Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 02:09 PM EST

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

This is a 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 (i) 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 (i)) were used in the production of this report:

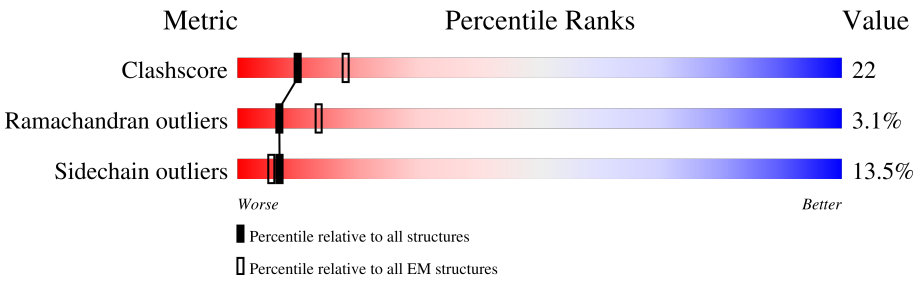
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 <=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	1058	27% 56% 32% 10% ••
2	B	1333	14% 62% 22% • 11%
2	C	1333	13% 63% 25% 5% 7%
3	D	448	9% 31% 28% 6% 35%
3	E	448	5% 30% 28% 7% 35%

2 Entry composition (i)

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

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

- Molecule 1 is a protein called Structural protein VP3.

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

- Molecule 2 is a protein called VP1.

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

- Molecule 3 is a protein called Structural protein VP5.

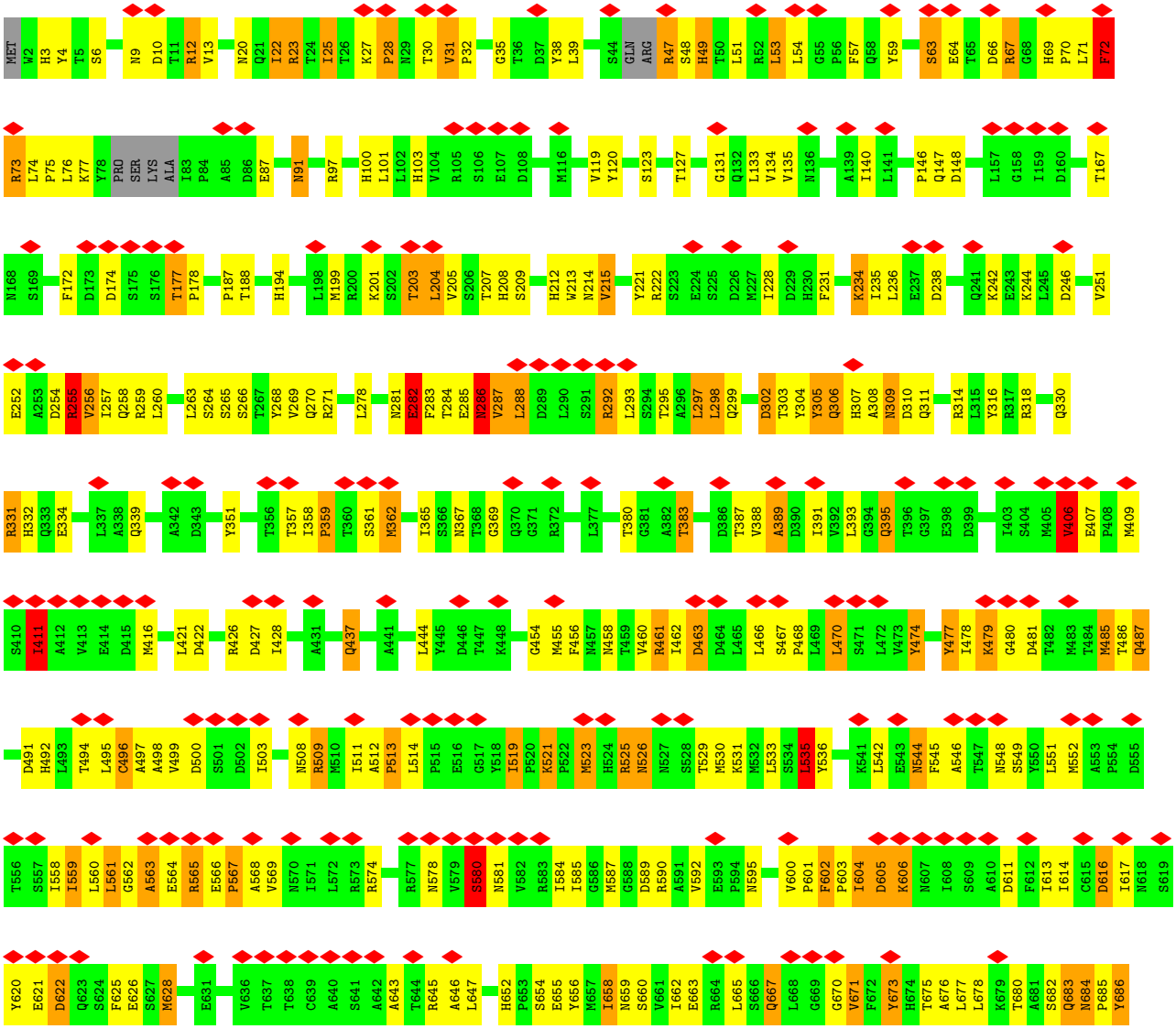
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	291	2276	1446	398	424	8	0	0
3	E	291	2276	1446	398	424	8	0	0

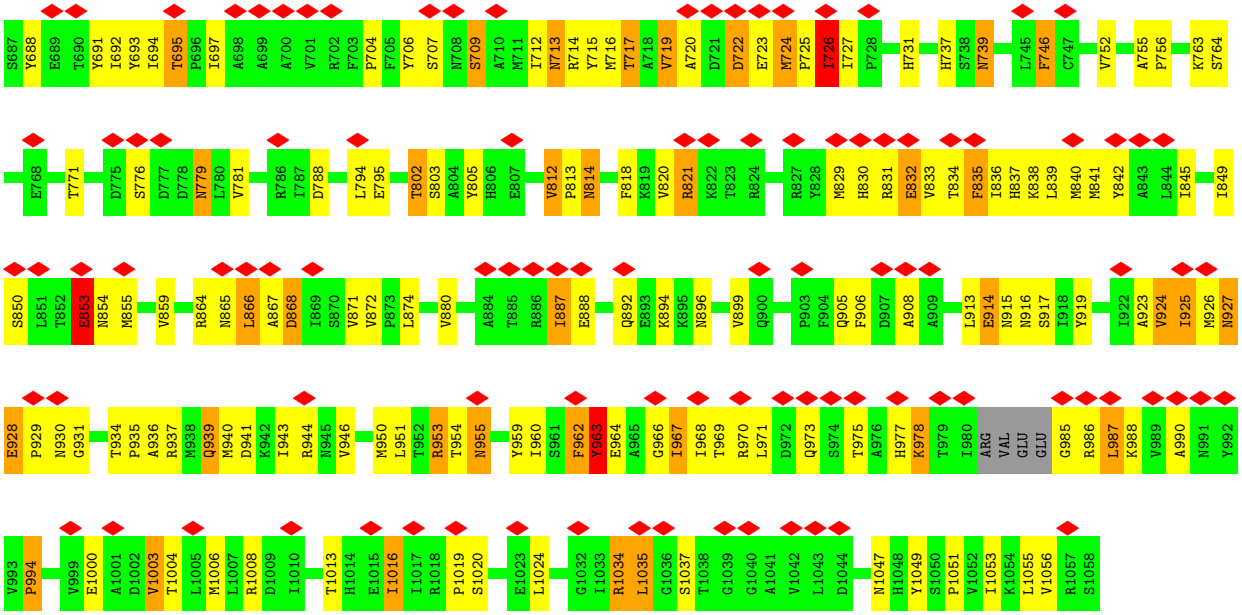
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Structural protein VP3

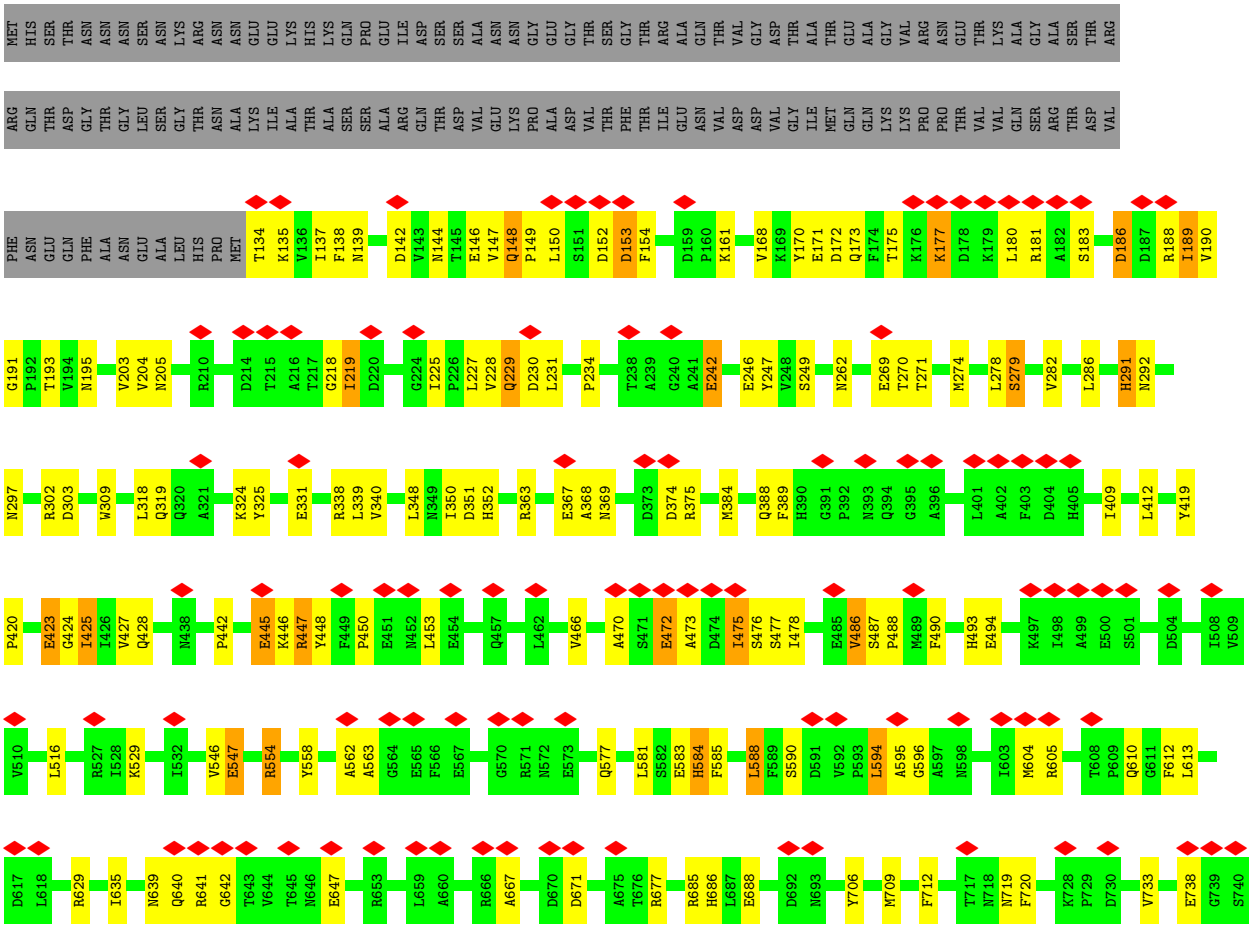
Chain A:

