



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:48 am GMT

PDB ID : 1I3Q
Title : RNA POLYMERASE II CRYSTAL FORM I AT 3.1 Å RESOLUTION
Authors : Cramer, P.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2001-02-15
Resolution : 3.10 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

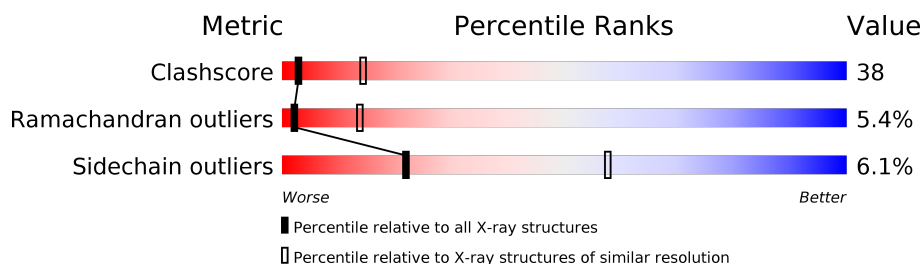
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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	1733	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	

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Mol	Chain	Length	Quality of chain
8	J	70	<div><div></div><div>29%56%6%7%</div></div>
9	K	120	<div><div></div><div>50%39%6%5%</div></div>
10	L	70	<div><div></div><div>19%34%11%34%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28161 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 DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1414	Total	C	N	O	S	0	0	0
			11114	7000	1947	2106	61			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1083	Total	C	N	O	S	0	0	0
			8624	5470	1501	1600	53			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

TIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total 2	Zn 2	0	0
11	L	1	Total 1	Zn 1	0	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

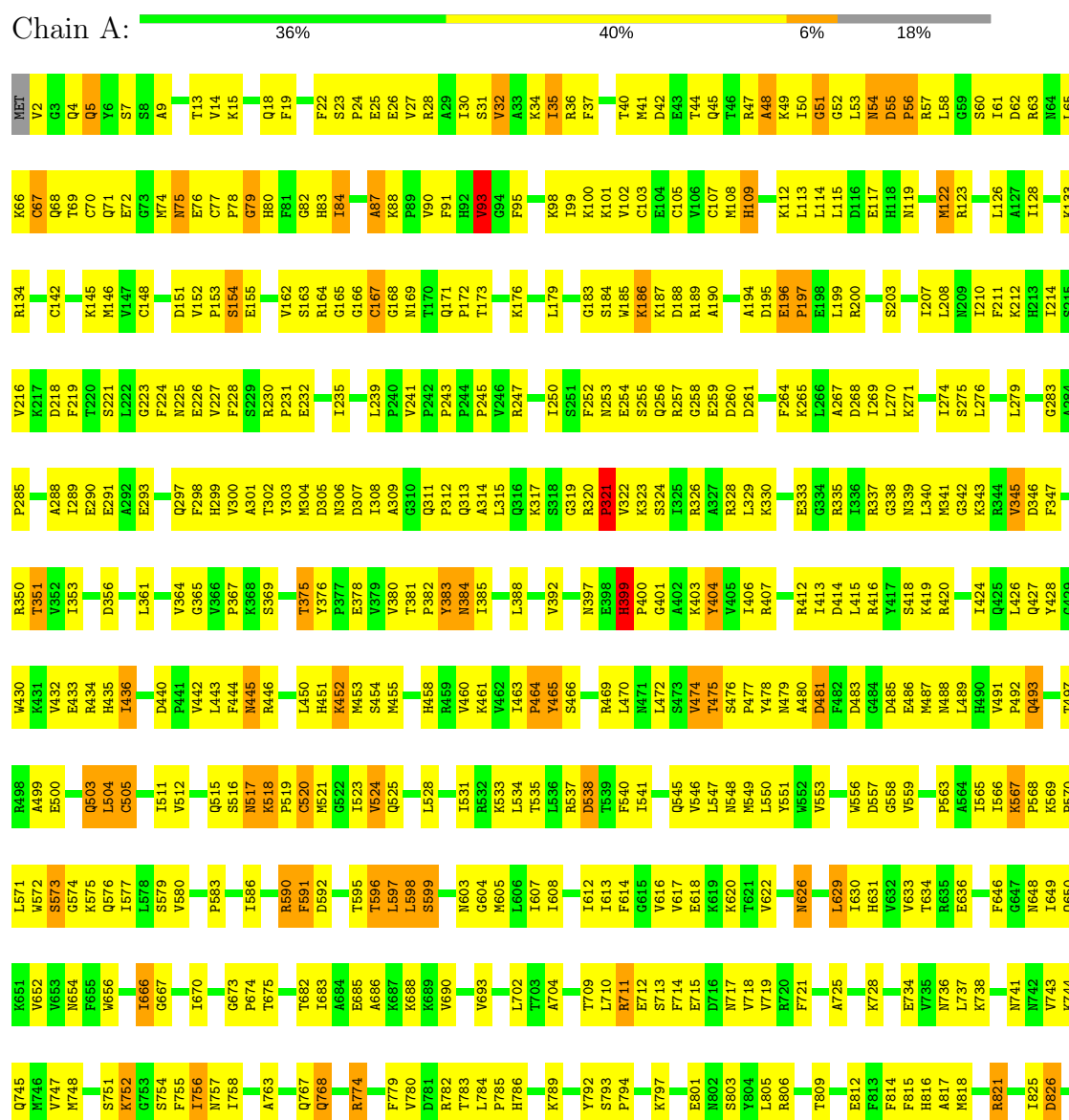
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

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

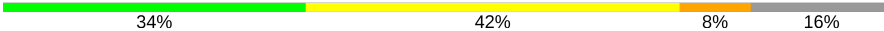
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

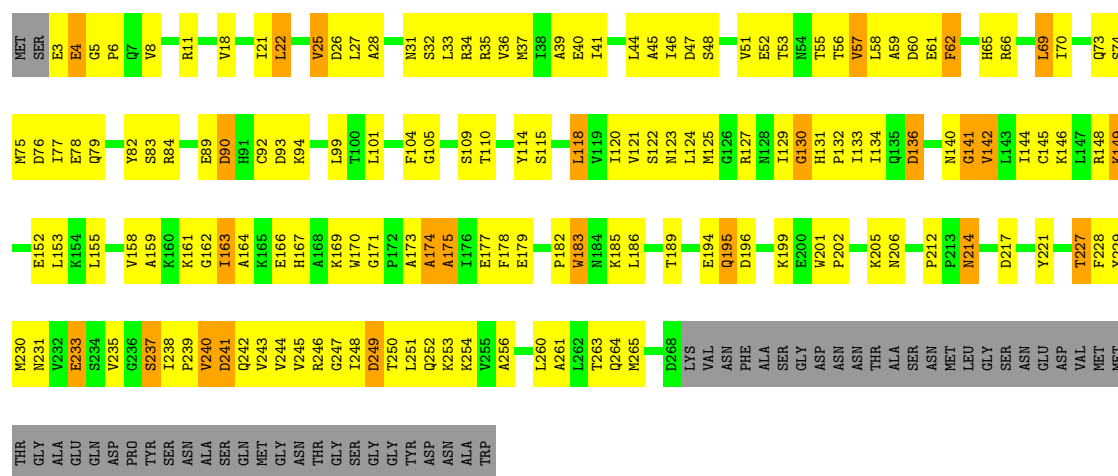


- Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE

R1222	F1146	T1077	M999	K934	Q862	A793	GLU	R654	R579	LYS	E437	Y351	T282	Y202	T136
D1223	L1147	K1078	P1000	R935	E863	N794	GLU	K655	V580	LEU	GLU	A352	V283	F203	Y137
F1224	K1148	G1079	F1001	D936	K864	L796	ASN	G656	F581	A509	ALA	K353	T284	I204	E138
	M1152	Q1084	A1003	S938	T871	Y797	LEU	I657	V585	P511	ASP	E359	T285	G206	ILE
	E1153	I1085	G1005	L941	E872	P799		K660	V586	R512	PHE	F360	R287	G207	ASP
	A1154	F1086	I1006	R942	T873	Q800	A726	L661	H587	Q513	ASN	L361	A288	S208	VAL
	D1156	F1087	V1007	S943	F874	R801		R662	G588	L514	MET	H363	E209	K209	PRO
	A1157	R1094	P1008	T944	R879	P802		T664	H590	H515	L446	L291	L291	V211	GLY
	F1158	L1095	E945	E946	T880	T805		E665	L596	T517	A447	T365	P293	L212	GLU
	R1159	L1096	N946	N947	N881	T806	R730	Y666	H597	H518	L448	Q366	D294	LEU	LEU
	V1160	H1097	G947	I948	L882	R807	S732	Q667	E598	G520	N449	L367	E295	E216	LYS
	H1161	M1098	M1013		R884	A808	H733	D668	T599	L521	A450	F370	E296	G220	TYR
	I1162	M1099	F1014	V952		M809	A735	I116	T599	V522	L453	L297	L297	G220	GLU
		D1100	H1015	L953	H887	E810	R736	GLU	L601	L522	L453	L298	N221	LEU	LEU
	I1165	D1101	A1016	V954	G888	Y811	T737	GLY	T602	Q531	T454	R373	E299	ILE	ILE
	C1166	G1167	I1017	T955	T889	L812	F738	GLY	L603	A532	S455	K374	H300	V225	ALA
	L1168	I1102	T956	T956	Y890	K813	T739	PHE	R604	G533	L461	A375	V305	F226	GLU
	M1169	H1104	S1019	N957	D891	R814	H740	GLU	R605	G534	A462	F377	N306	K228	SER
	T1170	A1105	Q958	Q958	K892	R815		ASP	L609	L535	T463	L378	D307	A229	GLU
	R1106	R1106	M1021	D959	L893	E816	I743	VAL	I609	V536	G464	K308	A230	A230	ASP
	V1171	T1022	G960	G960	G907	L817	H744		GLU	K537	N465	P231	L311	P231	ASP
	I1172	R1108	L961	L961	D896	R818	P745	E678	E512	M538	N466	L382	L311		SER
	A1173	G1109	K982	K982	G897	A819	S746	T679	V613		G467	L387	L314	I234	GLU
	K1174	P1110	F963	F963	L898	G820	M747	T680		L541	GLU	D391	K315	S235	SER
	L1175	E1028	N964	N964	L899	Q821	I748	W681	I616	M542	GLN	R392	P316	H236	GLY
	H1177	C1029	K965	K965	A900	N822		S682	D618		LYS	K393	C317	V237	K164
	V1178	L1030	V966	V966	P901	A823	V751	L684		L545	LYS	D392	D320	I240	F166
	Q1179	V1034	R969	R969	G902	T824		L685	I619	S546	ALA	K393	R241	R240	F166
	F1180	A1035	T970	T970	V903	W825	I755	L686		V547	MET	D394	G321	S242	G168
	E1181	R1036	R971	R971	R904	A826	I756	M686	E621	G548	SER	Q395	F322	S242	G168
	C1182	L1037	K972	K972	S906	T827	P757	E687		T549	SER	D396	A243	A243	R169
	G1183	E1041	P974	P974	G907	W830	P759	E688	L624	D550	ARG	D397	V323	L244	L170
	C1184	G1042	Q975	Q975	I911	N834	Q763	E690		P551	A477	R398	I324	P171	P171
	D1186	D1043	I976	I976	I912	Q835	S764	Y692	F627	M552	S480	G402	Q325	G247	I172
	M1187	A1044	G977	G977	G913	T840	P765	L693	T628	P553			D326	S248	M173
	I1194	S1045	D978	D978	K914	M841	P766	D694	G630	I554	L483	R405	T329	R249	R175
	H1195	P1046	K979	K979	T915	N842	T767	A695	R632	T556	N484	L408	A330	I251	N178
	I1196	I1050	F980	F980	T916	Q843	T768	E696	V633	F557	R485	L408	D332	S252	C179
	P1197	T1051	A981	A981	P917	S844	Q770	E697	R635	L568	Y486	A409	F333	T253	C179
		L1128	S982	S982	I918					S559	T487	F417	L334	L254	L181
	A1200	R1129	H983	H983	S919	S845	Q770	L701		G562	Y488	K418	G335	Y259	L181
	K1201	E1053	H984	H984	PR0	T846	M778	L702		M563	S490	F421	ARG	G260	T185
	Q1205	G1054	Q985	Q985	ASP	D847			F838	E564	S490	F421	ARG	R261	T185
	E1206	I1055	Q986	Q986	GLU	L850	V780	M705	I639	P565	H494	L424	GLY	R261	L189
	L1207	S1056	K987	K987	GLU	F851	L781	Q706	E641	L566	H494	L424	THR	R267	L190
		R1060	G988	G988	LEU	L854	L782	P707			R496	T425	ALA		
	M1210	C1137	T989	T989	GLY	F855	N784	D708	D642	Y569	T497	T425	LEU	L273	K193
	M1211	M1138	T990	T990	GLN	R856		D709	D643		T498	T425	GLY	P274	E194
	I1212	I1139	G991	G991	THR	R857		L710	E944	Q573	N499	F429	ILE	I276	C195
	A1140	A1140	S1066	S1066	ARG	R857		E711				R430	LYS	K277	P196
	R1215	H1141	R1067	R1067	ALA	S858		P712	K649	S574	I502	Y431	K345	E278	D198
		A1144	R995	R996	ALA	R859		ALA	E650	P575	ARG	M432	GLY	Q278	P196
	R1220	S1145	R996	R997	TYR	R860		GLU	L651	D576	ARG	T435	ALA	D279	D198
	S1221		D998	D998	HIS	M860		ALA	K652	P577	ASP	T436	R348	I280	G200
						D861		ASN	L652	T578	GLY	V436		G201	G200

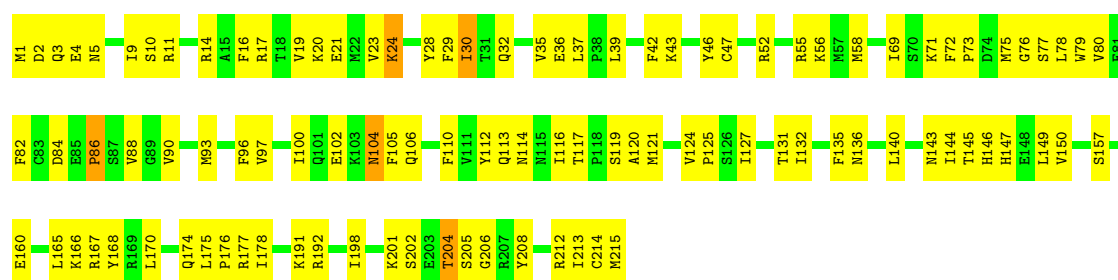
- Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

Chain C: 



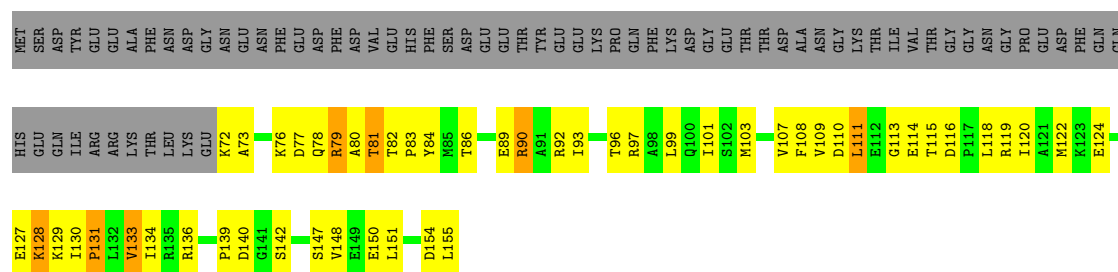
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

Chain E: 

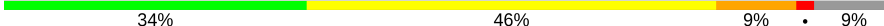


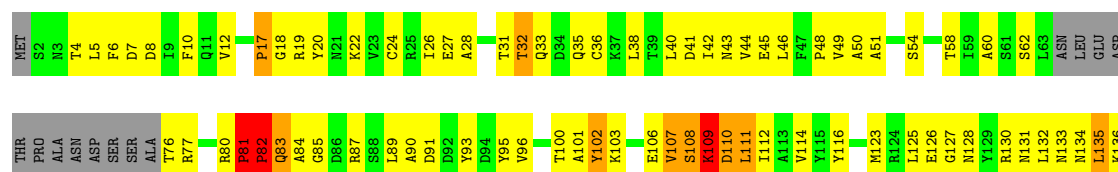
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F: 



• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

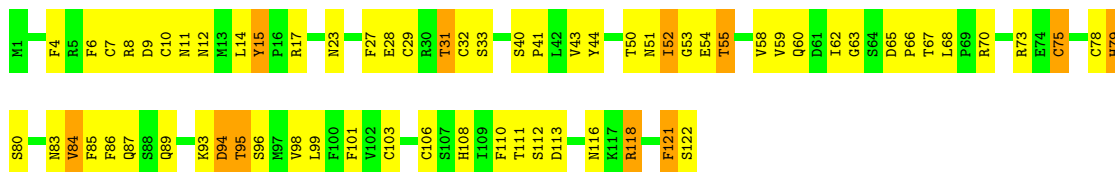
Chain H: 





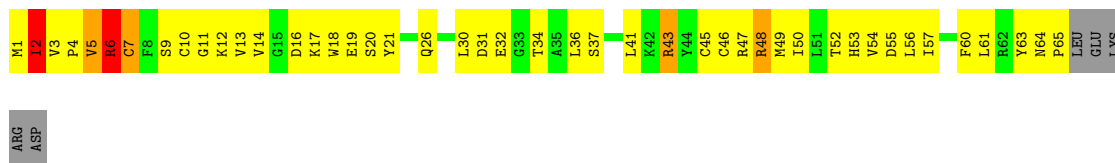
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I: 45% 46% 9%



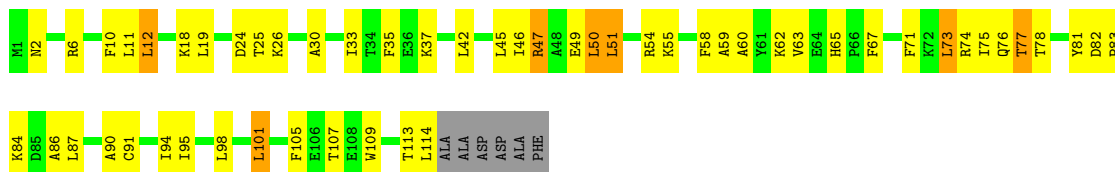
• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J: 29% 56% 6% 7%



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

Chain K: 50% 39% 6% 5%



• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

Chain L: 19% 34% 11% 34%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	130.70 Å 224.80 Å 369.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28161	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.40	1/11312 (0.0%)	0.70	2/15298 (0.0%)
2	B	0.40	0/8793	0.68	3/11857 (0.0%)
3	C	0.42	0/2133	0.72	1/2891 (0.0%)
4	E	0.37	0/1796	0.63	0/2416
5	F	0.42	0/691	0.66	0/933
6	H	0.59	2/1086 (0.2%)	0.91	6/1470 (0.4%)
7	I	0.41	0/1016	0.70	0/1365
8	J	0.43	0/541	0.85	1/727 (0.1%)
9	K	0.42	0/937	0.61	0/1265
10	L	0.41	0/366	0.66	0/485
All	All	0.41	3/28671 (0.0%)	0.70	13/38707 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	109	LYS	CD-CE	7.54	1.70	1.51
6	H	109	LYS	CE-NZ	5.69	1.63	1.49
1	A	520	CYS	CB-SG	-5.67	1.72	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	109	LYS	N-CA-C	7.39	130.95	111.00
1	A	452	LYS	N-CA-C	-6.74	92.80	111.00
6	H	109	LYS	CA-CB-CG	6.68	128.09	113.40
6	H	80	ARG	NE-CZ-NH1	-6.09	117.25	120.30
6	H	80	ARG	NE-CZ-NH2	5.97	123.28	120.30
2	B	1066	SER	N-CA-C	5.54	125.97	111.00
1	A	399	HIS	N-CA-C	5.53	125.93	111.00
3	C	183	TRP	N-CA-C	-5.49	96.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	819	ALA	N-CA-C	-5.44	96.31	111.00
2	B	937	ALA	N-CA-C	-5.36	96.54	111.00
8	J	5	VAL	N-CA-C	-5.28	96.74	111.00
6	H	81	PRO	N-CA-C	5.21	125.65	112.10
6	H	108	SER	CB-CA-C	5.17	119.92	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	11114	0	11193	945	0
2	B	8624	0	8642	736	1
3	C	2095	0	2051	177	0
4	E	1760	0	1788	103	0
5	F	679	0	701	56	0
6	H	1068	0	1040	93	0
7	I	997	0	955	71	0
8	J	532	0	542	78	0
9	K	919	0	929	62	0
10	L	364	0	388	47	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	1	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	1	0	0	0	0
All	All	28161	0	28229	2150	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 38.

