



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:41 AM UTC

PDB ID : 6ROW / pdb_00006row
EMDB ID : EMD-4975
Title : Haemonchus galactose containing glycoprotein complex
Authors : Scarff, C.A.; Thompson, R.F.; Newlands, G.F.J.; Jamson, H.; Kennaway, C.;
da Silva, V.J.; Rabelo, E.M.; Song, C.F.; Trinick, J.; Smith, W.D.; Muench,
S.P.
Deposited on : 2019-05-13
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

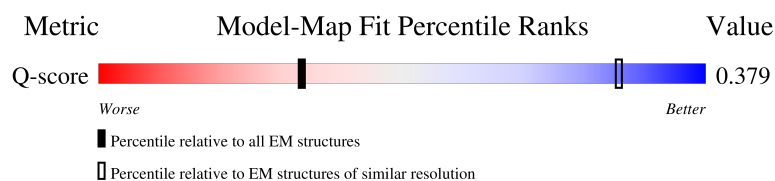
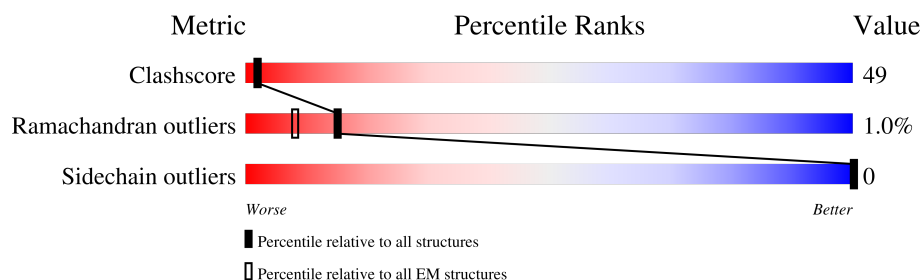
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

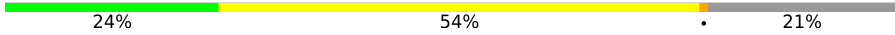
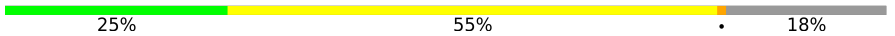
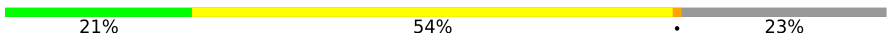
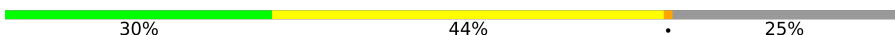
The reported resolution of this entry is 4.50 Å.

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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	755	
1	B	755	
1	C	755	
1	D	755	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	369	 56% 25% 19%
2	F	369	 59% 20% 21%
3	G	253	 63% . . 32%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43049 atoms, of which 20156 are hydrogens and 0 are deuteriums.

In the tables below, 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 Putative zinc metallopeptidase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	596	Total	C	H	N	O	S	0	0
			9475	3063	4638	824	919	31		
1	B	619	Total	C	H	N	O	S	0	0
			9828	3187	4817	845	946	33		
1	C	583	Total	C	H	N	O	S	0	0
			9290	3010	4556	801	893	30		
1	D	566	Total	C	H	N	O	S	0	0
			8988	2910	4413	777	860	28		

- Molecule 2 is a protein called Parasite pepsinogen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	299	Total	C	H	N	O	0	0
			2133	860	676	299	298		
2	F	293	Total	C	H	N	O	0	0
			2093	844	664	293	292		

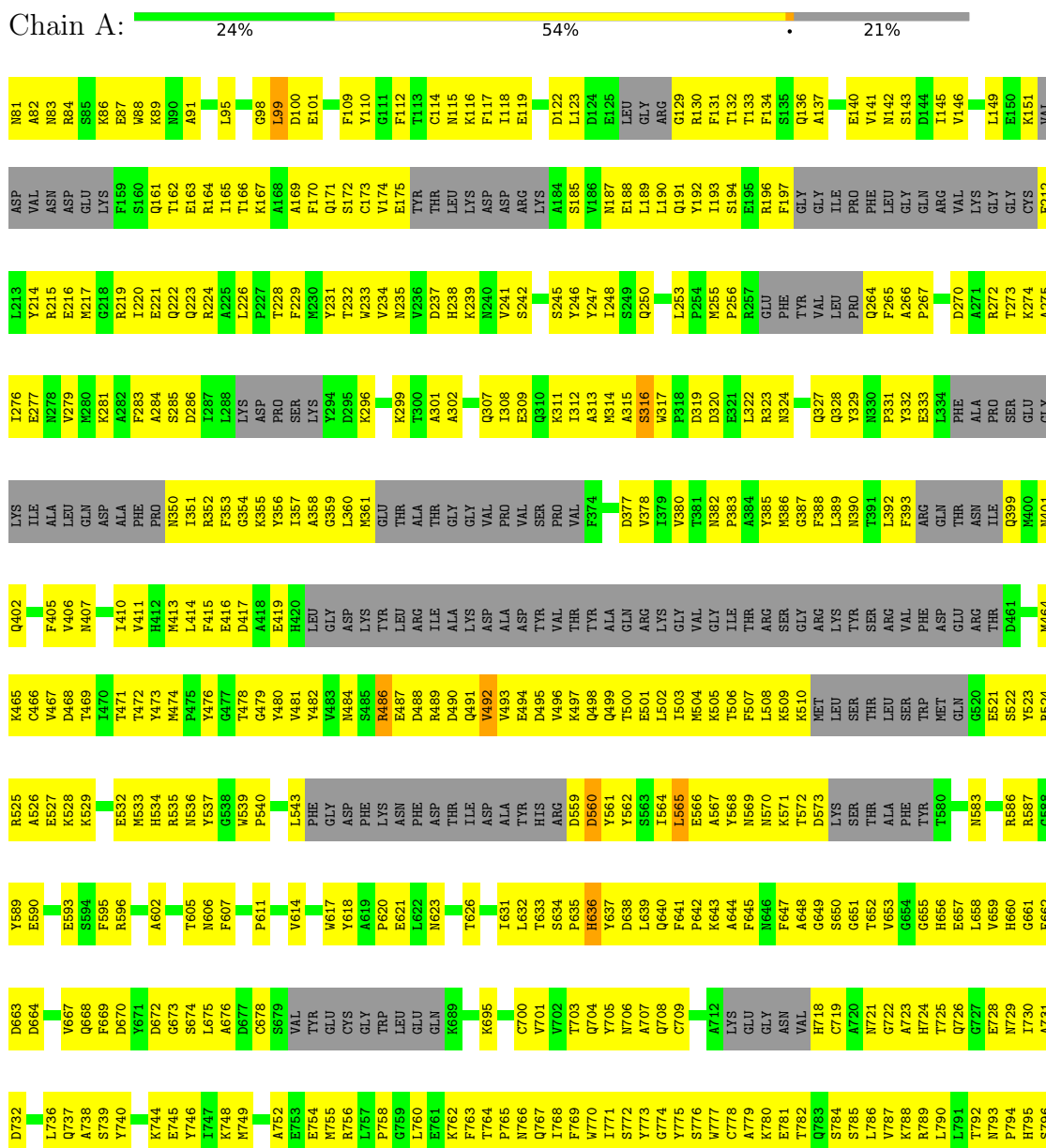
- Molecule 3 is a protein called Cysteine Protease.

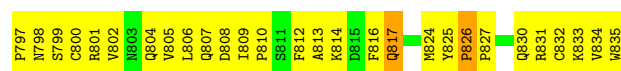
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	173	Total	C	H	N	O	0	0
			1242	504	392	173	173		

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

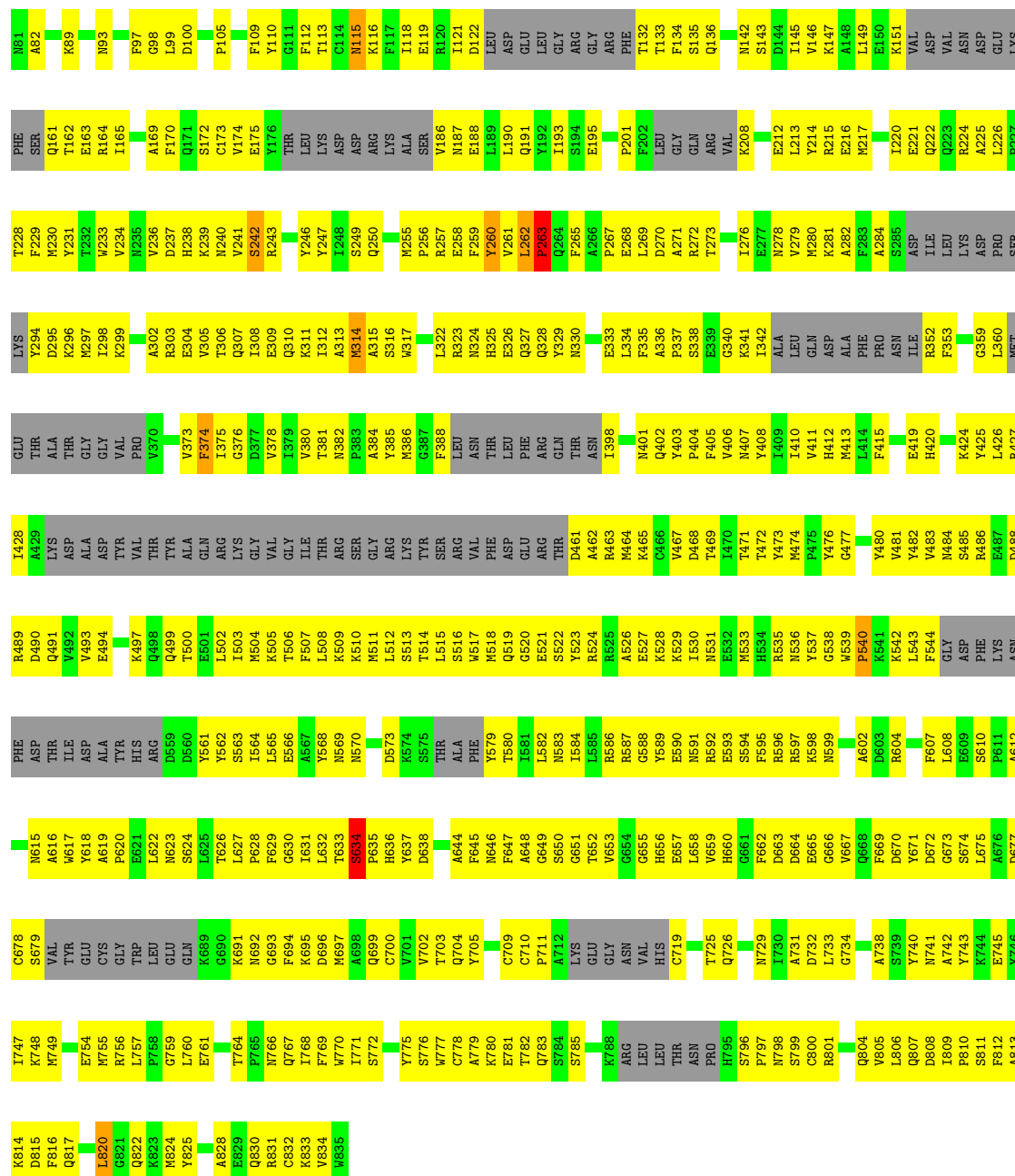
• Molecule 1: Putative zinc metallopeptidase





• Molecule 1: Putative zinc metalloproteinase

Chain B: 25% 55% 18%



• Molecule 1: Putative zinc metalloproteinase

Chain C: 21% 54% 23%



Q223	Q224	Q225	A226	A227	A228	A229	A230	A231	A232	A233	A234	A235	A236	A237	A238	A239	A240	A241	A242	A243	A244	A245	A246	A247	A248	A249	A250	A251	A252	A253	A254	A255	A256	A257	A258	A259	A260	A261	A262	A263	A264	A265	A266	A267	A268	A269	A270	A271	A272	A273	A274	A275	A276	A277	A278	A279	A280	A281	A282	A283	A284	A285	A286	A287	A288	A289	A290	A291	A292	A293	A294	A295	A296	A297	A298	A299	A300	A301	A302	A303	A304	A305	A306	A307	A308	A309	A310	A311	A312	A313	A314	A315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

T764	M697	T633	Y561	ASP	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
------	------	------	------	-----	-----	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

• Molecule 2: Parasite pepsinogen

Chain E:  56% 25% 19%

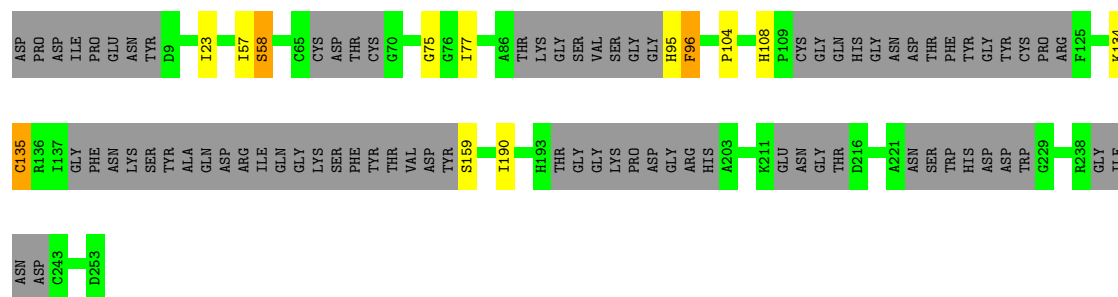
VAL	PHE	PRO	HIS	PRO	ILE	TYR	ASP	GLN	ASP	T770	L73	A74	K75	I76	T77	I78	GLY	ALA	PRO	G82	Q83	P85	L89	A94	N95	L96	N97	P99	N105	GLY	ARG	ARG	GLY	ALA	CYS	THR	THR	CYS	ASP	ARG	GLY	LEU	VAL	CYS	GLU	VAL	LEU	CYS	HIS
LYS	SER	CYS	GLU	ASP	ASP	VAL	ASN	ASN	PRO	ASP	GLU	ASN	P144	Y159	A160	G161	Y167	F168	E169	I170	Y171	Y172	G173	K178	G179	G182	N183	V186	R187	E191	G192	N193	V198	T202	V203	Q206	A207	V208	Q209	L223	A231	P238	R241	I242					
L245	P250	I251	F252	T253	Y254	Y255	G268	A269	A270	F271	Y273	Y287	V288	D289	E301	ALA	PHE	SER	ALA	GLY	TYR	LEU	SER	ILE	ARG	LYS	G313	I317	M325	G326	V327	V335	A336	D337	S338	Y339	G340	G341	Q342	Y343	D344	E345	M346	F347	I348	Y350	T351	I364	
E379	GLU	ASP	LYS	ASP	SER	CYS	MET	A388	M389	G398	P399	Q400	W401	I402	L403	C412	M413	I414	H415	D416	M417	M420	T421	I422	G423	E426	P427	G106	ARG	ARG	GLY	ALA	CYS	ARG	ILE	THR	THR	ASP	ARG	GLY	LEU	VAL	CYS	GLU	VAL	LEU	CYS	HIS	

• Molecule 2: Parasite pepsinogen

Chain F:  59% 20% 21%

VAL	PHE	PRO	HIS	PRO	PRO	ILE	TYR	ASP	GLN	ASP	T770	K775	I776	T777	I778	GLY	ALA	PRO	G82	Q83	S84	F85	H86	D90	T91	G92	S93	A94	N95	P99	D100	G106	ARG	ARG	GLY	ALA	CYS	ARG	ILE	THR	THR	ASP	ARG	GLY	LEU	VAL	CYS	GLU	VAL	LEU	CYS	HIS	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: Cysteine Protease



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	387.66003, 387.66003, 387.66003	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.88	0/4938	0.97	10/6653 (0.2%)
1	B	0.88	4/5122 (0.1%)	0.98	10/6903 (0.1%)
1	C	0.81	1/4835 (0.0%)	0.90	7/6513 (0.1%)
1	D	0.82	0/4674	1.04	11/6304 (0.2%)
2	E	0.31	0/1452	0.56	0/2003
2	F	0.47	0/1424	0.71	0/1965
3	G	1.20	0/841	1.88	9/1154 (0.8%)
All	All	0.82	5/23286 (0.0%)	0.99	47/31495 (0.1%)

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	5
1	B	0	4
1	C	0	6
1	D	0	1
All	All	0	16

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	PRO	N-CD	-13.90	1.28	1.47
1	C	816	PHE	CA-CB	-9.87	1.36	1.52
1	B	115	ASN	C-O	-9.64	1.12	1.24
1	B	540	PRO	N-CD	8.89	1.60	1.47
1	B	314	MET	CA-C	-6.36	1.38	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	96	PHE	N-CA-C	-11.46	93.68	110.64
3	G	58	SER	N-CA-C	-10.97	93.84	110.30
3	G	96	PHE	CB-CA-C	9.85	121.91	109.80
3	G	135	CYS	N-CA-C	-9.62	96.38	110.42
1	B	262	LEU	N-CA-C	9.37	130.52	109.81
3	G	58	SER	CB-CA-C	9.19	122.83	110.06
1	D	793	ASN	N-CA-C	7.84	115.04	108.07
3	G	135	CYS	CB-CA-C	7.52	120.16	109.71
3	G	159	SER	CA-C-N	7.25	124.81	120.24
3	G	159	SER	C-N-CA	7.25	124.81	120.24
1	A	636	HIS	N-CA-C	-7.00	105.67	114.56
1	B	472	THR	CA-C-N	-6.75	110.31	122.46
1	B	472	THR	C-N-CA	-6.75	110.31	122.46
1	B	644	ALA	N-CA-C	-6.46	104.24	111.28
1	C	261	VAL	N-CA-C	-6.46	104.61	113.00
1	A	316	SER	CA-C-N	-6.05	111.57	122.28
1	A	316	SER	C-N-CA	-6.05	111.57	122.28
1	A	129	GLY	N-CA-C	6.02	130.77	113.30
3	G	75	GLY	CA-C-O	-5.93	118.18	122.45
1	D	663	ASP	CA-C-N	5.93	129.71	120.82
1	D	663	ASP	C-N-CA	5.93	129.71	120.82
1	B	817	GLN	CA-C-N	-5.92	114.34	122.93
1	B	817	GLN	C-N-CA	-5.92	114.34	122.93
1	B	262	LEU	C-N-CD	-5.89	100.84	125.00
1	D	587	ARG	CB-CG-CD	5.82	124.69	111.30
1	C	147	LYS	CA-C-N	-5.77	111.50	121.66
1	C	147	LYS	C-N-CA	-5.77	111.50	121.66
1	A	99	LEU	N-CA-C	5.71	117.58	111.36
1	D	264	GLN	N-CA-C	5.71	115.06	108.49
1	B	256	PRO	CA-C-N	5.64	132.32	121.54
1	B	256	PRO	C-N-CA	5.64	132.32	121.54
1	A	565	LEU	CA-CB-CG	-5.48	97.13	116.30
1	A	99	LEU	CB-CA-C	-5.47	101.56	110.85
1	D	640	GLN	CA-C-N	-5.46	113.64	122.48
1	D	640	GLN	C-N-CA	-5.46	113.64	122.48
1	C	198	GLY	N-CA-C	5.43	117.05	111.56
1	B	260	TYR	N-CA-CB	-5.42	102.94	111.39
1	D	276	ILE	N-CA-C	-5.41	105.34	110.42
1	A	492	VAL	N-CA-C	-5.38	108.60	113.71
1	C	253	LEU	CA-CB-CG	-5.28	97.83	116.30
1	D	85	SER	CA-C-N	5.17	127.46	120.38
1	D	85	SER	C-N-CA	5.17	127.46	120.38
1	C	808	ASP	CA-C-N	-5.16	118.36	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	808	ASP	C-N-CA	-5.16	118.36	122.85
1	A	386	MET	CA-C-N	-5.11	111.39	121.41
1	A	386	MET	C-N-CA	-5.11	111.39	121.41
1	D	587	ARG	N-CA-CB	5.07	117.66	110.16

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	VAL	Peptide
1	A	486	ARG	Peptide
1	A	560	ASP	Peptide
1	A	676	ALA	Peptide
1	A	826	PRO	Peptide
1	B	242	SER	Peptide
1	B	634	SER	Peptide
1	B	820	LEU	Peptide
1	B	98	GLY	Peptide
1	C	200	ILE	Peptide
1	C	216	GLU	Peptide
1	C	294	TYR	Peptide
1	C	534	HIS	Peptide
1	C	571	LYS	Peptide
1	C	816	PHE	Peptide
1	D	634	SER	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	4837	4638	4636	544	0
1	B	5011	4817	4815	581	0
1	C	4734	4556	4555	507	0
1	D	4575	4413	4413	404	0
2	E	1457	676	676	63	0
2	F	1429	664	663	42	0
3	G	850	392	389	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22893	20156	20147	2127	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 49.

