



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:43 PM BST

PDB ID : 3J17
EMDB ID: : EMD-5376
Title : Structure of a transcribing cypovirus by cryo-electron microscopy
Authors : Yang, C.; Ji, G.; Liu, H.; Zhang, K.; Liu, G.; Sun, F.; Zhu, P.; Cheng, L.
Deposited on : 2011-12-25
Resolution : 4.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

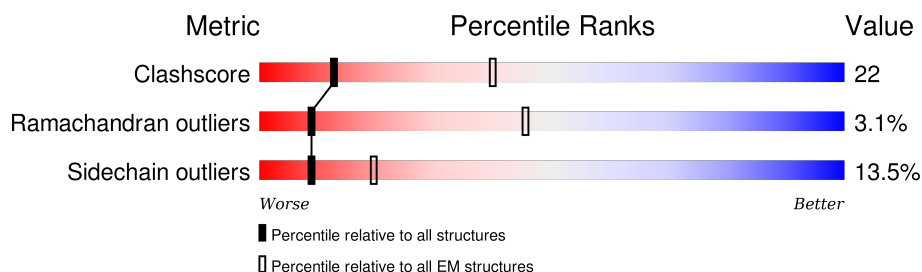
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1058	56% 32% 10% ..
2	B	1333	62% 22% • 11%
2	C	1333	63% 25% 5% 7%
3	D	448	31% 28% 6% 35%
3	E	448	30% 28% 7% 35%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32047 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Structural protein VP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1047	Total	C	N	O	P	S	0	0
			8372	5304	1444	1579	1	44		

- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1180	Total	C	N	O	S	0	0
			9317	5889	1621	1771	36		
2	C	1244	Total	C	N	O	S	0	0
			9806	6191	1704	1873	38		

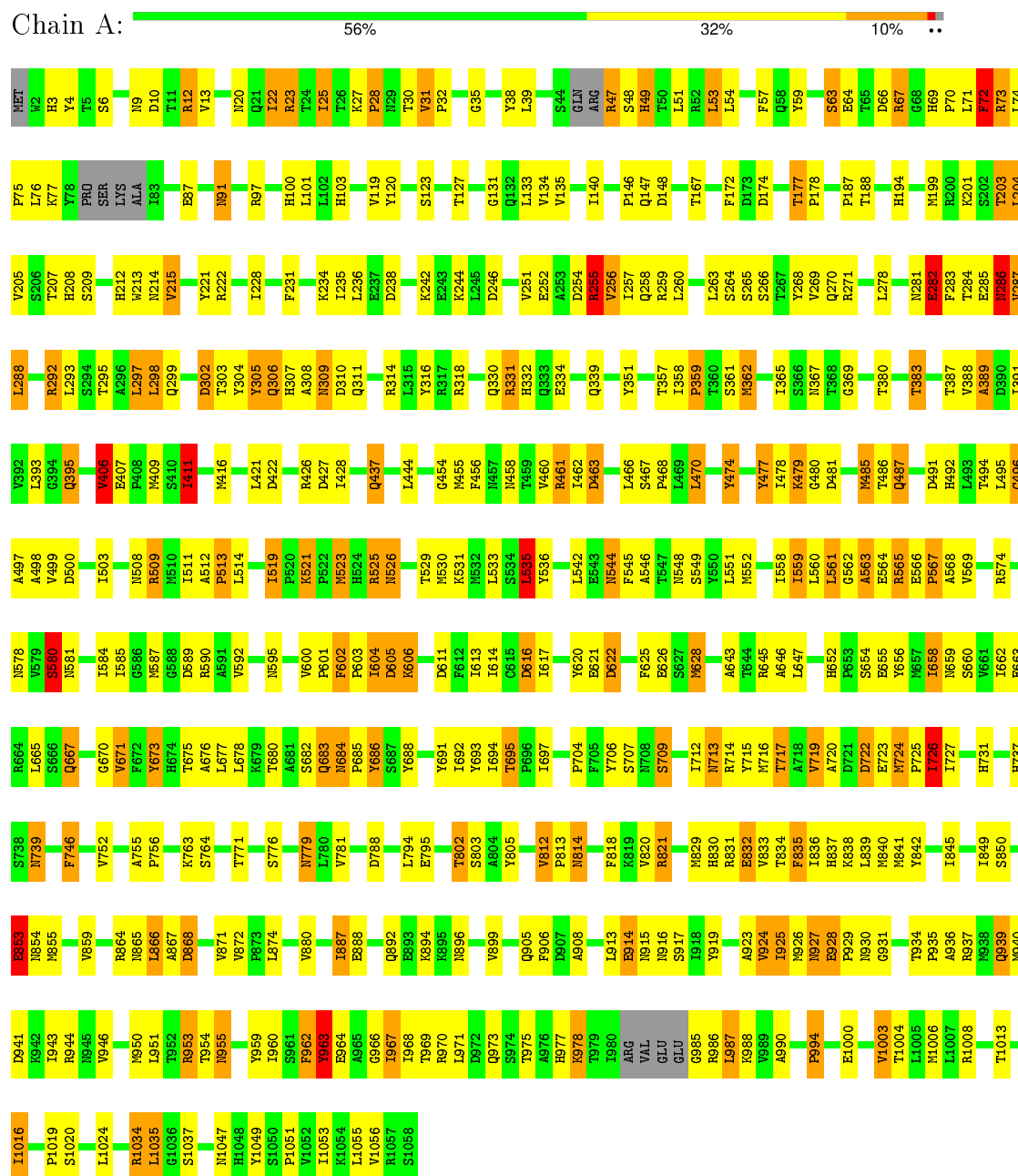
- Molecule 3 is a protein called Structural protein VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	291	Total	C	N	O	S	0	0
			2276	1446	398	424	8		
3	E	291	Total	C	N	O	S	0	0
			2276	1446	398	424	8		

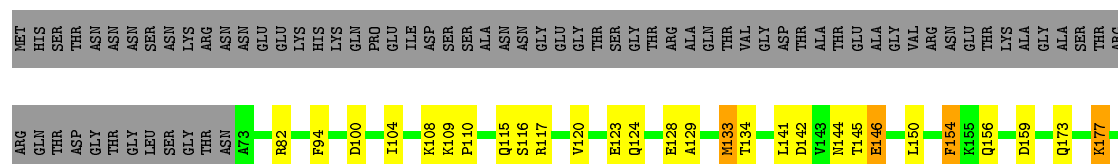
3 Residue-property plots [i](#)

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

- Molecule 1: Structural protein VP3




Chain B: 62% 22% 11%

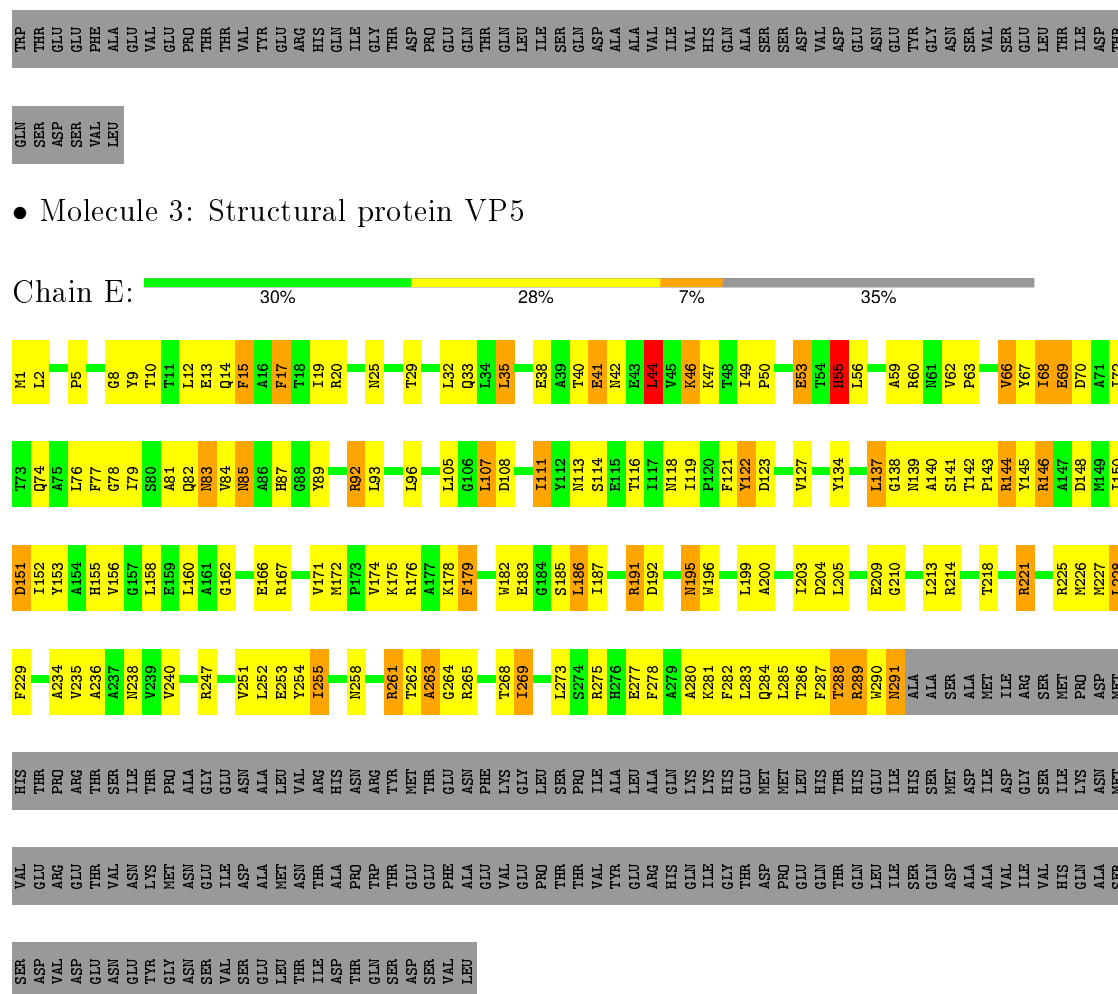


A185	T315	A563	R651	W764	R860	Q954	I1062	M1194	G1287
G191	R316	G564	R655	L767	R861	Q959	F1071	K1198	I1288
P192	M317	E565	L655	C768	R862	R959	F1071	K1198	E1292
V204	G326	S458	R666	Q769	L863	R968	V1074	L1201	V1293
I205	V337	L462	R667	C770	R864	R971	R1075	F1202	A86
I209	R338	V463	V668	T771	V868	P972	I1076	H1203	H1295
R210	L339	R469	Q669	Y772	D670	R980	L1079	D1208	I1296
R210	K341	S471	D670	F773	D671	R980	T1080	G1209	S1297
L221	R346	A472	R672	L774	R874	R985	P1086	E1214	T1306
D230	E473	A473	Q673	ARG	S878	P1088	D1083	E1309	I1309
L231	I478	I478	R674	GLN	R879	P1088	D1085	R1340	R1340
P234	S356	F589	R676	SER	Q882	R989	P1087	G1224	M1315
V237	L480	S590	R677	LYS	R883	T990	D1087	M1227	A1316
S249	N361	V592	V681	VAL	R883	R999	P1090	L1229	V1317
L255	M366	P693	L684	ASP	T890	L1000	P1090	L1229	E1318
L255	A372	L494	L684	ALA	H891	T1001	T1118	Q1234	R1319
D261	D373	V492	L687	SER	V892	L1002	H1121	P1235	M1321
I262	I376	R494	D688	ILE	V894	L1005	P1122	I1236	P1322
V265	M384	E495	T689	MET	V895	L1008	P1123	S1237	V1325
V265	I385	I600	Q690	GLU	L896	T1009	M1126	V1238	R1326
G268	S386	A499	R693	E790	Q898	R1020	A1127	M1242	A1333
Q268	T387	L512	T708	T799	R902	R1021	Y1128	R1243	
Q369	R387	M604	M709	L815	N903	I1022	S1130	A1244	
T270	Q388	R605	S710	P816	R1023	R1023	P1131	I1245	
T271	R389	F521	R711	I820	P1024	P1024	R1134	V1246	
T272	R390	F522	F712	I820	D1025	D1025	P1135	M1247	
T277	R391	E524	M713	D828	G1026	G1026	H1136	H1248	
I283	R393	L613	L714	V830	I1027	I1027	V1137	E1249	
I284	Q394	E527	R716	R831	V1028	V1028	R1144	E1250	
L286	R398	L528	F720	T834	R1030	R1030	D1153	R1263	
R287	I408	Q533	D730	Y835	Y1031	Y1031	D1153	A1267	
T288	I409	L536	Q731	Q836	F929	F929	I1156	S1262	
I290	L412	F624	E738	R837	N931	N931	V1164	Y1263	
R291	L422	R627	I745	E838	L934	L934	V1165	E1264	
I292	N430	F540	R746	A839	Q935	Q935	V1166	T1269	
I293	N430	M543	R747	D840	N936	N936	L1270	S1270	
V294	L440	P631	R747	D842	N937	N937	I1171	R1271	
I297	R441	Q632	E750	E845	N938	N938	T1174	R1272	
P298	P442	R634	T751	G846	R940	R940	A1175	M1273	
A299	K446	E547	T752	R847	E943	E943	E1176	G1274	
R302	R447	L552	T756	M849	E947	E947	P1180	P1280	
Q306	Y448	Q553	I757	R849	R948	R948	S1181	V1281	
W309	F449	R554	D759	D853	T951	T951	E1182	A1282	
	P450	T645	D759	Q854	P951	P951	H1187	ASN	
	E451	E647	I762	Y855	P952	P952		GLY	
	N452	A562	V763	L856	D953	D953		GLN	
								V1286	

