



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:21 pm GMT

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

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

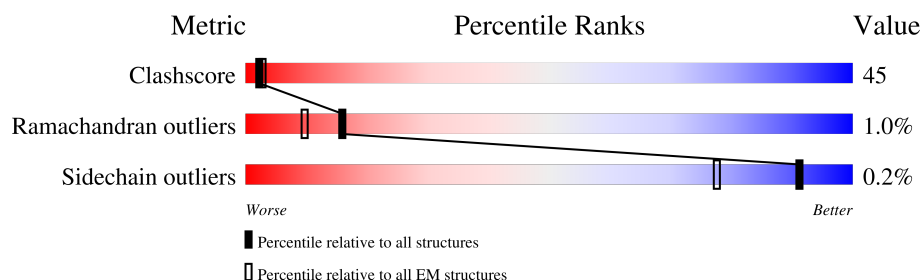
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	755	
1	B	755	
1	C	755	
1	D	755	
2	E	369	
2	F	369	
3	G	253	

## 2 Entry composition [i](#)

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

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

- Molecule 1 is a protein called Putative zinc metallopeptidase.

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

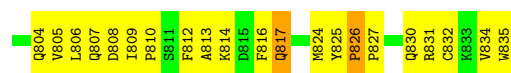
- Molecule 2 is a protein called Parasite pepsinogen.

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

- Molecule 3 is a protein called Cysteine Protease.

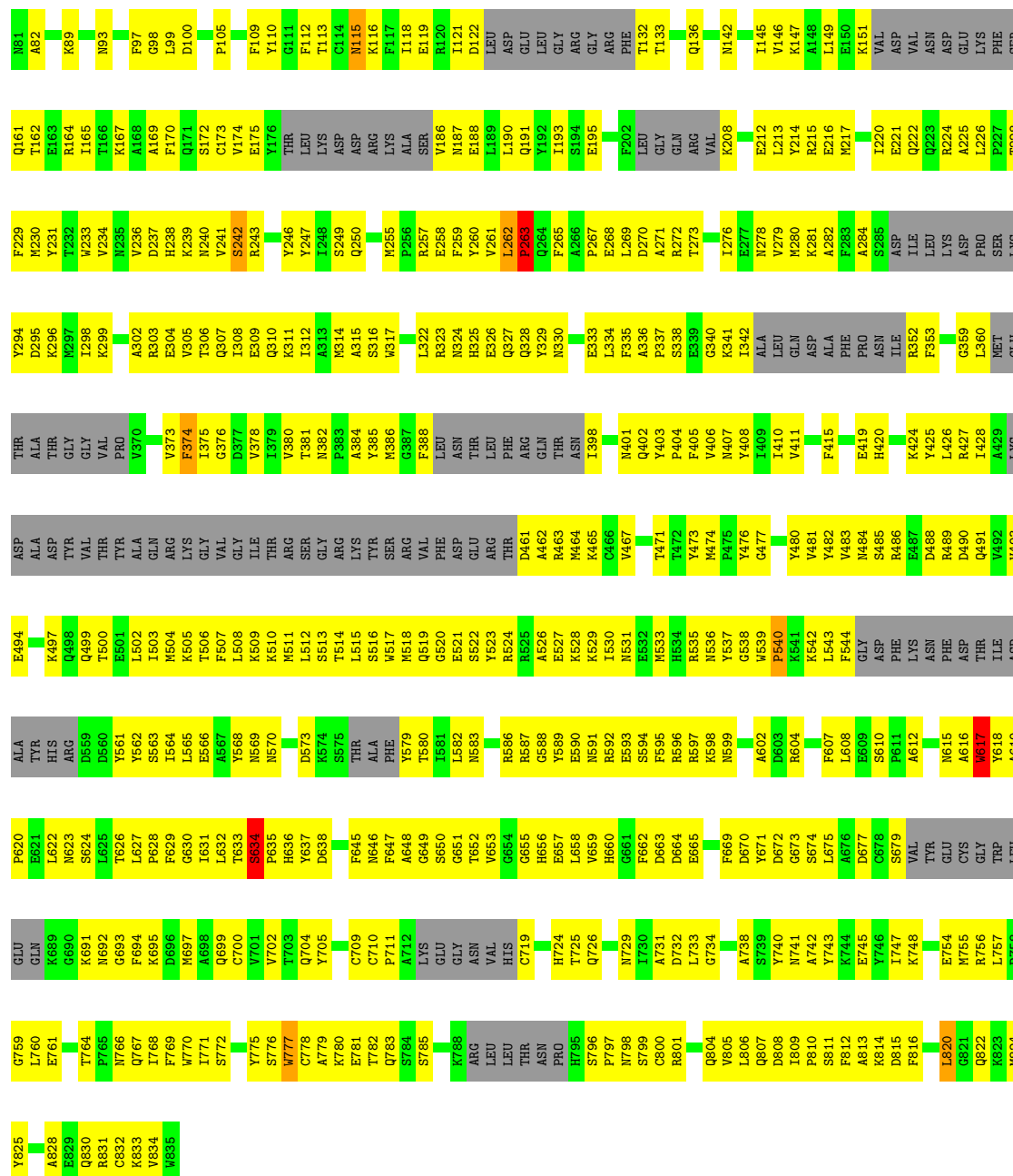
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	173	Total	C	H	N	O	0	0
			1242	504	392	173	173		





• Molecule 1: Putative zinc metallopeptidase

Chain B: 28% 53% 18%



• Molecule 1: Putative zinc metallopeptidase

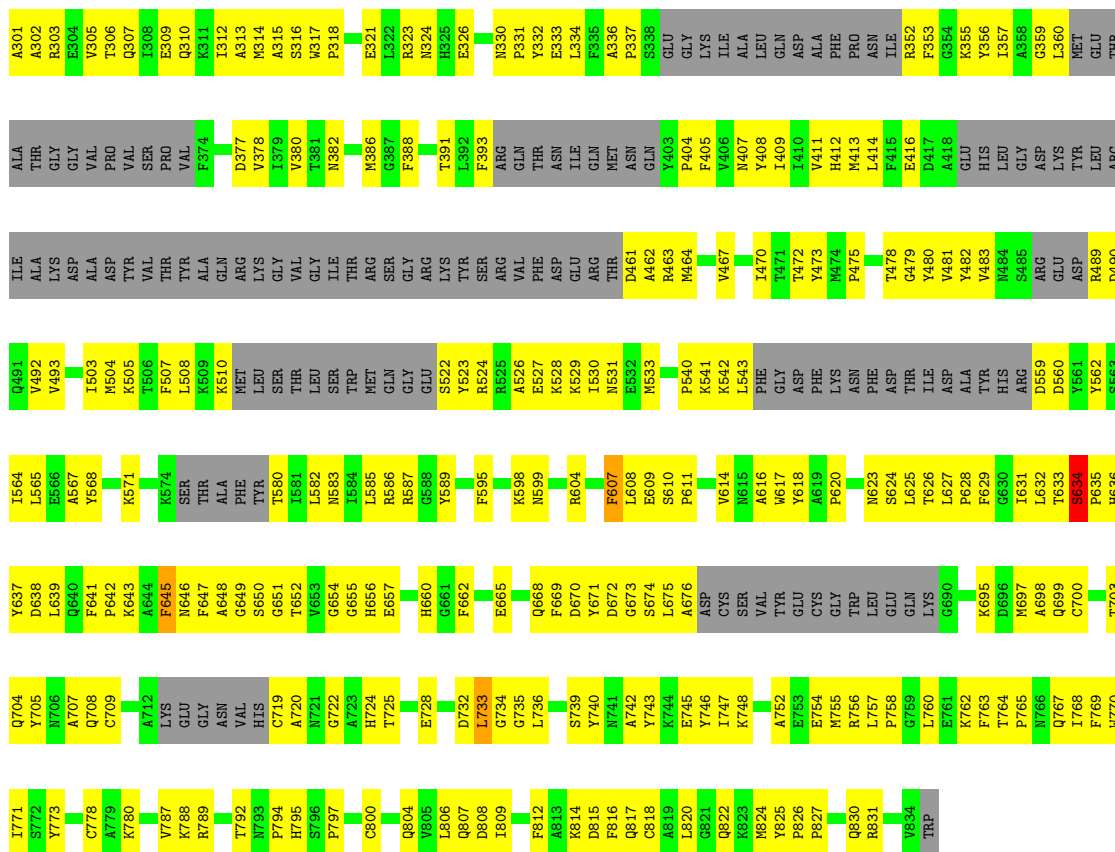
Chain C: 25% 51% 23%

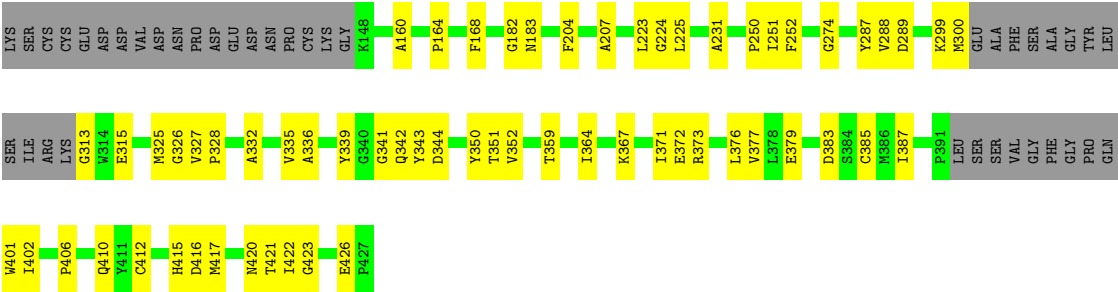
N798	L733	G666	S594	M533	I470	N407	GLN	E277	E216	N81
S799	L733	V667	F595	H534	T470	N407	ASP	E277	E216	N81
C800	Q668	Q668	R596	H534	T471	I409	ALA	M280	G218	S85
R801	L736	F669	R597	N536	T472	I410	PHE	A284	R219	K86
N803	Q737	ASP	K598	Y537	Y473	V411	ASN	K289	I220	E87
O804	A738	TYR	N599	G538	M474	H412	ASN	PRO	E221	W88
W805	S739	ASP	E600	W539	Y476	M413	ILE	ASP	Q222	K89
L806	Y740	GLY	F607	P540	Y476	L414	ARG	PRO	Q223	N90
Q807	N741	SER	L608	K541	T478	F415	F353	GLY	Q161	A91
D808	A742	LEU	E609	L543	G479	D417	G355	SER	T162	A92
L809	Y743	ALA	S610	F544	Y480	A418	K356	LYS	R164	N93
P810	K744	ASP	P611	G545	V481	GLU	Y356	Y294	I165	T94
E811	E745	CYS	A612	G545	Y482	GLU	I357	D295	T227	L95
F812	Y746	SER	S613	PHE	Y482	LEU	A358	D295	T228	L96
A813	I747	VAL	G614	ASP	Y483	LEU	G359	P297	K167	F97
K814	LYS	GLY	V614	LYS	N484	GLY	L360	T298	M230	G98
MET	GLY	TYR	W617	ASN	S485	ASP	ASP	K299	Y231	L99
LYS	LYS	CYS	V617	PHE	R486	LYS	T363	T380	T232	F170
GLY	GLY	GLY	V618	ASP	R486	LYS	T363	T380	W233	D100
ALA	TRP	ALA	A619	THR	E487	TYR	ALA	A301	V294	E101
GLU	GLU	LEU	P620	ILE	D488	LEU	THR	A302	M235	S102
E754	E621	GLU	E621	ASP	R489	ILE	GLY	R303	V236	V174
N755	L622	GLN	V493	ALA	V493	ILE	VAL	E304	D237	D104
R756	L622	GLN	E494	ALA	E494	LYS	VAL	V305	H238	P105
L757	G690	GLN	D495	THR	D495	ASP	PRO	T306	K239	C106
P758	P758	GLN	L625	HIS	V496	ASP	VAL	Q307	M240	E107
G759	M824	GLN	T626	D569	K497	ALA	SER	I308	V241	F108
L760	E761	GLN	L627	D569	Q498	ASP	PRO	E309	S242	O808
E761	K695	GLN	P628	Y562	Q499	TYR	V373	Q310	R243	Y110
K762	D696	ALA	PHE	S583	T500	THR	G376	K311	M244	G111
F763	M697	ALA	GLY	L564	E501	TYR	D377	L312	S245	
T764	A698	GLU	ILE	L565	L502	TYR	F378	A313	Y246	C114
P765	Q699	GLN	LEU	E566	I503	GLN	I379	M314	Y247	N115
N766	Q710	GLN	THR	A567	M504	ARG	V380	A315	I248	
Q767	Y705	GLN	SER	Y568	K506	LYS	N381	S316	Q249	D122
K832	W706	GLN	PRO	N569	T506	GLY	K382	K317	Q250	LEU
F768	A707	GLN	PRO	N570	T506	VAL	P383	P318	P251	ASP
W834	Q708	GLY	H636	N570	E501	VAL	P383	D319	T252	LEU
W835	C709	GLY	V637	K571	L502	GLY	A384	L322	L253	ASP
	C710	GLY	D638	T572	M511	ILE	Y385	Q327	P254	LEU
	Y711	GLY	L639	D573	L512	THR	K386	Q328	E258	GLY
	G711	GLY	L640	K574	S513	ARG	G387	Y329	F259	GLY
G774	Y711	GLY	F641	S575	T514	SER	G387	N324	Y261	ARG
Y775	S776	ALA	F641	S575	T514	SER	F388	H325	P256	ARG
T776	W777	LYS	F642	THR	L515	GLY	F388	H325	R257	GLY
C778	W777	GLY	K643	PHE	S516	ARG	ASN	Q327	E258	ARG
A779	W779	ASN	N646	Y579	W517	TYR	THR	LYS	F259	F131
	VAL	VAL	F647	T580	Q519	SER	PHE	Y329	Y261	T132
	H718	VAL	A648	S581	G520	THR	ARG	N330	V261	F133
T782	Q719	GLY	L648	L581	G520	THR	ARG	P331	L262	T134
Q783	A720	LYS	T652	L582	E521	VAL	GLN	Y332	P263	A137
S785	N721	GLY	N583	N583	S522	PHE	THR	E333	Q264	Q138
L786	G722	GLY	L584	L584	Y523	ASP	ASN	L334	F265	
	A723	GLY	E657	L585	R524	GLU	ILE	F335	A266	S143
		GLY	L658	R586	R525	ARG	GLN	A336	E268	I145
L790	H724	GLY	V659	R587	S526	THR	MET	P337	L269	V146
L791	T725	GLY	H660	G588	E527	ASP	ASN		D270	
T792	Q726	GLY	G661	Y589	K528	ASP	GLN	G340	A271	L149
N793	G727	GLY	F662	E590	K529	R463	TYR	LYS	R272	E150
P794	E728	GLY	D663	N591	I530	M464	PRO	ILE	T273	K151
H795	T729	GLY	D664	R592	N531	ALA	PHE	ALA	K274	VAL
	N720	GLY	E665	E592	E520	VAL	VAL	LEU	R215	

● Molecule 1: Putative zinc metallopeptidase

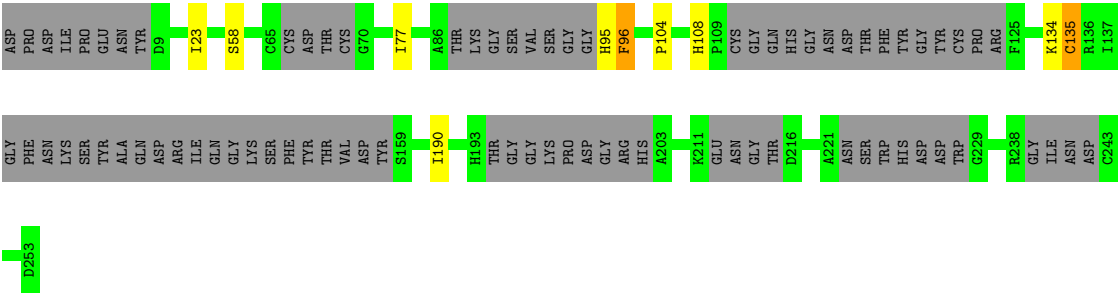
Chain D: 33% 42% 25%

R224	A225	L226	P227	T228	F229	M230	T231	T232	V236	D237	H238	Y241	Y246	Y247	Q250	E258	V261	L262	P263	Q264	P267	E268	L269	D270	A271	R272	T273	I276	E277	R278	V279	M280	F283	A284	SER	ASP	ILE	LEU	LYS	CYS	PRO	SER	LYS	TYR	D295	G296	M297	L298	K299	R300					
S160	Q161	T162	E163	R164	I165	T166	K167	Q171	V174	E175	THR	LEU	LYS	ASP	ASP	ARG	LYS	ALA	SER	VAL	ASN	GLU	LEU	GLN	GLM	TYR	ILE	SER	GLU	ARG	PHE	GLY	GLY	ILE	PRO	PHE	LEU	GLY	GLN	ARG	VAL	LYS	GLY	GLY	CYS	GLU	LEU	Y214	M217	G218	R219	I220	E221	Q222	Q223
N81	A82	N83	R84	S85	W88	F97	G98	L99	D100	E101	F109	F112	T113	C114	N115	K116	F117	I118	E119	R120	I121	D122	L123	ASP	GLU	LEU	GLY	GLY	ARG	G129	T132	T133	F134	S135	Q136	A137	Q138	L139	E140	V141	N142	S143	D144	I145	V146	K147	L148	L149	V154	ASN	ASP	GLU	LYS	PHE	





● Molecule 3: Cysteine Protease





## 4 Experimental information

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.91	3/4938 (0.1%)	0.76	4/6653 (0.1%)
1	B	0.88	7/5122 (0.1%)	0.77	3/6903 (0.0%)
1	C	0.82	5/4835 (0.1%)	0.73	2/6513 (0.0%)
1	D	0.78	2/4674 (0.0%)	0.71	2/6304 (0.0%)
2	E	0.32	0/1452	0.52	0/2003
2	F	0.39	0/1424	0.56	0/1965
3	G	0.80	0/841	0.91	5/1154 (0.4%)
All	All	0.81	17/23286 (0.1%)	0.73	16/31495 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	6
1	D	0	1
All	All	0	16

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	PRO	N-CD	-13.97	1.28	1.47
1	B	540	PRO	N-CD	8.81	1.60	1.47
1	C	816	PHE	CA-CB	-7.78	1.36	1.53
1	B	617	TRP	CB-CG	-7.30	1.37	1.50
1	A	617	TRP	CB-CG	-7.19	1.37	1.50
1	A	770	TRP	CB-CG	-6.74	1.38	1.50
1	C	317	TRP	CB-CG	-6.47	1.38	1.50
1	B	777	TRP	CB-CG	-6.03	1.39	1.50
1	B	770	TRP	CB-CG	-5.60	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	MET	CA-C	-5.56	1.38	1.52
1	B	115	ASN	C-O	-5.46	1.12	1.23
1	D	317	TRP	CB-CG	-5.43	1.40	1.50
1	C	88	TRP	CB-CG	-5.28	1.40	1.50
1	C	260	TYR	CD1-CE1	-5.20	1.31	1.39
1	C	260	TYR	CB-CG	-5.17	1.43	1.51
1	A	317	TRP	CB-CG	-5.11	1.41	1.50
1	D	645	PHE	CB-CG	-5.03	1.42	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	LEU	C-N-CD	-8.98	100.84	120.60
1	A	565	LEU	CA-CB-CG	-7.90	97.13	115.30
1	C	253	LEU	CA-CB-CG	-7.60	97.83	115.30
1	B	262	LEU	N-CA-C	7.23	130.52	111.00
1	A	129	GLY	N-CA-C	7.07	130.77	113.10
3	G	58	SER	CB-CA-C	6.70	122.83	110.10
3	G	96	PHE	N-CA-C	-6.42	93.68	111.00
3	G	58	SER	N-CA-C	-6.36	93.84	111.00
3	G	96	PHE	CB-CA-C	5.75	121.91	110.40
1	C	736	LEU	CA-CB-CG	-5.52	102.59	115.30
1	A	226	LEU	CA-CB-CG	-5.45	102.77	115.30
3	G	135	CYS	N-CA-C	-5.42	96.38	111.00
1	D	733	LEU	CA-CB-CG	-5.32	103.07	115.30
1	A	386	MET	C-N-CA	-5.20	111.39	122.30
1	B	262	LEU	CB-CA-C	-5.04	100.63	110.20
1	D	587	ARG	CB-CG-CD	5.03	124.69	111.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	VAL	Peptide
1	A	486	ARG	Peptide
1	A	560	ASP	Peptide
1	A	676	ALA	Peptide
1	A	826	PRO	Peptide
1	B	242	SER	Peptide
1	B	634	SER	Peptide
1	B	820	LEU	Peptide
1	B	98	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	200	ILE	Peptide
1	C	216	GLU	Peptide
1	C	294	TYR	Peptide
1	C	534	HIS	Peptide
1	C	571	LYS	Peptide
1	C	816	PHE	Peptide
1	D	634	SER	Peptide

## 5.2 Too-close contacts [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	4837	4638	4636	503	0
1	B	5011	4817	4815	524	0
1	C	4734	4556	4555	455	0
1	D	4575	4413	4413	355	0
2	E	1457	676	676	60	0
2	F	1429	664	663	41	0
3	G	850	392	389	2	0
All	All	22893	20156	20147	1925	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 45.

