



Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 03:41 PM JST

PDB ID : 7DL2
EMDB ID : EMD-30708
Title : Cryo-EM structure of human TSC complex
Authors : Yang, H.; Yu, Z.; Chen, X.; Li, J.; Li, N.; Cheng, J.; Gao, N.; Yuan, H.; Ye, D.; Guan, K.; Xu, Y.
Deposited on : 2020-11-25
Resolution : 4.40 Å(reported)

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

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

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:

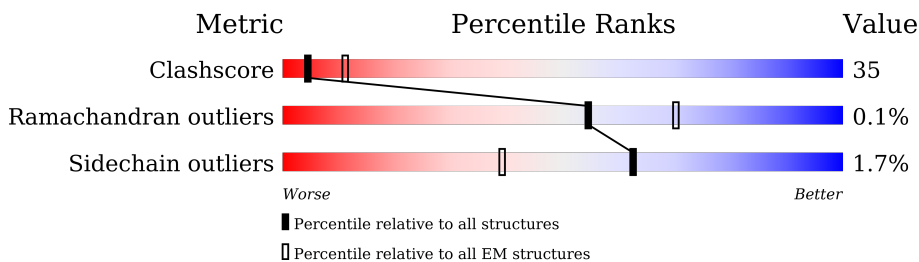
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 4.40 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	C	1164	
1	D	1164	
2	A	1692	
2	B	1692	
3	E	267	
4	F	261	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23285 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 Hamartin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	226	Total	C	N	O	S	0	0
			1575	973	294	305	3		
1	C	224	Total	C	N	O	S	0	0
			1558	962	291	302	3		

- Molecule 2 is a protein called Isoform 7 of Tuberin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	1127	Total	C	N	O	S	0	0
			9016	5785	1544	1632	55		
2	B	1042	Total	C	N	O	S	0	0
			7952	5079	1379	1455	39		

- Molecule 3 is a protein called TBC1 domain family member 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	267	Total	C	N	O	S	0	0
			2169	1403	364	387	15		

- Molecule 4 is a protein called unknown protein.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
4	F	203	Total	C	N	O	0	0
			1015	609	203	203		

PRO ALA GLU PRO THR PRO GLY TYR VAL VAL ARG MET ILE SER SER VAL VAL VAL ASP PHE THR PHE VAL

• Molecule 2: Isoform 7 of Tuberin

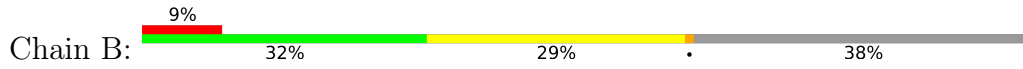
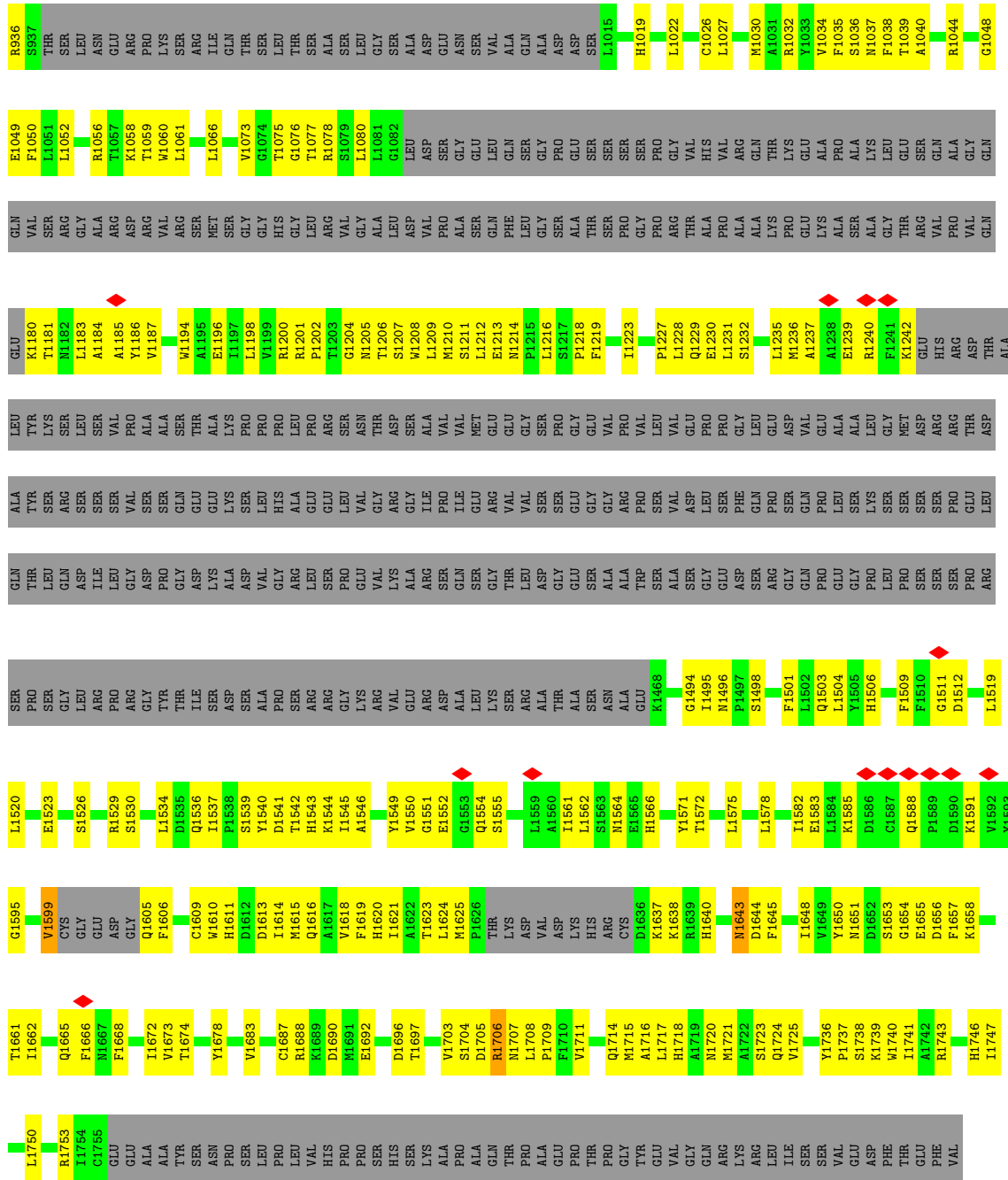
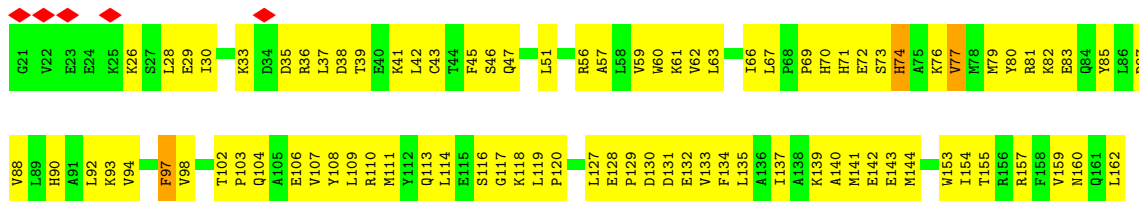
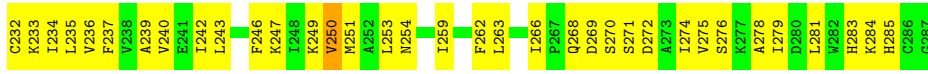
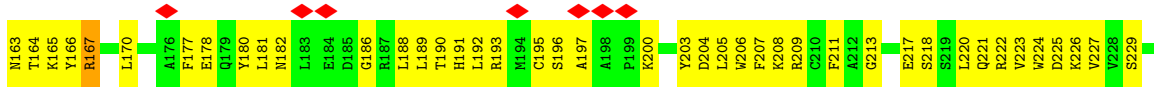


Table of amino acid residues for Chain B, including residue numbers and their corresponding three-letter codes, arranged in multiple rows.

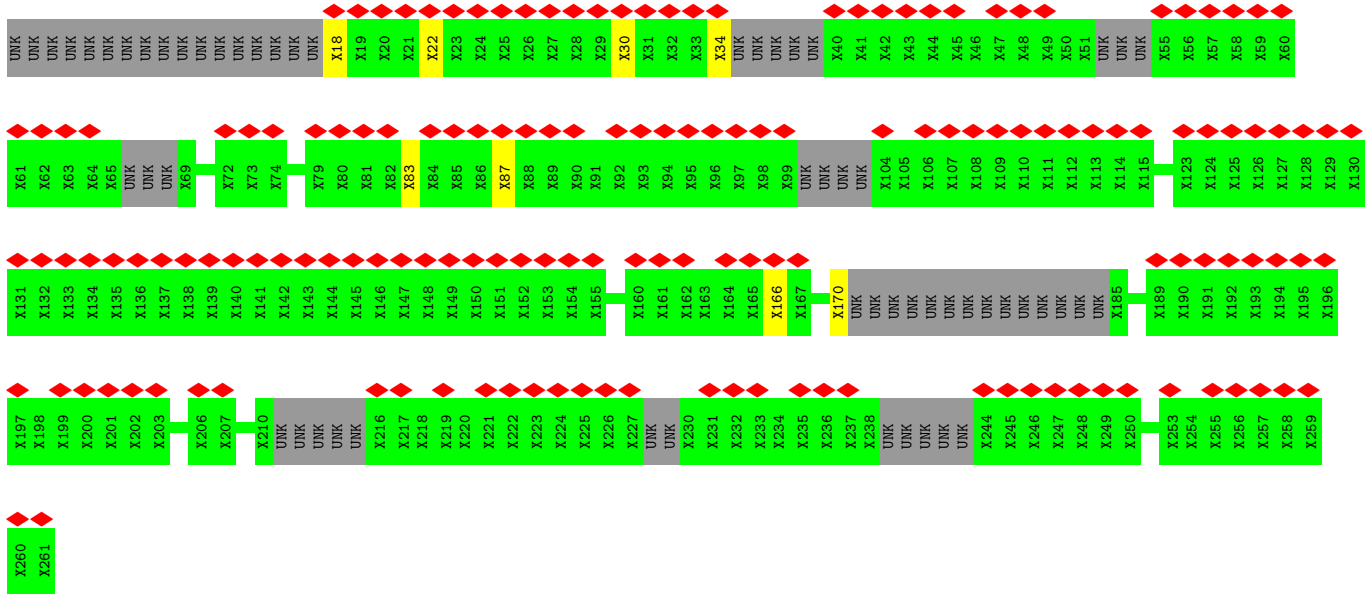
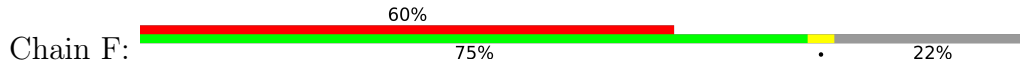


• Molecule 3: TBC1 domain family member 7





• Molecule 4: unknown protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	705.12, 705.12, 705.12	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.356, 1.356, 1.356	Depositor

5 Model quality i

5.1 Standard geometry i

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	C	0.47	0/1568	0.51	0/2126
1	D	0.47	0/1585	0.51	0/2148
2	A	0.34	0/9207	0.48	0/12489
2	B	0.33	0/8099	0.48	4/10996 (0.0%)
3	E	0.41	0/2221	0.47	0/3005
All	All	0.36	0/22680	0.48	4/30764 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	232	PRO	N-CA-CB	5.99	110.48	103.30
2	B	131	PRO	N-CA-CB	5.88	110.35	103.30
2	B	237	PRO	N-CA-CB	5.74	110.18	103.30
2	B	290	PRO	N-CA-CB	5.61	110.03	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1558	0	1313	189	0
1	D	1575	0	1329	178	0
2	A	9016	0	9119	622	0
2	B	7952	0	7731	528	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2169	0	2210	256	0
4	F	1015	0	231	4	0
All	All	23285	0	21933	1572	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 35.

