2	1:A:724:ARG:HH11	1.84	0.43
1:B:764:MET:HA	1:B:768:HIS:CG	2.54	0.43
1:C:13:ILE:HD13	1:C:13:ILE:HG21	1.83	0.43
1:C:504:ALA:HB2	1:C:511:TYR:HE1	1.82	0.43
1:C:590:ILE:CG2	1:C:636:VAL:HG22	2.49	0.43
1:C:679:MET:HE2	1:C:811:PHE:CD1	2.54	0.43
1:D:550:GLU:CD	1:D:556:HIS:H	2.26	0.43
1:D:601:ARG:NH2	1:D:784:GLN:OE1	2.52	0.43
1:A:20:GLY:N	1:A:21:VAL:HG22	2.34	0.42
1:A:379:VAL:HG22	1:A:380:ILE:HD13	2.01	0.42
1:A:680:LLP:H4'1	1:A:680:LLP:H5'1	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:O	1:B:276:SER:HB3	2.19	0.42
1:B:717:ASP:HA	1:B:720:ARG:HB2	2.00	0.42
1:C:59:VAL:O	1:C:62:HIS:HB2	2.19	0.42
1:C:204:GLY:HA3	1:C:218:THR:HG22	2.02	0.42
1:C:735:ILE:HA	1:C:736:PRO:HD3	1.83	0.42
1:D:168:GLN:HG2	1:D:175:GLN:HG3	2.00	0.42
1:A:227:ASP:OD1	1:A:242:ARG:HG3	2.19	0.42
1:A:230:VAL:CG2	1:A:239:ASN:HB2	2.50	0.42
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.53	0.42
1:B:446:ILE:O	1:B:478:LYS:HE3	2.18	0.42
1:B:569:ARG:HD2	1:B:574:LYS:HE3	2.01	0.42
1:C:13:ILE:CD1	1:D:31:PHE:HE1	2.32	0.42
1:C:224:MET:HB2	1:C:247:LYS:CE	2.49	0.42
1:D:92:GLY:H	1:D:129:ALA:HB3	1.83	0.42
1:D:204:GLY:HA3	1:D:218:THR:HG22	2.01	0.42
1:D:489:ARG:HD3	1:D:489:ARG:N	2.33	0.42
1:A:33:ARG:HH12	1:B:18:LEU:HD13	1.84	0.42
1:A:369:VAL:HG23	1:A:447:ALA:O	2.19	0.42
1:A:370:LYS:HA	1:A:450:HIS:HD2	1.84	0.42
1:A:782:LYS:HD3	1:A:785:GLU:OE2	2.18	0.42
1:B:165:ILE:HG12	1:B:279:LEU:HB3	2.01	0.42
1:C:355:ASP:OD1	1:C:398:ARG:NH1	2.53	0.42
1:D:446:ILE:O	1:D:478:LYS:NZ	2.52	0.42
1:A:289:LYS:HE3	1:A:289:LYS:HB2	1.80	0.42
1:C:631:ASN:OD1	1:C:641:ARG:HA	2.18	0.42
1:D:143:PHE:O	1:D:147:MET:HG3	2.20	0.42
1:A:336:GLN:CG	1:A:825:TRP:HE1	2.31	0.42
1:A:459:HIS:CG	1:A:673:ALA:HB1	2.54	0.42
1:A:791:TYR:HA	1:A:797:TRP:CD1	2.55	0.42
1:B:24:VAL:HG22	1:B:107:ALA:O	2.18	0.42
1:B:150:LEU:HB3	1:B:829:PRO:HB3	2.00	0.42
1:B:228:THR:HA	1:B:229:PRO:HD2	1.83	0.42
1:B:481:ASN:ND2	1:B:482:LYS:N	2.66	0.42
1:B:570:ILE:HG13	1:B:620:ILE:HD11	2.01	0.42
1:D:455:VAL:HG12	1:D:674:SER:CB	2.49	0.42
1:D:753:LYS:HE3	1:D:753:LYS:HB2	1.96	0.42
1:A:501:GLU:O	1:A:505:GLU:HG3	2.18	0.42
1:A:627:GLY:HA2	1:A:642:VAL:HB	2.00	0.42
1:B:159:ILE:CG1	1:B:299:VAL:HB	2.50	0.42
1:B:173:GLY:HA2	1:B:624:THR:CG2	2.49	0.42
1:B:713:MET:SD	1:B:718:VAL:CA	3.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:HD21	1:C:53:PHE:HB3	2.02	0.42
1:C:184:ARG:CZ	1:C:184:ARG:HB2	2.49	0.42
1:D:558:ASN:HB3	1:D:561:SER:H	1.84	0.42
1:A:201:HIS:HB2	1:A:218:THR:HB	2.01	0.42
1:B:73:HIS:NE2	1:B:834:LEU:HD11	2.35	0.42
1:C:220:VAL:O	1:C:249:PRO:HG3	2.20	0.42
1:C:626:ILE:HG22	1:C:642:VAL:HG21	2.01	0.42
1:C:689:ILE:HG23	1:C:689:ILE:O	2.19	0.42
1:A:150:LEU:HB3	1:A:829:PRO:HB2	2.01	0.42
1:A:206:VAL:HG13	1:A:398:ARG:HD2	2.01	0.42
1:C:214:LYS:HE3	1:C:214:LYS:HB2	1.73	0.42
1:C:292:ARG:O	1:C:296:GLU:HG3	2.20	0.42
1:C:741:ILE:HG22	1:C:744:GLN:CG	2.48	0.42
1:C:764:MET:SD	1:C:769:ASP:CA	3.04	0.42
1:D:490:ARG:HA	1:D:494:LEU:HD13	2.01	0.42
1:A:503:ILE:HG23	1:A:521:LEU:HD11	2.02	0.42
1:A:813:SER:O	1:A:817:ILE:HB	2.20	0.42
1:B:18:LEU:HD11	1:B:30:ASN:HD21	1.85	0.42
1:B:160:ARG:HG2	1:B:160:ARG:HH11	1.84	0.42
1:C:33:ARG:HG3	1:D:18:LEU:CG	2.50	0.42
1:C:49:ARG:HD3	1:C:185:TYR:CD2	2.55	0.42
1:D:60:ARG:O	1:D:64:VAL:HG22	2.19	0.42
1:D:515:LEU:HD23	1:D:812:SER:HB2	2.01	0.42
1:A:66:ARG:HG2	1:A:66:ARG:HH11	1.85	0.42