All (1925) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:PRO:HA	1:B:607:PHE:CZ	1.47	1.48
1:A:239:LYS:HD3	1:A:329:TYR:CE2	1.64	1.33
1:A:234:VAL:HG23	1:A:245:SER:O	1.20	1.29
1:D:760:LEU:HD11	1:D:763:PHE:CE2	1.67	1.29
1:A:474:MET:CE	1:A:586:ARG:HD2	1.64	1.27
1:A:237:ASP:OD1	1:A:245:SER:HB3	1.31	1.26
1:A:237:ASP:OD1	1:A:245:SER:CB	1.85	1.23
1:A:277:GLU:OE2	1:A:302:ALA:HB1	1.37	1.20
1:A:561:TYR:O	1:A:564:ILE:HG12	1.37	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ASN:HB2	1:A:589:TYR:CE1	1.80	1.16
1:B:812:PHE:HE2	1:B:824:MET:SD	1.70	1.15
1:A:98:GLY:HA2	1:A:116:LYS:HB2	1.25	1.11
1:A:242:SER:O	1:A:602:ALA:HB2	1.50	1.10
1:A:709:CYS:SG	1:A:719:CYS:HA	1.91	1.10
1:B:812:PHE:CE2	1:B:824:MET:SD	2.46	1.09
1:B:540:PRO:CA	1:B:607:PHE:CZ	2.37	1.08
1:A:277:GLU:HG3	1:A:302:ALA:HB2	1.32	1.07
1:A:402:GLN:O	1:A:406:VAL:HG22	1.52	1.07
1:B:809:ILE:HG22	1:B:811:SER:OG	1.55	1.07
1:B:796:SER:OG	1:B:797:PRO:HD2	1.54	1.06
1:D:97:PHE:O	1:D:116:LYS:HG2	1.55	1.06
1:B:579:TYR:HA	1:B:582:LEU:HD12	1.39	1.05
1:A:253:LEU:CD1	1:A:255:MET:O	2.04	1.04
1:D:757:LEU:HD11	1:D:760:LEU:HB3	1.37	1.04
1:D:101:GLU:CD	1:D:762:LYS:HZ3	1.58	1.04
1:A:474:MET:HE1	1:A:586:ARG:HD2	1.06	1.03
1:A:569:ASN:HB2	1:A:589:TYR:HE1	0.90	1.03
1:B:109:PHE:CE2	1:B:806:LEU:HD22	1.94	1.03
1:C:109:PHE:HB2	1:C:824:MET:HE2	1.35	1.03
1:A:118:ILE:HG12	1:A:780:LYS:HB2	1.37	1.02
1:B:109:PHE:CE2	1:B:806:LEU:CD2	2.42	1.02
1:B:709:CYS:SG	1:B:719:CYS:N	2.33	1.00
2:E:182:GLY:O	2:E:203:VAL:HA	1.61	1.00
1:D:160:SER:HB2	1:D:163:GLU:OE1	1.59	1.00
1:A:570:ASN:O	1:A:571:LYS:HG3	1.62	0.99
1:B:255:MET:HB3	1:B:260:TYR:OH	1.60	0.99
1:A:561:TYR:O	1:A:564:ILE:CG1	2.09	0.99
1:A:239:LYS:CD	1:A:329:TYR:CE2	2.45	0.98
1:A:253:LEU:HD12	1:A:255:MET:O	1.62	0.97
1:A:234:VAL:CG2	1:A:245:SER:O	2.11	0.97
1:C:592:ARG:HA	1:C:595:PHE:CE2	2.00	0.97
1:A:238:HIS:NE2	1:A:621:GLU:OE2	1.97	0.97
1:B:561:TYR:O	1:B:564:ILE:HG22	1.65	0.96
1:D:760:LEU:HD11	1:D:763:PHE:HE2	0.83	0.96
1:A:98:GLY:HA2	1:A:116:LYS:CB	1.95	0.95
1:A:569:ASN:CB	1:A:589:TYR:HE1	1.79	0.95
1:C:108:ASP:HB2	1:C:110:TYR:CE2	2.01	0.95
1:B:637:TYR:O	1:B:638:ASP:OD1	1.85	0.94
1:C:95:LEU:HD11	1:C:771:ILE:CG2	1.97	0.94
1:B:809:ILE:HG22	1:B:811:SER:HG	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASN:O	1:B:145:ILE:HG22	1.65	0.93
1:B:540:PRO:HA	1:B:607:PHE:HZ	1.34	0.92
1:C:798:ASN:O	1:C:801:ARG:N	2.03	0.91
1:B:810:PRO:HD2	1:B:831:ARG:HH11	1.33	0.91
1:B:109:PHE:CD2	1:B:806:LEU:HD23	2.05	0.91
1:A:277:GLU:OE2	1:A:302:ALA:CB	2.18	0.90
1:C:95:LEU:HD11	1:C:771:ILE:HG21	1.52	0.90
1:B:230:MET:HA	1:B:249:SER:O	1.70	0.90
1:C:103:VAL:CG1	1:C:108:ASP:OD1	2.20	0.90
1:C:583:ASN:ND2	1:C:587:ARG:HH12	1.71	0.89
1:A:238:HIS:CE1	1:A:621:GLU:OE2	2.26	0.89
1:B:380:VAL:CG1	1:B:385:TYR:HE2	1.86	0.89
1:C:331:PRO:HA	1:C:379:ILE:HG12	1.54	0.89
1:A:250:GLN:OE1	1:A:317:TRP:N	2.06	0.88
1:A:719:CYS:O	1:A:790:LEU:HD21	1.72	0.88
1:B:109:PHE:CD2	1:B:806:LEU:CD2	2.57	0.88
1:C:793:ASN:ND2	1:C:795:HIS:CE1	2.41	0.88
1:D:145:ILE:HD13	1:D:478:THR:HG23	1.56	0.87
1:C:243:ARG:HH22	1:C:376:GLY:HA2	1.39	0.87
1:A:242:SER:O	1:A:602:ALA:CB	2.23	0.86
1:A:277:GLU:CG	1:A:302:ALA:HB2	2.03	0.86
1:C:823:LYS:O	1:C:824:MET:HG2	1.74	0.86
1:A:239:LYS:HD3	1:A:329:TYR:HE2	1.34	0.86
1:B:262:LEU:CB	1:B:263:PRO:HD3	2.06	0.85
1:C:583:ASN:ND2	1:C:587:ARG:NH1	2.24	0.85
1:A:232:THR:OG1	1:A:247:TYR:O	1.94	0.85
1:A:474:MET:HE1	1:A:586:ARG:CD	2.01	0.85
1:C:114:CYS:HG	1:C:778:CYS:HG	0.94	0.85
1:A:709:CYS:HG	1:A:719:CYS:HG	1.19	0.85
1:A:273:THR:O	1:A:277:GLU:OE1	1.94	0.84
1:B:670:ASP:OD1	1:B:673:GLY:N	2.09	0.84
1:C:232:THR:HG22	1:C:248:ILE:HA	1.60	0.84
1:A:536:ASN:HB3	1:A:626:THR:HG22	1.59	0.84
1:B:743:TYR:CE1	1:B:747:ILE:HD13	2.12	0.83
1:B:262:LEU:HB3	1:B:263:PRO:HD3	1.59	0.83
1:D:631:ILE:O	1:D:633:THR:HG22	1.79	0.83
1:A:474:MET:CE	1:A:586:ARG:CD	2.54	0.83
1:D:404:PRO:O	1:D:407:ASN:ND2	2.10	0.83
1:B:540:PRO:HB3	1:B:607:PHE:CE2	2.14	0.83
1:A:782:THR:HB	1:A:785:SER:HB3	1.60	0.82
1:B:540:PRO:CB	1:B:607:PHE:CE2	2.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:760:LEU:CD1	1:D:763:PHE:HE2	1.80	0.82
1:A:569:ASN:CB	1:A:589:TYR:CE1	2.58	0.82
1:D:382:ASN:O	1:D:386:MET:HG2	1.80	0.82
1:B:214:TYR:O	1:B:217:MET:N	2.12	0.82
1:A:98:GLY:CA	1:A:116:LYS:HB2	2.10	0.82
1:C:643:LYS:NZ	1:C:746:TYR:OH	2.13	0.82
1:C:304:GLU:OE2	1:C:407:ASN:ND2	2.13	0.81
1:B:226:LEU:HD23	1:B:226:LEU:O	1.81	0.81
1:C:719:CYS:SG	1:C:720:ALA:N	2.52	0.81
1:B:169:ALA:O	1:B:172:SER:OG	1.99	0.81
1:C:109:PHE:HB2	1:C:824:MET:CE	2.10	0.81
1:B:208:LYS:N	1:B:403:TYR:HH	1.79	0.81
1:D:101:GLU:HG2	1:D:762:LYS:HZ1	1.45	0.80
1:C:569:ASN:HB3	1:C:589:TYR:HE1	1.44	0.80
1:B:608:LEU:HD11	1:B:619:ALA:HB2	1.62	0.80
1:A:474:MET:HE3	1:A:586:ARG:HD2	1.63	0.80
1:C:295:ASP:OD2	1:C:298:ILE:HG12	1.82	0.80
1:A:237:ASP:OD1	1:A:245:SER:HB2	1.80	0.80
1:C:317:TRP:CE3	1:C:382:ASN:OD1	2.35	0.80
1:D:145:ILE:CD1	1:D:478:THR:HG23	2.11	0.80
1:D:637:TYR:CG	1:D:646:ASN:OD1	2.35	0.80
1:B:622:LEU:HD12	1:B:623:ASN:N	1.97	0.80
1:B:796:SER:OG	1:B:797:PRO:CD	2.30	0.80
1:C:821:GLY:O	1:C:822:GLN:HG3	1.82	0.80
1:A:709:CYS:SG	1:A:719:CYS:CA	2.71	0.79
1:B:398:ILE:HG22	1:B:402:GLN:HG3	1.61	0.79
1:A:238:HIS:NE2	1:A:621:GLU:CG	2.45	0.79
1:A:469:THR:O	1:A:472:THR:OG1	2.00	0.79
1:A:234:VAL:HG22	1:A:235:ASN:N	1.96	0.79
1:A:301:ALA:HB1	1:A:407:ASN:HD21	1.47	0.79
1:B:588:GLY:HA3	1:B:592:ARG:HH21	1.45	0.79
1:C:764:THR:HB	1:C:765:PRO:HD2	1.64	0.79
1:A:764:THR:CG2	1:A:765:PRO:HD2	2.12	0.79
1:C:174:VAL:HG23	1:C:463:ARG:HG2	1.65	0.79
1:A:87:GLU:OE1	1:A:640:GLN:CB	2.31	0.79
1:A:196:ARG:HH12	1:A:219:ARG:HE	1.32	0.79
1:C:177:THR:O	1:C:181:ASP:N	2.13	0.79
1:B:246:TYR:HB2	1:B:378:VAL:HG13	1.65	0.78
1:B:342:ILE:O	1:B:352:ARG:NH1	2.16	0.78
1:D:101:GLU:CD	1:D:762:LYS:NZ	2.37	0.78
1:D:719:CYS:SG	1:D:787:VAL:HG23	2.22	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:GLU:O	1:D:312:ILE:N	2.17	0.78
1:B:489:ARG:HG3	1:B:490:ASP:H	1.49	0.78
1:A:253:LEU:HD11	1:A:255:MET:O	1.81	0.78
1:C:161:GLN:HB2	1:C:564:ILE:HD13	1.65	0.78
1:C:467:VAL:HA	1:C:470:ILE:HD12	1.64	0.78
1:A:507:PHE:CZ	1:A:659:VAL:HG12	2.18	0.78
1:C:482:TYR:O	1:C:485:SER:OG	2.01	0.78
1:A:718:HIS:O	1:A:719:CYS:SG	2.42	0.78
1:B:105:PRO:HA	1:B:112:PHE:CD1	2.19	0.78
1:B:583:ASN:HD21	1:B:587:ARG:HH21	1.28	0.78
1:D:760:LEU:CD1	1:D:763:PHE:CE2	2.60	0.78
1:B:579:TYR:HA	1:B:582:LEU:CD1	2.13	0.77
1:B:217:MET:HE2	1:B:230:MET:SD	2.24	0.77
1:B:512:LEU:HB2	1:B:523:TYR:HB2	1.65	0.77
1:C:515:LEU:HD22	1:C:518:MET:HG3	1.67	0.77
2:E:78:ILE:HA	2:E:186:VAL:HA	1.66	0.77
1:A:721:ASN:OD1	1:A:722:GLY:N	2.17	0.77
1:B:519:GLN:NE2	1:B:521:GLU:OE1	2.18	0.77
1:C:257:ARG:HH12	1:C:313:ALA:HB1	1.50	0.77
1:B:594:SER:HA	1:B:597:ARG:CZ	2.15	0.77
1:D:393:PHE:CE1	1:D:405:PHE:CE2	2.73	0.77
1:D:393:PHE:CD1	1:D:405:PHE:CE2	2.72	0.77
1:A:732:ASP:OD2	1:A:801:ARG:NH2	2.16	0.77
1:B:341:LYS:HE2	1:B:353:PHE:HE2	1.49	0.77
1:C:793:ASN:ND2	1:C:795:HIS:HE1	1.82	0.77
1:A:606:ASN:OD1	1:A:607:PHE:N	2.17	0.77
1:B:511:MET:N	1:B:514:THR:OG1	2.18	0.77
1:B:474:MET:SD	1:B:570:ASN:ND2	2.57	0.76
1:C:583:ASN:HD21	1:C:587:ARG:NH1	1.82	0.76
2:F:252:PHE:HA	2:F:274:GLY:H	1.51	0.76
1:A:385:TYR:O	1:A:388:PHE:N	2.18	0.76
1:D:380:VAL:CG1	1:D:386:MET:HG3	2.15	0.76
1:A:169:ALA:O	1:A:172:SER:OG	2.02	0.76
1:C:583:ASN:HD21	1:C:587:ARG:HH12	1.34	0.76
1:D:764:THR:OG1	1:D:767:GLN:HG2	1.85	0.76
1:A:253:LEU:HD12	1:A:253:LEU:C	2.06	0.76
1:C:280:MET:O	1:C:284:ALA:N	2.14	0.76
1:C:579:TYR:O	1:C:583:ASN:N	2.16	0.76
1:B:237:ASP:OD2	1:B:240:ASN:N	2.19	0.76
1:B:306:THR:O	1:B:309:GLU:N	2.18	0.76
1:B:323:ARG:NH1	1:B:665:GLU:OE2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:VAL:HG22	1:B:629:PHE:CD2	2.21	0.76
1:B:579:TYR:CA	1:B:582:LEU:HD12	2.16	0.76
1:B:743:TYR:CZ	1:B:747:ILE:HG21	2.21	0.76
1:A:264:GLN:HE22	1:A:314:MET:CE	1.99	0.76
1:A:764:THR:HG22	1:A:765:PRO:N	2.01	0.76
1:B:424:LYS:HA	1:B:427:ARG:HH21	1.51	0.76
1:B:489:ARG:HG3	1:B:490:ASP:N	2.00	0.76
1:B:407:ASN:O	1:B:410:ILE:HG22	1.85	0.76
1:D:88:TRP:CE3	1:D:642:PRO:HG3	2.21	0.76
1:B:705:TYR:CE2	1:B:729:ASN:CG	2.59	0.75
1:C:238:HIS:ND1	1:C:247:TYR:OH	2.18	0.75
1:A:656:HIS:ND1	1:A:732:ASP:OD1	2.19	0.75
1:A:825:TYR:HB3	1:A:827:PRO:HD2	1.67	0.75
1:C:238:HIS:HD1	1:C:247:TYR:HH	1.34	0.75
1:C:643:LYS:HD3	1:C:646:ASN:HD21	1.51	0.75
2:E:193:ASN:N	2:E:273:TYR:O	2.16	0.75
1:B:236:VAL:HG13	1:B:241:VAL:CG2	2.15	0.75
1:A:324:ASN:O	1:A:327:GLN:N	2.19	0.75
1:D:109:PHE:CE2	1:D:806:LEU:HD12	2.21	0.75
1:C:793:ASN:HD22	1:C:795:HIS:CE1	2.03	0.75
1:C:193:ILE:HG23	1:C:197:PHE:HE2	1.51	0.75
1:D:757:LEU:CD1	1:D:760:LEU:HB3	2.14	0.75
1:D:480:TYR:HB2	1:D:543:LEU:HD21	1.68	0.75
1:A:222:GLN:NE2	1:A:360:LEU:O	2.19	0.75
1:A:724:HIS:CE1	1:A:794:PRO:HA	2.22	0.75
1:C:218:GLY:HA3	1:C:356:TYR:HE1	1.51	0.75
1:A:267:PRO:O	1:A:270:ASP:N	2.20	0.74
1:A:827:PRO:O	1:A:830:GLN:NE2	2.20	0.74
1:B:259:PHE:CE1	1:B:263:PRO:HD2	2.22	0.74
1:B:518:MET:HG2	1:B:519:GLN:H	1.51	0.74
1:B:540:PRO:HA	1:B:607:PHE:CE1	2.20	0.74
1:A:226:LEU:HD13	1:A:416:GLU:OE2	1.87	0.74
1:A:327:GLN:O	1:A:329:TYR:N	2.18	0.74
1:A:494:GLU:O	1:A:498:GLN:N	2.20	0.74
1:B:491:GLN:O	1:B:494:GLU:HG2	1.86	0.74
1:C:810:PRO:O	1:C:813:ALA:N	2.15	0.74
1:B:236:VAL:HG13	1:B:241:VAL:HG23	1.67	0.74
1:C:179:LYS:NZ	1:C:462:ALA:O	2.20	0.74
1:A:253:LEU:HD12	1:A:253:LEU:O	1.87	0.74
1:D:309:GLU:O	1:D:312:ILE:HG22	1.87	0.74
1:B:419:GLU:HA	1:B:426:LEU:HG	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:ASN:OD1	1:C:722:GLY:N	2.21	0.74
1:A:130:ARG:HG2	1:A:781:GLU:CB	2.17	0.74
1:B:420:HIS:CE1	1:B:580:THR:HA	2.22	0.74
1:C:229:PHE:O	1:C:230:MET:HG3	1.87	0.74
1:C:114:CYS:HG	1:C:778:CYS:CB	2.01	0.73
1:C:272:ARG:NH2	1:C:309:GLU:OE2	2.19	0.73
1:D:162:THR:HA	1:D:165:ILE:HD12	1.71	0.73
1:A:634:SER:HB3	1:A:635:PRO:HD2	1.69	0.73
1:A:764:THR:HG22	1:A:765:PRO:CD	2.18	0.73
1:C:103:VAL:HG12	1:C:108:ASP:OD1	1.87	0.73
1:C:592:ARG:HA	1:C:595:PHE:HE2	1.50	0.73
1:D:100:ASP:O	1:D:112:PHE:CD1	2.41	0.73
1:A:277:GLU:CD	1:A:302:ALA:HB1	2.09	0.73
1:B:594:SER:HA	1:B:597:ARG:NE	2.03	0.73
1:C:134:PHE:O	1:C:138:GLN:N	2.17	0.73
1:D:258:GLU:HG2	1:D:258:GLU:O	1.89	0.73
2:E:288:VAL:O	2:E:422:ILE:N	2.18	0.73
1:A:764:THR:N	1:A:767:GLN:OE1	2.22	0.73
1:B:237:ASP:OD1	1:B:238:HIS:N	2.21	0.73
1:C:319:ASP:HA	1:C:322:LEU:HD12	1.68	0.73
1:A:491:GLN:HG2	1:A:492:VAL:HG13	1.69	0.73
1:B:622:LEU:CD1	1:B:624:SER:OG	2.37	0.73
1:C:333:GLU:O	1:C:335:PHE:N	2.22	0.73
1:A:134:PHE:HE1	1:A:636:HIS:CE1	2.07	0.72
1:C:571:LYS:NZ	1:C:572:THR:O	2.22	0.72
1:C:614:VAL:HG13	1:C:614:VAL:O	1.86	0.72
1:B:536:ASN:HB2	1:B:626:THR:HG22	1.70	0.72
1:A:281:LYS:O	1:A:284:ALA:N	2.22	0.72
1:C:215:ARG:O	1:C:219:ARG:NE	2.22	0.72
1:D:820:LEU:HA	1:D:825:TYR:HD2	1.53	0.72
1:A:495:ASP:OD2	1:A:637:TYR:OH	2.08	0.72
1:A:709:CYS:HG	1:A:719:CYS:CB	2.03	0.72
1:C:767:GLN:OE1	1:C:767:GLN:N	2.23	0.72
1:A:507:PHE:CE2	1:A:659:VAL:HG12	2.23	0.72
1:B:634:SER:O	1:B:636:HIS:N	2.23	0.72
1:C:705:TYR:O	1:C:708:GLN:N	2.21	0.72
1:A:789:ARG:HB3	1:A:793:ASN:OD1	1.90	0.72
1:B:743:TYR:O	1:B:747:ILE:HG12	1.90	0.72
1:D:133:THR:O	1:D:136:GLN:HB3	1.89	0.72
1:D:757:LEU:O	1:D:757:LEU:HD12	1.89	0.72
1:B:544:PHE:CD2	1:B:544:PHE:O	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:TYR:HE2	1:B:729:ASN:CG	1.93	0.72
1:C:256:PRO:HB3	1:C:792:THR:HG22	1.72	0.71
1:C:100:ASP:OD1	1:C:101:GLU:N	2.24	0.71
1:C:582:LEU:O	1:C:586:ARG:HG3	1.89	0.71
1:D:480:TYR:HD2	1:D:543:LEU:HG	1.56	0.71
2:E:183:ASN:HA	2:E:202:THR:O	1.88	0.71
2:F:75:LYS:HA	2:F:85:PHE:O	1.90	0.71
2:F:288:VAL:O	2:F:422:ILE:N	2.23	0.71
1:A:162:THR:O	1:A:165:ILE:N	2.22	0.71
1:A:722:GLY:O	1:A:725:THR:OG1	2.07	0.71
1:B:325:HIS:HA	1:B:328:GLN:HG2	1.72	0.71
1:A:130:ARG:HG2	1:A:781:GLU:HB2	1.72	0.71
1:A:764:THR:HG22	1:A:765:PRO:HD2	1.73	0.71
1:D:101:GLU:HG2	1:D:762:LYS:NZ	2.06	0.71
2:F:98:ILE:O	2:F:207:ALA:N	2.17	0.71
1:B:99:LEU:O	1:B:116:LYS:HG2	1.91	0.71
1:B:172:SER:O	1:B:175:GLU:N	2.24	0.71
1:D:380:VAL:HG11	1:D:386:MET:HG3	1.73	0.71
1:D:670:ASP:O	1:D:673:GLY:N	2.20	0.71
1:A:533:MET:HA	1:A:623:ASN:ND2	2.06	0.70
1:B:100:ASP:O	1:B:100:ASP:OD1	2.09	0.70
1:C:311:LYS:O	1:C:314:MET:N	2.24	0.70
1:B:812:PHE:CZ	1:B:824:MET:SD	2.84	0.70
1:D:163:GLU:HG3	1:D:481:VAL:HG22	1.73	0.70
1:D:100:ASP:O	1:D:112:PHE:CE1	2.44	0.70
2:E:344:ASP:N	2:E:349:ILE:O	2.24	0.70
1:A:506:THR:O	1:A:510:LYS:N	2.24	0.70
1:D:620:PRO:HB2	1:D:669:PHE:HD2	1.57	0.70
1:D:705:TYR:CZ	1:D:800:CYS:SG	2.84	0.70
2:E:412:CYS:H	2:E:426:GLU:HA	1.55	0.70
1:A:231:TYR:HH	1:A:233:TRP:HE1	1.27	0.70
2:E:169:GLU:HA	2:E:178:LYS:HA	1.72	0.70
1:A:277:GLU:CG	1:A:302:ALA:CB	2.69	0.70
1:C:566:GLU:OE2	1:C:596:ARG:NH2	2.25	0.70
1:D:489:ARG:O	1:D:492:VAL:HG12	1.91	0.70
1:A:175:GLU:N	1:A:175:GLU:OE2	2.24	0.70
1:B:308:ILE:O	1:B:311:LYS:N	2.25	0.69
1:A:583:ASN:OD1	1:A:586:ARG:NH2	2.25	0.69
1:B:481:VAL:O	1:B:485:SER:OG	2.10	0.69
1:D:101:GLU:CG	1:D:762:LYS:NZ	2.55	0.69
1:D:226:LEU:HD13	1:D:413:MET:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:GLN:N	1:A:824:MET:HE1	2.07	0.69
1:B:380:VAL:HG11	1:B:385:TYR:HE2	1.57	0.69
1:D:83:ASN:OD1	1:D:84:ARG:N	2.25	0.69
1:D:480:TYR:HB2	1:D:543:LEU:HD11	1.74	0.69
1:B:610:SER:O	1:B:612:ALA:N	2.25	0.69
1:C:162:THR:HB	1:C:564:ILE:HG12	1.74	0.69
1:A:634:SER:O	1:A:636:HIS:N	2.24	0.69
1:A:807:GLN:HA	1:A:824:MET:HE3	1.75	0.69
1:D:393:PHE:CD1	1:D:405:PHE:HE2	2.10	0.69
1:D:638:ASP:HB3	1:D:641:PHE:CZ	2.27	0.69
1:B:250:GLN:OE1	1:B:250:GLN:N	2.22	0.69
1:B:636:HIS:O	1:B:650:SER:N	2.21	0.69
1:B:147:LYS:O	1:B:151:LYS:NZ	2.26	0.69
1:D:122:ASP:OD1	1:D:123:LEU:N	2.26	0.69
1:B:402:GLN:O	1:B:405:PHE:HD2	1.76	0.69
1:D:334:LEU:HD23	1:D:334:LEU:O	1.92	0.69
1:D:109:PHE:CD2	1:D:806:LEU:HD12	2.27	0.68
1:D:674:SER:OG	1:D:675:LEU:N	2.24	0.68
1:A:232:THR:HG23	1:A:232:THR:O	1.93	0.68
1:A:648:ALA:O	1:A:652:THR:OG1	2.10	0.68
1:D:352:ARG:O	1:D:356:TYR:N	2.25	0.68
1:A:765:PRO:O	1:A:768:ILE:N	2.26	0.68
1:B:481:VAL:O	1:B:485:SER:CB	2.41	0.68
1:B:561:TYR:O	1:B:564:ILE:N	2.27	0.68
1:A:212:GLU:OE1	1:A:215:ARG:NH2	2.22	0.68
1:B:239:LYS:O	1:B:240:ASN:OD1	2.10	0.68
1:A:130:ARG:NH1	1:A:793:ASN:OD1	2.27	0.68
1:B:480:TYR:HB2	1:B:543:LEU:HD11	1.75	0.68
1:C:775:TYR:HA	1:C:778:CYS:SG	2.34	0.68
1:B:489:ARG:CG	1:B:490:ASP:H	2.07	0.68
1:B:511:MET:HG3	1:B:513:SER:H	1.58	0.68
1:B:511:MET:O	1:B:514:THR:OG1	2.09	0.68
1:B:808:ASP:O	1:B:831:ARG:NH1	2.27	0.68
1:B:334:LEU:HD12	1:B:335:PHE:N	2.09	0.67
1:B:186:VAL:HG23	1:B:187:ASN:H	1.59	0.67
1:D:241:VAL:HG11	1:D:672:ASP:O	1.92	0.67
1:B:631:ILE:O	1:B:633:THR:N	2.27	0.67
1:D:268:GLU:O	1:D:271:ALA:N	2.24	0.67
1:A:86:LYS:O	1:A:89:LYS:N	2.27	0.67
1:D:160:SER:CB	1:D:163:GLU:OE1	2.38	0.67
1:D:645:PHE:O	1:D:648:ALA:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:MET:CE	1:C:356:TYR:CE2	2.78	0.67
1:C:409:ILE:H	1:C:409:ILE:HD12	1.58	0.67
2:F:406:PRO:O	2:F:410:GLN:N	2.26	0.67
1:A:277:GLU:HG3	1:A:302:ALA:CB	2.18	0.67
1:B:540:PRO:HA	1:B:607:PHE:CE2	2.23	0.67
1:B:759:GLY:O	1:B:760:LEU:HG	1.94	0.67
1:B:757:LEU:CD1	1:B:768:ILE:HD13	2.24	0.67
1:D:595:PHE:O	1:D:598:LYS:HG2	1.95	0.67
2:F:90:ASP:N	2:F:223:LEU:O	2.19	0.67
1:B:151:LYS:N	1:B:151:LYS:HD2	2.10	0.66
1:B:691:LYS:O	1:B:694:PHE:N	2.28	0.66
2:E:78:ILE:O	2:E:83:GLN:N	2.27	0.66
1:A:285:SER:OG	1:A:286:ASP:OD1	2.12	0.66
1:B:764:THR:OG1	1:B:767:GLN:N	2.23	0.66
1:C:330:ASN:ND2	1:C:381:THR:O	2.28	0.66
1:C:535:ARG:HB3	1:C:537:TYR:OH	1.95	0.66
2:E:301:GLU:H	2:E:364:ILE:HA	1.59	0.66
1:A:323:ARG:NH1	1:A:664:ASP:OD1	2.28	0.66
1:A:101:GLU:OE1	1:A:112:PHE:CE1	2.49	0.66
1:A:238:HIS:CD2	1:A:621:GLU:HG2	2.30	0.66
1:A:419:GLU:OE1	1:A:419:GLU:N	2.28	0.66
1:A:491:GLN:HB2	1:A:639:LEU:HD13	1.76	0.66
2:E:98:ILE:O	2:E:207:ALA:N	2.25	0.66
1:A:471:THR:HA	1:A:478:THR:HG21	1.77	0.66
1:C:257:ARG:NH1	1:C:257:ARG:O	2.29	0.66
1:B:267:PRO:O	1:B:270:ASP:N	2.26	0.66
1:B:508:LEU:O	1:B:511:MET:HB3	1.96	0.66
1:C:181:ASP:OD1	1:C:182:ARG:N	2.28	0.66
1:B:583:ASN:HD21	1:B:587:ARG:NH2	1.92	0.66
1:D:483:VAL:HG22	1:D:629:PHE:CD2	2.30	0.66
1:A:387:GLY:O	1:A:390:ASN:N	2.29	0.66
1:A:472:THR:OG1	1:A:473:TYR:CD2	2.49	0.66
1:C:736:LEU:O	1:C:739:SER:OG	2.08	0.66
1:A:772:SER:O	1:A:775:TYR:N	2.29	0.66
1:C:224:ARG:NH2	1:C:416:GLU:OE1	2.29	0.66
1:D:163:GLU:HG3	1:D:481:VAL:CG2	2.26	0.66
1:A:559:ASP:OD1	1:A:560:ASP:N	2.29	0.65
1:B:278:ASN:OD1	1:B:279:VAL:HG23	1.96	0.65
1:B:583:ASN:OD1	1:B:587:ARG:NE	2.28	0.65
1:A:87:GLU:OE1	1:A:640:GLN:HB2	1.95	0.65
1:A:234:VAL:HG12	1:A:595:PHE:HD1	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:VAL:HB	1:A:631:ILE:HG22	1.77	0.65
1:B:162:THR:HA	1:B:165:ILE:HD12	1.79	0.65
1:B:239:LYS:O	1:B:239:LYS:HG2	1.96	0.65
1:C:264:GLN:HG2	1:C:265:PHE:HD1	1.60	0.65
1:A:193:ILE:O	1:A:197:PHE:N	2.29	0.65
1:B:116:LYS:O	1:B:119:GLU:N	2.29	0.65
1:C:527:GLU:HA	1:C:530:ILE:HD12	1.77	0.65
1:A:319:ASP:O	1:A:322:LEU:N	2.27	0.65
1:A:473:TYR:O	1:A:590:GLU:OE1	2.15	0.65
1:C:146:VAL:HA	1:C:149:LEU:HB2	1.77	0.65
1:C:475:PRO:HA	1:C:610:SER:HB2	1.78	0.65
1:D:237:ASP:OD1	1:D:238:HIS:N	2.29	0.65
1:B:280:MET:HA	1:B:284:ALA:HB3	1.78	0.65
1:C:249:SER:OG	1:C:250:GLN:N	2.28	0.65
1:A:466:CYS:O	1:A:469:THR:OG1	2.15	0.65
1:A:496:VAL:HA	1:A:499:GLN:HB2	1.79	0.65
1:A:614:VAL:CB	1:A:631:ILE:HG22	2.27	0.65
1:B:424:LYS:O	1:B:427:ARG:NE	2.30	0.65
1:A:214:TYR:HE2	1:A:353:PHE:HA	1.62	0.65
1:A:357:ILE:HG22	1:A:361:MET:HE1	1.79	0.65
1:A:507:PHE:CD1	1:A:738:ALA:HB2	2.32	0.65
1:B:312:ILE:O	1:B:315:ALA:N	2.26	0.65
1:B:700:CYS:O	1:B:704:GLN:HG2	1.97	0.65
1:B:756:ARG:NH2	1:B:761:GLU:OE2	2.29	0.65
1:D:522:SER:OG	1:D:523:TYR:N	2.30	0.65
2:F:412:CYS:H	2:F:426:GLU:HA	1.62	0.65
1:A:117:PHE:HE2	1:A:779:ALA:HA	1.62	0.65
1:B:540:PRO:CA	1:B:607:PHE:CE2	2.80	0.65
1:A:226:LEU:CD1	1:A:416:GLU:OE2	2.44	0.64
1:A:279:VAL:HG21	1:A:415:PHE:HD1	1.62	0.64
1:D:652:THR:HG23	1:D:736:LEU:HD13	1.78	0.64
1:D:675:LEU:HD12	1:D:676:ALA:N	2.12	0.64
2:F:335:VAL:O	2:F:339:TYR:N	2.29	0.64
2:F:77:THR:HA	2:F:84:SER:HA	1.79	0.64
2:F:93:SER:O	2:F:225:LEU:N	2.30	0.64
1:B:604:ARG:HH22	1:B:672:ASP:HA	1.62	0.64
1:C:327:GLN:OE1	1:D:310:GLN:NE2	2.31	0.64
1:C:720:ALA:HA	1:C:790:LEU:HD11	1.78	0.64
1:C:816:PHE:O	1:C:818:CYS:N	2.30	0.64
1:D:132:THR:O	1:D:135:SER:OG	2.13	0.64
1:A:226:LEU:HD13	1:A:416:GLU:CD	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:ASN:HA	1:C:586:ARG:CZ	2.27	0.64
1:D:268:GLU:O	1:D:270:ASP:N	2.30	0.64
1:A:276:ILE:HG23	1:A:411:VAL:HG21	1.79	0.64
1:A:764:THR:HG23	1:A:765:PRO:HD2	1.78	0.64
1:C:319:ASP:O	1:C:322:LEU:N	2.29	0.64
1:D:526:ALA:HB1	1:D:662:PHE:HE2	1.62	0.64
1:A:650:SER:OG	1:A:651:GLY:N	2.30	0.64
1:C:515:LEU:CD2	1:C:518:MET:HG3	2.28	0.64
1:D:656:HIS:NE2	1:D:728:GLU:OE1	2.28	0.64
1:B:255:MET:CB	1:B:260:TYR:OH	2.42	0.64
1:B:526:ALA:HB1	1:B:662:PHE:HE1	1.61	0.64
1:B:570:ASN:HA	1:B:589:TYR:CE2	2.32	0.64
1:D:98:GLY:O	1:D:116:LYS:HB3	1.98	0.64
2:E:252:PHE:O	2:E:414:ILE:HA	1.98	0.64
1:A:507:PHE:CZ	1:A:659:VAL:CG1	2.81	0.64
1:A:509:LYS:O	1:A:510:LYS:HG2	1.98	0.64
1:C:543:LEU:HD23	1:C:544:PHE:HB2	1.81	0.63
1:C:745:GLU:OE1	1:C:745:GLU:N	2.31	0.63
1:A:775:TYR:O	1:A:778:CYS:N	2.30	0.63
1:A:487:GLU:OE1	1:A:489:ARG:NH1	2.31	0.63
1:B:820:LEU:HB3	1:B:825:TYR:CE2	2.34	0.63
1:A:489:ARG:O	1:A:493:VAL:N	2.26	0.63
1:B:190:LEU:HA	1:B:193:ILE:HG12	1.79	0.63
1:C:470:ILE:O	1:C:474:MET:N	2.27	0.63
1:C:764:THR:OG1	1:C:767:GLN:NE2	2.32	0.63
1:D:132:THR:OG1	1:D:778:CYS:O	2.16	0.63
1:A:234:VAL:CG2	1:A:235:ASN:N	2.61	0.63
1:A:640:GLN:N	1:A:640:GLN:OE1	2.31	0.63
1:B:427:ARG:HG3	1:B:428:ILE:HG13	1.80	0.63
1:B:618:TYR:HD1	1:B:624:SER:O	1.82	0.63
1:D:246:TYR:OH	1:D:598:LYS:CD	2.47	0.63
1:A:214:TYR:OH	1:A:352:ARG:O	2.14	0.63
1:C:171:GLN:HA	1:C:174:VAL:HG12	1.80	0.63
1:C:588:GLY:O	1:C:592:ARG:HG3	1.98	0.63
1:D:97:PHE:CZ	1:D:120:ARG:HG2	2.33	0.63
1:D:614:VAL:HG13	1:D:614:VAL:O	1.98	0.63
2:E:335:VAL:O	2:E:339:TYR:N	2.32	0.63
1:C:519:GLN:O	1:C:522:SER:OG	2.15	0.63
1:D:280:MET:HA	1:D:283:PHE:CD2	2.33	0.63
1:A:638:ASP:OD1	1:A:639:LEU:N	2.32	0.63
1:D:479:GLY:HA3	1:D:611:PRO:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:O	1:A:136:GLN:HB3	1.99	0.62
1:A:570:ASN:O	1:A:571:LYS:CG	2.44	0.62
1:C:515:LEU:CD2	1:C:518:MET:CG	2.77	0.62
1:C:663:ASP:CG	1:C:730:ILE:HD11	2.20	0.62
1:A:322:LEU:HD23	1:A:328:GLN:OE1	2.00	0.62
1:A:782:THR:O	1:A:786:LEU:N	2.32	0.62
1:B:325:HIS:HA	1:B:328:GLN:CG	2.28	0.62
1:B:411:VAL:O	1:B:415:PHE:HB2	2.00	0.62
1:B:593:GLU:O	1:B:597:ARG:HG3	1.99	0.62
1:B:782:THR:O	1:B:785:SER:OG	2.12	0.62
1:C:100:ASP:HB2	1:C:115:ASN:HB3	1.80	0.62
1:D:770:TRP:CE3	1:D:770:TRP:HA	2.34	0.62
2:E:287:TYR:HA	2:E:423:GLY:HA2	1.81	0.62
1:A:166:THR:O	1:A:169:ALA:N	2.32	0.62
1:C:313:ALA:O	1:C:316:SER:N	2.31	0.62
1:D:567:ALA:HA	1:D:589:TYR:OH	1.98	0.62
1:C:510:LYS:HZ3	1:C:737:GLN:HG2	1.63	0.62
1:D:109:PHE:CE2	1:D:806:LEU:CD1	2.82	0.62
2:E:251:ILE:HA	2:E:415:HIS:O	1.99	0.62