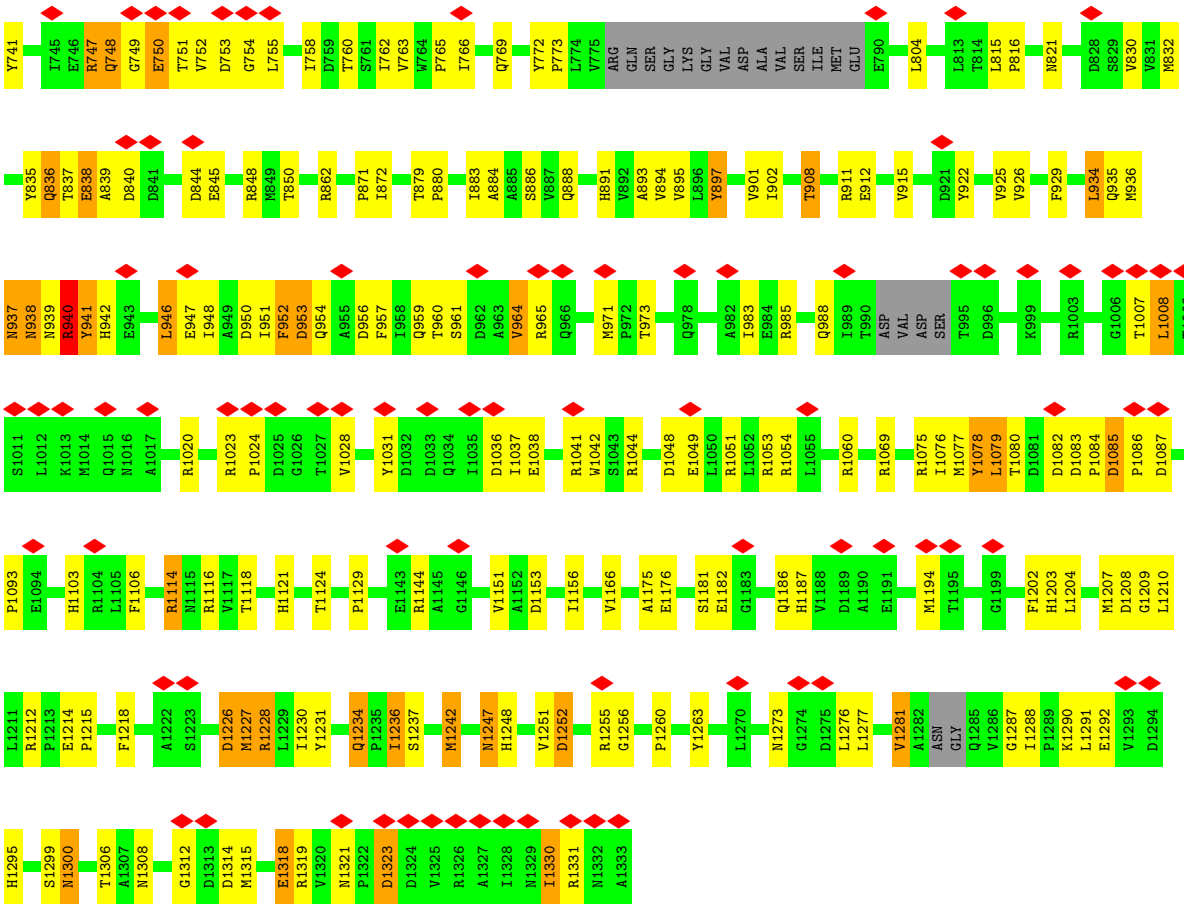




- Molecule 2: VP1

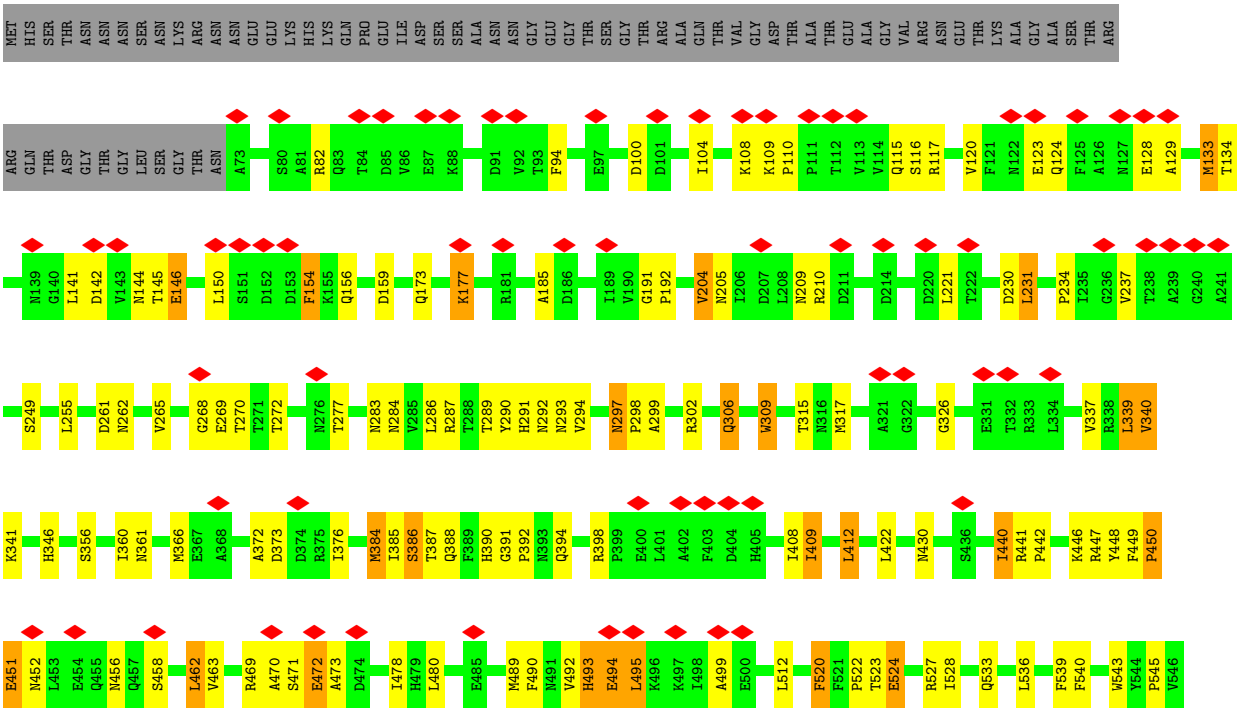
Chain B:

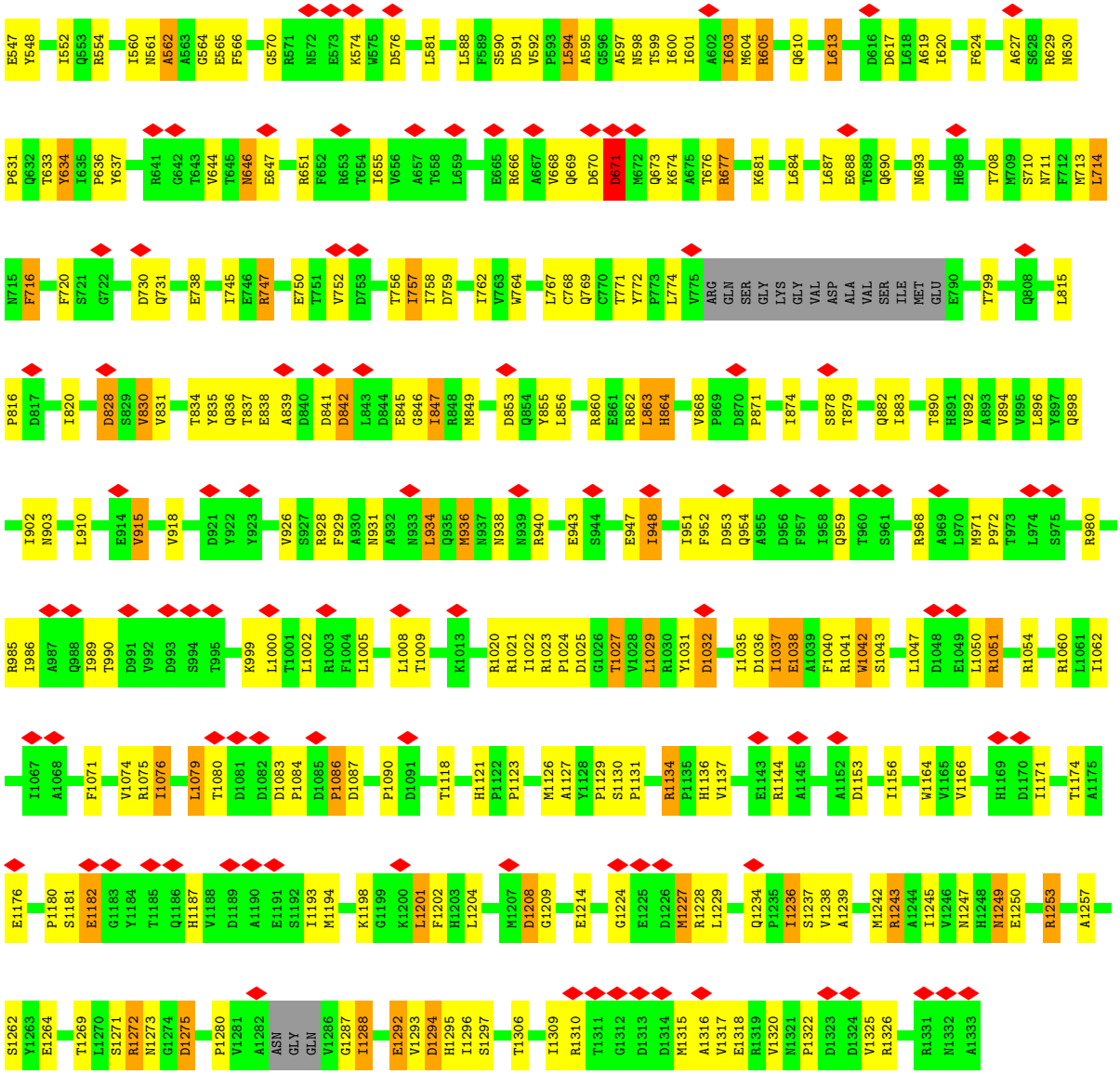




- Molecule 2: VP1

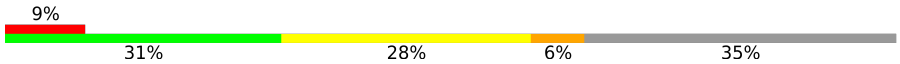
Chain C:

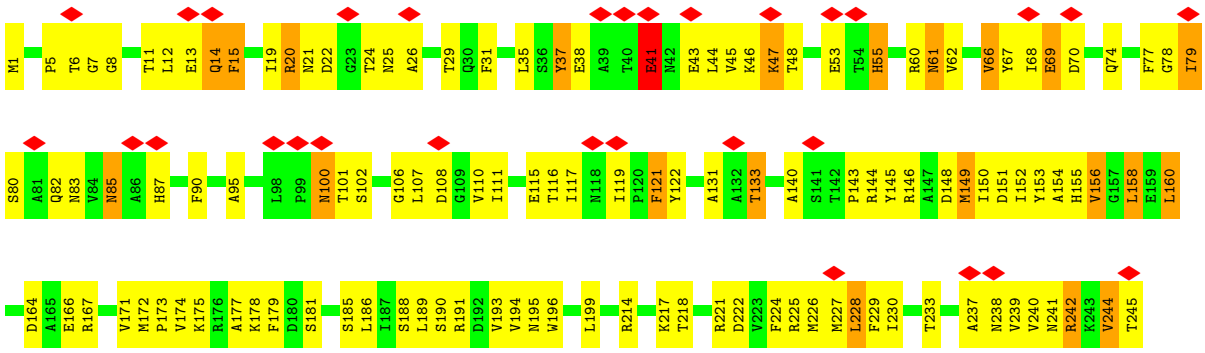


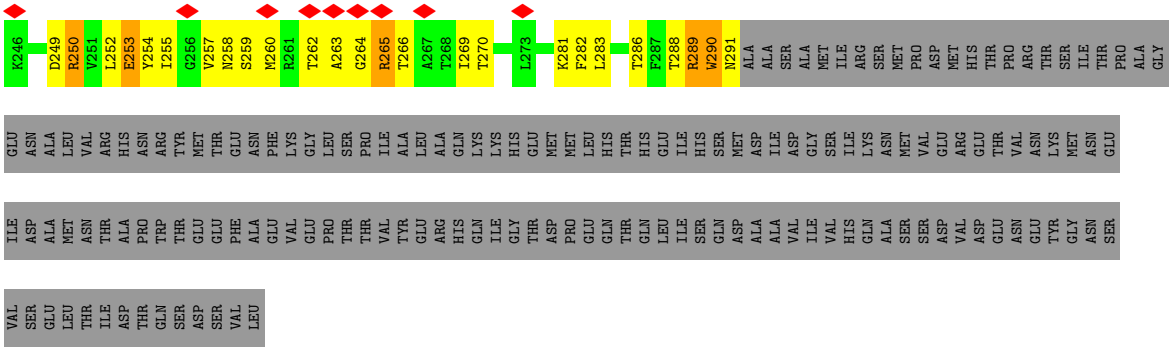


• Molecule 3: Structural protein VP5

Chain D:

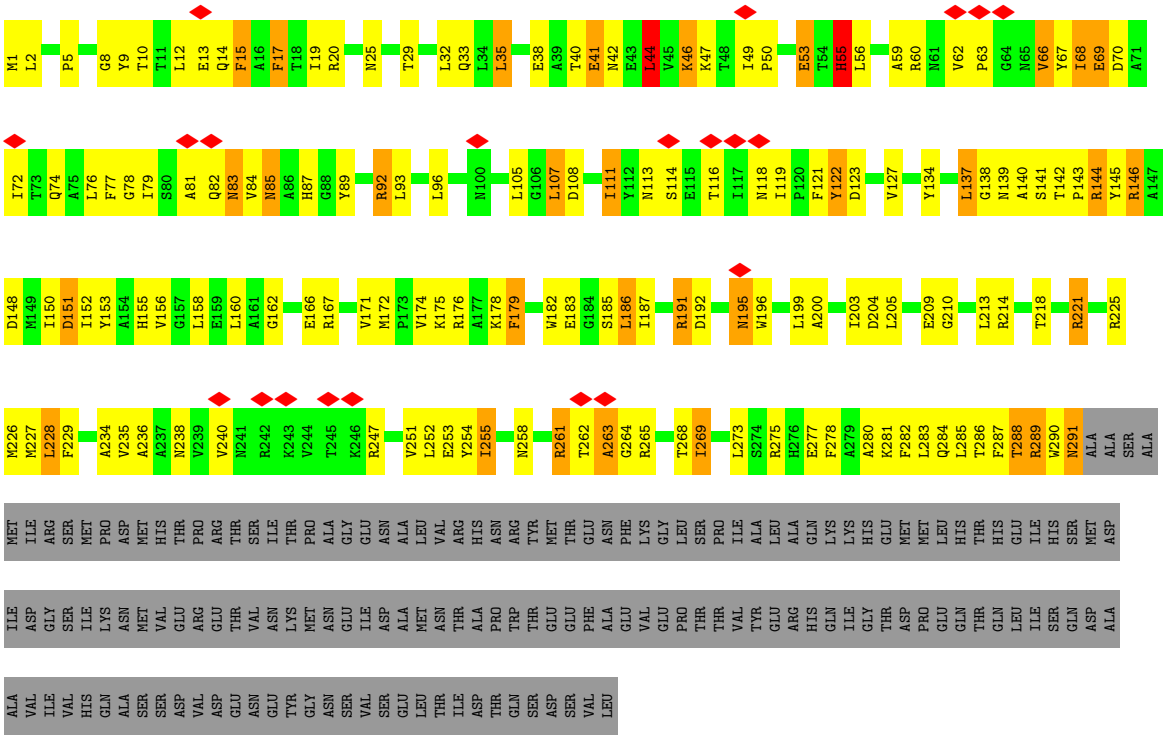






• Molecule 3: Structural protein VP5

Chain E: 5% 30% 28% 7% 35%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	each image	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125390	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	15.127	Depositor
Minimum map value	-10.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.6	Depositor
Map size (Å)	861.12, 861.12, 430.56	wwPDB
Map dimensions	720, 720, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.196, 1.196, 1.196	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: GPL

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

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	8372	0	8310	421	0
2	B	9317	0	9234	336	0
2	C	9806	0	9713	336	0
3	D	2276	0	2271	227	0
3	E	2276	0	2277	252	0
All	All	32047	0	31805	1392	0