All (2150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.59	1.17
7:I:111:THR:HG22	7:I:113:ASP:H	1.05	1.17
10:L:60:ARG:HG3	10:L:61:THR:H	1.04	1.12
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.32	1.11
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.06	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.24	1.09
1:A:47:ARG:HH22	1:A:255:SER:HA	1.13	1.08
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.26	1.08
1:A:308:ILE:HG22	1:A:309:ALA:H	1.13	1.07
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.32	1.07
1:A:381:THR:HG22	1:A:383:TYR:H	1.21	1.06
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.55	1.04
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.38	1.04
2:B:955:THR:HG22	2:B:956:THR:H	0.88	1.04
1:A:535:THR:HG21	1:A:617:VAL:H	1.23	1.04
2:B:806:THR:HG22	2:B:808:ALA:H	1.24	1.03
2:B:955:THR:HG22	2:B:956:THR:N	1.72	1.02
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.41	1.02
6:H:26:ILE:HD11	6:H:49:VAL:HG11	1.40	1.02
2:B:731:VAL:HG12	2:B:732:SER:H	1.26	1.01
10:L:60:ARG:CG	10:L:61:THR:H	1.72	1.01
1:A:313:GLN:HB2	1:A:320:ARG:HB3	1.42	1.01
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.42	1.01
2:B:405:ARG:NH1	2:B:632:ARG:HG2	1.75	1.00
2:B:955:THR:CG2	2:B:956:THR:H	1.70	1.00
1:A:40:THR:HG22	1:A:41:MET:HG3	1.40	1.00
2:B:708:GLU:HG3	2:B:709:ASP:H	1.27	0.99
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.98	0.97
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.27	0.97
2:B:871:THR:HG22	2:B:872:GLU:H	1.27	0.97
2:B:1165:ILE:HD12	2:B:1187:ASN:HD21	1.27	0.96
1:A:533:LYS:HE2	1:A:745:GLN:HE22	1.31	0.96
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.29	0.95
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.96	0.95
10:L:60:ARG:HG3	10:L:61:THR:N	1.79	0.95
1:A:869:GLY:O	4:E:204:THR:HG21	1.66	0.95
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.46	0.94
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.48	0.94
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.50	0.94
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.50	0.94
2:B:650:GLU:HG2	2:B:654:ARG:HH12	1.31	0.94
1:A:2:VAL:HG21	2:B:1157:ALA:HB3	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.96	0.93
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.49	0.93
2:B:642:ASP:HB3	2:B:649:LYS:HD3	1.51	0.93
1:A:849:MET:CE	1:A:1061:GLY:HA2	1.98	0.93
2:B:654:ARG:H	2:B:657:HIS:HD2	1.07	0.92
1:A:567:LYS:NZ	6:H:46:LEU:HB2	1.82	0.92
2:B:955:THR:HG23	10:L:54:ARG:O	1.68	0.92
2:B:680:THR:HG22	2:B:681:TRP:N	1.85	0.92
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.50	0.92
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.32	0.92
6:H:35:GLN:HB3	6:H:111:LEU:HD21	1.50	0.92
4:E:5:ASN:HD21	4:E:52:ARG:HG2	1.34	0.91
1:A:907:THR:HG22	1:A:908:LEU:H	1.36	0.91
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.51	0.90
2:B:174:LEU:O	2:B:175:ARG:HB2	1.69	0.90
1:A:1116:LEU:HD13	1:A:1311:VAL:HG13	1.53	0.90
2:B:345:LYS:HA	2:B:348:ARG:HE	1.35	0.90
6:H:109:LYS:CG	6:H:110:ASP:H	1.83	0.90
2:B:884:ARG:O	2:B:936:ASP:HB3	1.72	0.90
2:B:65:GLU:HG3	2:B:66:ASP:H	1.35	0.89
2:B:882:THR:HG21	2:B:935:ARG:HA	1.54	0.89
1:A:47:ARG:NH2	1:A:255:SER:HA	1.88	0.89
2:B:211:VAL:O	2:B:480:SER:HA	1.73	0.89
2:B:680:THR:HG22	2:B:681:TRP:H	1.37	0.89
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.21	0.89
2:B:801:LYS:O	8:J:52:THR:HG23	1.73	0.88
6:H:107:VAL:HG12	6:H:107:VAL:O	1.74	0.88
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.56	0.88
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.52	0.88
1:A:741:ASN:HD22	1:A:744:LYS:H	1.17	0.88
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.37	0.88
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.54	0.88
9:K:113:THR:O	9:K:114:LEU:HB2	1.73	0.87
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.55	0.87
2:B:311:LEU:HB3	7:I:4:PHE:HE2	1.40	0.87
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.09	0.87
5:F:111:LEU:H	5:F:111:LEU:HD12	1.38	0.87
6:H:4:THR:HA	6:H:60:ALA:HB2	1.57	0.87
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.90	0.86
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.55	0.86
1:A:313:GLN:CB	1:A:320:ARG:HB3	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:O	1:A:475:THR:HB	1.76	0.86
7:I:111:THR:HG22	7:I:113:ASP:N	1.89	0.85
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.77	0.85
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.57	0.85
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.59	0.84
1:A:32:VAL:HG21	1:A:68:GLN:NE2	1.91	0.84
1:A:1404:GLU:C	1:A:1406:VAL:H	1.80	0.84
1:A:590:ARG:HB3	1:A:605:MET:H	1.42	0.84
4:E:143:ASN:HB3	4:E:146:HIS:HD2	1.43	0.84
2:B:744:HIS:HD2	2:B:746:SER:H	1.25	0.84
2:B:363:HIS:O	2:B:364:ILE:HB	1.77	0.83
1:A:590:ARG:NH1	1:A:590:ARG:HG3	1.92	0.83
1:A:13:THR:HG23	1:A:1432:GLN:NE2	1.93	0.83
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.43	0.83
1:A:255:SER:O	1:A:256:GLN:HG3	1.78	0.83
2:B:559:SER:HA	2:B:563:MET:HB3	1.61	0.83
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.60	0.83
1:A:445:ASN:CB	1:A:455:MET:HG2	2.09	0.83
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.14	0.83
2:B:605:ARG:NH1	2:B:639:ILE:HD13	1.92	0.82
4:E:177:ARG:HD3	4:E:215:MET:SD	2.20	0.82
10:L:27:LEU:HD22	10:L:37:LYS:HD3	1.61	0.82
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	1.59	0.82
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.61	0.82
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.15	0.82
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.80	0.82
1:A:1329:THR:HG22	1:A:1331:SER:H	1.45	0.82
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.42	0.82
2:B:956:THR:HA	2:B:961:LEU:O	1.80	0.81
3:C:123:ASN:ND2	3:C:125:MET:HG2	1.95	0.81
2:B:542:MET:HE3	2:B:747:MET:HG3	1.62	0.81
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.60	0.81
1:A:412:ARG:NH2	2:B:1110:PRO:HD3	1.95	0.81
1:A:48:ALA:O	1:A:49:LYS:HG3	1.80	0.81
1:A:590:ARG:HB3	1:A:605:MET:N	1.95	0.81
1:A:315:LEU:HD12	1:A:321:PRO:HG2	1.60	0.81
6:H:89:LEU:C	6:H:91:ASP:H	1.82	0.81
3:C:174:ALA:O	8:J:10:CYS:HB2	1.81	0.80
10:L:54:ARG:HH11	10:L:54:ARG:HB2	1.46	0.80
1:A:308:ILE:HG22	1:A:309:ALA:N	1.95	0.80
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.45	0.80
8:J:32:GLU:CD	8:J:32:GLU:H	1.85	0.80
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.11	0.80
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.63	0.80
1:A:41:MET:HA	1:A:49:LYS:HA	1.64	0.80
2:B:680:THR:HG22	2:B:682:SER:H	1.45	0.80
3:C:134:ILE:HG12	3:C:141:GLY:HA3	1.64	0.80
7:I:17:ARG:HG3	7:I:28:GLU:HG2	1.64	0.80
1:A:650:GLN:O	1:A:654:ASN:HB2	1.82	0.80
1:A:913:LEU:HD12	1:A:914:GLU:H	1.46	0.79
2:B:1172:ILE:HD11	2:B:1183:LYS:HE2	1.65	0.79
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.11	0.79
10:L:55:ILE:HG13	10:L:56:LEU:H	1.47	0.79
2:B:871:THR:HG22	2:B:872:GLU:N	1.97	0.79
8:J:1:MET:N	8:J:56:LEU:HB2	1.97	0.79
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.22	0.79
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.63	0.79
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.17	0.79
2:B:54:PHE:HA	2:B:58:THR:HB	1.64	0.79
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.16	0.79
2:B:807:ARG:HG3	2:B:807:ARG:HH11	1.45	0.79
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.45	0.79
1:A:567:LYS:HB3	6:H:96:VAL:H	1.48	0.79
4:E:147:HIS:CD2	4:E:149:LEU:H	2.00	0.79
7:I:54:GLU:OE2	7:I:118:ARG:NH1	2.15	0.79
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.64	0.78
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.63	0.78
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.48	0.78
6:H:109:LYS:HG2	6:H:110:ASP:H	1.48	0.78
1:A:805:LEU:O	1:A:805:LEU:HD12	1.83	0.78
1:A:675:THR:HG21	1:A:736:ASN:ND2	1.97	0.78
1:A:1390:ASN:O	1:A:1391:ARG:HB2	1.84	0.78
1:A:535:THR:HG21	1:A:617:VAL:N	1.98	0.78
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.64	0.78
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.12	0.78
2:B:1002:THR:HG22	2:B:1006:ILE:N	1.99	0.77
2:B:601:ARG:O	2:B:605:ARG:HG3	1.82	0.77
1:A:524:VAL:HG12	1:A:525:GLN:H	1.48	0.77
2:B:991:GLY:O	2:B:992:ILE:HB	1.84	0.77
2:B:650:GLU:HG2	2:B:654:ARG:NH1	1.98	0.77
1:A:330:LYS:HA	1:A:333:GLU:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HD2	2:B:1220:ARG:HE	1.50	0.77
1:A:709:THR:HG22	1:A:711:ARG:H	1.48	0.77
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.31	0.77
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.99	0.77
1:A:675:THR:CG2	1:A:736:ASN:HD21	1.97	0.77
2:B:429:PHE:HA	2:B:432:MET:HE3	1.66	0.77
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.67	0.77
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.32	0.77
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.20	0.76
2:B:680:THR:CG2	2:B:681:TRP:H	1.97	0.76
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.20	0.76
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.67	0.76
3:C:66:ARG:NH2	8:J:5:VAL:HG23	2.00	0.76
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.67	0.76
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.50	0.76
2:B:702:LEU:CD2	2:B:737:THR:HG22	2.16	0.76
6:H:82:PRO:HG3	9:K:54:ARG:HG2	1.66	0.75
2:B:745:PRO:O	2:B:748:ILE:HG12	1.87	0.75
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.68	0.75
4:E:3:GLN:HG3	4:E:5:ASN:H	1.49	0.75
3:C:194:GLU:O	3:C:195:GLN:HG3	1.86	0.75
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.68	0.75
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.69	0.75
1:A:1431:GLY:HA2	2:B:1152:MET:CE	2.16	0.75
1:A:1399:ARG:O	1:A:1401:SER:N	2.20	0.75
1:A:1431:GLY:HA2	2:B:1152:MET:HE2	1.69	0.75
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.68	0.75
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.52	0.75
2:B:903:VAL:HG13	10:L:63:ARG:HH21	1.50	0.75
4:E:90:VAL:HA	4:E:120:ALA:HB2	1.67	0.75
1:A:567:LYS:HB3	6:H:96:VAL:N	2.02	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.21	0.74
1:A:1400:CYS:HB3	1:A:1405:THR:HG1	1.53	0.74
2:B:654:ARG:H	2:B:657:HIS:CD2	1.98	0.74
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.02	0.74
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.67	0.74
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.69	0.74
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.52	0.74
4:E:19:VAL:HG11	4:E:80:VAL:HG11	1.68	0.74
6:H:100:THR:HG23	6:H:138:GLU:HA	1.69	0.74
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:O	1:A:214:ILE:HG13	1.87	0.74
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.23	0.74
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.17	0.74
1:A:308:ILE:CG2	1:A:309:ALA:H	1.98	0.74
1:A:855:THR:HG21	1:A:857:ARG:HE	1.53	0.74
3:C:77:ILE:HD13	3:C:129:ILE:HD11	1.70	0.74
5:F:76:LYS:HA	5:F:79:ARG:HD2	1.69	0.74
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.69	0.74
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.69	0.74
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	1.87	0.73
1:A:219:PHE:HB3	1:A:224:PHE:HB2	1.69	0.73
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.69	0.73
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.69	0.73
2:B:737:THR:HG23	7:I:66:PRO:HB2	1.67	0.73
4:E:55:ARG:HB2	4:E:84:ASP:OD2	1.86	0.73
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.03	0.73
1:A:40:THR:HG23	1:A:54:ASN:OD1	1.89	0.73
2:B:487:THR:HG22	2:B:490:SER:H	1.53	0.73
4:E:17:ARG:O	4:E:21:GLU:HG3	1.88	0.73
2:B:120:ARG:CG	2:B:955:THR:HG21	2.18	0.73
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.70	0.73
2:B:35:SER:HA	2:B:811:TYR:HE2	1.53	0.73
1:A:1168:GLU:O	1:A:1172:LEU:HG	1.87	0.73
1:A:270:LEU:O	1:A:274:ILE:HG13	1.88	0.73
2:B:702:LEU:HD22	2:B:737:THR:HG22	1.71	0.73
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.71	0.72
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.18	0.72
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.19	0.72
2:B:879:ARG:HD2	2:B:883:LEU:HD22	1.68	0.72
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.87	0.72
1:A:317:LYS:HD2	1:A:321:PRO:HG3	1.72	0.72
1:A:31:SER:CB	1:A:83:HIS:HB2	2.19	0.72
2:B:680:THR:CG2	2:B:681:TRP:N	2.53	0.72
2:B:705:MET:H	2:B:710:LEU:HD12	1.54	0.72
6:H:109:LYS:CG	6:H:110:ASP:N	2.51	0.72
1:A:907:THR:HG22	1:A:908:LEU:N	2.05	0.72
2:B:98:THR:HG22	2:B:99:LYS:H	1.53	0.72
1:A:302:THR:OG1	1:A:312:PRO:HG3	1.90	0.72
1:A:590:ARG:HG2	1:A:604:GLY:HA2	1.72	0.72
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.72	0.72
2:B:737:THR:HG21	7:I:66:PRO:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG22	2:B:808:ALA:N	2.02	0.72
3:C:167:HIS:HD2	3:C:169:LYS:H	1.38	0.72
1:A:1370:LEU:HD12	1:A:1370:LEU:O	1.89	0.71
9:K:55:LYS:HD3	9:K:78:THR:HB	1.72	0.71
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.20	0.71
2:B:387:LEU:HD23	2:B:393:LYS:HD2	1.70	0.71
6:H:130:ARG:HB3	6:H:134:ASN:HD22	1.54	0.71
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.71	0.71
3:C:56:THR:HG22	3:C:58:LEU:H	1.54	0.71
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.25	0.71
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.10	0.71
2:B:234:ILE:H	2:B:234:ILE:HD12	1.55	0.71
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.73	0.71
4:E:43:LYS:O	4:E:47:CYS:HB2	1.91	0.71
1:A:535:THR:HG22	1:A:616:VAL:HA	1.72	0.71
1:A:61:ILE:HG22	1:A:62:ASP:H	1.56	0.71
2:B:654:ARG:N	2:B:657:HIS:HD2	1.86	0.71
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.73	0.71
1:A:901:LEU:HA	1:A:907:THR:HG23	1.72	0.71
1:A:1404:GLU:C	1:A:1406:VAL:N	2.40	0.71
2:B:709:ASP:O	2:B:710:LEU:HD23	1.89	0.71
2:B:642:ASP:O	2:B:644:GLU:N	2.24	0.71
2:B:25:ILE:HD11	2:B:653:VAL:O	1.91	0.71
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.05	0.71
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.06	0.71
1:A:913:LEU:HD12	1:A:914:GLU:N	2.06	0.71
9:K:65:HIS:HD2	9:K:67:PHE:H	1.37	0.71
1:A:434:ARG:HG3	1:A:435:HIS:O	1.91	0.70
1:A:57:ARG:HB3	1:A:68:GLN:HG3	1.72	0.70
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.72	0.70
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.06	0.70
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.71	0.70
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.06	0.70
1:A:535:THR:CG2	1:A:616:VAL:HA	2.21	0.70
2:B:58:THR:O	2:B:62:ILE:HG13	1.91	0.70
2:B:821:GLN:OE1	2:B:850:LEU:HD12	1.91	0.70
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.73	0.70
3:C:76:ASP:O	3:C:79:GLN:HG2	1.91	0.70
1:A:1189:SER:HB2	1:A:1190:PRO:HD2	1.73	0.70
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.57	0.70
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LEU:HB2	4:E:206:GLY:N	2.05	0.70
9:K:55:LYS:HD3	9:K:78:THR:CB	2.22	0.70
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.72	0.70
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.73	0.70
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.52	0.70
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.40	0.70
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.25	0.70
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.73	0.69
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.72	0.69
2:B:864:LYS:HD3	2:B:871:THR:HA	1.74	0.69
3:C:241:ASP:O	3:C:245:VAL:HG23	1.92	0.69
5:F:77:ASP:O	5:F:78:GLN:HB2	1.91	0.69
2:B:46:GLN:HG3	2:B:47:GLN:N	2.07	0.69
4:E:147:HIS:HD2	4:E:149:LEU:H	1.37	0.69
2:B:639:ILE:HD11	2:B:691:GLU:CG	2.16	0.69
1:A:711:ARG:HH12	7:I:95:THR:HG22	1.56	0.69
1:A:853:ASP:OD1	1:A:855:THR:HB	1.92	0.69
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.23	0.69
2:B:46:GLN:HG3	2:B:47:GLN:H	1.57	0.69
2:B:889:THR:HG22	2:B:891:ASP:H	1.55	0.69
5:F:81:THR:CG2	5:F:136:ARG:HH11	2.05	0.69
2:B:827:ILE:HD13	2:B:1017:ILE:HD11	1.73	0.69
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.58	0.69
1:A:1111:MET:HE1	1:A:1114:PRO:HA	1.75	0.69
1:A:367:PRO:HB3	1:A:466:SER:HA	1.75	0.69
1:A:751:SER:O	1:A:752:LYS:HB2	1.91	0.69
1:A:919:ILE:HD13	1:A:983:ILE:HD12	1.74	0.69
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.75	0.69
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.08	0.69
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.22	0.69
1:A:757:ASN:OD1	2:B:1021:MET:HE2	1.94	0.68
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.76	0.68
1:A:57:ARG:HB3	1:A:68:GLN:CG	2.23	0.68
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.23	0.68
6:H:111:LEU:HA	6:H:127:GLY:O	1.93	0.68
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.76	0.68
1:A:1400:CYS:HB3	1:A:1405:THR:OG1	1.93	0.68
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.23	0.68
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.23	0.68
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.75	0.68
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLY:H	2:B:298:LEU:HG	1.58	0.68
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.08	0.68
8:J:16:ASP:OD1	8:J:17:LYS:HG3	1.93	0.68
1:A:4:GLN:O	1:A:5:GLN:HB2	1.94	0.68
1:A:579:SER:OG	1:A:612:ILE:HG22	1.94	0.68
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.76	0.68
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.59	0.68
1:A:1039:LYS:O	1:A:1043:ASP:HB2	1.94	0.68
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.59	0.68
1:A:187:LYS:O	1:A:188:ASP:HB2	1.93	0.68
1:A:80:HIS:O	1:A:243:PRO:HB3	1.94	0.68
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.59	0.68
1:A:108:MET:O	1:A:109:HIS:HB2	1.93	0.67
1:A:1258:HIS:ND1	1:A:1262:LYS:HE3	2.09	0.67
1:A:185:TRP:O	1:A:186:LYS:HB2	1.93	0.67
1:A:741:ASN:ND2	1:A:744:LYS:H	1.92	0.67
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.29	0.67
1:A:913:LEU:HD11	1:A:981:LEU:O	1.95	0.67
3:C:66:ARG:CZ	8:J:5:VAL:HG23	2.24	0.67
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.23	0.67
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.94	0.67
1:A:982:THR:HG22	1:A:984:LYS:H	1.58	0.67
1:A:265:LYS:O	1:A:269:ILE:HG13	1.94	0.67
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.77	0.67
2:B:707:PRO:HG2	2:B:708:GLU:H	1.58	0.67
3:C:166:GLU:HG3	9:K:10:PHE:CZ	2.29	0.67
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.76	0.67
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.75	0.67
2:B:871:THR:CG2	2:B:872:GLU:H	2.05	0.67
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.29	0.67
2:B:995:ARG:HB3	2:B:997:GLU:OE2	1.94	0.67
1:A:474:VAL:HG13	1:A:478:TYR:CE1	2.29	0.67
1:A:879:GLU:O	1:A:955:PRO:HA	1.94	0.67
1:A:1422:ARG:HG2	2:B:1220:ARG:NH1	2.10	0.67
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.10	0.67
3:C:56:THR:HG22	3:C:57:VAL:N	2.09	0.67
4:E:29:PHE:O	4:E:30:ILE:HG13	1.94	0.67
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.75	0.67
1:A:31:SER:OG	1:A:83:HIS:HB2	1.94	0.67
6:H:12:VAL:HA	6:H:28:ALA:CB	2.25	0.67
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG22	2:B:884:ARG:H	1.60	0.67
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.77	0.67
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.25	0.66
2:B:780:VAL:HG21	8:J:56:LEU:HD11	1.76	0.66
2:B:392:ARG:NH2	7:I:52:ILE:HD11	2.10	0.66
7:I:111:THR:HG22	7:I:112:SER:N	2.10	0.66
1:A:711:ARG:NH1	7:I:95:THR:HG22	2.10	0.66
2:B:825:VAL:HG12	2:B:826:ALA:N	2.11	0.66
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.24	0.66
1:A:711:ARG:HH12	7:I:95:THR:CG2	2.07	0.66
1:A:345:VAL:HG11	2:B:1128:LEU:O	1.95	0.66
2:B:1166:CYS:O	2:B:1168:LEU:N	2.27	0.66
2:B:345:LYS:HA	2:B:348:ARG:NE	2.10	0.66
2:B:731:VAL:HG12	2:B:732:SER:N	2.04	0.66
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.94	0.66
1:A:1114:PRO:O	1:A:1115:SER:HB3	1.94	0.66
1:A:32:VAL:HB	1:A:57:ARG:HB2	1.77	0.66
2:B:165:VAL:HG13	2:B:446:LEU:HD21	1.76	0.66
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.76	0.66
10:L:60:ARG:CG	10:L:61:THR:N	2.45	0.66
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.76	0.66
1:A:709:THR:HB	1:A:712:GLU:HG3	1.77	0.66
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.76	0.66
2:B:542:MET:CE	2:B:747:MET:HG3	2.24	0.66
1:A:540:PHE:C	1:A:541:ILE:HD12	2.16	0.66
2:B:108:VAL:HG12	2:B:109:THR:H	1.60	0.66
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.25	0.66
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.77	0.66
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.11	0.66
1:A:806:ARG:HH12	2:B:729:ILE:HD11	1.61	0.66
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.78	0.66
2:B:515:HIS:CD2	2:B:517:THR:H	2.14	0.66
2:B:712:PRO:HD3	2:B:733:HIS:CD2	2.31	0.66
3:C:124:LEU:O	3:C:127:ARG:HG2	1.94	0.66
2:B:118:ARG:NH1	2:B:204:ILE:HD11	2.10	0.65
6:H:5:LEU:HB3	6:H:133:ASN:O	1.96	0.65
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.78	0.65
1:A:590:ARG:O	1:A:591:PHE:HB2	1.96	0.65
1:A:675:THR:CG2	1:A:736:ASN:ND2	2.59	0.65
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.79	0.65
1:A:783:THR:HG22	1:A:784:LEU:HG	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:SER:OG	5:F:150:GLU:HG3	1.96	0.65
1:A:24:PRO:HG2	1:A:25:GLU:OE2	1.96	0.65
1:A:74:MET:O	1:A:75:ASN:HB2	1.95	0.65
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.21	0.65
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.32	0.65
1:A:515:GLN:HG3	1:A:516:SER:N	2.12	0.65
2:B:378:LEU:O	2:B:382:ILE:HG13	1.97	0.65
1:A:1025:ARG:HD2	1:A:1030:ARG:HH12	1.61	0.65
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.78	0.65
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.32	0.65
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.78	0.65
4:E:46:TYR:CD2	4:E:58:MET:HG2	2.31	0.65
8:J:53:HIS:CD2	8:J:54:VAL:N	2.64	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.77	0.65
2:B:549:THR:HB	2:B:628:THR:HG22	1.78	0.65
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.79	0.65
4:E:69:ILE:HG23	4:E:73:PRO:HA	1.78	0.65
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.77	0.65
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.45	0.65
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.79	0.65
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.78	0.65
3:C:3:GLU:O	3:C:4:GLU:HB2	1.96	0.65
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.10	0.64
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.79	0.64
2:B:205:ILE:CD1	2:B:461:LEU:HB3	2.27	0.64
2:B:619:ILE:HD12	7:I:65:ASP:HB2	1.78	0.64
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.79	0.64
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.60	0.64
1:A:313:GLN:O	1:A:321:PRO:HD2	1.97	0.64
1:A:901:LEU:HD13	1:A:919:ILE:HG23	1.78	0.64
8:J:3:VAL:CG2	8:J:18:TRP:HB2	2.26	0.64
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.79	0.64
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.80	0.64
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.28	0.64
1:A:1113:THR:HG22	1:A:1113:THR:O	1.97	0.64
1:A:737:LEU:HD11	1:A:758:ILE:HG21	1.78	0.64
2:B:1002:THR:CG2	2:B:1006:ILE:H	2.10	0.64
3:C:244:VAL:O	3:C:248:ILE:HG13	1.98	0.64
1:A:337:ARG:HH22	1:A:1403:GLU:HA	1.61	0.64
1:A:451:HIS:O	2:B:1137:CYS:SG	2.54	0.64
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLN:NE2	2:B:496:ARG:HD3	2.13	0.64
3:C:175:ALA:HB2	8:J:10:CYS:HB2	1.80	0.64
1:A:65:LEU:O	1:A:71:GLN:HA	1.97	0.64
2:B:912:ILE:O	2:B:938:SER:HB2	1.97	0.64
1:A:1293:SER:OG	1:A:1295:THR:HG22	1.98	0.64
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.63
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.33	0.63
9:K:18:LYS:NZ	9:K:37:LYS:HB2	2.12	0.63
9:K:47:ARG:HG3	9:K:60:ALA:HA	1.79	0.63
1:A:122:MET:O	1:A:126:LEU:HG	1.98	0.63
1:A:311:GLN:HG2	1:A:313:GLN:HG3	1.80	0.63
1:A:58:LEU:HD22	1:A:80:HIS:O	1.99	0.63
6:H:106:GLU:C	6:H:108:SER:H	2.02	0.63
1:A:15:LYS:O	1:A:1421:CYS:HB2	1.98	0.63
1:A:100:LYS:HE2	1:A:176:LYS:HB2	1.79	0.63
1:A:305:ASP:OD1	1:A:306:ASN:N	2.32	0.63
1:A:49:LYS:CB	1:A:55:ASP:HB2	2.27	0.63
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.80	0.63
1:A:973:ILE:HG21	1:A:1036:ARG:O	1.97	0.63
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.34	0.63
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.27	0.63
1:A:1399:ARG:C	1:A:1401:SER:H	2.01	0.63
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.62	0.63
2:B:287:ARG:NH2	2:B:325:GLN:HE22	1.97	0.63
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.38	0.63
2:B:545:ILE:HG22	2:B:546:SER:O	1.98	0.63
2:B:35:SER:HA	2:B:811:TYR:CE2	2.32	0.63
3:C:33:LEU:HG	3:C:37:MET:CE	2.28	0.63
6:H:36:CYS:HA	6:H:126:GLU:O	1.99	0.63
8:J:57:ILE:O	8:J:61:LEU:HG	1.98	0.63
1:A:350:ARG:HD2	1:A:488:ASN:OD1	1.98	0.63
2:B:90:ILE:HA	2:B:133:LYS:O	1.99	0.63
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.79	0.63
5:F:111:LEU:H	5:F:111:LEU:CD1	2.11	0.63
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.80	0.63
1:A:567:LYS:NZ	6:H:46:LEU:CB	2.61	0.63
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.97	0.63
1:A:225:ASN:O	1:A:226:GLU:HG2	1.99	0.63
1:A:340:LEU:HD22	1:A:1425:SER:HB2	1.79	0.63
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.63
1:A:470:LEU:HD13	1:A:474:VAL:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:ALA:HB3	3:C:170:TRP:NE1	2.14	0.63
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.81	0.63
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.31	0.63
2:B:834:ASN:O	2:B:1013:ASN:HB2	1.99	0.63
1:A:98:LYS:NZ	1:A:1411:GLU:HG2	2.14	0.62
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.80	0.62
1:A:847:ASP:OD2	1:A:858:ASN:HB2	1.99	0.62
2:B:484:ASN:OD1	2:B:486:TYR:HE1	1.80	0.62
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.79	0.62
3:C:141:GLY:O	3:C:142:VAL:HB	1.98	0.62
3:C:66:ARG:NH2	8:J:3:VAL:O	2.32	0.62
1:A:173:THR:O	1:A:183:GLY:HA2	2.00	0.62
1:A:535:THR:O	1:A:575:LYS:HE3	1.99	0.62
2:B:515:HIS:HD2	2:B:517:THR:H	1.44	0.62
2:B:541:LEU:CB	2:B:747:MET:HE3	2.26	0.62
3:C:99:LEU:CD2	3:C:120:ILE:HG12	2.27	0.62
1:A:90:VAL:HG12	1:A:91:PHE:N	2.13	0.62
3:C:73:GLN:HE21	3:C:75:MET:H	1.44	0.62
6:H:138:GLU:HG2	6:H:139:ASN:N	2.13	0.62
1:A:100:LYS:NZ	1:A:176:LYS:HD2	2.13	0.62
1:A:605:MET:HE3	1:A:612:ILE:HG13	1.80	0.62
1:A:927:VAL:O	1:A:931:GLU:HG3	2.00	0.62
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.82	0.62
1:A:1333:ILE:O	1:A:1337:GLU:HG3	1.99	0.62
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.28	0.62
2:B:1166:CYS:HB2	2:B:1215:ARG:NH1	2.14	0.62
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.80	0.62
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.64	0.62
2:B:1185:CYS:O	2:B:1186:ASP:HB2	1.98	0.62
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.80	0.62
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.30	0.62
1:A:337:ARG:HH22	1:A:1403:GLU:CA	2.12	0.62
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.29	0.62
2:B:708:GLU:HG3	2:B:709:ASP:N	2.08	0.62
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.82	0.62
4:E:113:GLN:C	4:E:114:ASN:HD22	2.02	0.62
8:J:1:MET:H1	8:J:56:LEU:HB2	1.64	0.62
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.82	0.62
2:B:636:PRO:HA	2:B:691:GLU:O	2.00	0.62
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.12	0.62
1:A:88:LYS:HD2	1:A:293:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.64	0.62
3:C:235:VAL:HG13	8:J:13:VAL:HG23	1.81	0.62
4:E:192:ARG:HB2	4:E:215:MET:O	1.99	0.62
6:H:43:ASN:OD1	6:H:45:GLU:HB3	2.00	0.62
7:I:32:CYS:HG	11:I:2003:ZN:ZN	1.14	0.62
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.82	0.61
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.81	0.61
3:C:93:ASP:O	3:C:127:ARG:NH2	2.32	0.61
7:I:111:THR:CG2	7:I:112:SER:N	2.62	0.61
3:C:175:ALA:HB3	8:J:43:ARG:CZ	2.29	0.61
1:A:367:PRO:HB3	1:A:465:TYR:O	2.00	0.61
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.32	0.61
1:A:743:VAL:O	1:A:747:VAL:HG23	2.01	0.61
2:B:705:MET:H	2:B:710:LEU:CD1	2.13	0.61
9:K:55:LYS:O	9:K:77:THR:HG22	2.00	0.61
1:A:1025:ARG:HD2	1:A:1030:ARG:NH1	2.15	0.61
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.35	0.61
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.81	0.61
1:A:381:THR:HG22	1:A:383:TYR:N	2.06	0.61
1:A:596:THR:O	1:A:598:LEU:N	2.32	0.61
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.82	0.61
2:B:787:VAL:O	2:B:787:VAL:HG12	2.00	0.61
1:A:1120:LEU:HB3	1:A:1124:HIS:O	2.00	0.61
1:A:709:THR:HG21	7:I:93:LYS:O	2.00	0.61
2:B:315:LYS:N	2:B:316:PRO:HD2	2.15	0.61
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.34	0.61
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.83	0.61
2:B:860:MET:HG2	2:B:861:ASP:N	2.15	0.61
6:H:26:ILE:HD11	6:H:49:VAL:CG1	2.26	0.61
6:H:36:CYS:SG	6:H:130:ARG:NH2	2.73	0.61
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.36	0.61
10:L:38:LEU:O	10:L:39:SER:HB3	2.00	0.61
4:E:131:THR:HG21	4:E:191:LYS:HE2	1.82	0.61
10:L:43:THR:O	10:L:43:THR:HG22	2.01	0.61
1:A:252:PHE:HB2	1:A:256:GLN:OE1	2.00	0.61
1:A:646:PHE:O	1:A:650:GLN:HG3	2.00	0.61
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.82	0.61
7:I:78:CYS:O	7:I:80:SER:N	2.33	0.61
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.15	0.61
1:A:1116:LEU:CD1	1:A:1311:VAL:HG13	2.29	0.61
1:A:19:PHE:O	1:A:1416:ALA:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.82	0.61
1:A:786:HIS:CD2	1:A:786:HIS:N	2.66	0.61
2:B:970:THR:HG22	2:B:971:THR:N	2.14	0.61
3:C:242:GLN:OE1	3:C:242:GLN:HA	1.99	0.61
3:C:37:MET:HG2	3:C:243:VAL:HG12	1.83	0.61
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.36	0.61
6:H:26:ILE:CD1	6:H:49:VAL:HG11	2.22	0.61
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.83	0.61
4:E:2:ASP:O	4:E:3:GLN:HG2	2.01	0.61
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.36	0.61
6:H:4:THR:HA	6:H:60:ALA:CB	2.30	0.61
2:B:1183:LYS:O	2:B:1185:CYS:N	2.29	0.61
2:B:708:GLU:O	2:B:710:LEU:N	2.34	0.61
3:C:133:ILE:HD12	3:C:237:SER:HA	1.83	0.61
6:H:139:ASN:O	6:H:140:ALA:HB2	2.01	0.61
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.30	0.61
1:A:151:ASP:HA	1:A:162:VAL:O	2.01	0.60
1:A:50:ILE:C	1:A:52:GLY:H	2.04	0.60
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.47	0.60
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.83	0.60
6:H:82:PRO:O	6:H:84:ALA:N	2.34	0.60
9:K:18:LYS:HZ1	9:K:37:LYS:HB2	1.66	0.60
9:K:55:LYS:HD3	9:K:78:THR:OG1	2.01	0.60
1:A:313:GLN:HA	1:A:322:VAL:HG23	1.83	0.60
1:A:470:LEU:HD21	1:A:487:MET:CE	2.31	0.60
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.83	0.60
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.84	0.60
5:F:82:THR:HG22	5:F:84:TYR:H	1.66	0.60
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.82	0.60
1:A:537:ARG:HB2	6:H:20:TYR:CE2	2.36	0.60
1:A:844:ALA:HB2	1:A:1384:VAL:CG1	2.31	0.60
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.36	0.60
1:A:35:ILE:HD11	1:A:241:VAL:HG11	1.82	0.60
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.31	0.60
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.83	0.60
2:B:1051:THR:CG2	2:B:1053:GLU:H	2.14	0.60
2:B:807:ARG:HG3	2:B:807:ARG:NH1	2.17	0.60
7:I:121:PHE:O	7:I:122:SER:HB3	2.01	0.60
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.16	0.60
1:A:353:ILE:HD13	1:A:487:MET:CE	2.30	0.60
2:B:135:ARG:O	2:B:136:THR:CB	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.32	0.60
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.83	0.60
8:J:48:ARG:HE	8:J:49:MET:HE2	1.66	0.60
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.83	0.60
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.66	0.60
1:A:857:ARG:HD3	1:A:861:GLY:O	2.02	0.60
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.67	0.60
2:B:363:HIS:O	2:B:364:ILE:CB	2.49	0.60
4:E:32:GLN:HE21	4:E:36:GLU:HG3	1.67	0.60
6:H:18:GLY:O	6:H:19:ARG:HB2	2.02	0.60
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.84	0.60
8:J:45:CYS:O	8:J:48:ARG:HG3	2.01	0.60
9:K:46:ILE:HG22	9:K:50:LEU:CD1	2.29	0.60
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.37	0.60
2:B:914:LYS:HB3	2:B:937:ALA:O	2.01	0.60
3:C:75:MET:HG2	3:C:246:ARG:HH22	1.67	0.60
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.02	0.59
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.84	0.59
2:B:575:PRO:HG2	2:B:576:ASP:H	1.66	0.59
2:B:25:ILE:HD11	2:B:653:VAL:C	2.21	0.59
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.84	0.59
4:E:46:TYR:CE2	4:E:58:MET:HA	2.37	0.59
1:A:184:SER:HB3	1:A:199:LEU:CD2	2.32	0.59
1:A:190:ALA:HA	1:A:195:ASP:OD1	2.02	0.59
2:B:640:VAL:O	2:B:641:GLU:C	2.40	0.59
5:F:109:VAL:CG2	5:F:124:GLU:HG2	2.32	0.59
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.59
1:A:913:LEU:CD1	1:A:981:LEU:O	2.50	0.59
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.84	0.59
3:C:260:LEU:O	3:C:263:THR:HB	2.01	0.59
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.01	0.59
1:A:230:ARG:HB3	1:A:232:GLU:HG2	1.85	0.59
1:A:32:VAL:HG11	1:A:68:GLN:OE1	2.02	0.59
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.65	0.59
5:F:81:THR:HG22	5:F:82:THR:N	2.17	0.59
7:I:50:THR:HG22	7:I:51:ASN:N	2.17	0.59
1:A:34:LYS:HD2	1:A:36:ARG:NH2	2.17	0.59
1:A:465:TYR:CD1	1:A:465:TYR:N	2.71	0.59
2:B:1220:ARG:O	2:B:1222:ARG:N	2.34	0.59
2:B:733:HIS:O	2:B:735:ALA:N	2.35	0.59
1:A:1400:CYS:CB	1:A:1405:THR:HG1	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD11	1:A:485:ASP:HB2	1.83	0.59
1:A:741:ASN:HD22	1:A:744:LYS:N	1.96	0.59
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.20	0.59
2:B:429:PHE:HA	2:B:432:MET:CE	2.30	0.59
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.38	0.59
1:A:1004:ASN:CG	4:E:167:ARG:HD2	2.22	0.59
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.85	0.59
3:C:166:GLU:HG3	9:K:10:PHE:CE2	2.37	0.59
1:A:388:LEU:O	1:A:392:VAL:HG23	2.02	0.59
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.37	0.59
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.85	0.59
2:B:847:ASP:O	3:C:65:HIS:HE1	1.85	0.59
6:H:38:LEU:HD13	6:H:125:LEU:CD1	2.31	0.59
1:A:862:ASN:HA	4:E:174:GLN:HB3	1.85	0.59
8:J:1:MET:H3	8:J:56:LEU:HB2	1.68	0.59
9:K:47:ARG:HD2	9:K:51:LEU:HD22	1.83	0.59
1:A:49:LYS:HD3	1:A:54:ASN:O	2.03	0.59
1:A:528:LEU:HD23	1:A:751:SER:HB3	1.85	0.59
2:B:555:ILE:HD13	2:B:587:HIS:NE2	2.18	0.59
2:B:770:GLN:HB2	2:B:985:GLY:H	1.66	0.59
5:F:118:LEU:O	5:F:122:MET:HG3	2.03	0.59
1:A:548:ASN:OD1	9:K:60:ALA:HB1	2.03	0.59
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.85	0.59
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.85	0.59
2:B:871:THR:O	2:B:917:PRO:HD2	2.02	0.59
5:F:111:LEU:N	5:F:111:LEU:HD12	2.14	0.59
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.42	0.59
10:L:47:ARG:HG2	10:L:52:GLY:HA2	1.85	0.59
1:A:1436:ILE:O	1:A:1437:GLY:C	2.41	0.58
1:A:533:LYS:HE2	1:A:745:GLN:NE2	2.13	0.58
2:B:1148:LYS:HG2	2:B:1152:MET:HE3	1.85	0.58
2:B:1162:ILE:CD1	2:B:1194:ILE:HD13	2.32	0.58
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.31	0.58
3:C:32:SER:O	3:C:36:VAL:HG23	2.03	0.58
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.66	0.58
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.85	0.58
2:B:841:MET:HG3	2:B:1010:LEU:HD12	1.84	0.58
2:B:405:ARG:HH11	2:B:632:ARG:HG2	1.60	0.58
2:B:976:ILE:O	2:B:990:ILE:O	2.20	0.58
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.38	0.58