1:B:162:THR:H	1:B:564:ILE:HD13	1.65	0.62
1:B:380:VAL:CG1	1:B:385:TYR:CE2	2.77	0.62
1:B:562:TYR:O	1:B:565:LEU:HB3	2.00	0.62
1:C:618:TYR:CE1	1:C:620:PRO:HA	2.34	0.62
1:D:160:SER:O	1:D:163:GLU:OE1	2.17	0.62
1:D:809:ILE:HG22	1:D:812:PHE:H	1.65	0.62
2:E:168:PHE:N	2:E:179:GLY:O	2.32	0.62
1:D:121:ILE:O	1:D:780:LYS:NZ	2.32	0.62
1:A:764:THR:CG2	1:A:765:PRO:CD	2.78	0.62
1:B:269:LEU:O	1:B:272:ARG:HB3	2.00	0.62
1:A:163:GLU:OE2	1:A:480:TYR:CE2	2.53	0.62
1:B:208:LYS:HG2	1:B:403:TYR:OH	1.99	0.62
1:B:620:PRO:HB2	1:B:669:PHE:HD2	1.64	0.62
1:C:643:LYS:HA	1:C:646:ASN:ND2	2.15	0.62
1:D:660:HIS:NE2	1:D:728:GLU:OE2	2.30	0.62
1:B:279:VAL:O	1:B:282:ALA:N	2.31	0.62
1:C:214:TYR:HA	1:C:217:MET:HB3	1.82	0.62
2:E:250:PRO:O	2:E:417:MET:N	2.33	0.62
1:A:770:TRP:CZ2	1:A:812:PHE:HB2	2.35	0.61
1:B:295:ASP:O	1:B:298:ILE:N	2.33	0.61
1:B:544:PHE:O	1:B:544:PHE:CG	2.53	0.61
1:B:480:TYR:HE1	1:B:484:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:TYR:CZ	1:C:620:PRO:HA	2.35	0.61
2:F:300:MET:O	2:F:313:GLY:N	2.32	0.61
1:A:762:LYS:CD	1:C:817:GLN:N	2.63	0.61
1:B:669:PHE:HA	1:B:674:SER:O	2.00	0.61
1:C:310:GLN:O	1:C:314:MET:HG2	1.99	0.61
1:C:664:ASP:OD1	1:C:665:GLU:N	2.33	0.61
2:E:253:THR:HA	2:E:413:ASN:O	2.00	0.61
2:F:343:TYR:HA	2:F:350:TYR:HA	1.80	0.61
1:B:109:PHE:CG	1:B:806:LEU:HD23	2.35	0.61
1:B:272:ARG:NH1	1:B:272:ARG:HA	2.15	0.61
1:D:139:LEU:HD12	1:D:464:MET:SD	2.41	0.61
1:A:212:GLU:OE2	1:A:355:LYS:NZ	2.29	0.61
1:A:248:ILE:HB	1:A:380:VAL:HG22	1.83	0.61
1:B:645:PHE:HE1	1:B:768:ILE:HG22	1.66	0.61
1:B:742:ALA:O	1:B:745:GLU:N	2.34	0.61
1:C:224:ARG:NH2	1:C:417:ASP:OD1	2.33	0.61
1:A:238:HIS:NE2	1:A:621:GLU:CD	2.54	0.61
1:A:762:LYS:HD2	1:C:817:GLN:N	2.16	0.61
1:B:109:PHE:CZ	1:B:806:LEU:CD2	2.83	0.61
1:B:510:LYS:HA	1:B:514:THR:HG21	1.83	0.61
1:B:805:VAL:O	1:B:805:VAL:HG12	2.01	0.61
1:B:133:THR:O	1:B:136:GLN:HB2	2.00	0.61
1:B:809:ILE:HG22	1:B:809:ILE:O	1.98	0.61
1:A:709:CYS:SG	1:A:719:CYS:CB	2.87	0.61
1:D:228:THR:O	1:D:230:MET:N	2.32	0.61
1:B:341:LYS:CE	1:B:353:PHE:HE2	2.13	0.61
1:B:481:VAL:O	1:B:485:SER:HB3	2.01	0.61
1:B:538:GLY:HA2	1:B:629:PHE:H	1.65	0.61
1:C:238:HIS:CE1	1:C:247:TYR:HH	2.19	0.61
1:A:82:ALA:HB1	1:A:758:PRO:HB3	1.83	0.60
1:C:81:ASN:HB2	1:C:756:ARG:HB2	1.81	0.60
1:D:279:VAL:HG21	1:D:414:LEU:HD11	1.82	0.60
1:A:561:TYR:C	1:A:564:ILE:HG12	2.20	0.60
1:C:619:ALA:HB3	1:C:624:SER:OG	2.01	0.60
1:C:776:SER:O	1:C:776:SER:OG	2.20	0.60
1:B:174:VAL:HG23	1:B:175:GLU:HG2	1.82	0.60
1:A:87:GLU:OE1	1:A:640:GLN:CG	2.50	0.60
1:A:91:ALA:HB2	1:A:641:PHE:CE1	2.36	0.60
1:D:97:PHE:HZ	1:D:120:ARG:HG2	1.66	0.60
1:A:275:ALA:O	1:A:279:VAL:HG23	2.00	0.60
1:A:484:ASN:HA	1:A:487:GLU:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:ARG:O	1:D:604:ARG:HG3	1.99	0.60
1:B:622:LEU:HD13	1:B:624:SER:OG	2.00	0.60
1:C:298:ILE:O	1:C:301:ALA:N	2.35	0.60
1:B:217:MET:O	1:B:220:ILE:N	2.34	0.60
1:C:733:LEU:C	1:C:733:LEU:HD12	2.22	0.60
1:C:736:LEU:HD21	1:C:770:TRP:HZ3	1.67	0.60
1:C:793:ASN:CB	1:C:795:HIS:CE1	2.85	0.60
1:C:820:LEU:HA	1:C:825:TYR:O	2.02	0.60
2:E:345:GLU:H	2:E:348:GLU:HA	1.67	0.60
1:B:305:VAL:HG11	1:B:411:VAL:HG21	1.82	0.60
1:C:793:ASN:HB3	1:C:795:HIS:CE1	2.37	0.60
1:D:119:GLU:O	1:D:119:GLU:HG2	2.02	0.60
1:D:323:ARG:NH2	1:D:724:HIS:O	2.35	0.60
1:D:380:VAL:HG13	1:D:386:MET:HG3	1.82	0.60
1:D:407:ASN:O	1:D:411:VAL:HG23	2.01	0.60
1:D:820:LEU:C	1:D:820:LEU:HD12	2.21	0.60
2:E:289:ASP:HA	2:E:421:THR:HA	1.84	0.60
1:B:308:ILE:HG23	1:B:309:GLU:N	2.17	0.60
2:F:182:GLY:H	2:F:204:PHE:H	1.49	0.60
1:A:130:ARG:HG2	1:A:781:GLU:HB3	1.83	0.60
1:A:705:TYR:HE1	1:A:804:GLN:HG2	1.66	0.60
1:A:277:GLU:CD	1:A:302:ALA:CB	2.69	0.59
1:B:231:TYR:HD2	1:B:233:TRP:CZ3	2.20	0.59
1:C:182:ARG:HD3	1:C:580:THR:H	1.66	0.59
1:D:565:LEU:HA	1:D:568:TYR:HB2	1.84	0.59
1:D:631:ILE:HG23	1:D:632:LEU:N	2.17	0.59
1:A:91:ALA:HB2	1:A:641:PHE:CZ	2.37	0.59
1:C:663:ASP:OD1	1:C:730:ILE:HD11	2.02	0.59
1:D:238:HIS:ND1	1:D:247:TYR:OH	2.31	0.59
1:D:559:ASP:OD1	1:D:560:ASP:N	2.32	0.59
1:D:650:SER:OG	1:D:651:GLY:N	2.35	0.59
1:A:636:HIS:O	1:A:650:SER:N	2.21	0.59
1:B:121:ILE:O	1:B:780:LYS:HD3	2.02	0.59
1:B:705:TYR:HE2	1:B:729:ASN:OD1	1.85	0.59
1:B:757:LEU:HD12	1:B:768:ILE:HD13	1.83	0.59
1:C:569:ASN:HB3	1:C:589:TYR:CE1	2.31	0.59
1:A:648:ALA:HB2	1:A:769:PHE:CD1	2.37	0.59
1:B:333:GLU:O	1:B:336:ALA:N	2.35	0.59
1:C:767:GLN:HB2	1:C:816:PHE:CZ	2.37	0.59
1:D:492:VAL:HG13	1:D:493:VAL:N	2.17	0.59
1:A:99:LEU:HD13	1:A:760:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:GLU:HG3	1:B:597:ARG:HH21	1.67	0.59
1:B:660:HIS:HA	1:B:663:ASP:OD2	2.03	0.59
1:C:381:THR:O	1:C:383:PRO:HD3	2.02	0.59
1:C:779:ALA:HB3	1:C:798:ASN:OD1	2.02	0.59
1:D:273:THR:HA	1:D:276:ILE:HG22	1.83	0.59
1:C:621:GLU:H	1:C:621:GLU:CD	2.06	0.59
1:C:628:PRO:HG2	1:C:637:TYR:HE2	1.67	0.59
1:D:321:GLU:OE1	1:D:321:GLU:N	2.35	0.59
1:D:296:LYS:O	1:D:296:LYS:HD2	2.02	0.59
1:D:609:GLU:HB3	1:D:617:TRP:CH2	2.37	0.59
1:A:355:LYS:O	1:A:357:ILE:N	2.36	0.59
1:B:565:LEU:HA	1:B:568:TYR:HB2	1.85	0.59
1:B:798:ASN:O	1:B:801:ARG:N	2.35	0.59
1:A:773:TYR:HE1	1:A:777:TRP:HE1	1.51	0.59
1:D:352:ARG:HB3	1:D:355:LYS:HB2	1.85	0.59
1:D:820:LEU:HA	1:D:825:TYR:CD2	2.37	0.59
1:B:374:PHE:CD1	1:B:375:ILE:N	2.71	0.58
1:B:406:VAL:O	1:B:410:ILE:HG22	2.03	0.58
1:B:519:GLN:HE22	1:B:521:GLU:H	1.50	0.58
1:B:622:LEU:HD12	1:B:622:LEU:C	2.23	0.58
1:C:512:LEU:N	1:C:523:TYR:OH	2.36	0.58
1:D:331:PRO:HB2	1:D:377:ASP:CG	2.24	0.58
2:F:416:ASP:O	2:F:420:ASN:N	2.36	0.58
1:A:785:SER:HA	1:A:788:LYS:HD3	1.83	0.58
1:C:519:GLN:O	1:C:523:TYR:N	2.33	0.58
1:C:643:LYS:HA	1:C:646:ASN:HD21	1.67	0.58
1:D:719:CYS:SG	1:D:787:VAL:CG2	2.92	0.58
2:E:336:ALA:O	2:E:341:GLY:N	2.35	0.58
2:F:299:LYS:HA	2:F:315:GLU:HA	1.85	0.58
1:A:382:ASN:O	1:A:385:TYR:N	2.37	0.58
1:B:489:ARG:CZ	1:B:544:PHE:CE2	2.87	0.58
1:C:104:ASP:OD1	1:C:105:PRO:HD2	2.03	0.58
1:C:187:ASN:HA	1:C:190:LEU:HB2	1.84	0.58
1:C:722:GLY:O	1:C:724:HIS:N	2.36	0.58
1:A:238:HIS:CD2	1:A:621:GLU:CG	2.87	0.58
1:A:813:ALA:HB1	1:A:825:TYR:HE1	1.68	0.58
1:C:806:LEU:HD22	1:C:812:PHE:CG	2.38	0.58
1:A:234:VAL:HG12	1:A:595:PHE:CD1	2.38	0.58
1:A:656:HIS:HE1	1:A:728:GLU:HG3	1.69	0.58
1:C:600:GLU:N	1:C:600:GLU:OE1	2.35	0.58
1:A:617:TRP:NE1	1:A:626:THR:OG1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASN:O	1:B:282:ALA:N	2.36	0.58
1:B:591:ASN:HB2	1:B:595:PHE:CZ	2.38	0.58
1:C:151:LYS:O	1:C:167:LYS:NZ	2.27	0.58
1:C:167:LYS:O	1:C:171:GLN:HG2	2.04	0.58
1:C:273:THR:HG22	1:C:306:THR:HG21	1.84	0.58
1:A:109:PHE:O	1:A:112:PHE:N	2.36	0.58
1:A:476:TYR:OH	1:A:607:PHE:HB2	2.04	0.58
1:A:620:PRO:HB2	1:A:669:PHE:CD2	2.39	0.57
1:B:110:TYR:CD1	1:B:799:SER:HA	2.39	0.57
1:B:310:GLN:O	1:B:312:ILE:N	2.37	0.57
1:B:809:ILE:CG2	1:B:811:SER:OG	2.42	0.57
1:D:504:MET:HG3	1:D:530:ILE:CG2	2.34	0.57
1:A:332:TYR:N	1:A:377:ASP:OD1	2.37	0.57
1:B:485:SER:OG	1:B:486:ARG:HG2	2.04	0.57
1:C:573:ASP:OD1	1:C:574:LYS:N	2.37	0.57
1:D:250:GLN:OE1	1:D:382:ASN:OD1	2.22	0.57
1:A:238:HIS:NE2	1:A:621:GLU:HG2	2.19	0.57
1:A:583:ASN:O	1:A:587:ARG:HG2	2.04	0.57
1:B:170:PHE:HZ	1:B:463:ARG:HG2	1.69	0.57
1:B:259:PHE:CE2	1:B:265:PHE:HB3	2.38	0.57
1:B:516:SER:OG	1:B:517:TRP:N	2.37	0.57
1:B:629:PHE:HA	1:B:632:LEU:HD13	1.86	0.57
1:D:652:THR:O	1:D:655:GLY:N	2.37	0.57
1:B:112:PHE:HE2	1:B:816:PHE:HZ	1.53	0.57
1:B:341:LYS:HB3	1:B:352:ARG:HH12	1.67	0.57
1:C:229:PHE:H	1:C:251:PRO:HG3	1.70	0.57
2:E:241:ARG:O	2:E:245:LEU:N	2.32	0.57
2:F:90:ASP:O	2:F:225:LEU:N	2.37	0.57
1:A:479:GLY:O	1:A:482:TYR:N	2.37	0.57
1:B:118:ILE:O	1:B:780:LYS:HD2	2.04	0.57
1:B:420:HIS:NE2	1:B:580:THR:HA	2.19	0.57
1:B:462:ALA:HA	1:B:465:LYS:NZ	2.19	0.57
1:C:834:VAL:HG22	1:C:835:TRP:CD1	2.40	0.57
1:D:357:ILE:O	1:D:360:LEU:N	2.33	0.57
1:A:504:MET:HE1	1:A:535:ARG:NH1	2.20	0.57
1:B:670:ASP:OD1	1:B:672:ASP:N	2.36	0.57
1:B:732:ASP:OD2	1:B:801:ARG:HG2	2.04	0.57
1:C:510:LYS:NZ	1:C:737:GLN:HG2	2.19	0.57
1:D:804:GLN:O	1:D:807:GLN:N	2.38	0.57
1:A:101:GLU:OE1	1:A:112:PHE:HE1	1.86	0.57
1:A:196:ARG:NH1	1:A:219:ARG:HE	1.98	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:OG1	1:B:778:CYS:O	2.22	0.57
1:B:341:LYS:HE2	1:B:353:PHE:CE2	2.36	0.57
1:B:520:GLY:O	1:B:523:TYR:HB3	2.04	0.57
1:D:393:PHE:CE1	1:D:405:PHE:CD2	2.93	0.57
1:D:560:ASP:HB2	1:D:564:ILE:HD11	1.86	0.57
2:F:95:ASN:O	2:F:224:GLY:N	2.37	0.57
2:F:344:ASP:H	2:F:350:TYR:HA	1.68	0.57
1:B:186:VAL:HG23	1:B:187:ASN:N	2.19	0.57
1:B:629:PHE:O	1:B:632:LEU:N	2.33	0.57
1:B:633:THR:OG1	1:B:634:SER:N	2.37	0.57
1:A:389:LEU:N	1:A:389:LEU:HD12	2.19	0.57
1:B:278:ASN:HA	1:B:425:TYR:CZ	2.40	0.57
1:B:591:ASN:OD1	1:B:592:ARG:N	2.37	0.57
1:C:110:TYR:CD1	1:C:111:GLY:N	2.73	0.57
1:D:808:ASP:HA	1:D:831:ARG:HG3	1.87	0.57
2:E:78:ILE:H	2:E:83:GLN:H	1.53	0.57
1:B:208:LYS:N	1:B:403:TYR:OH	2.37	0.56
1:B:461:ASP:OD1	1:B:462:ALA:N	2.37	0.56
1:C:386:MET:HE1	1:D:391:THR:HG22	1.87	0.56
1:C:582:LEU:O	1:C:585:LEU:HB3	2.05	0.56
1:C:768:ILE:O	1:C:771:ILE:N	2.38	0.56
1:D:529:LYS:O	1:D:533:MET:HG3	2.04	0.56
1:A:705:TYR:O	1:A:708:GLN:N	2.30	0.56
1:B:407:ASN:O	1:B:411:VAL:HG23	2.05	0.56
1:B:533:MET:CE	1:B:658:LEU:HD11	2.35	0.56
1:B:732:ASP:HB3	1:B:805:VAL:HG21	1.87	0.56
1:C:806:LEU:O	1:C:809:ILE:N	2.31	0.56
1:D:530:ILE:HA	1:D:533:MET:SD	2.44	0.56
1:A:185:SER:HB2	1:A:188:GLU:CD	2.25	0.56
1:B:262:LEU:CB	1:B:263:PRO:CD	2.80	0.56
1:B:510:LYS:HZ3	1:B:510:LYS:HB2	1.71	0.56
1:C:95:LEU:HD11	1:C:771:ILE:HG22	1.85	0.56
1:C:134:PHE:O	1:C:137:ALA:N	2.38	0.56
1:C:245:SER:OG	1:C:246:TYR:N	2.37	0.56
1:D:241:VAL:HG23	1:D:241:VAL:O	2.05	0.56
1:D:636:HIS:O	1:D:649:GLY:HA3	2.04	0.56
2:F:328:PRO:O	2:F:332:ALA:N	2.36	0.56
1:B:515:LEU:HB2	1:B:518:MET:HE3	1.87	0.56
1:D:332:TYR:O	1:D:378:VAL:N	2.22	0.56
1:D:770:TRP:HE1	1:D:812:PHE:HA	1.71	0.56
1:C:95:LEU:CD1	1:C:771:ILE:CG2	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LYS:HD2	1:B:281:LYS:N	2.21	0.56
1:B:767:GLN:HE21	1:B:816:PHE:HA	1.70	0.56
1:B:809:ILE:O	1:B:812:PHE:N	2.34	0.56
1:C:617:TRP:NE1	1:C:626:THR:HB	2.20	0.56
1:D:116:LYS:O	1:D:119:GLU:N	2.37	0.56
1:D:770:TRP:HA	1:D:770:TRP:HE3	1.71	0.56
1:A:196:ARG:HH12	1:A:219:ARG:NE	2.02	0.56
1:A:272:ARG:HH21	1:A:276:ILE:HD11	1.70	0.56
1:A:637:TYR:OH	1:A:639:LEU:HA	2.05	0.56
1:B:637:TYR:O	1:B:638:ASP:CG	2.42	0.56
2:F:100:ASP:N	2:F:207:ALA:O	2.39	0.56
1:A:789:ARG:HA	1:A:792:THR:HG22	1.88	0.56
1:B:304:GLU:O	1:B:307:GLN:N	2.38	0.56
1:C:564:ILE:O	1:C:568:TYR:HB2	2.06	0.56
1:D:143:SER:O	1:D:147:LYS:HG2	2.05	0.56
2:F:251:ILE:HA	2:F:415:HIS:O	2.05	0.56
1:A:132:THR:HA	1:A:779:ALA:HB2	1.88	0.56
1:A:801:ARG:O	1:A:804:GLN:N	2.27	0.56
1:C:228:THR:O	1:C:229:PHE:HB2	2.06	0.56
3:G:95:HIS:O	3:G:96:PHE:C	2.44	0.56
1:B:542:LYS:N	1:B:542:LYS:HD2	2.20	0.56
1:C:234:VAL:HG12	1:C:594:SER:O	2.06	0.56
1:A:571:LYS:O	1:A:572:THR:OG1	2.23	0.55
1:B:188:GLU:O	1:B:191:GLN:HB3	2.06	0.55
1:A:703:THR:O	1:A:706:ASN:OD1	2.23	0.55
1:B:507:PHE:HA	1:B:510:LYS:NZ	2.22	0.55
1:D:583:ASN:HA	1:D:586:ARG:CZ	2.36	0.55
1:A:496:VAL:O	1:A:499:GLN:N	2.40	0.55
1:A:784:SER:O	1:A:788:LYS:HG3	2.07	0.55
1:B:493:VAL:O	1:B:497:LYS:HG3	2.07	0.55
1:C:305:VAL:HG11	1:C:411:VAL:HG21	1.88	0.55
1:C:767:GLN:O	1:C:771:ILE:HG13	2.05	0.55
1:A:762:LYS:HD2	1:C:817:GLN:HA	1.88	0.55
1:B:278:ASN:HA	1:B:425:TYR:CE2	2.42	0.55
1:D:83:ASN:OD1	1:D:85:SER:N	2.40	0.55
1:D:480:TYR:CD2	1:D:543:LEU:HG	2.39	0.55
1:A:87:GLU:OE1	1:A:640:GLN:HG2	2.07	0.55
1:A:264:GLN:HE22	1:A:314:MET:HE3	1.70	0.55
1:C:193:ILE:HG23	1:C:197:PHE:CE2	2.36	0.55
1:C:385:TYR:O	1:C:385:TYR:CG	2.60	0.55
2:F:289:ASP:HA	2:F:421:THR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:O	1:A:145:ILE:HB	2.07	0.55
1:A:468:ASP:O	1:A:471:THR:OG1	2.20	0.55
1:A:537:TYR:O	1:A:539:TRP:N	2.39	0.55
1:B:589:TYR:O	1:B:592:ARG:N	2.40	0.55
1:C:263:PRO:O	1:C:266:ALA:N	2.39	0.55
1:C:267:PRO:HG2	1:C:268:GLU:OE2	2.07	0.55
1:D:405:PHE:O	1:D:408:TYR:HB3	2.06	0.55
1:B:333:GLU:OE1	1:B:333:GLU:N	2.39	0.55
1:B:579:TYR:HA	1:B:582:LEU:CG	2.36	0.55
1:B:645:PHE:O	1:B:648:ALA:N	2.39	0.55
2:E:99:PRO:HA	2:E:207:ALA:HB3	1.89	0.55
1:A:499:GLN:O	1:A:503:ILE:HG13	2.07	0.55
1:A:762:LYS:HD2	1:C:817:GLN:CA	2.37	0.55
1:B:109:PHE:CZ	1:B:806:LEU:HD21	2.41	0.55
1:B:710:CYS:SG	1:B:711:PRO:HD3	2.47	0.55
1:B:809:ILE:O	1:B:811:SER:N	2.40	0.55
1:C:270:ASP:OD1	1:C:271:ALA:N	2.39	0.55
1:C:583:ASN:HD21	1:C:587:ARG:CZ	2.19	0.55
1:D:529:LYS:NZ	1:D:669:PHE:O	2.37	0.55
2:F:373:ARG:O	2:F:377:VAL:N	2.39	0.55
1:A:664:ASP:HA	1:A:667:VAL:HG12	1.89	0.55
1:A:670:ASP:OD2	1:A:674:SER:OG	2.24	0.55
1:B:617:TRP:NE1	1:B:626:THR:OG1	2.39	0.55
1:C:178:LEU:HD22	1:C:182:ARG:NH1	2.22	0.55
1:C:218:GLY:O	1:C:220:ILE:N	2.39	0.55
1:C:260:TYR:O	1:C:266:ALA:HA	2.06	0.55
1:D:336:ALA:N	1:D:337:PRO:CD	2.69	0.55
1:A:162:THR:HA	1:A:165:ILE:HG12	1.89	0.55
1:B:647:PHE:O	1:B:652:THR:N	2.40	0.55
1:C:657:GLU:O	1:C:660:HIS:N	2.39	0.55
1:A:754:GLU:HB3	1:A:765:PRO:HD2	1.88	0.54
2:E:192:GLY:H	2:E:273:TYR:H	1.55	0.54
1:A:417:ASP:OD1	1:A:417:ASP:N	2.40	0.54
1:A:705:TYR:CE1	1:A:804:GLN:HG2	2.43	0.54
1:B:242:SER:C	1:B:243:ARG:HG3	2.26	0.54
1:C:230:MET:HE2	1:C:356:TYR:CE2	2.41	0.54
1:C:306:THR:HA	1:C:309:GLU:HG3	1.88	0.54
1:C:535:ARG:HB3	1:C:537:TYR:CZ	2.42	0.54
1:C:761:GLU:OE1	1:C:761:GLU:N	2.40	0.54
1:B:146:VAL:O	1:B:149:LEU:HG	2.08	0.54
1:B:540:PRO:HD2	1:B:543:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:C	1:C:180:ASP:H	2.10	0.54
1:C:190:LEU:O	1:C:194:SER:OG	2.11	0.54
1:C:535:ARG:HB3	1:C:537:TYR:CE2	2.42	0.54
1:C:744:LYS:O	1:C:747:ILE:N	2.23	0.54
1:A:81:ASN:O	1:A:756:ARG:HB2	2.07	0.54
1:A:214:TYR:CE2	1:A:353:PHE:HA	2.42	0.54
1:B:483:VAL:HG11	1:B:539:TRP:CE3	2.42	0.54
1:C:222:GLN:HG3	1:C:360:LEU:HD22	1.90	0.54
1:C:277:GLU:HG3	1:C:299:LYS:NZ	2.22	0.54
1:D:740:TYR:HB2	1:D:769:PHE:HE2	1.71	0.54
2:F:364:ILE:O	2:F:367:LYS:CB	2.56	0.54
1:C:87:GLU:OE2	1:C:639:LEU:HD23	2.08	0.54
1:C:599:ASN:HB2	1:C:600:GLU:CD	2.28	0.54
1:D:160:SER:HB2	1:D:163:GLU:CD	2.28	0.54
1:D:634:SER:O	1:D:636:HIS:N	2.39	0.54
2:E:325:MET:O	2:E:389:MET:N	2.29	0.54
1:A:187:ASN:OD1	1:A:188:GLU:N	2.38	0.54
1:A:766:ASN:O	1:A:769:PHE:N	2.40	0.54
1:B:231:TYR:HD2	1:B:233:TRP:HZ3	1.55	0.54
1:B:269:LEU:HG	1:B:270:ASP:OD1	2.07	0.54
1:B:482:TYR:HE2	1:B:630:GLY:HA2	1.72	0.54
1:B:482:TYR:O	1:B:485:SER:OG	2.25	0.54
1:B:824:MET:O	1:B:824:MET:CG	2.55	0.54
1:A:355:LYS:C	1:A:357:ILE:H	2.11	0.54
1:A:524:ARG:O	1:A:527:GLU:N	2.40	0.54
1:A:533:MET:HG2	1:A:623:ASN:HD21	1.72	0.54
1:B:112:PHE:HE2	1:B:816:PHE:CZ	2.26	0.54
1:C:143:SER:OG	1:C:144:ASP:N	2.41	0.54
1:C:243:ARG:NH2	1:C:376:GLY:HA2	2.16	0.54
1:C:517:TRP:HE1	1:C:518:MET:HE2	1.73	0.54
1:D:814:LYS:O	1:D:817:GLN:N	2.39	0.54
1:D:822:GLN:O	1:D:824:MET:N	2.39	0.54
1:A:474:MET:HE3	1:A:586:ARG:CD	2.31	0.54
1:B:82:ALA:HB2	1:B:756:ARG:O	2.08	0.54
1:C:257:ARG:NH1	1:C:313:ALA:HB1	2.20	0.54
1:A:401:ASN:HB3	1:A:405:PHE:CD2	2.43	0.54
1:A:607:PHE:HE2	1:A:611:PRO:HB3	1.73	0.54
1:B:483:VAL:HG11	1:B:539:TRP:HE3	1.73	0.54
1:B:519:GLN:NE2	1:B:521:GLU:H	2.06	0.54
1:D:647:PHE:CD2	1:D:743:TYR:HB2	2.43	0.54
1:A:141:VAL:HG13	1:A:142:ASN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLU:HA	1:B:426:LEU:CG	2.37	0.53
1:B:507:PHE:HA	1:B:510:LYS:HZ3	1.73	0.53
1:C:262:LEU:O	1:C:266:ALA:N	2.41	0.53
2:F:327:VAL:HA	2:F:401:TRP:HA	1.89	0.53
1:A:265:PHE:CE1	1:A:266:ALA:HB2	2.42	0.53
1:A:500:THR:HA	1:A:503:ILE:HD12	1.90	0.53
1:A:509:LYS:O	1:A:510:LYS:CG	2.55	0.53
1:A:809:ILE:HG22	1:A:812:PHE:H	1.73	0.53
1:B:402:GLN:O	1:B:405:PHE:CD2	2.60	0.53
1:C:494:GLU:O	1:C:498:GLN:HG3	2.07	0.53
1:D:528:LYS:O	1:D:531:ASN:N	2.41	0.53
1:A:764:THR:CG2	1:A:765:PRO:N	2.72	0.53
1:B:236:VAL:HG13	1:B:241:VAL:HG21	1.90	0.53
1:C:164:ARG:HA	1:C:167:LYS:HG2	1.89	0.53
1:C:621:GLU:OE1	1:C:621:GLU:N	2.34	0.53
1:A:670:ASP:O	1:A:672:ASP:N	2.41	0.53
1:A:718:HIS:O	1:A:718:HIS:CG	2.62	0.53
1:B:241:VAL:HG13	1:B:241:VAL:O	2.09	0.53
1:B:270:ASP:C	1:B:272:ARG:H	2.10	0.53
1:C:471:THR:HG23	1:C:612:ALA:HB3	1.91	0.53
1:D:262:LEU:O	1:D:264:GLN:N	2.41	0.53
1:A:490:ASP:OD1	1:A:490:ASP:N	2.38	0.53
1:B:764:THR:O	1:B:768:ILE:HG13	2.08	0.53
1:C:220:ILE:HA	1:C:223:GLN:HB3	1.91	0.53
1:A:333:GLU:OE1	1:A:333:GLU:N	2.41	0.53
1:A:521:GLU:HA	1:A:524:ARG:HH12	1.73	0.53
1:C:241:VAL:O	1:C:241:VAL:HG23	2.09	0.53
2:E:73:LEU:O	2:E:268:GLY:HA3	2.09	0.53
2:E:325:MET:C	2:E:389:MET:H	2.12	0.53
1:A:534:HIS:CD2	1:A:605:THR:HG22	2.43	0.53
1:B:337:PRO:O	1:B:340:GLY:N	2.40	0.53
1:B:759:GLY:O	1:B:760:LEU:CG	2.55	0.53
1:C:218:GLY:O	1:C:221:GLU:N	2.41	0.53
1:C:325:HIS:HA	1:C:328:GLN:HB2	1.91	0.53
1:D:405:PHE:O	1:D:409:ILE:HD12	2.08	0.53
1:D:461:ASP:OD1	1:D:463:ARG:HG3	2.09	0.53
2:E:89:LEU:HA	2:E:223:LEU:O	2.08	0.53
1:D:808:ASP:CG	1:D:831:ARG:HB3	2.28	0.53
1:B:615:ASN:OD1	1:B:616:ALA:N	2.42	0.53
1:C:263:PRO:O	1:C:265:PHE:N	2.42	0.53
2:E:192:GLY:H	2:E:273:TYR:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:LYS:HG3	1:A:746:TYR:OH	2.09	0.53
1:A:668:GLN:O	1:A:675:LEU:CD1	2.56	0.53
1:D:353:PHE:HA	1:D:356:TYR:HB3	1.89	0.53
1:D:507:PHE:HA	1:D:510:LYS:NZ	2.23	0.53
1:D:530:ILE:HA	1:D:533:MET:HG3	1.91	0.53
1:D:608:LEU:HB3	1:D:617:TRP:NE1	2.24	0.53
1:B:334:LEU:HD12	1:B:334:LEU:C	2.29	0.52
1:C:273:THR:OG1	1:C:274:LYS:N	2.42	0.52
1:C:689:LYS:HE2	1:C:691:LYS:HE3	1.89	0.52
2:F:325:MET:N	2:F:387:ILE:O	2.42	0.52
1:B:333:GLU:O	1:B:335:PHE:N	2.43	0.52
1:B:561:TYR:O	1:B:564:ILE:CG2	2.50	0.52
1:C:574:LYS:HG3	1:C:574:LYS:O	2.09	0.52
2:E:398:GLY:O	2:E:400:GLN:N	2.42	0.52
2:F:250:PRO:O	2:F:417:MET:N	2.30	0.52
1:B:238:HIS:O	1:B:674:SER:HA	2.10	0.52
1:A:661:GLY:C	1:A:662:PHE:HD1	2.13	0.52
1:B:622:LEU:CD1	1:B:623:ASN:N	2.72	0.52
1:C:296:LYS:O	1:C:298:ILE:N	2.43	0.52
2:E:168:PHE:O	2:E:179:GLY:N	2.43	0.52
2:E:252:PHE:HA	2:E:272:THR:O	2.10	0.52
1:B:112:PHE:CE2	1:B:816:PHE:CZ	2.97	0.52
1:B:489:ARG:NH2	1:B:544:PHE:HE2	2.07	0.52
1:C:177:THR:HA	1:C:180:ASP:HB3	1.92	0.52
1:C:538:GLY:HA2	1:C:628:PRO:C	2.30	0.52
1:C:694:PHE:O	1:C:697:MET:N	2.43	0.52
1:A:234:VAL:HG22	1:A:235:ASN:H	1.74	0.52
1:A:752:ALA:HB1	1:A:754:GLU:OE2	2.10	0.52
1:B:503:ILE:HD11	1:B:651:GLY:HA2	1.92	0.52
1:B:725:THR:OG1	1:B:729:ASN:ND2	2.42	0.52
1:A:112:PHE:CG	1:A:112:PHE:O	2.62	0.52
1:A:226:LEU:HD22	1:A:413:MET:HA	1.91	0.52
1:A:781:GLU:OE2	1:A:786:LEU:HG	2.10	0.52
1:B:563:SER:O	1:B:566:GLU:N	2.43	0.52
1:C:257:ARG:HE	1:C:318:PRO:HD3	1.75	0.52
1:C:386:MET:CE	1:D:391:THR:HG22	2.39	0.52
1:C:595:PHE:O	1:C:598:LYS:N	2.31	0.52
1:D:226:LEU:HD21	1:D:412:HIS:HB3	1.92	0.52
1:A:618:TYR:CE2	1:A:661:GLY:HA3	2.45	0.52
1:B:536:ASN:CB	1:B:626:THR:HG22	2.39	0.52
1:B:591:ASN:O	1:B:594:SER:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LEU:CD1	1:C:771:ILE:HG22	2.39	0.52
1:C:625:LEU:CD2	1:C:627:LEU:HD11	2.39	0.52
1:A:95:LEU:CD2	1:A:760:LEU:HD12	2.39	0.52
1:A:265:PHE:CZ	1:A:266:ALA:HB2	2.45	0.52
1:A:566:GLU:OE1	1:A:596:ARG:NH2	2.42	0.52
1:B:589:TYR:O	1:B:590:GLU:C	2.47	0.52
1:B:776:SER:OG	1:B:777:TRP:N	2.42	0.52
1:C:255:MET:HB2	1:C:259:PHE:CZ	2.45	0.52
1:C:810:PRO:O	1:C:812:PHE:N	2.42	0.52
1:D:145:ILE:CD1	1:D:478:THR:CG2	2.87	0.52
1:D:560:ASP:O	1:D:564:ILE:HG12	2.10	0.52
2:E:178:LYS:O	2:E:208:VAL:N	2.42	0.52
3:G:134:LYS:O	3:G:135:CYS:C	2.48	0.52
1:A:810:PRO:O	1:A:813:ALA:HB3	2.10	0.52
1:A:813:ALA:HB1	1:A:825:TYR:CE1	2.44	0.52
1:B:89:LYS:O	1:B:93:ASN:OD1	2.28	0.52
1:B:526:ALA:HB1	1:B:662:PHE:CE1	2.42	0.52
1:B:664:ASP:OD1	1:B:664:ASP:N	2.39	0.52
1:B:705:TYR:CE2	1:B:729:ASN:ND2	2.78	0.52
1:C:407:ASN:OD1	1:C:408:TYR:N	2.43	0.52
2:F:336:ALA:O	2:F:341:GLY:N	2.31	0.52
1:A:239:LYS:CD	1:A:329:TYR:CD2	2.93	0.51
1:A:826:PRO:HB2	1:A:831:ARG:N	2.26	0.51
1:B:738:ALA:O	1:B:741:ASN:N	2.44	0.51
1:C:565:LEU:O	1:C:568:TYR:HB3	2.10	0.51
1:C:834:VAL:HG13	1:C:835:TRP:HD1	1.74	0.51
1:D:83:ASN:HB2	1:D:755:MET:HB3	1.91	0.51
1:D:101:GLU:CG	1:D:762:LYS:HZ1	2.14	0.51
1:D:137:ALA:O	1:D:140:GLU:N	2.42	0.51
1:A:826:PRO:HG2	1:A:831:ARG:HB3	1.92	0.51
1:B:510:LYS:HZ1	1:B:738:ALA:HB2	1.74	0.51
1:C:266:ALA:HB3	1:C:267:PRO:HD3	1.91	0.51
1:D:794:PRO:O	1:D:795:HIS:ND1	2.43	0.51
1:B:511:MET:O	1:B:515:LEU:N	2.43	0.51
1:A:313:ALA:O	1:A:316:SER:N	2.43	0.51
1:A:533:MET:O	1:A:535:ARG:HG3	2.10	0.51
1:B:573:ASP:OD1	1:B:573:ASP:N	2.42	0.51
1:B:814:LYS:O	1:B:816:PHE:N	2.43	0.51
1:D:313:ALA:O	1:D:316:SER:N	2.26	0.51
2:E:342:GLN:O	2:E:351:THR:N	2.43	0.51
2:F:372:GLU:O	2:F:376:LEU:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:THR:O	1:B:276:ILE:HG22	2.10	0.51
1:D:637:TYR:CD1	1:D:646:ASN:CG	2.83	0.51
1:A:133:THR:HG23	1:A:778:CYS:O	2.10	0.51
1:A:151:LYS:O	1:A:167:LYS:NZ	2.38	0.51
1:A:496:VAL:HG23	1:A:497:LYS:H	1.75	0.51
1:A:631:ILE:O	1:A:633:THR:N	2.44	0.51
1:A:773:TYR:OH	1:A:805:VAL:HG21	2.11	0.51
1:B:533:MET:HE1	1:B:658:LEU:HD11	1.92	0.51
1:B:726:GLN:O	1:B:729:ASN:HB2	2.11	0.51
1:B:814:LYS:HE2	1:D:101:GLU:OE1	2.11	0.51
1:D:139:LEU:CD1	1:D:464:MET:SD	2.98	0.51
1:A:526:ALA:O	1:A:529:LYS:HB3	2.11	0.51
1:A:232:THR:O	1:A:232:THR:CG2	2.59	0.51
