



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:38 am GMT

PDB ID : 5G5L
EMDB ID : EMD-3439
Title : RNA polymerase I-Rrn3 complex at 4.8 Å resolution
Authors : Engel, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-05-26
Resolution : 4.80 Å (reported)
Based on initial model : 4C2M

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

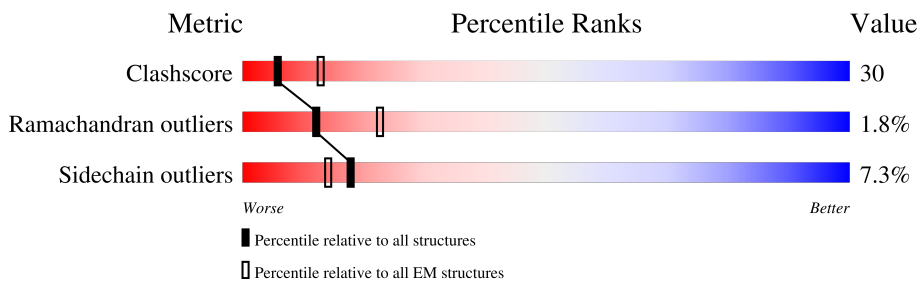
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	

2 Entry composition i

There are 16 unique types of molecules in this entry. The entry contains 37349 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1480	Total	C	N	O	S	0	0
			11686	7384	2030	2211	61		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1174	Total	C	N	O	S	0	0
			9327	5899	1635	1743	50		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	193	1520	982	259	274	5	0	0

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	131	1052	664	176	208	4	0	0

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	107	820	511	138	162	9	0	0

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	69	569	362	101	100	6	0	0

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	793	496	130	162	5	0	0

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	43	340	211	66	59	4	0	0

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	105	833	528	138	167	0	0

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

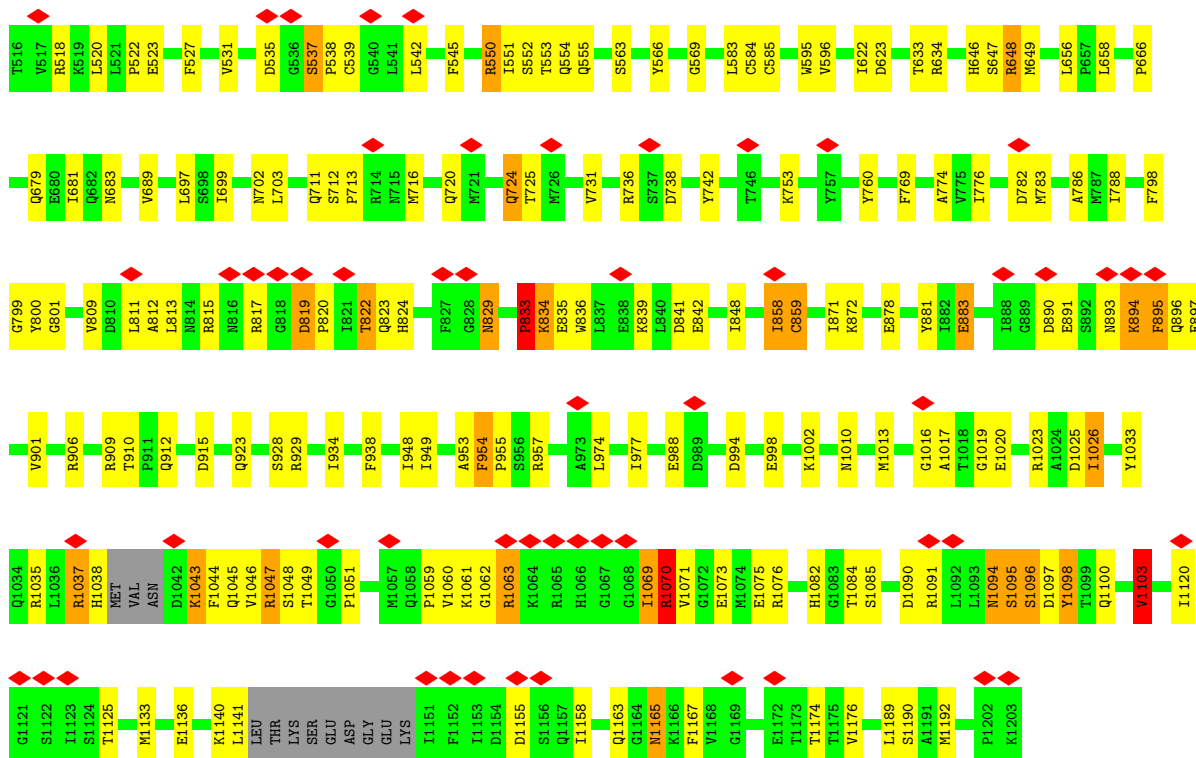
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	145	1151	735	188	224	4	0	0

- Molecule 15 is a protein called RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR RRN3.

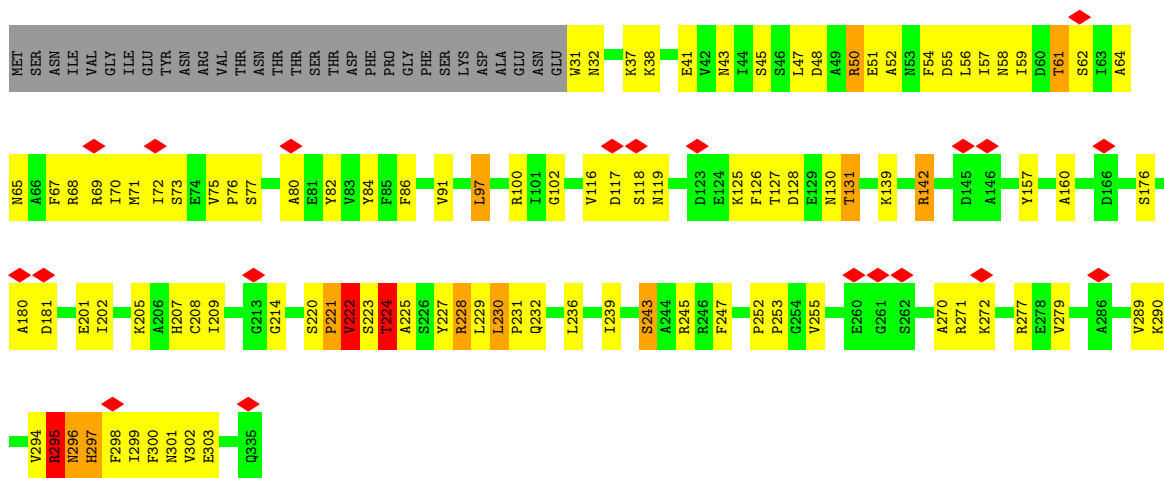
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	463	3811	2473	623	694	21	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

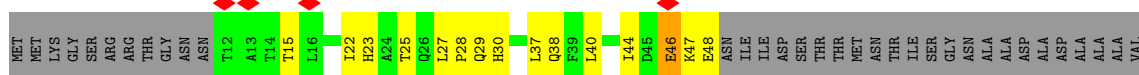
Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

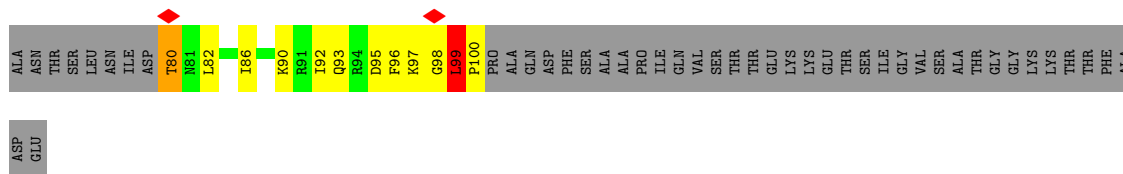


• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

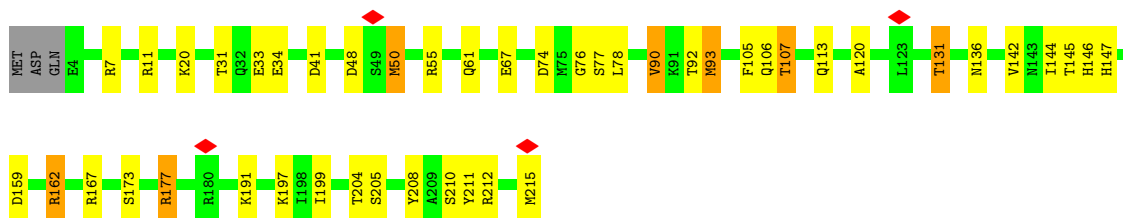
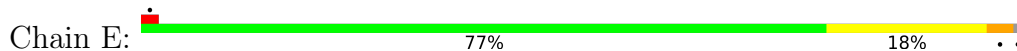


• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

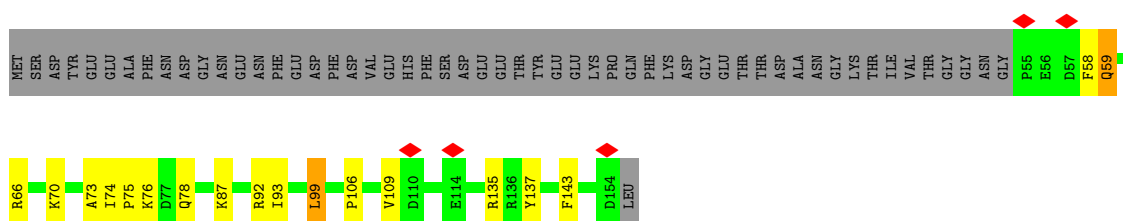




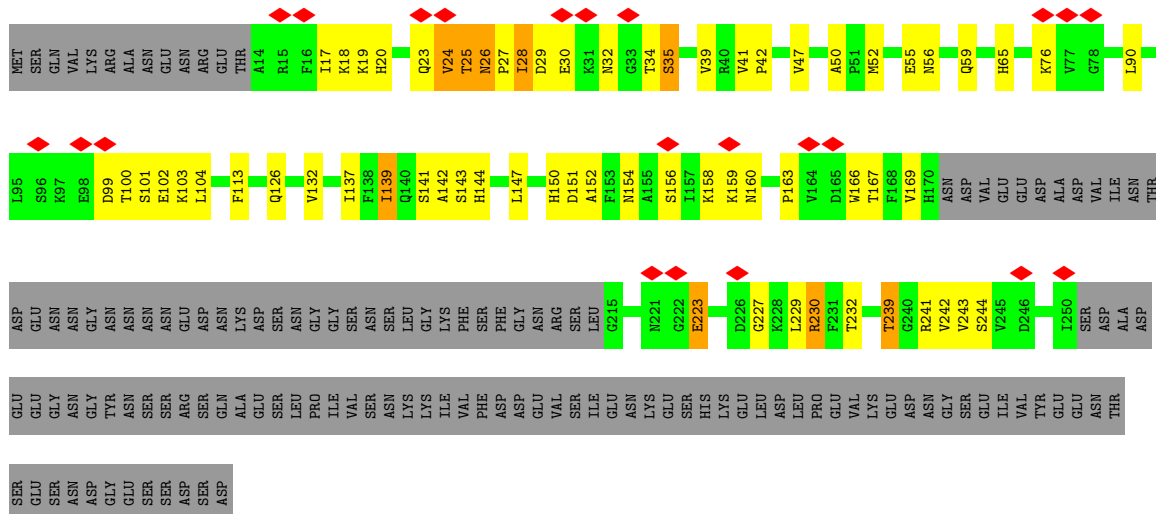
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

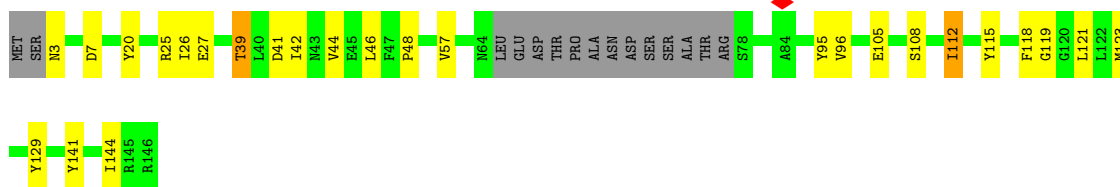


• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43



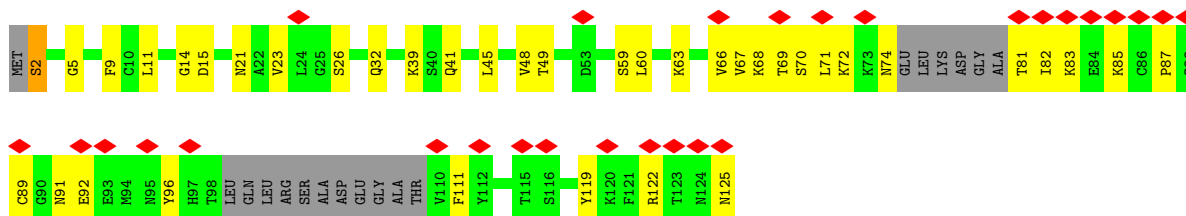
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:  72% 16% 10%




- Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain I:  22% 54% 30% 14%



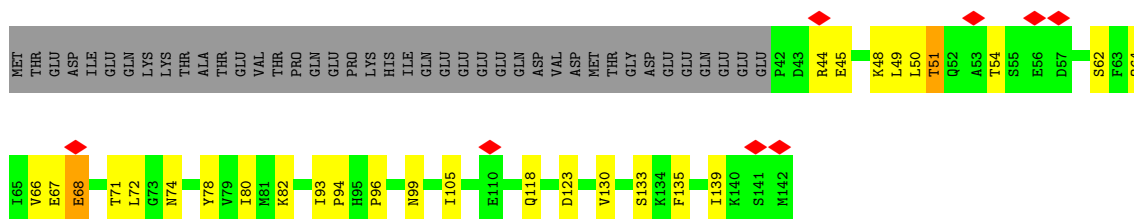
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:  79% 17% ...

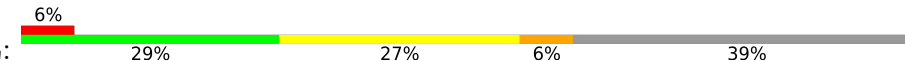


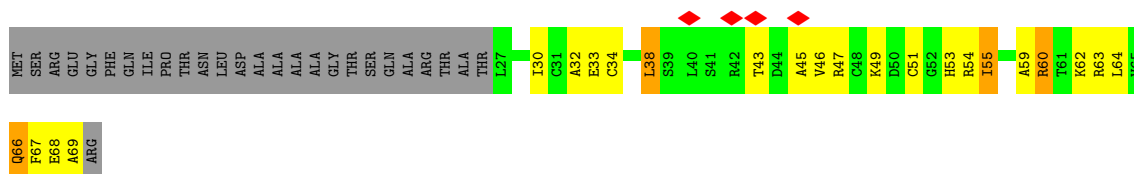
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K:  6% 51% 19% 29%

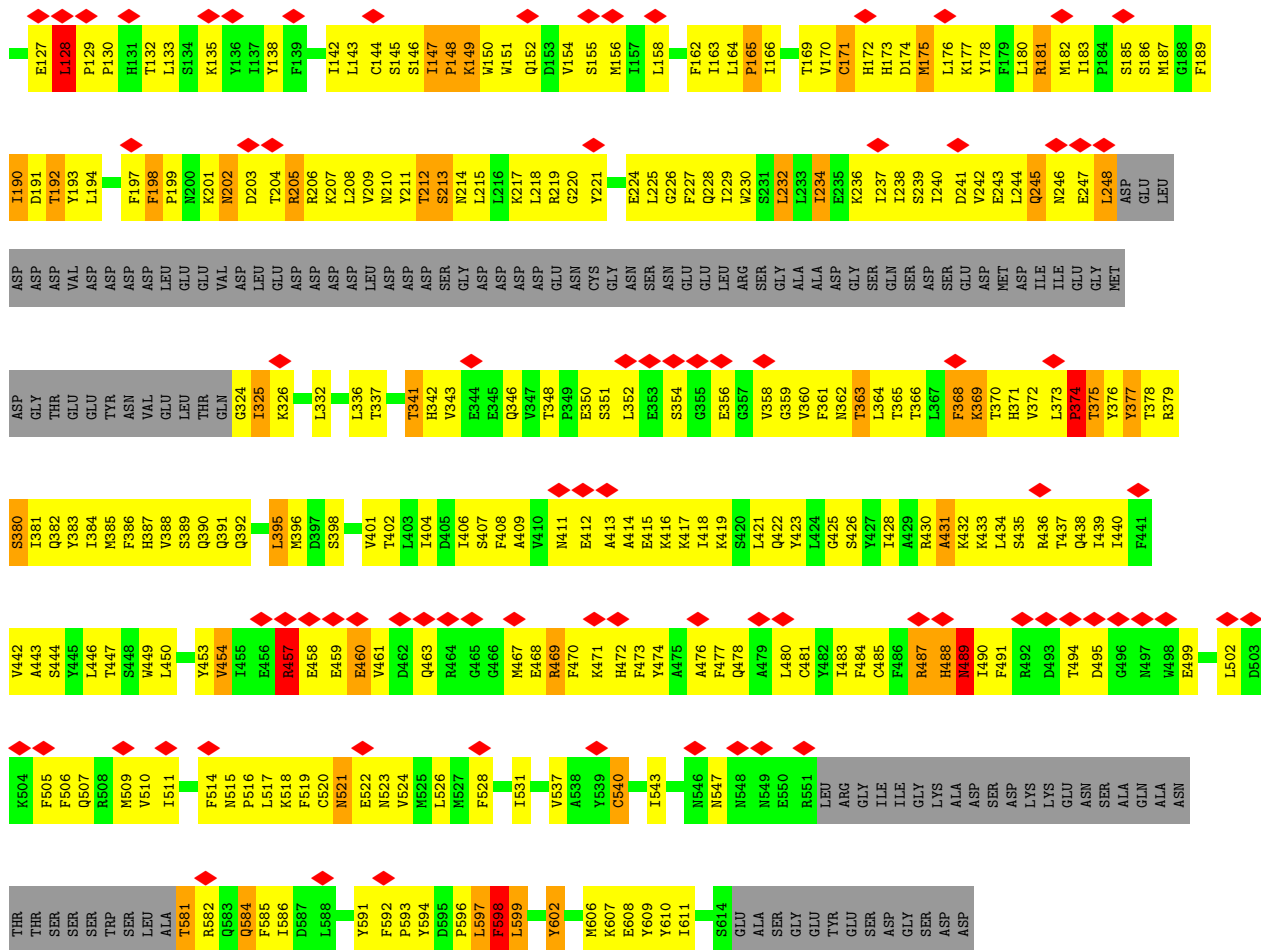


- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:  6% 29% 27% 6% 39%



- Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63445	Depositor
Resolution determination method	Not provided	
CTF correction method	RELION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (\AA)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.48	0/11900	0.72	22/16073 (0.1%)
2	B	0.49	1/9533 (0.0%)	0.77	25/12884 (0.2%)
3	C	0.43	0/2475	0.68	5/3354 (0.1%)
4	D	0.40	0/465	0.59	0/630
5	E	0.40	0/1771	0.66	3/2383 (0.1%)
6	F	0.45	0/838	0.58	0/1129
7	G	0.39	0/1558	0.60	3/2120 (0.1%)
8	H	0.42	0/1070	0.61	0/1449
9	I	0.42	0/831	0.57	0/1117
10	J	0.57	1/578 (0.2%)	0.59	0/775
11	K	0.46	0/804	0.79	3/1083 (0.3%)
12	L	0.38	0/342	0.55	0/454
13	M	0.42	0/849	0.56	1/1140 (0.1%)
14	N	0.40	0/1172	0.54	0/1580
15	O	0.38	1/3897 (0.0%)	0.58	3/5268 (0.1%)
All	All	0.45	3/38083 (0.0%)	0.69	65/51439 (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	1
15	O	0	5
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	10	CYS	CB-SG	7.64	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	198	PHE	C-N	-7.16	1.20	1.34
2	B	859	CYS	CB-SG	-6.12	1.71	1.82

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1023	ARG	NE-CZ-NH2	-13.90	113.35	120.30
2	B	452	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	397	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	A	329	ARG	NE-CZ-NH2	-13.12	113.74	120.30
2	B	448	ARG	NE-CZ-NH2	-12.97	113.81	120.30
1	A	329	ARG	NE-CZ-NH1	12.94	126.77	120.30
2	B	429	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	A	59	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	A	59	ARG	NE-CZ-NH2	-12.78	113.91	120.30
5	E	167	ARG	NE-CZ-NH1	12.52	126.56	120.30
5	E	167	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	A	416	ARG	NE-CZ-NH2	-12.41	114.09	120.30
11	K	44	ARG	NE-CZ-NH2	-12.29	114.15	120.30
2	B	448	ARG	NE-CZ-NH1	12.28	126.44	120.30
2	B	261	ARG	NE-CZ-NH1	12.22	126.41	120.30
2	B	452	ARG	NE-CZ-NH1	12.22	126.41	120.30
2	B	634	ARG	NE-CZ-NH2	-12.21	114.19	120.30
2	B	261	ARG	NE-CZ-NH2	-12.11	114.25	120.30
2	B	429	ARG	NE-CZ-NH1	12.07	126.33	120.30
11	K	44	ARG	NE-CZ-NH1	11.97	126.29	120.30
1	A	397	ARG	NE-CZ-NH2	-11.89	114.35	120.30
3	C	142	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	A	422	ARG	NE-CZ-NH2	-11.46	114.57	120.30
3	C	142	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	A	342	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	A	422	ARG	NE-CZ-NH1	11.12	125.86	120.30
2	B	634	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	A	416	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	230	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	A	230	ARG	NE-CZ-NH2	-10.79	114.91	120.30
2	B	648	ARG	NE-CZ-NH2	-10.72	114.94	120.30
2	B	550	ARG	NE-CZ-NH2	-10.51	115.04	120.30
2	B	550	ARG	NE-CZ-NH1	9.88	125.24	120.30
2	B	1023	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	342	ARG	NE-CZ-NH1	9.25	124.92	120.30
2	B	648	ARG	NE-CZ-NH1	9.09	124.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	460	GLU	N-CA-C	-7.44	90.91	111.00
2	B	261	ARG	CD-NE-CZ	6.91	133.28	123.60
1	A	397	ARG	CD-NE-CZ	6.90	133.25	123.60
15	O	598	PHE	N-CA-C	6.90	129.62	111.00
1	A	59	ARG	CD-NE-CZ	6.61	132.86	123.60
2	B	452	ARG	CD-NE-CZ	6.55	132.77	123.60
2	B	448	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	329	ARG	CD-NE-CZ	6.33	132.46	123.60
11	K	44	ARG	CD-NE-CZ	6.24	132.34	123.60
2	B	634	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	416	ARG	CD-NE-CZ	6.18	132.25	123.60
1	A	422	ARG	CD-NE-CZ	6.17	132.23	123.60
2	B	429	ARG	CD-NE-CZ	6.13	132.18	123.60
3	C	142	ARG	CD-NE-CZ	6.00	132.00	123.60
5	E	167	ARG	CD-NE-CZ	5.93	131.90	123.60
7	G	35	SER	O-C-N	5.92	132.17	122.70
1	A	1622	LEU	O-C-N	5.78	131.94	122.70
1	A	342	ARG	CD-NE-CZ	5.67	131.54	123.60
2	B	1103	VAL	CB-CA-C	-5.59	100.78	111.40
7	G	35	SER	CA-C-N	-5.54	105.02	117.20
2	B	550	ARG	CD-NE-CZ	5.45	131.23	123.60
2	B	648	ARG	CD-NE-CZ	5.39	131.15	123.60
2	B	1023	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	230	ARG	CD-NE-CZ	5.20	130.88	123.60
7	G	26	ASN	C-N-CD	5.12	139.16	128.40
15	O	128	LEU	C-N-CD	5.08	139.06	128.40
13	M	110	GLY	C-N-CD	5.06	139.03	128.40
3	C	220	SER	C-N-CD	5.05	139.00	128.40
3	C	230	LEU	C-N-CD	5.03	138.97	128.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1343	ASP	Peptide
15	O	374	PRO	Peptide
15	O	375	THR	Peptide
15	O	411	ASN	Peptide
15	O	598	PHE	Peptide
15	O	599	LEU	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	11686	0	11770	682	0
2	B	9327	0	9214	482	0
3	C	2423	0	2409	283	0
4	D	459	0	461	103	0
5	E	1735	0	1764	40	0
6	F	823	0	840	64	0
7	G	1520	0	1529	164	0
8	H	1052	0	1021	15	0
9	I	820	0	805	71	0
10	J	569	0	585	6	0
11	K	793	0	790	36	0
12	L	340	0	361	47	0
13	M	833	0	826	32	0
14	N	1151	0	1169	44	0
15	O	3811	0	3800	757	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	37349	0	37344	2258	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 30.

