



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:30 PM GMT

PDB ID : 1FQV
Title : Insights into scf ubiquitin ligases from the structure of the skp1-skp2 complex
Authors : Schulman, B.A.; Carrano, A.C.; Jeffrey, P.D.; Bowen, Z.; Kinnucan, E.R.; Finnin, M.S.; Elledge, S.J.; Harper, J.W.; Pagano, M.; Pavletich, N.P.
Deposited on : 2000-09-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

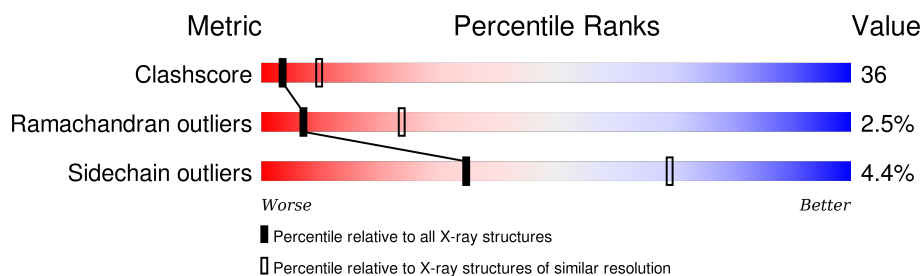
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	336	
1	C	336	
1	E	336	
1	G	336	
1	I	336	
1	K	336	
1	M	336	

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Mol	Chain	Length	Quality of chain
1	O	336	
2	B	149	
2	D	149	
2	F	149	
2	H	149	
2	J	149	
2	L	149	
2	N	149	
2	P	149	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SKP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	C	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	E	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	G	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	I	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	K	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	M	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	O	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			

- Molecule 2 is a protein called SKP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	D	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	F	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	H	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	J	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	L	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	P	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	GLY	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	PRO	DELETION	UNP P63208
B	?	-	PRO	DELETION	UNP P63208
B	?	-	PRO	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	ASN	DELETION	UNP P63208
B	?	-	LYS	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	LYS	DELETION	UNP P63208
B	?	-	ARG	DELETION	UNP P63208
B	?	-	THR	DELETION	UNP P63208
B	78	GLY	-	SEE REMARK 999	UNP P63208
B	79	GLY	-	SEE REMARK 999	UNP P63208
B	80	SER	-	SEE REMARK 999	UNP P63208
B	81	GLY	-	SEE REMARK 999	UNP P63208
B	82	THR	-	SEE REMARK 999	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208
D	?	-	GLY	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	PRO	DELETION	UNP P63208
D	?	-	PRO	DELETION	UNP P63208
D	?	-	PRO	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208
D	?	-	ASN	DELETION	UNP P63208
D	?	-	LYS	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208
D	?	-	LYS	DELETION	UNP P63208
D	?	-	ARG	DELETION	UNP P63208
D	?	-	THR	DELETION	UNP P63208
D	78	GLY	-	SEE REMARK 999	UNP P63208
D	79	GLY	-	SEE REMARK 999	UNP P63208
D	80	SER	-	SEE REMARK 999	UNP P63208
D	81	GLY	-	SEE REMARK 999	UNP P63208
D	82	THR	-	SEE REMARK 999	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	GLY	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	PRO	DELETION	UNP P63208
F	?	-	PRO	DELETION	UNP P63208
F	?	-	PRO	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	ASN	DELETION	UNP P63208
F	?	-	LYS	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	LYS	DELETION	UNP P63208
F	?	-	ARG	DELETION	UNP P63208
F	?	-	THR	DELETION	UNP P63208
F	78	GLY	-	SEE REMARK 999	UNP P63208
F	79	GLY	-	SEE REMARK 999	UNP P63208
F	80	SER	-	SEE REMARK 999	UNP P63208
F	81	GLY	-	SEE REMARK 999	UNP P63208
F	82	THR	-	SEE REMARK 999	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	GLY	DELETION	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ASP	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	PRO	DELETION	UNP P63208
H	?	-	PRO	DELETION	UNP P63208
H	?	-	PRO	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	ASN	DELETION	UNP P63208
H	?	-	LYS	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	LYS	DELETION	UNP P63208
H	?	-	ARG	DELETION	UNP P63208
H	?	-	THR	DELETION	UNP P63208
H	78	GLY	-	SEE REMARK 999	UNP P63208
H	79	GLY	-	SEE REMARK 999	UNP P63208
H	80	SER	-	SEE REMARK 999	UNP P63208
H	81	GLY	-	SEE REMARK 999	UNP P63208
H	82	THR	-	SEE REMARK 999	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	GLY	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	PRO	DELETION	UNP P63208
J	?	-	PRO	DELETION	UNP P63208
J	?	-	PRO	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	ASN	DELETION	UNP P63208
J	?	-	LYS	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	LYS	DELETION	UNP P63208
J	?	-	ARG	DELETION	UNP P63208
J	?	-	THR	DELETION	UNP P63208
J	78	GLY	-	SEE REMARK 999	UNP P63208
J	79	GLY	-	SEE REMARK 999	UNP P63208
J	80	SER	-	SEE REMARK 999	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
J	81	GLY	-	SEE REMARK 999	UNP P63208
J	82	THR	-	SEE REMARK 999	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	GLY	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	PRO	DELETION	UNP P63208
L	?	-	PRO	DELETION	UNP P63208
L	?	-	PRO	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	ASN	DELETION	UNP P63208
L	?	-	LYS	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	LYS	DELETION	UNP P63208
L	?	-	ARG	DELETION	UNP P63208
L	?	-	THR	DELETION	UNP P63208
L	78	GLY	-	SEE REMARK 999	UNP P63208
L	79	GLY	-	SEE REMARK 999	UNP P63208
L	80	SER	-	SEE REMARK 999	UNP P63208
L	81	GLY	-	SEE REMARK 999	UNP P63208
L	82	THR	-	SEE REMARK 999	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208
N	?	-	GLY	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	PRO	DELETION	UNP P63208
N	?	-	PRO	DELETION	UNP P63208
N	?	-	PRO	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208
N	?	-	ASN	DELETION	UNP P63208
N	?	-	LYS	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208

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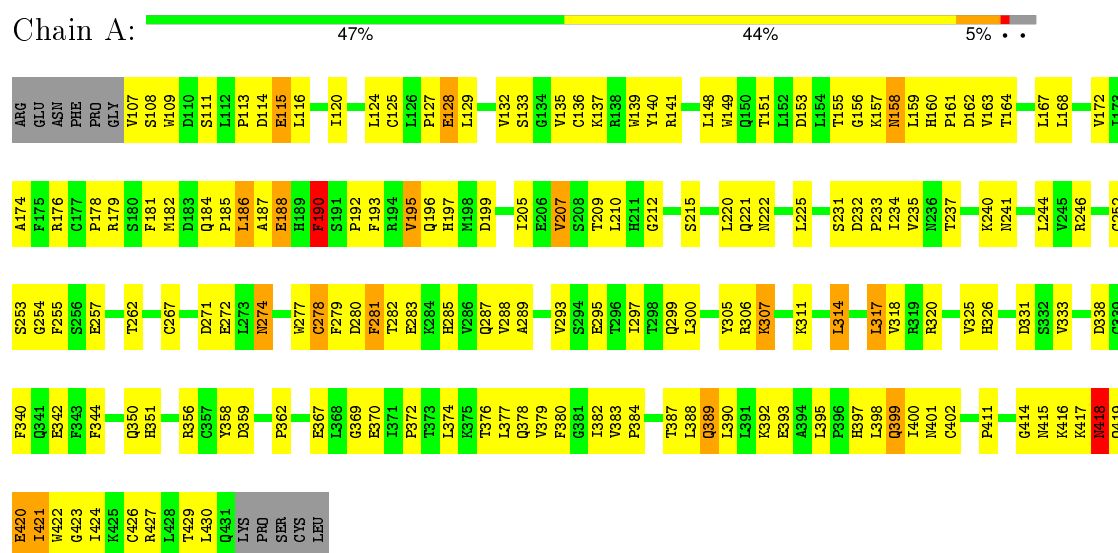
Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	DELETION	UNP P63208
N	?	-	ARG	DELETION	UNP P63208
N	?	-	THR	DELETION	UNP P63208
N	78	GLY	-	SEE REMARK 999	UNP P63208
N	79	GLY	-	SEE REMARK 999	UNP P63208
N	80	SER	-	SEE REMARK 999	UNP P63208
N	81	GLY	-	SEE REMARK 999	UNP P63208
N	82	THR	-	SEE REMARK 999	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
P	?	-	GLY	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	PRO	DELETION	UNP P63208
P	?	-	PRO	DELETION	UNP P63208
P	?	-	PRO	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
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P	?	-	ASP	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
P	?	-	ASN	DELETION	UNP P63208
P	?	-	LYS	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
P	?	-	LYS	DELETION	UNP P63208
P	?	-	ARG	DELETION	UNP P63208
P	?	-	THR	DELETION	UNP P63208
P	78	GLY	-	SEE REMARK 999	UNP P63208
P	79	GLY	-	SEE REMARK 999	UNP P63208
P	80	SER	-	SEE REMARK 999	UNP P63208
P	81	GLY	-	SEE REMARK 999	UNP P63208
P	82	THR	-	SEE REMARK 999	UNP P63208

3 Residue-property plots

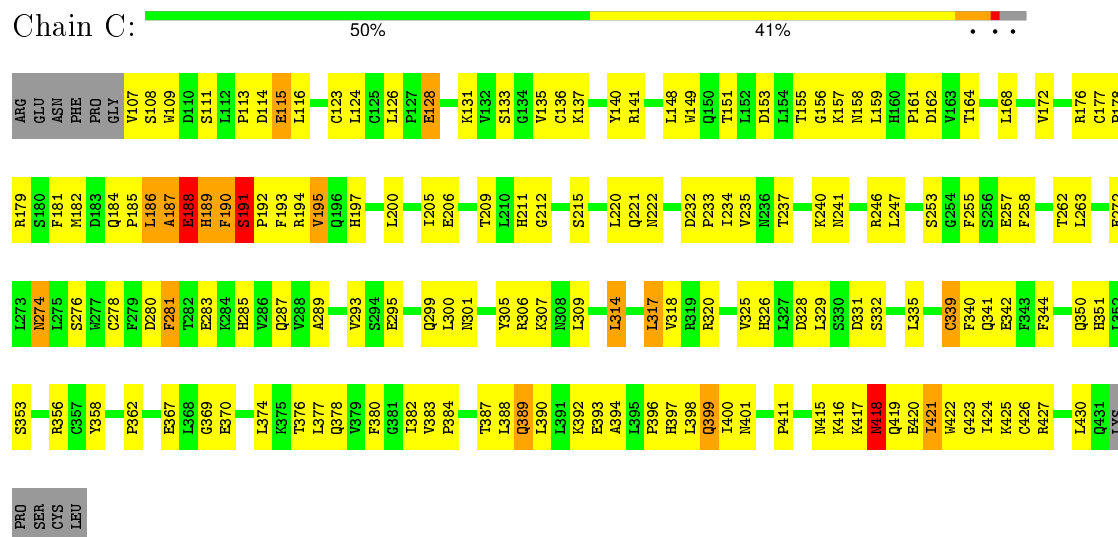
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: SKP2

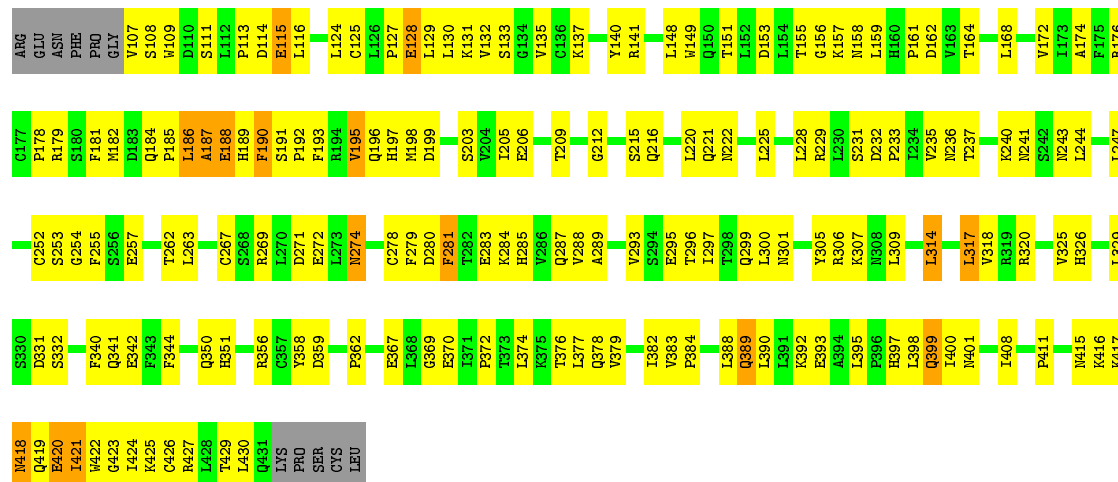


• Molecule 1: SKP2



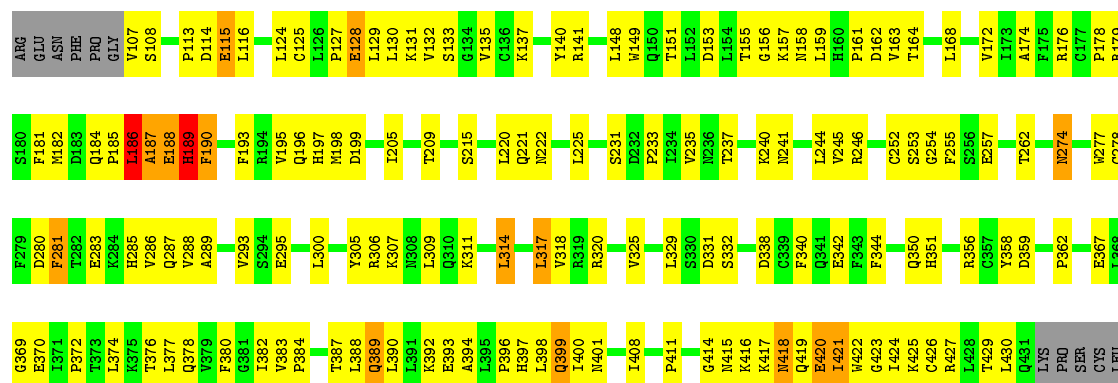
- Molecule 1: SKP2

Chain E: 46% 46% 5% .



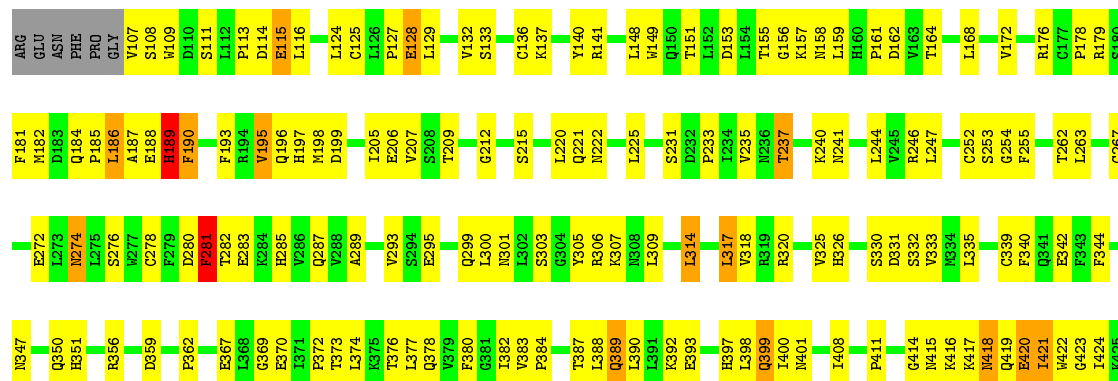
- Molecule 1: SKP2

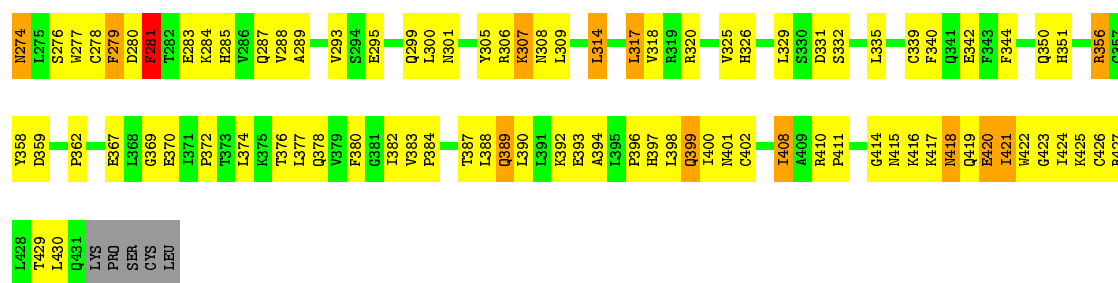
Chain G:  51% 41% . . .



- Molecule 1: SKP2

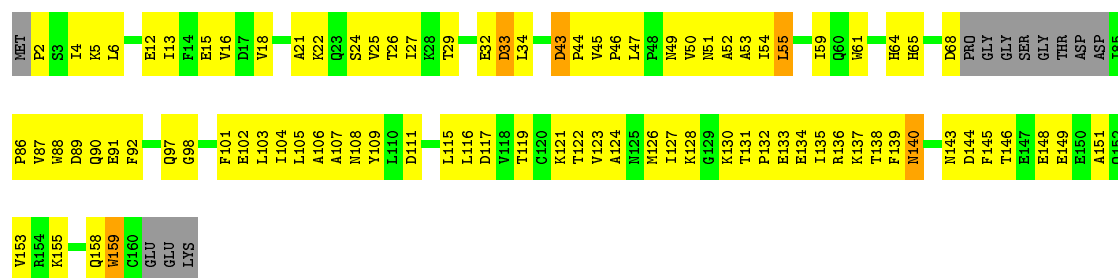
Chain I: 49% 43% . . .





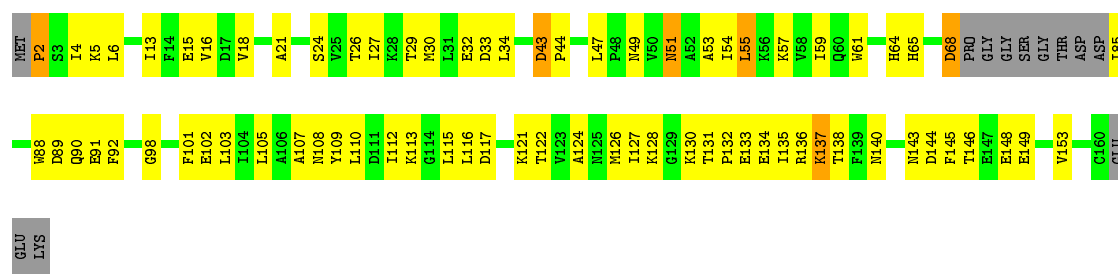
• Molecule 2: SKP1

Chain B: 33% 56% 8%



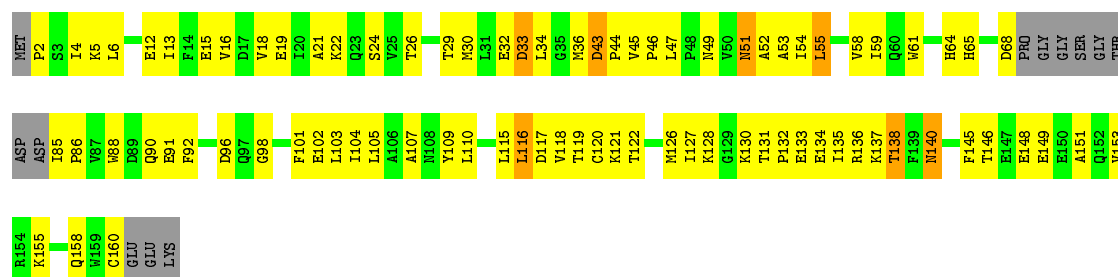
• Molecule 2: SKP1

Chain D: 42% 46% 8%



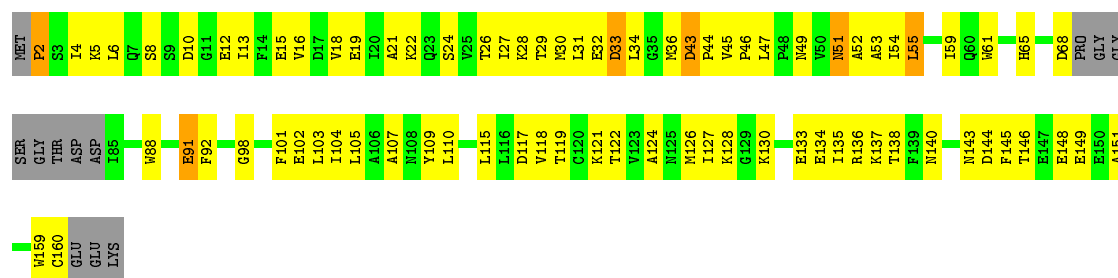
• Molecule 2: SKP1

Chain F: 36% 51% 5% 8%



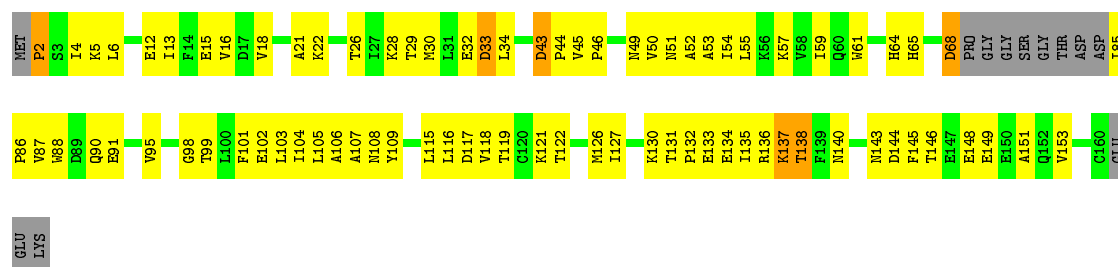
• Molecule 2: SKP1

Chain H: 39% 49% 8%



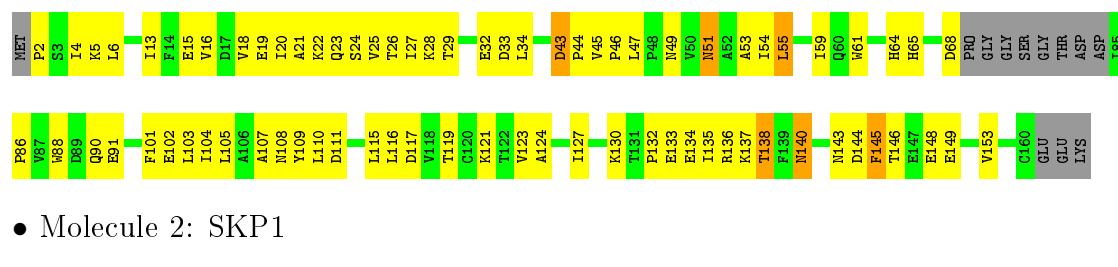
- Molecule 2: SKP1

Chain J: 38% 50% 8%



- Molecule 2: SKP1

Chain L: 42% 46% 8%



- Molecule 2: SKP1

Chain N: 38% 50% 8%



- Molecule 2: SKP1

Chain P: 38% 50% 8%



I85	I86	I87	I88	I89	I90	I91	I92	I93	I94	I95	I96	I97	I98	I99	F101	F102	F103	F104	F105	F106	F107	F108	F109	F110	F111	F112	F113	F114	F115	F116	F117	F118	F119	F120	F121	F122	F123	F124	F125	F126	F127	F128	F129	F130	F131	F132	F133	F134	F135	F136	F137	F138	F139	F140	F141	F142	F143	F144	F145	F146	F147	F148	F149	F150	F151	F152	F153	F154	F155	F156	F157	F158	F159	F160	F161	F162	F163	F164	F165	F166	F167	F168	F169	F170	F171	F172	F173	F174	F175	F176	F177	F178	F179	F180	F181	F182	F183	F184	F185	F186	F187	F188	F189	F190	F191	F192	F193	F194	F195	F196	F197	F198	F199	F200	F201	F202	F203	F204	F205	F206	F207	F208	F209	F210	F211	F212	F213	F214	F215	F216	F217	F218	F219	F220	F221	F222	F223	F224	F225	F226	F227	F228	F229	F230	F231	F232	F233	F234	F235	F236	F237	F238	F239	F240	F241	F242	F243	F244	F245	F246	F247	F248	F249	F250	F251	F252	F253	F254	F255	F256	F257	F258	F259	F260	F261	F262	F263	F264	F265	F266	F267	F268	F269	F270	F271	F272	F273	F274	F275	F276	F277	F278	F279	F280	F281	F282	F283	F284	F285	F286	F287	F288	F289	F290	F291	F292	F293	F294	F295	F296	F297	F298	F299	F300	F301	F302	F303	F304	F305	F306	F307	F308	F309	F310	F311	F312	F313	F314	F315	F316	F317	F318	F319	F320	F321	F322	F323	F324	F325	F326	F327	F328	F329	F330	F331	F332	F333	F334	F335	F336	F337	F338	F339	F340	F341	F342	F343	F344	F345	F346	F347	F348	F349	F350	F351	F352	F353	F354	F355	F356	F357	F358	F359	F360	F361	F362	F363	F364	F365	F366	F367	F368	F369	F370	F371	F372	F373	F374	F375	F376	F377	F378	F379	F380	F381	F382	F383	F384	F385	F386	F387	F388	F389	F390	F391	F392	F393	F394	F395	F396	F397	F398	F399	F400	F401	F402	F403	F404	F405	F406	F407	F408	F409	F410	F411	F412	F413	F414	F415	F416	F417	F418	F419	F420	F421	F422	F423	F424	F425	F426	F427	F428	F429	F430	F431	F432	F433	F434	F435	F436	F437	F438	F439	F440	F441	F442	F443	F444	F445	F446	F447	F448	F449	F450	F451	F452	F453	F454	F455	F456	F457	F458	F459	F460	F461	F462	F463	F464	F465	F466	F467	F468	F469	F470	F471	F472	F473	F474	F475	F476	F477	F478	F479	F480	F481	F482	F483	F484	F485	F486	F487	F488	F489	F490	F491	F492	F493	F494	F495	F496	F497	F498	F499	F500	F501	F502	F503	F504	F505	F506	F507	F508	F509	F510	F511	F512	F513	F514	F515	F516	F517	F518	F519	F520	F521	F522	F523	F524	F525	F526	F527	F528	F529	F530	F531	F532	F533	F534	F535	F536	F537	F538	F539	F540	F541	F542	F543	F544	F545	F546	F547	F548	F549	F550	F551	F552	F553	F554	F555	F556	F557	F558	F559	F560	F561	F562	F563	F564	F565	F566	F567	F568	F569	F570	F571	F572	F573	F574	F575	F576	F577	F578	F579	F580	F581	F582	F583	F584	F585	F586	F587	F588	F589	F590	F591	F592	F593	F594	F595	F596	F597	F598	F599	F600	F601	F602	F603	F604	F605	F606	F607	F608	F609	F610	F611	F612	F613	F614	F615	F616	F617	F618	F619	F620	F621	F622	F623	F624	F625	F626	F627	F628	F629	F630	F631	F632	F633	F634	F635	F636	F637	F638	F639	F640	F641	F642	F643	F644	F645	F646	F647	F648	F649	F650	F651	F652	F653	F654	F655	F656	F657	F658	F659	F660	F661	F662	F663	F664	F665	F666	F667	F668	F669	F670	F671	F672	F673	F674	F675	F676	F677	F678	F679	F680	F681	F682	F683	F684	F685	F686	F687	F688	F689	F690	F691	F692	F693	F694	F695	F696	F697	F698	F699	F700	F701	F702	F703	F704	F705	F706	F707	F708	F709	F710	F711	F712	F713	F714	F715	F716	F717	F718	F719	F720	F721	F722	F723	F724	F725	F726	F727	F728	F729	F730	F731	F732	F733	F734	F735	F736	F737	F738	F739	F740	F741	F742	F743	F744	F745	F746	F747	F748	F749	F750	F751	F752	F753	F754	F755	F756	F757	F758	F759	F760	F761	F762	F763	F764	F765	F766	F767	F768	F769	F770	F771	F772	F773	F774	F775	F776	F777	F778	F779	F780	F781	F782	F783	F784	F785	F786	F787	F788	F789	F790	F791	F792	F793	F794	F795	F796	F797	F798	F799	F800	F801	F802	F803	F804	F805	F806	F807	F808	F809	F810	F811	F812	F813	F814	F815	F816	F817	F818	F819	F820	F821	F822	F823	F824	F825	F826	F827	F828	F829	F830	F831	F832	F833	F834	F835	F836	F837	F838	F839	F840	F841	F842	F843	F844	F845	F846	F847	F848	F849	F850	F851	F852	F853	F854	F855	F856	F857	F858	F859	F860	F861	F862	F863	F864	F865	F866	F867	F868	F869	F870	F871	F872	F873	F874	F875	F876	F877	F878	F879	F880	F881	F882	F883	F884	F885	F886	F887	F888	F889	F890	F891	F892	F893	F894	F895	F896	F897	F898	F899	F900	F901	F902	F903	F904	F905	F906	F907	F908	F909	F910	F911	F912	F913	F914	F915	F916	F917	F918	F919	F920	F921	F922	F923	F924	F925	F926	F927	F928	F929	F930	F931	F932	F933	F934	F935	F936	F937	F938	F939	F940	F941	F942	F943	F944	F945	F946	F947	F948	F949	F950	F951	F952	F953	F954	F955	F956	F957	F958	F959	F960	F961	F962	F963	F964	F965	F966	F967	F968	F969	F970	F971	F972	F973	F974	F975	F976	F977	F978	F979	F980	F981	F982	F983	F984	F985	F986	F987	F988	F989	F990	F991	F992	F993	F994	F995	F996	F997	F998	F999	F1000	F1001	F1002	F1003	F1004	F1005	F1006	F1007	F1008	F1009	F1010	F1011	F1012	F1013	F1014	F1015	F1016	F1017	F1018	F1019	F1020	F1021	F1022	F1023	F1024	F1025	F1026	F1027	F1028	F1029	F1030	F1031	F1032	F1033	F1034	F1035	F1036	F1037	F1038	F1039	F1040	F1041	F1042	F1043	F1044	F1045	F1046	F1047	F1048	F1049	F1050	F1051	F1052	F1053	F1054	F1055	F1056	F1057	F1058	F1059	F1060	F1061	F1062	F1063	F1064	F1065	F1066	F1067	F1068	F1069	F1070	F1071	F1072	F1073	F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W159	C160	GLU	GLU	LYS
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4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.70 Å 148.20 Å 133.30 Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29256	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	1/2612 (0.0%)	0.80	3/3545 (0.1%)
1	C	0.63	4/2612 (0.2%)	0.88	7/3545 (0.2%)
1	E	0.52	0/2612	0.77	1/3545 (0.0%)
1	G	0.63	2/2612 (0.1%)	1.06	7/3545 (0.2%)
1	I	0.60	2/2612 (0.1%)	1.01	6/3545 (0.2%)
1	K	0.59	1/2612 (0.0%)	1.06	7/3545 (0.2%)
1	M	0.59	3/2612 (0.1%)	0.90	4/3545 (0.1%)
1	O	0.55	1/2612 (0.0%)	1.06	8/3545 (0.2%)
2	B	0.35	0/1111	0.61	1/1502 (0.1%)
2	D	0.42	0/1111	0.64	1/1502 (0.1%)
2	F	0.38	0/1111	0.63	1/1502 (0.1%)
2	H	0.58	0/1111	0.71	1/1502 (0.1%)
2	J	0.42	0/1111	0.66	1/1502 (0.1%)
2	L	0.44	0/1111	0.66	1/1502 (0.1%)
2	N	0.44	0/1111	0.65	1/1502 (0.1%)
2	P	0.54	0/1111	0.69	1/1502 (0.1%)
All	All	0.55	14/29784 (0.0%)	0.87	51/40376 (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	I	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	186	LEU	C-N	15.94	1.70	1.34
1	I	186	LEU	C-N	12.79	1.63	1.34
1	G	189	HIS	C-N	-9.35	1.12	1.34
1	K	189	HIS	C-N	-8.94	1.13	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	PHE	N-CA	-7.71	1.30	1.46
1	M	186	LEU	C-N	7.59	1.51	1.34
1	O	189	HIS	C-N	-7.04	1.17	1.34
1	C	189	HIS	C-N	-6.15	1.19	1.34
1	C	123	CYS	CB-SG	-5.89	1.72	1.81
1	M	190	PHE	N-CA	-5.85	1.34	1.46
1	C	190	PHE	C-N	-5.62	1.21	1.34
1	I	189	HIS	C-N	-5.60	1.21	1.34
1	M	189	HIS	CA-C	-5.55	1.38	1.52
1	C	339	CYS	CB-SG	-5.05	1.73	1.81