1:B:342:ILE:HB	1:B:352:ARG:NH1	2.26	0.51
1:C:88:TRP:CH2	1:C:642:PRO:HB3	2.46	0.51
1:A:740:TYR:HD2	1:A:769:PHE:CE2	2.28	0.51
1:C:264:GLN:HG2	1:C:265:PHE:CD1	2.41	0.51
1:C:309:GLU:O	1:C:310:GLN:C	2.49	0.51
1:C:756:ARG:HB3	1:C:761:GLU:HB2	1.93	0.51
1:D:270:ASP:O	1:D:273:THR:HG22	2.11	0.51
1:D:598:LYS:HG3	1:D:599:ASN:N	2.26	0.51
1:A:141:VAL:HG13	1:A:142:ASN:N	2.25	0.51
1:A:143:SER:O	1:A:146:VAL:N	2.44	0.51
1:B:810:PRO:HD2	1:B:831:ARG:NH1	2.14	0.51
1:D:228:THR:C	1:D:230:MET:H	2.09	0.51
1:D:330:ASN:OD1	1:D:330:ASN:N	2.43	0.51
1:D:633:THR:HG23	1:D:634:SER:N	2.26	0.51
1:B:269:LEU:CD1	1:B:303:ARG:HG2	2.41	0.50
1:C:175:GLU:HB2	1:C:178:LEU:HG	1.93	0.50
1:C:262:LEU:HB3	1:C:264:GLN:OE1	2.11	0.50
1:C:479:GLY:O	1:C:482:TYR:N	2.45	0.50
1:D:632:LEU:HD22	1:D:650:SER:HB3	1.92	0.50
1:A:83:ASN:HB2	1:A:755:MET:HG2	1.93	0.50
1:A:296:LYS:O	1:A:299:LYS:N	2.31	0.50
1:B:246:TYR:N	1:B:246:TYR:CD1	2.79	0.50
1:B:278:ASN:OD1	1:B:279:VAL:N	2.45	0.50
1:B:506:THR:O	1:B:509:LYS:HB3	2.10	0.50
1:B:536:ASN:O	1:B:537:TYR:HD1	1.94	0.50
1:B:754:GLU:CD	1:B:754:GLU:H	2.15	0.50
1:C:322:LEU:HD23	1:C:328:GLN:NE2	2.26	0.50
2:E:77:THR:O	2:E:187:ARG:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:O	1:A:192:TYR:N	2.45	0.50
1:C:145:ILE:O	1:C:149:LEU:HD23	2.11	0.50
1:D:246:TYR:OH	1:D:598:LYS:HD2	2.11	0.50
1:B:217:MET:HE2	1:B:230:MET:CE	2.42	0.50
1:C:309:GLU:O	1:C:312:ILE:HG22	2.12	0.50
1:C:497:LYS:NZ	1:C:501:GLU:HB2	2.26	0.50
1:D:770:TRP:O	1:D:773:TYR:N	2.45	0.50
1:A:468:ASP:O	1:A:472:THR:HG23	2.11	0.50
1:B:595:PHE:O	1:B:598:LYS:HB3	2.12	0.50
1:B:804:GLN:O	1:B:807:GLN:N	2.44	0.50
1:D:504:MET:HG3	1:D:530:ILE:HG21	1.94	0.50
1:B:213:LEU:HA	1:B:216:GLU:OE1	2.11	0.50
1:B:628:PRO:O	1:B:631:ILE:HG22	2.12	0.50
1:B:637:TYR:CG	1:B:638:ASP:N	2.80	0.50
1:C:414:LEU:C	1:C:416:GLU:H	2.14	0.50
1:D:113:THR:HG22	1:D:114:CYS:SG	2.51	0.50
1:D:768:ILE:O	1:D:771:ILE:N	2.44	0.50
1:A:350:ASN:OD1	1:A:351:ILE:N	2.45	0.50
1:B:489:ARG:NH2	1:B:544:PHE:CE2	2.80	0.50
1:B:633:THR:O	1:B:637:TYR:N	2.45	0.50
1:D:141:VAL:HG23	1:D:482:TYR:CZ	2.46	0.50
1:A:401:ASN:HB3	1:A:405:PHE:CE2	2.45	0.50
1:C:98:GLY:O	1:C:114:CYS:HA	2.11	0.50
1:C:765:PRO:O	1:C:768:ILE:HB	2.11	0.50
1:D:492:VAL:HG13	1:D:493:VAL:H	1.75	0.50
1:C:226:LEU:HD13	1:C:416:GLU:HG3	1.94	0.50
1:C:589:TYR:HA	1:C:592:ARG:HD2	1.92	0.50
1:C:739:SER:O	1:C:742:ALA:N	2.29	0.50
2:E:75:LYS:HA	2:E:85:PHE:O	2.12	0.50
1:A:775:TYR:O	1:A:776:SER:C	2.49	0.49
1:B:382:ASN:O	1:B:384:ALA:N	2.45	0.49
1:B:622:LEU:HD11	1:B:624:SER:OG	2.12	0.49
1:C:414:LEU:O	1:C:416:GLU:N	2.44	0.49
1:B:121:ILE:HG22	1:B:122:ASP:H	1.76	0.49
1:B:259:PHE:HZ	1:B:263:PRO:HB2	1.77	0.49
1:B:535:ARG:HD2	1:B:537:TYR:OH	2.12	0.49
1:C:260:TYR:HB2	1:C:262:LEU:HB2	1.94	0.49
1:D:475:PRO:O	1:D:610:SER:HA	2.12	0.49
1:D:541:LYS:C	1:D:542:LYS:HE2	2.32	0.49
1:D:632:LEU:CD2	1:D:650:SER:CB	2.90	0.49
1:A:500:THR:O	1:A:504:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLU:H	1:A:521:GLU:CD	2.15	0.49
1:B:132:THR:HB	1:B:779:ALA:HA	1.94	0.49
1:B:162:THR:CG2	1:B:477:GLY:HA2	2.43	0.49
1:C:525:ARG:HD3	1:C:691:LYS:HZ1	1.76	0.49
1:A:196:ARG:HH22	1:A:219:ARG:HE	1.60	0.49
1:A:636:HIS:HA	1:A:649:GLY:HA3	1.94	0.49
1:A:670:ASP:OD1	1:A:670:ASP:N	2.44	0.49
1:A:704:GLN:O	1:A:708:GLN:HG2	2.12	0.49
1:B:473:TYR:CZ	1:B:587:ARG:HG2	2.48	0.49
1:B:812:PHE:O	1:B:815:ASP:N	2.46	0.49
1:C:229:PHE:O	1:C:230:MET:CG	2.58	0.49
2:E:178:LYS:O	2:E:209:GLN:N	2.40	0.49
1:A:114:CYS:O	1:A:117:PHE:N	2.45	0.49
1:A:196:ARG:HH12	1:A:219:ARG:HH21	1.60	0.49
1:A:496:VAL:O	1:A:500:THR:N	2.45	0.49
1:B:228:THR:C	1:B:230:MET:H	2.16	0.49
1:B:401:ASN:C	1:B:404:PRO:HD2	2.32	0.49
1:B:570:ASN:HA	1:B:589:TYR:CZ	2.48	0.49
1:B:796:SER:HG	1:B:797:PRO:HD2	1.68	0.49
1:C:185:SER:O	1:C:185:SER:OG	2.24	0.49
1:C:248:ILE:O	1:C:380:VAL:HG23	2.13	0.49
2:E:399:PRO:O	2:E:401:TRP:N	2.45	0.49
1:B:250:GLN:HG3	1:B:316:SER:OG	2.12	0.49
1:B:401:ASN:HA	1:B:404:PRO:HG2	1.93	0.49
1:B:593:GLU:OE2	1:B:596:ARG:NH2	2.46	0.49
1:C:236:VAL:HA	1:C:244:ASN:HA	1.95	0.49
1:C:478:THR:O	1:C:481:VAL:HB	2.11	0.49
1:C:510:LYS:HZ1	1:C:738:ALA:HA	1.78	0.49
1:C:793:ASN:CG	1:C:795:HIS:CE1	2.85	0.49
1:D:236:VAL:HG22	1:D:237:ASP:O	2.12	0.49
1:D:620:PRO:HB2	1:D:669:PHE:CD2	2.42	0.49
1:A:382:ASN:HB3	1:A:385:TYR:H	1.78	0.49
1:A:495:ASP:O	1:A:499:GLN:N	2.31	0.49
1:A:507:PHE:HD1	1:A:738:ALA:HB2	1.76	0.49
1:A:736:LEU:O	1:A:739:SER:N	2.45	0.49
1:B:521:GLU:HG2	1:B:522:SER:N	2.28	0.49
1:D:232:THR:HG21	1:D:356:TYR:OH	2.13	0.49
1:D:614:VAL:HG23	1:D:631:ILE:HG13	1.94	0.49
1:D:757:LEU:HD12	1:D:757:LEU:C	2.32	0.49
1:D:770:TRP:NE1	1:D:812:PHE:HA	2.27	0.49
2:E:191:GLU:HA	2:E:271:PHE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:MET:HG2	1:A:658:LEU:HD22	1.94	0.49
1:A:527:GLU:OE1	1:A:528:LYS:N	2.45	0.49
1:A:657:GLU:O	1:A:660:HIS:N	2.45	0.49
1:A:704:GLN:HE22	1:A:832:CYS:N	2.10	0.49
1:A:807:GLN:HA	1:A:824:MET:CE	2.42	0.49
1:B:504:MET:HG2	1:B:658:LEU:HD22	1.94	0.49
1:B:540:PRO:HB3	1:B:607:PHE:CD2	2.48	0.49
1:B:831:ARG:O	1:B:833:LYS:N	2.46	0.49
1:C:246:TYR:HB3	1:C:248:ILE:HD11	1.95	0.49
1:C:265:PHE:O	1:C:268:GLU:N	2.45	0.49
2:F:251:ILE:HA	2:F:416:ASP:HA	1.94	0.49
1:A:246:TYR:CZ	1:A:595:PHE:HZ	2.30	0.49
1:A:273:THR:HG22	1:A:277:GLU:OE2	2.13	0.49
1:A:273:THR:C	1:A:277:GLU:OE1	2.51	0.49
1:A:567:ALA:HA	1:A:589:TYR:OH	2.12	0.49
1:A:659:VAL:O	1:A:662:PHE:N	2.36	0.49
1:B:660:HIS:HA	1:B:663:ASP:CG	2.33	0.49
1:C:216:GLU:O	1:C:218:GLY:N	2.46	0.49
1:C:475:PRO:HG2	1:C:476:TYR:CD2	2.47	0.49
1:D:333:GLU:OE1	1:D:333:GLU:N	2.42	0.49
1:D:789:ARG:HA	1:D:792:THR:HG22	1.94	0.49
1:A:471:THR:HG22	1:A:478:THR:HG21	1.95	0.49
1:A:652:THR:O	1:A:655:GLY:N	2.46	0.49
1:B:172:SER:O	1:B:174:VAL:N	2.46	0.49
1:B:561:TYR:C	1:B:564:ILE:HG22	2.31	0.49
1:B:647:PHE:HA	1:B:651:GLY:HA3	1.95	0.49
1:C:143:SER:O	1:C:146:VAL:HG12	2.13	0.49
1:C:277:GLU:HG3	1:C:299:LYS:HZ2	1.78	0.49
1:C:528:LYS:O	1:C:531:ASN:N	2.46	0.49
1:D:408:TYR:O	1:D:411:VAL:HB	2.13	0.49
1:A:239:LYS:HD3	1:A:329:TYR:CZ	2.37	0.48
1:B:142:ASN:O	1:B:145:ILE:N	2.46	0.48
1:B:579:TYR:HA	1:B:582:LEU:HB2	1.94	0.48
1:B:693:GLY:O	1:B:697:MET:HG2	2.13	0.48
1:B:756:ARG:HD2	1:B:761:GLU:O	2.13	0.48
1:C:483:VAL:CG1	1:C:489:ARG:HH11	2.26	0.48
1:A:392:LEU:C	1:A:393:PHE:HD1	2.16	0.48
1:A:499:GLN:HG2	1:A:647:PHE:HE1	1.77	0.48
1:A:614:VAL:HA	1:A:631:ILE:CG2	2.43	0.48
1:A:649:GLY:O	1:A:652:THR:N	2.46	0.48
1:A:814:LYS:O	1:A:816:PHE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:PHE:O	1:B:338:SER:OG	2.31	0.48
1:B:506:THR:HG21	1:B:742:ALA:HB2	1.94	0.48
1:B:530:ILE:HG12	1:B:662:PHE:HZ	1.79	0.48
1:C:517:TRP:CD1	1:C:518:MET:N	2.81	0.48
2:F:92:GLY:N	2:F:225:LEU:O	2.29	0.48
1:A:187:ASN:OD1	1:A:188:GLU:HG3	2.13	0.48
1:A:529:LYS:O	1:A:532:GLU:HB3	2.14	0.48
1:A:745:GLU:O	1:A:749:MET:HG2	2.13	0.48
1:B:173:CYS:HA	1:B:579:TYR:CE2	2.48	0.48
1:B:234:VAL:HG23	1:B:234:VAL:O	2.12	0.48
1:C:91:ALA:HB2	1:C:641:PHE:CD2	2.48	0.48
1:C:162:THR:HA	1:C:165:ILE:CD1	2.44	0.48
1:C:162:THR:HA	1:C:165:ILE:HD12	1.95	0.48
1:C:811:SER:O	1:C:814:LYS:N	2.47	0.48
1:D:734:GLY:O	1:D:735:GLY:C	2.51	0.48
1:A:100:ASP:O	1:A:112:PHE:HD1	1.96	0.48
1:A:174:VAL:O	1:A:174:VAL:HG12	2.12	0.48
1:A:632:LEU:O	1:A:637:TYR:HD2	1.96	0.48
1:B:146:VAL:HA	1:B:149:LEU:HG	1.94	0.48
1:B:268:GLU:O	1:B:272:ARG:HB2	2.14	0.48
1:B:308:ILE:O	1:B:309:GLU:C	2.52	0.48
1:B:529:LYS:NZ	1:B:669:PHE:O	2.46	0.48
1:B:569:ASN:O	1:B:589:TYR:OH	2.29	0.48
1:D:270:ASP:OD1	1:D:271:ALA:N	2.46	0.48
2:E:317:ILE:O	2:E:403:LEU:N	2.39	0.48
1:A:146:VAL:HG22	1:A:467:VAL:HG21	1.96	0.48
1:A:670:ASP:O	1:A:673:GLY:N	2.46	0.48
1:B:161:GLN:O	1:B:164:ARG:N	2.47	0.48
1:C:579:TYR:O	1:C:582:LEU:N	2.45	0.48
1:D:628:PRO:O	1:D:631:ILE:HG22	2.13	0.48
1:D:631:ILE:O	1:D:633:THR:N	2.47	0.48
2:E:345:GLU:N	2:E:348:GLU:HA	2.28	0.48
1:B:187:ASN:OD1	1:B:188:GLU:N	2.47	0.48
1:B:234:VAL:HG12	1:B:246:TYR:HA	1.94	0.48
1:C:483:VAL:HG13	1:C:489:ARG:HH11	1.79	0.48
1:C:537:TYR:O	1:C:539:TRP:N	2.45	0.48
1:D:122:ASP:O	1:D:780:LYS:NZ	2.43	0.48
1:D:560:ASP:N	1:D:560:ASP:OD1	2.45	0.48
1:D:632:LEU:CD2	1:D:650:SER:HB3	2.44	0.48
2:F:359:THR:HA	2:F:371:ILE:O	2.14	0.48
1:A:134:PHE:CE1	1:A:636:HIS:CE1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLN:OE1	1:A:399:GLN:N	2.46	0.48
1:A:489:ARG:O	1:A:493:VAL:HG22	2.14	0.48
1:A:490:ASP:OD1	1:A:491:GLN:N	2.45	0.48
1:B:222:GLN:HA	1:B:591:ASN:HD21	1.77	0.48
1:B:653:VAL:HA	1:B:656:HIS:HB3	1.94	0.48
1:C:239:LYS:HB2	1:C:329:TYR:OH	2.13	0.48
1:C:246:TYR:HD2	1:C:378:VAL:HG12	1.78	0.48
1:C:761:GLU:O	1:C:763:PHE:N	2.47	0.48
1:D:88:TRP:CD2	1:D:642:PRO:HG3	2.47	0.48
1:D:756:ARG:HB2	1:D:756:ARG:HH11	1.79	0.48
1:B:259:PHE:HE2	1:B:265:PHE:HB3	1.79	0.48
1:B:373:VAL:HG12	1:B:376:GLY:HA3	1.95	0.48
1:C:636:HIS:O	1:C:638:ASP:N	2.41	0.48
1:D:101:GLU:OE2	1:D:762:LYS:HE2	2.13	0.48
1:D:480:TYR:HB2	1:D:543:LEU:CD2	2.39	0.48
2:E:77:THR:HA	2:E:83:GLN:O	2.14	0.48
1:A:382:ASN:O	1:A:383:PRO:C	2.52	0.48
1:A:807:GLN:CA	1:A:824:MET:CE	2.91	0.48
1:C:161:GLN:O	1:C:165:ILE:HG13	2.14	0.48
1:C:515:LEU:HD21	1:C:523:TYR:CD2	2.49	0.48
1:C:541:LYS:O	1:C:542:LYS:HD3	2.14	0.48
2:E:167:TYR:O	2:E:169:GLU:N	2.41	0.48
2:F:94:ALA:CB	2:F:231:ALA:HA	2.44	0.48
1:A:242:SER:HA	1:A:602:ALA:HB3	1.96	0.48
1:A:313:ALA:O	1:A:315:ALA:N	2.47	0.48
1:A:620:PRO:HG2	1:A:669:PHE:CE2	2.49	0.48
1:B:467:VAL:O	1:B:471:THR:OG1	2.30	0.48
1:B:781:GLU:O	1:B:783:GLN:NE2	2.47	0.48
1:C:108:ASP:HB2	1:C:110:TYR:HE2	1.70	0.48
1:C:357:ILE:O	1:C:360:LEU:N	2.47	0.48
1:C:572:THR:HG21	1:C:582:LEU:HD22	1.95	0.48
1:D:324:ASN:OD1	1:D:326:GLU:N	2.47	0.48
1:A:161:GLN:O	1:A:164:ARG:HB3	2.13	0.47
1:A:537:TYR:N	1:A:537:TYR:CD1	2.82	0.47
1:C:412:HIS:O	1:C:415:PHE:N	2.47	0.47
1:C:562:TYR:O	1:C:565:LEU:N	2.41	0.47
1:C:646:ASN:OD1	1:C:647:PHE:N	2.47	0.47
1:C:793:ASN:HB3	1:C:795:HIS:ND1	2.28	0.47
1:D:414:LEU:O	1:D:416:GLU:N	2.47	0.47
2:E:416:ASP:O	2:E:420:ASN:N	2.46	0.47
1:A:237:ASP:CG	1:A:245:SER:HB2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:GLN:HA	1:A:729:ASN:HB2	1.95	0.47
1:B:324:ASN:O	1:B:327:GLN:HG2	2.14	0.47
1:B:583:ASN:O	1:B:586:ARG:N	2.46	0.47
1:C:163:GLU:O	1:C:166:THR:OG1	2.29	0.47
1:C:177:THR:O	1:C:180:ASP:N	2.43	0.47
1:C:197:PHE:HB3	1:C:216:GLU:HG3	1.94	0.47
1:C:317:TRP:CD2	1:C:382:ASN:OD1	2.67	0.47
1:C:473:TYR:O	1:C:475:PRO:HD3	2.15	0.47
1:D:637:TYR:OH	1:D:639:LEU:HA	2.14	0.47
1:B:757:LEU:HD11	1:B:768:ILE:HD13	1.94	0.47
1:C:96:LEU:HD13	1:C:760:LEU:HD23	1.95	0.47
1:C:246:TYR:HB2	1:C:378:VAL:HG12	1.95	0.47
1:C:261:VAL:HG11	1:D:323:ARG:HB3	1.94	0.47
1:C:775:TYR:O	1:C:777:TRP:N	2.46	0.47
1:D:298:ILE:HG13	1:D:299:LYS:N	2.30	0.47
1:D:331:PRO:HB2	1:D:377:ASP:OD1	2.14	0.47
1:D:641:PHE:N	1:D:641:PHE:CD1	2.81	0.47
1:D:709:CYS:SG	1:D:720:ALA:HB1	2.54	0.47
1:D:732:ASP:O	1:D:733:LEU:C	2.50	0.47
1:A:668:GLN:C	1:A:669:PHE:HD1	2.18	0.47
1:B:270:ASP:C	1:B:272:ARG:N	2.68	0.47
1:B:490:ASP:N	1:B:490:ASP:OD1	2.45	0.47
1:B:511:MET:HG3	1:B:513:SER:N	2.29	0.47
1:C:193:ILE:O	1:C:196:ARG:HB3	2.14	0.47
1:C:482:TYR:OH	1:C:486:ARG:NH2	2.47	0.47
1:C:733:LEU:HD12	1:C:733:LEU:O	2.15	0.47
1:C:764:THR:H	1:C:767:GLN:NE2	2.12	0.47
1:D:480:TYR:CB	1:D:543:LEU:HD21	2.41	0.47
1:A:146:VAL:HA	1:A:149:LEU:HD12	1.95	0.47
1:B:631:ILE:HD11	1:B:636:HIS:CD2	2.50	0.47
1:C:171:GLN:O	1:C:175:GLU:HG2	2.14	0.47
1:C:199:GLY:O	1:C:200:ILE:HG23	2.14	0.47
1:D:675:LEU:HD12	1:D:675:LEU:C	2.35	0.47
1:D:700:CYS:O	1:D:703:THR:OG1	2.33	0.47
1:D:756:ARG:HB2	1:D:756:ARG:NH1	2.29	0.47
1:A:256:PRO:HG3	1:A:792:THR:HB	1.95	0.47
1:A:562:TYR:N	1:A:562:TYR:CD1	2.79	0.47
1:B:341:LYS:CE	1:B:353:PHE:CE2	2.95	0.47
1:B:617:TRP:CD1	1:B:626:THR:OG1	2.68	0.47
1:B:747:ILE:HG13	1:B:748:LYS:N	2.29	0.47
1:D:704:GLN:HG2	1:D:831:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:379:GLU:O	2:F:383:ASP:HA	2.14	0.47
1:A:272:ARG:O	1:A:276:ILE:HG12	2.15	0.47
1:A:307:GLN:O	1:A:311:LYS:HD3	2.14	0.47
1:A:320:ASP:OD2	1:B:262:LEU:HD21	2.14	0.47
1:A:539:TRP:CD1	1:A:543:LEU:HD12	2.50	0.47
1:A:748:LYS:HB3	1:A:749:MET:HE1	1.96	0.47
1:B:172:SER:OG	1:B:173:CYS:N	2.48	0.47
1:B:488:ASP:OD1	1:B:488:ASP:N	2.46	0.47
1:B:569:ASN:HB3	1:B:589:TYR:OH	2.15	0.47
1:B:813:ALA:HB1	1:B:820:LEU:HD21	1.96	0.47
1:C:161:GLN:O	1:C:164:ARG:N	2.47	0.47
1:C:525:ARG:HH12	1:C:689:LYS:HZ1	1.62	0.47
1:C:770:TRP:HA	1:C:770:TRP:CE3	2.49	0.47
1:D:562:TYR:O	1:D:565:LEU:N	2.47	0.47
1:D:697:MET:O	1:D:700:CYS:HB3	2.14	0.47
1:D:752:ALA:C	1:D:754:GLU:H	2.17	0.47
1:A:745:GLU:O	1:A:749:MET:HE2	2.14	0.47
1:B:239:LYS:HE3	1:B:329:TYR:CE2	2.50	0.47
1:B:759:GLY:C	1:B:760:LEU:HG	2.34	0.47
1:D:218:GLY:O	1:D:219:ARG:C	2.53	0.47
1:D:637:TYR:CD1	1:D:646:ASN:OD1	2.67	0.47
1:A:478:THR:O	1:A:481:VAL:HB	2.15	0.47
1:A:498:GLN:O	1:A:502:LEU:HD23	2.15	0.47
1:A:503:ILE:O	1:A:504:MET:C	2.53	0.47
1:A:539:TRP:HA	1:A:607:PHE:CZ	2.50	0.47
1:B:759:GLY:O	1:B:760:LEU:HD23	2.15	0.47
1:D:725:THR:HG21	1:D:795:HIS:O	2.14	0.47
1:B:226:LEU:HD23	1:B:226:LEU:C	2.36	0.47
1:B:243:ARG:O	1:B:602:ALA:HB2	2.15	0.47
1:B:388:PHE:CE1	1:B:405:PHE:HZ	2.33	0.47
1:B:529:LYS:HG3	1:B:671:TYR:HA	1.97	0.47
1:B:604:ARG:NH2	1:B:672:ASP:HA	2.28	0.47
1:B:659:VAL:HG11	1:B:731:ALA:HA	1.97	0.47
1:B:810:PRO:CD	1:B:831:ARG:HD2	2.45	0.47
1:D:524:ARG:O	1:D:527:GLU:HB3	2.14	0.47
1:D:707:ALA:O	1:D:708:GLN:OE1	2.33	0.47
2:E:161:LYS:CB	2:E:183:ASN:H	2.28	0.47
1:A:234:VAL:CG2	1:A:235:ASN:H	2.25	0.46
1:A:352:ARG:HD2	1:A:393:PHE:CB	2.46	0.46
1:A:799:SER:O	1:A:800:CYS:C	2.54	0.46
1:B:329:TYR:O	1:B:330:ASN:OD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:HD22	1:B:520:GLY:HA2	1.97	0.46
1:B:540:PRO:HD2	1:B:543:LEU:HB2	1.98	0.46
1:C:108:ASP:OD1	1:C:108:ASP:O	2.32	0.46
1:C:322:LEU:O	1:C:323:ARG:HD3	2.14	0.46
1:D:393:PHE:HD1	1:D:405:PHE:CE2	2.30	0.46
1:D:540:PRO:HD3	1:D:607:PHE:CZ	2.49	0.46
1:D:745:GLU:O	1:D:748:LYS:N	2.49	0.46
1:D:808:ASP:HA	1:D:831:ARG:CG	2.45	0.46
1:A:88:TRP:CE2	1:A:642:PRO:HD3	2.51	0.46
1:A:787:VAL:O	1:A:790:LEU:HB3	2.14	0.46
1:B:294:TYR:N	1:B:294:TYR:CD1	2.79	0.46
1:B:405:PHE:O	1:B:408:TYR:N	2.48	0.46
1:B:759:GLY:O	1:B:760:LEU:CD2	2.63	0.46
1:B:809:ILE:HA	1:B:831:ARG:NH1	2.29	0.46
1:C:196:ARG:HG2	1:C:197:PHE:CE1	2.50	0.46
1:C:495:ASP:HA	1:C:498:GLN:OE1	2.14	0.46
1:C:696:ASP:O	1:C:699:GLN:HB3	2.15	0.46
1:A:796:SER:HB3	1:A:797:PRO:HD2	1.97	0.46
1:B:162:THR:HG21	1:B:477:GLY:HA2	1.98	0.46
1:C:487:GLU:HA	1:C:489:ARG:HG3	1.98	0.46
1:C:520:GLY:O	1:C:523:TYR:N	2.49	0.46
1:C:588:GLY:HA3	1:C:592:ARG:NH2	2.30	0.46
2:E:327:VAL:HA	2:E:401:TRP:HA	1.96	0.46
1:A:116:LYS:O	1:A:119:GLU:N	2.48	0.46
1:C:329:TYR:CD1	1:C:331:PRO:HD3	2.51	0.46
1:C:782:THR:OG1	1:C:783:GLN:N	2.49	0.46
1:A:572:THR:HG22	1:A:573:ASP:N	2.30	0.46
1:B:217:MET:O	1:B:220:ILE:HG22	2.15	0.46
1:B:231:TYR:CD2	1:B:233:TRP:CZ3	3.02	0.46
1:B:626:THR:O	1:B:627:LEU:HD23	2.16	0.46
1:C:172:SER:OG	1:C:173:CYS:N	2.48	0.46
1:C:218:GLY:O	1:C:221:GLU:HG2	2.16	0.46
1:C:515:LEU:HD23	1:C:518:MET:CG	2.44	0.46
1:C:739:SER:O	1:C:740:TYR:C	2.52	0.46
1:A:825:TYR:C	1:A:827:PRO:HD2	2.36	0.46
1:B:543:LEU:HD12	1:B:563:SER:HB3	1.98	0.46
1:B:595:PHE:O	1:B:598:LYS:N	2.39	0.46
1:C:268:GLU:O	1:C:271:ALA:HB3	2.15	0.46
1:C:570:ASN:O	1:C:571:LYS:HB2	2.15	0.46
1:D:508:LEU:HD11	1:D:527:GLU:HG3	1.97	0.46
1:A:332:TYR:O	1:A:378:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LYS:O	1:B:93:ASN:CG	2.54	0.46
1:B:482:TYR:C	1:B:485:SER:HG	2.18	0.46
1:C:353:PHE:O	1:C:356:TYR:HB3	2.15	0.46
1:C:766:ASN:O	1:C:769:PHE:HB3	2.16	0.46
1:C:823:LYS:O	1:C:824:MET:CG	2.53	0.46
1:D:149:LEU:HD11	1:D:167:LYS:HA	1.98	0.46
1:D:408:TYR:CE1	1:D:412:HIS:CD2	3.04	0.46
1:A:504:MET:HE2	1:A:504:MET:HB2	1.63	0.46
1:B:172:SER:HB2	1:B:579:TYR:HD2	1.81	0.46
1:B:259:PHE:CZ	1:B:263:PRO:HB2	2.51	0.46
1:C:500:THR:O	1:C:504:MET:HG2	2.15	0.46
1:D:118:ILE:HG23	1:D:780:LYS:HG3	1.97	0.46
1:D:261:VAL:HB	1:D:314:MET:CE	2.46	0.46
1:D:276:ILE:HG23	1:D:277:GLU:N	2.30	0.46
1:D:393:PHE:HE1	1:D:405:PHE:CD2	2.34	0.46
1:D:467:VAL:O	1:D:470:ILE:HB	2.16	0.46
1:D:582:LEU:O	1:D:583:ASN:C	2.55	0.46
1:D:739:SER:O	1:D:742:ALA:HB3	2.16	0.46
2:F:75:LYS:HA	2:F:86:HIS:HA	1.98	0.46
1:A:191:GLN:O	1:A:194:SER:OG	2.31	0.46
1:B:528:LYS:O	1:B:531:ASN:N	2.49	0.46
1:C:246:TYR:CD2	1:C:378:VAL:HG12	2.51	0.46
1:C:303:ARG:O	1:C:307:GLN:HB2	2.15	0.46
1:C:334:LEU:C	1:C:337:PRO:HD2	2.36	0.46
1:C:659:VAL:O	1:C:661:GLY:N	2.49	0.46
1:D:480:TYR:CD1	1:D:480:TYR:C	2.89	0.46
1:A:309:GLU:HA	1:A:312:ILE:HD12	1.97	0.46
1:A:352:ARG:HD2	1:A:393:PHE:HB2	1.98	0.46
1:A:413:MET:O	1:A:416:GLU:CG	2.64	0.46
1:A:533:MET:CG	1:A:623:ASN:HD21	2.28	0.46
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.72	0.46
1:B:539:TRP:HD1	1:B:540:PRO:O	1.97	0.46
1:C:306:THR:O	1:C:309:GLU:HB2	2.16	0.46
1:C:522:SER:O	1:C:525:ARG:HB3	2.16	0.46
1:C:786:LEU:HD12	1:C:786:LEU:HA	1.70	0.46
1:D:507:PHE:HD1	1:D:510:LYS:NZ	2.13	0.46
2:E:326:GLY:O	2:E:402:ILE:N	2.49	0.46
2:E:337:ASP:O	2:E:340:GLY:N	2.39	0.46
1:A:488:ASP:HB3	1:A:491:GLN:OE1	2.16	0.45
1:B:217:MET:C	1:B:217:MET:SD	2.94	0.45
1:B:239:LYS:HD3	1:B:675:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LYS:O	1:B:302:ALA:N	2.49	0.45
1:B:561:TYR:CA	1:B:564:ILE:HG22	2.45	0.45
1:B:729:ASN:O	1:B:732:ASP:HB2	2.16	0.45
1:C:150:GLU:OE1	1:C:150:GLU:N	2.40	0.45
1:C:234:VAL:HG23	1:C:245:SER:O	2.15	0.45
1:C:739:SER:OG	1:C:740:TYR:N	2.48	0.45
1:D:300:THR:OG1	1:D:301:ALA:N	2.49	0.45
1:D:631:ILE:HG23	1:D:632:LEU:HG	1.98	0.45
1:D:631:ILE:CG2	1:D:632:LEU:N	2.79	0.45
2:E:186:VAL:O	2:E:198:VAL:HA	2.16	0.45
1:A:98:GLY:CA	1:A:116:LYS:CB	2.81	0.45
1:A:657:GLU:O	1:A:658:LEU:C	2.55	0.45
1:A:661:GLY:O	1:A:662:PHE:HD1	1.98	0.45
1:A:721:ASN:ND2	1:A:724:HIS:HB3	2.31	0.45
1:B:303:ARG:O	1:B:306:THR:HB	2.16	0.45
1:B:523:TYR:O	1:B:524:ARG:C	2.54	0.45
1:C:758:PRO:O	1:C:760:LEU:N	2.48	0.45
1:D:503:ILE:HD11	1:D:651:GLY:HA2	1.98	0.45
2:F:287:TYR:HA	2:F:423:GLY:HA2	1.98	0.45
1:A:504:MET:HE1	1:A:535:ARG:HH12	1.81	0.45
1:A:786:LEU:C	1:A:786:LEU:HD23	2.36	0.45
1:B:386:MET:HG3	1:B:386:MET:O	2.14	0.45
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.65	0.45
1:C:705:TYR:CZ	1:C:729:ASN:ND2	2.85	0.45
1:D:273:THR:O	1:D:276:ILE:HG22	2.16	0.45
1:D:614:VAL:HG23	1:D:631:ILE:CG1	2.46	0.45
1:A:320:ASP:OD2	1:A:723:ALA:HB3	2.17	0.45
1:A:320:ASP:OD2	1:B:262:LEU:CD2	2.65	0.45
1:A:486:ARG:HH12	1:A:633:THR:HB	1.80	0.45
1:A:535:ARG:HB3	1:A:537:TYR:CE1	2.51	0.45
1:A:539:TRP:HB2	1:A:540:PRO:HD2	1.97	0.45
1:A:762:LYS:HD3	1:C:817:GLN:N	2.31	0.45
1:B:214:TYR:O	1:B:215:ARG:C	2.52	0.45
1:B:229:PHE:O	1:B:230:MET:HB3	2.16	0.45
1:B:659:VAL:HG12	1:B:663:ASP:OD1	2.16	0.45
1:B:805:VAL:O	1:B:805:VAL:CG1	2.63	0.45
1:C:167:LYS:HG3	1:C:168:ALA:N	2.31	0.45
1:C:234:VAL:HG23	1:C:245:SER:C	2.37	0.45
1:C:583:ASN:HD21	1:C:587:ARG:NH2	2.13	0.45
1:C:722:GLY:O	1:C:725:THR:HG23	2.16	0.45
1:A:766:ASN:O	1:A:767:GLN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:PHE:CE1	1:A:816:PHE:HD2	2.34	0.45
1:B:142:ASN:O	1:B:145:ILE:CG2	2.53	0.45
1:B:511:MET:HG2	1:B:513:SER:OG	2.17	0.45
1:C:216:GLU:O	1:C:219:ARG:HG3	2.16	0.45
1:C:614:VAL:O	1:C:614:VAL:CG1	2.61	0.45
1:D:480:TYR:HB2	1:D:543:LEU:CD1	2.43	0.45
1:A:540:PRO:HD3	1:A:607:PHE:CE2	2.51	0.45
1:A:560:ASP:OD1	1:A:561:TYR:N	2.49	0.45
1:B:259:PHE:O	1:B:259:PHE:CD2	2.70	0.45
1:B:419:GLU:O	1:B:426:LEU:HD11	2.17	0.45
1:B:832:CYS:O	1:B:834:VAL:N	2.49	0.45
1:C:106:CYS:HA	1:C:824:MET:HG3	1.99	0.45
1:C:511:MET:HA	1:C:514:THR:HG22	1.99	0.45
1:C:521:GLU:OE1	1:C:521:GLU:N	2.38	0.45
1:D:269:LEU:HD12	1:D:270:ASP:N	2.32	0.45
1:D:461:ASP:OD1	1:D:462:ALA:N	2.50	0.45
1:D:698:ALA:O	1:D:699:GLN:C	2.55	0.45
1:D:816:PHE:HB3	1:D:818:CYS:SG	2.57	0.45
1:A:253:LEU:CD1	1:A:253:LEU:C	2.80	0.45
1:A:319:ASP:HA	1:A:322:LEU:HD12	1.98	0.45
1:C:85:SER:C	1:C:89:LYS:HZ2	2.16	0.45
1:C:504:MET:SD	1:C:535:ARG:NH2	2.89	0.45
1:C:533:MET:HA	1:C:623:ASN:OD1	2.17	0.45
1:C:810:PRO:O	1:C:811:SER:C	2.55	0.45
1:D:760:LEU:HD11	1:D:763:PHE:CD2	2.38	0.45
1:B:221:GLU:O	1:B:225:ALA:N	2.36	0.45
1:B:231:TYR:CD2	1:B:233:TRP:CE3	3.05	0.45
1:B:652:THR:O	1:B:655:GLY:N	2.50	0.45
1:B:740:TYR:HA	1:B:769:PHE:HE2	1.82	0.45
1:C:166:THR:O	1:C:169:ALA:N	2.50	0.45
1:C:518:MET:HB2	1:C:522:SER:OG	2.16	0.45
1:C:666:GLY:C	1:C:668:GLN:H	2.20	0.45
1:C:821:GLY:O	1:C:822:GLN:CG	2.59	0.45
1:D:171:GLN:O	1:D:174:VAL:HG22	2.17	0.45
1:D:523:TYR:O	1:D:527:GLU:HB2	2.17	0.45
1:D:632:LEU:HD21	1:D:650:SER:HB2	1.98	0.45
1:B:636:HIS:O	1:B:649:GLY:HA3	2.17	0.45
1:B:732:ASP:CB	1:B:805:VAL:HG21	2.46	0.45
1:C:806:LEU:HA	1:C:806:LEU:HD23	1.69	0.45
1:A:762:LYS:O	1:A:763:PHE:CG	2.70	0.45
1:C:473:TYR:HA	1:C:590:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:ASN:ND2	1:C:589:TYR:CE1	2.85	0.45
1:D:670:ASP:O	1:D:672:ASP:N	2.50	0.45
1:D:768:ILE:O	1:D:769:PHE:C	2.55	0.45
1:B:317:TRP:CE3	1:B:382:ASN:ND2	2.86	0.44
1:B:598:LYS:HG3	1:B:599:ASN:N	2.31	0.44