1:A:170:ILE:HD13	1:A:175:GLN:HA	2.02	0.42
1:B:344:LEU:HA	1:B:347:PRO:HG2	2.01	0.42
1:C:208:HIS:O	1:C:209:THR:HG23	2.19	0.42
1:C:374:TYR:CD2	1:C:452:VAL:HG13	2.55	0.42
1:C:727:ASN:ND2	1:C:729:GLN:HB3	2.35	0.42
1:C:737:GLU:O	1:C:740:GLN:HB3	2.20	0.42
1:D:88:GLU:CG	1:D:132:GLY:HA2	2.50	0.42
1:D:536:LYS:O	1:D:539:GLN:N	2.53	0.42
1:D:561:SER:HB2	1:D:563:PHE:CE1	2.54	0.42
1:D:587:TYR:CE1	1:D:636:VAL:HG21	2.54	0.42
1:D:661:ASP:O	1:D:686:ALA:HA	2.20	0.42
1:A:64:VAL:HG12	1:A:67:TRP:HE3	1.84	0.41
1:A:782:LYS:HA	1:A:785:GLU:HG3	2.02	0.41
1:B:280:TYR:HA	1:B:281:PRO:HD3	1.87	0.41
1:B:381:PRO:HA	1:B:384:LEU:HD13	2.01	0.41
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.84	0.41
1:C:139:LEU:HD23	1:C:143:PHE:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:GLU:O	1:C:532:ARG:NH1	2.53	0.41
1:D:376:ASN:ND2	1:D:378:THR:H	2.18	0.41
1:D:490:ARG:HG2	1:D:491:TRP:CE2	2.54	0.41
1:A:71:GLN:O	1:A:74:TYR:N	2.54	0.41
1:A:266:VAL:O	1:A:269:ARG:HB2	2.19	0.41
1:B:165:ILE:HD13	1:B:165:ILE:HA	1.82	0.41
1:C:49:ARG:NH2	1:C:125:ILE:O	2.52	0.41
1:C:699:MET:O	1:C:708:PHE:CE1	2.73	0.41
1:D:168:GLN:HE22	1:D:170:ILE:HD11	1.85	0.41
1:D:293:LEU:CD2	1:D:391:LEU:HD23	2.51	0.41
1:D:366:GLU:HG2	1:D:370:LYS:HE3	2.02	0.41
1:D:457:ARG:HH12	1:D:698:GLU:HG2	1.85	0.41
1:D:706:GLU:H	1:D:706:GLU:CD	2.28	0.41
1:A:318:CYS:O	1:A:320:ASP:N	2.53	0.41
1:A:415:ALA:O	1:A:419:PRO:HG3	2.20	0.41
1:B:592:LYS:O	1:B:594:PRO:HD3	2.20	0.41
1:C:18:LEU:HG	1:D:33:ARG:CD	2.42	0.41
1:D:404:TYR:HE1	1:D:431:VAL:HG21	1.84	0.41
1:D:810:LYS:HA	1:D:815:ARG:CD	2.50	0.41
1:A:242:ARG:HG3	1:A:242:ARG:HH11	1.85	0.41
1:A:819:GLN:O	1:A:823:GLU:HB2	2.21	0.41
1:B:180:ASP:O	1:B:182:TRP:HD1	2.03	0.41
1:B:682:MET:HB3	1:B:808:SER:OG	2.21	0.41
1:C:18:LEU:HD22	1:C:18:LEU:HA	1.95	0.41
1:C:517:GLN:HG2	1:C:520:LYS:HE3	2.02	0.41
1:C:753:LYS:HB2	1:C:754:GLN:OE1	2.21	0.41
1:D:103:ALA:HA	1:D:234:ARG:NH1	2.35	0.41
1:D:589:ARG:NH2	1:D:785:GLU:OE2	2.53	0.41
1:D:629:VAL:O	1:D:633:ASP:HB2	2.21	0.41
1:D:717:ASP:HA	1:D:720:ARG:CG	2.50	0.41
1:A:128:ASP:OD1	1:A:651:SER:HB3	2.21	0.41
1:A:488:PRO:HG2	1:A:489:ARG:NH1	2.35	0.41
1:A:665:GLN:HE21	1:A:688:THR:HG23	1.84	0.41
1:A:718:VAL:HG23	1:A:772:LYS:HD3	2.01	0.41
1:A:793:ASN:H	1:A:794:PRO:HD3	1.84	0.41
1:B:664:GLU:HA	1:B:689:ILE:HG23	2.01	0.41
1:C:746:SER:OG	1:C:762:VAL:HG11	2.21	0.41
1:A:201:HIS:HB3	1:A:220:VAL:HA	2.03	0.41
1:A:344:LEU:HD21	1:A:441:MET:HE1	2.02	0.41
1:B:456:ALA:HA	1:B:483:THR:HG23	2.01	0.41
1:B:550:GLU:HG2	1:B:555:VAL:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:GLU:HA	1:B:701:GLU:HB3	2.02	0.41
1:C:269:ARG:O	1:C:273:GLU:HG3	2.20	0.41
1:C:571:HIS:CE1	1:C:573:TYR:HD2	2.38	0.41
1:C:575:ARG:HB3	1:C:578:LEU:HB3	2.03	0.41
1:D:21:VAL:CG1	1:D:22:GLU:N	2.71	0.41
1:D:146:SER:O	1:D:150:LEU:HD23	2.20	0.41
1:D:455:VAL:HG12	1:D:674:SER:OG	2.20	0.41
1:D:797:TRP:CZ3	1:D:801:VAL:HG21	2.55	0.41
1:A:414:VAL:CG1	1:A:428:MET:SD	3.09	0.41
1:A:689:ILE:HD12	1:A:784:GLN:HE21	1.84	0.41
1:A:703:ALA:HB1	1:A:804:ASN:ND2	2.34	0.41
1:A:720:ARG:HA	1:A:723:GLN:HB2	2.02	0.41
1:B:82:ILE:CD1	1:B:147:MET:SD	3.07	0.41
1:B:355:ASP:OD2	1:B:398:ARG:NH1	2.54	0.41
1:B:545:PHE:CE2	1:B:549:LEU:HD22	2.56	0.41
1:B:555:VAL:O	1:B:556:HIS:HB3	2.21	0.41
1:C:504:ALA:HA	1:C:508:GLY:O	2.20	0.41
1:D:221:VAL:HG22	1:D:272:ALA:HB1	2.02	0.41