3:C:145:CYS:SG	3:C:146:LYS:N	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:102:TYR:O	6:H:103:LYS:HG3	2.03	0.58
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.69	0.58
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.56	0.58
1:A:1144:LYS:HG3	1:A:1268:LEU:O	2.03	0.58
1:A:337:ARG:NH2	1:A:1403:GLU:HA	2.18	0.58
1:A:686:ALA:O	1:A:690:VAL:HG23	2.04	0.58
1:A:68:GLN:HE22	1:A:80:HIS:CB	2.16	0.58
2:B:680:THR:HG22	2:B:682:SER:N	2.18	0.58
2:B:879:ARG:HH11	2:B:883:LEU:HB3	1.67	0.58
1:A:537:ARG:HB2	6:H:20:TYR:HE2	1.68	0.58
10:L:49:LYS:O	10:L:50:ASP:HB2	2.03	0.58
1:A:184:SER:HB3	1:A:199:LEU:HD21	1.85	0.58
2:B:1139:ILE:HG13	2:B:1147:LEU:HD11	1.85	0.58
3:C:22:LEU:O	3:C:227:THR:HA	2.04	0.58
4:E:157:SER:OG	4:E:160:GLU:HG3	2.04	0.58
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.85	0.58
7:I:40:SER:HB2	7:I:41:PRO:HD2	1.86	0.58
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	2.19	0.58
2:B:100:PRO:HA	2:B:125:SER:O	2.03	0.58
9:K:82:ASP:OD1	9:K:84:LYS:HG3	2.04	0.58
1:A:474:VAL:O	1:A:477:PRO:HD2	2.03	0.58
2:B:234:ILE:N	2:B:234:ILE:HD12	2.19	0.58
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.69	0.58
2:B:1177:HIS:HB2	2:B:1179:GLN:HG3	1.86	0.58
8:J:7:CYS:SG	8:J:49:MET:HE3	2.44	0.58
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.04	0.58
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.01	0.58
1:A:225:ASN:HD22	1:A:228:PHE:HD1	1.51	0.58
1:A:567:LYS:HE3	6:H:46:LEU:CD1	2.34	0.58
1:A:1424:VAL:HA	1:A:1434:ALA:HB2	1.85	0.57
2:B:1060:ARG:O	2:B:1060:ARG:HD2	2.04	0.57
2:B:542:MET:HG3	2:B:747:MET:HE1	1.86	0.57
2:B:859:TYR:CD1	2:B:859:TYR:N	2.72	0.57
1:A:1138:ILE:CG2	1:A:1279:ILE:HG21	2.34	0.57
1:A:1376:THR:O	1:A:1378:GLN:N	2.37	0.57
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.85	0.57
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.34	0.57
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.04	0.57
2:B:780:VAL:CG2	2:B:799:PRO:HG2	2.34	0.57
3:C:51:VAL:HG11	3:C:60:ASP:OD2	2.03	0.57
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.40	0.57
10:L:27:LEU:HD13	10:L:37:LYS:CB	2.34	0.57
1:A:151:ASP:OD1	1:A:163:SER:HA	2.05	0.57
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.18	0.57
1:A:713:SER:O	1:A:717:ASN:ND2	2.38	0.57
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.35	0.57
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.45	0.57
2:B:43:LEU:HD11	2:B:811:TYR:O	2.05	0.57
5:F:77:ASP:O	5:F:78:GLN:CB	2.52	0.57
7:I:8:ARG:O	7:I:9:ASP:HB2	2.04	0.57
9:K:12:LEU:HD12	9:K:12:LEU:H	1.69	0.57
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.34	0.57
1:A:1169:ILE:O	1:A:1173:HIS:CD2	2.57	0.57
1:A:518:LYS:HB2	1:A:519:PRO:CD	2.26	0.57
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.34	0.57
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.68	0.57
2:B:484:ASN:ND2	2:B:486:TYR:CD1	2.72	0.57
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.70	0.57
10:L:36:SER:O	10:L:38:LEU:N	2.38	0.57
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.39	0.57
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.70	0.57
2:B:98:THR:O	2:B:126:SER:HB2	2.05	0.57
4:E:84:ASP:O	4:E:86:PRO:HD3	2.05	0.57
10:L:63:ARG:O	10:L:64:LEU:O	2.22	0.57
1:A:907:THR:CG2	1:A:908:LEU:H	2.15	0.57
2:B:332:ASP:O	2:B:334:ILE:N	2.37	0.57
2:B:882:THR:HB	2:B:934:LYS:O	2.05	0.57
3:C:148:ARG:CG	3:C:149:LYS:H	2.17	0.57
1:A:789:LYS:HE3	7:I:67:THR:OG1	2.05	0.57
1:A:474:VAL:HG13	1:A:478:TYR:CD1	2.40	0.57
2:B:693:ILE:HD11	2:B:740:HIS:NE2	2.19	0.57
2:B:737:THR:HG23	7:I:66:PRO:CB	2.35	0.57
2:B:30:SER:HB2	2:B:743:ILE:O	2.05	0.57
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.86	0.57
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.52	0.56
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.20	0.56
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.87	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.40	0.56
1:A:842:VAL:O	1:A:846:GLU:HB2	2.05	0.56
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.87	0.56
6:H:89:LEU:C	6:H:91:ASP:N	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:73:LEU:HD22	9:K:75:ILE:HG13	1.87	0.56
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.45	0.56
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.34	0.56
1:A:979:SER:OG	1:A:981:LEU:HB2	2.05	0.56
9:K:63:VAL:O	9:K:63:VAL:CG2	2.53	0.56
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.35	0.56
1:A:347:PHE:CZ	2:B:1109:GLY:HA2	2.40	0.56
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.87	0.56
2:B:463:THR:CG2	2:B:465:ASN:HD22	2.18	0.56
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.85	0.56
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.35	0.56
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.87	0.56
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.20	0.56
8:J:14:VAL:HG12	8:J:14:VAL:O	2.05	0.56
1:A:32:VAL:CB	1:A:57:ARG:HD2	2.35	0.56
2:B:521:LEU:HD21	2:B:635:ARG:HD3	1.88	0.56
2:B:764:SER:HB3	2:B:765:PRO:CD	2.36	0.56
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.36	0.56
1:A:443:LEU:HD13	1:A:455:MET:CE	2.35	0.56
1:A:49:LYS:HB3	1:A:55:ASP:CB	2.27	0.56
1:A:858:ASN:HD22	1:A:858:ASN:C	2.08	0.56
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.40	0.56
3:C:11:ARG:NH2	3:C:229:TYR:CD2	2.73	0.56
4:E:76:GLY:H	4:E:106:GLN:CD	2.08	0.56
7:I:73:ARG:H	7:I:83:ASN:ND2	2.04	0.56
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.88	0.56
1:A:108:MET:SD	1:A:210:ILE:HD13	2.46	0.56
1:A:276:LEU:HD11	1:A:293:GLU:HG3	1.87	0.56
4:E:46:TYR:HE2	4:E:58:MET:HA	1.69	0.56
2:B:120:ARG:CZ	10:L:54:ARG:HH12	2.18	0.56
1:A:283:GLY:O	1:A:285:PRO:HD3	2.06	0.56
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.34	0.56
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.05	0.56
1:A:901:LEU:HA	1:A:907:THR:CG2	2.35	0.56
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.19	0.56
2:B:642:ASP:CB	2:B:649:LYS:HA	2.35	0.56
3:C:40:GLU:OE1	3:C:254:LYS:HE3	2.06	0.56
1:A:146:MET:HA	1:A:171:GLN:HB2	1.88	0.56
1:A:187:LYS:CB	1:A:194:ALA:HB1	2.29	0.56
1:A:265:LYS:NZ	1:A:323:LYS:H	2.03	0.56
1:A:399:HIS:O	1:A:435:HIS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HD13	2:B:432:MET:HE1	1.87	0.56
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.46	0.56
1:A:1035:TYR:O	1:A:1037:LEU:N	2.39	0.56
1:A:590:ARG:HH21	1:A:620:LYS:HD3	1.70	0.56
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.74	0.56
2:B:484:ASN:HB2	2:B:494:HIS:ND1	2.20	0.56
2:B:706:GLN:HE22	2:B:730:ARG:NH1	2.04	0.56
1:A:84:ILE:CG2	1:A:239:LEU:HB3	2.35	0.55
2:B:1148:LYS:CG	2:B:1152:MET:HE3	2.35	0.55
2:B:305:VAL:HG12	2:B:305:VAL:O	2.06	0.55
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.86	0.55
1:A:1431:GLY:HA2	2:B:1152:MET:HE1	1.89	0.55
1:A:768:GLN:CG	1:A:816:HIS:HA	2.36	0.55
2:B:616:ILE:N	2:B:616:ILE:HD12	2.20	0.55
2:B:957:ASN:HD22	2:B:961:LEU:CD1	2.14	0.55
2:B:770:GLN:HB2	2:B:985:GLY:N	2.21	0.55
1:A:1384:VAL:O	1:A:1386:ARG:N	2.40	0.55
1:A:1390:ASN:O	1:A:1391:ARG:CB	2.54	0.55
2:B:1182:CYS:C	2:B:1183:LYS:HG3	2.27	0.55
2:B:784:ASN:O	2:B:788:ARG:HG3	2.07	0.55
1:A:369:SER:HB3	9:K:2:ASN:OD1	2.06	0.55
2:B:54:PHE:HA	2:B:58:THR:CB	2.34	0.55
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.89	0.55
2:B:864:LYS:HD3	2:B:871:THR:CA	2.37	0.55
2:B:999:MET:HA	2:B:999:MET:CE	2.37	0.55
1:A:792:TYR:CE1	7:I:87:GLN:NE2	2.75	0.55
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.06	0.55
1:A:207:ILE:HG22	1:A:235:ILE:HD11	1.89	0.55
1:A:445:ASN:HB2	1:A:454:SER:O	2.06	0.55
2:B:549:THR:CG2	2:B:550:ASP:N	2.69	0.55
2:B:787:VAL:O	2:B:787:VAL:CG1	2.54	0.55
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.88	0.55
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.37	0.55
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.20	0.55
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.20	0.55
2:B:1166:CYS:HB2	2:B:1215:ARG:HH11	1.70	0.55
2:B:979:LYS:HE2	2:B:987:LYS:HD2	1.88	0.55
1:A:381:THR:CG2	1:A:383:TYR:CD1	2.89	0.55
2:B:393:LYS:HE2	2:B:621:GLU:CD	2.27	0.55
4:E:168:TYR:HB3	4:E:170:LEU:HD21	1.88	0.55
7:I:10:CYS:O	7:I:12:ASN:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:14:VAL:HG12	8:J:50:ILE:HD11	1.89	0.55
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.42	0.55
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.71	0.55
2:B:542:MET:HG3	2:B:747:MET:CE	2.37	0.55
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.89	0.55
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.07	0.55
2:B:861:ASP:OD1	2:B:862:GLN:N	2.40	0.55
3:C:73:GLN:HE21	3:C:75:MET:HB2	1.71	0.55
4:E:71:LYS:HB3	4:E:72:PHE:CE1	2.41	0.55
1:A:974:ASP:HB2	6:H:136:LYS:HZ1	1.72	0.55
1:A:690:VAL:HG13	1:A:718:VAL:HG13	1.89	0.55
2:B:220:GLY:HA2	2:B:241:ARG:HB3	1.89	0.55
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.42	0.55
2:B:806:THR:CG2	2:B:808:ALA:H	2.08	0.55
3:C:101:LEU:HD13	3:C:118:LEU:CD1	2.36	0.55
5:F:90:ARG:HD3	5:F:155:LEU:CD1	2.37	0.55
2:B:903:VAL:CG1	10:L:63:ARG:HH21	2.18	0.55
1:A:381:THR:HG21	1:A:383:TYR:CE1	2.43	0.54
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.37	0.54
1:A:78:PRO:O	1:A:79:GLY:C	2.46	0.54
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.70	0.54
3:C:129:ILE:O	3:C:130:GLY:O	2.24	0.54
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.88	0.54
4:E:192:ARG:HH11	4:E:192:ARG:HG3	1.72	0.54
9:K:63:VAL:HG23	9:K:63:VAL:O	2.05	0.54
1:A:1202:MET:O	1:A:1205:LYS:O	2.24	0.54
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.89	0.54
2:B:165:VAL:CG1	2:B:446:LEU:HD21	2.37	0.54
2:B:579:ARG:HG3	2:B:581:PHE:HE1	1.73	0.54
2:B:705:MET:N	2:B:710:LEU:HD12	2.22	0.54
2:B:1022:THR:HG23	2:B:1022:THR:O	2.08	0.54
2:B:108:VAL:HG12	2:B:109:THR:N	2.22	0.54
2:B:242:SER:OG	2:B:252:SER:O	2.25	0.54
3:C:73:GLN:NE2	3:C:75:MET:H	2.04	0.54
4:E:166:LYS:NZ	4:E:167:ARG:HH21	2.04	0.54
2:B:597:MET:SD	2:B:624:LEU:HD11	2.48	0.54
2:B:654:ARG:C	2:B:656:GLY:H	2.11	0.54
2:B:813:LYS:HA	2:B:816:GLU:OE1	2.07	0.54
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.88	0.54
1:A:557:ASP:HA	9:K:26:LYS:HD2	1.90	0.54
1:A:25:GLU:CD	1:A:25:GLU:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ALA:O	1:A:803:SER:HB3	2.08	0.54
1:A:1009:ASN:OD1	1:A:1012:ARG:NH1	2.41	0.54
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.07	0.54
2:B:1065:GLN:O	2:B:1065:GLN:HG3	2.06	0.54
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.21	0.54
2:B:1182:CYS:O	2:B:1183:LYS:O	2.26	0.54
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.37	0.54
2:B:551:PRO:O	2:B:555:ILE:HG13	2.08	0.54
4:E:93:MET:O	4:E:97:VAL:HG23	2.08	0.54
6:H:76:THR:HG22	6:H:76:THR:O	2.08	0.54
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.38	0.54
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.42	0.54
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.08	0.54
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.88	0.54
1:A:383:TYR:O	1:A:384:ASN:HB3	2.06	0.54
1:A:412:ARG:NE	2:B:1110:PRO:HG3	2.22	0.54
2:B:864:LYS:HB3	2:B:871:THR:HA	1.89	0.54
3:C:253:LYS:O	3:C:256:ALA:HB3	2.08	0.54
10:L:32:ALA:HB3	10:L:55:ILE:CD1	2.38	0.54
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.23	0.54
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.88	0.54
3:C:84:ARG:CD	9:K:11:LEU:HD21	2.38	0.54
6:H:7:ASP:O	6:H:8:ASP:HB2	2.07	0.54
1:A:1220:PHE:O	1:A:1223:ASP:OD1	2.26	0.54
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.07	0.54
1:A:573:SER:O	1:A:576:GLN:HB2	2.07	0.54
1:A:626:ASN:O	1:A:631:HIS:CD2	2.61	0.54
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.38	0.54
1:A:855:THR:CG2	1:A:857:ARG:HE	2.20	0.54
1:A:963:ILE:HD12	1:A:1049:ILE:HG12	1.89	0.54
2:B:324:ILE:HG23	2:B:329:THR:HB	1.90	0.54
3:C:173:ALA:O	3:C:175:ALA:N	2.40	0.54
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.73	0.54
2:B:954:VAL:O	10:L:55:ILE:O	2.26	0.54
1:A:460:VAL:HG12	1:A:461:LYS:N	2.22	0.54
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.89	0.54
2:B:642:ASP:HB2	2:B:649:LYS:HA	1.90	0.54
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.73	0.54
2:B:850:LEU:HG	2:B:851:PHE:HD1	1.71	0.54
7:I:10:CYS:SG	7:I:31:THR:HG21	2.48	0.54
1:A:383:TYR:HB2	5:F:115:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:OG	2:B:172:ILE:HD11	2.07	0.53
3:C:148:ARG:HG2	3:C:149:LYS:H	1.73	0.53
1:A:1284:MET:HG2	1:A:1306:LEU:CD2	2.38	0.53
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.08	0.53
2:B:167:ILE:HD13	2:B:424:LEU:CD2	2.38	0.53
2:B:46:GLN:HE22	2:B:496:ARG:HD3	1.72	0.53
2:B:702:LEU:HD23	2:B:737:THR:HG22	1.89	0.53
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.37	0.53
1:A:13:THR:HG23	1:A:1432:GLN:CD	2.29	0.53
1:A:313:GLN:HB2	1:A:320:ARG:CB	2.27	0.53
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.41	0.53
1:A:375:THR:HG23	1:A:376:TYR:N	2.22	0.53
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.44	0.53
2:B:1172:ILE:O	2:B:1180:PHE:O	2.26	0.53
2:B:1079:LYS:CA	3:C:27:LEU:HD21	2.38	0.53
4:E:19:VAL:O	4:E:23:VAL:HG23	2.06	0.53
6:H:44:VAL:O	6:H:44:VAL:HG12	2.08	0.53
7:I:70:ARG:HG2	7:I:84:VAL:HG23	1.90	0.53
1:A:575:LYS:HB3	1:A:612:ILE:HG23	1.91	0.53
2:B:800:GLN:CB	8:J:52:THR:HG22	2.38	0.53
6:H:31:THR:O	6:H:32:THR:CB	2.55	0.53
1:A:337:ARG:HG2	1:A:341:MET:HE2	1.91	0.53
1:A:528:LEU:O	1:A:531:ILE:HG22	2.08	0.53
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.72	0.53
2:B:737:THR:HG23	2:B:737:THR:O	2.09	0.53
3:C:31:ASN:O	3:C:35:ARG:HG3	2.07	0.53
1:A:1342:GLU:CD	4:E:212:ARG:HH12	2.11	0.53
1:A:1206:ASP:HB2	1:A:1274:ARG:NH1	2.24	0.53
1:A:326:ARG:CZ	1:A:1406:VAL:HG11	2.38	0.53
1:A:187:LYS:HB2	1:A:194:ALA:CB	2.32	0.53
1:A:2:VAL:HG21	2:B:1157:ALA:CB	2.31	0.53
2:B:135:ARG:O	2:B:136:THR:HB	2.09	0.53
2:B:178:ASN:O	2:B:179:CYS:C	2.46	0.53
2:B:244:LEU:O	2:B:249:ARG:HG2	2.09	0.53
2:B:957:ASN:O	2:B:959:ASP:N	2.42	0.53
8:J:7:CYS:CA	8:J:49:MET:HE3	2.39	0.53
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.44	0.53
1:A:622:VAL:HG22	1:A:622:VAL:O	2.09	0.53
2:B:1183:LYS:C	2:B:1185:CYS:H	2.09	0.53
2:B:185:THR:O	2:B:189:LEU:HG	2.09	0.53
2:B:893:LEU:HD22	2:B:897:GLY:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.06	0.53
4:E:124:VAL:HA	4:E:132:ILE:HD12	1.90	0.53
6:H:83:GLN:C	6:H:85:GLY:H	2.12	0.53
1:A:517:ASN:O	1:A:517:ASN:OD1	2.27	0.53
1:A:878:ILE:HG21	1:A:955:PRO:HB2	1.91	0.53
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.01	0.53
2:B:25:ILE:HD11	2:B:653:VAL:HG12	1.91	0.53
2:B:512:ARG:NH2	2:B:535:LEU:HD11	2.24	0.53
2:B:873:THR:HG22	2:B:874:PHE:N	2.23	0.53
3:C:22:LEU:HD12	3:C:230:MET:HE3	1.90	0.53
8:J:12:LYS:O	8:J:14:VAL:HG23	2.09	0.53
8:J:18:TRP:O	8:J:21:TYR:HB3	2.08	0.53
3:C:66:ARG:CZ	8:J:2:ILE:HG21	2.39	0.53
1:A:1394:THR:CG2	1:A:1395:GLY:H	2.12	0.53
1:A:337:ARG:HH22	1:A:1403:GLU:N	2.06	0.53
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.44	0.53
2:B:897:GLY:O	2:B:898:LEU:HD23	2.09	0.53
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.44	0.53
1:A:55:ASP:N	1:A:56:PRO:HD2	2.24	0.52
1:A:685:GLU:HA	1:A:688:LYS:HD2	1.90	0.52
1:A:751:SER:O	1:A:752:LYS:CB	2.56	0.52
2:B:970:THR:HG22	2:B:971:THR:H	1.72	0.52
5:F:109:VAL:HG23	5:F:124:GLU:HG2	1.91	0.52
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.25	0.52
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.09	0.52
1:A:783:THR:HG21	1:A:815:PHE:HZ	1.74	0.52
1:A:996:ASN:O	1:A:997:LEU:C	2.47	0.52
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.92	0.52
3:C:89:GLU:O	3:C:90:ASP:CB	2.57	0.52
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.91	0.52
8:J:7:CYS:CB	8:J:49:MET:HE3	2.38	0.52
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.07	0.52
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.92	0.52
1:A:855:THR:HG22	1:A:857:ARG:HG3	1.91	0.52
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.91	0.52
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.43	0.52
2:B:547:VAL:N	2:B:612:GLU:OE2	2.41	0.52
2:B:650:GLU:HG3	2:B:651:LEU:N	2.24	0.52
3:C:109:SER:O	3:C:110:THR:HB	2.08	0.52
4:E:88:VAL:HG11	4:E:110:PHE:HE2	1.73	0.52
6:H:126:GLU:C	6:H:130:ARG:NH1	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:31:THR:O	6:H:32:THR:HB	2.10	0.52
1:A:412:ARG:HH21	2:B:1110:PRO:HD3	1.73	0.52
1:A:715:GLU:O	1:A:719:VAL:HG23	2.08	0.52
2:B:1207:LEU:O	2:B:1212:ILE:HB	2.09	0.52
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.24	0.52
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.39	0.52
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.90	0.52
2:B:914:LYS:O	2:B:937:ALA:O	2.27	0.52
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.92	0.52
1:A:148:CYS:HB3	1:A:167:CYS:O	2.09	0.52
1:A:306:ASN:OD1	1:A:312:PRO:HD2	2.10	0.52
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.44	0.52
2:B:547:VAL:H	2:B:612:GLU:CD	2.12	0.52
5:F:76:LYS:O	5:F:79:ARG:HD3	2.08	0.52
7:I:59:VAL:HG12	7:I:60:GLN:N	2.24	0.52
1:A:1161:THR:HG21	1:A:1163:ILE:HB	1.92	0.52
1:A:1375:MET:HG3	1:A:1382:THR:O	2.10	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
1:A:901:LEU:H	1:A:926:GLN:NE2	2.07	0.52
2:B:596:LEU:HD12	2:B:596:LEU:O	2.09	0.52
2:B:890:TYR:O	2:B:893:LEU:HB2	2.09	0.52
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.45	0.52
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.40	0.52
1:A:167:CYS:SG	1:A:167:CYS:O	2.68	0.52
2:B:1051:THR:CG2	2:B:1053:GLU:HB2	2.39	0.52
3:C:133:ILE:CD1	3:C:237:SER:HA	2.39	0.52
8:J:31:ASP:OD1	8:J:34:THR:HB	2.10	0.52
10:L:48:CYS:HB3	10:L:51:CYS:O	2.10	0.52
1:A:500:GLU:O	1:A:504:LEU:HB2	2.10	0.52
2:B:60:GLN:HA	2:B:95:ILE:HD12	1.91	0.52
3:C:121:VAL:HG12	3:C:121:VAL:O	2.10	0.52
5:F:109:VAL:HG12	5:F:110:ASP:N	2.25	0.52
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.09	0.52
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.58	0.52
2:B:324:ILE:HD11	2:B:333:PHE:CD1	2.45	0.52
2:B:393:LYS:CE	2:B:621:GLU:OE1	2.58	0.52
2:B:792:MET:HA	2:B:856:PHE:O	2.09	0.52
2:B:864:LYS:N	2:B:872:GLU:OE1	2.43	0.52
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.09	0.52
5:F:133:VAL:HG22	5:F:147:SER:HA	1.91	0.52
6:H:89:LEU:O	6:H:91:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:ARG:HH21	7:I:52:ILE:HD11	1.74	0.52
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.22	0.52
1:A:313:GLN:HG2	1:A:322:VAL:HG23	1.92	0.52
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.23	0.52
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.45	0.52
1:A:801:GLU:HG3	1:A:801:GLU:O	2.10	0.52
2:B:1013:ASN:OD1	2:B:1015:HIS:HB2	2.10	0.52
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.40	0.52
2:B:167:ILE:HG12	2:B:448:ILE:HG21	1.92	0.52
2:B:557:PHE:HZ	2:B:599:THR:HG21	1.74	0.52
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.39	0.52
3:C:205:LYS:O	3:C:205:LYS:HG2	2.10	0.52
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.92	0.52
1:A:517:ASN:HD22	1:A:1362:TYR:HE2	1.58	0.51
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.45	0.51
2:B:850:LEU:HG	2:B:851:PHE:CD1	2.46	0.51
2:B:605:ARG:NH1	2:B:639:ILE:HG21	2.25	0.51
3:C:134:ILE:HG23	3:C:136:ASP:OD1	2.09	0.51
6:H:91:ASP:C	6:H:93:TYR:H	2.14	0.51
7:I:73:ARG:H	7:I:83:ASN:HD22	1.59	0.51
1:A:1286:LYS:HE3	1:A:1304:TRP:CE2	2.44	0.51
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.93	0.51
2:B:914:LYS:H	2:B:938:SER:HB3	1.75	0.51
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.41	0.51
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.46	0.51
1:A:369:SER:CB	9:K:2:ASN:HD21	2.23	0.51
1:A:105:CYS:O	1:A:114:LEU:HG	2.11	0.51
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.10	0.51
1:A:1289:ARG:O	1:A:1291:VAL:HG23	2.10	0.51
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.40	0.51
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.46	0.51
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.93	0.51
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.74	0.51
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.22	0.51
7:I:55:THR:HG23	7:I:58:VAL:CG2	2.41	0.51
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.92	0.51
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.91	0.51
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.09	0.51
1:A:98:LYS:CE	1:A:1411:GLU:HG2	2.41	0.51
2:B:955:THR:CG2	2:B:956:THR:N	2.45	0.51
3:C:55:THR:O	3:C:55:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:LEU:HA	1:A:1273:LEU:CD2	2.41	0.51
1:A:549:MET:SD	1:A:577:ILE:HD11	2.51	0.51
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.91	0.51
2:B:23:ALA:HB3	2:B:655:LYS:HE2	1.92	0.51
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.76	0.51
2:B:549:THR:HB	2:B:628:THR:CG2	2.40	0.51
1:A:806:ARG:NH1	2:B:729:ILE:HD11	2.25	0.51
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.41	0.51
4:E:144:ILE:HG13	4:E:145:THR:N	2.25	0.51
5:F:72:LYS:N	5:F:142:SER:HA	2.25	0.51
7:I:7:CYS:SG	7:I:8:ARG:O	2.68	0.51
1:A:1286:LYS:HE3	1:A:1304:TRP:CZ2	2.46	0.51
1:A:329:LEU:HD11	2:B:1210:MET:CE	2.41	0.51
1:A:873:MET:O	1:A:1058:VAL:HG23	2.11	0.51
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.40	0.51
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.39	0.51
2:B:710:LEU:O	2:B:711:GLU:OE1	2.28	0.51
5:F:81:THR:HG21	5:F:136:ARG:CD	2.40	0.51
1:A:108:MET:O	1:A:109:HIS:CB	2.59	0.51
1:A:596:THR:C	1:A:598:LEU:N	2.64	0.51
2:B:707:PRO:HG2	2:B:708:GLU:N	2.26	0.51
2:B:841:MET:CE	2:B:1010:LEU:HD11	2.41	0.51
3:C:174:ALA:O	3:C:175:ALA:HB2	2.11	0.51
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.93	0.51
6:H:6:PHE:O	6:H:58:THR:HA	2.10	0.51
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.56	0.51
1:A:1415:SER:O	1:A:1417:GLU:N	2.44	0.51
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.45	0.51
1:A:326:ARG:CZ	1:A:1406:VAL:CG1	2.88	0.51
1:A:709:THR:HG22	1:A:710:LEU:N	2.26	0.51
1:A:839:ARG:NE	2:B:1133:MET:HE1	2.26	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.93	0.51
2:B:174:LEU:HD13	2:B:204:ILE:HG13	1.92	0.51
2:B:295:GLY:O	2:B:299:GLU:HG3	2.11	0.51
2:B:315:LYS:N	2:B:316:PRO:CD	2.74	0.51
2:B:589:VAL:HG12	2:B:590:HIS:N	2.26	0.51
9:K:10:PHE:CE1	9:K:11:LEU:HD13	2.46	0.51
1:A:1199:ARG:HG2	1:A:1203:ASN:HD21	1.76	0.51
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.10	0.51
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.93	0.51
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
7:I:78:CYS:SG	7:I:106:CYS:HB3	2.51	0.51
9:K:91:CYS:O	9:K:95:ILE:HG13	2.11	0.51
1:A:412:ARG:NH2	1:A:433:GLU:OE1	2.44	0.50
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.92	0.50
2:B:652:LYS:HE3	2:B:688:GLY:O	2.11	0.50
3:C:175:ALA:HB3	8:J:43:ARG:NH1	2.26	0.50
7:I:84:VAL:CG1	7:I:84:VAL:O	2.59	0.50
1:A:648:ASN:O	1:A:652:VAL:HG23	2.11	0.50
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.46	0.50
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.25	0.50
2:B:562:GLY:O	2:B:563:MET:C	2.50	0.50
2:B:613:VAL:HG13	2:B:627:PHE:O	2.10	0.50
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.46	0.50
3:C:115:SER:OG	3:C:141:GLY:O	2.15	0.50
1:A:1318:THR:OG1	4:E:11:ARG:NH1	2.44	0.50
6:H:112:ILE:HD12	6:H:131:ASN:HD21	1.76	0.50
6:H:126:GLU:C	6:H:130:ARG:HH12	2.14	0.50
8:J:53:HIS:CD2	8:J:54:VAL:H	2.28	0.50
1:A:1206:ASP:HB2	1:A:1274:ARG:HH11	1.77	0.50
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.41	0.50
1:A:264:PHE:CD1	1:A:315:LEU:HD22	2.46	0.50
1:A:337:ARG:HH22	1:A:1403:GLU:H	1.59	0.50
2:B:281:PRO:CG	2:B:284:ILE:HD12	2.41	0.50
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.93	0.50
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.46	0.50
6:H:10:PHE:O	6:H:54:SER:HA	2.11	0.50
1:A:541:ILE:HG12	1:A:549:MET:HE1	1.92	0.50
2:B:1107:ALA:O	2:B:1108:ARG:C	2.49	0.50
2:B:446:LEU:O	2:B:447:ALA:CB	2.59	0.50
3:C:183:TRP:HB2	3:C:185:LYS:HG3	1.94	0.50
7:I:7:CYS:HB2	7:I:29:CYS:HB2	1.93	0.50
1:A:1169:ILE:HD11	1:A:1229:SER:HB3	1.92	0.50
1:A:511:ILE:HG12	1:A:521:MET:HE2	1.92	0.50
1:A:90:VAL:HG12	1:A:91:PHE:H	1.74	0.50
2:B:167:ILE:HD13	2:B:424:LEU:HD21	1.94	0.50
3:C:175:ALA:HB3	8:J:43:ARG:NH2	2.27	0.50
7:I:31:THR:HG22	7:I:32:CYS:N	2.26	0.50
8:J:36:LEU:HD12	8:J:47:ARG:NH1	2.25	0.50
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.94	0.50
1:A:392:VAL:HG13	1:A:415:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLY:CA	1:A:241:VAL:HB	2.41	0.50
2:B:116:GLU:OE1	2:B:120:ARG:NH2	2.42	0.50
2:B:259:TYR:O	2:B:267:ARG:HG2	2.12	0.50
7:I:65:ASP:C	7:I:65:ASP:OD1	2.49	0.50
1:A:1074:GLU:H	1:A:1075:PRO:HD2	1.75	0.50
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.94	0.50
1:A:1145:SER:HB2	1:A:1205:LYS:NZ	2.26	0.50
1:A:1329:THR:HG22	1:A:1330:ASN:N	2.26	0.50
1:A:260:ASP:OD2	1:A:328:ARG:NH2	2.45	0.50
1:A:515:GLN:HG3	1:A:516:SER:H	1.76	0.50
1:A:994:GLN:HE21	1:A:1019:CYS:HB3	1.75	0.50
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.12	0.50
2:B:558:LEU:HD13	2:B:580:VAL:HG11	1.94	0.50
2:B:862:GLN:O	2:B:914:LYS:HE3	2.10	0.50
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.11	0.50
6:H:130:ARG:O	6:H:133:ASN:N	2.45	0.50
6:H:83:GLN:C	6:H:85:GLY:N	2.65	0.50
1:A:166:GLY:O	1:A:167:CYS:HB3	2.12	0.50
1:A:167:CYS:C	1:A:169:ASN:H	2.15	0.50
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.10	0.50
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.42	0.50
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.52	0.50
3:C:239:PRO:O	3:C:242:GLN:HB2	2.11	0.50
6:H:5:LEU:CD1	6:H:135:LEU:HG	2.41	0.50
1:A:35:ILE:HG12	1:A:52:GLY:O	2.11	0.50
1:A:434:ARG:HH21	1:A:440:ASP:CG	2.14	0.50
2:B:361:LEU:N	2:B:362:PRO:CD	2.74	0.50
2:B:25:ILE:CD1	2:B:653:VAL:HG12	2.41	0.50
1:A:406:ILE:HD11	1:A:412:ARG:NH1	2.27	0.49
3:C:101:LEU:HD13	3:C:118:LEU:HD12	1.94	0.49
3:C:22:LEU:HD12	3:C:230:MET:CE	2.42	0.49
6:H:123:MET:HE3	6:H:142:LEU:CD2	2.38	0.49
8:J:37:SER:OG	8:J:47:ARG:NH2	2.44	0.49
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.77	0.49
1:A:1376:THR:CG2	4:E:212:ARG:HH21	2.25	0.49
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.77	0.49
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.49
1:A:871:ASP:CG	4:E:204:THR:HG23	2.32	0.49
1:A:1066:VAL:HG11	2:B:1140:ALA:HB2	1.94	0.49
2:B:484:ASN:HD21	2:B:486:TYR:HD1	1.57	0.49
5:F:96:THR:O	5:F:99:LEU:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:LEU:O	10:L:39:SER:CB	2.59	0.49
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.00	0.49
1:A:1143:LEU:HA	1:A:1273:LEU:HD21	1.93	0.49
1:A:385:ILE:HD11	1:A:428:TYR:CE2	2.46	0.49
1:A:442:VAL:HG21	1:A:489:LEU:HD11	1.94	0.49
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.40	0.49
1:A:590:ARG:CB	1:A:605:MET:N	2.73	0.49
1:A:902:LEU:HG	1:A:926:GLN:CG	2.43	0.49
1:A:505:CYS:HB3	2:B:1141:HIS:CE1	2.47	0.49
2:B:220:GLY:O	2:B:221:ASN:HB2	2.12	0.49
4:E:213:ILE:O	4:E:213:ILE:HG23	2.12	0.49
9:K:90:ALA:O	9:K:94:ILE:HG13	2.12	0.49
1:A:24:PRO:HG2	1:A:25:GLU:CD	2.33	0.49
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.48	0.49
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.94	0.49
2:B:1103:ILE:O	2:B:1103:ILE:HG22	2.13	0.49
3:C:56:THR:CG2	3:C:57:VAL:N	2.73	0.49
3:C:248:ILE:CD1	9:K:101:LEU:HD22	2.43	0.49
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.93	0.49
1:A:1236:LEU:O	1:A:1237:ILE:HG13	2.13	0.49
1:A:1295:THR:CG2	1:A:1297:GLU:OE1	2.60	0.49
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.13	0.49
1:A:223:GLY:O	1:A:1415:SER:HA	2.12	0.49
1:A:243:PRO:C	1:A:245:PRO:HD2	2.33	0.49
1:A:275:SER:O	1:A:279:LEU:HG	2.13	0.49
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.39	0.49
1:A:783:THR:CG2	1:A:815:PHE:CZ	2.96	0.49
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.49
2:B:1037:LEU:HD11	2:B:1064:TYR:CD1	2.47	0.49
2:B:956:THR:HG21	2:B:960:GLY:HA2	1.95	0.49
1:A:1386:ARG:HG3	1:A:1386:ARG:O	2.12	0.49
1:A:1402:PHE:O	1:A:1404:GLU:HG3	2.13	0.49
1:A:469:ARG:HH21	2:B:976:ILE:HD13	1.78	0.49
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.13	0.49
1:A:901:LEU:H	1:A:926:GLN:HE21	1.60	0.49
1:A:757:ASN:HA	2:B:1021:MET:CE	2.43	0.49
2:B:1172:ILE:CD1	2:B:1183:LYS:HE2	2.41	0.49
2:B:228:LYS:HD3	2:B:234:ILE:HD13	1.95	0.49
2:B:365:THR:HG23	2:B:367:LEU:HG	1.94	0.49
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.12	0.49
1:A:100:LYS:O	1:A:103:CYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLY:N	1:A:674:PRO:HD2	2.28	0.49
2:B:65:GLU:HG3	2:B:66:ASP:N	2.15	0.49
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.94	0.49
1:A:1396:ALA:O	1:A:1397:LEU:HG	2.12	0.49
1:A:1406:VAL:HG12	1:A:1407:GLU:N	2.25	0.49
1:A:1063:MET:SD	1:A:1436:ILE:HB	2.53	0.49
1:A:321:PRO:O	1:A:322:VAL:HG23	2.12	0.49
3:C:141:GLY:O	3:C:142:VAL:CB	2.60	0.49
3:C:174:ALA:HB3	3:C:233:GLU:HB3	1.95	0.49
5:F:101:ILE:HD13	5:F:120:ILE:CG2	2.43	0.49
6:H:96:VAL:HG22	6:H:143:LEU:HD23	1.94	0.49
1:A:464:PRO:O	9:K:2:ASN:HB3	2.13	0.49
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.48	0.49
2:B:778:MET:SD	2:B:1094:ARG:HD3	2.53	0.49
2:B:794:ASN:C	2:B:795:ILE:HD12	2.33	0.49
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.49
1:A:1400:CYS:O	1:A:1401:SER:O	2.31	0.49
1:A:305:ASP:OD2	1:A:326:ARG:HD2	2.12	0.49
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.94	0.49
2:B:650:GLU:CG	2:B:654:ARG:HH12	2.15	0.49
2:B:863:GLU:O	2:B:864:LYS:O	2.31	0.49
2:B:976:ILE:O	2:B:990:ILE:HB	2.13	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
4:E:71:LYS:HB3	4:E:72:PHE:CD1	2.47	0.49
1:A:566:ILE:O	1:A:566:ILE:HG22	2.13	0.48
2:B:397:ASP:OD2	2:B:515:HIS:HE1	1.96	0.48
2:B:957:ASN:O	2:B:958:GLN:C	2.51	0.48
3:C:53:THR:O	3:C:153:LEU:HA	2.12	0.48
4:E:88:VAL:HG21	4:E:110:PHE:CE2	2.48	0.48
10:L:48:CYS:HB3	10:L:51:CYS:HB2	1.95	0.48
1:A:203:SER:O	1:A:207:ILE:HG12	2.13	0.48
1:A:42:ASP:O	1:A:50:ILE:HD11	2.13	0.48
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.48	0.48
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.71	0.48
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.95	0.48
2:B:130:VAL:HG12	2:B:131:ASP:N	2.27	0.48
2:B:635:ARG:HG3	2:B:635:ARG:HH11	1.77	0.48
2:B:959:ASP:O	2:B:961:LEU:HG	2.12	0.48
6:H:130:ARG:HB3	6:H:134:ASN:ND2	2.26	0.48
7:I:15:TYR:N	7:I:15:TYR:CD1	2.81	0.48
10:L:29:TYR:O	10:L:30:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.78	0.48
1:A:4:GLN:O	1:A:5:GLN:CB	2.61	0.48
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.36	0.48
1:A:95:PHE:O	1:A:98:LYS:HB2	2.14	0.48
2:B:1051:THR:HG21	2:B:1053:GLU:HB2	1.95	0.48
2:B:484:ASN:ND2	2:B:486:TYR:CE1	2.82	0.48
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.28	0.48
2:B:65:GLU:CG	2:B:66:ASP:H	2.15	0.48
3:C:77:ILE:CD1	3:C:129:ILE:HD11	2.40	0.48
5:F:81:THR:CG2	5:F:82:THR:N	2.75	0.48
2:B:1170:THR:O	2:B:1170:THR:HG22	2.14	0.48
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.95	0.48
2:B:896:ASP:OD2	10:L:58:LYS:HE3	2.13	0.48
7:I:63:GLY:O	7:I:70:ARG:NH2	2.47	0.48
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.13	0.48
9:K:113:THR:O	9:K:114:LEU:CB	2.52	0.48
1:A:493:GLN:HE21	1:A:493:GLN:HA	1.78	0.48
2:B:251:ILE:HG22	2:B:251:ILE:O	2.13	0.48
2:B:618:ASP:HB3	2:B:621:GLU:HB3	1.94	0.48
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.78	0.48
1:A:1338:VAL:O	4:E:144:ILE:HG21	2.13	0.48
1:A:50:ILE:C	1:A:52:GLY:N	2.67	0.48
1:A:69:THR:O	2:B:1174:LYS:HG2	2.14	0.48
2:B:1037:LEU:HD21	2:B:1064:TYR:CE1	2.48	0.48
2:B:166:PHE:O	2:B:167:ILE:HG13	2.13	0.48
2:B:612:GLU:O	2:B:632:ARG:NH2	2.46	0.48
1:A:871:ASP:CB	4:E:204:THR:HG23	2.44	0.48
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.53	0.48
1:A:276:LEU:HD11	1:A:293:GLU:CG	2.43	0.48
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.52	0.48
10:L:51:CYS:C	10:L:53:HIS:H	2.17	0.48
1:A:1264:GLU:OE2	7:I:44:TYR:HE2	1.97	0.48
1:A:326:ARG:NH1	1:A:1406:VAL:HG11	2.29	0.48
1:A:505:CYS:HB3	2:B:1141:HIS:ND1	2.29	0.48
1:A:500:GLU:OE2	2:B:1145:SER:HB3	2.13	0.48
2:B:40:GLU:OE1	2:B:680:THR:CG2	2.61	0.48
4:E:102:GLU:C	4:E:104:ASN:H	2.17	0.48
5:F:89:GLU:O	5:F:93:ILE:HG13	2.14	0.48
7:I:86:PHE:HD1	7:I:87:GLN:O	1.97	0.48
1:A:877:HIS:HB3	1:A:1056:SER:OG	2.13	0.48
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:CB	1:A:497:THR:HG22	2.44	0.48
1:A:814:PHE:O	1:A:817:ALA:HB3	2.14	0.48
2:B:25:ILE:HG22	2:B:26:THR:N	2.29	0.48
2:B:463:THR:HG22	2:B:465:ASN:N	2.29	0.48
2:B:34:ILE:HG12	2:B:542:MET:CE	2.44	0.48
2:B:690:VAL:HG12	2:B:691:GLU:N	2.28	0.48
4:E:75:MET:HA	4:E:106:GLN:HE22	1.78	0.48
5:F:109:VAL:CG1	5:F:110:ASP:N	2.77	0.48
7:I:121:PHE:O	7:I:122:SER:CB	2.61	0.48
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.96	0.48
10:L:32:ALA:CB	10:L:55:ILE:HD12	2.41	0.48
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.87	0.48
1:A:1066:VAL:CG1	2:B:1140:ALA:HB2	2.43	0.48
1:A:451:HIS:HB3	1:A:452:LYS:H	1.50	0.48
1:A:549:MET:SD	1:A:577:ILE:CD1	3.02	0.48
2:B:498:THR:HG22	2:B:499:ASN:N	2.29	0.48
2:B:563:MET:O	2:B:563:MET:HG3	2.14	0.48
10:L:27:LEU:HD23	10:L:27:LEU:N	2.29	0.48
2:B:902:GLY:O	10:L:65:VAL:HG21	2.14	0.48
1:A:1293:SER:HB2	1:A:1299:VAL:HG21	1.93	0.47
1:A:329:LEU:HD11	2:B:1210:MET:HE1	1.95	0.47
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.96	0.47
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.96	0.47
1:A:573:SER:H	1:A:576:GLN:HG3	1.78	0.47
1:A:608:ILE:HB	1:A:613:ILE:CD1	2.44	0.47
1:A:745:GLN:HA	1:A:748:MET:HE3	1.96	0.47
1:A:88:LYS:HD2	1:A:293:GLU:CD	2.35	0.47
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.95	0.47
2:B:796:LEU:O	2:B:799:PRO:HD3	2.14	0.47
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.74	0.47
3:C:171:GLY:O	8:J:6:ARG:NH2	2.47	0.47
4:E:177:ARG:O	4:E:212:ARG:HD3	2.14	0.47
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.47	0.47
1:A:399:HIS:O	1:A:435:HIS:CD2	2.67	0.47
2:B:1043:ASP:O	2:B:1050:ILE:HD12	2.14	0.47
2:B:321:GLY:C	2:B:323:VAL:H	2.17	0.47
2:B:393:LYS:HE2	2:B:621:GLU:OE2	2.14	0.47
2:B:825:VAL:CG1	2:B:826:ALA:N	2.77	0.47
3:C:166:GLU:OE1	10:L:70:ARG:NH2	2.43	0.47
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.96	0.47
2:B:827:ILE:CD1	2:B:1017:ILE:HD11	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:THR:CG2	2:B:499:ASN:N	2.77	0.47
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.96	0.47
1:A:754:SER:O	1:A:755:PHE:C	2.53	0.47
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.96	0.47
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.44	0.47
3:C:39:ALA:O	3:C:163:ILE:HG23	2.14	0.47
5:F:111:LEU:C	5:F:113:GLY:H	2.17	0.47
1:A:535:THR:CG2	1:A:535:THR:O	2.63	0.47
2:B:957:ASN:ND2	2:B:961:LEU:HD12	2.15	0.47
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.29	0.47
3:C:169:LYS:C	3:C:171:GLY:H	2.17	0.47
3:C:254:LYS:HD3	9:K:42:LEU:HD13	1.96	0.47
3:C:33:LEU:HG	3:C:37:MET:HE2	1.96	0.47
5:F:127:GLU:O	5:F:129:LYS:HG3	2.15	0.47
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.44	0.47
1:A:1205:LYS:O	1:A:1207:LEU:N	2.47	0.47
1:A:365:GLY:HA3	1:A:463:ILE:HD13	1.96	0.47
1:A:451:HIS:HB2	1:A:454:SER:OG	2.14	0.47
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.49	0.47
2:B:680:THR:O	2:B:683:SER:OG	2.32	0.47
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.96	0.47
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.14	0.47