1:B:669:PHE:HE1	1:B:675:LEU:HD21	1.81	0.44
1:B:824:MET:O	1:B:824:MET:HG2	2.17	0.44
1:C:230:MET:HE3	1:C:248:ILE:HG21	1.98	0.44
1:C:618:TYR:HE1	1:C:623:ASN:HA	1.82	0.44
1:C:627:LEU:HB3	1:C:628:PRO:HD2	1.99	0.44
1:D:480:TYR:HD2	1:D:543:LEU:CG	2.27	0.44
1:D:650:SER:O	1:D:651:GLY:C	2.56	0.44
2:F:342:GLN:O	2:F:351:THR:N	2.42	0.44
1:A:657:GLU:O	1:A:660:HIS:HB3	2.17	0.44
1:C:267:PRO:HG3	1:D:695:LYS:HE2	1.99	0.44
1:C:489:ARG:O	1:C:493:VAL:HG23	2.17	0.44
1:C:544:PHE:CG	1:C:545:GLY:N	2.85	0.44
1:C:770:TRP:CZ2	1:C:812:PHE:HB2	2.52	0.44
1:D:269:LEU:HD12	1:D:269:LEU:C	2.37	0.44
1:A:109:PHE:O	1:A:110:TYR:C	2.54	0.44
1:A:238:HIS:NE2	1:A:621:GLU:HG3	2.31	0.44
1:A:487:GLU:HB3	1:A:489:ARG:HH12	1.83	0.44
1:B:224:ARG:HA	1:B:224:ARG:HD3	1.71	0.44
1:B:268:GLU:O	1:B:272:ARG:CB	2.66	0.44
1:B:618:TYR:O	1:B:620:PRO:HD3	2.18	0.44
1:B:810:PRO:O	1:B:813:ALA:N	2.51	0.44
1:C:524:ARG:HA	1:C:527:GLU:HB3	1.99	0.44
1:C:618:TYR:HA	1:C:624:SER:O	2.17	0.44
1:C:746:TYR:CG	1:C:746:TYR:O	2.70	0.44
1:A:145:ILE:HD11	1:A:482:TYR:HB2	1.99	0.44
1:A:228:THR:O	1:A:229:PHE:HB2	2.18	0.44
1:A:273:THR:CG2	1:A:277:GLU:OE2	2.66	0.44
1:A:308:ILE:O	1:A:312:ILE:HG13	2.18	0.44
1:A:561:TYR:O	1:A:564:ILE:HG13	2.09	0.44
1:A:779:ALA:HB3	1:A:798:ASN:OD1	2.16	0.44
1:A:795:HIS:HD2	1:A:801:ARG:NH1	2.16	0.44
1:B:236:VAL:HG12	1:B:237:ASP:O	2.18	0.44
1:B:308:ILE:CG2	1:B:309:GLU:N	2.80	0.44
1:B:512:LEU:CD2	1:B:520:GLY:HA2	2.48	0.44
1:B:695:LYS:HD2	1:B:695:LYS:HA	1.64	0.44
1:C:260:TYR:CE1	1:C:314:MET:SD	3.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:CYS:SG	1:C:786:LEU:HD21	2.57	0.44
1:D:306:THR:O	1:D:309:GLU:HB2	2.18	0.44
1:D:504:MET:CG	1:D:530:ILE:CG2	2.95	0.44
1:D:665:GLU:O	1:D:668:GLN:N	2.43	0.44
1:A:704:GLN:HE22	1:A:832:CYS:H	1.66	0.44
1:B:670:ASP:CG	1:B:672:ASP:H	2.20	0.44
1:C:378:VAL:O	1:C:379:ILE:HG13	2.17	0.44
1:C:408:TYR:O	1:C:411:VAL:N	2.51	0.44
1:C:740:TYR:O	1:C:743:TYR:N	2.50	0.44
1:D:222:GLN:OE1	1:D:360:LEU:HA	2.17	0.44
1:D:705:TYR:OH	1:D:800:CYS:SG	2.45	0.44
1:D:763:PHE:HB3	1:D:767:GLN:HB2	1.99	0.44
1:A:137:ALA:O	1:A:140:GLU:N	2.51	0.44
1:C:260:TYR:CD2	1:C:262:LEU:HD12	2.53	0.44
1:A:173:CYS:O	1:A:175:GLU:N	2.51	0.44
1:B:221:GLU:OE2	1:B:226:LEU:N	2.51	0.44
1:B:533:MET:CE	1:B:658:LEU:CD1	2.95	0.44
1:C:302:ALA:O	1:C:306:THR:HG23	2.18	0.44
1:C:503:ILE:O	1:C:506:THR:OG1	2.23	0.44
1:C:803:ASN:O	1:C:805:VAL:N	2.51	0.44
1:C:806:LEU:O	1:C:807:GLN:C	2.56	0.44
1:D:222:GLN:HG3	1:D:359:GLY:O	2.18	0.44
1:A:166:THR:O	1:A:167:LYS:C	2.55	0.44
1:A:705:TYR:O	1:A:707:ALA:N	2.51	0.44
1:A:729:ASN:O	1:A:730:ILE:C	2.56	0.44
1:D:559:ASP:CG	1:D:560:ASP:H	2.20	0.44
1:D:580:THR:HB	1:D:583:ASN:OD1	2.18	0.44
1:D:675:LEU:CD1	1:D:676:ALA:N	2.81	0.44
1:D:770:TRP:CD1	1:D:812:PHE:HD1	2.36	0.44
1:A:265:PHE:CG	1:A:266:ALA:N	2.86	0.43
1:B:142:ASN:ND2	1:B:464:MET:SD	2.91	0.43
1:B:657:GLU:O	1:B:658:LEU:C	2.55	0.43
1:B:691:LYS:O	1:B:692:ASN:C	2.56	0.43
1:B:764:THR:HG1	1:B:767:GLN:H	1.58	0.43
1:D:246:TYR:HH	1:D:595:PHE:HE1	1.55	0.43
1:D:747:ILE:HD12	1:D:747:ILE:HA	1.83	0.43
2:F:416:ASP:O	2:F:420:ASN:CA	2.66	0.43
1:A:188:GLU:O	1:A:191:GLN:HB3	2.18	0.43
1:A:413:MET:O	1:A:416:GLU:HG2	2.17	0.43
1:A:606:ASN:CG	1:A:607:PHE:N	2.71	0.43
1:A:723:ALA:O	1:A:725:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:GLN:O	1:B:806:LEU:N	2.51	0.43
1:C:514:THR:HG23	1:C:518:MET:HE1	2.00	0.43
1:C:767:GLN:O	1:C:770:TRP:HB2	2.18	0.43
1:C:821:GLY:C	1:C:822:GLN:HG3	2.38	0.43
1:D:296:LYS:HE3	1:D:296:LYS:HB3	1.81	0.43
1:D:326:GLU:OE2	1:D:668:GLN:NE2	2.50	0.43
1:D:331:PRO:O	1:D:332:TYR:HD1	2.02	0.43
1:D:530:ILE:HA	1:D:533:MET:CG	2.48	0.43
1:D:618:TYR:HD1	1:D:624:SER:O	2.00	0.43
1:D:637:TYR:CB	1:D:646:ASN:OD1	2.66	0.43
1:A:494:GLU:O	1:A:497:LYS:N	2.51	0.43
1:A:496:VAL:HG11	1:A:632:LEU:HD21	1.99	0.43
1:A:663:ASP:N	1:A:663:ASP:OD1	2.49	0.43
1:C:317:TRP:CZ2	1:D:314:MET:SD	3.11	0.43
1:C:736:LEU:HD21	1:C:770:TRP:CZ3	2.51	0.43
1:A:264:GLN:HE22	1:A:314:MET:HE1	1.78	0.43
1:A:464:MET:O	1:A:465:LYS:C	2.57	0.43
1:A:521:GLU:HA	1:A:524:ARG:NH1	2.33	0.43
1:A:825:TYR:HA	1:A:826:PRO:HD3	1.84	0.43
1:B:310:GLN:C	1:B:312:ILE:N	2.72	0.43
1:B:822:GLN:O	1:B:824:MET:N	2.51	0.43
1:B:831:ARG:HE	1:B:833:LYS:HB2	1.83	0.43
1:C:185:SER:HA	1:C:187:ASN:ND2	2.34	0.43
1:C:267:PRO:O	1:C:270:ASP:N	2.40	0.43
1:C:497:LYS:HD2	1:C:497:LYS:HA	1.71	0.43
1:C:643:LYS:O	1:C:647:PHE:HB2	2.18	0.43
1:D:762:LYS:HE3	1:D:763:PHE:CZ	2.53	0.43
1:A:117:PHE:CE2	1:A:779:ALA:HA	2.48	0.43
1:A:358:ALA:O	1:A:361:MET:N	2.52	0.43
1:A:770:TRP:O	1:A:771:ILE:C	2.55	0.43
1:C:408:TYR:HA	1:C:411:VAL:HG23	1.99	0.43
1:C:705:TYR:O	1:C:707:ALA:N	2.51	0.43
1:D:142:ASN:HB3	1:D:467:VAL:HG11	2.00	0.43
1:D:261:VAL:HB	1:D:314:MET:HE3	2.01	0.43
1:D:270:ASP:O	1:D:272:ARG:N	2.51	0.43
1:D:643:LYS:HE3	1:D:746:TYR:OH	2.18	0.43
1:D:830:GLN:O	1:D:831:ARG:NH2	2.52	0.43
2:E:179:GLY:HA3	2:E:206:GLN:O	2.18	0.43
1:A:705:TYR:HD1	1:A:705:TYR:HA	1.57	0.43
1:A:705:TYR:HE2	1:A:729:ASN:CG	2.22	0.43
1:B:195:GLU:O	1:B:195:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:MET:C	1:B:281:LYS:HD2	2.38	0.43
1:B:296:LYS:H	1:B:296:LYS:HD3	1.82	0.43
1:B:743:TYR:CE1	1:B:747:ILE:HG21	2.51	0.43
1:B:800:CYS:O	1:B:801:ARG:C	2.57	0.43
1:C:253:LEU:HA	1:C:253:LEU:HD23	1.74	0.43
1:C:691:LYS:O	1:C:694:PHE:HB3	2.18	0.43
1:C:800:CYS:HA	1:C:804:GLN:HG2	2.00	0.43
1:D:825:TYR:CZ	1:D:827:PRO:HG3	2.54	0.43
1:A:489:ARG:HB3	1:A:493:VAL:CG1	2.48	0.43
1:A:618:TYR:OH	1:A:623:ASN:OD1	2.32	0.43
1:A:643:LYS:HG3	1:A:746:TYR:CZ	2.54	0.43
1:A:744:LYS:HD2	1:A:744:LYS:HA	1.45	0.43
1:B:403:TYR:O	1:B:406:VAL:HG12	2.19	0.43
1:B:806:LEU:HD11	1:B:812:PHE:CG	2.54	0.43
1:C:134:PHE:HD1	1:C:134:PHE:HA	1.61	0.43
1:C:175:GLU:O	1:C:178:LEU:HB2	2.19	0.43
1:C:257:ARG:HB3	1:C:258:GLU:OE2	2.17	0.43
1:C:316:SER:O	1:C:317:TRP:HD1	2.02	0.43
1:C:529:LYS:HB2	1:C:529:LYS:HE3	1.68	0.43
1:C:573:ASP:OD2	1:C:575:SER:OG	2.18	0.43
1:D:831:ARG:HA	1:D:831:ARG:NE	2.32	0.43
2:E:253:THR:HA	2:E:414:ILE:HA	2.01	0.43
1:A:270:ASP:O	1:A:273:THR:HB	2.18	0.43
1:A:385:TYR:O	1:A:387:GLY:N	2.51	0.43
1:A:644:ALA:O	1:A:645:PHE:C	2.57	0.43
1:B:151:LYS:HB2	1:B:167:LYS:HZ1	1.84	0.43
1:B:523:TYR:CE1	1:B:527:GLU:HB2	2.54	0.43
1:B:740:TYR:O	1:B:743:TYR:N	2.52	0.43
1:B:820:LEU:HB3	1:B:825:TYR:CD2	2.53	0.43
1:C:189:LEU:HD12	1:C:190:LEU:HD23	2.01	0.43
1:C:595:PHE:CD1	1:C:596:ARG:N	2.87	0.43
1:C:648:ALA:O	1:C:652:THR:HG22	2.19	0.43
1:D:309:GLU:O	1:D:310:GLN:C	2.57	0.43
1:D:654:GLY:O	1:D:657:GLU:N	2.48	0.43
1:A:162:THR:OG1	1:A:564:ILE:HG22	2.19	0.43
1:A:333:GLU:HB3	1:A:377:ASP:OD2	2.18	0.43
1:A:484:ASN:HA	1:A:487:GLU:OE2	2.18	0.43
1:B:324:ASN:ND2	1:B:326:GLU:HB3	2.34	0.43
1:B:740:TYR:HA	1:B:769:PHE:CE2	2.54	0.43
1:C:571:LYS:HG3	1:C:572:THR:N	2.33	0.43
1:D:528:LYS:O	1:D:529:LYS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:238:PRO:O	2:E:242:ALA:HB2	2.19	0.43
1:A:540:PRO:HD3	1:A:607:PHE:CZ	2.54	0.43
1:B:493:VAL:HG22	1:B:497:LYS:NZ	2.34	0.43
1:B:772:SER:O	1:B:775:TYR:HB3	2.19	0.43
1:B:812:PHE:O	1:B:813:ALA:C	2.56	0.43
1:C:111:GLY:O	1:C:115:ASN:HB2	2.18	0.43
1:D:161:GLN:O	1:D:165:ILE:HG13	2.18	0.43
1:D:764:THR:HG1	1:D:767:GLN:HG2	1.83	0.43
1:A:174:VAL:N	1:A:175:GLU:OE2	2.51	0.42
1:A:229:PHE:N	1:A:229:PHE:CD1	2.87	0.42
1:A:312:ILE:HG13	1:A:312:ILE:H	1.70	0.42
1:B:476:TYR:OH	1:B:607:PHE:HB2	2.19	0.42
1:B:523:TYR:CG	1:B:524:ARG:N	2.86	0.42
1:B:569:ASN:HB2	1:B:589:TYR:HE1	1.84	0.42
1:C:81:ASN:ND2	1:C:756:ARG:HH11	2.17	0.42
1:C:90:ASN:O	1:C:93:ASN:HB3	2.19	0.42
1:C:355:LYS:O	1:C:358:ALA:HB3	2.19	0.42
1:C:464:MET:O	1:C:467:VAL:N	2.52	0.42
1:D:163:GLU:CG	1:D:481:VAL:HG22	2.45	0.42
1:D:217:MET:CG	1:D:218:GLY:N	2.82	0.42
1:D:336:ALA:N	1:D:337:PRO:HD2	2.34	0.42
1:D:480:TYR:HB2	1:D:543:LEU:CG	2.49	0.42
1:D:503:ILE:O	1:D:504:MET:C	2.57	0.42
1:D:788:LYS:O	1:D:792:THR:HG22	2.18	0.42
1:A:276:ILE:HD13	1:A:276:ILE:HA	1.80	0.42
1:A:533:MET:HA	1:A:623:ASN:HD22	1.83	0.42
1:A:700:CYS:SG	1:A:701:VAL:N	2.92	0.42
1:B:82:ALA:CB	1:B:756:ARG:O	2.67	0.42
1:B:115:ASN:OD1	1:B:115:ASN:C	2.58	0.42
1:B:226:LEU:O	1:B:226:LEU:CD2	2.61	0.42
1:C:386:MET:CE	1:D:391:THR:CG2	2.96	0.42
1:C:483:VAL:HG21	1:C:543:LEU:HD22	2.00	0.42
1:C:510:LYS:NZ	1:C:738:ALA:HA	2.34	0.42
1:C:608:LEU:HG	1:C:608:LEU:O	2.18	0.42
2:E:325:MET:H	2:E:388:ALA:HA	1.83	0.42
1:A:196:ARG:HH22	1:A:219:ARG:NE	2.17	0.42
1:A:507:PHE:HB2	1:A:738:ALA:HB1	2.01	0.42
1:A:509:LYS:HA	1:A:523:TYR:OH	2.19	0.42
1:A:522:SER:O	1:A:523:TYR:C	2.55	0.42
1:A:539:TRP:HA	1:A:607:PHE:HZ	1.84	0.42
1:A:653:VAL:O	1:A:656:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ASP:O	1:A:809:ILE:HG13	2.18	0.42
1:B:262:LEU:HB2	1:B:263:PRO:HD3	1.98	0.42
1:B:388:PHE:HE1	1:B:405:PHE:CZ	2.37	0.42
1:B:407:ASN:O	1:B:410:ILE:CG2	2.62	0.42
1:B:593:GLU:HG3	1:B:597:ARG:NH2	2.33	0.42
1:C:86:LYS:HA	1:C:89:LYS:NZ	2.34	0.42
1:C:502:LEU:O	1:C:506:THR:HG23	2.20	0.42
1:C:725:THR:O	1:C:727:GLY:N	2.52	0.42
1:D:142:ASN:O	1:D:145:ILE:HG22	2.19	0.42
1:D:218:GLY:O	1:D:221:GLU:N	2.52	0.42
1:D:767:GLN:OE1	1:D:815:ASP:HB3	2.19	0.42
1:D:806:LEU:HB3	1:D:812:PHE:CE2	2.53	0.42
1:A:408:TYR:HH	1:A:412:HIS:CE1	2.38	0.42
1:A:533:MET:HG2	1:A:623:ASN:ND2	2.32	0.42
1:A:695:LYS:HA	1:A:695:LYS:HD2	1.81	0.42
1:B:588:GLY:O	1:B:592:ARG:HB2	2.19	0.42
1:B:733:LEU:HG	1:B:734:GLY:N	2.35	0.42
1:C:91:ALA:O	1:C:94:THR:HG22	2.19	0.42
1:C:593:GLU:HA	1:C:596:ARG:CZ	2.50	0.42
1:C:627:LEU:HD12	1:C:627:LEU:N	2.34	0.42
1:D:760:LEU:HG	1:D:763:PHE:HD2	1.85	0.42
1:A:131:PHE:CD2	1:A:131:PHE:O	2.72	0.42
1:A:524:ARG:O	1:A:525:ARG:C	2.58	0.42
1:A:614:VAL:HG23	1:A:614:VAL:O	2.19	0.42
1:A:705:TYR:CE2	1:A:729:ASN:CG	2.93	0.42
1:B:115:ASN:O	1:B:118:ILE:HB	2.19	0.42
1:B:518:MET:SD	1:B:523:TYR:HB2	2.59	0.42
1:C:103:VAL:CG1	1:C:108:ASP:CG	2.86	0.42
1:D:533:MET:HE2	1:D:625:LEU:CD1	2.49	0.42
2:E:94:ALA:HB1	2:E:231:ALA:HA	2.00	0.42
1:B:217:MET:CE	1:B:230:MET:CE	2.97	0.42
1:B:380:VAL:O	1:B:381:THR:C	2.57	0.42
1:B:407:ASN:O	1:B:408:TYR:C	2.57	0.42
1:B:499:GLN:OE1	1:B:500:THR:N	2.53	0.42
1:B:587:ARG:O	1:B:588:GLY:C	2.58	0.42
1:B:657:GLU:O	1:B:659:VAL:N	2.52	0.42
1:C:109:PHE:O	1:C:109:PHE:CD1	2.72	0.42
1:C:109:PHE:CB	1:C:824:MET:CE	2.91	0.42
1:C:305:VAL:HG11	1:C:411:VAL:HG11	2.01	0.42
1:C:385:TYR:O	1:C:386:MET:C	2.58	0.42
1:C:514:THR:HG23	1:C:518:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ALA:O	1:D:138:GLN:C	2.58	0.42
1:D:160:SER:CA	1:D:163:GLU:OE1	2.67	0.42
1:D:463:ARG:O	1:D:467:VAL:HG12	2.20	0.42
1:D:618:TYR:HB3	1:D:657:GLU:OE2	2.19	0.42
1:D:831:ARG:HA	1:D:831:ARG:CZ	2.49	0.42
1:A:669:PHE:O	1:A:678:CYS:HB2	2.20	0.42
1:B:296:LYS:HB2	1:B:296:LYS:HE2	1.82	0.42
1:B:499:GLN:O	1:B:502:LEU:HB2	2.20	0.42
1:B:512:LEU:HB2	1:B:523:TYR:CB	2.45	0.42
1:C:143:SER:O	1:C:144:ASP:C	2.58	0.42
1:D:136:GLN:O	1:D:139:LEU:HB3	2.19	0.42
1:D:505:LYS:O	1:D:508:LEU:HB3	2.19	0.42
1:D:508:LEU:O	1:D:510:LYS:N	2.52	0.42
1:A:98:GLY:HA2	1:A:116:LYS:HB3	1.93	0.42
1:A:239:LYS:HD2	1:A:329:TYR:CD2	2.54	0.42
1:A:509:LYS:C	1:A:510:LYS:HG2	2.39	0.42
1:A:572:THR:HG22	1:A:573:ASP:H	1.85	0.42
1:A:637:TYR:CG	1:A:638:ASP:N	2.88	0.42
1:D:472:THR:HG1	1:D:473:TYR:HD1	1.66	0.42
1:D:492:VAL:CG1	1:D:493:VAL:N	2.82	0.42
1:A:501:GLU:HA	1:A:504:MET:HE2	2.02	0.42
1:A:825:TYR:HB3	1:A:827:PRO:CD	2.44	0.42
1:B:325:HIS:O	1:B:328:GLN:N	2.52	0.42
1:B:462:ALA:HA	1:B:465:LYS:HZ3	1.85	0.42
1:B:507:PHE:HE2	1:B:662:PHE:CE2	2.38	0.42
1:B:620:PRO:O	1:B:669:PHE:CD2	2.72	0.42
1:C:171:GLN:CA	1:C:174:VAL:HG12	2.49	0.42
1:C:295:ASP:CG	1:C:298:ILE:HG12	2.40	0.42
1:C:782:THR:HG23	1:C:785:SER:H	1.83	0.42
1:D:507:PHE:HD1	1:D:510:LYS:HZ3	1.67	0.42
1:D:627:LEU:HD12	1:D:627:LEU:N	2.35	0.42
1:A:834:VAL:HG22	1:A:835:TRP:CE3	2.54	0.42
1:B:214:TYR:CD1	1:B:214:TYR:N	2.87	0.42
1:B:267:PRO:C	1:B:269:LEU:N	2.71	0.42
1:B:374:PHE:CE1	1:B:375:ILE:HB	2.55	0.42
1:B:503:ILE:O	1:B:504:MET:C	2.58	0.42
1:C:221:GLU:OE1	1:C:227:PRO:HB3	2.19	0.42
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.93	0.42
1:C:381:THR:OG1	1:C:382:ASN:N	2.52	0.42
1:C:511:MET:C	1:C:523:TYR:HE2	2.23	0.42
2:F:94:ALA:HB3	2:F:231:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:352:VAL:H	2:F:385:CYS:HA	1.85	0.42
1:A:95:LEU:HD22	1:A:760:LEU:HD12	2.02	0.41
1:A:231:TYR:OH	1:A:233:TRP:NE1	2.26	0.41
1:B:212:GLU:O	1:B:215:ARG:N	2.53	0.41
1:B:272:ARG:HA	1:B:272:ARG:CZ	2.50	0.41
1:B:764:THR:HG1	1:B:767:GLN:N	2.16	0.41
1:B:804:GLN:OE1	1:B:804:GLN:HA	2.15	0.41
1:C:87:GLU:HB3	1:C:641:PHE:CE1	2.56	0.41
1:C:768:ILE:O	1:C:769:PHE:C	2.56	0.41
1:D:305:VAL:HG11	1:D:411:VAL:HG21	2.01	0.41
1:A:631:ILE:C	1:A:633:THR:H	2.24	0.41
1:B:820:LEU:HD13	1:B:825:TYR:CE2	2.55	0.41
1:C:146:VAL:O	1:C:149:LEU:N	2.51	0.41
1:C:262:LEU:HD13	1:C:264:GLN:HE22	1.85	0.41
1:C:272:ARG:O	1:C:273:THR:C	2.58	0.41
1:C:311:LYS:O	1:C:312:ILE:C	2.58	0.41
1:C:771:ILE:O	1:C:774:GLY:N	2.53	0.41
1:D:300:THR:O	1:D:301:ALA:C	2.58	0.41
1:D:303:ARG:O	1:D:307:GLN:HG2	2.21	0.41
1:A:134:PHE:HE1	1:A:636:HIS:NE2	2.18	0.41
1:A:360:LEU:HA	1:A:360:LEU:HD23	1.73	0.41
1:A:414:LEU:O	1:A:416:GLU:N	2.54	0.41
1:A:705:TYR:C	1:A:707:ALA:N	2.73	0.41
1:A:728:GLU:O	1:A:731:ALA:HB3	2.20	0.41
1:B:828:ALA:O	1:B:830:GLN:N	2.53	0.41
1:C:100:ASP:OD1	1:C:102:SER:N	2.52	0.41
1:C:110:TYR:CG	1:C:111:GLY:N	2.89	0.41
1:C:470:ILE:HG23	1:C:474:MET:HB3	2.02	0.41
1:C:658:LEU:HD12	1:C:658:LEU:HA	1.65	0.41
1:D:134:PHE:O	1:D:135:SER:C	2.58	0.41
1:D:250:GLN:CD	1:D:382:ASN:OD1	2.58	0.41
1:A:84:ARG:HD3	1:A:84:ARG:HA	1.81	0.41
1:A:521:GLU:HB3	1:A:524:ARG:HH22	1.84	0.41
1:A:618:TYR:HE2	1:A:661:GLY:HA3	1.85	0.41
1:A:649:GLY:O	1:A:650:SER:C	2.59	0.41
1:B:322:LEU:HA	1:B:322:LEU:HD23	1.48	0.41
1:B:677:ASP:O	1:B:679:SER:N	2.53	0.41
1:B:725:THR:O	1:B:726:GLN:C	2.58	0.41
1:B:809:ILE:O	1:B:810:PRO:C	2.58	0.41
1:C:168:ALA:O	1:C:171:GLN:HB2	2.20	0.41
1:C:334:LEU:HB3	1:C:335:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:LYS:O	1:C:498:GLN:C	2.58	0.41
1:D:88:TRP:CD1	1:D:88:TRP:N	2.88	0.41
1:D:219:ARG:HA	1:D:219:ARG:HD3	1.90	0.41
1:D:277:GLU:HA	1:D:280:MET:HB3	2.01	0.41
1:D:318:PRO:HG2	1:D:321:GLU:OE1	2.19	0.41
1:D:504:MET:SD	1:D:530:ILE:HG22	2.60	0.41
1:D:752:ALA:O	1:D:754:GLU:N	2.53	0.41
1:D:800:CYS:O	1:D:804:GLN:HG2	2.21	0.41
1:A:83:ASN:HB3	1:A:88:TRP:CE3	2.55	0.41
1:A:725:THR:C	1:A:729:ASN:HD22	2.23	0.41
1:A:770:TRP:CE2	1:A:812:PHE:HB2	2.55	0.41
1:B:259:PHE:CZ	1:B:265:PHE:HB3	2.56	0.41
1:C:595:PHE:O	1:C:596:ARG:C	2.59	0.41
1:D:224:ARG:HA	1:D:224:ARG:HD2	1.73	0.41
1:D:313:ALA:O	1:D:315:ALA:N	2.53	0.41
1:D:571:LYS:HA	1:D:571:LYS:HD3	1.73	0.41
2:E:96:LEU:O	2:E:98:ILE:N	2.53	0.41
1:A:331:PRO:O	1:A:332:TYR:CD1	2.74	0.41
1:A:503:ILE:HG13	1:A:503:ILE:H	1.58	0.41
1:A:589:TYR:O	1:A:593:GLU:HB2	2.20	0.41
1:B:388:PHE:CE1	1:B:405:PHE:CZ	3.09	0.41
1:B:533:MET:HE2	1:B:658:LEU:CD1	2.50	0.41
1:C:162:THR:HG23	1:C:163:GLU:N	2.36	0.41
1:C:257:ARG:HH22	1:C:313:ALA:HB1	1.84	0.41
1:C:382:ASN:O	1:C:384:ALA:N	2.54	0.41
1:C:498:GLN:HG3	1:C:498:GLN:H	1.63	0.41
1:D:302:ALA:O	1:D:303:ARG:C	2.59	0.41
1:D:353:PHE:O	1:D:356:TYR:HB3	2.21	0.41
1:D:616:ALA:HA	1:D:626:THR:O	2.21	0.41
1:B:113:THR:HG23	1:B:771:ILE:HG23	2.01	0.41
1:B:398:ILE:HB	1:B:402:GLN:HE21	1.85	0.41
1:B:820:LEU:HD13	1:B:825:TYR:CZ	2.56	0.41
1:B:822:GLN:C	1:B:824:MET:H	2.23	0.41
1:C:536:ASN:HB3	1:C:607:PHE:CE1	2.56	0.41
1:D:533:MET:HA	1:D:623:ASN:ND2	2.36	0.41
1:A:274:LYS:HA	1:A:274:LYS:HD3	1.73	0.41
1:A:488:ASP:HB2	1:A:491:GLN:HE22	1.85	0.41
1:A:496:VAL:H	1:A:496:VAL:HG22	1.66	0.41
1:B:97:PHE:O	1:B:116:LYS:HB2	2.21	0.41
1:B:170:PHE:HE1	1:B:463:ARG:HA	1.84	0.41
1:B:631:ILE:C	1:B:633:THR:HG22	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:ALA:HB2	1:B:769:PHE:CD1	2.55	0.41
1:C:94:THR:HG23	1:C:95:LEU:N	2.36	0.41
1:D:270:ASP:O	1:D:273:THR:N	2.54	0.41
1:D:529:LYS:HA	1:D:671:TYR:HB3	2.03	0.41
1:D:582:LEU:HD12	1:D:582:LEU:N	2.36	0.41
2:E:94:ALA:CB	2:E:231:ALA:HA	2.50	0.41
1:A:122:ASP:OD1	1:A:123:LEU:N	2.54	0.41
1:A:134:PHE:CE1	1:A:636:HIS:NE2	2.89	0.41
1:A:378:VAL:O	1:A:378:VAL:HG13	2.20	0.41
1:A:410:ILE:O	1:A:411:VAL:C	2.59	0.41
1:A:564:ILE:O	1:A:568:TYR:N	2.54	0.41
1:A:565:LEU:HA	1:A:565:LEU:HD12	1.74	0.41
1:A:596:ARG:O	1:A:596:ARG:HG2	2.21	0.41
1:A:834:VAL:O	1:A:835:TRP:CG	2.74	0.41
1:B:190:LEU:HD23	1:B:193:ILE:HG13	2.01	0.41
1:B:233:TRP:O	1:B:247:TYR:HB2	2.20	0.41
1:B:269:LEU:HD11	1:B:303:ARG:HG2	2.03	0.41
1:B:462:ALA:HA	1:B:465:LYS:HZ2	1.84	0.41
1:B:669:PHE:CE1	1:B:675:LEU:HD21	2.55	0.41
1:B:798:ASN:O	1:B:799:SER:C	2.58	0.41
1:C:87:GLU:CD	1:C:639:LEU:HD23	2.42	0.41
1:C:191:GLN:O	1:C:192:TYR:C	2.59	0.41
1:C:197:PHE:HD1	1:C:216:GLU:OE2	2.04	0.41
1:C:471:THR:CG2	1:C:612:ALA:HB3	2.51	0.41
1:C:562:TYR:O	1:C:565:LEU:HB3	2.21	0.41
1:C:568:TYR:O	1:C:568:TYR:CG	2.73	0.41
1:C:595:PHE:CG	1:C:596:ARG:N	2.89	0.41
1:C:618:TYR:CE2	1:C:661:GLY:HA2	2.56	0.41
1:D:83:ASN:O	1:D:758:PRO:HB3	2.21	0.41
1:D:133:THR:H	1:D:133:THR:HG23	1.63	0.41
1:D:261:VAL:HG11	1:D:314:MET:HB2	2.02	0.41
1:D:473:TYR:O	1:D:475:PRO:HD3	2.21	0.41
1:D:540:PRO:HG3	1:D:607:PHE:CG	2.55	0.41
1:D:609:GLU:HB3	1:D:617:TRP:CZ3	2.55	0.41
1:A:283:PHE:O	1:A:285:SER:N	2.54	0.41
1:A:668:GLN:O	1:A:675:LEU:HD12	2.20	0.41
1:A:814:LYS:O	1:A:817:GLN:N	2.55	0.41
1:B:115:ASN:OD1	1:B:115:ASN:O	2.38	0.41
1:B:145:ILE:HG21	1:B:467:VAL:HG21	2.03	0.41
1:B:162:THR:N	1:B:564:ILE:HD13	2.33	0.41
1:B:359:GLY:O	1:B:360:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:GLN:CD	1:B:520:GLY:N	2.75	0.41
1:C:412:HIS:O	1:C:413:MET:C	2.58	0.41
1:C:621:GLU:CD	1:C:621:GLU:N	2.74	0.41
1:D:161:GLN:O	1:D:164:ARG:HB3	2.20	0.41
1:D:582:LEU:O	1:D:585:LEU:N	2.54	0.41
1:A:496:VAL:HG23	1:A:497:LYS:N	2.34	0.40
1:A:656:HIS:CG	1:A:732:ASP:OD1	2.74	0.40
1:B:341:LYS:HD2	1:B:352:ARG:HH22	1.85	0.40
1:B:700:CYS:HB3	1:B:832:CYS:HB3	1.97	0.40
1:C:85:SER:O	1:C:89:LYS:NZ	2.42	0.40
1:C:230:MET:CE	1:C:248:ILE:HG21	2.52	0.40
1:C:513:SER:C	1:C:515:LEU:H	2.25	0.40
1:D:219:ARG:HH12	1:D:359:GLY:HA2	1.86	0.40
1:D:764:THR:O	1:D:765:PRO:C	2.59	0.40
2:E:325:MET:O	2:E:388:ALA:HB1	2.21	0.40
2:F:326:GLY:O	2:F:402:ILE:N	2.54	0.40
1:A:324:ASN:HB3	1:A:327:GLN:HG2	2.02	0.40
1:A:355:LYS:O	1:A:357:ILE:HG12	2.21	0.40
1:A:501:GLU:HA	1:A:504:MET:CE	2.51	0.40
1:B:121:ILE:O	1:B:780:LYS:CD	2.69	0.40
1:B:268:GLU:HA	1:B:271:ALA:HB3	2.04	0.40
1:B:295:ASP:O	1:B:296:LYS:C	2.59	0.40
1:B:296:LYS:HD3	1:B:296:LYS:N	2.35	0.40
1:B:374:PHE:CG	1:B:375:ILE:N	2.89	0.40
1:C:273:THR:H	1:C:273:THR:HG23	1.62	0.40
1:C:305:VAL:HG23	1:C:306:THR:H	1.86	0.40
1:C:736:LEU:O	1:C:739:SER:N	2.53	0.40
1:D:119:GLU:O	1:D:119:GLU:CG	2.69	0.40
1:D:405:PHE:N	1:D:405:PHE:CD1	2.85	0.40
1:D:764:THR:O	1:D:768:ILE:HG12	2.21	0.40
1:D:814:LYS:C	1:D:814:LYS:HD3	2.42	0.40
1:A:196:ARG:NH2	1:A:219:ARG:HE	2.19	0.40
1:A:239:LYS:HB2	1:A:329:TYR:OH	2.21	0.40
1:A:484:ASN:HA	1:A:487:GLU:CG	2.50	0.40
1:A:495:ASP:O	1:A:498:GLN:HB3	2.20	0.40
1:B:398:ILE:HB	1:B:402:GLN:NE2	2.36	0.40
1:B:699:GLN:O	1:B:702:VAL:HB	2.22	0.40
1:B:754:GLU:O	1:B:755:MET:C	2.60	0.40
1:C:385:TYR:O	1:C:385:TYR:CD1	2.74	0.40
1:D:101:GLU:OE2	1:D:762:LYS:NZ	2.50	0.40
1:D:134:PHE:HE1	1:D:636:HIS:CE1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LEU:O	1:D:140:GLU:C	2.59	0.40
1:D:490:ASP:O	1:D:490:ASP:OD1	2.40	0.40
1:D:745:GLU:O	1:D:746:TYR:C	2.60	0.40
1:D:797:PRO:O	1:D:800:CYS:N	2.54	0.40
1:A:319:ASP:O	1:A:320:ASP:C	2.59	0.40
1:A:633:THR:HG23	1:A:634:SER:N	2.37	0.40
1:A:765:PRO:O	1:A:766:ASN:C	2.59	0.40
1:B:766:ASN:O	1:B:767:GLN:C	2.60	0.40
1:C:114:CYS:SG	1:C:778:CYS:CB	3.04	0.40
1:C:250:GLN:OE1	1:C:317:TRP:N	2.47	0.40
1:C:798:ASN:O	1:C:801:ARG:CA	2.67	0.40
1:D:167:LYS:O	1:D:171:GLN:OE1	2.39	0.40
1:A:99:LEU:HD13	1:A:760:LEU:CD1	2.50	0.40
1:A:219:ARG:HG3	1:A:359:GLY:HA2	2.03	0.40
1:A:246:TYR:HH	1:A:595:PHE:HZ	1.67	0.40
1:A:356:TYR:O	1:A:356:TYR:CG	2.72	0.40
1:A:505:LYS:HE2	1:A:509:LYS:HE2	2.03	0.40
1:A:559:ASP:CG	1:A:560:ASP:H	2.25	0.40
1:A:643:LYS:HA	1:A:643:LYS:HD3	1.92	0.40
1:B:505:LYS:O	1:B:508:LEU:N	2.55	0.40
1:B:515:LEU:HD12	1:B:518:MET:HE1	2.03	0.40
1:B:536:ASN:C	1:B:537:TYR:HD1	2.25	0.40
1:B:622:LEU:HD12	1:B:623:ASN:CA	2.51	0.40
1:B:767:GLN:O	1:B:771:ILE:HG13	2.22	0.40
1:C:132:THR:HA	1:C:779:ALA:HA	2.03	0.40
1:C:260:TYR:C	1:C:262:LEU:N	2.73	0.40
1:C:305:VAL:CG1	1:C:411:VAL:HG21	2.51	0.40
1:D:144:ASP:O	1:D:147:LYS:HB2	2.22	0.40
2:E:78:ILE:H	2:E:83:GLN:N	2.17	0.40
2:E:255:TYR:C	2:E:270:ALA:O	2.59	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	564/755 (75%)	375 (66%)	188 (33%)	1 (0%)	44	78
1	B	589/755 (78%)	385 (65%)	196 (33%)	8 (1%)	9	40
1	C	551/755 (73%)	364 (66%)	181 (33%)	6 (1%)	12	46
1	D	536/755 (71%)	378 (70%)	153 (28%)	5 (1%)	14	51
2	E	289/369 (78%)	217 (75%)	72 (25%)	0	100	100
2	F	283/369 (77%)	198 (70%)	81 (29%)	4 (1%)	9	40
3	G	155/253 (61%)	121 (78%)	29 (19%)	5 (3%)	3	21
All	All	2967/4011 (74%)	2038 (69%)	900 (30%)	29 (1%)	16	49