All (1572) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1534:LEU:HB2	2:B:1746:HIS:CE1	1.41	1.52
3:E:249:LYS:HG2	3:E:262:PHE:CE1	1.50	1.46
1:D:854:VAL:CG2	2:B:1235:LEU:HD11	1.54	1.38
1:D:854:VAL:HG22	2:B:1235:LEU:CD1	1.57	1.34
3:E:249:LYS:HG2	3:E:262:PHE:CD1	1.64	1.32
2:B:1625:MET:CB	2:B:1637:LYS:HG2	1.59	1.30
1:D:902:LEU:HB2	1:C:902:LEU:CD2	1.61	1.29
3:E:81:ARG:HD2	3:E:153:TRP:CD1	1.68	1.28
3:E:103:PRO:HD2	3:E:106:GLU:HB2	1.22	1.21
1:D:944:ALA:HB2	3:E:80:TYR:CE1	1.76	1.20
1:D:847:PHE:CZ	1:C:852:LEU:HD22	1.77	1.20
3:E:249:LYS:CG	3:E:262:PHE:CD1	2.25	1.19
3:E:141:MET:CE	3:E:154:ILE:CG2	2.21	1.18
3:E:249:LYS:CG	3:E:262:PHE:CE1	2.24	1.18
2:B:1534:LEU:CB	2:B:1746:HIS:CE1	2.31	1.14
1:D:909:ILE:HG21	1:C:908:ARG:NH1	1.62	1.14
2:A:1574:PHE:HE1	2:A:1709:PRO:HA	1.05	1.14
2:B:1605:GLN:N	2:B:1624:LEU:HD22	1.62	1.14
3:E:81:ARG:HG2	3:E:153:TRP:CE2	1.83	1.14
3:E:66:ILE:HD13	3:E:153:TRP:CB	1.76	1.13
3:E:141:MET:HE2	3:E:154:ILE:HG22	1.17	1.13
3:E:131:ASP:O	3:E:135:LEU:HG	1.48	1.12
2:A:1574:PHE:CE1	2:A:1709:PRO:HA	1.82	1.12
2:A:1574:PHE:HE1	2:A:1709:PRO:CA	1.60	1.12
1:D:909:ILE:HG21	1:C:908:ARG:HH11	1.00	1.12
1:D:847:PHE:CE2	1:C:852:LEU:HD22	1.84	1.10
1:D:899:THR:HG23	1:C:898:GLN:HE22	1.14	1.10
1:D:902:LEU:N	1:C:902:LEU:HD11	1.64	1.10
2:A:1584:LEU:HD21	2:A:1597:LEU:CA	1.80	1.10
3:E:66:ILE:CD1	3:E:153:TRP:HB3	1.81	1.09
2:A:1584:LEU:HD21	2:A:1597:LEU:HA	1.32	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:81:ARG:HB3	3:E:153:TRP:HE1	1.17	1.09
2:A:1584:LEU:CD2	2:A:1597:LEU:HA	1.82	1.07
2:B:1605:GLN:N	2:B:1624:LEU:HD13	1.68	1.07
3:E:141:MET:HE1	3:E:154:ILE:HG21	1.34	1.07
2:B:1625:MET:HB2	2:B:1637:LYS:HG2	1.36	1.07
3:E:141:MET:CE	3:E:154:ILE:HG21	1.83	1.06
2:A:1584:LEU:HD21	2:A:1597:LEU:O	1.54	1.05
3:E:102:THR:HG22	3:E:103:PRO:HD2	1.37	1.05
2:A:1524:SER:CB	2:A:1527:PHE:HD2	1.68	1.05
2:A:1584:LEU:HD11	2:A:1597:LEU:HG	1.37	1.04
1:D:955:THR:HG21	1:C:951:GLN:HE21	1.17	1.04
3:E:102:THR:HG22	3:E:103:PRO:CD	1.87	1.04
3:E:141:MET:CE	3:E:154:ILE:HG22	1.83	1.04
2:A:1081:LEU:HD22	1:C:847:PHE:HE1	1.18	1.04
2:B:1562:LEU:HD11	2:B:1662:ILE:CD1	1.87	1.04
3:E:141:MET:HE2	3:E:154:ILE:CG2	1.83	1.04
1:D:902:LEU:HB2	1:C:902:LEU:HD21	1.03	1.03
2:B:1625:MET:CG	2:B:1637:LYS:HG2	1.89	1.03
3:E:81:ARG:CG	3:E:153:TRP:NE1	2.22	1.02
2:A:1235:LEU:CD2	1:C:844:GLN:HB3	1.90	1.02
2:A:1584:LEU:HD21	2:A:1597:LEU:C	1.78	1.02
2:B:1546:ALA:HB2	2:B:1644:ASP:OD2	1.60	1.02
2:A:1574:PHE:CE1	2:A:1709:PRO:CA	2.40	1.01
3:E:109:LEU:CD2	3:E:135:LEU:HD21	1.90	1.01
3:E:141:MET:HE1	3:E:154:ILE:CG2	1.88	1.01
1:D:851:GLN:NE2	1:C:852:LEU:HD12	1.77	0.99
3:E:109:LEU:HD22	3:E:135:LEU:CD2	1.90	0.99
3:E:113:GLN:NE2	3:E:120:PRO:CD	2.26	0.99
2:A:1570:ARG:NH1	1:C:892:ARG:HH12	1.60	0.98
3:E:67:LEU:HD21	3:E:81:ARG:HH22	1.28	0.98
3:E:81:ARG:HG2	3:E:153:TRP:CZ2	1.99	0.98
1:D:899:THR:HG23	1:C:898:GLN:NE2	1.78	0.97
2:B:1615:MET:CE	2:B:1717:LEU:CD1	2.42	0.97
3:E:81:ARG:CB	3:E:153:TRP:HE1	1.75	0.97
1:D:902:LEU:HD13	1:C:902:LEU:HD22	1.46	0.97
2:A:629:LEU:CD1	1:C:900:GLN:NE2	2.28	0.97
2:A:1569:TYR:HH	1:C:884:TYR:HD2	0.97	0.97
1:C:918:LYS:O	1:C:922:LEU:HG	1.66	0.96
2:B:1534:LEU:HB2	2:B:1746:HIS:NE2	1.79	0.96
3:E:249:LYS:HB3	3:E:262:PHE:CZ	2.01	0.95
3:E:81:ARG:HD2	3:E:153:TRP:NE1	1.79	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:LEU:O	1:D:867:GLN:HG2	1.66	0.95
2:A:1571:TYR:HD1	2:A:1650:TYR:CD1	1.84	0.95
3:E:81:ARG:CD	3:E:153:TRP:NE1	2.31	0.94
2:A:722:LEU:O	2:A:725:THR:HG22	1.67	0.94
3:E:153:TRP:O	3:E:157:ARG:HG2	1.67	0.94
3:E:182:ASN:HA	3:E:189:LEU:CD1	1.97	0.94
2:A:478:GLN:CD	1:C:926:GLN:NE2	2.21	0.94
1:D:902:LEU:CB	1:C:902:LEU:HD21	1.96	0.94
1:D:944:ALA:CB	3:E:80:TYR:CE1	2.51	0.94
3:E:137:ILE:O	3:E:141:MET:HG2	1.68	0.93
3:E:81:ARG:CD	3:E:153:TRP:CD1	2.52	0.93
1:D:955:THR:HG21	1:C:951:GLN:NE2	1.83	0.93
1:D:868:ASN:ND2	1:C:870:HIS:HB2	1.84	0.93
2:A:1569:TYR:OH	1:C:884:TYR:HB2	1.69	0.92
2:B:1534:LEU:HA	2:B:1746:HIS:CD2	2.03	0.92
1:D:944:ALA:HB2	3:E:80:TYR:HE1	1.35	0.92
1:D:909:ILE:CG2	1:C:908:ARG:HH11	1.83	0.92
3:E:188:LEU:HD23	3:E:243:LEU:HB3	1.48	0.92
2:A:1524:SER:HB2	2:A:1527:PHE:CD2	2.05	0.91
2:A:1524:SER:HB2	2:A:1527:PHE:HD2	1.33	0.91
2:B:1534:LEU:HD12	2:B:1746:HIS:ND1	1.85	0.91
1:D:899:THR:CG2	1:C:898:GLN:NE2	2.33	0.91
3:E:92:LEU:CD2	3:E:110:ARG:HB3	1.99	0.91
2:A:629:LEU:CD1	1:C:900:GLN:HE22	1.83	0.90
2:A:1570:ARG:HH11	1:C:892:ARG:HH12	1.17	0.90
3:E:249:LYS:HG3	3:E:262:PHE:CD1	2.07	0.90
2:B:813:VAL:HG22	2:B:1707:ASN:ND2	1.87	0.89
3:E:182:ASN:HA	3:E:189:LEU:HD12	1.53	0.89
2:B:1605:GLN:N	2:B:1624:LEU:CD2	2.35	0.89
2:B:1615:MET:HE2	2:B:1717:LEU:CD1	2.02	0.89
2:A:1081:LEU:HD22	1:C:847:PHE:CE1	2.08	0.89
2:B:1615:MET:HE2	2:B:1717:LEU:HD11	1.56	0.88
3:E:113:GLN:NE2	3:E:120:PRO:HD2	1.86	0.88
2:A:1571:TYR:HD1	2:A:1650:TYR:CG	1.91	0.88
3:E:74:HIS:HA	3:E:77:VAL:HG23	1.56	0.88
1:D:947:ARG:HH21	3:E:80:TYR:HA	1.37	0.88
2:B:1625:MET:CB	2:B:1637:LYS:CG	2.50	0.88
2:A:1570:ARG:NH1	1:C:892:ARG:NH1	2.22	0.87
2:A:574:LYS:NZ	2:A:582:HIS:ND1	2.23	0.87
2:B:1562:LEU:HD11	2:B:1662:ILE:HD11	1.55	0.87
2:A:512:LEU:HD13	2:A:566:GLY:HA3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:98:VAL:HG21	3:E:107:VAL:HG23	1.57	0.86
2:B:1625:MET:HG2	2:B:1637:LYS:HG2	1.55	0.86
1:D:880:MET:O	1:C:884:TYR:HE2	1.59	0.85
2:B:857:TYR:OH	2:B:899:ARG:HG2	1.76	0.85
2:B:1562:LEU:HD11	2:B:1662:ILE:HD12	1.58	0.85
3:E:143:GLU:OE1	3:E:217:GLU:HB2	1.77	0.85
2:A:1584:LEU:CD2	2:A:1597:LEU:O	2.25	0.85
2:A:1524:SER:OG	2:A:1527:PHE:HD2	1.59	0.85
2:A:1524:SER:HG	2:A:1527:PHE:HD2	1.19	0.84
3:E:191:HIS:CG	3:E:251:MET:HE1	2.12	0.84
2:A:416:ASP:HA	2:A:418:ARG:HH21	1.42	0.84
2:B:1605:GLN:N	2:B:1624:LEU:CD1	2.39	0.84
1:C:895:VAL:O	1:C:899:THR:HG23	1.77	0.84
1:C:888:LEU:H	1:C:888:LEU:HD22	1.43	0.84
1:D:868:ASN:HD21	1:C:870:HIS:CA	1.90	0.84
2:B:1615:MET:CE	2:B:1717:LEU:HD12	2.07	0.83
2:A:1581:LEU:H	2:A:1581:LEU:HD23	1.43	0.83
3:E:67:LEU:HD21	3:E:81:ARG:NH2	1.92	0.83
2:B:1534:LEU:HG	2:B:1746:HIS:CG	2.12	0.83
2:A:1524:SER:CB	2:A:1527:PHE:CD2	2.58	0.83
3:E:188:LEU:CD2	3:E:243:LEU:HB3	2.09	0.83
3:E:191:HIS:CD2	3:E:195:CYS:SG	2.72	0.83
1:D:877:VAL:HG13	2:A:1606:PHE:CE1	2.14	0.83
3:E:251:MET:HA	3:E:251:MET:CE	2.09	0.83
3:E:92:LEU:HD21	3:E:110:ARG:HB3	1.60	0.82
2:B:1546:ALA:CB	2:B:1644:ASP:OD2	2.27	0.82
3:E:67:LEU:HD22	3:E:74:HIS:HB2	1.61	0.82
1:D:930:LEU:HD12	1:C:930:LEU:CD2	2.10	0.82
2:A:478:GLN:HG3	1:C:926:GLN:HE22	1.43	0.82
2:B:1615:MET:HE3	2:B:1717:LEU:CD1	2.09	0.82
1:D:926:GLN:OE1	1:C:923:LEU:HD12	1.79	0.82
1:D:868:ASN:ND2	1:C:870:HIS:CB	2.43	0.81
1:D:851:GLN:HE21	1:D:851:GLN:HA	1.43	0.81
2:B:1236:MET:CE	2:B:1236:MET:HA	2.11	0.81
1:D:930:LEU:HB2	1:C:930:LEU:HD21	1.60	0.81
2:A:279:LEU:HD22	2:A:322:SER:OG	1.80	0.81
3:E:251:MET:HA	3:E:251:MET:HE2	1.62	0.81
1:D:849:ASN:ND2	2:B:1050:PHE:CZ	2.47	0.81
2:A:1235:LEU:HD23	1:C:844:GLN:HB3	1.63	0.80
3:E:74:HIS:HA	3:E:77:VAL:CG2	2.11	0.80
1:D:944:ALA:CB	3:E:80:TYR:HE1	1.92	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1534:LEU:CA	2:B:1746:HIS:NE2	2.43	0.80
1:D:852:LEU:HD12	2:A:1241:PHE:HE1	1.45	0.80
2:A:343:THR:HG22	2:A:392:GLU:OE1	1.82	0.80
1:C:842:GLN:HA	1:C:842:GLN:HE21	1.45	0.80
2:A:1585:LYS:HG2	2:A:1587:CYS:SG	2.22	0.80
2:A:1680:CYS:HB2	2:A:1702:ILE:HD11	1.64	0.80
2:A:474:LEU:HA	2:A:477:ARG:HH22	1.47	0.79
1:D:868:ASN:HD22	1:C:870:HIS:HB2	1.48	0.79
2:A:1581:LEU:HB3	2:A:1608:TYR:HA	1.63	0.79
3:E:186:GLY:O	3:E:190:THR:HG23	1.82	0.79
1:D:902:LEU:CB	1:C:902:LEU:CD2	2.55	0.79
2:A:342:ILE:HD11	2:A:366:GLU:HB2	1.65	0.79
2:A:625:SER:H	2:A:629:LEU:HD22	1.47	0.78
1:D:902:LEU:H	1:C:902:LEU:HD11	1.44	0.78
1:D:902:LEU:HB2	1:C:902:LEU:HD22	1.65	0.78
1:D:951:GLN:HA	1:D:951:GLN:HE21	1.49	0.78
2:A:144:LYS:O	2:A:148:ASP:HB2	1.82	0.78
2:A:884:TYR:HB2	2:A:1725:VAL:HG11	1.64	0.78
2:B:1060:TRP:NE1	2:B:1519:LEU:HD13	1.99	0.78
3:E:66:ILE:HD13	3:E:153:TRP:HB3	0.87	0.78
2:A:1584:LEU:HD22	2:A:1597:LEU:HA	1.66	0.78
3:E:104:GLN:HE21	3:E:104:GLN:HA	1.48	0.78
3:E:113:GLN:NE2	3:E:120:PRO:HD3	1.96	0.78
1:D:854:VAL:HG22	2:B:1235:LEU:HD11	0.80	0.78
3:E:92:LEU:HB3	3:E:98:VAL:HG12	1.63	0.78
2:B:1216:LEU:HB2	2:B:1223:ILE:HD12	1.64	0.78
2:A:478:GLN:CG	1:C:926:GLN:NE2	2.47	0.78
3:E:81:ARG:CG	3:E:153:TRP:CE2	2.61	0.78
1:D:951:GLN:O	1:D:955:THR:CG2	2.33	0.77
2:B:1625:MET:HG2	2:B:1637:LYS:CG	2.14	0.77
3:E:81:ARG:HG2	3:E:153:TRP:NE1	1.94	0.77
1:D:847:PHE:CE2	1:C:852:LEU:CD2	2.67	0.77
2:A:1585:LYS:HE3	2:A:1587:CYS:SG	2.24	0.77
3:E:113:GLN:HE21	3:E:120:PRO:CD	1.94	0.77
3:E:88:VAL:HG23	3:E:114:LEU:HD23	1.66	0.77
2:A:1571:TYR:CD1	2:A:1650:TYR:CD1	2.73	0.77
2:B:1534:LEU:CB	2:B:1746:HIS:NE2	2.40	0.77
1:C:953:ARG:O	1:C:957:VAL:HG23	1.84	0.77
2:B:1212:LEU:HD23	2:B:1214:ASN:H	1.49	0.77
2:A:591:VAL:HG11	2:A:688:LEU:HB3	1.67	0.76
3:E:113:GLN:HE21	3:E:120:PRO:HD2	1.47	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:842:GLN:HA	1:C:842:GLN:NE2	1.99	0.76
2:A:1588:GLN:OE1	2:A:1592:VAL:HG22	1.85	0.76
2:A:1588:GLN:HE21	2:A:1588:GLN:HA	1.51	0.76
1:D:880:MET:SD	2:A:1576:THR:HG21	2.26	0.76
2:A:1569:TYR:OH	1:C:884:TYR:CB	2.34	0.76
2:A:1585:LYS:CG	2:A:1587:CYS:SG	2.74	0.76
2:B:1625:MET:HB3	2:B:1637:LYS:HG2	1.64	0.76
3:E:92:LEU:HD22	3:E:110:ARG:HB3	1.68	0.76
2:A:183:LEU:HB2	2:A:187:ASN:HB2	1.68	0.76
2:A:629:LEU:HD12	2:A:642:PRO:HB3	1.66	0.76
2:A:1235:LEU:HD21	1:C:844:GLN:HB3	1.67	0.76
1:D:848:LEU:HD21	2:A:1238:ALA:HB2	1.67	0.76
2:A:327:MET:SD	2:A:373:GLN:NE2	2.58	0.76
2:A:1516:LYS:HZ1	2:B:936:ARG:HB3	1.50	0.76
2:A:1025:THR:HG21	2:A:1741:ILE:HG13	1.67	0.75
2:A:1209:LEU:HB2	2:A:1240:ARG:HH11	1.51	0.75
2:A:1581:LEU:HD12	2:A:1606:PHE:HB3	1.68	0.75
2:A:1649:VAL:CG2	2:A:1672:ILE:HG12	2.16	0.75
3:E:249:LYS:HG3	3:E:262:PHE:CG	2.21	0.75
3:E:103:PRO:HD2	3:E:106:GLU:CB	2.11	0.75
2:A:1081:LEU:HD13	1:C:847:PHE:CE1	2.21	0.75
2:A:478:GLN:CG	1:C:926:GLN:HE22	1.99	0.75
2:A:1662:ILE:HG13	2:A:1664:GLY:H	1.52	0.75
1:D:868:ASN:HD21	1:C:870:HIS:N	1.83	0.75
1:D:902:LEU:CA	1:C:902:LEU:HD11	2.16	0.74
2:A:484:LEU:O	2:A:488:VAL:HG12	1.86	0.74
2:B:597:HIS:HD2	2:B:611:ARG:HE	1.35	0.74
2:B:717:LEU:HA	2:B:720:LYS:HB2	1.70	0.74
2:A:168:MET:HB3	2:A:195:ILE:HD13	1.70	0.74
2:B:1059:THR:HG23	2:B:1520:LEU:HD21	1.68	0.74
1:C:844:GLN:HA	1:C:844:GLN:HE21	1.52	0.74
3:E:181:LEU:HD13	3:E:240:VAL:HG13	1.68	0.74
3:E:141:MET:HG3	3:E:155:THR:OG1	1.88	0.74
2:A:811:CYS:O	2:A:815:MET:N	2.20	0.73
3:E:178:GLU:O	3:E:182:ASN:HB2	1.87	0.73
3:E:217:GLU:OE1	3:E:217:GLU:N	2.20	0.73
2:A:478:GLN:HG3	1:C:926:GLN:NE2	2.03	0.73
2:B:1562:LEU:N	2:B:1562:LEU:HD12	2.03	0.73
2:A:901:ARG:HG2	2:A:903:PRO:HD2	1.70	0.73
1:D:854:VAL:O	1:D:858:VAL:HG23	1.88	0.73
2:A:485:ILE:HA	2:A:488:VAL:CG1	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:629:LEU:HD12	1:C:900:GLN:NE2	2.03	0.73
1:D:926:GLN:OE1	1:C:923:LEU:CD1	2.36	0.73
1:D:962:ILE:CD1	1:C:958:PHE:HD1	2.02	0.73
2:B:1555:SER:HB2	2:B:1655:GLU:OE2	1.88	0.73
3:E:76:LYS:O	3:E:80:TYR:HD2	1.71	0.73
2:B:813:VAL:HG22	2:B:1707:ASN:HD21	1.54	0.73
3:E:103:PRO:CD	3:E:106:GLU:HB2	2.13	0.73
2:B:1657:PHE:CZ	2:B:1661:THR:HG21	2.24	0.72
1:D:899:THR:CG2	1:C:898:GLN:HE22	1.94	0.72
2:A:1235:LEU:CD2	1:C:844:GLN:CB	2.65	0.72
1:D:927:LYS:NZ	2:A:478:GLN:O	2.22	0.72
1:D:930:LEU:HD12	1:C:930:LEU:HD23	1.70	0.72
1:D:951:GLN:O	1:D:955:THR:HG23	1.89	0.72
2:A:1081:LEU:HD13	1:C:847:PHE:CZ	2.25	0.72
2:A:195:ILE:HG13	2:A:197:ARG:HG2	1.72	0.72
2:A:1571:TYR:CD1	2:A:1650:TYR:CG	2.76	0.72
1:D:849:ASN:ND2	2:B:1050:PHE:CE1	2.58	0.72
2:A:895:MET:SD	2:A:899:ARG:NH1	2.61	0.72
2:B:1562:LEU:CD1	2:B:1662:ILE:HD11	2.20	0.72
2:B:816:PRO:HB2	2:B:856:LEU:HD13	1.71	0.72
2:A:633:ASN:ND2	2:A:637:VAL:O	2.21	0.72
2:A:1570:ARG:HH11	1:C:892:ARG:NH1	1.81	0.72
2:B:1611:HIS:ND1	2:B:1616:GLN:OE1	2.23	0.71
2:A:1189:LEU:HD11	2:A:1216:LEU:HD22	1.72	0.71
2:B:512:LEU:HD13	2:B:566:GLY:HA3	1.71	0.71
2:A:218:SER:OG	2:A:222:LEU:N	2.23	0.71
2:A:929:GLU:HG2	2:B:1509:PHE:HA	1.73	0.71
2:B:1058:LYS:NZ	2:B:1498:SER:HB3	2.04	0.71
2:A:722:LEU:O	2:A:725:THR:CG2	2.37	0.71
1:D:850:ARG:CZ	2:B:1239:GLU:HA	2.21	0.71
1:C:888:LEU:HD22	1:C:888:LEU:N	2.05	0.71
2:A:1571:TYR:CD1	2:A:1650:TYR:CB	2.74	0.71
2:B:1060:TRP:CD1	2:B:1519:LEU:HB2	2.26	0.71
2:B:579:PRO:HB2	2:B:582:HIS:HD2	1.54	0.71
2:B:1551:GLY:H	2:B:1554:GLN:HB2	1.54	0.71
2:A:335:SER:O	2:A:339:VAL:HG12	1.90	0.71
1:D:902:LEU:CD1	1:C:902:LEU:HD22	2.19	0.70
3:E:133:VAL:O	3:E:137:ILE:HG13	1.90	0.70
1:D:953:ARG:NH1	3:E:117:GLY:HA3	2.06	0.70
1:D:875:LYS:HD2	1:D:875:LYS:N	2.07	0.70
2:A:1581:LEU:HD22	2:A:1608:TYR:CE1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:HIS:HD2	2:B:496:ILE:HG12	1.57	0.70
2:A:246:THR:O	2:A:250:LYS:NZ	2.24	0.70
3:E:102:THR:CG2	3:E:103:PRO:CD	2.67	0.70
2:B:805:VAL:HA	2:B:808:LEU:HD12	1.74	0.70
2:B:813:VAL:CG2	2:B:1707:ASN:HD21	2.04	0.70
2:B:1606:PHE:H	2:B:1624:LEU:HD13	1.55	0.70
1:C:923:LEU:HG	1:C:927:LYS:HE3	1.72	0.70
2:B:477:ARG:HA	2:B:481:GLU:HB2	1.72	0.69
1:C:904:THR:O	1:C:907:LYS:HG2	1.90	0.69
3:E:97:PHE:CZ	3:E:120:PRO:O	2.44	0.69
1:D:851:GLN:NE2	1:D:851:GLN:HA	2.06	0.69
1:D:877:VAL:HG13	2:A:1606:PHE:HE1	1.57	0.69
2:A:1533:LEU:HD12	2:A:1533:LEU:C	2.12	0.69
1:D:959:GLU:HG2	1:C:958:PHE:CE1	2.27	0.69
3:E:249:LYS:CB	3:E:262:PHE:CE1	2.75	0.69
2:A:1571:TYR:HA	2:A:1650:TYR:CE1	2.28	0.69
1:D:852:LEU:HD23	1:D:852:LEU:O	1.92	0.69
2:B:1657:PHE:CE1	2:B:1661:THR:HG21	2.28	0.69
1:D:902:LEU:CA	1:C:902:LEU:CD1	2.69	0.69
2:A:1533:LEU:HD11	2:A:1746:HIS:CD2	2.28	0.69
2:B:1599:VAL:HG13	2:B:1625:MET:O	1.93	0.69
1:D:948:TYR:CE2	1:D:952:LYS:HD2	2.28	0.69
2:B:1076:GLY:O	2:B:1080:LEU:HG	1.93	0.69
1:C:895:VAL:O	1:C:899:THR:CG2	2.40	0.69
3:E:249:LYS:CB	3:E:262:PHE:CZ	2.75	0.69
2:A:456:GLU:O	2:A:462:ARG:NH2	2.26	0.68
3:E:104:GLN:HA	3:E:104:GLN:NE2	2.06	0.68
2:B:734:CYS:HA	2:B:737:LEU:HD12	1.74	0.68
2:B:1564:ASN:ND2	2:B:1566:HIS:O	2.26	0.68
1:D:902:LEU:HA	1:C:902:LEU:HD13	1.73	0.68
2:A:1581:LEU:HD23	2:A:1581:LEU:N	2.08	0.68
2:B:1534:LEU:CD1	2:B:1746:HIS:ND1	2.55	0.68
3:E:203:TYR:O	3:E:207:PHE:N	2.27	0.68
2:A:1534:LEU:C	2:A:1534:LEU:HD23	2.14	0.68
2:A:1575:LEU:HD23	2:A:1575:LEU:O	1.93	0.68
2:B:1606:PHE:N	2:B:1624:LEU:HD13	2.08	0.68
3:E:233:LYS:O	3:E:236:VAL:HB	1.93	0.68
2:A:148:ASP:HA	2:A:160:LEU:HD11	1.76	0.68
2:B:1534:LEU:HA	2:B:1746:HIS:NE2	2.08	0.68
2:B:1599:VAL:CG1	2:B:1625:MET:O	2.42	0.68
3:E:88:VAL:HG11	3:E:111:MET:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:LEU:H	1:C:888:LEU:CD2	2.08	0.68
1:D:851:GLN:NE2	1:C:852:LEU:CD1	2.55	0.67
2:A:629:LEU:HD13	1:C:900:GLN:NE2	2.09	0.67
2:A:1081:LEU:CD2	1:C:847:PHE:HE1	2.00	0.67
2:A:1571:TYR:CD1	2:A:1650:TYR:HB2	2.29	0.67
2:B:1687:CYS:SG	2:B:1688:ARG:N	2.67	0.67
2:B:738:CYS:SG	2:B:784:LYS:NZ	2.67	0.67
2:B:1235:LEU:HD23	2:B:1235:LEU:O	1.94	0.67
3:E:81:ARG:CB	3:E:153:TRP:NE1	2.48	0.67
3:E:191:HIS:NE2	3:E:195:CYS:SG	2.67	0.67
2:A:578:LEU:HD21	1:C:908:ARG:HG3	1.76	0.67
2:A:1569:TYR:OH	1:C:884:TYR:CD2	2.44	0.67
2:A:1688:ARG:NH1	2:A:1690:ASP:OD2	2.28	0.67
2:A:136:LEU:HB3	2:A:139:ARG:HD2	1.76	0.67
2:A:830:LEU:HA	2:A:833:ILE:HD11	1.77	0.67
2:A:877:ASN:OD1	2:A:880:LYS:N	2.27	0.67
3:E:74:HIS:CA	3:E:77:VAL:HG23	2.24	0.67
2:A:1032:ARG:HH21	2:A:1040:ALA:HA	1.59	0.67
2:A:527:LEU:HD21	2:A:589:MET:HE1	1.77	0.67
2:A:1209:LEU:O	2:A:1240:ARG:NH1	2.27	0.67
2:A:1514:SER:HB2	2:B:1511:GLY:HA3	1.76	0.67
2:A:1584:LEU:HD13	2:A:1594:LEU:HD11	1.77	0.67
1:C:879:MET:O	1:C:883:ALA:N	2.25	0.67
2:A:559:ASP:OD1	2:A:560:VAL:N	2.27	0.67
2:A:1588:GLN:HA	2:A:1588:GLN:NE2	2.09	0.67
2:B:1625:MET:HG2	2:B:1637:LYS:HA	1.76	0.67
3:E:127:LEU:CD2	3:E:135:LEU:HD11	2.25	0.67
1:C:837:ASN:O	1:C:841:VAL:HG23	1.95	0.67
2:A:921:LEU:HA	2:A:924:PHE:HB3	1.76	0.66
2:B:813:VAL:HG22	2:B:1707:ASN:CG	2.15	0.66
2:A:577:THR:HG22	2:A:579:PRO:HD2	1.78	0.66
3:E:81:ARG:HB3	3:E:153:TRP:NE1	2.01	0.66
2:A:883:GLN:NE2	2:A:1736:TYR:OH	2.28	0.66
2:A:473:LEU:HD23	2:A:484:LEU:HD23	1.76	0.66
1:D:877:VAL:HG13	2:A:1606:PHE:CZ	2.30	0.66
2:B:530:ILE:HG21	2:B:567:LEU:HD21	1.78	0.66
2:B:1605:GLN:N	2:B:1624:LEU:CG	2.58	0.66
2:B:1625:MET:HB2	2:B:1637:LYS:CG	2.21	0.66
1:D:930:LEU:HD12	1:C:930:LEU:HD21	1.77	0.66
2:A:478:GLN:CD	1:C:926:GLN:HE22	1.98	0.66
1:D:899:THR:HG22	1:C:898:GLN:NE2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:205:LEU:HA	3:E:209:ARG:HB2	1.78	0.66
2:A:485:ILE:HA	2:A:488:VAL:HG12	1.76	0.66
2:A:835:ALA:HA	2:A:875:TYR:OH	1.96	0.66
1:D:852:LEU:HG	2:A:1241:PHE:CE1	2.30	0.65
2:A:485:ILE:O	2:A:489:VAL:HG12	1.96	0.65
2:A:1574:PHE:CE1	2:A:1709:PRO:CB	2.79	0.65
2:B:1606:PHE:H	2:B:1624:LEU:CD1	2.09	0.65
1:D:948:TYR:HE2	1:D:952:LYS:HD2	1.60	0.65
2:B:1534:LEU:C	2:B:1534:LEU:HD23	2.17	0.65
3:E:232:CYS:SG	3:E:233:LYS:NZ	2.65	0.65
1:D:912:LEU:HD13	1:C:912:LEU:HB2	1.77	0.65
2:B:840:ALA:HA	2:B:875:TYR:CE1	2.32	0.65
2:B:1060:TRP:CD1	2:B:1519:LEU:HA	2.31	0.65
2:B:1606:PHE:HZ	1:C:819:ASN:CB	2.09	0.65
3:E:51:LEU:O	3:E:56:ARG:NH1	2.29	0.65
2:A:1549:TYR:HB2	2:A:1571:TYR:CZ	2.31	0.65
2:A:1584:LEU:CD2	2:A:1597:LEU:C	2.61	0.65
1:D:868:ASN:ND2	1:C:870:HIS:CA	2.58	0.65
2:A:1574:PHE:CE1	2:A:1709:PRO:HB3	2.32	0.65
2:B:549:ASP:O	2:B:553:TYR:N	2.20	0.65
2:B:852:ARG:HH11	2:B:1714:GLN:HE22	1.43	0.65
2:B:1650:TYR:HD1	2:B:1673:VAL:HG23	1.62	0.65
3:E:246:PHE:O	3:E:250:VAL:HG12	1.96	0.65
2:A:456:GLU:HB3	2:A:462:ARG:HE	1.60	0.64
2:A:629:LEU:HD11	1:C:900:GLN:HE22	1.62	0.64
2:A:1588:GLN:OE1	2:A:1592:VAL:CG2	2.45	0.64
2:B:587:TYR:O	2:B:590:LEU:HB2	1.96	0.64
2:B:786:ARG:HD2	2:B:818:ILE:HG23	1.79	0.64
2:B:1625:MET:HG2	2:B:1637:LYS:CB	2.27	0.64
2:A:920:VAL:HG13	2:A:921:LEU:HG	1.80	0.64
