Full wwPDB EM Validation Report (i)

Feb 14, 2024 – 12:46 PM EST

PDB ID	:	3LU0
EMDB ID	:	EMD-5169
Title	:	Molecular model of Escherichia coli core RNA polymerase
Authors	:	Darst, S.A.
Deposited on	:	2010-02-16
Resolution	:	11.20 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:

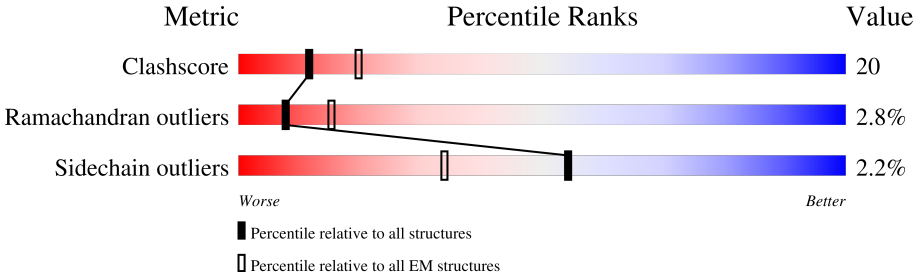
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 11.20 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	329	30% 45% 24% • 29%
1	B	329	32% 46% 25% • 29%
2	C	1342	19% 68% 30% • •
3	D	1407	21% 61% 32% • •
4	E	91	98% 20% 71% 5% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	235	1820	1132	323	358	7	0	0
1	B	235	1820	1132	323	358	7	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1335	10523	6602	1836	2042	43	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	conflict	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1364	10547	6624	1879	1994	50	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	89	697	424	132	140	1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	D	1	1	1	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

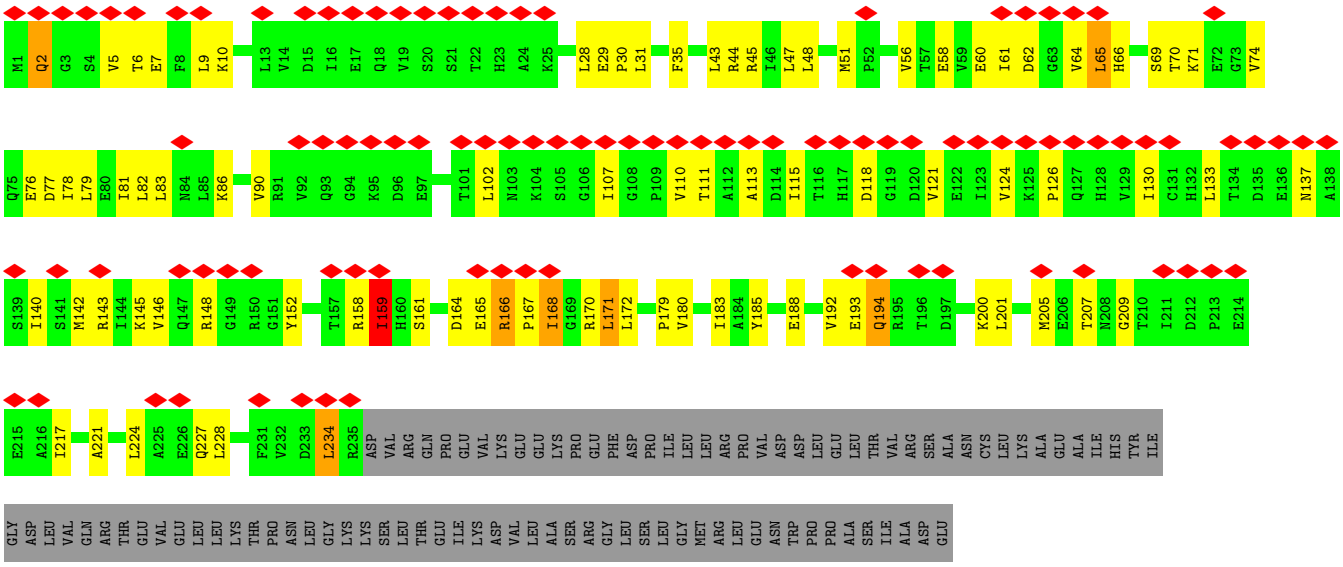
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
6	D	2	2	2	0

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.