• Molecule 3: Structural protein VP5

Chain D:  31% 28% 6% 35%

M1	A81	R167	L252	ARG
P5	Q82	V171	E253	TYR
T6	M83	M172	T254	MET
G7	V84	P173	I255	THR
G8	N85	V174	G256	GLU
T11	A86	K175	V257	ASN
L12	H87	R176	N258	PHE
E13	F90	A177	S259	LYS
Q14	A95	K178	M260	GLY
F15	T100	F179	T261	LEU
I19	S102	D180	T262	SER
R20	M100	S181	A263	PRO
N21	T101	S186	G264	ILE
D22	G106	I187	R265	ALA
G23	L107	L188	T266	LEU
T24	R108	I189	T269	GLN
N25	G109	L190	T270	LYS
A26	V110	D192	K281	HIS
T29	I111	V193	F282	GLU
Q30	E115	V194	L283	MET
F31	T116	M195	T286	LEU
L35	I117	W196	T287	THR
S36	M118	L199	R289	HIS
Y37	I119	R214	W290	GLU
E38	F121	ALA	N291	ILE
E41	Y122	SER	ALA	HIS
R42	A131	MET	ALA	SER
E43	I132	ASP	ALA	ASP
L44	T133	ILE	ILE	ASP
V45	A140	GLY	ARG	GLY
K46		SER	SER	SER
K47		MET	MET	ILE
T48		PRO	PRO	LYS
E53	P143	ASN	ASN	ASN
T54	R144	MET	MET	MET
H55	Y145	THR	THR	VAL
R60	R146	THR	THR	VAL
N61	A147	ARG	ARG	GLU
V62	M149	GLU	GLU	THR
V66	I150	THR	THR	THR
G67	D151	SER	SER	VAL
I68	I152	ASN	ASN	ASN
E69	Y153	LYS	LYS	LYS
D70	A154	MET	MET	ASN
Q74	H155	ASN	ASN	ILE
F77	V156	GLY	GLY	GLY
G78	G157	ILE	ILE	GLU
I79	L158	ALA	ALA	ASP
S80	E159	LEU	LEU	MET
	L160	VAL	VAL	ASN
	D164	THR	THR	THR
	A165	ALA	ALA	ALA
	I179	HIS	HIS	HIS
	V251	ASN	ASN	ASN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	8000	Depositor
Resolution determination method	feature based	Depositor
CTF correction method	each image	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	Gatan UltraScan4000 (model 895)	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.41	0/8520	0.59	1/11599 (0.0%)
2	B	0.35	0/9508	0.54	1/12941 (0.0%)
2	C	0.35	0/10006	0.55	4/13622 (0.0%)
3	D	0.37	0/2322	0.64	2/3156 (0.1%)
3	E	0.37	0/2322	0.74	5/3156 (0.2%)
All	All	0.37	0/32678	0.58	13/44474 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	E	59	ALA	CB-CA-C	-11.46	92.91	110.10
3	E	60	ARG	N-CA-CB	-7.76	96.63	110.60
3	D	7	GLY	N-CA-C	-6.60	96.61	113.10
3	E	263	ALA	N-CA-C	-5.96	94.91	111.00
1	A	535	LEU	CA-CB-CG	5.56	128.08	115.30
2	C	1201	LEU	CA-CB-CG	5.50	127.94	115.30
3	E	44	LEU	CA-CB-CG	5.41	127.73	115.30
3	D	41	GLU	N-CA-C	5.37	125.50	111.00
2	C	613	LEU	CA-CB-CG	5.22	127.31	115.30
3	E	60	ARG	N-CA-C	5.18	125.00	111.00
2	C	1079	LEU	CA-CB-CG	5.03	126.86	115.30
2	C	495	LEU	CA-CB-CG	5.03	126.86	115.30
2	B	934	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8372	0	8310	421	0
2	B	9317	0	9234	336	0
2	C	9806	0	9713	336	0
3	D	2276	0	2271	227	0
3	E	2276	0	2277	252	0
All	All	32047	0	31805	1392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1392) 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)
2:B:271:THR:CG2	2:C:237:VAL:HG23	1.34	1.53
1:A:194:HIS:CE1	3:D:146:ARG:NH1	1.74	1.53
3:E:46:LYS:HD3	3:E:155:HIS:CE1	1.49	1.45
3:E:53:GLU:HG2	3:E:145:TYR:CD1	1.57	1.37
2:B:271:THR:HG21	2:C:237:VAL:CG2	1.54	1.36
2:B:1044:ARG:NH2	3:D:266:THR:HG22	1.42	1.34
2:B:274:MET:CG	2:C:234:PRO:HD3	1.58	1.33
3:E:46:LYS:CD	3:E:155:HIS:HE1	1.40	1.31
3:D:253:GLU:OE1	3:D:254:TYR:CE2	1.83	1.30
3:D:253:GLU:HG3	3:D:254:TYR:CD2	1.68	1.29
1:A:194:HIS:CE1	3:D:146:ARG:HH11	1.37	1.29
2:B:271:THR:CG2	2:C:237:VAL:CG2	2.08	1.29
1:A:47:ARG:CZ	2:B:596:GLY:HA2	1.60	1.29
3:D:8:GLY:O	3:D:11:THR:HG22	1.34	1.27
3:D:253:GLU:OE1	3:D:254:TYR:HE2	1.03	1.27
3:E:32:LEU:O	3:E:35:LEU:CD1	1.84	1.24
1:A:47:ARG:NH2	2:B:596:GLY:CA	2.01	1.23
1:A:47:ARG:NE	2:B:595:ALA:O	1.71	1.23
1:A:47:ARG:HH21	2:B:596:GLY:N	1.35	1.22
3:E:68:ILE:C	3:E:68:ILE:HD13	1.56	1.22
1:A:194:HIS:NE2	3:D:146:ARG:NH1	1.88	1.22
3:D:5:PRO:O	3:D:6:THR:CG2	1.90	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:ASP:OD1	3:E:82:GLN:NE2	1.73	1.19
3:E:182:TRP:O	3:E:183:GLU:HG2	1.07	1.19
3:E:289:ARG:O	3:E:289:ARG:HD2	1.40	1.19
1:A:308:ALA:H	1:A:309:ASN:HB2	1.01	1.18
3:D:45:VAL:HG13	3:D:171:VAL:HG22	1.19	1.18
1:A:724:MET:HB3	1:A:725:PRO:CD	1.71	1.18
3:E:55:HIS:HD2	3:E:145:TYR:CE2	1.63	1.17
1:A:47:ARG:HH21	2:B:596:GLY:CA	1.58	1.17
1:A:47:ARG:NH2	2:B:596:GLY:HA2	1.58	1.17
3:D:5:PRO:O	3:D:6:THR:HG22	1.01	1.16
1:A:307:HIS:CB	1:A:308:ALA:HA	1.70	1.16
2:B:445:GLU:HB3	2:B:446:LYS:HA	1.17	1.15
2:B:388:GLN:OE1	2:C:499:ALA:HB1	1.41	1.15
3:E:107:LEU:HA	3:E:122:TYR:HE1	1.06	1.14
2:B:137:ILE:HD11	2:C:759:ASP:CG	1.67	1.14
3:E:158:LEU:O	3:E:162:GLY:HA3	1.48	1.13
2:B:1044:ARG:NE	3:D:266:THR:CG2	2.12	1.12
1:A:307:HIS:HB2	1:A:308:ALA:CA	1.79	1.12
3:E:205:LEU:HD13	3:E:205:LEU:O	1.49	1.12
3:D:217:LYS:HD3	3:D:290:TRP:CH2	1.82	1.12
3:E:175:LYS:HB2	3:E:255:ILE:CD1	1.80	1.11
1:A:308:ALA:N	1:A:309:ASN:HB2	1.66	1.10
3:E:137:LEU:HD23	3:E:137:LEU:C	1.72	1.09
3:E:49:ILE:HG23	3:E:50:PRO:HD2	1.35	1.08
3:D:149:MET:HE3	3:D:260:MET:HE1	1.15	1.08
1:A:127:THR:CG2	2:B:640:GLN:H	1.68	1.07
3:E:182:TRP:O	3:E:183:GLU:CG	2.01	1.07
3:D:217:LYS:HD3	3:D:290:TRP:CZ3	1.88	1.06
2:B:1044:ARG:CZ	3:D:266:THR:CG2	2.34	1.06
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.19	1.06
1:A:928:GLU:HB2	1:A:929:PRO:HD2	1.32	1.06
1:A:127:THR:HG21	2:B:640:GLN:N	1.70	1.05
2:B:1044:ARG:CZ	3:D:266:THR:HG22	1.84	1.04
2:B:338:ARG:HH21	2:C:1002:LEU:HD22	1.21	1.04
3:E:191:ARG:HG3	3:E:191:ARG:NH1	1.60	1.04
3:E:32:LEU:O	3:E:35:LEU:HD12	1.57	1.03
3:E:175:LYS:CB	3:E:255:ILE:HD11	1.86	1.03
3:E:107:LEU:HA	3:E:122:TYR:CE1	1.93	1.03
2:B:274:MET:HG3	2:C:234:PRO:HD3	1.06	1.03
3:E:1:MET:HE1	3:E:121:PHE:CE2	1.94	1.02
2:B:363:ARG:CZ	3:D:80:SER:OG	2.08	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:LEU:O	3:E:35:LEU:HD11	1.57	1.02
1:A:724:MET:CB	1:A:725:PRO:HD3	1.89	1.02
1:A:127:THR:HG21	2:B:640:GLN:H	0.91	1.02
3:E:191:ARG:HH11	3:E:191:ARG:CG	1.72	1.01
3:E:53:GLU:CG	3:E:145:TYR:HD1	1.73	1.01
2:C:82:ARG:HH22	2:C:209:ASN:ND2	1.57	1.01
3:E:262:THR:HG22	3:E:263:ALA:O	1.61	1.00
1:A:47:ARG:NE	2:B:596:GLY:HA2	1.75	1.00
1:A:486:THR:O	1:A:487:GLN:HG3	1.61	0.99
3:D:153:TYR:HA	3:D:156:VAL:HG12	1.42	0.99
2:C:337:VAL:HG22	3:E:187:ILE:HD12	1.42	0.99
2:B:271:THR:HG23	2:C:237:VAL:HG23	1.02	0.99
2:B:274:MET:HG3	2:C:234:PRO:CD	1.91	0.99
3:E:127:VAL:HG12	3:E:203:ILE:HD11	1.45	0.99
3:E:158:LEU:O	3:E:162:GLY:CA	2.10	0.98
3:D:253:GLU:CG	3:D:254:TYR:CD2	2.46	0.98
3:E:68:ILE:C	3:E:68:ILE:CD1	2.30	0.98
1:A:238:ASP:OD2	1:A:259:ARG:HG3	1.62	0.98
3:E:46:LYS:CD	3:E:155:HIS:CE1	2.25	0.98
1:A:47:ARG:HH21	2:B:595:ALA:C	1.66	0.98
3:D:149:MET:HE3	3:D:260:MET:CE	1.94	0.98
1:A:174:ASP:HB3	2:B:605:ARG:NH1	1.78	0.98
3:E:68:ILE:HD13	3:E:68:ILE:O	1.63	0.97
3:E:261:ARG:HH12	3:E:265:ARG:NH2	1.62	0.97
2:B:338:ARG:NH2	2:C:1002:LEU:HD22	1.80	0.97
3:E:53:GLU:CG	3:E:145:TYR:CD1	2.47	0.97
1:A:47:ARG:CZ	2:B:595:ALA:O	2.13	0.96
3:E:55:HIS:CD2	3:E:145:TYR:CE2	2.53	0.96
2:B:891:HIS:NE2	3:D:240:VAL:HG23	1.80	0.96
2:B:367:GLU:HG3	3:D:82:GLN:OE1	1.65	0.96
1:A:127:THR:CG2	2:B:640:GLN:N	2.28	0.96
1:A:409:MET:HB3	1:A:1034:ARG:HH12	1.31	0.96
2:C:449:PHE:CZ	2:C:463:VAL:HA	2.00	0.95
3:E:261:ARG:HH12	3:E:265:ARG:HH21	1.11	0.95
3:E:68:ILE:HD11	3:E:72:ILE:CD1	1.96	0.95
3:E:107:LEU:HD23	3:E:122:TYR:CE1	2.02	0.95
3:D:149:MET:CE	3:D:260:MET:HE1	1.97	0.95
2:C:1273:ASN:O	3:E:183:GLU:OE1	1.85	0.95
3:D:153:TYR:HA	3:D:156:VAL:CG1	1.96	0.95
3:E:53:GLU:HG2	3:E:145:TYR:HD1	0.80	0.94
2:B:274:MET:HG2	2:C:234:PRO:HD3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:191:ARG:HG3	3:E:191:ARG:HH11	0.79	0.94
3:D:262:THR:HG21	3:D:270:THR:HA	1.47	0.94
2:B:891:HIS:HA	3:D:242:ARG:HD2	1.50	0.94
2:B:1044:ARG:HH21	3:D:266:THR:HG22	1.15	0.94
3:D:253:GLU:CD	3:D:254:TYR:CE2	2.41	0.94
1:A:406:VAL:HB	1:A:407:GLU:HA	1.47	0.94
2:B:137:ILE:CD1	2:C:759:ASP:CG	2.37	0.93
2:B:445:GLU:HB3	2:B:446:LYS:CA	1.97	0.93
3:E:200:ALA:O	3:E:204:ASP:OD2	1.85	0.93
2:B:1044:ARG:HE	3:D:266:THR:HG21	1.31	0.92
3:E:1:MET:CE	3:E:121:PHE:CE2	2.53	0.92
2:B:748:GLN:O	2:B:748:GLN:HG2	1.69	0.92
2:C:448:TYR:HB3	2:C:768:CYS:SG	2.08	0.92
3:D:253:GLU:HG3	3:D:254:TYR:HD2	1.10	0.92
2:B:1044:ARG:NH2	3:D:266:THR:CG2	2.33	0.92
2:B:271:THR:HG21	2:C:237:VAL:HG21	1.50	0.91
1:A:481:ASP:HB3	1:A:511:ILE:HG12	1.51	0.91
3:D:214:ARG:O	3:D:218:THR:HG23	1.69	0.91
1:A:724:MET:HB3	1:A:725:PRO:HD3	0.92	0.90
2:B:891:HIS:CD2	3:D:240:VAL:CG2	2.55	0.90
3:D:44:LEU:HD11	3:D:154:ALA:HA	1.50	0.90
1:A:565:ARG:HB3	1:A:592:VAL:N	1.86	0.89
2:B:231:LEU:HB2	2:B:249:SER:HB2	1.52	0.89
2:B:1273:ASN:OD1	3:D:79:ILE:HG21	1.71	0.89
2:B:388:GLN:OE1	2:C:499:ALA:CB	2.20	0.89
3:D:156:VAL:HG23	3:D:228:LEU:CD2	2.02	0.89
2:C:337:VAL:HG22	3:E:187:ILE:CD1	2.02	0.89
3:D:149:MET:CE	3:D:260:MET:CE	2.50	0.88
3:E:160:LEU:HD11	3:E:229:PHE:HB2	1.55	0.88
3:D:8:GLY:O	3:D:11:THR:CG2	2.20	0.88
2:C:1273:ASN:HA	3:E:183:GLU:OE1	1.71	0.88
3:E:68:ILE:HD11	3:E:72:ILE:HD12	1.57	0.87
3:E:12:LEU:HG	3:E:14:GLN:HE21	1.38	0.87
3:E:289:ARG:C	3:E:289:ARG:HD2	1.87	0.87
1:A:127:THR:HG22	2:B:639:ASN:HB2	1.56	0.86
1:A:310:ASP:CG	1:A:311:GLN:H	1.76	0.86
2:B:939:ASN:O	2:B:940:ARG:HB3	1.73	0.86
2:C:104:ILE:HG23	2:C:1310:ARG:NH2	1.89	0.86
3:E:49:ILE:CG2	3:E:50:PRO:HD2	2.06	0.86
1:A:194:HIS:CG	3:D:146:ARG:HH11	1.94	0.85
1:A:406:VAL:CB	1:A:407:GLU:HA	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:160:LEU:CD1	3:E:229:PHE:HB2	2.05	0.85
2:B:445:GLU:CB	2:B:446:LYS:HA	2.06	0.85
1:A:59:TYR:HA	1:A:167:THR:HG21	1.57	0.85
3:D:153:TYR:O	3:D:156:VAL:HG13	1.74	0.85
1:A:914:GLU:HA	1:A:950:MET:HB3	1.59	0.85
1:A:47:ARG:NH2	2:B:596:GLY:N	2.19	0.85
1:A:194:HIS:CD2	3:D:146:ARG:NH1	2.44	0.84
3:E:69:GLU:CD	3:E:69:GLU:C	2.35	0.84
1:A:406:VAL:HB	1:A:407:GLU:CA	2.06	0.84
1:A:133:LEU:HD21	2:C:545:PRO:CB	2.06	0.84
2:B:137:ILE:CD1	2:C:759:ASP:OD1	2.25	0.84
1:A:308:ALA:H	1:A:309:ASN:CB	1.88	0.84
1:A:964:GLU:HA	1:A:968:ILE:HD13	1.59	0.84
2:C:1042:TRP:CG	2:C:1043:SER:HA	2.13	0.84
1:A:563:ALA:HA	1:A:564:GLU:HG3	1.58	0.84
3:E:175:LYS:HB2	3:E:255:ILE:HD11	0.90	0.84
1:A:27:LYS:HB3	1:A:28:PRO:HD3	1.57	0.84
3:D:172:MET:HE3	3:D:175:LYS:HG3	1.57	0.84
3:E:55:HIS:O	3:E:55:HIS:CG	2.30	0.83
1:A:281:ASN:O	1:A:283:PHE:N	2.11	0.83
3:E:146:ARG:CZ	3:E:277:GLU:OE2	2.26	0.83
2:B:862:ARG:HB3	2:B:952:PHE:CE2	2.13	0.83
3:D:5:PRO:C	3:D:6:THR:HG22	1.98	0.83
1:A:47:ARG:NH2	2:B:595:ALA:C	2.31	0.83
1:A:303:THR:HB	1:A:307:HIS:NE2	1.93	0.83
1:A:565:ARG:HB3	1:A:592:VAL:H	1.40	0.83
2:B:1273:ASN:OD1	3:D:191:ARG:HA	1.79	0.83
2:B:1044:ARG:HE	3:D:266:THR:CG2	1.84	0.83
2:C:104:ILE:HG23	2:C:1310:ARG:HH22	1.43	0.83
2:B:135:LYS:CG	2:C:470:ALA:O	2.26	0.82
1:A:986:ARG:HB3	1:A:994:PRO:CB	2.09	0.82
1:A:48:SER:O	1:A:49:HIS:HB3	1.78	0.82
1:A:222:ARG:HD2	2:B:720:PHE:CZ	2.13	0.82
3:E:69:GLU:HG2	3:E:199:LEU:HB2	1.61	0.82
3:D:181:SER:HB3	3:D:250:ARG:HG2	1.61	0.82
2:B:475:ILE:O	2:B:478:ILE:HG13	1.80	0.82
3:E:79:ILE:HA	3:E:269:ILE:HD13	1.62	0.82
1:A:135:VAL:HG11	2:C:669:GLN:OE1	1.80	0.82
3:E:166:GLU:OE2	3:E:171:VAL:O	1.97	0.81
1:A:917:SER:HB3	1:A:919:TYR:HE1	1.43	0.81
2:B:420:PRO:HB2	2:B:748:GLN:OE1	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:85:ASN:ND2	3:E:141:SER:HB3	1.95	0.81
2:B:642:GLY:HA2	2:C:670:ASP:OD2	1.80	0.81
3:D:100:ASN:H	3:D:100:ASN:HD22	1.24	0.81
1:A:308:ALA:CA	1:A:309:ASN:HB2	2.11	0.81
3:D:258:ASN:OD1	3:D:259:SER:O	1.98	0.81
1:A:222:ARG:HD2	2:B:720:PHE:HZ	1.41	0.81
2:B:891:HIS:CD2	3:D:240:VAL:HG23	2.16	0.81
2:C:1037:ILE:O	2:C:1038:GLU:HB3	1.79	0.80
1:A:670:GLY:O	1:A:671:VAL:HG22	1.81	0.80
1:A:318:ARG:NH1	3:D:43:GLU:HG2	1.95	0.80
3:D:41:GLU:HA	3:D:41:GLU:OE1	1.79	0.80
3:D:264:GLY:O	3:D:266:THR:N	2.14	0.80
2:B:891:HIS:NE2	3:D:240:VAL:CG2	2.44	0.80
1:A:566:GLU:HB2	1:A:567:PRO:HD2	1.60	0.80
3:D:253:GLU:CG	3:D:254:TYR:HD2	1.89	0.80
2:C:1272:ARG:HD2	3:E:247:ARG:HH22	1.44	0.80
3:D:153:TYR:O	3:D:156:VAL:CG1	2.30	0.80
1:A:565:ARG:HG3	1:A:590:ARG:O	1.81	0.80
1:A:426:ARG:HB2	1:A:707:SER:HB2	1.64	0.80
1:A:286:ASN:CG	1:A:287:VAL:H	1.85	0.80
2:B:271:THR:HG23	2:C:237:VAL:CG2	1.93	0.79
3:E:55:HIS:HD2	3:E:145:TYR:CZ	2.00	0.79
3:E:137:LEU:O	3:E:137:LEU:HD23	1.82	0.79
3:D:41:GLU:OE1	3:D:41:GLU:CA	2.30	0.79
3:E:40:THR:CG2	3:E:41:GLU:OE2	2.30	0.79
3:E:40:THR:HG23	3:E:41:GLU:OE2	1.83	0.79
2:C:154:PHE:HB3	2:C:262:ASN:HB2	1.63	0.79
2:C:1051:ARG:HG2	2:C:1051:ARG:HH11	1.47	0.79
2:B:367:GLU:CG	3:D:82:GLN:OE1	2.31	0.78
2:C:448:TYR:C	2:C:450:PRO:HD3	2.04	0.78
1:A:31:VAL:HG23	1:A:32:PRO:HD3	1.63	0.78
3:E:158:LEU:O	3:E:162:GLY:N	2.17	0.78
2:C:1042:TRP:CB	2:C:1043:SER:HA	2.14	0.78
2:B:134:THR:HG22	2:C:472:GLU:OE1	1.84	0.78
3:D:153:TYR:CA	3:D:156:VAL:HG12	2.12	0.78
2:C:141:LEU:HG	2:C:142:ASP:H	1.49	0.78
2:C:292:ASN:O	2:C:293:ASN:HB3	1.82	0.78
2:B:1084:PRO:HB3	2:B:1207:MET:HG3	1.66	0.77
2:C:565:GLU:HG2	2:C:566:PHE:N	1.98	0.77
2:B:1273:ASN:OD1	3:D:79:ILE:CG2	2.32	0.77
3:E:56:LEU:H	3:E:56:LEU:HD23	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:GLU:OE2	2:B:752:VAL:HG13	1.85	0.77
3:D:217:LYS:CD	3:D:290:TRP:CZ3	2.67	0.77
1:A:461:ARG:HG3	1:A:461:ARG:NH1	1.96	0.77
2:C:523:THR:O	2:C:524:GLU:HB3	1.85	0.77
2:B:747:ARG:O	2:B:747:ARG:HG3	1.83	0.77
2:C:673:GLN:O	2:C:677:ARG:HB2	1.85	0.77
1:A:268:TYR:OH	2:B:562:ALA:HB1	1.84	0.77
1:A:830:HIS:HD2	1:A:1034:ARG:HH11	1.33	0.77
3:D:107:LEU:O	3:D:108:ASP:CG	2.23	0.77
2:B:137:ILE:HD12	2:C:759:ASP:OD1	1.85	0.76
2:B:1236:ILE:CG1	2:B:1237:SER:H	1.99	0.76
2:C:146:GLU:HB2	2:C:1317:VAL:O	1.84	0.76
3:E:68:ILE:HD11	3:E:72:ILE:HD11	1.65	0.76
3:E:107:LEU:HD23	3:E:122:TYR:CZ	2.20	0.76
2:C:385:ILE:HG13	2:C:708:THR:HG22	1.68	0.76
3:D:45:VAL:HG13	3:D:171:VAL:CG2	2.10	0.76
3:E:262:THR:CG2	3:E:263:ALA:O	2.33	0.76
1:A:725:PRO:O	1:A:726:ILE:HG12	1.86	0.76
2:B:558:TYR:CE2	2:B:590:SER:HB3	2.21	0.76
3:E:42:ASN:HB2	3:E:174:VAL:HB	1.68	0.76
2:B:1044:ARG:NE	3:D:266:THR:HG21	1.89	0.76
2:B:1084:PRO:HG2	2:B:1209:GLY:HA3	1.68	0.76
3:E:68:ILE:HD13	3:E:69:GLU:N	2.00	0.76
2:B:1085:ASP:O	2:B:1208:ASP:HA	1.86	0.76
2:C:1180:PRO:HB3	2:C:1209:GLY:HA2	1.69	0.75
2:C:1050:LEU:HD12	2:C:1054:ARG:HH21	1.51	0.75
3:E:69:GLU:CG	3:E:199:LEU:HB2	2.17	0.75
1:A:986:ARG:HB3	1:A:994:PRO:HB3	1.69	0.75
2:B:177:LYS:HE3	2:B:177:LYS:H	1.51	0.75
2:C:442:PRO:HB3	2:C:473:ALA:HB1	1.68	0.75
1:A:917:SER:HB3	1:A:919:TYR:CE1	2.22	0.74
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	2.01	0.74
2:B:594:LEU:HD13	2:B:596:GLY:H	1.52	0.74
2:C:853:ASP:HB2	3:D:117:ILE:HD11	1.69	0.74
2:C:408:ILE:O	2:C:412:LEU:HB2	1.87	0.74
3:E:235:VAL:HG13	3:E:258:ASN:HD22	1.51	0.74
2:C:1042:TRP:CD1	2:C:1043:SER:HA	2.21	0.74
2:C:1273:ASN:CA	3:E:183:GLU:OE1	2.35	0.74
1:A:307:HIS:HB2	1:A:308:ALA:HA	0.82	0.74
2:C:287:ARG:HH21	2:C:326:GLY:HA3	1.52	0.74
2:C:82:ARG:NH2	2:C:209:ASN:ND2	2.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:O	1:A:28:PRO:HD2	1.88	0.73
2:B:183:SER:HB3	2:B:186:ASP:HB2	1.70	0.73
3:E:156:VAL:HG13	3:E:228:LEU:HD12	1.68	0.73
3:D:238:ASN:HB2	3:D:253:GLU:HB2	1.68	0.73
3:E:137:LEU:C	3:E:137:LEU:CD2	2.49	0.73
2:B:1080:THR:HB	2:B:1227:MET:HB3	1.70	0.73
3:D:172:MET:HG3	3:D:173:PRO:HD2	1.69	0.73
2:B:135:LYS:HG2	2:C:470:ALA:O	1.87	0.73
3:D:108:ASP:OD1	3:D:110:VAL:HG23	1.88	0.73
1:A:967:ILE:HD12	1:A:978:LYS:HB2	1.71	0.73
3:E:150:ILE:HG22	3:E:150:ILE:O	1.87	0.73
2:C:838:GLU:HG3	2:C:839:ALA:H	1.53	0.72
2:B:1023:ARG:HB2	2:B:1024:PRO:HD2	1.69	0.72
3:E:214:ARG:O	3:E:218:THR:HG23	1.89	0.72
2:C:376:ILE:HD11	2:C:1317:VAL:HG21	1.71	0.72
2:C:1025:ASP:OD1	3:D:95:ALA:HB1	1.89	0.72
3:E:182:TRP:C	3:E:183:GLU:HG2	2.05	0.72
1:A:967:ILE:HG23	1:A:968:ILE:HD12	1.72	0.72
3:D:282:PHE:O	3:D:286:THR:HG22	1.90	0.72
1:A:928:GLU:HB2	1:A:929:PRO:CD	2.17	0.72
2:B:926:VAL:HG21	2:B:936:MET:O	1.89	0.72
3:E:137:LEU:HD11	3:E:278:PHE:CZ	2.23	0.72
2:C:270:THR:HG22	2:C:291:HIS:HA	1.72	0.72
3:E:253:GLU:OE2	3:E:254:TYR:CZ	2.43	0.72
3:D:265:ARG:NE	3:D:265:ARG:HA	2.04	0.72
3:E:53:GLU:HG2	3:E:145:TYR:CE1	2.24	0.72
2:C:750:GLU:HG3	2:C:756:THR:HB	1.72	0.72
1:A:395:GLN:HA	1:A:395:GLN:HE21	1.55	0.72
2:C:494:GLU:O	2:C:757:ILE:HA	1.90	0.71
2:C:1042:TRP:HB3	2:C:1043:SER:CA	2.20	0.71
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.71	0.71
1:A:544:ASN:HD21	1:A:546:ALA:HB3	1.54	0.71
3:D:156:VAL:HG23	3:D:228:LEU:HD21	1.71	0.71
2:C:449:PHE:HE2	2:C:462:LEU:HD13	1.56	0.71
2:C:341:LYS:HG3	2:C:1306:THR:OG1	1.91	0.71