All (2258) 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)
15:O:162:PHE:CB	15:O:214:ASN:CB	1.76	1.62
3:C:75:VAL:HG11	3:C:221:PRO:CG	1.33	1.52
1:A:478:TYR:HA	2:B:1048:SER:CA	1.42	1.50
1:A:436:ALA:CB	1:A:443:ALA:HB2	1.43	1.46
1:A:83:VAL:HG21	1:A:427:PHE:CZ	1.50	1.46
15:O:458:GLU:HA	15:O:461:VAL:CG2	1.26	1.44
15:O:458:GLU:CA	15:O:461:VAL:HG23	1.28	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:454:VAL:CB	15:O:514:PHE:HE2	1.30	1.41
1:A:478:TYR:CA	2:B:1048:SER:HA	1.53	1.38
1:A:436:ALA:HB2	1:A:443:ALA:CB	1.54	1.37
2:B:207:ILE:HG13	2:B:503:VAL:CG2	1.54	1.37
15:O:408:PHE:CZ	15:O:446:LEU:CD1	2.06	1.37
15:O:408:PHE:CZ	15:O:446:LEU:HD11	1.59	1.37
15:O:471:LYS:HB2	15:O:585:PHE:CE1	1.58	1.37
1:A:83:VAL:HG11	1:A:427:PHE:CE2	1.59	1.36
15:O:138:TYR:CE2	15:O:142:ILE:HD11	1.56	1.36
3:C:31:TRP:CB	11:K:82:LYS:HD2	1.54	1.35
15:O:454:VAL:HB	15:O:514:PHE:CE2	1.61	1.35
1:A:437:PHE:CZ	1:A:456:VAL:HG23	1.62	1.35
7:G:242:VAL:HG11	15:O:185:SER:OG	1.22	1.35
1:A:437:PHE:CZ	1:A:456:VAL:CG2	2.11	1.34
2:B:42:VAL:CG1	2:B:46:ILE:HD11	1.57	1.33
3:C:75:VAL:HG11	3:C:221:PRO:CD	1.59	1.32
3:C:75:VAL:CG1	3:C:221:PRO:CG	2.07	1.31
3:C:54:PHE:CE2	3:C:300:PHE:HB2	1.66	1.30
3:C:55:ASP:CG	3:C:299:ILE:HG12	1.51	1.29
1:A:477:ASN:OD1	2:B:1059:PRO:HG3	1.13	1.29
3:C:84:TYR:HE2	12:L:66:GLN:OE1	1.16	1.29
15:O:198:PHE:CD2	15:O:232:LEU:HG	1.65	1.29
4:D:30:HIS:NE2	7:G:26:ASN:OD1	1.66	1.27
15:O:432:LYS:HG2	15:O:608:GLU:O	1.23	1.27
4:D:25:THR:CG2	6:F:59:GLN:HE21	1.45	1.27
3:C:75:VAL:CG1	3:C:221:PRO:CD	2.14	1.26
3:C:84:TYR:CE2	12:L:66:GLN:OE1	1.87	1.26
1:A:478:TYR:N	2:B:1048:SER:O	1.66	1.25
7:G:242:VAL:CG1	15:O:185:SER:OG	1.81	1.24
1:A:1008:ASP:OD2	1:A:1202:LEU:HD13	1.37	1.24
3:C:54:PHE:CE2	3:C:300:PHE:CB	2.20	1.24
15:O:431:ALA:CB	15:O:434:LEU:HD11	1.63	1.24
1:A:1348:VAL:HB	2:B:268:GLU:O	1.35	1.24
15:O:237:ILE:CB	15:O:381:ILE:HD12	1.68	1.24
7:G:158:LYS:CG	15:O:105:ASN:OD1	1.86	1.23
15:O:432:LYS:HB3	15:O:609:TYR:CA	1.69	1.23
1:A:756:LYS:HD3	9:I:85:LYS:NZ	1.51	1.23
2:B:769:PHE:CE1	2:B:798:PHE:CE1	2.26	1.22
4:D:30:HIS:CE1	7:G:26:ASN:OD1	1.92	1.22
15:O:432:LYS:CG	15:O:608:GLU:O	1.88	1.22
2:B:769:PHE:CE1	2:B:798:PHE:HE1	1.56	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1605:THR:O	1:A:1606:SER:O	1.57	1.22
3:C:230:LEU:CD2	3:C:294:VAL:HG21	1.67	1.22
3:C:54:PHE:CZ	3:C:300:PHE:HB3	1.73	1.22
15:O:454:VAL:CB	15:O:514:PHE:CE2	2.17	1.22
3:C:131:THR:HG23	3:C:209:ILE:CG2	1.69	1.21
15:O:352:LEU:HD23	15:O:358:VAL:CG2	1.69	1.21
15:O:373:LEU:HD11	15:O:416:LYS:CG	1.69	1.21
15:O:352:LEU:CD2	15:O:358:VAL:HG22	1.71	1.20
3:C:31:TRP:CD1	11:K:82:LYS:NZ	2.10	1.20
15:O:432:LYS:CB	15:O:609:TYR:HA	1.71	1.20
1:A:477:ASN:OD1	2:B:1059:PRO:CG	1.90	1.20
3:C:62:SER:HB2	11:K:74:ASN:ND2	1.51	1.20
15:O:426:SER:OG	15:O:594:TYR:HB2	1.42	1.19
1:A:1050:TYR:CE1	1:A:1185:VAL:HG11	1.76	1.19
15:O:247:GLU:OE1	15:O:325:ILE:HG12	1.42	1.19
15:O:390:GLN:O	15:O:609:TYR:CE1	1.94	1.19
3:C:55:ASP:HA	3:C:299:ILE:HA	1.20	1.18
3:C:54:PHE:O	3:C:300:PHE:N	1.76	1.18
15:O:237:ILE:CG2	15:O:381:ILE:HD12	1.73	1.18
1:A:1008:ASP:OD1	1:A:1202:LEU:HD22	1.43	1.18
7:G:141:SER:CB	15:O:138:TYR:OH	1.92	1.17
15:O:162:PHE:O	15:O:210:ASN:O	1.61	1.17
15:O:237:ILE:HB	15:O:381:ILE:HD12	1.22	1.17
1:A:437:PHE:CE1	1:A:456:VAL:HG23	1.78	1.17
2:B:207:ILE:CG1	2:B:503:VAL:CG2	2.22	1.17
1:A:1006:LEU:CD1	2:B:716:MET:SD	2.32	1.17
2:B:207:ILE:CG1	2:B:503:VAL:HG21	1.73	1.17
1:A:83:VAL:HG21	1:A:427:PHE:CE2	1.78	1.16
1:A:1006:LEU:HD11	2:B:716:MET:SD	1.85	1.16
7:G:158:LYS:CD	15:O:105:ASN:OD1	1.91	1.16
15:O:430:ARG:NH2	15:O:596:PRO:HD3	1.60	1.16
1:A:1048:PHE:CZ	5:E:211:TYR:HD1	1.64	1.16
1:A:1011:VAL:HG11	1:A:1201:THR:C	1.63	1.16
1:A:756:LYS:CD	9:I:85:LYS:NZ	2.07	1.16
2:B:207:ILE:HG13	2:B:503:VAL:HG22	1.26	1.16
3:C:59:ILE:HG23	3:C:298:PHE:CE1	1.79	1.15
4:D:92:ILE:HG12	7:G:152:ALA:HB2	1.29	1.15
7:G:158:LYS:HG2	15:O:105:ASN:OD1	1.43	1.15
1:A:1344:ILE:HD12	2:B:329:TYR:HE2	1.10	1.14
1:A:556:ALA:HB2	15:O:246:ASN:ND2	1.63	1.14
15:O:219:ARG:NH2	15:O:360:VAL:HG21	1.63	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:408:PHE:CE2	15:O:446:LEU:HD11	1.83	1.14
15:O:408:PHE:CZ	15:O:446:LEU:HD13	1.81	1.13
7:G:143:SER:HB2	15:O:104:ILE:H	1.06	1.13
15:O:454:VAL:HA	15:O:514:PHE:CZ	1.83	1.12
2:B:42:VAL:HB	2:B:46:ILE:CD1	1.77	1.12
7:G:28:ILE:HG22	7:G:29:ASP:H	1.02	1.12
1:A:1348:VAL:CB	2:B:268:GLU:O	1.97	1.12
15:O:247:GLU:OE1	15:O:325:ILE:CG1	1.97	1.12
3:C:58:ASN:HA	3:C:296:ASN:CB	1.79	1.11
2:B:42:VAL:CG1	2:B:46:ILE:CD1	2.26	1.11
3:C:54:PHE:CD2	3:C:300:PHE:HB2	1.85	1.11
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.12	1.11
15:O:370:THR:O	15:O:374:PRO:HD3	1.51	1.11
15:O:598:PHE:HB3	15:O:599:LEU:HD13	1.12	1.11
15:O:156:MET:HG3	15:O:197:PHE:CE2	1.83	1.11
15:O:454:VAL:CG2	15:O:514:PHE:HE2	1.62	1.11
2:B:42:VAL:CB	2:B:46:ILE:CD1	2.29	1.10
7:G:158:LYS:HB3	15:O:105:ASN:ND2	1.65	1.10
13:M:101:VAL:CG1	13:M:106:LYS:HG3	1.81	1.10
1:A:1226:VAL:O	1:A:1598:PHE:HD2	1.34	1.10
15:O:129:PRO:HD2	15:O:132:THR:HB	1.32	1.10
15:O:156:MET:SD	15:O:197:PHE:CZ	2.45	1.10
15:O:446:LEU:O	15:O:449:TRP:HB3	1.51	1.10
1:A:83:VAL:CG1	1:A:427:PHE:CE2	2.34	1.10
1:A:480:ALA:HB2	2:B:1046:VAL:HG23	1.23	1.10
15:O:240:ILE:HG21	15:O:332:LEU:HB2	1.24	1.10
1:A:1011:VAL:HG11	1:A:1201:THR:O	1.51	1.10
3:C:31:TRP:CE3	11:K:82:LYS:HG3	1.86	1.10
3:C:58:ASN:CA	3:C:296:ASN:HB2	1.81	1.10
4:D:25:THR:HG22	6:F:59:GLN:HE21	1.07	1.10
7:G:158:LYS:CB	15:O:105:ASN:ND2	2.15	1.10
1:A:475:ARG:HD2	2:B:1059:PRO:O	1.51	1.09
3:C:59:ILE:CG2	3:C:298:PHE:CD1	2.35	1.09
15:O:425:GLY:HA2	15:O:483:ILE:HD11	1.34	1.09
3:C:55:ASP:OD1	3:C:299:ILE:HG12	1.53	1.09
7:G:158:LYS:HA	15:O:105:ASN:HD21	1.08	1.09
15:O:447:THR:O	15:O:450:LEU:HB2	1.50	1.09
3:C:31:TRP:HB3	11:K:82:LYS:HD2	1.17	1.09
3:C:56:LEU:HB2	3:C:298:PHE:HB2	1.35	1.09
3:C:230:LEU:HD23	3:C:294:VAL:CG2	1.83	1.09
1:A:436:ALA:CB	1:A:443:ALA:CB	2.21	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ARG:CD	2:B:1059:PRO:O	2.00	1.08
3:C:230:LEU:HD12	3:C:231:PRO:CD	1.84	1.08
4:D:28:PRO:HG2	7:G:24:VAL:HG11	1.28	1.08
15:O:138:TYR:CE2	15:O:142:ILE:CD1	2.35	1.08
15:O:201:LYS:HD2	15:O:239:SER:OG	1.54	1.08
1:A:478:TYR:CZ	2:B:1049:THR:HG23	1.88	1.08
1:A:1011:VAL:CG1	1:A:1201:THR:O	2.00	1.08
2:B:42:VAL:CB	2:B:46:ILE:HD11	1.84	1.08
4:D:25:THR:HA	6:F:59:GLN:HG2	1.32	1.08
15:O:129:PRO:CD	15:O:132:THR:HB	1.83	1.08
3:C:75:VAL:HB	3:C:221:PRO:HD3	1.36	1.07
3:C:57:ILE:HA	3:C:297:HIS:HA	1.14	1.07
15:O:156:MET:SD	15:O:197:PHE:HZ	1.78	1.07
1:A:478:TYR:CZ	2:B:1049:THR:CG2	2.38	1.07
3:C:230:LEU:HD12	3:C:231:PRO:HD3	1.36	1.07
15:O:138:TYR:CZ	15:O:142:ILE:HD11	1.89	1.07
1:A:475:ARG:NH2	2:B:1061:LYS:HB2	1.70	1.06
1:A:1008:ASP:O	1:A:1011:VAL:HG23	1.53	1.06
13:M:101:VAL:HG11	13:M:106:LYS:HG3	1.27	1.06
4:D:80:THR:OG1	15:O:227:PHE:CG	2.08	1.06
15:O:245:GLN:HG3	15:O:378:THR:HA	1.15	1.06
2:B:42:VAL:HG12	2:B:46:ILE:CD1	1.84	1.06
15:O:431:ALA:HB3	15:O:434:LEU:HD11	1.37	1.06
3:C:41:GLU:HB3	3:C:57:ILE:CG2	1.83	1.06
15:O:198:PHE:CD1	15:O:236:LYS:HE3	1.90	1.06
15:O:240:ILE:HG22	15:O:332:LEU:HD22	1.08	1.06
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	1.88	1.06
3:C:75:VAL:HG11	3:C:221:PRO:HG2	1.06	1.05
7:G:158:LYS:NZ	15:O:108:GLU:CG	1.78	1.05
15:O:162:PHE:CA	15:O:214:ASN:CB	2.33	1.05
1:A:408:LYS:HA	1:A:411:VAL:CG1	1.85	1.05
15:O:152:GLN:HG2	15:O:193:TYR:OH	1.52	1.05
15:O:431:ALA:HB1	15:O:434:LEU:HD11	1.34	1.05
1:A:1179:ILE:HD11	1:A:1183:GLU:HG3	1.33	1.05
15:O:240:ILE:CG2	15:O:332:LEU:HD22	1.87	1.05
1:A:1048:PHE:CZ	5:E:211:TYR:CD1	2.44	1.05
15:O:198:PHE:CZ	15:O:236:LYS:HG3	1.92	1.05
3:C:75:VAL:CB	3:C:221:PRO:CD	2.35	1.04
15:O:488:HIS:CG	15:O:489:ASN:H	1.74	1.04
15:O:390:GLN:NE2	15:O:432:LYS:H	1.54	1.04
3:C:131:THR:HG23	3:C:209:ILE:HG22	1.08	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:241:ARG:CB	15:O:189:PHE:CE2	2.39	1.04
15:O:152:GLN:CG	15:O:193:TYR:OH	2.04	1.04
1:A:83:VAL:HG11	1:A:427:PHE:CD2	1.90	1.04
1:A:502:ALA:HB1	1:A:581:ILE:CG2	1.87	1.04
7:G:141:SER:HB2	15:O:138:TYR:OH	1.53	1.04
15:O:174:ASP:HA	15:O:177:LYS:HE2	1.40	1.03
15:O:435:SER:HB3	15:O:438:GLN:HG3	1.37	1.03
4:D:25:THR:CG2	6:F:59:GLN:NE2	2.21	1.03
15:O:237:ILE:HB	15:O:381:ILE:CD1	1.88	1.03
1:A:1003:ARG:NE	2:B:520:LEU:HB2	1.74	1.03
12:L:68:GLU:HG2	12:L:69:ALA:H	1.23	1.03
1:A:1050:TYR:CE1	1:A:1185:VAL:CG1	2.42	1.02
1:A:782:ASP:OD2	1:A:931:SER:O	1.78	1.02
2:B:472:SER:CB	2:B:476:LEU:HD12	1.88	1.02
2:B:1155:ASP:OD2	7:G:239:THR:OG1	1.76	1.02
3:C:59:ILE:CG2	3:C:298:PHE:CE1	2.43	1.02
1:A:413:LEU:HB3	1:A:417:ARG:NH2	1.75	1.02
15:O:241:ASP:OD1	15:O:378:THR:HG22	1.58	1.02
1:A:909:SER:OG	9:I:83:LYS:CE	2.08	1.01
3:C:51:GLU:HB3	3:C:303:GLU:HG2	1.42	1.01
15:O:369:LYS:O	15:O:373:LEU:N	1.91	1.01
1:A:392:THR:CG2	1:A:430:ILE:HB	1.88	1.01
1:A:480:ALA:CB	2:B:1046:VAL:HG23	1.90	1.01
3:C:56:LEU:CD1	3:C:300:PHE:CE1	2.44	1.01
7:G:158:LYS:HB3	15:O:105:ASN:CG	1.79	1.01
15:O:201:LYS:CD	15:O:239:SER:OG	2.09	1.01
2:B:42:VAL:C	2:B:46:ILE:HD12	1.82	1.00
15:O:428:ILE:HG23	15:O:439:ILE:HG21	1.38	1.00
3:C:45:SER:HB2	3:C:271:ARG:NH2	1.76	1.00
7:G:158:LYS:CA	15:O:105:ASN:HD21	1.75	1.00
1:A:408:LYS:HA	1:A:411:VAL:HG12	1.40	1.00
1:A:799:GLU:HG3	1:A:1062:HIS:CG	1.95	1.00
7:G:158:LYS:HZ3	15:O:108:GLU:CG	1.27	1.00
15:O:348:THR:HG22	15:O:351:SER:HB3	1.42	1.00
15:O:352:LEU:HA	15:O:358:VAL:HG23	1.44	1.00
1:A:756:LYS:CD	9:I:85:LYS:HZ2	1.70	1.00
1:A:782:ASP:OD1	1:A:783:LYS:N	1.93	1.00
15:O:240:ILE:HG21	15:O:332:LEU:CB	1.92	1.00
15:O:352:LEU:HD23	15:O:358:VAL:HG22	1.00	1.00
15:O:428:ILE:HD12	15:O:439:ILE:HG23	1.44	1.00
15:O:471:LYS:CB	15:O:585:PHE:CE1	2.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ASP:HB3	2:B:440:PHE:CE2	1.97	0.99
1:A:1055:ILE:HD12	1:A:1063:MET:CE	1.91	0.99
15:O:454:VAL:CG2	15:O:514:PHE:CE2	2.44	0.99
7:G:143:SER:CB	15:O:104:ILE:H	1.75	0.99
15:O:158:LEU:HD23	15:O:172:HIS:HD2	1.25	0.99
1:A:1006:LEU:HD12	2:B:716:MET:SD	2.01	0.99
7:G:158:LYS:CA	15:O:105:ASN:ND2	2.25	0.99
1:A:1344:ILE:HD12	2:B:329:TYR:CE2	1.97	0.98
2:B:70:GLU:CB	2:B:98:SER:HB3	1.93	0.98
2:B:1019:GLY:HA3	3:C:65:ASN:HB2	1.45	0.98
3:C:54:PHE:CZ	3:C:300:PHE:CB	2.41	0.98
3:C:84:TYR:CD2	12:L:66:GLN:HB2	1.99	0.98
2:B:70:GLU:HB3	2:B:98:SER:HB3	0.99	0.98
15:O:240:ILE:CG2	15:O:332:LEU:HD13	1.93	0.98
15:O:373:LEU:HD11	15:O:416:LYS:HG3	1.43	0.98
7:G:241:ARG:CB	15:O:189:PHE:HE2	1.76	0.98
15:O:598:PHE:CB	15:O:599:LEU:HD13	1.92	0.98
1:A:392:THR:HG21	1:A:430:ILE:CB	1.94	0.98
6:F:75:PRO:HG2	6:F:78:GLN:CB	1.92	0.98
1:A:909:SER:OG	9:I:83:LYS:HE2	1.62	0.97
1:A:83:VAL:CG2	1:A:427:PHE:CZ	2.47	0.97
4:D:96:PHE:HE1	7:G:150:HIS:HB3	1.28	0.97
15:O:423:TYR:HD1	15:O:594:TYR:CE2	1.82	0.97
13:M:105:SER:HA	13:M:108:LEU:HG	1.46	0.97
1:A:392:THR:HG21	1:A:430:ILE:HB	0.98	0.97
1:A:509:GLU:OE2	1:A:579:ARG:NE	1.97	0.97
1:A:953:GLU:HG2	1:A:1205:PHE:CE2	2.00	0.97
2:B:70:GLU:HB3	2:B:98:SER:CB	1.93	0.97
15:O:454:VAL:HB	15:O:514:PHE:HE2	0.99	0.96
1:A:476:VAL:HG11	2:B:1071:VAL:HG23	1.47	0.96
1:A:480:ALA:HB2	2:B:1046:VAL:CG2	1.95	0.96
1:A:1660:VAL:O	7:G:102:GLU:HA	1.65	0.96
3:C:59:ILE:HG22	3:C:298:PHE:CD1	1.98	0.96
1:A:83:VAL:CG2	1:A:427:PHE:CE2	2.48	0.96
1:A:966:LEU:HD22	1:A:997:PHE:CZ	2.00	0.96
2:B:769:PHE:CD1	2:B:798:PHE:HE1	1.83	0.96
15:O:156:MET:CG	15:O:197:PHE:CE2	2.48	0.96
1:A:1055:ILE:HG21	1:A:1060:GLU:HG3	1.47	0.95
1:A:1:MET:HG2	2:B:1098:TYR:CZ	2.01	0.95
1:A:502:ALA:HB1	1:A:581:ILE:HG21	1.46	0.95
7:G:158:LYS:HD3	15:O:105:ASN:OD1	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ILE:HG12	15:O:376:TYR:CE2	2.01	0.95
15:O:440:ILE:HG23	15:O:491:PHE:HE1	1.27	0.95
15:O:408:PHE:HZ	15:O:446:LEU:HD11	1.25	0.95
1:A:502:ALA:CB	1:A:581:ILE:HG21	1.97	0.95
2:B:1090:ASP:OD1	2:B:1095:SER:OG	1.85	0.95
15:O:454:VAL:HG23	15:O:514:PHE:CE2	2.01	0.95
1:A:1344:ILE:CD1	2:B:329:TYR:HE2	1.78	0.94
2:B:77:LYS:NZ	2:B:438:ILE:O	1.99	0.94
15:O:63:LEU:HD12	15:O:71:ILE:HG13	1.47	0.94
15:O:374:PRO:O	15:O:419:LYS:NZ	2.01	0.94
1:A:401:ASP:OD2	1:A:405:LYS:HE3	1.67	0.94
15:O:234:ILE:CG2	15:O:371:HIS:HD2	1.81	0.94
7:G:158:LYS:HD3	15:O:105:ASN:CG	1.88	0.94
3:C:75:VAL:HB	3:C:221:PRO:CD	1.94	0.94
1:A:799:GLU:HG3	1:A:1062:HIS:ND1	1.83	0.93
1:A:990:ILE:HA	1:A:994:GLU:OE1	1.69	0.93
2:B:894:LYS:H	12:L:54:ARG:NH2	1.66	0.93
15:O:342:HIS:CD2	15:O:346:GLN:HE21	1.85	0.93
15:O:417:LYS:HD2	15:O:472:HIS:CE1	2.02	0.93
1:A:878:ARG:HG2	9:I:67:VAL:HG11	1.48	0.93
15:O:241:ASP:CG	15:O:378:THR:HG22	1.88	0.93
2:B:209:GLN:HG2	2:B:210:ARG:H	1.31	0.93
2:B:211:ARG:HG2	2:B:401:GLU:OE1	1.68	0.93
3:C:57:ILE:HD12	3:C:297:HIS:ND1	1.82	0.93
15:O:198:PHE:HD2	15:O:232:LEU:HG	1.05	0.93
3:C:62:SER:CB	11:K:74:ASN:ND2	2.32	0.93
7:G:242:VAL:HG11	15:O:185:SER:HG	1.32	0.93
15:O:342:HIS:O	15:O:346:GLN:HG2	1.68	0.93
3:C:75:VAL:CG1	3:C:221:PRO:HG2	1.89	0.93
4:D:80:THR:OG1	15:O:227:PHE:CD2	2.20	0.93
15:O:358:VAL:O	15:O:362:ASN:ND2	2.00	0.93
1:A:413:LEU:HB3	1:A:417:ARG:HH21	1.29	0.93
4:D:92:ILE:HG22	4:D:96:PHE:CZ	2.03	0.93
7:G:158:LYS:CB	15:O:105:ASN:CG	2.35	0.93
7:G:158:LYS:CG	15:O:105:ASN:CG	2.37	0.93
3:C:75:VAL:CB	3:C:221:PRO:HD2	1.97	0.92
15:O:598:PHE:HB3	15:O:599:LEU:CD1	1.99	0.92
3:C:131:THR:CG2	3:C:209:ILE:HG22	1.98	0.92
7:G:154:ASN:HD21	15:O:182:MET:CE	1.82	0.92
1:A:83:VAL:HG21	1:A:427:PHE:HZ	1.13	0.92
15:O:224:GLU:OE1	15:O:224:GLU:N	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HD3	9:I:85:LYS:HZ1	1.19	0.92
3:C:71:MET:SD	3:C:225:ALA:HB1	2.10	0.92
15:O:147:ILE:O	15:O:149:LYS:N	2.03	0.92
14:N:85:HIS:HE1	14:N:141:GLU:CD	1.72	0.92
15:O:386:PHE:HD2	15:O:606:MET:CE	1.83	0.92
15:O:390:GLN:O	15:O:609:TYR:HE1	1.52	0.92
15:O:435:SER:CB	15:O:438:GLN:HG3	1.98	0.92
1:A:1658:ALA:O	7:G:104:LEU:HA	1.70	0.91
15:O:240:ILE:HG22	15:O:332:LEU:CD2	1.98	0.91
6:F:74:ILE:HG23	6:F:75:PRO:HD2	1.51	0.91
7:G:28:ILE:HG22	7:G:29:ASP:N	1.81	0.91
2:B:894:LYS:H	12:L:54:ARG:HH21	0.92	0.91
15:O:219:ARG:NH2	15:O:360:VAL:CG2	2.32	0.91
15:O:408:PHE:HZ	15:O:446:LEU:CD1	1.74	0.91
3:C:52:ALA:O	3:C:301:ASN:HA	1.69	0.91
3:C:253:PRO:HB2	14:N:180:PHE:CD1	2.06	0.91
15:O:390:GLN:NE2	15:O:609:TYR:HB3	1.86	0.91
1:A:478:TYR:C	2:B:1047:ARG:O	2.08	0.91
15:O:240:ILE:HG21	15:O:332:LEU:HD13	1.51	0.91
1:A:1036:ASN:O	1:A:1049:MET:HA	1.71	0.91
15:O:478:GLN:HE21	15:O:592:PHE:HZ	1.19	0.91
1:A:412:SER:O	1:A:416:ARG:N	2.03	0.90
2:B:42:VAL:HG11	2:B:46:ILE:HD11	1.52	0.90
2:B:894:LYS:N	12:L:54:ARG:HH21	1.69	0.90
2:B:472:SER:OG	2:B:476:LEU:HD12	1.71	0.90
3:C:230:LEU:HD23	3:C:294:VAL:HG21	0.91	0.90
15:O:342:HIS:CE1	15:O:346:GLN:HG3	2.05	0.90
15:O:426:SER:OG	15:O:594:TYR:CB	2.18	0.90
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.06	0.90
15:O:240:ILE:CG2	15:O:332:LEU:HB2	2.01	0.90
4:D:25:THR:HA	6:F:59:GLN:CG	1.99	0.90
15:O:454:VAL:HA	15:O:514:PHE:HZ	1.34	0.90
1:A:756:LYS:CD	9:I:85:LYS:HZ1	1.76	0.90
1:A:1048:PHE:HE2	5:E:211:TYR:H	1.11	0.90
15:O:471:LYS:HB2	15:O:585:PHE:HE1	1.00	0.90
1:A:516:ILE:HG21	15:O:376:TYR:OH	1.72	0.90
3:C:41:GLU:HB3	3:C:57:ILE:HG21	1.53	0.90
4:D:28:PRO:HG2	7:G:24:VAL:CG1	2.01	0.90
1:A:413:LEU:O	1:A:417:ARG:NE	2.05	0.90
3:C:75:VAL:HG11	3:C:221:PRO:HD2	1.54	0.90
15:O:158:LEU:HD23	15:O:172:HIS:CD2	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:426:SER:CB	15:O:594:TYR:HB2	2.01	0.90
15:O:432:LYS:HB2	15:O:609:TYR:C	1.93	0.90
3:C:31:TRP:CG	11:K:82:LYS:HD2	2.06	0.89
3:C:86:PHE:CE1	12:L:64:LEU:HD13	2.07	0.89
15:O:198:PHE:CG	15:O:236:LYS:HE3	2.06	0.89
1:A:1226:VAL:O	1:A:1598:PHE:CD2	2.24	0.89
7:G:158:LYS:HA	15:O:105:ASN:ND2	1.85	0.89
15:O:194:LEU:O	15:O:232:LEU:HD21	1.72	0.89
15:O:421:LEU:HD13	15:O:476:ALA:HB2	1.54	0.89
2:B:478:LEU:HD13	2:B:484:TYR:CE1	2.06	0.89
4:D:96:PHE:CE1	7:G:150:HIS:HB3	2.07	0.89
1:A:1050:TYR:HE1	1:A:1185:VAL:CG1	1.83	0.89
1:A:1179:ILE:HD11	1:A:1183:GLU:CG	2.01	0.89
4:D:80:THR:HG21	15:O:227:PHE:HB3	1.53	0.89
15:O:129:PRO:CG	15:O:132:THR:HB	2.01	0.89
3:C:37:LYS:HD2	11:K:130:VAL:HG22	1.54	0.89
2:B:42:VAL:CB	2:B:46:ILE:HD12	2.00	0.89
15:O:432:LYS:CB	15:O:609:TYR:CA	2.41	0.89
15:O:457:ARG:HA	15:O:460:GLU:HB2	1.54	0.89
15:O:219:ARG:HH21	15:O:360:VAL:CG2	1.85	0.89
1:A:891:ILE:CD1	9:I:71:LEU:HB2	2.03	0.89
13:M:102:SER:O	13:M:106:LYS:HB2	1.73	0.89
1:A:406:LEU:CD1	1:A:411:VAL:HB	2.03	0.88
6:F:66:ARG:CZ	7:G:90:LEU:HD13	2.02	0.88
2:B:894:LYS:HG2	12:L:47:ARG:CD	2.04	0.88
3:C:58:ASN:H	3:C:296:ASN:C	1.75	0.88
1:A:401:ASP:O	1:A:405:LYS:HB2	1.74	0.88
3:C:56:LEU:HD11	3:C:300:PHE:CE1	2.08	0.88
4:D:28:PRO:CG	7:G:24:VAL:HG11	2.03	0.88
1:A:83:VAL:CG1	1:A:427:PHE:HE2	1.80	0.88
1:A:1348:VAL:CG2	2:B:268:GLU:O	2.21	0.88
1:A:1038:ILE:HG12	1:A:1049:MET:O	1.74	0.88
15:O:521:ASN:HD22	15:O:524:VAL:H	1.22	0.88
3:C:230:LEU:CD1	3:C:231:PRO:CD	2.52	0.88
1:A:556:ALA:HB2	15:O:246:ASN:HD22	1.38	0.88
2:B:769:PHE:CE1	2:B:798:PHE:CZ	2.61	0.88
15:O:488:HIS:ND1	15:O:489:ASN:N	2.21	0.88
15:O:488:HIS:O	15:O:490:ILE:N	2.06	0.88
15:O:459:GLU:O	15:O:463:GLN:HG3	1.73	0.87
3:C:75:VAL:CB	3:C:221:PRO:HD3	2.01	0.87
1:A:1662:ASN:HA	7:G:101:SER:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:LEU:CD1	3:C:231:PRO:HD2	2.04	0.87
15:O:417:LYS:CD	15:O:472:HIS:CE1	2.57	0.87
1:A:756:LYS:HD2	9:I:85:LYS:NZ	1.86	0.87
15:O:198:PHE:HD2	15:O:232:LEU:CG	1.86	0.87
3:C:131:THR:CG2	3:C:209:ILE:CG2	2.51	0.87
1:A:475:ARG:HD3	2:B:1059:PRO:O	1.73	0.87
1:A:1055:ILE:HD12	1:A:1063:MET:SD	2.14	0.87
7:G:158:LYS:HZ3	15:O:108:GLU:HG2	1.39	0.87
1:A:1:MET:HA	2:B:1098:TYR:CD1	2.10	0.87
1:A:862:THR:O	9:I:67:VAL:HG12	1.73	0.87
3:C:70:ILE:HD11	11:K:71:THR:CG2	2.04	0.87
3:C:75:VAL:CG1	3:C:221:PRO:HG3	2.03	0.87
1:A:1660:VAL:HG22	7:G:103:LYS:O	1.75	0.86
4:D:25:THR:O	6:F:59:GLN:HG3	1.75	0.86
4:D:80:THR:CB	15:O:227:PHE:CD2	2.58	0.86
1:A:636:HIS:ND1	2:B:1091:ARG:NH2	2.22	0.86
1:A:1600:ARG:CD	1:A:1616:GLU:OE1	2.24	0.86
11:K:66:VAL:HG12	11:K:67:GLU:HG2	1.57	0.86
1:A:1348:VAL:HB	2:B:268:GLU:C	1.95	0.86
3:C:56:LEU:HG	3:C:300:PHE:CD1	2.10	0.86
1:A:408:LYS:CA	1:A:411:VAL:HG12	2.04	0.86
3:C:31:TRP:CD2	11:K:82:LYS:HG3	2.10	0.86
7:G:143:SER:HB2	15:O:104:ILE:N	1.89	0.86
1:A:475:ARG:HH22	2:B:1061:LYS:HB2	1.36	0.86
3:C:59:ILE:HG22	3:C:298:PHE:HD1	1.38	0.86
1:A:878:ARG:HE	9:I:67:VAL:CG1	1.87	0.86
1:A:1003:ARG:CZ	2:B:520:LEU:HB2	2.04	0.86
3:C:31:TRP:HB3	11:K:82:LYS:CD	2.03	0.86
15:O:366:THR:O	15:O:370:THR:HG23	1.75	0.86
15:O:417:LYS:HB3	15:O:472:HIS:NE2	1.91	0.86
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.07	0.86
4:D:80:THR:CG2	15:O:227:PHE:HB3	2.06	0.86
1:A:468:ARG:NE	1:A:1021:ARG:NH1	2.23	0.86
7:G:141:SER:CA	15:O:138:TYR:OH	2.24	0.86
15:O:521:ASN:ND2	15:O:523:ASN:H	1.74	0.86
15:O:457:ARG:O	15:O:460:GLU:HB2	1.76	0.85
15:O:458:GLU:CA	15:O:461:VAL:CG2	2.08	0.85
1:A:1008:ASP:OD1	1:A:1202:LEU:CD2	2.24	0.85
15:O:396:MET:HE1	15:O:434:LEU:HD12	1.57	0.85
15:O:181:ARG:CB	15:O:181:ARG:HH11	1.89	0.85
15:O:163:ILE:HG22	15:O:211:TYR:HB2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1661:PRO:C	7:G:101:SER:O	2.13	0.85
3:C:64:ALA:C	3:C:227:TYR:HE2	1.80	0.85
15:O:408:PHE:CE2	15:O:446:LEU:CD1	2.50	0.85
1:A:1060:GLU:HA	1:A:1063:MET:HG3	1.55	0.84
15:O:369:LYS:HB3	15:O:369:LYS:HZ3	1.37	0.84
1:A:392:THR:HB	1:A:430:ILE:HD13	1.59	0.84
2:B:472:SER:HB3	2:B:476:LEU:HD12	1.57	0.84
7:G:25:THR:HG22	7:G:26:ASN:H	1.40	0.84
15:O:181:ARG:HH11	15:O:181:ARG:HB2	1.41	0.84
15:O:237:ILE:HG22	15:O:381:ILE:HD12	1.60	0.84
15:O:361:PHE:O	15:O:365:THR:HG23	1.78	0.84
15:O:386:PHE:HD2	15:O:606:MET:HE1	1.41	0.84
1:A:1055:ILE:HG23	1:A:1063:MET:SD	2.17	0.84
3:C:253:PRO:HB2	14:N:180:PHE:HD1	1.41	0.84
15:O:243:GLU:HA	15:O:246:ASN:ND2	1.90	0.84
15:O:447:THR:HG22	15:O:480:LEU:HD22	1.58	0.84
1:A:436:ALA:HB2	1:A:443:ALA:HB2	0.86	0.84
1:A:1019:LEU:HD12	1:A:1227:MET:HG3	1.58	0.84
1:A:1600:ARG:HD2	1:A:1616:GLU:OE1	1.77	0.84
1:A:413:LEU:C	1:A:417:ARG:HH21	1.81	0.84
2:B:472:SER:CB	2:B:476:LEU:CD1	2.54	0.84
15:O:240:ILE:CB	15:O:332:LEU:HD13	2.07	0.84
2:B:37:LEU:HD13	2:B:760:TYR:CZ	2.12	0.84
2:B:42:VAL:O	2:B:46:ILE:HD12	1.76	0.84
4:D:96:PHE:HE1	7:G:150:HIS:CB	1.91	0.84
6:F:74:ILE:CG2	6:F:75:PRO:HD2	2.08	0.84
15:O:422:GLN:NE2	15:O:592:PHE:CE2	2.45	0.84
7:G:242:VAL:HG12	15:O:185:SER:OG	1.77	0.83
1:A:1008:ASP:CG	1:A:1202:LEU:HD13	1.98	0.83
2:B:894:LYS:O	2:B:896:GLN:N	2.11	0.83
15:O:398:SER:O	15:O:401:VAL:HG12	1.79	0.83
15:O:467:MET:HG3	15:O:519:PHE:CZ	2.13	0.83
1:A:436:ALA:CA	1:A:443:ALA:HB2	2.09	0.83
1:A:863:ASN:ND2	9:I:68:LYS:N	2.25	0.83
3:C:86:PHE:HE1	12:L:64:LEU:HD13	1.42	0.83
15:O:359:GLY:HA2	15:O:362:ASN:HD22	1.43	0.83
1:A:990:ILE:HB	1:A:994:GLU:HB2	1.61	0.83
1:A:990:ILE:CA	1:A:994:GLU:OE1	2.26	0.83
3:C:51:GLU:HB3	3:C:303:GLU:CG	2.08	0.83
15:O:240:ILE:HG21	15:O:332:LEU:CD1	2.08	0.83
15:O:156:MET:CG	15:O:197:PHE:CZ	2.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:370:THR:O	15:O:374:PRO:CD	2.25	0.83
2:B:207:ILE:HG12	2:B:503:VAL:HG21	1.59	0.83
15:O:242:VAL:HA	15:O:378:THR:HG21	1.60	0.83
15:O:390:GLN:NE2	15:O:432:LYS:N	2.25	0.83
1:A:1026:GLN:OE1	1:A:1603:MET:HB2	1.78	0.83
4:D:25:THR:CA	6:F:59:GLN:HG2	2.07	0.83
15:O:428:ILE:CG2	15:O:439:ILE:HG21	2.09	0.83
15:O:457:ARG:CA	15:O:460:GLU:HB2	2.09	0.83
1:A:1:MET:HA	2:B:1098:TYR:CE1	2.13	0.83
1:A:556:ALA:CB	15:O:246:ASN:HD22	1.90	0.83
15:O:454:VAL:CA	15:O:514:PHE:CE2	2.62	0.83
1:A:1654:PHE:CZ	6:F:92:ARG:HD3	2.14	0.83
3:C:253:PRO:HG2	14:N:180:PHE:HB3	1.61	0.83
1:A:1179:ILE:CD1	1:A:1183:GLU:HG3	2.09	0.83
1:A:1603:MET:HE2	1:A:1615:TYR:CD2	2.14	0.83
15:O:352:LEU:O	15:O:358:VAL:HG21	1.77	0.83
15:O:488:HIS:CG	15:O:489:ASN:N	2.40	0.83
1:A:1575:ILE:CG1	9:I:122:ARG:HH12	1.92	0.82
15:O:242:VAL:N	15:O:378:THR:HG21	1.94	0.82
15:O:440:ILE:HG23	15:O:491:PHE:CE1	2.13	0.82
3:C:31:TRP:CG	11:K:82:LYS:NZ	2.44	0.82
1:A:406:LEU:HD13	1:A:411:VAL:HB	1.60	0.82
15:O:246:ASN:OD1	15:O:247:GLU:N	2.11	0.82
3:C:55:ASP:HA	3:C:299:ILE:CA	2.07	0.82
7:G:158:LYS:HD3	15:O:105:ASN:CB	2.09	0.82
1:A:437:PHE:CZ	1:A:456:VAL:HG21	2.14	0.82
4:D:25:THR:HB	6:F:59:GLN:NE2	1.94	0.82
3:C:55:ASP:CA	3:C:299:ILE:HA	2.08	0.82
1:A:1:MET:HG2	2:B:1098:TYR:CE2	2.12	0.82
1:A:556:ALA:CB	15:O:246:ASN:ND2	2.41	0.82
4:D:95:ASP:OD2	7:G:150:HIS:HA	1.80	0.82
15:O:245:GLN:HG3	15:O:378:THR:CA	2.05	0.82
4:D:25:THR:CA	6:F:59:GLN:CG	2.57	0.82
7:G:158:LYS:NZ	15:O:108:GLU:HG2	1.95	0.82
4:D:25:THR:HB	6:F:59:GLN:CD	2.00	0.81
1:A:863:ASN:HD22	9:I:67:VAL:HA	1.45	0.81
15:O:386:PHE:CD2	15:O:606:MET:CE	2.62	0.81
15:O:457:ARG:C	15:O:460:GLU:HB2	2.01	0.81
2:B:472:SER:HB3	2:B:476:LEU:CD1	2.11	0.81
2:B:776:ILE:HB	2:B:1026:ILE:HD13	1.60	0.81
15:O:162:PHE:HA	15:O:214:ASN:CB	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:383:TYR:CD2	15:O:597:LEU:HD22	2.15	0.81
1:A:50:TYR:HE1	1:A:368:ARG:O	1.64	0.81
15:O:237:ILE:CG2	15:O:381:ILE:CD1	2.57	0.81
15:O:454:VAL:HA	15:O:514:PHE:CE2	2.15	0.81
1:A:1011:VAL:HG13	1:A:1201:THR:O	1.80	0.81
1:A:782:ASP:CG	1:A:931:SER:O	2.18	0.81
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.63	0.81
3:C:253:PRO:O	14:N:180:PHE:CD1	2.34	0.81
4:D:80:THR:HG21	15:O:227:PHE:CD2	2.16	0.81
15:O:369:LYS:HE2	15:O:370:THR:CG2	2.10	0.81
3:C:75:VAL:HG12	3:C:221:PRO:CG	2.11	0.81
15:O:458:GLU:HA	15:O:461:VAL:HG21	1.59	0.81
1:A:564:PRO:HG2	15:O:371:HIS:ND1	1.97	0.80
15:O:243:GLU:HA	15:O:246:ASN:HD21	1.46	0.80
1:A:966:LEU:HD22	1:A:997:PHE:HZ	1.44	0.80
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.21	0.80
15:O:387:HIS:HB2	15:O:606:MET:SD	2.21	0.80
1:A:1004:GLU:HA	1:A:1007:ILE:HD12	1.64	0.80
2:B:208:VAL:HG23	2:B:401:GLU:HG2	1.64	0.80
3:C:57:ILE:HA	3:C:297:HIS:CA	2.05	0.80
4:D:92:ILE:CG2	4:D:96:PHE:CZ	2.63	0.80
1:A:1000:MET:HG2	2:B:520:LEU:HD23	1.62	0.80
3:C:37:LYS:HD2	11:K:130:VAL:CG2	2.11	0.80
3:C:56:LEU:HD12	3:C:300:PHE:HE1	1.46	0.80
4:D:28:PRO:HD2	7:G:24:VAL:HG13	1.62	0.80
15:O:240:ILE:HG21	15:O:332:LEU:CG	2.11	0.80
7:G:141:SER:HA	15:O:138:TYR:OH	1.82	0.80
7:G:158:LYS:CD	15:O:105:ASN:CG	2.48	0.80
3:C:75:VAL:HG21	3:C:221:PRO:HD2	1.64	0.80
15:O:166:ILE:CD1	15:O:213:SER:OG	2.30	0.80
6:F:75:PRO:CG	6:F:78:GLN:HB2	2.05	0.79
1:A:478:TYR:CE1	2:B:1049:THR:HG23	2.16	0.79
1:A:996:TYR:O	1:A:1000:MET:HG3	1.83	0.79
3:C:71:MET:HE1	3:C:302:VAL:HG22	1.64	0.79
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	1.65	0.79
3:C:31:TRP:HB2	11:K:82:LYS:HD2	1.59	0.79
1:A:403:LEU:CD1	1:A:419:ILE:HG21	2.12	0.79
15:O:234:ILE:HG21	15:O:371:HIS:CD2	2.18	0.79
4:D:25:THR:CB	6:F:59:GLN:NE2	2.46	0.79
15:O:436:ARG:O	15:O:440:ILE:HG13	1.82	0.79
1:A:401:ASP:OD2	1:A:405:LYS:CE	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASP:O	1:A:405:LYS:CB	2.31	0.79
15:O:129:PRO:HG2	15:O:132:THR:HB	1.63	0.79
2:B:480:GLN:OE1	2:B:480:GLN:N	2.14	0.78
15:O:584:GLN:OE1	15:O:584:GLN:N	2.11	0.78
1:A:638:PRO:HA	2:B:1090:ASP:OD2	1.82	0.78
1:A:953:GLU:HA	1:A:1205:PHE:CD2	2.18	0.78
2:B:42:VAL:HG12	2:B:46:ILE:CG1	2.14	0.78
2:B:566:TYR:HD2	13:M:73:SER:OG	1.66	0.78
3:C:253:PRO:CB	14:N:180:PHE:HD1	1.95	0.78
15:O:243:GLU:O	15:O:246:ASN:OD1	1.99	0.78
15:O:372:VAL:C	15:O:374:PRO:HD2	2.04	0.78
15:O:478:GLN:NE2	15:O:592:PHE:HZ	1.81	0.78
1:A:249:THR:OG1	1:A:435:ASN:ND2	2.16	0.78
2:B:75:ASP:HB3	2:B:440:PHE:CZ	2.17	0.78
1:A:1348:VAL:HG11	2:B:268:GLU:HB2	1.66	0.78
15:O:174:ASP:CA	15:O:177:LYS:HE2	2.12	0.78
3:C:50:ARG:O	3:C:303:GLU:HA	1.84	0.78
1:A:1344:ILE:HG22	2:B:333:LYS:HB3	1.66	0.78
3:C:75:VAL:CG2	3:C:221:PRO:HD2	2.14	0.78
4:D:23:HIS:CD2	6:F:58:PHE:CE2	2.71	0.78
15:O:242:VAL:CA	15:O:378:THR:HG21	2.14	0.78
15:O:373:LEU:CD1	15:O:416:LYS:HG3	2.13	0.78
1:A:1604:GLU:O	1:A:1612:LYS:HE2	1.83	0.78
2:B:934:ILE:HG22	3:C:72:ILE:HB	1.66	0.78
15:O:129:PRO:HG2	15:O:132:THR:CB	2.14	0.78
15:O:430:ARG:NH2	15:O:596:PRO:CD	2.44	0.78