2:B:1643:ASN:ND2	2:B:1643:ASN:O	2.30	0.64
3:E:246:PHE:HB3	3:E:262:PHE:HZ	1.63	0.64
2:A:700:GLU:OE2	2:A:702:ASP:N	2.23	0.64
2:B:470:SER:HA	2:B:510:GLN:HE21	1.61	0.64
2:B:1537:ILE:O	2:B:1743:ARG:NH2	2.31	0.64
1:C:844:GLN:HA	1:C:844:GLN:NE2	2.12	0.64
1:D:944:ALA:HA	3:E:80:TYR:CD1	2.32	0.64
2:A:1503:GLN:HA	2:B:1201:ARG:HH22	1.63	0.64
1:D:951:GLN:HA	1:D:951:GLN:NE2	2.11	0.64
2:A:803:GLN:OE1	2:A:803:GLN:N	2.23	0.64
2:A:861:ALA:N	2:A:864:GLN:OE1	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:203:TYR:HA	3:E:206:TRP:HE3	1.62	0.64
2:A:1581:LEU:CD1	2:A:1606:PHE:HB3	2.27	0.64
2:A:1581:LEU:HD13	2:A:1608:TYR:CE2	2.33	0.64
2:B:534:VAL:HA	2:B:560:VAL:HG21	1.79	0.63
2:B:813:VAL:CG1	2:B:1707:ASN:HD21	2.11	0.63
2:B:1032:ARG:NH2	2:B:1038:PHE:O	2.31	0.63
2:B:890:HIS:CE1	2:B:1022:LEU:HB3	2.33	0.63
2:A:482:GLU:OE1	2:A:522:HIS:NE2	2.31	0.63
2:A:642:PRO:HB3	1:C:900:GLN:HE21	1.63	0.63
2:A:741:LEU:O	2:A:759:ARG:NH2	2.31	0.63
2:A:1575:LEU:HD23	2:A:1575:LEU:C	2.18	0.63
2:B:813:VAL:HG13	2:B:1707:ASN:HD21	1.63	0.63
3:E:271:SER:HA	3:E:274:ILE:HD12	1.79	0.63
1:D:898:GLN:HE22	1:C:899:THR:HG22	1.64	0.63
2:B:586:VAL:O	2:B:589:MET:HB3	1.97	0.63
2:B:1236:MET:HA	2:B:1236:MET:HE2	1.79	0.63
1:D:902:LEU:N	1:C:902:LEU:CD1	2.51	0.63
2:B:892:VAL:HA	2:B:895:MET:HG2	1.80	0.63
2:B:1027:LEU:HA	2:B:1030:MET:HE2	1.79	0.63
3:E:35:ASP:OD1	3:E:71:HIS:CD2	2.52	0.63
2:A:931:ASP:OD2	2:A:934:ARG:NH1	2.32	0.63
2:B:591:VAL:O	2:B:595:GLN:N	2.30	0.63
2:B:1060:TRP:HD1	2:B:1519:LEU:HA	1.64	0.63
2:B:1534:LEU:CA	2:B:1746:HIS:CD2	2.79	0.63
1:D:852:LEU:CD1	2:A:1241:PHE:HE1	2.11	0.63
2:B:582:HIS:O	2:B:585:ARG:HG3	1.99	0.63
2:B:813:VAL:CG2	2:B:1707:ASN:ND2	2.60	0.63
3:E:113:GLN:HE22	3:E:120:PRO:CD	2.10	0.63
1:D:849:ASN:ND2	2:B:1050:PHE:CE2	2.65	0.62
2:A:1240:ARG:HH12	2:B:1211:SER:N	1.96	0.62
2:A:1516:LYS:NZ	2:A:1517:PRO:O	2.27	0.62
2:B:1543:HIS:HB2	2:B:1616:GLN:O	1.99	0.62
3:E:76:LYS:O	3:E:80:TYR:CD2	2.51	0.62
2:A:245:ARG:HE	2:A:274:TYR:HA	1.64	0.62
1:D:909:ILE:HD11	1:C:905:SER:HA	1.80	0.62
2:B:1545:ILE:HD11	2:B:1648:ILE:HD11	1.82	0.62
2:A:185:LYS:NZ	2:A:185:LYS:O	2.32	0.62
4:F:30:UNK:O	4:F:34:UNK:N	2.32	0.62
2:A:168:MET:SD	2:A:168:MET:N	2.72	0.62
2:B:563:ALA:O	2:B:567:LEU:HG	1.99	0.62
3:E:98:VAL:HB	3:E:110:ARG:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:775:SER:HB2	2:A:1702:ILE:HG21	1.81	0.62
2:B:512:LEU:HD11	2:B:563:ALA:HA	1.79	0.62
1:C:947:ARG:NE	1:C:947:ARG:HA	2.13	0.62
2:A:343:THR:O	2:A:346:ILE:HG12	2.00	0.62
2:B:1060:TRP:HD1	2:B:1519:LEU:CA	2.13	0.62
3:E:279:ILE:O	3:E:283:HIS:ND1	2.30	0.62
2:B:418:ARG:NH1	2:B:420:GLU:O	2.32	0.62
2:B:813:VAL:CG2	2:B:1707:ASN:OD1	2.48	0.62
2:B:840:ALA:HA	2:B:875:TYR:HE1	1.65	0.62
2:A:1221:SER:OG	2:B:1037:ASN:ND2	2.31	0.62
2:B:466:LEU:HD21	2:B:506:LYS:HB3	1.81	0.62
3:E:85:TYR:HE2	3:E:108:TYR:HE1	1.47	0.61
1:D:962:ILE:CD1	1:C:958:PHE:CD1	2.82	0.61
2:A:409:GLU:O	2:A:413:ARG:NH2	2.34	0.61
2:A:1584:LEU:CD2	2:A:1597:LEU:CA	2.56	0.61
2:A:736:ALA:O	2:A:740:MET:N	2.27	0.61
2:A:1078:ARG:O	2:A:1082:GLY:N	2.33	0.61
2:B:1534:LEU:CG	2:B:1746:HIS:ND1	2.63	0.61
2:B:1625:MET:HG2	2:B:1637:LYS:CA	2.30	0.61
1:C:956:GLN:HA	1:C:956:GLN:OE1	2.00	0.61
2:A:486:ASN:HA	2:A:489:VAL:HG12	1.81	0.61
2:A:907:ASP:OD1	2:A:907:ASP:N	2.32	0.61
2:A:1584:LEU:HD11	2:A:1597:LEU:CG	2.23	0.61
2:A:478:GLN:NE2	1:C:926:GLN:NE2	2.47	0.61
2:B:734:CYS:O	2:B:737:LEU:HB2	2.00	0.61
2:B:861:ALA:N	2:B:864:GLN:OE1	2.31	0.61
3:E:102:THR:CG2	3:E:103:PRO:HD3	2.31	0.61
2:A:283:ARG:HH21	2:A:284:ALA:H	1.47	0.61
3:E:88:VAL:CG1	3:E:111:MET:HE3	2.31	0.61
1:D:852:LEU:HD23	1:D:852:LEU:C	2.20	0.61
1:D:878:GLU:HB3	1:D:881:LYS:HD2	1.83	0.61
1:D:847:PHE:HZ	1:C:852:LEU:HD22	1.57	0.61
2:A:462:ARG:NH1	2:A:498:GLU:OE2	2.34	0.61
2:A:1552:GLU:N	2:A:1552:GLU:OE1	2.31	0.61
2:B:1058:LYS:HZ3	2:B:1498:SER:HB3	1.64	0.61
2:A:478:GLN:CD	1:C:926:GLN:CD	2.60	0.60
2:B:1673:VAL:HG12	2:B:1683:VAL:HG22	1.83	0.60
2:A:1571:TYR:HD1	2:A:1650:TYR:CB	2.11	0.60
3:E:30:ILE:HG13	3:E:33:LYS:HD3	1.82	0.60
2:B:378:PRO:HA	2:B:381:ARG:HE	1.65	0.60
1:D:902:LEU:HA	1:C:902:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:937:ALA:HA	1:D:940:GLN:HE21	1.66	0.60
2:B:1235:LEU:HD23	2:B:1235:LEU:C	2.22	0.60
2:B:550:VAL:O	2:B:554:SER:HB2	2.02	0.60
2:B:1621:ILE:HG22	2:B:1623:THR:H	1.65	0.60
2:A:486:ASN:HA	2:A:489:VAL:CG1	2.31	0.60
2:A:1524:SER:OG	2:A:1527:PHE:CD2	2.42	0.60
2:A:1569:TYR:OH	1:C:884:TYR:HD2	1.76	0.60
2:B:890:HIS:HE1	2:B:1022:LEU:HB3	1.66	0.60
3:E:191:HIS:CD2	3:E:251:MET:CE	2.85	0.60
3:E:90:HIS:HA	3:E:93:LYS:HD3	1.83	0.60
1:D:851:GLN:HE22	1:C:852:LEU:HD12	1.60	0.60
1:D:951:GLN:O	1:D:955:THR:HG22	2.01	0.60
2:B:492:GLN:O	2:B:495:HIS:ND1	2.35	0.60
2:B:849:THR:HG22	2:B:1714:GLN:HG2	1.84	0.60
2:B:1585:LYS:O	2:B:1588:GLN:NE2	2.35	0.60
3:E:97:PHE:HZ	3:E:120:PRO:O	1.85	0.60
3:E:221:GLN:HA	3:E:224:TRP:HB2	1.83	0.60
1:D:876:GLU:HB2	1:D:879:MET:HG2	1.84	0.59
2:B:425:ASN:O	2:B:429:TYR:N	2.33	0.59
3:E:92:LEU:CD1	3:E:110:ARG:HB2	2.32	0.59
1:D:877:VAL:HG23	1:D:877:VAL:O	2.01	0.59
1:D:887:GLU:OE1	1:D:887:GLU:HA	2.02	0.59
2:B:462:ARG:HA	2:B:465:VAL:HG22	1.84	0.59
1:C:934:LYS:HB2	1:C:934:LYS:NZ	2.17	0.59
3:E:88:VAL:HG11	3:E:111:MET:HE2	1.84	0.59
3:E:234:ILE:HA	3:E:237:PHE:HD2	1.66	0.59
3:E:249:LYS:CG	3:E:262:PHE:CZ	2.85	0.59
2:A:1649:VAL:HG21	2:A:1672:ILE:HG12	1.83	0.59
2:B:496:ILE:HD11	2:B:533:LYS:HD3	1.84	0.59
2:B:730:VAL:O	2:B:733:LEU:HG	2.01	0.59
2:A:316:PRO:HG2	2:A:362:LEU:HD21	1.84	0.59
2:A:478:GLN:NE2	1:C:926:GLN:CD	2.55	0.59
2:A:1574:PHE:HE1	2:A:1709:PRO:N	1.99	0.59
2:B:343:THR:O	2:B:347:LYS:NZ	2.34	0.59
3:E:211:PHE:HE2	3:E:235:LEU:HD22	1.68	0.59
2:A:363:ASN:O	2:A:367:ARG:HG2	2.02	0.59
2:B:863:GLU:OE1	2:B:863:GLU:N	2.35	0.59
2:B:1059:THR:CG2	2:B:1520:LEU:HD21	2.32	0.59
1:D:920:ASP:HA	1:D:923:LEU:HD12	1.85	0.59
2:B:894:ALA:O	2:B:898:ILE:HG12	2.03	0.59
3:E:182:ASN:CA	3:E:189:LEU:CD1	2.78	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1614:ILE:CD1	2:B:1740:TRP:HZ2	2.15	0.59
3:E:109:LEU:HD22	3:E:135:LEU:HD21	0.93	0.59
3:E:127:LEU:HD21	3:E:135:LEU:HD11	1.85	0.59
2:B:527:LEU:HD23	2:B:530:ILE:HD12	1.85	0.59
3:E:92:LEU:HD13	3:E:110:ARG:HB2	1.83	0.59
2:A:1062:VAL:HG23	2:A:1063:GLY:H	1.67	0.58
2:B:561:LYS:O	2:B:565:LEU:HG	2.03	0.58
3:E:213:GLY:HA2	3:E:217:GLU:OE2	2.02	0.58
1:D:839:GLU:O	1:D:843:GLN:NE2	2.35	0.58
2:A:1078:ARG:HA	2:A:1081:LEU:HB2	1.85	0.58
2:A:1653:SER:HB3	2:A:1656:ASP:HB3	1.85	0.58
2:B:907:ASP:OD1	2:B:907:ASP:N	2.35	0.58
1:D:852:LEU:CG	2:A:1241:PHE:CE1	2.87	0.58
1:D:870:HIS:HE1	2:A:1580:ARG:HB2	1.69	0.58
2:B:590:LEU:O	2:B:594:ILE:N	2.34	0.58
2:B:824:PRO:O	2:B:828:VAL:HG23	2.03	0.58
2:B:1656:ASP:N	2:B:1656:ASP:OD1	2.36	0.58
2:B:1704:SER:OG	2:B:1706:ARG:NH1	2.37	0.58
3:E:137:ILE:HD12	3:E:159:VAL:HG22	1.85	0.58
3:E:205:LEU:HA	3:E:209:ARG:HD2	1.85	0.58
2:A:1636:ASP:O	2:A:1640:HIS:N	2.37	0.58
3:E:196:SER:O	3:E:200:LYS:NZ	2.36	0.58
3:E:246:PHE:O	3:E:250:VAL:CG1	2.51	0.58
2:A:245:ARG:HH21	2:A:274:TYR:HA	1.69	0.58
2:A:523:HIS:O	2:A:527:LEU:HB2	2.04	0.58
2:A:528:LEU:HA	2:A:531:ILE:HD12	1.85	0.58
2:B:1075:THR:HA	2:B:1078:ARG:HE	1.68	0.58
2:A:525:ASN:HA	2:A:528:LEU:HD12	1.86	0.58
2:A:1574:PHE:CD1	2:A:1709:PRO:HB3	2.39	0.58
2:B:1202:PRO:HA	2:B:1743:ARG:HD2	1.84	0.58
1:C:884:TYR:O	1:C:888:LEU:HD23	2.03	0.58
2:B:1651:ASN:HB2	2:B:1672:ILE:HG23	1.86	0.58
3:E:113:GLN:HB3	3:E:119:LEU:HA	1.86	0.58
2:A:415:ALA:O	2:A:418:ARG:NH2	2.37	0.58
2:A:1653:SER:OG	2:A:1654:GLY:N	2.36	0.58
2:B:416:ASP:OD2	2:B:451:ARG:NH2	2.37	0.58
2:A:574:LYS:HZ1	2:A:582:HIS:CG	2.20	0.57
2:B:477:ARG:NH1	2:B:478:GLN:HB2	2.18	0.57
2:A:1028:ASP:OD1	2:A:1201:ARG:NH2	2.37	0.57
2:A:1524:SER:OG	2:A:1527:PHE:HB2	2.04	0.57
2:B:1073:VAL:O	2:B:1078:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:286:MET:SD	2:A:286:MET:N	2.77	0.57
2:B:418:ARG:NH1	2:B:421:SER:OG	2.35	0.57
2:A:1044:ARG:NH1	2:A:1049:GLU:OE1	2.38	0.57
1:D:939:GLY:O	1:D:942:GLN:NE2	2.36	0.57
2:A:737:LEU:O	2:A:740:MET:HB3	2.05	0.57
2:A:1566:HIS:O	2:A:1566:HIS:ND1	2.38	0.57
2:B:320:LEU:HD13	2:B:365:ILE:HB	1.87	0.57
2:B:1059:THR:CG2	2:B:1520:LEU:HD11	2.34	0.57
2:B:1562:LEU:HD12	2:B:1562:LEU:H	1.70	0.57
2:B:1720:ASN:OD1	2:B:1724:GLN:NE2	2.35	0.57
3:E:188:LEU:CD2	3:E:243:LEU:O	2.52	0.57
2:A:511:LEU:CD2	2:A:526:SER:HB2	2.34	0.57
2:A:539:LEU:O	2:A:541:PRO:HD3	2.04	0.57
2:A:367:ARG:HE	2:A:370:GLN:HE21	1.51	0.57
3:E:67:LEU:HD23	3:E:81:ARG:HH12	1.69	0.57
2:A:481:GLU:O	2:A:485:ILE:N	2.34	0.57
2:B:327:MET:HG3	2:B:372:LEU:HD22	1.86	0.57
2:B:529:ASP:O	2:B:533:LYS:HG2	2.04	0.57
3:E:132:GLU:HB3	3:E:209:ARG:HH12	1.70	0.57
1:D:853:LEU:HD11	2:B:1077:THR:CG2	2.35	0.57
2:A:503:GLN:H	2:A:503:GLN:CD	2.08	0.57
2:B:293:ARG:O	2:B:297:PHE:N	2.33	0.57
2:A:714:PRO:HA	2:A:717:LEU:HD12	1.87	0.57
2:B:124:PHE:O	2:B:128:LYS:N	2.37	0.57
1:C:841:VAL:HG12	1:C:841:VAL:O	2.05	0.57
1:C:959:GLU:OE2	3:E:90:HIS:NE2	2.38	0.57
3:E:42:LEU:HD13	3:E:59:VAL:HG23	1.87	0.57
3:E:60:TRP:HA	3:E:63:LEU:HB2	1.87	0.57
3:E:159:VAL:O	3:E:163:ASN:ND2	2.38	0.57
2:B:500:LYS:O	2:B:503:GLN:NE2	2.38	0.56
2:B:1736:TYR:HD1	2:B:1738:SER:H	1.52	0.56
2:A:180:LEU:HD22	2:A:190:TYR:HE2	1.69	0.56
2:A:185:LYS:HZ3	2:A:188:SER:HG	1.47	0.56
2:A:359:ASP:HB2	2:A:362:LEU:HD12	1.86	0.56
2:B:1534:LEU:HD23	2:B:1534:LEU:O	2.04	0.56
2:A:148:ASP:O	2:A:151:ARG:NH1	2.38	0.56
2:A:587:TYR:HE2	2:A:685:PRO:HD2	1.69	0.56
2:B:167:TRP:O	2:B:171:GLY:N	2.39	0.56
2:B:607:ALA:HA	2:B:610:ILE:HD12	1.88	0.56
2:B:1572:THR:HA	2:B:1575:LEU:HD12	1.87	0.56
3:E:142:GLU:OE1	3:E:142:GLU:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:ALA:O	1:D:886:LYS:HG2	2.05	0.56
1:D:899:THR:CG2	1:C:898:GLN:HE21	2.19	0.56
2:A:801:ALA:O	2:A:805:VAL:HG23	2.06	0.56
2:A:1069:VAL:HG23	2:A:1497:PRO:HB2	1.88	0.56
2:B:430:ARG:HH22	2:B:448:LEU:HD22	1.70	0.56
2:A:1209:LEU:HB2	2:A:1240:ARG:NH1	2.19	0.56
2:B:550:VAL:HA	2:B:553:TYR:HB3	1.86	0.56
3:E:88:VAL:HG11	3:E:111:MET:HE3	1.88	0.56
2:A:713:LEU:O	2:A:716:SER:OG	2.21	0.56
2:A:824:PRO:O	2:A:828:VAL:HG23	2.05	0.56
3:E:103:PRO:HG2	3:E:106:GLU:CD	2.26	0.56
2:B:882:ASN:OD1	2:B:884:TYR:N	2.34	0.56
2:B:1059:THR:HG23	2:B:1520:LEU:CD2	2.36	0.56
3:E:181:LEU:HB2	3:E:240:VAL:HG22	1.87	0.56
2:A:917:ARG:HA	2:A:920:VAL:HG12	1.87	0.56
2:A:1055:GLY:HA3	2:A:1071:THR:O	2.06	0.56
2:B:1198:LEU:HD13	2:B:1207:SER:HB3	1.88	0.56
2:B:1534:LEU:CG	2:B:1746:HIS:CG	2.86	0.56
1:C:964:ASP:O	1:C:968:ARG:NH2	2.39	0.56
2:A:1571:TYR:CE1	2:A:1650:TYR:HB2	2.41	0.56
2:B:1562:LEU:CD1	2:B:1662:ILE:CD1	2.72	0.56
3:E:177:PHE:HA	3:E:236:VAL:HG13	1.87	0.56
1:D:857:GLU:OE2	1:C:859:ASN:ND2	2.38	0.55
2:A:378:PRO:HA	2:A:381:ARG:NE	2.22	0.55
2:A:545:LEU:HA	2:A:548:ARG:HB2	1.88	0.55
2:A:854:PRO:HA	2:A:857:TYR:CZ	2.41	0.55
2:A:1736:TYR:HB3	2:A:1742:ALA:HB2	1.88	0.55
2:A:916:LEU:HD22	2:A:1023:THR:HG23	1.87	0.55
2:B:367:ARG:HH21	2:B:407:TYR:HB3	1.71	0.55
2:B:1050:PHE:CE1	2:B:1076:GLY:HA3	2.41	0.55
2:B:1609:CYS:SG	2:B:1610:TRP:N	2.79	0.55
1:D:854:VAL:HG23	2:B:1235:LEU:HD11	1.74	0.55
1:D:953:ARG:HD2	3:E:117:GLY:HA2	1.88	0.55
2:A:574:LYS:HZ2	2:A:582:HIS:CB	2.20	0.55
2:A:1515:ASN:ND2	2:B:1512:ASP:OD1	2.39	0.55
2:A:1649:VAL:HG23	2:A:1672:ILE:HG12	1.87	0.55
2:B:523:HIS:HB2	2:B:582:HIS:CE1	2.41	0.55
2:B:1236:MET:HA	2:B:1236:MET:HE3	1.86	0.55
2:B:1526:SER:OG	2:B:1753:ARG:NH2	2.40	0.55
3:E:222:ARG:NH2	3:E:272:ASP:O	2.40	0.55
1:D:936:GLN:HB2	3:E:70:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:239:PHE:CG	2:A:240:ILE:N	2.74	0.55
2:A:492:GLN:HA	2:A:495:HIS:HD2	1.70	0.55
2:B:1582:ILE:HG13	2:B:1609:CYS:HB3	1.88	0.55
1:D:899:THR:HG22	1:C:898:GLN:HE21	1.70	0.55
1:D:936:GLN:OE1	3:E:70:HIS:ND1	2.39	0.55
2:A:738:CYS:O	2:A:742:SER:N	2.35	0.55
2:B:418:ARG:NH1	2:B:421:SER:HG	2.04	0.55
2:B:1077:THR:O	2:B:1080:LEU:HB2	2.05	0.55
2:B:1696:ASP:OD1	2:B:1697:THR:N	2.39	0.55
3:E:129:PRO:O	3:E:133:VAL:HG23	2.07	0.55
1:D:905:SER:HB2	1:C:905:SER:HB2	1.89	0.55
2:A:264:LEU:O	2:A:268:LEU:HG	2.07	0.55
2:B:910:PRO:HD3	2:B:934:ARG:HD2	1.88	0.55
2:B:1229:GLN:O	2:B:1232:SER:OG	2.21	0.55
2:B:1625:MET:HB3	2:B:1637:LYS:CG	2.28	0.55
1:D:927:LYS:HZ1	2:A:479:PHE:HB3	1.71	0.55
2:A:1516:LYS:HE2	2:B:936:ARG:HH11	1.71	0.55
2:B:482:GLU:HG2	2:B:483:GLU:H	1.72	0.55
2:B:1595:GLY:HA3	2:B:1620:HIS:NE2	2.22	0.55
2:A:370:GLN:HA	2:A:373:GLN:HB2	1.89	0.55
2:A:523:HIS:CE1	2:A:527:LEU:HD22	2.42	0.55
2:B:493:LEU:HA	2:B:495:HIS:CE1	2.42	0.55
2:B:1060:TRP:NE1	2:B:1519:LEU:HB2	2.22	0.55
3:E:191:HIS:CD2	3:E:251:MET:HE1	2.42	0.55
2:A:443:GLN:OE1	2:A:443:GLN:N	2.39	0.55
2:A:809:SER:O	2:A:813:VAL:HG23	2.07	0.55
2:A:1032:ARG:NH2	2:A:1039:THR:O	2.39	0.55
2:B:1575:LEU:HA	2:B:1578:LEU:HD12	1.87	0.55
1:D:951:GLN:HG3	1:C:951:GLN:HG3	1.88	0.54
2:A:553:TYR:O	2:A:557:LEU:HG	2.07	0.54
2:A:1581:LEU:CB	2:A:1608:TYR:HA	2.35	0.54
2:B:367:ARG:NH2	2:B:407:TYR:HB3	2.22	0.54
2:B:1213:GLU:N	2:B:1213:GLU:OE1	2.41	0.54
4:F:83:UNK:O	4:F:87:UNK:N	2.39	0.54
1:D:879:MET:SD	2:A:1576:THR:HG23	2.48	0.54
2:A:275:ASN:O	2:A:279:LEU:HG	2.07	0.54
2:A:482:GLU:O	2:A:486:ASN:ND2	2.40	0.54
2:A:782:LYS:HZ3	2:A:786:ARG:HE	1.54	0.54
2:A:1505:TYR:OH	2:B:1504:LEU:O	2.25	0.54
2:A:449:MET:HG3	2:A:454:ARG:HH12	1.71	0.54
2:A:527:LEU:O	2:A:531:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:555:ALA:HA	2:A:558:GLU:HG3	1.89	0.54
2:B:708:LEU:O	2:B:712:ARG:HG2	2.07	0.54
3:E:103:PRO:HG2	3:E:106:GLU:CG	2.37	0.54
1:D:866:LEU:O	1:D:870:HIS:N	2.40	0.54
2:A:508:ALA:O	2:A:512:LEU:HG	2.06	0.54
2:A:1622:ALA:HB3	2:A:1624:LEU:HG	1.88	0.54
2:B:340:LEU:O	2:B:343:THR:OG1	2.23	0.54
2:B:1615:MET:HE3	2:B:1717:LEU:HD13	1.89	0.54
1:D:842:GLN:OE1	1:D:843:GLN:NE2	2.37	0.54
2:B:1542:THR:O	2:B:1543:HIS:ND1	2.41	0.54
3:E:239:ALA:O	3:E:242:ILE:HG22	2.07	0.54
1:D:867:GLN:O	1:D:870:HIS:HB3	2.08	0.54
2:B:424:LEU:HA	2:B:427:ILE:HD13	1.90	0.54
2:B:841:VAL:HG22	2:B:885:ILE:HD11	1.90	0.54
2:B:899:ARG:HA	2:B:899:ARG:HH21	1.72	0.54
2:B:1060:TRP:CD1	2:B:1519:LEU:CB	2.90	0.54
3:E:160:ASN:O	3:E:164:THR:HG22	2.08	0.54
2:A:460:ALA:HA	2:A:463:ILE:HD12	1.89	0.54
2:A:805:VAL:HA	2:A:808:LEU:HD12	1.90	0.54
2:B:418:ARG:HH12	2:B:421:SER:HG	1.52	0.54
2:B:466:LEU:HG	2:B:510:GLN:HE22	1.73	0.54
2:B:693:LEU:HA	2:B:696:CYS:SG	2.48	0.54
2:A:500:LYS:HB3	2:A:503:GLN:NE2	2.22	0.54
2:A:700:GLU:OE2	2:A:701:SER:N	2.39	0.54
2:A:205:LEU:O	2:A:209:THR:HG23	2.07	0.54
2:A:539:LEU:HB3	2:A:602:TYR:CD1	2.42	0.54
2:A:622:ARG:O	2:A:631:LEU:N	2.40	0.54
2:B:913:THR:HA	2:B:916:LEU:HB2	1.89	0.54
1:C:907:LYS:HA	1:C:910:LEU:HD12	1.90	0.54
3:E:85:TYR:CE2	3:E:108:TYR:HE1	2.25	0.54
1:D:953:ARG:NH1	3:E:117:GLY:CA	2.71	0.54
3:E:206:TRP:HA	3:E:211:PHE:H	1.72	0.54
1:D:868:ASN:HD21	1:C:869:LYS:C	2.12	0.53
1:D:926:GLN:HE21	1:C:930:LEU:HD12	1.72	0.53
2:A:485:ILE:CA	2:A:488:VAL:HG12	2.39	0.53
2:B:1019:HIS:HA	2:B:1022:LEU:HD12	1.90	0.53
3:E:104:GLN:HE21	3:E:104:GLN:CA	2.13	0.53
1:D:902:LEU:HD11	1:C:901:ARG:HG2	1.90	0.53
2:A:1539:SER:O	2:A:1740:TRP:CD1	2.61	0.53
2:B:913:THR:HA	2:B:916:LEU:HD12	1.90	0.53
1:C:896:LEU:HA	1:C:899:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:715:GLU:OE1	2:B:715:GLU:N	2.32	0.53
1:D:920:ASP:O	1:D:924:LEU:HG	2.09	0.53
2:B:1534:LEU:CG	2:B:1746:HIS:CE1	2.90	0.53
1:D:844:GLN:HG3	1:C:845:MET:HG2	1.90	0.53
2:A:722:LEU:C	2:A:725:THR:HG22	2.28	0.53
2:B:1666:PHE:O	2:B:1668:PHE:N	2.41	0.53
1:C:886:LYS:O	1:C:886:LYS:HG3	2.08	0.53
3:E:191:HIS:CD2	3:E:251:MET:HE2	2.44	0.53
2:A:530:ILE:O	2:A:534:VAL:HG23	2.09	0.53
2:A:801:ALA:HA	2:A:804:CYS:SG	2.48	0.53
2:B:1236:MET:CE	2:B:1236:MET:CA	2.86	0.53
1:C:884:TYR:O	1:C:888:LEU:CD2	2.57	0.53
3:E:37:LEU:HB2	3:E:69:PRO:HA	1.91	0.53
2:B:813:VAL:HG21	2:B:1707:ASN:OD1	2.08	0.53
2:B:914:LYS:HA	2:B:917:ARG:HG2	1.89	0.53
2:A:151:ARG:HB2	2:A:156:LEU:HB3	1.91	0.53
2:A:1594:LEU:HD21	2:A:1597:LEU:HD12	1.90	0.53
2:A:1714:GLN:OE1	2:A:1718:HIS:NE2	2.41	0.53
2:B:392:GLU:HA	2:B:395:CYS:SG	2.49	0.53
2:B:1056:ARG:NH1	2:B:1495:ILE:O	2.41	0.53
1:C:943:ALA:O	1:C:947:ARG:HG2	2.09	0.53
3:E:46:SER:O	3:E:226:LYS:NZ	2.27	0.53
2:A:1058:LYS:HG3	2:A:1497:PRO:HG2	1.90	0.53
2:A:1240:ARG:HH12	2:B:1211:SER:H	1.54	0.53
3:E:131:ASP:O	3:E:135:LEU:CG	2.40	0.53
2:A:1055:GLY:HA2	2:A:1073:VAL:HG13	1.90	0.53
1:C:866:LEU:O	1:C:870:HIS:CB	2.57	0.53
2:A:496:ILE:HG21	2:A:532:GLU:HB3	1.92	0.52
2:A:515:LEU:HD12	2:A:523:HIS:HA	1.91	0.52
2:A:1578:LEU:HG	2:A:1619:PHE:HE2	1.74	0.52
2:B:1180:LYS:O	2:B:1184:ALA:N	2.38	0.52
2:A:528:LEU:HD23	2:A:531:ILE:HD12	1.91	0.52
2:B:339:VAL:O	2:B:343:THR:HG23	2.10	0.52
2:B:505:ARG:HB3	2:B:559:ASP:OD1	2.08	0.52
1:D:852:LEU:HG	2:A:1241:PHE:CD1	2.44	0.52
2:A:336:TYR:O	2:A:340:LEU:HG	2.08	0.52
2:A:400:PHE:HA	2:A:403:SER:HB3	1.91	0.52
1:D:852:LEU:HD12	2:A:1241:PHE:CE1	2.34	0.52
2:A:1570:ARG:HG3	2:A:1650:TYR:OH	2.09	0.52
2:B:1545:ILE:HG22	2:B:1618:VAL:O	2.10	0.52
3:E:269:ASP:OD1	3:E:270:SER:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:153:ILE:HG22	2:A:154:THR:H	1.75	0.52
2:A:722:LEU:HA	2:A:725:THR:HG22	1.92	0.52
2:A:763:HIS:O	2:A:767:VAL:HG23	2.10	0.52
2:A:1736:TYR:CG	2:A:1737:PRO:HD2	2.44	0.52
2:B:809:SER:O	2:B:812:SER:OG	2.21	0.52
2:B:843:LEU:O	2:B:847:LEU:HG	2.08	0.52
2:B:1060:TRP:CD1	2:B:1519:LEU:CA	2.92	0.52
2:B:1228:LEU:HA	2:B:1231:LEU:HB2	1.91	0.52
1:C:913:GLU:HA	1:C:916:LEU:HD12	1.91	0.52
1:D:875:LYS:N	1:D:875:LYS:CD	2.73	0.52
1:D:890:LYS:O	1:D:894:HIS:HB2	2.09	0.52
1:D:968:ARG:O	1:D:971:LYS:NZ	2.35	0.52
1:D:968:ARG:HD2	1:D:971:LYS:HZ1	1.74	0.52
2:A:218:SER:HG	2:A:222:LEU:N	2.06	0.52
2:A:802:SER:H	2:A:839:MET:HE1	1.74	0.52
2:A:816:PRO:O	2:A:820:ILE:HG13	2.09	0.52
2:A:1499:PHE:O	2:A:1503:GLN:HG2	2.09	0.52
1:C:934:LYS:NZ	1:C:934:LYS:CB	2.73	0.52