1:A:986:ARG:HB3	1:A:994:PRO:HB2	1.71	0.71
2:B:338:ARG:NH2	2:C:1002:LEU:CD2	2.54	0.71
2:B:950:ASP:CG	2:B:951:ILE:H	1.94	0.71
1:A:47:ARG:CZ	2:B:596:GLY:CA	2.49	0.70
2:B:891:HIS:CD2	3:D:240:VAL:HG21	2.26	0.70
2:B:1288:ILE:HD12	3:D:20:ARG:NH2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ASP:HA	2:B:189:ILE:HG22	1.73	0.70
1:A:133:LEU:HD21	2:C:545:PRO:HB3	1.74	0.70
1:A:647:LEU:HD21	1:A:691:TYR:HD2	1.56	0.70
2:B:363:ARG:NH2	3:D:80:SER:OG	2.24	0.70
3:E:192:ASP:OD1	3:E:192:ASP:C	2.30	0.70
1:A:928:GLU:CB	1:A:929:PRO:HD2	2.18	0.70
2:C:340:VAL:HG23	2:C:341:LYS:HG2	1.72	0.70
1:A:559:ILE:HG22	1:A:613:ILE:HG12	1.74	0.70
1:A:174:ASP:O	2:B:605:ARG:HD2	1.91	0.70
3:E:13:GLU:O	3:E:13:GLU:CD	2.30	0.70
3:D:47:LYS:HG3	3:D:48:THR:H	1.57	0.70
1:A:127:THR:CG2	2:B:639:ASN:HB2	2.21	0.70
3:E:13:GLU:C	3:E:13:GLU:OE1	2.30	0.69
2:B:279:SER:HA	2:C:1198:LYS:HE2	1.74	0.69
3:E:46:LYS:HD3	3:E:155:HIS:HE1	0.56	0.69
2:B:1084:PRO:HB3	2:B:1207:MET:CG	2.23	0.69
2:C:892:VAL:HG13	2:C:894:VAL:H	1.56	0.69
1:A:254:ASP:O	1:A:255:ARG:HB3	1.92	0.69
2:C:565:GLU:HG2	2:C:566:PHE:H	1.55	0.69
1:A:868:ASP:O	1:A:871:VAL:HG23	1.91	0.69
3:E:253:GLU:HG3	3:E:254:TYR:CD2	2.28	0.69
1:A:383:THR:HG21	1:A:805:TYR:HB3	1.74	0.69
3:E:69:GLU:CD	3:E:69:GLU:O	2.31	0.69
1:A:462:ILE:HG13	1:A:684:ASN:H	1.57	0.69
2:C:82:ARG:NH2	2:C:209:ASN:HD21	1.90	0.69
2:C:838:GLU:HB3	2:C:934:LEU:HB2	1.74	0.69
3:D:244:VAL:HG12	3:D:245:THR:H	1.57	0.69
2:C:853:ASP:HB2	3:D:117:ILE:CD1	2.23	0.69
3:D:61:ASN:OD1	3:D:61:ASN:C	2.30	0.69
2:B:1044:ARG:NE	3:D:266:THR:HG23	2.08	0.68
1:A:47:ARG:NH2	2:B:595:ALA:O	2.27	0.68
3:E:35:LEU:HB3	3:E:179:PHE:HB3	1.75	0.68
2:C:341:LYS:HD2	2:C:1306:THR:HG21	1.75	0.68
2:C:1280:PRO:HB3	2:C:1287:GLY:HA2	1.76	0.68
2:B:147:VAL:HG22	2:B:1315:MET:H	1.59	0.68
2:B:446:LYS:HB3	2:B:769:GLN:NE2	2.10	0.67
1:A:925:ILE:HD11	1:A:930:ASN:HA	1.75	0.67
1:A:764:SER:HA	1:A:795:GLU:HG3	1.76	0.67
2:C:269:GLU:HB3	2:C:292:ASN:CB	2.24	0.67
3:E:56:LEU:CD2	3:E:56:LEU:H	2.08	0.67
1:A:127:THR:HG23	2:B:640:GLN:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ILE:CG1	1:A:684:ASN:H	2.07	0.67
3:E:1:MET:HE1	3:E:121:PHE:HE2	1.54	0.67
3:E:153:TYR:HD1	3:E:156:VAL:HG21	1.59	0.67
3:E:139:ASN:C	3:E:139:ASN:OD1	2.33	0.67
3:E:68:ILE:CD1	3:E:72:ILE:HD12	2.24	0.67
1:A:286:ASN:HB2	1:A:814:ASN:HD21	1.60	0.67
3:D:78:GLY:O	3:D:269:ILE:HD11	1.95	0.67
3:E:162:GLY:HA2	3:E:172:MET:CE	2.24	0.67
2:C:841:ASP:O	2:C:842:ASP:HB2	1.93	0.67
2:C:1273:ASN:C	3:E:183:GLU:OE1	2.33	0.67
1:A:864:ARG:O	1:A:865:ASN:HB3	1.94	0.67
2:B:1121:HIS:HD2	2:B:1124:THR:HG22	1.60	0.67
2:B:733:VAL:HG21	2:B:741:TYR:CD1	2.31	0.66
1:A:562:GLY:HA3	1:A:563:ALA:O	1.96	0.66
1:A:427:ASP:HA	1:A:704:PRO:HD2	1.77	0.66
2:B:1044:ARG:CZ	3:D:266:THR:HG23	2.24	0.66
3:D:239:VAL:HG12	3:D:250:ARG:HH12	1.61	0.66
3:E:261:ARG:NH1	3:E:265:ARG:NH2	2.39	0.66
1:A:477:TYR:HA	1:A:480:GLY:O	1.94	0.66
3:D:178:LYS:O	3:D:178:LYS:HG3	1.96	0.66
2:B:1273:ASN:CG	3:D:79:ILE:CG2	2.64	0.66
1:A:310:ASP:CG	1:A:311:GLN:N	2.49	0.66
1:A:978:LYS:HG2	1:A:987:LEU:HD13	1.77	0.66
3:D:100:ASN:H	3:D:100:ASN:ND2	1.94	0.65
2:B:1084:PRO:HB2	2:B:1208:ASP:C	2.16	0.65
3:E:56:LEU:N	3:E:56:LEU:HD23	2.11	0.65
2:B:368:ALA:HA	3:D:83:ASN:ND2	2.11	0.65
3:E:69:GLU:OE1	3:E:70:ASP:N	2.30	0.65
3:E:247:ARG:HA	3:E:247:ARG:HE	1.62	0.65
1:A:462:ILE:HG12	1:A:684:ASN:HA	1.78	0.65
2:C:272:THR:HB	2:C:289:THR:HG22	1.78	0.65
3:E:221:ARG:HH11	3:E:225:ARG:HD2	1.60	0.65
2:C:1021:ARG:HD2	2:C:1032:ASP:HB2	1.79	0.65
1:A:71:LEU:HG	1:A:75:PRO:HG2	1.78	0.65
3:E:12:LEU:O	3:E:14:GLN:NE2	2.30	0.65
1:A:919:TYR:HB2	1:A:955:ASN:HB3	1.79	0.65
3:D:85:ASN:C	3:D:85:ASN:HD22	2.00	0.65
2:C:1051:ARG:NH1	2:C:1051:ARG:HG2	2.05	0.65
3:E:134:TYR:OH	3:E:286:THR:HG22	1.97	0.65
2:B:368:ALA:O	3:D:83:ASN:HB2	1.97	0.65
3:D:143:PRO:O	3:D:144:ARG:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:449:PHE:N	2:C:450:PRO:HD3	2.12	0.65
2:B:442:PRO:HG3	2:B:475:ILE:HD12	1.79	0.65
3:E:195:ASN:N	3:E:195:ASN:OD1	2.30	0.65
3:E:53:GLU:N	3:E:53:GLU:OE2	2.30	0.64
3:E:69:GLU:C	3:E:69:GLU:OE1	2.35	0.64
2:C:1042:TRP:HB3	2:C:1043:SER:HA	1.76	0.64
2:B:1236:ILE:HG12	2:B:1237:SER:H	1.63	0.64
1:A:667:GLN:NE2	1:A:667:GLN:H	1.94	0.64
1:A:174:ASP:HB3	2:B:605:ARG:HH12	1.58	0.64
2:C:269:GLU:HB3	2:C:292:ASN:HB3	1.78	0.64
2:C:390:HIS:HB2	2:C:1318:GLU:OE2	1.97	0.64
1:A:723:GLU:O	1:A:724:MET:HB2	1.98	0.64
2:B:926:VAL:O	2:B:926:VAL:HG12	1.97	0.64
1:A:174:ASP:HB3	2:B:605:ARG:HH11	1.58	0.64
3:D:144:ARG:O	3:D:144:ARG:HD2	1.98	0.64
2:B:1031:TYR:CE2	2:B:1041:ARG:HD3	2.33	0.64
3:D:55:HIS:ND1	3:D:55:HIS:C	2.50	0.64
3:E:191:ARG:NH1	3:E:191:ARG:CG	2.42	0.64
1:A:955:ASN:HD21	1:A:1055:LEU:HB3	1.60	0.64
1:A:887:ILE:HG22	1:A:888:GLU:H	1.63	0.64
2:C:838:GLU:HG3	2:C:839:ALA:N	2.12	0.64
1:A:462:ILE:HG21	1:A:682:SER:HA	1.80	0.64
3:E:284:GLN:O	3:E:288:THR:HG22	1.96	0.64
2:B:1181:SER:O	2:B:1182:GLU:HG2	1.98	0.64
3:E:68:ILE:CD1	3:E:69:GLU:N	2.59	0.64
2:B:748:GLN:CG	2:B:748:GLN:O	2.45	0.64
2:B:234:PRO:HD2	2:B:242:GLU:HB3	1.80	0.64
3:E:55:HIS:CD2	3:E:145:TYR:CZ	2.85	0.64
3:D:153:TYR:CA	3:D:156:VAL:CG1	2.72	0.64
1:A:133:LEU:HD22	2:C:545:PRO:HG3	1.80	0.64
3:E:55:HIS:ND1	3:E:55:HIS:O	2.30	0.64
3:D:41:GLU:N	3:D:41:GLU:OE1	2.30	0.64
3:D:22:ASP:C	3:D:22:ASP:OD1	2.36	0.64
3:E:137:LEU:HD23	3:E:138:GLY:N	2.13	0.63
2:C:449:PHE:HE1	2:C:463:VAL:HG22	1.60	0.63
3:D:100:ASN:N	3:D:100:ASN:HD22	1.92	0.63
2:C:837:THR:HG22	2:C:934:LEU:HD21	1.78	0.63
2:B:340:VAL:HG21	2:C:1008:LEU:HD23	1.80	0.63
1:A:962:PHE:CG	1:A:963:TYR:N	2.65	0.63
3:E:55:HIS:CD2	3:E:145:TYR:HE2	2.15	0.63
3:D:82:GLN:HA	3:D:82:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1086:PRO:HD3	2:C:1208:ASP:HA	1.80	0.63
2:C:837:THR:HA	2:C:936:MET:HG3	1.80	0.63
2:C:1272:ARG:HD2	3:E:247:ARG:NH2	2.13	0.63
2:C:1243:ARG:NH1	2:C:1243:ARG:HB3	2.14	0.63
2:C:82:ARG:HH22	2:C:209:ASN:HD21	1.39	0.63
3:E:234:ALA:O	3:E:263:ALA:HB2	1.98	0.63
3:D:242:ARG:CG	3:D:242:ARG:HH11	2.11	0.63
3:E:12:LEU:O	3:E:13:GLU:HB3	1.98	0.62
2:B:148:GLN:O	2:B:375:ARG:HD3	1.98	0.62
3:D:237:ALA:HB3	3:D:253:GLU:HG2	1.81	0.62
3:D:35:LEU:HD23	3:D:179:PHE:HB3	1.81	0.62
1:A:27:LYS:O	1:A:30:THR:HG23	1.99	0.62
2:C:1243:ARG:HH11	2:C:1243:ARG:HB3	1.64	0.62
3:E:77:PHE:CE1	3:E:227:MET:HB2	2.34	0.62
1:A:47:ARG:NE	2:B:596:GLY:CA	2.57	0.62
1:A:935:PRO:O	1:A:939:GLN:N	2.27	0.62
2:C:598:ASN:HA	2:C:601:ILE:HG22	1.82	0.62
3:D:107:LEU:O	3:D:108:ASP:OD2	2.17	0.62
2:C:269:GLU:CB	2:C:292:ASN:HB3	2.30	0.62
1:A:724:MET:CB	1:A:725:PRO:CD	2.60	0.62
3:E:1:MET:O	3:E:2:LEU:HB2	2.00	0.62
1:A:565:ARG:CB	1:A:592:VAL:HB	2.30	0.62
1:A:286:ASN:O	1:A:288:LEU:N	2.33	0.62
1:A:955:ASN:ND2	1:A:1055:LEU:HB3	2.15	0.62
3:E:235:VAL:HG13	3:E:258:ASN:ND2	2.14	0.62
1:A:255:ARG:O	1:A:256:VAL:HG12	2.00	0.62
1:A:51:LEU:HB3	1:A:172:PHE:HE1	1.64	0.61
3:E:42:ASN:CB	3:E:174:VAL:HB	2.29	0.61
2:C:449:PHE:CE1	2:C:463:VAL:HG22	2.35	0.61
3:E:209:GLU:O	3:E:213:LEU:HB2	2.00	0.61
2:C:449:PHE:CE1	2:C:463:VAL:HA	2.34	0.61
3:E:85:ASN:HD22	3:E:141:SER:HB3	1.65	0.61
1:A:864:ARG:O	1:A:864:ARG:HG2	2.00	0.61
3:D:21:ASN:O	3:D:22:ASP:CG	2.39	0.61
2:C:671:ASP:HA	2:C:674:LYS:HD3	1.82	0.61
3:E:66:VAL:HG23	3:E:89:TYR:CD2	2.36	0.61
2:B:350:ILE:HG22	2:B:351:ASP:H	1.64	0.61
1:A:133:LEU:HD21	2:C:545:PRO:HB2	1.81	0.61
2:C:1042:TRP:HB3	2:C:1043:SER:CB	2.31	0.61
2:B:193:THR:HG23	2:B:297:ASN:H	1.66	0.61
3:D:148:ASP:OD1	3:D:148:ASP:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1037:ILE:HG12	2:B:1038:GLU:H	1.65	0.61
2:B:862:ARG:CB	2:B:952:PHE:CZ	2.84	0.60
2:B:951:ILE:O	2:B:952:PHE:CB	2.49	0.60
3:E:40:THR:CG2	3:E:41:GLU:N	2.63	0.60
2:C:1118:THR:HG22	2:C:1129:PRO:HA	1.82	0.60
2:C:490:PHE:HA	2:C:745:ILE:HG22	1.83	0.60
2:C:520:PHE:HD1	2:C:520:PHE:H	1.49	0.60
3:E:40:THR:HG22	3:E:41:GLU:N	2.15	0.60
1:A:936:ALA:HA	1:A:939:GLN:HE21	1.67	0.60
2:B:472:GLU:H	2:B:472:GLU:CD	2.03	0.60
3:D:242:ARG:HG2	3:D:242:ARG:HH11	1.66	0.60
2:B:427:VAL:HG11	2:B:755:LEU:CD2	2.32	0.60
2:C:879:THR:O	2:C:883:ILE:HG12	2.01	0.60
2:C:231:LEU:CB	2:C:249:SER:HB2	2.32	0.60
1:A:395:GLN:HA	1:A:395:GLN:NE2	2.17	0.60
3:E:85:ASN:ND2	3:E:141:SER:CB	2.63	0.60
1:A:936:ALA:O	1:A:940:MET:HB3	2.00	0.60
2:B:1276:LEU:HD22	2:B:1300:ASN:HB2	1.83	0.60
3:E:46:LYS:HD2	3:E:155:HIS:CE1	2.34	0.60
2:B:137:ILE:HD11	2:C:759:ASP:CB	2.31	0.60
3:D:217:LYS:CE	3:D:290:TRP:CE3	2.85	0.60
3:E:85:ASN:HD21	3:E:141:SER:CB	2.14	0.60
2:B:1078:TYR:HE2	2:B:1080:THR:HG22	1.67	0.60
1:A:837:HIS:NE2	1:A:1047:ASN:HA	2.17	0.60
2:B:1114:ARG:HD3	2:B:1116:ARG:HH21	1.67	0.60
3:D:153:TYR:C	3:D:156:VAL:HG12	2.22	0.60
1:A:561:LEU:HD12	1:A:617:ILE:HD11	1.83	0.60
3:E:209:GLU:HG3	3:E:210:GLY:H	1.66	0.60
3:D:37:TYR:HD1	3:D:177:ALA:HB2	1.66	0.60
1:A:523:MET:HG2	1:A:574:ARG:NH2	2.16	0.60
1:A:940:MET:HA	1:A:943:ILE:HG12	1.83	0.59
3:D:224:PHE:O	3:D:228:LEU:HB2	2.02	0.59
2:C:841:ASP:H	2:C:940:ARG:HH12	1.51	0.59
2:C:1288:ILE:HD13	2:C:1288:ILE:H	1.67	0.59
2:C:286:LEU:CD2	2:C:290:TYR:HB3	2.31	0.59
2:C:392:PRO:HG2	2:C:1315:MET:HG3	1.84	0.59
3:D:5:PRO:O	3:D:6:THR:CB	2.50	0.59
2:B:1236:ILE:CG1	2:B:1237:SER:N	2.62	0.59
2:C:373:ASP:HB2	2:C:394:GLN:HG3	1.83	0.59
2:B:1236:ILE:HG12	2:B:1237:SER:N	2.16	0.59
2:C:341:LYS:CD	2:C:1306:THR:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:ARG:HB3	1:A:835:PHE:CE2	2.38	0.59
3:D:47:LYS:HG3	3:D:48:THR:N	2.18	0.59
3:E:68:ILE:CD1	3:E:72:ILE:CD1	2.77	0.59
3:E:67:TYR:HB3	3:E:70:ASP:HB3	1.85	0.59
3:E:1:MET:CE	3:E:121:PHE:CD2	2.85	0.59
3:E:262:THR:O	3:E:263:ALA:C	2.41	0.59
2:C:1042:TRP:CB	2:C:1043:SER:CA	2.79	0.59
2:B:862:ARG:HB3	2:B:952:PHE:CZ	2.37	0.59
1:A:529:THR:HG22	1:A:568:ALA:HB2	1.84	0.59
1:A:535:LEU:HD11	1:A:614:ILE:HG21	1.85	0.59
2:B:752:VAL:CG2	2:B:755:LEU:HB2	2.33	0.58
3:E:153:TYR:CD1	3:E:156:VAL:HG21	2.37	0.58
2:C:1080:THR:HG21	2:C:1227:MET:SD	2.43	0.58
1:A:717:THR:HG21	1:A:1020:SER:HB2	1.85	0.58
1:A:201:LYS:O	2:B:629:ARG:HG3	2.03	0.58
3:D:253:GLU:CD	3:D:254:TYR:CD2	2.76	0.58
1:A:486:THR:C	1:A:487:GLN:HG3	2.23	0.58
3:E:85:ASN:O	3:E:85:ASN:CG	2.41	0.58
1:A:565:ARG:HB2	1:A:592:VAL:HB	1.84	0.58
2:C:356:SER:O	2:C:360:ILE:HG12	2.04	0.58
1:A:549:SER:O	1:A:551:LEU:N	2.33	0.58
3:D:77:PHE:CZ	3:D:227:MET:HB2	2.39	0.58
2:B:612:PHE:CZ	2:B:635:ILE:HD11	2.39	0.58
2:C:910:LEU:HD13	2:C:915:VAL:HG23	1.86	0.58
2:C:1042:TRP:HB3	2:C:1043:SER:HB2	1.86	0.58
2:C:192:PRO:HG3	2:C:294:VAL:HB	1.86	0.58
1:A:268:TYR:CZ	2:B:562:ALA:HB1	2.38	0.58
1:A:519:ILE:H	1:A:519:ILE:HD13	1.69	0.58
1:A:303:THR:HA	1:A:307:HIS:CE1	2.39	0.58
1:A:481:ASP:CB	1:A:511:ILE:HG12	2.30	0.58
2:C:838:GLU:O	2:C:940:ARG:NH1	2.36	0.58
3:E:1:MET:HE3	3:E:121:PHE:CD2	2.39	0.58
3:D:217:LYS:CE	3:D:290:TRP:CZ3	2.87	0.58
2:B:950:ASP:CG	2:B:951:ILE:N	2.57	0.58
1:A:499:VAL:HB	1:A:503:ILE:HD11	1.86	0.58
1:A:283:PHE:HA	1:A:284:THR:C	2.24	0.58
2:B:139:ASN:O	2:C:757:ILE:HG22	2.03	0.57
2:B:960:THR:HG23	2:B:965:ARG:HH12	1.68	0.57
2:B:872:ILE:HG12	2:B:886:SER:HB2	1.85	0.57
3:D:217:LYS:HE2	3:D:290:TRP:CE3	2.38	0.57
1:A:47:ARG:NH2	2:B:596:GLY:HA3	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:673:GLN:HA	2:C:676:THR:HG22	1.84	0.57
1:A:604:ILE:O	1:A:605:ASP:HB3	2.04	0.57
1:A:64:GLU:HA	1:A:67:ARG:HG2	1.86	0.57
1:A:479:LYS:HA	1:A:514:LEU:HD12	1.86	0.57
1:A:318:ARG:HH11	3:D:43:GLU:HG2	1.65	0.57
3:D:85:ASN:C	3:D:85:ASN:ND2	2.55	0.57
2:C:446:LYS:HA	2:C:769:GLN:NE2	2.19	0.57
2:C:878:SER:HB3	2:C:903:ASN:HB2	1.85	0.57
2:C:1076:ILE:HG23	2:C:1166:VAL:HB	1.87	0.57
3:E:205:LEU:CD1	3:E:205:LEU:O	2.39	0.57
1:A:460:VAL:O	1:A:461:ARG:HD3	2.04	0.57
1:A:831:ARG:HB3	1:A:835:PHE:HE2	1.70	0.57
1:A:64:GLU:OE1	2:B:647:GLU:OE2	2.23	0.57
2:B:1228:ARG:HG2	2:B:1231:TYR:CE2	2.39	0.57
2:B:338:ARG:NH2	2:C:1005:LEU:HD11	2.20	0.56
2:C:1051:ARG:HH11	2:C:1051:ARG:CG	2.18	0.56
3:D:144:ARG:O	3:D:144:ARG:CD	2.52	0.56
1:A:495:LEU:HG	1:A:503:ILE:HD13	1.87	0.56
1:A:954:THR:HB	1:A:1056:VAL:HG23	1.87	0.56
1:A:286:ASN:CG	1:A:287:VAL:N	2.57	0.56
1:A:936:ALA:O	1:A:940:MET:CB	2.53	0.56
3:E:53:GLU:HB2	3:E:145:TYR:HE1	1.69	0.56
1:A:970:ARG:HH22	1:A:977:HIS:HA	1.70	0.56
1:A:913:LEU:HD22	1:A:919:TYR:CZ	2.41	0.56
2:C:269:GLU:C	2:C:292:ASN:HB2	2.26	0.56
2:B:1236:ILE:HG13	2:B:1237:SER:H	1.70	0.56
2:B:279:SER:OG	2:C:1198:LYS:HE2	2.05	0.56
1:A:256:VAL:HG13	1:A:257:ILE:HG13	1.88	0.56
2:B:352:HIS:HA	2:B:1300:ASN:OD1	2.05	0.56
1:A:500:ASP:HB2	1:A:521:LYS:O	2.04	0.56
1:A:133:LEU:CD2	2:C:545:PRO:CB	2.82	0.56
1:A:776:SER:HA	1:A:818:PHE:CE1	2.41	0.56
2:C:1271:SER:N	2:C:1275:ASP:O	2.39	0.56
3:E:44:LEU:HD13	3:E:172:MET:O	2.05	0.56
3:E:235:VAL:CG1	3:E:258:ASN:HA	2.36	0.56
2:B:583:GLU:O	2:B:584:HIS:HB2	2.05	0.56
1:A:936:ALA:O	1:A:940:MET:N	2.34	0.56
1:A:308:ALA:HB3	1:A:309:ASN:CG	2.26	0.56
2:B:368:ALA:O	3:D:83:ASN:CB	2.53	0.56
3:E:142:THR:HG23	3:E:143:PRO:HD2	1.87	0.56
1:A:494:THR:O	1:A:498:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:PHE:HB3	2:B:1151:VAL:HG21	1.88	0.56
2:C:902:ILE:HB	2:C:929:PHE:HB3	1.88	0.56
2:C:668:VAL:HG11	2:C:673:GLN:HB2	1.88	0.56
3:D:239:VAL:HG23	3:D:263:ALA:HB1	1.87	0.56
2:C:269:GLU:HB3	2:C:292:ASN:CG	2.26	0.56
1:A:308:ALA:N	1:A:309:ASN:CB	2.56	0.55
2:C:1031:TYR:O	2:C:1032:ASP:HB3	2.06	0.55
3:E:81:ALA:H	3:E:275:ARG:HH21	1.54	0.55
3:E:150:ILE:CG2	3:E:150:ILE:O	2.54	0.55
1:A:351:TYR:OH	3:D:150:ILE:HB	2.07	0.55
3:E:284:GLN:O	3:E:288:THR:CG2	2.54	0.55
3:E:85:ASN:OD1	3:E:85:ASN:C	2.44	0.55
2:C:154:PHE:HA	2:C:262:ASN:HD22	1.71	0.55
2:B:191:GLY:HA2	2:B:193:THR:N	2.22	0.55
1:A:201:LYS:C	2:B:629:ARG:HD3	2.27	0.55
1:A:388:VAL:HG22	1:A:389:ALA:H	1.71	0.55
1:A:486:THR:HA	1:A:491:ASP:OD2	2.07	0.55
2:B:494:GLU:HG2	2:B:577:GLN:HG3	1.88	0.55
3:E:209:GLU:O	3:E:213:LEU:CB	2.55	0.55
2:B:733:VAL:HG21	2:B:741:TYR:HD1	1.70	0.55
1:A:87:GLU:O	1:A:91:ASN:HB2	2.07	0.55
2:B:142:ASP:HB3	2:B:1318:GLU:HG2	1.89	0.55
1:A:602:PHE:H	1:A:602:PHE:HD1	1.54	0.55
1:A:820:VAL:HG12	1:A:821:ARG:H	1.72	0.55
2:C:539:PHE:O	2:C:543:TRP:HB3	2.06	0.55
1:A:318:ARG:NH1	3:D:43:GLU:CG	2.70	0.55
2:B:1087:ASP:OD2	2:B:1236:ILE:HG23	2.07	0.55
2:C:1071:PHE:HD1	2:C:1234:GLN:HG2	1.72	0.55
1:A:63:SER:OG	1:A:123:SER:HA	2.07	0.55
2:C:834:THR:HA	2:C:847:ILE:O	2.07	0.55
2:C:1325:VAL:HG12	2:C:1326:ARG:H	1.71	0.55
3:E:1:MET:O	3:E:121:PHE:O	2.24	0.55
1:A:605:ASP:O	1:A:606:LYS:HB2	2.07	0.55
1:A:1024:LEU:HD21	1:A:1035:LEU:HD21	1.89	0.55
1:A:562:GLY:HA2	1:A:616:ASP:O	2.07	0.54
1:A:47:ARG:HE	2:B:595:ALA:C	2.05	0.54
2:B:558:TYR:CE2	2:B:585:PHE:HB2	2.42	0.54
1:A:71:LEU:HD11	1:A:91:ASN:CG	2.27	0.54
2:C:1074:VAL:HG12	2:C:1171:ILE:HG21	1.88	0.54
3:E:285:LEU:O	3:E:288:THR:HG23	2.08	0.54
3:E:238:ASN:O	3:E:253:GLU:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:MET:HG2	1:A:574:ARG:HH22	1.73	0.54
3:E:262:THR:HG22	3:E:263:ALA:N	2.21	0.54
2:C:1035:ILE:HG22	2:C:1036:ASP:H	1.71	0.54
2:C:1153:ASP:HA	2:C:1156:ILE:HG22	1.90	0.54
2:B:1247:ASN:HD22	2:B:1247:ASN:H	1.55	0.54
3:E:1:MET:O	3:E:2:LEU:CB	2.55	0.54
2:C:594:LEU:HD12	2:C:597:ALA:HB3	1.88	0.54
2:B:1084:PRO:CG	2:B:1209:GLY:HA3	2.35	0.54
1:A:467:SER:N	1:A:468:PRO:HD2	2.23	0.54
3:E:107:LEU:HD23	3:E:122:TYR:HE1	1.70	0.54
3:D:290:TRP:C	3:D:290:TRP:HE3	2.11	0.54
3:E:253:GLU:O	3:E:254:TYR:CD1	2.61	0.54
1:A:569:VAL:HG11	1:A:595:ASN:HD21	1.73	0.54
2:B:338:ARG:HH21	2:C:1005:LEU:HD12	1.71	0.54
2:B:862:ARG:CB	2:B:952:PHE:CE2	2.89	0.54
2:C:141:LEU:H	2:C:141:LEU:HD23	1.73	0.54
1:A:559:ILE:CG2	1:A:613:ILE:HG12	2.38	0.54
3:D:25:ASN:C	3:D:25:ASN:OD1	2.45	0.54
2:C:440:ILE:HD12	2:C:478:ILE:HG21	1.88	0.54
2:B:1008:LEU:HD13	2:B:1008:LEU:H	1.73	0.54
2:C:287:ARG:HH21	2:C:326:GLY:CA	2.18	0.54
2:C:931:ASN:ND2	2:C:934:LEU:O	2.38	0.54
2:C:129:ALA:HB3	2:C:133:MET:HG2	1.90	0.54
1:A:531:LYS:HE2	1:A:683:GLN:NE2	2.23	0.54
3:D:156:VAL:HG23	3:D:228:LEU:HD23	1.88	0.53
3:E:229:PHE:CE1	3:E:252:LEU:CD1	2.90	0.53
2:C:146:GLU:O	2:C:1316:ALA:HA	2.08	0.53
1:A:719:VAL:HG13	1:A:720:ALA:N	2.23	0.53
1:A:293:LEU:O	1:A:297:LEU:HB2	2.09	0.53
3:E:14:GLN:N	3:E:14:GLN:CD	2.61	0.53
3:D:239:VAL:HG23	3:D:263:ALA:CB	2.38	0.53
3:D:178:LYS:CG	3:D:178:LYS:O	2.56	0.53