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	HIS	O-C-N	23.02	159.53	122.70
1	I	189	HIS	C-N-CA	-22.18	66.25	121.70
1	K	186	LEU	O-C-N	21.78	157.54	122.70
1	G	186	LEU	O-C-N	20.23	155.06	122.70
1	O	186	LEU	O-C-N	19.63	154.11	122.70
1	M	186	LEU	O-C-N	19.60	154.06	122.70
1	O	189	HIS	C-N-CA	-19.60	72.70	121.70
1	I	189	HIS	CA-C-N	-19.52	74.26	117.20
1	G	189	HIS	C-N-CA	-19.19	73.73	121.70
1	G	189	HIS	CA-C-N	-19.03	75.33	117.20
1	O	189	HIS	O-C-N	18.85	152.87	122.70
1	I	189	HIS	O-C-N	18.70	152.62	122.70
1	K	189	HIS	O-C-N	18.35	152.06	122.70
1	K	189	HIS	C-N-CA	-18.23	76.14	121.70
1	O	189	HIS	CA-C-N	-17.30	79.14	117.20
1	K	189	HIS	CA-C-N	-17.25	79.25	117.20
1	O	186	LEU	CA-C-N	-16.47	80.96	117.20
1	M	186	LEU	CA-C-N	-15.71	82.63	117.20
1	K	186	LEU	CA-C-N	-15.33	83.47	117.20
1	G	186	LEU	CA-C-N	-14.87	84.49	117.20
1	C	190	PHE	N-CA-CB	-14.73	84.09	110.60
1	I	186	LEU	O-C-N	12.12	142.09	122.70
1	I	186	LEU	CA-C-N	-9.06	97.27	117.20
1	G	186	LEU	C-N-CA	-8.29	100.98	121.70
1	O	186	LEU	C-N-CA	-8.23	101.12	121.70
1	A	281	PHE	N-CA-C	7.85	132.19	111.00
1	K	186	LEU	C-N-CA	-7.64	102.60	121.70
1	K	281	PHE	N-CA-C	7.59	131.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	PHE	N-CA-C	7.52	131.31	111.00
1	E	281	PHE	N-CA-C	7.45	131.10	111.00
1	G	281	PHE	N-CA-C	7.34	130.83	111.00
1	I	281	PHE	N-CA-C	7.26	130.60	111.00
1	M	281	PHE	N-CA-C	7.09	130.14	111.00
1	C	189	HIS	N-CA-C	6.89	129.61	111.00
1	O	281	PHE	N-CA-C	6.87	129.54	111.00
1	C	188	GLU	O-C-N	6.45	133.02	122.70
1	C	189	HIS	CB-CA-C	-6.32	97.75	110.40
1	C	191	SER	N-CA-C	6.32	128.06	111.00
1	M	186	LEU	C-N-CA	-6.20	106.20	121.70
2	N	2	PRO	N-CA-CB	5.75	110.20	103.30
2	D	2	PRO	N-CA-CB	5.64	110.07	103.30
2	F	2	PRO	N-CA-CB	5.51	109.91	103.30
2	J	2	PRO	N-CA-CB	5.51	109.91	103.30
2	L	2	PRO	N-CA-CB	5.50	109.90	103.30
2	B	2	PRO	N-CA-CB	5.50	109.89	103.30
1	O	356	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	H	2	PRO	N-CA-CB	5.26	109.61	103.30
2	P	2	PRO	N-CA-CB	5.21	109.55	103.30
1	C	188	GLU	CA-C-N	-5.21	105.75	117.20
1	A	278	CYS	N-CA-C	-5.17	97.03	111.00
1	A	158	ASN	N-CA-C	-5.07	97.32	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	189	HIS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2563	0	2598	214	0
1	C	2563	0	2597	206	0
1	E	2563	0	2598	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2563	0	2596	217	0
1	I	2563	0	2598	188	0
1	K	2563	0	2598	217	0
1	M	2563	0	2598	194	0
1	O	2563	0	2598	221	0
2	B	1094	0	1099	87	0
2	D	1094	0	1099	75	0
2	F	1094	0	1099	84	1
2	H	1094	0	1099	71	0
2	J	1094	0	1099	75	0
2	L	1094	0	1099	84	1
2	N	1094	0	1099	77	0
2	P	1094	0	1099	87	0
All	All	29256	0	29573	2115	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (2115) 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:G:186:LEU:C	1:G:187:ALA:N	1.70	1.40
1:M:189:HIS:O	1:M:190:PHE:O	1.58	1.17
1:K:417:LYS:CE	1:O:417:LYS:HG3	1.75	1.15
1:I:417:LYS:HG3	1:M:417:LYS:CE	1.77	1.14
2:L:43:ASP:HB2	2:L:44:PRO:HD3	1.29	1.14
1:I:416:LYS:HD2	1:I:417:LYS:HZ1	1.10	1.13
2:H:4:ILE:HG12	2:H:18:VAL:HG12	1.33	1.10
1:C:188:GLU:O	1:C:212:GLY:O	1.69	1.10
1:K:148:LEU:HA	1:K:427:ARG:HH22	1.14	1.09
1:A:417:LYS:HG3	1:E:417:LYS:CE	1.81	1.09
1:C:417:LYS:CE	1:G:417:LYS:HG3	1.84	1.07
1:E:215:SER:HA	1:E:237:THR:HG21	1.36	1.07
1:G:186:LEU:CA	1:G:187:ALA:N	2.18	1.07
2:N:65:HIS:HB3	2:N:68:ASP:HB2	1.31	1.07
1:M:189:HIS:O	1:M:190:PHE:C	1.88	1.06
1:O:416:LYS:HD2	1:O:417:LYS:HZ1	1.13	1.06
1:A:416:LYS:HB3	1:A:417:LYS:HE2	1.38	1.06
1:E:189:HIS:O	1:E:190:PHE:O	1.73	1.05
2:J:4:ILE:HG12	2:J:18:VAL:HG12	1.37	1.05
2:P:43:ASP:HB2	2:P:44:PRO:HD3	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:417:LYS:HD2	1:M:417:LYS:HG3	1.36	1.04
1:C:417:LYS:HE3	1:G:417:LYS:HG3	1.05	1.04
1:A:215:SER:HA	1:A:237:THR:HG21	1.39	1.04
2:B:43:ASP:HB2	2:B:44:PRO:HD3	1.40	1.04
2:N:43:ASP:HB2	2:N:44:PRO:HD3	1.38	1.04
2:B:65:HIS:HB3	2:B:68:ASP:HB2	1.35	1.04
1:K:416:LYS:HB3	1:K:417:LYS:HE2	1.37	1.03
1:O:416:LYS:HB3	1:O:417:LYS:HE2	1.39	1.03
2:J:43:ASP:HB2	2:J:44:PRO:HD3	1.40	1.03
2:F:65:HIS:HB3	2:F:68:ASP:HB2	1.40	1.03
2:L:65:HIS:HB3	2:L:68:ASP:HB2	1.41	1.03
2:P:4:ILE:HG12	2:P:18:VAL:HG12	1.39	1.03
2:P:65:HIS:HB3	2:P:68:ASP:HB2	1.38	1.02
2:D:4:ILE:HG12	2:D:18:VAL:HG12	1.39	1.02
2:F:43:ASP:HB2	2:F:44:PRO:HD3	1.37	1.02
1:K:153:ASP:OD1	1:K:155:THR:HG23	1.60	1.02
1:K:148:LEU:HA	1:K:427:ARG:NH2	1.74	1.02
2:D:43:ASP:HB2	2:D:44:PRO:HD3	1.41	1.02
2:F:96:ASP:OD1	1:O:284:LYS:HE3	1.59	1.02
2:B:4:ILE:HG12	2:B:18:VAL:HG12	1.41	1.02
1:C:416:LYS:HB3	1:C:417:LYS:HE2	1.39	1.01
1:C:162:ASP:HA	1:C:190:PHE:HZ	1.26	1.01
1:K:417:LYS:HG3	1:O:417:LYS:HD2	1.43	1.01
1:G:155:THR:HG22	1:G:178:PRO:HD2	1.42	1.01
1:C:148:LEU:HA	1:C:427:ARG:HH22	1.23	1.01
1:A:289:ALA:O	1:A:293:VAL:HG23	1.59	1.01
2:L:4:ILE:HG12	2:L:18:VAL:HG12	1.40	1.01
1:C:215:SER:HA	1:C:237:THR:HG21	1.40	1.00
2:H:43:ASP:HB2	2:H:44:PRO:HD3	1.38	1.00
1:M:189:HIS:C	1:M:190:PHE:O	1.91	1.00
1:I:417:LYS:CG	1:M:417:LYS:HE3	1.90	1.00
1:M:215:SER:HA	1:M:237:THR:HG21	1.44	1.00
2:F:4:ILE:HG12	2:F:18:VAL:HG12	1.42	1.00
1:E:162:ASP:HA	1:E:190:PHE:HZ	1.23	1.00
1:E:416:LYS:HB3	1:E:417:LYS:HE2	1.38	0.99
1:K:417:LYS:HE3	1:O:417:LYS:CG	1.90	0.99
1:A:417:LYS:CG	1:E:417:LYS:HE3	1.92	0.99
1:A:417:LYS:HG3	1:E:417:LYS:HE3	1.00	0.99
2:N:4:ILE:HG12	2:N:18:VAL:HG12	1.40	0.99
1:M:155:THR:HG22	1:M:178:PRO:HD2	1.44	0.99
1:C:417:LYS:HE3	1:G:417:LYS:CG	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:HA	1:C:427:ARG:NH2	1.77	0.98
1:A:417:LYS:HD2	1:E:417:LYS:HG3	1.45	0.98
1:G:416:LYS:HB3	1:G:417:LYS:HE2	1.44	0.97
1:M:416:LYS:HB3	1:M:417:LYS:HE2	1.44	0.97
1:O:215:SER:HA	1:O:237:THR:HG21	1.44	0.97
1:E:155:THR:HG22	1:E:178:PRO:HD2	1.45	0.97
1:I:416:LYS:HB3	1:I:417:LYS:HE2	1.44	0.97
1:K:417:LYS:HE3	1:O:417:LYS:HG3	0.97	0.96
1:G:215:SER:HA	1:G:237:THR:HG21	1.45	0.96
1:G:176:ARG:CZ	1:G:419:GLN:H	1.79	0.95
1:G:416:LYS:HD2	1:G:417:LYS:HZ1	1.25	0.95
1:C:155:THR:HG22	1:C:178:PRO:HD2	1.48	0.95
1:A:416:LYS:HD2	1:A:417:LYS:HZ1	1.32	0.94
1:I:417:LYS:HG3	1:M:417:LYS:HE3	0.94	0.94
1:A:155:THR:HG22	1:A:178:PRO:HD2	1.48	0.94
1:I:417:LYS:CD	1:M:417:LYS:HG3	1.97	0.93
1:I:215:SER:HA	1:I:237:THR:HG21	1.45	0.93
1:K:399:GLN:HE21	1:K:399:GLN:HA	1.34	0.93
2:D:65:HIS:HB3	2:D:68:ASP:HB2	1.48	0.92
1:M:156:GLY:HA2	1:M:179:ARG:O	1.70	0.92
1:C:113:PRO:HD2	1:C:116:LEU:HD12	1.50	0.91
1:I:416:LYS:HD2	1:I:417:LYS:NZ	1.84	0.91
1:K:215:SER:HA	1:K:237:THR:HG21	1.52	0.91
1:K:253:SER:HB2	1:K:280:ASP:HB2	1.53	0.91
1:K:197:HIS:HD2	1:K:222:ASN:HD22	1.19	0.90
1:K:417:LYS:HG3	1:O:417:LYS:CD	2.00	0.90
1:A:113:PRO:HD2	1:A:116:LEU:HD12	1.53	0.90
1:O:176:ARG:CZ	1:O:419:GLN:H	1.84	0.89
2:H:65:HIS:HB3	2:H:68:ASP:HB2	1.54	0.89
1:O:416:LYS:HD2	1:O:417:LYS:NZ	1.87	0.89
1:O:155:THR:HG22	1:O:178:PRO:HD2	1.55	0.89
1:C:253:SER:HB2	1:C:280:ASP:HB2	1.52	0.88
1:A:156:GLY:HA2	1:A:179:ARG:O	1.72	0.88
1:I:289:ALA:O	1:I:293:VAL:HG23	1.73	0.88
2:H:107:ALA:HB2	2:H:115:LEU:HD12	1.55	0.88
1:I:155:THR:HG22	1:I:178:PRO:HD2	1.51	0.88
1:K:116:LEU:HD21	2:L:108:ASN:CG	1.95	0.88
1:M:253:SER:HB2	1:M:280:ASP:HB2	1.54	0.88
1:G:289:ALA:O	1:G:293:VAL:HG23	1.74	0.88
1:I:113:PRO:HD2	1:I:116:LEU:HD12	1.54	0.88
2:D:5:LYS:HG2	2:D:15:GLU:HG2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:414:GLY:HA2	1:M:416:LYS:NZ	1.89	0.87
1:A:197:HIS:CD2	1:A:222:ASN:HD22	1.92	0.87
1:G:197:HIS:HD2	1:G:222:ASN:HD22	1.21	0.87
1:O:109:TRP:HA	2:P:101:PHE:HE2	1.38	0.87
2:B:107:ALA:HB2	2:B:115:LEU:HD12	1.54	0.87
1:C:153:ASP:OD1	1:C:155:THR:HG23	1.76	0.86
1:I:414:GLY:HA2	1:M:416:LYS:HZ2	1.40	0.86
2:F:5:LYS:HG2	2:F:15:GLU:HG2	1.58	0.86
1:A:137:LYS:HE3	2:B:144:ASP:O	1.75	0.86
1:C:253:SER:CB	1:C:280:ASP:HB2	2.05	0.86
2:P:107:ALA:HB2	2:P:115:LEU:HD12	1.55	0.86
1:E:389:GLN:O	1:E:393:GLU:HG2	1.77	0.85
1:O:389:GLN:O	1:O:393:GLU:HG2	1.76	0.85
1:K:113:PRO:HD2	1:K:116:LEU:HD12	1.56	0.85
2:J:65:HIS:HB3	2:J:68:ASP:HB2	1.56	0.85
1:O:128:GLU:HG2	2:P:128:LYS:HG2	1.59	0.85
1:G:186:LEU:C	1:G:187:ALA:CA	2.44	0.85
1:C:215:SER:HA	1:C:237:THR:CG2	2.07	0.85
1:E:215:SER:HA	1:E:237:THR:CG2	2.07	0.85
1:K:417:LYS:HG3	1:O:417:LYS:CE	2.07	0.84
1:I:415:ASN:O	1:I:417:LYS:HG2	1.76	0.84
1:K:155:THR:HG22	1:K:178:PRO:HD2	1.57	0.84
1:M:197:HIS:HD2	1:M:222:ASN:HD22	1.22	0.84
1:M:289:ALA:O	1:M:293:VAL:HG23	1.77	0.84
1:G:416:LYS:HD2	1:G:417:LYS:NZ	1.92	0.84
1:E:156:GLY:HA2	1:E:179:ARG:O	1.78	0.84
1:A:220:LEU:H	1:A:241:ASN:HD22	1.26	0.84
1:C:289:ALA:O	1:C:293:VAL:HG23	1.77	0.84
1:O:220:LEU:H	1:O:241:ASN:HD22	1.26	0.84
1:O:415:ASN:O	1:O:417:LYS:HG2	1.78	0.84
1:K:416:LYS:CB	1:K:417:LYS:HE2	2.07	0.84
1:E:283:GLU:O	1:E:287:GLN:HG3	1.78	0.83
1:I:156:GLY:HA2	1:I:179:ARG:O	1.78	0.83
1:E:189:HIS:C	1:E:190:PHE:O	2.14	0.83
1:A:197:HIS:HD2	1:A:222:ASN:HD22	1.26	0.83
1:E:416:LYS:CB	1:E:417:LYS:HE2	2.08	0.83
1:I:253:SER:CB	1:I:280:ASP:HB2	2.08	0.83
1:A:417:LYS:CD	1:E:417:LYS:HG3	2.09	0.83
1:M:215:SER:HA	1:M:237:THR:CG2	2.08	0.83
1:O:253:SER:HB2	1:O:280:ASP:HB2	1.58	0.83
1:K:253:SER:CB	1:K:280:ASP:HB2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:SER:CB	1:E:280:ASP:HB2	2.09	0.83
1:A:416:LYS:HD2	1:A:417:LYS:NZ	1.94	0.82
1:E:253:SER:HB2	1:E:280:ASP:HB2	1.61	0.82
1:K:136:CYS:HB2	2:L:144:ASP:OD2	1.79	0.82
1:A:253:SER:CB	1:A:280:ASP:HB2	2.09	0.82
1:I:253:SER:HB2	1:I:280:ASP:HB2	1.61	0.82
1:K:162:ASP:HA	1:K:190:PHE:HZ	1.44	0.82
2:J:5:LYS:HG2	2:J:15:GLU:HG2	1.61	0.82
1:G:113:PRO:HD2	1:G:116:LEU:HD12	1.59	0.82
1:O:148:LEU:HA	1:O:427:ARG:HH22	1.44	0.81
1:C:162:ASP:HA	1:C:190:PHE:CZ	2.15	0.81
1:A:415:ASN:O	1:A:417:LYS:HG2	1.80	0.81
1:C:417:LYS:HG3	1:G:417:LYS:HD2	1.60	0.81
1:E:189:HIS:O	1:E:190:PHE:C	2.17	0.81
1:A:389:GLN:O	1:A:393:GLU:HG2	1.80	0.81
1:O:289:ALA:O	1:O:293:VAL:HG23	1.79	0.81
1:M:113:PRO:HD2	1:M:116:LEU:HD12	1.61	0.81
1:C:191:SER:HB3	1:C:192:PRO:HD2	1.62	0.81
1:K:283:GLU:O	1:K:287:GLN:HG3	1.80	0.81
1:K:281:PHE:HB2	1:K:285:HIS:CG	2.16	0.81
1:G:176:ARG:CD	1:G:419:GLN:HA	2.11	0.81
1:G:148:LEU:HA	1:G:427:ARG:HH22	1.46	0.81
1:C:416:LYS:CB	1:C:417:LYS:HE2	2.10	0.80
1:M:148:LEU:HA	1:M:427:ARG:HH22	1.46	0.80
1:C:220:LEU:HB2	1:C:241:ASN:HD22	1.46	0.80
1:A:253:SER:HB2	1:A:280:ASP:HB2	1.62	0.80
2:N:5:LYS:HG2	2:N:15:GLU:HG2	1.60	0.80
1:E:148:LEU:HA	1:E:427:ARG:HH22	1.44	0.80
1:G:162:ASP:HA	1:G:190:PHE:HZ	1.45	0.80
1:E:281:PHE:HB2	1:E:285:HIS:ND1	1.96	0.80
1:K:220:LEU:H	1:K:241:ASN:HD22	1.26	0.80
1:M:253:SER:CB	1:M:280:ASP:HB2	2.12	0.80
1:I:220:LEU:HB2	1:I:241:ASN:ND2	1.97	0.80
1:O:162:ASP:HA	1:O:190:PHE:HZ	1.47	0.80
1:K:151:THR:HB	1:K:426:CYS:HA	1.64	0.79
1:E:416:LYS:HD2	1:E:417:LYS:NZ	1.96	0.79
1:A:414:GLY:HA2	1:E:416:LYS:NZ	1.97	0.79
1:I:215:SER:HA	1:I:237:THR:CG2	2.12	0.79
1:G:253:SER:CB	1:G:280:ASP:HB2	2.13	0.79
2:P:5:LYS:HG2	2:P:15:GLU:HG2	1.64	0.79
1:K:389:GLN:O	1:K:393:GLU:HG2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:LYS:HG2	2:B:15:GLU:HG2	1.63	0.79
1:C:389:GLN:O	1:C:393:GLU:HG2	1.82	0.79
1:K:189:HIS:O	1:K:190:PHE:O	1.60	0.79
1:I:389:GLN:O	1:I:393:GLU:HG2	1.83	0.79
1:O:113:PRO:HD2	1:O:116:LEU:HD12	1.64	0.79
1:O:215:SER:HA	1:O:237:THR:CG2	2.13	0.79
1:K:281:PHE:HB2	1:K:285:HIS:ND1	1.98	0.79
1:O:351:HIS:HD2	1:O:376:THR:OG1	1.66	0.79
1:C:137:LYS:HE3	2:D:144:ASP:O	1.83	0.79
1:E:197:HIS:HD2	1:E:222:ASN:HD22	1.27	0.79
1:K:215:SER:HA	1:K:237:THR:CG2	2.12	0.78
1:E:113:PRO:HD2	1:E:116:LEU:HD12	1.65	0.78
2:F:107:ALA:HB2	2:F:115:LEU:HD12	1.66	0.78
1:I:417:LYS:CE	1:M:417:LYS:HG3	2.12	0.78
1:M:415:ASN:O	1:M:417:LYS:HG2	1.84	0.78
1:E:162:ASP:HA	1:E:190:PHE:CZ	2.13	0.78
1:E:281:PHE:HB2	1:E:285:HIS:CG	2.19	0.78
1:G:159:LEU:HD23	1:G:164:THR:HG22	1.65	0.78
1:E:159:LEU:HD23	1:E:164:THR:HG22	1.65	0.78
1:O:131:LYS:HD3	2:P:130:LYS:O	1.83	0.78
1:G:281:PHE:HB2	1:G:285:HIS:CG	2.19	0.78
1:I:351:HIS:HD2	1:I:376:THR:OG1	1.66	0.77
2:H:4:ILE:CG1	2:H:18:VAL:HG12	2.13	0.77
1:G:148:LEU:HA	1:G:427:ARG:NH2	1.99	0.77
1:M:389:GLN:O	1:M:393:GLU:HG2	1.84	0.77
1:G:281:PHE:HB2	1:G:285:HIS:ND1	2.00	0.77
1:A:281:PHE:HB2	1:A:285:HIS:CG	2.19	0.77
1:O:253:SER:CB	1:O:280:ASP:HB2	2.14	0.77
2:N:107:ALA:HB2	2:N:115:LEU:HD12	1.64	0.77
1:G:215:SER:HA	1:G:237:THR:CG2	2.12	0.77
1:K:197:HIS:CD2	1:K:222:ASN:HD22	2.03	0.77
2:L:146:THR:HG22	2:L:148:GLU:H	1.49	0.77
1:O:182:MET:O	1:O:205:ILE:HA	1.84	0.77
1:K:116:LEU:HD21	2:L:108:ASN:OD1	1.85	0.77
1:M:220:LEU:H	1:M:241:ASN:HD22	1.30	0.77
1:I:197:HIS:HD2	1:I:222:ASN:HD22	1.32	0.77
1:G:253:SER:HB2	1:G:280:ASP:HB2	1.67	0.77
2:P:4:ILE:CG1	2:P:18:VAL:HG12	2.15	0.76
1:C:220:LEU:HB2	1:C:241:ASN:ND2	1.99	0.76
1:K:416:LYS:NZ	1:O:414:GLY:HA2	2.00	0.76
1:G:153:ASP:OD1	1:G:155:THR:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:220:LEU:HB2	1:I:241:ASN:HD22	1.47	0.76
1:I:197:HIS:CD2	1:I:222:ASN:HD22	2.03	0.76
1:C:415:ASN:O	1:C:417:LYS:HG2	1.85	0.76
1:O:153:ASP:OD1	1:O:155:THR:HG23	1.86	0.76
1:O:281:PHE:HB2	1:O:285:HIS:ND1	1.99	0.76
1:G:415:ASN:O	1:G:417:LYS:HG2	1.84	0.76
1:G:197:HIS:CD2	1:G:222:ASN:HD22	2.04	0.76
1:G:156:GLY:HA2	1:G:179:ARG:O	1.85	0.76
1:E:176:ARG:CZ	1:E:419:GLN:H	1.98	0.76
1:G:131:LYS:HD3	2:H:130:LYS:O	1.85	0.76
1:K:415:ASN:O	1:K:417:LYS:HG2	1.84	0.76
1:E:215:SER:CA	1:E:237:THR:HG21	2.14	0.76
1:M:281:PHE:HB2	1:M:285:HIS:CG	2.21	0.76
1:O:109:TRP:HZ3	2:P:104:ILE:HD12	1.49	0.76
1:E:220:LEU:H	1:E:241:ASN:HD22	1.34	0.76
1:K:155:THR:HG21	1:K:176:ARG:NH1	2.00	0.76
1:C:281:PHE:HB2	1:C:285:HIS:ND1	2.01	0.76
1:M:416:LYS:CB	1:M:417:LYS:HE2	2.17	0.75
1:K:161:PRO:HB3	1:K:209:THR:HG23	1.65	0.75
1:C:416:LYS:NZ	1:G:414:GLY:HA2	2.00	0.75
1:M:148:LEU:HA	1:M:427:ARG:NH2	2.01	0.75
1:G:189:HIS:O	1:G:190:PHE:O	1.68	0.75
1:O:156:GLY:HA2	1:O:179:ARG:O	1.85	0.75
1:I:350:GLN:HA	1:I:374:LEU:HA	1.69	0.75
2:H:5:LYS:HG2	2:H:15:GLU:HG2	1.67	0.75
2:L:43:ASP:HB2	2:L:44:PRO:CD	2.11	0.75
1:C:389:GLN:NE2	1:C:392:LYS:HD2	2.02	0.75
1:M:215:SER:CA	1:M:237:THR:HG21	2.17	0.75
2:N:133:GLU:O	2:N:137:LYS:HG3	1.88	0.74
1:I:281:PHE:HB2	1:I:285:HIS:CG	2.22	0.74
1:C:197:HIS:HD2	1:C:222:ASN:HD22	1.33	0.74
1:G:220:LEU:HB2	1:G:241:ASN:ND2	2.03	0.74
1:M:399:GLN:HA	1:M:399:GLN:HE21	1.51	0.74
1:A:153:ASP:OD1	1:A:155:THR:HG23	1.88	0.74
2:B:86:PRO:O	2:B:90:GLN:HG3	1.86	0.74
1:A:215:SER:HA	1:A:237:THR:CG2	2.15	0.74
1:O:281:PHE:HB2	1:O:285:HIS:CG	2.23	0.74
1:M:159:LEU:HD23	1:M:164:THR:HG22	1.69	0.74
1:C:281:PHE:HB2	1:C:285:HIS:CG	2.22	0.74
1:G:176:ARG:HD3	1:G:419:GLN:HA	1.67	0.73
2:H:107:ALA:HB2	2:H:115:LEU:CD1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:ALA:O	1:E:293:VAL:HG23	1.88	0.73
1:E:399:GLN:HE21	1:E:399:GLN:HA	1.51	0.73
1:A:417:LYS:CE	1:E:417:LYS:HG3	2.19	0.73
1:M:155:THR:HG21	1:M:176:ARG:NH1	2.02	0.73
1:I:367:GLU:O	1:I:370:GLU:HG2	1.86	0.73
1:I:417:LYS:HD2	1:M:417:LYS:CG	2.15	0.73
2:B:88:TRP:O	2:B:91:GLU:HG3	1.89	0.73
1:O:281:PHE:CE1	1:O:305:TYR:CE2	2.76	0.73
1:E:148:LEU:HA	1:E:427:ARG:NH2	2.03	0.73
2:J:49:ASN:HB2	2:J:109:TYR:CE2	2.23	0.73
1:K:289:ALA:O	1:K:293:VAL:HG23	1.88	0.73
2:J:88:TRP:O	2:J:91:GLU:HG3	1.87	0.73
1:A:176:ARG:CZ	1:A:419:GLN:H	2.01	0.73
1:C:416:LYS:HD2	1:C:417:LYS:NZ	2.03	0.73
1:A:148:LEU:HA	1:A:427:ARG:HH22	1.54	0.73
1:G:220:LEU:H	1:G:241:ASN:HD22	1.35	0.73
1:G:350:GLN:HA	1:G:374:LEU:HA	1.70	0.73
1:C:399:GLN:HE21	1:C:399:GLN:HA	1.53	0.73
1:M:191:SER:HB3	1:M:192:PRO:HD2	1.70	0.73
1:A:155:THR:HG21	1:A:176:ARG:NH1	2.04	0.73
1:C:215:SER:CA	1:C:237:THR:HG21	2.17	0.73
1:E:415:ASN:O	1:E:417:LYS:HG2	1.89	0.73
1:K:417:LYS:CG	1:O:417:LYS:HD2	2.18	0.72
1:C:176:ARG:CZ	1:C:419:GLN:H	2.01	0.72
1:I:176:ARG:CZ	1:I:419:GLN:H	2.01	0.72
1:O:367:GLU:O	1:O:370:GLU:HG2	1.89	0.72
1:C:351:HIS:HD2	1:C:376:THR:OG1	1.72	0.72
1:E:168:LEU:HD22	1:E:195:VAL:CG2	2.19	0.72
1:C:159:LEU:HD23	1:C:164:THR:HG22	1.70	0.72
1:O:176:ARG:CD	1:O:419:GLN:HA	2.19	0.72
1:C:376:THR:HG22	1:C:399:GLN:HB3	1.70	0.72
2:J:117:ASP:OD1	2:J:121:LYS:HE3	1.89	0.72
1:O:137:LYS:HE3	2:P:144:ASP:O	1.88	0.72
2:N:130:LYS:HE3	2:N:138:THR:HG21	1.71	0.72
1:M:128:GLU:HG2	2:N:128:LYS:HG2	1.71	0.72
1:K:220:LEU:HB2	1:K:241:ASN:ND2	2.05	0.72
1:I:220:LEU:H	1:I:241:ASN:HD22	1.33	0.72
1:E:351:HIS:HD2	1:E:376:THR:OG1	1.72	0.72
1:M:197:HIS:CD2	1:M:222:ASN:HD22	2.05	0.72
2:D:146:THR:HB	2:D:149:GLU:HG3	1.72	0.72
1:G:389:GLN:O	1:G:393:GLU:HG2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:376:THR:HG22	1:O:399:GLN:HB3	1.72	0.72
2:J:26:THR:O	2:J:29:THR:HG22	1.89	0.72
2:F:49:ASN:HB2	2:F:109:TYR:CE2	2.25	0.72
2:B:49:ASN:HB2	2:B:109:TYR:CE2	2.25	0.71
1:E:397:HIS:CE1	1:E:398:LEU:HG	2.25	0.71
2:P:26:THR:O	2:P:29:THR:HG22	1.89	0.71
1:O:161:PRO:HB3	1:O:209:THR:HG23	1.70	0.71
2:L:5:LYS:HG2	2:L:15:GLU:HG2	1.72	0.71
1:O:215:SER:CA	1:O:237:THR:HG21	2.20	0.71
1:O:283:GLU:O	1:O:287:GLN:HG3	1.91	0.71
1:E:197:HIS:CD2	1:E:222:ASN:HD22	2.08	0.71
1:A:356:ARG:HG2	1:A:358:TYR:OH	1.91	0.71
2:L:107:ALA:HB2	2:L:115:LEU:HD12	1.72	0.71
1:A:399:GLN:HE21	1:A:399:GLN:HA	1.54	0.71
1:E:220:LEU:HB2	1:E:241:ASN:ND2	2.06	0.71
1:C:350:GLN:HA	1:C:374:LEU:HA	1.73	0.71
1:E:220:LEU:HB2	1:E:241:ASN:HD22	1.56	0.71
1:M:176:ARG:CZ	1:M:419:GLN:H	2.03	0.71
1:O:220:LEU:HB2	1:O:241:ASN:ND2	2.06	0.71
1:C:109:TRP:CD2	2:D:101:PHE:HD2	2.09	0.71
2:N:107:ALA:HB2	2:N:115:LEU:CD1	2.20	0.71
2:J:107:ALA:HB2	2:J:115:LEU:HD12	1.73	0.71
1:O:350:GLN:HA	1:O:374:LEU:HA	1.71	0.71
1:M:416:LYS:HD2	1:M:417:LYS:NZ	2.05	0.71
1:C:197:HIS:CD2	1:C:222:ASN:HD22	2.08	0.71
2:P:22:LYS:CG	2:P:28:LYS:HZ3	2.03	0.71
1:I:181:PHE:CD1	1:K:384:PRO:HG3	2.26	0.71
1:M:164:THR:HG21	1:M:182:MET:SD	2.32	0.70
1:E:376:THR:HG22	1:E:399:GLN:HB3	1.73	0.70
1:M:176:ARG:HD3	1:M:419:GLN:HA	1.73	0.70
1:O:109:TRP:HA	2:P:101:PHE:CE2	2.24	0.70
1:I:283:GLU:O	1:I:287:GLN:HG3	1.92	0.70
1:K:164:THR:HG21	1:K:182:MET:SD	2.31	0.70
1:K:416:LYS:HD2	1:K:417:LYS:NZ	2.06	0.70
2:F:98:GLY:HA3	1:O:284:LYS:NZ	2.06	0.70
2:P:22:LYS:HG2	2:P:28:LYS:HZ3	1.57	0.70
1:A:417:LYS:HD2	1:E:417:LYS:CG	2.18	0.70
2:L:54:ILE:HG23	2:L:103:LEU:HD23	1.73	0.70
1:M:176:ARG:CD	1:M:419:GLN:HA	2.22	0.70
2:H:130:LYS:HE3	2:H:138:THR:HG21	1.73	0.70
1:C:164:THR:HG21	1:C:182:MET:SD	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:GLU:O	1:G:370:GLU:HG2	1.92	0.70
1:K:109:TRP:HA	2:L:101:PHE:HE2	1.57	0.70
1:K:156:GLY:HA2	1:K:179:ARG:O	1.92	0.70
1:K:367:GLU:O	1:K:370:GLU:HG2	1.90	0.70
1:C:161:PRO:HB3	1:C:209:THR:HG23	1.72	0.70
1:K:215:SER:CA	1:K:237:THR:HG21	2.22	0.69
1:A:389:GLN:NE2	1:A:392:LYS:HD2	2.06	0.69
1:M:389:GLN:NE2	1:M:392:LYS:HD2	2.07	0.69
1:A:351:HIS:HD2	1:A:376:THR:OG1	1.75	0.69
1:C:417:LYS:HG3	1:G:417:LYS:CE	2.22	0.69
1:M:281:PHE:HB2	1:M:285:HIS:ND1	2.07	0.69
1:G:137:LYS:HE3	2:H:144:ASP:O	1.92	0.69
2:D:107:ALA:HB2	2:D:115:LEU:HD12	1.74	0.69
1:C:274:ASN:C	1:C:274:ASN:HD22	1.94	0.69
1:C:168:LEU:HD22	1:C:195:VAL:HG21	1.73	0.69
1:E:168:LEU:HD22	1:E:195:VAL:HG21	1.71	0.69
1:G:215:SER:CA	1:G:237:THR:HG21	2.21	0.69
1:A:281:PHE:CE1	1:A:305:TYR:CE2	2.80	0.69
2:D:130:LYS:HE3	2:D:138:THR:HG21	1.75	0.69
1:C:417:LYS:HG3	1:G:417:LYS:CD	2.22	0.69
2:B:130:LYS:HE3	2:B:138:THR:HG21	1.73	0.69
1:K:397:HIS:CE1	1:K:398:LEU:HG	2.28	0.69
2:F:43:ASP:HB2	2:F:44:PRO:CD	2.21	0.69
1:I:215:SER:CA	1:I:237:THR:HG21	2.22	0.69
2:L:146:THR:HB	2:L:149:GLU:HG3	1.74	0.68
1:C:367:GLU:O	1:C:370:GLU:HG2	1.92	0.68
1:C:109:TRP:CZ2	2:D:101:PHE:HB2	2.29	0.68
1:E:376:THR:HG22	1:E:399:GLN:CB	2.24	0.68
1:K:109:TRP:CD2	2:L:101:PHE:HD2	2.11	0.68
1:E:188:GLU:O	1:E:212:GLY:O	2.12	0.68
1:A:295:GLU:HG2	1:A:320:ARG:O	1.94	0.68
1:A:414:GLY:HA2	1:E:416:LYS:HZ2	1.57	0.68
1:E:350:GLN:HA	1:E:374:LEU:HA	1.76	0.68
1:M:295:GLU:HG2	1:M:320:ARG:O	1.93	0.68
1:O:197:HIS:HD2	1:O:222:ASN:HD22	1.42	0.68
1:I:281:PHE:HB2	1:I:285:HIS:ND1	2.09	0.68
1:A:148:LEU:HA	1:A:427:ARG:NH2	2.09	0.68
2:H:146:THR:HG22	2:H:148:GLU:H	1.59	0.68
1:O:164:THR:HG21	1:O:182:MET:SD	2.33	0.68
1:C:281:PHE:CE1	1:C:305:TYR:CE2	2.81	0.68
1:I:295:GLU:HG2	1:I:320:ARG:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:86:PRO:O	2:L:90:GLN:HG3	1.94	0.68
1:M:331:ASP:OD2	1:M:356:ARG:NH1	2.27	0.68
1:G:383:VAL:HG12	1:G:388:LEU:HB2	1.76	0.68
1:K:140:TYR:CE2	2:L:153:VAL:HG22	2.29	0.67
1:A:378:GLN:NE2	1:A:401:ASN:HA	2.09	0.67
1:G:155:THR:HG21	1:G:176:ARG:NH1	2.09	0.67
1:G:416:LYS:O	1:G:417:LYS:HD3	1.94	0.67
1:K:314:LEU:O	1:K:318:VAL:HG23	1.94	0.67
1:A:176:ARG:HD3	1:A:419:GLN:HA	1.76	0.67
2:N:86:PRO:O	2:N:90:GLN:HG3	1.95	0.67
1:E:367:GLU:O	1:E:370:GLU:HG2	1.95	0.67
1:M:367:GLU:O	1:M:370:GLU:HG2	1.94	0.67
1:C:415:ASN:O	1:C:416:LYS:HB3	1.95	0.67
1:K:351:HIS:HD2	1:K:376:THR:OG1	1.76	0.67
1:M:116:LEU:HD21	2:N:108:ASN:CG	2.15	0.67
1:E:231:SER:OG	1:E:233:PRO:HD2	1.94	0.67
2:H:133:GLU:O	2:H:137:LYS:HG3	1.94	0.67
2:H:88:TRP:O	2:H:91:GLU:HG3	1.93	0.67
1:E:153:ASP:OD1	1:E:155:THR:HG23	1.95	0.67
1:I:389:GLN:NE2	1:I:392:LYS:HD2	2.09	0.67
2:L:130:LYS:HE3	2:L:138:THR:HG21	1.76	0.67
2:P:43:ASP:HB2	2:P:44:PRO:CD	2.22	0.67
1:O:399:GLN:HA	1:O:399:GLN:HE21	1.59	0.67
1:O:193:PHE:HB3	1:O:195:VAL:HG23	1.76	0.67
1:A:176:ARG:CD	1:A:419:GLN:HA	2.25	0.67
1:G:384:PRO:HD2	1:G:387:THR:OG1	1.95	0.67
1:G:220:LEU:HB2	1:G:241:ASN:HD22	1.60	0.67
1:G:397:HIS:CE1	1:G:398:LEU:HG	2.30	0.67
2:P:143:ASN:OD1	2:P:145:PHE:HB2	1.95	0.66
1:M:376:THR:HG22	1:M:399:GLN:HB3	1.76	0.66
2:P:117:ASP:OD1	2:P:121:LYS:HE3	1.95	0.66
2:J:130:LYS:HE3	2:J:138:THR:HG21	1.76	0.66
1:O:415:ASN:O	1:O:416:LYS:HB3	1.95	0.66
1:M:153:ASP:OD1	1:M:155:THR:HG23	1.95	0.66
1:A:344:PHE:CE2	1:A:370:GLU:HB2	2.31	0.66
1:E:137:LYS:HE3	2:F:145:PHE:HA	1.76	0.66
1:C:148:LEU:CA	1:C:427:ARG:HH22	2.04	0.66
1:O:376:THR:HG22	1:O:399:GLN:CB	2.24	0.66
1:G:168:LEU:HD22	1:G:195:VAL:HG21	1.76	0.66
1:E:416:LYS:HD2	1:E:417:LYS:HZ1	1.58	0.66
2:H:43:ASP:CB	2:H:44:PRO:HD3	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:GLU:HG2	1:C:320:ARG:O	1.95	0.66
1:K:415:ASN:O	1:K:416:LYS:HB3	1.95	0.66
1:E:215:SER:O	1:E:240:LYS:NZ	2.29	0.66
2:F:4:ILE:CG1	2:F:18:VAL:HG12	2.22	0.66
1:O:197:HIS:CD2	1:O:222:ASN:HD22	2.13	0.66
1:K:350:GLN:HA	1:K:374:LEU:HA	1.76	0.66
2:B:107:ALA:HB2	2:B:115:LEU:CD1	2.25	0.66
1:A:220:LEU:HB2	1:A:241:ASN:ND2	2.11	0.66
1:O:344:PHE:CE2	1:O:370:GLU:HB2	2.31	0.66
1:O:137:LYS:HG3	2:P:144:ASP:HB2	1.77	0.66
1:A:162:ASP:HA	1:A:190:PHE:HZ	1.60	0.66
1:C:376:THR:HG22	1:C:399:GLN:CB	2.25	0.66
1:A:159:LEU:HD23	1:A:164:THR:HG22	1.77	0.66
1:A:383:VAL:HG12	1:A:388:LEU:HB2	1.77	0.66
1:A:225:LEU:O	1:A:252:CYS:SG	2.54	0.65
1:K:158:ASN:HA	1:K:181:PHE:HB2	1.77	0.65
1:A:281:PHE:HB2	1:A:285:HIS:ND1	2.12	0.65
1:O:158:ASN:HA	1:O:181:PHE:HB2	1.78	0.65
1:M:182:MET:O	1:M:205:ILE:HA	1.95	0.65
1:O:397:HIS:CE1	1:O:398:LEU:HG	2.30	0.65
1:G:351:HIS:HD2	1:G:376:THR:OG1	1.79	0.65
2:N:104:ILE:HG12	2:N:119:THR:HB	1.79	0.65
2:B:43:ASP:HB2	2:B:44:PRO:CD	2.23	0.65
1:M:161:PRO:HB3	1:M:209:THR:HG23	1.78	0.65
1:O:176:ARG:HD3	1:O:419:GLN:HA	1.77	0.65
1:O:148:LEU:HA	1:O:427:ARG:NH2	2.10	0.65
2:L:101:PHE:CE1	2:L:105:LEU:HD11	2.31	0.65
2:B:146:THR:HB	2:B:149:GLU:HG3	1.78	0.65
2:F:26:THR:O	2:F:29:THR:HG22	1.97	0.65
1:I:415:ASN:O	1:I:416:LYS:HB3	1.95	0.65
2:F:107:ALA:HB2	2:F:115:LEU:CD1	2.26	0.65
1:A:367:GLU:O	1:A:370:GLU:HG2	1.97	0.65
1:M:350:GLN:HA	1:M:374:LEU:HA	1.77	0.65
1:K:176:ARG:CZ	1:K:419:GLN:H	2.10	0.65
1:K:220:LEU:H	1:K:241:ASN:ND2	1.95	0.65
1:I:274:ASN:HD22	1:I:274:ASN:C	2.00	0.65
1:M:155:THR:CG2	1:M:178:PRO:HD2	2.25	0.65
1:A:137:LYS:HG3	2:B:144:ASP:HB2	1.78	0.65
1:E:295:GLU:HG2	1:E:320:ARG:O	1.96	0.65
1:A:215:SER:CA	1:A:237:THR:HG21	2.21	0.64
1:K:182:MET:O	1:K:205:ILE:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:416:LYS:C	1:O:417:LYS:HD3	2.18	0.64
1:C:253:SER:HB2	1:C:280:ASP:CB	2.25	0.64
1:O:220:LEU:HB2	1:O:241:ASN:HD22	1.60	0.64
1:I:159:LEU:HD23	1:I:164:THR:HG22	1.78	0.64
1:I:362:PRO:HG3	1:I:382:ILE:O	1.97	0.64
1:C:131:LYS:NZ	2:D:127:ILE:O	2.29	0.64
1:A:350:GLN:HA	1:A:374:LEU:HA	1.79	0.64
1:G:186:LEU:HA	1:G:187:ALA:N	2.13	0.64
2:N:43:ASP:CB	2:N:44:PRO:HD3	2.22	0.64
1:G:419:GLN:NE2	1:G:426:CYS:O	2.31	0.64
1:K:253:SER:HB2	1:K:280:ASP:CB	2.26	0.64
1:I:220:LEU:CB	1:I:241:ASN:HD22	2.11	0.64
1:K:344:PHE:CE2	1:K:370:GLU:HB2	2.33	0.64
1:E:383:VAL:HG12	1:E:388:LEU:HB2	1.78	0.64
1:K:356:ARG:HG2	1:K:358:TYR:OH	1.98	0.64
1:K:109:TRP:CE2	2:L:101:PHE:HD2	2.16	0.64
2:P:133:GLU:O	2:P:137:LYS:HG3	1.98	0.64
2:J:101:PHE:CE1	2:J:105:LEU:HD11	2.33	0.64
1:A:397:HIS:CE1	1:A:398:LEU:HG	2.33	0.64
2:N:43:ASP:HB2	2:N:44:PRO:CD	2.22	0.64
1:E:389:GLN:NE2	1:E:392:LYS:HD2	2.13	0.64
1:I:148:LEU:HA	1:I:427:ARG:HH22	1.62	0.64
2:P:61:TRP:CD2	2:P:115:LEU:HD23	2.33	0.63
1:I:414:GLY:CA	1:M:416:LYS:NZ	2.60	0.63
1:C:186:LEU:O	1:C:188:GLU:N	2.30	0.63
1:A:416:LYS:C	1:A:417:LYS:HD3	2.18	0.63
2:P:107:ALA:HB2	2:P:115:LEU:CD1	2.28	0.63
2:P:61:TRP:CG	2:P:115:LEU:HD23	2.32	0.63
1:O:159:LEU:HD23	1:O:164:THR:HG22	1.80	0.63
1:C:416:LYS:HD2	1:C:417:LYS:HZ1	1.63	0.63
2:D:146:THR:HG22	2:D:148:GLU:H	1.61	0.63
2:B:16:VAL:CG2	2:B:21:ALA:HB2	2.29	0.63
2:F:133:GLU:O	2:F:137:LYS:HG3	1.99	0.63
1:M:151:THR:HB	1:M:426:CYS:HA	1.79	0.63
1:E:176:ARG:CD	1:E:419:GLN:HA	2.29	0.63
1:K:220:LEU:HB2	1:K:241:ASN:HD22	1.63	0.63
2:D:117:ASP:OD1	2:D:121:LYS:HE3	1.99	0.63
1:A:415:ASN:O	1:A:416:LYS:HB3	1.98	0.63
1:K:162:ASP:HA	1:K:190:PHE:CZ	2.30	0.63
2:L:51:ASN:ND2	2:L:53:ALA:H	1.95	0.63
1:G:415:ASN:O	1:G:416:LYS:HB3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:384:PRO:HD2	1:K:387:THR:OG1	1.98	0.63
1:G:128:GLU:HG2	2:H:128:LYS:HG2	1.80	0.63
1:O:295:GLU:HG2	1:O:320:ARG:O	1.97	0.63
1:O:274:ASN:C	1:O:274:ASN:HD22	2.01	0.63
2:J:104:ILE:HG12	2:J:119:THR:HB	1.79	0.63
1:E:415:ASN:O	1:E:416:LYS:HB3	1.99	0.63
1:G:416:LYS:C	1:G:417:LYS:HD3	2.19	0.63
1:A:231:SER:HA	1:A:254:GLY:O	1.99	0.63
1:C:362:PRO:HG3	1:C:382:ILE:O	1.99	0.63
2:D:43:ASP:HB2	2:D:44:PRO:CD	2.24	0.62
1:O:220:LEU:H	1:O:241:ASN:ND2	1.96	0.62
1:C:417:LYS:CG	1:G:417:LYS:HD2	2.29	0.62
1:I:155:THR:HG21	1:I:176:ARG:NH1	2.13	0.62
2:P:61:TRP:CE3	2:P:115:LEU:HB2	2.34	0.62
1:M:377:LEU:O	1:M:400:ILE:HA	1.99	0.62
2:P:43:ASP:CB	2:P:44:PRO:HD3	2.23	0.62
1:E:176:ARG:HD3	1:E:419:GLN:HA	1.81	0.62
1:G:168:LEU:HD22	1:G:195:VAL:CG2	2.28	0.62
1:C:128:GLU:HG2	2:D:128:LYS:HG2	1.81	0.62
1:C:156:GLY:HA2	1:C:179:ARG:O	2.00	0.62
1:A:253:SER:HB2	1:A:280:ASP:CB	2.29	0.62
2:B:26:THR:O	2:B:29:THR:HG22	1.99	0.62
1:O:362:PRO:HG3	1:O:382:ILE:O	1.99	0.62
1:O:257:GLU:HB2	1:O:288:VAL:HG21	1.81	0.62
1:E:155:THR:HG21	1:E:176:ARG:NH1	2.14	0.62
1:I:376:THR:HG22	1:I:399:GLN:HB3	1.81	0.62
1:O:325:VAL:HG13	1:O:350:GLN:HG2	1.81	0.62
1:O:411:PRO:HG3	1:O:422:TRP:CH2	2.34	0.62
1:A:184:GLN:CB	1:A:185:PRO:HD2	2.29	0.62
1:M:220:LEU:HB2	1:M:241:ASN:ND2	2.15	0.62
1:C:378:GLN:NE2	1:C:401:ASN:HA	2.14	0.62
1:K:176:ARG:CD	1:K:419:GLN:HA	2.30	0.62
1:C:220:LEU:H	1:C:241:ASN:HD22	1.48	0.62
2:L:16:VAL:CG2	2:L:21:ALA:HB2	2.30	0.62
1:I:162:ASP:HA	1:I:190:PHE:HZ	1.65	0.62
1:I:253:SER:HB2	1:I:280:ASP:CB	2.30	0.62
1:M:397:HIS:CE1	1:M:398:LEU:HG	2.35	0.62
2:J:4:ILE:CG1	2:J:18:VAL:HG12	2.23	0.62
1:A:419:GLN:O	1:A:419:GLN:HG2	2.00	0.62
1:O:155:THR:CG2	1:O:178:PRO:HD2	2.29	0.62
1:E:158:ASN:HA	1:E:181:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:376:THR:HG22	1:I:399:GLN:CB	2.30	0.62
1:O:155:THR:HG21	1:O:176:ARG:NH1	2.14	0.61
2:J:49:ASN:HB2	2:J:109:TYR:CZ	2.35	0.61
1:I:309:LEU:HD23	1:I:332:SER:OG	1.99	0.61
1:K:168:LEU:HD22	1:K:195:VAL:HG21	1.82	0.61
1:C:411:PRO:HG3	1:C:422:TRP:CH2	2.35	0.61
1:C:158:ASN:HA	1:C:181:PHE:HB2	1.82	0.61
2:B:4:ILE:CG1	2:B:18:VAL:HG12	2.24	0.61
1:O:253:SER:HB2	1:O:280:ASP:CB	2.30	0.61
1:C:137:LYS:H	2:D:144:ASP:HB2	1.65	0.61
1:M:356:ARG:HG2	1:M:358:TYR:OH	1.99	0.61
2:J:22:LYS:HD3	2:J:22:LYS:O	2.01	0.61
1:I:153:ASP:OD1	1:I:155:THR:HG23	2.00	0.61
1:E:253:SER:HB2	1:E:280:ASP:CB	2.29	0.61
2:J:86:PRO:O	2:J:90:GLN:HG3	1.99	0.61
2:H:26:THR:O	2:H:29:THR:HG22	2.00	0.61
2:H:51:ASN:ND2	2:H:53:ALA:H	1.98	0.61
2:F:43:ASP:CB	2:F:44:PRO:HD3	2.23	0.61
1:E:362:PRO:HG3	1:E:382:ILE:O	2.00	0.61
2:D:4:ILE:CG1	2:D:18:VAL:HG12	2.22	0.61
2:L:4:ILE:CG1	2:L:18:VAL:HG12	2.23	0.61
2:J:107:ALA:HB2	2:J:115:LEU:CD1	2.31	0.61
2:J:127:ILE:HG23	2:J:135:ILE:CD1	2.30	0.61
2:F:54:ILE:HG23	2:F:103:LEU:HD23	1.83	0.61
1:O:416:LYS:CB	1:O:417:LYS:HE2	2.24	0.61
2:J:43:ASP:CB	2:J:44:PRO:HD3	2.22	0.61
1:K:191:SER:HB3	1:K:192:PRO:HD2	1.82	0.61
1:C:283:GLU:O	1:C:287:GLN:HG3	2.01	0.61
1:E:128:GLU:HG2	2:F:128:LYS:HG2	1.83	0.61
1:M:314:LEU:O	1:M:318:VAL:HG23	2.01	0.61
2:H:43:ASP:HB2	2:H:44:PRO:CD	2.21	0.61
2:L:107:ALA:HB2	2:L:115:LEU:CD1	2.31	0.61
1:I:158:ASN:HA	1:I:181:PHE:HB2	1.81	0.61
1:M:415:ASN:O	1:M:416:LYS:HB3	2.00	0.61
1:A:116:LEU:HD13	2:B:104:ILE:HG22	1.81	0.61
1:M:253:SER:HB2	1:M:280:ASP:CB	2.27	0.61
1:A:164:THR:HG21	1:A:182:MET:SD	2.40	0.61
1:A:168:LEU:HD22	1:A:195:VAL:HG21	1.83	0.61
2:N:146:THR:HG22	2:N:148:GLU:H	1.66	0.61
2:N:16:VAL:CG2	2:N:21:ALA:HB2	2.31	0.61
2:B:101:PHE:CE1	2:B:105:LEU:HD11	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:TRP:CZ2	2:L:101:PHE:HB2	2.36	0.61
2:D:16:VAL:CG2	2:D:21:ALA:HB2	2.31	0.61
1:G:344:PHE:CE2	1:G:370:GLU:HB2	2.36	0.60
1:O:168:LEU:HD22	1:O:195:VAL:HG21	1.83	0.60
2:F:16:VAL:CG2	2:F:21:ALA:HB2	2.31	0.60
1:I:231:SER:HA	1:I:254:GLY:O	2.01	0.60
1:K:399:GLN:HE21	1:K:399:GLN:CA	2.11	0.60
1:K:281:PHE:CB	1:K:285:HIS:CG	2.84	0.60
1:C:281:PHE:CB	1:C:285:HIS:CG	2.84	0.60
2:N:12:GLU:OE2	2:N:52:ALA:HB1	2.02	0.60
1:I:399:GLN:HA	1:I:399:GLN:HE21	1.66	0.60
1:A:382:ILE:HG13	1:A:383:VAL:HG23	1.83	0.60
1:I:416:LYS:C	1:I:417:LYS:HD3	2.22	0.60
1:A:416:LYS:O	1:A:417:LYS:HD3	2.02	0.60
1:G:416:LYS:CB	1:G:417:LYS:HE2	2.27	0.60
1:O:109:TRP:CZ3	2:P:104:ILE:HD12	2.33	0.60
2:J:16:VAL:CG2	2:J:21:ALA:HB2	2.30	0.60
1:G:274:ASN:HD22	1:G:274:ASN:C	2.05	0.60
1:A:124:LEU:HB3	1:A:128:GLU:HB3	1.83	0.60
1:M:383:VAL:HG12	1:M:388:LEU:HB2	1.82	0.60
1:O:389:GLN:NE2	1:O:392:LYS:HD2	2.17	0.60
1:M:351:HIS:HD2	1:M:376:THR:OG1	1.84	0.60
1:K:325:VAL:HG13	1:K:350:GLN:HG2	1.84	0.60
1:G:295:GLU:HG2	1:G:320:ARG:O	2.02	0.60
1:K:276:SER:HB3	1:K:301:ASN:OD1	2.01	0.60
1:C:417:LYS:HG3	1:G:417:LYS:HZ2	1.67	0.60
1:A:281:PHE:CB	1:A:285:HIS:CG	2.85	0.60
1:I:281:PHE:CB	1:I:285:HIS:CG	2.85	0.60
1:C:344:PHE:CE2	1:C:370:GLU:HB2	2.36	0.60
2:J:16:VAL:HG21	2:J:21:ALA:HB2	1.84	0.60
1:C:215:SER:O	1:C:240:LYS:NZ	2.35	0.60
1:M:159:LEU:CD2	1:M:164:THR:HG22	2.32	0.60
1:M:181:PHE:CD1	1:O:384:PRO:HG3	2.37	0.60
1:E:325:VAL:HG13	1:E:350:GLN:HG2	1.82	0.60
2:H:49:ASN:HB2	2:H:109:TYR:CE2	2.37	0.60
1:M:137:LYS:HE3	2:N:145:PHE:HA	1.84	0.60
2:D:16:VAL:HG21	2:D:21:ALA:HB2	1.84	0.60
1:O:132:VAL:CG1	2:P:127:ILE:HG21	2.32	0.59
1:O:419:GLN:OE1	1:O:429:THR:HG21	2.02	0.59
1:C:168:LEU:HD22	1:C:195:VAL:CG2	2.32	0.59
2:P:54:ILE:HG23	2:P:103:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:101:PHE:CE1	2:H:105:LEU:HD11	2.37	0.59
2:P:101:PHE:CE1	2:P:105:LEU:HD11	2.37	0.59
1:E:281:PHE:CB	1:E:285:HIS:CG	2.85	0.59
1:G:281:PHE:CB	1:G:285:HIS:CG	2.85	0.59
1:I:181:PHE:CE1	1:K:384:PRO:HA	2.37	0.59
2:H:146:THR:HB	2:H:149:GLU:HG3	1.83	0.59
1:I:149:TRP:O	1:I:172:VAL:HA	2.02	0.59
2:D:43:ASP:CB	2:D:44:PRO:HD3	2.25	0.59
1:C:151:THR:HB	1:C:426:CYS:HA	1.84	0.59
1:K:281:PHE:CE1	1:K:305:TYR:CE2	2.91	0.59
1:K:168:LEU:HD22	1:K:195:VAL:CG2	2.32	0.59
2:B:127:ILE:HG23	2:B:135:ILE:CD1	2.32	0.59
2:F:88:TRP:O	2:F:91:GLU:HG3	2.01	0.59
1:E:115:GLU:OE1	1:E:115:GLU:N	2.36	0.59
1:G:162:ASP:HA	1:G:190:PHE:CZ	2.31	0.59
2:B:43:ASP:CB	2:B:44:PRO:HD3	2.25	0.59
1:C:176:ARG:CD	1:C:419:GLN:HA	2.32	0.59
2:J:115:LEU:O	2:J:115:LEU:HD13	2.01	0.59
2:F:146:THR:HG22	2:F:148:GLU:H	1.67	0.59
1:I:184:GLN:CB	1:I:185:PRO:HD2	2.32	0.59
2:L:127:ILE:HG23	2:L:135:ILE:CD1	2.33	0.59
1:C:383:VAL:HG12	1:C:388:LEU:HB2	1.85	0.59
2:P:130:LYS:HE3	2:P:138:THR:HG21	1.85	0.59
2:P:16:VAL:CG1	2:P:59:ILE:HD13	2.33	0.59
1:K:416:LYS:HZ3	1:O:414:GLY:HA2	1.68	0.59