4:D:28:PRO:CG	7:G:24:VAL:CG1	2.62	0.77
2:B:68:ILE:HD11	2:B:414:LYS:HG3	1.66	0.77
2:B:1043:LYS:HD3	2:B:1063:ARG:NH2	1.97	0.77
1:A:1344:ILE:HG22	2:B:333:LYS:CB	2.15	0.77
7:G:154:ASN:HD21	15:O:182:MET:HE3	1.48	0.77
1:A:1:MET:HB2	2:B:1098:TYR:CG	2.19	0.77
1:A:475:ARG:CZ	2:B:1061:LYS:HB2	2.14	0.77
2:B:467:THR:HB	2:B:469:ASN:ND2	2.00	0.77
15:O:186:SER:O	15:O:190:ILE:HG22	1.84	0.77
15:O:414:ALA:O	15:O:418:ILE:HD12	1.85	0.77
1:A:1028:GLU:HG3	1:A:1029:GLY:N	2.00	0.77
15:O:234:ILE:CG2	15:O:371:HIS:CD2	2.66	0.77
15:O:386:PHE:CD2	15:O:606:MET:HE1	2.20	0.77
1:A:1603:MET:CE	1:A:1615:TYR:CD2	2.68	0.76
1:A:1662:ASN:CA	7:G:101:SER:HB2	2.13	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:VAL:HG12	3:C:221:PRO:HG3	1.63	0.76
9:I:60:LEU:HA	9:I:63:LYS:HG3	1.65	0.76
15:O:359:GLY:O	15:O:363:THR:HG22	1.85	0.76
15:O:425:GLY:HA2	15:O:483:ILE:CD1	2.13	0.76
2:B:878:GLU:OE2	2:B:909:ARG:NH1	2.17	0.76
15:O:174:ASP:O	15:O:177:LYS:HG2	1.85	0.76
15:O:240:ILE:HB	15:O:332:LEU:HD13	1.66	0.76
1:A:437:PHE:HZ	1:A:456:VAL:CG2	1.98	0.76
3:C:56:LEU:CD1	3:C:300:PHE:HE1	1.95	0.76
15:O:360:VAL:O	15:O:364:LEU:HG	1.83	0.76
2:B:328:GLN:HE22	13:M:109:ARG:HH21	1.31	0.76
3:C:75:VAL:CG1	3:C:221:PRO:HD3	2.10	0.76
15:O:62:ASP:HB3	15:O:67:ASP:OD2	1.86	0.76
1:A:438:ILE:HG23	2:B:1192:MET:HG2	1.68	0.76
3:C:55:ASP:OD1	3:C:299:ILE:CG1	2.34	0.76
15:O:432:LYS:CB	15:O:609:TYR:C	2.54	0.76
15:O:484:PHE:CE1	15:O:502:LEU:CD1	2.69	0.76
1:A:502:ALA:HB1	1:A:581:ILE:HG22	1.64	0.76
1:A:641:GLU:HB2	6:F:99:LEU:HD13	1.68	0.76
2:B:1069:ILE:HG22	2:B:1070:ARG:H	1.50	0.76
15:O:158:LEU:CD2	15:O:172:HIS:CD2	2.67	0.76
1:A:478:TYR:CE2	2:B:1049:THR:CG2	2.68	0.76
15:O:454:VAL:CA	15:O:514:PHE:CZ	2.67	0.76
3:C:131:THR:HG23	3:C:209:ILE:HG23	1.68	0.76
7:G:159:LYS:H	15:O:105:ASN:HD22	1.32	0.76
1:A:1055:ILE:CG2	1:A:1060:GLU:HG3	2.16	0.76
3:C:70:ILE:HD11	11:K:71:THR:HG21	1.67	0.76
7:G:154:ASN:OD1	15:O:183:ILE:HG12	1.85	0.76
1:A:1052:GLY:O	5:E:205:SER:HB2	1.85	0.76
1:A:878:ARG:NE	9:I:67:VAL:CG1	2.48	0.75
1:A:1050:TYR:CD1	1:A:1185:VAL:HG11	2.20	0.75
2:B:769:PHE:HE1	2:B:798:PHE:CZ	2.03	0.75
15:O:219:ARG:HH22	15:O:360:VAL:HG21	1.47	0.75
15:O:371:HIS:C	15:O:374:PRO:HD2	2.06	0.75
6:F:66:ARG:NH2	7:G:90:LEU:HD13	2.01	0.75
15:O:359:GLY:HA2	15:O:362:ASN:ND2	2.01	0.75
1:A:1019:LEU:CD1	1:A:1227:MET:HG3	2.17	0.75
15:O:166:ILE:HD13	15:O:213:SER:OG	1.86	0.75
1:A:891:ILE:HD13	9:I:71:LEU:HB2	1.68	0.75
1:A:1048:PHE:HE2	5:E:211:TYR:N	1.83	0.75
15:O:428:ILE:HD12	15:O:439:ILE:CG2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:PHE:CE2	5:E:211:TYR:N	2.53	0.75
2:B:42:VAL:HB	2:B:46:ILE:HD11	1.51	0.75
2:B:207:ILE:CG1	2:B:503:VAL:HG22	2.04	0.75
3:C:131:THR:HG22	3:C:208:CYS:O	1.86	0.75
4:D:44:ILE:HG21	4:D:90:LYS:HE3	1.69	0.75
15:O:230:TRP:CE2	15:O:364:LEU:HD21	2.20	0.75
7:G:154:ASN:HD21	15:O:182:MET:HE1	1.51	0.75
15:O:198:PHE:CE2	15:O:232:LEU:HG	2.22	0.75
15:O:342:HIS:NE2	15:O:346:GLN:NE2	2.34	0.75
3:C:31:TRP:CB	11:K:82:LYS:CD	2.51	0.74
1:A:437:PHE:CE1	1:A:456:VAL:CG2	2.58	0.74
15:O:101:SER:HB3	15:O:142:ILE:HD12	1.69	0.74
15:O:440:ILE:CG2	15:O:491:PHE:HE1	2.01	0.74
15:O:484:PHE:CE1	15:O:502:LEU:HD12	2.21	0.74
1:A:1348:VAL:CG1	2:B:268:GLU:HB2	2.18	0.74
3:C:45:SER:CB	3:C:271:ARG:NH2	2.49	0.74
4:D:96:PHE:HE1	7:G:150:HIS:CG	2.04	0.74
1:A:556:ALA:HB1	15:O:243:GLU:OE2	1.88	0.74
1:A:1575:ILE:HG12	9:I:122:ARG:HH12	1.52	0.74
15:O:241:ASP:OD1	15:O:378:THR:CG2	2.33	0.74
3:C:64:ALA:O	3:C:227:TYR:HE2	1.69	0.74
15:O:369:LYS:HE2	15:O:370:THR:HG23	1.67	0.74
4:D:25:THR:HG22	6:F:59:GLN:NE2	1.93	0.74
15:O:143:LEU:HD11	15:O:150:TRP:CD1	2.22	0.74
15:O:374:PRO:HG2	15:O:375:THR:HG23	1.69	0.74
15:O:484:PHE:HE1	15:O:502:LEU:HD12	1.52	0.74
3:C:82:TYR:CD1	12:L:68:GLU:HG3	2.22	0.74
15:O:238:ILE:HD11	15:O:371:HIS:HB3	1.70	0.74
15:O:390:GLN:HE22	15:O:432:LYS:N	1.86	0.74
15:O:421:LEU:CD1	15:O:476:ALA:HB2	2.18	0.74
2:B:401:GLU:HG3	2:B:402:VAL:N	2.03	0.74
15:O:407:SER:HB2	15:O:408:PHE:CD1	2.22	0.74
1:A:411:VAL:HG22	1:A:412:SER:H	1.52	0.73
2:B:42:VAL:HB	2:B:46:ILE:HD12	1.59	0.73
2:B:518:ARG:NH2	2:B:537:SER:O	2.21	0.73
15:O:371:HIS:O	15:O:374:PRO:HD2	1.88	0.73
1:A:1048:PHE:HB2	5:E:208:TYR:OH	1.89	0.73
4:D:37:LEU:HD22	4:D:97:LYS:HE3	1.70	0.73
15:O:245:GLN:HA	15:O:245:GLN:HE21	1.51	0.73
15:O:423:TYR:CD1	15:O:594:TYR:CE2	2.72	0.73
1:A:527:PRO:O	1:A:580:HIS:CE1	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:ALA:C	3:C:227:TYR:CE2	2.60	0.73
4:D:25:THR:HB	6:F:59:GLN:CG	2.19	0.73
15:O:432:LYS:HG2	15:O:608:GLU:C	2.07	0.73
2:B:478:LEU:HD13	2:B:484:TYR:HE1	1.50	0.73
3:C:55:ASP:OD1	3:C:299:ILE:HG23	1.88	0.73
2:B:1020:GLU:HG2	3:C:61:THR:HG21	1.70	0.73
3:C:253:PRO:O	14:N:180:PHE:CE1	2.41	0.73
7:G:143:SER:OG	15:O:101:SER:O	2.06	0.73
7:G:144:HIS:NE2	15:O:145:SER:CB	2.51	0.73
15:O:120:ILE:CD1	15:O:150:TRP:CE3	2.71	0.73
15:O:194:LEU:CD2	15:O:225:LEU:HD11	2.19	0.73
7:G:28:ILE:CG2	7:G:29:ASP:H	1.89	0.73
15:O:201:LYS:HD3	15:O:239:SER:OG	1.88	0.73
15:O:241:ASP:C	15:O:378:THR:HG21	2.08	0.73
15:O:373:LEU:HD11	15:O:416:LYS:HG2	1.65	0.73
15:O:237:ILE:HG22	15:O:381:ILE:HB	1.71	0.73
15:O:356:GLU:O	15:O:360:VAL:HG23	1.88	0.73
3:C:56:LEU:HG	3:C:300:PHE:HD1	1.53	0.73
4:D:92:ILE:HG12	7:G:152:ALA:CB	2.16	0.73
1:A:1305:GLU:OE2	9:I:63:LYS:NZ	2.16	0.72
2:B:552:SER:O	2:B:647:SER:N	2.21	0.72
15:O:152:GLN:HG3	15:O:193:TYR:OH	1.89	0.72
15:O:156:MET:SD	15:O:197:PHE:CE2	2.82	0.72
15:O:348:THR:CG2	15:O:351:SER:HB3	2.19	0.72
1:A:50:TYR:CE1	1:A:368:ARG:O	2.42	0.72
15:O:162:PHE:O	15:O:210:ASN:C	2.27	0.72
15:O:234:ILE:HG22	15:O:371:HIS:HD2	1.53	0.72
15:O:447:THR:O	15:O:450:LEU:CB	2.33	0.72
15:O:390:GLN:HE21	15:O:432:LYS:H	1.38	0.72
1:A:509:GLU:CD	1:A:579:ARG:HE	1.92	0.72
2:B:207:ILE:CD1	2:B:503:VAL:CG2	2.68	0.72
15:O:352:LEU:CA	15:O:358:VAL:HG23	2.19	0.72
4:D:23:HIS:CD2	6:F:58:PHE:CZ	2.78	0.72
1:A:413:LEU:CB	1:A:417:ARG:HH21	2.03	0.72
14:N:85:HIS:CE1	14:N:141:GLU:CD	2.60	0.72
15:O:488:HIS:CD2	15:O:489:ASN:OD1	2.42	0.72
1:A:878:ARG:HE	9:I:67:VAL:HG12	1.53	0.72
1:A:1056:ASP:OD1	1:A:1179:ILE:HD13	1.90	0.72
2:B:938:PHE:CE1	3:C:68:ARG:CZ	2.73	0.72
2:B:938:PHE:CZ	3:C:68:ARG:HD2	2.24	0.72
2:B:207:ILE:CD1	2:B:503:VAL:HG21	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:LEU:CB	3:C:298:PHE:HB2	2.17	0.72
4:D:23:HIS:HD2	6:F:58:PHE:CZ	2.07	0.72
15:O:225:LEU:O	15:O:225:LEU:HD13	1.89	0.72
1:A:478:TYR:CA	2:B:1048:SER:CA	2.34	0.71
3:C:45:SER:CB	3:C:271:ARG:HH22	2.03	0.71
12:L:68:GLU:HG2	12:L:69:ALA:N	2.01	0.71
15:O:432:LYS:HB3	15:O:609:TYR:HA	0.81	0.71
1:A:1055:ILE:CD1	1:A:1063:MET:CE	2.67	0.71
2:B:152:LEU:HD13	2:B:443:LYS:HG3	1.71	0.71
3:C:54:PHE:O	3:C:299:ILE:HA	1.90	0.71
15:O:158:LEU:HD22	15:O:172:HIS:HA	1.71	0.71
1:A:411:VAL:HG22	1:A:412:SER:N	2.05	0.71
1:A:527:PRO:O	1:A:580:HIS:HE1	1.73	0.71
1:A:1003:ARG:HD2	2:B:520:LEU:H	1.56	0.71
2:B:281:CYS:HA	2:B:323:ARG:HD2	1.72	0.71
2:B:1069:ILE:HD12	2:B:1069:ILE:N	2.05	0.71
15:O:361:PHE:CE1	15:O:365:THR:HG21	2.24	0.71
1:A:524:ILE:O	1:A:554:ARG:NH1	2.23	0.71
2:B:1069:ILE:HG22	2:B:1070:ARG:N	2.03	0.71
3:C:52:ALA:O	3:C:301:ASN:OD1	2.07	0.71
1:A:478:TYR:CD1	2:B:1048:SER:HB2	2.25	0.71
1:A:1048:PHE:CD2	5:E:210:SER:HA	2.26	0.71
4:D:92:ILE:CG1	7:G:152:ALA:HB2	2.16	0.71
15:O:128:LEU:HB3	15:O:129:PRO:CD	2.21	0.71
15:O:163:ILE:HA	15:O:211:TYR:N	1.97	0.71
1:A:468:ARG:NE	1:A:1021:ARG:HH12	1.89	0.71
1:A:1038:ILE:HD11	1:A:1050:TYR:HA	1.71	0.71
3:C:62:SER:HB2	11:K:74:ASN:CG	2.10	0.71
1:A:83:VAL:CG2	1:A:427:PHE:HE2	2.03	0.71
2:B:211:ARG:NH2	2:B:239:VAL:HG21	2.06	0.71
3:C:31:TRP:CE3	11:K:82:LYS:CG	2.69	0.71
3:C:70:ILE:HD11	11:K:71:THR:HG23	1.71	0.71
6:F:106:PRO:HG2	7:G:55:GLU:HG3	1.73	0.71
15:O:352:LEU:O	15:O:358:VAL:CG2	2.39	0.71
1:A:990:ILE:HB	1:A:994:GLU:CB	2.21	0.70
2:B:470:LEU:HB2	2:B:484:TYR:CE2	2.26	0.70
2:B:1165:ASN:OD1	2:B:1165:ASN:N	2.24	0.70
3:C:54:PHE:CE2	3:C:300:PHE:CG	2.78	0.70
15:O:198:PHE:CE1	15:O:236:LYS:HG3	2.25	0.70
15:O:152:GLN:HG2	15:O:193:TYR:HH	1.53	0.70
15:O:459:GLU:O	15:O:463:GLN:CG	2.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:ALA:CB	3:C:298:PHE:CE2	2.73	0.70
9:I:2:SER:HB2	9:I:11:LEU:HD21	1.72	0.70
15:O:373:LEU:N	15:O:374:PRO:CD	2.54	0.70
15:O:447:THR:CG2	15:O:480:LEU:HD22	2.21	0.70
1:A:891:ILE:HD12	9:I:71:LEU:HB2	1.71	0.70
3:C:71:MET:HE1	3:C:225:ALA:CB	2.21	0.70
7:G:158:LYS:HD3	15:O:105:ASN:HB3	1.72	0.70
1:A:438:ILE:HG23	2:B:1192:MET:HE3	1.73	0.70
2:B:894:LYS:N	12:L:54:ARG:NH2	2.34	0.70
7:G:159:LYS:H	15:O:105:ASN:ND2	1.89	0.70
4:D:80:THR:HG21	15:O:227:PHE:HD2	1.56	0.70
15:O:225:LEU:O	15:O:227:PHE:N	2.24	0.70
15:O:428:ILE:O	15:O:487:ARG:NE	2.24	0.70
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.25	0.70
15:O:373:LEU:HD12	15:O:373:LEU:O	1.91	0.70
1:A:436:ALA:HB1	1:A:443:ALA:CB	2.19	0.70
1:A:478:TYR:CE2	2:B:1049:THR:HG22	2.27	0.70
15:O:426:SER:HG	15:O:594:TYR:HB2	1.54	0.70
3:C:223:SER:O	3:C:224:THR:HB	1.92	0.70
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.74	0.70
1:A:436:ALA:O	1:A:440:SER:HA	1.91	0.69
1:A:1055:ILE:CD1	1:A:1063:MET:HE3	2.20	0.69
2:B:64:GLY:O	2:B:68:ILE:HG13	1.92	0.69
3:C:54:PHE:N	3:C:300:PHE:O	2.21	0.69
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.73	0.69
15:O:369:LYS:HB3	15:O:369:LYS:NZ	2.04	0.69
1:A:406:LEU:CD1	1:A:411:VAL:CB	2.71	0.69
1:A:438:ILE:CG2	2:B:1192:MET:HG2	2.23	0.69
1:A:782:ASP:OD1	1:A:931:SER:O	2.10	0.69
1:A:1348:VAL:HG23	2:B:268:GLU:O	1.91	0.69
1:A:1049:MET:HG2	1:A:1050:TYR:H	1.55	0.69
2:B:42:VAL:HG12	2:B:46:ILE:HG13	1.73	0.69
2:B:211:ARG:CG	2:B:401:GLU:OE1	2.39	0.69
1:A:99:ARG:O	1:A:109:ARG:NH2	2.24	0.69
2:B:300:SER:OG	9:I:49:THR:HG22	1.92	0.69
7:G:156:SER:CB	15:O:146:SER:HA	2.22	0.69
15:O:220:GLY:O	15:O:221:TYR:CD1	2.46	0.69
1:A:1:MET:CA	2:B:1098:TYR:CD1	2.75	0.69
4:D:99:LEU:HB3	4:D:100:PRO:CD	2.22	0.69
15:O:369:LYS:O	15:O:373:LEU:CB	2.41	0.69
1:A:478:TYR:CA	2:B:1047:ARG:O	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:TRP:CG	11:K:82:LYS:CD	2.76	0.69
3:C:41:GLU:HB3	3:C:57:ILE:HG22	1.74	0.69
3:C:253:PRO:HB2	14:N:180:PHE:CB	2.22	0.69
1:A:982:VAL:HG13	1:A:994:GLU:OE2	1.92	0.69
1:A:1573:TYR:O	9:I:122:ARG:NH2	2.26	0.69
15:O:417:LYS:HD3	15:O:472:HIS:HE1	1.57	0.69
1:A:1348:VAL:HG23	2:B:269:TYR:HA	1.75	0.68
4:D:48:GLU:CG	4:D:86:ILE:CD1	2.71	0.68
2:B:769:PHE:CD1	2:B:798:PHE:CE1	2.68	0.68
2:B:1002:LYS:HD2	14:N:166:LEU:HB2	1.74	0.68
4:D:25:THR:CB	6:F:59:GLN:CG	2.71	0.68
15:O:174:ASP:HA	15:O:177:LYS:CE	2.22	0.68
2:B:566:TYR:HB3	13:M:74:ASN:OD1	1.94	0.68
15:O:390:GLN:CB	15:O:609:TYR:CD1	2.76	0.68
1:A:432:ASN:HD21	1:A:444:GLN:H	1.38	0.68
3:C:64:ALA:HB1	3:C:227:TYR:CE2	2.29	0.68
3:C:71:MET:CE	3:C:225:ALA:CB	2.71	0.68
15:O:430:ARG:HH21	15:O:596:PRO:HD3	1.55	0.68
2:B:934:ILE:CG2	3:C:73:SER:HB3	2.24	0.68
3:C:55:ASP:HB3	3:C:297:HIS:CD2	2.28	0.68
2:B:1043:LYS:HG3	2:B:1063:ARG:NE	2.09	0.68
4:D:80:THR:CG2	15:O:227:PHE:CD2	2.76	0.68
15:O:241:ASP:CG	15:O:380:SER:HB2	2.14	0.68
15:O:430:ARG:HH22	15:O:596:PRO:HD3	1.58	0.68
1:A:35:PRO:HA	1:A:390:LEU:CD1	2.24	0.68
1:A:209:THR:HG21	5:E:173:SER:OG	1.93	0.68
3:C:54:PHE:O	3:C:299:ILE:C	2.32	0.68
15:O:343:VAL:CG1	15:O:388:VAL:CG2	2.71	0.68
2:B:207:ILE:HD11	2:B:503:VAL:CG1	2.25	0.68
3:C:52:ALA:O	3:C:301:ASN:CG	2.31	0.68
15:O:237:ILE:CB	15:O:381:ILE:CD1	2.57	0.68
1:A:572:THR:HA	7:G:52:MET:CE	2.23	0.67
2:B:938:PHE:CE1	3:C:68:ARG:NE	2.61	0.67
15:O:368:PHE:O	15:O:372:VAL:HG23	1.94	0.67
3:C:57:ILE:HD12	3:C:297:HIS:CE1	2.29	0.67
15:O:474:TYR:HB3	15:O:520:CYS:SG	2.33	0.67
2:B:566:TYR:CE2	13:M:70:SER:HA	2.30	0.67
3:C:57:ILE:CD1	3:C:297:HIS:ND1	2.56	0.67
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.76	0.67
15:O:458:GLU:HG3	15:O:514:PHE:CZ	2.28	0.67
3:C:71:MET:HE1	3:C:225:ALA:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:66:ASN:HD22	15:O:66:ASN:N	1.89	0.67
1:A:381:SER:HB2	1:A:453:ILE:CG2	2.24	0.67
1:A:436:ALA:HB2	1:A:443:ALA:HB1	1.66	0.67
2:B:1043:LYS:CG	2:B:1063:ARG:CZ	2.68	0.67
15:O:241:ASP:C	15:O:378:THR:CG2	2.63	0.67
15:O:431:ALA:HB1	15:O:434:LEU:CD1	2.20	0.67
1:A:81:LEU:HB2	1:A:358:ASP:O	1.94	0.67
4:D:48:GLU:HG2	4:D:86:ILE:HD11	1.76	0.67
1:A:1006:LEU:HB3	2:B:539:CYS:SG	2.34	0.67
15:O:471:LYS:HB2	15:O:585:PHE:CZ	2.25	0.67
1:A:1344:ILE:HG21	2:B:333:LYS:HG3	1.76	0.67
1:A:1556:GLU:OE2	5:E:212:ARG:NH1	2.28	0.67
3:C:71:MET:O	3:C:222:VAL:HG21	1.94	0.67
15:O:371:HIS:O	15:O:374:PRO:HG2	1.95	0.67
1:A:356:PHE:C	1:A:357:MET:HG3	2.14	0.67
1:A:406:LEU:HD12	1:A:406:LEU:O	1.94	0.67
1:A:1011:VAL:C	1:A:1201:THR:HG21	2.15	0.67
3:C:84:TYR:HD2	12:L:66:GLN:HB2	1.59	0.67
15:O:108:GLU:HB2	15:O:147:ILE:HD11	1.76	0.67
1:A:1027:LEU:O	1:A:1028:GLU:HG2	1.95	0.66
2:B:470:LEU:HD22	2:B:484:TYR:OH	1.95	0.66
3:C:86:PHE:HE1	12:L:64:LEU:CD1	2.08	0.66
3:C:253:PRO:CG	14:N:180:PHE:HB3	2.25	0.66
15:O:371:HIS:O	15:O:374:PRO:CG	2.43	0.66
2:B:207:ILE:HD11	2:B:503:VAL:HG11	1.76	0.66
15:O:240:ILE:CG2	15:O:332:LEU:CD1	2.67	0.66
15:O:390:GLN:CD	15:O:609:TYR:HB3	2.15	0.66
1:A:1050:TYR:CE1	1:A:1185:VAL:HG12	2.29	0.66
3:C:131:THR:CG2	3:C:209:ILE:HG23	2.25	0.66
4:D:25:THR:CA	6:F:59:GLN:HG3	2.24	0.66
13:M:101:VAL:HG12	13:M:106:LYS:HG3	1.72	0.66
15:O:390:GLN:HB3	15:O:609:TYR:CD1	2.30	0.66
1:A:113:VAL:HG21	1:A:178:LEU:HD13	1.77	0.66
3:C:223:SER:HB2	3:C:303:GLU:HB3	1.76	0.66
1:A:863:ASN:HD22	9:I:67:VAL:CA	2.07	0.66
4:D:96:PHE:CE1	7:G:150:HIS:CG	2.83	0.66
15:O:240:ILE:CG2	15:O:332:LEU:CD2	2.63	0.66
1:A:437:PHE:O	1:A:455:GLY:HA3	1.96	0.66
7:G:242:VAL:HG21	15:O:183:ILE:CG2	2.26	0.66
15:O:434:LEU:HD12	15:O:434:LEU:N	2.10	0.66
1:A:403:LEU:HD12	1:A:419:ILE:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:428:ILE:HG23	15:O:439:ILE:CG2	2.23	0.66
1:A:1000:MET:CG	2:B:520:LEU:HD23	2.26	0.66
1:A:1344:ILE:CG2	2:B:333:LYS:HG3	2.26	0.66
1:A:109:ARG:NH1	1:A:230:ARG:O	2.29	0.66
15:O:454:VAL:HG23	15:O:458:GLU:HG3	1.77	0.66
1:A:403:LEU:CD1	1:A:419:ILE:CG2	2.74	0.66
15:O:247:GLU:OE1	15:O:325:ILE:HG13	1.95	0.66
2:B:209:GLN:HG2	2:B:210:ARG:N	2.07	0.65
2:B:209:GLN:O	2:B:401:GLU:N	2.27	0.65
1:A:1000:MET:HG2	2:B:520:LEU:CD2	2.25	0.65
3:C:52:ALA:O	3:C:301:ASN:CA	2.42	0.65
15:O:422:GLN:NE2	15:O:592:PHE:CD2	2.65	0.65
1:A:478:TYR:CA	2:B:1048:SER:O	2.44	0.65
1:A:756:LYS:HD3	9:I:85:LYS:HZ2	1.32	0.65
2:B:300:SER:OG	9:I:49:THR:CG2	2.44	0.65
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.78	0.65
3:C:230:LEU:CG	3:C:294:VAL:HG21	2.26	0.65
15:O:108:GLU:HG3	15:O:108:GLU:O	1.96	0.65
15:O:146:SER:O	15:O:148:PRO:HD3	1.95	0.65
15:O:219:ARG:HH21	15:O:360:VAL:HG22	1.60	0.65
2:B:891:GLU:HA	12:L:54:ARG:NE	2.12	0.65
3:C:272:LYS:HG2	14:N:175:TYR:CD1	2.32	0.65
4:D:48:GLU:HG3	4:D:86:ILE:HD12	1.78	0.65
15:O:458:GLU:CG	15:O:514:PHE:CZ	2.79	0.65
1:A:799:GLU:HG3	1:A:1062:HIS:CE1	2.32	0.65
1:A:1034:TYR:CD1	1:A:1181:PRO:HG2	2.32	0.65
2:B:566:TYR:CD2	13:M:73:SER:OG	2.48	0.65
2:B:938:PHE:CZ	3:C:68:ARG:CD	2.80	0.65
4:D:99:LEU:HB3	4:D:100:PRO:HD3	1.78	0.65
15:O:343:VAL:CG1	15:O:388:VAL:HG23	2.27	0.65
1:A:406:LEU:CD1	1:A:411:VAL:CG2	2.74	0.65
2:B:341:SER:OG	2:B:343:ASP:OD1	2.13	0.65
4:D:25:THR:HG21	6:F:59:GLN:NE2	2.12	0.65
1:A:502:ALA:CB	1:A:581:ILE:CG2	2.63	0.65
3:C:222:VAL:C	3:C:224:THR:N	2.49	0.65
15:O:241:ASP:CB	15:O:380:SER:HB2	2.26	0.65
15:O:488:HIS:NE2	15:O:489:ASN:OD1	2.29	0.65
1:A:782:ASP:CG	1:A:783:LYS:N	2.50	0.65
1:A:1651:THR:OG1	2:B:1085:SER:OG	2.14	0.65
3:C:59:ILE:HG23	3:C:298:PHE:HE1	1.54	0.65
7:G:144:HIS:NE2	15:O:145:SER:HB2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:241:ASP:HA	15:O:380:SER:HB2	1.78	0.65
1:A:406:LEU:HD11	1:A:411:VAL:HG21	1.78	0.65
1:A:438:ILE:HG23	2:B:1192:MET:CE	2.26	0.65
1:A:1053:ASP:O	1:A:1054:ALA:HB3	1.97	0.65
2:B:915:ASP:OD1	2:B:1038:HIS:HD2	1.78	0.65
2:B:923:GLN:NE2	2:B:953:ALA:O	2.30	0.65
15:O:343:VAL:HG11	15:O:388:VAL:CG2	2.27	0.65
1:A:953:GLU:C	1:A:1205:PHE:CB	2.66	0.64
7:G:156:SER:HB2	15:O:146:SER:HA	1.78	0.64
15:O:417:LYS:CD	15:O:472:HIS:HE1	2.10	0.64
15:O:428:ILE:HD12	15:O:439:ILE:HD12	1.79	0.64
1:A:1575:ILE:HG13	9:I:122:ARG:HH12	1.60	0.64
15:O:374:PRO:CG	15:O:375:THR:HG23	2.27	0.64
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.30	0.64
1:A:1262:LEU:CD2	1:A:1497:ILE:HG12	2.28	0.64
2:B:1120:ILE:HD12	15:O:117:GLN:HE22	1.63	0.64
3:C:54:PHE:CE1	3:C:300:PHE:HB3	2.31	0.64
7:G:159:LYS:HB3	15:O:103:ASN:OD1	1.98	0.64
15:O:510:VAL:HG13	15:O:517:LEU:HD11	1.79	0.64
2:B:623:ASP:O	2:B:648:ARG:NH1	2.25	0.64
1:A:1023:LEU:HD23	1:A:1598:PHE:CD1	2.32	0.64
1:A:1344:ILE:CD1	2:B:329:TYR:CE2	2.71	0.64
2:B:469:ASN:HA	2:B:481:VAL:O	1.97	0.64
3:C:86:PHE:CE1	12:L:64:LEU:CD1	2.79	0.64
1:A:83:VAL:CB	1:A:427:PHE:CE2	2.81	0.64
1:A:413:LEU:O	1:A:417:ARG:NH2	2.30	0.64
1:A:480:ALA:CB	2:B:1046:VAL:CG2	2.63	0.64
1:A:1036:ASN:HB3	1:A:1049:MET:HG3	1.78	0.64
3:C:82:TYR:HE1	12:L:68:GLU:OE1	1.80	0.64
7:G:144:HIS:NE2	15:O:145:SER:HB3	2.13	0.64
1:A:1038:ILE:CG1	1:A:1049:MET:O	2.44	0.64
1:A:1273:THR:HG23	9:I:48:VAL:HG22	1.79	0.64
2:B:699:ILE:HD13	2:B:760:TYR:CE1	2.32	0.64
15:O:240:ILE:CG2	15:O:332:LEU:CG	2.76	0.64
1:A:995:TYR:O	1:A:999:CYS:HB2	1.98	0.64
1:A:1055:ILE:CG2	1:A:1063:MET:SD	2.85	0.64
3:C:73:SER:O	3:C:214:GLY:N	2.31	0.64
5:E:20:LYS:HE2	5:E:34:GLU:HG2	1.80	0.64
15:O:170:VAL:HG13	15:O:171:CYS:N	2.12	0.64
1:A:478:TYR:OH	2:B:1049:THR:HG21	1.97	0.64
3:C:54:PHE:O	3:C:299:ILE:CA	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:CD2	1:A:423:LEU:HA	2.28	0.64
1:A:953:GLU:C	1:A:1205:PHE:HB3	2.18	0.64
1:A:1021:ARG:HD3	2:B:1073:GLU:OE1	1.98	0.64
15:O:368:PHE:CE2	15:O:382:GLN:HA	2.33	0.64
15:O:383:TYR:CE2	15:O:597:LEU:HD22	2.33	0.64
1:A:1055:ILE:HD12	1:A:1063:MET:HE3	1.74	0.63
4:D:25:THR:CB	6:F:59:GLN:HE21	2.06	0.63
1:A:1322:ILE:HD12	1:A:1457:ILE:HD11	1.79	0.63
8:H:44:VAL:HG22	8:H:48:PRO:HA	1.81	0.63
15:O:454:VAL:HG23	15:O:458:GLU:CG	2.28	0.63
1:A:476:VAL:HG11	2:B:1071:VAL:CG2	2.25	0.63
1:A:478:TYR:N	2:B:1048:SER:C	2.52	0.63
1:A:1654:PHE:CE2	6:F:92:ARG:HD3	2.33	0.63
3:C:41:GLU:CB	3:C:57:ILE:CG2	2.70	0.63
15:O:392:GLN:HB2	15:O:395:LEU:HD22	1.79	0.63
15:O:426:SER:OG	15:O:594:TYR:CA	2.46	0.63
1:A:1026:GLN:HE22	1:A:1603:MET:HA	1.61	0.63
15:O:454:VAL:HG23	15:O:458:GLU:OE2	1.98	0.63
2:B:281:CYS:HA	2:B:323:ARG:CD	2.29	0.63
3:C:75:VAL:CG1	3:C:221:PRO:HD2	2.06	0.63
7:G:141:SER:CB	15:O:138:TYR:CZ	2.81	0.63
1:A:888:LYS:HE2	9:I:69:THR:HG22	1.79	0.63
1:A:1600:ARG:NE	1:A:1616:GLU:OE1	2.30	0.63
2:B:475:GLY:O	2:B:476:LEU:HB2	1.98	0.63
15:O:155:SER:HA	15:O:158:LEU:HD12	1.81	0.63
15:O:379:ARG:CB	15:O:382:GLN:HE22	2.12	0.63
1:A:401:ASP:OD2	1:A:405:LYS:NZ	2.32	0.63
1:A:402:ASP:O	1:A:406:LEU:HD23	1.99	0.63
1:A:408:LYS:HA	1:A:411:VAL:HG11	1.79	0.63
1:A:1655:ASP:N	6:F:135:ARG:O	2.28	0.63
4:D:80:THR:CG2	15:O:227:PHE:CB	2.75	0.63
6:F:70:LYS:HG3	7:G:94:PRO:HB2	1.80	0.63
15:O:373:LEU:N	15:O:374:PRO:HD2	2.14	0.63
1:A:1060:GLU:O	1:A:1060:GLU:HG2	1.98	0.63
4:D:23:HIS:HD2	6:F:58:PHE:CE2	2.16	0.63
7:G:158:LYS:CE	15:O:105:ASN:OD1	2.47	0.63
15:O:245:GLN:HA	15:O:245:GLN:NE2	2.14	0.63
15:O:471:LYS:HG3	15:O:472:HIS:N	2.14	0.63
1:A:436:ALA:O	1:A:440:SER:CA	2.46	0.62
1:A:509:GLU:HG2	1:A:579:ARG:HG2	1.81	0.62
3:C:75:VAL:HG12	3:C:76:PRO:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:142:ALA:O	15:O:102:SER:O	2.16	0.62
12:L:68:GLU:CG	12:L:69:ALA:H	2.05	0.62
1:A:83:VAL:CG2	1:A:427:PHE:HZ	2.01	0.62
1:A:991:LYS:N	1:A:994:GLU:OE1	2.31	0.62
15:O:181:ARG:HH11	15:O:181:ARG:CG	2.12	0.62
1:A:1050:TYR:HB2	1:A:1179:ILE:HG21	1.81	0.62
2:B:42:VAL:CA	2:B:46:ILE:HD12	2.29	0.62
15:O:151:TRP:CZ2	15:O:176:LEU:HD23	2.35	0.62
1:A:572:THR:HA	7:G:52:MET:HE1	1.80	0.62
3:C:41:GLU:O	3:C:57:ILE:HG22	1.99	0.62
15:O:98:ASP:OD2	15:O:135:LYS:HD3	1.99	0.62
15:O:386:PHE:CD2	15:O:606:MET:HE2	2.34	0.62
15:O:225:LEU:HD13	15:O:225:LEU:C	2.19	0.62
15:O:457:ARG:HA	15:O:460:GLU:CB	2.30	0.62
2:B:40:GLU:OE1	2:B:550:ARG:NH2	2.32	0.62
7:G:142:ALA:C	15:O:102:SER:O	2.38	0.62
15:O:447:THR:HA	15:O:450:LEU:HD12	1.80	0.62
1:A:406:LEU:HD12	1:A:411:VAL:HB	1.82	0.62
1:A:1011:VAL:C	1:A:1201:THR:CG2	2.68	0.62
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.79	0.62
1:A:1028:GLU:CG	1:A:1029:GLY:N	2.62	0.62
1:A:1657:LEU:HD21	6:F:135:ARG:CZ	2.30	0.62
2:B:554:GLN:HA	2:B:646:HIS:CD2	2.34	0.62
2:B:1043:LYS:HG3	2:B:1063:ARG:CD	2.29	0.62
3:C:58:ASN:N	3:C:296:ASN:O	2.30	0.62
15:O:460:GLU:O	15:O:469:ARG:NH1	2.32	0.62
1:A:891:ILE:CD1	9:I:71:LEU:CB	2.77	0.62
3:C:59:ILE:O	3:C:298:PHE:HE1	1.83	0.62
3:C:222:VAL:C	3:C:224:THR:H	2.03	0.62
15:O:343:VAL:HG12	15:O:388:VAL:HG23	1.82	0.62
15:O:435:SER:HB3	15:O:438:GLN:CG	2.23	0.62
3:C:62:SER:CB	11:K:74:ASN:HD21	2.12	0.62
15:O:368:PHE:CE2	15:O:385:MET:HB2	2.34	0.62
15:O:581:THR:HA	15:O:584:GLN:NE2	2.15	0.62
2:B:934:ILE:HG23	3:C:73:SER:HB3	1.82	0.61
3:C:55:ASP:OD2	3:C:299:ILE:HG12	1.97	0.61
4:D:47:LYS:HD2	4:D:82:LEU:HD21	1.82	0.61
15:O:100:LEU:HD22	15:O:107:ILE:HD11	1.82	0.61
15:O:144:CYS:O	15:O:148:PRO:HG3	2.00	0.61
12:L:30:ILE:CD1	12:L:59:ALA:HB2	2.29	0.61
15:O:431:ALA:HB3	15:O:434:LEU:CD1	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:447:THR:CG2	15:O:480:LEU:CD2	2.79	0.61
15:O:450:LEU:O	15:O:454:VAL:HG12	1.99	0.61
3:C:71:MET:CE	3:C:302:VAL:HG22	2.29	0.61
3:C:131:THR:CG2	3:C:208:CYS:O	2.48	0.61
15:O:158:LEU:HB3	15:O:172:HIS:HB3	1.82	0.61
1:A:406:LEU:HD13	1:A:411:VAL:CB	2.27	0.61
1:A:1025:LYS:HZ2	2:B:1076:ARG:NH1	1.98	0.61
2:B:481:VAL:O	2:B:481:VAL:HG12	2.01	0.61
1:A:1662:ASN:N	7:G:101:SER:O	2.32	0.61
2:B:769:PHE:HE1	2:B:798:PHE:HZ	1.48	0.61
7:G:141:SER:HB3	15:O:138:TYR:OH	1.95	0.61
15:O:447:THR:HG22	15:O:480:LEU:CD2	2.28	0.61
1:A:413:LEU:O	1:A:417:ARG:CZ	2.47	0.61
1:A:478:TYR:H	2:B:1048:SER:C	2.03	0.61
2:B:1069:ILE:O	2:B:1070:ARG:HB2	2.00	0.61
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.36	0.61
15:O:181:ARG:HB2	15:O:181:ARG:NH1	2.12	0.61
15:O:369:LYS:HG3	15:O:406:ILE:HD11	1.83	0.61
15:O:396:MET:SD	15:O:434:LEU:HA	2.41	0.61
1:A:1050:TYR:CB	1:A:1179:ILE:HG21	2.31	0.61
2:B:923:GLN:NE2	2:B:957:ARG:HD2	2.16	0.61
3:C:71:MET:CE	3:C:225:ALA:HB1	2.30	0.61
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.82	0.61
15:O:67:ASP:OD1	15:O:69:THR:HB	2.00	0.61
1:A:509:GLU:HG3	1:A:579:ARG:HD3	1.81	0.61
1:A:1660:VAL:CG2	7:G:103:LYS:HB2	2.30	0.61
3:C:71:MET:SD	3:C:225:ALA:CB	2.88	0.61
4:D:44:ILE:HD13	4:D:90:LYS:HG3	1.82	0.61
15:O:408:PHE:CE1	15:O:446:LEU:HD13	2.35	0.61
15:O:454:VAL:HG23	15:O:458:GLU:CD	2.20	0.61
1:A:564:PRO:HB2	15:O:371:HIS:CE1	2.36	0.61
15:O:56:VAL:HG21	15:O:99:ILE:HD12	1.82	0.61
15:O:371:HIS:O	15:O:374:PRO:CD	2.49	0.61
1:A:479:ALA:HB2	2:B:1091:ARG:HH22	1.65	0.60
2:B:552:SER:OG	2:B:647:SER:N	2.35	0.60
8:H:25:ARG:NH1	8:H:27:GLU:OE2	2.34	0.60
15:O:457:ARG:O	15:O:460:GLU:CB	2.47	0.60
15:O:467:MET:HG3	15:O:519:PHE:CE2	2.36	0.60
15:O:582:ARG:O	15:O:586:ILE:HG13	2.01	0.60
1:A:932:GLY:O	9:I:125:ASN:ND2	2.34	0.60
1:A:1344:ILE:HG22	2:B:333:LYS:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1651:THR:OG1	2:B:1085:SER:CB	2.49	0.60
1:A:1052:GLY:O	5:E:205:SER:CB	2.48	0.60
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.82	0.60
15:O:487:ARG:HH11	15:O:487:ARG:CG	2.14	0.60
1:A:799:GLU:OE2	1:A:1062:HIS:HB2	2.01	0.60
2:B:938:PHE:CD1	3:C:68:ARG:CZ	2.83	0.60
1:A:1261:VAL:HG13	1:A:1265:GLU:CD	2.22	0.60
1:A:1261:VAL:HG13	1:A:1265:GLU:OE1	2.01	0.60
2:B:1020:GLU:CG	3:C:61:THR:HG21	2.32	0.60
3:C:272:LYS:CG	14:N:175:TYR:CE1	2.83	0.60
4:D:80:THR:HG21	15:O:227:PHE:CB	2.28	0.60
7:G:143:SER:CB	15:O:101:SER:O	2.48	0.60
1:A:1034:TYR:HA	1:A:1181:PRO:CG	2.32	0.60
2:B:1090:ASP:O	2:B:1095:SER:N	2.34	0.60
1:A:246:ASP:HB3	1:A:248:PHE:H	1.66	0.60
1:A:1226:VAL:HG12	1:A:1227:MET:HG2	1.83	0.60
1:A:449:GLY:O	1:A:451:VAL:N	2.34	0.60
1:A:996:TYR:HE1	1:A:1000:MET:CE	2.14	0.60
2:B:228:SER:HB2	2:B:253:LEU:HD23	1.84	0.60
15:O:241:ASP:OD1	15:O:379:ARG:C	2.39	0.60
1:A:84:PRO:HG2	1:A:318:THR:HG22	1.84	0.60
1:A:477:ASN:O	1:A:478:TYR:HB2	2.01	0.60
2:B:699:ILE:CD1	2:B:760:TYR:CE1	2.85	0.60
1:A:87:ASN:HB2	1:A:357:MET:SD	2.42	0.60
15:O:98:ASP:OD2	15:O:135:LYS:NZ	2.35	0.60
1:A:1026:GLN:OE1	1:A:1603:MET:CB	2.48	0.59
3:C:55:ASP:HB3	3:C:297:HIS:NE2	2.17	0.59
1:A:1008:ASP:O	1:A:1011:VAL:CG2	2.41	0.59
1:A:1034:TYR:HA	1:A:1181:PRO:HG3	1.84	0.59
1:A:1054:ALA:O	1:A:1178:LEU:HD23	2.02	0.59
2:B:1019:GLY:HA3	3:C:65:ASN:CB	2.27	0.59
15:O:198:PHE:CD1	15:O:236:LYS:CE	2.78	0.59
1:A:406:LEU:HD13	1:A:411:VAL:CG2	2.31	0.59
6:F:106:PRO:HG2	7:G:55:GLU:CG	2.30	0.59
1:A:699:CYS:O	1:A:815:ARG:NH1	2.35	0.59
2:B:207:ILE:O	2:B:207:ILE:HG22	2.02	0.59
1:A:35:PRO:HA	1:A:390:LEU:HD12	1.84	0.59
1:A:1027:LEU:HD21	1:A:1588:MET:HG2	1.84	0.59
1:A:878:ARG:HG2	9:I:67:VAL:CG1	2.29	0.59
2:B:211:ARG:HB3	2:B:239:VAL:CG1	2.32	0.59
2:B:551:ILE:HA	2:B:648:ARG:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:566:TYR:HB2	13:M:73:SER:OG	2.03	0.59
1:A:720:PHE:CE2	8:H:141:TYR:HE2	2.21	0.59
4:D:80:THR:OG1	15:O:227:PHE:CD1	2.55	0.59
5:E:55:ARG:NH2	5:E:113:GLN:OE1	2.36	0.59
15:O:374:PRO:HB2	15:O:375:THR:HG23	1.85	0.59
15:O:390:GLN:HB2	15:O:609:TYR:CD1	2.37	0.59
1:A:509:GLU:O	1:A:576:LYS:HA	2.03	0.59
1:A:863:ASN:ND2	9:I:68:LYS:H	2.01	0.59
15:O:101:SER:HB3	15:O:142:ILE:CD1	2.33	0.59
1:A:516:ILE:HG21	15:O:376:TYR:CZ	2.38	0.59
1:A:581:ILE:HG13	1:A:582:LYS:H	1.68	0.59
2:B:328:GLN:NE2	13:M:109:ARG:HH21	1.99	0.59
2:B:829:ASN:OD1	2:B:829:ASN:N	2.36	0.59
2:B:110:ASN:O	2:B:112:GLY:N	2.35	0.59
2:B:209:GLN:O	2:B:401:GLU:HG2	2.03	0.59
2:B:563:SER:CB	13:M:73:SER:HB3	2.33	0.59
3:C:231:PRO:HG2	3:C:270:ALA:HB1	1.83	0.59
3:C:272:LYS:HG2	14:N:175:TYR:CE1	2.38	0.59
15:O:369:LYS:HD3	15:O:373:LEU:HD22	1.85	0.59