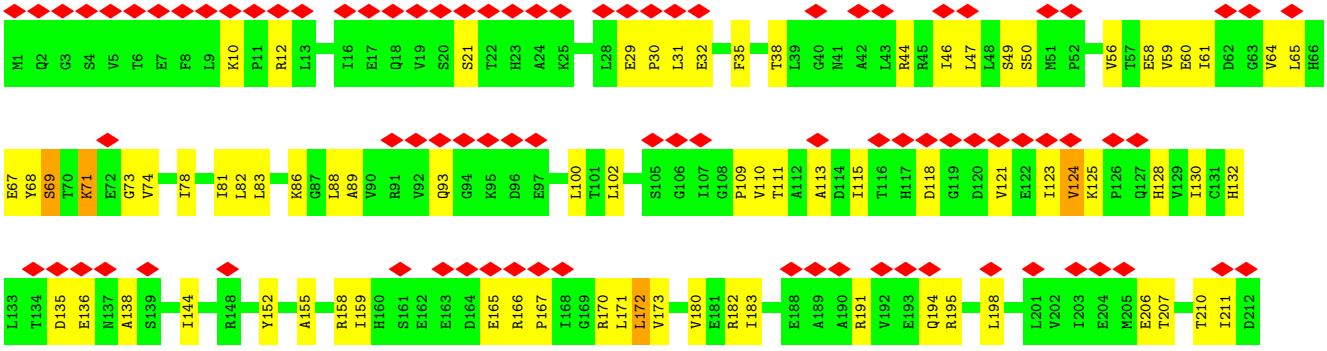
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



P213 E214 E215 A216 I217 R218 R219 A220 A221 T222 I223 L224 A225 E226 Q227 L228 E229 V232 D233 L234 R235 ASP VAL ARG GLN PRO GLU VAL LYS GLU GLU LYS PRO GLU PHE ASP PRO ILE LEU LEU ARG PRO VAL ASP ASP LEU GLU LEU THR VAL ARG SER ALA ASN CYS LEU LYS ALA GLU

ALA ILE HIS TYR ILE GLY ASP LEU VAL GLN ARG THR GLU VAL GLU LEU LEU LYS THR PRO ASN LEU GLY LYS LYS SER LEU THR GLU ILE LYS ASP VAL LEU ALA SER ARG GLY LEU SER LEU GLY MET ARG LEU GLU ASN TRP PRO PRO ALA SER ILE ALA ASP GLU

- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 19% 68% 30%

MET VAL TYR SER TYR THR GLU K8 I11 R12 K13 K17 L22 D23 L27 L28 S29 I30 Q31 E40 Q41 D42 P43 E44 L49 E50 F53 V56 F57 P58 I59 G64 L68 Y73 R74 L75 G76 E77 P78 V79 F80 D81 E84 I87 R88 Y92

S93 R97 V98 K99 L100 R101 L102 E108 A109 P110 E111 G112 K118 E119 Q120 E121 G125 E126 T131 D132 N133 G134 I138 N139 G140 T141 E142 R143 V144 I145 Q148 L149 H150 R151 S152 P153 G154 V155 F156 F157 D158 S159 D160 K161 K169 V170 L171 Y172 N173 A174 R175 I176

I177 P178 Y179 R180 W183 L184 D185 F188 D189 P190 L194 R197 I198 D199 A212 T216 T217 E218 Q219 I220 L221 D222 L223 F224 F225 F230 R233 K236 L237 Q238 L241 R245 L246 A257 Y262 V263 E264 K265 G266 R267 R268 I269 T270 A271 R272 R275

Q276 L277 E278 K279 D280 D281 I285 I292 V297 A298 K299 E316 L317 L322 L325 I333 L336 F337 T338 D342 H343 G344 P345 Y346 I347 R352 P355 R359 L363 V364 E365 R368 M369 E374 P375 E382 S383 L384 L388 L397 S398 A399

V400 M403 K404 F405 N406 R407 S408 L409 L410 R411 I414 E415 I426 D427 V428 M429 K430 D434 I435 R436 N437 G438 K439 G440 E441 V442 D443 D444 I445 D446 H447 L448 R451 R452 I453 R454 S455 V456 Q463 F464 L468 E472 K476 E477 R478 L481 G482 D483 L487