2:D:107:ALA:HB2	2:D:115:LEU:CD1	2.32	0.59
1:G:399:GLN:HA	1:G:399:GLN:HE21	1.68	0.59
2:L:26:THR:O	2:L:29:THR:HG22	2.02	0.59
1:I:225:LEU:O	1:I:252:CYS:SG	2.61	0.59
2:H:117:ASP:OD1	2:H:121:LYS:HE3	2.03	0.59
1:C:416:LYS:HZ2	1:G:414:GLY:HA2	1.68	0.59
1:G:325:VAL:HG13	1:G:350:GLN:HG2	1.84	0.59
1:G:376:THR:HG22	1:G:399:GLN:CB	2.33	0.59
1:A:184:GLN:HB3	1:A:185:PRO:HD2	1.84	0.59
1:K:417:LYS:CE	1:O:417:LYS:CG	2.65	0.59
1:G:153:ASP:HB3	1:G:429:THR:HG22	1.85	0.59
1:E:419:GLN:OE1	1:E:429:THR:HG21	2.02	0.59
2:N:149:GLU:O	2:N:153:VAL:HG23	2.02	0.59
2:P:16:VAL:CG2	2:P:21:ALA:HB2	2.33	0.59
2:L:43:ASP:CB	2:L:44:PRO:HD3	2.20	0.58
1:C:419:GLN:NE2	1:C:426:CYS:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:419:GLN:NE2	1:I:426:CYS:O	2.36	0.58
1:I:220:LEU:H	1:I:241:ASN:ND2	2.00	0.58
1:C:136:CYS:HB2	2:D:144:ASP:OD2	2.03	0.58
2:B:87:VAL:HG21	1:E:296:THR:HA	1.83	0.58
2:N:26:THR:O	2:N:29:THR:HG22	2.02	0.58
2:H:148:GLU:O	2:H:151:ALA:HB3	2.04	0.58
1:A:374:LEU:HG	1:A:398:LEU:HD21	1.86	0.58
1:O:383:VAL:HG12	1:O:388:LEU:HB2	1.85	0.58
1:C:187:ALA:C	1:C:212:GLY:HA3	2.23	0.58
1:E:137:LYS:HG2	2:F:145:PHE:CE2	2.39	0.58
2:P:146:THR:HB	2:P:149:GLU:HG3	1.84	0.58
1:K:416:LYS:HZ2	1:O:414:GLY:HA2	1.68	0.58
2:J:43:ASP:HB2	2:J:44:PRO:CD	2.24	0.58
1:O:377:LEU:O	1:O:400:ILE:HA	2.04	0.58
1:K:424:ILE:HD12	1:K:424:ILE:N	2.18	0.58
1:K:419:GLN:OE1	1:K:429:THR:HG21	2.04	0.58
1:E:155:THR:CG2	1:E:178:PRO:HD2	2.26	0.58
1:K:383:VAL:HG12	1:K:388:LEU:HB2	1.86	0.58
1:K:151:THR:CB	1:K:426:CYS:HA	2.32	0.58
1:A:220:LEU:N	1:A:241:ASN:HD22	2.01	0.58
1:K:331:ASP:OD2	1:K:356:ARG:NH1	2.37	0.58
1:I:149:TRP:O	1:I:172:VAL:HG22	2.03	0.58
2:P:33:ASP:O	2:P:34:LEU:HD23	2.02	0.58
1:K:411:PRO:HG3	1:K:422:TRP:CH2	2.39	0.58
1:A:237:THR:HG23	1:A:240:LYS:HE3	1.86	0.58
1:C:176:ARG:HD3	1:C:419:GLN:HA	1.85	0.58
1:A:120:ILE:HD13	2:B:123:VAL:HG11	1.85	0.58
2:J:146:THR:HB	2:J:149:GLU:HG3	1.85	0.58
2:N:4:ILE:CG1	2:N:18:VAL:HG12	2.25	0.58
1:M:419:GLN:OE1	1:M:429:THR:HG21	2.03	0.58
1:M:124:LEU:HB3	1:M:128:GLU:HB3	1.86	0.58
1:A:325:VAL:HG13	1:A:350:GLN:HG2	1.85	0.58
2:P:88:TRP:O	2:P:91:GLU:HG3	2.02	0.58
2:D:88:TRP:O	2:D:91:GLU:HG3	2.04	0.58
2:D:133:GLU:O	2:D:137:LYS:HG3	2.04	0.58
1:C:188:GLU:O	1:C:212:GLY:C	2.42	0.58
1:I:155:THR:CG2	1:I:178:PRO:HD2	2.28	0.58
2:P:127:ILE:HG23	2:P:135:ILE:CD1	2.34	0.58
1:E:220:LEU:H	1:E:241:ASN:ND2	2.01	0.58
1:G:389:GLN:NE2	1:G:392:LYS:HD2	2.18	0.58
1:K:378:GLN:NE2	1:K:401:ASN:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:LEU:HD23	1:E:332:SER:OG	2.04	0.58
1:C:184:GLN:CB	1:C:185:PRO:HD2	2.34	0.58
1:E:153:ASP:HB3	1:E:429:THR:HG22	1.85	0.58
1:I:383:VAL:HG12	1:I:388:LEU:HB2	1.85	0.58
1:K:362:PRO:HG3	1:K:382:ILE:O	2.04	0.58
1:K:225:LEU:O	1:K:252:CYS:SG	2.62	0.58
1:M:225:LEU:O	1:M:252:CYS:SG	2.62	0.58
1:E:184:GLN:CB	1:E:185:PRO:HD2	2.34	0.57
1:A:283:GLU:O	1:A:287:GLN:HG3	2.04	0.57
1:A:115:GLU:N	1:A:115:GLU:OE1	2.37	0.57
1:G:186:LEU:C	1:G:187:ALA:C	2.62	0.57
1:I:389:GLN:HE22	1:I:392:LYS:NZ	2.02	0.57
1:M:168:LEU:HD22	1:M:195:VAL:HG21	1.85	0.57
2:F:86:PRO:O	2:F:90:GLN:HG3	2.03	0.57
1:C:155:THR:CG2	1:C:178:PRO:HD2	2.31	0.57
1:O:419:GLN:NE2	1:O:426:CYS:O	2.37	0.57
2:D:51:ASN:ND2	2:D:53:ALA:H	2.03	0.57
1:M:300:LEU:HD23	1:M:317:LEU:HD11	1.85	0.57
1:K:419:GLN:NE2	1:K:426:CYS:O	2.38	0.57
2:B:127:ILE:HG23	2:B:135:ILE:HD13	1.86	0.57
2:B:64:HIS:CE1	1:E:269:ARG:NH2	2.73	0.57
1:K:116:LEU:HD11	2:L:108:ASN:ND2	2.19	0.57
1:A:411:PRO:HG3	1:A:422:TRP:CH2	2.40	0.57
1:I:416:LYS:CD	1:I:417:LYS:HZ1	2.01	0.57
1:E:281:PHE:CE1	1:E:305:TYR:CE2	2.92	0.57
1:O:309:LEU:HD21	1:O:329:LEU:HD22	1.86	0.57
1:I:176:ARG:HD3	1:I:419:GLN:HA	1.85	0.57
1:E:231:SER:HA	1:E:254:GLY:O	2.05	0.57
1:O:123:CYS:SG	2:P:121:LYS:HG2	2.45	0.57
2:N:89:ASP:O	2:N:92:PHE:HB3	2.04	0.57
1:M:384:PRO:HD2	1:M:387:THR:OG1	2.05	0.57
2:N:65:HIS:CB	2:N:68:ASP:HB2	2.21	0.57
2:P:101:PHE:HE1	2:P:105:LEU:HD11	1.70	0.57
2:F:146:THR:HB	2:F:149:GLU:HG3	1.86	0.57
1:I:148:LEU:HA	1:I:427:ARG:NH2	2.20	0.57
1:A:161:PRO:HB3	1:A:209:THR:HG23	1.86	0.57
2:J:133:GLU:O	2:J:137:LYS:HG3	2.05	0.57
1:G:161:PRO:HB3	1:G:209:THR:HG23	1.86	0.57
2:B:49:ASN:HB2	2:B:109:TYR:CZ	2.39	0.57
2:L:104:ILE:HG12	2:L:119:THR:HB	1.86	0.57
2:J:101:PHE:HE1	2:J:105:LEU:HD11	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:151:THR:HG22	1:M:174:ALA:HB3	1.86	0.57
1:O:161:PRO:HB3	1:O:209:THR:CG2	2.34	0.57
1:G:157:LYS:HD2	1:G:430:LEU:HD12	1.86	0.57
1:I:378:GLN:NE2	1:I:401:ASN:HA	2.20	0.57
1:K:215:SER:O	1:K:240:LYS:NZ	2.38	0.56
1:A:220:LEU:H	1:A:241:ASN:ND2	2.01	0.56
1:A:220:LEU:HB2	1:A:241:ASN:HD22	1.69	0.56
1:I:220:LEU:N	1:I:241:ASN:HD22	2.03	0.56
1:A:419:GLN:OE1	1:A:429:THR:HG21	2.05	0.56
1:O:220:LEU:N	1:O:241:ASN:HD22	1.99	0.56
1:C:182:MET:O	1:C:205:ILE:HA	2.05	0.56
1:K:159:LEU:HD23	1:K:164:THR:HG22	1.87	0.56
1:C:421:ILE:O	1:C:421:ILE:HG23	2.05	0.56
1:C:309:LEU:HD21	1:C:329:LEU:HD22	1.87	0.56
1:G:378:GLN:NE2	1:G:401:ASN:HA	2.20	0.56
1:C:416:LYS:NZ	1:G:414:GLY:CA	2.68	0.56
1:O:124:LEU:HB3	1:O:128:GLU:HB3	1.86	0.56
1:A:370:GLU:O	1:A:372:PRO:HD3	2.05	0.56
1:A:181:PHE:CD1	1:C:384:PRO:HG3	2.40	0.56
1:G:376:THR:HG22	1:G:399:GLN:HB3	1.86	0.56
2:F:16:VAL:HG21	2:F:21:ALA:HB2	1.88	0.56
2:P:146:THR:HG22	2:P:148:GLU:H	1.70	0.56
2:J:146:THR:HG22	2:J:148:GLU:H	1.70	0.56
1:M:421:ILE:HG23	1:M:424:ILE:HB	1.87	0.56
1:O:378:GLN:NE2	1:O:401:ASN:HA	2.19	0.56
1:K:320:ARG:HB2	1:K:320:ARG:HH11	1.71	0.56
1:G:199:ASP:OD1	1:G:411:PRO:HG2	2.06	0.56
1:K:161:PRO:HB3	1:K:209:THR:CG2	2.36	0.56
2:H:130:LYS:HB3	2:H:134:GLU:HB2	1.86	0.56
1:C:159:LEU:CD2	1:C:164:THR:HG22	2.34	0.56
1:M:374:LEU:HG	1:M:398:LEU:HD21	1.87	0.56
2:B:16:VAL:HG21	2:B:21:ALA:HB2	1.88	0.56
1:M:283:GLU:O	1:M:287:GLN:HG3	2.04	0.56
1:K:148:LEU:CA	1:K:427:ARG:HH22	2.04	0.56
1:E:419:GLN:HG2	1:E:419:GLN:O	2.06	0.56
1:A:331:ASP:OD2	1:A:356:ARG:NH1	2.39	0.56
1:G:124:LEU:HB3	1:G:128:GLU:HB3	1.86	0.56
1:K:193:PHE:HB3	1:K:195:VAL:HG23	1.88	0.56
1:M:420:GLU:O	1:M:423:GLY:N	2.37	0.56
1:O:300:LEU:HD23	1:O:317:LEU:HD11	1.87	0.56
2:L:49:ASN:HB2	2:L:109:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:49:ASN:HB2	2:N:109:TYR:CE2	2.41	0.56
1:O:299:GLN:HG2	1:O:326:HIS:HB2	1.88	0.56
1:G:159:LEU:CD2	1:G:164:THR:HG22	2.35	0.56
1:G:309:LEU:HD21	1:G:329:LEU:HD22	1.88	0.56
1:A:125:CYS:SG	1:A:127:PRO:HG2	2.45	0.56
1:C:140:TYR:CE2	2:D:153:VAL:HG22	2.40	0.56
1:I:397:HIS:CE1	1:I:398:LEU:HG	2.41	0.56
1:M:124:LEU:HD23	2:N:124:ALA:HB1	1.88	0.56
1:C:309:LEU:HD23	1:C:332:SER:OG	2.06	0.56
2:N:65:HIS:HA	2:N:68:ASP:OD1	2.05	0.56
1:E:159:LEU:CD2	1:E:164:THR:HG22	2.35	0.56
1:M:376:THR:HG22	1:M:399:GLN:CB	2.35	0.56
2:L:127:ILE:HG23	2:L:135:ILE:HD13	1.88	0.56
1:G:419:GLN:OE1	1:G:429:THR:HG21	2.05	0.56
1:G:253:SER:HB2	1:G:280:ASP:CB	2.35	0.56
1:M:281:PHE:CE1	1:M:305:TYR:CE2	2.94	0.56
1:E:300:LEU:HD23	1:E:317:LEU:HD11	1.88	0.56
1:G:283:GLU:O	1:G:287:GLN:HG3	2.06	0.56
1:O:215:SER:O	1:O:240:LYS:NZ	2.39	0.56
1:A:108:SER:OG	2:B:140:ASN:ND2	2.34	0.56
1:A:417:LYS:HZ2	1:E:417:LYS:HG3	1.71	0.55
1:E:220:LEU:CB	1:E:241:ASN:HD22	2.18	0.55
1:A:149:TRP:O	1:A:172:VAL:HG22	2.06	0.55
1:M:362:PRO:HG3	1:M:382:ILE:O	2.06	0.55
2:N:47:LEU:HD12	2:N:55:LEU:HD11	1.88	0.55
1:A:137:LYS:H	2:B:144:ASP:HB2	1.71	0.55
1:K:141:ARG:HB3	1:K:141:ARG:HH11	1.72	0.55
1:M:128:GLU:CG	2:N:128:LYS:HG2	2.35	0.55
1:E:374:LEU:HG	1:E:398:LEU:HD21	1.88	0.55
1:O:314:LEU:O	1:O:318:VAL:HG23	2.05	0.55
1:E:274:ASN:C	1:E:274:ASN:HD22	2.10	0.55
1:G:158:ASN:HA	1:G:181:PHE:HB2	1.89	0.55
2:J:98:GLY:O	2:J:102:GLU:HG2	2.06	0.55
2:H:12:GLU:OE2	2:H:52:ALA:HB1	2.06	0.55
1:G:377:LEU:O	1:G:400:ILE:HA	2.07	0.55
1:E:344:PHE:CE2	1:E:370:GLU:HB2	2.41	0.55
1:O:416:LYS:O	1:O:417:LYS:HD3	2.06	0.55
1:K:389:GLN:NE2	1:K:392:LYS:HD2	2.21	0.55
1:E:182:MET:O	1:E:205:ILE:HA	2.06	0.55
1:G:309:LEU:HD23	1:G:332:SER:OG	2.07	0.55
2:D:122:THR:O	2:D:126:MET:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:335:LEU:HD22	1:O:339:CYS:SG	2.47	0.55
2:H:16:VAL:CG2	2:H:21:ALA:HB2	2.36	0.55
2:H:43:ASP:O	2:H:45:VAL:N	2.39	0.55
1:A:182:MET:O	1:A:205:ILE:HA	2.06	0.55
2:N:16:VAL:HG21	2:N:21:ALA:HB2	1.88	0.55
2:H:98:GLY:O	2:H:102:GLU:HG2	2.07	0.55
1:E:141:ARG:HH11	1:E:141:ARG:HB3	1.71	0.55
1:A:151:THR:HB	1:A:426:CYS:HA	1.87	0.55
1:I:220:LEU:CB	1:I:241:ASN:ND2	2.68	0.55
1:M:281:PHE:CB	1:M:285:HIS:CG	2.89	0.55
1:C:424:ILE:HD12	1:C:424:ILE:N	2.22	0.55
1:M:257:GLU:HB2	1:M:288:VAL:HG21	1.88	0.55
1:K:176:ARG:HD3	1:K:419:GLN:HA	1.87	0.55
1:A:155:THR:CG2	1:A:178:PRO:HD2	2.31	0.55
1:G:378:GLN:HE21	1:G:380:PHE:HE1	1.54	0.55
2:B:98:GLY:O	2:B:102:GLU:HG2	2.07	0.55
1:E:149:TRP:O	1:E:172:VAL:HG22	2.07	0.55
1:I:417:LYS:CD	1:M:417:LYS:CG	2.80	0.55
1:M:416:LYS:HD2	1:M:417:LYS:HZ1	1.68	0.55
1:G:151:THR:HB	1:G:426:CYS:HA	1.87	0.55
2:D:101:PHE:CE1	2:D:105:LEU:HD11	2.42	0.55
2:H:47:LEU:HD12	2:H:55:LEU:HD11	1.89	0.55
2:F:98:GLY:HA3	1:O:284:LYS:HZ3	1.71	0.54
2:B:101:PHE:HE1	2:B:105:LEU:HD11	1.71	0.54
2:H:61:TRP:HB2	2:H:92:PHE:CZ	2.43	0.54
1:C:220:LEU:CB	1:C:241:ASN:HD22	2.18	0.54
1:E:157:LYS:NZ	1:E:430:LEU:HD13	2.22	0.54
1:M:158:ASN:HA	1:M:181:PHE:HB2	1.89	0.54
1:I:182:MET:O	1:I:205:ILE:HA	2.07	0.54
1:O:309:LEU:HD23	1:O:332:SER:OG	2.07	0.54
2:N:88:TRP:O	2:N:91:GLU:HG3	2.07	0.54
2:D:54:ILE:HG13	2:D:102:GLU:HB3	1.87	0.54
1:E:257:GLU:HB2	1:E:288:VAL:HG21	1.88	0.54
2:F:12:GLU:OE2	2:F:52:ALA:HB1	2.07	0.54
1:K:419:GLN:HG2	1:K:419:GLN:O	2.07	0.54
1:I:176:ARG:CD	1:I:419:GLN:HA	2.37	0.54
1:M:220:LEU:HB2	1:M:241:ASN:HD22	1.72	0.54
1:G:374:LEU:HG	1:G:398:LEU:HD21	1.89	0.54
1:M:196:GLN:HB3	1:M:221:GLN:HE21	1.73	0.54
1:C:155:THR:HG21	1:C:176:ARG:NH1	2.23	0.54
2:L:20:ILE:HA	2:L:23:GLN:HE21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:420:GLU:O	1:K:420:GLU:CG	2.55	0.54
1:G:141:ARG:HB3	1:G:141:ARG:HH11	1.71	0.54
1:C:187:ALA:O	1:C:188:GLU:C	2.46	0.54
1:C:397:HIS:CE1	1:C:398:LEU:HG	2.43	0.54
1:G:362:PRO:HG3	1:G:382:ILE:O	2.08	0.54
1:G:257:GLU:HB2	1:G:288:VAL:HG21	1.89	0.54
1:M:215:SER:O	1:M:240:LYS:NZ	2.39	0.54
1:M:131:LYS:HD3	2:N:130:LYS:O	2.08	0.54
1:G:182:MET:O	1:G:205:ILE:HA	2.08	0.54
1:A:362:PRO:HG3	1:A:382:ILE:O	2.08	0.54
1:C:340:PHE:CD1	1:C:340:PHE:N	2.74	0.54
1:I:414:GLY:CA	1:M:416:LYS:HZ2	2.14	0.54
2:P:65:HIS:CB	2:P:68:ASP:HB2	2.25	0.54
1:M:370:GLU:O	1:M:372:PRO:HD3	2.08	0.54
1:M:420:GLU:CG	1:M:420:GLU:O	2.56	0.54
2:N:22:LYS:O	2:N:22:LYS:HD3	2.06	0.54
1:A:277:TRP:HZ2	1:A:331:ASP:OD2	1.90	0.54
1:K:109:TRP:CD2	2:L:101:PHE:CD2	2.95	0.54
1:K:320:ARG:CB	1:K:320:ARG:NH1	2.71	0.54
2:F:130:LYS:HE3	2:F:138:THR:HG21	1.88	0.54
2:F:98:GLY:HA3	1:O:284:LYS:HZ1	1.73	0.54
1:O:281:PHE:HE1	1:O:305:TYR:CE2	2.24	0.54
2:F:133:GLU:HG3	2:F:137:LYS:HE2	1.90	0.54
2:H:16:VAL:HG21	2:H:21:ALA:HB2	1.89	0.54
1:K:220:LEU:N	1:K:241:ASN:HD22	2.01	0.54
2:L:24:SER:OG	2:L:110:LEU:HB3	2.07	0.54
1:A:377:LEU:O	1:A:400:ILE:HA	2.08	0.54
1:I:424:ILE:HD12	1:I:424:ILE:N	2.23	0.54
1:C:184:GLN:HB3	1:C:185:PRO:HD2	1.89	0.53
1:K:126:LEU:HD23	1:K:430:LEU:CD2	2.38	0.53
2:D:61:TRP:CD2	2:D:115:LEU:HD23	2.44	0.53
1:K:137:LYS:HE3	2:L:145:PHE:HA	1.91	0.53
1:A:380:PHE:CE2	1:A:401:ASN:HB3	2.43	0.53
1:A:158:ASN:HA	1:A:181:PHE:HB2	1.88	0.53
1:O:141:ARG:HH11	1:O:141:ARG:HB3	1.73	0.53
1:I:417:LYS:CG	1:M:417:LYS:CE	2.67	0.53
1:E:419:GLN:NE2	1:E:426:CYS:O	2.40	0.53
1:E:164:THR:HG21	1:E:182:MET:SD	2.49	0.53
1:M:420:GLU:O	1:M:420:GLU:HG3	2.08	0.53
1:G:420:GLU:O	1:G:420:GLU:CG	2.56	0.53
1:I:115:GLU:N	1:I:115:GLU:OE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLU:N	1:C:115:GLU:OE1	2.41	0.53
2:H:54:ILE:HG23	2:H:103:LEU:HD23	1.89	0.53
1:G:186:LEU:N	1:G:187:ALA:N	2.55	0.53
1:M:153:ASP:HB3	1:M:429:THR:HG22	1.90	0.53
1:A:197:HIS:CD2	1:A:222:ASN:ND2	2.72	0.53
1:O:281:PHE:CB	1:O:285:HIS:CG	2.91	0.53
1:C:325:VAL:HG13	1:C:350:GLN:HG2	1.89	0.53
1:C:276:SER:HB3	1:C:301:ASN:OD1	2.08	0.53
2:B:47:LEU:HD12	2:B:55:LEU:HD11	1.89	0.53
1:G:418:ASN:ND2	1:G:418:ASN:C	2.62	0.53
2:B:146:THR:HG22	2:B:148:GLU:H	1.73	0.53
2:B:149:GLU:O	2:B:153:VAL:HG23	2.08	0.53
1:K:133:SER:O	1:K:140:TYR:HB2	2.08	0.53
1:G:300:LEU:HD23	1:G:317:LEU:HD11	1.91	0.53
1:O:231:SER:OG	1:O:233:PRO:HD2	2.09	0.53
1:K:124:LEU:HB3	1:K:128:GLU:HB3	1.91	0.53
1:E:420:GLU:O	1:E:420:GLU:CG	2.56	0.53
1:G:419:GLN:HG2	1:G:419:GLN:O	2.08	0.53
1:O:220:LEU:CB	1:O:241:ASN:HD22	2.22	0.53
1:E:157:LYS:HD2	1:E:430:LEU:HD12	1.89	0.53
2:L:16:VAL:HG21	2:L:21:ALA:HB2	1.90	0.53
1:I:231:SER:OG	1:I:233:PRO:HD2	2.08	0.53
2:F:101:PHE:CE1	2:F:105:LEU:HD11	2.44	0.53
1:E:189:HIS:HA	1:E:216:GLN:NE2	2.24	0.53
1:M:151:THR:CB	1:M:426:CYS:HA	2.39	0.53
1:G:157:LYS:HD2	1:G:430:LEU:CD1	2.39	0.53
1:E:157:LYS:HD2	1:E:430:LEU:CD1	2.38	0.53
1:G:370:GLU:O	1:G:372:PRO:HD3	2.09	0.53
1:C:384:PRO:HD2	1:C:387:THR:OG1	2.08	0.53
2:J:54:ILE:O	2:J:57:LYS:HB2	2.09	0.53
1:E:378:GLN:NE2	1:E:401:ASN:HA	2.24	0.53
1:E:418:ASN:C	1:E:418:ASN:ND2	2.61	0.53
1:I:416:LYS:O	1:I:417:LYS:HD3	2.08	0.53
2:P:115:LEU:HD13	2:P:115:LEU:O	2.09	0.53
1:C:131:LYS:HD3	2:D:130:LYS:O	2.09	0.53
1:C:124:LEU:HB3	1:C:128:GLU:HB3	1.90	0.53
1:O:420:GLU:O	1:O:420:GLU:CG	2.57	0.53
1:A:246:ARG:NE	1:A:272:GLU:OE2	2.41	0.53
1:A:300:LEU:HD23	1:A:317:LEU:HD11	1.89	0.53
1:I:390:LEU:HA	1:I:393:GLU:HG2	1.89	0.53
1:M:149:TRP:O	1:M:172:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:GLN:CB	1:G:185:PRO:HD2	2.39	0.53
2:B:61:TRP:CE3	2:B:115:LEU:HB2	2.44	0.53
2:P:133:GLU:HA	2:P:136:ARG:NH1	2.24	0.53
1:M:109:TRP:CD2	2:N:101:PHE:HD2	2.27	0.53
1:M:418:ASN:C	1:M:418:ASN:HD22	2.11	0.53
1:I:416:LYS:CB	1:I:417:LYS:HE2	2.29	0.52
1:A:416:LYS:CB	1:A:417:LYS:HE2	2.26	0.52
2:F:61:TRP:CG	2:F:115:LEU:HD23	2.44	0.52
1:G:157:LYS:HG2	1:G:159:LEU:HD13	1.90	0.52
2:N:16:VAL:CG1	2:N:59:ILE:HD13	2.39	0.52
1:I:331:ASP:OD1	1:I:356:ARG:NH1	2.36	0.52
1:A:274:ASN:HD22	1:A:274:ASN:C	2.13	0.52
1:K:186:LEU:O	1:K:188:GLU:N	2.42	0.52
1:E:184:GLN:HB3	1:E:185:PRO:HD2	1.91	0.52
1:I:137:LYS:HE3	2:J:144:ASP:O	2.08	0.52
1:M:235:VAL:HG21	1:M:255:PHE:CG	2.45	0.52
1:I:300:LEU:HD23	1:I:317:LEU:HD11	1.91	0.52
1:K:274:ASN:HD22	1:K:274:ASN:C	2.11	0.52
2:F:22:LYS:O	2:F:22:LYS:HD3	2.09	0.52
1:K:417:LYS:HG3	1:O:417:LYS:NZ	2.25	0.52
1:C:417:LYS:HG3	1:G:417:LYS:NZ	2.24	0.52
1:I:351:HIS:CD2	1:I:376:THR:OG1	2.56	0.52
1:I:157:LYS:HG2	1:I:159:LEU:HD13	1.91	0.52
2:J:85:ILE:HG22	2:J:90:GLN:HG3	1.92	0.52
2:J:127:ILE:HG23	2:J:135:ILE:HD11	1.90	0.52
1:E:124:LEU:HB3	1:E:128:GLU:HB3	1.91	0.52
1:O:314:LEU:HD23	1:O:314:LEU:O	2.09	0.52
1:M:125:CYS:SG	1:M:127:PRO:HG2	2.49	0.52
1:A:420:GLU:O	1:A:420:GLU:CG	2.58	0.52
1:A:414:GLY:HA2	1:E:416:LYS:HZ3	1.74	0.52
1:I:190:PHE:N	1:I:190:PHE:CD1	2.78	0.52
1:I:196:GLN:HB3	1:I:221:GLN:HE21	1.74	0.52
2:F:117:ASP:OD1	2:F:121:LYS:HE3	2.09	0.52
1:C:417:LYS:CD	1:G:417:LYS:HD2	2.40	0.52
1:G:155:THR:CG2	1:G:178:PRO:HD2	2.27	0.52
1:O:168:LEU:HD22	1:O:195:VAL:CG2	2.40	0.52
2:N:26:THR:HB	2:N:110:LEU:HA	1.92	0.52
1:G:420:GLU:O	1:G:423:GLY:N	2.39	0.52
1:I:420:GLU:O	1:I:423:GLY:N	2.40	0.52
1:C:257:GLU:OE2	1:C:257:GLU:N	2.36	0.52
1:G:420:GLU:O	1:G:420:GLU:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:ASN:C	1:E:418:ASN:HD22	2.12	0.52
1:M:378:GLN:NE2	1:M:401:ASN:HA	2.25	0.52
2:B:54:ILE:HG21	2:B:106:ALA:HB2	1.92	0.52
1:C:141:ARG:HB3	1:C:141:ARG:HH11	1.74	0.52
1:M:237:THR:HG23	1:M:240:LYS:HE3	1.92	0.52
1:I:325:VAL:HG13	1:I:350:GLN:HG2	1.92	0.52
1:C:374:LEU:HG	1:C:398:LEU:HD21	1.91	0.52
1:E:130:LEU:HD12	2:F:160:CYS:SG	2.50	0.52
1:K:149:TRP:O	1:K:172:VAL:HG22	2.09	0.52
1:E:235:VAL:HG21	1:E:255:PHE:CG	2.45	0.52
2:L:133:GLU:O	2:L:137:LYS:HG3	2.10	0.52
1:I:272:GLU:HG2	1:I:299:GLN:HB2	1.92	0.52
1:M:411:PRO:HG3	1:M:422:TRP:CH2	2.45	0.52
1:K:399:GLN:NE2	1:K:399:GLN:HA	2.13	0.52
1:G:193:PHE:HB3	1:G:195:VAL:HG23	1.92	0.52
1:I:159:LEU:HD23	1:I:164:THR:CG2	2.39	0.52
2:H:143:ASN:OD1	2:H:145:PHE:HB2	2.09	0.52
1:M:418:ASN:C	1:M:418:ASN:ND2	2.62	0.52
1:C:377:LEU:O	1:C:400:ILE:HA	2.10	0.52
1:C:247:LEU:HD21	1:C:263:LEU:HD21	1.92	0.52
1:A:314:LEU:O	1:A:318:VAL:HG23	2.10	0.52
1:K:416:LYS:HZ3	1:O:414:GLY:CA	2.23	0.51
1:C:419:GLN:HG2	1:C:419:GLN:O	2.10	0.51
2:L:26:THR:HB	2:L:110:LEU:HA	1.92	0.51
1:G:418:ASN:HD22	1:G:418:ASN:C	2.12	0.51
2:L:136:ARG:CZ	2:L:143:ASN:ND2	2.73	0.51
1:I:161:PRO:HB3	1:I:209:THR:HG23	1.91	0.51
1:K:235:VAL:HG21	1:K:255:PHE:CG	2.45	0.51
1:A:418:ASN:C	1:A:418:ASN:HD22	2.13	0.51
1:G:115:GLU:N	1:G:115:GLU:OE1	2.43	0.51
2:P:127:ILE:HG23	2:P:135:ILE:HD13	1.93	0.51
2:L:101:PHE:HE1	2:L:105:LEU:HD11	1.75	0.51
1:K:109:TRP:HZ3	2:L:104:ILE:HD12	1.74	0.51
1:M:161:PRO:HB3	1:M:209:THR:CG2	2.40	0.51
1:M:109:TRP:CZ2	2:N:101:PHE:HB2	2.46	0.51
1:I:124:LEU:HB3	1:I:128:GLU:HB3	1.92	0.51
1:E:159:LEU:HD23	1:E:164:THR:CG2	2.38	0.51
1:M:220:LEU:H	1:M:241:ASN:ND2	2.05	0.51
2:H:124:ALA:O	2:H:128:LYS:HG3	2.11	0.51
2:B:12:GLU:OE2	2:B:52:ALA:HB1	2.11	0.51
1:A:340:PHE:CD1	1:A:340:PHE:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:49:ASN:HB2	2:P:109:TYR:CE2	2.45	0.51
1:C:416:LYS:HZ3	1:G:414:GLY:CA	2.23	0.51
1:G:419:GLN:HG3	1:G:426:CYS:HB2	1.91	0.51
1:I:419:GLN:OE1	1:I:429:THR:HG21	2.11	0.51
1:C:191:SER:HB3	1:C:192:PRO:CD	2.35	0.51
1:O:420:GLU:O	1:O:423:GLY:N	2.42	0.51
1:A:418:ASN:C	1:A:418:ASN:ND2	2.63	0.51
2:F:104:ILE:HG12	2:F:119:THR:HB	1.93	0.51
1:C:299:GLN:HG2	1:C:326:HIS:HB2	1.91	0.51
1:E:151:THR:HB	1:E:426:CYS:HA	1.92	0.51
1:C:151:THR:CB	1:C:426:CYS:HA	2.40	0.51
1:M:116:LEU:HD21	2:N:108:ASN:OD1	2.10	0.51
2:F:61:TRP:CD2	2:F:115:LEU:HD23	2.46	0.51
1:G:159:LEU:HD23	1:G:164:THR:CG2	2.36	0.51
1:G:383:VAL:CG1	1:G:388:LEU:HB2	2.40	0.51
1:E:133:SER:O	1:E:140:TYR:HB2	2.10	0.51
1:E:420:GLU:O	1:E:423:GLY:N	2.42	0.51
1:M:378:GLN:HE21	1:M:380:PHE:HE1	1.58	0.51
2:D:26:THR:O	2:D:29:THR:HG22	2.11	0.51
1:K:418:ASN:C	1:K:418:ASN:HD22	2.14	0.51
1:A:421:ILE:O	1:A:421:ILE:HG23	2.10	0.51
2:N:24:SER:OG	2:N:110:LEU:HB3	2.09	0.51
1:G:149:TRP:O	1:G:172:VAL:HA	2.11	0.51
1:A:237:THR:CG2	1:A:240:LYS:HE3	2.40	0.51
1:O:419:GLN:HG2	1:O:419:GLN:O	2.10	0.51
1:O:351:HIS:CD2	1:O:376:THR:OG1	2.55	0.51
1:G:157:LYS:NZ	1:G:430:LEU:HD13	2.26	0.51
1:C:351:HIS:CD2	1:C:376:THR:OG1	2.60	0.51
1:A:181:PHE:CE1	1:C:384:PRO:HA	2.45	0.51
1:O:418:ASN:ND2	1:O:418:ASN:C	2.64	0.51
1:C:415:ASN:C	1:C:417:LYS:H	2.14	0.51
1:O:153:ASP:HB3	1:O:429:THR:HG22	1.91	0.51
1:C:281:PHE:HE1	1:C:305:TYR:CE2	2.28	0.51
2:D:61:TRP:CE3	2:D:115:LEU:HB2	2.45	0.51
1:G:351:HIS:CD2	1:G:376:THR:OG1	2.62	0.51
2:H:16:VAL:CG1	2:H:59:ILE:HD13	2.40	0.51
2:L:132:PRO:O	2:L:136:ARG:HG3	2.10	0.51
1:O:149:TRP:O	1:O:172:VAL:HA	2.10	0.51
1:A:417:LYS:NZ	1:E:417:LYS:HG3	2.25	0.51
2:B:61:TRP:CG	2:B:115:LEU:HD23	2.45	0.51
1:I:420:GLU:O	1:I:420:GLU:CG	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:394:ALA:O	1:O:396:PRO:HD2	2.11	0.51
1:G:189:HIS:H	1:G:190:PHE:HD1	1.58	0.51
1:K:417:LYS:CD	1:O:417:LYS:HD2	2.41	0.51
2:F:98:GLY:O	2:F:102:GLU:HG2	2.11	0.51
1:K:376:THR:HG22	1:K:399:GLN:CB	2.41	0.51
1:K:320:ARG:CZ	1:K:320:ARG:HB3	2.41	0.51
1:M:231:SER:HA	1:M:254:GLY:O	2.11	0.51
1:M:130:LEU:HD11	2:N:159:TRP:CZ2	2.46	0.51
1:I:133:SER:O	1:I:140:TYR:HB2	2.11	0.51
2:J:87:VAL:HG21	1:M:296:THR:HA	1.92	0.51
1:O:115:GLU:OE1	1:O:115:GLU:N	2.44	0.51
1:A:419:GLN:HG3	1:A:426:CYS:HB2	1.94	0.50
1:I:215:SER:O	1:I:240:LYS:NZ	2.44	0.50
1:K:184:GLN:CB	1:K:185:PRO:HD2	2.41	0.50
1:A:181:PHE:CG	1:C:384:PRO:HG3	2.45	0.50
1:I:162:ASP:OD2	1:I:186:LEU:HD12	2.11	0.50
1:K:382:ILE:HG13	1:K:383:VAL:HG23	1.93	0.50
2:J:132:PRO:O	2:J:136:ARG:HG3	2.10	0.50
1:E:424:ILE:HD12	1:E:424:ILE:N	2.26	0.50
2:P:86:PRO:O	2:P:90:GLN:HG3	2.10	0.50
1:C:149:TRP:O	1:C:172:VAL:HG22	2.11	0.50
1:O:220:LEU:CB	1:O:241:ASN:ND2	2.74	0.50
1:K:189:HIS:H	1:K:190:PHE:HD1	1.59	0.50
1:C:137:LYS:HE3	2:D:145:PHE:HA	1.91	0.50
1:I:274:ASN:ND2	1:I:274:ASN:C	2.65	0.50
2:D:54:ILE:HG23	2:D:103:LEU:HD23	1.93	0.50
2:D:24:SER:OG	2:D:110:LEU:HB3	2.11	0.50
2:B:22:LYS:HD3	2:B:22:LYS:O	2.11	0.50
1:M:184:GLN:CB	1:M:185:PRO:HD2	2.41	0.50
1:O:284:LYS:O	1:O:288:VAL:HG23	2.12	0.50
1:A:424:ILE:N	1:A:424:ILE:HD12	2.26	0.50
1:E:220:LEU:N	1:E:241:ASN:HD22	2.05	0.50
1:M:325:VAL:HG13	1:M:350:GLN:HG2	1.93	0.50
2:F:85:ILE:HG22	2:F:90:GLN:HG3	1.93	0.50
1:A:107:VAL:HG12	1:A:108:SER:N	2.26	0.50
1:C:126:LEU:HD23	1:C:430:LEU:HG	1.93	0.50
1:E:253:SER:HB3	1:E:280:ASP:HB2	1.92	0.50
1:A:376:THR:HG22	1:A:399:GLN:HB3	1.93	0.50
1:K:370:GLU:O	1:K:372:PRO:HD3	2.11	0.50
2:J:127:ILE:HG23	2:J:135:ILE:HD13	1.92	0.50
2:D:98:GLY:O	2:D:102:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:51:ASN:ND2	2:J:53:ALA:H	2.09	0.50
1:C:417:LYS:CE	1:G:417:LYS:CG	2.71	0.50
1:K:419:GLN:O	1:K:425:LYS:HA	2.10	0.50
1:A:417:LYS:HD2	1:E:417:LYS:CD	2.40	0.50
2:D:65:HIS:CB	2:D:68:ASP:HB2	2.32	0.50
1:K:237:THR:HG23	1:K:240:LYS:HE3	1.92	0.50
1:A:220:LEU:CB	1:A:241:ASN:ND2	2.75	0.50
1:A:278:CYS:HB2	1:A:281:PHE:CE2	2.47	0.50
2:P:16:VAL:HG23	2:P:21:ALA:HB2	1.93	0.50
1:E:377:LEU:O	1:E:400:ILE:HA	2.11	0.50
1:E:196:GLN:HB3	1:E:221:GLN:HE21	1.76	0.50
1:C:418:ASN:C	1:C:418:ASN:HD22	2.15	0.50
1:G:314:LEU:CD2	1:G:314:LEU:O	2.59	0.50
1:A:414:GLY:CA	1:E:416:LYS:NZ	2.72	0.50
1:M:419:GLN:NE2	1:M:426:CYS:O	2.44	0.50
1:K:197:HIS:CD2	1:K:222:ASN:ND2	2.78	0.50
1:E:220:LEU:CB	1:E:241:ASN:ND2	2.75	0.50
1:G:220:LEU:N	1:G:241:ASN:HD22	2.07	0.50
1:A:157:LYS:HG2	1:A:159:LEU:HD13	1.93	0.50
1:C:418:ASN:C	1:C:418:ASN:ND2	2.64	0.50
1:K:416:LYS:NZ	1:O:414:GLY:CA	2.73	0.50
2:D:61:TRP:CG	2:D:115:LEU:HD23	2.47	0.50
1:A:384:PRO:HG3	1:C:181:PHE:CD1	2.47	0.50
1:O:196:GLN:HB3	1:O:221:GLN:HE21	1.77	0.50
2:F:64:HIS:HD2	2:F:65:HIS:CE1	2.29	0.50
1:M:164:THR:O	1:M:168:LEU:HG	2.11	0.50
1:I:159:LEU:CD2	1:I:164:THR:HG22	2.42	0.50
2:D:130:LYS:HB3	2:D:134:GLU:HB2	1.93	0.50
1:M:331:ASP:CG	1:M:356:ARG:HH11	2.13	0.50
1:A:378:GLN:HE22	1:A:401:ASN:HA	1.74	0.50
1:O:314:LEU:O	1:O:314:LEU:CD2	2.59	0.50
2:H:122:THR:O	2:H:126:MET:HG3	2.12	0.50
2:P:12:GLU:OE2	2:P:52:ALA:HB1	2.12	0.50
2:F:127:ILE:HG23	2:F:135:ILE:CD1	2.42	0.50
1:K:115:GLU:N	1:K:115:GLU:OE1	2.45	0.50
1:I:340:PHE:CD1	1:I:340:PHE:N	2.78	0.50
1:G:281:PHE:CE1	1:G:305:TYR:CE2	2.99	0.49
1:I:164:THR:HG21	1:I:182:MET:SD	2.52	0.49
2:B:130:LYS:CE	2:B:138:THR:HG21	2.40	0.49
1:A:133:SER:O	1:A:140:TYR:HB2	2.12	0.49
2:L:22:LYS:HD3	2:L:22:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:ARG:NH1	2:N:156:GLU:HA	2.27	0.49
1:C:314:LEU:O	1:C:314:LEU:CD2	2.60	0.49
2:B:25:VAL:HB	2:B:111:ASP:OD2	2.12	0.49
1:E:331:ASP:OD2	1:E:356:ARG:NH1	2.45	0.49
1:M:415:ASN:C	1:M:417:LYS:H	2.14	0.49
2:B:61:TRP:CD1	2:B:115:LEU:HD23	2.47	0.49
2:J:61:TRP:CE3	2:J:115:LEU:HB2	2.48	0.49
1:A:383:VAL:CG1	1:A:388:LEU:HB2	2.41	0.49
2:B:133:GLU:O	2:B:137:LYS:HG3	2.12	0.49
1:A:188:GLU:O	1:A:212:GLY:O	2.28	0.49
2:F:47:LEU:HD12	2:F:55:LEU:HD11	1.94	0.49
1:E:244:LEU:HD12	1:E:267:CYS:SG	2.53	0.49
1:A:417:LYS:CD	1:E:417:LYS:CG	2.86	0.49
1:G:153:ASP:HB2	1:G:426:CYS:HB2	1.92	0.49
1:M:419:GLN:HG2	1:M:419:GLN:O	2.13	0.49
2:H:107:ALA:CB	2:H:115:LEU:HD12	2.33	0.49
1:G:195:VAL:HG11	1:G:198:MET:CE	2.42	0.49
1:E:187:ALA:O	1:E:188:GLU:C	2.49	0.49
1:M:344:PHE:CE2	1:M:370:GLU:HB2	2.48	0.49
1:A:193:PHE:HB3	1:A:195:VAL:HG23	1.93	0.49
1:C:420:GLU:O	1:C:420:GLU:CG	2.59	0.49
2:B:133:GLU:HG3	2:B:137:LYS:HE2	1.93	0.49
1:K:247:LEU:HD21	1:K:263:LEU:HD21	1.95	0.49
1:C:274:ASN:C	1:C:274:ASN:ND2	2.65	0.49
2:J:16:VAL:CG1	2:J:59:ILE:HD13	2.42	0.49
1:K:418:ASN:C	1:K:418:ASN:ND2	2.65	0.49
1:A:136:CYS:SG	1:A:139:TRP:CD1	3.05	0.49
1:K:220:LEU:CB	1:K:241:ASN:ND2	2.75	0.49
2:N:133:GLU:HG3	2:N:137:LYS:HE2	1.93	0.49
2:J:61:TRP:CG	2:J:115:LEU:HD23	2.47	0.49
2:H:127:ILE:HG23	2:H:135:ILE:CD1	2.42	0.49
1:A:184:GLN:CB	1:A:185:PRO:CD	2.90	0.49
1:I:184:GLN:CG	1:I:185:PRO:HD2	2.42	0.49
1:G:320:ARG:HB2	1:G:320:ARG:HH11	1.76	0.49
2:D:49:ASN:HB2	2:D:109:TYR:CE2	2.47	0.49
1:E:107:VAL:HG12	1:E:108:SER:N	2.27	0.49
2:H:6:LEU:O	2:H:13:ILE:HA	2.12	0.49
2:B:6:LEU:O	2:B:13:ILE:HA	2.13	0.49
1:O:279:PHE:CD1	1:O:279:PHE:C	2.86	0.49
1:A:153:ASP:HB3	1:A:429:THR:HG22	1.94	0.49
1:E:181:PHE:CD1	1:G:384:PRO:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:GLU:O	1:C:423:GLY:N	2.44	0.49
2:J:54:ILE:HG21	2:J:106:ALA:HB2	1.93	0.49
2:F:127:ILE:HG23	2:F:135:ILE:HD13	1.93	0.49
1:G:162:ASP:OD2	1:G:186:LEU:HD12	2.12	0.49
1:G:184:GLN:CG	1:G:185:PRO:HD2	2.43	0.49
1:K:197:HIS:HD2	1:K:222:ASN:ND2	2.00	0.49
1:I:370:GLU:O	1:I:372:PRO:HD3	2.12	0.49
1:I:189:HIS:H	1:I:190:PHE:HD1	1.60	0.49
1:O:232:ASP:HB2	1:O:233:PRO:HD3	1.93	0.49
1:G:107:VAL:HG12	1:G:108:SER:N	2.28	0.49
2:H:61:TRP:CG	2:H:115:LEU:HD23	2.48	0.49
1:A:220:LEU:CB	1:A:241:ASN:HD22	2.25	0.49
1:C:205:ILE:O	1:C:206:GLU:C	2.51	0.49
2:D:54:ILE:O	2:D:57:LYS:HB2	2.13	0.49
1:E:420:GLU:O	1:E:420:GLU:HG3	2.13	0.49
1:I:168:LEU:HD22	1:I:195:VAL:HG21	1.93	0.49
1:K:415:ASN:C	1:K:417:LYS:H	2.15	0.49
1:I:418:ASN:C	1:I:418:ASN:HD22	2.16	0.49
2:B:61:TRP:HB2	2:B:92:PHE:CZ	2.47	0.49
1:I:344:PHE:CE2	1:I:370:GLU:HB2	2.47	0.49
1:E:370:GLU:O	1:E:372:PRO:HD3	2.12	0.49
1:A:311:LYS:HE3	1:A:338:ASP:O	2.13	0.49
2:P:61:TRP:CZ3	2:P:115:LEU:HB2	2.47	0.49
1:I:389:GLN:HE21	1:I:392:LYS:HD2	1.77	0.49
1:G:220:LEU:H	1:G:241:ASN:ND2	2.06	0.49
1:O:195:VAL:HG11	1:O:198:MET:CE	2.43	0.49
2:P:133:GLU:HG3	2:P:137:LYS:HE2	1.94	0.49
1:A:187:ALA:O	1:A:188:GLU:C	2.51	0.49
1:E:225:LEU:O	1:E:252:CYS:SG	2.71	0.49
2:H:104:ILE:HG12	2:H:119:THR:HB	1.94	0.49
1:C:278:CYS:HB2	1:C:281:PHE:CZ	2.48	0.48
1:G:389:GLN:HE22	1:G:392:LYS:NZ	2.11	0.48
1:O:418:ASN:HD22	1:O:418:ASN:N	2.10	0.48
1:O:163:VAL:O	1:O:167:LEU:HG	2.13	0.48
2:L:117:ASP:OD1	2:L:121:LYS:HE3	2.13	0.48
1:G:153:ASP:HB2	1:G:426:CYS:CB	2.42	0.48
1:O:190:PHE:CD1	1:O:190:PHE:N	2.81	0.48
1:E:137:LYS:CE	2:F:149:GLU:OE1	2.61	0.48
2:B:55:LEU:HD22	2:B:59:ILE:HD11	1.94	0.48
2:H:101:PHE:HE1	2:H:105:LEU:HD11	1.77	0.48
1:A:161:PRO:HB3	1:A:209:THR:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:ARG:NE	1:G:419:GLN:H	2.10	0.48
1:M:129:LEU:O	1:M:132:VAL:HG22	2.14	0.48
1:C:193:PHE:HB3	1:C:195:VAL:HG23	1.93	0.48
2:N:130:LYS:CE	2:N:138:THR:HG21	2.42	0.48
2:P:133:GLU:HA	2:P:136:ARG:HH11	1.76	0.48
1:E:130:LEU:HD12	2:F:160:CYS:CB	2.44	0.48
1:G:149:TRP:O	1:G:172:VAL:HG22	2.13	0.48
2:F:51:ASN:ND2	2:F:53:ALA:H	2.11	0.48
1:K:417:LYS:CG	1:O:417:LYS:CD	2.81	0.48
1:O:184:GLN:CB	1:O:185:PRO:HD2	2.43	0.48
1:C:390:LEU:HA	1:C:393:GLU:HG2	1.95	0.48
1:A:376:THR:HG22	1:A:399:GLN:CB	2.43	0.48
1:M:284:LYS:O	1:M:288:VAL:HG23	2.13	0.48
2:F:24:SER:OG	2:F:110:LEU:HB3	2.13	0.48
2:H:22:LYS:O	2:H:22:LYS:HD3	2.13	0.48
1:E:301:ASN:HB2	1:E:408:ILE:HD12	1.94	0.48
1:K:416:LYS:CG	1:K:417:LYS:HE2	2.43	0.48
1:A:417:LYS:CG	1:E:417:LYS:CE	2.70	0.48
1:M:168:LEU:HD22	1:M:195:VAL:CG2	2.44	0.48
1:O:418:ASN:HD22	1:O:418:ASN:C	2.17	0.48
1:G:314:LEU:O	1:G:318:VAL:HG23	2.13	0.48
1:E:331:ASP:CG	1:E:356:ARG:HH11	2.17	0.48
2:J:95:VAL:CG2	2:J:99:THR:HB	2.43	0.48
1:K:417:LYS:CG	1:O:417:LYS:CE	2.87	0.48
1:G:390:LEU:HA	1:G:393:GLU:HG2	1.95	0.48
1:A:159:LEU:CD2	1:A:164:THR:HG22	2.42	0.48
2:F:133:GLU:HA	2:F:136:ARG:NH1	2.28	0.48
1:K:309:LEU:HD21	1:K:329:LEU:HD22	1.96	0.48
1:M:115:GLU:OE1	1:M:115:GLU:N	2.46	0.48
1:C:416:LYS:HZ3	1:G:414:GLY:HA2	1.77	0.48
1:K:231:SER:HA	1:K:254:GLY:O	2.14	0.48
1:K:161:PRO:HG3	1:K:184:GLN:O	2.13	0.48
1:M:220:LEU:N	1:M:241:ASN:HD22	2.06	0.48
1:I:320:ARG:CZ	1:I:320:ARG:HB3	2.43	0.48
1:C:378:GLN:HE22	1:C:401:ASN:HA	1.78	0.48
1:M:382:ILE:HG13	1:M:383:VAL:HG23	1.94	0.48
2:J:149:GLU:O	2:J:153:VAL:HG23	2.14	0.48
1:C:135:VAL:HG13	2:D:136:ARG:HG2	1.94	0.48
2:F:101:PHE:HE1	2:F:105:LEU:HD11	1.78	0.48
2:B:51:ASN:ND2	2:B:53:ALA:H	2.11	0.48
1:M:133:SER:O	1:M:140:TYR:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:LEU:O	1:G:252:CYS:SG	2.72	0.48
1:C:419:GLN:HG3	1:C:426:CYS:HB2	1.95	0.48
2:P:61:TRP:HB2	2:P:92:PHE:CZ	2.48	0.48
1:G:231:SER:OG	1:G:233:PRO:HD2	2.13	0.48
1:C:133:SER:O	1:C:140:TYR:HB2	2.13	0.48
2:B:16:VAL:CG1	2:B:59:ILE:HD13	2.44	0.48
2:F:16:VAL:CG1	2:F:59:ILE:HD13	2.44	0.48
2:P:102:GLU:HA	2:P:102:GLU:OE2	2.14	0.48
1:E:421:ILE:O	1:E:421:ILE:HG23	2.13	0.48
2:J:122:THR:O	2:J:126:MET:HG3	2.14	0.48
2:N:6:LEU:O	2:N:13:ILE:HA	2.13	0.48
1:O:159:LEU:CD2	1:O:164:THR:HG22	2.44	0.48
1:O:384:PRO:HD2	1:O:387:THR:OG1	2.14	0.48
1:O:374:LEU:HG	1:O:398:LEU:HD21	1.96	0.48
1:G:137:LYS:HE3	2:H:145:PHE:HA	1.96	0.48
2:D:127:ILE:HG23	2:D:135:ILE:CD1	2.44	0.48
1:E:186:LEU:O	1:E:188:GLU:N	2.47	0.48
1:A:395:LEU:HD13	1:A:398:LEU:HD12	1.96	0.48
2:L:47:LEU:HD12	2:L:55:LEU:HD11	1.96	0.48
1:G:125:CYS:SG	1:G:127:PRO:HG2	2.54	0.48
1:K:231:SER:HB2	1:K:233:PRO:HD2	1.96	0.48
1:I:418:ASN:C	1:I:418:ASN:ND2	2.65	0.48
1:A:241:ASN:O	1:A:244:LEU:HG	2.13	0.48
1:G:231:SER:HA	1:G:254:GLY:O	2.14	0.48
1:M:367:GLU:C	1:M:369:GLY:H	2.17	0.48
2:N:146:THR:HB	2:N:149:GLU:HG3	1.94	0.48
1:E:309:LEU:HD21	1:E:329:LEU:HD22	1.95	0.48
1:M:274:ASN:C	1:M:274:ASN:HD22	2.17	0.48
1:I:137:LYS:HG3	2:J:144:ASP:HB2	1.96	0.47
1:E:418:ASN:HD22	1:E:418:ASN:N	2.12	0.47
2:B:124:ALA:O	2:B:128:LYS:HG3	2.13	0.47
1:O:340:PHE:N	1:O:340:PHE:CD1	2.81	0.47
2:B:117:ASP:OD1	2:B:121:LYS:HE3	2.14	0.47
1:A:419:GLN:NE2	1:A:426:CYS:O	2.47	0.47
1:A:253:SER:HB2	1:A:280:ASP:CG	2.34	0.47
2:D:131:THR:OG1	2:D:134:GLU:HG3	2.14	0.47
1:E:370:GLU:HA	1:E:370:GLU:OE1	2.14	0.47
1:C:340:PHE:N	1:C:340:PHE:HD1	2.13	0.47
1:K:126:LEU:HD23	1:K:430:LEU:HG	1.96	0.47
1:C:314:LEU:O	1:C:314:LEU:HD23	2.15	0.47
2:L:65:HIS:HA	2:L:68:ASP:OD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:PHE:CD1	1:K:190:PHE:N	2.81	0.47
1:E:148:LEU:CA	1:E:427:ARG:HH22	2.21	0.47
2:L:25:VAL:HB	2:L:111:ASP:OD2	2.13	0.47
1:G:419:GLN:O	1:G:425:LYS:HA	2.15	0.47
1:C:148:LEU:CA	1:C:427:ARG:NH2	2.65	0.47
1:I:418:ASN:HD22	1:I:418:ASN:N	2.11	0.47
1:I:419:GLN:HG2	1:I:419:GLN:O	2.14	0.47
2:J:50:VAL:HG23	2:J:109:TYR:CE2	2.50	0.47
1:M:131:LYS:HZ1	2:N:128:LYS:HA	1.78	0.47
2:P:24:SER:HB3	2:P:27:ILE:HB	1.96	0.47
1:I:164:THR:HG21	1:I:182:MET:CE	2.44	0.47
1:G:235:VAL:HG21	1:G:255:PHE:CG	2.48	0.47
1:I:301:ASN:HB2	1:I:408:ILE:HD12	1.96	0.47
1:K:107:VAL:HG12	1:K:108:SER:N	2.30	0.47
1:K:278:CYS:HB2	1:K:281:PHE:CE2	2.49	0.47
2:N:132:PRO:O	2:N:136:ARG:HG3	2.14	0.47
1:C:107:VAL:HG12	1:C:108:SER:N	2.29	0.47
1:A:196:GLN:OE1	1:A:221:GLN:NE2	2.48	0.47
1:E:415:ASN:C	1:E:417:LYS:H	2.18	0.47
2:D:61:TRP:HB2	2:D:92:PHE:CZ	2.49	0.47
2:H:127:ILE:HG23	2:H:135:ILE:HD13	1.97	0.47
2:L:130:LYS:CE	2:L:138:THR:HG21	2.44	0.47
1:E:137:LYS:HG2	2:F:145:PHE:CD2	2.50	0.47
2:P:16:VAL:HG21	2:P:21:ALA:HB2	1.95	0.47
1:G:340:PHE:CD1	1:G:340:PHE:N	2.82	0.47
1:G:190:PHE:CD1	1:G:190:PHE:N	2.83	0.47
1:M:176:ARG:NE	1:M:419:GLN:H	2.12	0.47
1:K:231:SER:CB	1:K:233:PRO:HD2	2.44	0.47
2:B:115:LEU:O	2:B:115:LEU:HD13	2.13	0.47
2:B:148:GLU:O	2:B:151:ALA:HB3	2.15	0.47
1:K:220:LEU:CB	1:K:241:ASN:HD22	2.27	0.47
1:G:278:CYS:HB2	1:G:281:PHE:CE2	2.50	0.47
1:G:220:LEU:CB	1:G:241:ASN:HD22	2.27	0.47
1:M:159:LEU:N	1:M:181:PHE:O	2.42	0.47
1:G:137:LYS:CE	2:H:144:ASP:O	2.62	0.47
1:E:382:ILE:HG13	1:E:383:VAL:HG23	1.96	0.47
2:B:16:VAL:HG23	2:B:21:ALA:HB2	1.96	0.47
1:C:420:GLU:O	1:C:421:ILE:C	2.53	0.47
2:P:54:ILE:O	2:P:57:LYS:HB2	2.15	0.47
1:C:418:ASN:N	1:C:418:ASN:HD22	2.12	0.47
1:I:193:PHE:HB3	1:I:195:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG21	1:A:255:PHE:CG	2.49	0.47
1:G:277:TRP:HZ2	1:G:331:ASP:OD2	1.97	0.47
1:O:276:SER:HB3	1:O:301:ASN:OD1	2.14	0.47
1:O:301:ASN:HB2	1:O:408:ILE:HD12	1.97	0.47
2:J:6:LEU:O	2:J:13:ILE:HA	2.15	0.47
1:K:377:LEU:O	1:K:400:ILE:HA	2.15	0.47
1:A:257:GLU:HB2	1:A:288:VAL:HG21	1.96	0.47
1:I:153:ASP:HB3	1:I:429:THR:HG22	1.96	0.47
1:G:367:GLU:C	1:G:369:GLY:H	2.18	0.47
2:N:101:PHE:CE1	2:N:105:LEU:HD11	2.49	0.47
2:P:122:THR:O	2:P:126:MET:HG3	2.15	0.47
2:D:85:ILE:HG22	2:D:90:GLN:HG3	1.95	0.47
1:I:107:VAL:HG12	1:I:108:SER:N	2.29	0.47