15:O:428:ILE:CD1	15:O:439:ILE:HD12	2.33	0.59
1:A:990:ILE:CB	1:A:994:GLU:OE1	2.51	0.58
2:B:538:PRO:HB2	2:B:542:LEU:HG	1.84	0.58
15:O:241:ASP:O	15:O:378:THR:CG2	2.51	0.58
15:O:348:THR:HG23	15:O:351:SER:H	1.67	0.58
15:O:607:LYS:HG3	15:O:608:GLU:N	2.17	0.58
1:A:1048:PHE:HZ	5:E:211:TYR:CD1	2.18	0.58
3:C:253:PRO:CB	14:N:180:PHE:HB3	2.33	0.58
7:G:159:LYS:N	15:O:105:ASN:HD22	2.01	0.58
1:A:827:THR:OG1	1:A:828:CYS:N	2.36	0.58
7:G:30:GLU:HA	7:G:32:ASN:N	2.18	0.58
15:O:129:PRO:CG	15:O:132:THR:CB	2.74	0.58
15:O:164:LEU:O	15:O:165:PRO:O	2.20	0.58
15:O:369:LYS:CE	15:O:370:THR:HG22	2.33	0.58
1:A:415:ASP:HA	1:A:418:VAL:HG12	1.84	0.58
1:A:1055:ILE:HD11	1:A:1174:TYR:CD2	2.39	0.58
1:A:1074:TYR:HE2	1:A:1159:ASP:HB3	1.68	0.58
1:A:1660:VAL:HG23	7:G:103:LYS:HB2	1.85	0.58
2:B:328:GLN:HE22	13:M:109:ARG:NH2	1.99	0.58
2:B:415:GLU:OE2	2:B:474:SER:OG	2.21	0.58
1:A:437:PHE:CZ	1:A:456:VAL:HG22	2.28	0.58
4:D:48:GLU:HG3	4:D:86:ILE:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:68:GLU:HG2	11:K:72:LEU:HD23	1.86	0.58
15:O:454:VAL:CG2	15:O:458:GLU:OE2	2.51	0.58
1:A:468:ARG:HE	1:A:1021:ARG:NH1	2.00	0.58
2:B:1019:GLY:CA	3:C:65:ASN:HB2	2.28	0.58
3:C:221:PRO:O	3:C:222:VAL:HG13	2.04	0.58
4:D:25:THR:HG21	6:F:59:GLN:HE21	1.57	0.58
4:D:27:LEU:HD22	7:G:23:GLN:O	2.03	0.58
3:C:253:PRO:HB2	14:N:180:PHE:HB3	1.85	0.58
15:O:386:PHE:HD2	15:O:606:MET:HE2	1.62	0.58
15:O:484:PHE:CD1	15:O:502:LEU:HD13	2.38	0.58
7:G:159:LYS:N	15:O:105:ASN:ND2	2.51	0.58
2:B:923:GLN:HG2	2:B:949:ILE:HD11	1.84	0.58
2:B:1016:GLY:O	3:C:69:ARG:HD2	2.04	0.58
13:M:10:ILE:HB	14:N:70:LEU:HB3	1.86	0.58
1:A:406:LEU:CD1	1:A:411:VAL:HG21	2.34	0.58
2:B:117:VAL:HG13	2:B:117:VAL:O	2.03	0.58
4:D:25:THR:C	6:F:59:GLN:HG3	2.24	0.58
4:D:48:GLU:OE1	4:D:90:LYS:NZ	2.37	0.58
12:L:38:LEU:HD12	12:L:49:LYS:HG3	1.85	0.58
15:O:421:LEU:HD13	15:O:476:ALA:CB	2.31	0.58
15:O:423:TYR:HD1	15:O:594:TYR:CZ	2.20	0.58
12:L:33:GLU:HG3	12:L:53:HIS:CE1	2.39	0.57
14:N:69:SER:OG	14:N:70:LEU:N	2.37	0.57
15:O:174:ASP:O	15:O:177:LYS:CG	2.52	0.57
1:A:407:GLN:O	1:A:411:VAL:HG12	2.04	0.57
1:A:581:ILE:HG13	1:A:582:LYS:N	2.19	0.57
14:N:89:ILE:HG12	14:N:139:VAL:HG22	1.85	0.57
3:C:56:LEU:CG	3:C:300:PHE:CD1	2.86	0.57
15:O:369:LYS:O	15:O:373:LEU:HB3	2.04	0.57
1:A:476:VAL:CG1	2:B:1071:VAL:HG23	2.30	0.57
1:A:1055:ILE:HG22	1:A:1060:GLU:HB2	1.87	0.57
2:B:467:THR:C	2:B:469:ASN:H	2.07	0.57
15:O:247:GLU:HB3	15:O:325:ILE:HD11	1.86	0.57
15:O:471:LYS:CB	15:O:585:PHE:HE1	1.94	0.57
2:B:848:ILE:HB	12:L:60:ARG:HG3	1.86	0.57
3:C:51:GLU:CB	3:C:303:GLU:CG	2.80	0.57
15:O:487:ARG:O	15:O:490:ILE:HB	2.03	0.57
1:A:493:ASN:HB3	1:A:654:ASP:OD1	2.04	0.57
1:A:782:ASP:O	1:A:784:SER:N	2.38	0.57
1:A:953:GLU:HA	1:A:1205:PHE:CG	2.40	0.57
2:B:207:ILE:HD11	2:B:503:VAL:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:893:ASN:HA	12:L:54:ARG:NH2	2.20	0.57
6:F:66:ARG:CZ	7:G:90:LEU:CD1	2.80	0.57
7:G:143:SER:HB3	15:O:103:ASN:N	2.20	0.57
15:O:173:HIS:CD2	15:O:217:LYS:HG2	2.39	0.57
15:O:391:GLN:OE1	15:O:609:TYR:OH	2.23	0.57
1:A:1003:ARG:NE	2:B:520:LEU:CB	2.61	0.57
1:A:1348:VAL:CG2	2:B:268:GLU:C	2.72	0.57
15:O:128:LEU:HD22	15:O:129:PRO:HD3	1.86	0.57
15:O:190:ILE:HA	15:O:193:TYR:CD2	2.39	0.57
15:O:417:LYS:HB3	15:O:472:HIS:CE1	2.39	0.57
15:O:484:PHE:CE1	15:O:502:LEU:HD13	2.39	0.57
1:A:468:ARG:NE	1:A:1021:ARG:CZ	2.63	0.57
1:A:1235:THR:O	1:A:1544:ASN:ND2	2.38	0.57
2:B:833:PRO:HG2	2:B:836:TRP:CE2	2.40	0.57
15:O:230:TRP:CZ2	15:O:364:LEU:HD11	2.39	0.57
15:O:422:GLN:NE2	15:O:592:PHE:CZ	2.69	0.57
1:A:18:ILE:HD12	1:A:354:SER:HB3	1.85	0.57
1:A:478:TYR:HA	2:B:1048:SER:C	2.18	0.57
1:A:727:THR:HG21	8:H:119:GLY:O	2.05	0.57
1:A:988:SER:HB2	2:B:988:GLU:HG2	1.87	0.57
2:B:1043:LYS:HG3	2:B:1063:ARG:HD2	1.85	0.57
1:A:1048:PHE:O	1:A:1049:MET:HB2	2.04	0.57
3:C:56:LEU:CG	3:C:300:PHE:CE1	2.88	0.57
4:D:48:GLU:CG	4:D:86:ILE:HD11	2.35	0.57
15:O:158:LEU:HD22	15:O:172:HIS:CB	2.35	0.57
1:A:563:THR:HA	15:O:375:THR:HG21	1.87	0.56
2:B:894:LYS:HG2	12:L:47:ARG:HD2	1.86	0.56
2:B:894:LYS:HG2	12:L:47:ARG:NE	2.19	0.56
2:B:1020:GLU:CG	3:C:61:THR:OG1	2.53	0.56
15:O:154:VAL:O	15:O:158:LEU:HG	2.04	0.56
1:A:412:SER:HB3	1:A:414:GLU:H	1.70	0.56
1:A:799:GLU:CD	1:A:1062:HIS:HB2	2.25	0.56
2:B:207:ILE:HD11	2:B:503:VAL:HG21	1.87	0.56
2:B:800:TYR:CD1	2:B:801:GLY:N	2.73	0.56
3:C:82:TYR:CE1	12:L:68:GLU:OE1	2.58	0.56
4:D:28:PRO:HD2	7:G:24:VAL:CG1	2.35	0.56
5:E:145:THR:C	5:E:147:HIS:H	2.08	0.56
6:F:75:PRO:HG2	6:F:78:GLN:CG	2.34	0.56
7:G:20:HIS:O	7:G:20:HIS:ND1	2.38	0.56
1:A:1050:TYR:CG	1:A:1179:ILE:HG21	2.40	0.56
2:B:338:PHE:HZ	2:B:357:ILE:HD12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:890:ASP:O	12:L:54:ARG:NE	2.38	0.56
2:B:1013:MET:SD	2:B:1026:ILE:HG12	2.45	0.56
3:C:223:SER:HB2	3:C:303:GLU:CB	2.35	0.56
5:E:90:VAL:HG13	5:E:120:ALA:HA	1.88	0.56
7:G:56:ASN:HB3	7:G:59:GLN:HB3	1.86	0.56
7:G:143:SER:CB	15:O:104:ILE:N	2.57	0.56
15:O:66:ASN:N	15:O:66:ASN:ND2	2.53	0.56
15:O:109:SER:OG	15:O:111:ARG:HG3	2.05	0.56
1:A:966:LEU:CD2	1:A:997:PHE:CZ	2.83	0.56
3:C:56:LEU:HD12	3:C:300:PHE:CE1	2.23	0.56
11:K:49:LEU:HD23	11:K:51:THR:HG23	1.86	0.56
15:O:458:GLU:HG2	15:O:514:PHE:CZ	2.40	0.56
2:B:1020:GLU:HG2	3:C:61:THR:OG1	2.06	0.56
3:C:86:PHE:HE2	3:C:205:LYS:HG3	1.69	0.56
12:L:63:ARG:HG3	12:L:64:LEU:H	1.69	0.56
1:A:477:ASN:OD1	2:B:1047:ARG:NH1	2.39	0.56
2:B:208:VAL:HG23	2:B:401:GLU:CG	2.35	0.56
2:B:554:GLN:CA	2:B:646:HIS:CD2	2.89	0.56
7:G:141:SER:HB3	15:O:138:TYR:CZ	2.41	0.56
15:O:98:ASP:CG	15:O:135:LYS:HD3	2.26	0.56
15:O:396:MET:HE1	15:O:434:LEU:CD1	2.32	0.56
15:O:432:LYS:HG3	15:O:608:GLU:O	1.96	0.56
15:O:447:THR:HA	15:O:450:LEU:CG	2.35	0.56
1:A:990:ILE:HB	1:A:994:GLU:OE1	2.06	0.56
15:O:191:ASP:O	15:O:194:LEU:HB2	2.06	0.56
15:O:205:ARG:O	15:O:209:VAL:HG12	2.05	0.56
2:B:480:GLN:HB3	2:B:507:SER:OG	2.05	0.56
3:C:71:MET:CE	3:C:225:ALA:HB2	2.33	0.56
13:M:15:VAL:HG22	13:M:90:LEU:HB2	1.88	0.56
15:O:63:LEU:HD23	15:O:111:ARG:HD2	1.87	0.56
1:A:35:PRO:HA	1:A:390:LEU:HD13	1.88	0.56
1:A:797:LEU:HD13	1:A:809:VAL:HG21	1.87	0.56
1:A:1655:ASP:CG	6:F:137:TYR:CE2	2.76	0.56
15:O:129:PRO:HG2	15:O:132:THR:OG1	2.06	0.56
15:O:440:ILE:CG2	15:O:491:PHE:CE1	2.82	0.56
15:O:447:THR:C	15:O:450:LEU:H	2.09	0.56
15:O:458:GLU:CB	15:O:461:VAL:CG2	2.80	0.56
15:O:484:PHE:CD1	15:O:502:LEU:CD1	2.89	0.56
1:A:468:ARG:CZ	1:A:1021:ARG:NH1	2.65	0.56
1:A:1482:LYS:HE2	2:B:304:ASP:CG	2.26	0.56
1:A:1655:ASP:CB	6:F:135:ARG:HB3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:LEU:HB3	2:B:481:VAL:HG13	1.87	0.56
3:C:64:ALA:CB	3:C:298:PHE:CD2	2.89	0.56
1:A:87:ASN:CB	1:A:357:MET:SD	2.94	0.55
1:A:478:TYR:OH	2:B:1049:THR:CG2	2.51	0.55
2:B:1020:GLU:HG2	3:C:61:THR:CG2	2.34	0.55
1:A:1:MET:CG	2:B:1098:TYR:CE2	2.88	0.55
2:B:470:LEU:HB2	2:B:484:TYR:HE2	1.66	0.55
15:O:166:ILE:HD11	15:O:213:SER:OG	2.06	0.55
15:O:343:VAL:CG1	15:O:388:VAL:HG21	2.36	0.55
15:O:369:LYS:HE2	15:O:370:THR:HG22	1.87	0.55
1:A:1162:ASN:HD21	1:A:1164:LYS:HB2	1.71	0.55
1:A:916:THR:O	1:A:919:LYS:NZ	2.40	0.55
1:A:1038:ILE:HG12	1:A:1049:MET:C	2.27	0.55
1:A:1049:MET:C	1:A:1051:GLY:H	2.09	0.55
1:A:1575:ILE:HG13	9:I:122:ARG:HH22	1.71	0.55
2:B:236:ILE:HD13	2:B:377:MET:HE1	1.88	0.55
2:B:934:ILE:CG2	3:C:72:ILE:HB	2.35	0.55
3:C:84:TYR:CE2	12:L:66:GLN:CD	2.77	0.55
15:O:359:GLY:CA	15:O:362:ASN:HD22	2.16	0.55
15:O:447:THR:O	15:O:450:LEU:N	2.39	0.55
15:O:447:THR:HA	15:O:450:LEU:HG	1.88	0.55
1:A:389:VAL:HA	1:A:430:ILE:HD11	1.88	0.55
1:A:1050:TYR:CD2	1:A:1179:ILE:HG21	2.41	0.55
1:A:1348:VAL:N	2:B:268:GLU:O	2.37	0.55
2:B:859:CYS:HB3	2:B:872:LYS:HB2	1.88	0.55
10:J:10:CYS:HB3	10:J:43:ARG:NH1	2.21	0.55
13:M:11:GLU:N	13:M:86:LYS:O	2.36	0.55
15:O:432:LYS:HB2	15:O:610:TYR:N	2.20	0.55
1:A:437:PHE:CE2	1:A:456:VAL:CG2	2.85	0.55
1:A:1657:LEU:HD22	7:G:104:LEU:HD13	1.89	0.55
3:C:139:LYS:HG2	3:C:201:GLU:HB3	1.89	0.55
5:E:144:ILE:O	5:E:147:HIS:HB2	2.07	0.55
15:O:343:VAL:HG11	15:O:388:VAL:HG21	1.89	0.55
15:O:447:THR:HA	15:O:450:LEU:CD1	2.36	0.55
15:O:517:LEU:HD12	15:O:543:ILE:HG21	1.88	0.55
1:A:405:LYS:HG2	1:A:405:LYS:O	2.07	0.55
5:E:159:ASP:OD1	5:E:162:ARG:NH1	2.38	0.55
7:G:143:SER:HB3	15:O:101:SER:O	2.06	0.55
1:A:1024:THR:O	1:A:1028:GLU:HB3	2.07	0.55
1:A:1162:ASN:HD22	1:A:1165:LYS:HG3	1.71	0.55
2:B:322:ASN:HB3	2:B:325:GLN:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:LEU:HG	3:C:300:PHE:CE1	2.41	0.55
15:O:164:LEU:HB3	15:O:165:PRO:HD2	1.89	0.55
15:O:432:LYS:CB	15:O:608:GLU:O	2.55	0.55
7:G:25:THR:HG22	7:G:26:ASN:N	2.17	0.55
7:G:28:ILE:CG2	7:G:29:ASP:N	2.56	0.55
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.89	0.55
2:B:373:MET:O	2:B:377:MET:HG3	2.08	0.55
3:C:45:SER:HB2	3:C:271:ARG:CZ	2.35	0.55
3:C:57:ILE:CG1	3:C:297:HIS:ND1	2.70	0.55
15:O:158:LEU:HD22	15:O:172:HIS:CA	2.36	0.55
15:O:369:LYS:HD2	15:O:369:LYS:C	2.27	0.55
1:A:863:ASN:HD21	9:I:68:LYS:N	2.05	0.54
15:O:147:ILE:O	15:O:147:ILE:HG22	2.07	0.54
1:A:996:TYR:CE1	1:A:1000:MET:CE	2.90	0.54
2:B:42:VAL:HG21	2:B:190:ILE:HB	1.89	0.54
7:G:143:SER:HA	15:O:103:ASN:HA	1.90	0.54
1:A:479:ALA:HB2	2:B:1091:ARG:NH2	2.22	0.54
1:A:800:VAL:HG23	1:A:1068:PHE:CZ	2.41	0.54
3:C:253:PRO:HB2	14:N:180:PHE:CG	2.42	0.54
1:A:412:SER:C	1:A:414:GLU:N	2.56	0.54
15:O:158:LEU:CD2	15:O:172:HIS:HD2	2.01	0.54
15:O:487:ARG:NH2	15:O:611:ILE:HD12	2.22	0.54
15:O:488:HIS:C	15:O:490:ILE:H	2.10	0.54
1:A:399:LEU:HD11	1:A:423:LEU:HG	1.89	0.54
1:A:402:ASP:HA	1:A:405:LYS:HB3	1.88	0.54
2:B:401:GLU:HG3	2:B:402:VAL:H	1.69	0.54
2:B:799:GLY:O	2:B:1035:ARG:NH1	2.39	0.54
4:D:48:GLU:HG2	4:D:86:ILE:CD1	2.36	0.54
7:G:158:LYS:HZ2	15:O:108:GLU:CG	2.03	0.54
7:G:229:LEU:HD12	7:G:230:ARG:H	1.72	0.54
15:O:241:ASP:CA	15:O:380:SER:HB2	2.38	0.54
15:O:360:VAL:O	15:O:363:THR:HG23	2.06	0.54
15:O:372:VAL:C	15:O:374:PRO:CD	2.76	0.54
1:A:478:TYR:CA	2:B:1048:SER:C	2.74	0.54
1:A:1008:ASP:OD1	1:A:1202:LEU:HB3	2.07	0.54
1:A:1446:ARG:O	1:A:1450:ILE:HG13	2.08	0.54
2:B:284:SER:OG	2:B:287:GLU:HG3	2.07	0.54
3:C:58:ASN:HA	3:C:296:ASN:HB2	0.84	0.54
3:C:253:PRO:CA	14:N:180:PHE:HD1	2.20	0.54
1:A:589:MET:HE1	1:A:614:LEU:HD13	1.89	0.54
1:A:878:ARG:CZ	9:I:66:VAL:HG23	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:ALA:HA	2:B:269:TYR:CE1	2.43	0.54
3:C:59:ILE:HG22	3:C:298:PHE:CE1	2.31	0.54
15:O:169:THR:HA	15:O:172:HIS:ND1	2.22	0.54
15:O:426:SER:HB3	15:O:594:TYR:HD2	1.72	0.54
1:A:1344:ILE:CG2	2:B:333:LYS:CG	2.86	0.54
9:I:71:LEU:HG	9:I:72:LYS:O	2.08	0.54
1:A:1651:THR:OG1	2:B:1085:SER:HB2	2.07	0.54
3:C:253:PRO:CB	14:N:180:PHE:CD1	2.79	0.54
15:O:100:LEU:HD22	15:O:107:ILE:CD1	2.38	0.54
15:O:423:TYR:CD1	15:O:594:TYR:CZ	2.95	0.54
1:A:556:ALA:CA	15:O:246:ASN:HD22	2.20	0.54
2:B:21:ARG:NH1	2:B:22:GLU:OE1	2.40	0.54
2:B:1043:LYS:CG	2:B:1063:ARG:NE	2.70	0.54
7:G:132:VAL:HG22	7:G:232:THR:HG22	1.90	0.54
15:O:391:GLN:NE2	15:O:609:TYR:CE2	2.76	0.54
2:B:788:ILE:HB	2:B:948:ILE:HB	1.89	0.53
1:A:389:VAL:HA	1:A:430:ILE:CD1	2.38	0.53
1:A:413:LEU:C	1:A:417:ARG:NH2	2.56	0.53
1:A:1136:VAL:HG22	1:A:1174:TYR:CG	2.44	0.53
3:C:55:ASP:CB	3:C:297:HIS:HE2	2.21	0.53
3:C:97:LEU:HD11	3:C:202:ILE:HD13	1.90	0.53
15:O:368:PHE:CZ	15:O:385:MET:HB2	2.43	0.53
1:A:641:GLU:HB2	6:F:99:LEU:CD1	2.36	0.53
1:A:1660:VAL:HG22	7:G:103:LYS:C	2.28	0.53
3:C:55:ASP:OD1	3:C:299:ILE:CG2	2.56	0.53
9:I:96:TYR:HA	9:I:111:PHE:O	2.09	0.53
15:O:69:THR:O	15:O:73:ILE:HG13	2.07	0.53
1:A:572:THR:HA	7:G:52:MET:HE3	1.90	0.53
2:B:398:GLN:HG2	2:B:398:GLN:O	2.06	0.53
15:O:147:ILE:HG22	15:O:149:LYS:HB3	1.90	0.53
1:A:91:PHE:CD2	1:A:249:THR:HG22	2.43	0.53
1:A:1655:ASP:HB2	6:F:135:ARG:CB	2.38	0.53
1:A:1482:LYS:HE2	2:B:304:ASP:OD2	2.08	0.53
2:B:470:LEU:O	2:B:481:VAL:CG1	2.56	0.53
4:D:37:LEU:CD2	4:D:97:LYS:HE3	2.38	0.53
13:M:75:GLN:HB2	14:N:60:SER:HA	1.91	0.53
15:O:63:LEU:CD2	15:O:111:ARG:HD2	2.38	0.53
15:O:342:HIS:O	15:O:346:GLN:CG	2.51	0.53
1:A:1008:ASP:OD1	1:A:1202:LEU:CG	2.56	0.53
2:B:563:SER:HA	13:M:73:SER:OG	2.08	0.53
2:B:934:ILE:HG21	3:C:73:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:PHE:O	3:C:71:MET:HG3	2.08	0.53
15:O:156:MET:HE2	15:O:193:TYR:CE1	2.44	0.53
15:O:218:LEU:HD23	15:O:229:ILE:HD11	1.90	0.53
15:O:238:ILE:CD1	15:O:371:HIS:HB3	2.37	0.53
15:O:390:GLN:HB2	15:O:609:TYR:CG	2.43	0.53
1:A:248:PHE:CD1	1:A:442:LYS:O	2.62	0.53
1:A:1289:SER:HB3	1:A:1475:GLU:HG2	1.91	0.53
1:A:1344:ILE:CG2	2:B:333:LYS:CB	2.86	0.53
2:B:317:TYR:HB3	2:B:320:LEU:HD12	1.89	0.53
4:D:28:PRO:CD	7:G:24:VAL:HG13	2.35	0.53
4:D:92:ILE:HG22	4:D:96:PHE:CE2	2.41	0.53
11:K:48:LYS:HE2	11:K:64:GLN:NE2	2.23	0.53
15:O:374:PRO:CB	15:O:375:THR:HG23	2.39	0.53
1:A:408:LYS:C	1:A:411:VAL:HG12	2.29	0.53
2:B:472:SER:O	2:B:474:SER:N	2.41	0.53
3:C:131:THR:HG21	3:C:207:HIS:HB3	1.91	0.53
4:D:23:HIS:CD2	6:F:58:PHE:CD2	2.97	0.53
7:G:30:GLU:HA	7:G:32:ASN:H	1.74	0.53
13:M:12:ILE:HD12	14:N:67:LEU:HB2	1.90	0.53
15:O:189:PHE:CD1	15:O:190:ILE:N	2.76	0.53
15:O:520:CYS:O	15:O:521:ASN:O	2.27	0.53
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	1.90	0.53
2:B:207:ILE:CD1	2:B:503:VAL:HG22	2.36	0.53
2:B:211:ARG:NH2	2:B:243:GLN:OE1	2.42	0.53
2:B:566:TYR:HD2	13:M:73:SER:HG	1.56	0.53
3:C:272:LYS:HG3	14:N:175:TYR:CE1	2.44	0.53
2:B:555:GLN:HB2	2:B:646:HIS:CE1	2.44	0.52
1:A:477:ASN:OD1	2:B:1059:PRO:HG2	1.99	0.52
1:A:800:VAL:HG23	1:A:1068:PHE:HZ	1.73	0.52
2:B:894:LYS:HG2	12:L:47:ARG:HD3	1.89	0.52
3:C:64:ALA:CB	3:C:227:TYR:CE2	2.92	0.52
15:O:459:GLU:C	15:O:461:VAL:N	2.61	0.52
2:B:33:SER:C	2:B:35:PHE:H	2.12	0.52
3:C:64:ALA:HB3	3:C:298:PHE:CE2	2.44	0.52
15:O:371:HIS:C	15:O:374:PRO:CD	2.78	0.52
15:O:499:GLU:O	15:O:502:LEU:HG	2.09	0.52
3:C:127:THR:H	3:C:130:ASN:HB2	1.74	0.52
7:G:142:ALA:HB3	15:O:102:SER:HA	1.91	0.52
9:I:59:SER:O	9:I:63:LYS:HG3	2.09	0.52
15:O:337:THR:O	15:O:341:THR:OG1	2.27	0.52
2:B:22:GLU:O	2:B:26:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:242:VAL:HG21	15:O:183:ILE:HG21	1.91	0.52
9:I:59:SER:O	9:I:63:LYS:CG	2.57	0.52
1:A:509:GLU:HG3	1:A:579:ARG:CD	2.39	0.52
1:A:969:PHE:CE2	1:A:978:ALA:HA	2.44	0.52
2:B:527:PHE:CE1	2:B:666:PRO:HG3	2.45	0.52
2:B:915:ASP:OD1	2:B:1038:HIS:CD2	2.61	0.52
15:O:348:THR:HG22	15:O:351:SER:CB	2.26	0.52
2:B:833:PRO:O	2:B:834:LYS:HB3	2.10	0.52
3:C:82:TYR:CE1	12:L:68:GLU:HG3	2.44	0.52
15:O:155:SER:HB2	15:O:176:LEU:HD21	1.91	0.52
15:O:156:MET:HG3	15:O:197:PHE:HE2	1.60	0.52
15:O:373:LEU:CD1	15:O:416:LYS:CG	2.62	0.52
1:A:441:THR:HG22	1:A:441:THR:O	2.10	0.52
2:B:42:VAL:O	2:B:46:ILE:CD1	2.52	0.52
2:B:134:ARG:HD2	2:B:160:GLY:HA3	1.91	0.52
4:D:37:LEU:HD22	4:D:97:LYS:CE	2.39	0.52
13:M:105:SER:HA	13:M:108:LEU:CG	2.29	0.52
15:O:175:MET:HE2	15:O:175:MET:HA	1.92	0.52
15:O:206:ARG:HA	15:O:209:VAL:HG12	1.90	0.52
15:O:402:THR:O	15:O:406:ILE:HG13	2.10	0.52
15:O:458:GLU:CG	15:O:514:PHE:CE2	2.92	0.52
3:C:51:GLU:CB	3:C:303:GLU:HG3	2.40	0.52
7:G:26:ASN:HD21	7:G:126:GLN:HE21	1.56	0.52
15:O:459:GLU:HG3	15:O:460:GLU:N	2.25	0.52
1:A:497:VAL:HG21	1:A:605:VAL:HG13	1.92	0.51
1:A:722:PRO:HG2	8:H:46:LEU:HD13	1.90	0.51
2:B:37:LEU:CD1	2:B:760:TYR:CZ	2.90	0.51
15:O:415:GLU:O	15:O:419:LYS:HG3	2.10	0.51
15:O:518:LYS:HD3	15:O:519:PHE:CZ	2.45	0.51
1:A:636:HIS:CE1	2:B:1091:ARG:HH21	2.28	0.51
2:B:307:GLU:OE2	2:B:311:ARG:NH1	2.43	0.51
2:B:938:PHE:CD1	3:C:68:ARG:NE	2.78	0.51
2:B:1069:ILE:N	2:B:1069:ILE:CD1	2.73	0.51
2:B:1120:ILE:CD1	15:O:117:GLN:HE22	2.23	0.51
3:C:47:LEU:HD23	3:C:48:ASP:N	2.25	0.51
15:O:241:ASP:O	15:O:378:THR:HG23	2.10	0.51
15:O:426:SER:HB3	15:O:594:TYR:HB2	1.88	0.51
15:O:478:GLN:OE1	15:O:521:ASN:HB2	2.10	0.51
15:O:377:TYR:O	15:O:378:THR:OG1	2.20	0.51
1:A:87:ASN:HA	1:A:357:MET:SD	2.50	0.51
15:O:98:ASP:OD2	15:O:135:LYS:CE	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:457:ARG:O	15:O:461:VAL:HG23	2.10	0.51
1:A:1003:ARG:CD	2:B:520:LEU:N	2.73	0.51
1:A:1603:MET:HE1	1:A:1615:TYR:CD2	2.43	0.51
1:A:1657:LEU:HB3	7:G:104:LEU:HB3	1.93	0.51
2:B:1047:ARG:NH2	2:B:1051:PRO:O	2.43	0.51
3:C:64:ALA:O	3:C:227:TYR:CE2	2.58	0.51
15:O:158:LEU:HD22	15:O:172:HIS:CD2	2.46	0.51
15:O:383:TYR:CZ	15:O:597:LEU:HB2	2.46	0.51
1:A:392:THR:CB	1:A:430:ILE:HD13	2.37	0.51
2:B:527:PHE:CD1	2:B:666:PRO:HG3	2.46	0.51
4:D:95:ASP:OD2	7:G:150:HIS:CA	2.56	0.51
15:O:151:TRP:HZ2	15:O:176:LEU:HA	1.76	0.51
15:O:379:ARG:CB	15:O:382:GLN:NE2	2.74	0.51
15:O:487:ARG:CG	15:O:487:ARG:NH1	2.73	0.51
1:A:401:ASP:O	1:A:405:LYS:HB3	2.09	0.51
1:A:1028:GLU:CG	1:A:1029:GLY:H	2.24	0.51
1:A:1056:ASP:OD2	1:A:1179:ILE:HA	2.11	0.51
2:B:472:SER:O	2:B:473:GLN:C	2.48	0.51
3:C:31:TRP:CD2	11:K:82:LYS:CG	2.91	0.51
15:O:247:GLU:OE1	15:O:325:ILE:CD1	2.57	0.51
1:A:954:GLY:N	1:A:1205:PHE:HB3	2.25	0.51
1:A:1655:ASP:CG	6:F:137:TYR:HE2	2.14	0.51
2:B:300:SER:CB	9:I:49:THR:HG22	2.41	0.51
2:B:819:ASP:CG	2:B:820:PRO:HD2	2.31	0.51
3:C:229:LEU:HD22	3:C:295:ARG:O	2.11	0.51
15:O:369:LYS:CE	15:O:370:THR:CG2	2.86	0.51
1:A:475:ARG:HB3	2:B:1059:PRO:HB2	1.90	0.51
1:A:840:ASN:O	1:A:844:THR:HG23	2.11	0.51
2:B:769:PHE:CZ	2:B:798:PHE:CE1	2.91	0.51
3:C:131:THR:HG22	3:C:208:CYS:N	2.26	0.51
7:G:244:SER:HB2	15:O:148:PRO:HD2	1.91	0.51
15:O:198:PHE:CD2	15:O:232:LEU:CG	2.60	0.51
1:A:527:PRO:C	1:A:580:HIS:HE1	2.14	0.51
1:A:1003:ARG:CD	2:B:520:LEU:H	2.23	0.51
1:A:1450:ILE:HD12	1:A:1460:TYR:CD2	2.46	0.51
2:B:934:ILE:HG21	3:C:69:ARG:O	2.10	0.51
15:O:248:LEU:HD23	15:O:248:LEU:O	2.10	0.51
1:A:509:GLU:OE2	1:A:579:ARG:CZ	2.58	0.50
1:A:880:GLN:OE1	2:B:633:THR:O	2.27	0.50
1:A:991:LYS:HB3	1:A:993:GLN:OE1	2.11	0.50
1:A:1048:PHE:CE2	5:E:211:TYR:HD1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:VAL:O	7:G:103:LYS:N	2.39	0.50
2:B:934:ILE:HG21	3:C:73:SER:CB	2.41	0.50
3:C:57:ILE:O	3:C:58:ASN:HB2	2.12	0.50
3:C:296:ASN:O	3:C:297:HIS:HB2	2.11	0.50
4:D:28:PRO:CD	7:G:24:VAL:CG1	2.89	0.50
15:O:444:SER:O	15:O:447:THR:OG1	2.23	0.50
15:O:446:LEU:O	15:O:449:TRP:CB	2.42	0.50
1:A:478:TYR:HD1	2:B:1048:SER:HB2	1.76	0.50
1:A:564:PRO:HB2	15:O:371:HIS:HE1	1.76	0.50
1:A:1660:VAL:N	7:G:103:LYS:O	2.41	0.50
4:D:80:THR:HG23	15:O:227:PHE:HB3	1.88	0.50
10:J:1:MET:HG2	10:J:57:ILE:HB	1.93	0.50
1:A:1326:GLU:OE2	1:A:1454:HIS:HB3	2.11	0.50
2:B:894:LYS:HD3	12:L:47:ARG:NH1	2.26	0.50
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.93	0.50
15:O:591:TYR:CE2	15:O:593:PRO:HG3	2.46	0.50
1:A:970:LYS:HG2	1:A:973:GLU:HG2	1.92	0.50
2:B:469:ASN:CA	2:B:481:VAL:O	2.60	0.50
2:B:1002:LYS:CD	14:N:166:LEU:HB2	2.40	0.50
6:F:74:ILE:CG2	6:F:75:PRO:CD	2.87	0.50
1:A:437:PHE:CE2	1:A:456:VAL:HG23	2.36	0.50
1:A:1003:ARG:CD	2:B:520:LEU:HB2	2.41	0.50
2:B:68:ILE:HD11	2:B:414:LYS:CG	2.39	0.50
2:B:293:ILE:HG12	2:B:306:LEU:HD13	1.94	0.50
2:B:472:SER:HB3	2:B:476:LEU:HD11	1.92	0.50
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.93	0.50
15:O:242:VAL:HA	15:O:378:THR:CG2	2.37	0.50
15:O:352:LEU:HD22	15:O:358:VAL:HG22	1.81	0.50
2:B:203:ILE:HG21	2:B:405:GLY:HA2	1.93	0.50
2:B:284:SER:HB2	9:I:14:GLY:HA3	1.93	0.50
3:C:230:LEU:HD11	3:C:231:PRO:HD2	1.92	0.50
4:D:44:ILE:CG2	4:D:90:LYS:HE3	2.40	0.50
5:E:145:THR:C	5:E:147:HIS:N	2.65	0.50
14:N:87:TYR:CE1	14:N:141:GLU:OE1	2.64	0.50
15:O:359:GLY:CA	15:O:362:ASN:ND2	2.73	0.50
15:O:488:HIS:O	15:O:491:PHE:N	2.37	0.50
1:A:505:LEU:HD12	1:A:581:ILE:HD13	1.93	0.50
3:C:100:ARG:NH2	10:J:3:VAL:O	2.44	0.50
15:O:208:LEU:O	15:O:212:THR:HG23	2.12	0.50
1:A:953:GLU:CA	1:A:1205:PHE:CG	2.95	0.50
2:B:328:GLN:NE2	13:M:109:ARG:NH2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LEU:HD23	3:C:48:ASP:H	1.77	0.50
3:C:222:VAL:O	3:C:224:THR:N	2.44	0.50
3:C:231:PRO:HG2	3:C:270:ALA:CB	2.42	0.50
1:A:1025:LYS:NZ	2:B:1076:ARG:NH1	2.59	0.50
1:A:1048:PHE:CE2	5:E:210:SER:HA	2.46	0.50
1:A:1056:ASP:HB2	1:A:1177:SER:O	2.11	0.50
2:B:858:ILE:HD13	2:B:872:LYS:O	2.11	0.50
15:O:352:LEU:CA	15:O:358:VAL:CG2	2.90	0.50
1:A:863:ASN:HD22	9:I:67:VAL:C	2.15	0.49
1:A:1003:ARG:HD2	2:B:520:LEU:N	2.23	0.49
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.47	0.49
14:N:85:HIS:CE1	14:N:141:GLU:OE1	2.64	0.49
15:O:368:PHE:C	15:O:368:PHE:CD1	2.85	0.49
15:O:453:TYR:CE1	15:O:473:PHE:HB2	2.47	0.49
1:A:1006:LEU:HD21	2:B:535:ASP:CB	2.42	0.49
7:G:143:SER:HB3	15:O:103:ASN:CA	2.42	0.49
15:O:324:GLY:O	15:O:326:LYS:N	2.44	0.49
15:O:368:PHE:CD2	15:O:385:MET:HG2	2.47	0.49
15:O:468:GLU:C	15:O:470:PHE:N	2.65	0.49
1:A:381:SER:HB2	1:A:453:ILE:HG21	1.93	0.49
2:B:338:PHE:CE1	2:B:353:VAL:HG22	2.47	0.49
2:B:1019:GLY:CA	3:C:65:ASN:CG	2.81	0.49
4:D:23:HIS:CG	6:F:58:PHE:CD2	3.00	0.49
7:G:242:VAL:HG21	15:O:183:ILE:HG23	1.93	0.49
9:I:91:ASN:OD1	9:I:92:GLU:N	2.45	0.49
1:A:412:SER:H	1:A:415:ASP:HB2	1.76	0.49
1:A:507:TYR:HB2	1:A:637:PHE:CE2	2.47	0.49
1:A:1053:ASP:HB2	5:E:204:THR:CG2	2.43	0.49
1:A:1622:LEU:HD21	2:B:1189:LEU:HD22	1.94	0.49
2:B:1043:LYS:HE2	2:B:1063:ARG:CD	2.42	0.49
2:B:1120:ILE:HD12	15:O:117:GLN:NE2	2.27	0.49
3:C:71:MET:HE1	3:C:225:ALA:HB1	1.90	0.49
3:C:71:MET:CE	3:C:302:VAL:CG2	2.90	0.49
15:O:430:ARG:O	15:O:431:ALA:O	2.31	0.49
1:A:995:TYR:O	1:A:999:CYS:N	2.35	0.49
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	1.92	0.49
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.77	0.49
4:D:30:HIS:HE2	7:G:26:ASN:CG	2.11	0.49
12:L:45:ALA:O	12:L:47:ARG:N	2.46	0.49
15:O:173:HIS:CE1	15:O:217:LYS:HB3	2.47	0.49
1:A:1034:TYR:HA	1:A:1181:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1500:GLN:HG2	1:A:1501:ILE:N	2.28	0.49
15:O:173:HIS:CD2	15:O:217:LYS:CG	2.95	0.49
15:O:488:HIS:C	15:O:490:ILE:N	2.59	0.49
15:O:488:HIS:CE1	15:O:489:ASN:H	2.27	0.49
1:A:1026:GLN:NE2	1:A:1603:MET:HA	2.26	0.49
15:O:177:LYS:HG3	15:O:178:TYR:N	2.26	0.49
15:O:443:ALA:O	15:O:447:THR:HG23	2.12	0.49
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.28	0.49
6:F:75:PRO:HG3	6:F:78:GLN:NE2	2.27	0.49
15:O:361:PHE:CD1	15:O:361:PHE:C	2.86	0.49
15:O:507:GLN:O	15:O:511:ILE:HG23	2.12	0.49
1:A:249:THR:HG1	1:A:435:ASN:HD21	1.58	0.49
1:A:476:VAL:O	2:B:1059:PRO:HG2	2.13	0.49
1:A:795:HIS:NE2	1:A:1062:HIS:HE1	2.11	0.49
1:A:982:VAL:HG13	1:A:994:GLU:CD	2.33	0.49
1:A:1661:PRO:CA	7:G:101:SER:O	2.61	0.49
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.44	0.49
2:B:262:PHE:CD1	2:B:357:ILE:HD13	2.48	0.49
13:M:65:TYR:CE1	13:M:97:VAL:HB	2.48	0.49
15:O:234:ILE:O	15:O:238:ILE:HG13	2.12	0.49
1:A:91:PHE:CZ	1:A:249:THR:HA	2.46	0.49
1:A:582:LYS:O	1:A:585:ASP:HB2	2.12	0.49
1:A:1662:ASN:N	7:G:101:SER:HB2	2.28	0.49
15:O:163:ILE:HG22	15:O:207:LYS:O	2.12	0.49
15:O:434:LEU:CD1	15:O:434:LEU:N	2.75	0.49
1:A:1053:ASP:HB2	5:E:204:THR:HG22	1.95	0.48
2:B:281:CYS:HA	2:B:323:ARG:NE	2.28	0.48
15:O:390:GLN:C	15:O:609:TYR:CE1	2.81	0.48
15:O:396:MET:HE1	15:O:433:LYS:C	2.34	0.48
15:O:468:GLU:C	15:O:470:PHE:H	2.15	0.48
1:A:475:ARG:NH1	2:B:1061:LYS:HB2	2.28	0.48
2:B:225:ARG:NH2	2:B:261:ARG:HD3	2.27	0.48
4:D:95:ASP:OD1	7:G:151:ASP:HB2	2.12	0.48
7:G:137:ILE:HG13	7:G:227:GLY:O	2.13	0.48
8:H:112:ILE:HD12	8:H:129:TYR:HB2	1.93	0.48
15:O:591:TYR:HE2	15:O:593:PRO:HG3	1.77	0.48
1:A:996:TYR:HE1	1:A:1000:MET:HE1	1.78	0.48
1:A:1050:TYR:HE1	1:A:1185:VAL:HG12	1.67	0.48
1:A:1055:ILE:CG2	1:A:1060:GLU:HB2	2.43	0.48
1:A:1260:LYS:HE2	1:A:1262:LEU:HD11	1.95	0.48
2:B:209:GLN:CG	2:B:210:ARG:H	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1043:LYS:HG3	2:B:1063:ARG:CZ	2.43	0.48
15:O:391:GLN:HE22	15:O:609:TYR:HE2	1.61	0.48
1:A:50:TYR:CD1	1:A:365:THR:HG23	2.47	0.48
1:A:440:SER:C	1:A:442:LYS:H	2.17	0.48
5:E:145:THR:O	5:E:147:HIS:N	2.46	0.48
15:O:91:LYS:HG3	15:O:92:ASN:N	2.28	0.48
15:O:383:TYR:CG	15:O:597:LEU:HD22	2.47	0.48
15:O:597:LEU:HD12	15:O:598:PHE:H	1.77	0.48
1:A:1606:SER:HB3	1:A:1611:MET:HE2	1.96	0.48
2:B:471:VAL:O	2:B:471:VAL:HG12	2.13	0.48
2:B:929:ARG:HH22	11:K:96:PRO:HB2	1.77	0.48
15:O:199:PRO:HB2	15:O:208:LEU:HD23	1.95	0.48
1:A:365:THR:O	1:A:368:ARG:N	2.37	0.48
1:A:413:LEU:CA	1:A:417:ARG:HH21	2.27	0.48
1:A:721:LYS:HB3	8:H:96:VAL:HB	1.95	0.48
1:A:932:GLY:C	9:I:125:ASN:HD21	2.16	0.48
2:B:550:ARG:O	2:B:649:MET:HA	2.14	0.48
2:B:800:TYR:CD1	2:B:800:TYR:C	2.87	0.48
4:D:48:GLU:CD	4:D:90:LYS:NZ	2.66	0.48
14:N:111:VAL:HG13	14:N:122:ALA:HB2	1.96	0.48
15:O:241:ASP:OD1	15:O:380:SER:HB2	2.13	0.48
15:O:408:PHE:CD2	15:O:449:TRP:CE2	3.02	0.48
15:O:440:ILE:HD13	15:O:491:PHE:CD1	2.48	0.48
15:O:484:PHE:O	15:O:488:HIS:HB3	2.14	0.48
1:A:399:LEU:HD22	1:A:423:LEU:HA	1.95	0.48
1:A:597:LYS:HB2	2:B:1082:HIS:CE1	2.48	0.48
1:A:1003:ARG:HD2	2:B:520:LEU:CB	2.43	0.48
1:A:40:ASN:N	1:A:40:ASN:OD1	2.44	0.48
1:A:480:ALA:CA	2:B:1046:VAL:HG23	2.42	0.48
1:A:684:ASP:OD1	8:H:20:TYR:HB3	2.13	0.48
1:A:747:ILE:HD13	1:A:748:ASN:H	1.77	0.48
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.94	0.48
4:D:92:ILE:CD1	7:G:152:ALA:CB	2.92	0.48
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.61	0.48
15:O:369:LYS:HE2	15:O:370:THR:N	2.28	0.48
15:O:477:PHE:CE2	15:O:481:CYS:SG	3.07	0.48
1:A:869:PRO:HG2	1:A:872:ASP:HB2	1.96	0.48
1:A:1006:LEU:CD2	2:B:535:ASP:HB2	2.43	0.48
1:A:1023:LEU:CD2	1:A:1598:PHE:CD1	2.97	0.48
1:A:1162:ASN:ND2	1:A:1165:LYS:HG3	2.29	0.48
2:B:552:SER:O	2:B:647:SER:CA	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1133:MET:CE	7:G:17:ILE:HD13	2.44	0.48
15:O:369:LYS:HD2	15:O:370:THR:HA	1.95	0.48
15:O:446:LEU:C	15:O:449:TRP:HB3	2.31	0.48
1:A:1055:ILE:CG2	1:A:1060:GLU:CG	2.90	0.48
1:A:1312:GLU:O	1:A:1316:VAL:HG23	2.13	0.48
2:B:70:GLU:CB	2:B:97:VAL:O	2.62	0.48
2:B:894:LYS:HD3	12:L:47:ARG:CZ	2.44	0.48
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.95	0.48
15:O:146:SER:C	15:O:148:PRO:HD3	2.34	0.48
1:A:747:ILE:HD13	1:A:748:ASN:N	2.29	0.47
4:D:92:ILE:HD11	7:G:152:ALA:HB1	1.95	0.47
7:G:158:LYS:HE2	15:O:105:ASN:OD1	2.14	0.47
15:O:151:TRP:CZ2	15:O:176:LEU:HA	2.49	0.47
15:O:225:LEU:HD12	15:O:229:ILE:HG13	1.96	0.47
1:A:959:VAL:HG22	1:A:965:THR:HG22	1.95	0.47