1:A:1415:SER:O	1:A:1416:ALA:C	2.52	0.47
1:A:225:ASN:C	1:A:227:VAL:H	2.16	0.47
1:A:337:ARG:NH2	1:A:1400:CYS:O	2.47	0.47
1:A:53:LEU:O	1:A:56:PRO:HD2	2.14	0.47
2:B:463:THR:HG22	2:B:464:GLY:N	2.29	0.47
2:B:778:MET:HG2	2:B:794:ASN:CB	2.41	0.47
3:C:75:MET:HG2	3:C:246:ARG:NH2	2.29	0.47
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.55	0.47
1:A:32:VAL:HB	1:A:57:ARG:CB	2.45	0.47
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.50	0.47
1:A:844:ALA:C	1:A:845:LEU:HD23	2.34	0.47
1:A:839:ARG:NE	2:B:1133:MET:CE	2.78	0.47
2:B:331:LEU:HD21	2:B:353:LYS:HG2	1.96	0.47
2:B:424:LEU:O	2:B:428:ILE:HG13	2.15	0.47
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.47	0.47
2:B:794:ASN:O	2:B:795:ILE:HD12	2.15	0.47
3:C:70:ILE:HG21	3:C:115:SER:HB2	1.96	0.47
4:E:204:THR:HG22	4:E:205:SER:N	2.30	0.47
1:A:1155:ASP:CG	1:A:1162:VAL:HG23	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:PHE:C	1:A:1404:GLU:N	2.66	0.47
1:A:535:THR:CG2	1:A:617:VAL:H	2.10	0.47
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.97	0.47
2:B:563:MET:HE1	2:B:588:GLY:N	2.30	0.47
2:B:959:ASP:O	2:B:961:LEU:N	2.48	0.47
3:C:77:ILE:C	3:C:79:GLN:H	2.17	0.47
1:A:1376:THR:CG2	4:E:212:ARG:NH2	2.78	0.47
1:A:1433:MET:HE1	5:F:92:ARG:NH1	2.30	0.47
1:A:1126:ALA:O	1:A:1128:GLN:N	2.48	0.47
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.15	0.47
1:A:1223:ASP:HA	1:A:1243:VAL:HG13	1.97	0.47
1:A:1152:ILE:CG2	1:A:1260:LEU:HD23	2.44	0.47
1:A:13:THR:HG23	1:A:1432:GLN:HE22	1.76	0.47
1:A:1402:PHE:C	1:A:1404:GLU:H	2.17	0.47
1:A:460:VAL:CG1	1:A:461:LYS:N	2.78	0.47
1:A:71:GLN:O	1:A:72:GLU:HB2	2.15	0.47
1:A:974:ASP:HB2	6:H:136:LYS:NZ	2.29	0.47
1:A:994:GLN:NE2	1:A:1019:CYS:HB3	2.30	0.47
1:A:1431:GLY:O	2:B:1148:LYS:HE3	2.15	0.47
3:C:99:LEU:HD12	3:C:118:LEU:HD23	1.96	0.47
4:E:117:THR:HG22	4:E:119:SER:H	1.79	0.47
5:F:76:LYS:CA	5:F:79:ARG:HD2	2.44	0.47
1:A:1031:VAL:HG12	1:A:1031:VAL:O	2.14	0.47
1:A:873:MET:C	1:A:1058:VAL:HG23	2.35	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:HG3	1.79	0.47
1:A:216:VAL:HA	1:A:219:PHE:CD1	2.50	0.47
1:A:565:ILE:O	1:A:570:PRO:HA	2.15	0.47
1:A:534:LEU:HD13	1:A:656:TRP:CD1	2.50	0.47
1:A:77:CYS:O	1:A:79:GLY:N	2.48	0.47
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.80	0.47
2:B:708:GLU:C	2:B:710:LEU:H	2.18	0.47
2:B:780:VAL:HG22	2:B:799:PRO:HG2	1.97	0.47
2:B:904:ARG:NH2	2:B:948:ILE:HD11	2.30	0.47
3:C:136:ASP:OD2	8:J:16:ASP:HB2	2.14	0.47
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.36	0.47
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.97	0.47
1:A:1198:ASP:OD1	1:A:1200:ALA:N	2.46	0.46
2:B:25:ILE:HG22	2:B:26:THR:H	1.79	0.46
2:B:791:THR:O	2:B:792:MET:HB2	2.15	0.46
4:E:88:VAL:HG21	4:E:110:PHE:HE2	1.80	0.46
1:A:1441:PHE:HZ	5:F:89:GLU:HA	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASP:O	1:A:196:GLU:O	2.33	0.46
1:A:364:VAL:O	1:A:364:VAL:HG13	2.15	0.46
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.98	0.46
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.15	0.46
2:B:815:ARG:NE	2:B:1041:GLU:OE2	2.48	0.46
7:I:17:ARG:HG3	7:I:28:GLU:CG	2.40	0.46
2:B:212:LEU:HD13	2:B:409:ALA:HA	1.96	0.46
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.44	0.46
2:B:946:ASN:CG	2:B:946:ASN:O	2.54	0.46
7:I:99:LEU:O	7:I:111:THR:HG23	2.15	0.46
7:I:53:GLY:O	7:I:89:GLN:HB2	2.15	0.46
1:A:783:THR:HG22	1:A:784:LEU:N	2.31	0.46
2:B:167:ILE:CG2	2:B:453:ILE:HD12	2.46	0.46
2:B:405:ARG:HA	2:B:631:GLY:O	2.15	0.46
3:C:37:MET:HG2	3:C:243:VAL:CG1	2.45	0.46
2:B:969:ARG:HH21	3:C:59:ALA:HB1	1.81	0.46
9:K:73:LEU:HD22	9:K:75:ILE:CG1	2.46	0.46
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.45	0.46
1:A:99:ILE:HG23	1:A:211:PHE:CZ	2.50	0.46
1:A:313:GLN:HB3	1:A:320:ARG:C	2.35	0.46
1:A:338:GLY:O	1:A:343:LYS:HB2	2.15	0.46
1:A:346:ASP:HB3	1:A:347:PHE:CD1	2.51	0.46
1:A:577:ILE:O	1:A:580:VAL:HB	2.15	0.46
1:A:897:TYR:CD1	1:A:897:TYR:N	2.84	0.46
1:A:670:ILE:HD13	2:B:1067:ARG:NH2	2.30	0.46
1:A:821:ARG:HH21	2:B:534:GLY:HA2	1.80	0.46
2:B:549:THR:HG22	2:B:550:ASP:N	2.29	0.46
2:B:707:PRO:CG	2:B:708:GLU:H	2.26	0.46
3:C:240:VAL:O	3:C:242:GLN:N	2.48	0.46
4:E:77:SER:HB2	4:E:105:PHE:HD2	1.81	0.46
5:F:154:ASP:O	5:F:155:LEU:HB2	2.15	0.46
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.96	0.46
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.35	0.46
1:A:134:ARG:HD3	1:A:221:SER:O	2.16	0.46
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.36	0.46
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.45	0.46
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.46
2:B:98:THR:HG22	2:B:99:LYS:N	2.26	0.46
3:C:105:GLY:O	3:C:149:LYS:O	2.34	0.46
3:C:131:HIS:O	3:C:132:PRO:C	2.54	0.46
3:C:134:ILE:HG23	3:C:141:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:40:LEU:HD12	6:H:41:ASP:H	1.80	0.46
1:A:119:ASN:O	1:A:123:ARG:HG3	2.16	0.46
1:A:1429:ILE:O	1:A:1429:ILE:HG22	2.16	0.46
1:A:313:GLN:HB3	1:A:321:PRO:N	2.30	0.46
1:A:361:LEU:HD21	1:A:521:MET:CE	2.46	0.46
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.15	0.46
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.46
1:A:901:LEU:HD23	1:A:907:THR:CG2	2.44	0.46
2:B:287:ARG:NH2	2:B:325:GLN:NE2	2.63	0.46
2:B:618:ASP:CB	2:B:621:GLU:HB3	2.46	0.46
2:B:618:ASP:O	2:B:621:GLU:N	2.48	0.46
2:B:781:PHE:O	2:B:782:LEU:HG	2.16	0.46
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.80	0.46
1:A:857:ARG:CZ	5:F:139:PRO:HG3	2.45	0.46
8:J:48:ARG:O	8:J:52:THR:HB	2.16	0.46
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.97	0.46
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.19	0.46
1:A:41:MET:HB3	1:A:48:ALA:O	2.16	0.46
1:A:596:THR:C	1:A:598:LEU:H	2.18	0.46
1:A:786:HIS:HD2	1:A:786:HIS:N	2.12	0.46
1:A:839:ARG:HE	2:B:1133:MET:HE1	1.80	0.46
2:B:240:ILE:O	2:B:240:ILE:HG23	2.16	0.46
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.51	0.46
5:F:107:VAL:HG12	5:F:109:VAL:H	1.80	0.46
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.15	0.46
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.51	0.46
1:A:35:ILE:HD13	1:A:53:LEU:HD23	1.98	0.46
1:A:605:MET:CE	1:A:612:ILE:HG13	2.43	0.46
1:A:575:LYS:HG2	1:A:612:ILE:HD13	1.96	0.46
1:A:774:ARG:HB2	1:A:797:LYS:O	2.15	0.46
2:B:121:ASN:HA	2:B:207:GLY:CA	2.46	0.46
2:B:531:GLN:HG3	2:B:532:ALA:H	1.80	0.46
2:B:216:GLU:OE1	2:B:537:LYS:HE2	2.16	0.46
2:B:570:VAL:CG2	2:B:573:GLN:HB2	2.46	0.46
3:C:177:GLU:O	3:C:230:MET:HA	2.16	0.46
6:H:126:GLU:N	6:H:130:ARG:HH12	2.14	0.46
3:C:6:PRO:HB2	9:K:101:LEU:HB2	1.98	0.46
9:K:55:LYS:CD	9:K:78:THR:HB	2.43	0.46
10:L:45:ALA:O	10:L:46:VAL:CG2	2.64	0.46
1:A:849:MET:HE3	1:A:1061:GLY:HA2	1.90	0.46
1:A:1153:TYR:CD1	1:A:1163:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASP:C	1:A:414:ASP:OD1	2.53	0.46
1:A:55:ASP:O	1:A:56:PRO:C	2.54	0.46
1:A:62:ASP:O	1:A:63:ARG:HB2	2.16	0.46
1:A:858:ASN:ND2	1:A:858:ASN:C	2.69	0.46
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.30	0.46
2:B:650:GLU:HG3	2:B:651:LEU:H	1.80	0.46
2:B:665:GLU:O	2:B:668:ASP:HB2	2.16	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.16	0.46
2:B:978:ASP:O	2:B:989:THR:HA	2.16	0.46
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.81	0.45
1:A:1114:PRO:O	1:A:1330:ASN:OD1	2.34	0.45
1:A:1152:ILE:HD11	1:A:1260:LEU:O	2.16	0.45
1:A:128:ILE:HG21	1:A:133:LYS:HB3	1.98	0.45
1:A:44:THR:HG22	1:A:44:THR:O	2.17	0.45
1:A:50:ILE:HG22	1:A:51:GLY:N	2.31	0.45
2:B:1152:MET:HG2	2:B:1153:GLU:N	2.32	0.45
2:B:1158:PHE:O	2:B:1195:HIS:HA	2.16	0.45
2:B:235:SER:OG	2:B:236:HIS:HD2	1.99	0.45
2:B:314:LEU:C	2:B:316:PRO:HD2	2.36	0.45
2:B:40:GLU:O	2:B:40:GLU:HG3	2.16	0.45
2:B:859:TYR:H	2:B:859:TYR:HD1	1.64	0.45
4:E:176:PRO:O	4:E:212:ARG:HA	2.16	0.45
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.98	0.45
2:B:843:GLN:HG3	9:K:6:ARG:NH2	2.31	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HB	2.47	0.45
1:A:1220:PHE:O	1:A:1221:LYS:C	2.55	0.45
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.98	0.45
1:A:214:ILE:CG2	1:A:218:ASP:HB2	2.46	0.45
1:A:289:ILE:O	1:A:291:GLU:N	2.49	0.45
1:A:517:ASN:O	1:A:517:ASN:CG	2.54	0.45
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.51	0.45
1:A:922:ASP:HB3	1:A:925:LEU:HB2	1.97	0.45
1:A:1342:GLU:CG	4:E:198:ILE:HD13	2.46	0.45
7:I:4:PHE:HE1	7:I:6:PHE:CZ	2.34	0.45
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.16	0.45
1:A:404:TYR:HA	1:A:413:ILE:O	2.16	0.45
1:A:412:ARG:CZ	2:B:1110:PRO:HD3	2.44	0.45
2:B:332:ASP:C	2:B:334:ILE:N	2.68	0.45
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.16	0.45
2:B:463:THR:HG22	2:B:465:ASN:H	1.80	0.45
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.51	0.45
1:A:1115:SER:O	1:A:1329:THR:HG23	2.16	0.45
1:A:1189:SER:HB2	1:A:1190:PRO:CD	2.44	0.45
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.16	0.45
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.46	0.45
1:A:50:ILE:O	1:A:52:GLY:N	2.49	0.45
4:E:192:ARG:HG3	4:E:192:ARG:NH1	2.31	0.45
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.16	0.45
1:A:185:TRP:O	1:A:197:PRO:HA	2.16	0.45
1:A:329:LEU:CD1	2:B:1210:MET:HE1	2.46	0.45
1:A:598:LEU:O	1:A:599:SER:C	2.54	0.45
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.46	0.45
2:B:805:THR:HA	2:B:809:MET:HE1	1.98	0.45
7:I:84:VAL:O	7:I:84:VAL:HG13	2.16	0.45
1:A:1261:LYS:C	1:A:1263:ILE:N	2.69	0.45
1:A:225:ASN:ND2	1:A:228:PHE:CD1	2.84	0.45
1:A:736:ASN:O	1:A:737:LEU:C	2.54	0.45
2:B:654:ARG:O	2:B:656:GLY:N	2.49	0.45
2:B:906:SER:O	2:B:907:GLY:C	2.54	0.45
3:C:33:LEU:HD11	3:C:248:ILE:HG12	1.99	0.45
4:E:205:SER:O	4:E:206:GLY:C	2.54	0.45
1:A:1370:LEU:C	1:A:1370:LEU:HD12	2.35	0.45
1:A:1383:SER:HB3	1:A:1387:HIS:CD2	2.51	0.45
1:A:49:LYS:NZ	1:A:60:SER:HA	2.31	0.45
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.50	0.45
2:B:1103:ILE:O	2:B:1104:HIS:C	2.55	0.45
2:B:212:LEU:HD12	2:B:409:ALA:CB	2.46	0.45
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.46	0.45
2:B:666:TYR:C	2:B:668:ASP:H	2.19	0.45
5:F:127:GLU:O	5:F:129:LYS:N	2.50	0.45
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.50	0.45
1:A:466:SER:HB2	2:B:1103:ILE:HD13	1.98	0.45
2:B:1155:SER:O	2:B:1156:ASP:O	2.34	0.45
2:B:282:ILE:O	2:B:286:PHE:HD1	2.00	0.45
2:B:564:GLU:HA	2:B:565:PRO:HD2	1.70	0.45
1:A:1106:ASN:OD1	1:A:1385:THR:HB	2.16	0.45
1:A:1199:ARG:HA	1:A:1236:LEU:CD1	2.47	0.45
1:A:343:LYS:O	1:A:345:VAL:HG22	2.17	0.45
1:A:474:VAL:HG13	1:A:478:TYR:HE1	1.77	0.45
2:B:172:ILE:HD13	2:B:178:ASN:HB2	1.99	0.45
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:109:LYS:HG3	6:H:110:ASP:N	2.30	0.45
6:H:5:LEU:O	6:H:133:ASN:HB3	2.17	0.45
7:I:50:THR:HG22	7:I:52:ILE:H	1.80	0.45
1:A:380:VAL:HG12	1:A:381:THR:N	2.32	0.45
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.52	0.45
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.31	0.45
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.45	0.45
1:A:553:VAL:HG22	1:A:652:VAL:HG22	1.99	0.45
1:A:826:ASP:O	1:A:830:LYS:N	2.45	0.45
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.47	0.45
1:A:886:ILE:CG1	1:A:943:LEU:HB3	2.47	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.45
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.99	0.45
4:E:177:ARG:HD3	4:E:215:MET:CE	2.46	0.45
1:A:709:THR:HG23	7:I:94:ASP:HA	1.99	0.45
1:A:1389:PHE:CD1	1:A:1389:PHE:N	2.84	0.44
1:A:34:LYS:CD	1:A:36:ARG:NH2	2.79	0.44
1:A:867:ILE:HG13	4:E:208:TYR:HE1	1.81	0.44
2:B:915:THR:HG22	2:B:916:THR:N	2.33	0.44
3:C:48:SER:HB3	3:C:158:VAL:HB	1.99	0.44
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.57	0.44
8:J:19:GLU:O	8:J:20:SER:C	2.54	0.44
8:J:30:LEU:HD13	8:J:34:THR:HG22	1.99	0.44
10:L:55:ILE:HG13	10:L:56:LEU:N	2.24	0.44
1:A:114:LEU:HD22	1:A:171:GLN:HE22	1.80	0.44
1:A:32:VAL:HG11	1:A:68:GLN:CD	2.38	0.44
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.99	0.44
2:B:1099:VAL:C	2:B:1101:ASP:H	2.20	0.44
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.17	0.44
6:H:91:ASP:C	6:H:93:TYR:N	2.70	0.44
8:J:32:GLU:CD	8:J:32:GLU:N	2.62	0.44
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.99	0.44
1:A:1066:VAL:O	1:A:1067:LEU:C	2.54	0.44
1:A:1197:LEU:HD12	1:A:1209:MET:SD	2.57	0.44
2:B:864:LYS:CG	2:B:871:THR:HG23	2.47	0.44
2:B:990:ILE:HG22	2:B:992:ILE:H	1.82	0.44
4:E:10:SER:O	4:E:14:ARG:HG3	2.17	0.44
6:H:42:ILE:CG2	6:H:43:ASN:N	2.80	0.44
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.99	0.44
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.32	0.44
1:A:269:ILE:HD11	1:A:303:TYR:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:PHE:HA	1:A:595:THR:CB	2.48	0.44
1:A:66:LYS:O	1:A:67:CYS:HB2	2.17	0.44
1:A:783:THR:CG2	1:A:815:PHE:CE2	3.00	0.44
1:A:903:ASN:O	1:A:904:THR:C	2.55	0.44
3:C:238:ILE:HG23	3:C:242:GLN:CB	2.48	0.44
4:E:43:LYS:HA	4:E:47:CYS:SG	2.57	0.44
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.70	0.44
1:A:90:VAL:CG1	1:A:91:PHE:N	2.79	0.44
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.83	0.44
2:B:575:PRO:HG2	2:B:576:ASP:N	2.32	0.44
2:B:603:LEU:O	2:B:609:ILE:N	2.49	0.44
2:B:627:PHE:CB	2:B:632:ARG:HH11	2.30	0.44
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.52	0.44
2:B:864:LYS:HD3	2:B:871:THR:OG1	2.18	0.44
2:B:969:ARG:NH2	3:C:59:ALA:HB1	2.32	0.44
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.79	0.44
4:E:39:LEU:HG	4:E:43:LYS:HE3	1.99	0.44
4:E:56:LYS:HG3	4:E:84:ASP:HB2	1.99	0.44
6:H:139:ASN:O	6:H:140:ALA:CB	2.65	0.44
1:A:341:MET:CE	1:A:343:LYS:HE3	2.48	0.44
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.98	0.44
1:A:591:PHE:HA	1:A:595:THR:HB	1.99	0.44
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.17	0.44
4:E:35:VAL:C	4:E:37:LEU:H	2.20	0.44
8:J:7:CYS:HA	8:J:49:MET:HE3	2.00	0.44
1:A:465:TYR:HA	9:K:2:ASN:O	2.17	0.44
1:A:317:LYS:HD2	1:A:321:PRO:CG	2.45	0.44
2:B:1135:ARG:HG3	2:B:1147:LEU:HD22	2.00	0.44
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.83	0.44
2:B:200:GLY:HA2	2:B:202:TYR:CD2	2.53	0.44
2:B:226:PHE:CE2	2:B:398:ARG:HG2	2.53	0.44
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.45	0.44
3:C:196:ASP:OD2	3:C:199:LYS:HG3	2.18	0.44
6:H:138:GLU:O	6:H:139:ASN:C	2.56	0.44
7:I:28:GLU:HG3	7:I:28:GLU:O	2.17	0.44
7:I:94:ASP:OD1	7:I:94:ASP:N	2.50	0.44
10:L:54:ARG:NH1	10:L:54:ARG:HB2	2.23	0.44
1:A:442:VAL:CB	1:A:489:LEU:HD11	2.48	0.44
1:A:780:VAL:O	1:A:782:ARG:HG2	2.17	0.44
1:A:825:ILE:HD11	2:B:512:ARG:O	2.18	0.44
2:B:247:GLY:O	2:B:248:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASN:O	2:B:308:TRP:N	2.48	0.44
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.99	0.44
2:B:377:PHE:O	2:B:378:LEU:C	2.56	0.44
6:H:43:ASN:C	6:H:45:GLU:H	2.21	0.44
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.33	0.44
2:B:618:ASP:HB3	2:B:621:GLU:CB	2.48	0.44
2:B:979:LYS:HB3	2:B:1095:LEU:HB2	1.99	0.44
3:C:74:SER:HB3	3:C:77:ILE:HG13	1.99	0.44
8:J:17:LYS:O	8:J:18:TRP:C	2.55	0.44
1:A:1106:ASN:HA	1:A:1383:SER:OG	2.18	0.43
1:A:1425:SER:HA	1:A:1428:VAL:HG23	1.98	0.43
1:A:154:SER:HB3	1:A:162:VAL:HG23	2.00	0.43
1:A:403:LYS:O	1:A:404:TYR:O	2.35	0.43
1:A:499:ALA:O	1:A:503:GLN:HB2	2.18	0.43
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.62	0.43
1:A:534:LEU:O	1:A:574:GLY:HA3	2.18	0.43
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.86	0.43
2:B:864:LYS:CB	2:B:871:THR:HA	2.48	0.43
3:C:56:THR:HG21	3:C:145:CYS:SG	2.57	0.43
3:C:62:PHE:C	3:C:62:PHE:HD2	2.21	0.43
4:E:3:GLN:HG3	4:E:4:GLU:N	2.33	0.43
8:J:6:ARG:HD2	8:J:13:VAL:HG22	1.99	0.43
1:A:1161:THR:HG23	1:A:1239:ARG:HH21	1.82	0.43
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.99	0.43
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.47	0.43
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.98	0.43
2:B:446:LEU:O	2:B:446:LEU:HG	2.18	0.43
3:C:110:THR:O	3:C:110:THR:HG22	2.18	0.43
4:E:116:ILE:HG22	4:E:121:MET:HG2	2.00	0.43
1:A:1365:TYR:HD2	4:E:204:THR:HG1	1.65	0.43
4:E:88:VAL:HG11	4:E:110:PHE:CE2	2.54	0.43
10:L:29:TYR:HD1	10:L:39:SER:HA	1.82	0.43
1:A:1401:SER:O	1:A:1402:PHE:CB	2.65	0.43
1:A:172:PRO:HA	1:A:184:SER:O	2.19	0.43
1:A:849:MET:HE2	1:A:1061:GLY:CA	2.49	0.43
2:B:168:GLY:H	2:B:450:ALA:HB1	1.83	0.43
2:B:634:TYR:CD1	2:B:634:TYR:C	2.92	0.43
7:I:78:CYS:SG	7:I:103:CYS:SG	3.15	0.43
10:L:39:SER:O	10:L:40:LEU:HD23	2.18	0.43
1:A:119:ASN:HB3	1:A:122:MET:HB3	2.01	0.43
1:A:1230:GLU:O	1:A:1232:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:ILE:HD13	1:A:756:ILE:HA	1.90	0.43
2:B:130:VAL:HG12	2:B:131:ASP:H	1.83	0.43
2:B:25:ILE:HG22	2:B:29:ASP:HB2	1.99	0.43
2:B:659:ALA:O	2:B:663:ALA:HB2	2.19	0.43
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.48	0.43
3:C:56:THR:HG22	3:C:57:VAL:H	1.79	0.43
3:C:69:LEU:HB3	8:J:5:VAL:HG11	1.99	0.43
1:A:1143:LEU:N	1:A:1273:LEU:HD22	2.33	0.43
1:A:300:VAL:O	1:A:304:MET:HG3	2.18	0.43
1:A:179:LEU:HD21	1:A:308:ILE:HD13	2.01	0.43
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.50	0.43
3:C:77:ILE:HG22	3:C:161:LYS:HE3	1.99	0.43
1:A:1135:ARG:HG3	1:A:1282:VAL:CG1	2.48	0.43
1:A:123:ARG:NH2	1:A:155:GLU:OE2	2.50	0.43
1:A:392:VAL:HG21	1:A:426:LEU:HD11	2.00	0.43
1:A:537:ARG:NH2	1:A:599:SER:O	2.51	0.43
2:B:1128:LEU:O	2:B:1128:LEU:HG	2.18	0.43
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.59	0.43
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.52	0.43
2:B:765:PRO:O	2:B:766:ARG:C	2.56	0.43
3:C:62:PHE:CD2	3:C:62:PHE:C	2.91	0.43
4:E:29:PHE:C	4:E:30:ILE:HG13	2.38	0.43
1:A:219:PHE:CD2	1:A:231:PRO:HG2	2.54	0.43
1:A:474:VAL:O	1:A:478:TYR:HD1	2.02	0.43
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.00	0.43
1:A:675:THR:CB	1:A:736:ASN:HD21	2.31	0.43
1:A:805:LEU:C	1:A:805:LEU:HD12	2.39	0.43
1:A:855:THR:HG21	1:A:857:ARG:NE	2.28	0.43
2:B:999:MET:CG	2:B:1008:PRO:HG2	2.48	0.43
2:B:51:PHE:O	2:B:54:PHE:HB3	2.19	0.43
2:B:522:VAL:HG13	2:B:537:LYS:HB3	2.01	0.43
2:B:566:LEU:HB2	2:B:588:GLY:HA2	2.00	0.43
2:B:654:ARG:C	2:B:656:GLY:N	2.70	0.43
2:B:880:THR:O	2:B:881:ASN:HB2	2.19	0.43
2:B:856:PHE:CD2	2:B:969:ARG:HB2	2.53	0.43
3:C:11:ARG:NH2	3:C:229:TYR:HD2	2.13	0.43
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.84	0.43
7:I:32:CYS:SG	7:I:33:SER:N	2.92	0.43
8:J:6:ARG:HG3	8:J:11:GLY:O	2.18	0.43
8:J:3:VAL:O	8:J:4:PRO:C	2.55	0.43
1:A:1222:ASN:O	1:A:1223:ASP:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:HA	1:A:302:THR:HB	2.00	0.43
1:A:265:LYS:HZ2	1:A:323:LYS:H	1.65	0.43
1:A:704:ALA:CB	1:A:710:LEU:HD12	2.42	0.43
2:B:577:ALA:HB1	2:B:589:VAL:HG12	2.00	0.43
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.83	0.43
2:B:63:ILE:CG1	2:B:95:ILE:HD11	2.48	0.43
1:A:298:PHE:CZ	1:A:312:PRO:HB3	2.54	0.43
1:A:592:ASP:N	1:A:595:THR:OG1	2.50	0.43
1:A:72:GLU:OE2	1:A:76:GLU:HB3	2.19	0.43
2:B:193:LYS:HZ3	8:J:65:PRO:HG2	1.84	0.43
2:B:640:VAL:HG12	2:B:640:VAL:O	2.18	0.43
2:B:973:ILE:HA	2:B:974:PRO:HD2	1.87	0.43
3:C:120:ILE:HD11	3:C:130:GLY:O	2.18	0.43
4:E:127:ILE:O	4:E:127:ILE:HG13	2.19	0.43
5:F:150:GLU:O	5:F:151:LEU:C	2.57	0.43
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.02	0.43
10:L:28:LYS:H	10:L:39:SER:HB2	1.83	0.43
10:L:30:ILE:O	10:L:56:LEU:HA	2.18	0.43
1:A:1060:PRO:HD2	5:F:86:THR:HG21	2.01	0.43
1:A:1398:MET:O	1:A:1399:ARG:C	2.57	0.43
1:A:1404:GLU:O	1:A:1406:VAL:N	2.52	0.43
1:A:115:LEU:HD21	1:A:145:LYS:CE	2.49	0.43
1:A:57:ARG:O	1:A:68:GLN:HG3	2.18	0.43
2:B:291:ILE:HD12	2:B:375:ALA:HB1	2.00	0.43
2:B:393:LYS:HE2	2:B:621:GLU:OE1	2.19	0.43
2:B:397:ASP:OD2	2:B:515:HIS:CE1	2.72	0.43
3:C:136:ASP:OD1	3:C:141:GLY:HA2	2.19	0.43
1:A:1151:GLU:HA	7:I:44:TYR:O	2.19	0.43
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.19	0.42
1:A:345:VAL:CG2	2:B:1106:ARG:HH11	2.31	0.42
1:A:399:HIS:HE1	1:A:436:ILE:O	2.01	0.42
1:A:512:VAL:HG23	1:A:634:THR:HG21	2.01	0.42
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.59	0.42
3:C:33:LEU:HG	3:C:37:MET:HE3	2.00	0.42
4:E:1:MET:C	4:E:3:GLN:H	2.21	0.42
7:I:111:THR:CG2	7:I:112:SER:H	2.32	0.42
7:I:50:THR:HG22	7:I:51:ASN:H	1.84	0.42
1:A:1127:ASP:C	1:A:1129:GLU:N	2.72	0.42
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	2.00	0.42
1:A:128:ILE:HG21	1:A:133:LYS:CB	2.49	0.42
1:A:342:GLY:HA3	2:B:1130:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:HG2	1:A:388:LEU:HD11	2.00	0.42
1:A:44:THR:O	1:A:45:GLN:HB2	2.18	0.42
1:A:541:ILE:N	1:A:541:ILE:HD12	2.34	0.42
1:A:68:GLN:HE22	1:A:80:HIS:HB2	1.83	0.42
1:A:75:ASN:O	1:A:76:GLU:HB2	2.18	0.42
1:A:774:ARG:H	1:A:774:ARG:HG2	1.62	0.42
2:B:203:PHE:O	2:B:209:GLU:HA	2.19	0.42
2:B:376:PHE:O	2:B:586:TRP:HZ3	2.01	0.42
2:B:690:VAL:CG1	2:B:691:GLU:N	2.82	0.42
2:B:651:LEU:HD11	2:B:707:PRO:HB3	2.01	0.42
2:B:488:TYR:CD1	2:B:817:LEU:HD12	2.54	0.42
3:C:179:GLU:CD	3:C:206:ASN:HD22	2.22	0.42
4:E:102:GLU:C	4:E:104:ASN:N	2.72	0.42
1:A:250:ILE:N	1:A:258:GLY:O	2.53	0.42
1:A:335:ARG:O	1:A:339:ASN:ND2	2.52	0.42
2:B:841:MET:HE2	2:B:1010:LEU:HD11	2.00	0.42
2:B:193:LYS:NZ	8:J:65:PRO:HG2	2.35	0.42
9:K:35:PHE:N	9:K:35:PHE:CD1	2.87	0.42
1:A:547:LEU:HD22	9:K:58:PHE:CE1	2.54	0.42
1:A:1130:GLN:HG3	1:A:1130:GLN:O	2.20	0.42
1:A:453:MET:HG2	1:A:520:CYS:SG	2.60	0.42
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.19	0.42
1:A:928:LEU:HD23	1:A:928:LEU:HA	1.93	0.42
2:B:179:CYS:C	2:B:181:LEU:H	2.23	0.42
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.53	0.42
2:B:332:ASP:O	2:B:333:PHE:C	2.58	0.42
2:B:435:THR:O	2:B:435:THR:HG22	2.19	0.42
2:B:822:ASN:O	8:J:48:ARG:NH1	2.53	0.42
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.20	0.42
2:B:63:ILE:HD13	2:B:95:ILE:HD11	2.01	0.42
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.54	0.42
1:A:1004:ASN:OD1	4:E:167:ARG:HD2	2.19	0.42
6:H:40:LEU:HD21	6:H:142:LEU:HD21	2.00	0.42
8:J:36:LEU:HD22	8:J:41:LEU:HD12	2.01	0.42
9:K:101:LEU:HD23	9:K:101:LEU:O	2.19	0.42
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.35	0.42
1:A:252:PHE:O	1:A:253:ASN:C	2.58	0.42
1:A:436:ILE:CD1	1:A:491:VAL:HG21	2.47	0.42
2:B:170:LEU:O	2:B:171:PRO:C	2.55	0.42
2:B:345:LYS:CA	2:B:348:ARG:HE	2.18	0.42
2:B:446:LEU:N	2:B:446:LEU:HD23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:LEU:O	2:B:599:THR:HB	2.20	0.42
3:C:136:ASP:OD1	3:C:136:ASP:N	2.50	0.42
1:A:1077:THR:HG22	1:A:1077:THR:O	2.20	0.42
1:A:586:ILE:HD12	1:A:633:VAL:HG22	2.02	0.42
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.83	0.42
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.19	0.42
2:B:365:THR:CG2	2:B:367:LEU:H	2.33	0.42
2:B:806:THR:C	2:B:808:ALA:N	2.72	0.42
4:E:166:LYS:CE	4:E:167:ARG:HH21	2.31	0.42
5:F:116:ASP:HB3	5:F:119:ARG:HB2	2.00	0.42
5:F:101:ILE:HD13	5:F:120:ILE:HG21	2.02	0.42
9:K:83:PRO:O	9:K:86:ALA:HB3	2.20	0.42
10:L:28:LYS:N	10:L:39:SER:HB2	2.34	0.42
1:A:100:LYS:O	1:A:102:VAL:N	2.53	0.42
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.83	0.42
1:A:849:MET:CE	1:A:1061:GLY:CA	2.84	0.42
1:A:855:THR:CG2	1:A:856:THR:N	2.82	0.42
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.48	0.42
2:B:570:VAL:HB	2:B:573:GLN:HB2	2.01	0.42
2:B:765:PRO:O	2:B:768:THR:N	2.51	0.42
2:B:899:ILE:HG22	2:B:900:ALA:N	2.34	0.42
4:E:77:SER:HB2	4:E:105:PHE:CD2	2.54	0.42
6:H:42:ILE:HG22	6:H:43:ASN:N	2.35	0.42
6:H:49:VAL:HG12	6:H:50:ALA:N	2.34	0.42
7:I:50:THR:CG2	7:I:51:ASN:N	2.82	0.42
8:J:30:LEU:HD22	8:J:34:THR:HG21	2.01	0.42
8:J:5:VAL:O	8:J:6:ARG:CB	2.66	0.42
10:L:45:ALA:C	10:L:46:VAL:HG23	2.40	0.42
1:A:569:LYS:HG2	1:A:571:LEU:CD1	2.49	0.42
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.01	0.42
2:B:274:PRO:HG3	2:B:359:GLU:O	2.19	0.42
2:B:864:LYS:HD3	2:B:871:THR:CB	2.50	0.42
3:C:239:PRO:HD2	3:C:242:GLN:HG3	2.02	0.42
3:C:264:GLN:H	3:C:264:GLN:HG3	1.64	0.42
1:A:1001:ARG:O	1:A:1002:GLY:C	2.58	0.42
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.20	0.42
1:A:1425:SER:HA	1:A:1428:VAL:CG2	2.50	0.42
1:A:261:ASP:OD1	1:A:315:LEU:HD13	2.19	0.42
1:A:815:PHE:O	1:A:818:MET:HB2	2.20	0.42
2:B:682:SER:O	2:B:686:ASN:ND2	2.53	0.42
2:B:744:HIS:CD2	2:B:746:SER:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:755:ILE:HG22	2:B:755:ILE:O	2.20	0.42
2:B:956:THR:HG23	2:B:961:LEU:N	2.35	0.42
4:E:39:LEU:O	4:E:42:PHE:HB3	2.20	0.42
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.20	0.42
1:A:551:TYR:CE2	9:K:62:LYS:HE2	2.54	0.42
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.84	0.42
1:A:100:LYS:CE	1:A:176:LYS:HB2	2.48	0.42
1:A:306:ASN:ND2	1:A:322:VAL:CG1	2.83	0.42
1:A:418:SER:O	1:A:420:ARG:N	2.53	0.42
1:A:714:PHE:O	1:A:718:VAL:HG23	2.20	0.42
2:B:486:TYR:CD2	2:B:1096:ARG:CZ	3.03	0.42
3:C:31:ASN:O	3:C:34:ARG:HB3	2.20	0.42
3:C:265:MET:HE1	9:K:19:LEU:O	2.19	0.42
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.87	0.41
1:A:1359:ASP:C	1:A:1361:SER:H	2.23	0.41
1:A:112:LYS:NZ	1:A:165:GLY:H	2.18	0.41
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.46	0.41
1:A:7:SER:C	1:A:9:ALA:H	2.24	0.41
1:A:992:ASP:O	1:A:995:GLU:HB2	2.20	0.41
2:B:1177:HIS:O	2:B:1179:GLN:HG3	2.20	0.41
2:B:1183:LYS:C	2:B:1185:CYS:N	2.72	0.41
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.84	0.41
2:B:627:PHE:HB3	2:B:632:ARG:HH11	1.84	0.41
8:J:1:MET:O	8:J:2:ILE:O	2.38	0.41
3:C:146:LYS:HB2	8:J:57:ILE:CD1	2.50	0.41
10:L:46:VAL:O	10:L:47:ARG:HG3	2.19	0.41
1:A:1045:VAL:O	1:A:1046:LEU:C	2.56	0.41
1:A:1436:ILE:O	1:A:1436:ILE:HG13	2.20	0.41
1:A:23:SER:O	1:A:27:VAL:HG23	2.20	0.41
1:A:289:ILE:C	1:A:291:GLU:H	2.24	0.41
1:A:179:LEU:HD21	1:A:308:ILE:CD1	2.50	0.41
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.19	0.41
2:B:225:VAL:HA	2:B:237:VAL:O	2.20	0.41
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.53	0.41
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.41
4:E:5:ASN:O	4:E:9:ILE:HG13	2.19	0.41
5:F:147:SER:O	5:F:148:VAL:C	2.58	0.41
8:J:9:SER:OG	8:J:48:ARG:NH2	2.53	0.41
1:A:1064:VAL:O	1:A:1064:VAL:HG12	2.21	0.41
1:A:225:ASN:ND2	1:A:228:PHE:HD1	2.16	0.41
1:A:252:PHE:CD1	1:A:252:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ALA:O	1:A:271:LYS:HG3	2.19	0.41
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.50	0.41
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.50	0.41
1:A:845:LEU:N	1:A:845:LEU:HD23	2.35	0.41
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	2.01	0.41
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.02	0.41
2:B:532:ALA:HB1	2:B:536:VAL:HG23	2.02	0.41
2:B:914:LYS:N	2:B:938:SER:HB3	2.35	0.41
3:C:75:MET:CG	3:C:246:ARG:HH22	2.30	0.41
4:E:165:LEU:HD21	4:E:175:LEU:HD11	2.02	0.41
4:E:178:ILE:HG23	4:E:214:CYS:HA	2.03	0.41
8:J:52:THR:HG22	8:J:52:THR:O	2.19	0.41
2:B:784:ASN:HB3	8:J:63:TYR:CZ	2.56	0.41
9:K:18:LYS:HA	9:K:18:LYS:HD3	1.85	0.41
1:A:1364:ASN:HD21	1:A:1366:ARG:H	1.64	0.41
1:A:1364:ASN:CG	1:A:1366:ARG:HH11	2.24	0.41
1:A:311:GLN:HA	1:A:312:PRO:HD2	1.90	0.41
1:A:319:GLY:O	1:A:321:PRO:HD3	2.19	0.41
1:A:399:HIS:C	1:A:401:GLY:N	2.73	0.41
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.21	0.41
2:B:737:THR:CG2	2:B:737:THR:O	2.69	0.41
2:B:871:THR:CG2	2:B:872:GLU:N	2.68	0.41
2:B:873:THR:CG2	2:B:874:PHE:N	2.84	0.41
2:B:879:ARG:HD2	2:B:883:LEU:CD2	2.47	0.41
3:C:66:ARG:CZ	8:J:2:ILE:CG2	2.98	0.41
6:H:82:PRO:HG3	9:K:54:ARG:CG	2.43	0.41
8:J:43:ARG:HG2	8:J:43:ARG:H	1.67	0.41
9:K:49:GLU:HG3	9:K:94:ILE:HG12	2.01	0.41
1:A:1009:ASN:HA	1:A:1012:ARG:NH1	2.36	0.41
1:A:315:LEU:HD12	1:A:321:PRO:CG	2.41	0.41
1:A:503:GLN:HG3	5:F:90:ARG:HH21	1.84	0.41
2:B:205:ILE:HD11	2:B:461:LEU:HD23	2.02	0.41
2:B:551:PRO:HG2	2:B:552:MET:SD	2.60	0.41
2:B:43:LEU:CD1	2:B:812:LEU:HD23	2.49	0.41
2:B:825:VAL:HG12	2:B:826:ALA:H	1.83	0.41
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.35	0.41
3:C:77:ILE:C	3:C:79:GLN:N	2.73	0.41
4:E:78:LEU:C	4:E:78:LEU:HD23	2.41	0.41
1:A:1141:THR:HG21	1:A:1207:LEU:HD11	2.03	0.41
1:A:1173:HIS:O	1:A:1174:PHE:CG	2.74	0.41
1:A:1391:ARG:HB3	1:A:1392:SER:H	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.39	0.41
1:A:550:LEU:HD23	1:A:550:LEU:HA	1.88	0.41
1:A:702:LEU:HD23	1:A:702:LEU:HA	1.87	0.41
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.86	0.41
3:C:248:ILE:HG23	9:K:98:LEU:HD22	2.03	0.41
3:C:82:TYR:O	3:C:83:SER:C	2.59	0.41
5:F:127:GLU:O	5:F:128:LYS:C	2.59	0.41
6:H:84:ALA:HA	6:H:87:ARG:CG	2.50	0.41
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	2.21	0.41
1:A:1193:LEU:HB2	1:A:1260:LEU:CD1	2.45	0.41
1:A:1215:ARG:NH1	1:A:1273:LEU:O	2.53	0.41
1:A:1140:HIS:CE1	1:A:1272:THR:HG23	2.55	0.41
1:A:1300:LYS:NZ	1:A:1300:LYS:HB3	2.36	0.41
1:A:152:VAL:HG23	1:A:164:ARG:HD3	2.01	0.41
1:A:511:ILE:HG12	1:A:521:MET:CE	2.51	0.41
1:A:535:THR:HG23	1:A:575:LYS:HE3	2.03	0.41
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.49	0.41
1:A:974:ASP:HB3	6:H:136:LYS:HZ3	1.85	0.41
1:A:486:GLU:OE1	2:B:1102:LYS:HD3	2.20	0.41
1:A:505:CYS:HB3	2:B:1141:HIS:CG	2.56	0.41
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.55	0.41
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.33	0.41
3:C:56:THR:CG2	3:C:57:VAL:H	2.34	0.41
3:C:69:LEU:HA	3:C:69:LEU:HD12	1.83	0.41
4:E:191:LYS:O	4:E:192:ARG:C	2.59	0.41
4:E:82:PHE:N	4:E:82:PHE:CD1	2.89	0.41
5:F:111:LEU:HD23	5:F:114:GLU:O	2.20	0.41
5:F:130:ILE:HA	5:F:131:PRO:HD2	1.83	0.41
5:F:82:THR:HA	5:F:83:PRO:HD3	1.75	0.41
1:A:254:GLU:O	1:A:255:SER:OG	2.35	0.41
1:A:67:CYS:O	1:A:70:CYS:SG	2.79	0.41
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.56	0.41
2:B:484:ASN:CG	2:B:486:TYR:CE1	2.94	0.41
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.41
3:C:127:ARG:HG2	3:C:127:ARG:H	1.70	0.41
1:A:868:TYR:CE2	1:A:1058:VAL:HG21	2.56	0.41
1:A:100:LYS:CE	1:A:176:LYS:HD2	2.50	0.41
1:A:214:ILE:HG22	1:A:218:ASP:HB2	2.02	0.41
1:A:734:GLU:HA	1:A:737:LEU:HD12	2.03	0.41
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.56	0.41
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ALA:HB3	2:B:655:LYS:CE	2.51	0.41
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.02	0.41
2:B:806:THR:N	2:B:809:MET:HE3	2.35	0.41
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.86	0.41
4:E:24:LYS:HE3	4:E:30:ILE:O	2.21	0.41
7:I:78:CYS:O	7:I:79:HIS:C	2.59	0.41
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.55	0.41
1:A:1035:TYR:O	1:A:1036:ARG:C	2.59	0.41
1:A:148:CYS:O	1:A:168:GLY:HA2	2.21	0.41
1:A:22:PHE:HD2	1:A:26:GLU:HG2	1.86	0.41
1:A:751:SER:OG	2:B:1015:HIS:HE1	2.04	0.41
2:B:112:LEU:HD12	2:B:113:TYR:H	1.86	0.41
2:B:345:LYS:HB3	2:B:346:GLU:H	1.57	0.41
2:B:254:LEU:HD22	2:B:361:LEU:HD13	2.03	0.41
2:B:59:LEU:HD11	2:B:417:PHE:CZ	2.56	0.41
2:B:707:PRO:CG	2:B:708:GLU:N	2.84	0.41
7:I:96:SER:OG	7:I:98:VAL:HG23	2.20	0.41
1:A:1199:ARG:HG2	1:A:1203:ASN:ND2	2.36	0.41
1:A:519:PRO:HD3	1:A:631:HIS:CG	2.56	0.41
1:A:608:ILE:HB	1:A:613:ILE:HD11	2.03	0.41
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.21	0.41
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.50	0.41
2:B:1182:CYS:C	2:B:1183:LYS:O	2.59	0.41
2:B:1222:ARG:HG2	2:B:1223:ASP:N	2.36	0.41
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.56	0.41
2:B:520:GLY:HA2	2:B:748:ILE:HG22	2.02	0.41
2:B:782:LEU:HD23	2:B:782:LEU:HA	1.85	0.41
2:B:806:THR:C	2:B:808:ALA:H	2.24	0.41
3:C:182:PRO:HB3	3:C:206:ASN:HB2	2.01	0.41
2:B:997:GLU:HB2	3:C:35:ARG:HH21	1.86	0.41
7:I:10:CYS:SG	7:I:31:THR:CG2	3.09	0.41
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.21	0.40
1:A:1116:LEU:HD12	1:A:1329:THR:OG1	2.21	0.40
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.70	0.40
1:A:538:ASP:OD1	6:H:22:LYS:HG3	2.22	0.40
1:A:629:LEU:O	1:A:633:VAL:HG23	2.21	0.40
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.54	0.40
1:A:948:VAL:HG12	1:A:948:VAL:O	2.20	0.40
2:B:1152:MET:HG2	2:B:1153:GLU:H	1.86	0.40
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.56	0.40
2:B:510:LYS:N	2:B:511:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:575:PRO:CG	2:B:576:ASP:H	2.34	0.40
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.50	0.40
2:B:984:HIS:CD2	2:B:1025:HIS:CA	3.03	0.40
3:C:40:GLU:O	3:C:250:THR:HG21	2.21	0.40
6:H:130:ARG:C	6:H:132:LEU:N	2.72	0.40
9:K:63:VAL:HG12	9:K:71:PHE:HB3	2.03	0.40
1:A:107:CYS:SG	1:A:148:CYS:CB	3.04	0.40
2:B:1037:LEU:HD11	2:B:1064:TYR:CE1	2.56	0.40
2:B:202:TYR:CD2	2:B:483:LEU:HD22	2.56	0.40
2:B:597:MET:HE3	2:B:600:LEU:HD12	2.03	0.40
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.56	0.40
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.84	0.40
1:A:326:ARG:HD3	1:A:1406:VAL:HG11	2.03	0.40
1:A:475:THR:CG2	1:A:476:SER:N	2.85	0.40
1:A:613:ILE:O	1:A:614:PHE:HB3	2.22	0.40
1:A:61:ILE:HG22	1:A:62:ASP:N	2.30	0.40
1:A:809:THR:H	1:A:812:GLU:HB2	1.86	0.40
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.57	0.40
2:B:23:ALA:HB3	2:B:655:LYS:CD	2.51	0.40
2:B:701:ILE:HB	2:B:739:THR:OG1	2.21	0.40
2:B:842:ASN:HD22	2:B:845:SER:CB	2.34	0.40
2:B:859:TYR:CE2	2:B:942:ARG:HG3	2.56	0.40
2:B:959:ASP:O	2:B:960:GLY:C	2.59	0.40
4:E:116:ILE:CG2	4:E:121:MET:HG2	2.52	0.40
4:E:72:PHE:CD1	4:E:72:PHE:N	2.89	0.40
1:A:1001:ARG:HB2	5:F:80:ALA:O	2.21	0.40
6:H:84:ALA:HA	6:H:87:ARG:CB	2.51	0.40
7:I:101:PHE:CD1	7:I:101:PHE:N	2.89	0.40
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.56	0.40
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.03	0.40
1:A:1332:PHE:CD1	1:A:1381:LEU:HD13	2.56	0.40
1:A:1391:ARG:O	1:A:1392:SER:HB3	2.22	0.40
1:A:189:ARG:O	1:A:190:ALA:HB3	2.21	0.40
1:A:545:GLN:O	1:A:549:MET:HG3	2.21	0.40
1:A:666:ILE:O	1:A:667:GLY:C	2.59	0.40
1:A:683:ILE:O	1:A:686:ALA:HB3	2.21	0.40
2:B:1050:ILE:CG2	2:B:1055:ILE:HD11	2.52	0.40
2:B:1180:PHE:O	2:B:1181:GLU:O	2.39	0.40
2:B:121:ASN:HD22	2:B:121:ASN:N	2.19	0.40
2:B:348:ARG:O	2:B:351:TYR:HB3	2.21	0.40
2:B:603:LEU:HD23	2:B:603:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:693:ILE:HD13	2:B:701:ILE:HD13	2.04	0.40
2:B:893:LEU:HA	2:B:893:LEU:HD23	1.91	0.40
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.36	0.40
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.88	0.40
3:C:175:ALA:CB	8:J:43:ARG:NH1	2.84	0.40
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.22	0.40
1:A:1129:GLU:O	1:A:1132:LYS:HB2	2.21	0.40
1:A:269:ILE:HD11	1:A:303:TYR:HB3	2.03	0.40
1:A:341:MET:HE3	1:A:343:LYS:HE3	2.04	0.40
2:B:292:ILE:N	2:B:293:PRO:HD2	2.36	0.40
3:C:167:HIS:HE1	10:L:70:ARG:O	2.05	0.40
3:C:62:PHE:HD2	3:C:62:PHE:O	2.05	0.40
3:C:77:ILE:O	3:C:79:GLN:N	2.54	0.40
3:C:92:CYS:C	3:C:94:LYS:H	2.24	0.40
4:E:112:TYR:CZ	4:E:136:ASN:HB2	2.57	0.40
1:A:946:VAL:HG22	4:E:201:LYS:HD2	2.04	0.40
6:H:44:VAL:HG13	6:H:48:PRO:HA	2.03	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:B:106:ASP:OD1	2:B:106:ASP:OD1[2_655]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1138 (81%)	203 (14%)	65 (5%)	3	17
2	B	1061/1224 (87%)	868 (82%)	128 (12%)	65 (6%)	2	11
3	C	264/318 (83%)	210 (80%)	35 (13%)	19 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	213/215 (99%)	184 (86%)	27 (13%)	2 (1%)	20	60
5	F	82/155 (53%)	63 (77%)	15 (18%)	4 (5%)	2	16
6	H	129/146 (88%)	91 (70%)	22 (17%)	16 (12%)	0	1
7	I	120/122 (98%)	97 (81%)	17 (14%)	6 (5%)	2	16
8	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	2	16
9	K	112/120 (93%)	106 (95%)	5 (4%)	1 (1%)	20	60
10	L	44/70 (63%)	28 (64%)	9 (20%)	7 (16%)	0	0
All	All	3494/4173 (84%)	2838 (81%)	468 (13%)	188 (5%)	2	14