1:K:155:THR:CG2	1:K:178:PRO:HD2	2.39	0.47
1:A:176:ARG:NE	1:A:419:GLN:H	2.12	0.47
1:M:132:VAL:CG1	2:N:127:ILE:HG21	2.45	0.47
1:C:161:PRO:HB3	1:C:209:THR:CG2	2.41	0.47
2:B:131:THR:O	2:B:135:ILE:HG13	2.15	0.47
2:B:155:LYS:HA	2:B:158:GLN:HG3	1.96	0.47
1:E:340:PHE:N	1:E:340:PHE:CD1	2.81	0.47
1:A:417:LYS:CE	1:E:417:LYS:CG	2.93	0.47
1:C:419:GLN:O	1:C:425:LYS:HA	2.15	0.47
1:K:162:ASP:OD2	1:K:186:LEU:HD12	2.15	0.47
1:C:164:THR:O	1:C:168:LEU:HG	2.14	0.47
1:G:420:GLU:HG3	1:G:423:GLY:HA2	1.96	0.47
2:L:133:GLU:HG3	2:L:137:LYS:HE2	1.96	0.47
1:A:232:ASP:HB2	1:A:233:PRO:HD3	1.96	0.47
2:P:139:PHE:O	2:P:140:ASN:O	2.33	0.47
1:E:278:CYS:HB2	1:E:281:PHE:CZ	2.49	0.46
1:A:420:GLU:HG3	1:A:423:GLY:HA2	1.96	0.46
1:M:185:PRO:O	1:M:186:LEU:HB2	2.15	0.46
1:G:416:LYS:CD	1:G:417:LYS:NZ	2.74	0.46
2:F:96:ASP:OD1	1:O:284:LYS:CE	2.48	0.46
1:O:162:ASP:OD2	1:O:186:LEU:HD12	2.16	0.46
2:F:133:GLU:HA	2:F:136:ARG:HH11	1.80	0.46
1:A:254:GLY:H	1:A:280:ASP:CG	2.19	0.46
1:C:389:GLN:HE21	1:C:392:LYS:HD2	1.76	0.46
1:O:132:VAL:O	1:O:135:VAL:HG23	2.15	0.46
1:I:278:CYS:HB2	1:I:281:PHE:CZ	2.50	0.46
1:C:159:LEU:HD23	1:C:164:THR:CG2	2.41	0.46
1:G:320:ARG:CB	1:G:320:ARG:NH1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG11	2:B:159:TRP:CG	2.51	0.46
1:I:235:VAL:HG21	1:I:255:PHE:CG	2.50	0.46
1:I:335:LEU:HD22	1:I:339:CYS:SG	2.55	0.46
1:I:347:ASN:O	1:I:373:THR:HG21	2.15	0.46
1:G:164:THR:HG21	1:G:182:MET:SD	2.55	0.46
1:M:390:LEU:HA	1:M:393:GLU:HG2	1.97	0.46
1:G:220:LEU:CB	1:G:241:ASN:ND2	2.77	0.46
2:L:130:LYS:HB3	2:L:134:GLU:HB2	1.96	0.46
2:F:148:GLU:O	2:F:151:ALA:HB3	2.14	0.46
1:E:356:ARG:HG2	1:E:358:TYR:OH	2.15	0.46
2:F:30:MET:HB3	2:F:36:MET:CE	2.46	0.46
1:G:356:ARG:HG2	1:G:358:TYR:OH	2.15	0.46
1:I:417:LYS:CE	1:M:417:LYS:CG	2.91	0.46
1:O:185:PRO:O	1:O:186:LEU:HB2	2.15	0.46
1:O:189:HIS:HA	1:O:216:GLN:NE2	2.30	0.46
1:G:424:ILE:HD12	1:G:424:ILE:N	2.31	0.46
1:O:246:ARG:HG2	1:O:272:GLU:HB2	1.98	0.46
1:A:141:ARG:HB3	1:A:141:ARG:HH11	1.79	0.46
1:K:416:LYS:HD2	1:K:417:LYS:HZ1	1.81	0.46
2:N:65:HIS:HB3	2:N:68:ASP:CB	2.22	0.46
1:G:215:SER:O	1:G:240:LYS:NZ	2.49	0.46
1:K:186:LEU:C	1:K:188:GLU:N	2.69	0.46
1:O:189:HIS:H	1:O:190:PHE:HD1	1.64	0.46
2:B:49:ASN:HB2	2:B:109:TYR:CD2	2.51	0.46
1:C:341:GLN:HA	1:C:344:PHE:CD1	2.51	0.46
2:D:132:PRO:O	2:D:136:ARG:HG3	2.16	0.46
2:D:26:THR:HB	2:D:110:LEU:HA	1.97	0.46
1:G:184:GLN:HG2	1:G:185:PRO:HD2	1.98	0.46
1:I:417:LYS:HD2	1:M:417:LYS:CD	2.46	0.46
1:A:215:SER:O	1:A:240:LYS:NZ	2.49	0.46
2:B:64:HIS:HD2	2:B:65:HIS:CE1	2.34	0.46
2:F:65:HIS:CB	2:F:68:ASP:HB2	2.29	0.46
2:B:104:ILE:HG12	2:B:119:THR:HB	1.96	0.46
1:O:390:LEU:HA	1:O:393:GLU:HG2	1.97	0.46
1:E:278:CYS:HB2	1:E:281:PHE:CE2	2.51	0.46
1:I:374:LEU:HG	1:I:398:LEU:HD21	1.97	0.46
2:J:61:TRP:CD2	2:J:115:LEU:HD23	2.51	0.46
1:O:420:GLU:O	1:O:421:ILE:C	2.52	0.46
2:L:16:VAL:CG1	2:L:59:ILE:HD13	2.45	0.46
1:I:199:ASP:OD1	1:I:411:PRO:HG2	2.14	0.46
1:O:107:VAL:HG12	1:O:108:SER:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:ARG:CZ	1:E:253:SER:OG	2.64	0.46
1:I:278:CYS:HB2	1:I:281:PHE:CE2	2.51	0.46
1:M:331:ASP:CG	1:M:356:ARG:NH1	2.69	0.46
2:F:132:PRO:O	2:F:136:ARG:HG3	2.16	0.46
1:O:246:ARG:NE	1:O:272:GLU:OE2	2.48	0.46
1:K:272:GLU:HG2	1:K:299:GLN:HB2	1.98	0.46
2:F:6:LEU:O	2:F:13:ILE:HA	2.15	0.46
1:C:328:ASP:HA	1:C:353:SER:HB2	1.98	0.46
1:O:331:ASP:OD2	1:O:356:ARG:NH1	2.49	0.46
1:I:414:GLY:CA	1:M:416:LYS:HZ3	2.29	0.46
1:I:415:ASN:O	1:I:417:LYS:HE2	2.15	0.46
1:C:184:GLN:CB	1:C:185:PRO:CD	2.94	0.46
1:K:244:LEU:HD12	1:K:267:CYS:SG	2.56	0.46
1:E:131:LYS:NZ	2:F:128:LYS:HA	2.30	0.46
1:G:378:GLN:NE2	1:G:380:PHE:CE1	2.83	0.46
1:K:320:ARG:NH1	1:K:320:ARG:HB3	2.31	0.46
1:E:141:ARG:CB	1:E:141:ARG:NH1	2.79	0.46
1:I:411:PRO:HG3	1:I:422:TRP:CH2	2.50	0.46
1:E:314:LEU:O	1:E:318:VAL:HG23	2.16	0.46
2:B:33:ASP:O	2:B:34:LEU:HD23	2.16	0.46
1:A:307:LYS:C	1:A:307:LYS:HD2	2.36	0.46
2:N:122:THR:O	2:N:126:MET:HG3	2.16	0.46
1:A:151:THR:HG22	1:A:174:ALA:HB3	1.98	0.46
1:A:157:LYS:NZ	1:A:430:LEU:HD13	2.31	0.46
2:N:27:ILE:HG12	2:N:47:LEU:HD21	1.98	0.46
1:A:196:GLN:HB3	1:A:221:GLN:HE21	1.81	0.46
2:H:24:SER:OG	2:H:110:LEU:HB3	2.15	0.46
2:F:122:THR:O	2:F:126:MET:HG3	2.15	0.46
1:G:286:VAL:O	1:G:289:ALA:HB3	2.16	0.45
1:I:253:SER:HB2	1:I:280:ASP:CG	2.37	0.45
2:P:127:ILE:HG23	2:P:135:ILE:HD11	1.97	0.45
1:M:137:LYS:HE3	2:N:144:ASP:O	2.16	0.45
2:J:136:ARG:CZ	2:J:143:ASN:ND2	2.79	0.45
1:O:277:TRP:HZ2	1:O:331:ASP:OD2	2.00	0.45
1:A:129:LEU:O	1:A:132:VAL:HG22	2.17	0.45
2:H:19:GLU:OE2	2:H:19:GLU:HA	2.16	0.45
2:B:65:HIS:HB3	2:B:68:ASP:CB	2.26	0.45
1:C:237:THR:HG23	1:C:240:LYS:HE3	1.99	0.45
1:O:278:CYS:HB2	1:O:281:PHE:CE2	2.51	0.45
1:I:159:LEU:N	1:I:181:PHE:O	2.42	0.45
1:O:195:VAL:HG11	1:O:198:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:SER:HB3	1:I:301:ASN:OD1	2.16	0.45
1:M:353:SER:O	1:M:354:LEU:HD23	2.17	0.45
1:O:415:ASN:O	1:O:417:LYS:HE2	2.16	0.45
1:C:185:PRO:O	1:C:186:LEU:HB2	2.16	0.45
1:M:153:ASP:OD2	1:M:419:GLN:HB2	2.17	0.45
1:E:155:THR:HG22	1:E:178:PRO:CD	2.32	0.45
1:E:395:LEU:HD13	1:E:398:LEU:HD12	1.99	0.45
1:E:320:ARG:HB3	1:E:320:ARG:CZ	2.46	0.45
1:A:185:PRO:O	1:A:186:LEU:HB2	2.17	0.45
2:H:33:ASP:O	2:H:34:LEU:HD23	2.16	0.45
1:M:245:VAL:HG12	1:M:246:ARG:HG3	1.99	0.45
1:O:424:ILE:HD12	1:O:424:ILE:N	2.32	0.45
2:H:61:TRP:CD2	2:H:115:LEU:HD23	2.51	0.45
1:O:157:LYS:HG2	1:O:159:LEU:HD13	1.97	0.45
1:I:184:GLN:HB3	1:I:185:PRO:HD2	1.96	0.45
2:P:55:LEU:HD22	2:P:59:ILE:HD11	1.96	0.45
1:K:380:PHE:CE2	1:K:401:ASN:HB3	2.51	0.45
1:K:149:TRP:O	1:K:172:VAL:HA	2.17	0.45
1:K:309:LEU:HD23	1:K:332:SER:OG	2.16	0.45
1:O:356:ARG:HG2	1:O:358:TYR:OH	2.16	0.45
1:M:141:ARG:HB3	1:M:141:ARG:HH11	1.81	0.45
1:E:416:LYS:CG	1:E:417:LYS:HE2	2.47	0.45
2:L:61:TRP:CG	2:L:115:LEU:HD23	2.52	0.45
2:J:22:LYS:HG2	2:J:28:LYS:HZ2	1.82	0.45
1:K:141:ARG:NH1	1:K:141:ARG:CB	2.79	0.45
1:I:303:SER:HB2	1:I:330:SER:O	2.17	0.45
2:L:136:ARG:NH2	2:L:143:ASN:ND2	2.64	0.45
2:H:32:GLU:O	2:H:34:LEU:N	2.50	0.45
1:I:415:ASN:C	1:I:417:LYS:H	2.20	0.45
1:G:153:ASP:OD2	1:G:419:GLN:HB2	2.16	0.45
1:C:220:LEU:CB	1:C:241:ASN:ND2	2.77	0.45
1:E:131:LYS:HZ1	2:F:128:LYS:HA	1.81	0.45
1:G:411:PRO:HG3	1:G:422:TRP:CH2	2.52	0.45
1:C:417:LYS:HD3	1:C:417:LYS:HA	1.87	0.45
1:M:419:GLN:O	1:M:425:LYS:HA	2.17	0.45
1:O:162:ASP:HA	1:O:190:PHE:CZ	2.37	0.45
2:P:130:LYS:HB3	2:P:134:GLU:HB2	1.98	0.45
1:M:159:LEU:HD23	1:M:164:THR:CG2	2.42	0.45
1:I:181:PHE:CG	1:K:384:PRO:HG3	2.50	0.45
2:P:98:GLY:O	2:P:102:GLU:HG2	2.17	0.45
2:F:130:LYS:HB3	2:F:134:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:TRP:CZ3	1:K:167:LEU:HD22	2.52	0.45
2:D:30:MET:C	2:D:32:GLU:H	2.20	0.45
1:K:232:ASP:HB2	1:K:233:PRO:HD3	1.99	0.45
1:A:367:GLU:C	1:A:369:GLY:H	2.20	0.45
2:L:55:LEU:HD22	2:L:59:ILE:HD11	1.98	0.45
1:G:378:GLN:NE2	1:G:380:PHE:HE1	2.14	0.45
1:M:109:TRP:HA	2:N:101:PHE:HE2	1.82	0.45
2:H:32:GLU:C	2:H:34:LEU:H	2.19	0.45
1:E:191:SER:HB3	1:E:192:PRO:HD2	1.99	0.45
1:E:161:PRO:HB3	1:E:209:THR:HG23	1.97	0.45
1:A:415:ASN:O	1:A:417:LYS:HE2	2.17	0.45
1:A:421:ILE:HG23	1:A:424:ILE:HB	1.99	0.45
2:J:130:LYS:CE	2:J:138:THR:HG21	2.45	0.45
2:D:136:ARG:CZ	2:D:143:ASN:ND2	2.80	0.45
2:J:143:ASN:OD1	2:J:145:PHE:HB2	2.17	0.45
1:G:378:GLN:HE22	1:G:401:ASN:HA	1.81	0.45
1:C:272:GLU:HG2	1:C:299:GLN:HB2	1.98	0.45
1:C:232:ASP:HB2	1:C:233:PRO:HD3	1.98	0.45
1:K:340:PHE:N	1:K:340:PHE:CD1	2.83	0.45
2:P:131:THR:OG1	2:P:134:GLU:HG3	2.17	0.45
1:A:278:CYS:HB2	1:A:281:PHE:CZ	2.52	0.45
1:E:168:LEU:HD22	1:E:195:VAL:HG22	1.97	0.45
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.82	0.45
1:A:159:LEU:N	1:A:181:PHE:O	2.47	0.45
2:D:133:GLU:HA	2:D:136:ARG:NH1	2.32	0.45
2:L:22:LYS:HG2	2:L:28:LYS:HZ2	1.82	0.45
2:H:8:SER:C	2:H:10:ASP:H	2.20	0.45
1:O:415:ASN:C	1:O:417:LYS:H	2.19	0.44
1:G:151:THR:HG22	1:G:174:ALA:HB3	1.99	0.44
1:G:164:THR:O	1:G:168:LEU:HG	2.17	0.44
1:E:193:PHE:HB3	1:E:195:VAL:HG23	1.98	0.44
2:B:50:VAL:HG23	2:B:109:TYR:CD2	2.53	0.44
1:K:159:LEU:CD2	1:K:164:THR:HG22	2.46	0.44
1:E:140:TYR:CE2	2:F:153:VAL:HG22	2.52	0.44
2:L:25:VAL:HG21	2:L:111:ASP:OD2	2.17	0.44
1:E:314:LEU:O	1:E:314:LEU:CD2	2.65	0.44
1:A:132:VAL:O	1:A:135:VAL:HG23	2.16	0.44
1:C:331:ASP:OD2	1:C:356:ARG:NH1	2.50	0.44
1:O:417:LYS:HD3	1:O:417:LYS:N	2.31	0.44
1:O:109:TRP:C	1:O:111:SER:H	2.20	0.44
1:E:389:GLN:HE21	1:E:392:LYS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:SER:HB2	1:E:280:ASP:CG	2.37	0.44
1:A:253:SER:HB3	1:A:280:ASP:HB2	1.95	0.44
1:G:241:ASN:O	1:G:244:LEU:HG	2.17	0.44
2:D:127:ILE:HG23	2:D:135:ILE:HD11	1.98	0.44
1:E:184:GLN:CB	1:E:185:PRO:CD	2.96	0.44
1:I:136:CYS:HB2	2:J:144:ASP:OD2	2.16	0.44
2:D:88:TRP:HE3	2:D:89:ASP:OD2	1.99	0.44
1:M:424:ILE:HD12	1:M:424:ILE:N	2.32	0.44
1:C:257:GLU:OE1	1:C:258:PHE:CE1	2.71	0.44
2:D:32:GLU:C	2:D:34:LEU:H	2.21	0.44
1:E:299:GLN:HA	1:E:326:HIS:HB2	1.99	0.44
1:O:244:LEU:HD12	1:O:267:CYS:SG	2.57	0.44
1:M:107:VAL:HG12	1:M:108:SER:N	2.31	0.44
1:I:116:LEU:HD21	2:J:108:ASN:CG	2.38	0.44
1:E:376:THR:HG22	1:E:399:GLN:HB2	1.98	0.44
1:I:185:PRO:O	1:I:186:LEU:HB2	2.17	0.44
2:P:32:GLU:C	2:P:34:LEU:H	2.20	0.44
1:C:335:LEU:HD22	1:C:339:CYS:SG	2.57	0.44
1:C:235:VAL:HG21	1:C:255:PHE:CG	2.52	0.44
1:C:417:LYS:NZ	1:G:417:LYS:HG3	2.29	0.44
2:L:18:VAL:HG23	2:L:19:GLU:N	2.32	0.44
1:K:281:PHE:HB2	1:K:285:HIS:CE1	2.51	0.44
1:K:390:LEU:HA	1:K:393:GLU:HG2	1.99	0.44
2:P:58:VAL:HG11	2:P:110:LEU:HD12	1.98	0.44
1:O:420:GLU:O	1:O:422:TRP:N	2.50	0.44
2:D:16:VAL:CG1	2:D:59:ILE:HD13	2.47	0.44
1:M:421:ILE:O	1:M:421:ILE:HG23	2.17	0.44
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.86	0.44
2:N:20:ILE:O	2:N:23:GLN:HB2	2.17	0.44
1:O:153:ASP:HB2	1:O:426:CYS:HB2	1.99	0.44
2:P:124:ALA:O	2:P:128:LYS:HG3	2.16	0.44
1:K:160:HIS:CE1	1:K:161:PRO:HG2	2.52	0.44
1:O:184:GLN:CG	1:O:185:PRO:HD2	2.47	0.44
1:O:157:LYS:HD2	1:O:430:LEU:HD12	1.99	0.44
1:C:109:TRP:CH2	2:D:101:PHE:HA	2.52	0.44
1:K:109:TRP:CH2	2:L:101:PHE:HA	2.51	0.44
1:A:320:ARG:HB3	1:A:320:ARG:CZ	2.47	0.44
2:N:16:VAL:HG23	2:N:21:ALA:HB2	2.00	0.44
1:I:314:LEU:HD23	1:I:314:LEU:O	2.17	0.44
1:K:176:ARG:NE	1:K:419:GLN:H	2.16	0.44
1:G:148:LEU:CA	1:G:427:ARG:HH22	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:424:ILE:HD12	1:K:424:ILE:H	1.83	0.44
1:A:160:HIS:CE1	1:A:161:PRO:HG2	2.52	0.44
2:B:22:LYS:C	2:B:22:LYS:HD3	2.38	0.44
1:M:166:ARG:HH12	2:N:156:GLU:HA	1.83	0.44
1:E:331:ASP:CG	1:E:356:ARG:NH1	2.71	0.44
1:A:271:ASP:O	1:A:297:ILE:HD12	2.17	0.44
2:J:12:GLU:OE2	2:J:52:ALA:HB1	2.17	0.44
1:M:340:PHE:N	1:M:340:PHE:CD1	2.83	0.44
1:M:162:ASP:HA	1:M:190:PHE:CZ	2.53	0.44
2:H:2:PRO:C	2:H:18:VAL:HG13	2.38	0.44
1:E:419:GLN:HG3	1:E:426:CYS:HB2	2.00	0.44
1:O:370:GLU:O	1:O:372:PRO:HD3	2.18	0.44
2:P:22:LYS:C	2:P:22:LYS:HD3	2.38	0.44
2:H:133:GLU:HA	2:H:136:ARG:NH1	2.33	0.44
1:A:182:MET:HB2	1:A:205:ILE:HG12	1.99	0.44
1:G:320:ARG:CZ	1:G:320:ARG:HB3	2.47	0.44
2:N:22:LYS:C	2:N:22:LYS:HD3	2.38	0.44
1:M:418:ASN:HD22	1:M:418:ASN:N	2.14	0.44
1:I:314:LEU:O	1:I:318:VAL:HG23	2.18	0.44
1:I:244:LEU:HD12	1:I:267:CYS:SG	2.58	0.44
1:M:126:LEU:HD23	1:M:430:LEU:HG	1.98	0.44
1:G:186:LEU:O	1:G:188:GLU:N	2.51	0.44
1:K:416:LYS:HD2	1:K:417:LYS:HZ3	1.81	0.44
2:J:2:PRO:C	2:J:18:VAL:HG13	2.38	0.44
2:N:2:PRO:C	2:N:18:VAL:HG13	2.37	0.44
1:E:390:LEU:HA	1:E:393:GLU:HG2	1.99	0.44
1:E:351:HIS:CD2	1:E:376:THR:OG1	2.61	0.44
1:G:132:VAL:HA	1:G:135:VAL:HG23	2.00	0.44
2:B:136:ARG:CZ	2:B:143:ASN:ND2	2.80	0.44
1:K:126:LEU:HD23	1:K:430:LEU:HD21	1.99	0.44
2:L:136:ARG:CZ	2:L:143:ASN:HD22	2.30	0.44
2:F:33:ASP:O	2:F:34:LEU:HD23	2.17	0.44
1:I:129:LEU:O	1:I:132:VAL:HG22	2.17	0.44
1:M:419:GLN:HG3	1:M:426:CYS:HB2	2.00	0.44
1:O:237:THR:HG23	1:O:240:LYS:HE3	1.99	0.44
1:A:331:ASP:CG	1:A:356:ARG:NH1	2.71	0.44
1:K:140:TYR:HB2	2:L:145:PHE:HZ	1.82	0.44
2:J:54:ILE:HG23	2:J:103:LEU:HD23	1.99	0.44
1:K:299:GLN:HG2	1:K:326:HIS:HB2	2.00	0.44
1:I:377:LEU:O	1:I:400:ILE:HA	2.18	0.44
1:O:237:THR:CG2	1:O:240:LYS:HE3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:151:THR:HB	1:O:426:CYS:HA	1.99	0.43
1:K:241:ASN:O	1:K:244:LEU:HG	2.18	0.43
1:I:370:GLU:OE1	1:I:370:GLU:HA	2.18	0.43
2:J:49:ASN:HB2	2:J:109:TYR:CD2	2.53	0.43
1:M:320:ARG:CZ	1:M:320:ARG:HB3	2.47	0.43
1:A:172:VAL:O	1:A:195:VAL:HA	2.18	0.43
1:A:184:GLN:CG	1:A:185:PRO:HD2	2.47	0.43
2:J:85:ILE:HA	2:J:86:PRO:HD3	1.87	0.43
2:F:16:VAL:HG23	2:F:21:ALA:HB2	1.99	0.43
2:B:54:ILE:HG23	2:B:103:LEU:HD23	2.00	0.43
1:O:415:ASN:O	1:O:416:LYS:CB	2.64	0.43
1:A:414:GLY:CA	1:E:416:LYS:HZ3	2.30	0.43
2:D:64:HIS:HD2	2:D:65:HIS:CE1	2.37	0.43
1:O:153:ASP:OD2	1:O:419:GLN:HB2	2.18	0.43
1:I:419:GLN:HG3	1:I:426:CYS:HB2	2.00	0.43
1:M:241:ASN:O	1:M:244:LEU:HG	2.18	0.43
2:F:49:ASN:HB2	2:F:109:TYR:CD2	2.53	0.43
1:E:383:VAL:HA	1:E:384:PRO:HD3	1.90	0.43
2:H:30:MET:HB3	2:H:36:MET:CE	2.49	0.43
1:E:128:GLU:CG	2:F:128:LYS:HG2	2.48	0.43
1:G:418:ASN:N	1:G:418:ASN:HD22	2.16	0.43
2:L:6:LEU:O	2:L:13:ILE:HA	2.18	0.43
1:G:311:LYS:HE3	1:G:338:ASP:O	2.17	0.43
2:N:25:VAL:HB	2:N:111:ASP:OD2	2.19	0.43
1:C:246:ARG:HG3	1:C:246:ARG:HH11	1.82	0.43
1:K:417:LYS:HG3	1:O:417:LYS:HZ2	1.82	0.43
1:E:417:LYS:HA	1:E:417:LYS:HD3	1.88	0.43
1:E:185:PRO:O	1:E:186:LEU:HB2	2.18	0.43
1:G:382:ILE:HG13	1:G:383:VAL:HG23	2.00	0.43
1:O:420:GLU:HG3	1:O:420:GLU:O	2.18	0.43
1:I:137:LYS:HE2	2:J:149:GLU:OE2	2.18	0.43
2:L:49:ASN:HB2	2:L:109:TYR:CD2	2.53	0.43
2:B:133:GLU:HA	2:B:136:ARG:NH1	2.33	0.43
1:G:141:ARG:NH1	1:G:141:ARG:CB	2.81	0.43
1:I:161:PRO:HB3	1:I:209:THR:CG2	2.48	0.43
2:F:30:MET:C	2:F:32:GLU:H	2.22	0.43
1:A:109:TRP:NE1	2:B:139:PHE:HD2	2.16	0.43
1:I:416:LYS:HD2	1:I:417:LYS:CE	2.47	0.43
2:P:18:VAL:HG23	2:P:19:GLU:N	2.34	0.43
2:P:130:LYS:CE	2:P:138:THR:HG21	2.47	0.43
2:B:55:LEU:HD22	2:B:59:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:24:SER:HB3	2:L:27:ILE:HB	2.00	0.43
2:D:133:GLU:HA	2:D:136:ARG:HH11	1.83	0.43
1:M:378:GLN:NE2	1:M:380:PHE:CE1	2.86	0.43
1:K:417:LYS:NZ	1:O:417:LYS:HG3	2.31	0.43
1:I:416:LYS:CD	1:I:417:LYS:NZ	2.69	0.43
2:H:43:ASP:CB	2:H:44:PRO:CD	2.89	0.43
1:G:278:CYS:HB2	1:G:281:PHE:CZ	2.54	0.43
1:M:278:CYS:HB2	1:M:281:PHE:CE2	2.54	0.43
1:C:194:ARG:O	1:C:195:VAL:C	2.56	0.43
2:B:50:VAL:HG23	2:B:109:TYR:CE2	2.54	0.43
1:G:129:LEU:O	1:G:132:VAL:HG22	2.18	0.43
1:G:274:ASN:ND2	1:G:274:ASN:C	2.71	0.43
2:L:25:VAL:HB	2:L:111:ASP:HB3	2.01	0.43
1:O:178:PRO:O	1:O:179:ARG:HB2	2.18	0.43
1:G:254:GLY:H	1:G:280:ASP:CG	2.21	0.43
2:F:61:TRP:HB2	2:F:92:PHE:CZ	2.54	0.43
1:M:220:LEU:CB	1:M:241:ASN:HD22	2.31	0.43
1:C:399:GLN:HE21	1:C:399:GLN:CA	2.26	0.43
1:E:187:ALA:C	1:E:212:GLY:HA3	2.39	0.43
1:A:379:VAL:N	1:A:401:ASN:OD1	2.41	0.43
2:P:133:GLU:HA	2:P:133:GLU:OE2	2.19	0.43
1:M:420:GLU:O	1:M:421:ILE:C	2.56	0.43
1:K:420:GLU:O	1:K:423:GLY:N	2.50	0.43
1:E:411:PRO:HG3	1:E:422:TRP:CH2	2.53	0.43
1:M:149:TRP:CZ3	1:M:167:LEU:HD22	2.53	0.43
1:A:420:GLU:O	1:A:423:GLY:N	2.51	0.43
1:K:307:LYS:HD2	1:K:307:LYS:C	2.39	0.43
1:O:416:LYS:CD	1:O:417:LYS:NZ	2.72	0.43
1:M:415:ASN:C	1:M:417:LYS:N	2.71	0.43
1:A:153:ASP:OD2	1:A:419:GLN:HB2	2.19	0.43
2:P:24:SER:OG	2:P:110:LEU:HB3	2.18	0.43
1:C:128:GLU:OE2	2:D:128:LYS:HA	2.19	0.43
1:G:320:ARG:HB2	1:G:320:ARG:NH1	2.33	0.43
2:P:54:ILE:HG13	2:P:102:GLU:HB3	2.01	0.43
1:I:380:PHE:CE2	1:I:401:ASN:HB3	2.54	0.43
1:A:299:GLN:HG2	1:A:326:HIS:HB2	2.01	0.43
1:A:418:ASN:N	1:A:418:ASN:HD22	2.16	0.43
1:G:314:LEU:O	1:G:314:LEU:HD23	2.18	0.43
1:E:109:TRP:C	1:E:111:SER:H	2.21	0.43
1:E:132:VAL:O	1:E:135:VAL:HG23	2.19	0.43
1:G:394:ALA:O	1:G:396:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:43:ASP:CB	2:N:44:PRO:CD	2.91	0.43
2:L:104:ILE:HD11	2:L:123:VAL:HG21	2.00	0.43
1:E:367:GLU:C	1:E:369:GLY:H	2.22	0.43
1:C:380:PHE:CE2	1:C:401:ASN:HB3	2.54	0.43
2:L:127:ILE:HG23	2:L:135:ILE:HD11	2.00	0.43
2:P:55:LEU:HD22	2:P:59:ILE:CD1	2.48	0.43
1:O:299:GLN:HG2	1:O:326:HIS:ND1	2.34	0.43
2:F:22:LYS:C	2:F:22:LYS:HD3	2.39	0.43
2:B:32:GLU:C	2:B:34:LEU:H	2.22	0.43
1:I:125:CYS:SG	1:I:127:PRO:HG2	2.59	0.43
1:M:184:GLN:CG	1:M:185:PRO:HD2	2.49	0.43
2:H:18:VAL:HG23	2:H:19:GLU:N	2.34	0.43
1:E:419:GLN:O	1:E:425:LYS:HA	2.19	0.43
1:O:176:ARG:NE	1:O:419:GLN:H	2.16	0.43
1:A:244:LEU:HD12	1:A:267:CYS:SG	2.58	0.43
1:A:389:GLN:HE22	1:A:392:LYS:NZ	2.16	0.43
2:N:127:ILE:HG23	2:N:135:ILE:CD1	2.49	0.43
2:P:26:THR:HB	2:P:110:LEU:HA	2.00	0.43
1:M:370:GLU:OE1	1:M:370:GLU:HA	2.19	0.43
2:L:16:VAL:HG23	2:L:21:ALA:HB2	2.00	0.43
2:D:133:GLU:HG3	2:D:137:LYS:HE2	2.01	0.43
1:K:141:ARG:HH11	1:K:141:ARG:CB	2.31	0.43
1:I:420:GLU:O	1:I:422:TRP:N	2.52	0.43
2:F:32:GLU:C	2:F:34:LEU:H	2.22	0.43
1:K:300:LEU:HD23	1:K:317:LEU:HD11	2.01	0.43
2:L:43:ASP:CB	2:L:44:PRO:CD	2.87	0.43
1:A:151:THR:CB	1:A:426:CYS:HA	2.49	0.43
1:O:419:GLN:HG3	1:O:426:CYS:HB2	2.01	0.43
1:O:131:LYS:NZ	2:P:127:ILE:O	2.51	0.43
1:O:205:ILE:O	1:O:206:GLU:C	2.57	0.43
1:C:274:ASN:ND2	1:C:276:SER:H	2.16	0.43
1:M:420:GLU:HG3	1:M:423:GLY:HA2	2.00	0.43
1:E:130:LEU:CD1	2:F:160:CYS:HB2	2.48	0.43
1:O:331:ASP:CG	1:O:356:ARG:HH11	2.21	0.43
2:N:117:ASP:OD1	2:N:121:LYS:HE3	2.19	0.43
1:E:232:ASP:O	1:E:236:ASN:ND2	2.52	0.43
2:B:64:HIS:CD2	2:B:88:TRP:CE3	3.07	0.42
1:A:137:LYS:HE2	2:B:149:GLU:OE2	2.18	0.42
2:N:124:ALA:O	2:N:128:LYS:HG3	2.19	0.42
1:K:109:TRP:C	1:K:111:SER:H	2.23	0.42
1:E:383:VAL:HG11	1:E:388:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:331:ASP:CG	1:K:356:ARG:HH11	2.22	0.42
1:A:384:PRO:HD2	1:A:387:THR:OG1	2.19	0.42
2:J:22:LYS:C	2:J:22:LYS:HD3	2.40	0.42
1:G:274:ASN:HB2	1:G:408:ILE:HG22	2.01	0.42
1:O:141:ARG:NH1	1:O:141:ARG:HB3	2.34	0.42
2:D:6:LEU:O	2:D:13:ILE:HA	2.19	0.42
2:J:131:THR:HG23	2:J:134:GLU:OE2	2.18	0.42
1:M:271:ASP:O	1:M:297:ILE:HD12	2.19	0.42
2:J:32:GLU:C	2:J:34:LEU:H	2.23	0.42
2:F:155:LYS:HA	2:F:158:GLN:HG3	2.00	0.42
1:I:389:GLN:HE22	1:I:392:LYS:HZ1	1.67	0.42
1:E:159:LEU:N	1:E:181:PHE:O	2.44	0.42
1:C:278:CYS:HB2	1:C:281:PHE:CE2	2.54	0.42
1:M:399:GLN:HE21	1:M:399:GLN:CA	2.25	0.42
1:C:109:TRP:C	1:C:111:SER:H	2.22	0.42
1:K:370:GLU:HA	1:K:370:GLU:OE1	2.18	0.42
1:A:320:ARG:NH1	1:A:320:ARG:CB	2.82	0.42
1:E:384:PRO:HG3	1:G:181:PHE:CD2	2.54	0.42
1:C:124:LEU:HD23	2:D:124:ALA:HB1	2.01	0.42
1:K:378:GLN:HE22	1:K:401:ASN:HA	1.81	0.42
2:B:143:ASN:OD1	2:B:145:PHE:HB2	2.19	0.42
1:E:420:GLU:O	1:E:422:TRP:N	2.52	0.42
1:A:272:GLU:HG2	1:A:299:GLN:HB2	2.00	0.42
1:G:130:LEU:HD12	2:H:160:CYS:SG	2.59	0.42
1:C:420:GLU:O	1:C:422:TRP:N	2.52	0.42
1:E:420:GLU:O	1:E:421:ILE:C	2.58	0.42
1:O:307:LYS:HE3	1:O:308:ASN:OD1	2.19	0.42
1:M:162:ASP:OD2	1:M:186:LEU:HD12	2.20	0.42
1:O:416:LYS:CD	1:O:417:LYS:HZ1	2.05	0.42
1:C:415:ASN:C	1:C:417:LYS:N	2.72	0.42
1:G:415:ASN:O	1:G:417:LYS:HE2	2.19	0.42
2:F:18:VAL:HG23	2:F:19:GLU:N	2.34	0.42
1:I:281:PHE:CE1	1:I:305:TYR:CE2	3.08	0.42
2:P:149:GLU:O	2:P:153:VAL:HG23	2.19	0.42
2:F:131:THR:O	2:F:135:ILE:HG13	2.18	0.42
2:H:24:SER:HB3	2:H:27:ILE:HB	2.02	0.42
1:M:272:GLU:HG2	1:M:299:GLN:HB2	2.00	0.42
1:G:245:VAL:HG12	1:G:246:ARG:HG3	2.01	0.42
2:B:24:SER:HB3	2:B:27:ILE:HB	2.01	0.42
2:N:32:GLU:C	2:N:34:LEU:H	2.23	0.42
2:N:33:ASP:O	2:N:34:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:379:VAL:HG23	1:K:379:VAL:O	2.19	0.42
2:P:45:VAL:HA	2:P:46:PRO:HD3	1.88	0.42
1:A:415:ASN:O	1:A:416:LYS:CB	2.66	0.42
1:C:416:LYS:CG	1:C:417:LYS:HE2	2.49	0.42
1:G:153:ASP:OD2	1:G:419:GLN:HG3	2.19	0.42
1:I:151:THR:HB	1:I:426:CYS:HA	2.01	0.42
1:M:278:CYS:HB2	1:M:281:PHE:CZ	2.55	0.42
1:M:191:SER:HB3	1:M:192:PRO:CD	2.45	0.42
1:A:164:THR:O	1:A:168:LEU:HG	2.19	0.42
1:K:277:TRP:HZ2	1:K:331:ASP:OD2	2.03	0.42
1:K:131:LYS:NZ	2:L:127:ILE:O	2.52	0.42
1:O:378:GLN:HE21	1:O:380:PHE:HE1	1.68	0.42
2:B:132:PRO:O	2:B:136:ARG:HG3	2.19	0.42
2:F:130:LYS:CE	2:F:138:THR:HG21	2.50	0.42
2:D:24:SER:HB3	2:D:27:ILE:HB	2.01	0.42
1:M:231:SER:OG	1:M:233:PRO:HD2	2.19	0.42
1:A:187:ALA:O	1:A:188:GLU:O	2.38	0.42
2:D:47:LEU:HD12	2:D:55:LEU:HD11	2.00	0.42
1:K:394:ALA:O	1:K:396:PRO:HD2	2.20	0.42
2:N:102:GLU:OE2	2:N:102:GLU:HA	2.20	0.42
1:K:415:ASN:C	1:K:417:LYS:N	2.72	0.42
1:K:419:GLN:HG3	1:K:426:CYS:HB2	2.00	0.42
1:O:376:THR:HG22	1:O:399:GLN:HB2	2.00	0.42
1:E:195:VAL:HG11	1:E:198:MET:CE	2.49	0.42
1:I:378:GLN:HE21	1:I:380:PHE:HE1	1.67	0.42
1:E:284:LYS:O	1:E:288:VAL:HG23	2.19	0.42
1:K:418:ASN:HD22	1:K:418:ASN:N	2.17	0.42
1:C:314:LEU:O	1:C:318:VAL:HG23	2.19	0.42
2:L:25:VAL:CB	2:L:111:ASP:OD2	2.67	0.42
1:E:272:GLU:HG2	1:E:299:GLN:HB2	2.00	0.42
2:D:112:ILE:O	2:D:112:ILE:HG22	2.20	0.42
1:C:389:GLN:HE22	1:C:392:LYS:NZ	2.16	0.42
1:G:132:VAL:CG1	2:H:127:ILE:HG21	2.50	0.42
1:O:383:VAL:CG1	1:O:388:LEU:HB2	2.48	0.42
1:C:421:ILE:HG23	1:C:424:ILE:HB	2.02	0.42
2:P:148:GLU:O	2:P:151:ALA:HB3	2.18	0.42
1:A:199:ASP:OD1	1:A:411:PRO:HG2	2.20	0.42
1:E:314:LEU:O	1:E:314:LEU:HD23	2.20	0.42
1:A:271:ASP:C	1:A:297:ILE:HD12	2.40	0.42
2:F:116:LEU:O	2:F:120:CYS:SG	2.71	0.42
1:K:376:THR:HG22	1:K:399:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:HD21	2:D:108:ASN:CG	2.40	0.42
1:O:109:TRP:CZ2	2:P:101:PHE:HB2	2.55	0.42
1:O:132:VAL:HG12	2:P:127:ILE:HG21	2.01	0.42
2:N:100:LEU:O	2:N:104:ILE:HG13	2.20	0.42
1:C:420:GLU:HG3	1:C:420:GLU:O	2.20	0.42
1:G:329:LEU:O	1:G:332:SER:OG	2.32	0.42
1:G:421:ILE:HG23	1:G:424:ILE:HB	2.02	0.42
1:I:421:ILE:HG23	1:I:421:ILE:O	2.18	0.42
1:C:141:ARG:NH1	1:C:141:ARG:CB	2.83	0.42
1:O:125:CYS:SG	1:O:127:PRO:HG2	2.60	0.42
2:F:45:VAL:HA	2:F:46:PRO:HD3	1.81	0.42
1:E:279:PHE:C	1:E:279:PHE:CD1	2.93	0.42
1:O:389:GLN:HE22	1:O:392:LYS:NZ	2.18	0.42
2:J:49:ASN:ND2	2:J:109:TYR:CE1	2.86	0.42
2:D:130:LYS:CE	2:D:138:THR:HG21	2.47	0.42
1:E:231:SER:CB	1:E:233:PRO:HD2	2.49	0.42
1:I:382:ILE:HG13	1:I:383:VAL:HG23	2.01	0.42
1:O:320:ARG:HB3	1:O:320:ARG:CZ	2.50	0.42
1:I:330:SER:O	1:I:331:ASP:HB2	2.20	0.42
1:I:299:GLN:HG2	1:I:326:HIS:HB2	2.02	0.42
1:A:340:PHE:HD1	1:A:340:PHE:N	2.18	0.42
1:M:299:GLN:HG2	1:M:326:HIS:HB2	2.01	0.42
1:C:331:ASP:CG	1:C:356:ARG:HH11	2.23	0.42
1:C:177:CYS:HB3	1:C:200:LEU:HD23	2.02	0.42
2:L:64:HIS:HD2	2:L:65:HIS:CE1	2.38	0.42
1:C:374:LEU:HG	1:C:398:LEU:CD2	2.50	0.42
1:O:274:ASN:C	1:O:274:ASN:ND2	2.69	0.42
2:J:16:VAL:HG12	2:J:59:ILE:HG21	2.02	0.42
2:J:148:GLU:O	2:J:151:ALA:HB3	2.19	0.42
1:G:420:GLU:O	1:G:421:ILE:C	2.59	0.42
1:E:271:ASP:C	1:E:297:ILE:HD12	2.40	0.42
1:C:186:LEU:HA	1:C:186:LEU:HD23	1.91	0.41
1:E:243:ASN:HA	1:E:269:ARG:HD2	2.02	0.41
1:E:151:THR:HG22	1:E:174:ALA:HB3	2.02	0.41
1:K:351:HIS:CD2	1:K:376:THR:OG1	2.65	0.41
2:H:65:HIS:CB	2:H:68:ASP:HB2	2.37	0.41
1:O:109:TRP:C	1:O:111:SER:N	2.74	0.41
1:K:220:LEU:HD13	1:K:223:LEU:HD22	2.02	0.41
2:D:146:THR:HB	2:D:149:GLU:CG	2.48	0.41
1:G:367:GLU:C	1:G:369:GLY:N	2.73	0.41
1:K:367:GLU:C	1:K:369:GLY:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:197:HIS:CD2	1:O:222:ASN:ND2	2.85	0.41
1:M:367:GLU:C	1:M:369:GLY:N	2.74	0.41
2:P:55:LEU:O	2:P:59:ILE:HG13	2.20	0.41
2:P:33:ASP:O	2:P:34:LEU:CD2	2.68	0.41
1:K:420:GLU:HG3	1:K:420:GLU:O	2.20	0.41
2:P:85:ILE:HG22	2:P:90:GLN:HG3	2.01	0.41
1:G:130:LEU:HD11	2:H:159:TRP:CZ2	2.55	0.41
1:O:419:GLN:O	1:O:425:LYS:HA	2.20	0.41
1:K:185:PRO:O	1:K:186:LEU:HB2	2.20	0.41
1:O:184:GLN:HG2	1:O:185:PRO:HD2	2.02	0.41
1:A:351:HIS:CD2	1:A:376:THR:OG1	2.65	0.41
1:A:168:LEU:HD22	1:A:195:VAL:CG2	2.48	0.41
2:B:136:ARG:O	2:B:140:ASN:HA	2.20	0.41
1:O:141:ARG:CB	1:O:141:ARG:NH1	2.83	0.41
1:K:196:GLN:HB3	1:K:221:GLN:HE21	1.86	0.41
1:I:187:ALA:C	1:I:212:GLY:HA3	2.40	0.41
1:E:416:LYS:CD	1:E:417:LYS:NZ	2.75	0.41
1:A:116:LEU:HD21	2:B:108:ASN:HB2	2.01	0.41
1:O:278:CYS:C	1:O:280:ASP:N	2.74	0.41
1:A:390:LEU:HA	1:A:393:GLU:HG2	2.01	0.41
1:M:164:THR:HG21	1:M:182:MET:CE	2.51	0.41
2:L:55:LEU:HD22	2:L:59:ILE:CD1	2.49	0.41
2:B:127:ILE:HG23	2:B:135:ILE:HD11	2.01	0.41
1:I:378:GLN:HE22	1:I:401:ASN:HA	1.85	0.41
1:A:420:GLU:O	1:A:420:GLU:HG3	2.20	0.41
1:I:420:GLU:O	1:I:420:GLU:HG3	2.20	0.41
1:K:235:VAL:HG21	1:K:255:PHE:CB	2.50	0.41
1:M:157:LYS:HD2	1:M:430:LEU:HD12	2.02	0.41
2:J:30:MET:O	2:J:34:LEU:HB2	2.21	0.41
1:C:394:ALA:O	1:C:396:PRO:HD2	2.21	0.41
2:N:158:GLN:O	2:N:160:CYS:N	2.53	0.41
1:O:410:ARG:HG3	1:O:410:ARG:NH1	2.35	0.41
1:K:327:LEU:O	1:K:352:LEU:HD12	2.21	0.41
1:G:186:LEU:C	1:G:188:GLU:N	2.74	0.41
2:L:45:VAL:HA	2:L:46:PRO:HD3	1.86	0.41
1:A:415:ASN:C	1:A:417:LYS:H	2.24	0.41
1:K:229:ARG:CZ	1:K:253:SER:OG	2.68	0.41
1:O:390:LEU:HA	1:O:393:GLU:CG	2.51	0.41
2:J:64:HIS:HD2	2:J:65:HIS:CE1	2.38	0.41
1:G:253:SER:HB2	1:G:280:ASP:CG	2.41	0.41
1:C:390:LEU:HA	1:C:393:GLU:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:281:PHE:HB2	1:M:285:HIS:CE1	2.56	0.41
2:F:136:ARG:O	2:F:140:ASN:HA	2.20	0.41
1:E:199:ASP:OD1	1:E:411:PRO:HG2	2.20	0.41
1:O:149:TRP:O	1:O:172:VAL:HG22	2.20	0.41
1:A:207:VAL:O	1:A:234:ILE:HD11	2.20	0.41
2:N:25:VAL:HG21	2:N:111:ASP:OD2	2.20	0.41
1:C:211:HIS:HB2	1:C:234:ILE:HG12	2.01	0.41
2:D:65:HIS:HD2	2:D:68:ASP:OD2	2.03	0.41
2:L:146:THR:HB	2:L:149:GLU:CG	2.47	0.41
2:D:61:TRP:CZ3	2:D:115:LEU:HB2	2.56	0.41
2:F:149:GLU:O	2:F:153:VAL:HG23	2.19	0.41
2:H:29:THR:HG23	2:H:30:MET:N	2.36	0.41
2:F:54:ILE:O	2:F:58:VAL:HG23	2.20	0.41
2:H:28:LYS:HG2	2:H:32:GLU:OE2	2.21	0.41
1:M:246:ARG:HG2	1:M:272:GLU:HB2	2.01	0.41
1:O:191:SER:HB3	1:O:192:PRO:HD2	2.01	0.41
1:I:417:LYS:NZ	1:M:417:LYS:HG3	2.35	0.41
2:P:19:GLU:HA	2:P:19:GLU:OE2	2.21	0.41
2:D:2:PRO:C	2:D:18:VAL:HG13	2.40	0.41
2:B:61:TRP:CD2	2:B:115:LEU:HD23	2.55	0.41
1:A:137:LYS:CG	2:B:144:ASP:HB2	2.47	0.41
1:K:390:LEU:O	1:K:393:GLU:HB2	2.21	0.41
2:N:133:GLU:HA	2:N:136:ARG:NH1	2.35	0.41
1:O:367:GLU:C	1:O:369:GLY:H	2.24	0.41
2:J:133:GLU:HG3	2:J:137:LYS:HE2	2.01	0.41
1:O:378:GLN:HE22	1:O:402:CYS:N	2.19	0.41
1:M:109:TRP:C	1:M:111:SER:H	2.23	0.41
1:M:309:LEU:HD23	1:M:332:SER:OG	2.20	0.41
2:L:32:GLU:C	2:L:34:LEU:H	2.24	0.41
1:G:196:GLN:HB3	1:G:221:GLN:HE21	1.86	0.41
1:I:176:ARG:NH2	1:I:418:ASN:HB2	2.36	0.41
1:I:253:SER:HB3	1:I:280:ASP:HB2	1.96	0.41
1:O:159:LEU:HD23	1:O:164:THR:CG2	2.47	0.41
1:M:193:PHE:HB3	1:M:195:VAL:HG23	2.03	0.41
2:P:88:TRP:HA	2:P:91:GLU:HG3	2.02	0.41
1:G:415:ASN:O	1:G:416:LYS:CB	2.66	0.41
2:B:89:ASP:O	2:B:92:PHE:HB3	2.20	0.41
1:O:159:LEU:N	1:O:181:PHE:O	2.42	0.41
1:I:367:GLU:C	1:I:369:GLY:H	2.24	0.41
2:F:49:ASN:HB2	2:F:109:TYR:CZ	2.55	0.41
2:J:61:TRP:CD1	2:J:115:LEU:HD23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:ILE:O	1:I:206:GLU:C	2.59	0.41
1:K:182:MET:HB2	1:K:205:ILE:HG23	2.02	0.41
1:K:341:GLN:HA	1:K:344:PHE:CD1	2.56	0.41
1:E:341:GLN:HA	1:E:344:PHE:CD1	2.55	0.41
1:A:159:LEU:HD23	1:A:164:THR:CG2	2.48	0.41
1:E:384:PRO:HA	1:G:181:PHE:CE1	2.56	0.41
1:K:421:ILE:O	1:K:421:ILE:HG23	2.21	0.41
1:K:124:LEU:HD23	2:L:124:ALA:HB1	2.02	0.41
2:L:136:ARG:NE	2:L:143:ASN:ND2	2.69	0.41
1:M:354:LEU:O	1:M:357:CYS:SG	2.79	0.41
1:C:300:LEU:HD23	1:C:317:LEU:HD11	2.02	0.41
2:N:54:ILE:O	2:N:57:LYS:HB2	2.21	0.41
1:G:185:PRO:O	1:G:186:LEU:HB2	2.21	0.41
1:C:417:LYS:HE3	1:G:417:LYS:CD	2.49	0.41
1:G:195:VAL:HG11	1:G:198:MET:HE2	2.03	0.41
1:O:164:THR:HG21	1:O:182:MET:CE	2.51	0.41
2:P:22:LYS:C	2:P:24:SER:H	2.24	0.41
2:L:54:ILE:HG13	2:L:102:GLU:HB3	2.01	0.41
1:G:135:VAL:O	2:H:136:ARG:NE	2.54	0.41
2:F:85:ILE:HA	2:F:86:PRO:HD3	1.94	0.41
1:K:420:GLU:O	1:K:421:ILE:C	2.58	0.41
1:M:378:GLN:NE2	1:M:380:PHE:HE1	2.19	0.41
1:C:356:ARG:HG2	1:C:358:TYR:OH	2.21	0.41
1:E:109:TRP:C	1:E:111:SER:N	2.74	0.41
2:J:33:ASP:O	2:J:34:LEU:HD23	2.20	0.41
1:A:279:PHE:C	1:A:279:PHE:CD1	2.94	0.41
2:P:6:LEU:O	2:P:13:ILE:HA	2.21	0.41
1:K:415:ASN:O	1:K:416:LYS:CB	2.64	0.41
2:L:43:ASP:O	2:L:45:VAL:N	2.54	0.41
2:H:4:ILE:HG21	2:H:31:LEU:HD11	2.02	0.41
1:C:162:ASP:OD2	1:C:186:LEU:HD12	2.21	0.41
1:E:237:THR:HG23	1:E:240:LYS:HE3	2.03	0.41
1:I:390:LEU:HA	1:I:393:GLU:CG	2.51	0.41
1:C:140:TYR:HB2	2:D:145:PHE:HZ	1.85	0.41
1:E:157:LYS:HG2	1:E:159:LEU:HD13	2.02	0.41
1:E:205:ILE:O	1:E:206:GLU:C	2.60	0.41
1:G:278:CYS:CB	1:G:281:PHE:CE2	3.04	0.41
1:C:370:GLU:OE1	1:C:370:GLU:HA	2.21	0.41
1:E:421:ILE:HG23	1:E:424:ILE:HB	2.04	0.41
1:G:235:VAL:HG21	1:G:255:PHE:CB	2.51	0.41
1:A:210:LEU:HB3	1:A:234:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:HA	1:A:297:ILE:HD12	1.97	0.41
1:E:203:SER:O	1:E:228:LEU:CD2	2.69	0.41
1:I:247:LEU:HD21	1:I:263:LEU:HD21	2.02	0.41
2:B:45:VAL:HA	2:B:46:PRO:HD3	1.81	0.41
1:K:253:SER:HB2	1:K:280:ASP:CG	2.41	0.40
1:O:278:CYS:C	1:O:280:ASP:H	2.23	0.40
1:M:220:LEU:CB	1:M:241:ASN:ND2	2.82	0.40
2:N:136:ARG:O	2:N:140:ASN:HA	2.20	0.40
1:A:149:TRP:CZ3	1:A:167:LEU:HD22	2.56	0.40
1:I:109:TRP:C	1:I:111:SER:H	2.24	0.40
1:O:382:ILE:HG13	1:O:383:VAL:HG23	2.03	0.40
1:I:137:LYS:H	2:J:144:ASP:HB2	1.85	0.40
1:E:141:ARG:HH11	1:E:141:ARG:CB	2.34	0.40
2:L:133:GLU:HA	2:L:136:ARG:NH1	2.36	0.40
2:H:22:LYS:HG2	2:H:28:LYS:HZ3	1.85	0.40
1:O:410:ARG:HH11	1:O:410:ARG:HG3	1.86	0.40
1:G:133:SER:O	1:G:140:TYR:HB2	2.20	0.40
1:I:141:ARG:HB3	1:I:141:ARG:HH11	1.85	0.40
1:G:176:ARG:NE	1:G:419:GLN:HA	2.36	0.40
2:L:19:GLU:HA	2:L:19:GLU:OE2	2.21	0.40
1:C:253:SER:HB3	1:C:280:ASP:HB2	1.95	0.40
1:E:181:PHE:CE1	1:G:384:PRO:HG3	2.57	0.40
1:C:157:LYS:HG2	1:C:159:LEU:HD13	2.04	0.40
1:A:399:GLN:CG	1:A:402:CYS:SG	3.10	0.40
1:I:109:TRP:HZ3	2:J:104:ILE:HD12	1.86	0.40
1:O:421:ILE:O	1:O:421:ILE:HG23	2.21	0.40
1:K:126:LEU:HD23	1:K:430:LEU:CG	2.52	0.40
2:L:22:LYS:HD3	2:L:22:LYS:C	2.41	0.40
2:J:45:VAL:HA	2:J:46:PRO:HD3	1.82	0.40
1:I:384:PRO:HD2	1:I:387:THR:OG1	2.21	0.40
1:M:415:ASN:O	1:M:416:LYS:CB	2.68	0.40
1:C:189:HIS:O	1:C:190:PHE:C	2.59	0.40
2:D:43:ASP:CB	2:D:44:PRO:CD	2.93	0.40
1:A:151:THR:CG2	1:A:424:ILE:HG21	2.52	0.40
1:O:109:TRP:CD2	2:P:101:PHE:HD2	2.40	0.40
2:N:134:GLU:HA	2:N:137:LYS:HD2	2.03	0.40
1:I:281:PHE:CD2	1:I:285:HIS:CD2	3.09	0.40
1:C:197:HIS:CE1	1:C:221:GLN:HE21	2.39	0.40
1:C:109:TRP:C	1:C:111:SER:N	2.74	0.40
1:C:109:TRP:CE2	2:D:101:PHE:HD2	2.38	0.40
1:E:137:LYS:HA	2:F:145:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:320:ARG:CB	1:K:320:ARG:CZ	2.99	0.40
2:L:136:ARG:O	2:L:140:ASN:HA	2.21	0.40
1:M:299:GLN:HG2	1:M:326:HIS:ND1	2.36	0.40
1:A:109:TRP:HE1	2:B:97:GLN:HB3	1.86	0.40
1:G:163:VAL:HG11	2:H:159:TRP:CG	2.57	0.40
1:K:416:LYS:CD	1:K:417:LYS:HZ3	2.34	0.40
2:H:45:VAL:HA	2:H:46:PRO:HD3	1.85	0.40
1:K:399:GLN:CG	1:K:402:CYS:SG	3.10	0.40
1:A:116:LEU:CD1	2:B:105:LEU:HD23	2.52	0.40
2:N:131:THR:O	2:N:135:ILE:HG13	2.21	0.40
2:N:131:THR:OG1	2:N:134:GLU:HG3	2.21	0.40
2:J:50:VAL:HG23	2:J:109:TYR:CD2	2.56	0.40
1:K:179:ARG:HA	1:K:202:ASN:O	2.22	0.40
2:B:130:LYS:HB3	2:B:134:GLU:HB2	2.03	0.40
1:C:367:GLU:C	1:C:369:GLY:H	2.24	0.40
1:E:137:LYS:HE2	2:F:149:GLU:OE1	2.21	0.40
1:K:181:PHE:HA	1:K:204:VAL:O	2.21	0.40
1:A:325:VAL:CG1	1:A:350:GLN:HG2	2.50	0.40
2:J:133:GLU:HA	2:J:136:ARG:HH11	1.87	0.40
1:G:141:ARG:HB3	1:G:141:ARG:NH1	2.36	0.40
1:I:420:GLU:O	1:I:421:ILE:C	2.60	0.40
1:C:141:ARG:NH1	1:C:141:ARG:HB3	2.37	0.40
1:I:195:VAL:HG11	1:I:198:MET:CE	2.52	0.40
1:A:141:ARG:CB	1:A:141:ARG:NH1	2.84	0.40
2:N:54:ILE:O	2:N:58:VAL:HG23	2.22	0.40
1:K:129:LEU:O	1:K:132:VAL:HG22	2.22	0.40
1:O:260:LEU:O	1:O:264:LEU:HG	2.22	0.40
2:L:88:TRP:O	2:L:91:GLU:HG3	2.21	0.40
1:E:379:VAL:O	1:E:379:VAL:HG23	2.22	0.40
1:E:247:LEU:HD21	1:E:263:LEU:HD21	2.02	0.40
1:O:415:ASN:C	1:O:417:LYS:N	2.75	0.40
1:G:415:ASN:C	1:G:417:LYS:H	2.25	0.40
2:N:43:ASP:O	2:N:45:VAL:N	2.54	0.40
1:G:237:THR:HG23	1:G:240:LYS:HE3	2.04	0.40
1:K:376:THR:HG22	1:K:399:GLN:HB2	2.01	0.40
1:K:254:GLY:H	1:K:280:ASP:CG	2.24	0.40
1:O:184:GLN:O	1:O:209:THR:OG1	2.39	0.40
1:G:281:PHE:HB2	1:G:285:HIS:CE1	2.56	0.40
2:H:101:PHE:O	2:H:105:LEU:HG	2.21	0.40
1:I:420:GLU:HG3	1:I:423:GLY:HA2	2.02	0.40
1:I:246:ARG:HG2	1:I:272:GLU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TRP:C	1:A:111:SER:H	2.23	0.40
1:E:129:LEU:O	1:E:132:VAL:HG22	2.21	0.40
2:B:122:THR:O	2:B:126:MET:HG3	2.20	0.40
1:E:125:CYS:SG	1:E:127:PRO:HG2	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:ASN:ND2	2:L:43:ASP:OD1[2_656]	1.93	0.27