1:A:960:MET:SD	2:B:522:PRO:HB2	2.54	0.47
2:B:73:ILE:HB	2:B:425:ILE:HD12	1.96	0.47
4:D:80:THR:HG21	15:O:227:PHE:CG	2.48	0.47
15:O:369:LYS:O	15:O:373:LEU:CA	2.60	0.47
15:O:478:GLN:NE2	15:O:592:PHE:CZ	2.69	0.47
2:B:73:ILE:HD12	2:B:425:ILE:HG23	1.95	0.47
2:B:208:VAL:CG2	2:B:401:GLU:CG	2.92	0.47
3:C:230:LEU:CG	3:C:294:VAL:CG2	2.92	0.47
15:O:120:ILE:HD13	15:O:150:TRP:CE3	2.49	0.47
1:A:1348:VAL:HB	2:B:268:GLU:CA	2.43	0.47
2:B:552:SER:O	2:B:647:SER:HA	2.14	0.47
2:B:584:CYS:HB3	2:B:596:VAL:HG23	1.95	0.47
10:J:6:ARG:HD2	10:J:11:GLY:O	2.13	0.47
1:A:1048:PHE:CE1	5:E:211:TYR:CD1	3.01	0.47
1:A:1261:VAL:HG12	1:A:1262:LEU:N	2.28	0.47
1:A:1482:LYS:HE2	2:B:304:ASP:OD1	2.15	0.47
1:A:1605:THR:C	1:A:1606:SER:O	2.37	0.47
5:E:48:ASP:OD1	5:E:50:MET:HB3	2.13	0.47
1:A:258:GLU:HA	1:A:261:ILE:HD12	1.97	0.47
2:B:338:PHE:CZ	2:B:357:ILE:HD12	2.49	0.47
2:B:470:LEU:O	2:B:481:VAL:HG13	2.15	0.47
15:O:107:ILE:O	15:O:109:SER:N	2.46	0.47
1:A:439:ASP:HB3	1:A:442:LYS:HD2	1.96	0.47
1:A:741:PRO:HA	1:A:742:PRO:HD3	1.68	0.47
1:A:1573:TYR:HB3	9:I:122:ARG:NH2	2.30	0.47
2:B:812:ALA:HA	2:B:815:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1020:GLU:HG2	3:C:61:THR:CB	2.44	0.47
3:C:126:PHE:HD1	3:C:131:THR:HG1	1.62	0.47
15:O:237:ILE:CG2	15:O:381:ILE:CG1	2.93	0.47
15:O:460:GLU:O	15:O:469:ARG:NH2	2.47	0.47
15:O:471:LYS:CG	15:O:472:HIS:N	2.75	0.47
15:O:521:ASN:ND2	15:O:523:ASN:N	2.54	0.47
1:A:19:LEU:HD11	2:B:1190:SER:HB2	1.96	0.47
2:B:396:ALA:HB1	2:B:523:GLU:HG3	1.96	0.47
3:C:247:PHE:HE1	3:C:289:VAL:HG21	1.80	0.47
1:A:479:ALA:HB2	1:A:636:HIS:ND1	2.29	0.47
3:C:31:TRP:NE1	11:K:82:LYS:NZ	2.54	0.47
3:C:86:PHE:CD1	12:L:64:LEU:HD13	2.46	0.47
13:M:109:ARG:HH22	13:M:112:LYS:HG3	1.79	0.47
15:O:170:VAL:CG1	15:O:171:CYS:N	2.78	0.47
15:O:176:LEU:HD13	15:O:218:LEU:HD13	1.96	0.47
1:A:55:GLY:HA2	1:A:62:CYS:SG	2.56	0.47
2:B:413:LEU:O	2:B:417:ILE:HG13	2.14	0.47
15:O:129:PRO:O	15:O:133:LEU:CB	2.62	0.47
15:O:602:TYR:O	15:O:606:MET:HG2	2.15	0.47
1:A:863:ASN:HD22	9:I:68:LYS:N	2.08	0.46
2:B:203:ILE:CG2	2:B:405:GLY:HA2	2.45	0.46
2:B:470:LEU:N	2:B:481:VAL:O	2.47	0.46
2:B:569:GLY:HA2	14:N:140:SER:OG	2.15	0.46
2:B:1103:VAL:HG22	2:B:1176:VAL:HG22	1.97	0.46
3:C:231:PRO:CG	3:C:270:ALA:O	2.62	0.46
3:C:239:ILE:HG23	3:C:243:SER:HB3	1.96	0.46
15:O:138:TYR:CD2	15:O:142:ILE:CD1	2.92	0.46
15:O:488:HIS:O	15:O:489:ASN:C	2.54	0.46
1:A:364:PRO:HB2	1:A:367:PHE:CD2	2.51	0.46
1:A:403:LEU:CD2	1:A:423:LEU:HD11	2.45	0.46
1:A:1320:GLN:HE21	1:A:1320:GLN:HB2	1.56	0.46
2:B:681:ILE:O	14:N:154:ARG:NE	2.36	0.46
2:B:736:ARG:HD3	2:B:738:ASP:OD2	2.15	0.46
4:D:46:GLU:OE1	4:D:47:LYS:HE2	2.15	0.46
4:D:95:ASP:HB2	7:G:151:ASP:HB3	1.97	0.46
15:O:170:VAL:HG13	15:O:171:CYS:H	1.79	0.46
15:O:206:ARG:HA	15:O:209:VAL:CG1	2.44	0.46
15:O:388:VAL:HG13	15:O:389:SER:N	2.31	0.46
1:A:412:SER:C	1:A:414:GLU:H	2.17	0.46
1:A:492:THR:HG23	1:A:811:SER:OG	2.14	0.46
1:A:996:TYR:CE1	1:A:1000:MET:HE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:ASP:O	1:A:1054:ALA:CB	2.62	0.46
1:A:1060:GLU:HA	1:A:1063:MET:CG	2.37	0.46
1:A:1258:ILE:HB	1:A:1501:ILE:HD12	1.97	0.46
1:A:1440:ASN:HA	1:A:1443:GLN:HB2	1.96	0.46
3:C:231:PRO:HG3	3:C:270:ALA:O	2.16	0.46
15:O:181:ARG:CG	15:O:181:ARG:NH1	2.77	0.46
2:B:679:GLN:HG3	14:N:155:VAL:O	2.14	0.46
3:C:71:MET:HE1	3:C:302:VAL:CG2	2.40	0.46
9:I:23:VAL:O	9:I:39:LYS:NZ	2.48	0.46
11:K:93:ILE:HA	11:K:94:PRO:HD2	1.75	0.46
15:O:74:ILE:O	15:O:78:VAL:HG13	2.16	0.46
15:O:148:PRO:HB3	15:O:183:ILE:HD13	1.98	0.46
15:O:433:LYS:HG3	15:O:433:LYS:O	2.16	0.46
1:A:211:THR:HG23	5:E:177:ARG:CZ	2.45	0.46
2:B:280:LEU:HD13	2:B:371:PHE:N	2.30	0.46
4:D:95:ASP:HB2	7:G:151:ASP:CB	2.46	0.46
15:O:506:PHE:HD2	15:O:537:VAL:CG1	2.28	0.46
1:A:411:VAL:CG2	1:A:412:SER:N	2.76	0.46
1:A:507:TYR:HB2	1:A:637:PHE:CZ	2.51	0.46
2:B:467:THR:O	2:B:469:ASN:N	2.49	0.46
7:G:141:SER:HB2	15:O:138:TYR:CZ	2.43	0.46
7:G:143:SER:HB3	15:O:102:SER:C	2.35	0.46
15:O:352:LEU:HA	15:O:358:VAL:CG2	2.31	0.46
1:A:94:LEU:HD11	1:A:356:PHE:CZ	2.51	0.46
1:A:1003:ARG:CD	2:B:520:LEU:CB	2.93	0.46
1:A:1028:GLU:HG3	1:A:1637:PRO:HG2	1.97	0.46
2:B:265:ARG:NH2	2:B:339:GLN:OE1	2.48	0.46
2:B:822:THR:HB	2:B:823:GLN:HG3	1.98	0.46
4:D:48:GLU:CG	4:D:86:ILE:HD12	2.39	0.46
2:B:202:LEU:HD13	2:B:500:PHE:CE1	2.51	0.46
3:C:50:ARG:O	3:C:303:GLU:CA	2.58	0.46
3:C:57:ILE:CA	3:C:297:HIS:HA	2.09	0.46
4:D:25:THR:CB	6:F:59:GLN:HG2	2.39	0.46
15:O:447:THR:HB	15:O:505:PHE:CE2	2.51	0.46
15:O:459:GLU:O	15:O:463:GLN:CB	2.63	0.46
1:A:5:LYS:HB3	1:A:5:LYS:HE2	1.68	0.46
1:A:184:LYS:HA	1:A:187:GLU:HG2	1.98	0.46
1:A:438:ILE:CG2	2:B:1192:MET:CE	2.92	0.46
1:A:1575:ILE:HG13	9:I:122:ARG:NH1	2.29	0.46
2:B:774:ALA:HB1	2:B:1026:ILE:HD11	1.97	0.46
2:B:890:ASP:HB3	2:B:896:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1120:ILE:CD1	15:O:117:GLN:NE2	2.79	0.46
3:C:31:TRP:NE1	11:K:78:TYR:OH	2.46	0.46
5:E:131:THR:HG21	5:E:191:LYS:CE	2.45	0.46
15:O:239:SER:O	15:O:243:GLU:HG2	2.16	0.46
1:A:412:SER:HB3	1:A:414:GLU:HB3	1.96	0.46
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.50	0.46
2:B:293:ILE:CD1	2:B:302:LEU:HB3	2.46	0.46
2:B:554:GLN:C	2:B:646:HIS:CD2	2.90	0.46
4:D:92:ILE:CD1	7:G:152:ALA:HB1	2.45	0.46
15:O:467:MET:HE1	15:O:470:PHE:HE2	1.81	0.46
1:A:1019:LEU:CD1	1:A:1227:MET:CG	2.91	0.45
1:A:1608:SER:OG	1:A:1632:GLU:OE2	2.20	0.45
2:B:292:ILE:HB	2:B:306:LEU:HD11	1.98	0.45
2:B:724:GLN:O	2:B:1037:ARG:HG3	2.17	0.45
4:D:28:PRO:CB	7:G:24:VAL:HG11	2.46	0.45
13:M:26:PHE:CE1	13:M:98:SER:HB2	2.51	0.45
15:O:428:ILE:CG2	15:O:439:ILE:CG2	2.86	0.45
15:O:506:PHE:CG	15:O:528:PHE:HZ	2.34	0.45
1:A:436:ALA:O	1:A:440:SER:N	2.49	0.45
1:A:954:GLY:N	1:A:1205:PHE:CB	2.79	0.45
2:B:552:SER:C	2:B:647:SER:H	2.16	0.45
4:D:40:LEU:HD13	4:D:93:GLN:HB2	1.98	0.45
9:I:89:CYS:SG	9:I:91:ASN:HB2	2.56	0.45
11:K:80:ILE:HD13	11:K:105:ILE:HD11	1.98	0.45
15:O:458:GLU:HG3	15:O:514:PHE:CE2	2.51	0.45
15:O:485:CYS:SG	15:O:531:ILE:HD12	2.56	0.45
2:B:68:ILE:CD1	2:B:414:LYS:HG3	2.41	0.45
2:B:480:GLN:CB	2:B:507:SER:OG	2.64	0.45
3:C:54:PHE:CD1	3:C:300:PHE:O	2.69	0.45
3:C:228:ARG:HG3	3:C:299:ILE:HB	1.98	0.45
15:O:69:THR:HG22	15:O:70:GLN:N	2.31	0.45
15:O:190:ILE:HD13	15:O:190:ILE:C	2.37	0.45
15:O:245:GLN:O	15:O:248:LEU:N	2.39	0.45
15:O:370:THR:O	15:O:374:PRO:CG	2.63	0.45
15:O:459:GLU:O	15:O:463:GLN:N	2.50	0.45
1:A:1237:GLN:H	1:A:1544:ASN:HB2	1.81	0.45
2:B:841:ASP:OD1	2:B:842:GLU:N	2.40	0.45
2:B:1020:GLU:HG3	3:C:61:THR:OG1	2.17	0.45
3:C:294:VAL:O	3:C:294:VAL:HG12	2.15	0.45
3:C:295:ARG:HD3	3:C:295:ARG:HA	1.66	0.45
7:G:143:SER:CB	15:O:103:ASN:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:169:THR:O	15:O:170:VAL:C	2.54	0.45
1:A:782:ASP:O	1:A:785:GLN:N	2.27	0.45
1:A:863:ASN:ND2	9:I:67:VAL:C	2.70	0.45
1:A:953:GLU:HG2	1:A:1205:PHE:CD2	2.50	0.45
1:A:1006:LEU:HD21	2:B:535:ASP:HB2	1.98	0.45
1:A:1048:PHE:HZ	5:E:211:TYR:HB2	1.81	0.45
1:A:1657:LEU:HD22	7:G:104:LEU:CD1	2.45	0.45
2:B:61:LEU:HA	2:B:61:LEU:HD23	1.76	0.45
2:B:646:HIS:O	2:B:647:SER:HB2	2.16	0.45
7:G:242:VAL:HG12	15:O:185:SER:CB	2.46	0.45
15:O:372:VAL:CG1	15:O:423:TYR:OH	2.64	0.45
1:A:891:ILE:CD1	9:I:71:LEU:N	2.80	0.45
1:A:1348:VAL:CA	2:B:268:GLU:O	2.63	0.45
2:B:585:CYS:HB2	2:B:595:TRP:CZ3	2.51	0.45
4:D:80:THR:CG2	15:O:227:PHE:CG	2.99	0.45
6:F:75:PRO:HG3	6:F:78:GLN:CD	2.37	0.45
15:O:148:PRO:HB3	15:O:183:ILE:CD1	2.46	0.45
15:O:407:SER:CB	15:O:408:PHE:CD1	2.95	0.45
15:O:521:ASN:HD22	15:O:523:ASN:H	1.59	0.45
1:A:799:GLU:CG	1:A:1062:HIS:CG	2.85	0.45
1:A:799:GLU:CG	1:A:1062:HIS:ND1	2.69	0.45
1:A:1154:LEU:O	1:A:1158:SER:HB2	2.17	0.45
1:A:1291:VAL:HG22	1:A:1473:LYS:HG3	1.99	0.45
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.98	0.45
2:B:205:MET:HE1	2:B:500:PHE:O	2.16	0.45
3:C:117:ASP:OD1	3:C:119:ASN:ND2	2.44	0.45
3:C:176:SER:O	3:C:180:ALA:HB2	2.16	0.45
13:M:65:TYR:HE1	13:M:97:VAL:HB	1.81	0.45
15:O:369:LYS:HE3	15:O:370:THR:HG22	1.99	0.45
15:O:384:ILE:HA	15:O:602:TYR:OH	2.16	0.45
15:O:408:PHE:HZ	15:O:446:LEU:CD2	2.30	0.45
15:O:468:GLU:O	15:O:470:PHE:N	2.49	0.45
1:A:878:ARG:NE	9:I:67:VAL:HG13	2.30	0.45
2:B:1158:ILE:HA	2:B:1167:PHE:O	2.17	0.45
5:E:7:ARG:O	5:E:11:ARG:HG3	2.17	0.45
15:O:98:ASP:OD2	15:O:135:LYS:CD	2.64	0.45
15:O:237:ILE:HG22	15:O:381:ILE:CB	2.44	0.45
1:A:1463:ASP:HB2	1:A:1469:TRP:CE2	2.52	0.45
3:C:57:ILE:HG13	3:C:296:ASN:O	2.17	0.45
11:K:49:LEU:HG	11:K:54:THR:HG21	1.98	0.45
3:C:71:MET:CB	3:C:225:ALA:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:22:ILE:O	7:G:76:LYS:HG2	2.17	0.45
5:E:144:ILE:HG13	5:E:145:THR:N	2.32	0.45
13:M:61:GLU:OE2	13:M:106:LYS:NZ	2.43	0.45
1:A:878:ARG:NH2	9:I:66:VAL:HG23	2.32	0.44
1:A:1054:ALA:HB1	1:A:1178:LEU:HD22	1.98	0.44
3:C:231:PRO:HG2	3:C:270:ALA:C	2.37	0.44
7:G:163:PRO:HG2	7:G:166:TRP:CD1	2.53	0.44
15:O:426:SER:OG	15:O:594:TYR:C	2.54	0.44
15:O:426:SER:HB3	15:O:594:TYR:CD2	2.50	0.44
1:A:54:LEU:HD13	1:A:368:ARG:NH2	2.33	0.44
1:A:799:GLU:HG3	1:A:1062:HIS:CD2	2.49	0.44
2:B:470:LEU:HD22	2:B:478:LEU:HD12	1.99	0.44
2:B:683:ASN:HA	14:N:150:TYR:CZ	2.53	0.44
15:O:143:LEU:HD11	15:O:150:TRP:HD1	1.77	0.44
15:O:156:MET:CE	15:O:193:TYR:CE1	3.00	0.44
1:A:437:PHE:CE2	1:A:456:VAL:HG21	2.52	0.44
1:A:480:ALA:HA	2:B:1046:VAL:HA	1.97	0.44
2:B:833:PRO:HG2	2:B:836:TRP:CZ2	2.52	0.44
5:E:78:LEU:HD13	5:E:107:THR:HB	1.98	0.44
5:E:177:ARG:HD3	5:E:215:MET:HB2	1.99	0.44
7:G:154:ASN:ND2	15:O:182:MET:HE1	2.26	0.44
15:O:488:HIS:CE1	15:O:489:ASN:OD1	2.71	0.44
1:A:35:PRO:CA	1:A:390:LEU:HD13	2.47	0.44
1:A:257:ASN:OD1	1:A:258:GLU:N	2.51	0.44
1:A:1441:LYS:HB3	1:A:1441:LYS:HE2	1.75	0.44
2:B:107:PRO:HG2	2:B:133:TYR:CZ	2.52	0.44
2:B:468:GLY:O	2:B:484:TYR:HD2	2.01	0.44
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.98	0.44
2:B:1020:GLU:OE2	3:C:61:THR:HG21	2.18	0.44
3:C:131:THR:HG22	3:C:208:CYS:C	2.35	0.44
3:C:230:LEU:CG	3:C:231:PRO:HD2	2.48	0.44
3:C:272:LYS:HA	14:N:175:TYR:CE2	2.53	0.44
1:A:37:VAL:HG12	1:A:38:LEU:HG	2.00	0.44
1:A:891:ILE:HD13	9:I:71:LEU:CB	2.44	0.44
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.52	0.44
1:A:1229:ALA:HB3	1:A:1597:ALA:HB2	1.99	0.44
1:A:1600:ARG:NH2	1:A:1617:THR:OG1	2.48	0.44
2:B:399:HIS:C	2:B:400:GLN:CG	2.86	0.44
3:C:252:PRO:HD2	3:C:255:VAL:HG21	1.99	0.44
4:D:48:GLU:OE2	4:D:90:LYS:NZ	2.51	0.44
10:J:36:LEU:HD13	10:J:47:ARG:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:163:ILE:CG2	15:O:211:TYR:HB2	2.38	0.44
15:O:368:PHE:HE2	15:O:382:GLN:HA	1.81	0.44
15:O:391:GLN:CD	15:O:609:TYR:OH	2.55	0.44
1:A:1313:LEU:O	1:A:1317:ILE:HD12	2.18	0.44
1:A:1654:PHE:HA	6:F:135:ARG:O	2.17	0.44
2:B:190:ILE:HG13	2:B:191:GLY:N	2.32	0.44
2:B:910:THR:OG1	2:B:912:GLN:NE2	2.51	0.44
2:B:954:PHE:H	2:B:955:PRO:HD2	1.83	0.44
2:B:974:LEU:O	10:J:47:ARG:NH1	2.50	0.44
12:L:63:ARG:HA	12:L:63:ARG:HD2	1.74	0.44
15:O:158:LEU:HD22	15:O:172:HIS:CG	2.52	0.44
15:O:237:ILE:HG22	15:O:381:ILE:CD1	2.34	0.44
15:O:581:THR:HA	15:O:584:GLN:CD	2.37	0.44
1:A:1:MET:CB	2:B:1098:TYR:CG	2.98	0.44
1:A:509:GLU:CG	1:A:579:ARG:HE	2.31	0.44
1:A:1023:LEU:CD2	1:A:1598:PHE:CE1	3.01	0.44
2:B:938:PHE:CD1	3:C:68:ARG:NH2	2.86	0.44
4:D:28:PRO:HB2	7:G:24:VAL:CG1	2.47	0.44
5:E:93:MET:CG	5:E:120:ALA:HB1	2.46	0.44
15:O:78:VAL:HA	15:O:88:ILE:HG22	2.00	0.44
1:A:782:ASP:O	1:A:783:LYS:C	2.56	0.44
1:A:1660:VAL:O	7:G:102:GLU:CA	2.50	0.44
2:B:78:PRO:O	2:B:79:LEU:HB3	2.17	0.44
15:O:128:LEU:HB3	15:O:129:PRO:HD2	1.97	0.44
15:O:237:ILE:HD13	15:O:384:ILE:HD11	2.00	0.44
1:A:507:TYR:CD2	1:A:508:PRO:O	2.70	0.44
3:C:55:ASP:CG	3:C:299:ILE:CG1	2.47	0.44
15:O:76:ASN:O	15:O:80:LEU:HD13	2.18	0.44
15:O:412:GLU:OE1	15:O:412:GLU:HA	2.18	0.44
15:O:458:GLU:CB	15:O:461:VAL:HG21	2.47	0.44
15:O:515:ASN:N	15:O:516:PRO:HD3	2.33	0.44
1:A:1:MET:CB	2:B:1098:TYR:CD1	3.01	0.43
1:A:34:ASN:C	1:A:390:LEU:HD13	2.38	0.43
1:A:509:GLU:OE2	1:A:579:ARG:NH2	2.51	0.43
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.18	0.43
3:C:230:LEU:CG	3:C:231:PRO:CD	2.96	0.43
4:D:96:PHE:CE1	7:G:150:HIS:CD2	3.06	0.43
6:F:75:PRO:CG	6:F:78:GLN:CD	2.87	0.43
6:F:76:LYS:C	6:F:78:GLN:H	2.22	0.43
15:O:56:VAL:CG2	15:O:99:ILE:HD12	2.48	0.43
15:O:174:ASP:C	15:O:177:LYS:HG2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:607:LYS:HE2	15:O:607:LYS:HB2	1.88	0.43
1:A:1028:GLU:HA	1:A:1187:ILE:HG12	2.00	0.43
1:A:1261:VAL:HG21	1:A:1306:TYR:HB3	2.00	0.43
2:B:563:SER:HB2	13:M:73:SER:HB3	2.00	0.43
9:I:26:SER:O	9:I:39:LYS:HB2	2.18	0.43
15:O:194:LEU:HD21	15:O:225:LEU:HD11	1.96	0.43
15:O:458:GLU:HA	15:O:461:VAL:HG23	0.48	0.43
1:A:36:THR:HG22	1:A:45:VAL:HG21	2.00	0.43
1:A:403:LEU:HD12	1:A:403:LEU:HA	1.79	0.43
1:A:436:ALA:HA	1:A:443:ALA:HB2	1.99	0.43
1:A:509:GLU:OE1	1:A:509:GLU:HA	2.18	0.43
1:A:718:THR:HG21	8:H:118:PHE:O	2.18	0.43
1:A:782:ASP:C	1:A:784:SER:N	2.71	0.43
2:B:203:ILE:HB	2:B:405:GLY:HA3	2.00	0.43
2:B:1069:ILE:CG2	2:B:1070:ARG:N	2.73	0.43
14:N:87:TYR:CD1	14:N:141:GLU:HA	2.53	0.43
15:O:413:ALA:HB1	15:O:415:GLU:OE1	2.18	0.43
1:A:535:GLN:HA	1:A:546:LEU:HG	1.99	0.43
3:C:64:ALA:HB2	3:C:298:PHE:CE2	2.51	0.43
15:O:245:GLN:CG	15:O:378:THR:HG23	2.48	0.43
15:O:383:TYR:O	15:O:386:PHE:N	2.51	0.43
15:O:460:GLU:O	15:O:469:ARG:CZ	2.66	0.43
1:A:1606:SER:HB3	1:A:1611:MET:CE	2.47	0.43
2:B:209:GLN:CG	2:B:210:ARG:N	2.76	0.43
3:C:84:TYR:CZ	12:L:66:GLN:OE1	2.60	0.43
13:M:8:SER:O	14:N:71:PRO:HA	2.19	0.43
14:N:40:LEU:HD12	14:N:40:LEU:HA	1.84	0.43
14:N:94:ASP:HB3	14:N:99:LEU:HG	2.00	0.43
15:O:173:HIS:HE1	15:O:214:ASN:O	2.02	0.43
15:O:431:ALA:HB3	15:O:434:LEU:HD21	2.00	0.43
15:O:434:LEU:HD23	15:O:439:ILE:HG13	2.00	0.43
2:B:236:ILE:HG21	2:B:377:MET:HE1	1.99	0.43
2:B:893:ASN:O	2:B:895:PHE:HD1	2.01	0.43
15:O:66:ASN:CG	15:O:111:ARG:NH1	2.72	0.43
15:O:189:PHE:HA	15:O:192:THR:HG23	1.99	0.43
15:O:232:LEU:HA	15:O:232:LEU:HD12	1.74	0.43
15:O:352:LEU:HD23	15:O:358:VAL:HG23	1.85	0.43
1:A:399:LEU:CD1	1:A:423:LEU:HG	2.44	0.43
15:O:377:TYR:O	15:O:377:TYR:CD2	2.70	0.43
1:A:1600:ARG:NH2	1:A:1621:PHE:CE2	2.86	0.43
2:B:29:PRO:O	2:B:177:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:699:ILE:O	2:B:703:LEU:HG	2.19	0.43
2:B:923:GLN:HG2	2:B:949:ILE:CD1	2.47	0.43
7:G:29:ASP:OD1	7:G:30:GLU:N	2.52	0.43
15:O:356:GLU:OE1	15:O:356:GLU:HA	2.19	0.43
15:O:412:GLU:O	15:O:413:ALA:C	2.57	0.43
15:O:487:ARG:NH1	15:O:487:ARG:HG3	2.34	0.43
1:A:1305:GLU:CD	9:I:63:LYS:HE3	2.39	0.43
2:B:399:HIS:O	2:B:400:GLN:HG2	2.18	0.43
2:B:555:GLN:N	2:B:646:HIS:NE2	2.67	0.43
2:B:1017:ALA:C	3:C:65:ASN:ND2	2.72	0.43
4:D:80:THR:HB	15:O:227:PHE:CD2	2.50	0.43
15:O:48:SER:O	15:O:49:ALA:C	2.57	0.43
15:O:169:THR:O	15:O:172:HIS:N	2.52	0.43
1:A:407:GLN:HB3	1:A:409:ASP:OD2	2.19	0.43
1:A:1575:ILE:HG12	9:I:122:ARG:NH1	2.28	0.43
1:A:1657:LEU:HD21	6:F:135:ARG:NH2	2.34	0.43
2:B:742:TYR:CE2	2:B:1037:ARG:HD3	2.54	0.43
15:O:124:LYS:O	15:O:127:GLU:HB2	2.18	0.43
15:O:225:LEU:C	15:O:225:LEU:CD1	2.86	0.43
1:A:1070:LEU:C	1:A:1072:ASN:H	2.21	0.42
1:A:1172:LEU:O	1:A:1176:ARG:HG2	2.19	0.42
2:B:883:GLU:HG3	2:B:906:ARG:HB2	2.01	0.42
14:N:63:ASP:OD2	14:N:66:LYS:NZ	2.35	0.42
15:O:390:GLN:NE2	15:O:431:ALA:HA	2.34	0.42
2:B:550:ARG:HA	2:B:550:ARG:HD3	1.80	0.42
6:F:66:ARG:NH1	7:G:90:LEU:CD1	2.82	0.42
12:L:32:ALA:HB3	12:L:55:ILE:HG23	2.01	0.42
15:O:96:LEU:O	15:O:100:LEU:HG	2.20	0.42
15:O:156:MET:HG2	15:O:197:PHE:CZ	2.53	0.42
15:O:199:PRO:HD3	15:O:211:TYR:CG	2.54	0.42
15:O:457:ARG:HA	15:O:460:GLU:CG	2.49	0.42
1:A:550:SER:OG	1:A:553:GLN:HG3	2.19	0.42
1:A:938:VAL:HG22	9:I:82:ILE:HD13	2.00	0.42
1:A:953:GLU:CA	1:A:1205:PHE:CD2	2.97	0.42
2:B:300:SER:OG	9:I:49:THR:HG23	2.17	0.42
2:B:569:GLY:CA	14:N:140:SER:OG	2.66	0.42
3:C:55:ASP:HB3	3:C:297:HIS:HE2	1.80	0.42
15:O:173:HIS:NE2	15:O:217:LYS:HB3	2.35	0.42
15:O:336:LEU:HD11	15:O:380:SER:O	2.19	0.42
1:A:998:HIS:NE2	2:B:712:SER:N	2.55	0.42
1:A:1034:TYR:HA	1:A:1181:PRO:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:ILE:HB	3:C:297:HIS:CE1	2.55	0.42
6:F:93:ILE:HA	6:F:93:ILE:HD13	1.70	0.42
14:N:70:LEU:HA	14:N:71:PRO:HD3	1.84	0.42
15:O:404:ILE:CD1	15:O:442:VAL:HG11	2.49	0.42
15:O:430:ARG:HH22	15:O:596:PRO:CD	2.25	0.42
15:O:515:ASN:HD21	15:O:547:ASN:HD21	1.67	0.42
2:B:211:ARG:CB	2:B:239:VAL:CG1	2.98	0.42
2:B:809:VAL:HG13	2:B:901:VAL:HB	2.01	0.42
2:B:1082:HIS:HB3	2:B:1084:THR:HG23	2.01	0.42
3:C:31:TRP:CE3	11:K:82:LYS:CB	3.02	0.42
4:D:44:ILE:HG21	4:D:90:LYS:CE	2.45	0.42
7:G:160:ASN:OD1	7:G:160:ASN:N	2.52	0.42
9:I:60:LEU:CA	9:I:63:LYS:HG3	2.45	0.42
15:O:369:LYS:C	15:O:369:LYS:CD	2.86	0.42
1:A:475:ARG:NH1	2:B:1061:LYS:HA	2.35	0.42
1:A:990:ILE:CB	1:A:994:GLU:HB2	2.41	0.42
1:A:1655:ASP:HB2	6:F:135:ARG:CG	2.49	0.42
2:B:57:ASP:OD1	2:B:57:ASP:N	2.52	0.42
2:B:399:HIS:C	2:B:400:GLN:HG3	2.40	0.42
2:B:890:ASP:O	12:L:54:ARG:CD	2.68	0.42
15:O:124:LYS:HD3	15:O:127:GLU:OE2	2.20	0.42
15:O:202:ASN:N	15:O:202:ASN:OD1	2.52	0.42
15:O:234:ILE:HA	15:O:234:ILE:HD13	1.74	0.42
15:O:468:GLU:HG2	15:O:469:ARG:N	2.33	0.42
1:A:999:CYS:SG	2:B:531:VAL:HG22	2.59	0.42
7:G:159:LYS:HD2	15:O:103:ASN:CG	2.39	0.42
11:K:50:LEU:O	11:K:54:THR:HG23	2.20	0.42
13:M:102:SER:O	13:M:106:LYS:CB	2.56	0.42
15:O:413:ALA:C	15:O:415:GLU:N	2.72	0.42
1:A:478:TYR:HA	2:B:1048:SER:HA	0.57	0.42
1:A:1003:ARG:HD2	2:B:520:LEU:HB3	2.02	0.42
1:A:1575:ILE:CG1	9:I:122:ARG:HH22	2.32	0.42
2:B:469:ASN:HA	2:B:482:SER:HA	2.00	0.42
2:B:478:LEU:HB3	2:B:484:TYR:OH	2.20	0.42
2:B:697:LEU:HB2	2:B:702:ASN:ND2	2.35	0.42
2:B:938:PHE:CE2	3:C:68:ARG:HD2	2.54	0.42
15:O:447:THR:HB	15:O:505:PHE:CZ	2.55	0.42
15:O:447:THR:HG21	15:O:480:LEU:HD21	2.02	0.42
1:A:660:PRO:O	1:A:1057:ILE:HG21	2.20	0.42
2:B:881:TYR:CZ	12:L:67:PHE:HE1	2.37	0.42
3:C:116:VAL:HG11	3:C:125:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:66:ASN:ND2	15:O:111:ARG:CZ	2.83	0.42
15:O:77:GLN:HG2	15:O:88:ILE:HB	2.01	0.42
15:O:129:PRO:HD2	15:O:132:THR:CB	2.25	0.42
15:O:409:ALA:O	15:O:417:LYS:HE2	2.20	0.42
15:O:467:MET:CG	15:O:519:PHE:CZ	2.96	0.42
1:A:953:GLU:C	1:A:1205:PHE:CG	2.94	0.42
2:B:938:PHE:CE1	3:C:68:ARG:CD	3.03	0.42
2:B:1017:ALA:O	3:C:65:ASN:ND2	2.53	0.42
3:C:57:ILE:HG13	3:C:297:HIS:HB2	2.02	0.42
4:D:28:PRO:CB	7:G:24:VAL:CG1	2.98	0.42
5:E:67:GLU:CD	5:E:67:GLU:H	2.23	0.42
15:O:370:THR:O	15:O:374:PRO:HG3	2.19	0.42
1:A:365:THR:C	1:A:367:PHE:N	2.73	0.41
1:A:478:TYR:O	2:B:1047:ARG:O	2.37	0.41
1:A:692:TYR:O	1:A:696:ILE:HG12	2.19	0.41
1:A:1648:ASN:O	1:A:1652:GLY:O	2.38	0.41
2:B:211:ARG:HH21	2:B:239:VAL:HG21	1.81	0.41
3:C:236:LEU:HD11	3:C:290:LYS:HG3	2.02	0.41
15:O:173:HIS:CG	15:O:217:LYS:HG3	2.55	0.41
15:O:417:LYS:HD3	15:O:472:HIS:CE1	2.33	0.41
1:A:385:LEU:HA	1:A:385:LEU:HD23	1.88	0.41
1:A:437:PHE:C	1:A:439:ASP:H	2.22	0.41
1:A:507:TYR:CE2	1:A:508:PRO:O	2.73	0.41
1:A:874:GLU:OE2	1:A:878:ARG:HD2	2.20	0.41
2:B:1020:GLU:CD	3:C:61:THR:HG21	2.40	0.41
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	2.02	0.41
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.84	0.41
14:N:81:THR:HG22	14:N:86:ASP:HB3	2.01	0.41
15:O:56:VAL:HG23	15:O:57:LYS:N	2.35	0.41
15:O:430:ARG:O	15:O:610:TYR:HA	2.20	0.41
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.95	0.41
1:A:680:LEU:O	1:A:728:GLY:HA3	2.21	0.41
2:B:478:LEU:CB	2:B:484:TYR:OH	2.69	0.41
2:B:656:LEU:HD21	2:B:689:VAL:HG12	2.01	0.41
3:C:64:ALA:HB1	3:C:298:PHE:CD2	2.56	0.41
15:O:150:TRP:O	15:O:154:VAL:HG23	2.21	0.41
15:O:234:ILE:HG22	15:O:371:HIS:CD2	2.42	0.41
15:O:458:GLU:HG2	15:O:461:VAL:HG21	2.02	0.41
15:O:592:PHE:HA	15:O:593:PRO:HD3	1.91	0.41
1:A:854:GLY:HA3	1:A:974:THR:O	2.21	0.41
1:A:891:ILE:HD12	9:I:71:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:ASP:OD1	1:A:1517:ARG:NH1	2.49	0.41
1:A:1499:ARG:HG2	1:A:1500:GLN:N	2.35	0.41
2:B:143:TRP:CE3	2:B:446:MET:HG3	2.54	0.41
2:B:321:GLN:HB3	9:I:32:GLN:HE21	1.84	0.41
2:B:401:GLU:C	2:B:402:VAL:HG23	2.41	0.41
2:B:553:THR:C	2:B:646:HIS:HD2	2.23	0.41
2:B:1094:ASN:O	2:B:1096:SER:N	2.41	0.41
3:C:41:GLU:C	3:C:57:ILE:HG22	2.41	0.41
7:G:223:GLU:H	7:G:223:GLU:HG3	1.71	0.41
15:O:108:GLU:HB2	15:O:147:ILE:CD1	2.47	0.41
15:O:201:LYS:H	15:O:201:LYS:HG3	1.59	0.41
15:O:352:LEU:CD2	15:O:358:VAL:CG2	2.56	0.41
15:O:423:TYR:CE1	15:O:593:PRO:HB2	2.55	0.41
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	2.01	0.41
1:A:1348:VAL:HA	1:A:1349:PRO:HD3	1.93	0.41
2:B:464:PHE:O	2:B:468:GLY:N	2.49	0.41
3:C:84:TYR:CE2	12:L:66:GLN:HB2	2.47	0.41
3:C:84:TYR:HD2	12:L:66:GLN:CB	2.30	0.41
4:D:82:LEU:O	4:D:86:ILE:HG23	2.20	0.41
7:G:24:VAL:O	7:G:25:THR:O	2.39	0.41
7:G:154:ASN:ND2	15:O:182:MET:HE3	2.27	0.41
1:A:1:MET:HB2	2:B:1098:TYR:CD2	2.54	0.41
1:A:248:PHE:HD1	1:A:442:LYS:O	2.01	0.41
1:A:1056:ASP:HB3	1:A:1059:LYS:HB2	2.02	0.41
1:A:1305:GLU:HG3	9:I:60:LEU:HG	2.03	0.41
2:B:211:ARG:O	2:B:212:ASN:HB2	2.21	0.41
2:B:286:ARG:HD2	2:B:286:ARG:HA	1.88	0.41
3:C:272:LYS:HG3	14:N:175:TYR:CZ	2.55	0.41
7:G:139:ILE:CD1	15:O:178:TYR:OH	2.68	0.41
14:N:25:ILE:HA	14:N:26:PRO:HD3	1.84	0.41
1:A:1063:MET:HE2	1:A:1063:MET:HB3	1.85	0.41
2:B:206:LEU:HD23	2:B:206:LEU:HA	1.81	0.41
3:C:80:ALA:HB3	3:C:102:GLY:HA2	2.03	0.41
7:G:28:ILE:HG23	7:G:34:THR:O	2.20	0.41
8:H:95:TYR:HD2	8:H:144:ILE:HD12	1.86	0.41
12:L:33:GLU:HG3	12:L:53:HIS:ND1	2.36	0.41
15:O:241:ASP:HA	15:O:380:SER:CB	2.46	0.41
1:A:1049:MET:C	1:A:1051:GLY:N	2.74	0.41
1:A:1179:ILE:HD11	1:A:1183:GLU:CD	2.40	0.41
3:C:57:ILE:HB	3:C:297:HIS:ND1	2.35	0.41
4:D:23:HIS:CD2	6:F:58:PHE:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:54:THR:HG22	11:K:62:SER:H	1.86	0.41
15:O:107:ILE:O	15:O:107:ILE:CG2	2.69	0.41
15:O:115:LEU:O	15:O:119:ILE:HG13	2.21	0.41
15:O:237:ILE:HG21	15:O:381:ILE:CG1	2.51	0.41
1:A:315:ILE:HG13	1:A:319:GLU:HB2	2.03	0.41
1:A:440:SER:C	1:A:442:LYS:N	2.74	0.41
1:A:509:GLU:CG	1:A:579:ARG:CD	2.99	0.41
1:A:1074:TYR:CE2	1:A:1159:ASP:HB3	2.54	0.41
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.03	0.41
1:A:1262:LEU:HD22	1:A:1497:ILE:HG12	2.03	0.41
1:A:1317:ILE:O	1:A:1322:ILE:HG12	2.21	0.41
1:A:1575:ILE:HG13	9:I:122:ARG:NH2	2.36	0.41
2:B:262:PHE:CE1	2:B:357:ILE:HD13	2.56	0.41
2:B:279:ALA:HB2	2:B:326:VAL:HG12	2.03	0.41
2:B:527:PHE:CE2	2:B:666:PRO:HA	2.55	0.41
2:B:545:PHE:CZ	2:B:551:ILE:HD11	2.56	0.41
2:B:1043:LYS:HE2	2:B:1063:ARG:HD2	2.01	0.41
2:B:1094:ASN:C	2:B:1096:SER:H	2.24	0.41
7:G:50:ALA:HA	7:G:113:PHE:CD2	2.56	0.41
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.02	0.41
9:I:2:SER:HA	9:I:9:PHE:O	2.21	0.41
15:O:107:ILE:CD1	15:O:115:LEU:HD23	2.51	0.41
15:O:147:ILE:HG22	15:O:149:LYS:CB	2.51	0.41
15:O:163:ILE:HD12	15:O:207:LYS:HG2	2.02	0.41
15:O:369:LYS:HZ3	15:O:369:LYS:CB	2.21	0.41
1:A:700:ILE:HD13	1:A:700:ILE:HA	1.81	0.41
1:A:964:LYS:HB3	1:A:964:LYS:HE2	1.83	0.41
1:A:1037:SER:HA	1:A:1049:MET:HA	2.03	0.41
2:B:42:VAL:O	2:B:46:ILE:CG1	2.69	0.41
2:B:371:PHE:CE2	2:B:375:LEU:HD11	2.56	0.41
2:B:401:GLU:CG	2:B:402:VAL:N	2.73	0.41
2:B:699:ILE:HD13	2:B:760:TYR:CD1	2.55	0.41
2:B:736:ARG:NH1	2:B:738:ASP:OD1	2.54	0.41
2:B:1069:ILE:CG2	2:B:1070:ARG:H	2.20	0.41
15:O:194:LEU:O	15:O:232:LEU:CD2	2.57	0.41
15:O:447:THR:O	15:O:450:LEU:CA	2.68	0.41
1:A:411:VAL:CG2	1:A:412:SER:H	2.26	0.40
1:A:1006:LEU:CD2	2:B:535:ASP:CB	2.99	0.40
2:B:416:LYS:HA	2:B:416:LYS:HD3	1.87	0.40
15:O:198:PHE:HD2	15:O:232:LEU:CD2	2.32	0.40
1:A:356:PHE:C	1:A:357:MET:CG	2.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:O	1:A:367:PHE:N	2.54	0.40
1:A:516:ILE:HG12	15:O:376:TYR:HE2	1.73	0.40
1:A:556:ALA:HA	15:O:246:ASN:HD22	1.85	0.40
1:A:1055:ILE:HG21	1:A:1060:GLU:CG	2.34	0.40
1:A:1229:ALA:HB1	1:A:1595:TYR:CE2	2.56	0.40
2:B:219:ARG:HA	2:B:220:PRO:HD2	1.73	0.40
2:B:427:GLN:OE1	2:B:452:ARG:NH1	2.54	0.40
2:B:555:GLN:CB	2:B:646:HIS:CE1	3.04	0.40
7:G:41:VAL:HA	7:G:42:PRO:HD3	1.92	0.40
8:H:7:ASP:HA	8:H:57:VAL:O	2.21	0.40
11:K:135:PHE:CE2	11:K:139:ILE:HD11	2.56	0.40
12:L:68:GLU:CG	12:L:69:ALA:N	2.73	0.40
15:O:128:LEU:HD13	15:O:132:THR:HG22	2.02	0.40
15:O:244:LEU:HD23	15:O:244:LEU:O	2.20	0.40
1:A:487:ASP:HB2	1:A:615:ARG:HB3	2.02	0.40
1:A:756:LYS:HD2	9:I:85:LYS:HZ2	1.61	0.40
1:A:1008:ASP:OD1	1:A:1202:LEU:HD13	2.19	0.40
1:A:1661:PRO:HA	7:G:101:SER:O	2.21	0.40
3:C:128:ASP:OD1	3:C:128:ASP:N	2.54	0.40
4:D:25:THR:HB	6:F:59:GLN:HG3	2.02	0.40
15:O:505:PHE:O	15:O:509:MET:HG2	2.21	0.40
1:A:601:MET:HE1	1:A:656:GLN:HB2	2.03	0.40
2:B:467:THR:HB	2:B:469:ASN:HD21	1.81	0.40
2:B:491:ILE:HB	2:B:495:ARG:HD2	2.03	0.40
3:C:45:SER:HB3	3:C:271:ARG:HH22	1.80	0.40
15:O:237:ILE:HB	15:O:381:ILE:HD11	1.92	0.40
15:O:422:GLN:HB3	15:O:593:PRO:HD3	2.02	0.40
1:A:389:VAL:O	1:A:393:SER:HB2	2.22	0.40
1:A:498:PRO:HA	1:A:499:PRO:HD3	1.81	0.40
1:A:1048:PHE:HD2	5:E:210:SER:HG	1.69	0.40
2:B:168:ASN:O	2:B:169:ARG:HD3	2.21	0.40
4:D:23:HIS:CB	6:F:58:PHE:CD2	3.04	0.40
7:G:17:ILE:C	7:G:19:LYS:H	2.25	0.40
8:H:39:THR:O	8:H:123:MET:HA	2.22	0.40
9:I:87:PRO:HG2	9:I:119:TYR:CE2	2.56	0.40
15:O:342:HIS:NE2	15:O:346:GLN:HG3	2.34	0.40
15:O:376:TYR:O	15:O:377:TYR:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1464/1664 (88%)	1370 (94%)	82 (6%)	12 (1%)	19	59
2	B	1166/1203 (97%)	1086 (93%)	56 (5%)	24 (2%)	7	38
3	C	303/335 (90%)	278 (92%)	18 (6%)	7 (2%)	6	36
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	3	27
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	15	53
6	F	98/155 (63%)	94 (96%)	4 (4%)	0	100	100
7	G	189/326 (58%)	171 (90%)	13 (7%)	5 (3%)	5	34
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	101/125 (81%)	89 (88%)	9 (9%)	3 (3%)	4	31
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	41/70 (59%)	32 (78%)	6 (15%)	3 (7%)	1	16
13	M	103/415 (25%)	93 (90%)	8 (8%)	2 (2%)	8	40
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	6	37
15	O	457/627 (73%)	400 (88%)	38 (8%)	19 (4%)	3	25
All	All	4618/5863 (79%)	4259 (92%)	277 (6%)	82 (2%)	12	41