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

All (1392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1037:ILE:HG12	2:B:1038:GLU:H	1.65	0.61
2:B:862:ARG:CB	2:B:952:PHE:CZ	2.84	0.60
2:B:951:ILE:O	2:B:952:PHE:CB	2.49	0.60
2:C:490:PHE:HA	2:C:745:ILE:HG22	1.83	0.60
2:C:520:PHE:HD1	2:C:520:PHE:H	1.49	0.60
2:C:1118:THR:HG22	2:C:1129:PRO:HA	1.82	0.60
3:E:40:THR:CG2	3:E:41:GLU:N	2.63	0.60
1:A:936:ALA:HA	1:A:939:GLN:HE21	1.67	0.60
3:E:40:THR:HG22	3:E:41:GLU:N	2.15	0.60
2:B:472:GLU:CD	2:B:472:GLU:H	2.03	0.60
2:B:427:VAL:HG11	2:B:755:LEU:CD2	2.32	0.60
2:C:231:LEU:CB	2:C:249:SER:HB2	2.32	0.60
2:C:879:THR:O	2:C:883:ILE:HG12	2.01	0.60
3:D:242:ARG:HH11	3:D:242:ARG:HG2	1.66	0.60
1:A:395:GLN:HA	1:A:395:GLN:NE2	2.17	0.60
1:A:936:ALA:O	1:A:940:MET:HB3	2.00	0.60
2:B:1276:LEU:HD22	2:B:1300:ASN:HB2	1.83	0.60
3:E:85:ASN:ND2	3:E:141:SER:CB	2.63	0.60
1:A:837:HIS:NE2	1:A:1047:ASN:HA	2.17	0.60
2:B:137:ILE:HD11	2:C:759:ASP:CB	2.31	0.60
2:B:1078:TYR:HE2	2:B:1080:THR:HG22	1.67	0.60
2:B:1114:ARG:HD3	2:B:1116:ARG:HH21	1.67	0.60
3:D:217:LYS:CE	3:D:290:TRP:CE3	2.85	0.60
3:E:46:LYS:HD2	3:E:155:HIS:CE1	2.34	0.60
3:E:85:ASN:HD21	3:E:141:SER:CB	2.14	0.60
1:A:561:LEU:HD12	1:A:617:ILE:HD11	1.83	0.60
3:D:153:TYR:C	3:D:156:VAL:HG12	2.22	0.60
3:D:37:TYR:HD1	3:D:177:ALA:HB2	1.66	0.60
3:E:209:GLU:HG3	3:E:210:GLY:H	1.66	0.60
1:A:523:MET:HG2	1:A:574:ARG:NH2	2.16	0.60
1:A:940:MET:HA	1:A:943:ILE:HG12	1.83	0.59
2:C:286:LEU:CD2	2:C:290:TYR:HB3	2.31	0.59
2:C:841:ASP:H	2:C:940:ARG:HH12	1.51	0.59
2:C:1288:ILE:HD13	2:C:1288:ILE:H	1.67	0.59
3:D:224:PHE:O	3:D:228:LEU:HB2	2.02	0.59
2:C:392:PRO:HG2	2:C:1315:MET:HG3	1.84	0.59
2:B:1236:ILE:CG1	2:B:1237:SER:N	2.62	0.59
2:C:373:ASP:HB2	2:C:394:GLN:HG3	1.83	0.59
3:D:5:PRO:O	3:D:6:THR:CB	2.50	0.59
1:A:831:ARG:HB3	1:A:835:PHE:CE2	2.38	0.59
2:B:1236:ILE:HG12	2:B:1237:SER:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:341:LYS:CD	2:C:1306:THR:HG21	2.32	0.59
3:D:47:LYS:HG3	3:D:48:THR:N	2.18	0.59
3:E:68:ILE:CD1	3:E:72:ILE:CD1	2.77	0.59
3:E:67:TYR:HB3	3:E:70:ASP:HB3	1.85	0.59
1:A:529:THR:HG22	1:A:568:ALA:HB2	1.84	0.59
1:A:535:LEU:HD11	1:A:614:ILE:HG21	1.85	0.59
2:B:862:ARG:HB3	2:B:952:PHE:CZ	2.37	0.59
2:C:1042:TRP:CB	2:C:1043:SER:CA	2.79	0.59
3:E:1:MET:CE	3:E:121:PHE:CD2	2.85	0.59
3:E:262:THR:O	3:E:263:ALA:C	2.41	0.59
2:B:752:VAL:CG2	2:B:755:LEU:HB2	2.33	0.58
2:C:1080:THR:HG21	2:C:1227:MET:SD	2.43	0.58
3:E:153:TYR:CD1	3:E:156:VAL:HG21	2.37	0.58
1:A:201:LYS:O	2:B:629:ARG:HG3	2.03	0.58
1:A:717:THR:HG21	1:A:1020:SER:HB2	1.85	0.58
1:A:486:THR:C	1:A:487:GLN:HG3	2.23	0.58
3:D:253:GLU:CD	3:D:254:TYR:CD2	2.76	0.58
3:E:85:ASN:CG	3:E:85:ASN:O	2.41	0.58
1:A:565:ARG:HB2	1:A:592:VAL:HB	1.84	0.58
2:C:356:SER:O	2:C:360:ILE:HG12	2.04	0.58
1:A:549:SER:O	1:A:551:LEU:N	2.33	0.58
2:B:612:PHE:CZ	2:B:635:ILE:HD11	2.39	0.58
2:C:910:LEU:HD13	2:C:915:VAL:HG23	1.86	0.58
3:D:77:PHE:CZ	3:D:227:MET:HB2	2.39	0.58
1:A:268:TYR:CZ	2:B:562:ALA:HB1	2.38	0.58
1:A:519:ILE:HD13	1:A:519:ILE:H	1.69	0.58
2:C:192:PRO:HG3	2:C:294:VAL:HB	1.86	0.58
2:C:1042:TRP:HB3	2:C:1043:SER:HB2	1.86	0.58
1:A:303:THR:HA	1:A:307:HIS:CE1	2.39	0.58
1:A:481:ASP:CB	1:A:511:ILE:HG12	2.30	0.58
2:C:838:GLU:O	2:C:940:ARG:NH1	2.36	0.58
2:B:950:ASP:CG	2:B:951:ILE:N	2.57	0.58
3:D:217:LYS:CE	3:D:290:TRP:CZ3	2.87	0.58
3:E:1:MET:HE3	3:E:121:PHE:CD2	2.39	0.58
1:A:499:VAL:HB	1:A:503:ILE:HD11	1.86	0.58
1:A:283:PHE:HA	1:A:284:THR:C	2.24	0.58
2:B:139:ASN:O	2:C:757:ILE:HG22	2.03	0.57
2:B:872:ILE:HG12	2:B:886:SER:HB2	1.85	0.57
2:B:960:THR:HG23	2:B:965:ARG:HH12	1.68	0.57
3:D:217:LYS:HE2	3:D:290:TRP:CE3	2.38	0.57
1:A:47:ARG:NH2	2:B:596:GLY:HA3	2.12	0.57