1:D:402:ILE:O	1:D:406:ILE:HG13	2.20	0.41
1:D:459:HIS:HE1	1:D:463:LEU:HD21	1.85	0.41
1:D:703:ALA:O	1:D:707:ASN:ND2	2.53	0.41
1:D:753:LYS:HE3	1:D:754:GLN:OE1	2.20	0.41
1:D:786:ARG:O	1:D:790:LEU:HB3	2.21	0.41
1:A:112:THR:OG1	1:A:119:MET:HB2	2.21	0.41
1:A:150:LEU:HD12	1:A:817:ILE:CG2	2.49	0.41
1:A:236:ASN:HB2	1:A:834:LEU:O	2.21	0.41
1:A:469:LYS:HE2	1:A:469:LYS:HB2	1.83	0.41
1:A:724:ARG:NH2	1:A:730:GLU:OE1	2.54	0.41
1:B:187:ASN:HD22	1:B:189:TRP:H	1.66	0.41
1:C:67:TRP:O	1:C:71:GLN:HG2	2.20	0.41
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.20	0.41
1:C:384:LEU:HD21	1:C:468:PHE:HE1	1.85	0.41
1:C:557:ILE:HG23	1:C:559:PRO:HD3	2.03	0.41
1:C:633:ASP:C	1:C:635:VAL:H	2.28	0.41
1:D:106:ASN:HA	1:D:109:ASP:HB3	2.02	0.41
1:A:21:VAL:HG12	1:A:24:VAL:HG11	2.02	0.41
1:A:170:ILE:HD13	1:A:170:ILE:HA	1.87	0.41
1:A:584:ILE:HG21	1:A:750:PHE:CE2	2.56	0.41
1:A:654:GLU:O	1:A:658:PRO:HD2	2.20	0.41
1:A:661:ASP:HB3	1:A:797:TRP:CZ2	2.56	0.41
1:B:102:LEU:O	1:B:103:ALA:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASN:O	1:B:254:LEU:HD23	2.21	0.41
1:B:271:LEU:HA	1:B:274:ASN:ND2	2.36	0.41
1:B:322:VAL:HG23	1:B:323:ARG:NH2	2.35	0.41
1:B:355:ASP:OD1	1:B:398:ARG:NH1	2.54	0.41
1:B:685:GLY:CA	1:B:801:VAL:HG13	2.51	0.41
1:B:685:GLY:HA2	1:B:801:VAL:HG13	2.03	0.41
1:B:692:MET:CE	1:B:697:VAL:HA	2.50	0.41
1:B:713:MET:HB2	1:B:776:ASP:OD1	2.21	0.41
1:C:60:ARG:O	1:C:64:VAL:HG13	2.21	0.41
1:C:322:VAL:HG13	1:C:325:ASN:CB	2.49	0.41
1:C:389:VAL:HG12	1:C:439:ILE:HG13	2.02	0.41
1:C:571:HIS:ND1	1:C:573:TYR:CD2	2.88	0.41
1:D:235:ASN:OD1	1:D:237:VAL:HG12	2.20	0.41
1:D:256:ASP:O	1:D:257:PHE:HB2	2.21	0.41
1:D:257:PHE:HD1	1:D:257:PHE:HA	1.81	0.41
1:D:304:LEU:O	1:D:308:ILE:HG13	2.21	0.41
1:D:742:ILE:HD13	1:D:742:ILE:HA	1.94	0.41
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.84	0.41
1:A:446:ILE:HD11	1:A:468:PHE:CE2	2.56	0.41
1:A:461:GLU:C	1:A:465:LYS:HE2	2.46	0.41
1:A:566:GLN:O	1:A:605:ILE:HA	2.21	0.41
1:B:271:LEU:HA	1:B:274:ASN:CB	2.47	0.41
1:B:738:LEU:HD12	1:B:738:LEU:HA	1.82	0.41
1:C:81:ARG:HA	1:C:153:ALA:O	2.20	0.41
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.85	0.41
1:C:462:ILE:HA	1:C:465:LYS:HB2	2.02	0.41
1:C:573:TYR:CE1	1:C:574:LYS:HE3	2.57	0.41
1:D:110:GLU:HG2	1:D:114:GLN:NE2	2.36	0.41
1:D:326:PHE:O	1:D:330:PRO:HD3	2.21	0.41
1:D:613:TYR:CD2	1:D:616:ALA:HB3	2.56	0.41
1:D:756:ASP:O	1:D:759:LYS:HB2	2.21	0.41
1:A:83:TYR:CE1	1:A:310:ARG:NH1	2.89	0.40
1:C:19:ALA:C	1:C:21:VAL:N	2.74	0.40
1:C:262:TYR:HD1	1:C:262:TYR:HA	1.71	0.40
1:D:325:ASN:CG	1:D:326:PHE:H	2.29	0.40
1:D:538:LYS:O	1:D:542:LYS:HG3	2.21	0.40
1:A:99:MET:HE1	1:A:119:MET:CE	2.51	0.40
1:A:353:LEU:O	1:A:357:GLU:HB2	2.21	0.40
1:A:564:ASP:HB3	1:A:603:VAL:HA	2.02	0.40
1:D:100:VAL:HG23	1:D:101:ASN:N	2.37	0.40
1:D:206:VAL:HG21	1:D:401:GLN:HE22	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ILE:O	1:D:265:ALA:N	2.54	0.40
1:D:456:ALA:HA	1:D:483:THR:HG23	2.02	0.40
1:D:698:GLU:HA	1:D:701:GLU:HB3	2.03	0.40
1:A:461:GLU:HB3	1:A:465:LYS:HE2	2.03	0.40
1:A:761:ILE:HD13	1:A:761:ILE:HG21	1.86	0.40
1:B:279:LEU:HD22	1:B:280:TYR:H	1.86	0.40
1:B:344:LEU:HD13	1:B:396:LEU:HD21	2.02	0.40
1:B:455:VAL:H	1:B:459:HIS:HD2	1.69	0.40
1:C:10:ARG:NH2	1:D:43:ARG:O	2.55	0.40
1:C:138:ARG:HD3	1:C:138:ARG:O	2.21	0.40
1:C:205:ARG:HG3	1:C:217:ASP:HB2	2.03	0.40