1:D:926:GLN:HE22	1:C:927:LYS:N	2.08	0.52
2:A:1534:LEU:O	2:A:1537:ILE:HG12	2.10	0.52
2:B:565:LEU:O	2:B:569:VAL:HG23	2.10	0.52
2:B:597:HIS:CD2	2:B:611:ARG:HE	2.21	0.52
2:B:760:THR:HA	2:B:799:ARG:HH21	1.74	0.52
3:E:266:ILE:O	3:E:268:GLN:NE2	2.41	0.52
2:A:730:VAL:HG23	2:A:733:LEU:HD21	1.91	0.52
2:A:1506:HIS:O	2:A:1506:HIS:ND1	2.41	0.52
2:B:882:ASN:OD1	2:B:883:GLN:N	2.42	0.52
3:E:119:LEU:HD12	3:E:120:PRO:HD2	1.91	0.52
2:A:309:LEU:HD12	2:A:311:SER:H	1.75	0.52
2:A:1679:GLU:O	2:A:1705:ASP:HB2	2.08	0.52
3:E:211:PHE:HB2	3:E:220:LEU:HD21	1.91	0.52
1:D:862:TYR:CE2	1:D:866:LEU:HD11	2.45	0.52
2:A:274:TYR:C	2:A:278:HIS:HD1	2.13	0.52
2:B:1657:PHE:HB3	2:B:1672:ILE:CD1	2.40	0.52
1:C:842:GLN:HE21	1:C:842:GLN:CA	2.16	0.52
2:A:419:PRO:HB3	2:A:458:ARG:NH1	2.25	0.51
2:A:710:LEU:HD12	2:A:769:VAL:HG21	1.90	0.51
2:A:822:ALA:O	2:A:826:LEU:HG	2.10	0.51
2:B:527:LEU:HD22	2:B:586:VAL:HG11	1.90	0.51
3:E:74:HIS:HA	3:E:77:VAL:HG21	1.92	0.51
1:D:875:LYS:HD2	1:D:875:LYS:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:TYR:CE2	2:B:699:GLN:HB3	2.46	0.51
2:B:1658:LYS:O	2:B:1661:THR:HG23	2.10	0.51
3:E:72:GLU:N	3:E:72:GLU:OE1	2.43	0.51
2:A:568:LEU:HD11	2:A:617:PHE:CG	2.44	0.51
2:A:717:LEU:O	2:A:776:TYR:OH	2.25	0.51
2:A:1521:PRO:HB2	2:A:1524:SER:HB3	1.93	0.51
2:B:505:ARG:NE	2:B:558:GLU:OE2	2.43	0.51
3:E:188:LEU:HD22	3:E:247:LYS:HG2	1.93	0.51
2:A:336:TYR:O	2:A:339:VAL:HG13	2.10	0.51
2:A:367:ARG:HH22	2:A:409:GLU:N	2.09	0.51
2:B:343:THR:HG22	2:B:392:GLU:OE1	2.11	0.51
2:B:616:ASP:OD1	2:B:712:ARG:NH2	2.43	0.51
2:B:688:LEU:O	2:B:692:VAL:HG23	2.11	0.51
2:B:1218:PRO:HG2	2:B:1219:PHE:CE1	2.46	0.51
3:E:191:HIS:CG	3:E:251:MET:CE	2.91	0.51
3:E:246:PHE:HE2	3:E:274:ILE:HD11	1.74	0.51
2:A:1057:THR:OG1	2:A:1069:VAL:O	2.22	0.51
2:A:1057:THR:HB	2:A:1070:THR:HG23	1.92	0.51
2:A:1501:PHE:HZ	2:A:1517:PRO:HB3	1.75	0.51
2:A:1581:LEU:N	2:A:1581:LEU:CD2	2.73	0.51
2:B:760:THR:HA	2:B:799:ARG:NH2	2.25	0.51
1:D:897:GLN:HB3	1:D:901:ARG:HH21	1.76	0.51
2:A:767:VAL:O	2:A:771:THR:HG23	2.10	0.51
2:A:1186:TYR:CD2	2:A:1231:LEU:HD23	2.45	0.51
2:A:1539:SER:O	2:A:1740:TRP:NE1	2.44	0.51
2:B:733:LEU:O	2:B:737:LEU:N	2.29	0.51
2:B:801:ALA:HB1	2:B:804:CYS:HB3	1.93	0.51
2:B:1040:ALA:HB1	2:B:1204:GLY:HA3	1.92	0.51
2:A:418:ARG:H	2:A:418:ARG:HE	1.59	0.51
2:A:1206:THR:OG1	2:B:1503:GLN:NE2	2.44	0.51
2:B:317:THR:HG23	2:B:320:LEU:HD12	1.91	0.51
2:B:495:HIS:CD2	2:B:496:ILE:H	2.28	0.51
1:C:866:LEU:O	1:C:870:HIS:HB3	2.11	0.51
2:A:900:CYS:O	2:A:905:ARG:NH2	2.42	0.51
2:B:876:THR:OG1	2:B:919:ASN:ND2	2.44	0.51
3:E:222:ARG:NH2	3:E:275:VAL:HB	2.26	0.51
2:B:597:HIS:HA	2:B:602:TYR:CZ	2.46	0.51
2:B:1555:SER:HB2	2:B:1655:GLU:CD	2.31	0.51
1:C:851:GLN:HA	1:C:854:VAL:HG22	1.93	0.51
1:D:936:GLN:O	1:D:940:GLN:HG2	2.10	0.51
3:E:92:LEU:HD22	3:E:110:ARG:CB	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:959:GLU:HG2	1:C:958:PHE:CZ	2.46	0.50
2:A:408:PHE:O	2:A:411:VAL:HG12	2.11	0.50
2:A:526:SER:O	2:A:530:ILE:HG13	2.12	0.50
2:B:1610:TRP:CZ3	2:B:1615:MET:CE	2.94	0.50
2:B:1544:LYS:HA	2:B:1618:VAL:HG23	1.93	0.50
3:E:81:ARG:HA	3:E:153:TRP:HZ2	1.76	0.50
1:D:926:GLN:HG2	1:C:930:LEU:HD11	1.92	0.50
2:A:200:GLN:OE1	2:A:200:GLN:N	2.44	0.50
2:A:522:HIS:O	2:A:526:SER:OG	2.24	0.50
2:A:574:LYS:HZ2	2:A:582:HIS:HB2	1.76	0.50
2:B:1077:THR:HA	2:B:1080:LEU:HD12	1.91	0.50
2:B:1236:MET:HE3	2:B:1236:MET:CA	2.41	0.50
2:B:1546:ALA:O	2:B:1648:ILE:N	2.31	0.50
1:C:896:LEU:CA	1:C:899:THR:HG23	2.41	0.50
3:E:204:ASP:OD1	3:E:205:LEU:N	2.40	0.50
3:E:206:TRP:HB3	3:E:211:PHE:CE1	2.46	0.50
2:A:817:ASP:OD1	2:A:818:ILE:N	2.43	0.50
2:A:1047:VAL:HG21	2:A:1244:HIS:CE1	2.46	0.50
2:A:1078:ARG:HD3	1:C:844:GLN:OE1	2.10	0.50
2:A:1711:VAL:O	2:A:1715:MET:HG3	2.12	0.50
2:B:429:TYR:O	2:B:432:GLN:NE2	2.44	0.50
2:B:906:LYS:HD3	2:B:934:ARG:HH12	1.75	0.50
3:E:237:PHE:CE1	3:E:285:HIS:HB2	2.47	0.50
2:A:223:ASP:OD1	2:A:224:ALA:N	2.42	0.50
2:A:827:VAL:HA	2:A:830:LEU:HB2	1.92	0.50
2:B:537:ARG:HH11	2:B:538:SER:H	1.60	0.50
2:B:588:GLU:HA	2:B:591:VAL:HG22	1.94	0.50
2:B:852:ARG:NH1	2:B:1714:GLN:HE22	2.07	0.50
2:A:1504:LEU:HD21	2:B:1208:TRP:CZ3	2.47	0.50
2:A:1569:TYR:CE2	1:C:884:TYR:HD2	2.30	0.50
2:B:710:LEU:O	2:B:714:PRO:HD3	2.12	0.50
3:E:70:HIS:O	3:E:73:SER:OG	2.27	0.50
3:E:159:VAL:HA	3:E:162:LEU:HD12	1.92	0.50
2:A:1534:LEU:HB2	2:A:1746:HIS:CE1	2.47	0.50
2:B:877:ASN:OD1	2:B:880:LYS:N	2.28	0.50
2:B:917:ARG:HA	2:B:920:VAL:HG12	1.92	0.50
2:B:1539:SER:O	2:B:1614:ILE:HD12	2.11	0.50
1:C:896:LEU:HA	1:C:899:THR:CG2	2.42	0.50
1:C:959:GLU:OE2	3:E:90:HIS:CE1	2.64	0.50
2:A:1585:LYS:HG3	2:A:1587:CYS:SG	2.52	0.50
2:B:873:LEU:HD13	2:B:915:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:127:LEU:HD23	3:E:135:LEU:HD11	1.91	0.50
1:D:840:SER:HA	1:D:843:GLN:HG2	1.94	0.50
1:D:902:LEU:O	1:D:906:GLN:HG3	2.11	0.50
2:A:223:ASP:HA	2:A:226:VAL:HG22	1.94	0.50
2:A:363:ASN:CG	2:A:405:GLU:HG2	2.32	0.50
2:A:734:CYS:O	2:A:737:LEU:HB2	2.12	0.50
2:B:609:SER:HA	2:B:612:LEU:HG	1.94	0.50
2:B:1594:LEU:CD1	2:B:1640:HIS:CD2	2.95	0.50
2:A:1574:PHE:CE1	2:A:1708:LEU:HG	2.47	0.49
2:B:731:ASP:OD1	2:B:732:GLN:N	2.45	0.49
2:B:1561:ILE:HG22	2:B:1562:LEU:HD12	1.94	0.49
2:A:819:ILE:O	2:A:823:LEU:HG	2.12	0.49
2:B:520:HIS:O	2:B:522:HIS:ND1	2.24	0.49
2:B:830:LEU:O	2:B:833:ILE:HG12	2.11	0.49
2:B:1030:MET:O	2:B:1034:VAL:N	2.43	0.49
2:B:1606:PHE:CZ	1:C:819:ASN:CB	2.93	0.49
1:D:852:LEU:CD1	2:A:1241:PHE:CE1	2.94	0.49
2:A:759:ARG:O	2:A:763:HIS:HD2	1.96	0.49
1:C:865:GLN:OE1	1:C:865:GLN:HA	2.11	0.49
1:D:841:VAL:O	1:D:844:GLN:HB3	2.11	0.49
2:A:227:CYS:O	2:A:231:LEU:HG	2.13	0.49
2:A:264:LEU:HB3	2:A:298:PHE:CE1	2.48	0.49
2:A:917:ARG:HE	2:A:928:PRO:HB2	1.77	0.49
2:A:1656:ASP:OD1	2:A:1657:PHE:N	2.45	0.49
2:B:485:ILE:HG22	2:B:525:ASN:HD22	1.78	0.49
2:A:503:GLN:OE1	2:A:503:GLN:N	2.37	0.49
2:B:435:HIS:CD2	2:B:468:VAL:HG13	2.48	0.49
2:B:713:LEU:O	2:B:717:LEU:HG	2.13	0.49
2:B:839:MET:O	2:B:843:LEU:HG	2.12	0.49
2:B:1562:LEU:N	2:B:1562:LEU:CD1	2.74	0.49
1:C:888:LEU:N	1:C:888:LEU:CD2	2.73	0.49
3:E:224:TRP:HA	3:E:227:VAL:HB	1.95	0.49
1:D:853:LEU:HD11	2:B:1077:THR:HG22	1.93	0.49
2:A:151:ARG:HD3	2:A:151:ARG:H	1.78	0.49
2:B:1534:LEU:HD11	2:B:1747:ILE:HG13	1.93	0.49
2:B:1614:ILE:HG13	2:B:1740:TRP:CZ2	2.48	0.49
2:A:643:TYR:HE1	1:C:907:LYS:HD2	1.77	0.49
2:A:905:ARG:HG2	2:A:1034:VAL:HG23	1.94	0.49
2:A:1574:PHE:CE1	2:A:1709:PRO:N	2.76	0.49
2:B:851:ALA:HB2	2:B:896:TRP:CE2	2.47	0.49
2:B:1605:GLN:O	2:B:1605:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:109:LEU:HD13	3:E:134:PHE:CD1	2.47	0.49
1:D:877:VAL:HG22	2:A:1606:PHE:HZ	1.78	0.49
2:B:819:ILE:O	2:B:823:LEU:HG	2.13	0.49
2:B:1534:LEU:CB	2:B:1746:HIS:CD2	2.95	0.49
3:E:62:VAL:HG22	3:E:67:LEU:HB2	1.93	0.49
2:A:297:PHE:HB2	2:A:337:GLU:OE1	2.12	0.49
2:A:731:ASP:OD1	2:A:732:GLN:N	2.46	0.49
2:B:363:ASN:O	2:B:366:GLU:HG3	2.13	0.49
2:B:500:LYS:HB3	2:B:502:HIS:NE2	2.28	0.49
1:C:945:GLU:O	1:C:949:GLU:HG2	2.13	0.49
3:E:26:LYS:O	3:E:29:GLU:HG3	2.12	0.49
4:F:18:UNK:O	4:F:22:UNK:N	2.46	0.49
1:D:947:ARG:HG2	1:C:948:TYR:CE1	2.48	0.48
2:A:1560:ALA:O	2:A:1564:ASN:HB2	2.13	0.48
2:A:343:THR:HA	2:A:346:ILE:CD1	2.43	0.48
2:A:482:GLU:OE2	2:A:486:ASN:ND2	2.39	0.48
2:A:882:ASN:OD1	2:A:883:GLN:N	2.44	0.48
2:A:1585:LYS:CE	2:A:1587:CYS:SG	2.99	0.48
2:A:1657:PHE:HB3	2:A:1672:ILE:CD1	2.43	0.48
2:A:367:ARG:HE	2:A:370:GLN:NE2	2.12	0.48
2:B:1227:PRO:HB2	2:B:1230:GLU:OE2	2.13	0.48
1:D:862:TYR:HE2	1:D:866:LEU:HD11	1.79	0.48
2:A:1657:PHE:HB3	2:A:1672:ILE:HD13	1.95	0.48
2:B:449:MET:O	2:B:453:PHE:HB2	2.13	0.48
2:B:477:ARG:HH11	2:B:478:GLN:HB2	1.78	0.48
1:C:926:GLN:NE2	1:C:926:GLN:HA	2.29	0.48
3:E:188:LEU:HG	3:E:243:LEU:HD23	1.94	0.48
2:A:633:ASN:HD22	2:A:637:VAL:C	2.15	0.48
2:A:1502:LEU:O	2:A:1506:HIS:HB2	2.14	0.48
2:B:758:SER:O	2:B:762:LEU:N	2.38	0.48
2:B:841:VAL:O	2:B:845:GLU:HG3	2.14	0.48
3:E:35:ASP:HA	3:E:71:HIS:CD2	2.48	0.48
2:A:625:SER:N	2:A:629:LEU:HD22	2.21	0.48
2:A:767:VAL:HG21	2:A:800:CYS:HB2	1.94	0.48
2:A:1081:LEU:CD1	1:C:847:PHE:CZ	2.96	0.48
2:A:1569:TYR:CE2	1:C:884:TYR:CD2	3.02	0.48
2:A:1662:ILE:HG21	2:A:1670:HIS:CE1	2.48	0.48
2:B:281:GLU:H	2:B:303:LEU:HA	1.78	0.48
2:B:450:GLU:HG2	2:B:454:ARG:HH12	1.78	0.48
2:B:767:VAL:O	2:B:771:THR:OG1	2.26	0.48
2:B:1200:ARG:HG2	2:B:1205:ASN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1614:ILE:HD11	2:B:1740:TRP:HZ2	1.79	0.48
1:D:878:GLU:OE2	1:D:878:GLU:HA	2.13	0.48
2:B:558:GLU:O	2:B:561:LYS:HG2	2.14	0.48
2:B:896:TRP:O	2:B:900:CYS:N	2.45	0.48
3:E:191:HIS:CD2	3:E:195:CYS:HG	2.30	0.48
2:A:179:VAL:O	2:A:183:LEU:HG	2.13	0.48
2:A:568:LEU:HD11	2:A:617:PHE:CD1	2.49	0.48
2:B:502:HIS:O	2:B:506:LYS:HG2	2.13	0.48
1:D:930:LEU:CB	1:C:930:LEU:HD21	2.39	0.48
2:A:1524:SER:HG	2:A:1527:PHE:HB2	1.77	0.48
2:A:1582:ILE:HG23	2:A:1582:ILE:O	2.14	0.48
2:A:1673:VAL:HG23	2:A:1683:VAL:HG12	1.96	0.48
2:B:1594:LEU:HD12	2:B:1640:HIS:CD2	2.49	0.48
3:E:88:VAL:CG1	3:E:111:MET:CE	2.89	0.48
3:E:92:LEU:CD2	3:E:110:ARG:CB	2.81	0.48
2:A:239:PHE:O	2:A:241:VAL:HG13	2.14	0.48
2:A:710:LEU:HA	2:A:713:LEU:HD12	1.96	0.48
3:E:39:THR:O	3:E:43:CYS:N	2.45	0.48
3:E:57:ALA:O	3:E:61:LYS:HG3	2.13	0.48
3:E:83:GLU:O	3:E:87:ASP:CG	2.52	0.48
3:E:204:ASP:O	3:E:209:ARG:N	2.36	0.48
2:A:574:LYS:NZ	2:A:582:HIS:CB	2.77	0.47
2:A:1750:LEU:O	2:A:1754:ILE:HG13	2.13	0.47
2:B:361:LEU:O	2:B:365:ILE:HG12	2.14	0.47
2:B:550:VAL:O	2:B:554:SER:CB	2.61	0.47
2:B:1061:LEU:HD13	2:B:1066:LEU:HA	1.95	0.47
2:B:1583:GLU:HG3	2:B:1585:LYS:HG2	1.96	0.47
2:B:1707:ASN:O	2:B:1711:VAL:HG12	2.14	0.47
2:A:1552:GLU:HA	2:A:1653:SER:HB2	1.96	0.47
1:C:874:THR:O	1:C:875:LYS:HG2	2.14	0.47
2:A:221:VAL:O	2:A:225:VAL:HG23	2.14	0.47
2:A:279:LEU:HD13	2:A:322:SER:HB2	1.96	0.47
2:A:917:ARG:CZ	2:A:930:LYS:HG3	2.45	0.47
2:B:446:GLN:O	2:B:449:MET:HG2	2.14	0.47
3:E:281:LEU:HD13	3:E:284:LYS:HE3	1.95	0.47
1:D:855:LEU:HD13	2:A:1241:PHE:HB3	1.96	0.47
1:D:902:LEU:CD1	1:C:901:ARG:HG2	2.44	0.47
1:D:909:ILE:HD13	1:C:908:ARG:CZ	2.44	0.47
2:A:303:LEU:HG	2:A:345:LEU:HD13	1.96	0.47
2:A:417:GLN:OE1	2:A:426:LEU:HD11	2.14	0.47
2:A:597:HIS:CE1	2:A:607:ALA:HB1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:622:ARG:HD2	2:A:719:TYR:CZ	2.49	0.47
2:B:444:ASN:O	2:B:448:LEU:HG	2.15	0.47
2:A:170:VAL:HB	2:A:197:ARG:NH2	2.28	0.47
2:A:334:VAL:HG23	2:A:335:SER:H	1.80	0.47
2:A:760:THR:O	2:A:764:LEU:HG	2.15	0.47
2:A:1581:LEU:HB2	2:A:1606:PHE:O	2.14	0.47
2:B:363:ASN:O	2:B:367:ARG:HG3	2.14	0.47
2:B:598:TYR:CZ	2:B:696:CYS:HA	2.49	0.47
2:B:897:PHE:HE2	2:B:1030:MET:HA	1.80	0.47
2:B:1186:TYR:OH	2:B:1230:GLU:OE2	2.32	0.47
3:E:223:VAL:O	3:E:227:VAL:HG23	2.14	0.47
1:D:952:LYS:HA	1:D:955:THR:HG23	1.96	0.47
2:A:231:LEU:O	2:A:234:GLU:HG3	2.14	0.47
2:A:315:SER:O	2:A:318:SER:OG	2.32	0.47
2:A:430:ARG:HD2	2:A:431:ALA:N	2.30	0.47
2:B:424:LEU:HD13	2:B:458:ARG:HG2	1.96	0.47
2:B:541:PRO:HD3	2:B:553:TYR:HH	1.79	0.47
2:B:722:LEU:O	2:B:725:THR:OG1	2.33	0.47
2:B:857:TYR:OH	2:B:899:ARG:CG	2.54	0.47
2:B:1534:LEU:HD12	2:B:1746:HIS:CE1	2.45	0.47
1:C:964:ASP:OD1	1:C:968:ARG:NH2	2.44	0.47
2:A:890:HIS:CE1	2:A:1022:LEU:HB3	2.50	0.47
2:A:1034:VAL:HG13	2:A:1035:PHE:HD2	1.79	0.47
2:A:1562:LEU:HD23	2:A:1641:LEU:HD21	1.97	0.47
2:B:574:LYS:HA	2:B:574:LYS:HD3	1.80	0.47
2:B:806:VAL:O	2:B:809:SER:OG	2.23	0.47
2:B:1058:LYS:HD3	2:B:1060:TRP:HZ2	1.78	0.47
2:B:1541:ASP:N	2:B:1614:ILE:O	2.48	0.47
2:B:1594:LEU:HD12	2:B:1640:HIS:HD2	1.79	0.47
2:B:1668:PHE:HA	2:B:1688:ARG:HH21	1.80	0.47
3:E:66:ILE:HD11	3:E:153:TRP:C	2.35	0.47
3:E:167:ARG:HA	3:E:170:LEU:HG	1.97	0.47
3:E:190:THR:HA	3:E:193:ARG:HH11	1.80	0.47
3:E:205:LEU:O	3:E:211:PHE:N	2.46	0.47
1:D:887:GLU:HB3	1:C:888:LEU:HD12	1.97	0.47
2:A:336:TYR:O	2:A:339:VAL:CG1	2.62	0.47
2:A:575:LEU:HA	2:A:583:ALA:HB2	1.97	0.47
2:A:1643:ASN:HA	2:A:1666:PHE:HB2	1.97	0.47
2:B:1668:PHE:HD1	2:B:1688:ARG:HH21	1.61	0.47
2:A:594:ILE:O	2:A:597:HIS:HB3	2.15	0.47
2:A:730:VAL:O	2:A:733:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:890:HIS:ND1	2:A:1022:LEU:HD12	2.30	0.47
2:A:890:HIS:HE1	2:A:1022:LEU:HB3	1.79	0.47
2:A:1245:ARG:HG3	1:C:851:GLN:HE22	1.79	0.47
2:A:1584:LEU:C	2:A:1584:LEU:HD12	2.35	0.47
2:B:813:VAL:CG2	2:B:1707:ASN:CG	2.83	0.47
2:B:823:LEU:HB2	2:B:824:PRO:HD3	1.97	0.47
1:C:856:GLY:O	1:C:860:GLU:HG2	2.15	0.47
2:A:1569:TYR:CZ	1:C:884:TYR:HD2	2.33	0.47
2:B:557:LEU:O	2:B:560:VAL:HG12	2.15	0.47
3:E:192:LEU:HD12	3:E:197:ALA:HB3	1.97	0.47
1:D:951:GLN:HG3	1:C:951:GLN:CG	2.45	0.46
2:A:473:LEU:O	2:A:477:ARG:NH1	2.47	0.46
2:A:586:VAL:HA	2:A:589:MET:HE2	1.97	0.46
2:A:594:ILE:HD11	2:A:611:ARG:HG3	1.97	0.46
2:B:549:ASP:O	2:B:552:ALA:N	2.48	0.46
2:B:616:ASP:HA	2:B:712:ARG:CZ	2.44	0.46
2:B:700:GLU:HG2	2:B:746:THR:HA	1.97	0.46
3:E:59:VAL:HG13	3:E:60:TRP:HD1	1.80	0.46
2:A:301:MET:SD	2:A:308:ARG:N	2.84	0.46
2:A:439:ASP:OD1	2:A:439:ASP:N	2.48	0.46
2:A:733:LEU:O	2:A:736:ALA:HB3	2.15	0.46
2:A:1078:ARG:HA	2:A:1081:LEU:HD12	1.97	0.46
2:B:427:ILE:H	2:B:427:ILE:HD12	1.80	0.46
2:B:600:HIS:HB2	2:B:602:TYR:CE1	2.51	0.46
2:B:823:LEU:O	2:B:827:VAL:HG23	2.15	0.46
3:E:251:MET:C	3:E:253:LEU:H	2.19	0.46
2:A:574:LYS:NZ	2:A:582:HIS:CG	2.83	0.46
2:A:1081:LEU:CD1	1:C:847:PHE:CE1	2.97	0.46
2:B:502:HIS:HA	2:B:505:ARG:CZ	2.45	0.46
1:C:934:LYS:HB2	1:C:934:LYS:HZ2	1.78	0.46
1:D:893:SER:O	1:D:897:GLN:HG3	2.15	0.46
2:A:331:ASN:HB2	2:A:334:VAL:HG22	1.97	0.46
2:A:374:THR:O	2:A:378:PRO:HD3	2.14	0.46
2:A:450:GLU:HG2	2:A:454:ARG:HH21	1.80	0.46
2:A:623:ALA:HB2	2:A:722:LEU:HD21	1.98	0.46
2:B:383:ILE:O	2:B:387:LEU:HB2	2.15	0.46
2:B:1653:SER:OG	2:B:1654:GLY:N	2.49	0.46
2:B:1688:ARG:HB3	2:B:1690:ASP:OD1	2.15	0.46
3:E:81:ARG:CD	3:E:153:TRP:CE2	2.97	0.46
4:F:166:UNK:O	4:F:170:UNK:N	2.28	0.46
2:A:202:ILE:HG22	2:A:205:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:309:LEU:HD13	2:A:312:LEU:HD23	1.97	0.46
2:B:502:HIS:O	2:B:505:ARG:HG2	2.15	0.46
2:B:782:LYS:O	2:B:786:ARG:HD3	2.15	0.46
2:B:784:LYS:HD2	2:B:784:LYS:HA	1.74	0.46
2:B:918:SER:HA	2:B:921:LEU:HG	1.98	0.46
2:B:1237:ALA:HA	2:B:1240:ARG:NH1	2.30	0.46
3:E:128:GLU:HB2	3:E:130:ASP:OD1	2.16	0.46
3:E:222:ARG:HH21	3:E:272:ASP:HA	1.80	0.46
2:A:206:CYS:O	2:A:209:THR:OG1	2.21	0.46
2:A:410:LEU:HD12	2:A:429:TYR:HA	1.97	0.46
2:A:606:ILE:O	2:A:610:ILE:HG12	2.15	0.46
2:B:765:ALA:C	2:B:768:PRO:HD2	2.36	0.46
3:E:37:LEU:N	3:E:69:PRO:O	2.35	0.46
3:E:181:LEU:C	3:E:189:LEU:HD11	2.35	0.46
1:D:856:GLY:O	1:D:860:GLU:HG2	2.15	0.46
1:D:925:GLU:O	1:D:928:LYS:HG2	2.15	0.46
2:A:495:HIS:ND1	2:A:507:LEU:HD13	2.31	0.46
2:A:1620:HIS:HB3	2:A:1621:ILE:HD12	1.96	0.46
2:B:705:VAL:HA	2:B:708:LEU:HD12	1.98	0.46
2:B:796:LEU:HD21	2:B:808:LEU:HD11	1.97	0.46
2:B:1183:LEU:O	2:B:1187:VAL:HG23	2.15	0.46
2:B:1657:PHE:HB3	2:B:1672:ILE:HD13	1.96	0.46
3:E:271:SER:O	3:E:275:VAL:HG23	2.16	0.46
2:A:1212:LEU:HD22	2:B:1208:TRP:HD1	1.80	0.46
2:B:435:HIS:HD2	2:B:468:VAL:HG13	1.79	0.46
3:E:140:ALA:O	3:E:144:MET:HG2	2.16	0.46
2:A:396:ASP:OD2	2:A:397:GLN:NE2	2.47	0.46
2:A:642:PRO:HD2	1:C:907:LYS:NZ	2.30	0.46
2:A:902:LEU:HB2	2:A:903:PRO:HD3	1.97	0.46
2:B:460:ALA:HA	2:B:463:ILE:HD12	1.98	0.46
2:B:1543:HIS:CD2	2:B:1717:LEU:HG	2.50	0.46
2:B:1721:MET:O	2:B:1725:VAL:HG23	2.16	0.46
3:E:76:LYS:HB3	3:E:80:TYR:HE2	1.81	0.46
1:D:918:LYS:O	1:D:922:LEU:HG	2.16	0.46
2:A:243:LEU:HA	2:A:246:THR:HG22	1.97	0.46
2:A:1611:HIS:NE2	2:A:1616:GLN:OE1	2.50	0.46
2:B:620:LEU:HA	2:B:622:ARG:NH1	2.31	0.46
2:B:1058:LYS:HD3	2:B:1060:TRP:CZ2	2.51	0.46
2:B:1690:ASP:OD1	2:B:1690:ASP:N	2.49	0.46
3:E:59:VAL:O	3:E:63:LEU:N	2.38	0.46
1:D:887:GLU:CB	1:C:888:LEU:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:339:VAL:HA	2:A:342:ILE:HG22	1.98	0.45
2:A:852:ARG:HH22	2:A:891:HIS:HE1	1.63	0.45
2:B:338:ILE:O	2:B:342:ILE:HG12	2.16	0.45
2:B:1540:TYR:CE1	2:B:1613:ASP:O	2.68	0.45
2:B:1643:ASN:HA	2:B:1665:GLN:HB2	1.97	0.45
2:A:263:LEU:O	2:A:267:HIS:HB2	2.15	0.45
2:B:600:HIS:CD2	2:B:602:TYR:HE1	2.34	0.45
2:B:816:PRO:O	2:B:820:ILE:HG13	2.16	0.45
3:E:192:LEU:CD1	3:E:197:ALA:HB3	2.46	0.45
2:A:132:SER:O	2:A:132:SER:OG	2.30	0.45
2:A:485:ILE:HG21	2:A:522:HIS:CG	2.52	0.45
2:A:897:PHE:CE2	2:A:1030:MET:HA	2.51	0.45
2:A:1213:GLU:N	2:A:1213:GLU:OE1	2.49	0.45
2:B:568:LEU:HD22	2:B:617:PHE:HD1	1.81	0.45
2:A:1021:GLU:CD	2:A:1745:ARG:HE	2.19	0.45
2:A:1078:ARG:CG	1:C:844:GLN:HE22	2.28	0.45
2:A:1533:LEU:HD12	2:A:1533:LEU:O	2.16	0.45
2:B:1196:GLU:OE2	2:B:1207:SER:HB2	2.16	0.45
1:C:908:ARG:HA	1:C:911:GLU:HG2	1.98	0.45
3:E:47:GLN:HA	3:E:226:LYS:HG2	1.99	0.45
1:D:952:LYS:CA	1:D:955:THR:HG23	2.46	0.45
2:A:316:PRO:O	2:A:319:VAL:HG22	2.16	0.45
2:B:770:LEU:HA	2:B:773:LEU:HB3	1.99	0.45
2:B:1526:SER:HA	2:B:1529:ARG:NH1	2.31	0.45
2:B:1708:LEU:HD12	2:B:1709:PRO:HD3	1.98	0.45
2:A:413:ARG:O	2:A:417:GLN:N	2.49	0.45
2:A:441:TRP:HA	2:A:443:GLN:HE22	1.82	0.45
2:A:631:LEU:HD22	2:A:640:PHE:HA	1.99	0.45
2:B:766:VAL:O	2:B:769:VAL:HG22	2.16	0.45
2:B:813:VAL:HG22	2:B:1707:ASN:OD1	2.15	0.45
3:E:43:CYS:HA	3:E:229:SER:HG	1.82	0.45
3:E:103:PRO:HG2	3:E:106:GLU:HG3	1.98	0.45
3:E:188:LEU:HD13	3:E:247:LYS:HG2	1.98	0.45
2:A:133:ASN:HA	2:A:163:PHE:CE1	2.52	0.45
2:A:1212:LEU:HD22	2:B:1208:TRP:CD1	2.52	0.45
2:A:1657:PHE:HZ	2:A:1662:ILE:HB	1.81	0.45
2:B:1060:TRP:CD1	2:B:1519:LEU:HD13	2.52	0.45
3:E:232:CYS:SG	3:E:233:LYS:N	2.90	0.45
2:A:366:GLU:HA	2:A:369:LEU:HB2	1.98	0.45
2:A:1582:ILE:HG12	2:A:1588:GLN:NE2	2.31	0.45
2:B:394:LEU:HD23	2:B:426:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:ARG:HB3	2:B:615:PHE:CZ	2.51	0.45
2:B:747:LEU:HD21	2:B:759:ARG:HG2	1.98	0.45
2:B:841:VAL:HB	2:B:842:PRO:HD3	1.99	0.45
2:B:845:GLU:O	2:B:848:SER:OG	2.28	0.45
2:B:1026:CYS:SG	2:B:1027:LEU:N	2.89	0.45