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	817	GLN
1	C	820	LEU
2	F	168	PHE
3	G	104	PRO
1	C	107	GLU
1	C	817	GLN
1	C	824	MET
2	F	160	ALA
3	G	77	ILE
1	B	258	GLU
1	B	635	PRO
1	C	334	LEU
1	B	374	PHE
1	B	634	SER
2	F	183	ASN
1	B	257	ARG
1	B	263	PRO
1	B	646	ASN
1	D	634	SER
1	D	635	PRO
2	F	164	PRO
3	G	108	HIS
1	C	821	GLY
1	B	261	VAL
1	D	826	PRO
1	D	722	GLY

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Mol	Chain	Res	Type
3	G	190	ILE
1	D	267	PRO
3	G	23	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	521/655 (80%)	521 (100%)	0	100	100
1	B	538/655 (82%)	536 (100%)	2 (0%)	89	90
1	C	510/655 (78%)	510 (100%)	0	100	100
1	D	492/655 (75%)	490 (100%)	2 (0%)	89	90
All	All	2061/2620 (79%)	2057 (100%)	4 (0%)	91	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	617	TRP
1	B	724	HIS
1	D	388	PHE
1	D	607	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	327	GLN
1	A	407	ASN
1	A	704	GLN
1	A	804	GLN
1	B	729	ASN
1	B	830	GLN
1	C	382	ASN
1	C	536	ASN