1:D:386:ARG:HG2	1:D:440:ASN:HA	2.03	0.40
1:D:487:THR:HA	1:D:488:PRO:HD3	1.78	0.40
1:A:381:PRO:O	1:A:384:LEU:HB2	2.22	0.40
1:A:396:LEU:HB3	1:A:399:HIS:HB2	2.03	0.40
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.56	0.40
1:A:748:GLY:HA3	1:A:755:PRO:HA	2.03	0.40
1:B:135:GLY:HA2	1:B:138:ARG:HB3	2.03	0.40
1:B:666:ILE:H	1:B:666:ILE:HG13	1.77	0.40
1:B:810:LYS:HD3	1:B:811:PHE:CE1	2.57	0.40
1:B:822:ARG:NH1	1:B:828:GLU:OE1	2.54	0.40
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.36	0.40
1:C:665:GLN:HG2	1:C:678:ASN:ND2	2.33	0.40
1:D:69:ARG:HA	1:D:72:GLN:HB2	2.03	0.40
1:D:577:LEU:HD22	1:D:765:LEU:HD11	2.03	0.40
1:A:97:ASN:HA	1:A:100:VAL:HG22	2.04	0.40
1:A:603:VAL:HG23	1:A:642:VAL:HA	2.03	0.40
1:A:798:THR:O	1:A:802:ILE:HG13	2.21	0.40
1:B:622:LEU:HD22	1:B:626:ILE:HG13	2.04	0.40
1:B:778:GLU:O	1:B:782:LYS:HE3	2.21	0.40
1:C:133:ASN:ND2	1:C:165:ILE:HG13	2.37	0.40
1:C:262:TYR:HB3	1:C:264:GLN:HG2	2.03	0.40
1:C:433:GLU:HB3	1:C:437:LYS:HG3	2.02	0.40
1:D:296:GLU:O	1:D:299:VAL:HG12	2.21	0.40
1:D:326:PHE:CD2	1:D:326:PHE:N	2.88	0.40
1:D:382:GLU:HG3	1:D:382:GLU:H	1.64	0.40
1:D:570:ILE:HG23	1:D:576:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

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	816/842 (97%)	651 (80%)	112 (14%)	53 (6%)	1	3
1	B	816/842 (97%)	669 (82%)	107 (13%)	40 (5%)	1	6
1	C	818/842 (97%)	678 (83%)	102 (12%)	38 (5%)	2	7
1	D	818/842 (97%)	643 (79%)	124 (15%)	51 (6%)	1	3
All	All	3268/3368 (97%)	2641 (81%)	445 (14%)	182 (6%)	1	4

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	21	VAL
1	A	152	LEU
1	A	166	PHE
1	A	236	ASN
1	A	256	ASP
1	A	257	PHE
1	A	319	ARG
1	A	321	PRO
1	A	322	VAL
1	A	342	PRO
1	A	358	ARG
1	A	465	LYS
1	A	510	GLU
1	A	555	VAL
1	A	610	ALA
1	A	793	ASN
1	A	809	GLY
1	A	836	ALA
1	B	21	VAL
1	B	166	PHE
1	B	271	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	321	PRO
1	B	360	ASP
1	B	380	ILE
1	B	490	ARG
1	B	553	TYR
1	B	835	PRO
1	C	16	ARG
1	C	22	GLU
1	C	166	PHE
1	C	250	ASN
1	C	323	ARG
1	C	553	TYR
1	C	555	VAL
1	C	556	HIS
1	C	599	VAL
1	C	609	ALA
1	C	610	ALA
1	C	625	ALA
1	C	658	PRO
1	C	793	ASN
1	D	22	GLU
1	D	93	ARG
1	D	166	PHE
1	D	234	ARG
1	D	253	ASN
1	D	254	LEU
1	D	256	ASP
1	D	264	GLN
1	D	315	LYS
1	D	321	PRO
1	D	322	VAL
1	D	358	ARG
1	D	559	PRO
1	D	561	SER
1	D	610	ALA
1	D	658	PRO
1	D	674	SER
1	D	757	LEU
1	A	22	GLU
1	A	253	ASN
1	A	273	GLU
1	A	288	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	492	LEU
1	A	529	ALA
1	A	827	VAL
1	B	17	GLY
1	B	92	GLY
1	B	253	ASN
1	B	256	ASP
1	B	379	VAL
1	B	554	LYS
1	B	610	ALA
1	C	19	ALA
1	C	92	GLY
1	C	95	LEU
1	C	256	ASP
1	C	493	VAL
1	C	694	GLY
1	C	783	CYS
1	D	19	ALA
1	D	103	ALA
1	D	260	GLY
1	D	429	SER
1	D	596	LYS
1	D	712	GLY
1	D	730	GLU
1	D	836	ALA
1	A	88	GLU
1	A	91	MET
1	A	318	CYS
1	A	464	LYS
1	A	473	GLU
1	A	484	ASN
1	A	556	HIS
1	A	675	GLY
1	A	730	GLU
1	A	823	GLU
1	B	153	ALA
1	B	210	SER
1	B	258	ASN
1	B	339	ASP
1	B	341	HIS
1	B	350	MET
1	B	384	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	517	GLN
1	B	625	ALA
1	B	808	SER
1	C	40	VAL
1	C	93	ARG
1	C	254	LEU
1	C	321	PRO
1	C	383	ALA
1	C	561	SER
1	C	723	GLN
1	C	809	GLY
1	D	21	VAL
1	D	179	ALA
1	D	262	TYR
1	D	273	GLU
1	D	715	VAL
1	D	721	LEU
1	D	725	GLY
1	D	777	TYR
1	D	783	CYS
1	D	809	GLY
1	A	625	ALA
1	A	783	CYS
1	A	808	SER
1	A	826	GLY
1	B	93	ARG