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/336 (96%)	294 (91%)	21 (6%)	8 (2%)	7	24
1	C	323/336 (96%)	292 (90%)	24 (7%)	7 (2%)	8	28
1	E	323/336 (96%)	289 (90%)	27 (8%)	7 (2%)	8	28
1	G	323/336 (96%)	292 (90%)	24 (7%)	7 (2%)	8	28
1	I	323/336 (96%)	295 (91%)	21 (6%)	7 (2%)	8	28
1	K	323/336 (96%)	291 (90%)	24 (7%)	8 (2%)	7	24
1	M	323/336 (96%)	293 (91%)	25 (8%)	5 (2%)	13	40
1	O	323/336 (96%)	294 (91%)	21 (6%)	8 (2%)	7	24
2	B	133/149 (89%)	117 (88%)	12 (9%)	4 (3%)	5	18
2	D	133/149 (89%)	118 (89%)	10 (8%)	5 (4%)	4	13
2	F	133/149 (89%)	118 (89%)	11 (8%)	4 (3%)	5	18
2	H	133/149 (89%)	118 (89%)	12 (9%)	3 (2%)	8	26
2	J	133/149 (89%)	120 (90%)	8 (6%)	5 (4%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	133/149 (89%)	119 (90%)	9 (7%)	5 (4%)	4	13
2	N	133/149 (89%)	116 (87%)	13 (10%)	4 (3%)	5	18
2	P	133/149 (89%)	117 (88%)	11 (8%)	5 (4%)	4	13
All	All	3648/3880 (94%)	3283 (90%)	273 (8%)	92 (2%)	7	24