2:C:1131:PRO:HA	2:C:1134:ARG:NH1	2.23	0.53
1:A:236:LEU:HD13	1:A:236:LEU:O	2.08	0.53
3:E:76:LEU:HD12	3:E:76:LEU:H	1.73	0.53
2:C:1273:ASN:O	3:E:183:GLU:CD	2.46	0.53
1:A:830:HIS:HD2	1:A:1034:ARG:NH1	2.03	0.53
2:B:862:ARG:HB3	2:B:952:PHE:HE2	1.70	0.53
2:B:635:ILE:HG22	2:B:706:TYR:HB3	1.90	0.53
1:A:194:HIS:CG	3:D:146:ARG:NH1	2.62	0.53
3:E:142:THR:HG22	3:E:144:ARG:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:868:VAL:HB	2:C:890:THR:HA	1.89	0.53
3:D:242:ARG:NH1	3:D:242:ARG:HG2	2.23	0.53
1:A:667:GLN:CD	1:A:667:GLN:N	2.62	0.53
2:C:554:ARG:O	2:C:570:GLY:HA2	2.09	0.53
1:A:722:ASP:CG	1:A:723:GLU:H	2.11	0.53
1:A:426:ARG:HG3	1:A:428:ILE:H	1.74	0.53
3:E:214:ARG:O	3:E:218:THR:CG2	2.57	0.53
1:A:407:GLU:OE1	1:A:1034:ARG:HG2	2.08	0.53
1:A:563:ALA:HA	1:A:564:GLU:CG	2.33	0.53
2:C:853:ASP:HB2	3:D:117:ILE:CG1	2.39	0.53
2:C:841:ASP:N	2:C:940:ARG:HH12	2.06	0.53
2:C:862:ARG:HG2	2:C:952:PHE:HE1	1.72	0.53
2:C:716:PHE:CD1	2:C:716:PHE:N	2.76	0.53
3:D:172:MET:CE	3:D:175:LYS:HG3	2.33	0.53
2:C:838:GLU:CB	2:C:934:LEU:HB2	2.39	0.53
2:C:841:ASP:CG	2:C:842:ASP:H	2.12	0.53
2:B:147:VAL:HG22	2:B:1315:MET:N	2.22	0.53
2:B:546:VAL:HG13	2:B:547:GLU:HG3	1.91	0.53
2:B:1060:ARG:HH12	2:B:1292:GLU:HA	1.74	0.53
1:A:926:MET:HG2	1:A:927:ASN:H	1.74	0.53
2:B:954:GLN:NE2	3:D:240:VAL:CG1	2.71	0.53
3:E:229:PHE:HE1	3:E:252:LEU:HD12	1.73	0.53
1:A:59:TYR:CA	1:A:167:THR:HG21	2.36	0.53
1:A:880:VAL:HB	1:A:899:VAL:HG12	1.91	0.53
1:A:673:TYR:CD2	1:A:694:ILE:HG23	2.44	0.53
1:A:127:THR:HG23	2:B:641:ARG:H	1.74	0.52
1:A:283:PHE:HA	1:A:285:GLU:N	2.24	0.52
1:A:318:ARG:HH12	3:D:43:GLU:CD	2.12	0.52
2:C:309:TRP:CD1	2:C:1253:ARG:HB3	2.44	0.52
3:D:111:ILE:HG23	3:D:111:ILE:O	2.07	0.52
1:A:53:LEU:HD13	1:A:57:PHE:HB3	1.91	0.52
2:C:339:LEU:C	2:C:341:LYS:H	2.12	0.52
1:A:203:THR:H	2:B:629:ARG:HG2	1.73	0.52
3:D:189:LEU:HB3	3:D:230:ILE:HD11	1.91	0.52
1:A:755:ALA:N	1:A:756:PRO:HD2	2.23	0.52
2:B:448:TYR:CZ	2:B:470:ALA:HB1	2.45	0.52
1:A:943:ILE:HA	1:A:946:VAL:HB	1.92	0.52
2:C:387:THR:HA	2:C:1322:PRO:HD3	1.92	0.52
2:C:1087:ASP:HB3	2:C:1236:ILE:HG13	1.92	0.52
1:A:559:ILE:HG12	1:A:585:ILE:HB	1.92	0.52
1:A:474:TYR:O	1:A:477:TYR:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:HB2	1:A:251:VAL:HG22	1.90	0.52
3:E:74:GLN:O	3:E:78:GLY:HA3	2.10	0.52
3:E:240:VAL:O	3:E:251:VAL:HG22	2.09	0.52
3:E:107:LEU:HD23	3:E:122:TYR:OH	2.09	0.52
2:B:138:PHE:O	2:C:759:ASP:OD1	2.27	0.52
1:A:926:MET:HB2	1:A:931:GLY:HA3	1.91	0.52
2:B:338:ARG:HH21	2:C:1005:LEU:CD1	2.21	0.52
2:B:1048:ASP:HB3	2:B:1051:ARG:HB2	1.91	0.52
1:A:271:ARG:HG3	1:A:316:TYR:OH	2.10	0.52
1:A:367:ASN:HD22	1:A:369:GLY:H	1.56	0.52
1:A:127:THR:HG22	2:B:639:ASN:CB	2.36	0.52
2:C:520:PHE:N	2:C:520:PHE:CD1	2.78	0.52
3:D:115:GLU:N	3:D:115:GLU:OE2	2.30	0.52
2:C:669:GLN:O	2:C:670:ASP:HB2	2.09	0.52
1:A:22:ILE:HG12	1:A:25:ILE:HD11	1.91	0.52
2:B:1118:THR:HG22	2:B:1129:PRO:HA	1.90	0.52
3:D:217:LYS:HE2	3:D:290:TRP:CZ3	2.45	0.51
1:A:282:GLU:O	1:A:285:GLU:HA	2.10	0.51
2:C:828:ASP:O	2:C:948:ILE:HA	2.10	0.51
1:A:731:HIS:HB2	1:A:746:PHE:HB3	1.91	0.51
3:E:290:TRP:HD1	3:E:291:ASN:HB3	1.75	0.51
3:E:1:MET:HE2	3:E:123:ASP:HA	1.92	0.51
1:A:282:GLU:HG3	1:A:286:ASN:OD1	2.11	0.51
1:A:832:GLU:CD	1:A:833:VAL:H	2.13	0.51
1:A:422:ASP:HB3	1:A:677:LEU:HD12	1.93	0.51
1:A:723:GLU:O	1:A:724:MET:CB	2.59	0.51
2:B:338:ARG:NH2	2:C:1005:LEU:CD1	2.73	0.51
1:A:406:VAL:CB	1:A:407:GLU:CA	2.79	0.51
1:A:966:GLY:O	1:A:970:ARG:HD3	2.10	0.51
2:C:261:ASP:O	2:C:1054:ARG:NH1	2.43	0.51
1:A:146:PRO:O	1:A:147:GLN:HB3	2.10	0.51
3:D:153:TYR:C	3:D:156:VAL:CG1	2.79	0.51
2:B:368:ALA:CA	3:D:83:ASN:HD22	2.24	0.51
2:C:1264:GLU:HA	2:C:1297:SER:HA	1.93	0.51
3:E:53:GLU:HB2	3:E:145:TYR:CE1	2.45	0.51
3:E:83:ASN:OD1	3:E:83:ASN:N	2.43	0.51
3:E:262:THR:O	3:E:263:ALA:HB3	2.10	0.51
3:D:214:ARG:O	3:D:218:THR:CG2	2.51	0.51
3:D:44:LEU:HD11	3:D:154:ALA:CA	2.31	0.51
1:A:292:ARG:HG2	1:A:295:THR:CG2	2.40	0.51
3:E:290:TRP:C	3:E:290:TRP:CD1	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:CG2	1:A:407:GLU:HA	2.40	0.51
2:C:448:TYR:HB3	2:C:768:CYS:HG	1.72	0.51
1:A:201:LYS:HA	2:B:629:ARG:HD3	1.92	0.51
1:A:508:ASN:HB2	1:A:509:ARG:HH11	1.74	0.51
1:A:437:GLN:HB3	1:A:656:TYR:HB2	1.92	0.51
3:E:82:GLN:HG2	3:E:83:ASN:OD1	2.10	0.51
3:D:21:ASN:O	3:D:24:THR:O	2.29	0.51
3:E:283:LEU:O	3:E:287:PHE:HB2	2.11	0.51
2:B:153:ASP:HB3	2:B:154:PHE:HD1	1.75	0.51
3:D:153:TYR:HA	3:D:156:VAL:HG11	1.86	0.51
2:B:134:THR:CG2	2:C:472:GLU:CD	2.79	0.51
2:C:931:ASN:OD1	2:C:934:LEU:HD22	2.11	0.51
2:B:279:SER:CA	2:C:1198:LYS:HE2	2.41	0.51
2:B:269:GLU:O	2:B:291:HIS:CD2	2.63	0.51
2:C:255:LEU:HD23	2:C:1062:ILE:HD13	1.93	0.51
1:A:59:TYR:HA	1:A:167:THR:CG2	2.38	0.51
3:D:149:MET:CE	3:D:260:MET:HE2	2.38	0.51
3:E:160:LEU:HD11	3:E:229:PHE:CB	2.36	0.51
1:A:133:LEU:CD2	2:C:545:PRO:HB3	2.41	0.51
2:C:339:LEU:O	2:C:340:VAL:HG22	2.09	0.51
1:A:47:ARG:HE	2:B:596:GLY:CA	2.22	0.50
3:D:290:TRP:C	3:D:290:TRP:CE3	2.85	0.50
1:A:926:MET:SD	1:A:930:ASN:O	2.69	0.50
3:E:12:LEU:HD23	3:E:15:PHE:CZ	2.46	0.50
2:B:368:ALA:O	3:D:83:ASN:ND2	2.41	0.50
1:A:605:ASP:O	1:A:606:LYS:CB	2.60	0.50
3:D:250:ARG:HB3	3:D:250:ARG:HH11	1.76	0.50
2:C:412:LEU:HD11	2:C:714:LEU:HD23	1.93	0.50
2:C:871:PRO:HB2	2:C:896:LEU:HD23	1.93	0.50
2:C:716:PHE:N	2:C:716:PHE:HD1	2.09	0.50
1:A:567:PRO:O	1:A:568:ALA:HB3	2.12	0.50
1:A:709:SER:HB2	1:A:712:ILE:HB	1.94	0.50
3:E:62:VAL:HG23	3:E:63:PRO:HD2	1.93	0.50
1:A:840:MET:SD	1:A:1019:PRO:HB2	2.51	0.50
3:E:289:ARG:CD	3:E:289:ARG:O	2.35	0.50
3:E:236:ALA:O	3:E:263:ALA:HA	2.10	0.50
3:D:153:TYR:O	3:D:156:VAL:HG12	2.11	0.50
2:B:747:ARG:CG	2:B:747:ARG:O	2.58	0.50
2:B:926:VAL:O	2:B:926:VAL:CG1	2.59	0.50
2:C:835:TYR:O	2:C:846:GLY:HA3	2.12	0.50
2:C:1126:MET:HG3	2:C:1127:ALA:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:836:GLN:HE22	2:B:844:ASP:HA	1.75	0.50
3:D:289:ARG:NE	3:D:289:ARG:HA	2.24	0.50
3:D:291:ASN:OD1	3:D:291:ASN:C	2.50	0.50
2:B:862:ARG:HH12	2:B:948:ILE:HD13	1.77	0.50
2:C:520:PHE:N	2:C:520:PHE:HD1	2.10	0.50
2:B:1263:TYR:CG	2:B:1295:HIS:HD2	2.29	0.50
3:E:41:GLU:OE1	3:E:41:GLU:O	2.30	0.50
2:B:1078:TYR:CE2	2:B:1080:THR:HG22	2.46	0.50
1:A:298:LEU:CD1	2:B:563:ALA:HB3	2.42	0.50
2:B:941:TYR:CD1	2:B:941:TYR:O	2.65	0.50
1:A:208:HIS:HB3	1:A:260:LEU:HA	1.93	0.50
2:C:522:PRO:HG3	2:C:636:PRO:HB2	1.94	0.50
3:D:15:PHE:CD1	3:D:15:PHE:N	2.80	0.50
2:C:298:PRO:O	2:C:299:ALA:HB3	2.12	0.50
3:E:69:GLU:O	3:E:69:GLU:OE2	2.30	0.50
1:A:308:ALA:CB	1:A:309:ASN:HB2	2.41	0.50
3:D:153:TYR:CE2	3:D:258:ASN:ND2	2.80	0.50
1:A:283:PHE:CA	1:A:284:THR:C	2.80	0.50
1:A:76:LEU:HB2	1:A:172:PHE:CE2	2.47	0.50
2:C:1037:ILE:O	2:C:1038:GLU:CB	2.58	0.50
2:C:384:MET:HA	2:C:708:THR:HG21	1.93	0.50
2:C:853:ASP:O	3:D:117:ILE:HD11	2.12	0.50
3:E:10:THR:HG23	3:E:17:PHE:HZ	1.77	0.50
2:B:135:LYS:HG3	2:C:470:ALA:O	2.09	0.49
2:B:953:ASP:OD1	3:D:241:ASN:OD1	2.30	0.49
1:A:395:GLN:CA	1:A:395:GLN:HE21	2.20	0.49
1:A:351:TYR:CE1	3:D:150:ILE:HG21	2.47	0.49
1:A:845:ILE:O	1:A:849:ILE:HG12	2.11	0.49
2:B:1276:LEU:HB3	2:B:1290:LYS:HD3	1.95	0.49
2:B:269:GLU:HB3	2:B:292:ASN:HD22	1.76	0.49
2:B:225:ILE:HG23	2:B:247:TYR:CD2	2.46	0.49
2:C:284:ASN:N	2:C:284:ASN:OD1	2.44	0.49
3:E:13:GLU:C	3:E:13:GLU:CD	2.71	0.49
2:C:293:ASN:CG	2:C:294:VAL:H	2.16	0.49
1:A:64:GLU:CG	2:B:647:GLU:OE1	2.60	0.49
2:C:270:THR:HA	2:C:292:ASN:H	1.77	0.49
3:D:107:LEU:HD23	3:D:122:TYR:CE1	2.47	0.49
2:C:853:ASP:HB2	3:D:117:ILE:HG13	1.93	0.49
2:C:1280:PRO:HB3	2:C:1287:GLY:CA	2.41	0.49
1:A:188:THR:HG21	3:D:144:ARG:HG2	1.93	0.49
1:A:64:GLU:HG3	2:B:647:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:PHE:N	1:A:602:PHE:HD1	2.11	0.49
1:A:416:MET:HG2	1:A:466:LEU:HD21	1.94	0.49
1:A:662:ILE:HG12	1:A:675:THR:HG21	1.93	0.49
1:A:254:ASP:O	1:A:255:ARG:CB	2.61	0.49
1:A:213:TRP:O	1:A:215:VAL:N	2.36	0.49
3:E:20:ARG:HD2	3:E:25:ASN:HB3	1.94	0.49
1:A:307:HIS:HD2	1:A:308:ALA:HB2	1.77	0.49
2:B:862:ARG:HB2	2:B:952:PHE:CZ	2.48	0.49
3:E:84:VAL:HG23	3:E:85:ASN:N	2.28	0.49
2:C:931:ASN:HB2	2:C:936:MET:SD	2.53	0.49
3:D:21:ASN:O	3:D:22:ASP:OD1	2.31	0.49
3:D:164:ASP:HA	3:D:167:ARG:HG2	1.94	0.49
1:A:242:LYS:O	1:A:246:ASP:HB2	2.12	0.49
3:D:172:MET:HG3	3:D:173:PRO:CD	2.42	0.49
3:D:181:SER:HB2	3:D:185:SER:OG	2.13	0.49
3:E:85:ASN:OD1	3:E:85:ASN:O	2.30	0.49
2:B:139:ASN:O	2:C:757:ILE:CG2	2.61	0.49
3:E:139:ASN:OD1	3:E:139:ASN:O	2.30	0.49
2:C:1238:VAL:HG23	2:C:1239:ALA:H	1.77	0.49
2:C:1144:ARG:HD2	2:C:1194:MET:HA	1.95	0.49
2:C:1180:PRO:CB	2:C:1209:GLY:HA2	2.41	0.49
2:C:624:PHE:CE2	2:C:713:MET:HG2	2.48	0.49
3:E:53:GLU:O	3:E:53:GLU:OE2	2.30	0.49
1:A:503:ILE:N	1:A:503:ILE:HD12	2.28	0.49
3:E:92:ARG:HD3	3:E:92:ARG:O	2.12	0.49
3:E:72:ILE:O	3:E:76:LEU:CD1	2.61	0.48
2:B:234:PRO:HD2	2:B:242:GLU:CB	2.43	0.48
3:E:66:VAL:HG13	3:E:111:ILE:CG2	2.42	0.48
1:A:351:TYR:CZ	3:D:150:ILE:HG21	2.48	0.48
3:E:38:GLU:HB3	3:E:176:ARG:HB3	1.95	0.48
1:A:409:MET:CB	1:A:1034:ARG:HH12	2.12	0.48
2:B:148:GLN:HA	2:B:148:GLN:OE1	2.13	0.48
1:A:866:LEU:O	1:A:867:ALA:HB3	2.13	0.48
3:E:49:ILE:CG2	3:E:50:PRO:CD	2.84	0.48
3:E:12:LEU:HG	3:E:14:GLN:HG2	1.95	0.48
2:C:878:SER:HB3	2:C:903:ASN:CB	2.43	0.48
2:C:533:GLN:HG2	2:C:588:LEU:HD23	1.95	0.48
3:D:121:PHE:N	3:D:121:PHE:CD1	2.82	0.48
2:C:528:ILE:HD11	2:C:758:ILE:HD12	1.96	0.48
1:A:461:ARG:CG	1:A:461:ARG:NH1	2.73	0.48
1:A:64:GLU:OE1	2:B:647:GLU:OE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:12:LEU:HG	3:E:14:GLN:NE2	2.18	0.48
3:E:13:GLU:O	3:E:13:GLU:OE1	2.30	0.48
1:A:76:LEU:HB2	1:A:172:PHE:CD2	2.48	0.48
2:B:577:GLN:HB2	2:B:747:ARG:HH21	1.78	0.48
2:C:1025:ASP:OD1	3:D:95:ALA:CB	2.61	0.48
1:A:236:LEU:HD13	1:A:236:LEU:C	2.34	0.48
2:C:619:ALA:HB2	2:C:711:ASN:HB2	1.95	0.48
2:B:1234:GLN:HA	2:B:1234:GLN:HE21	1.79	0.48
2:C:150:LEU:HD12	2:C:150:LEU:H	1.78	0.48
2:B:1214:GLU:HB2	2:B:1215:PRO:HD2	1.96	0.48
3:E:122:TYR:CD1	3:E:122:TYR:N	2.82	0.48
1:A:286:ASN:HB2	1:A:814:ASN:ND2	2.27	0.48
2:B:836:GLN:NE2	2:B:845:GLU:H	2.11	0.48
2:B:709:MET:HA	2:B:712:PHE:HD2	1.78	0.48
3:D:166:GLU:OE2	3:D:166:GLU:HA	2.13	0.48
2:C:210:ARG:HG3	2:C:210:ARG:O	2.13	0.48
2:C:297:ASN:ND2	2:C:298:PRO:O	2.46	0.48
2:B:751:THR:HG22	2:B:753:ASP:H	1.78	0.48
1:A:1004:THR:O	1:A:1008:ARG:HG2	2.13	0.48
3:E:33:GLN:C	3:E:35:LEU:H	2.17	0.48
1:A:28:PRO:C	1:A:30:THR:H	2.17	0.48
3:D:244:VAL:HG12	3:D:245:THR:N	2.28	0.48
1:A:835:PHE:O	1:A:839:LEU:HG	2.14	0.48
2:B:1077:MET:SD	2:B:1079:LEU:HB2	2.53	0.48
3:D:255:ILE:HG13	3:D:255:ILE:O	2.13	0.48
3:E:1:MET:SD	3:E:121:PHE:CZ	3.06	0.48
3:D:77:PHE:HE1	3:D:227:MET:O	1.96	0.48
2:C:109:LYS:HZ2	2:C:110:PRO:HD2	1.78	0.48
3:D:60:ARG:O	3:D:62:VAL:HG23	2.14	0.48
3:E:5:PRO:HB2	3:E:8:GLY:O	2.14	0.48
1:A:12:ARG:HD3	1:A:12:ARG:O	2.14	0.48
3:D:242:ARG:HH11	3:D:242:ARG:CB	2.27	0.48
1:A:407:GLU:CD	1:A:1034:ARG:HG2	2.34	0.48
2:C:292:ASN:OD1	2:C:293:ASN:N	2.47	0.48
1:A:544:ASN:ND2	1:A:546:ALA:HB3	2.24	0.48
3:E:192:ASP:O	3:E:192:ASP:OD1	2.31	0.48
1:A:667:GLN:CD	1:A:667:GLN:H	2.16	0.48
1:A:602:PHE:N	1:A:602:PHE:CD1	2.80	0.48
2:B:908:THR:HA	2:B:911:ARG:HE	1.78	0.48
3:E:196:TRP:HH2	3:E:226:MET:HG2	1.79	0.48
3:D:190:SER:O	3:D:194:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:385:ILE:O	2:C:386:SER:HB3	2.13	0.47
2:C:855:TYR:HB2	2:C:918:VAL:HG11	1.96	0.47
1:A:305:TYR:HD2	1:A:316:TYR:HE2	1.62	0.47
1:A:937:ARG:O	1:A:941:ASP:HB2	2.13	0.47
1:A:959:TYR:HB2	1:A:1051:PRO:HD2	1.96	0.47
1:A:308:ALA:HB3	1:A:309:ASN:ND2	2.29	0.47
3:D:221:ARG:NH1	3:D:225:ARG:HH21	2.12	0.47
3:E:191:ARG:HA	3:E:191:ARG:HD2	1.60	0.47
1:A:462:ILE:HG12	1:A:684:ASN:CA	2.44	0.47
2:C:687:LEU:HD11	2:C:764:TRP:HZ3	1.79	0.47
2:C:492:VAL:HG22	2:C:747:ARG:HA	1.95	0.47
1:A:645:ARG:HG3	1:A:695:THR:HG22	1.96	0.47
3:D:152:ILE:O	3:D:155:HIS:HB2	2.14	0.47
3:D:185:SER:O	3:D:188:SER:N	2.43	0.47
2:C:629:ARG:HA	2:C:1037:ILE:HG12	1.95	0.47
1:A:462:ILE:HG22	1:A:463:ASP:N	2.27	0.47
3:D:143:PRO:O	3:D:144:ARG:CB	2.63	0.47
1:A:302:ASP:O	1:A:305:TYR:HB3	2.14	0.47
2:B:902:ILE:HD11	2:B:929:PHE:HE1	1.79	0.47
1:A:962:PHE:HB3	1:A:1049:TYR:CD1	2.49	0.47
2:B:951:ILE:O	2:B:952:PHE:HB2	2.14	0.47
2:C:268:GLY:O	2:C:269:GLU:HB2	2.14	0.47
2:C:841:ASP:O	2:C:842:ASP:CB	2.61	0.47
1:A:613:ILE:HG13	1:A:643:ALA:HB2	1.96	0.47
2:B:1041:ARG:HG3	2:B:1042:TRP:CD1	2.49	0.47
2:B:1263:TYR:CG	2:B:1295:HIS:CD2	3.02	0.47
1:A:298:LEU:HD13	2:B:563:ALA:HB3	1.95	0.47
3:E:166:GLU:CD	3:E:171:VAL:O	2.53	0.47
2:C:523:THR:O	2:C:524:GLU:CB	2.60	0.47
1:A:908:ALA:HB2	1:A:943:ILE:HB	1.95	0.47
2:C:231:LEU:HB2	2:C:249:SER:HB2	1.97	0.47
2:C:554:ARG:NH2	2:C:594:LEU:HD23	2.29	0.47
2:B:893:ALA:HB1	2:B:915:VAL:HG12	1.95	0.47
2:B:424:GLY:O	2:B:428:GLN:HB2	2.15	0.47
1:A:487:GLN:HE22	1:A:548:ASN:HA	1.80	0.47
2:B:427:VAL:HG11	2:B:755:LEU:HD21	1.97	0.47
2:C:836:GLN:HB3	2:C:940:ARG:HH11	1.79	0.47
1:A:467:SER:HA	1:A:470:LEU:HD22	1.96	0.47
2:B:961:SER:O	2:B:964:VAL:HG12	2.14	0.47
2:B:765:PRO:HA	2:B:769:GLN:HB2	1.96	0.47
3:D:37:TYR:HD1	3:D:177:ALA:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:105:LEU:O	3:E:121:PHE:HB2	2.15	0.47
1:A:409:MET:HB3	1:A:1034:ARG:NH1	2.13	0.47
2:B:368:ALA:CA	3:D:83:ASN:ND2	2.78	0.47
1:A:91:ASN:HD22	1:A:91:ASN:HA	1.56	0.47
2:B:466:VAL:O	2:B:470:ALA:HB2	2.15	0.47
3:E:288:THR:HG23	3:E:289:ARG:H	1.80	0.47
3:E:49:ILE:HG23	3:E:50:PRO:CD	2.24	0.47
2:C:668:VAL:HG22	2:C:669:GLN:H	1.80	0.47
1:A:667:GLN:NE2	1:A:667:GLN:N	2.62	0.47
3:E:148:ASP:OD1	3:E:151:ASP:HB2	2.15	0.47
3:D:67:TYR:CD1	3:D:110:VAL:HG22	2.50	0.46
1:A:833:VAL:O	1:A:837:HIS:N	2.43	0.46
2:C:230:ASP:HB3	2:C:985:ARG:HE	1.79	0.46
3:E:53:GLU:OE1	3:E:145:TYR:CD1	2.69	0.46
2:C:449:PHE:CE2	2:C:462:LEU:HD13	2.43	0.46
1:A:565:ARG:HB3	1:A:592:VAL:HB	1.95	0.46
1:A:567:PRO:O	1:A:568:ALA:CB	2.63	0.46
1:A:834:THR:O	1:A:838:LYS:HG3	2.15	0.46
1:A:580:SER:HB2	1:A:581:ASN:H	1.61	0.46
1:A:303:THR:HB	1:A:307:HIS:CE1	2.50	0.46
3:D:44:LEU:HB2	3:D:174:VAL:HG23	1.97	0.46
1:A:833:VAL:HA	1:A:836:ILE:HB	1.97	0.46
2:B:419:TYR:CE1	2:B:1007:THR:HA	2.51	0.46
1:A:456:PHE:HB3	1:A:686:TYR:HE1	1.79	0.46
2:B:748:GLN:HE21	2:B:748:GLN:HB3	1.59	0.46
1:A:643:ALA:HB3	1:A:646:ALA:HB2	1.97	0.46
1:A:69:HIS:CB	1:A:70:PRO:HD3	2.45	0.46
2:C:552:ILE:HD13	2:C:552:ILE:HA	1.84	0.46
2:B:425:ILE:HD13	2:B:425:ILE:H	1.80	0.46
3:E:33:GLN:C	3:E:35:LEU:N	2.69	0.46
2:B:935:GLN:O	2:B:940:ARG:NH1	2.49	0.46
1:A:559:ILE:HD11	1:A:587:MET:HG2	1.97	0.46
1:A:495:LEU:HA	1:A:503:ILE:HD13	1.97	0.46
2:B:667:ALA:HB3	2:B:677:ARG:HD3	1.97	0.46
3:E:113:ASN:C	3:E:114:SER:HG	2.13	0.46
2:C:185:ALA:HB3	2:C:277:THR:O	2.15	0.46
3:E:1:MET:SD	3:E:121:PHE:CE2	3.09	0.46
3:E:162:GLY:HA2	3:E:172:MET:HE2	1.95	0.46
1:A:926:MET:HB2	1:A:931:GLY:N	2.30	0.46
2:B:1051:ARG:HG2	2:B:1054:ARG:HH12	1.80	0.46
1:A:802:THR:HG23	1:A:803:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1242:MET:SD	2:B:1260:PRO:HG3	2.55	0.46
2:B:1175:ALA:HB2	2:B:1204:LEU:HB2	1.98	0.46
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.97	0.46
2:B:939:ASN:O	2:B:940:ARG:CB	2.56	0.46
2:C:141:LEU:HG	2:C:142:ASP:N	2.26	0.46
1:A:560:LEU:HD23	1:A:614:ILE:HB	1.96	0.46
3:D:53:GLU:HG2	3:D:145:TYR:HE1	1.81	0.46
2:C:815:LEU:N	2:C:816:PRO:HD2	2.31	0.46
2:C:1075:ARG:HD2	2:C:1090:PRO:HD2	1.97	0.46
1:A:676:ALA:O	1:A:693:TYR:HB3	2.15	0.46
2:B:581:LEU:H	2:B:581:LEU:HD23	1.81	0.46
1:A:285:GLU:HG2	1:A:286:ASN:N	2.31	0.46
3:D:66:VAL:O	3:D:111:ILE:HG22	2.16	0.46
1:A:462:ILE:HG12	1:A:685:PRO:HD3	1.97	0.46
1:A:204:LEU:HA	1:A:264:SER:O	2.15	0.46
1:A:519:ILE:O	1:A:519:ILE:HG12	2.15	0.46
1:A:64:GLU:OE1	2:B:647:GLU:CD	2.55	0.46
2:C:828:ASP:N	2:C:828:ASP:OD2	2.49	0.46
2:B:1277:LEU:HD13	2:B:1287:GLY:HA3	1.96	0.46
2:C:388:GLN:HB3	2:C:1320:VAL:HG23	1.97	0.46
1:A:255:ARG:HD3	1:A:258:GLN:CD	2.36	0.46
2:C:231:LEU:HB3	2:C:249:SER:HB2	1.97	0.46
2:B:154:PHE:CD1	2:B:154:PHE:N	2.84	0.46
3:E:53:GLU:CD	3:E:53:GLU:O	2.55	0.45
3:D:217:LYS:O	3:D:221:ARG:HB3	2.15	0.45
2:B:1273:ASN:CG	3:D:79:ILE:HG21	2.30	0.45
1:A:27:LYS:CB	1:A:28:PRO:HD3	2.39	0.45
2:B:1084:PRO:HB2	2:B:1209:GLY:N	2.31	0.45
1:A:73:ARG:HG3	1:A:74:LEU:HD12	1.97	0.45
2:B:154:PHE:HD1	2:B:154:PHE:N	2.14	0.45