All (188) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	35	ILE
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	87	ALA
1	A	167	CYS
1	A	196	GLU
1	A	257	ARG
1	A	314	ALA
1	A	384	ASN
1	A	404	TYR
1	A	465	TYR
1	A	567	LYS
1	A	597	LEU
1	A	904	THR
1	A	998	LEU
1	A	1036	ARG
1	A	1114	PRO
1	A	1122	PRO
1	A	1127	ASP
1	A	1223	ASP
1	A	1377	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1401	SER

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Mol	Chain	Res	Type
1	A	1416	ALA
2	B	65	GLU
2	B	136	THR
2	B	175	ARG
2	B	367	LEU
2	B	436	VAL
2	B	480	SER
2	B	531	GLN
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	734	HIS
2	B	864	LYS
2	B	884	ARG
2	B	943	SER
2	B	958	GLN
2	B	992	ILE
2	B	1108	ARG
2	B	1156	ASP
2	B	1167	GLY
2	B	1176	ASN
2	B	1181	GLU
2	B	1183	LYS
2	B	1221	SER
2	B	1222	ARG
3	C	90	ASP
3	C	141	GLY
3	C	174	ALA
5	F	73	ALA
5	F	128	LYS
6	H	81	PRO
6	H	83	GLN
6	H	140	ALA
7	I	11	ASN
7	I	79	HIS
8	J	2	ILE
10	L	38	LEU
10	L	64	LEU
1	A	54	ASN
1	A	67	CYS
1	A	75	ASN
1	A	109	HIS