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Mol	Chain	Res	Type
1	C	583	ASN
1	C	793	ASN
1	C	795	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

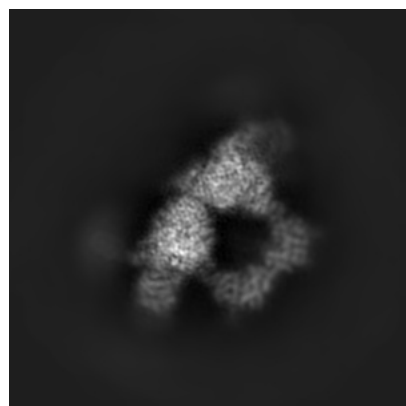
## 6 Map visualisation [i](#)

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

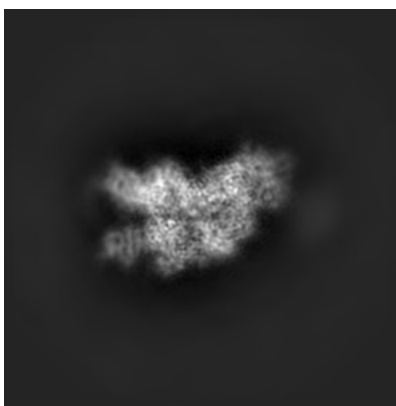
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

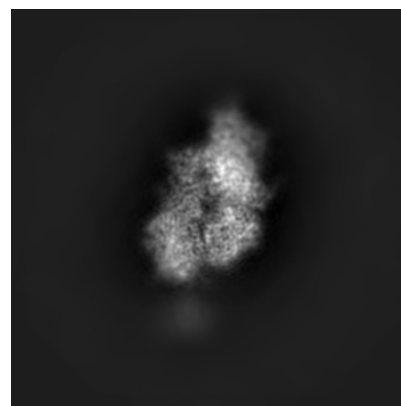
#### 6.1.1 Primary map



X

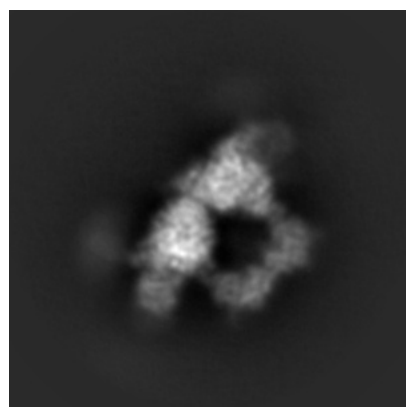


Y

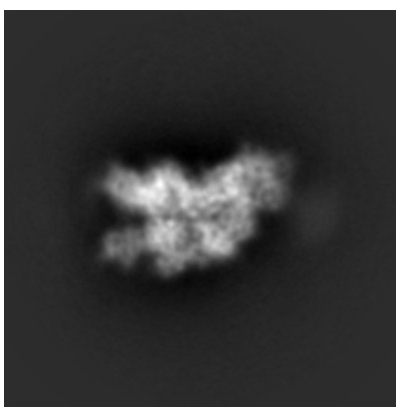


Z

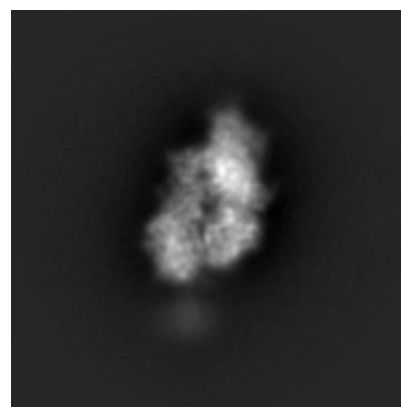
#### 6.1.2 Raw map



X



Y

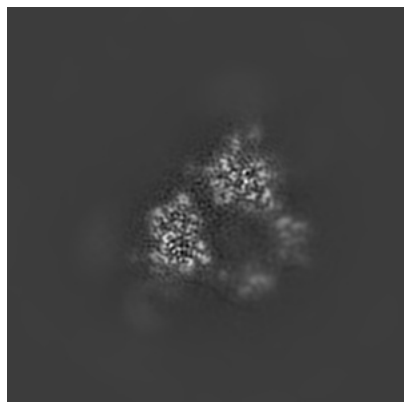


Z

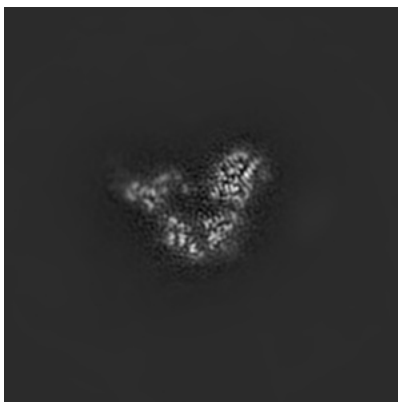
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

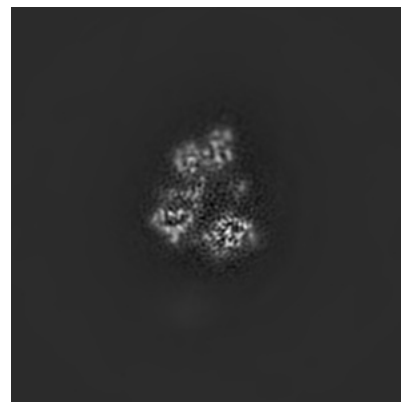
### 6.2.1 Primary map



X Index: 182

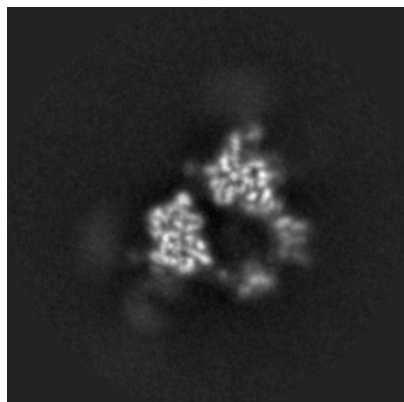


Y Index: 182

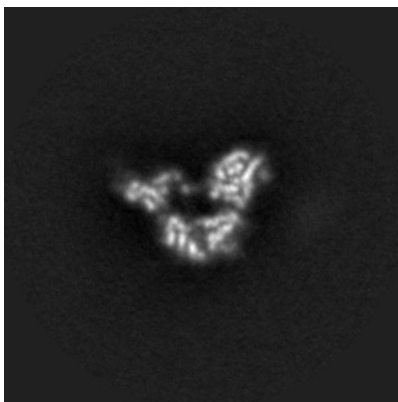


Z Index: 182

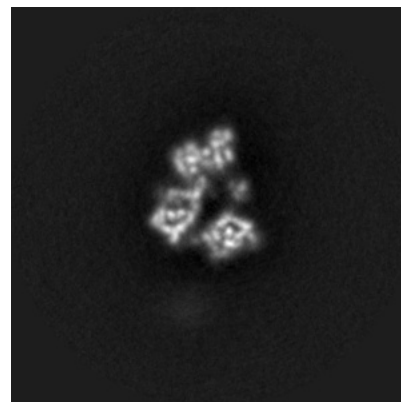
### 6.2.2 Raw map



X Index: 182



Y Index: 182



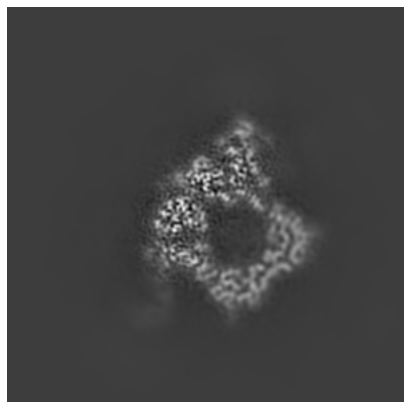
Z Index: 182

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

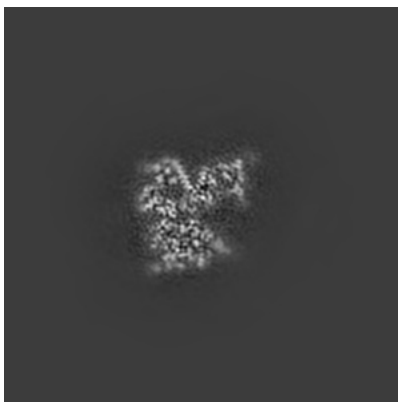


## 6.3 Largest variance slices [i](#)

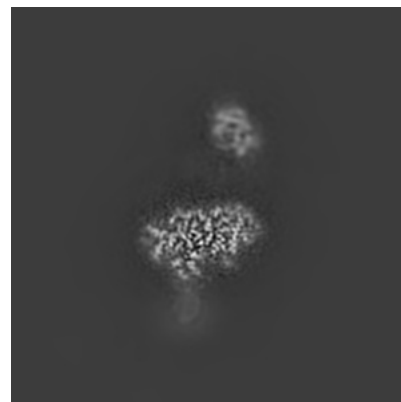
### 6.3.1 Primary map



X Index: 199

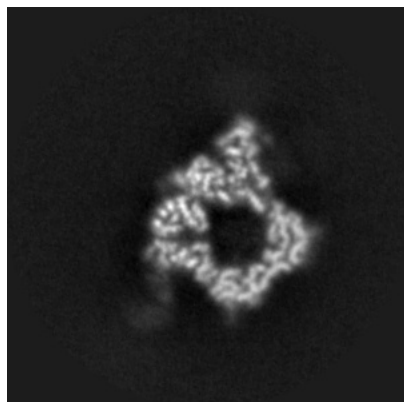


Y Index: 166

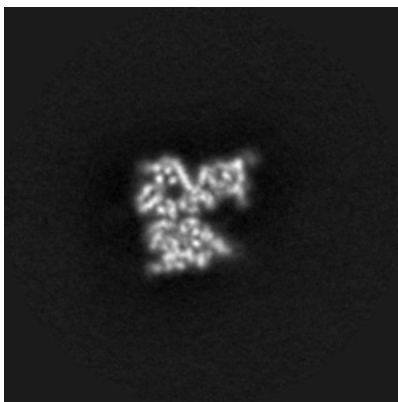


Z Index: 143

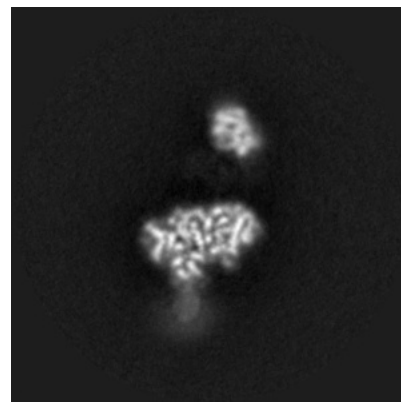
### 6.3.2 Raw map



X Index: 198



Y Index: 166

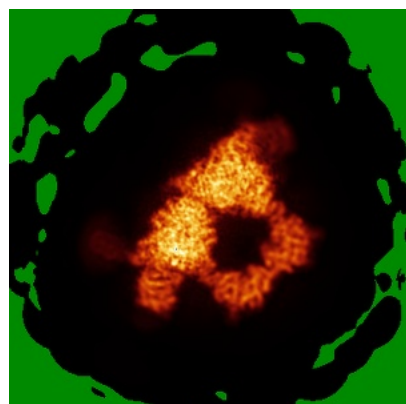


Z Index: 142

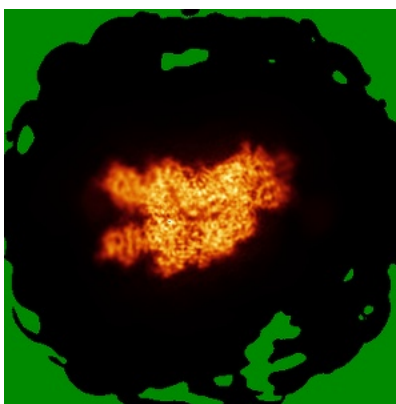
The images above show the largest variance slices of the map in three orthogonal directions.