2:C:302:ARG:HD2	2:C:315:THR:HG22	1.98	0.45
2:B:278:LEU:HB2	2:B:282:VAL:HG13	1.97	0.45
2:C:561:ASN:O	2:C:562:ALA:HB3	2.16	0.45
2:B:1273:ASN:ND2	3:D:79:ILE:CG2	2.79	0.45
1:A:314:ARG:O	1:A:318:ARG:HB2	2.16	0.45
2:C:144:ASN:HA	2:C:1318:GLU:HB3	1.98	0.45
2:B:144:ASN:HB2	2:B:1318:GLU:HA	1.98	0.45
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.97	0.45
1:A:496:CYS:SG	1:A:497:ALA:N	2.90	0.45
2:C:94:PHE:HA	2:C:104:ILE:HG21	1.98	0.45
1:A:967:ILE:HB	1:A:978:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:SER:HA	1:A:663:GLU:HB3	1.99	0.45
1:A:940:MET:O	1:A:944:ARG:HB2	2.16	0.45
1:A:64:GLU:HA	1:A:67:ARG:CG	2.45	0.45
1:A:456:PHE:HB3	1:A:686:TYR:CE1	2.51	0.45
2:B:493:HIS:CG	2:B:758:ILE:HD13	2.52	0.45
2:C:1060:ARG:HH22	2:C:1292:GLU:HA	1.81	0.45
3:D:181:SER:CB	3:D:250:ARG:HG2	2.41	0.45
2:C:838:GLU:CG	2:C:839:ALA:H	2.23	0.45
2:C:934:LEU:HD13	2:C:934:LEU:H	1.81	0.45
1:A:934:THR:N	1:A:935:PRO:HD2	2.31	0.45
1:A:673:TYR:CE2	1:A:694:ILE:HG22	2.51	0.45
2:C:1027:THR:HG22	3:D:102:SER:OG	2.16	0.45
3:D:140:ALA:HA	3:D:281:LYS:HG3	1.97	0.45
1:A:308:ALA:HB3	1:A:309:ASN:CB	2.47	0.45
3:E:229:PHE:HE1	3:E:252:LEU:CD1	2.29	0.45
2:C:1035:ILE:O	2:C:1036:ASP:HB3	2.17	0.45
2:C:1038:GLU:O	2:C:1041:ARG:HB2	2.17	0.45
2:B:368:ALA:C	3:D:83:ASN:HD22	2.17	0.45
1:A:658:ILE:HD11	1:A:692:ILE:HD11	1.99	0.45
1:A:894:LYS:C	1:A:896:ASN:H	2.19	0.45
1:A:411:ILE:HD13	1:A:411:ILE:N	2.31	0.45
2:B:763:VAL:HA	2:B:766:ILE:HD12	1.98	0.45
2:B:218:GLY:C	2:B:219:ILE:HG12	2.36	0.45
3:E:70:ASP:O	3:E:70:ASP:OD2	2.35	0.45
3:E:166:GLU:HG3	3:E:172:MET:SD	2.57	0.45
1:A:208:HIS:HB3	1:A:260:LEU:HD23	1.99	0.45
2:B:1255:ARG:HB3	2:B:1256:GLY:H	1.56	0.45
1:A:752:VAL:HG12	1:A:812:VAL:HG23	1.98	0.45
2:B:639:ASN:HB3	2:B:641:ARG:HG3	1.99	0.45
3:D:110:VAL:HG12	3:D:111:ILE:N	2.32	0.45
2:B:279:SER:CB	2:C:1198:LYS:HE2	2.47	0.45
1:A:463:ASP:OD2	1:A:530:MET:HB3	2.16	0.45
3:D:178:LYS:HD2	3:D:249:ASP:HB3	1.99	0.45
2:C:286:LEU:HD21	2:C:290:TYR:HB3	1.98	0.45
2:C:372:ALA:HB1	2:C:1315:MET:HE3	1.97	0.45
3:D:131:ALA:C	3:D:133:THR:H	2.19	0.45
2:B:180:LEU:HB3	2:B:195:ASN:HD21	1.82	0.45
2:B:135:LYS:O	2:C:471:SER:HA	2.16	0.45
1:A:926:MET:HG2	1:A:927:ASN:N	2.31	0.45
2:C:451:GLU:O	2:C:452:ASN:HB3	2.17	0.45
1:A:27:LYS:HB3	1:A:28:PRO:CD	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:VAL:HG23	2:B:375:ARG:HH11	1.82	0.45
2:C:1071:PHE:CD1	2:C:1234:GLN:HG2	2.50	0.45
2:C:627:ALA:H	2:C:716:PHE:HB2	1.82	0.45
2:B:835:TYR:CE1	2:B:941:TYR:CD2	3.05	0.45
3:D:106:GLY:HA2	3:D:121:PHE:HB3	1.98	0.45
3:E:148:ASP:O	3:E:280:ALA:HB1	2.16	0.45
3:E:53:GLU:CG	3:E:145:TYR:CE1	2.93	0.45
1:A:565:ARG:N	1:A:590:ARG:O	2.50	0.45
2:B:134:THR:HG21	2:C:472:GLU:CD	2.37	0.45
2:C:409:ILE:HD11	2:C:1040:PHE:CZ	2.52	0.45
2:C:306:GLN:N	2:C:306:GLN:HE21	2.14	0.45
2:B:884:ALA:O	2:B:888:GLN:HG2	2.16	0.45
3:D:185:SER:HB3	3:D:186:LEU:H	1.50	0.44
2:B:753:ASP:N	2:B:754:GLY:HA2	2.32	0.44
2:C:1137:VAL:HG22	2:C:1164:TRP:CE2	2.51	0.44
1:A:308:ALA:HB3	1:A:309:ASN:HB2	1.98	0.44
3:D:221:ARG:HH12	3:D:225:ARG:HH21	1.64	0.44
1:A:953:ARG:HH12	1:A:1055:LEU:HD23	1.81	0.44
1:A:670:GLY:O	1:A:671:VAL:CG2	2.60	0.44
2:C:863:LEU:HD11	2:C:871:PRO:HD3	1.99	0.44
2:B:348:LEU:HD23	2:B:350:ILE:HD11	1.98	0.44
2:B:583:GLU:HA	2:B:583:GLU:OE1	2.17	0.44
2:B:709:MET:HA	2:B:712:PHE:CD2	2.52	0.44
3:E:116:THR:HG21	3:E:119:ILE:HD12	1.99	0.44
2:C:980:ARG:HH21	2:C:999:LYS:HE2	1.82	0.44
1:A:331:ARG:HD3	1:A:331:ARG:H	1.82	0.44
3:D:238:ASN:H	3:D:253:GLU:HB3	1.82	0.44
1:A:127:THR:CG2	2:B:639:ASN:CB	2.91	0.44
1:A:222:ARG:NH1	2:B:613:LEU:HD13	2.31	0.44
1:A:959:TYR:O	1:A:960:ILE:HG13	2.17	0.44
1:A:358:ILE:HB	1:A:359:PRO:HA	1.99	0.44
1:A:926:MET:HB2	1:A:931:GLY:CA	2.47	0.44
2:C:449:PHE:N	2:C:450:PRO:CD	2.79	0.44
2:C:192:PRO:HG3	2:C:294:VAL:CG2	2.48	0.44
2:C:385:ILE:O	2:C:386:SER:CB	2.65	0.44
2:C:624:PHE:CD2	2:C:713:MET:HG2	2.53	0.44
2:B:888:GLN:NE2	3:D:38:GLU:OE1	2.51	0.44
1:A:127:THR:HG23	2:B:640:GLN:CA	2.47	0.44
1:A:926:MET:SD	1:A:928:GLU:HG2	2.58	0.44
3:E:42:ASN:HB3	3:E:174:VAL:CG2	2.48	0.44
1:A:663:GLU:O	1:A:667:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:33:GLN:O	3:E:35:LEU:N	2.51	0.44
3:E:68:ILE:HD13	3:E:69:GLU:CA	2.47	0.44
1:A:988:LYS:HD2	1:A:994:PRO:HD3	2.00	0.44
3:D:14:GLN:NE2	3:D:107:LEU:HD13	2.32	0.44
2:C:837:THR:CG2	2:C:934:LEU:HD21	2.46	0.44
1:A:351:TYR:CE1	3:D:150:ILE:CG2	3.01	0.44
3:D:150:ILE:HG22	3:D:151:ASP:N	2.33	0.44
1:A:470:LEU:HD21	1:A:525:ARG:HD2	1.99	0.44
3:D:25:ASN:OD1	3:D:26:ALA:N	2.51	0.44
1:A:659:ASN:HD21	1:A:706:TYR:H	1.65	0.44
1:A:526:ASN:OD1	1:A:526:ASN:N	2.49	0.44
1:A:303:THR:CA	1:A:307:HIS:CE1	3.00	0.44
2:B:473:ALA:HA	2:B:765:PRO:HG3	1.98	0.44
2:B:291:HIS:HB3	2:B:292:ASN:H	1.55	0.44
3:E:46:LYS:CG	3:E:155:HIS:CE1	3.00	0.44
2:C:564:GLY:O	2:C:565:GLU:HB3	2.17	0.44
1:A:525:ARG:HE	1:A:525:ARG:HB2	1.42	0.44
3:D:116:THR:OG1	3:D:119:ILE:HD12	2.18	0.44
3:E:2:LEU:HD11	3:E:107:LEU:CD1	2.48	0.44
2:C:838:GLU:HA	2:C:940:ARG:NE	2.33	0.44
2:B:146:GLU:OE2	2:B:1314:ASP:HB3	2.18	0.44
1:A:842:TYR:HA	1:A:845:ILE:HG22	2.00	0.43
3:D:255:ILE:CG1	3:D:255:ILE:O	2.65	0.43
1:A:625:PHE:HA	1:A:628:MET:HB3	2.00	0.43
3:D:160:LEU:HD23	3:D:229:PHE:HA	2.00	0.43
2:B:1306:THR:HG23	2:B:1308:ASN:H	1.83	0.43
2:B:554:ARG:HH21	2:B:594:LEU:HD23	1.83	0.43
3:E:286:THR:O	3:E:290:TRP:CB	2.65	0.43
1:A:133:LEU:CD2	2:C:545:PRO:HG3	2.48	0.43
1:A:963:TYR:CE2	1:A:985:GLY:HA2	2.53	0.43
2:B:862:ARG:NH1	2:B:948:ILE:HD13	2.33	0.43
2:B:1078:TYR:CD2	2:B:1078:TYR:C	2.91	0.43
3:D:144:ARG:O	3:D:144:ARG:CG	2.64	0.43
2:B:154:PHE:HA	2:B:262:ASN:HD22	1.83	0.43
2:B:883:ILE:HG21	2:B:915:VAL:HG21	2.00	0.43
2:C:204:VAL:CG2	2:C:1242:MET:HG2	2.48	0.43
2:B:172:ASP:HA	2:B:175:THR:HG22	2.00	0.43
3:E:93:LEU:O	3:E:96:LEU:HB2	2.18	0.43
3:E:186:LEU:HD13	3:E:186:LEU:HA	1.60	0.43
2:C:390:HIS:O	2:C:1317:VAL:HG23	2.18	0.43
2:C:1121:HIS:ND1	2:C:1123:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:590:SER:HB2	2:C:592:VAL:HG12	2.00	0.43
2:B:959:GLN:OE1	2:B:959:GLN:HA	2.17	0.43
3:E:122:TYR:CE2	3:E:203:ILE:HG21	2.53	0.43
1:A:406:VAL:HB	1:A:407:GLU:C	2.39	0.43
2:C:191:GLY:H	2:C:192:PRO:HD2	1.84	0.43
2:C:627:ALA:HB2	2:C:716:PHE:CD2	2.54	0.43
2:B:1082:ASP:OD2	2:B:1226:ASP:HB2	2.18	0.43
1:A:853:GLU:HG3	1:A:853:GLU:H	1.69	0.43
2:B:1083:ASP:OD2	2:B:1083:ASP:N	2.51	0.43
2:C:856:LEU:HD11	3:D:117:ILE:HD12	2.00	0.43
3:E:253:GLU:HG3	3:E:254:TYR:CE2	2.54	0.43
1:A:602:PHE:HB2	1:A:603:PRO:HD2	2.00	0.43
2:B:389:PHE:CE1	2:B:1319:ARG:HG2	2.53	0.43
1:A:265:SER:HB2	1:A:269:VAL:HG21	2.00	0.43
3:E:152:ILE:HD12	3:E:152:ILE:H	1.83	0.43
2:C:1293:VAL:O	2:C:1294:ASP:HB2	2.18	0.43
3:D:46:LYS:HE3	3:D:158:LEU:HD22	2.00	0.43
1:A:512:ALA:HA	1:A:513:PRO:HA	1.74	0.43
1:A:292:ARG:HG2	1:A:295:THR:HG21	2.01	0.43
2:B:423:GLU:HB3	2:B:490:PHE:CE2	2.53	0.43
2:B:168:VAL:HG23	2:B:204:VAL:HG12	2.00	0.43
1:A:131:GLY:O	1:A:134:VAL:HG12	2.19	0.43
1:A:977:HIS:O	1:A:988:LYS:HB3	2.19	0.43
1:A:282:GLU:O	1:A:283:PHE:CG	2.72	0.43
2:C:837:THR:HA	2:C:936:MET:HB2	2.00	0.43
2:B:612:PHE:CE1	2:B:635:ILE:HD11	2.53	0.43
1:A:853:GLU:CD	1:A:854:ASN:H	2.22	0.43
2:C:297:ASN:HD22	2:C:298:PRO:N	2.16	0.43
2:C:630:ASN:HA	2:C:631:PRO:HD3	1.87	0.43
3:D:74:GLN:OE1	3:D:74:GLN:HA	2.19	0.43
3:E:282:PHE:CZ	3:E:286:THR:HG21	2.53	0.43
2:C:450:PRO:HB2	2:C:451:GLU:H	1.59	0.43
3:D:14:GLN:HE22	3:D:107:LEU:HD13	1.84	0.43
2:C:1031:TYR:O	2:C:1032:ASP:CB	2.67	0.43
1:A:535:LEU:HD13	1:A:536:TYR:N	2.34	0.43
2:C:115:GLN:HG3	2:C:116:SER:H	1.84	0.43
1:A:850:SER:HB3	1:A:872:VAL:HG11	2.00	0.43
3:E:162:GLY:O	3:E:167:ARG:NH1	2.48	0.42
2:B:937:ASN:C	2:B:939:ASN:H	2.22	0.42
3:D:241:ASN:HB3	3:D:250:ARG:HD2	2.01	0.42
3:D:66:VAL:HG23	3:D:67:TYR:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:210:GLY:O	3:E:214:ARG:HG3	2.18	0.42
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.90	0.42
3:D:53:GLU:CG	3:D:145:TYR:HE1	2.31	0.42
2:C:772:TYR:C	2:C:774:LEU:H	2.21	0.42
1:A:654:SER:HB3	1:A:715:TYR:HE2	1.84	0.42
1:A:1016:ILE:HD13	1:A:1016:ILE:H	1.84	0.42
3:E:32:LEU:O	3:E:35:LEU:CG	2.58	0.42
2:B:137:ILE:HB	2:C:471:SER:HB3	2.00	0.42
2:C:860:ARG:O	2:C:864:HIS:HB2	2.19	0.42
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.54	0.42
3:E:268:THR:OG1	3:E:269:ILE:N	2.48	0.42
2:C:855:TYR:CZ	2:C:896:LEU:HD21	2.54	0.42
2:C:594:LEU:HD22	2:C:595:ALA:H	1.84	0.42
2:B:772:TYR:HB3	2:B:773:PRO:HD2	2.01	0.42
1:A:855:MET:HA	1:A:916:ASN:HB3	2.01	0.42
2:C:493:HIS:NE2	2:C:527:ARG:HD2	2.35	0.42
3:D:217:LYS:HE2	3:D:290:TRP:O	2.18	0.42
2:B:641:ARG:O	2:C:670:ASP:OD2	2.36	0.42
2:C:440:ILE:HD13	2:C:441:ARG:N	2.35	0.42
2:C:1130:SER:O	2:C:1134:ARG:HD3	2.20	0.42
1:A:292:ARG:HG2	1:A:295:THR:HG22	2.02	0.42
1:A:12:ARG:HD3	1:A:12:ARG:C	2.40	0.42
2:B:318:LEU:HD11	2:B:325:TYR:HB2	1.99	0.42
2:C:1083:ASP:HA	2:C:1084:PRO:HD2	1.75	0.42
1:A:487:GLN:OE1	1:A:548:ASN:HB3	2.19	0.42
1:A:955:ASN:HD21	1:A:1055:LEU:HD23	1.84	0.42
1:A:752:VAL:HG23	1:A:779:ASN:O	2.20	0.42
1:A:739:ASN:HD22	1:A:739:ASN:HA	1.70	0.42
3:E:32:LEU:HD13	3:E:225:ARG:NH1	2.35	0.42
3:E:1:MET:CE	3:E:123:ASP:HA	2.49	0.42
2:B:937:ASN:O	2:B:939:ASN:N	2.52	0.42
2:C:1020:ARG:HD2	2:C:1031:TYR:HA	2.01	0.42
2:B:153:ASP:HB3	2:B:154:PHE:CD1	2.54	0.42
2:B:172:ASP:O	2:B:173:GLN:HB3	2.19	0.42
1:A:713:ASN:HA	1:A:716:MET:HB2	2.01	0.42
3:D:149:MET:HE2	3:D:260:MET:CE	2.43	0.42
1:A:222:ARG:NH1	2:B:613:LEU:CD1	2.82	0.42
2:C:1035:ILE:HG22	2:C:1036:ASP:N	2.33	0.42
1:A:395:GLN:CA	1:A:395:GLN:NE2	2.79	0.42
2:C:372:ALA:HA	2:C:398:ARG:HD3	2.02	0.42
1:A:147:GLN:HG3	1:A:215:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:MET:HG3	1:A:205:VAL:HG21	2.02	0.42
2:C:540:PHE:O	2:C:548:TYR:HB2	2.19	0.42
2:C:651:ARG:O	2:C:655:ILE:HG12	2.20	0.42
2:B:188:ARG:NH1	2:C:237:VAL:HG13	2.34	0.42
3:E:158:LEU:CD2	3:E:172:MET:HB3	2.49	0.42
2:B:363:ARG:NH1	3:D:80:SER:OG	2.50	0.42
1:A:71:LEU:HB3	1:A:72:PHE:H	1.67	0.42
2:B:274:MET:HG2	2:C:234:PRO:CD	2.35	0.42
2:B:748:GLN:O	2:B:750:GLU:HB3	2.20	0.42
3:D:239:VAL:CG1	3:D:250:ARG:HH12	2.30	0.42
2:C:1036:ASP:O	2:C:1037:ILE:HB	2.19	0.42
3:D:193:VAL:HG11	3:D:230:ILE:HD12	2.02	0.42
2:C:1249:ASN:HA	2:C:1250:GLU:HA	1.48	0.42
2:B:760:THR:C	2:B:762:ILE:H	2.22	0.42
3:E:32:LEU:CD1	3:E:225:ARG:NE	2.83	0.42
3:E:140:ALA:HB1	3:E:281:LYS:HG3	2.02	0.42
3:E:247:ARG:HA	3:E:247:ARG:NE	2.30	0.42
2:C:292:ASN:O	2:C:293:ASN:CB	2.58	0.42
2:C:1243:ARG:NH1	2:C:1257:ALA:HA	2.34	0.42
1:A:939:GLN:HE21	1:A:939:GLN:HB3	1.66	0.42
1:A:204:LEU:HD13	1:A:221:TYR:HB2	2.02	0.42
1:A:454:GLY:C	1:A:456:PHE:H	2.22	0.42
2:B:815:LEU:HB3	2:B:816:PRO:HD3	2.01	0.42
1:A:1000:GLU:O	1:A:1003:VAL:HG12	2.20	0.42
1:A:101:LEU:HD21	1:A:119:VAL:HG23	2.02	0.42
2:C:448:TYR:CA	2:C:450:PRO:HD3	2.49	0.41
1:A:962:PHE:HE2	1:A:966:GLY:HA3	1.85	0.41
1:A:72:PHE:CD1	1:A:72:PHE:N	2.87	0.41
2:B:835:TYR:CE1	2:B:925:VAL:HG21	2.55	0.41
1:A:208:HIS:NE2	1:A:234:GPL:O1P	2.53	0.41
2:B:1156:ILE:HD11	2:B:1194:MET:HG3	2.02	0.41
1:A:306:GLN:HA	1:A:306:GLN:OE1	2.18	0.41
2:C:1136:HIS:O	2:C:1136:HIS:CD2	2.73	0.41
3:E:69:GLU:HG3	3:E:199:LEU:HB2	1.98	0.41
1:A:308:ALA:CA	1:A:309:ASN:CB	2.92	0.41
3:E:2:LEU:HD11	3:E:107:LEU:HD11	2.02	0.41
1:A:566:GLU:HB2	1:A:567:PRO:CD	2.41	0.41
1:A:673:TYR:CE2	1:A:694:ILE:CG2	3.03	0.41
3:E:72:ILE:O	3:E:76:LEU:HD12	2.20	0.41
3:E:76:LEU:HD21	3:E:282:PHE:CD2	2.55	0.41
1:A:1013:THR:O	1:A:1055:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:LEU:HD23	3:D:14:GLN:HB2	2.01	0.41
2:C:968:ARG:O	2:C:971:MET:HB2	2.20	0.41
2:C:986:ILE:O	2:C:989:ILE:HG22	2.20	0.41
2:C:871:PRO:HG3	2:C:892:VAL:HG11	2.01	0.41
1:A:776:SER:HA	1:A:818:PHE:HE1	1.85	0.41
2:B:583:GLU:O	2:B:584:HIS:CB	2.69	0.41
1:A:677:LEU:HB3	1:A:692:ILE:HD13	2.02	0.41
2:B:149:PRO:HB3	2:B:1312:GLY:HA2	2.01	0.41
3:D:69:GLU:HB2	3:D:199:LEU:HD11	2.02	0.41
2:B:150:LEU:O	2:B:804:LEU:HD13	2.20	0.41
1:A:47:ARG:HB2	2:B:595:ALA:O	2.20	0.41
3:E:205:LEU:CD1	3:E:289:ARG:HG3	2.50	0.41
2:B:954:GLN:NE2	3:D:240:VAL:HG12	2.35	0.41
2:C:451:GLU:O	2:C:452:ASN:CB	2.69	0.41
1:A:23:ARG:HH21	1:A:27:LYS:HB3	1.85	0.41
2:B:228:VAL:HG22	2:B:229:GLN:H	1.84	0.41
2:B:838:GLU:HG3	2:B:839:ALA:H	1.84	0.41
1:A:49:HIS:NE2	1:A:172:PHE:CD1	2.75	0.41
2:B:475:ILE:O	2:B:477:SER:N	2.53	0.41
1:A:665:LEU:N	1:A:667:GLN:HE22	2.17	0.41
2:B:908:THR:HA	2:B:911:ARG:HH21	1.85	0.41
3:D:69:GLU:HG3	3:D:199:LEU:HG	2.02	0.41
2:B:871:PRO:HG3	2:B:894:VAL:HG13	2.02	0.41
2:B:487:SER:HA	2:B:488:PRO:HD3	1.94	0.41
1:A:530:MET:HA	1:A:533:LEU:HB2	2.02	0.41
1:A:203:THR:HG23	1:A:204:LEU:H	1.86	0.41
3:D:152:ILE:HG21	3:D:283:LEU:HB3	2.01	0.41
2:C:204:VAL:HG23	2:C:1242:MET:HG2	2.02	0.41
2:B:588:LEU:HD22	2:B:604:MET:CE	2.51	0.41
1:A:361:SER:HB3	1:A:362:MET:H	1.62	0.41
3:E:182:TRP:CD1	3:E:185:SER:HB3	2.55	0.41
2:B:269:GLU:O	2:B:291:HIS:HD2	2.04	0.41
2:B:486:VAL:HG21	2:B:709:MET:HB3	2.03	0.41
1:A:892:GLN:C	1:A:894:LYS:H	2.24	0.41
2:B:946:LEU:HD22	2:B:947:GLU:H	1.85	0.41
2:C:926:VAL:CG2	2:C:938:ASN:HB2	2.50	0.41
2:C:82:ARG:CZ	2:C:210:ARG:HB3	2.51	0.41
2:B:420:PRO:HB2	2:B:748:GLN:CD	2.39	0.41
1:A:511:ILE:HD12	1:A:511:ILE:O	2.21	0.41
3:E:140:ALA:CB	3:E:281:LYS:HG3	2.51	0.41
1:A:71:LEU:O	1:A:73:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:66:VAL:HG13	3:E:111:ILE:HG21	2.03	0.41
2:C:597:ALA:O	2:C:600:ILE:HG22	2.20	0.41
2:B:837:THR:O	2:B:838:GLU:CB	2.68	0.41
2:B:228:VAL:O	2:B:246:GLU:HB2	2.20	0.41
2:B:1321:ASN:C	2:B:1323:ASP:H	2.24	0.41
2:C:1181:SER:O	2:C:1182:GLU:HB3	2.21	0.41
1:A:35:GLY:H	1:A:38:TYR:HE1	1.67	0.41
1:A:303:THR:CB	1:A:307:HIS:NE2	2.76	0.41
1:A:725:PRO:C	1:A:726:ILE:HG12	2.39	0.41
1:A:491:ASP:OD1	1:A:491:ASP:C	2.60	0.41
3:D:258:ASN:OD1	3:D:259:SER:N	2.53	0.41
2:C:293:ASN:CG	2:C:294:VAL:N	2.73	0.41
2:C:1325:VAL:HG12	2:C:1326:ARG:N	2.36	0.41
1:A:600:VAL:HA	1:A:601:PRO:C	2.40	0.41
2:C:633:THR:HG21	2:C:710:SER:OG	2.21	0.41
2:B:1330:ILE:HD13	2:B:1330:ILE:H	1.86	0.41
1:A:194:HIS:ND1	3:D:146:ARG:HD2	2.35	0.40
2:B:445:GLU:HG3	2:B:447:ARG:HG2	2.03	0.40
2:B:954:GLN:HB3	2:B:956:ASP:O	2.20	0.40
2:C:1042:TRP:CE3	2:C:1042:TRP:HA	2.56	0.40
2:B:862:ARG:C	2:B:952:PHE:HZ	2.24	0.40
2:B:612:PHE:CZ	2:B:1331:ARG:HD2	2.56	0.40
2:B:941:TYR:HD1	2:B:941:TYR:O	2.04	0.40
2:B:450:PRO:HG3	2:B:686:HIS:HB2	2.04	0.40
3:D:29:THR:HG22	3:D:222:ASP:OD1	2.21	0.40
2:C:617:ASP:HA	2:C:620:ILE:HG22	2.03	0.40
2:B:821:ASN:HA	2:B:821:ASN:HD22	1.73	0.40
1:A:406:VAL:HG23	1:A:407:GLU:HA	2.03	0.40
1:A:967:ILE:HA	1:A:970:ARG:HB3	2.02	0.40
2:C:856:LEU:HA	2:C:860:ARG:HB2	2.03	0.40
3:E:209:GLU:CG	3:E:210:GLY:H	2.29	0.40
1:A:201:LYS:CA	2:B:629:ARG:HD3	2.51	0.40
1:A:513:PRO:HB2	1:A:514:LEU:H	1.62	0.40
2:C:948:ILE:O	2:C:948:ILE:HG22	2.21	0.40
2:C:317:MET:SD	2:C:1262:SER:HB3	2.61	0.40
2:C:159:ASP:OD2	2:C:291:HIS:HE1	2.04	0.40
2:C:835:TYR:HB2	2:C:847:ILE:HD11	2.03	0.40
2:C:999:LYS:HD3	2:C:1009:THR:HG22	2.04	0.40
3:E:70:ASP:OD2	3:E:70:ASP:C	2.60	0.40
3:E:140:ALA:O	3:E:146:ARG:HA	2.22	0.40
3:E:264:GLY:H	3:E:268:THR:CG2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:142:THR:HG23	3:E:143:PRO:CD	2.50	0.40
2:B:172:ASP:O	2:B:173:GLN:CB	2.70	0.40
1:A:177:THR:HA	1:A:178:PRO:HD3	1.95	0.40
2:B:1076:ILE:HB	2:B:1166:VAL:HG23	2.03	0.40
3:E:53:GLU:CB	3:E:145:TYR:CE1	3.05	0.40
2:B:274:MET:CG	2:C:234:PRO:CD	2.55	0.40
2:B:134:THR:HG22	2:C:472:GLU:CD	2.36	0.40
2:B:1031:TYR:CD2	2:B:1041:ARG:HD3	2.57	0.40
2:C:372:ALA:HB1	2:C:1315:MET:CE	2.51	0.40
1:A:604:ILE:H	1:A:604:ILE:HD13	1.86	0.40
2:B:225:ILE:HG22	2:B:227:LEU:HG	2.04	0.40
1:A:421:LEU:HD12	1:A:678:LEU:HB3	2.02	0.40
2:C:447:ARG:HE	2:C:690:GLN:NE2	2.20	0.40
2:C:603:ILE:C	2:C:605:ARG:H	2.25	0.40
2:C:610:GLN:O	2:C:634:TYR:CE2	2.75	0.40
2:C:177:LYS:HD3	2:C:177:LYS:H	1.86	0.40
3:D:257:VAL:O	3:D:257:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1038/1058 (98%)	813 (78%)	161 (16%)	64 (6%)	2	27
2	B	1172/1333 (88%)	958 (82%)	186 (16%)	28 (2%)	7	49
2	C	1238/1333 (93%)	1018 (82%)	192 (16%)	28 (2%)	8	50
3	D	289/448 (64%)	253 (88%)	33 (11%)	3 (1%)	19	65
3	E	289/448 (64%)	254 (88%)	34 (12%)	1 (0%)	46	82
All	All	4026/4620 (87%)	3296 (82%)	606 (15%)	124 (3%)	9	44