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1606	SER
2	B	111	ASP
2	B	117	VAL
2	B	895	PHE
2	B	1069	ILE
3	C	224	THR
4	D	99	LEU
7	G	25	THR

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Mol	Chain	Res	Type
9	I	41	GLN
15	O	165	PRO
15	O	226	GLY
15	O	325	ILE
15	O	380	SER
15	O	431	ALA
15	O	489	ASN
15	O	521	ASN
1	A	448	SER
1	A	783	LYS
1	A	1533	GLU
2	B	473	GLN
2	B	817	ARG
2	B	1140	LYS
4	D	98	GLY
5	E	50	MET
7	G	27	PRO
9	I	5	GLY
12	L	62	LYS
15	O	374	PRO
15	O	488	HIS
15	O	540	CYS
1	A	450	LYS
1	A	1050	TYR
2	B	34	ALA
2	B	78	PRO
2	B	208	VAL
2	B	209	GLN
2	B	1044	PHE
2	B	1070	ARG
2	B	1095	SER
2	B	1098	TYR
3	C	297	HIS
5	E	146	HIS
7	G	99	ASP
9	I	21	ASN
12	L	46	VAL
13	M	85	LYS
15	O	82	SER
15	O	130	PRO
15	O	457	ARG
15	O	469	ARG