M488 P489 Q490 D491 M492 I493 N494 A495 K496 P497 F506 F506 G507 L511 Q517 N518 N519 P520 L521 S522 E523 H526 K527 R528 L533 R540 G544 D549 V550 H551 P552 T553 H554 R557 V558 C559 P560 I561 E562 I572 N573 S574 L575 S576 V577 Y578 A579 Q580 T581 N582

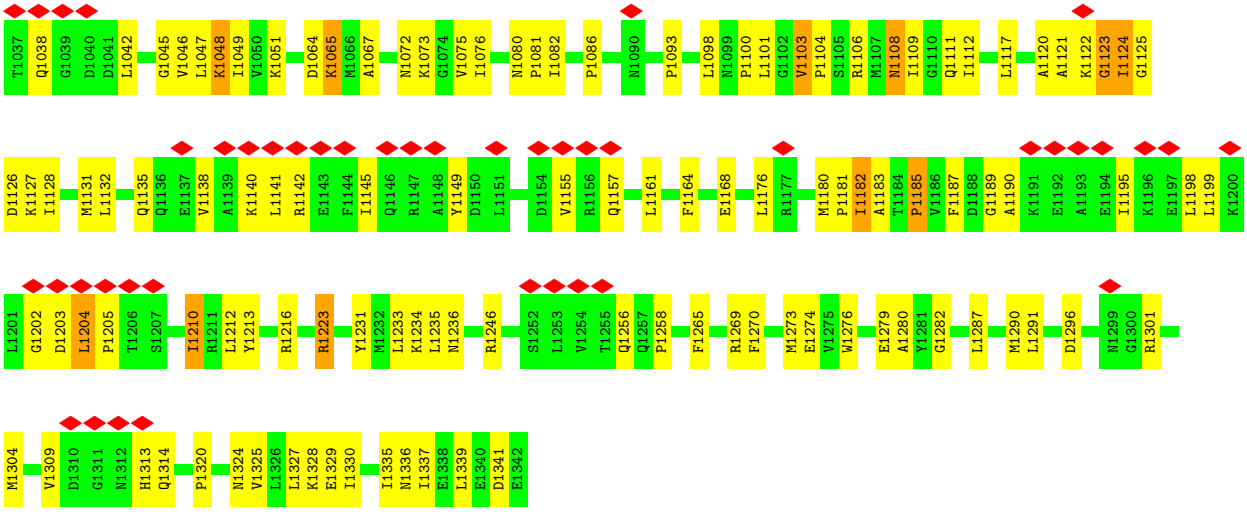
E583 Y584 L587 E588 T589 P590 Y591 V598 I603 H604 Y605 L606 S607 I616 G627 V630 E631 D632 L633 V634 T635 C636 R637 L644 F645 S646 R647 Y652 Q658 S662 E672 H673 L680 M681 M685 Q688 A689 V690 P691 T692 L693 R694 P698 L699 V700

E705 R706 A718 V724 I732 K735 A746 L753 T754 K755 S759 N760 I765 V771 S772 L773 R779 L783 P787 S788 E793 L794 A795 L796 G797 Q798 P806 W807 Y810 N811 F812 E813 D814 S815 I816 L817 V818 S819 E820 R821 V822 V823 D826

R827 F828 I831 L836 S840 R841 D842 T843 K844 L845 G846 P847 E848 E849 D853 I854 P855 N856 V857 G858 E859 A860 A861 L862 S863 K864 I865 D866 E867 I870 V871 G874 T878 G879 G880 D881 V887 T888 P889 K890 G891 E892 T893 Q894 L895 T896 P897 E898 E899 K900 L901