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	PHE
1	A	306	ARG
1	C	187	ALA
1	C	306	ARG
1	C	421	ILE
1	E	187	ALA
1	E	190	PHE
1	E	306	ARG
1	G	188	GLU
1	G	190	PHE
1	G	306	ARG
2	H	33	ASP
1	I	190	PHE
1	I	306	ARG
1	I	421	ILE
1	K	188	GLU
1	K	190	PHE
1	K	306	ARG
2	L	145	PHE
1	M	188	GLU
1	M	190	PHE
1	M	306	ARG
1	O	190	PHE
1	O	306	ARG
1	O	421	ILE
1	A	188	GLU
1	A	421	ILE
2	B	33	ASP
2	D	33	ASP
1	E	188	GLU
1	E	421	ILE
1	G	189	HIS
1	G	421	ILE

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Mol	Chain	Res	Type
1	I	188	GLU
1	K	187	ALA
1	K	421	ILE
2	L	33	ASP
1	M	421	ILE
2	N	33	ASP
2	N	159	TRP
1	O	188	GLU
2	P	33	ASP
2	P	140	ASN
1	A	186	LEU
1	C	186	LEU
1	C	188	GLU
1	C	418	ASN
1	E	186	LEU
2	F	33	ASP
2	F	140	ASN
2	H	140	ASN
2	J	33	ASP
1	O	189	HIS
2	B	140	ASN
2	D	43	ASP
2	D	113	LYS
2	D	140	ASN
1	G	187	ALA
2	H	43	ASP
1	I	189	HIS
1	I	333	VAL
1	K	189	HIS
2	L	43	ASP
2	L	140	ASN
1	M	187	ALA
2	N	43	ASP
1	O	279	PHE
2	P	43	ASP
2	P	159	TRP
1	A	418	ASN
2	B	43	ASP
2	B	159	TRP
2	D	137	LYS
2	F	43	ASP
1	G	186	LEU