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Mol	Chain	Res	Type
2	B	834	LYS
2	B	1094	ASN
3	C	295	ARG
7	G	100	THR
12	L	43	THR
13	M	36	THR
14	N	115	SER
15	O	148	PRO
15	O	187	MET
1	A	439	ASP
1	A	451	VAL
1	A	564	PRO
1	A	581	ILE
1	A	1049	MET
2	B	80	ASN
2	B	1062	GLY
2	B	1096	SER
3	C	32	ASN
3	C	296	ASN
15	O	377	TYR
1	A	1512	PRO
2	B	1063	ARG
3	C	222	VAL
15	O	147	ILE
3	C	221	PRO
14	N	70	LEU
15	O	128	LEU
2	B	468	GLY
14	N	39	PRO
7	G	28	ILE
2	B	833	PRO
2	B	954	PHE

5.3.2 Protein sidechains [i](#)

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	1307/1465 (89%)	1221 (93%)	86 (7%)	16	43
2	B	1027/1053 (98%)	956 (93%)	71 (7%)	15	42
3	C	269/296 (91%)	249 (93%)	20 (7%)	13	40
4	D	55/116 (47%)	49 (89%)	6 (11%)	6	25
5	E	194/197 (98%)	180 (93%)	14 (7%)	14	41
6	F	90/137 (66%)	86 (96%)	4 (4%)	28	54
7	G	170/291 (58%)	158 (93%)	12 (7%)	14	41
8	H	115/128 (90%)	111 (96%)	4 (4%)	36	60
9	I	97/110 (88%)	91 (94%)	6 (6%)	18	45
10	J	64/65 (98%)	57 (89%)	7 (11%)	6	25
11	K	91/130 (70%)	84 (92%)	7 (8%)	13	39
12	L	38/57 (67%)	34 (90%)	4 (10%)	7	26
13	M	95/371 (26%)	85 (90%)	10 (10%)	7	26
14	N	135/220 (61%)	129 (96%)	6 (4%)	28	54
15	O	427/576 (74%)	378 (88%)	49 (12%)	5	23
All	All	4174/5212 (80%)	3868 (93%)	306 (7%)	18	40

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	40	ASN
1	A	83	VAL
1	A	90	PHE
1	A	117	ARG
1	A	136	LEU
1	A	174	SER
1	A	186	SER
1	A	202	THR
1	A	230	ARG
1	A	257	ASN
1	A	271	ARG
1	A	272	GLN
1	A	273	ASP
1	A	312	SER
1	A	315	ILE
1	A	346	SER
1	A	357	MET

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	379	GLU
1	A	393	SER
1	A	409	ASP
1	A	412	SER
1	A	413	LEU
1	A	439	ASP
1	A	446	ARG
1	A	447	THR
1	A	451	VAL
1	A	503	VAL
1	A	555	LYS
1	A	582	LYS
1	A	611	GLU
1	A	627	ASP
1	A	656	GLN
1	A	661	THR
1	A	666	VAL
1	A	670	ILE
1	A	684	ASP
1	A	708	THR
1	A	709	ARG
1	A	739	VAL
1	A	747	ILE
1	A	758	GLU
1	A	783	LYS
1	A	957	VAL
1	A	966	LEU
1	A	988	SER
1	A	999	CYS
1	A	1004	GLU
1	A	1026	GLN
1	A	1033	SER
1	A	1056	ASP
1	A	1085	LEU
1	A	1098	SER
1	A	1118	VAL
1	A	1123	VAL
1	A	1131	LYS
1	A	1159	ASP
1	A	1162	ASN
1	A	1204	THR

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Mol	Chain	Res	Type
1	A	1215	VAL
1	A	1226	VAL
1	A	1273	THR
1	A	1275	THR
1	A	1276	THR
1	A	1304	GLU
1	A	1310	LYS
1	A	1314	GLN
1	A	1320	GLN
1	A	1441	LYS
1	A	1455	ARG
1	A	1509	HIS
1	A	1531	ASP
1	A	1533	GLU
1	A	1536	ILE
1	A	1571	SER
1	A	1601	GLN
1	A	1604	GLU
1	A	1605	THR
1	A	1607	THR
1	A	1609	SER
1	A	1611	MET
1	A	1632	GLU
1	A	1633	GLN
1	A	1635	ASP
1	A	1645	LYS
2	B	13	THR
2	B	17	ARG
2	B	22	GLU
2	B	53	THR
2	B	57	ASP
2	B	65	VAL
2	B	70	GLU
2	B	79	LEU
2	B	81	SER
2	B	87	ASN
2	B	150	GLU
2	B	187	SER
2	B	202	LEU
2	B	211	ARG
2	B	221	SER
2	B	225	ARG

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Mol	Chain	Res	Type
2	B	228	SER
2	B	231	HIS
2	B	239	VAL
2	B	281	CYS
2	B	300	SER
2	B	305	ARG
2	B	306	LEU
2	B	311	ARG
2	B	315	LYS
2	B	379	ARG
2	B	459	SER
2	B	486	VAL
2	B	537	SER
2	B	583	LEU
2	B	622	ILE
2	B	658	LEU
2	B	720	GLN
2	B	724	GLN
2	B	725	THR
2	B	731	VAL
2	B	753	LYS
2	B	782	ASP
2	B	811	LEU
2	B	813	LEU
2	B	819	ASP
2	B	822	THR
2	B	824	HIS
2	B	829	ASN
2	B	833	PRO
2	B	835	GLU
2	B	839	LYS
2	B	858	ILE
2	B	871	ILE
2	B	883	GLU
2	B	894	LYS
2	B	897	GLU
2	B	977	ILE
2	B	998	GLU
2	B	1026	ILE
2	B	1033	TYR
2	B	1037	ARG
2	B	1043	LYS