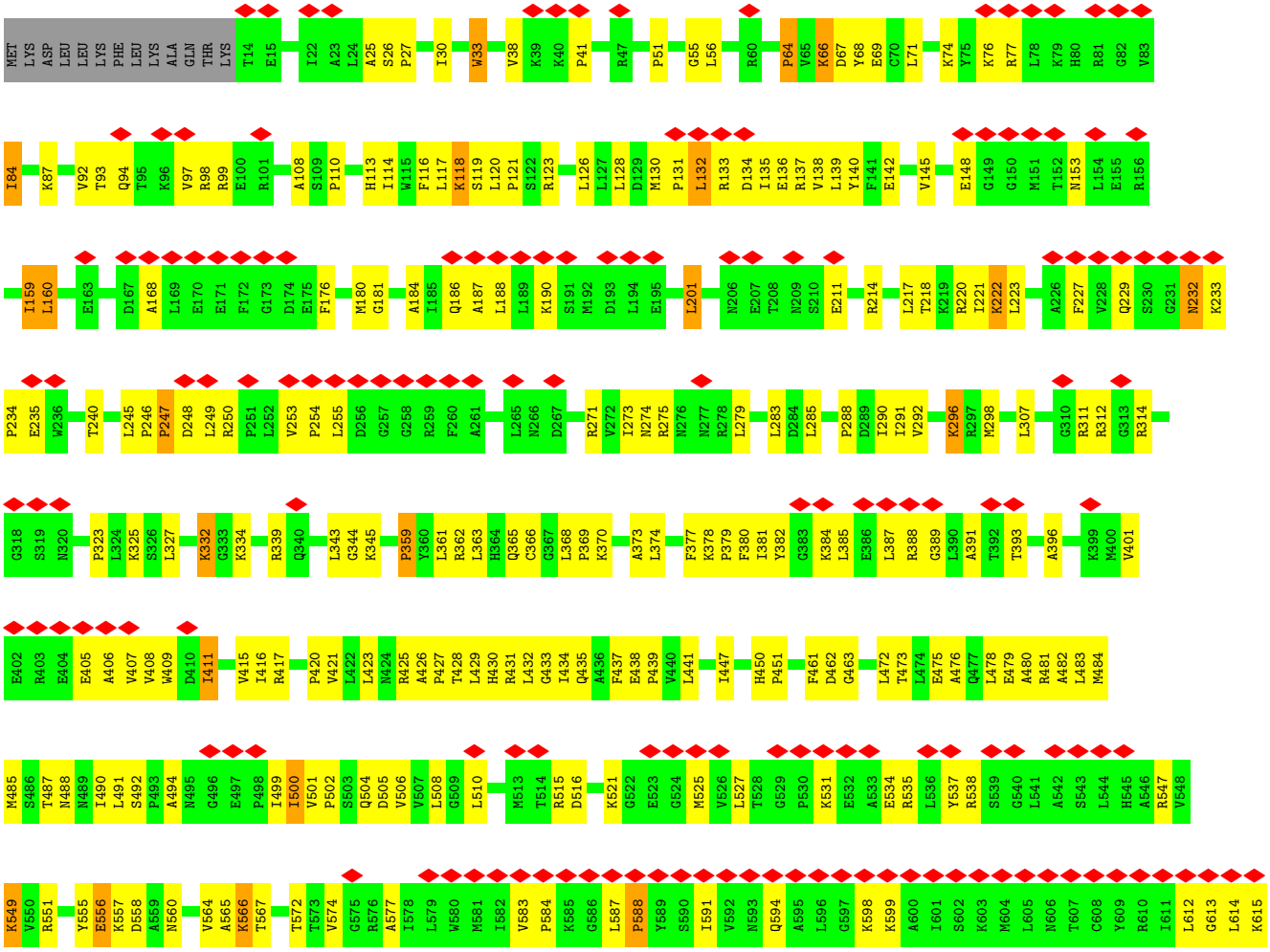
F906 G907 E908 K909 A910 S911 D912 V913 K914 D915 S916 S917 L918 R919 Q932 V933 F934 T935 R936 D937 G938 V939 E940 K941 D942 K943 R944 A945 L946 E947 I948 E949 E950 M951 Q952 L953 K954 Q955 A956 K957 K958 D959 L960 S961 E962 E963 L964 Q965 I966 L967 E968 A969 G970 L971 F972 S973 R974 I975 R976