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:PHE:HB3	2:B:1151:VAL:HG21	1.88	0.56
2:C:902:ILE:HB	2:C:929:PHE:HB3	1.88	0.56
2:C:269:GLU:HB3	2:C:292:ASN:CG	2.26	0.56
2:C:668:VAL:HG11	2:C:673:GLN:HB2	1.88	0.56
3:D:239:VAL:HG23	3:D:263:ALA:HB1	1.87	0.56
1:A:308:ALA:N	1:A:309:ASN:CB	2.56	0.55
2:C:1031:TYR:O	2:C:1032:ASP:HB3	2.06	0.55
3:E:81:ALA:H	3:E:275:ARG:HH21	1.54	0.55
1:A:351:TYR:OH	3:D:150:ILE:HB	2.07	0.55
3:E:150:ILE:O	3:E:150:ILE:CG2	2.54	0.55
1:A:201:LYS:C	2:B:629:ARG:HD3	2.27	0.55
1:A:388:VAL:HG22	1:A:389:ALA:H	1.71	0.55
2:B:191:GLY:HA2	2:B:193:THR:N	2.22	0.55
2:C:154:PHE:HA	2:C:262:ASN:HD22	1.71	0.55
3:E:85:ASN:C	3:E:85:ASN:OD1	2.44	0.55
3:E:284:GLN:O	3:E:288:THR:CG2	2.54	0.55
1:A:87:GLU:O	1:A:91:ASN:HB2	2.07	0.55
1:A:486:THR:HA	1:A:491:ASP:OD2	2.07	0.55
1:A:602:PHE:HD1	1:A:602:PHE:H	1.54	0.55
1:A:820:VAL:HG12	1:A:821:ARG:H	1.72	0.55
2:B:142:ASP:HB3	2:B:1318:GLU:HG2	1.89	0.55
2:B:494:GLU:HG2	2:B:577:GLN:HG3	1.88	0.55
2:B:733:VAL:HG21	2:B:741:TYR:HD1	1.70	0.55
2:C:539:PHE:O	2:C:543:TRP:HB3	2.06	0.55
3:E:209:GLU:O	3:E:213:LEU:CB	2.55	0.55
1:A:63:SER:OG	1:A:123:SER:HA	2.07	0.55
1:A:318:ARG:NH1	3:D:43:GLU:CG	2.70	0.55
2:B:1087:ASP:OD2	2:B:1236:ILE:HG23	2.07	0.55
2:C:834:THR:HA	2:C:847:ILE:O	2.07	0.55
2:C:1071:PHE:HD1	2:C:1234:GLN:HG2	1.72	0.55
2:C:1325:VAL:HG12	2:C:1326:ARG:H	1.71	0.55
1:A:605:ASP:O	1:A:606:LYS:HB2	2.07	0.55
1:A:1024:LEU:HD21	1:A:1035:LEU:HD21	1.89	0.55
3:E:1:MET:O	3:E:121:PHE:O	2.24	0.55
1:A:562:GLY:HA2	1:A:616:ASP:O	2.07	0.54
1:A:47:ARG:HE	2:B:595:ALA:C	2.05	0.54
1:A:71:LEU:HD11	1:A:91:ASN:CG	2.27	0.54
2:B:558:TYR:CE2	2:B:585:PHE:HB2	2.42	0.54
2:C:1074:VAL:HG12	2:C:1171:ILE:HG21	1.88	0.54
1:A:523:MET:HG2	1:A:574:ARG:HH22	1.73	0.54
3:E:238:ASN:O	3:E:253:GLU:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:285:LEU:O	3:E:288:THR:HG23	2.08	0.54
2:B:1247:ASN:HD22	2:B:1247:ASN:H	1.55	0.54
2:C:1035:ILE:HG22	2:C:1036:ASP:H	1.71	0.54
2:C:1153:ASP:HA	2:C:1156:ILE:HG22	1.90	0.54
3:E:262:THR:HG22	3:E:263:ALA:N	2.21	0.54
2:C:594:LEU:HD12	2:C:597:ALA:HB3	1.88	0.54
3:E:1:MET:O	3:E:2:LEU:CB	2.55	0.54
1:A:467:SER:N	1:A:468:PRO:HD2	2.23	0.54
2:B:1084:PRO:CG	2:B:1209:GLY:HA3	2.35	0.54
1:A:569:VAL:HG11	1:A:595:ASN:HD21	1.73	0.54
3:D:290:TRP:HE3	3:D:290:TRP:C	2.11	0.54
3:E:107:LEU:HD23	3:E:122:TYR:HE1	1.70	0.54
3:E:253:GLU:O	3:E:254:TYR:CD1	2.61	0.54
1:A:559:ILE:CG2	1:A:613:ILE:HG12	2.38	0.54
2:B:338:ARG:HH21	2:C:1005:LEU:HD12	1.71	0.54
2:B:862:ARG:CB	2:B:952:PHE:CE2	2.89	0.54
2:C:141:LEU:HD23	2:C:141:LEU:H	1.73	0.54
2:C:440:ILE:HD12	2:C:478:ILE:HG21	1.88	0.54
3:D:25:ASN:C	3:D:25:ASN:OD1	2.45	0.54
2:B:1008:LEU:HD13	2:B:1008:LEU:H	1.73	0.54
1:A:531:LYS:HE2	1:A:683:GLN:NE2	2.23	0.54
2:C:129:ALA:HB3	2:C:133:MET:HG2	1.90	0.54
2:C:287:ARG:HH21	2:C:326:GLY:CA	2.18	0.54
2:C:931:ASN:ND2	2:C:934:LEU:O	2.38	0.54
1:A:293:LEU:O	1:A:297:LEU:HB2	2.09	0.53
1:A:719:VAL:HG13	1:A:720:ALA:N	2.23	0.53
2:C:146:GLU:O	2:C:1316:ALA:HA	2.08	0.53
3:D:156:VAL:HG23	3:D:228:LEU:HD23	1.88	0.53
3:E:229:PHE:CE1	3:E:252:LEU:CD1	2.90	0.53
1:A:236:LEU:HD13	1:A:236:LEU:O	2.08	0.53
2:C:1131:PRO:HA	2:C:1134:ARG:NH1	2.23	0.53
3:D:178:LYS:O	3:D:178:LYS:CG	2.56	0.53
3:D:239:VAL:HG23	3:D:263:ALA:CB	2.38	0.53
3:E:14:GLN:N	3:E:14:GLN:CD	2.61	0.53
1:A:830:HIS:HD2	1:A:1034:ARG:NH1	2.03	0.53
2:B:635:ILE:HG22	2:B:706:TYR:HB3	1.90	0.53
2:B:862:ARG:HB3	2:B:952:PHE:HE2	1.70	0.53
2:C:1273:ASN:O	3:E:183:GLU:CD	2.46	0.53
3:E:76:LEU:HD12	3:E:76:LEU:H	1.73	0.53
1:A:194:HIS:CG	3:D:146:ARG:NH1	2.62	0.53
2:C:868:VAL:HB	2:C:890:THR:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:142:THR:HG22	3:E:144:ARG:H	1.73	0.53
1:A:667:GLN:CD	1:A:667:GLN:N	2.62	0.53
2:C:554:ARG:O	2:C:570:GLY:HA2	2.09	0.53
3:D:242:ARG:HG2	3:D:242:ARG:NH1	2.23	0.53
1:A:426:ARG:HG3	1:A:428:ILE:H	1.74	0.53
1:A:722:ASP:CG	1:A:723:GLU:H	2.11	0.53
3:E:214:ARG:O	3:E:218:THR:CG2	2.57	0.53
1:A:407:GLU:OE1	1:A:1034:ARG:HG2	2.08	0.53
1:A:563:ALA:HA	1:A:564:GLU:CG	2.33	0.53
2:C:716:PHE:CD1	2:C:716:PHE:N	2.76	0.53
2:C:841:ASP:N	2:C:940:ARG:HH12	2.06	0.53
2:C:853:ASP:HB2	3:D:117:ILE:CG1	2.39	0.53
2:C:862:ARG:HG2	2:C:952:PHE:HE1	1.72	0.53
2:B:147:VAL:HG22	2:B:1315:MET:N	2.22	0.53
2:B:546:VAL:HG13	2:B:547:GLU:HG3	1.91	0.53
2:B:1060:ARG:HH12	2:B:1292:GLU:HA	1.74	0.53
2:C:838:GLU:CB	2:C:934:LEU:HB2	2.39	0.53
2:C:841:ASP:CG	2:C:842:ASP:H	2.12	0.53
3:D:172:MET:CE	3:D:175:LYS:HG3	2.33	0.53
1:A:59:TYR:CA	1:A:167:THR:HG21	2.36	0.53
1:A:673:TYR:CD2	1:A:694:ILE:HG23	2.44	0.53
1:A:880:VAL:HB	1:A:899:VAL:HG12	1.91	0.53
1:A:926:MET:HG2	1:A:927:ASN:H	1.74	0.53
2:B:954:GLN:NE2	3:D:240:VAL:CG1	2.71	0.53
3:E:229:PHE:HE1	3:E:252:LEU:HD12	1.73	0.53
1:A:127:THR:HG23	2:B:641:ARG:H	1.74	0.52
1:A:283:PHE:HA	1:A:285:GLU:N	2.24	0.52
1:A:318:ARG:HH12	3:D:43:GLU:CD	2.12	0.52
2:C:309:TRP:CD1	2:C:1253:ARG:HB3	2.44	0.52
1:A:53:LEU:HD13	1:A:57:PHE:HB3	1.91	0.52
3:D:111:ILE:O	3:D:111:ILE:HG23	2.07	0.52
1:A:203:THR:H	2:B:629:ARG:HG2	1.73	0.52
1:A:755:ALA:N	1:A:756:PRO:HD2	2.23	0.52
2:C:339:LEU:C	2:C:341:LYS:H	2.12	0.52
3:D:189:LEU:HB3	3:D:230:ILE:HD11	1.91	0.52
2:B:448:TYR:CZ	2:B:470:ALA:HB1	2.45	0.52
1:A:943:ILE:HA	1:A:946:VAL:HB	1.92	0.52
2:C:387:THR:HA	2:C:1322:PRO:HD3	1.92	0.52
2:C:1087:ASP:HB3	2:C:1236:ILE:HG13	1.92	0.52
1:A:6:SER:HB2	1:A:251:VAL:HG22	1.90	0.52
1:A:474:TYR:O	1:A:477:TYR:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ILE:HG12	1:A:585:ILE:HB	1.92	0.52
3:E:74:GLN:O	3:E:78:GLY:HA3	2.10	0.52
3:E:240:VAL:O	3:E:251:VAL:HG22	2.09	0.52
1:A:271:ARG:HG3	1:A:316:TYR:OH	2.10	0.52
1:A:367:ASN:HD22	1:A:369:GLY:H	1.56	0.52
1:A:926:MET:HB2	1:A:931:GLY:HA3	1.91	0.52
2:B:138:PHE:O	2:C:759:ASP:OD1	2.27	0.52
2:B:338:ARG:HH21	2:C:1005:LEU:CD1	2.21	0.52
2:B:1048:ASP:HB3	2:B:1051:ARG:HB2	1.91	0.52
3:E:107:LEU:HD23	3:E:122:TYR:OH	2.09	0.52
1:A:127:THR:HG22	2:B:639:ASN:CB	2.36	0.52
2:C:520:PHE:CD1	2:C:520:PHE:N	2.78	0.52
3:D:115:GLU:OE2	3:D:115:GLU:N	2.30	0.52
1:A:22:ILE:HG12	1:A:25:ILE:HD11	1.91	0.52
2:B:1118:THR:HG22	2:B:1129:PRO:HA	1.90	0.52
2:C:669:GLN:O	2:C:670:ASP:HB2	2.09	0.52
1:A:282:GLU:O	1:A:285:GLU:HA	2.10	0.51
1:A:731:HIS:HB2	1:A:746:PHE:HB3	1.91	0.51
2:C:828:ASP:O	2:C:948:ILE:HA	2.10	0.51
3:D:217:LYS:HE2	3:D:290:TRP:CZ3	2.45	0.51
1:A:282:GLU:HG3	1:A:286:ASN:OD1	2.11	0.51
1:A:422:ASP:HB3	1:A:677:LEU:HD12	1.93	0.51
1:A:832:GLU:CD	1:A:833:VAL:H	2.13	0.51
3:E:1:MET:HE2	3:E:123:ASP:HA	1.92	0.51
3:E:290:TRP:HD1	3:E:291:ASN:HB3	1.75	0.51
1:A:146:PRO:O	1:A:147:GLN:HB3	2.10	0.51
1:A:406:VAL:CB	1:A:407:GLU:CA	2.79	0.51
1:A:723:GLU:O	1:A:724:MET:CB	2.59	0.51
1:A:966:GLY:O	1:A:970:ARG:HD3	2.10	0.51
2:B:338:ARG:NH2	2:C:1005:LEU:CD1	2.73	0.51
2:C:261:ASP:O	2:C:1054:ARG:NH1	2.43	0.51
2:B:368:ALA:CA	3:D:83:ASN:HD22	2.24	0.51
2:C:1264:GLU:HA	2:C:1297:SER:HA	1.93	0.51
3:D:153:TYR:C	3:D:156:VAL:CG1	2.79	0.51
1:A:292:ARG:HG2	1:A:295:THR:CG2	2.40	0.51
3:D:44:LEU:HD11	3:D:154:ALA:CA	2.31	0.51
3:D:214:ARG:O	3:D:218:THR:CG2	2.51	0.51
3:E:53:GLU:HB2	3:E:145:TYR:CE1	2.45	0.51
3:E:83:ASN:OD1	3:E:83:ASN:N	2.43	0.51
3:E:262:THR:O	3:E:263:ALA:HB3	2.10	0.51
1:A:201:LYS:HA	2:B:629:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:CG2	1:A:407:GLU:HA	2.40	0.51
1:A:437:GLN:HB3	1:A:656:TYR:HB2	1.92	0.51
1:A:508:ASN:HB2	1:A:509:ARG:HH11	1.74	0.51
2:C:448:TYR:HB3	2:C:768:CYS:HG	1.72	0.51
3:E:290:TRP:CD1	3:E:290:TRP:C	2.84	0.51
2:B:153:ASP:HB3	2:B:154:PHE:HD1	1.75	0.51
3:D:21:ASN:O	3:D:24:THR:O	2.29	0.51
3:E:82:GLN:HG2	3:E:83:ASN:OD1	2.10	0.51
3:E:283:LEU:O	3:E:287:PHE:HB2	2.11	0.51
2:B:134:THR:CG2	2:C:472:GLU:CD	2.79	0.51
2:B:269:GLU:O	2:B:291:HIS:CD2	2.63	0.51
2:B:279:SER:CA	2:C:1198:LYS:HE2	2.41	0.51
2:C:255:LEU:HD23	2:C:1062:ILE:HD13	1.93	0.51
2:C:931:ASN:OD1	2:C:934:LEU:HD22	2.11	0.51
3:D:153:TYR:HA	3:D:156:VAL:HG11	1.86	0.51
1:A:59:TYR:HA	1:A:167:THR:CG2	2.38	0.51
1:A:133:LEU:CD2	2:C:545:PRO:HB3	2.41	0.51
2:C:339:LEU:O	2:C:340:VAL:HG22	2.09	0.51
3:D:149:MET:CE	3:D:260:MET:HE2	2.38	0.51
3:E:160:LEU:HD11	3:E:229:PHE:CB	2.36	0.51
1:A:47:ARG:HE	2:B:596:GLY:CA	2.22	0.50
1:A:926:MET:SD	1:A:930:ASN:O	2.69	0.50
3:D:290:TRP:CE3	3:D:290:TRP:C	2.85	0.50
3:E:12:LEU:HD23	3:E:15:PHE:CZ	2.46	0.50
1:A:605:ASP:O	1:A:606:LYS:CB	2.60	0.50
2:B:368:ALA:O	3:D:83:ASN:ND2	2.41	0.50
2:C:412:LEU:HD11	2:C:714:LEU:HD23	1.93	0.50
2:C:716:PHE:N	2:C:716:PHE:HD1	2.09	0.50
2:C:871:PRO:HB2	2:C:896:LEU:HD23	1.93	0.50
3:D:250:ARG:HB3	3:D:250:ARG:HH11	1.76	0.50
1:A:567:PRO:O	1:A:568:ALA:HB3	2.12	0.50
1:A:709:SER:HB2	1:A:712:ILE:HB	1.94	0.50
1:A:840:MET:SD	1:A:1019:PRO:HB2	2.51	0.50
3:E:62:VAL:HG23	3:E:63:PRO:HD2	1.93	0.50
2:B:747:ARG:O	2:B:747:ARG:CG	2.58	0.50
2:B:836:GLN:HE22	2:B:844:ASP:HA	1.75	0.50
2:B:926:VAL:O	2:B:926:VAL:CG1	2.59	0.50
2:C:835:TYR:O	2:C:846:GLY:HA3	2.12	0.50
2:C:1126:MET:HG3	2:C:1127:ALA:H	1.76	0.50
3:D:153:TYR:O	3:D:156:VAL:HG12	2.11	0.50
3:D:289:ARG:HA	3:D:289:ARG:NE	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:291:ASN:OD1	3:D:291:ASN:C	2.50	0.50
3:E:236:ALA:O	3:E:263:ALA:HA	2.10	0.50
3:E:289:ARG:O	3:E:289:ARG:CD	2.35	0.50
2:B:862:ARG:HH12	2:B:948:ILE:HD13	1.77	0.50
2:B:1263:TYR:CG	2:B:1295:HIS:HD2	2.29	0.50
2:C:520:PHE:HD1	2:C:520:PHE:N	2.10	0.50
1:A:298:LEU:CD1	2:B:563:ALA:HB3	2.42	0.50
2:B:941:TYR:O	2:B:941:TYR:CD1	2.65	0.50
2:B:1078:TYR:CE2	2:B:1080:THR:HG22	2.46	0.50
3:E:41:GLU:O	3:E:41:GLU:OE1	2.30	0.50
1:A:208:HIS:HB3	1:A:260:LEU:HA	1.93	0.50
2:C:298:PRO:O	2:C:299:ALA:HB3	2.12	0.50
2:C:522:PRO:HG3	2:C:636:PRO:HB2	1.94	0.50
3:D:15:PHE:N	3:D:15:PHE:CD1	2.80	0.50
1:A:76:LEU:HB2	1:A:172:PHE:CE2	2.47	0.50
1:A:283:PHE:CA	1:A:284:THR:C	2.80	0.50
1:A:308:ALA:CB	1:A:309:ASN:HB2	2.41	0.50
2:C:384:MET:HA	2:C:708:THR:HG21	1.93	0.50
2:C:853:ASP:O	3:D:117:ILE:HD11	2.12	0.50
2:C:1037:ILE:O	2:C:1038:GLU:CB	2.58	0.50
3:D:153:TYR:CE2	3:D:258:ASN:ND2	2.80	0.50
3:E:10:THR:HG23	3:E:17:PHE:HZ	1.77	0.50
3:E:69:GLU:O	3:E:69:GLU:OE2	2.30	0.50
1:A:351:TYR:CE1	3:D:150:ILE:HG21	2.47	0.49
1:A:395:GLN:HE21	1:A:395:GLN:CA	2.20	0.49
1:A:845:ILE:O	1:A:849:ILE:HG12	2.11	0.49
2:B:135:LYS:HG3	2:C:470:ALA:O	2.09	0.49
2:B:953:ASP:OD1	3:D:241:ASN:OD1	2.30	0.49
2:B:225:ILE:HG23	2:B:247:TYR:CD2	2.46	0.49
2:B:269:GLU:HB3	2:B:292:ASN:HD22	1.76	0.49
2:B:1276:LEU:HB3	2:B:1290:LYS:HD3	1.95	0.49
2:C:284:ASN:OD1	2:C:284:ASN:N	2.44	0.49
1:A:64:GLU:CG	2:B:647:GLU:OE1	2.60	0.49
2:C:293:ASN:CG	2:C:294:VAL:H	2.16	0.49
3:E:13:GLU:CD	3:E:13:GLU:C	2.71	0.49
1:A:64:GLU:HG3	2:B:647:GLU:OE1	2.12	0.49
1:A:188:THR:HG21	3:D:144:ARG:HG2	1.93	0.49
1:A:416:MET:HG2	1:A:466:LEU:HD21	1.94	0.49
1:A:602:PHE:HD1	1:A:602:PHE:N	2.11	0.49
1:A:662:ILE:HG12	1:A:675:THR:HG21	1.93	0.49
2:C:270:THR:HA	2:C:292:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:853:ASP:HB2	3:D:117:ILE:HG13	1.93	0.49
2:C:1280:PRO:HB3	2:C:1287:GLY:CA	2.41	0.49
3:D:107:LEU:HD23	3:D:122:TYR:CE1	2.47	0.49
1:A:213:TRP:O	1:A:215:VAL:N	2.36	0.49
1:A:254:ASP:O	1:A:255:ARG:CB	2.61	0.49
3:E:20:ARG:HD2	3:E:25:ASN:HB3	1.94	0.49
1:A:307:HIS:HD2	1:A:308:ALA:HB2	1.77	0.49
2:B:862:ARG:HB2	2:B:952:PHE:CZ	2.48	0.49
2:C:931:ASN:HB2	2:C:936:MET:SD	2.53	0.49
3:D:21:ASN:O	3:D:22:ASP:OD1	2.31	0.49
3:D:164:ASP:HA	3:D:167:ARG:HG2	1.94	0.49
3:E:84:VAL:HG23	3:E:85:ASN:N	2.28	0.49
1:A:242:LYS:O	1:A:246:ASP:HB2	2.12	0.49
2:B:139:ASN:O	2:C:757:ILE:CG2	2.61	0.49
2:C:1144:ARG:HD2	2:C:1194:MET:HA	1.95	0.49
2:C:1238:VAL:HG23	2:C:1239:ALA:H	1.77	0.49
3:D:172:MET:HG3	3:D:173:PRO:CD	2.42	0.49
3:D:181:SER:HB2	3:D:185:SER:OG	2.13	0.49
3:E:85:ASN:O	3:E:85:ASN:OD1	2.30	0.49
3:E:139:ASN:OD1	3:E:139:ASN:O	2.30	0.49
2:C:624:PHE:CE2	2:C:713:MET:HG2	2.48	0.49
2:C:1180:PRO:CB	2:C:1209:GLY:HA2	2.41	0.49
1:A:503:ILE:N	1:A:503:ILE:HD12	2.28	0.49
3:E:53:GLU:OE2	3:E:53:GLU:O	2.30	0.49
3:E:92:ARG:O	3:E:92:ARG:HD3	2.12	0.49
1:A:351:TYR:CZ	3:D:150:ILE:HG21	2.48	0.48
2:B:234:PRO:HD2	2:B:242:GLU:CB	2.43	0.48
3:E:38:GLU:HB3	3:E:176:ARG:HB3	1.95	0.48
3:E:66:VAL:HG13	3:E:111:ILE:CG2	2.42	0.48
3:E:72:ILE:O	3:E:76:LEU:CD1	2.61	0.48
1:A:409:MET:CB	1:A:1034:ARG:HH12	2.12	0.48
1:A:866:LEU:O	1:A:867:ALA:HB3	2.13	0.48
2:B:148:GLN:HA	2:B:148:GLN:OE1	2.13	0.48
2:C:528:ILE:HD11	2:C:758:ILE:HD12	1.96	0.48
2:C:533:GLN:HG2	2:C:588:LEU:HD23	1.95	0.48
2:C:878:SER:HB3	2:C:903:ASN:CB	2.43	0.48
3:D:121:PHE:N	3:D:121:PHE:CD1	2.82	0.48
3:E:12:LEU:HG	3:E:14:GLN:HG2	1.95	0.48
3:E:49:ILE:CG2	3:E:50:PRO:CD	2.84	0.48
1:A:64:GLU:OE1	2:B:647:GLU:OE1	2.31	0.48
1:A:461:ARG:NH1	1:A:461:ARG:CG	2.73	0.48