All (2127) 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:B:540:PRO:HA	1:B:607:PHE:CZ	1.47	1.48
1:A:239:LYS:HD3	1:A:329:TYR:CE2	1.64	1.33
1:A:234:VAL:HG23	1:A:245:SER:O	1.20	1.29
1:D:760:LEU:HD11	1:D:763:PHE:CE2	1.67	1.29
1:A:474:MET:CE	1:A:586:ARG:HD2	1.64	1.27
1:A:237:ASP:OD1	1:A:245:SER:HB3	1.31	1.26
1:A:237:ASP:OD1	1:A:245:SER:CB	1.85	1.23
1:A:277:GLU:OE2	1:A:302:ALA:HB1	1.37	1.20
1:A:561:TYR:O	1:A:564:ILE:HG12	1.37	1.18
1:A:569:ASN:HB2	1:A:589:TYR:CE1	1.80	1.16
1:B:812:PHE:HE2	1:B:824:MET:SD	1.70	1.15
1:A:474:MET:HE1	1:A:586:ARG:HD2	1.16	1.12
1:A:98:GLY:HA2	1:A:116:LYS:HB2	1.25	1.11
1:A:242:SER:O	1:A:602:ALA:HB2	1.50	1.10
1:A:709:CYS:SG	1:A:719:CYS:HA	1.91	1.10
1:D:101:GLU:CD	1:D:762:LYS:HZ3	1.58	1.09
1:B:812:PHE:CE2	1:B:824:MET:SD	2.46	1.09
1:B:540:PRO:CA	1:B:607:PHE:CZ	2.37	1.08
1:A:277:GLU:HG3	1:A:302:ALA:HB2	1.32	1.07
1:A:402:GLN:O	1:A:406:VAL:HG22	1.52	1.07
1:B:809:ILE:HG22	1:B:811:SER:OG	1.55	1.07
1:B:796:SER:OG	1:B:797:PRO:HD2	1.54	1.06
1:D:97:PHE:O	1:D:116:LYS:HG2	1.55	1.06
1:B:579:TYR:HA	1:B:582:LEU:HD12	1.39	1.05
1:A:253:LEU:CD1	1:A:255:MET:O	2.04	1.04
1:D:757:LEU:HD11	1:D:760:LEU:HB3	1.37	1.04
1:A:569:ASN:HB2	1:A:589:TYR:HE1	0.90	1.03
1:B:109:PHE:CE2	1:B:806:LEU:HD22	1.94	1.03
1:A:118:ILE:HG12	1:A:780:LYS:HB2	1.37	1.02
1:B:109:PHE:CE2	1:B:806:LEU:CD2	2.42	1.02
1:B:709:CYS:SG	1:B:719:CYS:N	2.33	1.00
2:E:182:GLY:O	2:E:203:VAL:HA	1.61	1.00
1:D:160:SER:HB2	1:D:163:GLU:OE1	1.59	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLN:HE22	1:A:314:MET:HE1	1.22	0.99
1:A:570:ASN:O	1:A:571:LYS:HG3	1.62	0.99
1:B:255:MET:HB3	1:B:260:TYR:OH	1.60	0.99
1:A:561:TYR:O	1:A:564:ILE:CG1	2.09	0.99
1:A:239:LYS:CD	1:A:329:TYR:CE2	2.45	0.98
1:A:253:LEU:HD12	1:A:255:MET:O	1.62	0.97
1:A:234:VAL:CG2	1:A:245:SER:O	2.11	0.97
1:C:592:ARG:HA	1:C:595:PHE:CE2	2.00	0.97
1:A:238:HIS:NE2	1:A:621:GLU:OE2	1.97	0.97
1:B:561:TYR:O	1:B:564:ILE:HG22	1.65	0.96
1:D:760:LEU:HD11	1:D:763:PHE:HE2	0.83	0.96
1:A:98:GLY:HA2	1:A:116:LYS:CB	1.95	0.95
1:A:569:ASN:CB	1:A:589:TYR:HE1	1.79	0.95
1:C:108:ASP:HB2	1:C:110:TYR:CE2	2.01	0.95
1:B:637:TYR:O	1:B:638:ASP:OD1	1.85	0.94
1:C:95:LEU:HD11	1:C:771:ILE:CG2	1.97	0.94
1:B:217:MET:HE2	1:B:230:MET:HE3	1.49	0.93
1:B:142:ASN:O	1:B:145:ILE:HG22	1.65	0.93
1:B:809:ILE:HG22	1:B:811:SER:HG	1.30	0.93
1:B:540:PRO:HA	1:B:607:PHE:HZ	1.34	0.92
1:C:798:ASN:O	1:C:801:ARG:N	2.03	0.91
1:B:810:PRO:HD2	1:B:831:ARG:HH11	1.33	0.91
1:B:109:PHE:CD2	1:B:806:LEU:HD23	2.05	0.91
1:A:474:MET:HE3	1:A:586:ARG:HD2	1.53	0.91
1:A:277:GLU:OE2	1:A:302:ALA:CB	2.18	0.90
1:C:95:LEU:HD11	1:C:771:ILE:HG21	1.52	0.90
1:B:230:MET:HA	1:B:249:SER:O	1.70	0.90
1:C:103:VAL:CG1	1:C:108:ASP:OD1	2.20	0.90
1:C:583:ASN:ND2	1:C:587:ARG:HH12	1.71	0.89
1:A:238:HIS:CE1	1:A:621:GLU:OE2	2.26	0.89
1:B:380:VAL:CG1	1:B:385:TYR:HE2	1.86	0.89
1:C:331:PRO:HA	1:C:379:ILE:HG12	1.54	0.89
1:A:250:GLN:OE1	1:A:317:TRP:N	2.06	0.88
1:A:719:CYS:O	1:A:790:LEU:HD21	1.72	0.88
1:B:109:PHE:CD2	1:B:806:LEU:CD2	2.57	0.88
1:C:793:ASN:ND2	1:C:795:HIS:CE1	2.41	0.88
1:D:145:ILE:HD13	1:D:478:THR:HG23	1.56	0.87
1:C:243:ARG:HH22	1:C:376:GLY:HA2	1.39	0.87
1:A:242:SER:O	1:A:602:ALA:CB	2.23	0.86
1:A:277:GLU:CG	1:A:302:ALA:HB2	2.03	0.86
1:C:823:LYS:O	1:C:824:MET:HG2	1.74	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HD3	1:A:329:TYR:HE2	1.34	0.86
1:B:262:LEU:CB	1:B:263:PRO:HD3	2.06	0.85
1:C:583:ASN:ND2	1:C:587:ARG:NH1	2.24	0.85
1:A:232:THR:OG1	1:A:247:TYR:O	1.94	0.85
1:C:114:CYS:HG	1:C:778:CYS:HG	0.94	0.85
1:A:501:GLU:HA	1:A:504:MET:HE2	1.59	0.85
1:A:709:CYS:HG	1:A:719:CYS:HG	1.19	0.85
1:A:273:THR:O	1:A:277:GLU:OE1	1.94	0.84
1:B:217:MET:HE2	1:B:230:MET:CE	2.06	0.84
1:B:670:ASP:OD1	1:B:673:GLY:N	2.09	0.84
1:C:232:THR:HG22	1:C:248:ILE:HA	1.60	0.84
1:A:536:ASN:HB3	1:A:626:THR:HG22	1.59	0.84
1:A:357:ILE:HG22	1:A:361:MET:HE1	1.59	0.83
1:B:743:TYR:CE1	1:B:747:ILE:HD13	2.12	0.83
1:B:262:LEU:HB3	1:B:263:PRO:HD3	1.59	0.83
1:D:631:ILE:O	1:D:633:THR:HG22	1.79	0.83
1:A:474:MET:CE	1:A:586:ARG:CD	2.54	0.83
1:D:404:PRO:O	1:D:407:ASN:ND2	2.10	0.83
1:B:540:PRO:HB3	1:B:607:PHE:CE2	2.14	0.83
1:A:782:THR:HB	1:A:785:SER:HB3	1.60	0.82
1:B:540:PRO:CB	1:B:607:PHE:CE2	2.62	0.82
1:A:807:GLN:N	1:A:824:MET:HE1	1.94	0.82
1:D:101:GLU:CD	1:D:762:LYS:NZ	2.37	0.82
1:D:760:LEU:CD1	1:D:763:PHE:HE2	1.80	0.82
1:A:569:ASN:CB	1:A:589:TYR:CE1	2.58	0.82
1:D:382:ASN:O	1:D:386:MET:HG2	1.80	0.82
1:B:214:TYR:O	1:B:217:MET:N	2.12	0.82
1:A:98:GLY:CA	1:A:116:LYS:HB2	2.10	0.82
1:C:643:LYS:NZ	1:C:746:TYR:OH	2.13	0.82
1:C:304:GLU:OE2	1:C:407:ASN:ND2	2.13	0.81
1:B:226:LEU:HD23	1:B:226:LEU:O	1.81	0.81
1:C:719:CYS:SG	1:C:720:ALA:N	2.52	0.81
1:B:169:ALA:O	1:B:172:SER:OG	1.99	0.81
1:C:109:PHE:HB2	1:C:824:MET:CE	2.10	0.81
1:B:208:LYS:N	1:B:403:TYR:HH	1.79	0.81
1:A:253:LEU:HD12	1:A:253:LEU:C	2.06	0.81
1:D:101:GLU:HG2	1:D:762:LYS:HZ1	1.45	0.80
1:C:569:ASN:HB3	1:C:589:TYR:HE1	1.44	0.80
1:B:608:LEU:HD11	1:B:619:ALA:HB2	1.62	0.80
1:A:264:GLN:NE2	1:A:314:MET:HE1	1.96	0.80
1:B:705:TYR:CE2	1:B:729:ASN:CG	2.59	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASP:OD2	1:C:298:ILE:HG12	1.82	0.80
1:A:237:ASP:OD1	1:A:245:SER:HB2	1.80	0.80
1:C:317:TRP:CE3	1:C:382:ASN:OD1	2.35	0.80
1:D:145:ILE:CD1	1:D:478:THR:HG23	2.11	0.80
1:D:637:TYR:CG	1:D:646:ASN:OD1	2.35	0.80
1:B:622:LEU:HD12	1:B:623:ASN:N	1.97	0.80
1:B:796:SER:OG	1:B:797:PRO:CD	2.30	0.80
1:C:821:GLY:O	1:C:822:GLN:HG3	1.82	0.80
1:A:709:CYS:SG	1:A:719:CYS:CA	2.71	0.79
1:B:398:ILE:HG22	1:B:402:GLN:HG3	1.61	0.79
1:A:238:HIS:NE2	1:A:621:GLU:CG	2.45	0.79
1:A:469:THR:O	1:A:472:THR:OG1	2.00	0.79
1:A:234:VAL:HG22	1:A:235:ASN:N	1.96	0.79
1:A:301:ALA:HB1	1:A:407:ASN:HD21	1.47	0.79
1:B:588:GLY:HA3	1:B:592:ARG:HH21	1.45	0.79
1:C:764:THR:HB	1:C:765:PRO:HD2	1.64	0.79
1:A:764:THR:CG2	1:A:765:PRO:HD2	2.12	0.79
1:C:174:VAL:HG23	1:C:463:ARG:HG2	1.65	0.79
1:A:87:GLU:OE1	1:A:640:GLN:CB	2.31	0.79
1:A:196:ARG:HH12	1:A:219:ARG:HE	1.32	0.79
1:C:177:THR:O	1:C:181:ASP:N	2.13	0.79
1:B:246:TYR:HB2	1:B:378:VAL:HG13	1.65	0.78
1:B:342:ILE:O	1:B:352:ARG:NH1	2.16	0.78
1:D:719:CYS:SG	1:D:787:VAL:HG23	2.22	0.78
1:D:309:GLU:O	1:D:312:ILE:N	2.17	0.78
1:B:489:ARG:HG3	1:B:490:ASP:H	1.49	0.78
1:A:253:LEU:HD11	1:A:255:MET:O	1.81	0.78
1:C:161:GLN:HB2	1:C:564:ILE:HD13	1.65	0.78
1:C:467:VAL:HA	1:C:470:ILE:HD12	1.64	0.78
1:A:277:GLU:CD	1:A:302:ALA:HB1	2.09	0.78
1:A:507:PHE:CZ	1:A:659:VAL:HG12	2.18	0.78
1:C:482:TYR:O	1:C:485:SER:OG	2.01	0.78
1:A:718:HIS:O	1:A:719:CYS:SG	2.42	0.78
1:B:105:PRO:HA	1:B:112:PHE:CD1	2.19	0.78
1:B:583:ASN:HD21	1:B:587:ARG:HH21	1.28	0.78
1:D:760:LEU:CD1	1:D:763:PHE:CE2	2.60	0.78
1:B:579:TYR:HA	1:B:582:LEU:CD1	2.13	0.77
1:B:512:LEU:HB2	1:B:523:TYR:HB2	1.65	0.77
1:C:515:LEU:HD22	1:C:518:MET:HG3	1.67	0.77
2:E:78:ILE:HA	2:E:186:VAL:HA	1.66	0.77
1:A:721:ASN:OD1	1:A:722:GLY:N	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:GLN:NE2	1:B:521:GLU:OE1	2.18	0.77
1:C:257:ARG:HH12	1:C:313:ALA:HB1	1.50	0.77
1:B:594:SER:HA	1:B:597:ARG:CZ	2.15	0.77
1:D:393:PHE:CE1	1:D:405:PHE:CE2	2.73	0.77
1:D:393:PHE:CD1	1:D:405:PHE:CE2	2.72	0.77
1:A:732:ASP:OD2	1:A:801:ARG:NH2	2.16	0.77
1:B:341:LYS:HE2	1:B:353:PHE:HE2	1.49	0.77
1:B:533:MET:HE1	1:B:658:LEU:CD1	2.15	0.77
1:C:793:ASN:ND2	1:C:795:HIS:HE1	1.82	0.77
1:A:606:ASN:OD1	1:A:607:PHE:N	2.17	0.77
1:B:511:MET:N	1:B:514:THR:OG1	2.18	0.77
1:B:474:MET:SD	1:B:570:ASN:ND2	2.57	0.76
1:B:533:MET:HE1	1:B:658:LEU:HD11	1.66	0.76
1:C:583:ASN:HD21	1:C:587:ARG:NH1	1.82	0.76
2:F:252:PHE:HA	2:F:274:GLY:H	1.51	0.76
1:B:705:TYR:HE2	1:B:729:ASN:CG	1.93	0.76
1:A:385:TYR:O	1:A:388:PHE:N	2.18	0.76
1:D:380:VAL:CG1	1:D:386:MET:HG3	2.15	0.76
1:A:169:ALA:O	1:A:172:SER:OG	2.02	0.76
1:C:583:ASN:HD21	1:C:587:ARG:HH12	1.34	0.76
1:D:764:THR:OG1	1:D:767:GLN:HG2	1.85	0.76
1:C:280:MET:O	1:C:284:ALA:N	2.14	0.76
1:C:579:TYR:O	1:C:583:ASN:N	2.16	0.76
1:B:237:ASP:OD2	1:B:240:ASN:N	2.19	0.76
1:B:306:THR:O	1:B:309:GLU:N	2.18	0.76
1:B:323:ARG:NH1	1:B:665:GLU:OE2	2.19	0.76
1:B:483:VAL:HG22	1:B:629:PHE:CD2	2.21	0.76
1:B:579:TYR:CA	1:B:582:LEU:HD12	2.16	0.76
1:B:743:TYR:CZ	1:B:747:ILE:HG21	2.21	0.76
1:A:264:GLN:HE22	1:A:314:MET:CE	1.99	0.76
1:A:764:THR:HG22	1:A:765:PRO:N	2.01	0.76
1:B:424:LYS:HA	1:B:427:ARG:HH21	1.51	0.76
1:B:407:ASN:O	1:B:410:ILE:HG22	1.85	0.76
1:D:88:TRP:CE3	1:D:642:PRO:HG3	2.21	0.76
1:C:238:HIS:ND1	1:C:247:TYR:OH	2.18	0.75
1:A:656:HIS:ND1	1:A:732:ASP:OD1	2.19	0.75
1:A:825:TYR:HB3	1:A:827:PRO:HD2	1.67	0.75
1:C:238:HIS:HD1	1:C:247:TYR:HH	1.34	0.75
1:C:643:LYS:HD3	1:C:646:ASN:HD21	1.51	0.75
2:E:193:ASN:N	2:E:273:TYR:O	2.16	0.75
1:B:236:VAL:HG13	1:B:241:VAL:CG2	2.15	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASN:O	1:A:327:GLN:N	2.19	0.75
1:D:109:PHE:CE2	1:D:806:LEU:HD12	2.21	0.75
1:C:793:ASN:HD22	1:C:795:HIS:CE1	2.03	0.75
1:C:193:ILE:HG23	1:C:197:PHE:HE2	1.51	0.75
1:D:757:LEU:CD1	1:D:760:LEU:HB3	2.14	0.75
1:D:480:TYR:HB2	1:D:543:LEU:HD21	1.68	0.75
1:A:222:GLN:NE2	1:A:360:LEU:O	2.19	0.75
1:A:724:HIS:CE1	1:A:794:PRO:HA	2.22	0.75
1:C:218:GLY:HA3	1:C:356:TYR:HE1	1.51	0.75
1:A:267:PRO:O	1:A:270:ASP:N	2.20	0.74
1:A:827:PRO:O	1:A:830:GLN:NE2	2.20	0.74
1:B:259:PHE:CE1	1:B:263:PRO:HD2	2.22	0.74
1:B:518:MET:HG2	1:B:519:GLN:H	1.51	0.74
1:B:540:PRO:HA	1:B:607:PHE:CE1	2.20	0.74
1:A:226:LEU:HD13	1:A:416:GLU:OE2	1.87	0.74
1:A:327:GLN:O	1:A:329:TYR:N	2.18	0.74
1:A:494:GLU:O	1:A:498:GLN:N	2.20	0.74
1:B:491:GLN:O	1:B:494:GLU:HG2	1.86	0.74
1:C:810:PRO:O	1:C:813:ALA:N	2.15	0.74
1:B:236:VAL:HG13	1:B:241:VAL:HG23	1.67	0.74
1:C:179:LYS:NZ	1:C:462:ALA:O	2.20	0.74
1:A:748:LYS:HB3	1:A:749:MET:HE2	1.70	0.74
1:A:253:LEU:HD12	1:A:253:LEU:O	1.87	0.74
1:D:309:GLU:O	1:D:312:ILE:HG22	1.87	0.74
1:B:419:GLU:HA	1:B:426:LEU:HG	1.68	0.74
1:C:721:ASN:OD1	1:C:722:GLY:N	2.21	0.74
1:A:130:ARG:HG2	1:A:781:GLU:CB	2.17	0.74
1:B:420:HIS:CE1	1:B:580:THR:HA	2.22	0.74
1:C:229:PHE:O	1:C:230:MET:HG3	1.87	0.74
1:C:114:CYS:HG	1:C:778:CYS:CB	2.01	0.73
1:C:272:ARG:NH2	1:C:309:GLU:OE2	2.19	0.73
1:C:517:TRP:HE1	1:C:518:MET:HE2	1.53	0.73
1:D:162:THR:HA	1:D:165:ILE:HD12	1.71	0.73
1:A:634:SER:HB3	1:A:635:PRO:HD2	1.69	0.73
1:A:764:THR:HG22	1:A:765:PRO:CD	2.18	0.73
1:C:103:VAL:HG12	1:C:108:ASP:OD1	1.87	0.73
1:C:592:ARG:HA	1:C:595:PHE:HE2	1.50	0.73
1:D:100:ASP:O	1:D:112:PHE:CD1	2.41	0.73
1:B:594:SER:HA	1:B:597:ARG:NE	2.03	0.73
1:C:134:PHE:O	1:C:138:GLN:N	2.17	0.73
2:E:288:VAL:O	2:E:422:ILE:N	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:THR:N	1:A:767:GLN:OE1	2.22	0.73
1:B:237:ASP:OD1	1:B:238:HIS:N	2.21	0.73
1:B:489:ARG:HG3	1:B:490:ASP:N	2.00	0.73
1:C:319:ASP:HA	1:C:322:LEU:HD12	1.68	0.73
1:D:258:GLU:HG2	1:D:258:GLU:O	1.89	0.73
1:A:491:GLN:HG2	1:A:492:VAL:HG13	1.69	0.73
1:B:622:LEU:CD1	1:B:624:SER:OG	2.37	0.73
1:C:333:GLU:O	1:C:335:PHE:N	2.22	0.73
1:A:134:PHE:HE1	1:A:636:HIS:CE1	2.07	0.72
1:C:571:LYS:NZ	1:C:572:THR:O	2.22	0.72
1:C:614:VAL:HG13	1:C:614:VAL:O	1.86	0.72
1:B:217:MET:HE2	1:B:230:MET:SD	2.28	0.72
1:B:536:ASN:HB2	1:B:626:THR:HG22	1.70	0.72
1:A:281:LYS:O	1:A:284:ALA:N	2.22	0.72
1:C:215:ARG:O	1:C:219:ARG:NE	2.22	0.72
1:D:820:LEU:HA	1:D:825:TYR:HD2	1.53	0.72
1:A:495:ASP:OD2	1:A:637:TYR:OH	2.08	0.72
1:A:709:CYS:HG	1:A:719:CYS:CB	2.03	0.72
1:C:767:GLN:OE1	1:C:767:GLN:N	2.23	0.72
1:A:507:PHE:CE2	1:A:659:VAL:HG12	2.23	0.72
1:B:634:SER:O	1:B:636:HIS:N	2.23	0.72
1:C:705:TYR:O	1:C:708:GLN:N	2.21	0.72
1:A:789:ARG:HB3	1:A:793:ASN:OD1	1.90	0.72
1:B:743:TYR:O	1:B:747:ILE:HG12	1.90	0.72
1:D:133:THR:O	1:D:136:GLN:HB3	1.89	0.72
1:D:757:LEU:O	1:D:757:LEU:HD12	1.89	0.72
1:B:544:PHE:CD2	1:B:544:PHE:O	2.43	0.72
1:C:256:PRO:HB3	1:C:792:THR:HG22	1.72	0.71
1:C:100:ASP:OD1	1:C:101:GLU:N	2.24	0.71
1:C:582:LEU:O	1:C:586:ARG:HG3	1.89	0.71
1:D:480:TYR:HD2	1:D:543:LEU:HG	1.56	0.71
1:C:109:PHE:HB2	1:C:824:MET:HE1	1.72	0.71
2:E:183:ASN:HA	2:E:202:THR:O	1.88	0.71
2:F:75:LYS:HA	2:F:85:PHE:O	1.90	0.71
2:F:288:VAL:O	2:F:422:ILE:N	2.23	0.71
1:A:162:THR:O	1:A:165:ILE:N	2.22	0.71
1:A:722:GLY:O	1:A:725:THR:OG1	2.07	0.71
1:B:325:HIS:HA	1:B:328:GLN:HG2	1.72	0.71
1:A:130:ARG:HG2	1:A:781:GLU:HB2	1.72	0.71
1:A:764:THR:HG22	1:A:765:PRO:HD2	1.73	0.71
1:D:101:GLU:HG2	1:D:762:LYS:NZ	2.06	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ILE:O	2:F:207:ALA:N	2.17	0.71
1:B:99:LEU:O	1:B:116:LYS:HG2	1.91	0.71
1:B:172:SER:O	1:B:175:GLU:N	2.24	0.71
1:D:380:VAL:HG11	1:D:386:MET:HG3	1.73	0.71
1:D:670:ASP:O	1:D:673:GLY:N	2.20	0.71
1:A:533:MET:HA	1:A:623:ASN:ND2	2.06	0.70
1:B:100:ASP:O	1:B:100:ASP:OD1	2.09	0.70
1:C:311:LYS:O	1:C:314:MET:N	2.24	0.70
1:B:812:PHE:CZ	1:B:824:MET:SD	2.84	0.70
1:D:163:GLU:HG3	1:D:481:VAL:HG22	1.73	0.70
1:D:100:ASP:O	1:D:112:PHE:CE1	2.44	0.70
2:E:344:ASP:N	2:E:349:ILE:O	2.24	0.70
1:A:506:THR:O	1:A:510:LYS:N	2.24	0.70
1:C:386:MET:HE3	1:D:391:THR:CG2	2.21	0.70
1:D:620:PRO:HB2	1:D:669:PHE:HD2	1.57	0.70
1:D:705:TYR:CZ	1:D:800:CYS:SG	2.84	0.70
2:E:412:CYS:H	2:E:426:GLU:HA	1.55	0.70
2:E:169:GLU:HA	2:E:178:LYS:HA	1.72	0.70
1:A:277:GLU:CG	1:A:302:ALA:CB	2.69	0.70
1:C:525:ARG:HD3	1:C:691:LYS:HZ1	1.56	0.70
1:C:566:GLU:OE2	1:C:596:ARG:NH2	2.25	0.70
1:D:489:ARG:O	1:D:492:VAL:HG12	1.91	0.70
1:A:175:GLU:N	1:A:175:GLU:OE2	2.24	0.70
1:B:308:ILE:O	1:B:311:LYS:N	2.25	0.69
1:A:583:ASN:OD1	1:A:586:ARG:NH2	2.25	0.69
1:B:481:VAL:O	1:B:485:SER:OG	2.10	0.69
1:D:101:GLU:CG	1:D:762:LYS:NZ	2.55	0.69
1:D:226:LEU:HD13	1:D:413:MET:HA	1.74	0.69
1:B:380:VAL:HG11	1:B:385:TYR:HE2	1.57	0.69
1:D:83:ASN:OD1	1:D:84:ARG:N	2.25	0.69
1:D:480:TYR:HB2	1:D:543:LEU:HD11	1.74	0.69
1:B:610:SER:O	1:B:612:ALA:N	2.25	0.69
1:C:162:THR:HB	1:C:564:ILE:HG12	1.74	0.69
1:A:634:SER:O	1:A:636:HIS:N	2.24	0.69
1:D:393:PHE:CD1	1:D:405:PHE:HE2	2.10	0.69
1:D:638:ASP:HB3	1:D:641:PHE:CZ	2.27	0.69
1:A:226:LEU:HD13	1:A:416:GLU:CD	2.18	0.69
1:B:250:GLN:OE1	1:B:250:GLN:N	2.22	0.69
1:B:636:HIS:O	1:B:650:SER:N	2.21	0.69
1:B:147:LYS:O	1:B:151:LYS:NZ	2.26	0.69
1:D:122:ASP:OD1	1:D:123:LEU:N	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:GLN:CA	1:A:824:MET:HE1	2.23	0.69
1:B:402:GLN:O	1:B:405:PHE:HD2	1.76	0.69
1:D:334:LEU:HD23	1:D:334:LEU:O	1.92	0.69
1:D:109:PHE:CD2	1:D:806:LEU:HD12	2.27	0.68
1:A:232:THR:HG23	1:A:232:THR:O	1.93	0.68
1:A:648:ALA:O	1:A:652:THR:OG1	2.10	0.68
1:D:352:ARG:O	1:D:356:TYR:N	2.25	0.68
1:A:231:TYR:OH	1:A:233:TRP:NE1	2.26	0.68
1:A:765:PRO:O	1:A:768:ILE:N	2.26	0.68
1:B:481:VAL:O	1:B:485:SER:CB	2.41	0.68
1:B:561:TYR:O	1:B:564:ILE:N	2.27	0.68
1:A:212:GLU:OE1	1:A:215:ARG:NH2	2.22	0.68
1:B:239:LYS:O	1:B:240:ASN:OD1	2.10	0.68
1:A:130:ARG:NH1	1:A:793:ASN:OD1	2.27	0.68
1:B:480:TYR:HB2	1:B:543:LEU:HD11	1.75	0.68
1:C:775:TYR:HA	1:C:778:CYS:SG	2.34	0.68
1:B:489:ARG:CG	1:B:490:ASP:H	2.07	0.68
1:B:511:MET:HG3	1:B:513:SER:H	1.58	0.68
1:B:511:MET:O	1:B:514:THR:OG1	2.09	0.68
1:B:808:ASP:O	1:B:831:ARG:NH1	2.27	0.68
1:B:334:LEU:HD12	1:B:335:PHE:N	2.09	0.67
1:C:109:PHE:HB2	1:C:824:MET:HE2	1.76	0.67
1:B:186:VAL:HG23	1:B:187:ASN:H	1.59	0.67
1:D:241:VAL:HG11	1:D:672:ASP:O	1.92	0.67
1:B:631:ILE:O	1:B:633:THR:N	2.27	0.67
1:D:268:GLU:O	1:D:271:ALA:N	2.24	0.67
1:A:86:LYS:O	1:A:89:LYS:N	2.27	0.67
1:C:663:ASP:CG	1:C:730:ILE:HD11	2.20	0.67
1:D:160:SER:CB	1:D:163:GLU:OE1	2.38	0.67
1:D:645:PHE:O	1:D:648:ALA:N	2.28	0.67
1:C:230:MET:CE	1:C:356:TYR:CE2	2.78	0.67
1:C:386:MET:HE3	1:D:391:THR:HG21	1.77	0.67
1:C:409:ILE:H	1:C:409:ILE:HD12	1.58	0.67
2:F:406:PRO:O	2:F:410:GLN:N	2.26	0.67
1:A:277:GLU:HG3	1:A:302:ALA:CB	2.18	0.67
1:B:540:PRO:HA	1:B:607:PHE:CE2	2.23	0.67
1:B:759:GLY:O	1:B:760:LEU:HG	1.94	0.67
1:A:474:MET:HE3	1:A:586:ARG:CD	2.20	0.67
1:B:757:LEU:CD1	1:B:768:ILE:HD13	2.24	0.67
1:D:595:PHE:O	1:D:598:LYS:HG2	1.95	0.67
2:F:90:ASP:N	2:F:223:LEU:O	2.19	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:N	1:B:151:LYS:HD2	2.10	0.66
1:B:691:LYS:O	1:B:694:PHE:N	2.28	0.66
2:E:78:ILE:O	2:E:83:GLN:N	2.27	0.66
1:A:285:SER:OG	1:A:286:ASP:OD1	2.12	0.66
1:B:764:THR:OG1	1:B:767:GLN:N	2.23	0.66
1:C:330:ASN:ND2	1:C:381:THR:O	2.28	0.66
1:C:535:ARG:HB3	1:C:537:TYR:OH	1.95	0.66
2:E:301:GLU:H	2:E:364:ILE:HA	1.59	0.66
1:A:323:ARG:NH1	1:A:664:ASP:OD1	2.28	0.66
1:A:101:GLU:OE1	1:A:112:PHE:CE1	2.49	0.66
1:A:238:HIS:CD2	1:A:621:GLU:HG2	2.30	0.66
1:A:419:GLU:OE1	1:A:419:GLU:N	2.28	0.66
1:A:491:GLN:HB2	1:A:639:LEU:HD13	1.76	0.66
2:E:98:ILE:O	2:E:207:ALA:N	2.25	0.66
1:A:471:THR:HA	1:A:478:THR:HG21	1.77	0.66
1:C:257:ARG:NH1	1:C:257:ARG:O	2.29	0.66
1:B:267:PRO:O	1:B:270:ASP:N	2.26	0.66
1:B:508:LEU:O	1:B:511:MET:HB3	1.96	0.66
1:C:151:LYS:O	1:C:167:LYS:NZ	2.27	0.66
1:C:181:ASP:OD1	1:C:182:ARG:N	2.28	0.66
1:B:583:ASN:HD21	1:B:587:ARG:NH2	1.92	0.66
1:D:483:VAL:HG22	1:D:629:PHE:CD2	2.30	0.66
1:A:238:HIS:NE2	1:A:621:GLU:CD	2.54	0.66
1:A:387:GLY:O	1:A:390:ASN:N	2.29	0.66
1:A:472:THR:OG1	1:A:473:TYR:CD2	2.49	0.66
1:C:736:LEU:O	1:C:739:SER:OG	2.08	0.66
1:A:772:SER:O	1:A:775:TYR:N	2.29	0.66
1:C:224:ARG:NH2	1:C:416:GLU:OE1	2.29	0.66
1:D:163:GLU:HG3	1:D:481:VAL:CG2	2.26	0.66
1:A:559:ASP:OD1	1:A:560:ASP:N	2.29	0.65
1:B:278:ASN:OD1	1:B:279:VAL:HG23	1.96	0.65
1:B:583:ASN:OD1	1:B:587:ARG:NE	2.28	0.65
1:A:87:GLU:OE1	1:A:640:GLN:HB2	1.95	0.65
1:A:234:VAL:HG12	1:A:595:PHE:HD1	1.62	0.65
1:A:614:VAL:HB	1:A:631:ILE:HG22	1.77	0.65
1:B:162:THR:HA	1:B:165:ILE:HD12	1.79	0.65
1:C:264:GLN:HG2	1:C:265:PHE:HD1	1.60	0.65
1:A:193:ILE:O	1:A:197:PHE:N	2.29	0.65
1:A:561:TYR:C	1:A:564:ILE:HG12	2.20	0.65
1:B:116:LYS:O	1:B:119:GLU:N	2.29	0.65
1:C:527:GLU:HA	1:C:530:ILE:HD12	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:O	1:A:322:LEU:N	2.27	0.65
1:A:473:TYR:O	1:A:590:GLU:OE1	2.15	0.65
1:C:146:VAL:HA	1:C:149:LEU:HB2	1.77	0.65
1:C:475:PRO:HA	1:C:610:SER:HB2	1.78	0.65
1:D:237:ASP:OD1	1:D:238:HIS:N	2.29	0.65
1:D:820:LEU:C	1:D:820:LEU:HD12	2.21	0.65
1:B:280:MET:HA	1:B:284:ALA:HB3	1.78	0.65
1:C:249:SER:OG	1:C:250:GLN:N	2.28	0.65
1:A:466:CYS:O	1:A:469:THR:OG1	2.15	0.65
1:A:496:VAL:HA	1:A:499:GLN:HB2	1.79	0.65
1:A:614:VAL:CB	1:A:631:ILE:HG22	2.27	0.65
1:B:424:LYS:O	1:B:427:ARG:NE	2.30	0.65
1:C:514:THR:HG23	1:C:518:MET:HE3	1.79	0.65
1:A:214:TYR:HE2	1:A:353:PHE:HA	1.62	0.65
1:A:507:PHE:CD1	1:A:738:ALA:HB2	2.32	0.65
1:B:312:ILE:O	1:B:315:ALA:N	2.26	0.65
1:B:700:CYS:O	1:B:704:GLN:HG2	1.97	0.65
1:B:756:ARG:NH2	1:B:761:GLU:OE2	2.29	0.65
2:F:412:CYS:H	2:F:426:GLU:HA	1.62	0.65
1:A:117:PHE:HE2	1:A:779:ALA:HA	1.62	0.65
1:B:540:PRO:CA	1:B:607:PHE:CE2	2.80	0.65
1:A:226:LEU:CD1	1:A:416:GLU:OE2	2.44	0.64
1:A:279:VAL:HG21	1:A:415:PHE:HD1	1.62	0.64
1:D:652:THR:HG23	1:D:736:LEU:HD13	1.78	0.64
1:D:675:LEU:HD12	1:D:676:ALA:N	2.12	0.64
2:F:335:VAL:O	2:F:339:TYR:N	2.29	0.64
1:B:239:LYS:O	1:B:239:LYS:HG2	1.96	0.64
2:F:77:THR:HA	2:F:84:SER:HA	1.79	0.64
1:A:277:GLU:CD	1:A:302:ALA:CB	2.69	0.64
2:F:93:SER:O	2:F:225:LEU:N	2.30	0.64
1:B:604:ARG:HH22	1:B:672:ASP:HA	1.62	0.64
1:C:327:GLN:OE1	1:D:310:GLN:NE2	2.31	0.64
1:C:720:ALA:HA	1:C:790:LEU:HD11	1.78	0.64
1:C:816:PHE:O	1:C:818:CYS:N	2.30	0.64
1:D:132:THR:O	1:D:135:SER:OG	2.13	0.64
1:B:745:GLU:HG3	1:B:749:MET:HE2	1.79	0.64
1:C:583:ASN:HA	1:C:586:ARG:CZ	2.27	0.64
1:D:268:GLU:O	1:D:270:ASP:N	2.30	0.64
1:A:276:ILE:HG23	1:A:411:VAL:HG21	1.79	0.64
1:A:764:THR:HG23	1:A:765:PRO:HD2	1.78	0.64
1:C:319:ASP:O	1:C:322:LEU:N	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:ALA:HB1	1:D:662:PHE:HE2	1.62	0.64
1:A:650:SER:OG	1:A:651:GLY:N	2.30	0.64
1:C:515:LEU:CD2	1:C:518:MET:HG3	2.28	0.64
1:C:621:GLU:H	1:C:621:GLU:CD	2.06	0.64
1:D:656:HIS:NE2	1:D:728:GLU:OE1	2.28	0.64
1:B:255:MET:CB	1:B:260:TYR:OH	2.42	0.64
1:B:526:ALA:HB1	1:B:662:PHE:HE1	1.61	0.64
1:B:570:ASN:HA	1:B:589:TYR:CE2	2.32	0.64
1:D:98:GLY:O	1:D:116:LYS:HB3	1.98	0.64
2:E:252:PHE:O	2:E:414:ILE:HA	1.98	0.64
1:A:507:PHE:CZ	1:A:659:VAL:CG1	2.81	0.64
1:A:509:LYS:O	1:A:510:LYS:HG2	1.98	0.64
1:C:733:LEU:C	1:C:733:LEU:HD12	2.22	0.64
1:C:543:LEU:HD23	1:C:544:PHE:HB2	1.81	0.63
1:C:745:GLU:OE1	1:C:745:GLU:N	2.31	0.63
1:A:775:TYR:O	1:A:778:CYS:N	2.30	0.63
1:A:487:GLU:OE1	1:A:489:ARG:NH1	2.31	0.63
1:B:820:LEU:HB3	1:B:825:TYR:CE2	2.34	0.63
1:A:489:ARG:O	1:A:493:VAL:N	2.26	0.63
1:B:190:LEU:HA	1:B:193:ILE:HG12	1.79	0.63
1:B:622:LEU:HD12	1:B:622:LEU:C	2.23	0.63
1:D:331:PRO:HB2	1:D:377:ASP:CG	2.24	0.63
1:C:470:ILE:O	1:C:474:MET:N	2.27	0.63
1:C:764:THR:OG1	1:C:767:GLN:NE2	2.32	0.63
1:D:132:THR:OG1	1:D:778:CYS:O	2.16	0.63
1:A:234:VAL:CG2	1:A:235:ASN:N	2.61	0.63
1:A:640:GLN:N	1:A:640:GLN:OE1	2.31	0.63
1:B:427:ARG:HG3	1:B:428:ILE:HG13	1.80	0.63
1:B:618:TYR:HD1	1:B:624:SER:O	1.82	0.63
1:D:246:TYR:OH	1:D:598:LYS:CD	2.47	0.63
1:A:214:TYR:OH	1:A:352:ARG:O	2.14	0.63
1:C:171:GLN:HA	1:C:174:VAL:HG12	1.80	0.63
1:C:588:GLY:O	1:C:592:ARG:HG3	1.98	0.63
1:D:97:PHE:CZ	1:D:120:ARG:HG2	2.33	0.63
1:D:614:VAL:HG13	1:D:614:VAL:O	1.98	0.63
2:E:335:VAL:O	2:E:339:TYR:N	2.32	0.63
1:C:519:GLN:O	1:C:522:SER:OG	2.15	0.63
1:D:280:MET:HA	1:D:283:PHE:CD2	2.33	0.63
1:A:638:ASP:OD1	1:A:639:LEU:N	2.32	0.63
1:D:479:GLY:HA3	1:D:611:PRO:HG2	1.80	0.63
1:A:133:THR:O	1:A:136:GLN:HB3	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ASN:O	1:A:571:LYS:CG	2.44	0.62
1:C:515:LEU:CD2	1:C:518:MET:CG	2.77	0.62
1:A:322:LEU:HD23	1:A:328:GLN:OE1	2.00	0.62
1:A:782:THR:O	1:A:786:LEU:N	2.32	0.62
1:B:325:HIS:HA	1:B:328:GLN:CG	2.28	0.62
1:B:411:VAL:O	1:B:415:PHE:HB2	2.00	0.62
1:B:593:GLU:O	1:B:597:ARG:HG3	1.99	0.62
1:B:782:THR:O	1:B:785:SER:OG	2.12	0.62
1:C:100:ASP:HB2	1:C:115:ASN:HB3	1.80	0.62
1:D:770:TRP:CE3	1:D:770:TRP:HA	2.34	0.62
2:E:287:TYR:HA	2:E:423:GLY:HA2	1.81	0.62
1:A:166:THR:O	1:A:169:ALA:N	2.32	0.62
1:C:313:ALA:O	1:C:316:SER:N	2.31	0.62
1:D:567:ALA:HA	1:D:589:TYR:OH	1.98	0.62
1:C:510:LYS:HZ3	1:C:737:GLN:HG2	1.63	0.62
1:D:109:PHE:CE2	1:D:806:LEU:CD1	2.82	0.62
2:E:251:ILE:HA	2:E:415:HIS:O	1.99	0.62
1:B:162:THR:H	1:B:564:ILE:HD13	1.65	0.62
1:B:380:VAL:CG1	1:B:385:TYR:CE2	2.77	0.62
1:B:562:TYR:O	1:B:565:LEU:HB3	2.00	0.62
1:C:618:TYR:CE1	1:C:620:PRO:HA	2.34	0.62
1:D:160:SER:O	1:D:163:GLU:OE1	2.17	0.62
1:D:809:ILE:HG22	1:D:812:PHE:H	1.65	0.62
2:E:168:PHE:N	2:E:179:GLY:O	2.32	0.62
1:C:109:PHE:CB	1:C:824:MET:HE1	2.28	0.62
1:A:317:TRP:CH2	1:B:314:MET:HE2	2.35	0.62
1:A:764:THR:CG2	1:A:765:PRO:CD	2.78	0.62
1:B:269:LEU:O	1:B:272:ARG:HB3	2.00	0.62
1:A:163:GLU:OE2	1:A:480:TYR:CE2	2.53	0.62
1:B:208:LYS:HG2	1:B:403:TYR:OH	1.99	0.62
1:B:620:PRO:HB2	1:B:669:PHE:HD2	1.64	0.62
1:C:643:LYS:HA	1:C:646:ASN:ND2	2.15	0.62
1:D:660:HIS:NE2	1:D:728:GLU:OE2	2.30	0.62
1:D:674:SER:OG	1:D:675:LEU:N	2.24	0.62
1:B:279:VAL:O	1:B:282:ALA:N	2.31	0.62
1:C:214:TYR:HA	1:C:217:MET:HB3	1.82	0.62
2:E:250:PRO:O	2:E:417:MET:N	2.33	0.62
1:A:770:TRP:CZ2	1:A:812:PHE:HB2	2.35	0.61
1:B:295:ASP:O	1:B:298:ILE:N	2.33	0.61
1:B:544:PHE:O	1:B:544:PHE:CG	2.53	0.61
1:B:480:TYR:HE1	1:B:484:ASN:HD22	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:TYR:CZ	1:C:620:PRO:HA	2.35	0.61
2:F:300:MET:O	2:F:313:GLY:N	2.32	0.61