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	49	HIS
1	A	72	PHE
1	A	255	ARG
1	A	282	GLU
1	A	287	VAL
1	A	309	ASN
1	A	330	GLN
1	A	359	PRO
1	A	395	GLN
1	A	485	MET
1	A	513	PRO
1	A	724	MET
1	A	813	PRO
1	A	915	ASN
1	A	924	VAL
1	A	962	PHE
2	B	838	GLU
2	B	940	ARG
2	B	1281	VAL
2	C	972	PRO
1	A	187	PRO
1	A	387	THR
1	A	391	ILE
1	A	606	LYS
1	A	697	ILE
1	A	726	ILE
1	A	832	GLU
1	A	923	ALA
1	A	994	PRO
2	B	242	GLU
2	B	279	SER
2	B	749	GLY
2	B	901	VAL
2	B	973	THR
2	B	1299	SER
2	C	340	VAL
2	C	450	PRO
2	C	666	ARG
2	C	752	VAL
2	C	842	ASP
2	C	1032	ASP

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Mol	Chain	Res	Type
2	C	1037	ILE
3	D	244	VAL
1	A	214	ASN
1	A	286	ASN
1	A	305	TYR
1	A	496	CYS
1	A	580	SER
1	A	622	ASP
1	A	671	VAL
1	A	686	TYR
1	A	688	TYR
1	A	802	THR
1	A	853	GLU
1	A	1037	SER
2	B	291	HIS
2	B	584	HIS
2	B	897	TYR
2	B	937	ASN
2	B	952	PHE
2	B	1086	PRO
2	C	386	SER
2	C	948	ILE
2	C	1038	GLU
2	C	1047	LEU
3	D	253	GLU
1	A	28	PRO
1	A	209	SER
1	A	212	HIS
1	A	263	LEU
1	A	684	ASN
1	A	829	MET
1	A	914	GLU
1	A	963	TYR
2	B	229	GLN
2	C	671	ASP
2	C	831	VAL
2	C	1029	LEU
2	C	1208	ASP
2	C	1237	SER
3	D	265	ARG
1	A	203	THR
1	A	266	SER