1	B	342	PRO
1	B	436	VAL
1	B	638	ASP
1	B	751	SER
1	C	21	VAL
1	C	436	VAL
1	C	835	PRO
1	D	436	VAL
1	D	484	ASN
1	D	509	GLU
1	D	735	ILE
1	D	829	PRO
1	A	93	ARG
1	A	263	ILE
1	A	269	ARG
1	A	436	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	553	TYR
1	A	570	ILE
1	B	16	ARG
1	B	183	LEU
1	C	551	ARG
1	C	554	LYS
1	C	724	ARG
1	D	104	LEU
1	D	525	VAL
1	D	697	VAL
1	A	92	GLY
1	A	346	ILE
1	A	477	HIS
1	B	628	ASP
1	B	798	THR
1	D	91	MET
1	D	105	GLU
1	D	628	ASP
1	B	20	GLY
1	B	666	ILE
1	C	559	PRO
1	D	151	GLY
1	D	320	ASP
1	A	824	ILE
1	B	637	GLY
1	B	658	PRO
1	B	836	ALA
1	C	263	ILE
1	C	685	GLY
1	D	502	ILE
1	A	594	PRO
1	A	755	PRO
1	D	40	VAL
1	A	488	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	711/730 (97%)	578 (81%)	133 (19%)	1	5
1	B	711/730 (97%)	565 (80%)	146 (20%)	1	4
1	C	710/730 (97%)	575 (81%)	135 (19%)	1	5
1	D	711/730 (97%)	522 (73%)	189 (27%)	0	1
All	All	2843/2920 (97%)	2240 (79%)	603 (21%)	1	4

All (603) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	15	VAL
1	A	16	ARG
1	A	29	LYS
1	A	30	ASN
1	A	35	LEU
1	A	43	ARG
1	A	44	ASN
1	A	47	THR
1	A	63	LEU
1	A	75	TYR
1	A	78	ASP
1	A	82	ILE
1	A	87	LEU
1	A	104	LEU
1	A	128	ASP
1	A	131	LEU
1	A	139	LEU
1	A	144	LEU
1	A	149	THR
1	A	165	ILE
1	A	169	LYS
1	A	177	GLU
1	A	191	LYS
1	A	195	GLU
1	A	196	PHE
1	A	214	LYS
1	A	224	MET
1	A	231	PRO
1	A	235	ASN
1	A	237	VAL
1	A	240	THR
1	A	241	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	LEU
1	A	254	LEU
1	A	255	LYS
1	A	269	ARG
1	A	271	LEU
1	A	274	ASN
1	A	279	LEU
1	A	287	GLU
1	A	292	ARG
1	A	296	GLU
1	A	299	VAL
1	A	303	THR
1	A	304	LEU
1	A	308	ILE
1	A	319	ARG
1	A	321	PRO
1	A	323	ARG
1	A	324	THR
1	A	327	ASP
1	A	333	VAL
1	A	359	LEU
1	A	361	TRP
1	A	366	GLU
1	A	370	LYS
1	A	379	VAL
1	A	385	GLU
1	A	392	LEU
1	A	396	LEU
1	A	400	LEU
1	A	423	ASP
1	A	425	LEU
1	A	430	LEU
1	A	440	ASN
1	A	445	CYS
1	A	453	ASN
1	A	455	VAL
1	A	461	GLU
1	A	467	ILE
1	A	469	LYS
1	A	471	PHE
1	A	474	LEU
1	A	486	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	492	LEU
1	A	494	LEU
1	A	502	ILE
1	A	506	ARG
1	A	516	ASP
1	A	517	GLN
1	A	528	GLU
1	A	540	GLU
1	A	543	LEU
1	A	551	ARG
1	A	553	TYR
1	A	554	LYS
1	A	565	VAL
1	A	567	VAL
1	A	574	LYS
1	A	576	GLN
1	A	584	ILE
1	A	586	LEU
1	A	589	ARG
1	A	596	LYS
1	A	622	LEU
1	A	636	VAL
1	A	640	LEU
1	A	649	ARG
1	A	650	VAL
1	A	652	LEU
1	A	662	LEU
1	A	692	MET
1	A	697	VAL
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	714	ARG
1	A	723	GLN
1	A	727	ASN
1	A	733	ASP
1	A	740	GLN
1	A	741	ILE
1	A	743	GLU
1	A	751	SER
1	A	755	PRO
1	A	756	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	757	LEU
1	A	759	LYS
1	A	764	MET
1	A	765	LEU
1	A	766	MET
1	A	783	CYS
1	A	787	VAL
1	A	790	LEU
1	A	792	LYS
1	A	800	MET
1	A	807	THR
1	A	817	ILE
1	A	824	ILE
1	A	833	ARG
1	A	834	LEU
1	A	837	PRO
1	B	10	ARG
1	B	16	ARG
1	B	21	VAL
1	B	22	GLU
1	B	23	ASN
1	B	35	LEU
1	B	39	LEU
1	B	45	VAL
1	B	55	LEU
1	B	63	LEU
1	B	72	GLN
1	B	73	HIS
1	B	82	ILE
1	B	94	THR
1	B	95	LEU
1	B	105	GLU
1	B	112	THR
1	B	114	GLN
1	B	119	MET
1	B	128	ASP
1	B	131	LEU
1	B	136	LEU
1	B	155	TYR
1	B	165	ILE
1	B	177	GLU
1	B	187	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	195	GLU
1	B	209	THR
1	B	214	LYS
1	B	216	VAL
1	B	230	VAL
1	B	240	THR
1	B	241	MET
1	B	249	PRO
1	B	250	ASN
1	B	259	VAL
1	B	264	GLN
1	B	275	ILE
1	B	278	VAL
1	B	279	LEU
1	B	289	LYS