1:A:762:LYS:CD	1:C:817:GLN:N	2.63	0.61
1:B:669:PHE:HA	1:B:674:SER:O	2.00	0.61
1:C:310:GLN:O	1:C:314:MET:HG2	1.99	0.61
1:C:664:ASP:OD1	1:C:665:GLU:N	2.33	0.61
2:E:253:THR:HA	2:E:413:ASN:O	2.00	0.61
2:F:343:TYR:HA	2:F:350:TYR:HA	1.80	0.61
1:B:109:PHE:CG	1:B:806:LEU:HD23	2.35	0.61
1:B:272:ARG:NH1	1:B:272:ARG:HA	2.15	0.61
1:D:139:LEU:HD12	1:D:464:MET:SD	2.41	0.61
1:D:261:VAL:HB	1:D:314:MET:HE3	1.83	0.61
1:A:185:SER:HB2	1:A:188:GLU:CD	2.25	0.61
1:A:212:GLU:OE2	1:A:355:LYS:NZ	2.29	0.61
1:A:248:ILE:HB	1:A:380:VAL:HG22	1.83	0.61
1:B:645:PHE:HE1	1:B:768:ILE:HG22	1.66	0.61
1:B:742:ALA:O	1:B:745:GLU:N	2.34	0.61
1:C:224:ARG:NH2	1:C:417:ASP:OD1	2.33	0.61
1:A:762:LYS:HD2	1:C:817:GLN:N	2.16	0.61
1:B:109:PHE:CZ	1:B:806:LEU:CD2	2.83	0.61
1:B:510:LYS:HA	1:B:514:THR:HG21	1.83	0.61
1:B:805:VAL:O	1:B:805:VAL:HG12	2.01	0.61
1:B:133:THR:O	1:B:136:GLN:HB2	2.00	0.61
1:B:809:ILE:HG22	1:B:809:ILE:O	1.98	0.61
1:A:709:CYS:SG	1:A:719:CYS:CB	2.87	0.61
1:B:637:TYR:O	1:B:638:ASP:CG	2.42	0.61
1:D:228:THR:O	1:D:230:MET:N	2.32	0.61
1:B:341:LYS:CE	1:B:353:PHE:HE2	2.13	0.61
1:B:481:VAL:O	1:B:485:SER:HB3	2.01	0.61
1:B:538:GLY:HA2	1:B:629:PHE:H	1.65	0.61
1:C:238:HIS:CE1	1:C:247:TYR:HH	2.19	0.61
1:A:82:ALA:HB1	1:A:758:PRO:HB3	1.83	0.60
1:C:81:ASN:HB2	1:C:756:ARG:HB2	1.81	0.60
1:D:279:VAL:HG21	1:D:414:LEU:HD11	1.82	0.60
1:C:619:ALA:HB3	1:C:624:SER:OG	2.01	0.60
1:C:776:SER:O	1:C:776:SER:OG	2.20	0.60
1:B:174:VAL:HG23	1:B:175:GLU:HG2	1.82	0.60
3:G:95:HIS:O	3:G:96:PHE:C	2.44	0.60
1:A:87:GLU:OE1	1:A:640:GLN:CG	2.50	0.60
1:A:91:ALA:HB2	1:A:641:PHE:CE1	2.36	0.60
1:D:97:PHE:HZ	1:D:120:ARG:HG2	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ALA:O	1:A:279:VAL:HG23	2.00	0.60
1:A:484:ASN:HA	1:A:487:GLU:HG2	1.84	0.60
1:D:604:ARG:O	1:D:604:ARG:HG3	1.99	0.60
1:B:622:LEU:HD13	1:B:624:SER:OG	2.00	0.60
1:C:298:ILE:O	1:C:301:ALA:N	2.35	0.60
1:B:217:MET:O	1:B:220:ILE:N	2.34	0.60
1:C:736:LEU:HD21	1:C:770:TRP:HZ3	1.67	0.60
1:C:793:ASN:CB	1:C:795:HIS:CE1	2.85	0.60
1:C:820:LEU:HA	1:C:825:TYR:O	2.02	0.60
2:E:345:GLU:H	2:E:348:GLU:HA	1.67	0.60
1:B:305:VAL:HG11	1:B:411:VAL:HG21	1.82	0.60
1:C:793:ASN:HB3	1:C:795:HIS:CE1	2.37	0.60
1:D:119:GLU:O	1:D:119:GLU:HG2	2.02	0.60
1:D:323:ARG:NH2	1:D:724:HIS:O	2.35	0.60
1:D:380:VAL:HG13	1:D:386:MET:HG3	1.82	0.60
1:D:407:ASN:O	1:D:411:VAL:HG23	2.01	0.60
2:E:289:ASP:HA	2:E:421:THR:HA	1.84	0.60
1:B:308:ILE:HG23	1:B:309:GLU:N	2.17	0.60
2:F:182:GLY:H	2:F:204:PHE:H	1.49	0.60
1:A:130:ARG:HG2	1:A:781:GLU:HB3	1.83	0.60
1:A:705:TYR:HE1	1:A:804:GLN:HG2	1.66	0.60
1:B:231:TYR:HD2	1:B:233:TRP:CZ3	2.20	0.59
1:C:182:ARG:HD3	1:C:580:THR:H	1.66	0.59
1:D:565:LEU:HA	1:D:568:TYR:HB2	1.84	0.59
1:D:631:ILE:HG23	1:D:632:LEU:N	2.17	0.59
1:A:91:ALA:HB2	1:A:641:PHE:CZ	2.37	0.59
1:C:663:ASP:OD1	1:C:730:ILE:HD11	2.02	0.59
1:D:238:HIS:ND1	1:D:247:TYR:OH	2.31	0.59
1:D:559:ASP:OD1	1:D:560:ASP:N	2.32	0.59
1:A:636:HIS:O	1:A:650:SER:N	2.21	0.59
1:B:121:ILE:O	1:B:780:LYS:HD3	2.02	0.59
1:B:705:TYR:HE2	1:B:729:ASN:OD1	1.85	0.59
1:B:757:LEU:HD12	1:B:768:ILE:HD13	1.83	0.59
1:C:569:ASN:HB3	1:C:589:TYR:CE1	2.31	0.59
1:A:648:ALA:HB2	1:A:769:PHE:CD1	2.37	0.59
1:B:333:GLU:O	1:B:336:ALA:N	2.35	0.59
1:C:177:THR:C	1:C:180:ASP:H	2.10	0.59
1:C:767:GLN:HB2	1:C:816:PHE:CZ	2.37	0.59
1:D:492:VAL:HG13	1:D:493:VAL:N	2.17	0.59
1:D:650:SER:OG	1:D:651:GLY:N	2.35	0.59
1:A:99:LEU:HD13	1:A:760:LEU:HD13	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:GLU:HG3	1:B:597:ARG:HH21	1.67	0.59
1:B:660:HIS:HA	1:B:663:ASP:OD2	2.03	0.59
1:C:381:THR:O	1:C:383:PRO:HD3	2.02	0.59
1:C:779:ALA:HB3	1:C:798:ASN:OD1	2.02	0.59
1:D:273:THR:HA	1:D:276:ILE:HG22	1.83	0.59
1:B:242:SER:C	1:B:243:ARG:HG3	2.26	0.59
1:C:628:PRO:HG2	1:C:637:TYR:HE2	1.67	0.59
1:D:321:GLU:OE1	1:D:321:GLU:N	2.35	0.59
1:D:296:LYS:O	1:D:296:LYS:HD2	2.02	0.59
1:D:609:GLU:HB3	1:D:617:TRP:CH2	2.37	0.59
1:A:355:LYS:O	1:A:357:ILE:N	2.36	0.59
1:B:565:LEU:HA	1:B:568:TYR:HB2	1.85	0.59
1:B:798:ASN:O	1:B:801:ARG:N	2.35	0.59
1:A:773:TYR:HE1	1:A:777:TRP:HE1	1.51	0.59
1:D:160:SER:HB2	1:D:163:GLU:CD	2.28	0.59
1:D:352:ARG:HB3	1:D:355:LYS:HB2	1.85	0.59
1:D:820:LEU:HA	1:D:825:TYR:CD2	2.37	0.59
1:B:374:PHE:CD1	1:B:375:ILE:N	2.71	0.58
1:A:355:LYS:C	1:A:357:ILE:H	2.11	0.58
1:B:406:VAL:O	1:B:410:ILE:HG22	2.03	0.58
1:B:519:GLN:HE22	1:B:521:GLU:H	1.50	0.58
1:C:512:LEU:N	1:C:523:TYR:OH	2.36	0.58
2:F:416:ASP:O	2:F:420:ASN:N	2.36	0.58
1:A:785:SER:HA	1:A:788:LYS:HD3	1.83	0.58
1:C:519:GLN:O	1:C:523:TYR:N	2.33	0.58
1:C:643:LYS:HA	1:C:646:ASN:HD21	1.67	0.58
1:D:719:CYS:SG	1:D:787:VAL:CG2	2.92	0.58
2:E:336:ALA:O	2:E:341:GLY:N	2.35	0.58
2:F:299:LYS:HA	2:F:315:GLU:HA	1.85	0.58
1:A:382:ASN:O	1:A:385:TYR:N	2.37	0.58
1:B:489:ARG:CZ	1:B:544:PHE:CE2	2.87	0.58
1:C:104:ASP:OD1	1:C:105:PRO:HD2	2.03	0.58
1:C:187:ASN:HA	1:C:190:LEU:HB2	1.84	0.58
1:C:599:ASN:HB2	1:C:600:GLU:CD	2.28	0.58
1:C:722:GLY:O	1:C:724:HIS:N	2.36	0.58
1:A:238:HIS:CD2	1:A:621:GLU:CG	2.87	0.58
1:A:813:ALA:HB1	1:A:825:TYR:HE1	1.68	0.58
1:C:806:LEU:HD22	1:C:812:PHE:CG	2.38	0.58
1:D:808:ASP:CG	1:D:831:ARG:HB3	2.28	0.58
1:A:234:VAL:HG12	1:A:595:PHE:CD1	2.38	0.58
1:A:656:HIS:HE1	1:A:728:GLU:HG3	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:GLU:N	1:C:600:GLU:OE1	2.35	0.58
1:A:617:TRP:NE1	1:A:626:THR:OG1	2.37	0.58
1:B:278:ASN:O	1:B:282:ALA:N	2.36	0.58
1:B:591:ASN:HB2	1:B:595:PHE:CZ	2.38	0.58
1:C:167:LYS:O	1:C:171:GLN:HG2	2.04	0.58
1:C:273:THR:HG22	1:C:306:THR:HG21	1.84	0.58
2:E:325:MET:C	2:E:389:MET:H	2.12	0.58
1:A:109:PHE:O	1:A:112:PHE:N	2.36	0.58
1:A:476:TYR:OH	1:A:607:PHE:HB2	2.04	0.58
1:A:620:PRO:HB2	1:A:669:PHE:CD2	2.39	0.57
1:B:110:TYR:CD1	1:B:799:SER:HA	2.39	0.57
1:B:270:ASP:C	1:B:272:ARG:H	2.10	0.57
1:B:310:GLN:O	1:B:312:ILE:N	2.37	0.57
1:B:809:ILE:CG2	1:B:811:SER:OG	2.42	0.57
1:C:85:SER:C	1:C:89:LYS:HZ2	2.12	0.57
1:D:504:MET:HG3	1:D:530:ILE:CG2	2.34	0.57
1:A:332:TYR:N	1:A:377:ASP:OD1	2.37	0.57
1:B:485:SER:OG	1:B:486:ARG:HG2	2.04	0.57
1:C:573:ASP:OD1	1:C:574:LYS:N	2.37	0.57
1:D:250:GLN:OE1	1:D:382:ASN:OD1	2.22	0.57
1:A:238:HIS:NE2	1:A:621:GLU:HG2	2.19	0.57
1:A:583:ASN:O	1:A:587:ARG:HG2	2.04	0.57
1:B:170:PHE:HZ	1:B:463:ARG:HG2	1.69	0.57
1:B:259:PHE:CE2	1:B:265:PHE:HB3	2.38	0.57
1:B:629:PHE:HA	1:B:632:LEU:HD13	1.86	0.57
1:D:121:ILE:O	1:D:780:LYS:NZ	2.32	0.57
1:D:652:THR:O	1:D:655:GLY:N	2.37	0.57
1:B:112:PHE:HE2	1:B:816:PHE:HZ	1.53	0.57
1:B:201:PRO:HA	1:B:297:MET:HE1	1.87	0.57
1:B:341:LYS:HB3	1:B:352:ARG:HH12	1.67	0.57
1:C:229:PHE:H	1:C:251:PRO:HG3	1.70	0.57
1:C:517:TRP:NE1	1:C:518:MET:HE2	2.19	0.57
2:E:241:ARG:O	2:E:245:LEU:N	2.32	0.57
2:F:90:ASP:O	2:F:225:LEU:N	2.37	0.57
1:A:479:GLY:O	1:A:482:TYR:N	2.37	0.57
1:B:118:ILE:O	1:B:780:LYS:HD2	2.04	0.57
1:B:334:LEU:HD12	1:B:334:LEU:C	2.29	0.57
1:B:420:HIS:NE2	1:B:580:THR:HA	2.19	0.57
1:B:462:ALA:HA	1:B:465:LYS:NZ	2.19	0.57
1:C:834:VAL:HG22	1:C:835:TRP:CD1	2.40	0.57
1:D:357:ILE:O	1:D:360:LEU:N	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:ASP:OD1	1:B:672:ASP:N	2.36	0.57
1:B:732:ASP:OD2	1:B:801:ARG:HG2	2.04	0.57
1:C:510:LYS:NZ	1:C:737:GLN:HG2	2.19	0.57
1:D:804:GLN:O	1:D:807:GLN:N	2.38	0.57
1:A:101:GLU:OE1	1:A:112:PHE:HE1	1.86	0.57
1:A:196:ARG:NH1	1:A:219:ARG:HE	1.98	0.57
1:B:133:THR:OG1	1:B:778:CYS:O	2.22	0.57
1:B:341:LYS:HE2	1:B:353:PHE:CE2	2.36	0.57
1:B:520:GLY:O	1:B:523:TYR:HB3	2.04	0.57
1:D:393:PHE:CE1	1:D:405:PHE:CD2	2.93	0.57
1:D:560:ASP:HB2	1:D:564:ILE:HD11	1.86	0.57
2:F:95:ASN:O	2:F:224:GLY:N	2.37	0.57
2:F:344:ASP:H	2:F:350:TYR:HA	1.68	0.57
1:A:661:GLY:C	1:A:662:PHE:HD1	2.13	0.57
1:B:186:VAL:HG23	1:B:187:ASN:N	2.19	0.57
1:B:629:PHE:O	1:B:632:LEU:N	2.33	0.57
1:C:538:GLY:HA2	1:C:628:PRO:C	2.30	0.57
1:A:389:LEU:N	1:A:389:LEU:HD12	2.19	0.57
1:B:278:ASN:HA	1:B:425:TYR:CZ	2.40	0.57
1:B:591:ASN:OD1	1:B:592:ARG:N	2.37	0.57
1:C:110:TYR:CD1	1:C:111:GLY:N	2.73	0.57
1:D:808:ASP:HA	1:D:831:ARG:HG3	1.87	0.57
2:E:78:ILE:H	2:E:83:GLN:H	1.53	0.57
1:B:208:LYS:N	1:B:403:TYR:OH	2.37	0.56
1:B:461:ASP:OD1	1:B:462:ALA:N	2.37	0.56
1:C:582:LEU:O	1:C:585:LEU:HB3	2.05	0.56
1:C:768:ILE:O	1:C:771:ILE:N	2.38	0.56
1:D:529:LYS:O	1:D:533:MET:HG3	2.04	0.56
1:A:705:TYR:O	1:A:708:GLN:N	2.30	0.56
1:B:407:ASN:O	1:B:411:VAL:HG23	2.05	0.56
1:B:732:ASP:HB3	1:B:805:VAL:HG21	1.87	0.56
1:C:806:LEU:O	1:C:809:ILE:N	2.31	0.56
1:D:530:ILE:HA	1:D:533:MET:SD	2.44	0.56
1:B:262:LEU:CB	1:B:263:PRO:CD	2.80	0.56
1:B:589:TYR:O	1:B:590:GLU:C	2.47	0.56
1:B:755:MET:H	1:B:755:MET:HE2	1.71	0.56
1:C:95:LEU:HD11	1:C:771:ILE:HG22	1.85	0.56
1:C:134:PHE:O	1:C:137:ALA:N	2.38	0.56
1:C:245:SER:OG	1:C:246:TYR:N	2.37	0.56
1:D:241:VAL:HG23	1:D:241:VAL:O	2.05	0.56
1:D:636:HIS:O	1:D:649:GLY:HA3	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:PRO:O	2:F:332:ALA:N	2.36	0.56
3:G:134:LYS:O	3:G:135:CYS:C	2.48	0.56
1:D:332:TYR:O	1:D:378:VAL:N	2.22	0.56
1:D:770:TRP:HE1	1:D:812:PHE:HA	1.71	0.56
1:C:95:LEU:CD1	1:C:771:ILE:CG2	2.78	0.56
1:B:281:LYS:HD2	1:B:281:LYS:N	2.21	0.56
1:B:767:GLN:HE21	1:B:816:PHE:HA	1.70	0.56
1:B:809:ILE:O	1:B:812:PHE:N	2.34	0.56
1:C:617:TRP:NE1	1:C:626:THR:HB	2.20	0.56
1:D:116:LYS:O	1:D:119:GLU:N	2.37	0.56
1:D:770:TRP:HA	1:D:770:TRP:HE3	1.71	0.56
1:A:196:ARG:HH12	1:A:219:ARG:NE	2.02	0.56
1:A:272:ARG:HH21	1:A:276:ILE:HD11	1.70	0.56
1:A:637:TYR:OH	1:A:639:LEU:HA	2.05	0.56
2:F:100:ASP:N	2:F:207:ALA:O	2.39	0.56
1:A:789:ARG:HA	1:A:792:THR:HG22	1.88	0.56
1:B:99:LEU:O	1:B:116:LYS:NZ	2.38	0.56
1:B:304:GLU:O	1:B:307:GLN:N	2.38	0.56
1:C:564:ILE:O	1:C:568:TYR:HB2	2.06	0.56
1:D:143:SER:O	1:D:147:LYS:HG2	2.05	0.56
1:D:637:TYR:CD1	1:D:646:ASN:CG	2.83	0.56
2:F:251:ILE:HA	2:F:415:HIS:O	2.05	0.56
1:A:132:THR:HA	1:A:779:ALA:HB2	1.88	0.56
1:A:801:ARG:O	1:A:804:GLN:N	2.27	0.56
1:B:542:LYS:N	1:B:542:LYS:HD2	2.20	0.56
1:C:234:VAL:HG12	1:C:594:SER:O	2.06	0.56
1:A:571:LYS:O	1:A:572:THR:OG1	2.23	0.55
1:B:188:GLU:O	1:B:191:GLN:HB3	2.06	0.55
1:A:703:THR:O	1:A:706:ASN:OD1	2.23	0.55
1:B:507:PHE:HA	1:B:510:LYS:NZ	2.22	0.55
1:C:309:GLU:O	1:C:310:GLN:C	2.49	0.55
1:D:583:ASN:HA	1:D:586:ARG:CZ	2.36	0.55
1:A:496:VAL:O	1:A:499:GLN:N	2.40	0.55
1:A:784:SER:O	1:A:788:LYS:HG3	2.07	0.55
1:B:401:ASN:C	1:B:404:PRO:HD2	2.32	0.55
1:B:493:VAL:O	1:B:497:LYS:HG3	2.07	0.55
1:C:305:VAL:HG11	1:C:411:VAL:HG21	1.88	0.55
1:C:767:GLN:O	1:C:771:ILE:HG13	2.05	0.55
1:D:228:THR:C	1:D:230:MET:H	2.09	0.55
1:A:762:LYS:HD2	1:C:817:GLN:HA	1.88	0.55
1:B:278:ASN:HA	1:B:425:TYR:CE2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASN:OD1	1:D:85:SER:N	2.40	0.55
1:D:480:TYR:CD2	1:D:543:LEU:HG	2.39	0.55
1:A:87:GLU:OE1	1:A:640:GLN:HG2	2.07	0.55
1:C:193:ILE:HG23	1:C:197:PHE:CE2	2.36	0.55
1:C:385:TYR:O	1:C:385:TYR:CG	2.60	0.55
2:F:289:ASP:HA	2:F:421:THR:HA	1.87	0.55
1:A:142:ASN:O	1:A:145:ILE:HB	2.07	0.55
1:A:468:ASP:O	1:A:471:THR:OG1	2.20	0.55
1:A:537:TYR:O	1:A:539:TRP:N	2.39	0.55
1:B:589:TYR:O	1:B:592:ARG:N	2.40	0.55
1:C:263:PRO:O	1:C:266:ALA:N	2.39	0.55
1:C:267:PRO:HG2	1:C:268:GLU:OE2	2.07	0.55
1:D:405:PHE:O	1:D:408:TYR:HB3	2.06	0.55
1:B:333:GLU:OE1	1:B:333:GLU:N	2.39	0.55
1:B:510:LYS:HZ3	1:B:510:LYS:HB2	1.72	0.55
1:B:579:TYR:HA	1:B:582:LEU:CG	2.36	0.55
1:B:645:PHE:O	1:B:648:ALA:N	2.39	0.55
1:C:228:THR:O	1:C:229:PHE:HB2	2.06	0.55
2:E:99:PRO:HA	2:E:207:ALA:HB3	1.89	0.55
1:A:499:GLN:O	1:A:503:ILE:HG13	2.07	0.55
1:A:762:LYS:HD2	1:C:817:GLN:CA	2.37	0.55
1:B:109:PHE:CZ	1:B:806:LEU:HD21	2.41	0.55
1:B:710:CYS:SG	1:B:711:PRO:HD3	2.47	0.55
1:B:809:ILE:O	1:B:811:SER:N	2.40	0.55
1:C:270:ASP:OD1	1:C:271:ALA:N	2.39	0.55
1:C:583:ASN:HD21	1:C:587:ARG:CZ	2.19	0.55
1:D:529:LYS:NZ	1:D:669:PHE:O	2.37	0.55
2:F:373:ARG:O	2:F:377:VAL:N	2.39	0.55
1:A:664:ASP:HA	1:A:667:VAL:HG12	1.89	0.55
1:A:670:ASP:OD2	1:A:674:SER:OG	2.24	0.55
1:B:617:TRP:NE1	1:B:626:THR:OG1	2.39	0.55
1:C:178:LEU:HD22	1:C:182:ARG:NH1	2.22	0.55
1:C:218:GLY:O	1:C:220:ILE:N	2.39	0.55
1:C:260:TYR:O	1:C:266:ALA:HA	2.06	0.55
1:D:336:ALA:N	1:D:337:PRO:CD	2.69	0.55
1:A:162:THR:HA	1:A:165:ILE:HG12	1.89	0.55
1:B:647:PHE:O	1:B:652:THR:N	2.40	0.55
1:C:414:LEU:C	1:C:416:GLU:H	2.14	0.55
1:C:657:GLU:O	1:C:660:HIS:N	2.39	0.55
1:A:754:GLU:HB3	1:A:765:PRO:HD2	1.88	0.54
1:B:533:MET:CE	1:B:658:LEU:HD11	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:GLY:H	2:E:273:TYR:H	1.55	0.54
1:A:417:ASP:OD1	1:A:417:ASP:N	2.40	0.54
1:A:705:TYR:CE1	1:A:804:GLN:HG2	2.43	0.54
1:C:306:THR:HA	1:C:309:GLU:HG3	1.88	0.54
1:C:535:ARG:HB3	1:C:537:TYR:CZ	2.42	0.54
1:C:761:GLU:OE1	1:C:761:GLU:N	2.40	0.54
1:A:775:TYR:O	1:A:776:SER:C	2.49	0.54
1:B:146:VAL:O	1:B:149:LEU:HG	2.08	0.54
1:B:540:PRO:HD2	1:B:543:LEU:HD22	1.88	0.54
1:C:190:LEU:O	1:C:194:SER:OG	2.11	0.54
1:C:535:ARG:HB3	1:C:537:TYR:CE2	2.42	0.54
1:C:744:LYS:O	1:C:747:ILE:N	2.23	0.54
1:A:81:ASN:O	1:A:756:ARG:HB2	2.07	0.54
1:A:214:TYR:CE2	1:A:353:PHE:HA	2.42	0.54
1:B:483:VAL:HG11	1:B:539:TRP:CE3	2.42	0.54
1:B:754:GLU:CD	1:B:754:GLU:H	2.15	0.54
1:C:222:GLN:HG3	1:C:360:LEU:HD22	1.90	0.54
1:C:277:GLU:HG3	1:C:299:LYS:NZ	2.22	0.54
1:D:541:LYS:C	1:D:542:LYS:HE2	2.32	0.54
1:D:740:TYR:HB2	1:D:769:PHE:HE2	1.71	0.54
2:F:364:ILE:O	2:F:367:LYS:CB	2.56	0.54
1:C:87:GLU:OE2	1:C:639:LEU:HD23	2.08	0.54
1:D:634:SER:O	1:D:636:HIS:N	2.39	0.54
2:E:325:MET:O	2:E:389:MET:N	2.29	0.54
1:A:187:ASN:OD1	1:A:188:GLU:N	2.38	0.54
1:A:766:ASN:O	1:A:769:PHE:N	2.40	0.54
1:B:231:TYR:HD2	1:B:233:TRP:HZ3	1.55	0.54
1:B:269:LEU:HG	1:B:270:ASP:OD1	2.07	0.54
1:B:482:TYR:HE2	1:B:630:GLY:HA2	1.72	0.54
1:B:482:TYR:O	1:B:485:SER:OG	2.25	0.54
1:B:516:SER:OG	1:B:517:TRP:N	2.37	0.54
1:A:524:ARG:O	1:A:527:GLU:N	2.40	0.54
1:A:533:MET:HG2	1:A:623:ASN:HD21	1.72	0.54
1:B:112:PHE:HE2	1:B:816:PHE:CZ	2.26	0.54
1:C:143:SER:OG	1:C:144:ASP:N	2.41	0.54
1:C:243:ARG:NH2	1:C:376:GLY:HA2	2.16	0.54
1:C:501:GLU:HA	1:C:504:MET:HE3	1.88	0.54
1:C:793:ASN:CG	1:C:795:HIS:CE1	2.85	0.54
1:D:814:LYS:O	1:D:817:GLN:N	2.39	0.54
1:D:822:GLN:O	1:D:824:MET:N	2.39	0.54
1:A:521:GLU:H	1:A:521:GLU:CD	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ALA:HB2	1:B:756:ARG:O	2.08	0.54
1:C:257:ARG:NH1	1:C:313:ALA:HB1	2.20	0.54
1:D:522:SER:OG	1:D:523:TYR:N	2.30	0.54
1:D:757:LEU:HD12	1:D:757:LEU:C	2.32	0.54
1:A:401:ASN:HB3	1:A:405:PHE:CD2	2.43	0.54
1:A:607:PHE:HE2	1:A:611:PRO:HB3	1.73	0.54
1:B:483:VAL:HG11	1:B:539:TRP:HE3	1.73	0.54
1:B:519:GLN:NE2	1:B:521:GLU:H	2.06	0.54
1:D:647:PHE:CD2	1:D:743:TYR:HB2	2.43	0.54
1:A:141:VAL:HG13	1:A:142:ASN:H	1.73	0.53
1:A:273:THR:C	1:A:277:GLU:OE1	2.51	0.53
1:B:419:GLU:HA	1:B:426:LEU:CG	2.37	0.53
1:B:660:HIS:HA	1:B:663:ASP:CG	2.33	0.53
1:C:262:LEU:O	1:C:266:ALA:N	2.41	0.53
2:F:327:VAL:HA	2:F:401:TRP:HA	1.89	0.53
1:A:265:PHE:CE1	1:A:266:ALA:HB2	2.42	0.53
1:A:500:THR:HA	1:A:503:ILE:HD12	1.90	0.53
1:A:509:LYS:O	1:A:510:LYS:CG	2.55	0.53
1:A:809:ILE:HG22	1:A:812:PHE:H	1.73	0.53
1:B:402:GLN:O	1:B:405:PHE:CD2	2.60	0.53
1:B:561:TYR:C	1:B:564:ILE:HG22	2.31	0.53
1:C:494:GLU:O	1:C:498:GLN:HG3	2.07	0.53
1:D:528:LYS:O	1:D:531:ASN:N	2.41	0.53
1:A:764:THR:CG2	1:A:765:PRO:N	2.72	0.53
1:B:228:THR:C	1:B:230:MET:H	2.16	0.53
1:B:236:VAL:HG13	1:B:241:VAL:HG21	1.90	0.53
1:C:164:ARG:HA	1:C:167:LYS:HG2	1.89	0.53
1:C:621:GLU:OE1	1:C:621:GLU:N	2.34	0.53
1:A:392:LEU:C	1:A:393:PHE:HD1	2.16	0.53
1:A:670:ASP:O	1:A:672:ASP:N	2.41	0.53
1:A:718:HIS:O	1:A:718:HIS:CG	2.62	0.53
1:B:241:VAL:HG13	1:B:241:VAL:O	2.09	0.53
1:C:471:THR:HG23	1:C:612:ALA:HB3	1.91	0.53
1:D:262:LEU:O	1:D:264:GLN:N	2.41	0.53
1:A:490:ASP:OD1	1:A:490:ASP:N	2.38	0.53
1:B:764:THR:O	1:B:768:ILE:HG13	2.08	0.53
1:C:220:ILE:HA	1:C:223:GLN:HB3	1.91	0.53
1:D:734:GLY:O	1:D:735:GLY:C	2.51	0.53
1:A:333:GLU:OE1	1:A:333:GLU:N	2.41	0.53
1:A:521:GLU:HA	1:A:524:ARG:HH12	1.73	0.53
1:B:308:ILE:O	1:B:309:GLU:C	2.52	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:VAL:O	1:C:241:VAL:HG23	2.09	0.53
2:E:73:LEU:O	2:E:268:GLY:HA3	2.09	0.53
1:A:534:HIS:CD2	1:A:605:THR:HG22	2.43	0.53
1:B:337:PRO:O	1:B:340:GLY:N	2.40	0.53
1:B:759:GLY:O	1:B:760:LEU:CG	2.55	0.53
1:C:218:GLY:O	1:C:221:GLU:N	2.41	0.53
1:C:325:HIS:HA	1:C:328:GLN:HB2	1.91	0.53
1:D:405:PHE:O	1:D:409:ILE:HD12	2.08	0.53
1:D:461:ASP:OD1	1:D:463:ARG:HG3	2.09	0.53
2:E:89:LEU:HA	2:E:223:LEU:O	2.08	0.53
1:B:615:ASN:OD1	1:B:616:ALA:N	2.42	0.53
1:C:263:PRO:O	1:C:265:PHE:N	2.42	0.53
2:E:192:GLY:H	2:E:273:TYR:N	2.06	0.53
1:A:643:LYS:HG3	1:A:746:TYR:OH	2.09	0.53
1:A:668:GLN:O	1:A:675:LEU:CD1	2.56	0.53
1:B:824:MET:O	1:B:824:MET:CG	2.55	0.53
1:D:353:PHE:HA	1:D:356:TYR:HB3	1.89	0.53
1:D:507:PHE:HA	1:D:510:LYS:NZ	2.23	0.53
1:D:530:ILE:HA	1:D:533:MET:HG3	1.91	0.53
1:D:608:LEU:HB3	1:D:617:TRP:NE1	2.24	0.53
1:A:382:ASN:O	1:A:383:PRO:C	2.52	0.52
1:C:689:LYS:HE2	1:C:691:LYS:HE3	1.89	0.52
2:F:325:MET:N	2:F:387:ILE:O	2.42	0.52
1:B:333:GLU:O	1:B:335:PHE:N	2.43	0.52
1:B:561:TYR:O	1:B:564:ILE:CG2	2.50	0.52
1:C:574:LYS:HG3	1:C:574:LYS:O	2.09	0.52
2:E:398:GLY:O	2:E:400:GLN:N	2.42	0.52
2:F:250:PRO:O	2:F:417:MET:N	2.30	0.52
1:B:238:HIS:O	1:B:674:SER:HA	2.10	0.52
1:A:237:ASP:CG	1:A:245:SER:HB2	2.34	0.52
1:B:622:LEU:CD1	1:B:623:ASN:N	2.72	0.52
1:C:296:LYS:O	1:C:298:ILE:N	2.43	0.52
2:E:168:PHE:O	2:E:179:GLY:N	2.43	0.52
2:E:252:PHE:HA	2:E:272:THR:O	2.10	0.52
1:B:112:PHE:CE2	1:B:816:PHE:CZ	2.97	0.52
1:B:489:ARG:NH2	1:B:544:PHE:HE2	2.07	0.52
1:C:177:THR:HA	1:C:180:ASP:HB3	1.92	0.52
1:C:694:PHE:O	1:C:697:MET:N	2.43	0.52
1:D:732:ASP:O	1:D:733:LEU:C	2.50	0.52
1:A:234:VAL:HG22	1:A:235:ASN:H	1.74	0.52
1:A:668:GLN:C	1:A:669:PHE:HD1	2.18	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ALA:HB1	1:A:754:GLU:OE2	2.10	0.52
1:B:503:ILE:HD11	1:B:651:GLY:HA2	1.92	0.52
1:B:725:THR:OG1	1:B:729:ASN:ND2	2.42	0.52
1:A:112:PHE:CG	1:A:112:PHE:O	2.62	0.52
1:A:226:LEU:HD22	1:A:413:MET:HA	1.91	0.52
1:A:781:GLU:OE2	1:A:786:LEU:HG	2.10	0.52
1:B:563:SER:O	1:B:566:GLU:N	2.43	0.52
1:C:169:ALA:O	1:C:172:SER:OG	2.25	0.52
1:C:257:ARG:HE	1:C:318:PRO:HD3	1.75	0.52
1:C:386:MET:CE	1:D:391:THR:HG22	2.39	0.52
1:C:595:PHE:O	1:C:598:LYS:N	2.31	0.52
1:D:226:LEU:HD21	1:D:412:HIS:HB3	1.92	0.52
1:D:675:LEU:HD12	1:D:675:LEU:C	2.35	0.52
1:A:618:TYR:CE2	1:A:661:GLY:HA3	2.45	0.52
1:B:536:ASN:CB	1:B:626:THR:HG22	2.39	0.52
1:B:591:ASN:O	1:B:594:SER:N	2.43	0.52
1:C:95:LEU:CD1	1:C:771:ILE:HG22	2.39	0.52
1:C:625:LEU:CD2	1:C:627:LEU:HD11	2.39	0.52
1:D:752:ALA:C	1:D:754:GLU:H	2.17	0.52
1:A:95:LEU:CD2	1:A:760:LEU:HD12	2.39	0.52
1:A:265:PHE:CZ	1:A:266:ALA:HB2	2.45	0.52
1:A:566:GLU:OE1	1:A:596:ARG:NH2	2.42	0.52
1:C:255:MET:HB2	1:C:259:PHE:CZ	2.45	0.52
1:C:810:PRO:O	1:C:812:PHE:N	2.42	0.52
1:D:145:ILE:CD1	1:D:478:THR:CG2	2.87	0.52
1:D:560:ASP:O	1:D:564:ILE:HG12	2.10	0.52
2:E:178:LYS:O	2:E:208:VAL:N	2.42	0.52
1:A:810:PRO:O	1:A:813:ALA:HB3	2.10	0.52
1:A:813:ALA:HB1	1:A:825:TYR:CE1	2.44	0.52
1:B:89:LYS:O	1:B:93:ASN:OD1	2.28	0.52
1:B:526:ALA:HB1	1:B:662:PHE:CE1	2.42	0.52
1:B:664:ASP:OD1	1:B:664:ASP:N	2.39	0.52
1:C:407:ASN:OD1	1:C:408:TYR:N	2.43	0.52
2:F:336:ALA:O	2:F:341:GLY:N	2.31	0.52
1:A:239:LYS:CD	1:A:329:TYR:CD2	2.93	0.51
1:A:826:PRO:HB2	1:A:831:ARG:N	2.26	0.51
1:B:738:ALA:O	1:B:741:ASN:N	2.44	0.51
1:B:759:GLY:C	1:B:760:LEU:HG	2.34	0.51
1:B:776:SER:OG	1:B:777:TRP:N	2.42	0.51
1:C:273:THR:OG1	1:C:274:LYS:N	2.42	0.51
1:C:565:LEU:O	1:C:568:TYR:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:834:VAL:HG13	1:C:835:TRP:HD1	1.74	0.51
1:D:83:ASN:HB2	1:D:755:MET:HB3	1.91	0.51
1:D:101:GLU:CG	1:D:762:LYS:HZ1	2.14	0.51
1:D:137:ALA:O	1:D:140:GLU:N	2.42	0.51
1:D:218:GLY:O	1:D:219:ARG:C	2.53	0.51
1:A:503:ILE:O	1:A:504:MET:C	2.53	0.51
1:A:826:PRO:HG2	1:A:831:ARG:HB3	1.92	0.51
1:C:266:ALA:HB3	1:C:267:PRO:HD3	1.91	0.51
1:C:525:ARG:HH12	1:C:689:LYS:HZ1	1.57	0.51
1:D:794:PRO:O	1:D:795:HIS:ND1	2.43	0.51
1:A:253:LEU:CD1	1:A:253:LEU:C	2.80	0.51
1:B:226:LEU:HD23	1:B:226:LEU:C	2.36	0.51
1:B:511:MET:O	1:B:515:LEU:N	2.43	0.51
1:A:313:ALA:O	1:A:316:SER:N	2.43	0.51
1:A:533:MET:O	1:A:535:ARG:HG3	2.10	0.51
1:A:799:SER:O	1:A:800:CYS:C	2.54	0.51
1:B:814:LYS:O	1:B:816:PHE:N	2.43	0.51
1:D:313:ALA:O	1:D:316:SER:N	2.26	0.51
2:E:342:GLN:O	2:E:351:THR:N	2.43	0.51
2:F:372:GLU:O	2:F:376:LEU:N	2.42	0.51
1:B:273:THR:O	1:B:276:ILE:HG22	2.10	0.51
1:A:133:THR:HG23	1:A:778:CYS:O	2.10	0.51
1:A:151:LYS:O	1:A:167:LYS:NZ	2.38	0.51
1:A:496:VAL:HG23	1:A:497:LYS:H	1.75	0.51
1:A:631:ILE:O	1:A:633:THR:N	2.44	0.51
1:A:773:TYR:OH	1:A:805:VAL:HG21	2.11	0.51
1:B:573:ASP:OD1	1:B:573:ASP:N	2.42	0.51
1:B:726:GLN:O	1:B:729:ASN:HB2	2.11	0.51
1:B:814:LYS:HE2	1:D:101:GLU:OE1	2.11	0.51
1:D:139:LEU:CD1	1:D:464:MET:SD	2.98	0.51
1:A:526:ALA:O	1:A:529:LYS:HB3	2.11	0.51
1:B:705:TYR:CE2	1:B:729:ASN:ND2	2.78	0.51
1:C:739:SER:O	1:C:740:TYR:C	2.52	0.51
1:A:232:THR:O	1:A:232:THR:CG2	2.59	0.51
1:B:342:ILE:HB	1:B:352:ARG:NH1	2.26	0.51
1:C:88:TRP:CH2	1:C:642:PRO:HB3	2.46	0.51
1:A:740:TYR:HD2	1:A:769:PHE:CE2	2.28	0.51
1:A:825:TYR:C	1:A:827:PRO:HD2	2.36	0.51
1:C:264:GLN:HG2	1:C:265:PHE:CD1	2.41	0.51
1:C:756:ARG:HB3	1:C:761:GLU:HB2	1.93	0.51
1:D:270:ASP:O	1:D:273:THR:HG22	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:LYS:HG3	1:D:599:ASN:N	2.26	0.51
1:A:141:VAL:HG13	1:A:142:ASN:N	2.25	0.51
1:A:143:SER:O	1:A:146:VAL:N	2.44	0.51
1:B:810:PRO:HD2	1:B:831:ARG:NH1	2.14	0.51
1:C:105:PRO:O	1:C:824:MET:HE2	2.10	0.51
1:D:633:THR:HG23	1:D:634:SER:N	2.26	0.51
1:B:89:LYS:O	1:B:93:ASN:CG	2.54	0.50
1:B:269:LEU:CD1	1:B:303:ARG:HG2	2.41	0.50
1:C:175:GLU:HB2	1:C:178:LEU:HG	1.93	0.50
1:C:262:LEU:HB3	1:C:264:GLN:OE1	2.11	0.50
1:C:479:GLY:O	1:C:482:TYR:N	2.45	0.50
1:D:582:LEU:O	1:D:583:ASN:C	2.55	0.50
1:D:632:LEU:HD22	1:D:650:SER:HB3	1.92	0.50
1:A:83:ASN:HB2	1:A:755:MET:HG2	1.93	0.50
1:A:296:LYS:O	1:A:299:LYS:N	2.31	0.50
1:B:246:TYR:N	1:B:246:TYR:CD1	2.79	0.50
1:B:278:ASN:OD1	1:B:279:VAL:N	2.45	0.50
1:B:506:THR:O	1:B:509:LYS:HB3	2.10	0.50
1:B:536:ASN:O	1:B:537:TYR:HD1	1.94	0.50
1:C:322:LEU:HD23	1:C:328:GLN:NE2	2.26	0.50
1:D:480:TYR:CD1	1:D:480:TYR:C	2.89	0.50
2:E:77:THR:O	2:E:187:ARG:N	2.45	0.50
1:A:189:LEU:O	1:A:192:TYR:N	2.45	0.50
1:B:217:MET:C	1:B:217:MET:SD	2.94	0.50
1:C:145:ILE:O	1:C:149:LEU:HD23	2.11	0.50
1:D:246:TYR:OH	1:D:598:LYS:HD2	2.11	0.50
1:B:482:TYR:C	1:B:485:SER:HG	2.19	0.50
1:C:309:GLU:O	1:C:312:ILE:HG22	2.12	0.50
1:C:497:LYS:NZ	1:C:501:GLU:HB2	2.26	0.50
1:D:770:TRP:O	1:D:773:TYR:N	2.45	0.50
1:A:468:ASP:O	1:A:472:THR:HG23	2.11	0.50
1:A:474:MET:HE1	1:A:586:ARG:CD	2.11	0.50
1:A:657:GLU:O	1:A:658:LEU:C	2.55	0.50
1:B:523:TYR:O	1:B:524:ARG:C	2.54	0.50
1:B:595:PHE:O	1:B:598:LYS:HB3	2.12	0.50
1:B:804:GLN:O	1:B:807:GLN:N	2.44	0.50
1:D:463:ARG:HB2	1:D:464:MET:HE2	1.94	0.50
1:D:504:MET:HG3	1:D:530:ILE:HG21	1.94	0.50
1:A:786:LEU:C	1:A:786:LEU:HD23	2.36	0.50
1:B:213:LEU:HA	1:B:216:GLU:OE1	2.11	0.50
1:B:628:PRO:O	1:B:631:ILE:HG22	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:TYR:CG	1:B:638:ASP:N	2.80	0.50
1:D:113:THR:HG22	1:D:114:CYS:SG	2.51	0.50
1:D:768:ILE:O	1:D:771:ILE:N	2.44	0.50
1:A:350:ASN:OD1	1:A:351:ILE:N	2.45	0.50
1:B:214:TYR:O	1:B:215:ARG:C	2.52	0.50