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1175:ALA:HB2	2:B:1204:LEU:HB2	1.98	0.46
2:B:1242:MET:SD	2:B:1260:PRO:HG3	2.55	0.46
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.97	0.46
1:A:560:LEU:HD23	1:A:614:ILE:HB	1.96	0.46
1:A:676:ALA:O	1:A:693:TYR:HB3	2.15	0.46
2:B:581:LEU:HD23	2:B:581:LEU:H	1.81	0.46
2:B:939:ASN:O	2:B:940:ARG:CB	2.56	0.46
2:C:141:LEU:HG	2:C:142:ASP:N	2.26	0.46
2:C:815:LEU:N	2:C:816:PRO:HD2	2.31	0.46
2:C:1075:ARG:HD2	2:C:1090:PRO:HD2	1.97	0.46
3:D:53:GLU:HG2	3:D:145:TYR:HE1	1.81	0.46
1:A:64:GLU:OE1	2:B:647:GLU:CD	2.55	0.46
1:A:204:LEU:HA	1:A:264:SER:O	2.15	0.46
1:A:285:GLU:HG2	1:A:286:ASN:N	2.31	0.46
1:A:462:ILE:HG12	1:A:685:PRO:HD3	1.97	0.46
1:A:519:ILE:HG12	1:A:519:ILE:O	2.15	0.46
2:B:1277:LEU:HD13	2:B:1287:GLY:HA3	1.96	0.46
2:C:388:GLN:HB3	2:C:1320:VAL:HG23	1.97	0.46
2:C:828:ASP:OD2	2:C:828:ASP:N	2.49	0.46
3:D:66:VAL:O	3:D:111:ILE:HG22	2.16	0.46
1:A:255:ARG:HD3	1:A:258:GLN:CD	2.36	0.46
2:B:154:PHE:CD1	2:B:154:PHE:N	2.84	0.46
2:C:231:LEU:HB3	2:C:249:SER:HB2	1.97	0.46
1:A:27:LYS:CB	1:A:28:PRO:HD3	2.39	0.45
1:A:73:ARG:HG3	1:A:74:LEU:HD12	1.97	0.45
2:B:154:PHE:HD1	2:B:154:PHE:N	2.14	0.45
2:B:278:LEU:HB2	2:B:282:VAL:HG13	1.97	0.45
2:B:1084:PRO:HB2	2:B:1209:GLY:N	2.31	0.45
2:B:1273:ASN:CG	3:D:79:ILE:HG21	2.30	0.45
2:C:302:ARG:HD2	2:C:315:THR:HG22	1.98	0.45
2:C:561:ASN:O	2:C:562:ALA:HB3	2.16	0.45
3:D:217:LYS:O	3:D:221:ARG:HB3	2.15	0.45
3:E:53:GLU:O	3:E:53:GLU:CD	2.55	0.45
1:A:314:ARG:O	1:A:318:ARG:HB2	2.16	0.45
1:A:496:CYS:SG	1:A:497:ALA:N	2.90	0.45
2:B:144:ASN:HB2	2:B:1318:GLU:HA	1.98	0.45
2:B:1273:ASN:ND2	3:D:79:ILE:CG2	2.79	0.45
2:C:144:ASN:HA	2:C:1318:GLU:HB3	1.98	0.45
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.97	0.45
1:A:64:GLU:HA	1:A:67:ARG:CG	2.45	0.45
1:A:456:PHE:HB3	1:A:686:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:SER:HA	1:A:663:GLU:HB3	1.99	0.45
1:A:940:MET:O	1:A:944:ARG:HB2	2.16	0.45
1:A:967:ILE:HB	1:A:978:LYS:HD3	1.98	0.45
2:B:493:HIS:CG	2:B:758:ILE:HD13	2.52	0.45
2:C:94:PHE:HA	2:C:104:ILE:HG21	1.98	0.45
2:C:1060:ARG:HH22	2:C:1292:GLU:HA	1.81	0.45
1:A:673:TYR:CE2	1:A:694:ILE:HG22	2.51	0.45
1:A:934:THR:N	1:A:935:PRO:HD2	2.31	0.45
2:C:838:GLU:CG	2:C:839:ALA:H	2.23	0.45
2:C:934:LEU:HD13	2:C:934:LEU:H	1.81	0.45
2:C:1027:THR:HG22	3:D:102:SER:OG	2.16	0.45
3:D:140:ALA:HA	3:D:281:LYS:HG3	1.97	0.45
3:D:181:SER:CB	3:D:250:ARG:HG2	2.41	0.45
1:A:308:ALA:HB3	1:A:309:ASN:CB	2.47	0.45
1:A:411:ILE:HD13	1:A:411:ILE:N	2.31	0.45
1:A:658:ILE:HD11	1:A:692:ILE:HD11	1.99	0.45
1:A:894:LYS:C	1:A:896:ASN:H	2.19	0.45
2:B:218:GLY:C	2:B:219:ILE:HG12	2.36	0.45
2:B:368:ALA:C	3:D:83:ASN:HD22	2.17	0.45
2:B:763:VAL:HA	2:B:766:ILE:HD12	1.98	0.45
2:C:1035:ILE:O	2:C:1036:ASP:HB3	2.17	0.45
2:C:1038:GLU:O	2:C:1041:ARG:HB2	2.17	0.45
3:E:229:PHE:HE1	3:E:252:LEU:CD1	2.29	0.45
1:A:208:HIS:HB3	1:A:260:LEU:HD23	1.99	0.45
3:E:70:ASP:O	3:E:70:ASP:OD2	2.35	0.45
3:E:166:GLU:HG3	3:E:172:MET:SD	2.57	0.45
1:A:752:VAL:HG12	1:A:812:VAL:HG23	1.98	0.45
2:B:1255:ARG:HB3	2:B:1256:GLY:H	1.56	0.45
1:A:463:ASP:OD2	1:A:530:MET:HB3	2.16	0.45
2:B:180:LEU:HB3	2:B:195:ASN:HD21	1.82	0.45
2:B:279:SER:CB	2:C:1198:LYS:HE2	2.47	0.45
2:B:639:ASN:HB3	2:B:641:ARG:HG3	1.99	0.45
2:C:286:LEU:HD21	2:C:290:TYR:HB3	1.98	0.45
2:C:372:ALA:HB1	2:C:1315:MET:HE3	1.97	0.45
3:D:110:VAL:HG12	3:D:111:ILE:N	2.32	0.45
3:D:131:ALA:C	3:D:133:THR:H	2.19	0.45
3:D:178:LYS:HD2	3:D:249:ASP:HB3	1.99	0.45
1:A:27:LYS:HB3	1:A:28:PRO:CD	2.36	0.45
1:A:926:MET:HG2	1:A:927:ASN:N	2.31	0.45
2:B:135:LYS:O	2:C:471:SER:HA	2.16	0.45
2:B:147:VAL:HG23	2:B:375:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:TYR:CE1	2:B:941:TYR:CD2	3.05	0.45
2:C:451:GLU:O	2:C:452:ASN:HB3	2.17	0.45
2:C:627:ALA:H	2:C:716:PHE:HB2	1.82	0.45
2:C:1071:PHE:CD1	2:C:1234:GLN:HG2	2.50	0.45
3:D:106:GLY:HA2	3:D:121:PHE:HB3	1.98	0.45
3:E:148:ASP:O	3:E:280:ALA:HB1	2.16	0.45
1:A:565:ARG:N	1:A:590:ARG:O	2.50	0.45
2:B:134:THR:HG21	2:C:472:GLU:CD	2.37	0.45
2:B:884:ALA:O	2:B:888:GLN:HG2	2.16	0.45
2:C:306:GLN:HE21	2:C:306:GLN:N	2.14	0.45
2:C:409:ILE:HD11	2:C:1040:PHE:CZ	2.52	0.45
3:E:53:GLU:CG	3:E:145:TYR:CE1	2.93	0.45
2:B:753:ASP:N	2:B:754:GLY:HA2	2.32	0.44
2:C:1137:VAL:HG22	2:C:1164:TRP:CE2	2.51	0.44
3:D:185:SER:HB3	3:D:186:LEU:H	1.50	0.44
1:A:308:ALA:HB3	1:A:309:ASN:HB2	1.98	0.44
1:A:331:ARG:HD3	1:A:331:ARG:H	1.82	0.44
1:A:670:GLY:O	1:A:671:VAL:CG2	2.60	0.44
1:A:953:ARG:HH12	1:A:1055:LEU:HD23	1.81	0.44
2:B:348:LEU:HD23	2:B:350:ILE:HD11	1.98	0.44
2:B:583:GLU:HA	2:B:583:GLU:OE1	2.17	0.44
2:B:709:MET:HA	2:B:712:PHE:CD2	2.52	0.44
2:C:863:LEU:HD11	2:C:871:PRO:HD3	1.99	0.44
2:C:980:ARG:HH21	2:C:999:LYS:HE2	1.82	0.44
3:D:221:ARG:HH12	3:D:225:ARG:HH21	1.64	0.44
3:E:116:THR:HG21	3:E:119:ILE:HD12	1.99	0.44
1:A:127:THR:CG2	2:B:639:ASN:CB	2.91	0.44
1:A:222:ARG:NH1	2:B:613:LEU:HD13	2.31	0.44
1:A:358:ILE:HB	1:A:359:PRO:HA	1.99	0.44
1:A:959:TYR:O	1:A:960:ILE:HG13	2.17	0.44
3:D:238:ASN:H	3:D:253:GLU:HB3	1.82	0.44
1:A:926:MET:HB2	1:A:931:GLY:CA	2.47	0.44
2:B:888:GLN:NE2	3:D:38:GLU:OE1	2.51	0.44
2:C:192:PRO:HG3	2:C:294:VAL:CG2	2.48	0.44
2:C:385:ILE:O	2:C:386:SER:CB	2.65	0.44
2:C:449:PHE:N	2:C:450:PRO:CD	2.79	0.44
2:C:624:PHE:CD2	2:C:713:MET:HG2	2.53	0.44
1:A:127:THR:HG23	2:B:640:GLN:CA	2.47	0.44
1:A:663:GLU:O	1:A:667:GLN:NE2	2.51	0.44
1:A:926:MET:SD	1:A:928:GLU:HG2	2.58	0.44
3:E:42:ASN:HB3	3:E:174:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:CE1	3:D:150:ILE:CG2	3.01	0.44
1:A:470:LEU:HD21	1:A:525:ARG:HD2	1.99	0.44
1:A:526:ASN:OD1	1:A:526:ASN:N	2.49	0.44
1:A:659:ASN:HD21	1:A:706:TYR:H	1.65	0.44
1:A:988:LYS:HD2	1:A:994:PRO:HD3	2.00	0.44
2:C:837:THR:CG2	2:C:934:LEU:HD21	2.46	0.44
3:D:14:GLN:NE2	3:D:107:LEU:HD13	2.32	0.44
3:D:25:ASN:OD1	3:D:26:ALA:N	2.51	0.44
3:D:150:ILE:HG22	3:D:151:ASP:N	2.33	0.44
3:E:33:GLN:O	3:E:35:LEU:N	2.51	0.44
3:E:68:ILE:HD13	3:E:69:GLU:CA	2.47	0.44
1:A:303:THR:CA	1:A:307:HIS:CE1	3.00	0.44
2:B:291:HIS:HB3	2:B:292:ASN:H	1.55	0.44
2:B:473:ALA:HA	2:B:765:PRO:HG3	1.98	0.44
1:A:525:ARG:HE	1:A:525:ARG:HB2	1.42	0.44
2:C:564:GLY:O	2:C:565:GLU:HB3	2.17	0.44
3:D:116:THR:OG1	3:D:119:ILE:HD12	2.18	0.44
3:E:46:LYS:CG	3:E:155:HIS:CE1	3.00	0.44
2:B:146:GLU:OE2	2:B:1314:ASP:HB3	2.18	0.44
2:C:838:GLU:HA	2:C:940:ARG:NE	2.33	0.44
3:E:2:LEU:HD11	3:E:107:LEU:CD1	2.48	0.44
1:A:625:PHE:HA	1:A:628:MET:HB3	2.00	0.43
1:A:842:TYR:HA	1:A:845:ILE:HG22	2.00	0.43
2:B:1306:THR:HG23	2:B:1308:ASN:H	1.83	0.43
3:D:160:LEU:HD23	3:D:229:PHE:HA	2.00	0.43
3:D:255:ILE:O	3:D:255:ILE:CG1	2.65	0.43
1:A:133:LEU:CD2	2:C:545:PRO:HG3	2.48	0.43
1:A:963:TYR:CE2	1:A:985:GLY:HA2	2.53	0.43
2:B:154:PHE:HA	2:B:262:ASN:HD22	1.83	0.43
2:B:172:ASP:HA	2:B:175:THR:HG22	2.00	0.43
2:B:554:ARG:HH21	2:B:594:LEU:HD23	1.83	0.43
2:B:862:ARG:NH1	2:B:948:ILE:HD13	2.33	0.43
2:B:883:ILE:HG21	2:B:915:VAL:HG21	2.00	0.43
2:B:1078:TYR:C	2:B:1078:TYR:CD2	2.91	0.43
2:C:204:VAL:CG2	2:C:1242:MET:HG2	2.48	0.43
3:D:144:ARG:O	3:D:144:ARG:CG	2.64	0.43
3:E:93:LEU:O	3:E:96:LEU:HB2	2.18	0.43
3:E:186:LEU:HD13	3:E:186:LEU:HA	1.60	0.43
3:E:286:THR:O	3:E:290:TRP:CB	2.65	0.43
2:B:959:GLN:HA	2:B:959:GLN:OE1	2.17	0.43
2:C:390:HIS:O	2:C:1317:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:590:SER:HB2	2:C:592:VAL:HG12	2.00	0.43
2:C:1121:HIS:ND1	2:C:1123:PRO:HD2	2.33	0.43
1:A:406:VAL:HB	1:A:407:GLU:C	2.39	0.43
1:A:853:GLU:H	1:A:853:GLU:HG3	1.69	0.43
2:B:1082:ASP:OD2	2:B:1226:ASP:HB2	2.18	0.43
2:B:1083:ASP:OD2	2:B:1083:ASP:N	2.51	0.43
2:C:191:GLY:H	2:C:192:PRO:HD2	1.84	0.43
2:C:627:ALA:HB2	2:C:716:PHE:CD2	2.54	0.43
3:E:122:TYR:CE2	3:E:203:ILE:HG21	2.53	0.43
1:A:265:SER:HB2	1:A:269:VAL:HG21	2.00	0.43
1:A:602:PHE:HB2	1:A:603:PRO:HD2	2.00	0.43
2:B:389:PHE:CE1	2:B:1319:ARG:HG2	2.53	0.43
2:C:856:LEU:HD11	3:D:117:ILE:HD12	2.00	0.43
2:C:1293:VAL:O	2:C:1294:ASP:HB2	2.18	0.43
3:E:152:ILE:H	3:E:152:ILE:HD12	1.83	0.43
3:E:253:GLU:HG3	3:E:254:TYR:CE2	2.54	0.43
3:D:46:LYS:HE3	3:D:158:LEU:HD22	2.00	0.43
1:A:131:GLY:O	1:A:134:VAL:HG12	2.19	0.43
1:A:292:ARG:HG2	1:A:295:THR:HG21	2.01	0.43
1:A:512:ALA:HA	1:A:513:PRO:HA	1.74	0.43
2:B:168:VAL:HG23	2:B:204:VAL:HG12	2.00	0.43
2:B:423:GLU:HB3	2:B:490:PHE:CE2	2.53	0.43
1:A:282:GLU:O	1:A:283:PHE:CG	2.72	0.43
1:A:853:GLU:CD	1:A:854:ASN:H	2.22	0.43
1:A:977:HIS:O	1:A:988:LYS:HB3	2.19	0.43
2:B:612:PHE:CE1	2:B:635:ILE:HD11	2.53	0.43
2:C:837:THR:HA	2:C:936:MET:HB2	2.00	0.43
2:C:297:ASN:HD22	2:C:298:PRO:N	2.16	0.43
2:C:630:ASN:HA	2:C:631:PRO:HD3	1.87	0.43
3:D:74:GLN:OE1	3:D:74:GLN:HA	2.19	0.43
1:A:535:LEU:HD13	1:A:536:TYR:N	2.34	0.43
1:A:850:SER:HB3	1:A:872:VAL:HG11	2.00	0.43