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Mol	Chain	Res	Type
1	A	304	TYR
1	A	406	VAL
1	A	563	ALA
1	A	709	SER
1	A	722	ASP
1	A	821	ARG
1	A	887	ILE
1	A	990	ALA
2	B	476	SER
2	B	938	ASN
2	B	1234	GLN
2	C	562	ALA
2	C	845	GLU
2	C	951	ILE
2	C	1182	GLU
1	A	389	ALA
1	A	455	MET
1	A	567	PRO
1	A	975	THR
2	B	190	VAL
2	B	840	ASP
2	B	1085	ASP
2	B	1252	ASP
2	C	646	ASN
2	C	757	ILE
3	E	55	HIS
1	A	411	ILE
2	B	830	VAL
2	C	1086	PRO
1	A	25	ILE
2	C	830	VAL
1	A	928	GLU
2	B	880	PRO
2	B	1236	ILE
2	C	1224	GLY
1	A	478	ILE
2	B	1093	PRO
2	C	644	VAL
2	C	1245	ILE
2	B	983	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	932/942 (99%)	778 (84%)	154 (16%)	3	21
2	B	1029/1155 (89%)	920 (89%)	109 (11%)	8	40
2	C	1085/1155 (94%)	950 (88%)	135 (12%)	6	33
3	D	240/379 (63%)	205 (85%)	35 (15%)	4	26
3	E	240/379 (63%)	198 (82%)	42 (18%)	2	18
All	All	3526/4010 (88%)	3051 (86%)	475 (14%)	9	30