1:B:489:ARG:NH2	1:B:544:PHE:CE2	2.80	0.50
1:B:633:THR:O	1:B:637:TYR:N	2.45	0.50
1:B:796:SER:HG	1:B:797:PRO:HD2	1.68	0.50
1:C:234:VAL:HG23	1:C:245:SER:C	2.37	0.50
1:D:141:VAL:HG23	1:D:482:TYR:CZ	2.46	0.50
1:A:401:ASN:HB3	1:A:405:PHE:CE2	2.45	0.50
1:A:766:ASN:O	1:A:767:GLN:C	2.54	0.50
1:B:670:ASP:CG	1:B:672:ASP:H	2.20	0.50
1:C:98:GLY:O	1:C:114:CYS:HA	2.11	0.50
1:C:765:PRO:O	1:C:768:ILE:HB	2.11	0.50
1:D:492:VAL:HG13	1:D:493:VAL:H	1.75	0.50
1:C:226:LEU:HD13	1:C:416:GLU:HG3	1.94	0.50
1:C:589:TYR:HA	1:C:592:ARG:HD2	1.92	0.50
1:C:739:SER:O	1:C:742:ALA:N	2.29	0.50
1:C:810:PRO:O	1:C:811:SER:C	2.55	0.50
1:D:698:ALA:O	1:D:699:GLN:C	2.55	0.50
2:E:75:LYS:HA	2:E:85:PHE:O	2.12	0.50
1:B:382:ASN:O	1:B:384:ALA:N	2.45	0.49
1:B:622:LEU:HD11	1:B:624:SER:OG	2.12	0.49
1:C:334:LEU:C	1:C:337:PRO:HD2	2.36	0.49
1:C:414:LEU:O	1:C:416:GLU:N	2.44	0.49
1:B:121:ILE:HG22	1:B:122:ASP:H	1.76	0.49
1:B:259:PHE:HZ	1:B:263:PRO:HB2	1.77	0.49
1:B:535:ARG:HD2	1:B:537:TYR:OH	2.12	0.49
1:C:260:TYR:HB2	1:C:262:LEU:HB2	1.94	0.49
1:D:475:PRO:O	1:D:610:SER:HA	2.12	0.49
1:D:632:LEU:CD2	1:D:650:SER:CB	2.90	0.49
1:A:500:THR:O	1:A:504:MET:HG3	2.12	0.49
1:B:132:THR:HB	1:B:779:ALA:HA	1.94	0.49
1:B:162:THR:CG2	1:B:477:GLY:HA2	2.43	0.49
1:C:666:GLY:C	1:C:668:GLN:H	2.20	0.49
1:A:196:ARG:HH22	1:A:219:ARG:HE	1.60	0.49
1:A:636:HIS:HA	1:A:649:GLY:HA3	1.94	0.49
1:A:670:ASP:OD1	1:A:670:ASP:N	2.44	0.49
1:A:704:GLN:O	1:A:708:GLN:HG2	2.12	0.49
1:B:473:TYR:CZ	1:B:587:ARG:HG2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:812:PHE:O	1:B:815:ASP:N	2.46	0.49
1:C:229:PHE:O	1:C:230:MET:CG	2.58	0.49
1:D:768:ILE:O	1:D:769:PHE:C	2.55	0.49
2:E:178:LYS:O	2:E:209:GLN:N	2.40	0.49
1:A:114:CYS:O	1:A:117:PHE:N	2.45	0.49
1:A:196:ARG:HH12	1:A:219:ARG:HH21	1.60	0.49
1:A:496:VAL:O	1:A:500:THR:N	2.45	0.49
1:B:570:ASN:HA	1:B:589:TYR:CZ	2.48	0.49
1:C:248:ILE:O	1:C:380:VAL:HG23	2.13	0.49
2:E:399:PRO:O	2:E:401:TRP:N	2.45	0.49
1:B:250:GLN:HG3	1:B:316:SER:OG	2.12	0.49
1:B:401:ASN:HA	1:B:404:PRO:HG2	1.93	0.49
1:B:593:GLU:OE2	1:B:596:ARG:NH2	2.46	0.49
1:C:236:VAL:HA	1:C:244:ASN:HA	1.95	0.49
1:C:478:THR:O	1:C:481:VAL:HB	2.11	0.49
1:C:510:LYS:HZ1	1:C:738:ALA:HA	1.78	0.49
1:D:236:VAL:HG22	1:D:237:ASP:O	2.12	0.49
1:D:507:PHE:HA	1:D:510:LYS:HZ2	1.77	0.49
1:D:620:PRO:HB2	1:D:669:PHE:CD2	2.42	0.49
1:D:650:SER:O	1:D:651:GLY:C	2.56	0.49
1:A:382:ASN:HB3	1:A:385:TYR:H	1.78	0.49
1:A:495:ASP:O	1:A:499:GLN:N	2.31	0.49
1:A:507:PHE:HD1	1:A:738:ALA:HB2	1.76	0.49
1:A:736:LEU:O	1:A:739:SER:N	2.45	0.49
1:B:521:GLU:HG2	1:B:522:SER:N	2.28	0.49
1:D:232:THR:HG21	1:D:356:TYR:OH	2.13	0.49
1:D:269:LEU:C	1:D:269:LEU:HD12	2.37	0.49
1:D:614:VAL:HG23	1:D:631:ILE:HG13	1.94	0.49
1:D:770:TRP:NE1	1:D:812:PHE:HA	2.27	0.49
2:E:191:GLU:HA	2:E:271:PHE:O	2.13	0.49
1:A:109:PHE:O	1:A:110:TYR:C	2.54	0.49
1:A:504:MET:HG2	1:A:658:LEU:HD22	1.94	0.49
1:A:527:GLU:OE1	1:A:528:LYS:N	2.45	0.49
1:A:657:GLU:O	1:A:660:HIS:N	2.45	0.49
1:A:704:GLN:HE22	1:A:832:CYS:N	2.10	0.49
1:A:807:GLN:HA	1:A:824:MET:CE	2.42	0.49
1:B:504:MET:HG2	1:B:658:LEU:HD22	1.94	0.49
1:B:540:PRO:HB3	1:B:607:PHE:CD2	2.48	0.49
1:B:831:ARG:O	1:B:833:LYS:N	2.46	0.49
1:C:246:TYR:HB3	1:C:248:ILE:HD11	1.95	0.49
1:C:265:PHE:O	1:C:268:GLU:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:251:ILE:HA	2:F:416:ASP:HA	1.94	0.49
1:A:246:TYR:CZ	1:A:595:PHE:HZ	2.30	0.49
1:A:273:THR:HG22	1:A:277:GLU:OE2	2.13	0.49
1:A:567:ALA:HA	1:A:589:TYR:OH	2.12	0.49
1:A:659:VAL:O	1:A:662:PHE:N	2.36	0.49
1:C:201:PRO:HB3	1:C:297:MET:HE1	1.95	0.49
1:C:216:GLU:O	1:C:218:GLY:N	2.46	0.49
1:C:230:MET:HE1	1:C:356:TYR:CE2	2.47	0.49
1:C:475:PRO:HG2	1:C:476:TYR:CD2	2.47	0.49
1:D:333:GLU:OE1	1:D:333:GLU:N	2.42	0.49
1:D:789:ARG:HA	1:D:792:THR:HG22	1.94	0.49
1:A:471:THR:HG22	1:A:478:THR:HG21	1.95	0.49
1:A:652:THR:O	1:A:655:GLY:N	2.46	0.49
1:B:172:SER:O	1:B:174:VAL:N	2.46	0.49
1:B:462:ALA:HA	1:B:465:LYS:HZ3	1.78	0.49
1:B:647:PHE:HA	1:B:651:GLY:HA3	1.95	0.49
1:C:143:SER:O	1:C:146:VAL:HG12	2.13	0.49
1:C:277:GLU:HG3	1:C:299:LYS:HZ2	1.78	0.49
1:C:528:LYS:O	1:C:531:ASN:N	2.46	0.49
1:D:408:TYR:O	1:D:411:VAL:HB	2.13	0.49
1:A:239:LYS:HD3	1:A:329:TYR:CZ	2.37	0.48
1:B:142:ASN:O	1:B:145:ILE:N	2.46	0.48
1:B:579:TYR:HA	1:B:582:LEU:HB2	1.94	0.48
1:B:693:GLY:O	1:B:697:MET:HG2	2.13	0.48
1:B:756:ARG:HD2	1:B:761:GLU:O	2.13	0.48
1:C:333:GLU:C	1:C:335:PHE:H	2.20	0.48
1:C:483:VAL:CG1	1:C:489:ARG:HH11	2.26	0.48
1:A:499:GLN:HG2	1:A:647:PHE:HE1	1.77	0.48
1:A:614:VAL:HA	1:A:631:ILE:CG2	2.43	0.48
1:A:649:GLY:O	1:A:652:THR:N	2.46	0.48
1:A:814:LYS:O	1:A:816:PHE:N	2.46	0.48
1:B:335:PHE:O	1:B:338:SER:OG	2.31	0.48
1:B:506:THR:HG21	1:B:742:ALA:HB2	1.94	0.48
1:B:530:ILE:HG12	1:B:662:PHE:HZ	1.79	0.48
1:C:517:TRP:CD1	1:C:518:MET:N	2.81	0.48
1:C:806:LEU:O	1:C:807:GLN:C	2.56	0.48
2:F:92:GLY:N	2:F:225:LEU:O	2.29	0.48
1:A:166:THR:O	1:A:167:LYS:C	2.55	0.48
1:A:187:ASN:OD1	1:A:188:GLU:HG3	2.13	0.48
1:A:529:LYS:O	1:A:532:GLU:HB3	2.14	0.48
1:A:729:ASN:O	1:A:730:ILE:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:GLU:O	1:A:749:MET:HG2	2.13	0.48
1:B:173:CYS:HA	1:B:579:TYR:CE2	2.48	0.48
1:B:234:VAL:HG23	1:B:234:VAL:O	2.12	0.48
1:C:91:ALA:HB2	1:C:641:PHE:CD2	2.48	0.48
1:C:162:THR:HA	1:C:165:ILE:CD1	2.44	0.48
1:C:162:THR:HA	1:C:165:ILE:HD12	1.95	0.48
1:C:811:SER:O	1:C:814:LYS:N	2.47	0.48
1:D:559:ASP:CG	1:D:560:ASP:H	2.20	0.48
1:A:100:ASP:O	1:A:112:PHE:HD1	1.96	0.48
1:A:174:VAL:O	1:A:174:VAL:HG12	2.12	0.48
1:A:632:LEU:O	1:A:637:TYR:HD2	1.96	0.48
1:B:146:VAL:HA	1:B:149:LEU:HG	1.94	0.48
1:B:268:GLU:O	1:B:272:ARG:HB2	2.14	0.48
1:B:529:LYS:NZ	1:B:669:PHE:O	2.46	0.48
1:B:569:ASN:O	1:B:589:TYR:OH	2.29	0.48
1:B:657:GLU:O	1:B:658:LEU:C	2.55	0.48
1:B:691:LYS:O	1:B:692:ASN:C	2.56	0.48
1:D:270:ASP:OD1	1:D:271:ALA:N	2.46	0.48
2:E:317:ILE:O	2:E:403:LEU:N	2.39	0.48
1:A:146:VAL:HG22	1:A:467:VAL:HG21	1.96	0.48
1:A:606:ASN:CG	1:A:607:PHE:N	2.71	0.48
1:A:670:ASP:O	1:A:673:GLY:N	2.46	0.48
1:B:161:GLN:O	1:B:164:ARG:N	2.47	0.48
1:C:579:TYR:O	1:C:582:LEU:N	2.45	0.48
1:C:821:GLY:C	1:C:822:GLN:HG3	2.38	0.48
1:D:628:PRO:O	1:D:631:ILE:HG22	2.13	0.48
1:D:631:ILE:O	1:D:633:THR:N	2.47	0.48
2:E:345:GLU:N	2:E:348:GLU:HA	2.28	0.48
1:B:187:ASN:OD1	1:B:188:GLU:N	2.47	0.48
1:B:234:VAL:HG12	1:B:246:TYR:HA	1.94	0.48
1:C:483:VAL:HG13	1:C:489:ARG:HH11	1.79	0.48
1:C:537:TYR:O	1:C:539:TRP:N	2.45	0.48
1:C:625:LEU:C	1:C:626:THR:HG1	2.20	0.48
1:D:122:ASP:O	1:D:780:LYS:NZ	2.43	0.48
1:D:560:ASP:N	1:D:560:ASP:OD1	2.45	0.48
1:D:632:LEU:CD2	1:D:650:SER:HB3	2.44	0.48
2:F:359:THR:HA	2:F:371:ILE:O	2.14	0.48
1:A:134:PHE:CE1	1:A:636:HIS:CE1	2.96	0.48
1:A:399:GLN:OE1	1:A:399:GLN:N	2.46	0.48
1:A:464:MET:O	1:A:465:LYS:C	2.57	0.48
1:A:489:ARG:O	1:A:493:VAL:HG22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ASP:OD1	1:A:491:GLN:N	2.45	0.48
1:B:222:GLN:HA	1:B:591:ASN:HD21	1.77	0.48
1:B:653:VAL:HA	1:B:656:HIS:HB3	1.94	0.48
1:C:239:LYS:HB2	1:C:329:TYR:OH	2.13	0.48
1:C:246:TYR:HD2	1:C:378:VAL:HG12	1.78	0.48
1:C:386:MET:HE3	1:D:391:THR:HG22	1.91	0.48
1:C:761:GLU:O	1:C:763:PHE:N	2.47	0.48
1:D:88:TRP:CD2	1:D:642:PRO:HG3	2.47	0.48
1:D:756:ARG:HB2	1:D:756:ARG:HH11	1.79	0.48
1:A:705:TYR:HE2	1:A:729:ASN:CG	2.22	0.48
1:B:259:PHE:HE2	1:B:265:PHE:HB3	1.79	0.48
1:B:373:VAL:HG12	1:B:376:GLY:HA3	1.95	0.48
1:C:636:HIS:O	1:C:638:ASP:N	2.41	0.48
1:D:101:GLU:OE2	1:D:762:LYS:HE2	2.13	0.48
1:D:480:TYR:HB2	1:D:543:LEU:CD2	2.39	0.48
2:E:77:THR:HA	2:E:83:GLN:O	2.14	0.48
1:A:807:GLN:CA	1:A:824:MET:CE	2.91	0.48
1:B:800:CYS:O	1:B:801:ARG:C	2.57	0.48
1:C:161:GLN:O	1:C:165:ILE:HG13	2.14	0.48
1:C:515:LEU:HD21	1:C:523:TYR:CD2	2.49	0.48
1:C:541:LYS:O	1:C:542:LYS:HD3	2.14	0.48
2:E:167:TYR:O	2:E:169:GLU:N	2.41	0.48
2:F:94:ALA:CB	2:F:231:ALA:HA	2.44	0.48
1:A:242:SER:HA	1:A:602:ALA:HB3	1.96	0.48
1:A:313:ALA:O	1:A:315:ALA:N	2.47	0.48
1:A:620:PRO:HG2	1:A:669:PHE:CE2	2.49	0.48
1:B:280:MET:C	1:B:281:LYS:HD2	2.38	0.48
1:B:467:VAL:O	1:B:471:THR:OG1	2.30	0.48
1:B:507:PHE:HA	1:B:510:LYS:HZ3	1.79	0.48
1:B:781:GLU:O	1:B:783:GLN:NE2	2.47	0.48
1:C:108:ASP:HB2	1:C:110:TYR:HE2	1.70	0.48
1:C:357:ILE:O	1:C:360:LEU:N	2.47	0.48
1:C:572:THR:HG21	1:C:582:LEU:HD22	1.95	0.48
1:D:324:ASN:OD1	1:D:326:GLU:N	2.47	0.48
1:A:161:GLN:O	1:A:164:ARG:HB3	2.13	0.47
1:A:537:TYR:N	1:A:537:TYR:CD1	2.82	0.47
1:A:644:ALA:O	1:A:645:PHE:C	2.57	0.47
1:C:412:HIS:O	1:C:415:PHE:N	2.47	0.47
1:C:562:TYR:O	1:C:565:LEU:N	2.41	0.47
1:C:646:ASN:OD1	1:C:647:PHE:N	2.47	0.47
1:C:793:ASN:HB3	1:C:795:HIS:ND1	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:GLU:O	1:D:310:GLN:C	2.57	0.47
1:D:414:LEU:O	1:D:416:GLU:N	2.47	0.47
2:E:416:ASP:O	2:E:420:ASN:N	2.46	0.47
1:A:726:GLN:HA	1:A:729:ASN:HB2	1.95	0.47
1:B:324:ASN:O	1:B:327:GLN:HG2	2.14	0.47
1:B:583:ASN:O	1:B:586:ARG:N	2.46	0.47
1:C:163:GLU:O	1:C:166:THR:OG1	2.29	0.47
1:C:177:THR:O	1:C:180:ASP:N	2.43	0.47
1:C:197:PHE:HB3	1:C:216:GLU:HG3	1.94	0.47
1:C:317:TRP:CD2	1:C:382:ASN:OD1	2.67	0.47
1:C:473:TYR:O	1:C:475:PRO:HD3	2.15	0.47
1:D:528:LYS:O	1:D:529:LYS:C	2.56	0.47
1:D:637:TYR:OH	1:D:639:LEU:HA	2.14	0.47
1:B:757:LEU:HD11	1:B:768:ILE:HD13	1.94	0.47
1:C:96:LEU:HD13	1:C:760:LEU:HD23	1.95	0.47
1:C:246:TYR:HB2	1:C:378:VAL:HG12	1.95	0.47
1:C:261:VAL:HG11	1:D:323:ARG:HB3	1.94	0.47
1:C:775:TYR:O	1:C:777:TRP:N	2.46	0.47
1:D:298:ILE:HG13	1:D:299:LYS:N	2.30	0.47
1:D:331:PRO:HB2	1:D:377:ASP:OD1	2.14	0.47
1:D:641:PHE:N	1:D:641:PHE:CD1	2.81	0.47
1:D:709:CYS:SG	1:D:720:ALA:HB1	2.54	0.47
1:B:490:ASP:N	1:B:490:ASP:OD1	2.45	0.47
1:B:511:MET:HG3	1:B:513:SER:N	2.29	0.47
1:B:515:LEU:HB2	1:B:518:MET:HE3	1.96	0.47
1:B:696:ASP:HB3	1:B:697:MET:HE2	1.95	0.47
1:C:193:ILE:O	1:C:196:ARG:HB3	2.14	0.47
1:C:482:TYR:OH	1:C:486:ARG:NH2	2.47	0.47
1:C:733:LEU:HD12	1:C:733:LEU:O	2.15	0.47
1:C:764:THR:H	1:C:767:GLN:NE2	2.12	0.47
1:D:480:TYR:CB	1:D:543:LEU:HD21	2.41	0.47
1:D:503:ILE:O	1:D:504:MET:C	2.57	0.47
1:A:146:VAL:HA	1:A:149:LEU:HD12	1.95	0.47
1:A:770:TRP:O	1:A:771:ILE:C	2.55	0.47
1:B:115:ASN:C	1:B:115:ASN:OD1	2.58	0.47
1:B:310:GLN:C	1:B:312:ILE:N	2.72	0.47
1:B:631:ILE:HD11	1:B:636:HIS:CD2	2.50	0.47
1:C:171:GLN:O	1:C:175:GLU:HG2	2.14	0.47
1:C:199:GLY:O	1:C:200:ILE:HG23	2.14	0.47
1:D:756:ARG:HB2	1:D:756:ARG:NH1	2.29	0.47
1:A:256:PRO:HG3	1:A:792:THR:HB	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LYS:C	1:A:510:LYS:HG2	2.39	0.47
1:A:522:SER:O	1:A:523:TYR:C	2.55	0.47
1:A:562:TYR:N	1:A:562:TYR:CD1	2.79	0.47
1:B:270:ASP:C	1:B:272:ARG:N	2.68	0.47
1:B:341:LYS:CE	1:B:353:PHE:CE2	2.95	0.47
1:B:617:TRP:CD1	1:B:626:THR:OG1	2.68	0.47
1:B:747:ILE:HG13	1:B:748:LYS:N	2.29	0.47
1:D:704:GLN:HG2	1:D:831:ARG:NH1	2.30	0.47
2:F:379:GLU:O	2:F:383:ASP:HA	2.14	0.47
1:A:272:ARG:O	1:A:276:ILE:HG12	2.15	0.47
1:A:307:GLN:O	1:A:311:LYS:HD3	2.14	0.47
1:A:320:ASP:OD2	1:B:262:LEU:HD21	2.14	0.47
1:A:539:TRP:CD1	1:A:543:LEU:HD12	2.50	0.47
1:A:705:TYR:CE2	1:A:729:ASN:CG	2.93	0.47
1:B:172:SER:OG	1:B:173:CYS:N	2.48	0.47
1:B:407:ASN:O	1:B:408:TYR:C	2.57	0.47
1:B:488:ASP:OD1	1:B:488:ASP:N	2.46	0.47
1:B:569:ASN:HB3	1:B:589:TYR:OH	2.15	0.47
1:B:812:PHE:O	1:B:813:ALA:C	2.56	0.47
1:B:813:ALA:HB1	1:B:820:LEU:HD21	1.96	0.47
1:C:103:VAL:CG1	1:C:108:ASP:CG	2.86	0.47
1:C:161:GLN:O	1:C:164:ARG:N	2.47	0.47
1:C:503:ILE:O	1:C:506:THR:OG1	2.23	0.47
1:C:770:TRP:HA	1:C:770:TRP:CE3	2.49	0.47
1:D:562:TYR:O	1:D:565:LEU:N	2.47	0.47
1:D:697:MET:O	1:D:700:CYS:HB3	2.14	0.47
1:B:239:LYS:HE3	1:B:329:TYR:CE2	2.50	0.47
1:B:380:VAL:O	1:B:381:THR:C	2.57	0.47
1:B:587:ARG:O	1:B:588:GLY:C	2.58	0.47
1:C:385:TYR:O	1:C:386:MET:C	2.58	0.47
1:D:137:ALA:O	1:D:138:GLN:C	2.58	0.47
1:D:637:TYR:CD1	1:D:646:ASN:OD1	2.67	0.47
1:A:478:THR:O	1:A:481:VAL:HB	2.15	0.47
1:A:498:GLN:O	1:A:502:LEU:HD23	2.15	0.47
1:A:539:TRP:HA	1:A:607:PHE:CZ	2.50	0.47
1:B:759:GLY:O	1:B:760:LEU:HD23	2.15	0.47
1:C:230:MET:HE2	1:C:356:TYR:CE2	2.49	0.47
1:D:725:THR:HG21	1:D:795:HIS:O	2.14	0.47
1:B:243:ARG:O	1:B:602:ALA:HB2	2.15	0.47
1:B:388:PHE:CE1	1:B:405:PHE:HZ	2.33	0.47
1:B:529:LYS:HG3	1:B:671:TYR:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:ARG:NH2	1:B:672:ASP:HA	2.28	0.47
1:B:659:VAL:HG11	1:B:731:ALA:HA	1.97	0.47
1:B:810:PRO:CD	1:B:831:ARG:HD2	2.45	0.47
1:D:524:ARG:O	1:D:527:GLU:HB3	2.14	0.47
1:D:707:ALA:O	1:D:708:GLN:OE1	2.33	0.47
2:E:161:LYS:CB	2:E:183:ASN:H	2.28	0.47
1:A:234:VAL:CG2	1:A:235:ASN:H	2.25	0.46
1:A:352:ARG:HD2	1:A:393:PHE:CB	2.46	0.46
1:A:705:TYR:C	1:A:707:ALA:N	2.73	0.46
1:B:329:TYR:O	1:B:330:ASN:OD1	2.33	0.46
1:B:512:LEU:HD22	1:B:520:GLY:HA2	1.97	0.46
1:B:540:PRO:HD2	1:B:543:LEU:HB2	1.98	0.46
1:C:108:ASP:OD1	1:C:108:ASP:O	2.32	0.46
1:C:295:ASP:CG	1:C:298:ILE:HG12	2.40	0.46
1:C:322:LEU:O	1:C:323:ARG:HD3	2.14	0.46
1:D:393:PHE:HD1	1:D:405:PHE:CE2	2.30	0.46
1:D:540:PRO:HD3	1:D:607:PHE:CZ	2.49	0.46
1:D:745:GLU:O	1:D:748:LYS:N	2.49	0.46
1:D:808:ASP:HA	1:D:831:ARG:CG	2.45	0.46
1:A:88:TRP:CE2	1:A:642:PRO:HD3	2.51	0.46
1:A:725:THR:C	1:A:729:ASN:HD22	2.23	0.46
1:A:787:VAL:O	1:A:790:LEU:HB3	2.14	0.46
1:B:267:PRO:C	1:B:269:LEU:N	2.71	0.46
1:B:294:TYR:N	1:B:294:TYR:CD1	2.79	0.46
1:B:405:PHE:O	1:B:408:TYR:N	2.48	0.46
1:B:503:ILE:O	1:B:504:MET:C	2.58	0.46
1:B:759:GLY:O	1:B:760:LEU:CD2	2.63	0.46
1:B:809:ILE:HA	1:B:831:ARG:NH1	2.29	0.46
1:C:196:ARG:HG2	1:C:197:PHE:CE1	2.50	0.46
1:C:495:ASP:HA	1:C:498:GLN:OE1	2.14	0.46
1:C:696:ASP:O	1:C:699:GLN:HB3	2.15	0.46
1:C:768:ILE:O	1:C:769:PHE:C	2.56	0.46
1:A:524:ARG:O	1:A:525:ARG:C	2.58	0.46
1:A:796:SER:HB3	1:A:797:PRO:HD2	1.97	0.46
1:B:162:THR:HG21	1:B:477:GLY:HA2	1.98	0.46
1:C:260:TYR:C	1:C:262:LEU:N	2.73	0.46
1:C:487:GLU:HA	1:C:489:ARG:HG3	1.98	0.46
1:C:520:GLY:O	1:C:523:TYR:N	2.49	0.46
1:C:588:GLY:HA3	1:C:592:ARG:NH2	2.30	0.46
2:E:327:VAL:HA	2:E:401:TRP:HA	1.96	0.46
1:A:116:LYS:O	1:A:119:GLU:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ILE:C	1:A:633:THR:H	2.24	0.46
1:C:143:SER:O	1:C:144:ASP:C	2.58	0.46
1:C:311:LYS:O	1:C:312:ILE:C	2.58	0.46
1:C:329:TYR:CD1	1:C:331:PRO:HD3	2.51	0.46
1:C:782:THR:OG1	1:C:783:GLN:N	2.49	0.46
1:D:300:THR:O	1:D:301:ALA:C	2.58	0.46
1:A:572:THR:HG22	1:A:573:ASP:N	2.30	0.46
1:B:217:MET:O	1:B:220:ILE:HG22	2.15	0.46
1:B:231:TYR:CD2	1:B:233:TRP:CZ3	3.02	0.46
1:B:626:THR:O	1:B:627:LEU:HD23	2.16	0.46
1:C:218:GLY:O	1:C:221:GLU:HG2	2.16	0.46
1:C:515:LEU:HD23	1:C:518:MET:CG	2.44	0.46
1:D:134:PHE:O	1:D:135:SER:C	2.58	0.46
1:D:250:GLN:CD	1:D:382:ASN:OD1	2.58	0.46
1:A:504:MET:HB2	1:A:504:MET:HE3	1.65	0.46
1:A:649:GLY:O	1:A:650:SER:C	2.59	0.46
1:B:543:LEU:HD12	1:B:563:SER:HB3	1.98	0.46
1:B:595:PHE:O	1:B:598:LYS:N	2.39	0.46
1:B:725:THR:O	1:B:726:GLN:C	2.58	0.46
1:B:809:ILE:O	1:B:810:PRO:C	2.58	0.46
1:C:268:GLU:O	1:C:271:ALA:HB3	2.15	0.46
1:C:497:LYS:O	1:C:498:GLN:C	2.58	0.46
1:C:570:ASN:O	1:C:571:LYS:HB2	2.15	0.46
1:D:508:LEU:HD11	1:D:527:GLU:HG3	1.97	0.46
1:A:332:TYR:O	1:A:378:VAL:HG12	2.15	0.46
1:C:353:PHE:O	1:C:356:TYR:HB3	2.15	0.46
1:C:511:MET:C	1:C:523:TYR:HE2	2.23	0.46
1:C:595:PHE:O	1:C:596:ARG:C	2.59	0.46
1:C:766:ASN:O	1:C:769:PHE:HB3	2.16	0.46
1:C:823:LYS:O	1:C:824:MET:CG	2.53	0.46
1:D:149:LEU:HD11	1:D:167:LYS:HA	1.98	0.46
1:D:408:TYR:CE1	1:D:412:HIS:CD2	3.04	0.46
1:B:172:SER:HB2	1:B:579:TYR:HD2	1.81	0.46
1:B:259:PHE:CZ	1:B:263:PRO:HB2	2.51	0.46
1:B:631:ILE:C	1:B:633:THR:HG22	2.41	0.46
1:C:500:THR:O	1:C:504:MET:HG2	2.15	0.46
1:D:118:ILE:HG23	1:D:780:LYS:HG3	1.97	0.46
1:D:261:VAL:HB	1:D:314:MET:CE	2.46	0.46
1:D:276:ILE:HG23	1:D:277:GLU:N	2.30	0.46
1:D:302:ALA:O	1:D:303:ARG:C	2.59	0.46
1:D:330:ASN:OD1	1:D:330:ASN:N	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:PHE:HE1	1:D:405:PHE:CD2	2.34	0.46
1:D:467:VAL:O	1:D:470:ILE:HB	2.16	0.46
1:D:739:SER:O	1:D:742:ALA:HB3	2.16	0.46
2:F:75:LYS:HA	2:F:86:HIS:HA	1.98	0.46
1:A:191:GLN:O	1:A:194:SER:OG	2.31	0.46
1:B:279:VAL:C	1:B:282:ALA:H	2.24	0.46
1:B:528:LYS:O	1:B:531:ASN:N	2.49	0.46
1:B:822:GLN:C	1:B:824:MET:H	2.23	0.46
1:C:246:TYR:CD2	1:C:378:VAL:HG12	2.51	0.46
1:C:303:ARG:O	1:C:307:GLN:HB2	2.15	0.46
1:C:659:VAL:O	1:C:661:GLY:N	2.49	0.46
1:A:309:GLU:HA	1:A:312:ILE:HD12	1.97	0.46
1:A:352:ARG:HD2	1:A:393:PHE:HB2	1.98	0.46
1:A:355:LYS:C	1:A:357:ILE:N	2.74	0.46
1:A:413:MET:O	1:A:416:GLU:CG	2.64	0.46
1:A:533:MET:CG	1:A:623:ASN:HD21	2.28	0.46
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.72	0.46
1:B:539:TRP:HD1	1:B:540:PRO:O	1.97	0.46
1:C:306:THR:O	1:C:309:GLU:HB2	2.16	0.46
1:C:522:SER:O	1:C:525:ARG:HB3	2.16	0.46
1:C:786:LEU:HD12	1:C:786:LEU:HA	1.70	0.46
1:D:507:PHE:HD1	1:D:510:LYS:NZ	2.13	0.46
2:E:326:GLY:O	2:E:402:ILE:N	2.49	0.46
2:E:337:ASP:O	2:E:340:GLY:N	2.39	0.46
1:A:488:ASP:HB3	1:A:491:GLN:OE1	2.16	0.45
1:B:239:LYS:HD3	1:B:675:LEU:HB2	1.97	0.45
1:B:299:LYS:O	1:B:302:ALA:N	2.49	0.45
1:B:561:TYR:CA	1:B:564:ILE:HG22	2.45	0.45
1:B:729:ASN:O	1:B:732:ASP:HB2	2.16	0.45
1:C:150:GLU:OE1	1:C:150:GLU:N	2.40	0.45
1:C:234:VAL:HG23	1:C:245:SER:O	2.15	0.45
1:D:224:ARG:HH11	1:D:413:MET:HE2	1.80	0.45
1:D:631:ILE:HG23	1:D:632:LEU:HG	1.98	0.45
1:D:631:ILE:CG2	1:D:632:LEU:N	2.79	0.45
2:E:186:VAL:O	2:E:198:VAL:HA	2.16	0.45
1:A:98:GLY:CA	1:A:116:LYS:CB	2.81	0.45
1:A:661:GLY:O	1:A:662:PHE:HD1	1.98	0.45
1:A:721:ASN:ND2	1:A:724:HIS:HB3	2.31	0.45
1:B:303:ARG:O	1:B:306:THR:HB	2.16	0.45
1:B:519:GLN:CD	1:B:520:GLY:N	2.75	0.45
1:B:798:ASN:O	1:B:799:SER:C	2.58	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLU:CD	1:C:639:LEU:HD23	2.42	0.45
1:C:191:GLN:O	1:C:192:TYR:C	2.59	0.45
1:C:758:PRO:O	1:C:760:LEU:N	2.48	0.45
1:D:503:ILE:HD11	1:D:651:GLY:HA2	1.98	0.45
2:F:287:TYR:HA	2:F:423:GLY:HA2	1.98	0.45
1:B:386:MET:HG3	1:B:386:MET:O	2.14	0.45
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.65	0.45
1:C:621:GLU:CD	1:C:621:GLU:N	2.74	0.45
1:C:705:TYR:CZ	1:C:729:ASN:ND2	2.85	0.45
1:D:273:THR:O	1:D:276:ILE:HG22	2.16	0.45
1:D:614:VAL:HG23	1:D:631:ILE:CG1	2.46	0.45
1:A:320:ASP:OD2	1:A:723:ALA:HB3	2.17	0.45
1:A:320:ASP:OD2	1:B:262:LEU:CD2	2.65	0.45
1:A:486:ARG:HH12	1:A:633:THR:HB	1.80	0.45
1:A:535:ARG:HB3	1:A:537:TYR:CE1	2.51	0.45
1:A:539:TRP:HB2	1:A:540:PRO:HD2	1.97	0.45
1:A:762:LYS:HD3	1:C:817:GLN:N	2.31	0.45
1:B:659:VAL:HG12	1:B:663:ASP:OD1	2.16	0.45
1:B:805:VAL:O	1:B:805:VAL:CG1	2.63	0.45
1:C:167:LYS:HG3	1:C:168:ALA:N	2.31	0.45
1:C:513:SER:C	1:C:515:LEU:H	2.25	0.45
1:C:583:ASN:HD21	1:C:587:ARG:NH2	2.13	0.45
1:C:722:GLY:O	1:C:725:THR:HG23	2.16	0.45
1:D:300:THR:OG1	1:D:301:ALA:N	2.49	0.45
1:A:812:PHE:CE1	1:A:816:PHE:HD2	2.34	0.45
1:B:142:ASN:O	1:B:145:ILE:CG2	2.53	0.45
1:B:295:ASP:O	1:B:296:LYS:C	2.59	0.45
1:B:510:LYS:HZ1	1:B:738:ALA:HB2	1.81	0.45
1:B:511:MET:HG2	1:B:513:SER:OG	2.17	0.45
1:C:216:GLU:O	1:C:219:ARG:HG3	2.16	0.45
1:C:614:VAL:O	1:C:614:VAL:CG1	2.61	0.45
1:C:739:SER:OG	1:C:740:TYR:N	2.48	0.45
1:D:480:TYR:HB2	1:D:543:LEU:CD1	2.43	0.45
1:A:540:PRO:HD3	1:A:607:PHE:CE2	2.51	0.45
1:A:560:ASP:OD1	1:A:561:TYR:N	2.49	0.45
1:B:259:PHE:O	1:B:259:PHE:CD2	2.70	0.45
1:B:419:GLU:O	1:B:426:LEU:HD11	2.17	0.45
1:B:754:GLU:O	1:B:755:MET:C	2.60	0.45
1:B:832:CYS:O	1:B:834:VAL:N	2.49	0.45
1:C:106:CYS:HA	1:C:824:MET:HG3	1.99	0.45
1:C:511:MET:HA	1:C:514:THR:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:GLU:OE1	1:C:521:GLU:N	2.38	0.45
1:D:269:LEU:HD12	1:D:270:ASP:N	2.32	0.45
1:D:461:ASP:OD1	1:D:462:ALA:N	2.50	0.45
1:D:745:GLU:O	1:D:746:TYR:C	2.60	0.45
1:D:816:PHE:HB3	1:D:818:CYS:SG	2.57	0.45
1:A:319:ASP:O	1:A:320:ASP:C	2.59	0.45
1:A:319:ASP:HA	1:A:322:LEU:HD12	1.98	0.45
1:A:765:PRO:O	1:A:766:ASN:C	2.59	0.45
1:B:766:ASN:O	1:B:767:GLN:C	2.60	0.45
1:B:770:TRP:CD1	1:B:770:TRP:H	2.35	0.45
1:C:504:MET:SD	1:C:535:ARG:NH2	2.89	0.45
1:C:533:MET:HA	1:C:623:ASN:OD1	2.17	0.45
1:D:139:LEU:O	1:D:140:GLU:C	2.59	0.45
1:D:760:LEU:HD11	1:D:763:PHE:CD2	2.38	0.45
1:A:559:ASP:CG	1:A:560:ASP:H	2.25	0.45
1:B:221:GLU:O	1:B:225:ALA:N	2.36	0.45
1:B:231:TYR:CD2	1:B:233:TRP:CE3	3.05	0.45
1:B:536:ASN:C	1:B:537:TYR:HD1	2.25	0.45
1:B:652:THR:O	1:B:655:GLY:N	2.50	0.45
1:B:740:TYR:HA	1:B:769:PHE:HE2	1.82	0.45
1:C:166:THR:O	1:C:169:ALA:N	2.50	0.45
1:C:518:MET:HB2	1:C:522:SER:OG	2.16	0.45
1:C:821:GLY:O	1:C:822:GLN:CG	2.59	0.45
1:D:171:GLN:O	1:D:174:VAL:HG22	2.17	0.45
1:D:523:TYR:O	1:D:527:GLU:HB2	2.17	0.45
1:D:632:LEU:HD21	1:D:650:SER:HB2	1.98	0.45
1:D:814:LYS:C	1:D:814:LYS:HD3	2.42	0.45
2:E:255:TYR:C	2:E:270:ALA:O	2.59	0.45
1:B:636:HIS:O	1:B:649:GLY:HA3	2.17	0.45
1:B:732:ASP:CB	1:B:805:VAL:HG21	2.46	0.45
1:C:536:ASN:C	1:C:537:TYR:CG	2.95	0.45
1:C:806:LEU:HA	1:C:806:LEU:HD23	1.69	0.45
1:A:762:LYS:O	1:A:763:PHE:CG	2.70	0.45
1:B:424:LYS:C	1:B:427:ARG:HE	2.24	0.45
1:C:473:TYR:HA	1:C:590:GLU:HG3	1.99	0.45
1:C:570:ASN:ND2	1:C:589:TYR:CE1	2.85	0.45
1:D:270:ASP:O	1:D:271:ALA:C	2.59	0.45
1:D:670:ASP:O	1:D:672:ASP:N	2.50	0.45
1:B:317:TRP:CE3	1:B:382:ASN:ND2	2.86	0.44
1:B:598:LYS:HG3	1:B:599:ASN:N	2.31	0.44
1:B:669:PHE:HE1	1:B:675:LEU:HD21	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:824:MET:O	1:B:824:MET:HG2	2.17	0.44
1:A:489:ARG:C	1:A:493:VAL:HG22	2.42	0.44
1:C:618:TYR:HE1	1:C:623:ASN:HA	1.82	0.44
1:C:627:LEU:HB3	1:C:628:PRO:HD2	1.99	0.44
1:D:480:TYR:HD2	1:D:543:LEU:CG	2.27	0.44
2:F:342:GLN:O	2:F:351:THR:N	2.42	0.44
1:A:499:GLN:O	1:A:500:THR:C	2.61	0.44
1:A:657:GLU:O	1:A:660:HIS:HB3	2.17	0.44
1:B:382:ASN:C	1:B:384:ALA:N	2.75	0.44
1:C:172:SER:OG	1:C:173:CYS:N	2.48	0.44
1:C:267:PRO:HG3	1:D:695:LYS:HE2	1.99	0.44
1:C:412:HIS:O	1:C:413:MET:C	2.58	0.44
1:C:489:ARG:O	1:C:493:VAL:HG23	2.17	0.44
1:C:544:PHE:CG	1:C:545:GLY:N	2.85	0.44
1:C:770:TRP:CZ2	1:C:812:PHE:HB2	2.52	0.44
1:D:764:THR:O	1:D:765:PRO:C	2.59	0.44
1:D:806:LEU:C	1:D:824:MET:HE1	2.41	0.44
1:A:223:GLN:C	1:A:224:ARG:HG2	2.42	0.44
1:A:238:HIS:NE2	1:A:621:GLU:HG3	2.31	0.44
1:A:487:GLU:HB3	1:A:489:ARG:HH12	1.83	0.44
1:B:224:ARG:HA	1:B:224:ARG:HD3	1.71	0.44
1:B:229:PHE:O	1:B:230:MET:HB3	2.16	0.44
1:B:268:GLU:O	1:B:272:ARG:CB	2.66	0.44
1:B:618:TYR:O	1:B:620:PRO:HD3	2.18	0.44
1:B:649:GLY:O	1:B:650:SER:C	2.60	0.44
1:B:810:PRO:O	1:B:813:ALA:N	2.51	0.44
1:C:382:ASN:O	1:C:383:PRO:C	2.60	0.44
1:C:524:ARG:HA	1:C:527:GLU:HB3	1.99	0.44
1:C:526:ALA:O	1:C:527:GLU:C	2.60	0.44
1:C:618:TYR:HA	1:C:624:SER:O	2.17	0.44
1:C:704:GLN:O	1:C:705:TYR:C	2.60	0.44
1:C:746:TYR:CG	1:C:746:TYR:O	2.70	0.44
1:A:145:ILE:HD11	1:A:482:TYR:HB2	1.99	0.44
1:A:273:THR:CG2	1:A:277:GLU:OE2	2.66	0.44
1:A:308:ILE:O	1:A:312:ILE:HG13	2.18	0.44
1:A:561:TYR:O	1:A:564:ILE:HG13	2.09	0.44
1:A:723:ALA:C	1:A:725:THR:N	2.74	0.44
1:A:779:ALA:HB3	1:A:798:ASN:OD1	2.16	0.44
1:A:795:HIS:HD2	1:A:801:ARG:NH1	2.16	0.44
1:B:236:VAL:HG12	1:B:237:ASP:O	2.18	0.44
1:B:308:ILE:CG2	1:B:309:GLU:N	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:CD2	1:B:520:GLY:HA2	2.48	0.44
1:B:563:SER:C	1:B:565:LEU:N	2.75	0.44
1:B:695:LYS:HD2	1:B:695:LYS:HA	1.64	0.44
1:C:260:TYR:CE1	1:C:314:MET:SD	3.11	0.44
1:C:698:ALA:O	1:C:699:GLN:C	2.60	0.44
1:C:710:CYS:SG	1:C:786:LEU:HD21	2.57	0.44
1:D:306:THR:O	1:D:309:GLU:HB2	2.18	0.44