1	B	291	LEU
1	B	299	VAL
1	B	300	VAL
1	B	305	GLN
1	B	308	ILE
1	B	309	ARG
1	B	314	SER
1	B	316	PHE
1	B	318	CYS
1	B	319	ARG
1	B	321	PRO
1	B	325	ASN
1	B	337	LEU
1	B	341	HIS
1	B	351	ARG
1	B	356	LEU
1	B	360	ASP
1	B	382	GLU
1	B	400	LEU
1	B	401	GLN
1	B	409	ARG
1	B	413	ARG
1	B	425	LEU
1	B	430	LEU
1	B	439	ILE
1	B	441	MET
1	B	444	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	453	ASN
1	B	455	VAL
1	B	458	ILE
1	B	460	SER
1	B	474	LEU
1	B	481	ASN
1	B	482	LYS
1	B	483	THR
1	B	492	LEU
1	B	493	VAL
1	B	502	ILE
1	B	505	GLU
1	B	510	GLU
1	B	512	ILE
1	B	522	LEU
1	B	532	ARG
1	B	539	GLN
1	B	544	LYS
1	B	550	GLU
1	B	552	GLU
1	B	553	TYR
1	B	554	LYS
1	B	557	ILE
1	B	565	VAL
1	B	567	VAL
1	B	569	ARG
1	B	596	LYS
1	B	621	LYS
1	B	622	LEU
1	B	634	PRO
1	B	636	VAL
1	B	639	ARG
1	B	640	LEU
1	B	643	ILE
1	B	650	VAL
1	B	651	SER
1	B	652	LEU
1	B	656	VAL
1	B	658	PRO
1	B	665	GLN
1	B	672	GLU
1	B	676	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	679	MET
1	B	688	THR
1	B	689	ILE
1	B	692	MET
1	B	702	GLU
1	B	705	GLU
1	B	708	PHE
1	B	715	VAL
1	B	717	ASP
1	B	721	LEU
1	B	729	GLN
1	B	738	LEU
1	B	742	ILE
1	B	743	GLU
1	B	745	LEU
1	B	754	GLN
1	B	756	ASP
1	B	760	ASP
1	B	768	HIS
1	B	773	VAL
1	B	781	VAL
1	B	782	LYS
1	B	784	GLN
1	B	792	LYS
1	B	794	PRO
1	B	796	GLU
1	B	798	THR
1	B	799	ARG
1	B	803	ARG
1	B	808	SER
1	B	814	ASP
1	B	819	GLN
1	B	832	GLN
1	B	833	ARG
1	B	834	LEU
1	B	837	PRO
1	C	12	GLN
1	C	15	VAL
1	C	18	LEU
1	C	29	LYS
1	C	31	PHE
1	C	40	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	45	VAL
1	C	48	PRO
1	C	49	ARG
1	C	53	PHE
1	C	58	THR
1	C	70	THR
1	C	76	GLU
1	C	82	ILE
1	C	87	LEU
1	C	91	MET
1	C	95	LEU
1	C	100	VAL
1	C	104	LEU
1	C	105	GLU
1	C	117	LEU
1	C	120	GLU
1	C	125	ILE
1	C	136	LEU
1	C	138	ARG
1	C	139	LEU
1	C	150	LEU
1	C	162	GLU
1	C	165	ILE
1	C	169	LYS
1	C	175	GLN
1	C	178	GLU
1	C	183	LEU
1	C	190	GLU
1	C	198	LEU
1	C	211	GLN
1	C	234	ARG
1	C	235	ASN
1	C	237	VAL
1	C	242	ARG
1	C	243	LEU
1	C	251	ASP
1	C	256	ASP
1	C	262	TYR
1	C	267	LEU
1	C	269	ARG
1	C	270	ASN
1	C	271	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	274	ASN
1	C	281	PRO
1	C	291	LEU
1	C	292	ARG
1	C	304	LEU
1	C	319	ARG
1	C	321	PRO
1	C	332	LYS
1	C	337	LEU
1	C	339	ASP
1	C	356	LEU
1	C	372	CYS
1	C	382	GLU
1	C	390	HIS
1	C	391	LEU
1	C	395	LEU
1	C	396	LEU
1	C	398	ARG
1	C	400	LEU
1	C	433	GLU
1	C	437	LYS
1	C	439	ILE
1	C	444	LEU
1	C	457	ARG
1	C	460	SER
1	C	464	LYS
1	C	466	THR
1	C	469	LYS
1	C	474	LEU
1	C	486	ILE
1	C	492	LEU
1	C	494	LEU
1	C	499	LEU
1	C	506	ARG
1	C	518	LEU
1	C	525	VAL
1	C	533	ASP
1	C	536	LYS
1	C	537	VAL
1	C	538	LYS
1	C	549	LEU
1	C	554	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	565	VAL
1	C	569	ARG
1	C	574	LYS
1	C	576	GLN
1	C	584	ILE
1	C	586	LEU
1	C	591	LYS
1	C	596	LYS
1	C	598	VAL
1	C	599	VAL
1	C	623	ILE
1	C	629	VAL
1	C	630	VAL
1	C	640	LEU
1	C	649	ARG
1	C	654	GLU
1	C	655	LYS
1	C	656	VAL
1	C	658	PRO
1	C	662	LEU
1	C	663	SER
1	C	665	GLN
1	C	667	SER
1	C	678	ASN
1	C	683	LEU
1	C	692	MET
1	C	716	GLU
1	C	719	ASP
1	C	723	GLN
1	C	724	ARG
1	C	727	ASN
1	C	741	ILE
1	C	745	LEU
1	C	753	LYS
1	C	759	LYS
1	C	764	MET
1	C	782	LYS
1	C	792	LYS
1	C	795	ARG
1	C	797	TRP
1	C	813	SER
1	C	822	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	832	GLN
1	C	833	ARG
1	C	834	LEU
1	D	10	ARG
1	D	12	GLN
1	D	13	ILE
1	D	14	SER
1	D	16	ARG
1	D	18	LEU
1	D	22	GLU