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Mol	Chain	Res	Type
2	J	43	ASP
2	J	138	THR
2	J	140	ASN
1	K	418	ASN
2	L	138	THR
2	N	138	THR
1	O	195	VAL
2	F	138	THR
2	J	137	LYS
2	P	138	THR
1	C	195	VAL
1	E	195	VAL
1	I	195	VAL
1	A	195	VAL
1	A	333	VAL
1	O	408	ILE
1	K	195	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/311 (96%)	282 (94%)	17 (6%)	25	58
1	C	299/311 (96%)	286 (96%)	13 (4%)	35	70
1	E	299/311 (96%)	285 (95%)	14 (5%)	32	67
1	G	299/311 (96%)	285 (95%)	14 (5%)	32	67
1	I	299/311 (96%)	281 (94%)	18 (6%)	24	56
1	K	299/311 (96%)	287 (96%)	12 (4%)	38	73
1	M	299/311 (96%)	284 (95%)	15 (5%)	30	64
1	O	299/311 (96%)	283 (95%)	16 (5%)	27	60
2	B	124/134 (92%)	122 (98%)	2 (2%)	70	93
2	D	124/134 (92%)	120 (97%)	4 (3%)	46	80
2	F	124/134 (92%)	120 (97%)	4 (3%)	46	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	124/134 (92%)	120 (97%)	4 (3%)	46	80
2	J	124/134 (92%)	120 (97%)	4 (3%)	46	80
2	L	124/134 (92%)	121 (98%)	3 (2%)	57	87
2	N	124/134 (92%)	122 (98%)	2 (2%)	70	93
2	P	124/134 (92%)	117 (94%)	7 (6%)	26	59
All	All	3384/3560 (95%)	3235 (96%)	149 (4%)	35	69