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Mol	Chain	Res	Type
1	A	154	SER
1	A	186	LYS
1	A	290	GLU
1	A	920	LEU
1	A	986	ILE
1	A	1224	LEU
1	A	1231	ASP
1	A	1392	SER
2	B	55	VAL
2	B	174	LEU
2	B	200	GLY
2	B	247	GLY
2	B	333	PHE
2	B	347	LYS
2	B	364	ILE
2	B	575	PRO
2	B	649	LYS
2	B	887	HIS
2	B	901	PRO
2	B	907	GLY
2	B	960	GLY
2	B	996	ARG
2	B	1066	SER
2	B	1104	HIS
2	B	1154	ALA
3	C	4	GLU
3	C	5	GLY
3	C	130	GLY
3	C	142	VAL
3	C	195	GLN
3	C	241	ASP
6	H	17	PRO
6	H	32	THR
6	H	82	PRO
6	H	128	ASN
6	H	139	ASN
7	I	116	ASN
8	J	26	GLN
10	L	37	LYS
10	L	39	SER
1	A	79	GLY
1	A	101	LYS

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Mol	Chain	Res	Type
1	A	324	SER
1	A	419	LYS
1	A	464	PRO
1	A	1221	LYS
1	A	1280	GLU
2	B	21	GLU
2	B	47	GLN
2	B	641	GLU
2	B	1109	GLY
3	C	175	ALA
3	C	202	PRO
3	C	212	PRO
3	C	227	THR
3	C	237	SER
6	H	51	ALA
6	H	62	SER
6	H	90	ALA
6	H	138	GLU
7	I	121	PHE
1	A	197	PRO
1	A	307	ASP
1	A	321	PRO
1	A	399	HIS
1	A	591	PHE
1	A	958	VAL
1	A	1172	LEU
2	B	466	TRP
2	B	619	ILE
2	B	655	LYS
2	B	731	VAL
2	B	791	THR
2	B	792	MET
2	B	813	LYS
2	B	1046	PRO
3	C	78	GLU
3	C	149	LYS
6	H	77	ARG
6	H	111	LEU
6	H	135	LEU
7	I	23	ASN
8	J	6	ARG
9	K	107	THR