1	D	26	GLU
1	D	28	LYS
1	D	29	LYS
1	D	30	ASN
1	D	33	ARG
1	D	39	LEU
1	D	40	VAL
1	D	43	ARG
1	D	44	ASN
1	D	47	THR
1	D	63	LEU
1	D	71	GLN
1	D	77	LYS
1	D	82	ILE
1	D	85	LEU
1	D	87	LEU
1	D	90	TYR
1	D	91	MET
1	D	95	LEU
1	D	98	THR
1	D	102	LEU
1	D	104	LEU
1	D	106	ASN
1	D	115	LEU
1	D	117	LEU
1	D	121	GLU
1	D	131	LEU
1	D	136	LEU
1	D	162	GLU
1	D	167	ASN
1	D	177	GLU
1	D	191	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	194	PRO
1	D	198	LEU
1	D	199	PRO
1	D	229	PRO
1	D	234	ARG
1	D	237	VAL
1	D	242	ARG
1	D	245	SER
1	D	247	LYS
1	D	255	LYS
1	D	257	PHE
1	D	262	TYR
1	D	264	GLN
1	D	266	VAL
1	D	267	LEU
1	D	273	GLU
1	D	274	ASN
1	D	279	LEU
1	D	289	LYS
1	D	291	LEU
1	D	292	ARG
1	D	296	GLU
1	D	300	VAL
1	D	305	GLN
1	D	319	ARG
1	D	321	PRO
1	D	323	ARG
1	D	324	THR
1	D	327	ASP
1	D	332	LYS
1	D	336	GLN
1	D	337	LEU
1	D	340	THR
1	D	341	HIS
1	D	344	LEU
1	D	374	TYR
1	D	380	ILE
1	D	382	GLU
1	D	391	LEU
1	D	394	THR
1	D	395	LEU
1	D	396	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	400	LEU
1	D	409	ARG
1	D	413	ARG
1	D	421	ASP
1	D	425	LEU
1	D	426	ARG
1	D	430	LEU
1	D	431	VAL
1	D	432	GLU
1	D	437	LYS
1	D	439	ILE
1	D	444	LEU
1	D	458	ILE
1	D	460	SER
1	D	462	ILE
1	D	467	ILE
1	D	474	LEU
1	D	483	THR
1	D	486	ILE
1	D	492	LEU
1	D	505	GLU
1	D	510	GLU
1	D	511	TYR
1	D	516	ASP
1	D	517	GLN
1	D	526	ASP
1	D	533	ASP
1	D	538	LYS
1	D	539	GLN
1	D	541	ASN
1	D	543	LEU
1	D	544	LYS
1	D	549	LEU
1	D	552	GLU
1	D	554	LYS
1	D	555	VAL
1	D	557	ILE
1	D	558	ASN
1	D	560	ASN
1	D	562	LEU
1	D	566	GLN
1	D	569	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	571	HIS
1	D	573	TYR
1	D	579	ASN
1	D	585	THR
1	D	589	ARG
1	D	590	ILE
1	D	596	LYS
1	D	598	VAL
1	D	603	VAL
1	D	604	MET
1	D	605	ILE
1	D	608	LYS
1	D	618	MET
1	D	622	LEU
1	D	630	VAL
1	D	640	LEU
1	D	642	VAL
1	D	643	ILE
1	D	649	ARG
1	D	650	VAL
1	D	652	LEU
1	D	654	GLU
1	D	656	VAL
1	D	658	PRO
1	D	662	LEU
1	D	667	SER
1	D	668	THR
1	D	676	THR
1	D	681	PHE
1	D	682	MET
1	D	683	LEU
1	D	688	THR
1	D	689	ILE
1	D	692	MET
1	D	705	GLU
1	D	706	GLU
1	D	709	PHE
1	D	715	VAL
1	D	722	ASP
1	D	724	ARG
1	D	730	GLU
1	D	740	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	745	LEU
1	D	753	LYS
1	D	755	PRO
1	D	756	ASP
1	D	761	ILE
1	D	765	LEU
1	D	766	MET
1	D	770	ARG
1	D	773	VAL
1	D	787	VAL
1	D	788	SER
1	D	790	LEU
1	D	792	LYS
1	D	793	ASN
1	D	798	THR
1	D	800	MET
1	D	802	ILE
1	D	807	THR
1	D	808	SER
1	D	816	THR
1	D	819	GLN
1	D	823	GLU
1	D	832	GLN
1	D	834	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	36	HIS
1	A	71	GLN
1	A	168	GLN
1	A	201	HIS
1	A	235	ASN
1	A	239	ASN
1	A	250	ASN
1	A	377	HIS
1	A	390	HIS
1	A	401	GLN
1	A	412	ASN
1	A	480	GLN
1	A	481	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	582	HIS
1	A	647	ASN
1	A	665	GLN
1	A	684	ASN
1	A	744	GLN
1	A	754	GLN
1	A	784	GLN
1	A	804	ASN
1	B	23	ASN
1	B	44	ASN
1	B	72	GLN
1	B	167	ASN
1	B	168	GLN
1	B	187	ASN
1	B	201	HIS
1	B	264	GLN
1	B	274	ASN
1	B	295	GLN
1	B	336	GLN
1	B	377	HIS
1	B	453	ASN
1	B	459	HIS
1	B	480	GLN
1	B	481	ASN
1	B	566	GLN
1	B	576	GLN
1	B	582	HIS
1	B	665	GLN
1	B	678	ASN
1	B	723	GLN
1	B	727	ASN
1	B	744	GLN
1	B	754	GLN
1	C	36	HIS
1	C	44	ASN
1	C	62	HIS
1	C	106	ASN
1	C	264	GLN
1	C	274	ASN
1	C	336	GLN
1	C	338	ASN
1	C	377	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	399	HIS
1	C	459	HIS
1	C	480	GLN
1	C	566	GLN
1	C	576	GLN
1	C	579	ASN