1:D:504:MET:CG	1:D:530:ILE:CG2	2.95	0.44
1:D:533:MET:HE2	1:D:625:LEU:CD1	2.47	0.44
1:D:665:GLU:O	1:D:668:GLN:N	2.43	0.44
1:A:704:GLN:HE22	1:A:832:CYS:H	1.66	0.44
1:C:218:GLY:C	1:C:220:ILE:N	2.76	0.44
1:C:378:VAL:O	1:C:379:ILE:HG13	2.17	0.44
1:C:408:TYR:O	1:C:411:VAL:N	2.51	0.44
1:C:740:TYR:O	1:C:743:TYR:N	2.50	0.44
1:D:222:GLN:OE1	1:D:360:LEU:HA	2.17	0.44
1:D:464:MET:O	1:D:465:LYS:C	2.58	0.44
1:D:705:TYR:OH	1:D:800:CYS:SG	2.45	0.44
1:D:763:PHE:HB3	1:D:767:GLN:HB2	1.99	0.44
1:A:137:ALA:O	1:A:140:GLU:N	2.51	0.44
1:A:723:ALA:C	1:A:725:THR:H	2.26	0.44
1:A:812:PHE:O	1:A:813:ALA:C	2.60	0.44
1:B:810:PRO:O	1:B:811:SER:C	2.59	0.44
1:C:171:GLN:O	1:C:172:SER:C	2.59	0.44
1:C:260:TYR:CD2	1:C:262:LEU:HD12	2.53	0.44
1:C:272:ARG:O	1:C:273:THR:C	2.58	0.44
1:D:410:ILE:O	1:D:411:VAL:C	2.61	0.44
1:D:772:SER:O	1:D:773:TYR:C	2.60	0.44
3:G:57:ILE:O	3:G:58:SER:C	2.59	0.44
1:A:173:CYS:O	1:A:175:GLU:N	2.51	0.44
1:B:161:GLN:C	1:B:163:GLU:N	2.73	0.44
1:B:221:GLU:OE2	1:B:226:LEU:N	2.51	0.44
1:B:388:PHE:CD1	1:B:388:PHE:C	2.95	0.44
1:C:302:ALA:O	1:C:306:THR:HG23	2.18	0.44
1:C:520:GLY:O	1:C:521:GLU:C	2.61	0.44
1:C:803:ASN:O	1:C:805:VAL:N	2.51	0.44
1:D:222:GLN:HG3	1:D:359:GLY:O	2.18	0.44
1:A:705:TYR:O	1:A:707:ALA:N	2.51	0.44
1:B:659:VAL:O	1:B:660:HIS:C	2.61	0.44
1:B:806:LEU:O	1:B:807:GLN:C	2.59	0.44
1:C:230:MET:HE1	1:C:356:TYR:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ALA:C	1:D:315:ALA:N	2.75	0.44
1:D:580:THR:HB	1:D:583:ASN:OD1	2.18	0.44
1:D:660:HIS:C	1:D:662:PHE:H	2.26	0.44
1:D:675:LEU:CD1	1:D:676:ALA:N	2.81	0.44
1:D:770:TRP:CD1	1:D:812:PHE:HD1	2.36	0.44
2:E:159:TYR:C	2:E:161:LYS:H	2.25	0.44
1:A:265:PHE:CG	1:A:266:ALA:N	2.86	0.43
1:A:652:THR:O	1:A:653:VAL:C	2.62	0.43
1:B:142:ASN:ND2	1:B:464:MET:SD	2.91	0.43
1:B:764:THR:HG1	1:B:767:GLN:H	1.58	0.43
1:C:313:ALA:O	1:C:314:MET:C	2.61	0.43
1:D:560:ASP:O	1:D:561:TYR:C	2.61	0.43
1:D:657:GLU:O	1:D:658:LEU:C	2.61	0.43
1:D:747:ILE:HD12	1:D:747:ILE:HA	1.83	0.43
2:F:416:ASP:O	2:F:420:ASN:CA	2.66	0.43
1:A:188:GLU:O	1:A:191:GLN:HB3	2.18	0.43
1:A:413:MET:O	1:A:416:GLU:HG2	2.17	0.43
1:A:723:ALA:O	1:A:725:THR:N	2.52	0.43
1:B:740:TYR:O	1:B:741:ASN:C	2.60	0.43
1:B:804:GLN:O	1:B:806:LEU:N	2.51	0.43
1:C:767:GLN:O	1:C:770:TRP:HB2	2.18	0.43
1:D:246:TYR:HH	1:D:595:PHE:HE1	1.55	0.43
1:D:296:LYS:HE3	1:D:296:LYS:HB3	1.81	0.43
1:D:326:GLU:OE2	1:D:668:GLN:NE2	2.50	0.43
1:D:331:PRO:O	1:D:332:TYR:HD1	2.02	0.43
1:D:530:ILE:HA	1:D:533:MET:CG	2.48	0.43
1:D:618:TYR:HD1	1:D:624:SER:O	2.00	0.43
1:D:637:TYR:CB	1:D:646:ASN:OD1	2.66	0.43
1:D:770:TRP:O	1:D:771:ILE:C	2.60	0.43
1:A:494:GLU:O	1:A:497:LYS:N	2.51	0.43
1:A:496:VAL:HG11	1:A:632:LEU:HD21	1.99	0.43
1:A:663:ASP:N	1:A:663:ASP:OD1	2.49	0.43
1:B:217:MET:CE	1:B:230:MET:HE3	2.34	0.43
1:B:527:GLU:CD	1:B:527:GLU:C	2.86	0.43
1:B:694:PHE:CD1	1:B:694:PHE:C	2.96	0.43
1:C:235:ASN:CG	1:C:236:VAL:H	2.26	0.43
1:C:317:TRP:CZ2	1:D:314:MET:SD	3.11	0.43
1:C:736:LEU:HD21	1:C:770:TRP:CZ3	2.51	0.43
1:A:521:GLU:HA	1:A:524:ARG:NH1	2.33	0.43
1:A:825:TYR:HA	1:A:826:PRO:HD3	1.84	0.43
1:B:410:ILE:O	1:B:411:VAL:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:HIS:C	1:B:662:PHE:H	2.26	0.43
1:B:743:TYR:CD1	1:B:743:TYR:C	2.95	0.43
1:B:822:GLN:O	1:B:824:MET:N	2.51	0.43
1:B:831:ARG:HE	1:B:833:LYS:HB2	1.83	0.43
1:C:185:SER:HA	1:C:187:ASN:ND2	2.34	0.43
1:C:267:PRO:O	1:C:270:ASP:N	2.40	0.43
1:C:295:ASP:CG	1:C:296:LYS:N	2.76	0.43
1:C:497:LYS:HD2	1:C:497:LYS:HA	1.71	0.43
1:C:643:LYS:O	1:C:647:PHE:HB2	2.18	0.43
1:D:762:LYS:HE3	1:D:763:PHE:CZ	2.53	0.43
2:F:365:GLY:C	2:F:367:LYS:H	2.26	0.43
1:A:117:PHE:CE2	1:A:779:ALA:HA	2.48	0.43
1:A:162:THR:O	1:A:163:GLU:C	2.61	0.43
1:A:220:ILE:O	1:A:221:GLU:C	2.59	0.43
1:A:358:ALA:O	1:A:361:MET:N	2.52	0.43
1:A:772:SER:O	1:A:773:TYR:C	2.61	0.43
1:B:272:ARG:O	1:B:273:THR:C	2.61	0.43
1:C:408:TYR:HA	1:C:411:VAL:HG23	1.99	0.43
1:C:705:TYR:O	1:C:707:ALA:N	2.51	0.43
1:D:142:ASN:HB3	1:D:467:VAL:HG11	2.00	0.43
1:D:270:ASP:O	1:D:272:ARG:N	2.51	0.43
1:D:584:ILE:O	1:D:585:LEU:C	2.60	0.43
1:D:643:LYS:HE3	1:D:746:TYR:OH	2.18	0.43
1:D:812:PHE:O	1:D:813:ALA:C	2.62	0.43
1:D:830:GLN:O	1:D:831:ARG:NH2	2.52	0.43
2:E:179:GLY:HA3	2:E:206:GLN:O	2.18	0.43
1:A:527:GLU:O	1:A:528:LYS:C	2.61	0.43
1:A:705:TYR:HD1	1:A:705:TYR:HA	1.57	0.43
1:B:195:GLU:O	1:B:195:GLU:HG2	2.18	0.43
1:B:296:LYS:H	1:B:296:LYS:HD3	1.82	0.43
1:B:742:ALA:O	1:B:743:TYR:C	2.60	0.43
1:B:743:TYR:CE1	1:B:747:ILE:HG21	2.51	0.43
1:C:253:LEU:HA	1:C:253:LEU:HD23	1.74	0.43
1:C:691:LYS:O	1:C:694:PHE:HB3	2.18	0.43
1:C:800:CYS:HA	1:C:804:GLN:HG2	2.00	0.43
1:D:658:LEU:C	1:D:658:LEU:HD23	2.43	0.43
1:D:825:TYR:CZ	1:D:827:PRO:HG3	2.54	0.43
1:A:354:GLY:O	1:A:355:LYS:C	2.62	0.43
1:A:489:ARG:HB3	1:A:493:VAL:CG1	2.48	0.43
1:A:618:TYR:OH	1:A:623:ASN:OD1	2.32	0.43
1:A:643:LYS:HG3	1:A:746:TYR:CZ	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:TYR:C	1:A:707:ALA:H	2.27	0.43
1:A:744:LYS:HD2	1:A:744:LYS:HA	1.45	0.43
1:B:403:TYR:O	1:B:406:VAL:HG12	2.19	0.43
1:B:517:TRP:CD1	1:B:517:TRP:H	2.35	0.43
1:B:670:ASP:OD1	1:B:670:ASP:C	2.62	0.43
1:B:806:LEU:HD11	1:B:812:PHE:CG	2.54	0.43
1:C:134:PHE:HD1	1:C:134:PHE:HA	1.61	0.43
1:C:161:GLN:O	1:C:162:THR:C	2.62	0.43
1:C:175:GLU:O	1:C:178:LEU:HB2	2.19	0.43
1:C:257:ARG:HB3	1:C:258:GLU:OE2	2.17	0.43
1:C:316:SER:O	1:C:317:TRP:HD1	2.02	0.43
1:C:378:VAL:C	1:C:379:ILE:HG13	2.44	0.43
1:C:529:LYS:HB2	1:C:529:LYS:HE3	1.68	0.43
1:D:122:ASP:CG	1:D:123:LEU:H	2.23	0.43
1:D:831:ARG:HA	1:D:831:ARG:NE	2.32	0.43
2:E:253:THR:HA	2:E:414:ILE:HA	2.01	0.43
1:A:270:ASP:O	1:A:273:THR:HB	2.18	0.43
1:A:385:TYR:O	1:A:387:GLY:N	2.51	0.43
1:B:523:TYR:CE1	1:B:527:GLU:HB2	2.54	0.43
1:B:740:TYR:O	1:B:743:TYR:N	2.52	0.43
1:B:820:LEU:HB3	1:B:825:TYR:CD2	2.53	0.43
1:C:189:LEU:HD12	1:C:190:LEU:HD23	2.01	0.43
1:C:595:PHE:CD1	1:C:596:ARG:N	2.87	0.43
1:C:648:ALA:O	1:C:652:THR:HG22	2.19	0.43
1:D:654:GLY:O	1:D:657:GLU:N	2.48	0.43
1:A:162:THR:OG1	1:A:564:ILE:HG22	2.19	0.43
1:A:283:PHE:C	1:A:285:SER:N	2.77	0.43
1:A:333:GLU:HB3	1:A:377:ASP:OD2	2.18	0.43
1:A:484:ASN:HA	1:A:487:GLU:OE2	2.18	0.43
1:A:718:HIS:C	1:A:719:CYS:SG	3.01	0.43
1:B:212:GLU:O	1:B:213:LEU:C	2.62	0.43
1:B:324:ASN:ND2	1:B:326:GLU:HB3	2.34	0.43
1:B:740:TYR:HA	1:B:769:PHE:CE2	2.54	0.43
1:C:134:PHE:C	1:C:136:GLN:N	2.75	0.43
1:C:571:LYS:HG3	1:C:572:THR:N	2.33	0.43
1:C:655:GLY:O	1:C:656:HIS:C	2.61	0.43
1:C:775:TYR:C	1:C:777:TRP:H	2.26	0.43
2:E:238:PRO:O	2:E:242:ALA:HB2	2.19	0.43
2:E:344:ASP:C	2:E:346:MET:H	2.27	0.43
1:A:540:PRO:HD3	1:A:607:PHE:CZ	2.54	0.43
1:B:493:VAL:HG22	1:B:497:LYS:NZ	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:772:SER:O	1:B:775:TYR:HB3	2.19	0.43
1:C:111:GLY:O	1:C:115:ASN:HB2	2.18	0.43
1:D:161:GLN:O	1:D:165:ILE:HG13	2.18	0.43
1:D:217:MET:SD	1:D:230:MET:HE3	2.59	0.43
1:D:764:THR:HG1	1:D:767:GLN:HG2	1.83	0.43
1:D:767:GLN:O	1:D:768:ILE:C	2.62	0.43
1:A:174:VAL:N	1:A:175:GLU:OE2	2.51	0.42
1:A:229:PHE:N	1:A:229:PHE:CD1	2.87	0.42
1:A:312:ILE:HG13	1:A:312:ILE:H	1.70	0.42
1:B:476:TYR:OH	1:B:607:PHE:HB2	2.19	0.42
1:B:523:TYR:CG	1:B:524:ARG:N	2.86	0.42
1:B:569:ASN:HB2	1:B:589:TYR:HE1	1.84	0.42
1:C:81:ASN:ND2	1:C:756:ARG:HH11	2.17	0.42
1:C:90:ASN:O	1:C:93:ASN:HB3	2.19	0.42
1:C:355:LYS:O	1:C:358:ALA:HB3	2.19	0.42
1:C:464:MET:O	1:C:467:VAL:N	2.52	0.42
1:D:163:GLU:CG	1:D:481:VAL:HG22	2.45	0.42
1:D:217:MET:CG	1:D:218:GLY:N	2.82	0.42
1:D:336:ALA:N	1:D:337:PRO:HD2	2.34	0.42
1:D:480:TYR:HB2	1:D:543:LEU:CG	2.49	0.42
1:D:649:GLY:O	1:D:650:SER:C	2.62	0.42
1:D:788:LYS:O	1:D:792:THR:HG22	2.18	0.42
1:A:276:ILE:HD13	1:A:276:ILE:HA	1.80	0.42
1:A:533:MET:HA	1:A:623:ASN:HD22	1.83	0.42
1:A:700:CYS:SG	1:A:701:VAL:N	2.92	0.42
1:B:82:ALA:CB	1:B:756:ARG:O	2.67	0.42
1:B:226:LEU:O	1:B:226:LEU:CD2	2.61	0.42
1:C:163:GLU:O	1:C:164:ARG:C	2.60	0.42
1:C:216:GLU:O	1:C:217:MET:C	2.61	0.42
1:C:314:MET:O	1:C:315:ALA:C	2.62	0.42
1:C:414:LEU:C	1:C:416:GLU:N	2.75	0.42
1:C:483:VAL:HG21	1:C:543:LEU:HD22	2.00	0.42
1:C:510:LYS:NZ	1:C:738:ALA:HA	2.34	0.42
1:C:540:PRO:C	1:C:541:LYS:HE2	2.45	0.42
1:C:608:LEU:HG	1:C:608:LEU:O	2.18	0.42
1:C:729:ASN:C	1:C:731:ALA:N	2.77	0.42
1:D:645:PHE:O	1:D:646:ASN:C	2.61	0.42
2:E:325:MET:H	2:E:388:ALA:HA	1.83	0.42
1:A:196:ARG:HH22	1:A:219:ARG:NE	2.17	0.42
1:A:507:PHE:HB2	1:A:738:ALA:HB1	2.01	0.42
1:A:509:LYS:HA	1:A:523:TYR:OH	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:TRP:HA	1:A:607:PHE:HZ	1.84	0.42
1:A:653:VAL:O	1:A:656:HIS:HB3	2.19	0.42
1:A:808:ASP:O	1:A:809:ILE:HG13	2.18	0.42
1:B:262:LEU:HB2	1:B:263:PRO:HD3	1.98	0.42
1:B:388:PHE:HE1	1:B:405:PHE:CZ	2.37	0.42
1:B:407:ASN:O	1:B:410:ILE:CG2	2.62	0.42
1:B:593:GLU:HG3	1:B:597:ARG:NH2	2.33	0.42
1:B:663:ASP:C	1:B:665:GLU:N	2.77	0.42
1:C:86:LYS:HA	1:C:89:LYS:NZ	2.34	0.42
1:C:502:LEU:O	1:C:506:THR:HG23	2.20	0.42
1:C:725:THR:O	1:C:727:GLY:N	2.52	0.42
1:C:767:GLN:H	1:C:767:GLN:CD	2.26	0.42
1:D:142:ASN:O	1:D:145:ILE:HG22	2.19	0.42
1:D:160:SER:C	1:D:163:GLU:OE1	2.61	0.42
1:D:218:GLY:O	1:D:221:GLU:N	2.52	0.42
1:D:767:GLN:OE1	1:D:815:ASP:HB3	2.19	0.42
1:D:806:LEU:HB3	1:D:812:PHE:CE2	2.53	0.42
1:A:114:CYS:O	1:A:115:ASN:C	2.62	0.42
1:A:216:GLU:O	1:A:217:MET:C	2.61	0.42
1:A:228:THR:O	1:A:229:PHE:HB2	2.18	0.42
1:A:533:MET:HG2	1:A:623:ASN:ND2	2.32	0.42
1:A:533:MET:HE3	1:A:618:TYR:CE1	2.55	0.42
1:A:695:LYS:HA	1:A:695:LYS:HD2	1.81	0.42
1:B:588:GLY:O	1:B:592:ARG:HB2	2.19	0.42
1:B:733:LEU:HG	1:B:734:GLY:N	2.35	0.42
1:C:91:ALA:O	1:C:94:THR:HG22	2.19	0.42
1:C:593:GLU:HA	1:C:596:ARG:CZ	2.50	0.42
1:C:627:LEU:HD12	1:C:627:LEU:N	2.34	0.42
1:D:760:LEU:HG	1:D:763:PHE:HD2	1.85	0.42
1:A:131:PHE:CD2	1:A:131:PHE:O	2.72	0.42
1:A:504:MET:O	1:A:505:LYS:C	2.60	0.42
1:A:614:VAL:HG23	1:A:614:VAL:O	2.19	0.42
1:B:115:ASN:O	1:B:118:ILE:HB	2.19	0.42
1:B:518:MET:SD	1:B:523:TYR:HB2	2.59	0.42
1:B:731:ALA:O	1:B:732:ASP:C	2.59	0.42
1:D:329:TYR:CD1	1:D:329:TYR:C	2.98	0.42
1:D:806:LEU:C	1:D:808:ASP:H	2.26	0.42
2:E:94:ALA:HB1	2:E:231:ALA:HA	2.00	0.42
1:A:189:LEU:O	1:A:190:LEU:C	2.63	0.42
1:A:308:ILE:O	1:A:309:GLU:C	2.59	0.42
1:B:499:GLN:OE1	1:B:500:THR:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:ASN:O	1:B:584:ILE:C	2.63	0.42
1:B:657:GLU:O	1:B:659:VAL:N	2.52	0.42
1:C:109:PHE:O	1:C:109:PHE:CD1	2.72	0.42
1:C:305:VAL:HG11	1:C:411:VAL:HG11	2.01	0.42
1:D:160:SER:CA	1:D:163:GLU:OE1	2.67	0.42
1:D:165:ILE:O	1:D:166:THR:C	2.62	0.42
1:D:463:ARG:O	1:D:467:VAL:HG12	2.20	0.42
1:D:618:TYR:HB3	1:D:657:GLU:OE2	2.19	0.42
1:D:831:ARG:HA	1:D:831:ARG:CZ	2.49	0.42
1:A:163:GLU:CD	1:A:480:TYR:CE2	2.97	0.42
1:A:311:LYS:O	1:A:312:ILE:C	2.63	0.42
1:A:669:PHE:O	1:A:678:CYS:HB2	2.20	0.42
1:B:296:LYS:HB2	1:B:296:LYS:HE2	1.82	0.42
1:B:499:GLN:O	1:B:502:LEU:HB2	2.20	0.42
1:B:512:LEU:HB2	1:B:523:TYR:CB	2.45	0.42
1:B:515:LEU:HD12	1:B:518:MET:HE1	2.02	0.42
1:C:267:PRO:C	1:C:269:LEU:N	2.76	0.42
1:D:136:GLN:O	1:D:139:LEU:HB3	2.19	0.42
1:D:505:LYS:O	1:D:508:LEU:HB3	2.19	0.42
1:D:508:LEU:O	1:D:510:LYS:N	2.52	0.42
1:A:98:GLY:HA2	1:A:116:LYS:HB3	1.93	0.42
1:A:239:LYS:HD2	1:A:329:TYR:CD2	2.54	0.42
1:A:572:THR:HG22	1:A:573:ASP:H	1.85	0.42
1:A:637:TYR:CG	1:A:638:ASP:N	2.88	0.42
1:D:492:VAL:CG1	1:D:493:VAL:N	2.82	0.42
1:A:508:LEU:HD23	1:A:508:LEU:C	2.44	0.42
1:A:825:TYR:HB3	1:A:827:PRO:CD	2.44	0.42
1:B:325:HIS:O	1:B:328:GLN:N	2.52	0.42
1:B:507:PHE:HE2	1:B:662:PHE:CE2	2.38	0.42
1:B:620:PRO:O	1:B:669:PHE:CD2	2.72	0.42
1:C:171:GLN:CA	1:C:174:VAL:HG12	2.49	0.42
1:C:278:ASN:O	1:C:279:VAL:C	2.62	0.42
1:C:782:THR:HG23	1:C:785:SER:H	1.83	0.42
1:D:627:LEU:HD12	1:D:627:LEU:N	2.35	0.42
1:D:659:VAL:O	1:D:660:HIS:C	2.61	0.42
1:A:170:PHE:O	1:A:171:GLN:C	2.61	0.42
1:A:804:GLN:HE22	1:A:807:GLN:CD	2.28	0.42
1:A:834:VAL:HG22	1:A:835:TRP:CE3	2.54	0.42
1:B:214:TYR:CD1	1:B:214:TYR:N	2.87	0.42
1:B:242:SER:C	1:B:243:ARG:CG	2.92	0.42
1:B:374:PHE:CE1	1:B:375:ILE:HB	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:GLY:C	1:B:592:ARG:HE	2.28	0.42
1:B:633:THR:OG1	1:B:634:SER:N	2.37	0.42
1:C:221:GLU:OE1	1:C:227:PRO:HB3	2.19	0.42
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.93	0.42
1:C:381:THR:OG1	1:C:382:ASN:N	2.52	0.42
1:C:793:ASN:CG	1:C:795:HIS:HE1	2.24	0.42
1:D:163:GLU:O	1:D:164:ARG:C	2.62	0.42
1:D:173:CYS:C	1:D:175:GLU:H	2.27	0.42
2:E:171:VAL:C	2:E:173:GLY:H	2.28	0.42
2:F:94:ALA:HB3	2:F:231:ALA:HA	2.02	0.42
2:F:352:VAL:H	2:F:385:CYS:HA	1.85	0.42
1:A:95:LEU:HD22	1:A:760:LEU:HD12	2.02	0.41
1:A:410:ILE:O	1:A:411:VAL:C	2.59	0.41
1:A:774:GLY:O	1:A:775:TYR:C	2.61	0.41
1:A:801:ARG:O	1:A:802:VAL:C	2.63	0.41
1:B:212:GLU:O	1:B:215:ARG:N	2.53	0.41
1:B:272:ARG:HA	1:B:272:ARG:CZ	2.50	0.41
1:B:310:GLN:C	1:B:312:ILE:H	2.28	0.41
1:B:666:GLY:O	1:B:667:VAL:C	2.63	0.41
1:B:764:THR:HG1	1:B:767:GLN:N	2.16	0.41
1:B:804:GLN:OE1	1:B:804:GLN:HA	2.15	0.41
1:C:87:GLU:HB3	1:C:641:PHE:CE1	2.56	0.41
1:D:305:VAL:HG11	1:D:411:VAL:HG21	2.01	0.41
1:D:414:LEU:C	1:D:416:GLU:N	2.77	0.41
1:B:412:HIS:O	1:B:413:MET:C	2.61	0.41
1:B:820:LEU:HD13	1:B:825:TYR:CE2	2.55	0.41
1:C:146:VAL:O	1:C:149:LEU:N	2.51	0.41
1:C:262:LEU:HD13	1:C:264:GLN:HE22	1.85	0.41
1:C:514:THR:HG23	1:C:518:MET:CE	2.49	0.41
1:C:583:ASN:O	1:C:584:ILE:C	2.63	0.41
1:C:771:ILE:O	1:C:774:GLY:N	2.53	0.41
1:D:303:ARG:O	1:D:307:GLN:HG2	2.21	0.41
1:A:134:PHE:HE1	1:A:636:HIS:NE2	2.18	0.41
1:A:360:LEU:HA	1:A:360:LEU:HD23	1.73	0.41
1:A:414:LEU:O	1:A:416:GLU:N	2.54	0.41
1:A:728:GLU:O	1:A:731:ALA:HB3	2.20	0.41
1:B:677:ASP:O	1:B:678:CYS:C	2.64	0.41
1:B:828:ALA:O	1:B:830:GLN:N	2.53	0.41
1:C:100:ASP:OD1	1:C:102:SER:N	2.52	0.41
1:C:110:TYR:CG	1:C:111:GLY:N	2.89	0.41
1:C:276:ILE:O	1:C:277:GLU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ILE:HG23	1:C:474:MET:HB3	2.02	0.41
1:C:495:ASP:O	1:C:496:VAL:C	2.63	0.41
1:C:658:LEU:HD12	1:C:658:LEU:HA	1.65	0.41
1:D:409:ILE:O	1:D:410:ILE:C	2.62	0.41
1:A:84:ARG:HD3	1:A:84:ARG:HA	1.81	0.41
1:A:521:GLU:HB3	1:A:524:ARG:HH22	1.84	0.41
1:A:618:TYR:HE2	1:A:661:GLY:HA3	1.85	0.41
1:A:722:GLY:O	1:A:723:ALA:C	2.64	0.41
1:A:736:LEU:O	1:A:737:GLN:C	2.62	0.41
1:B:322:LEU:HA	1:B:322:LEU:HD23	1.48	0.41
1:B:677:ASP:O	1:B:679:SER:N	2.53	0.41
1:C:168:ALA:O	1:C:171:GLN:HB2	2.20	0.41
1:C:334:LEU:HB3	1:C:335:PHE:CE1	2.55	0.41
1:C:528:LYS:O	1:C:529:LYS:C	2.63	0.41
1:C:571:LYS:NZ	1:C:572:THR:C	2.78	0.41
1:D:88:TRP:CD1	1:D:88:TRP:N	2.88	0.41
1:D:219:ARG:HA	1:D:219:ARG:HD3	1.90	0.41
1:D:277:GLU:HA	1:D:280:MET:HB3	2.01	0.41
1:D:318:PRO:HG2	1:D:321:GLU:OE1	2.19	0.41
1:D:412:HIS:O	1:D:413:MET:C	2.63	0.41
1:D:474:MET:C	1:D:476:TYR:H	2.28	0.41
1:D:504:MET:SD	1:D:530:ILE:HG22	2.60	0.41
1:D:568:TYR:C	1:D:570:ASN:N	2.79	0.41
1:D:697:MET:HE2	1:D:697:MET:N	2.35	0.41
1:D:752:ALA:O	1:D:754:GLU:N	2.53	0.41
1:D:800:CYS:O	1:D:804:GLN:HG2	2.21	0.41
1:A:83:ASN:HB3	1:A:88:TRP:CE3	2.55	0.41
1:A:242:SER:C	1:A:602:ALA:CB	2.91	0.41
1:A:770:TRP:CE2	1:A:812:PHE:HB2	2.55	0.41
1:B:228:THR:C	1:B:230:MET:N	2.78	0.41
1:B:259:PHE:CZ	1:B:265:PHE:HB3	2.56	0.41
1:B:279:VAL:C	1:B:281:LYS:N	2.75	0.41
1:C:81:ASN:HA	1:C:755:MET:HE3	2.03	0.41
1:C:166:THR:O	1:C:167:LYS:C	2.63	0.41
1:C:565:LEU:HD23	1:C:565:LEU:C	2.46	0.41
1:D:224:ARG:HA	1:D:224:ARG:HD2	1.73	0.41
1:D:313:ALA:O	1:D:315:ALA:N	2.53	0.41
1:D:324:ASN:OD1	1:D:324:ASN:C	2.63	0.41
1:D:571:LYS:HA	1:D:571:LYS:HD3	1.73	0.41
2:E:96:LEU:O	2:E:98:ILE:N	2.53	0.41
1:A:331:PRO:O	1:A:332:TYR:CD1	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HG13	1:A:503:ILE:H	1.58	0.41
1:A:536:ASN:CG	1:A:607:PHE:HE1	2.29	0.41
1:A:559:ASP:CG	1:A:560:ASP:N	2.78	0.41
1:A:589:TYR:O	1:A:593:GLU:HB2	2.20	0.41
1:A:832:CYS:O	1:A:833:LYS:C	2.62	0.41
1:B:134:PHE:O	1:B:135:SER:C	2.64	0.41
1:B:388:PHE:CE1	1:B:405:PHE:CZ	3.09	0.41
1:B:652:THR:O	1:B:653:VAL:C	2.62	0.41
1:C:162:THR:HG23	1:C:163:GLU:N	2.36	0.41
1:C:257:ARG:HH22	1:C:313:ALA:HB1	1.84	0.41
1:C:382:ASN:O	1:C:384:ALA:N	2.54	0.41
1:C:498:GLN:HG3	1:C:498:GLN:H	1.63	0.41
1:D:321:GLU:C	1:D:323:ARG:H	2.28	0.41
1:D:353:PHE:O	1:D:356:TYR:HB3	2.21	0.41
1:D:616:ALA:HA	1:D:626:THR:O	2.21	0.41
1:A:361:MET:HE2	1:A:361:MET:HB2	1.73	0.41
1:B:113:THR:HG23	1:B:771:ILE:HG23	2.01	0.41
1:B:398:ILE:HB	1:B:402:GLN:HE21	1.85	0.41
1:B:595:PHE:C	1:B:597:ARG:N	2.74	0.41
1:B:820:LEU:HD13	1:B:825:TYR:CZ	2.56	0.41
1:C:536:ASN:HB3	1:C:607:PHE:CE1	2.56	0.41
1:C:773:TYR:O	1:C:774:GLY:C	2.64	0.41
1:C:805:VAL:O	1:C:806:LEU:C	2.61	0.41
1:D:265:PHE:C	1:D:267:PRO:HD3	2.46	0.41
1:D:407:ASN:O	1:D:408:TYR:C	2.63	0.41
1:D:533:MET:HA	1:D:623:ASN:ND2	2.36	0.41
1:D:699:GLN:O	1:D:700:CYS:C	2.62	0.41
1:A:274:LYS:HA	1:A:274:LYS:HD3	1.73	0.41
1:A:488:ASP:HB2	1:A:491:GLN:HE22	1.85	0.41
1:A:496:VAL:H	1:A:496:VAL:HG22	1.66	0.41
1:A:507:PHE:O	1:A:508:LEU:C	2.64	0.41
1:A:617:TRP:CD1	1:A:617:TRP:C	2.98	0.41
1:A:769:PHE:O	1:A:770:TRP:C	2.64	0.41
1:A:804:GLN:O	1:A:805:VAL:C	2.62	0.41
1:B:97:PHE:O	1:B:116:LYS:HB2	2.21	0.41
1:B:170:PHE:HE1	1:B:463:ARG:HA	1.84	0.41
1:B:405:PHE:O	1:B:406:VAL:C	2.60	0.41
1:B:648:ALA:HB2	1:B:769:PHE:CD1	2.55	0.41
1:C:94:THR:HG23	1:C:95:LEU:N	2.36	0.41
1:D:270:ASP:O	1:D:273:THR:N	2.54	0.41
1:D:529:LYS:HA	1:D:671:TYR:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:582:LEU:HD12	1:D:582:LEU:N	2.36	0.41
2:E:94:ALA:CB	2:E:231:ALA:HA	2.50	0.41
1:A:122:ASP:OD1	1:A:123:LEU:N	2.54	0.41
1:A:134:PHE:CE1	1:A:636:HIS:NE2	2.89	0.41
1:A:378:VAL:O	1:A:378:VAL:HG13	2.20	0.41
1:A:493:VAL:HG23	1:A:494:GLU:CD	2.46	0.41
1:A:494:GLU:O	1:A:495:ASP:C	2.64	0.41
1:A:564:ILE:O	1:A:568:TYR:N	2.54	0.41
1:A:565:LEU:HA	1:A:565:LEU:HD12	1.74	0.41
1:A:596:ARG:O	1:A:596:ARG:HG2	2.21	0.41
1:A:798:ASN:O	1:A:799:SER:C	2.63	0.41
1:A:834:VAL:O	1:A:835:TRP:CG	2.74	0.41
1:B:190:LEU:HD23	1:B:193:ILE:HG13	2.01	0.41
1:B:233:TRP:O	1:B:247:TYR:HB2	2.20	0.41
1:B:269:LEU:HD11	1:B:303:ARG:HG2	2.03	0.41
1:B:313:ALA:C	1:B:315:ALA:H	2.29	0.41
1:B:413:MET:HE3	1:B:413:MET:HB3	1.95	0.41
1:B:536:ASN:C	1:B:537:TYR:CD1	2.98	0.41
1:B:669:PHE:CE1	1:B:675:LEU:HD21	2.55	0.41
1:B:703:THR:O	1:B:704:GLN:C	2.63	0.41
1:B:767:GLN:O	1:B:768:ILE:C	2.64	0.41
1:B:804:GLN:C	1:B:806:LEU:N	2.77	0.41
1:C:197:PHE:HD1	1:C:216:GLU:OE2	2.04	0.41
1:C:471:THR:CG2	1:C:612:ALA:HB3	2.51	0.41
1:C:562:TYR:O	1:C:565:LEU:HB3	2.21	0.41
1:C:568:TYR:O	1:C:568:TYR:CG	2.73	0.41
1:C:595:PHE:CG	1:C:596:ARG:N	2.89	0.41
1:C:618:TYR:CE2	1:C:661:GLY:HA2	2.56	0.41
1:C:742:ALA:O	1:C:743:TYR:C	2.62	0.41
1:C:770:TRP:O	1:C:771:ILE:C	2.63	0.41
1:C:803:ASN:C	1:C:805:VAL:N	2.79	0.41
1:D:83:ASN:O	1:D:758:PRO:HB3	2.21	0.41
1:D:133:THR:H	1:D:133:THR:HG23	1.63	0.41
1:D:261:VAL:HG11	1:D:314:MET:HB2	2.02	0.41
1:D:473:TYR:O	1:D:475:PRO:HD3	2.21	0.41
1:D:540:PRO:HG3	1:D:607:PHE:CG	2.55	0.41
1:D:562:TYR:O	1:D:563:SER:C	2.63	0.41
1:D:609:GLU:HB3	1:D:617:TRP:CZ3	2.55	0.41
1:D:696:ASP:HB3	1:D:697:MET:HE2	2.02	0.41
1:D:725:THR:C	1:D:727:GLY:N	2.77	0.41
1:A:283:PHE:O	1:A:285:SER:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:GLN:O	1:A:675:LEU:HD12	2.20	0.41
1:A:814:LYS:O	1:A:817:GLN:N	2.55	0.41
1:B:115:ASN:OD1	1:B:115:ASN:O	2.38	0.41
1:B:145:ILE:HG21	1:B:467:VAL:HG21	2.03	0.41
1:B:162:THR:N	1:B:564:ILE:HD13	2.33	0.41
1:B:337:PRO:C	1:B:340:GLY:H	2.26	0.41
1:B:359:GLY:O	1:B:360:LEU:HD23	2.21	0.41
1:D:161:GLN:O	1:D:164:ARG:HB3	2.20	0.41
1:D:270:ASP:C	1:D:272:ARG:N	2.77	0.41
1:D:582:LEU:O	1:D:585:LEU:N	2.54	0.41
1:A:496:VAL:HG23	1:A:497:LYS:N	2.34	0.40
1:A:656:HIS:CG	1:A:732:ASP:OD1	2.74	0.40
1:B:142:ASN:O	1:B:143:SER:C	2.63	0.40
1:B:313:ALA:C	1:B:315:ALA:N	2.78	0.40
1:B:341:LYS:HD2	1:B:352:ARG:HH22	1.85	0.40
1:B:407:ASN:C	1:B:411:VAL:HG23	2.45	0.40
1:B:700:CYS:HB3	1:B:832:CYS:HB3	1.97	0.40
1:C:230:MET:CE	1:C:248:ILE:HG21	2.52	0.40
1:C:413:MET:HB2	1:C:413:MET:HE3	1.76	0.40
1:C:607:PHE:C	1:C:609:GLU:H	2.29	0.40
1:D:219:ARG:HH12	1:D:359:GLY:HA2	1.86	0.40
1:D:470:ILE:O	1:D:471:THR:C	2.65	0.40
2:E:325:MET:O	2:E:388:ALA:HB1	2.21	0.40
2:F:326:GLY:O	2:F:402:ILE:N	2.54	0.40
1:A:86:LYS:O	1:A:87:GLU:C	2.62	0.40
1:A:324:ASN:HB3	1:A:327:GLN:HG2	2.02	0.40
1:A:355:LYS:O	1:A:357:ILE:HG12	2.21	0.40
1:B:121:ILE:O	1:B:780:LYS:CD	2.69	0.40
1:B:268:GLU:HA	1:B:271:ALA:HB3	2.04	0.40
1:B:296:LYS:HD3	1:B:296:LYS:N	2.35	0.40
1:B:374:PHE:CG	1:B:375:ILE:N	2.89	0.40
1:B:645:PHE:C	1:B:647:PHE:N	2.79	0.40
1:C:230:MET:HE3	1:C:248:ILE:HG21	2.02	0.40
1:C:273:THR:H	1:C:273:THR:HG23	1.62	0.40
1:C:274:LYS:O	1:C:275:ALA:C	2.62	0.40
1:C:305:VAL:HG23	1:C:306:THR:H	1.86	0.40
1:C:736:LEU:O	1:C:739:SER:N	2.53	0.40
1:D:119:GLU:O	1:D:119:GLU:CG	2.69	0.40
1:D:321:GLU:N	1:D:321:GLU:CD	2.80	0.40
1:D:405:PHE:N	1:D:405:PHE:CD1	2.85	0.40
1:D:738:ALA:O	1:D:739:SER:C	2.63	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:THR:O	1:D:768:ILE:HG12	2.21	0.40
1:A:196:ARG:NH2	1:A:219:ARG:HE	2.19	0.40
1:A:239:LYS:HB2	1:A:329:TYR:OH	2.21	0.40
1:A:484:ASN:HA	1:A:487:GLU:CG	2.50	0.40
1:A:495:ASP:O	1:A:498:GLN:HB3	2.20	0.40
1:A:536:ASN:C	1:A:537:TYR:HD1	2.30	0.40
1:B:309:GLU:O	1:B:310:GLN:C	2.64	0.40
1:B:312:ILE:O	1:B:313:ALA:C	2.63	0.40
1:B:398:ILE:HB	1:B:402:GLN:NE2	2.36	0.40
1:B:468:ASP:O	1:B:469:THR:C	2.64	0.40
1:B:699:GLN:O	1:B:702:VAL:HB	2.22	0.40
1:C:319:ASP:O	1:C:320:ASP:C	2.64	0.40
1:C:385:TYR:O	1:C:385:TYR:CD1	2.74	0.40
1:D:101:GLU:OE2	1:D:762:LYS:NZ	2.50	0.40
1:D:134:PHE:HE1	1:D:636:HIS:CE1	2.40	0.40
1:D:490:ASP:O	1:D:490:ASP:OD1	2.40	0.40
1:D:618:TYR:HD1	1:D:624:SER:C	2.30	0.40
1:D:797:PRO:O	1:D:800:CYS:N	2.54	0.40
1:A:322:LEU:C	1:A:323:ARG:HG2	2.46	0.40
1:A:633:THR:HG23	1:A:634:SER:N	2.37	0.40
1:B:733:LEU:O	1:B:734:GLY:C	2.63	0.40
1:C:114:CYS:SG	1:C:778:CYS:CB	3.04	0.40
1:C:235:ASN:O	1:C:236:VAL:C	2.65	0.40
1:C:250:GLN:OE1	1:C:317:TRP:N	2.47	0.40
1:C:798:ASN:O	1:C:801:ARG:CA	2.67	0.40
1:D:167:LYS:O	1:D:171:GLN:OE1	2.39	0.40
1:A:99:LEU:HD13	1:A:760:LEU:CD1	2.50	0.40
1:A:219:ARG:HG3	1:A:359:GLY:HA2	2.03	0.40
1:A:356:TYR:O	1:A:356:TYR:CG	2.72	0.40
1:A:496:VAL:C	1:A:498:GLN:N	2.80	0.40
1:A:505:LYS:HE2	1:A:509:LYS:HE2	2.03	0.40
1:A:643:LYS:HA	1:A:643:LYS:HD3	1.92	0.40
1:B:505:LYS:O	1:B:508:LEU:N	2.55	0.40
1:B:622:LEU:HD12	1:B:623:ASN:CA	2.51	0.40
1:B:767:GLN:O	1:B:771:ILE:HG13	2.22	0.40
1:B:828:ALA:C	1:B:830:GLN:N	2.80	0.40
1:C:132:THR:HA	1:C:779:ALA:HA	2.03	0.40
1:C:305:VAL:CG1	1:C:411:VAL:HG21	2.51	0.40
1:D:132:THR:O	1:D:133:THR:C	2.65	0.40
1:D:144:ASP:O	1:D:147:LYS:HB2	2.22	0.40
1:D:568:TYR:C	1:D:570:ASN:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:TYR:CD1	1:D:743:TYR:C	2.99	0.40
1:D:806:LEU:C	1:D:808:ASP:N	2.78	0.40
2:E:78:ILE:H	2:E:83:GLN:N	2.17	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	564/755 (75%)	375 (66%)	188 (33%)	1 (0%)	43	77
1	B	589/755 (78%)	385 (65%)	196 (33%)	8 (1%)	9	39
1	C	551/755 (73%)	364 (66%)	181 (33%)	6 (1%)	11	45
1	D	536/755 (71%)	378 (70%)	153 (28%)	5 (1%)	14	49
2	E	289/369 (78%)	217 (75%)	72 (25%)	0	100	100
2	F	283/369 (77%)	198 (70%)	81 (29%)	4 (1%)	9	39
3	G	155/253 (61%)	121 (78%)	29 (19%)	5 (3%)	3	21
All	All	2967/4011 (74%)	2038 (69%)	900 (30%)	29 (1%)	15	47