2:B:1506:HIS:O	2:B:1506:HIS:ND1	2.48	0.45
3:E:135:LEU:O	3:E:139:LYS:HG3	2.17	0.45
1:D:962:ILE:HD11	1:C:958:PHE:HD1	1.80	0.45
2:A:449:MET:O	2:A:453:PHE:N	2.50	0.45
2:A:1725:VAL:O	2:A:1729:ARG:HB2	2.16	0.45
2:B:690:PHE:O	2:B:694:LEU:HG	2.17	0.45
2:B:1194:TRP:HE3	2:B:1209:LEU:HD11	1.81	0.45
2:B:1549:TYR:HB2	2:B:1571:TYR:CE2	2.52	0.45
2:A:902:LEU:HD23	2:A:905:ARG:NH2	2.32	0.45
2:A:1552:GLU:HG2	2:A:1553:GLY:H	1.81	0.45
2:A:1637:LYS:HA	2:A:1640:HIS:HB2	1.99	0.45
2:A:1659:LEU:N	2:A:1686:GLN:OE1	2.50	0.45
2:B:569:VAL:O	2:B:573:THR:HG23	2.17	0.45
2:B:1605:GLN:CA	2:B:1624:LEU:HD13	2.45	0.45
2:B:1724:GLN:HB3	2:B:1737:PRO:HG3	1.99	0.45
1:C:860:GLU:O	1:C:864:GLU:HG2	2.17	0.45
2:A:208:ARG:O	2:A:211:SER:OG	2.23	0.44
2:A:397:GLN:O	2:A:400:PHE:HB3	2.17	0.44
2:A:525:ASN:OD1	2:A:525:ASN:N	2.48	0.44
2:A:629:LEU:HD21	2:A:631:LEU:HD11	1.98	0.44
2:A:1588:GLN:NE2	2:A:1588:GLN:CA	2.76	0.44
2:A:360:ILE:HG23	2:A:361:LEU:HD22	1.97	0.44
2:A:1580:ARG:O	2:A:1609:CYS:O	2.34	0.44
2:B:1645:PHE:O	2:B:1668:PHE:N	2.50	0.44
3:E:188:LEU:HD22	3:E:243:LEU:O	2.18	0.44
1:D:935:LEU:O	1:D:938:ARG:HG2	2.17	0.44
1:D:958:PHE:O	1:D:962:ILE:HG13	2.17	0.44
2:A:202:ILE:HD12	2:A:202:ILE:H	1.82	0.44
2:A:492:GLN:HA	2:A:495:HIS:CD2	2.50	0.44
2:A:629:LEU:HD12	1:C:900:GLN:HE21	1.79	0.44
2:A:1546:ALA:O	2:A:1647:SER:HA	2.17	0.44
2:B:882:ASN:HB3	2:B:885:ILE:H	1.81	0.44
2:B:906:LYS:HB2	2:B:934:ARG:CZ	2.48	0.44
2:B:1705:ASP:O	2:B:1708:LEU:HG	2.17	0.44
3:E:102:THR:HG22	3:E:106:GLU:HB2	1.99	0.44
2:A:722:LEU:CA	2:A:725:THR:HG22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1062:VAL:HG23	2:A:1063:GLY:N	2.31	0.44
2:B:195:ILE:O	2:B:199:VAL:N	2.50	0.44
3:E:56:ARG:HG2	3:E:60:TRP:CE2	2.53	0.44
1:D:854:VAL:HG22	2:B:1235:LEU:HD13	1.77	0.44
2:A:283:ARG:NH2	2:A:284:ALA:H	2.15	0.44
2:A:768:PRO:O	2:A:771:THR:OG1	2.27	0.44
2:B:564:VAL:O	2:B:568:LEU:HG	2.18	0.44
2:B:691:ARG:HA	2:B:694:LEU:HD12	1.99	0.44
2:A:268:LEU:HA	2:A:274:TYR:CZ	2.53	0.44
2:A:694:LEU:HD11	2:A:733:LEU:HB3	2.00	0.44
2:A:771:THR:O	2:A:774:ILE:HG22	2.18	0.44
2:A:1558:GLU:OE2	2:A:1662:ILE:HD12	2.18	0.44
2:B:738:CYS:O	2:B:741:LEU:HB3	2.17	0.44
1:D:852:LEU:C	1:D:852:LEU:CD2	2.86	0.44
2:A:198:MET:SD	2:A:236:LEU:HD21	2.58	0.44
2:A:449:MET:HG3	2:A:454:ARG:NH1	2.32	0.44
2:A:777:HIS:CG	2:A:778:ASN:N	2.85	0.44
2:A:920:VAL:HG22	2:A:921:LEU:H	1.82	0.44
2:A:1232:SER:OG	1:C:841:VAL:CG2	2.66	0.44
2:B:390:THR:O	2:B:394:LEU:HG	2.18	0.44
2:B:413:ARG:O	2:B:417:GLN:HG3	2.17	0.44
2:B:530:ILE:HD13	2:B:567:LEU:HD21	2.00	0.44
2:B:579:PRO:HB2	2:B:582:HIS:CD2	2.44	0.44
2:B:721:VAL:HA	2:B:1678:TYR:HE1	1.83	0.44
2:B:1235:LEU:C	2:B:1235:LEU:CD2	2.86	0.44
2:B:1687:CYS:SG	2:B:1692:GLU:N	2.91	0.44
3:E:144:MET:HE1	3:E:220:LEU:HB3	2.00	0.44
2:A:256:CYS:SG	2:A:259:LEU:HB2	2.58	0.44
2:A:392:GLU:HA	2:A:395:CYS:SG	2.58	0.44
2:A:501:ASP:O	2:A:504:VAL:HG22	2.17	0.44
2:A:701:SER:O	2:A:701:SER:OG	2.35	0.44
2:A:1516:LYS:NZ	2:B:936:ARG:HE	2.15	0.44
2:A:1574:PHE:HD1	2:A:1709:PRO:HD3	1.83	0.44
2:B:454:ARG:HA	2:B:462:ARG:HH22	1.83	0.44
2:B:873:LEU:O	2:B:876:THR:OG1	2.23	0.44
1:C:926:GLN:HA	1:C:926:GLN:HE21	1.83	0.44
3:E:38:ASP:OD2	3:E:41:LYS:N	2.33	0.44
3:E:133:VAL:HA	3:E:209:ARG:HG2	2.00	0.44
3:E:203:TYR:HA	3:E:206:TRP:CE3	2.49	0.44
2:A:179:VAL:HA	2:A:182:ASN:HD22	1.82	0.44
2:A:765:ALA:O	2:A:768:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:870:ALA:O	2:A:874:PRO:HD3	2.17	0.44
2:A:1035:PHE:HE1	2:B:1496:ASN:HD22	1.65	0.44
2:A:1569:TYR:CZ	1:C:884:TYR:CB	3.01	0.44
2:B:453:PHE:C	2:B:454:ARG:HD3	2.38	0.44
2:B:723:ILE:HG23	2:B:726:SER:HB3	2.00	0.44
2:B:1060:TRP:HE1	2:B:1519:LEU:HB2	1.82	0.44
2:B:1545:ILE:HG22	2:B:1619:PHE:HA	2.00	0.44
1:D:847:PHE:CZ	1:C:849:ASN:HA	2.53	0.43
2:A:1551:GLY:H	2:A:1554:GLN:HB2	1.83	0.43
2:A:1615:MET:HE3	2:A:1717:LEU:HD12	2.00	0.43
2:B:530:ILE:O	2:B:534:VAL:HG13	2.18	0.43
2:B:1048:GLY:O	2:B:1052:LEU:HG	2.18	0.43
2:B:1530:SER:OG	2:B:1750:LEU:HD11	2.18	0.43
3:E:165:LYS:HE3	3:E:166:TYR:CZ	2.52	0.43
2:A:133:ASN:HA	2:A:163:PHE:CZ	2.53	0.43
2:A:303:LEU:HG	2:A:345:LEU:HD22	2.00	0.43
2:A:495:HIS:CE1	2:A:507:LEU:HD13	2.53	0.43
2:A:822:ALA:C	2:A:826:LEU:HG	2.38	0.43
2:A:1193:GLY:O	2:A:1212:LEU:HD23	2.18	0.43
2:A:1210:MET:SD	2:B:1210:MET:HG2	2.58	0.43
2:A:1533:LEU:HD11	2:A:1746:HIS:NE2	2.33	0.43
2:A:1550:VAL:HG23	2:A:1651:ASN:O	2.18	0.43
2:A:1573:GLU:O	2:A:1576:THR:OG1	2.31	0.43
2:B:500:LYS:O	2:B:504:VAL:HG23	2.18	0.43
2:B:763:HIS:HA	2:B:766:VAL:HG12	2.00	0.43
2:B:816:PRO:O	2:B:819:ILE:HG22	2.18	0.43
1:C:878:GLU:HA	1:C:878:GLU:OE1	2.18	0.43
3:E:67:LEU:CD2	3:E:81:ARG:HH12	2.31	0.43
1:D:953:ARG:HG3	3:E:114:LEU:CD1	2.48	0.43
2:A:343:THR:HA	2:A:346:ILE:HD11	1.99	0.43
2:A:451:ARG:HA	2:A:451:ARG:HD2	1.80	0.43
2:B:485:ILE:HG21	2:B:522:HIS:HB3	2.00	0.43
2:B:729:SER:O	2:B:732:GLN:HG2	2.18	0.43
2:B:801:ALA:O	2:B:805:VAL:N	2.46	0.43
1:D:906:GLN:O	1:D:910:LEU:HG	2.18	0.43
2:A:642:PRO:HD2	1:C:907:LYS:HZ2	1.82	0.43
2:A:767:VAL:HB	2:A:768:PRO:HD3	2.00	0.43
2:A:816:PRO:O	2:A:819:ILE:HG22	2.18	0.43
2:A:1081:LEU:CD2	1:C:847:PHE:CE1	2.87	0.43
2:A:1235:LEU:HD23	1:C:844:GLN:CB	2.39	0.43
2:B:374:THR:O	2:B:378:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:LYS:HB2	2:B:503:GLN:HE21	1.84	0.43
2:B:593:HIS:O	2:B:597:HIS:HB2	2.18	0.43
2:B:1534:LEU:C	2:B:1534:LEU:CD2	2.86	0.43
2:B:1668:PHE:HD1	2:B:1688:ARG:HD2	1.81	0.43
2:A:348:LYS:HD3	2:A:358:TRP:CE2	2.53	0.43
2:A:427:ILE:O	2:A:430:ARG:HG3	2.19	0.43
2:A:720:LYS:HB3	2:A:724:PHE:CE2	2.52	0.43
2:B:580:ALA:O	2:B:584:THR:HG23	2.18	0.43
2:B:1235:LEU:HD22	2:B:1236:MET:HE3	1.99	0.43
2:B:1542:THR:H	2:B:1739:LYS:HE3	1.83	0.43
1:D:848:LEU:HD13	1:C:848:LEU:HD22	2.00	0.43
2:A:1529:ARG:HB2	2:A:1529:ARG:NH1	2.33	0.43
2:A:1751:ARG:HA	2:A:1754:ILE:HD12	2.00	0.43
3:E:251:MET:CE	3:E:251:MET:CA	2.85	0.43
2:A:416:ASP:HA	2:A:418:ARG:NH2	2.21	0.43
2:A:931:ASP:HB2	2:A:933:PHE:HD2	1.83	0.43
2:A:1219:PHE:CZ	2:B:1613:ASP:HA	2.54	0.43
2:A:1584:LEU:HD12	2:A:1585:LYS:N	2.34	0.43
2:A:1585:LYS:HG3	2:A:1587:CYS:H	1.84	0.43
2:A:1636:ASP:N	2:A:1636:ASP:OD1	2.49	0.43
2:B:515:LEU:HD12	2:B:518:GLY:HA3	2.00	0.43
2:B:584:THR:O	2:B:587:TYR:HB3	2.19	0.43
2:B:900:CYS:O	2:B:905:ARG:NH2	2.51	0.43
1:D:962:ILE:HD12	1:C:958:PHE:CD1	2.52	0.43
2:A:781:ASP:O	2:A:785:GLN:N	2.31	0.43
2:B:344:ARG:HA	2:B:344:ARG:HD3	1.84	0.43
2:B:911:PHE:O	2:B:914:LYS:HB3	2.19	0.43
2:B:1539:SER:HB3	2:B:1740:TRP:HE1	1.83	0.43
3:E:180:TYR:HD2	3:E:236:VAL:HG11	1.84	0.43
3:E:204:ASP:O	3:E:208:LYS:N	2.51	0.43
2:A:575:LEU:HG	2:A:641:SER:OG	2.19	0.43
2:A:1045:SER:HB2	2:A:1243:GLU:H	1.84	0.43
2:B:435:HIS:CE1	2:B:438:LYS:HD3	2.53	0.43
2:B:705:VAL:O	2:B:709:VAL:HG13	2.18	0.43
1:C:962:ILE:O	1:C:965:LEU:HG	2.19	0.43
1:D:843:GLN:OE1	2:B:1242:LYS:HE2	2.18	0.43
2:A:241:VAL:HB	2:A:244:CYS:HB3	2.01	0.43
2:A:389:THR:O	2:A:392:GLU:HB3	2.19	0.43
2:A:435:HIS:HB3	2:A:436:PRO:HD3	2.01	0.43
2:A:1078:ARG:HG3	1:C:844:GLN:NE2	2.34	0.43
2:A:1214:ASN:HD21	2:B:1206:THR:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:VAL:HG13	2:B:385:HIS:ND1	2.34	0.43
2:B:394:LEU:HD21	2:B:423:LEU:HD22	2.00	0.43
2:B:1218:PRO:HG2	2:B:1219:PHE:CD1	2.54	0.43
2:B:1594:LEU:CD1	2:B:1640:HIS:HD2	2.32	0.43
2:A:245:ARG:CZ	2:A:277:CYS:HB2	2.49	0.42
2:A:553:TYR:O	2:A:556:SER:OG	2.20	0.42
2:A:570:ILE:O	2:A:574:LYS:HB3	2.19	0.42
2:A:597:HIS:NE2	2:A:607:ALA:HB1	2.34	0.42
2:B:482:GLU:O	2:B:486:ASN:ND2	2.52	0.42
2:B:515:LEU:HD12	2:B:515:LEU:HA	1.90	0.42
1:C:926:GLN:HE21	1:C:926:GLN:CA	2.31	0.42
2:A:343:THR:O	2:A:346:ILE:CG1	2.67	0.42
2:A:374:THR:O	2:A:377:SER:OG	2.36	0.42
2:A:630:GLY:O	2:A:631:LEU:HD23	2.18	0.42
2:A:640:PHE:HB3	1:C:907:LYS:HZ1	1.84	0.42
2:A:1648:ILE:HA	2:A:1671:VAL:HG23	2.01	0.42
2:B:841:VAL:HG12	2:B:845:GLU:OE1	2.18	0.42
2:B:1059:THR:HG23	2:B:1520:LEU:CG	2.49	0.42
2:B:1545:ILE:CG2	2:B:1619:PHE:HA	2.49	0.42
2:B:1549:TYR:HB2	2:B:1571:TYR:CZ	2.54	0.42
2:B:1711:VAL:O	2:B:1715:MET:HG2	2.19	0.42
3:E:90:HIS:O	3:E:94:VAL:HG23	2.19	0.42
1:D:953:ARG:HD2	3:E:114:LEU:O	2.19	0.42
2:A:575:LEU:HD13	2:A:583:ALA:HB1	2.02	0.42
2:A:1568:SER:OG	2:A:1570:ARG:HG2	2.19	0.42
2:B:561:LYS:HB2	2:B:610:ILE:HG12	2.01	0.42
2:B:598:TYR:HE2	2:B:699:GLN:HB3	1.85	0.42
2:B:610:ILE:HA	2:B:613:GLN:NE2	2.33	0.42
2:B:1032:ARG:HH22	2:B:1039:THR:C	2.23	0.42
2:B:1561:ILE:HD12	2:B:1661:THR:HB	2.01	0.42
1:C:867:GLN:O	1:C:871:SER:OG	2.23	0.42
3:E:116:SER:HB2	3:E:118:LYS:HE3	2.02	0.42
3:E:207:PHE:CZ	3:E:236:VAL:HA	2.54	0.42
3:E:259:ILE:O	3:E:263:LEU:HG	2.19	0.42
1:D:927:LYS:HE3	2:A:479:PHE:HD2	1.85	0.42
2:A:457:SER:OG	2:A:458:ARG:HD3	2.19	0.42
2:A:561:LYS:HG3	2:A:610:ILE:HD11	2.01	0.42
2:A:640:PHE:O	1:C:907:LYS:NZ	2.53	0.42
2:A:1558:GLU:OE2	2:A:1663:LYS:N	2.36	0.42
2:A:1704:SER:OG	2:A:1705:ASP:N	2.52	0.42
2:B:397:GLN:HG2	2:B:429:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1036:SER:OG	2:B:1037:ASN:N	2.53	0.42
2:A:439:ASP:HB3	1:C:929:TYR:OH	2.20	0.42
2:A:449:MET:CE	2:A:491:SER:HB3	2.49	0.42
2:A:1523:GLU:O	2:A:1525:GLN:N	2.53	0.42
2:B:428:SER:O	2:B:464:LYS:HE3	2.18	0.42
2:B:857:TYR:HB2	2:B:860:PHE:CE2	2.54	0.42
2:B:1645:PHE:HB3	2:B:1723:SER:HB2	2.02	0.42
2:A:279:LEU:HD22	2:A:322:SER:CB	2.49	0.42
2:A:316:PRO:O	2:A:320:LEU:HG	2.20	0.42
2:A:622:ARG:NH2	2:A:633:ASN:HD21	2.18	0.42
2:A:1584:LEU:HD13	2:A:1594:LEU:CD1	2.48	0.42
2:A:1625:MET:HB3	2:A:1626:PRO:HD3	2.02	0.42
2:B:907:ASP:O	2:B:910:PRO:HD2	2.19	0.42
3:E:35:ASP:HA	3:E:71:HIS:HD2	1.82	0.42
2:A:229:ASN:O	2:A:232:PRO:HD2	2.20	0.42
2:A:245:ARG:NH2	2:A:273:ILE:HG23	2.35	0.42
2:A:546:GLU:C	2:A:548:ARG:H	2.23	0.42
2:A:1196:GLU:OE2	2:A:1198:LEU:HB2	2.19	0.42
2:A:1534:LEU:HD11	2:A:1747:ILE:HD11	2.02	0.42
2:B:502:HIS:CG	2:B:503:GLN:H	2.38	0.42
2:B:1653:SER:OG	2:B:1655:GLU:HG3	2.20	0.42
1:C:959:GLU:O	1:C:962:ILE:HB	2.20	0.42
3:E:79:MET:O	3:E:83:GLU:HG3	2.20	0.42
2:A:618:LEU:HD23	2:A:618:LEU:HA	1.89	0.42
2:A:643:TYR:CE1	1:C:907:LYS:HD2	2.54	0.42
2:A:1242:LYS:O	2:A:1243:GLU:HG2	2.20	0.42
2:A:1500:VAL:O	2:A:1503:GLN:HB2	2.20	0.42
2:A:1543:HIS:O	2:A:1617:ALA:HA	2.18	0.42
2:A:1575:LEU:C	2:A:1575:LEU:CD2	2.86	0.42
2:B:607:ALA:O	2:B:611:ARG:HG3	2.19	0.42
2:B:884:TYR:HB2	2:B:1725:VAL:HG11	2.01	0.42
2:B:1571:TYR:CE2	2:B:1575:LEU:HD11	2.54	0.42
3:E:113:GLN:HE21	3:E:120:PRO:HD3	1.68	0.42
2:A:153:ILE:HG22	2:A:154:THR:N	2.35	0.42
2:A:723:ILE:H	2:A:723:ILE:HD12	1.85	0.42
2:A:932:SER:O	2:A:932:SER:OG	2.37	0.42
2:A:1199:VAL:HG22	2:A:1201:ARG:HG3	2.02	0.42
2:B:838:SER:OG	2:B:839:MET:N	2.53	0.42
2:B:839:MET:O	2:B:842:PRO:HD2	2.20	0.42
2:B:1186:TYR:CE1	2:B:1227:PRO:HD2	2.55	0.42
2:B:1625:MET:CG	2:B:1637:LYS:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1638:LYS:H	2:B:1638:LYS:HG3	1.65	0.42
2:B:1739:LYS:H	2:B:1739:LYS:HG2	1.52	0.42
3:E:188:LEU:HD11	3:E:250:VAL:HG22	2.02	0.42
1:D:853:LEU:HD11	2:B:1077:THR:HG21	2.02	0.42
2:A:427:ILE:HD12	2:A:464:LYS:HZ1	1.84	0.42
2:A:1534:LEU:CD1	2:A:1747:ILE:HD11	2.50	0.42
2:A:1589:PRO:C	2:A:1591:LYS:H	2.24	0.42
2:B:598:TYR:OH	2:B:699:GLN:O	2.37	0.42
2:B:610:ILE:HA	2:B:613:GLN:CD	2.41	0.42
2:B:800:CYS:SG	2:B:801:ALA:N	2.92	0.42
2:B:1056:ARG:HH22	2:B:1494:GLY:N	2.17	0.42
2:B:1614:ILE:CD1	2:B:1740:TRP:CZ2	3.00	0.42
1:D:944:ALA:CA	3:E:80:TYR:CD1	3.03	0.41
1:D:959:GLU:HA	1:D:962:ILE:HD12	2.01	0.41
2:A:276:MET:O	2:A:280:MET:HG2	2.20	0.41
2:A:504:VAL:HA	2:A:507:LEU:HD12	2.02	0.41
2:A:815:MET:HB3	2:A:818:ILE:CG2	2.50	0.41
2:A:1524:SER:OG	2:A:1524:SER:O	2.38	0.41
2:A:1534:LEU:C	2:A:1534:LEU:CD2	2.85	0.41
2:A:1534:LEU:HD23	2:A:1534:LEU:O	2.20	0.41
2:B:358:TRP:HD1	2:B:359:ASP:O	2.03	0.41
1:C:845:MET:SD	1:C:845:MET:C	2.98	0.41
3:E:29:GLU:O	3:E:33:LYS:HG3	2.20	0.41
3:E:251:MET:O	3:E:251:MET:SD	2.78	0.41
1:D:880:MET:O	1:C:884:TYR:CE2	2.52	0.41
2:A:367:ARG:NH1	2:A:408:PHE:HB2	2.34	0.41
2:A:931:ASP:HB2	2:A:933:PHE:CD2	2.55	0.41
2:B:465:VAL:O	2:B:469:LEU:HG	2.21	0.41
2:B:860:PHE:HD1	2:B:860:PHE:HA	1.74	0.41
2:B:1703:VAL:HG13	2:B:1708:LEU:HB3	2.01	0.41
2:B:1708:LEU:N	2:B:1709:PRO:HD2	2.35	0.41
2:A:858:ARG:HG2	2:A:859:ASN:OD1	2.19	0.41
2:A:1515:ASN:HD21	2:B:1512:ASP:N	2.19	0.41
2:A:1581:LEU:HD13	2:A:1608:TYR:CD2	2.54	0.41
2:A:1610:TRP:CD1	2:A:1611:HIS:N	2.88	0.41
2:B:606:ILE:O	2:B:610:ILE:HG13	2.20	0.41
2:B:733:LEU:HA	2:B:736:ALA:HB3	2.02	0.41
2:B:1034:VAL:HG13	2:B:1035:PHE:HD2	1.85	0.41
2:B:1615:MET:O	2:B:1615:MET:SD	2.79	0.41
1:C:844:GLN:NE2	1:C:844:GLN:CA	2.74	0.41
3:E:278:ALA:HA	3:E:281:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:527:LEU:HA	2:A:530:ILE:HD12	2.02	0.41
2:A:702:ASP:OD1	2:A:705:VAL:HB	2.20	0.41
2:A:1531:VAL:O	2:A:1534:LEU:HB3	2.21	0.41
2:A:1542:THR:HG23	2:A:1593:TYR:CE1	2.56	0.41
2:A:1552:GLU:HG2	2:A:1553:GLY:N	2.34	0.41
2:B:1545:ILE:HD11	2:B:1716:ALA:HB1	2.02	0.41
2:B:1738:SER:OG	2:B:1741:ILE:HB	2.19	0.41
1:D:865:GLN:NE2	1:D:869:LYS:HB2	2.35	0.41
1:D:868:ASN:HD21	1:C:870:HIS:HA	1.78	0.41
2:A:461:VAL:O	2:A:465:VAL:HG12	2.21	0.41
2:B:391:VAL:HA	2:B:394:LEU:HD12	2.02	0.41
2:B:1066:LEU:HD21	2:B:1200:ARG:HH11	1.85	0.41
1:D:870:HIS:ND1	2:A:1580:ARG:HD3	2.35	0.41
1:D:902:LEU:CB	1:C:902:LEU:HD22	2.39	0.41
2:A:211:SER:HA	2:A:214:ASP:OD2	2.20	0.41
2:A:709:VAL:HG13	2:A:710:LEU:HD22	2.03	0.41
2:B:496:ILE:N	2:B:497:PRO:HD2	2.36	0.41
3:E:28:LEU:HB2	3:E:45:PHE:CZ	2.55	0.41
3:E:222:ARG:O	3:E:225:ASP:HB2	2.20	0.41
1:D:867:GLN:HE22	2:B:1218:PRO:HB3	1.85	0.41
2:A:324:TYR:HD2	2:A:369:LEU:HD22	1.84	0.41
2:A:1191:THR:HA	2:A:1194:TRP:CZ3	2.56	0.41
2:A:1589:PRO:HG2	2:A:1591:LYS:HB3	2.03	0.41
1:C:845:MET:SD	1:C:845:MET:O	2.79	0.41
3:E:67:LEU:CD2	3:E:81:ARG:HH22	2.15	0.41
3:E:130:ASP:OD1	3:E:130:ASP:N	2.53	0.41
2:A:501:ASP:OD1	2:A:502:HIS:N	2.49	0.41
2:A:544:GLU:OE1	2:A:544:GLU:N	2.52	0.41
2:A:806:VAL:O	2:A:809:SER:OG	2.28	0.41
2:A:877:ASN:CA	2:A:919:ASN:HD21	2.34	0.41
2:A:921:LEU:HD11	2:A:928:PRO:HG3	2.03	0.41
2:B:485:ILE:O	2:B:489:VAL:HG12	2.21	0.41
2:B:1523:GLU:N	2:B:1523:GLU:OE1	2.54	0.41
2:B:1651:ASN:HD22	2:B:1674:THR:HB	1.86	0.41
2:A:184:VAL:HG23	2:A:185:LYS:H	1.85	0.41
2:A:410:LEU:HD13	2:A:410:LEU:HA	1.95	0.41
2:A:412:GLU:HB2	2:A:413:ARG:NH2	2.36	0.41
2:A:480:TYR:HD1	2:A:480:TYR:HA	1.75	0.41
2:A:493:LEU:HA	2:A:529:ASP:OD1	2.21	0.41
2:A:524:PHE:O	2:A:528:LEU:HG	2.20	0.41
2:A:1499:PHE:O	2:A:1502:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:THR:HG23	2:B:799:ARG:HE	1.86	0.41
2:B:1044:ARG:NE	2:B:1049:GLU:OE2	2.47	0.41
2:B:1205:ASN:OD1	2:B:1205:ASN:N	2.54	0.41
2:B:1552:GLU:HA	2:B:1653:SER:HB2	2.02	0.41
3:E:111:MET:HE2	3:E:111:MET:HB3	1.97	0.41
3:E:223:VAL:HB	3:E:275:VAL:HG13	2.03	0.41
3:E:223:VAL:HG23	3:E:234:ILE:HD13	2.02	0.41
3:E:276:SER:HA	3:E:279:ILE:HD12	2.03	0.41
2:A:688:LEU:H	2:A:688:LEU:HG	1.69	0.41
2:A:706:LEU:O	2:A:707:LYS:C	2.59	0.41
2:A:1061:LEU:HD11	2:A:1751:ARG:HB2	2.02	0.41
2:B:390:THR:HA	2:B:393:GLU:CD	2.42	0.41
2:B:1060:TRP:CZ3	2:B:1501:PHE:HB2	2.55	0.41
2:B:1715:MET:HA	2:B:1718:HIS:HD2	1.86	0.41
3:E:88:VAL:HG22	3:E:111:MET:HG2	2.03	0.41
3:E:195:CYS:HA	3:E:254:ASN:ND2	2.36	0.41
3:E:251:MET:C	3:E:253:LEU:N	2.74	0.41
1:D:877:VAL:CG2	2:A:1606:PHE:HZ	2.35	0.40
2:A:154:THR:O	2:A:157:GLU:HG3	2.21	0.40
2:A:221:VAL:HG13	2:A:222:LEU:N	2.37	0.40
2:A:935:ALA:HB3	2:A:936:ARG:NH1	2.35	0.40
2:A:1564:ASN:OD1	2:A:1565:GLU:N	2.55	0.40
2:A:1691:MET:H	2:A:1691:MET:HG2	1.67	0.40
2:B:320:LEU:HB3	2:B:365:ILE:HG21	2.04	0.40
2:B:482:GLU:HG2	2:B:483:GLU:N	2.34	0.40
2:B:686:TYR:CZ	2:B:722:LEU:HB2	2.56	0.40
2:B:1714:GLN:OE1	2:B:1718:HIS:NE2	2.54	0.40
3:E:35:ASP:O	3:E:70:HIS:HA	2.22	0.40
3:E:188:LEU:HD11	3:E:250:VAL:CG2	2.51	0.40
2:A:136:LEU:HG	2:A:137:HIS:H	1.86	0.40
2:A:477:ARG:NE	2:A:477:ARG:HA	2.36	0.40
2:A:488:VAL:CG2	2:A:492:GLN:NE2	2.84	0.40
2:A:687:SER:N	2:A:726:SER:OG	2.53	0.40
2:B:438:LYS:HA	2:B:438:LYS:HD2	1.84	0.40
2:B:1720:ASN:O	2:B:1724:GLN:HG3	2.20	0.40
1:C:746:ASP:O	1:C:750:TRP:N	2.48	0.40
3:E:66:ILE:O	3:E:81:ARG:NH1	2.54	0.40
2:A:426:LEU:HA	2:A:426:LEU:HD13	1.87	0.40
2:A:486:ASN:CA	2:A:489:VAL:HG12	2.50	0.40
2:B:504:VAL:O	2:B:507:LEU:HG	2.21	0.40
2:B:905:ARG:HE	2:B:905:ARG:HB2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:166:TYR:O	3:E:170:LEU:HG	2.20	0.40
2:A:413:ARG:H	2:A:413:ARG:HG2	1.64	0.40
2:A:585:ARG:O	2:A:589:MET:HG3	2.21	0.40
2:A:629:LEU:HD23	2:A:629:LEU:O	2.21	0.40
2:A:1529:ARG:HB2	2:A:1529:ARG:CZ	2.51	0.40
2:B:331:ASN:HB3	2:B:334:VAL:HG22	2.03	0.40
2:B:912:ILE:HG21	2:B:1030:MET:SD	2.62	0.40
2:B:1032:ARG:HH22	2:B:1040:ALA:HA	1.86	0.40
2:B:1181:THR:O	2:B:1185:ALA:CB	2.70	0.40
2:B:1606:PHE:N	2:B:1624:LEU:CD1	2.77	0.40
2:B:1643:ASN:ND2	2:B:1643:ASN:C	2.73	0.40
1:D:849:ASN:ND2	2:B:1050:PHE:CD1	2.88	0.40
2:A:218:SER:HG	2:A:222:LEU:H	1.58	0.40
2:A:224:ALA:HA	2:A:227:CYS:SG	2.61	0.40
2:A:362:LEU:O	2:A:366:GLU:HG3	2.20	0.40
2:A:500:LYS:HA	2:A:500:LYS:HD2	1.72	0.40
2:A:582:HIS:O	2:A:586:VAL:HG23	2.22	0.40
2:A:786:ARG:HG3	2:A:818:ILE:HD11	2.02	0.40
2:B:912:ILE:O	2:B:916:LEU:N	2.54	0.40
2:B:1541:ASP:HA	2:B:1739:LYS:HE3	2.04	0.40
2:B:1550:VAL:HG11	2:B:1657:PHE:CE1	2.56	0.40
3:E:128:GLU:O	3:E:131:ASP:HB2	2.21	0.40
3:E:180:TYR:HA	3:E:285:HIS:CE1	2.57	0.40
3:E:237:PHE:O	3:E:240:VAL:HB	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	C	222/1164 (19%)	215 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	224/1164 (19%)	216 (96%)	7 (3%)	1 (0%)	34	72
2	A	1107/1692 (65%)	960 (87%)	147 (13%)	0	100	100
2	B	1008/1692 (60%)	900 (89%)	106 (10%)	2 (0%)	47	81
3	E	265/267 (99%)	246 (93%)	18 (7%)	1 (0%)	34	72
All	All	2826/5979 (47%)	2537 (90%)	285 (10%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	881	LYS
3	E	218	SER
2	B	1536	GLN
2	B	289	ALA