2:C:115:GLN:HG3	2:C:116:SER:H	1.84	0.43
2:C:450:PRO:HB2	2:C:451:GLU:H	1.59	0.43
2:C:1031:TYR:O	2:C:1032:ASP:CB	2.67	0.43
3:D:14:GLN:HE22	3:D:107:LEU:HD13	1.84	0.43
3:E:282:PHE:CZ	3:E:286:THR:HG21	2.53	0.43
1:A:654:SER:HB3	1:A:715:TYR:HE2	1.84	0.42
1:A:1016:ILE:HD13	1:A:1016:ILE:H	1.84	0.42
2:B:937:ASN:C	2:B:939:ASN:H	2.22	0.42
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:772:TYR:C	2:C:774:LEU:H	2.21	0.42
3:D:53:GLU:CG	3:D:145:TYR:HE1	2.31	0.42
3:D:66:VAL:HG23	3:D:67:TYR:N	2.33	0.42
3:D:241:ASN:HB3	3:D:250:ARG:HD2	2.01	0.42
3:E:162:GLY:O	3:E:167:ARG:NH1	2.48	0.42
3:E:210:GLY:O	3:E:214:ARG:HG3	2.18	0.42
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.54	0.42
2:B:137:ILE:HB	2:C:471:SER:HB3	2.00	0.42
2:C:860:ARG:O	2:C:864:HIS:HB2	2.19	0.42
3:E:32:LEU:O	3:E:35:LEU:CG	2.58	0.42
1:A:855:MET:HA	1:A:916:ASN:HB3	2.01	0.42
2:B:772:TYR:HB3	2:B:773:PRO:HD2	2.01	0.42
2:C:493:HIS:NE2	2:C:527:ARG:HD2	2.35	0.42
2:C:594:LEU:HD22	2:C:595:ALA:H	1.84	0.42
2:C:855:TYR:CZ	2:C:896:LEU:HD21	2.54	0.42
3:E:268:THR:OG1	3:E:269:ILE:N	2.48	0.42
1:A:12:ARG:HD3	1:A:12:ARG:C	2.40	0.42
1:A:292:ARG:HG2	1:A:295:THR:HG22	2.02	0.42
2:B:318:LEU:HD11	2:B:325:TYR:HB2	1.99	0.42
2:B:641:ARG:O	2:C:670:ASP:OD2	2.36	0.42
2:C:440:ILE:HD13	2:C:441:ARG:N	2.35	0.42
2:C:1083:ASP:HA	2:C:1084:PRO:HD2	1.75	0.42
2:C:1130:SER:O	2:C:1134:ARG:HD3	2.20	0.42
3:D:217:LYS:HE2	3:D:290:TRP:O	2.18	0.42
1:A:487:GLN:OE1	1:A:548:ASN:HB3	2.19	0.42
1:A:739:ASN:HD22	1:A:739:ASN:HA	1.70	0.42
1:A:752:VAL:HG23	1:A:779:ASN:O	2.20	0.42
1:A:955:ASN:HD21	1:A:1055:LEU:HD23	1.84	0.42
1:A:713:ASN:HA	1:A:716:MET:HB2	2.01	0.42
2:B:153:ASP:HB3	2:B:154:PHE:CD1	2.54	0.42
2:B:172:ASP:O	2:B:173:GLN:HB3	2.19	0.42
2:B:937:ASN:O	2:B:939:ASN:N	2.52	0.42
2:C:1020:ARG:HD2	2:C:1031:TYR:HA	2.01	0.42
3:E:1:MET:CE	3:E:123:ASP:HA	2.49	0.42
3:E:32:LEU:HD13	3:E:225:ARG:NH1	2.35	0.42
1:A:147:GLN:HG3	1:A:215:VAL:HG13	2.01	0.42
1:A:199:MET:HG3	1:A:205:VAL:HG21	2.02	0.42
1:A:222:ARG:NH1	2:B:613:LEU:CD1	2.82	0.42
1:A:395:GLN:NE2	1:A:395:GLN:CA	2.79	0.42
2:C:372:ALA:HA	2:C:398:ARG:HD3	2.02	0.42
2:C:540:PHE:O	2:C:548:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:651:ARG:O	2:C:655:ILE:HG12	2.20	0.42
2:C:1035:ILE:HG22	2:C:1036:ASP:N	2.33	0.42
3:D:149:MET:HE2	3:D:260:MET:CE	2.43	0.42
1:A:71:LEU:HB3	1:A:72:PHE:H	1.67	0.42
2:B:188:ARG:NH1	2:C:237:VAL:HG13	2.34	0.42
2:B:363:ARG:NH1	3:D:80:SER:OG	2.50	0.42
3:E:158:LEU:CD2	3:E:172:MET:HB3	2.49	0.42
2:B:274:MET:HG2	2:C:234:PRO:CD	2.35	0.42
2:B:748:GLN:O	2:B:750:GLU:HB3	2.20	0.42
2:B:760:THR:C	2:B:762:ILE:H	2.22	0.42
2:C:1036:ASP:O	2:C:1037:ILE:HB	2.19	0.42
2:C:1249:ASN:HA	2:C:1250:GLU:HA	1.48	0.42
3:D:193:VAL:HG11	3:D:230:ILE:HD12	2.02	0.42
3:D:239:VAL:CG1	3:D:250:ARG:HH12	2.30	0.42
1:A:101:LEU:HD21	1:A:119:VAL:HG23	2.02	0.42
1:A:204:LEU:HD13	1:A:221:TYR:HB2	2.02	0.42
1:A:454:GLY:C	1:A:456:PHE:H	2.22	0.42
1:A:939:GLN:HE21	1:A:939:GLN:HB3	1.66	0.42
1:A:1000:GLU:O	1:A:1003:VAL:HG12	2.20	0.42
2:B:815:LEU:HB3	2:B:816:PRO:HD3	2.01	0.42
2:C:292:ASN:O	2:C:293:ASN:CB	2.58	0.42
2:C:1243:ARG:NH1	2:C:1257:ALA:HA	2.34	0.42
3:E:32:LEU:CD1	3:E:225:ARG:NE	2.83	0.42
3:E:140:ALA:HB1	3:E:281:LYS:HG3	2.02	0.42
3:E:247:ARG:HA	3:E:247:ARG:NE	2.30	0.42
1:A:72:PHE:CD1	1:A:72:PHE:N	2.87	0.41
1:A:208:HIS:NE2	1:A:234:GPL:O1P	2.53	0.41
1:A:306:GLN:HA	1:A:306:GLN:OE1	2.18	0.41
1:A:962:PHE:HE2	1:A:966:GLY:HA3	1.85	0.41
2:B:835:TYR:CE1	2:B:925:VAL:HG21	2.55	0.41
2:B:1156:ILE:HD11	2:B:1194:MET:HG3	2.02	0.41
2:C:448:TYR:CA	2:C:450:PRO:HD3	2.49	0.41
2:C:1136:HIS:CD2	2:C:1136:HIS:O	2.73	0.41
1:A:308:ALA:CA	1:A:309:ASN:CB	2.92	0.41
1:A:566:GLU:HB2	1:A:567:PRO:CD	2.41	0.41
1:A:673:TYR:CE2	1:A:694:ILE:CG2	3.03	0.41
3:E:2:LEU:HD11	3:E:107:LEU:HD11	2.02	0.41
3:E:69:GLU:HG3	3:E:199:LEU:HB2	1.98	0.41
1:A:1013:THR:O	1:A:1055:LEU:HD12	2.20	0.41
2:C:968:ARG:O	2:C:971:MET:HB2	2.20	0.41
2:C:986:ILE:O	2:C:989:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:LEU:HD23	3:D:14:GLN:HB2	2.01	0.41
3:E:72:ILE:O	3:E:76:LEU:HD12	2.20	0.41
3:E:76:LEU:HD21	3:E:282:PHE:CD2	2.55	0.41
1:A:677:LEU:HB3	1:A:692:ILE:HD13	2.02	0.41
1:A:776:SER:HA	1:A:818:PHE:HE1	1.85	0.41
2:B:149:PRO:HB3	2:B:1312:GLY:HA2	2.01	0.41
2:B:150:LEU:O	2:B:804:LEU:HD13	2.20	0.41
2:B:583:GLU:O	2:B:584:HIS:CB	2.69	0.41
2:C:871:PRO:HG3	2:C:892:VAL:HG11	2.01	0.41
3:D:69:GLU:HB2	3:D:199:LEU:HD11	2.02	0.41
1:A:23:ARG:HH21	1:A:27:LYS:HB3	1.85	0.41
1:A:47:ARG:HB2	2:B:595:ALA:O	2.20	0.41
2:B:228:VAL:HG22	2:B:229:GLN:H	1.84	0.41
2:B:838:GLU:HG3	2:B:839:ALA:H	1.84	0.41
2:B:954:GLN:NE2	3:D:240:VAL:HG12	2.35	0.41
2:C:451:GLU:O	2:C:452:ASN:CB	2.69	0.41
3:E:205:LEU:CD1	3:E:289:ARG:HG3	2.50	0.41
1:A:49:HIS:NE2	1:A:172:PHE:CD1	2.75	0.41
1:A:665:LEU:N	1:A:667:GLN:HE22	2.17	0.41
2:B:475:ILE:O	2:B:477:SER:N	2.53	0.41
2:B:487:SER:HA	2:B:488:PRO:HD3	1.94	0.41
2:B:871:PRO:HG3	2:B:894:VAL:HG13	2.02	0.41
2:B:908:THR:HA	2:B:911:ARG:HH21	1.85	0.41
3:D:69:GLU:HG3	3:D:199:LEU:HG	2.02	0.41
1:A:203:THR:HG23	1:A:204:LEU:H	1.86	0.41
1:A:361:SER:HB3	1:A:362:MET:H	1.62	0.41
1:A:530:MET:HA	1:A:533:LEU:HB2	2.02	0.41
2:B:588:LEU:HD22	2:B:604:MET:CE	2.51	0.41
2:C:204:VAL:HG23	2:C:1242:MET:HG2	2.02	0.41
3:D:152:ILE:HG21	3:D:283:LEU:HB3	2.01	0.41
1:A:892:GLN:C	1:A:894:LYS:H	2.24	0.41
2:B:269:GLU:O	2:B:291:HIS:HD2	2.04	0.41
2:B:486:VAL:HG21	2:B:709:MET:HB3	2.03	0.41
2:B:946:LEU:HD22	2:B:947:GLU:H	1.85	0.41
2:C:926:VAL:CG2	2:C:938:ASN:HB2	2.50	0.41
3:E:182:TRP:CD1	3:E:185:SER:HB3	2.55	0.41
1:A:35:GLY:H	1:A:38:TYR:HE1	1.67	0.41
1:A:71:LEU:O	1:A:73:ARG:N	2.53	0.41
1:A:511:ILE:O	1:A:511:ILE:HD12	2.21	0.41
2:B:228:VAL:O	2:B:246:GLU:HB2	2.20	0.41
2:B:420:PRO:HB2	2:B:748:GLN:CD	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:837:THR:O	2:B:838:GLU:CB	2.68	0.41
2:B:1321:ASN:C	2:B:1323:ASP:H	2.24	0.41
2:C:82:ARG:CZ	2:C:210:ARG:HB3	2.51	0.41
2:C:597:ALA:O	2:C:600:ILE:HG22	2.20	0.41
2:C:1181:SER:O	2:C:1182:GLU:HB3	2.21	0.41
3:E:66:VAL:HG13	3:E:111:ILE:HG21	2.03	0.41
3:E:140:ALA:CB	3:E:281:LYS:HG3	2.51	0.41
1:A:303:THR:CB	1:A:307:HIS:NE2	2.76	0.41
1:A:491:ASP:OD1	1:A:491:ASP:C	2.60	0.41
1:A:600:VAL:HA	1:A:601:PRO:C	2.40	0.41
1:A:725:PRO:C	1:A:726:ILE:HG12	2.39	0.41
2:B:1330:ILE:H	2:B:1330:ILE:HD13	1.86	0.41
2:C:293:ASN:CG	2:C:294:VAL:N	2.73	0.41
2:C:633:THR:HG21	2:C:710:SER:OG	2.21	0.41
2:C:1325:VAL:HG12	2:C:1326:ARG:N	2.36	0.41
3:D:258:ASN:OD1	3:D:259:SER:N	2.53	0.41
1:A:194:HIS:ND1	3:D:146:ARG:HD2	2.35	0.40
2:B:445:GLU:HG3	2:B:447:ARG:HG2	2.03	0.40
2:B:450:PRO:HG3	2:B:686:HIS:HB2	2.04	0.40
2:B:612:PHE:CZ	2:B:1331:ARG:HD2	2.56	0.40
2:B:821:ASN:HD22	2:B:821:ASN:HA	1.73	0.40
2:B:862:ARG:C	2:B:952:PHE:HZ	2.24	0.40
2:B:941:TYR:O	2:B:941:TYR:HD1	2.04	0.40
2:B:954:GLN:HB3	2:B:956:ASP:O	2.20	0.40
2:C:617:ASP:HA	2:C:620:ILE:HG22	2.03	0.40
2:C:1042:TRP:CE3	2:C:1042:TRP:HA	2.56	0.40
3:D:29:THR:HG22	3:D:222:ASP:OD1	2.21	0.40
1:A:201:LYS:CA	2:B:629:ARG:HD3	2.51	0.40
1:A:406:VAL:HG23	1:A:407:GLU:HA	2.03	0.40
1:A:513:PRO:HB2	1:A:514:LEU:H	1.62	0.40
1:A:967:ILE:HA	1:A:970:ARG:HB3	2.02	0.40
2:C:317:MET:SD	2:C:1262:SER:HB3	2.61	0.40
2:C:856:LEU:HA	2:C:860:ARG:HB2	2.03	0.40
2:C:948:ILE:HG22	2:C:948:ILE:O	2.21	0.40
3:E:209:GLU:CG	3:E:210:GLY:H	2.29	0.40
2:C:159:ASP:OD2	2:C:291:HIS:HE1	2.04	0.40
2:C:835:TYR:HB2	2:C:847:ILE:HD11	2.03	0.40
2:C:999:LYS:HD3	2:C:1009:THR:HG22	2.04	0.40
1:A:177:THR:HA	1:A:178:PRO:HD3	1.95	0.40
2:B:172:ASP:O	2:B:173:GLN:CB	2.70	0.40
2:B:1076:ILE:HB	2:B:1166:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:70:ASP:OD2	3:E:70:ASP:C	2.60	0.40
3:E:140:ALA:O	3:E:146:ARG:HA	2.22	0.40
3:E:142:THR:HG23	3:E:143:PRO:CD	2.50	0.40
3:E:264:GLY:H	3:E:268:THR:CG2	2.34	0.40
1:A:421:LEU:HD12	1:A:678:LEU:HB3	2.02	0.40
1:A:604:ILE:HD13	1:A:604:ILE:H	1.86	0.40
2:B:134:THR:HG22	2:C:472:GLU:CD	2.36	0.40
2:B:225:ILE:HG22	2:B:227:LEU:HG	2.04	0.40
2:B:274:MET:CG	2:C:234:PRO:CD	2.55	0.40
2:B:1031:TYR:CD2	2:B:1041:ARG:HD3	2.57	0.40
2:C:177:LYS:H	2:C:177:LYS:HD3	1.86	0.40
2:C:372:ALA:HB1	2:C:1315:MET:CE	2.51	0.40
2:C:447:ARG:HE	2:C:690:GLN:NE2	2.20	0.40
2:C:603:ILE:C	2:C:605:ARG:H	2.25	0.40
2:C:610:GLN:O	2:C:634:TYR:CE2	2.75	0.40
3:D:257:VAL:O	3:D:257:VAL:HG12	2.21	0.40
3:E:53:GLU:CB	3:E:145:TYR:CE1	3.05	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	1038/1058 (98%)	813 (78%)	161 (16%)	64 (6%)	1 19
2	B	1172/1333 (88%)	958 (82%)	186 (16%)	28 (2%)	6 35
2	C	1238/1333 (93%)	1018 (82%)	192 (16%)	28 (2%)	6 36
3	D	289/448 (64%)	253 (88%)	33 (11%)	3 (1%)	15 52
3	E	289/448 (64%)	254 (88%)	34 (12%)	1 (0%)	41 75
All	All	4026/4620 (87%)	3296 (82%)	606 (15%)	124 (3%)	7 31