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	817	GLN
1	C	820	LEU
2	F	168	PHE
3	G	104	PRO
1	C	107	GLU
1	C	817	GLN
1	C	824	MET
2	F	160	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	77	ILE
1	B	258	GLU
1	B	635	PRO
1	C	334	LEU
1	B	374	PHE
1	B	634	SER
2	F	183	ASN
1	B	257	ARG
1	B	263	PRO
1	B	646	ASN
1	D	634	SER
1	D	635	PRO
2	F	164	PRO
3	G	108	HIS
1	C	821	GLY
1	B	261	VAL
1	D	826	PRO
1	D	722	GLY
3	G	190	ILE
1	D	267	PRO
3	G	23	ILE

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 PDB entries followed by that with respect to all EM entries.

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	521/655 (80%)	521 (100%)	0	100	100
1	B	538/655 (82%)	538 (100%)	0	100	100
1	C	510/655 (78%)	510 (100%)	0	100	100
1	D	492/655 (75%)	492 (100%)	0	100	100
All	All	2061/2620 (79%)	2061 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	327	GLN
1	A	407	ASN
1	A	499	GLN
1	A	692	ASN
1	A	704	GLN
1	A	804	GLN
1	B	244	ASN
1	B	402	GLN
1	B	729	ASN
1	B	830	GLN
1	C	138	GLN
1	C	142	ASN
1	C	382	ASN
1	C	536	ASN
1	C	583	ASN
1	C	783	GLN
1	C	793	ASN
1	C	795	HIS
1	C	803	ASN
1	D	115	ASN
1	D	328	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