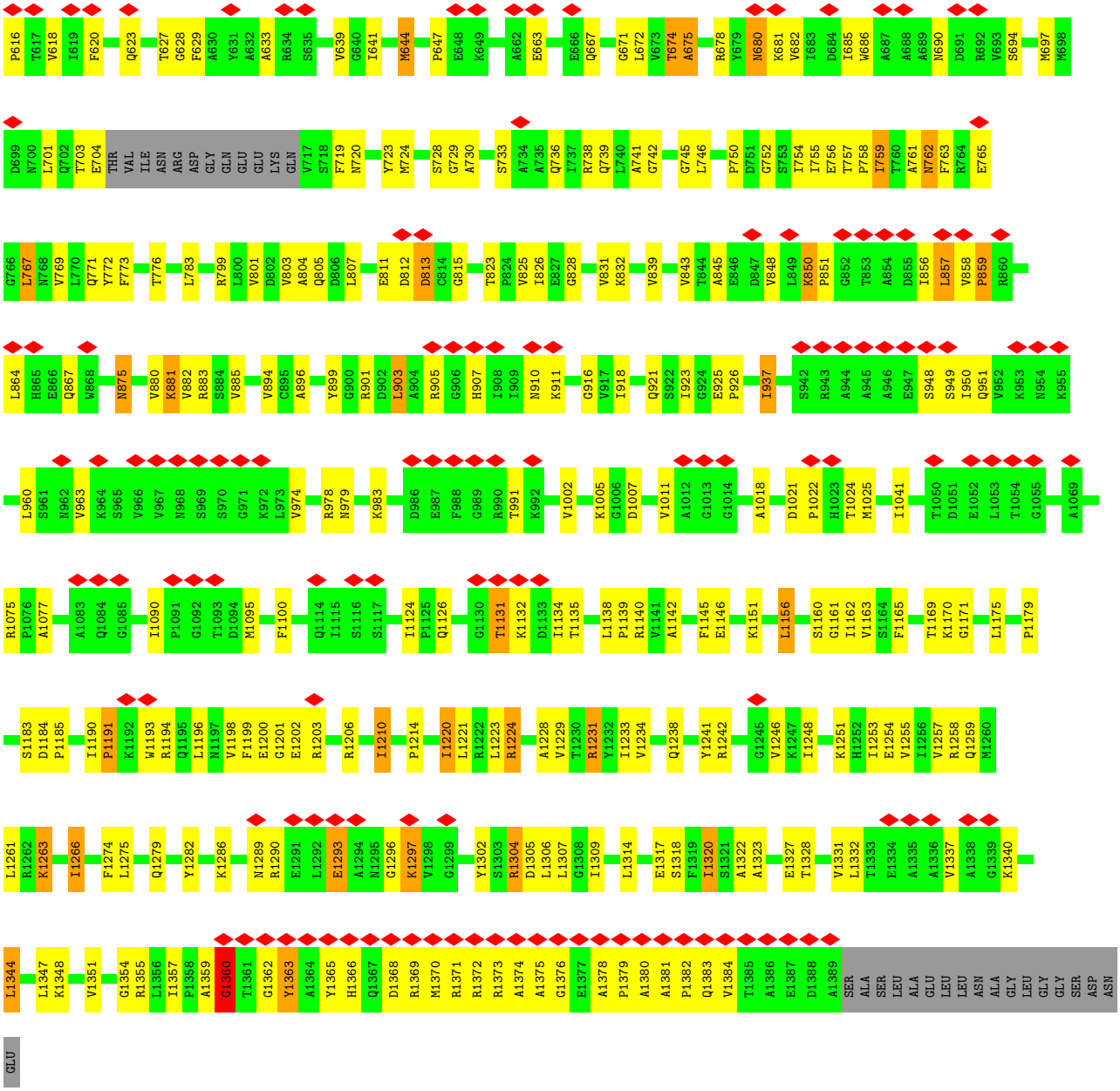
A977 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020 L1021 K1022 H1023 E1024 F1025 E1026 K1027 K1028 L1029 E1030 A1031 K1032 R1033 R1034 K1035 I1036



- Molecule 3: DNA-directed RNA polymerase subunit beta'

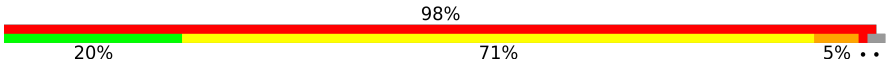
Chain D:

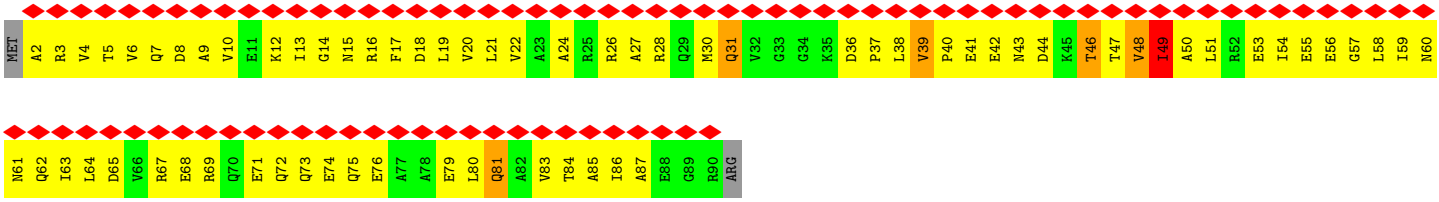




- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42000	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	69.984	Depositor
Minimum map value	-1.475	Depositor
Average map value	0.803	Depositor
Map value standard deviation	3.186	Depositor
Recommended contour level	11.0	Depositor
Map size (Å)	252, 252, 252	wwPDB
Map dimensions	90, 90, 90	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.8, 2.8, 2.8	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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.19	0/1842	0.37	0/2495
1	B	0.19	0/1842	0.36	0/2495
2	C	0.21	1/10690 (0.0%)	0.34	0/14422
3	D	0.26	0/10710	0.63	3/14470 (0.0%)
4	E	1.09	2/699 (0.3%)	1.79	4/942 (0.4%)
All	All	0.29	3/25783 (0.0%)	0.56	7/34824 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	49	ILE	C-N	5.62	1.47	1.34
2	C	951	MET	CG-SD	5.51	1.95	1.81
4	E	49	ILE	CA-C	5.30	1.66	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1360	GLY	CA-C-N	-50.05	7.09	117.20
4	E	81	GLN	CG-CD-OE1	-38.65	44.30	121.60
3	D	1360	GLY	C-N-CA	-31.89	41.97	121.70
4	E	81	GLN	CG-CD-NE2	-9.65	93.55	116.70
4	E	49	ILE	C-N-CA	8.22	142.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	81	GLN	OE1-CD-NE2	6.93	137.85	121.90
3	D	1363	TYR	CA-CB-CG	-6.59	100.88	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1360	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1820	0	1850	78	0
1	B	1820	0	1850	59	0
2	C	10523	0	10551	327	0
3	D	10547	0	10751	495	0
4	E	697	0	706	209	0
5	D	1	0	0	0	0
6	D	2	0	0	0	0
All	All	25410	0	25708	1011	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 20.