All (124) Ramachandran outliers are listed below:

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

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

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

5.3.2 Protein sidechains (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	932/942 (99%)	778 (84%)	154 (16%)	2	14
2	B	1029/1155 (89%)	920 (89%)	109 (11%)	6	27
2	C	1085/1155 (94%)	950 (88%)	135 (12%)	4	22
3	D	240/379 (63%)	205 (85%)	35 (15%)	3	18
3	E	240/379 (63%)	198 (82%)	42 (18%)	2	12
All	All	3526/4010 (88%)	3051 (86%)	475 (14%)	7	20

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	GPL	A	234	1	29,34,35	2.41	2 (6%)	29,49,51	1.53	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GPL	A	234	1	-	6/15/37/39	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GPL	P-NZ	11.92	1.74	1.61
1	A	234	GPL	C6-N1	-2.45	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	GPL	P-NZ-CE	-5.04	117.47	124.67
1	A	234	GPL	C3'-C2'-C1'	2.92	105.38	100.98
1	A	234	GPL	C5-C6-N1	2.54	118.44	113.95
1	A	234	GPL	C8-N7-C5	2.47	107.69	102.99

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	234	GPL	N-CA-CB-CG
1	A	234	GPL	CG-CD-CE-NZ
1	A	234	GPL	C5'-O5'-P-O1P
1	A	234	GPL	CE-NZ-P-O1P
1	A	234	GPL	O4'-C4'-C5'-O5'
1	A	234	GPL	C5'-O5'-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no 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.

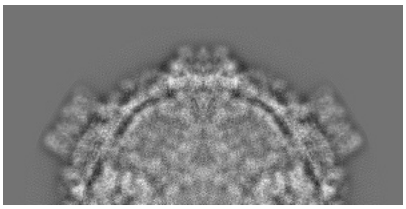
6 Map visualisation (i)

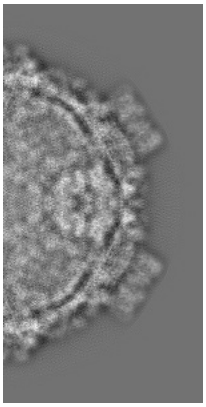
This section contains visualisations of the EMDB entry EMD-5376. These allow visual inspection of the internal detail of the map and identification of artifacts.

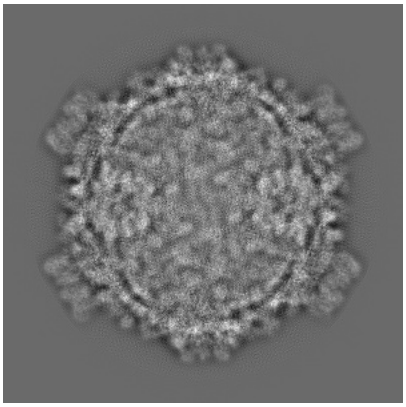
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

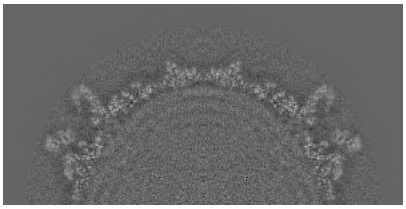

Y

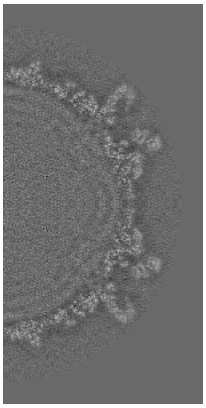

Z

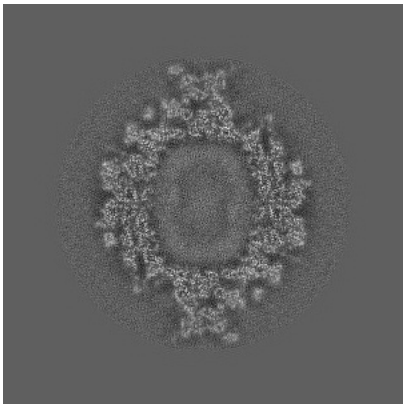
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 360

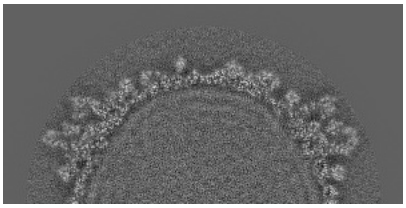

Y Index: 360


Z Index: 180

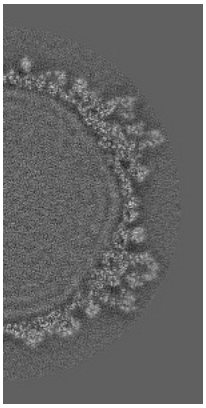
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

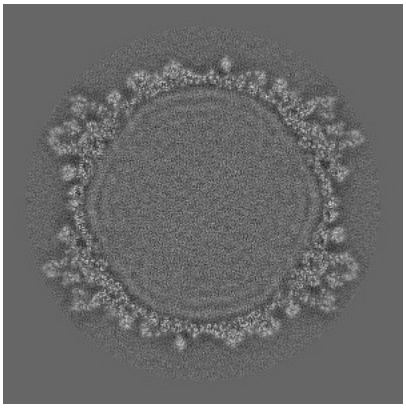
6.3.1 Primary map



X Index: 336



Y Index: 384



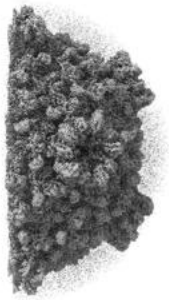
Z Index: 24

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 2.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

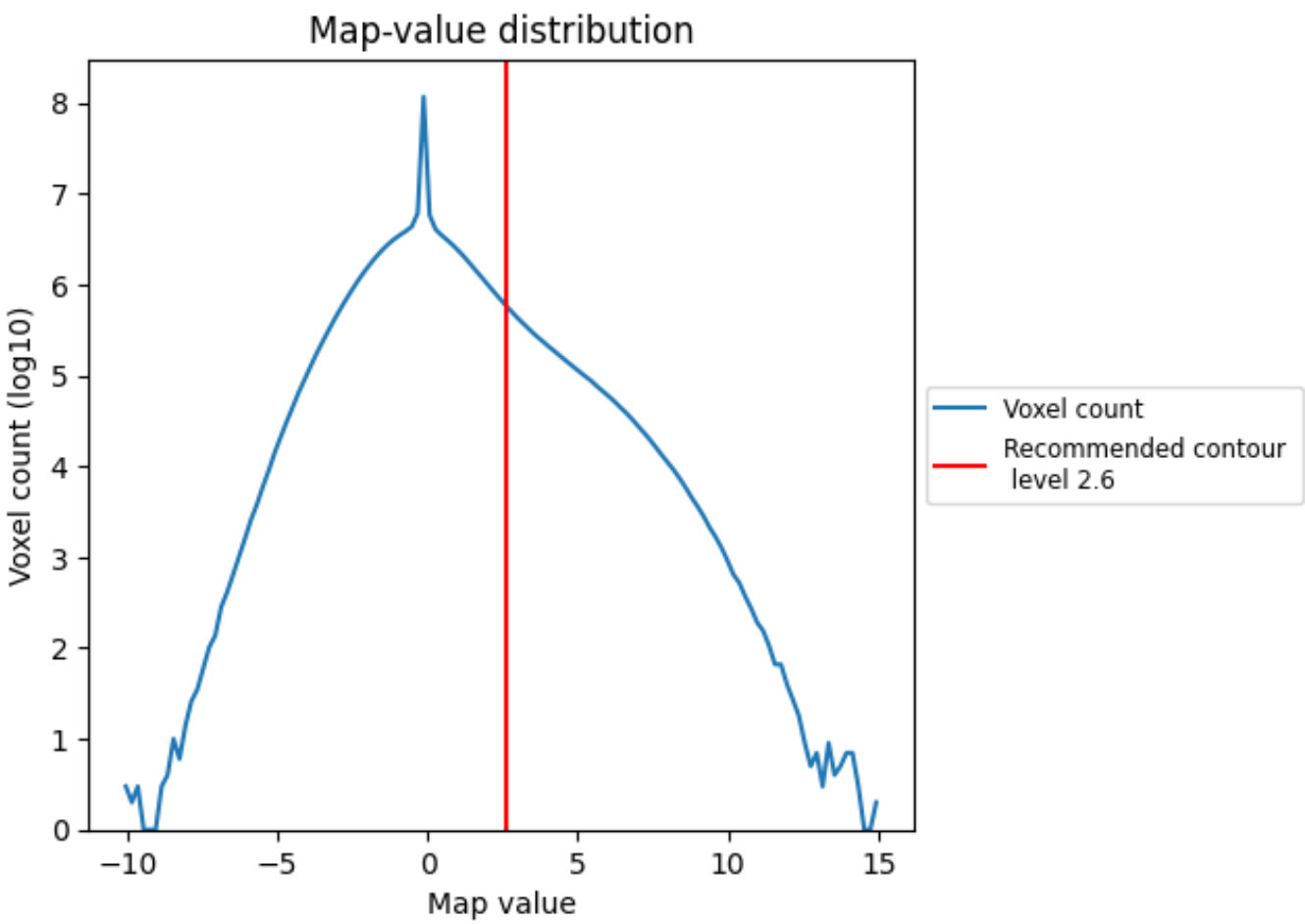
6.5 Mask visualisation (i)