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	C	120/1033 (12%)	116 (97%)	4 (3%)	38	61
1	D	121/1033 (12%)	117 (97%)	4 (3%)	38	61
2	A	1017/1480 (69%)	1003 (99%)	14 (1%)	67	81
2	B	832/1480 (56%)	821 (99%)	11 (1%)	69	82
3	E	243/243 (100%)	236 (97%)	7 (3%)	42	64
All	All	2333/5269 (44%)	2293 (98%)	40 (2%)	62	78

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	880	MET
1	D	894	HIS
1	D	907	LYS
1	D	955	THR

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Mol	Chain	Res	Type
2	A	139	ARG
2	A	144	LYS
2	A	151	ARG
2	A	400	PHE
2	A	418	ARG
2	A	611	ARG
2	A	634	LYS
2	A	702	ASP
2	A	799	ARG
2	A	1032	ARG
2	A	1533	LEU
2	A	1576	THR
2	A	1584	LEU
2	A	1748	LYS
2	B	454	ARG
2	B	477	ARG
2	B	786	ARG
2	B	799	ARG
2	B	815	MET
2	B	860	PHE
2	B	899	ARG
2	B	1591	LYS
2	B	1599	VAL
2	B	1643	ASN
2	B	1706	ARG
1	C	877	VAL
1	C	896	LEU
1	C	899	THR
1	C	954	ILE
3	E	36	ARG
3	E	74	HIS
3	E	77	VAL
3	E	82	LYS
3	E	97	PHE
3	E	167	ARG
3	E	250	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	851	GLN
1	D	868	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	D	870	HIS
1	D	897	GLN
1	D	926	GLN
1	D	936	GLN
1	D	940	GLN
1	D	956	GLN
2	A	182	ASN
2	A	248	ASN
2	A	331	ASN
2	A	370	GLN
2	A	476	ASN
2	A	495	HIS
2	A	523	HIS
2	A	763	HIS
2	A	883	GLN
2	A	891	HIS
2	A	1064	ASN
2	A	1192	GLN
2	B	363	ASN
2	B	486	ASN
2	B	495	HIS
2	B	503	GLN
2	B	525	ASN
2	B	582	HIS
2	B	597	HIS
2	B	600	HIS
2	B	763	HIS
2	B	832	HIS
2	B	890	HIS
2	B	1182	ASN
2	B	1503	GLN
2	B	1554	GLN
2	B	1651	ASN
2	B	1727	HIS
1	C	842	GLN
1	C	844	GLN
1	C	898	GLN
1	C	900	GLN
1	C	906	GLN
1	C	926	GLN
1	C	951	GLN
3	E	71	HIS