All (1011) 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)
3:D:615:LYS:CD	4:E:5:THR:CA	1.80	1.59
3:D:615:LYS:CE	4:E:5:THR:HA	1.37	1.53
3:D:615:LYS:CD	4:E:5:THR:HA	1.34	1.46
3:D:615:LYS:HD3	4:E:5:THR:C	1.31	1.46
3:D:615:LYS:HD3	4:E:5:THR:CA	1.34	1.45
3:D:618:VAL:HG21	4:E:2:ALA:CB	1.50	1.39
3:D:615:LYS:NZ	4:E:5:THR:HA	1.39	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:615:LYS:HD3	4:E:6:VAL:N	1.46	1.28
3:D:614:LEU:N	4:E:7:GLN:OE1	1.65	1.27
3:D:615:LYS:HD2	4:E:5:THR:N	1.48	1.26
3:D:614:LEU:H	4:E:7:GLN:CG	1.53	1.20
3:D:614:LEU:H	4:E:7:GLN:CD	1.45	1.19
2:C:1282:GLY:HA3	4:E:17:PHE:HE2	1.04	1.19
3:D:618:VAL:CG2	4:E:2:ALA:HB2	1.72	1.17
3:D:618:VAL:CG2	4:E:2:ALA:CB	2.22	1.16
3:D:615:LYS:CD	4:E:5:THR:N	2.08	1.11
3:D:615:LYS:NZ	4:E:5:THR:CA	2.12	1.11
4:E:73:GLN:HB3	4:E:75:GLN:HG2	1.30	1.09
2:C:1282:GLY:HA3	4:E:17:PHE:CE2	1.88	1.07
2:C:1282:GLY:CA	4:E:17:PHE:HE2	1.68	1.06
3:D:618:VAL:HG21	4:E:2:ALA:HB3	1.05	1.02
4:E:13:ILE:HD13	4:E:19:LEU:HG	1.38	1.02
3:D:615:LYS:CD	4:E:6:VAL:N	2.25	0.98
3:D:481:ARG:O	4:E:3:ARG:HD3	1.67	0.94
3:D:615:LYS:HD2	4:E:5:THR:H	1.14	0.92
3:D:615:LYS:NZ	4:E:5:THR:CB	2.32	0.91
4:E:44:ASP:CB	4:E:48:VAL:HG21	2.01	0.90
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.52	0.90
1:A:166:ARG:HB2	1:A:167:PRO:HD3	1.52	0.89
3:D:614:LEU:N	4:E:7:GLN:CG	2.35	0.89
3:D:615:LYS:HD2	4:E:5:THR:CA	1.83	0.88
3:D:1375:ALA:O	3:D:1379:PRO:HD3	1.75	0.86
3:D:1370:MET:SD	4:E:22:VAL:HG13	2.15	0.86
3:D:478:LEU:HD12	4:E:24:ALA:HA	1.56	0.86
3:D:614:LEU:N	4:E:7:GLN:CD	2.18	0.86
4:E:13:ILE:HB	4:E:19:LEU:HD11	1.58	0.86
4:E:13:ILE:CD1	4:E:19:LEU:HG	2.05	0.85
3:D:615:LYS:HZ2	4:E:5:THR:CA	1.88	0.85
4:E:63:ILE:HG12	4:E:64:LEU:CD1	2.06	0.85
2:C:1180:MET:HB3	2:C:1181:PRO:HD3	1.59	0.85
4:E:63:ILE:HG12	4:E:64:LEU:HD12	1.58	0.84
3:D:618:VAL:HG22	4:E:2:ALA:HB2	1.58	0.84
1:B:58:GLU:HG3	1:B:170:ARG:HH21	1.43	0.84
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.57	0.84
3:D:615:LYS:CG	4:E:6:VAL:H	1.91	0.83
4:E:17:PHE:O	4:E:20:VAL:HG12	1.78	0.83
4:E:10:VAL:HA	4:E:19:LEU:HD21	1.59	0.82
1:B:195:ARG:HG3	1:B:198:LEU:HD21	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:13:ILE:HB	4:E:19:LEU:CD1	2.10	0.82
3:D:1370:MET:CE	4:E:61:ASN:HB3	2.10	0.81
4:E:3:ARG:NH2	4:E:51:LEU:HD22	1.96	0.81
3:D:1378:ALA:O	3:D:1382:PRO:HD2	1.81	0.81
1:A:234:LEU:HD13	1:A:234:LEU:H	1.46	0.80
3:D:1366:HIS:CE1	4:E:17:PHE:HB2	2.16	0.80
3:D:614:LEU:HB3	4:E:7:GLN:HG2	1.62	0.80
1:B:172:LEU:HD13	1:B:172:LEU:H	1.46	0.80
3:D:615:LYS:HZ2	4:E:5:THR:HA	1.41	0.80
3:D:615:LYS:CD	4:E:6:VAL:H	1.92	0.80
2:C:1330:ILE:HG23	2:C:1335:ILE:HG13	1.65	0.79
4:E:10:VAL:HA	4:E:19:LEU:CD2	2.12	0.79
2:C:403:MET:HG3	2:C:414:ILE:HB	1.64	0.79