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

7 Map analysis (i)

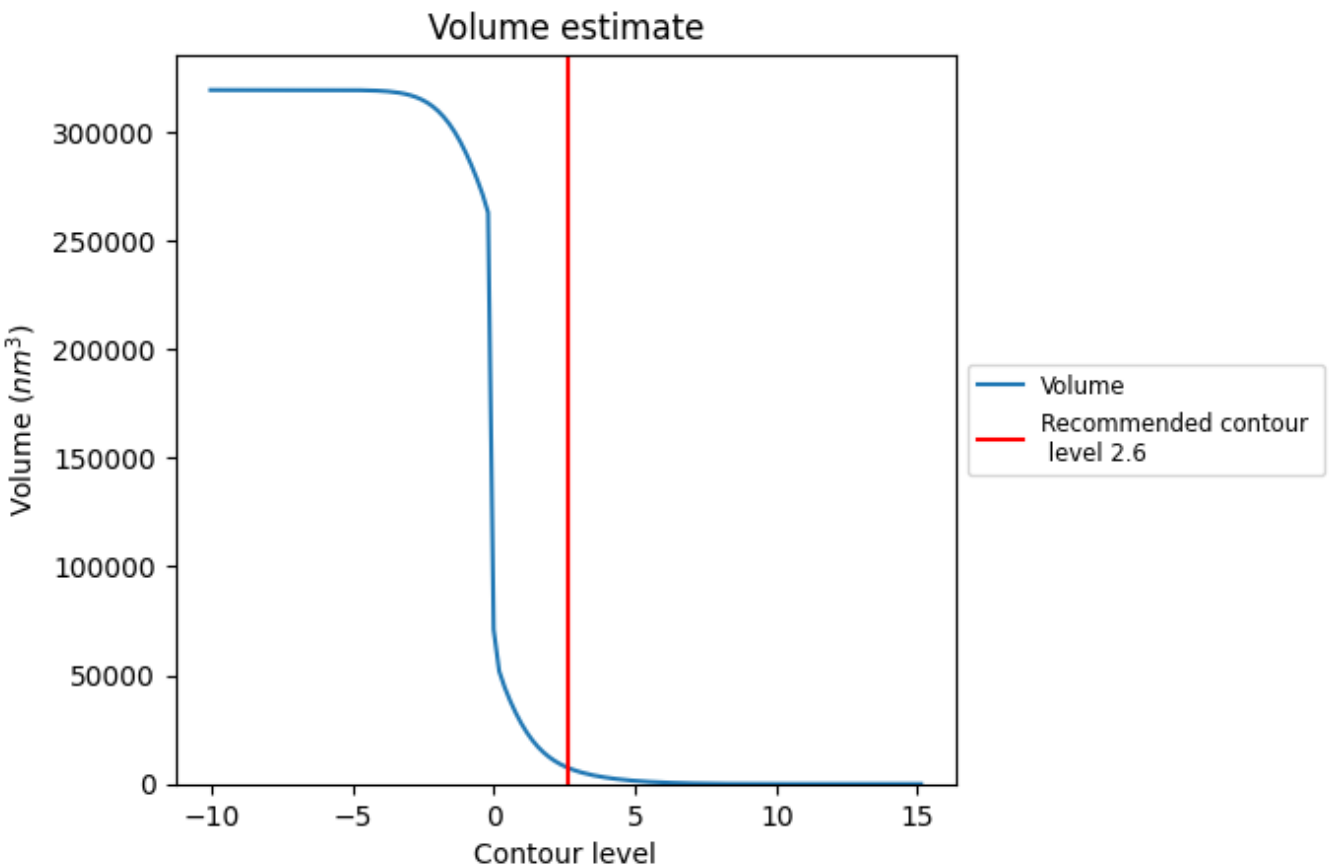
This section contains the results of statistical analysis of the map.

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 7585 nm^3; this corresponds to an approximate mass of 6852 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation (i)

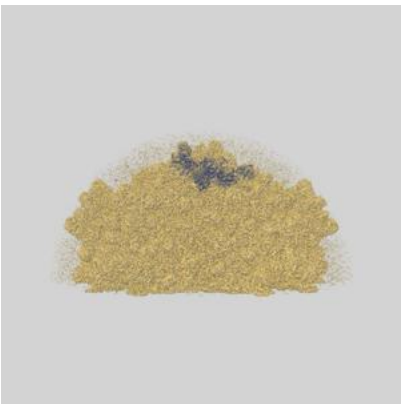
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

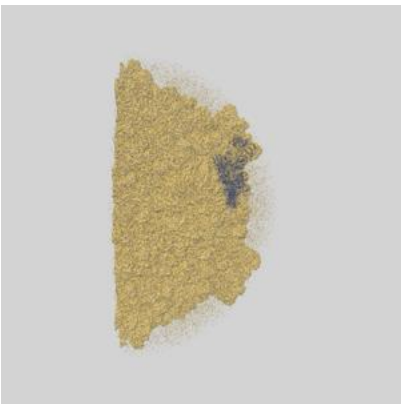
This section contains information regarding the fit between EMDB map EMD-5376 and PDB model 3J17. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

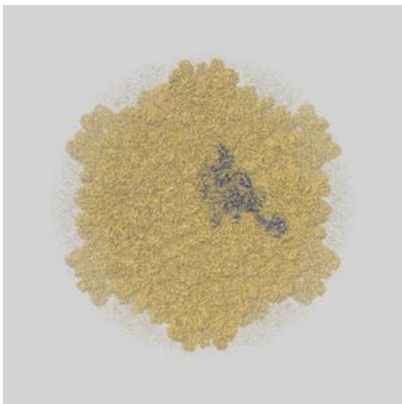
9.1.1 Map-model overlay (i)



X

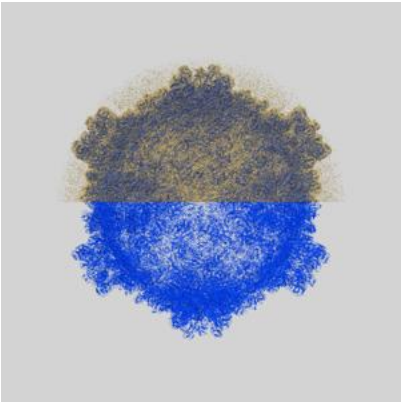


Y

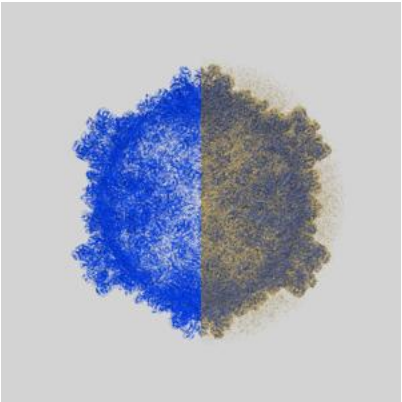


Z

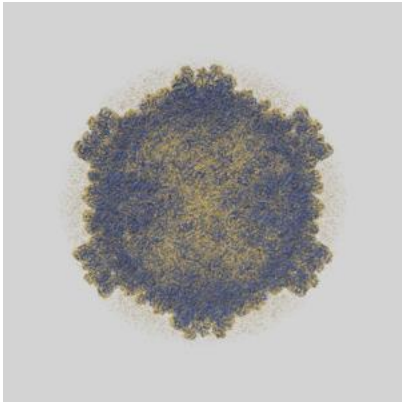
9.1.2 Map-model assembly overlay (i)



X



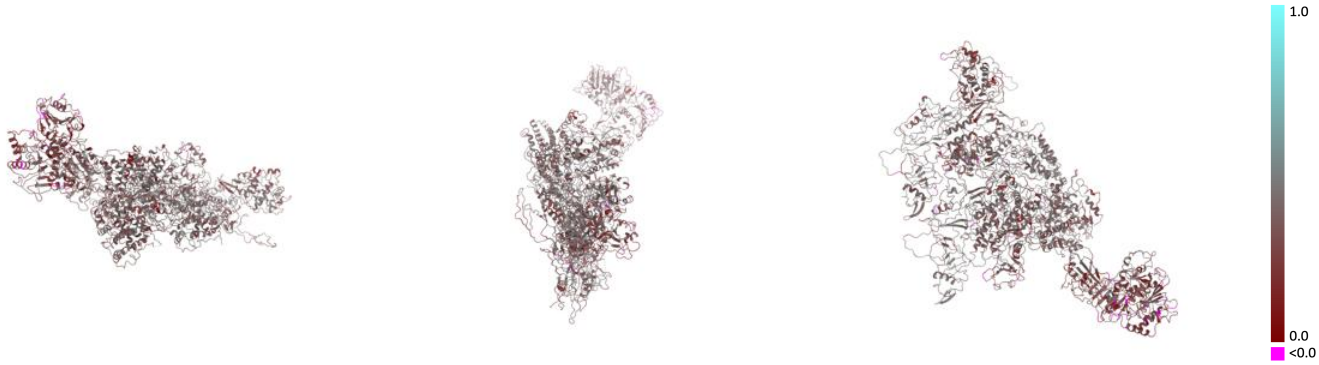
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.6 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.

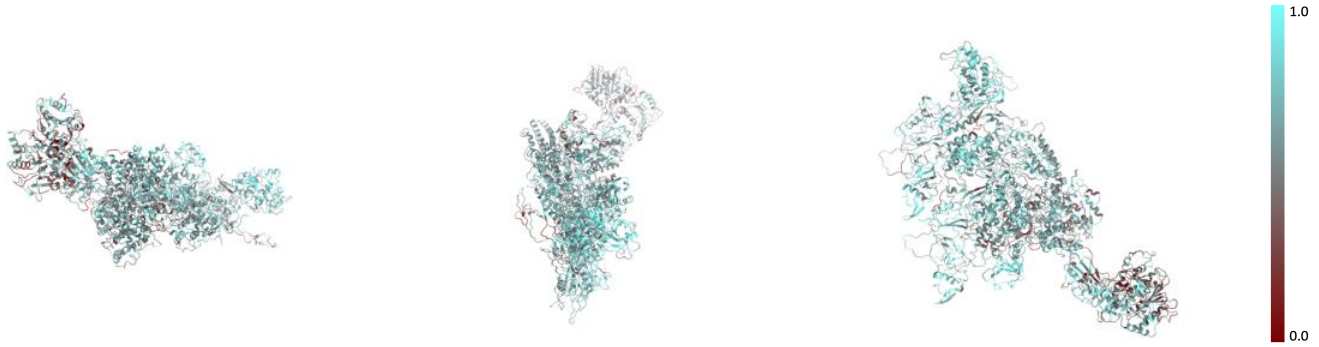
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

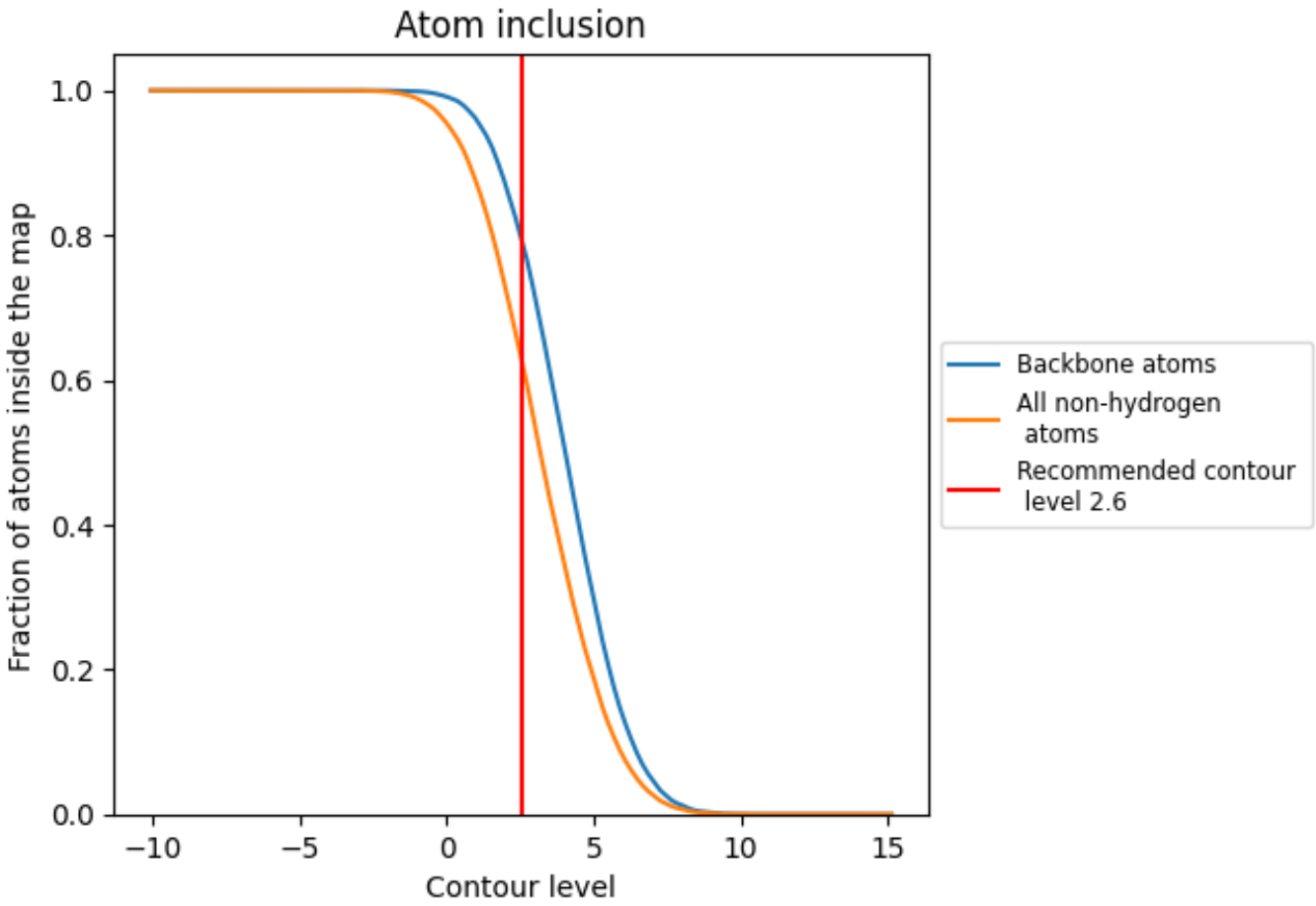
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.6).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6195	0.3550
A	0.5525	0.3190
B	0.6200	0.3700
C	0.6507	0.3760
D	0.6431	0.3500
E	0.7052	0.3340