All (475) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	TYR
1	A	9	ASN
1	A	10	ASP
1	A	12	ARG
1	A	20	ASN
1	A	22	ILE
1	A	23	ARG
1	A	31	VAL
1	A	39	LEU
1	A	47	ARG
1	A	53	LEU
1	A	54	LEU
1	A	63	SER
1	A	66	ASP
1	A	67	ARG
1	A	72	PHE
1	A	73	ARG
1	A	77	LYS
1	A	91	ASN
1	A	97	ARG
1	A	100	HIS
1	A	103	HIS
1	A	120	TYR

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Mol	Chain	Res	Type
1	A	140	ILE
1	A	148	ASP
1	A	177	THR
1	A	204	LEU
1	A	207	THR
1	A	215	VAL
1	A	228	ILE
1	A	231	PHE
1	A	235	ILE
1	A	244	LYS
1	A	252	GLU
1	A	255	ARG
1	A	256	VAL
1	A	270	GLN
1	A	278	LEU
1	A	282	GLU
1	A	286	ASN
1	A	288	LEU
1	A	292	ARG
1	A	297	LEU
1	A	298	LEU
1	A	299	GLN
1	A	302	ASP
1	A	306	GLN
1	A	331	ARG
1	A	332	HIS
1	A	334	GLU
1	A	339	GLN
1	A	357	THR
1	A	362	MET
1	A	365	ILE
1	A	380	THR
1	A	383	THR
1	A	393	LEU
1	A	406	VAL
1	A	411	ILE
1	A	437	GLN
1	A	444	LEU
1	A	458	ASN
1	A	461	ARG
1	A	463	ASP
1	A	470	LEU

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Mol	Chain	Res	Type
1	A	474	TYR
1	A	477	TYR
1	A	479	LYS
1	A	485	MET
1	A	487	GLN
1	A	492	HIS
1	A	509	ARG
1	A	519	ILE
1	A	521	LYS
1	A	523	MET
1	A	525	ARG
1	A	526	ASN
1	A	535	LEU
1	A	542	LEU
1	A	544	ASN
1	A	545	PHE
1	A	552	MET
1	A	558	ILE
1	A	559	ILE
1	A	561	LEU
1	A	565	ARG
1	A	578	ASN
1	A	580	SER
1	A	584	ILE
1	A	589	ASP
1	A	602	PHE
1	A	604	ILE
1	A	605	ASP
1	A	611	ASP
1	A	616	ASP
1	A	620	TYR
1	A	621	GLU
1	A	622	ASP
1	A	626	GLU
1	A	628	MET
1	A	652	HIS
1	A	655	GLU
1	A	658	ILE
1	A	667	GLN
1	A	673	TYR
1	A	680	THR
1	A	683	GLN

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Mol	Chain	Res	Type
1	A	695	THR
1	A	713	ASN
1	A	714	ARG
1	A	717	THR
1	A	719	VAL
1	A	726	ILE
1	A	727	ILE
1	A	737	HIS
1	A	739	ASN
1	A	746	PHE
1	A	763	LYS
1	A	771	THR
1	A	779	ASN
1	A	781	VAL
1	A	788	ASP
1	A	794	LEU
1	A	812	VAL
1	A	814	ASN
1	A	835	PHE
1	A	841	MET
1	A	853	GLU
1	A	859	VAL
1	A	866	LEU
1	A	868	ASP
1	A	874	LEU
1	A	905	GLN
1	A	906	PHE
1	A	924	VAL
1	A	925	ILE
1	A	927	ASN
1	A	939	GLN
1	A	951	LEU
1	A	953	ARG
1	A	955	ASN
1	A	963	TYR
1	A	967	ILE
1	A	969	THR
1	A	971	LEU
1	A	973	GLN
1	A	978	LYS
1	A	987	LEU
1	A	1003	VAL

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Mol	Chain	Res	Type
1	A	1006	MET
1	A	1016	ILE
1	A	1034	ARG
1	A	1035	LEU
1	A	1053	ILE
2	B	148	GLN
2	B	152	ASP
2	B	153	ASP
2	B	161	LYS
2	B	170	TYR
2	B	171	GLU
2	B	177	LYS
2	B	181	ARG
2	B	186	ASP
2	B	189	ILE
2	B	203	VAL
2	B	205	ASN
2	B	219	ILE
2	B	230	ASP
2	B	270	THR
2	B	286	LEU
2	B	302	ARG
2	B	303	ASP
2	B	309	TRP
2	B	319	GLN
2	B	324	LYS
2	B	331	GLU
2	B	339	LEU
2	B	369	ASN
2	B	374	ASP
2	B	384	MET
2	B	409	ILE
2	B	412	LEU
2	B	423	GLU
2	B	425	ILE
2	B	445	GLU
2	B	447	ARG
2	B	453	LEU
2	B	472	GLU
2	B	475	ILE
2	B	486	VAL
2	B	516	LEU

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Mol	Chain	Res	Type
2	B	529	LYS
2	B	547	GLU
2	B	554	ARG
2	B	588	LEU
2	B	594	LEU
2	B	610	GLN
2	B	671	ASP
2	B	685	ARG
2	B	688	GLU
2	B	719	ASN
2	B	738	GLU
2	B	747	ARG
2	B	748	GLN
2	B	750	GLU
2	B	832	MET
2	B	836	GLN
2	B	848	ARG
2	B	850	THR
2	B	879	THR
2	B	895	VAL
2	B	897	TYR
2	B	908	THR
2	B	912	GLU
2	B	922	TYR
2	B	934	LEU
2	B	938	ASN
2	B	940	ARG
2	B	941	TYR
2	B	942	HIS
2	B	946	LEU
2	B	953	ASP
2	B	957	PHE
2	B	964	VAL
2	B	971	MET
2	B	985	ARG
2	B	988	GLN
2	B	1008	LEU
2	B	1020	ARG
2	B	1028	VAL
2	B	1036	ASP
2	B	1049	GLU
2	B	1053	ARG

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Mol	Chain	Res	Type
2	B	1069	ARG
2	B	1075	ARG
2	B	1078	TYR
2	B	1079	LEU
2	B	1092	VAL
2	B	1103	HIS
2	B	1114	ARG
2	B	1144	ARG
2	B	1153	ASP
2	B	1176	GLU
2	B	1186	GLN
2	B	1187	HIS
2	B	1202	PHE
2	B	1203	HIS
2	B	1210	LEU
2	B	1212	ARG
2	B	1218	PHE
2	B	1226	ASP
2	B	1227	MET
2	B	1228	ARG
2	B	1230	ILE
2	B	1242	MET
2	B	1247	ASN
2	B	1252	ASP
2	B	1281	VAL
2	B	1291	LEU
2	B	1300	ASN
2	B	1318	GLU
2	B	1323	ASP
2	B	1330	ILE
2	C	108	LYS
2	C	117	ARG
2	C	120	VAL
2	C	123	GLU
2	C	124	GLN
2	C	128	GLU
2	C	133	MET
2	C	134	THR
2	C	145	THR
2	C	146	GLU
2	C	154	PHE
2	C	156	GLN

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Mol	Chain	Res	Type
2	C	173	GLN
2	C	177	LYS
2	C	204	VAL
2	C	205	ASN
2	C	221	LEU
2	C	231	LEU
2	C	265	VAL
2	C	283	ASN
2	C	297	ASN
2	C	306	GLN
2	C	309	TRP
2	C	339	LEU
2	C	346	HIS
2	C	361	ASN
2	C	366	MET
2	C	384	MET
2	C	409	ILE
2	C	412	LEU
2	C	422	LEU
2	C	430	ASN
2	C	440	ILE
2	C	451	GLU
2	C	456	ASN
2	C	458	SER
2	C	462	LEU
2	C	469	ARG
2	C	472	GLU
2	C	480	LEU
2	C	489	MET
2	C	493	HIS
2	C	494	GLU
2	C	495	LEU
2	C	512	LEU
2	C	520	PHE
2	C	524	GLU
2	C	536	LEU
2	C	547	GLU
2	C	560	ILE
2	C	574	LYS
2	C	576	ASP
2	C	581	LEU
2	C	591	ASP

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Mol	Chain	Res	Type
2	C	594	LEU
2	C	599	THR
2	C	603	ILE
2	C	604	MET
2	C	605	ARG
2	C	613	LEU
2	C	634	TYR
2	C	637	TYR
2	C	646	ASN
2	C	647	GLU
2	C	671	ASP
2	C	677	ARG
2	C	681	LYS
2	C	684	LEU
2	C	688	GLU
2	C	693	ASN
2	C	714	LEU
2	C	716	PHE
2	C	720	PHE
2	C	730	ASP
2	C	731	GLN
2	C	738	GLU
2	C	747	ARG
2	C	762	ILE
2	C	767	LEU
2	C	771	THR
2	C	799	THR
2	C	820	ILE
2	C	828	ASP
2	C	830	VAL
2	C	847	ILE
2	C	849	MET
2	C	863	LEU
2	C	864	HIS
2	C	874	ILE
2	C	882	GLN
2	C	898	GLN
2	C	915	VAL
2	C	928	ARG
2	C	934	LEU
2	C	936	MET
2	C	943	GLU

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Mol	Chain	Res	Type
2	C	947	GLU
2	C	953	ASP
2	C	954	GLN
2	C	959	GLN
2	C	990	THR
2	C	1000	LEU
2	C	1022	ILE
2	C	1027	THR
2	C	1029	LEU
2	C	1042	TRP
2	C	1051	ARG
2	C	1076	ILE
2	C	1079	LEU
2	C	1134	ARG
2	C	1174	THR
2	C	1176	GLU
2	C	1187	HIS
2	C	1193	ILE
2	C	1201	LEU
2	C	1202	PHE
2	C	1204	LEU
2	C	1214	GLU
2	C	1227	MET
2	C	1228	ARG
2	C	1229	LEU
2	C	1236	ILE
2	C	1243	ARG
2	C	1247	ASN
2	C	1249	ASN
2	C	1253	ARG
2	C	1269	THR
2	C	1272	ARG
2	C	1275	ASP
2	C	1288	ILE
2	C	1292	GLU
2	C	1294	ASP
2	C	1295	HIS
2	C	1296	ILE
2	C	1309	ILE
3	D	1	MET
3	D	13	GLU
3	D	14	GLN

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Mol	Chain	Res	Type
3	D	15	PHE
3	D	20	ARG
3	D	37	TYR
3	D	41	GLU
3	D	47	LYS
3	D	55	HIS
3	D	61	ASN
3	D	66	VAL
3	D	68	ILE
3	D	69	GLU
3	D	70	ASP
3	D	79	ILE
3	D	85	ASN
3	D	87	HIS
3	D	90	PHE
3	D	100	ASN
3	D	101	THR
3	D	121	PHE
3	D	133	THR
3	D	149	MET
3	D	156	VAL
3	D	158	LEU
3	D	160	LEU
3	D	195	ASN
3	D	196	TRP
3	D	226	MET
3	D	228	LEU
3	D	242	ARG
3	D	250	ARG
3	D	288	THR
3	D	289	ARG
3	D	290	TRP
3	E	9	TYR
3	E	15	PHE
3	E	17	PHE
3	E	19	ILE
3	E	29	THR
3	E	35	LEU
3	E	41	GLU
3	E	44	LEU
3	E	46	LYS
3	E	47	LYS

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Mol	Chain	Res	Type
3	E	53	GLU
3	E	55	HIS
3	E	66	VAL
3	E	68	ILE
3	E	69	GLU
3	E	83	ASN
3	E	85	ASN
3	E	87	HIS
3	E	92	ARG
3	E	107	LEU
3	E	108	ASP
3	E	111	ILE
3	E	118	ASN
3	E	122	TYR
3	E	137	LEU
3	E	144	ARG
3	E	146	ARG
3	E	151	ASP
3	E	178	LYS
3	E	179	PHE
3	E	186	LEU
3	E	191	ARG
3	E	195	ASN
3	E	221	ARG
3	E	228	LEU
3	E	255	ILE
3	E	261	ARG
3	E	269	ILE
3	E	273	LEU
3	E	288	THR
3	E	289	ARG
3	E	291	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	29	ASN
1	A	91	ASN
1	A	136	ASN
1	A	212	HIS
1	A	241	GLN

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Mol	Chain	Res	Type
1	A	367	ASN
1	A	395	GLN
1	A	434	GLN
1	A	437	GLN
1	A	548	ASN
1	A	578	ASN
1	A	581	ASN
1	A	607	ASN
1	A	659	ASN
1	A	667	GLN
1	A	674	HIS
1	A	683	GLN
1	A	737	HIS
1	A	739	ASN
1	A	814	ASN
1	A	830	HIS
1	A	857	GLN
1	A	916	ASN
1	A	939	GLN
1	A	955	ASN
1	A	1047	ASN
1	A	1048	HIS
2	B	195	ASN
2	B	205	ASN
2	B	292	ASN
2	B	430	ASN
2	B	610	GLN
2	B	623	ASN
2	B	632	GLN
2	B	640	GLN
2	B	646	ASN
2	B	693	ASN
2	B	701	HIS
2	B	731	GLN
2	B	769	GLN
2	B	821	ASN
2	B	836	GLN
2	B	935	GLN
2	B	1015	GLN
2	B	1103	HIS
2	B	1121	HIS
2	B	1203	HIS

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Mol	Chain	Res	Type
2	B	1247	ASN
2	C	115	GLN
2	C	122	ASN
2	C	173	GLN
2	C	195	ASN
2	C	205	ASN
2	C	209	ASN
2	C	283	ASN
2	C	291	HIS
2	C	297	ASN
2	C	306	GLN
2	C	311	ASN
2	C	316	ASN
2	C	320	GLN
2	C	349	ASN
2	C	394	GLN
2	C	430	ASN
2	C	646	ASN
2	C	690	GLN
2	C	693	ASN
2	C	711	ASN
2	C	731	GLN
2	C	836	GLN
2	C	854	GLN
2	C	867	ASN
2	C	882	GLN
2	C	954	GLN
2	C	959	GLN
2	C	988	GLN
2	C	1136	HIS
2	C	1205	GLN
2	C	1247	ASN
2	C	1249	ASN
3	D	3	GLN
3	D	14	GLN
3	D	83	ASN
3	D	100	ASN
3	D	139	ASN
3	D	238	ASN
3	D	241	ASN
3	E	14	GLN
3	E	55	HIS

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Mol	Chain	Res	Type
3	E	85	ASN
3	E	155	HIS
3	E	258	ASN
3	E	291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	GPL	A	234	1	28,34,35	2.62	3 (10%)	30,49,51	1.69	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GPL	A	234	1	-	0/14/37/39	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GPL	C5-C4	3.01	1.47	1.40
1	A	234	GPL	C6-C5	3.50	1.48	1.41
1	A	234	GPL	P-NZ	12.45	1.74	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	234	GPL	C5-C6-N1	-3.89	118.44	123.52
1	A	234	GPL	N3-C2-N1	-3.21	123.19	127.56
1	A	234	GPL	C6-C5-C4	-2.88	117.57	120.86
1	A	234	GPL	O4'-C1'-N9	2.06	112.00	108.11
1	A	234	GPL	O5'-P-NZ	2.30	113.81	106.93
1	A	234	GPL	C6-N1-C2	4.86	121.58	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	234	GPL	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.