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

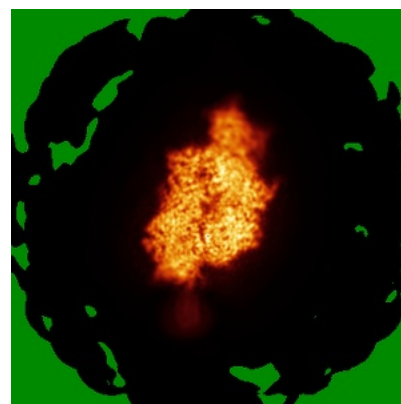
### 6.4.1 Primary map



X



Y



Z

### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



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

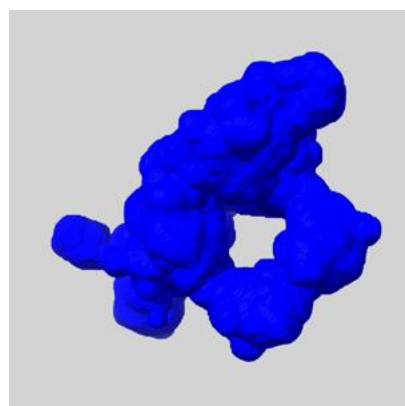
## 6.6 Mask visualisation [i](#)

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

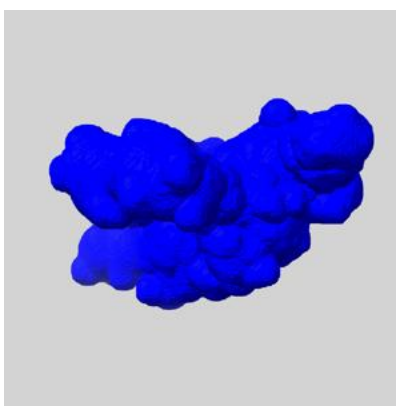
A mask typically either:

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

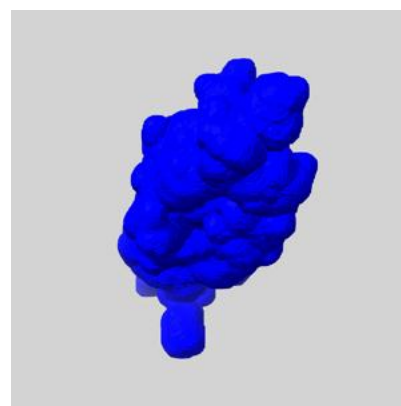
### 6.6.1 emd\_4975\_msk\_1.map [i](#)



X



Y

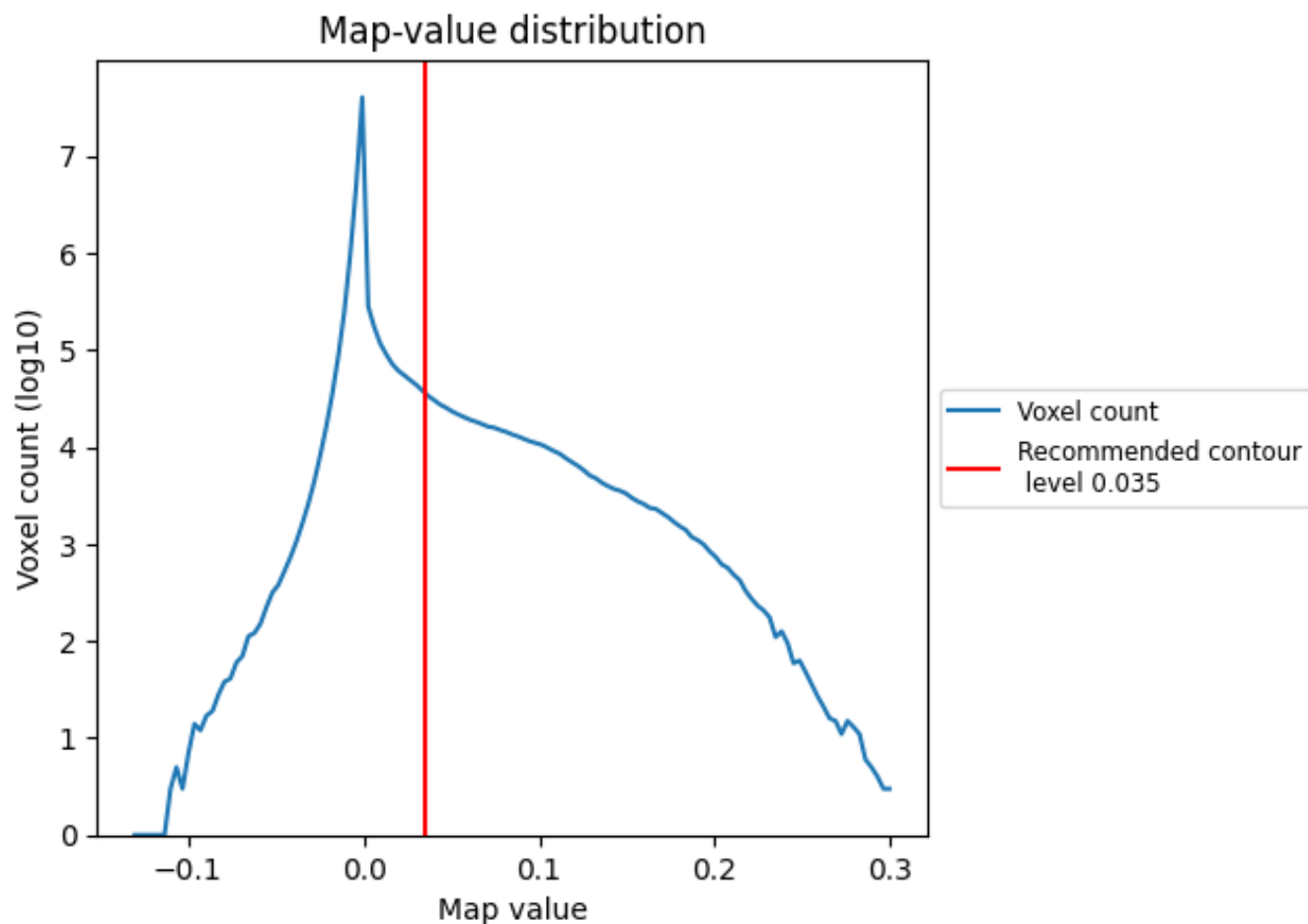


Z

## 7 Map analysis [i](#)

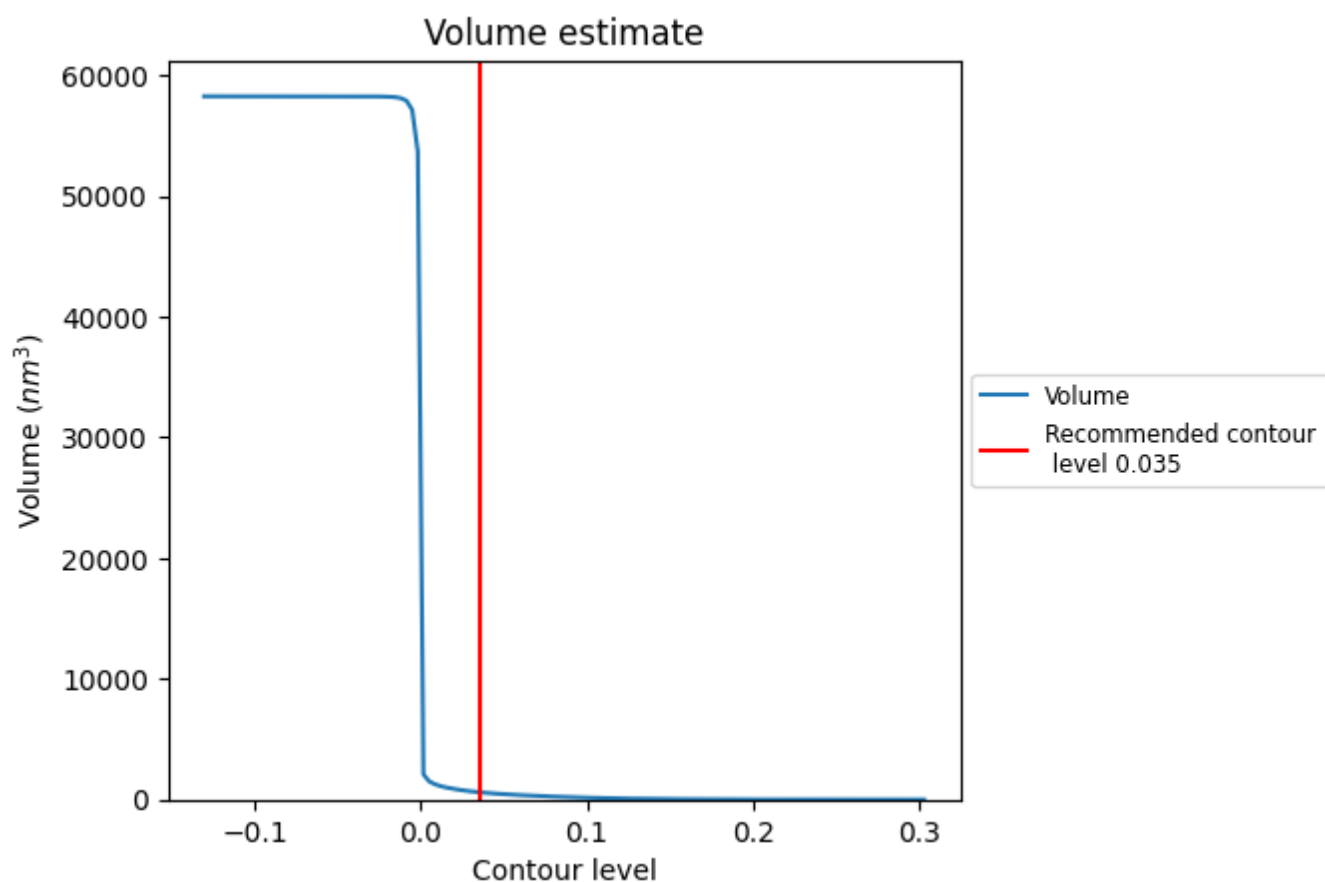
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

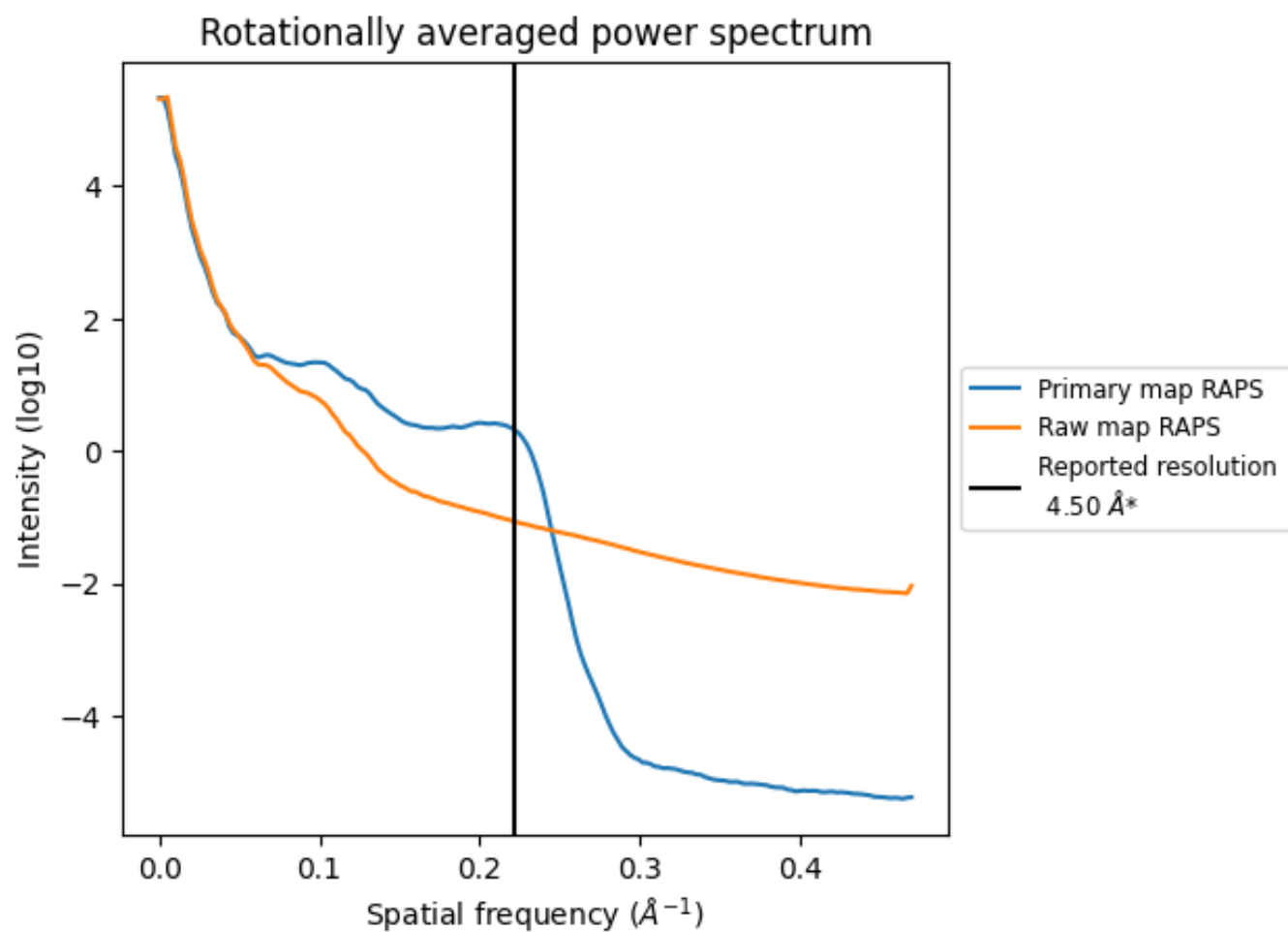
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 607 nm<sup>3</sup>; this corresponds to an approximate mass of 548 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

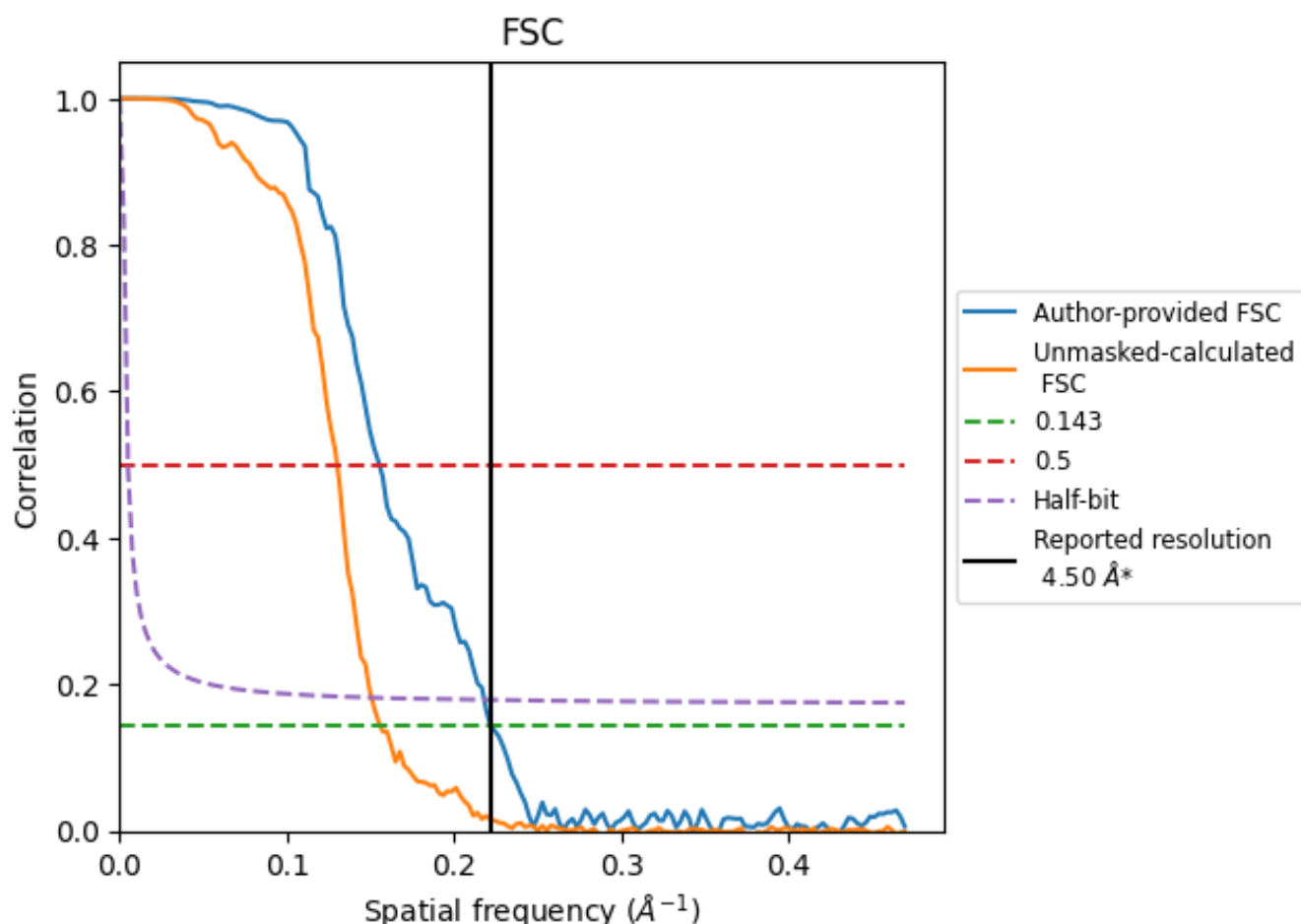


\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

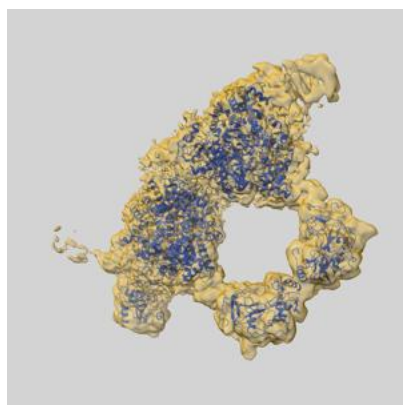
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.44	4.59
Unmasked-calculated*	6.41	7.69	6.64

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

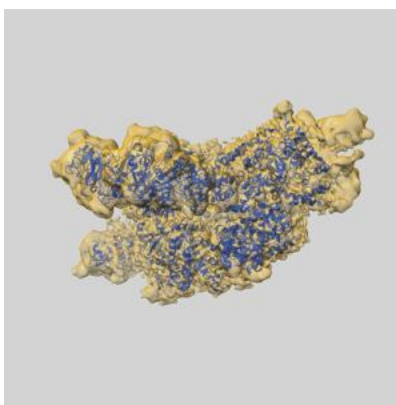
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4975 and PDB model 6ROW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

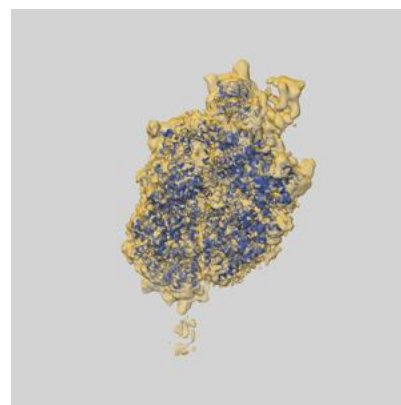
### 9.1 Map-model overlay [i](#)



X



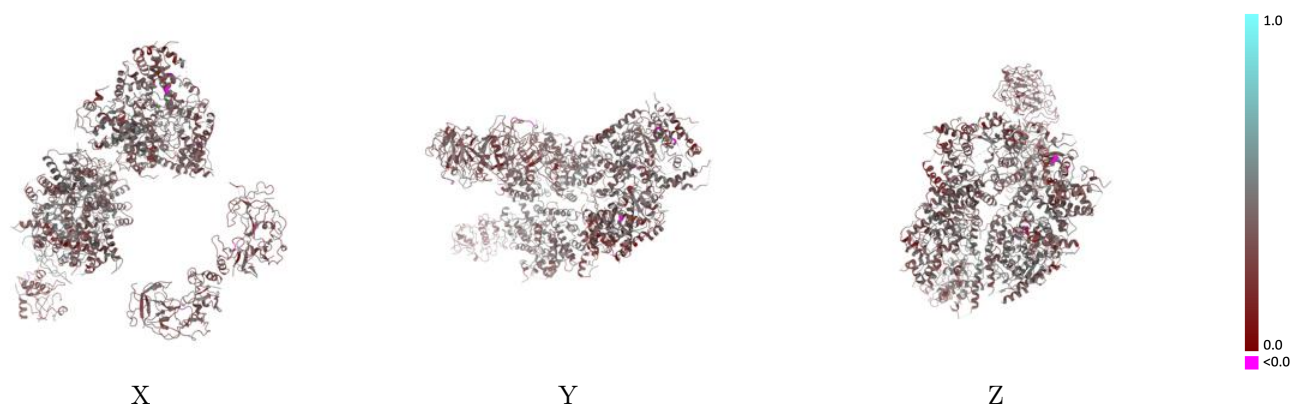
Y



Z

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

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



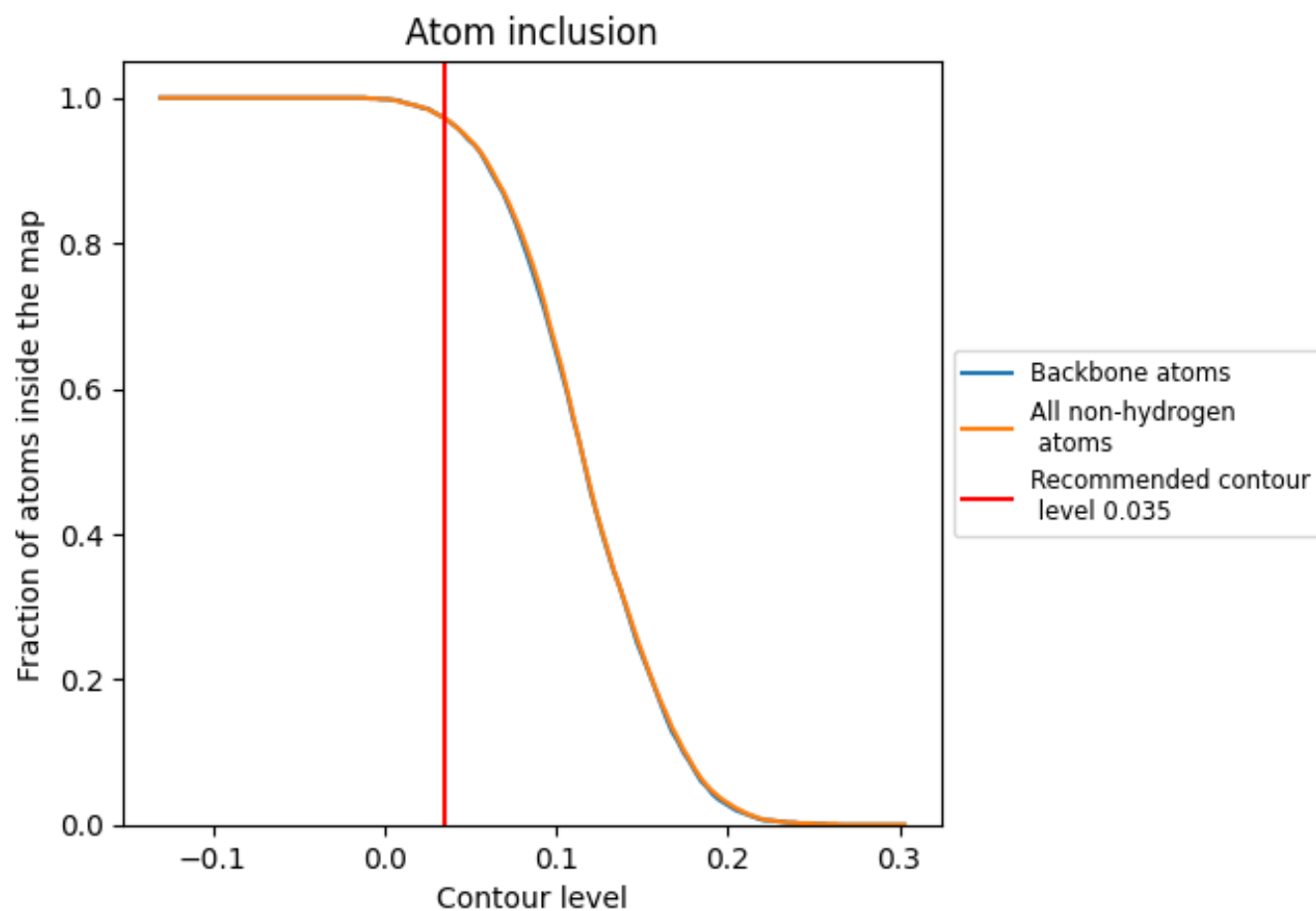
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

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

1.0

0.0

<0.0