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	115	GLU
1	A	128	GLU
1	A	192	PRO
1	A	207	VAL
1	A	262	THR
1	A	274	ASN
1	A	282	THR
1	A	307	LYS
1	A	314	LEU
1	A	317	LEU
1	A	342	GLU
1	A	359	ASP
1	A	389	GLN
1	A	399	GLN
1	A	418	ASN
1	A	420	GLU
2	B	55	LEU
2	B	116	LEU
1	C	114	ASP
1	C	115	GLU
1	C	128	GLU
1	C	191	SER
1	C	262	THR
1	C	274	ASN
1	C	307	LYS
1	C	314	LEU
1	C	317	LEU
1	C	342	GLU
1	C	389	GLN

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Mol	Chain	Res	Type
1	C	399	GLN
1	C	418	ASN
2	D	51	ASN
2	D	55	LEU
2	D	68	ASP
2	D	116	LEU
1	E	114	ASP
1	E	115	GLU
1	E	128	GLU
1	E	262	THR
1	E	274	ASN
1	E	307	LYS
1	E	314	LEU
1	E	317	LEU
1	E	342	GLU
1	E	359	ASP
1	E	389	GLN
1	E	399	GLN
1	E	418	ASN
1	E	420	GLU
2	F	51	ASN
2	F	55	LEU
2	F	116	LEU
2	F	118	VAL
1	G	114	ASP
1	G	115	GLU
1	G	128	GLU
1	G	262	THR
1	G	274	ASN
1	G	307	LYS
1	G	314	LEU
1	G	317	LEU
1	G	342	GLU
1	G	359	ASP
1	G	389	GLN
1	G	399	GLN
1	G	418	ASN
1	G	420	GLU
2	H	51	ASN
2	H	55	LEU
2	H	91	GLU
2	H	118	VAL

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Mol	Chain	Res	Type
1	I	114	ASP
1	I	115	GLU
1	I	128	GLU
1	I	207	VAL
1	I	237	THR
1	I	262	THR
1	I	274	ASN
1	I	281	PHE
1	I	282	THR
1	I	307	LYS
1	I	314	LEU
1	I	317	LEU
1	I	342	GLU
1	I	359	ASP
1	I	389	GLN
1	I	399	GLN
1	I	418	ASN
1	I	420	GLU
2	J	55	LEU
2	J	68	ASP
2	J	116	LEU
2	J	118	VAL
1	K	114	ASP
1	K	115	GLU
1	K	128	GLU
1	K	207	VAL
1	K	262	THR
1	K	274	ASN
1	K	307	LYS
1	K	314	LEU
1	K	317	LEU
1	K	342	GLU
1	K	399	GLN
1	K	418	ASN
2	L	51	ASN
2	L	55	LEU
2	L	116	LEU
1	M	114	ASP
1	M	115	GLU
1	M	128	GLU
1	M	207	VAL
1	M	262	THR

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Mol	Chain	Res	Type
1	M	274	ASN
1	M	282	THR
1	M	307	LYS
1	M	314	LEU
1	M	317	LEU
1	M	342	GLU
1	M	389	GLN
1	M	399	GLN
1	M	418	ASN
1	M	420	GLU
2	N	55	LEU
2	N	116	LEU
1	O	114	ASP
1	O	115	GLU
1	O	128	GLU
1	O	207	VAL
1	O	262	THR
1	O	274	ASN
1	O	281	PHE
1	O	307	LYS
1	O	314	LEU
1	O	317	LEU
1	O	342	GLU
1	O	359	ASP
1	O	389	GLN
1	O	399	GLN
1	O	418	ASN
1	O	420	GLU
2	P	33	ASP
2	P	51	ASN
2	P	55	LEU
2	P	89	ASP
2	P	91	GLU
2	P	116	LEU
2	P	118	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	197	HIS
1	A	221	GLN

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Mol	Chain	Res	Type
1	A	241	ASN
1	A	261	GLN
1	A	274	ASN
1	A	341	GLN
1	A	350	GLN
1	A	351	HIS
1	A	378	GLN
1	A	389	GLN
1	A	399	GLN
1	A	431	GLN
2	B	7	GLN
2	B	23	GLN
2	B	51	ASN
2	B	60	GLN
2	B	64	HIS
2	B	90	GLN
2	B	125	ASN
2	B	140	ASN
1	C	196	GLN
1	C	197	HIS
1	C	221	GLN
1	C	241	ASN
1	C	261	GLN
1	C	274	ASN
1	C	351	HIS
1	C	378	GLN
1	C	389	GLN
1	C	399	GLN
1	C	431	GLN
2	D	7	GLN
2	D	23	GLN
2	D	51	ASN
2	D	60	GLN
2	D	64	HIS
2	D	65	HIS
2	D	90	GLN
2	D	125	ASN
1	E	196	GLN
1	E	197	HIS
1	E	211	HIS
1	E	221	GLN
1	E	236	ASN

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Mol	Chain	Res	Type
1	E	241	ASN
1	E	261	GLN
1	E	274	ASN
1	E	351	HIS
1	E	389	GLN
1	E	399	GLN
1	E	431	GLN
2	F	7	GLN
2	F	60	GLN
2	F	64	HIS
2	F	90	GLN
2	F	125	ASN
1	G	196	GLN
1	G	197	HIS
1	G	211	HIS
1	G	221	GLN
1	G	241	ASN
1	G	261	GLN
1	G	274	ASN
1	G	350	GLN
1	G	351	HIS
1	G	378	GLN
1	G	389	GLN
1	G	399	GLN
2	H	7	GLN
2	H	23	GLN
2	H	51	ASN
2	H	60	GLN
2	H	64	HIS
2	H	90	GLN
2	H	125	ASN
1	I	196	GLN
1	I	197	HIS
1	I	211	HIS
1	I	221	GLN
1	I	241	ASN
1	I	261	GLN
1	I	274	ASN
1	I	351	HIS
1	I	378	GLN
1	I	389	GLN
1	I	399	GLN

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Mol	Chain	Res	Type
1	I	431	GLN
2	J	7	GLN
2	J	23	GLN
2	J	51	ASN
2	J	60	GLN
2	J	64	HIS
2	J	90	GLN
2	J	125	ASN
1	K	196	GLN
1	K	197	HIS
1	K	211	HIS
1	K	221	GLN
1	K	241	ASN
1	K	261	GLN
1	K	274	ASN
1	K	350	GLN
1	K	351	HIS
1	K	378	GLN
1	K	389	GLN
1	K	397	HIS
1	K	399	GLN
1	K	431	GLN
2	L	7	GLN
2	L	23	GLN
2	L	51	ASN
2	L	60	GLN
2	L	64	HIS
2	L	90	GLN
2	L	108	ASN
2	L	125	ASN
2	L	143	ASN
1	M	196	GLN
1	M	197	HIS
1	M	216	GLN
1	M	221	GLN
1	M	241	ASN
1	M	261	GLN
1	M	274	ASN
1	M	351	HIS
1	M	378	GLN
1	M	389	GLN
1	M	399	GLN

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Mol	Chain	Res	Type
1	M	431	GLN
2	N	7	GLN
2	N	23	GLN
2	N	60	GLN
2	N	64	HIS
2	N	90	GLN
2	N	125	ASN
1	O	196	GLN
1	O	197	HIS
1	O	221	GLN
1	O	241	ASN
1	O	261	GLN
1	O	274	ASN
1	O	350	GLN
1	O	351	HIS
1	O	378	GLN
1	O	389	GLN
1	O	399	GLN
1	O	431	GLN
2	P	7	GLN
2	P	23	GLN
2	P	60	GLN
2	P	64	HIS
2	P	90	GLN
2	P	125	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.