1	C	582	HIS
1	C	678	ASN
1	C	727	ASN
1	C	784	GLN
1	D	12	GLN
1	D	72	GLN
1	D	97	ASN
1	D	106	ASN
1	D	133	ASN
1	D	167	ASN
1	D	168	GLN
1	D	175	GLN
1	D	250	ASN
1	D	264	GLN
1	D	377	HIS
1	D	401	GLN
1	D	412	ASN
1	D	450	HIS
1	D	459	HIS
1	D	481	ASN
1	D	484	ASN
1	D	560	ASN
1	D	576	GLN
1	D	647	ASN
1	D	665	GLN
1	D	767	HIS
1	D	793	ASN
1	D	804	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	B	680	1	23,24,25	1.49	5 (21%)	25,32,34	1.47	3 (12%)
1	LLP	D	680	1	23,24,25	1.84	5 (21%)	25,32,34	1.34	2 (8%)
1	LLP	C	680	1	23,24,25	1.50	3 (13%)	25,32,34	2.12	2 (8%)
1	LLP	A	680	1	23,24,25	1.61	4 (17%)	25,32,34	1.21	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	680	1	-	2/16/17/19	0/1/1/1
1	LLP	D	680	1	-	8/16/17/19	0/1/1/1
1	LLP	C	680	1	-	0/16/17/19	0/1/1/1
1	LLP	A	680	1	-	2/16/17/19	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	680	LLP	C3-C2	-5.61	1.35	1.41
1	A	680	LLP	C3-C2	-4.68	1.36	1.41
1	D	680	LLP	C4-C4'	3.43	1.53	1.46
1	A	680	LLP	C4-C5	-3.42	1.37	1.42
1	C	680	LLP	C3-C2	-3.30	1.37	1.41
1	C	680	LLP	C4-C4'	3.00	1.53	1.46
1	B	680	LLP	C4'-NZ	2.93	1.37	1.27
1	C	680	LLP	C4'-NZ	2.88	1.36	1.27
1	D	680	LLP	C4'-NZ	2.85	1.36	1.27
1	B	680	LLP	C4-C5	-2.83	1.38	1.42
1	B	680	LLP	C3-C2	-2.76	1.38	1.41
1	B	680	LLP	P-OP2	-2.46	1.45	1.54
1	A	680	LLP	P-OP3	-2.28	1.46	1.54
1	B	680	LLP	C2-N1	2.25	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	680	LLP	C2'-C2	-2.23	1.46	1.50
1	A	680	LLP	C4'-NZ	2.23	1.34	1.27
1	D	680	LLP	P-OP3	-2.07	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	680	LLP	OP4-C5'-C5	8.90	126.03	109.36
1	B	680	LLP	OP4-C5'-C5	5.13	118.98	109.36
1	D	680	LLP	OP4-C5'-C5	4.68	118.14	109.36
1	C	680	LLP	CD-CE-NZ	-3.23	102.28	110.83
1	A	680	LLP	CG-CD-CE	-2.55	104.49	113.38
1	A	680	LLP	CD-CE-NZ	-2.37	104.56	110.83
1	D	680	LLP	CG-CD-CE	-2.37	105.13	113.38
1	B	680	LLP	OP2-P-OP4	-2.10	101.19	106.67
1	A	680	LLP	C5-C6-N1	-2.07	120.47	123.83
1	A	680	LLP	OP2-P-OP4	-2.06	101.30	106.67
1	A	680	LLP	C5-C4-C4'	-2.03	118.33	121.47
1	B	680	LLP	OP3-P-OP2	2.01	115.33	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	C4-C5-C5'-OP4
1	D	680	LLP	C5'-OP4-P-OP1
1	D	680	LLP	C5'-OP4-P-OP2
1	D	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	CE-CD-CG-CB
1	B	680	LLP	C5'-OP4-P-OP2
1	D	680	LLP	C6-C5-C5'-OP4
1	D	680	LLP	CG-CD-CE-NZ
1	A	680	LLP	C4-C5-C5'-OP4
1	A	680	LLP	N-CA-CB-CG
1	D	680	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	680	LLP	2	0
1	D	680	LLP	4	0
1	C	680	LLP	2	0
1	A	680	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	902	-	4,4,4	0.29	0	6,6,6	0.67	0
2	SO4	A	901	-	4,4,4	0.58	0	6,6,6	0.37	0
2	SO4	D	902	-	4,4,4	0.45	0	6,6,6	0.30	0
2	SO4	B	901	-	4,4,4	0.69	0	6,6,6	0.25	0
2	SO4	C	901	-	4,4,4	0.40	0	6,6,6	0.32	0
2	SO4	D	901	-	4,4,4	0.61	0	6,6,6	0.52	0
2	SO4	C	900	-	4,4,4	0.63	0	6,6,6	0.33	0
2	SO4	B	902	-	4,4,4	0.28	0	6,6,6	0.51	0
2	SO4	D	900	-	4,4,4	0.54	0	6,6,6	0.41	0
2	SO4	B	900	-	4,4,4	0.35	0	6,6,6	0.52	0
2	SO4	A	900	-	4,4,4	0.31	0	6,6,6	0.47	0
2	SO4	A	902	-	4,4,4	0.53	0	6,6,6	0.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SO4	1	0
2	D	902	SO4	1	0
2	C	900	SO4	4	0
2	B	902	SO4	1	0
2	D	900	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	18:LEU	C	19:ALA	N	22.68
1	B	18:LEU	C	19:ALA	N	19.70

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.