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Mol	Chain	Res	Type
3	E	104	GLN
3	E	113	GLN
3	E	163	ASN
3	E	191	HIS
3	E	254	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

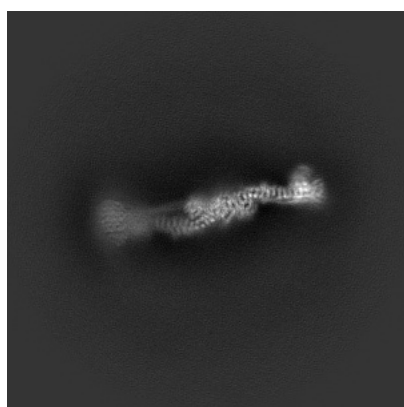
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30708. These allow visual inspection of the internal detail of the map and identification of artifacts.

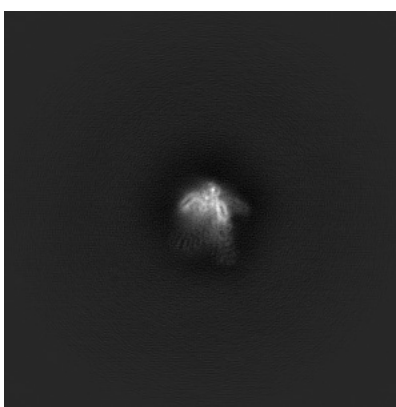
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

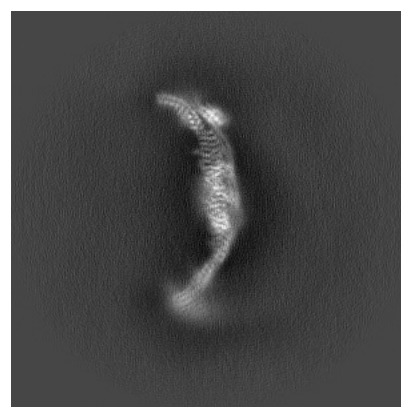
6.1.1 Primary map



X



Y



Z

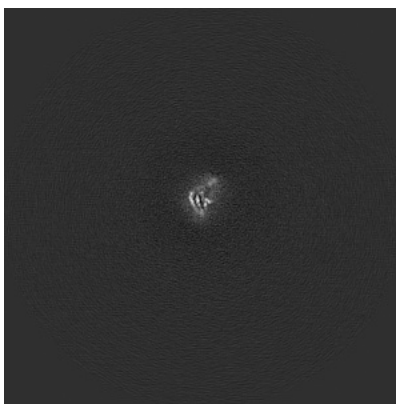
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 260



Y Index: 260

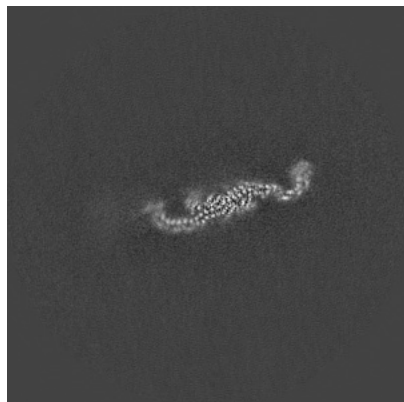


Z Index: 260

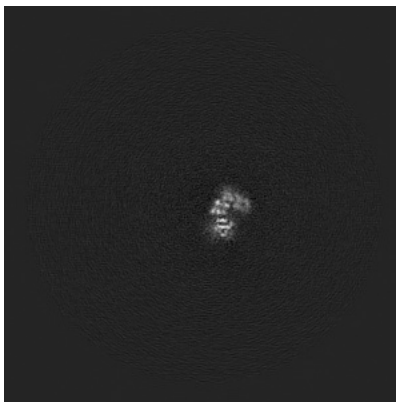
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

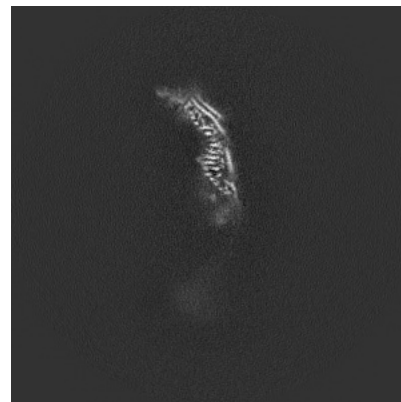
6.3.1 Primary map



X Index: 267



Y Index: 382

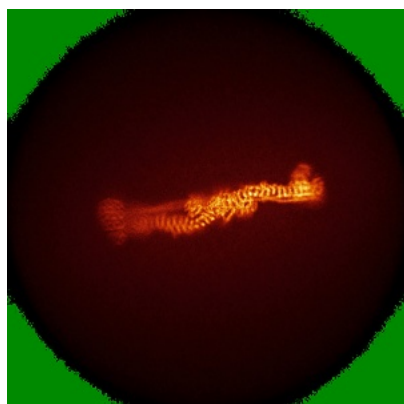


Z Index: 278

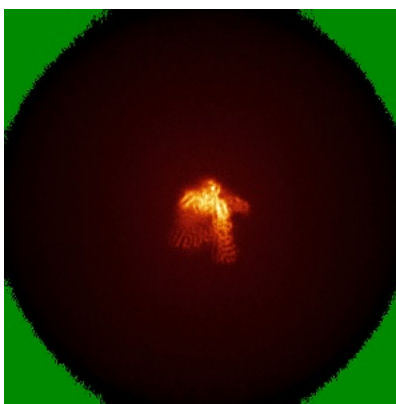
The images above show the largest variance slices of the map in three orthogonal directions.