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Mol	Chain	Res	Type
10	L	56	LEU
1	A	51	GLY
1	A	84	ILE
1	A	424	ILE
1	A	599	SER
1	A	752	LYS
1	A	875	ALA
1	A	1397	LEU
1	A	1437	GLY
2	B	90	ILE
2	B	179	CYS
2	B	180	TYR
2	B	707	PRO
2	B	938	SER
2	B	1017	ILE
3	C	28	ALA
3	C	214	ASN
5	F	81	THR
10	L	26	THR
2	B	168	GLY
2	B	1018	PRO
4	E	86	PRO
5	F	131	PRO
6	H	107	VAL
10	L	45	ALA
2	B	565	PRO
7	I	62	ILE
2	B	1184	GLY
4	E	30	ILE
2	B	167	ILE
3	C	240	VAL
1	A	1242	VAL
2	B	100	PRO
1	A	93	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	1234/1520 (81%)	1165 (94%)	69 (6%)	25	61
2	B	942/1061 (89%)	884 (94%)	58 (6%)	21	57
3	C	234/274 (85%)	221 (94%)	13 (6%)	25	61
4	E	197/197 (100%)	193 (98%)	4 (2%)	60	86
5	F	74/137 (54%)	67 (90%)	7 (10%)	10	37
6	H	117/128 (91%)	108 (92%)	9 (8%)	15	48
7	I	116/116 (100%)	107 (92%)	9 (8%)	15	48
8	J	60/65 (92%)	54 (90%)	6 (10%)	9	33
9	K	99/102 (97%)	90 (91%)	9 (9%)	11	39
10	L	40/57 (70%)	35 (88%)	5 (12%)	5	22
All	All	3113/3657 (85%)	2924 (94%)	189 (6%)	22	58