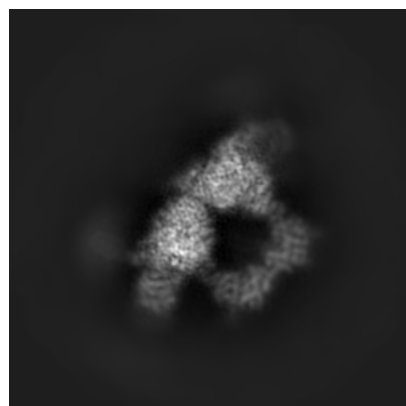
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4975. These allow visual inspection of the internal detail of the map and identification of artifacts.

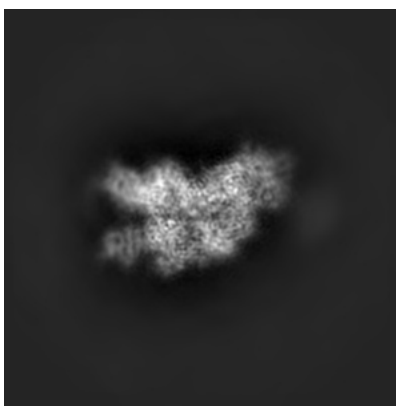
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

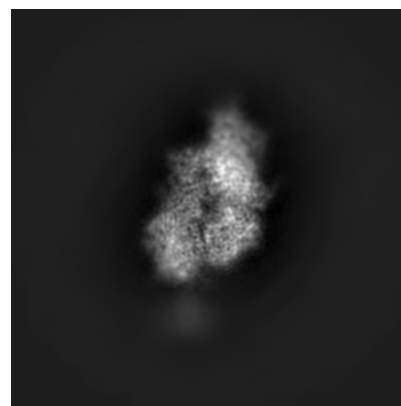
6.1.1 Primary map



X

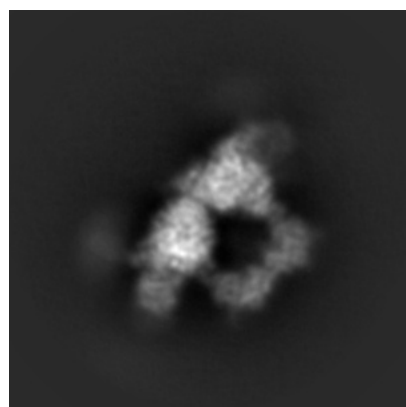


Y

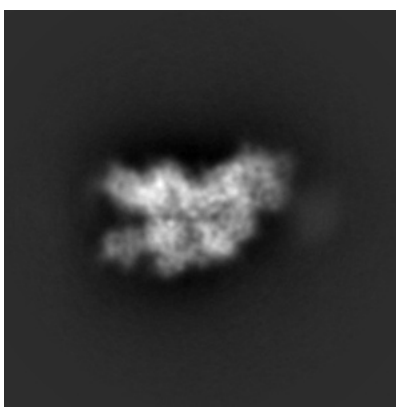


Z

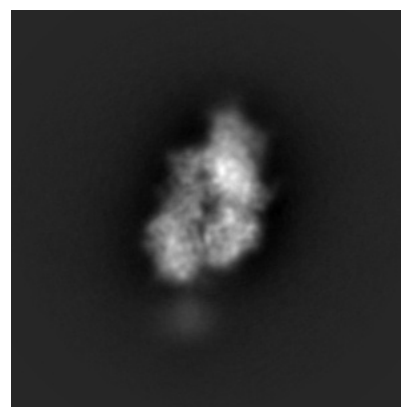
6.1.2 Raw map



X



Y

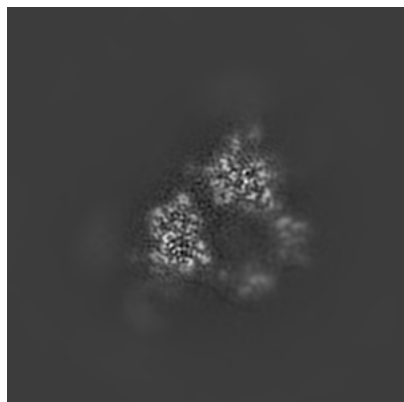


Z

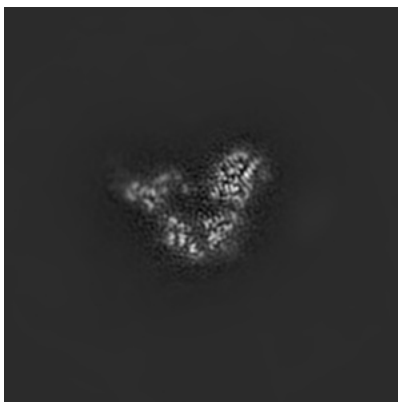
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

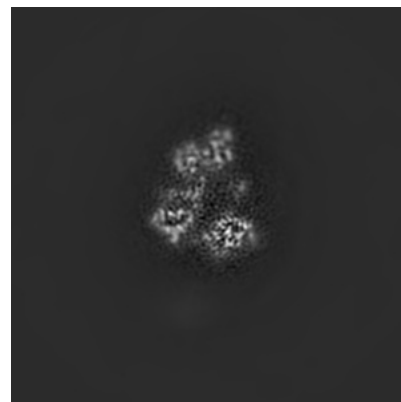
6.2.1 Primary map



X Index: 182

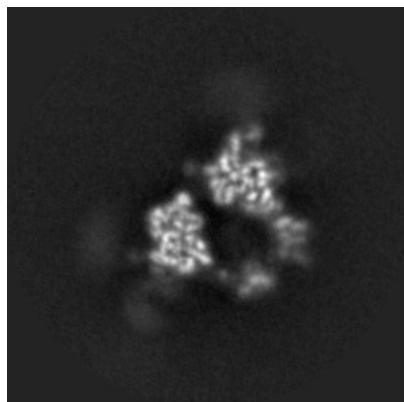


Y Index: 182

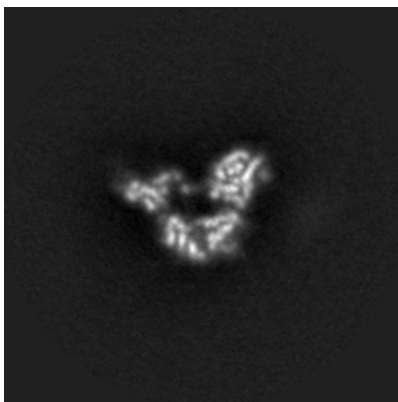


Z Index: 182

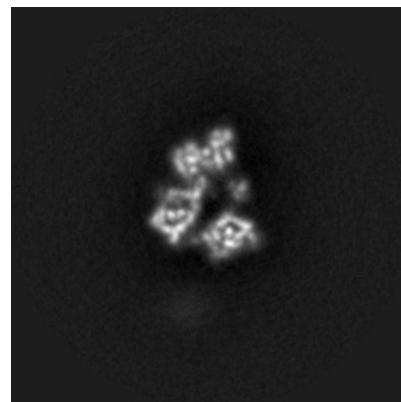
6.2.2 Raw map



X Index: 182



Y Index: 182

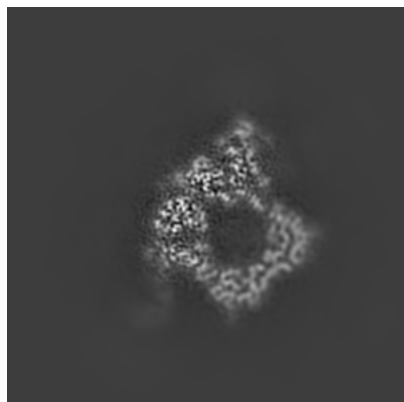


Z Index: 182

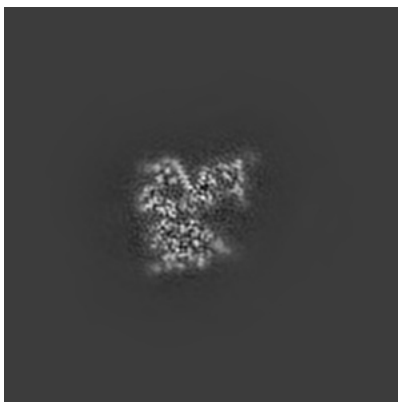
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