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

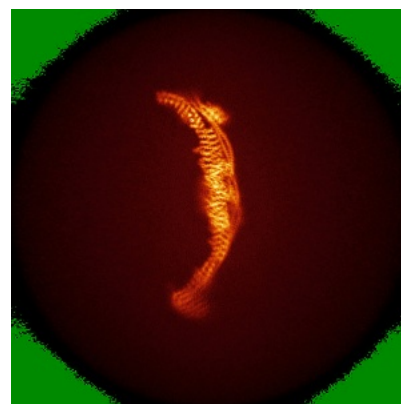
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

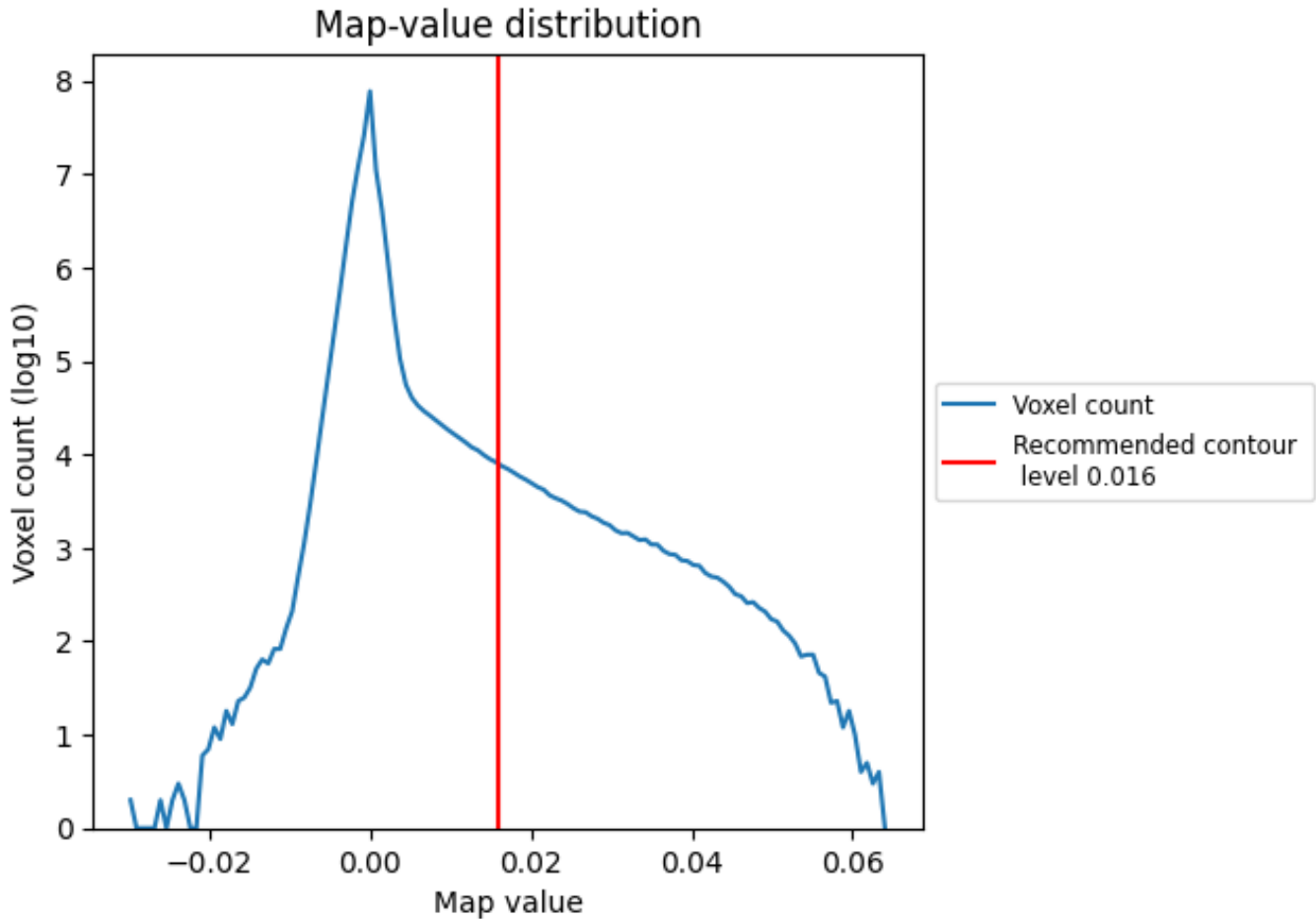
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

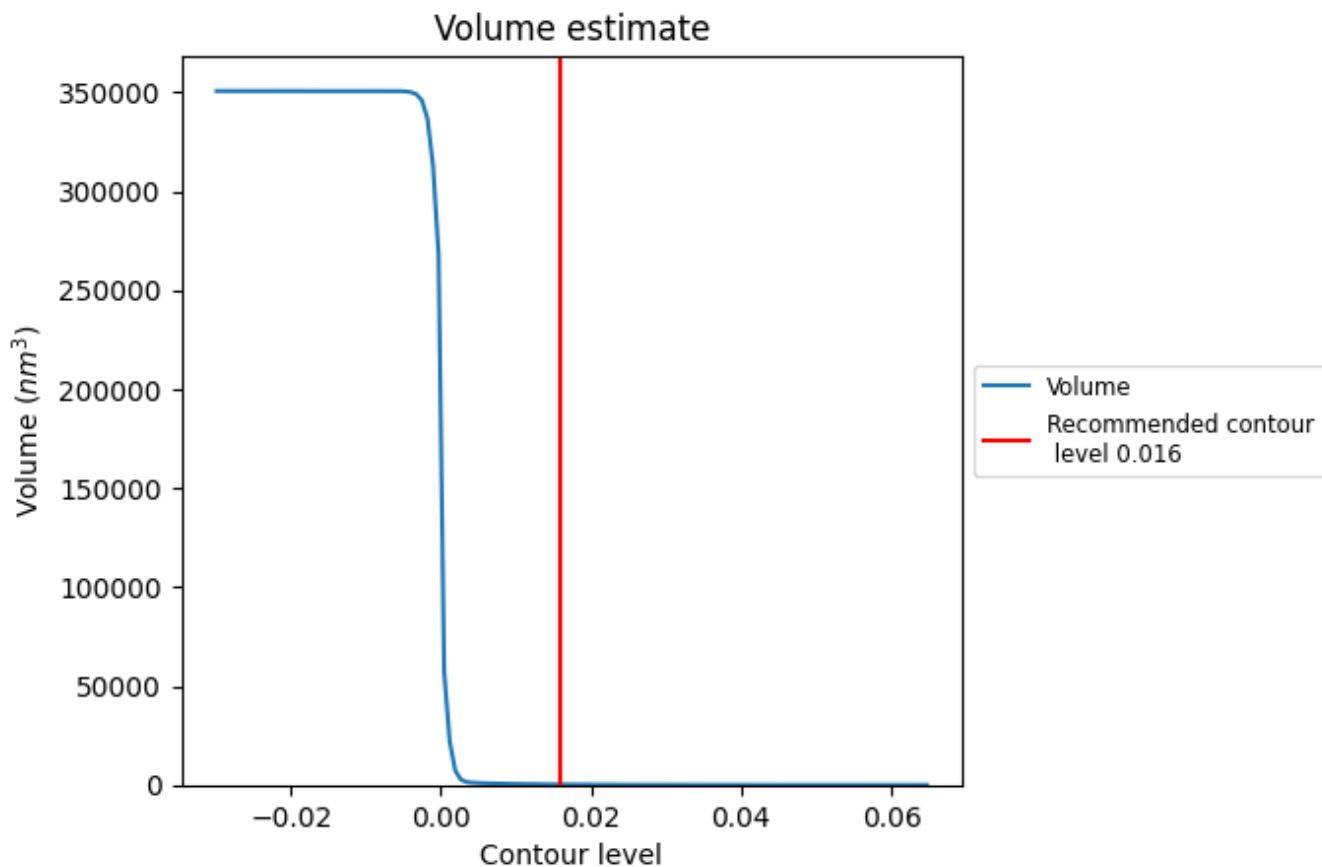
This section contains the results of statistical analysis of the map.

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.

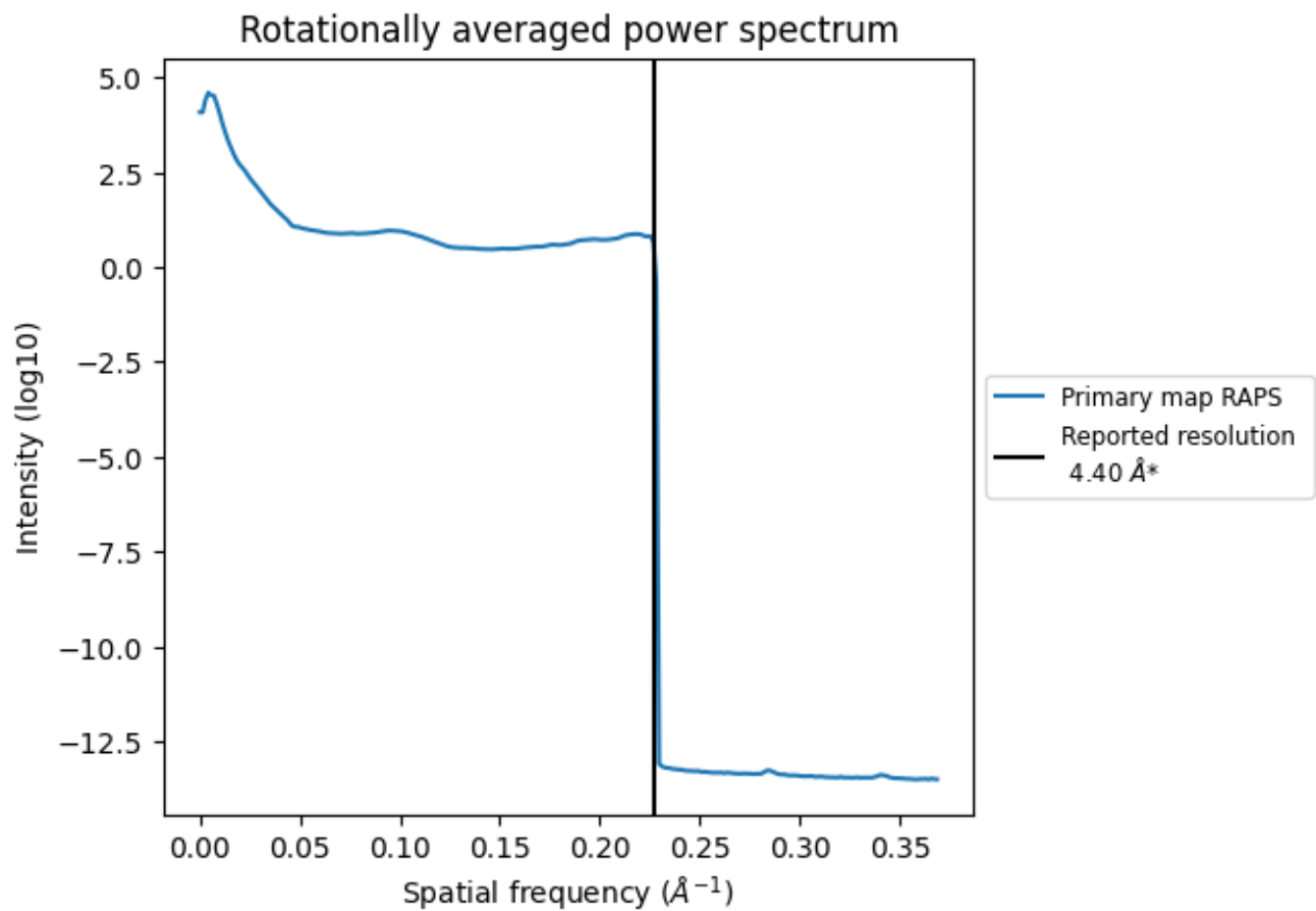
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 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 0.227 Å⁻¹

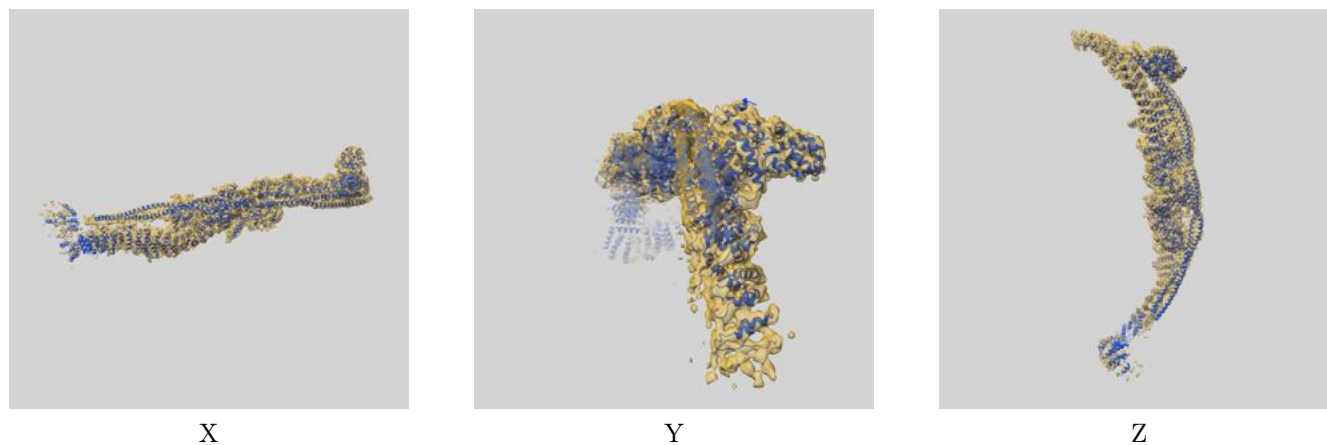
8 Fourier-Shell correlation

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-30708 and PDB model 7DL2. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



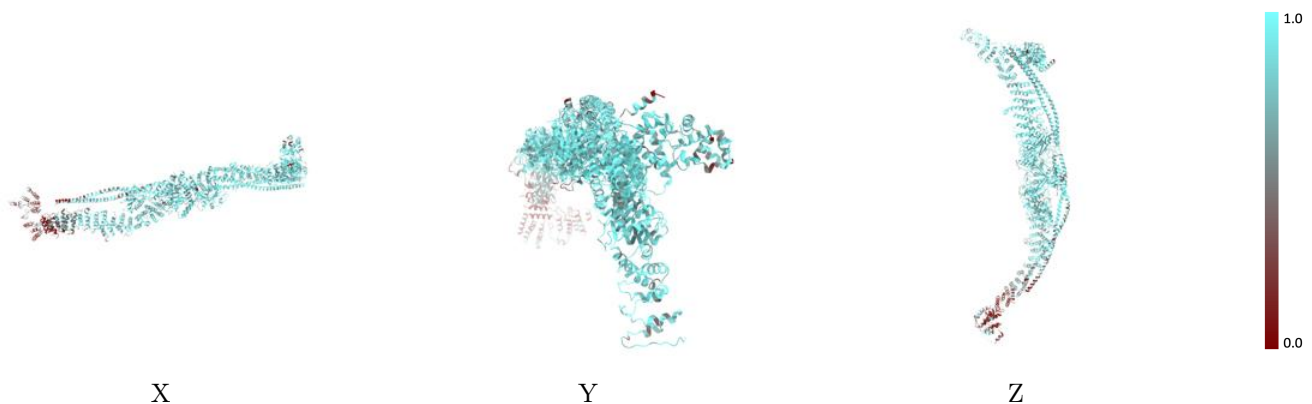
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



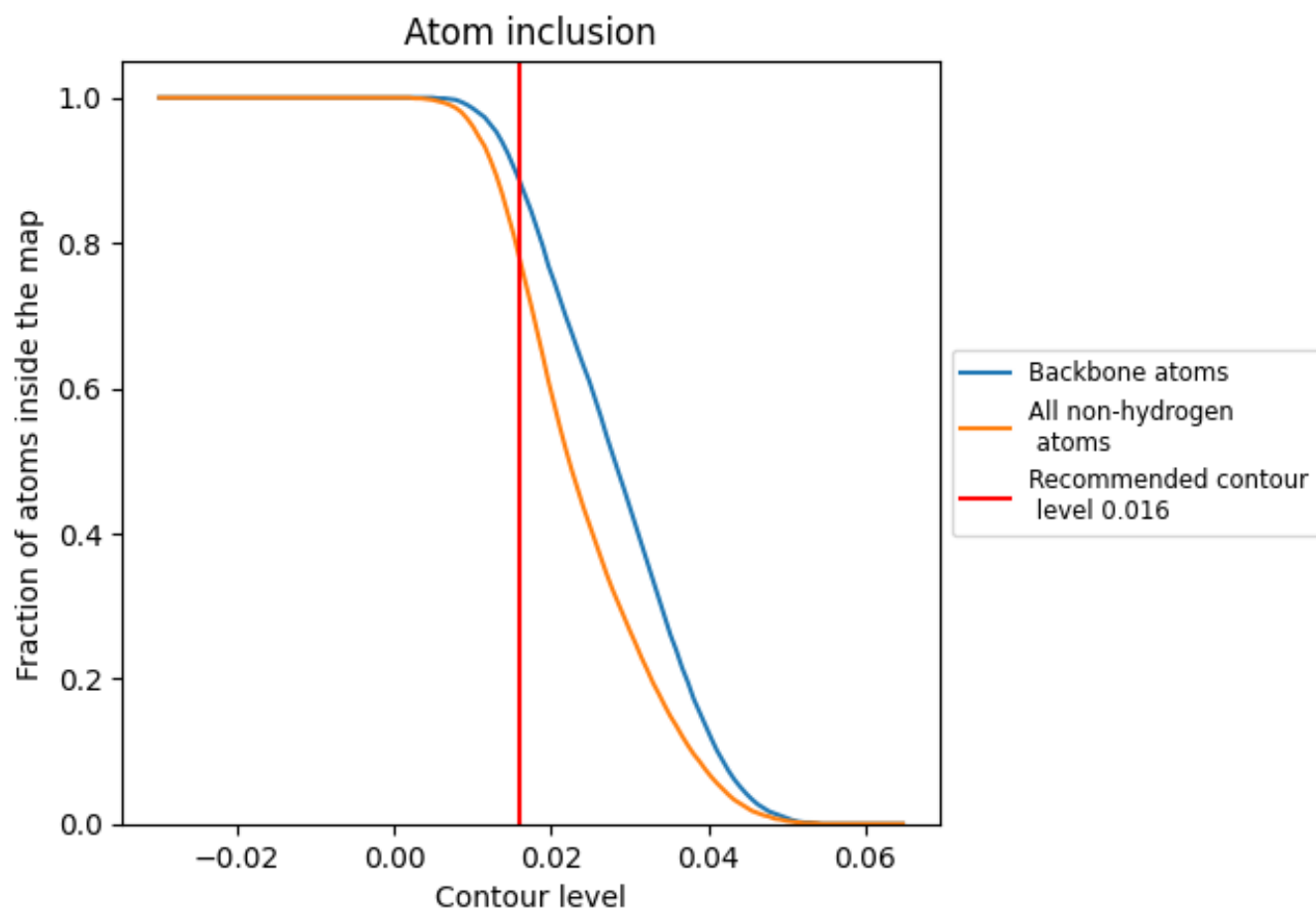
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).















9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7780	 0.3030
A	 0.8560	 0.3380
B	 0.7500	 0.3040
C	 0.7780	 0.2320
D	 0.7650	 0.2370
E	 0.8080	 0.2620
F	 0.2780	 0.2850