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	93	VAL
1	A	117	GLU
1	A	122	MET
1	A	247	ARG
1	A	321	PRO
1	A	345	VAL
1	A	351	THR
1	A	375	THR
1	A	383	TYR
1	A	397	ASN
1	A	436	ILE
1	A	445	ASN
1	A	450	LEU
1	A	474	VAL
1	A	475	THR
1	A	479	ASN
1	A	481	ASP
1	A	493	GLN
1	A	503	GLN
1	A	504	LEU
1	A	505	CYS
1	A	517	ASN
1	A	518	LYS

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Mol	Chain	Res	Type
1	A	524	VAL
1	A	538	ASP
1	A	573	SER
1	A	590	ARG
1	A	596	THR
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	666	ILE
1	A	711	ARG
1	A	756	ILE
1	A	768	GLN
1	A	774	ARG
1	A	821	ARG
1	A	826	ASP
1	A	845	LEU
1	A	854	ASN
1	A	855	THR
1	A	858	ASN
1	A	867	ILE
1	A	897	TYR
1	A	919	ILE
1	A	1035	TYR
1	A	1043	ASP
1	A	1055	ARG
1	A	1110	ASN
1	A	1122	PRO
1	A	1135	ARG
1	A	1208	THR
1	A	1257	ASP
1	A	1258	HIS
1	A	1264	GLU
1	A	1273	LEU
1	A	1295	THR
1	A	1308	THR
1	A	1331	SER
1	A	1345	ARG
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG

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Mol	Chain	Res	Type
1	A	1370	LEU
1	A	1387	HIS
1	A	1438	THR
2	B	20	ASP
2	B	63	ILE
2	B	121	ASN
2	B	174	LEU
2	B	194	GLU
2	B	199	MET
2	B	234	ILE
2	B	261	ARG
2	B	278	GLN
2	B	320	ASP
2	B	331	LEU
2	B	376	PHE
2	B	391	ASP
2	B	394	ASP
2	B	455	SER
2	B	466	TRP
2	B	480	SER
2	B	485	ARG
2	B	486	TYR
2	B	487	THR
2	B	513	GLN
2	B	538	ASN
2	B	547	VAL
2	B	559	SER
2	B	570	VAL
2	B	601	ARG
2	B	602	THR
2	B	616	ILE
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
2	B	678	GLU
2	B	679	TYR
2	B	685	LEU
2	B	737	THR
2	B	769	TYR
2	B	780	VAL
2	B	790	ASP
2	B	791	THR

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Mol	Chain	Res	Type
2	B	807	ARG
2	B	857	ARG
2	B	859	TYR
2	B	860	MET
2	B	901	PRO
2	B	969	ARG
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	997	GLU
2	B	999	MET
2	B	1028	GLU
2	B	1065	GLN
2	B	1145	SER
2	B	1159	ARG
2	B	1175	LEU
2	B	1183	LYS
2	B	1185	CYS
2	B	1211	ASN
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	57	VAL
3	C	62	PHE
3	C	69	LEU
3	C	118	LEU
3	C	122	SER
3	C	136	ASP
3	C	163	ILE
3	C	186	LEU
3	C	233	GLU
3	C	249	ASP
4	E	24	LYS
4	E	104	ASN
4	E	202	SER
4	E	204	THR
5	F	79	ARG
5	F	90	ARG
5	F	103	MET
5	F	108	PHE
5	F	111	LEU
5	F	133	VAL

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Mol	Chain	Res	Type
5	F	140	ASP
6	H	17	PRO
6	H	27	GLU
6	H	33	GLN
6	H	82	PRO
6	H	102	TYR
6	H	109	LYS
6	H	110	ASP
6	H	114	VAL
6	H	143	LEU
7	I	15	TYR
7	I	31	THR
7	I	52	ILE
7	I	55	THR
7	I	75	CYS
7	I	84	VAL
7	I	94	ASP
7	I	95	THR
7	I	118	ARG
8	J	2	ILE
8	J	6	ARG
8	J	7	CYS
8	J	43	ARG
8	J	48	ARG
8	J	55	ASP
9	K	12	LEU
9	K	25	THR
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	73	LEU
9	K	74	ARG
9	K	77	THR
9	K	101	LEU
10	L	38	LEU
10	L	50	ASP
10	L	54	ARG
10	L	58	LYS
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	92	HIS
1	A	169	ASN
1	A	225	ASN
1	A	281	HIS
1	A	297	GLN
1	A	399	HIS
1	A	435	HIS
1	A	445	ASN
1	A	479	ASN
1	A	493	GLN
1	A	631	HIS
1	A	654	ASN
1	A	698	GLN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	926	GLN
1	A	935	GLN
1	A	994	GLN
1	A	1078	GLN
1	A	1140	HIS
1	A	1203	ASN
1	A	1270	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	115	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS

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Mol	Chain	Res	Type
2	B	686	ASN
2	B	706	GLN
2	B	744	HIS
2	B	822	ASN
2	B	842	ASN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1179	GLN
2	B	1187	ASN
3	C	65	HIS
3	C	73	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
4	E	5	ASN
4	E	32	GLN
4	E	61	GLN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
4	E	114	ASN
4	E	146	HIS
4	E	147	HIS
6	H	11	GLN
6	H	128	ASN
6	H	131	ASN
6	H	134	ASN
7	I	12	ASN
7	I	83	ASN
8	J	53	HIS
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.