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Mol	Chain	Res	Type
2	B	1047	ARG
2	B	1060	VAL
2	B	1070	ARG
2	B	1075	GLU
2	B	1097	ASP
2	B	1100	GLN
2	B	1103	VAL
2	B	1125	THR
2	B	1136	GLU
2	B	1141	LEU
2	B	1163	GLN
2	B	1165	ASN
2	B	1174	THR
3	C	38	LYS
3	C	43	ASN
3	C	50	ARG
3	C	61	THR
3	C	77	SER
3	C	91	VAL
3	C	97	LEU
3	C	118	SER
3	C	131	THR
3	C	142	ARG
3	C	181	ASP
3	C	222	VAL
3	C	224	THR
3	C	228	ARG
3	C	232	GLN
3	C	243	SER
3	C	245	ARG
3	C	277	ARG
3	C	279	VAL
3	C	295	ARG
4	D	15	THR
4	D	29	GLN
4	D	38	GLN
4	D	46	GLU
4	D	80	THR
4	D	99	LEU
5	E	31	THR
5	E	33	GLU
5	E	41	ASP

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Mol	Chain	Res	Type
5	E	74	ASP
5	E	77	SER
5	E	90	VAL
5	E	92	THR
5	E	93	MET
5	E	107	THR
5	E	131	THR
5	E	136	ASN
5	E	142	VAL
5	E	162	ARG
5	E	177	ARG
6	F	59	GLN
6	F	87	LYS
6	F	99	LEU
6	F	109	VAL
7	G	18	LYS
7	G	24	VAL
7	G	35	SER
7	G	39	VAL
7	G	139	ILE
7	G	147	LEU
7	G	167	THR
7	G	169	VAL
7	G	223	GLU
7	G	230	ARG
7	G	239	THR
7	G	243	VAL
8	H	3	ASN
8	H	39	THR
8	H	108	SER
8	H	112	ILE
9	I	2	SER
9	I	15	ASP
9	I	45	LEU
9	I	70	SER
9	I	74	ASN
9	I	81	THR
10	J	3	VAL
10	J	9	SER
10	J	10	CYS
10	J	14	VAL
10	J	27	GLU

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Mol	Chain	Res	Type
10	J	45	CYS
10	J	48	ARG
11	K	45	GLU
11	K	51	THR
11	K	68	GLU
11	K	99	ASN
11	K	118	GLN
11	K	123	ASP
11	K	133	SER
12	L	38	LEU
12	L	55	ILE
12	L	60	ARG
12	L	66	GLN
13	M	17	ASP
13	M	18	GLN
13	M	31	ARG
13	M	44	LYS
13	M	48	LYS
13	M	65	TYR
13	M	77	VAL
13	M	84	GLU
13	M	98	SER
13	M	109	ARG
14	N	51	GLN
14	N	124	THR
14	N	135	LYS
14	N	153	VAL
14	N	167	LYS
14	N	178	GLU
15	O	66	ASN
15	O	67	ASP
15	O	69	THR
15	O	78	VAL
15	O	80	LEU
15	O	87	ARG
15	O	101	SER
15	O	111	ARG
15	O	117	GLN
15	O	149	LYS
15	O	171	CYS
15	O	175	MET
15	O	180	LEU

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Mol	Chain	Res	Type
15	O	181	ARG
15	O	190	ILE
15	O	192	THR
15	O	202	ASN
15	O	203	ASP
15	O	204	THR
15	O	205	ARG
15	O	212	THR
15	O	213	SER
15	O	215	LEU
15	O	228	GLN
15	O	232	LEU
15	O	234	ILE
15	O	245	GLN
15	O	248	LEU
15	O	341	THR
15	O	350	GLU
15	O	354	SER
15	O	363	THR
15	O	368	PHE
15	O	369	LYS
15	O	395	LEU
15	O	437	THR
15	O	454	VAL
15	O	457	ARG
15	O	487	ARG
15	O	489	ASN
15	O	494	THR
15	O	495	ASP
15	O	522	GLU
15	O	526	LEU
15	O	540	CYS
15	O	581	THR
15	O	584	GLN
15	O	597	LEU
15	O	602	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	ASN
1	A	580	HIS

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Mol	Chain	Res	Type
1	A	863	ASN
1	A	1162	ASN
2	B	328	GLN
2	B	462	GLN
2	B	646	HIS
2	B	912	GLN
2	B	1038	HIS
2	B	1163	GLN
4	D	23	HIS
4	D	93	GLN
6	F	59	GLN
6	F	78	GLN
7	G	126	GLN
7	G	150	HIS
7	G	154	ASN
9	I	32	GLN
12	L	66	GLN
14	N	85	HIS
15	O	66	ASN
15	O	70	GLN
15	O	105	ASN
15	O	117	GLN
15	O	172	HIS
15	O	173	HIS
15	O	245	GLN
15	O	346	GLN
15	O	362	ASN
15	O	371	HIS
15	O	390	GLN
15	O	472	HIS
15	O	497	ASN
15	O	507	GLN
15	O	521	ASN
15	O	547	ASN
15	O	549	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

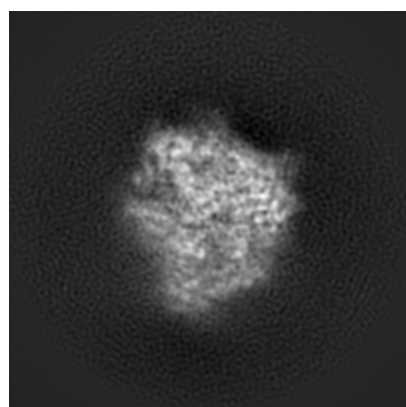
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3439. These allow visual inspection of the internal detail of the map and identification of artifacts.

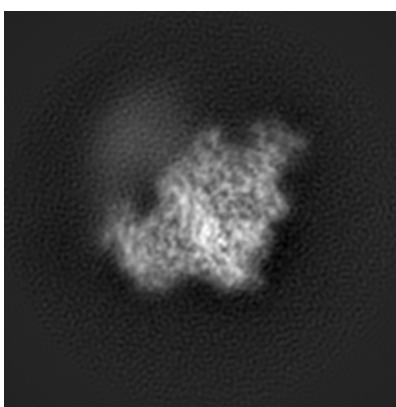
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

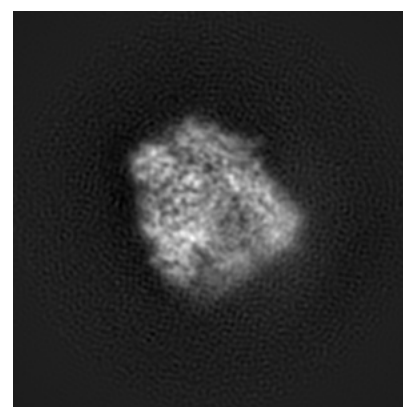
6.1.1 Primary map



X



Y

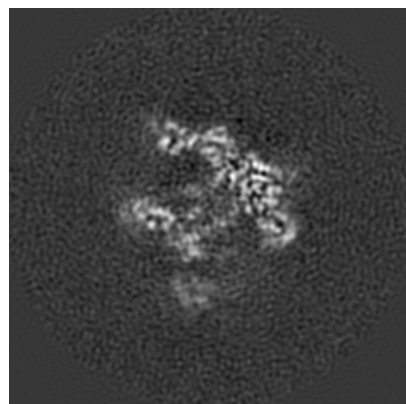


Z

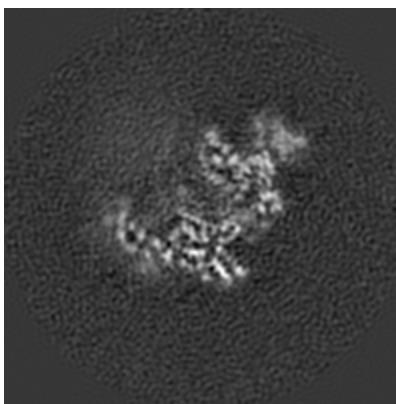
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

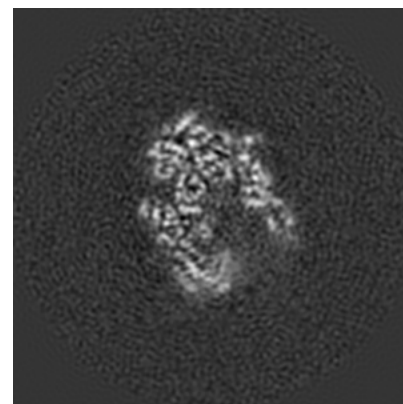
6.2.1 Primary map



X Index: 120



Y Index: 120

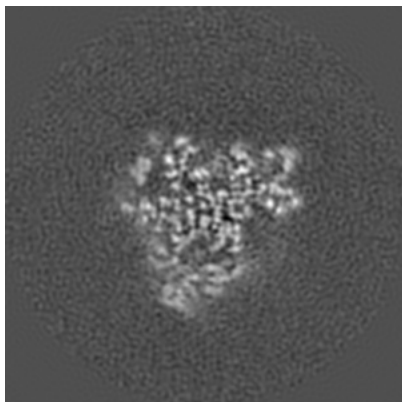


Z Index: 120

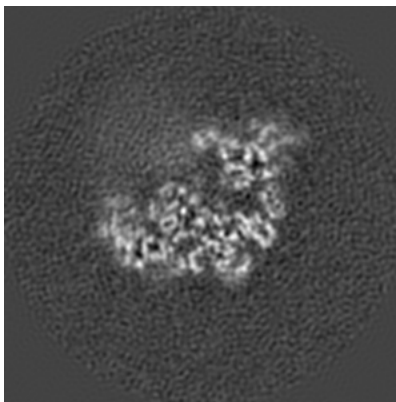
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

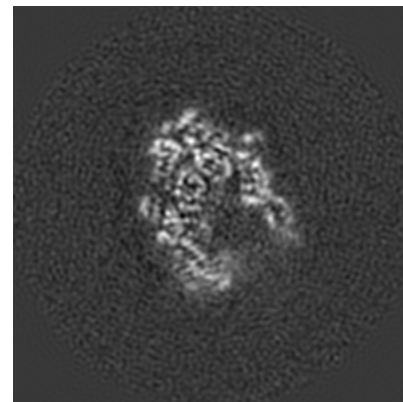
6.3.1 Primary map



X Index: 106



Y Index: 106

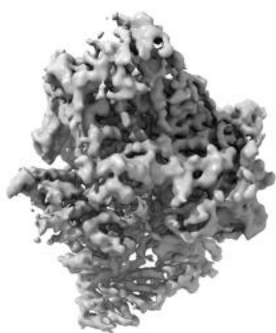


Z Index: 121

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

6.4 Orthogonal surface views [i](#)

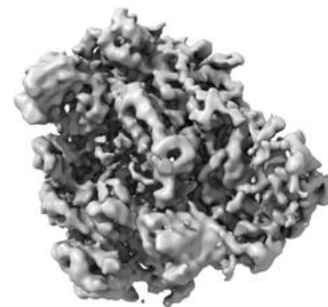
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

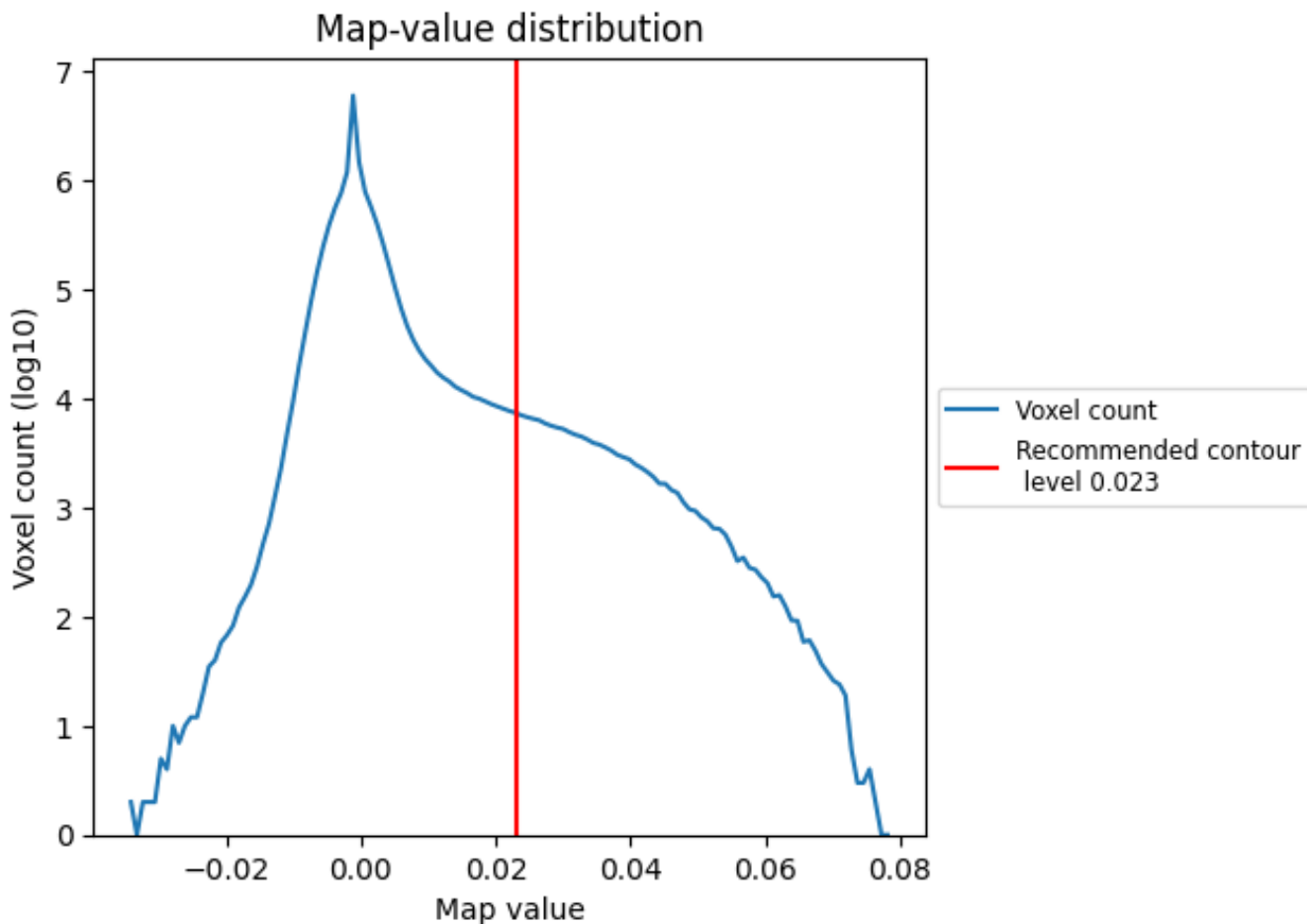
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

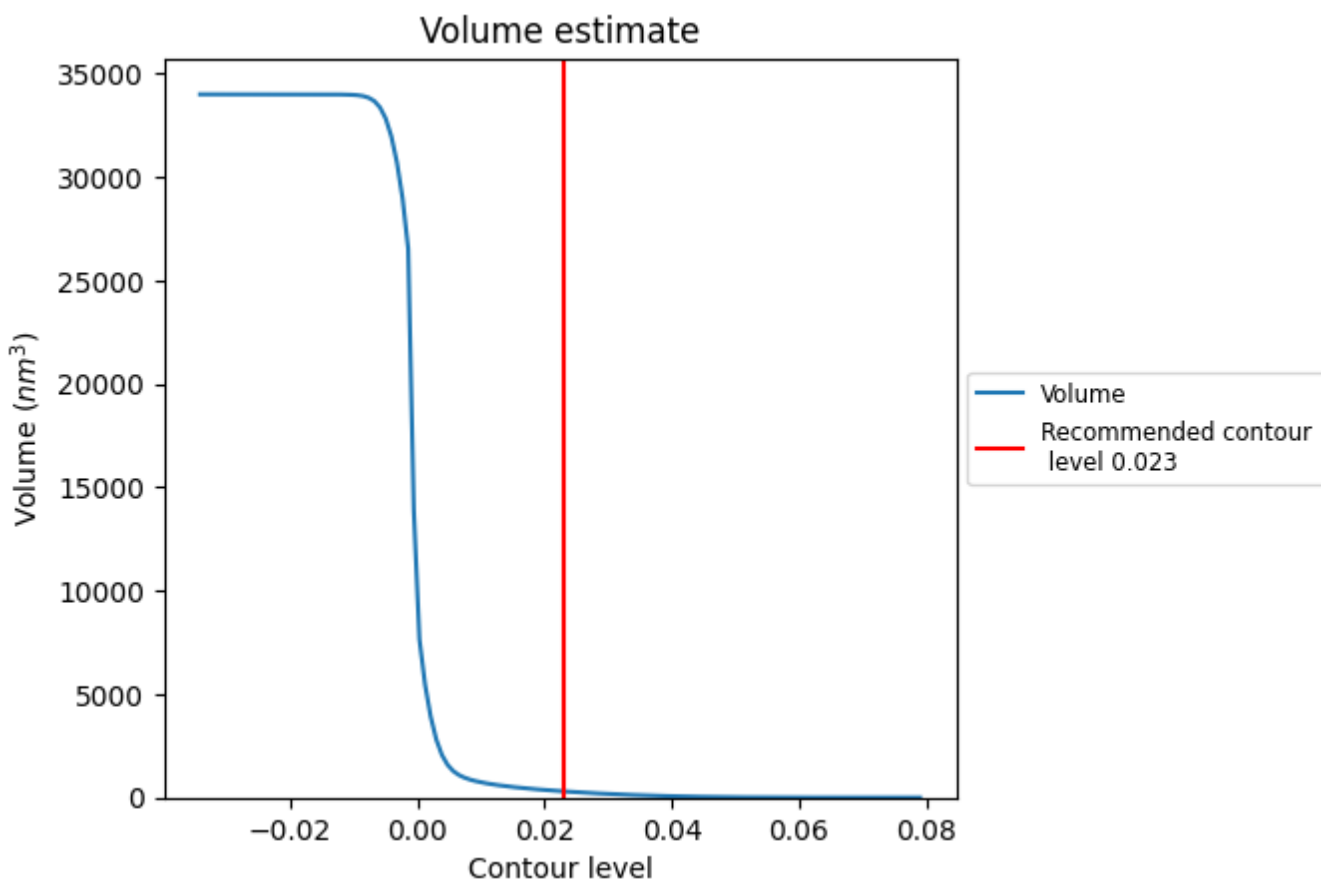
This section contains the results of statistical analysis of the map.

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.

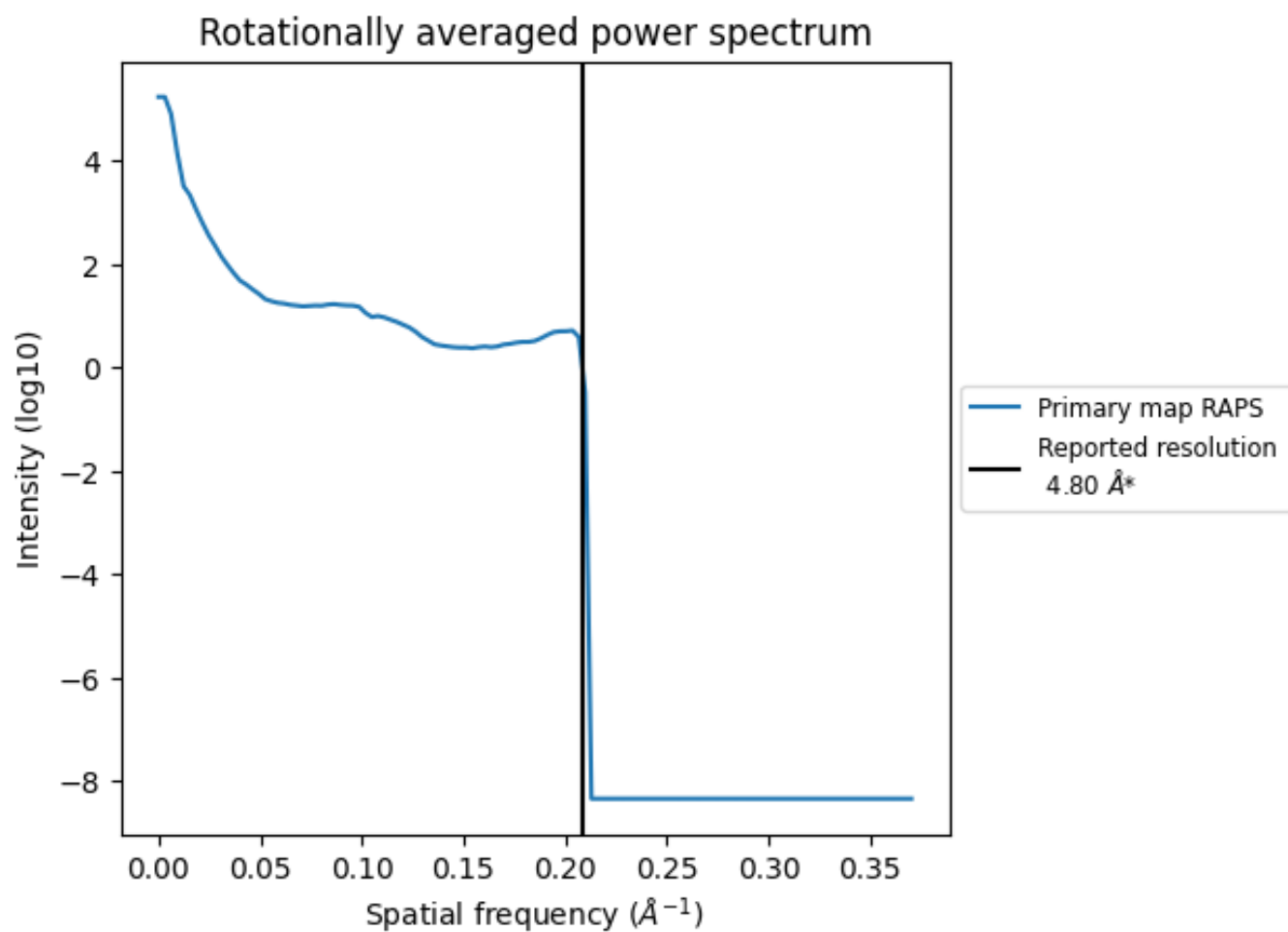
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 300 nm³; this corresponds to an approximate mass of 271 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

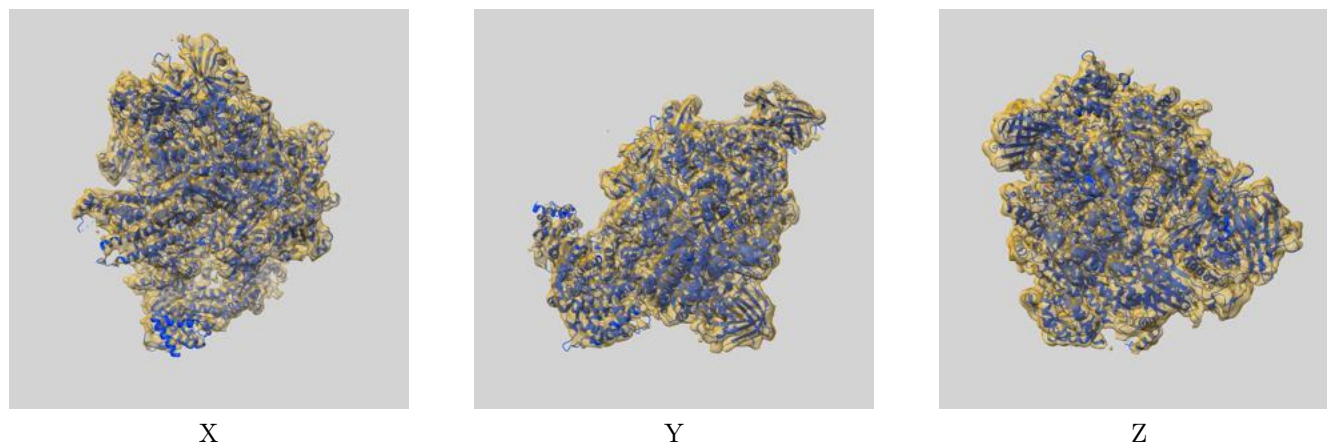
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

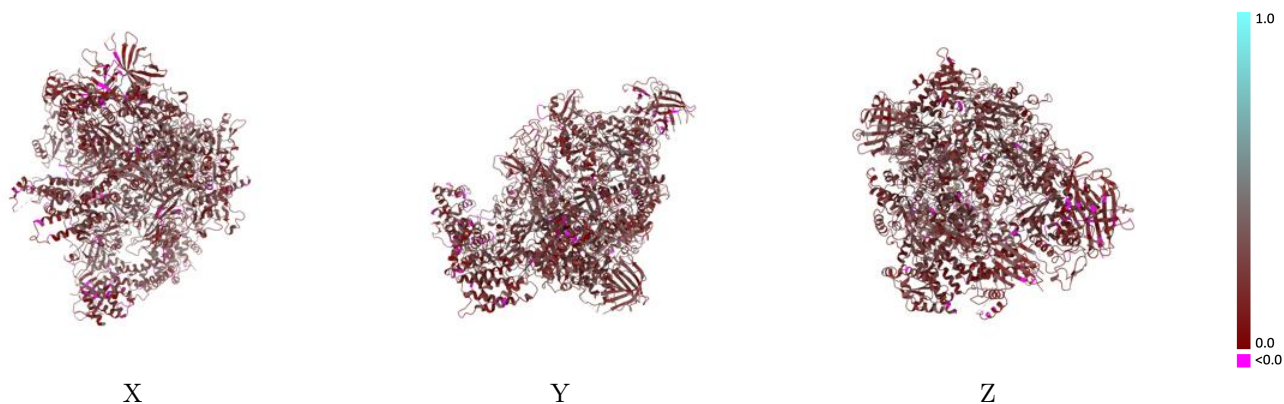
This section contains information regarding the fit between EMDB map EMD-3439 and PDB model 5G5L. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



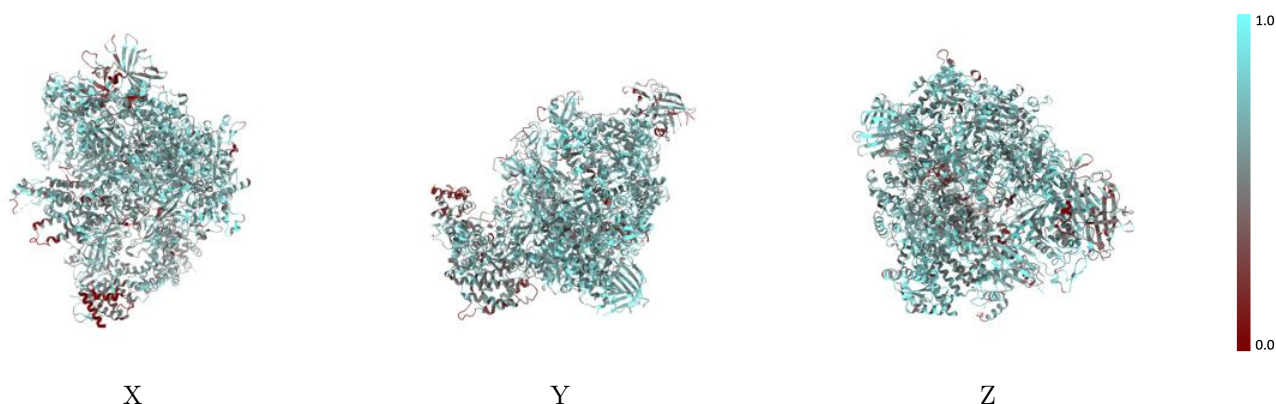
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



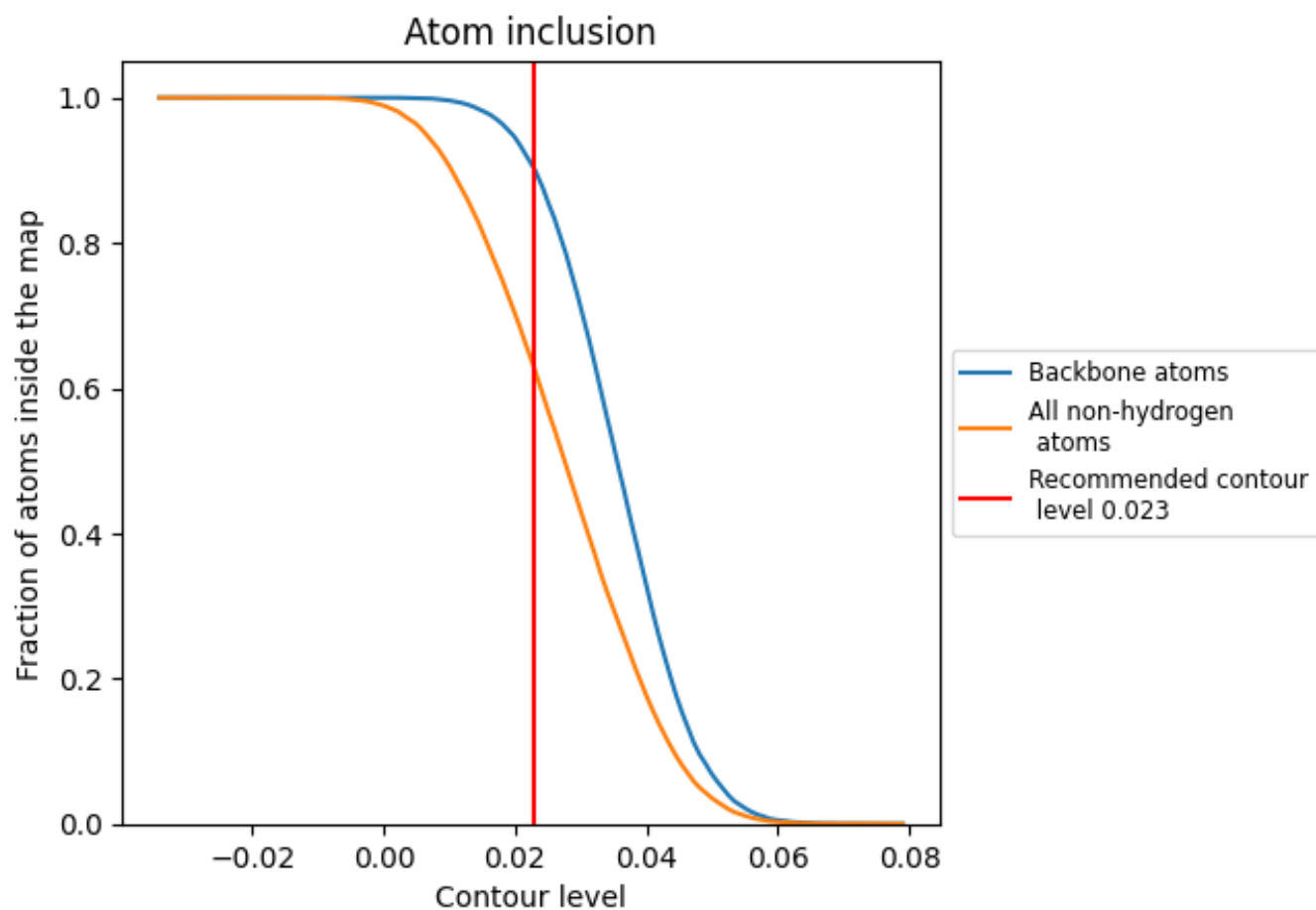
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 63% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6252	 0.2290
A	 0.6393	 0.2330
B	 0.6486	 0.2420
C	 0.6936	 0.2360
D	 0.6022	 0.2160
E	 0.7098	 0.2390
F	 0.6604	 0.2600
G	 0.6352	 0.2230
H	 0.7135	 0.2510
I	 0.5270	 0.2350
J	 0.6793	 0.2400
K	 0.6620	 0.2310
L	 0.6727	 0.2440
M	 0.4988	 0.1990
N	 0.4506	 0.1930
O	 0.4924	 0.1840