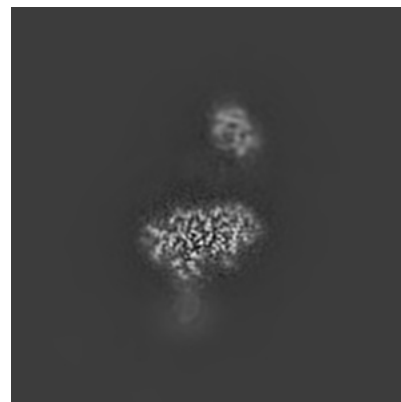
6.3.1 Primary map



X Index: 199

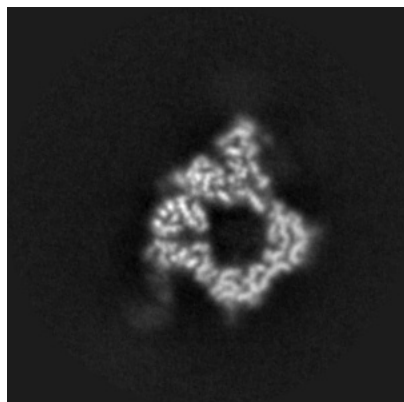


Y Index: 166

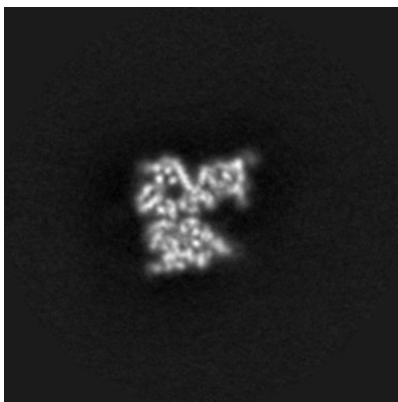


Z Index: 143

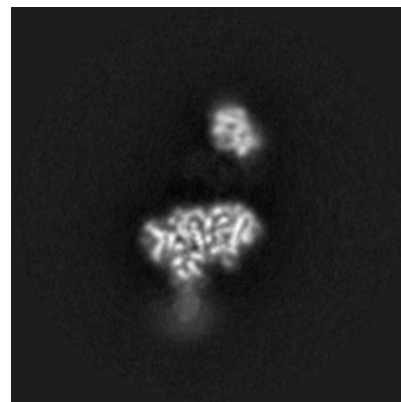
6.3.2 Raw map



X Index: 198



Y Index: 166

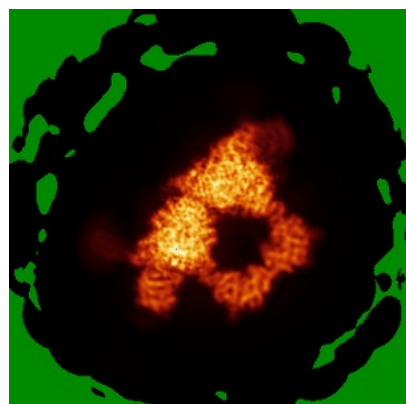


Z Index: 142

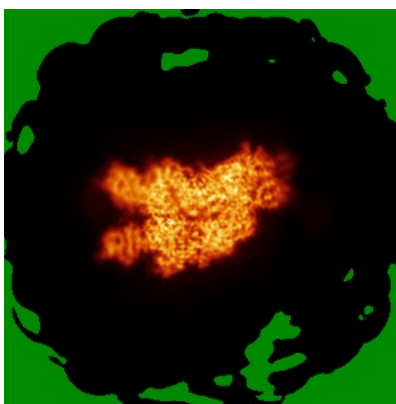
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

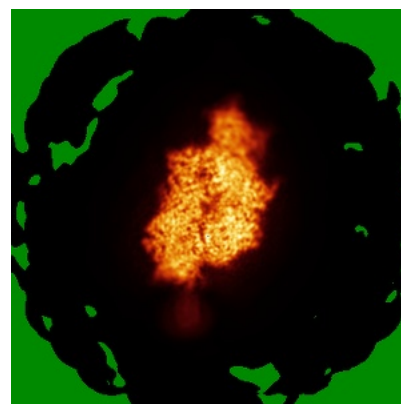
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

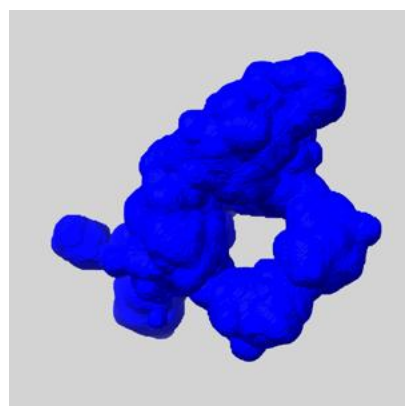
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

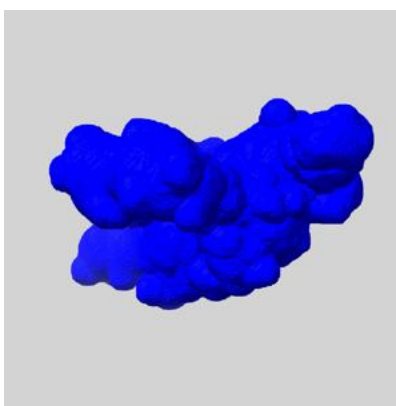
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

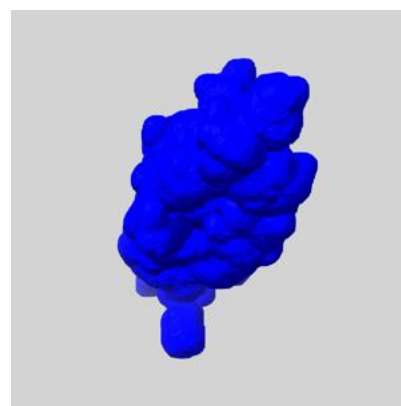
6.6.1 emd_4975_msk_1.map [i](#)



X



Y

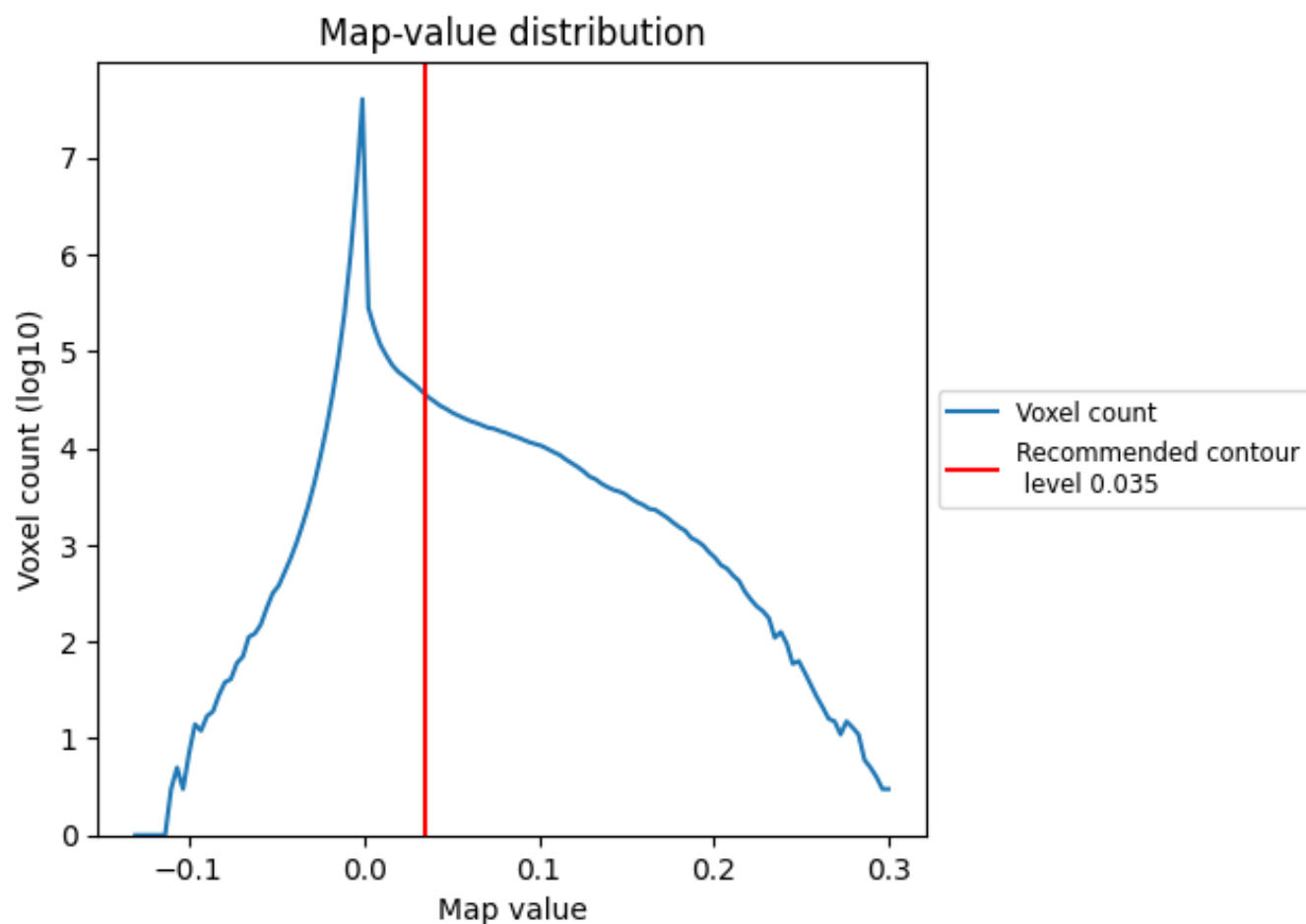


Z

7 Map analysis [i](#)

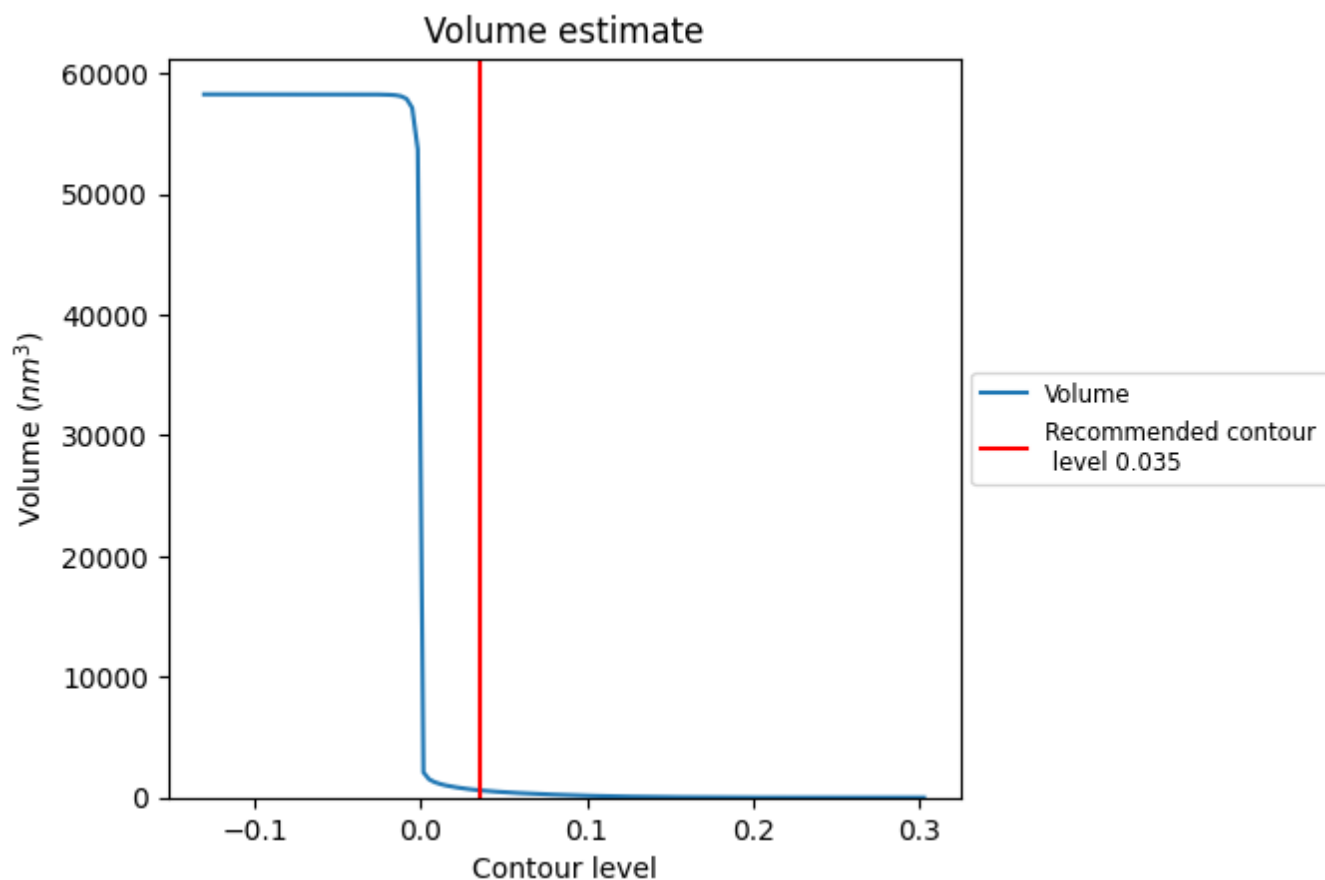
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

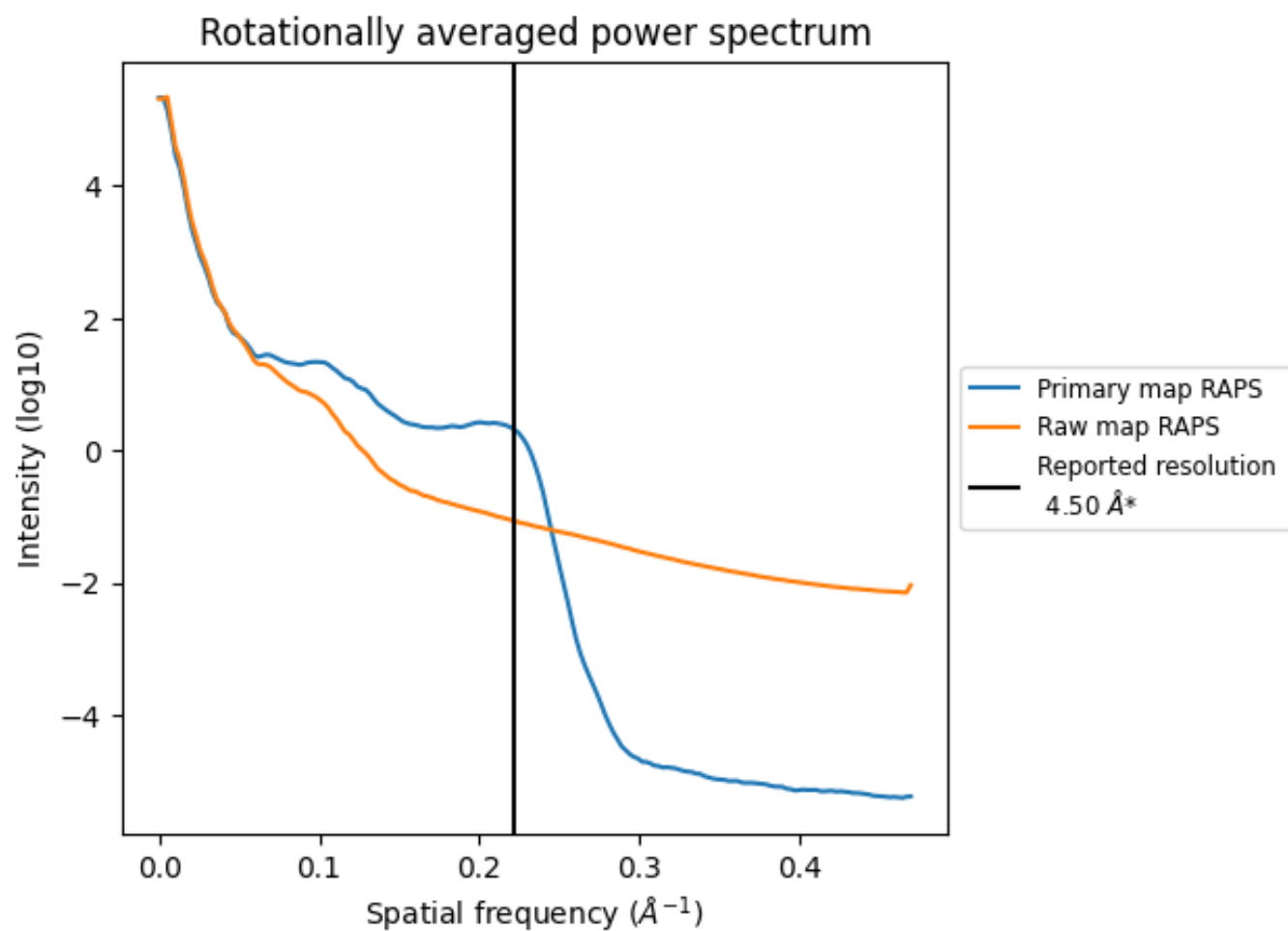
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 607 nm³; this corresponds to an approximate mass of 548 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

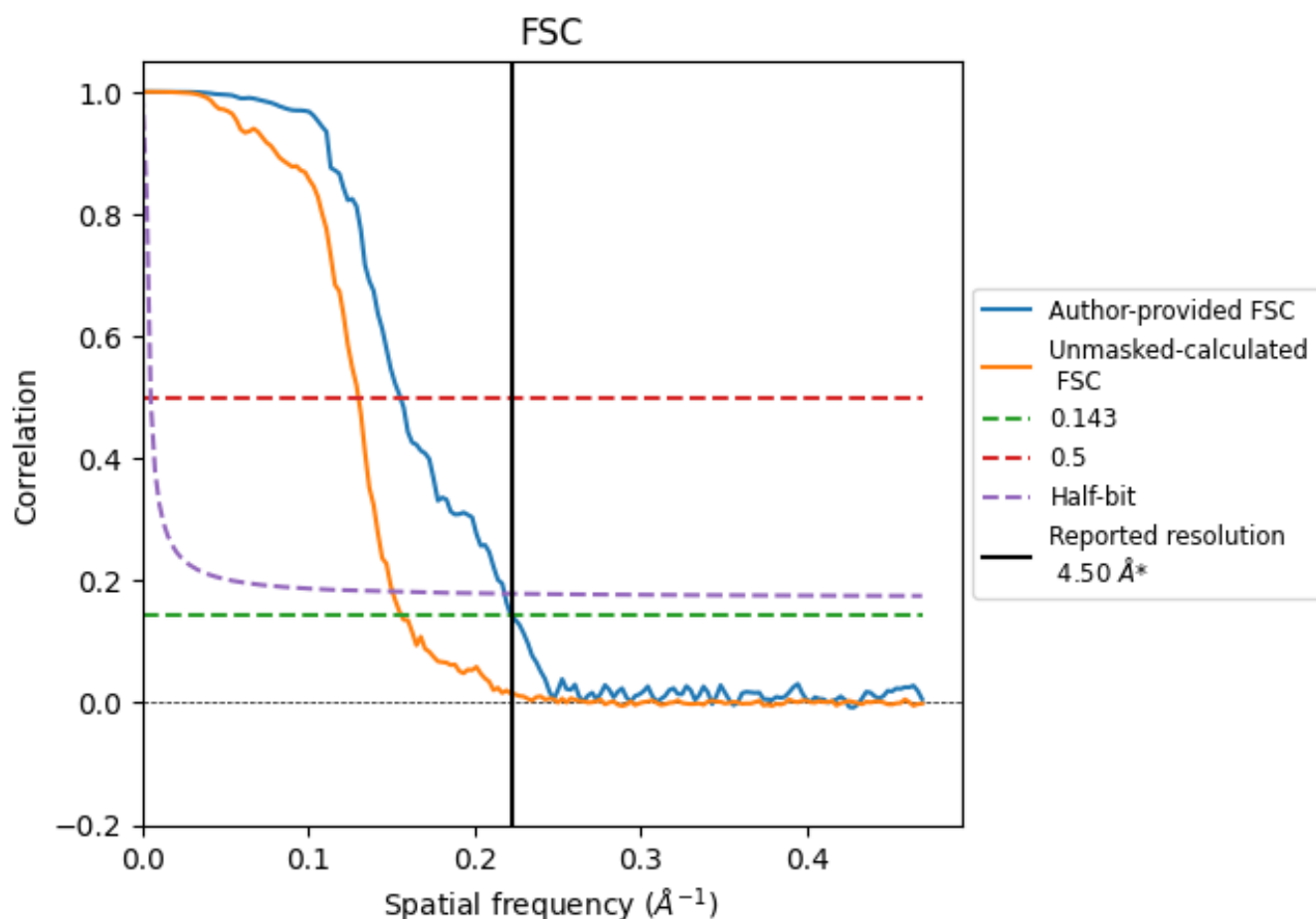


*Reported resolution corresponds to spatial frequency of $0.222 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

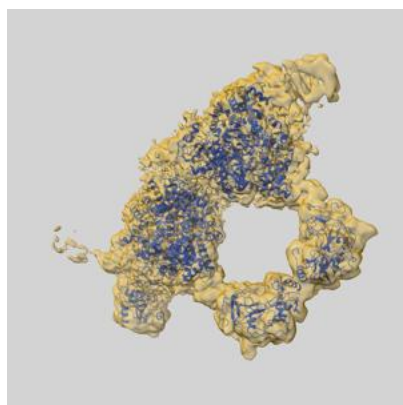
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.44	4.59
Unmasked-calculated*	6.41	7.69	6.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.5 by more than 10 %

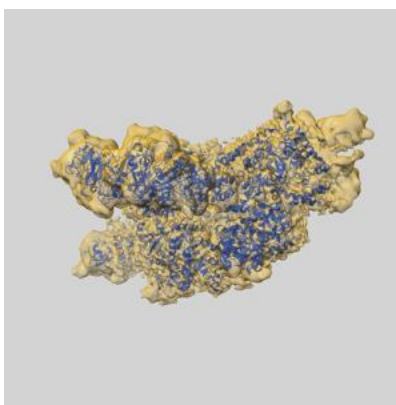
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4975 and PDB model 6ROW. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

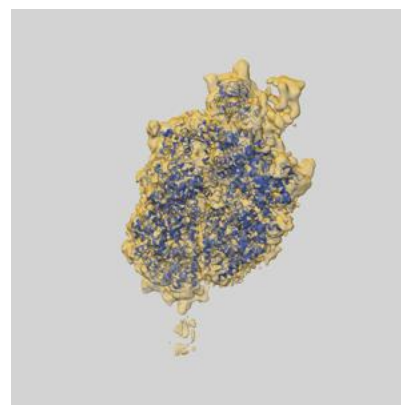
9.1 Map-model overlay [i](#)



X



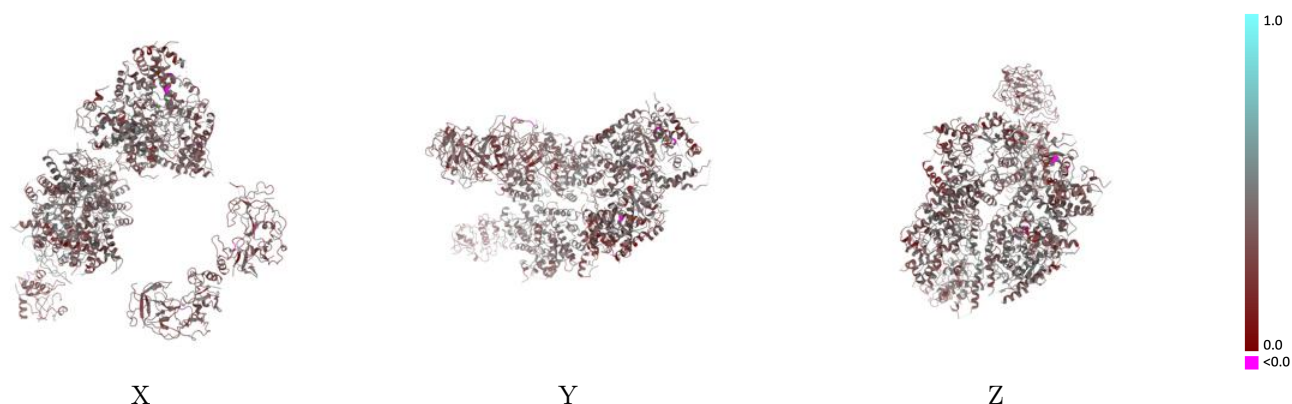
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



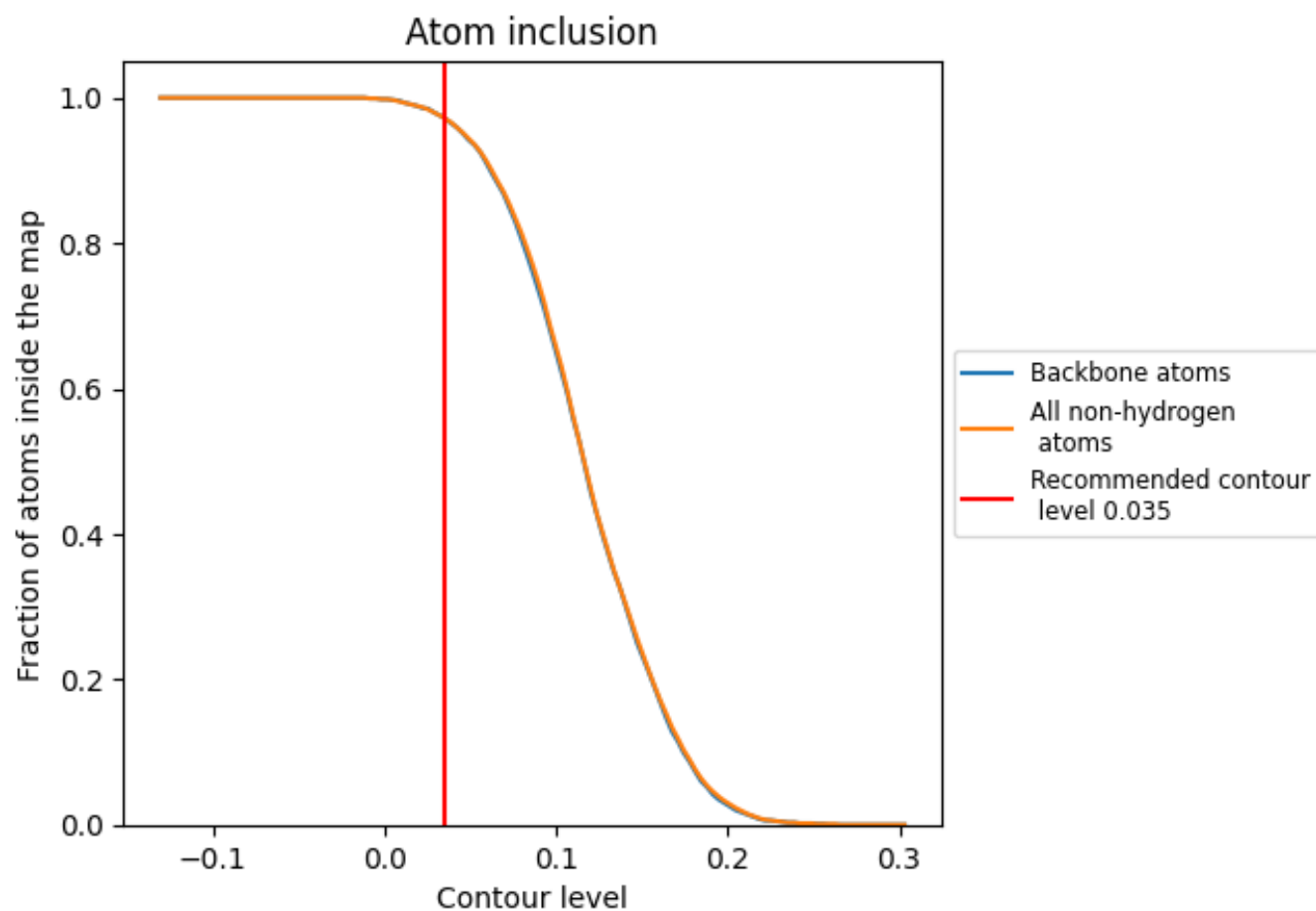
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.3790
A	0.9760	0.4040
B	0.9660	0.3870
C	0.9730	0.3890
D	0.9620	0.3650
E	1.0000	0.3610
F	1.0000	0.3400
G	0.9980	0.2980

1.0

0.0

<0.0