3:D:618:VAL:CG2	4:E:2:ALA:HB3	1.96	0.79
3:D:615:LYS:HD3	4:E:6:VAL:H	1.46	0.78
4:E:63:ILE:C	4:E:64:LEU:HD12	2.03	0.78
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.65	0.78
3:D:1263:LYS:H	3:D:1263:LYS:HD2	1.47	0.78
4:E:6:VAL:O	4:E:10:VAL:HG23	1.82	0.78
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.65	0.78
3:D:132:LEU:HD13	3:D:132:LEU:H	1.49	0.78
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.64	0.77
4:E:13:ILE:HG22	4:E:15:ASN:H	1.47	0.77
2:C:765:ILE:HG13	2:C:787:PRO:HG3	1.66	0.77
3:D:1156:LEU:HD13	3:D:1156:LEU:H	1.49	0.77
3:D:1373:ARG:HB3	4:E:58:LEU:HD11	1.66	0.77
4:E:31:GLN:HE21	4:E:31:GLN:HA	1.50	0.77
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.67	0.77
4:E:44:ASP:HB2	4:E:48:VAL:HG21	1.66	0.77
3:D:500:ILE:H	3:D:500:ILE:HD13	1.51	0.76
2:C:1123:GLY:HA2	2:C:1127:LYS:HD2	1.66	0.76
4:E:13:ILE:HD13	4:E:19:LEU:CG	2.16	0.75
3:D:288:PRO:HG2	3:D:291:ILE:HD12	1.68	0.75
3:D:1382:PRO:HG2	4:E:80:LEU:HD11	1.69	0.75
3:D:1371:ARG:O	4:E:59:ILE:HD12	1.86	0.75
2:C:487:LEU:HD23	2:C:487:LEU:H	1.51	0.75
2:C:1181:PRO:O	2:C:1182:ILE:HG13	1.86	0.74
3:D:615:LYS:HZ2	4:E:5:THR:CB	1.94	0.74
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.68	0.74
2:C:1065:LYS:H	2:C:1065:LYS:HD3	1.53	0.74
1:A:124:VAL:HG11	1:A:209:GLY:HA3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:549:LYS:H	3:D:549:LYS:HD2	1.52	0.74
4:E:5:THR:OG1	4:E:8:ASP:HB2	1.87	0.73
3:D:1370:MET:HE1	4:E:61:ASN:HB3	1.69	0.73
3:D:99:ARG:HE	3:D:248:ASP:HB2	1.53	0.73
3:D:1380:ALA:O	3:D:1383:GLN:HG2	1.88	0.73
2:C:1282:GLY:CA	4:E:17:PHE:CE2	2.61	0.73
3:D:674:THR:HG23	3:D:675:ALA:H	1.52	0.73
3:D:1380:ALA:O	3:D:1384:VAL:HG23	1.89	0.73
3:D:615:LYS:NZ	4:E:5:THR:OG1	2.22	0.73
3:D:615:LYS:HZ3	4:E:5:THR:CA	2.01	0.73
1:A:28:LEU:HG	1:A:31:LEU:HD21	1.69	0.72
1:B:152:TYR:HB3	3:D:567:THR:HG21	1.71	0.72
2:C:223:LEU:HD13	2:C:426:ILE:HD13	1.72	0.72
3:D:615:LYS:CD	4:E:5:THR:C	2.27	0.72
1:B:67:GLU:HG3	1:B:82:LEU:HD12	1.72	0.71
3:D:614:LEU:H	4:E:7:GLN:HG3	1.51	0.71
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.71	0.71
3:D:492:SER:HB3	3:D:499:ILE:HG13	1.71	0.71
3:D:368:LEU:HD21	3:D:439:PRO:HB3	1.72	0.71
3:D:615:LYS:HD3	4:E:5:THR:N	1.93	0.71
3:D:361:LEU:HD21	3:D:366:CYS:HA	1.73	0.71
3:D:615:LYS:HZ3	4:E:5:THR:CB	1.96	0.71
3:D:1320:ILE:HD13	3:D:1320:ILE:H	1.56	0.71
3:D:1372:ARG:HG3	3:D:1375:ALA:H	1.56	0.70
2:C:633:LEU:HD23	2:C:633:LEU:H	1.55	0.70
3:D:478:LEU:HD11	4:E:27:ALA:CB	2.21	0.70
4:E:62:GLN:HG3	4:E:63:ILE:H	1.55	0.70
3:D:755:ILE:HG22	3:D:757:THR:H	1.56	0.70
3:D:479:GLU:CB	4:E:20:VAL:HG21	2.20	0.70
3:D:831:VAL:HG23	3:D:832:LYS:H	1.55	0.70
3:D:222:LYS:HD3	3:D:223:LEU:HG	1.73	0.70
3:D:949:SER:HB2	3:D:951:GLN:HE22	1.56	0.69
3:D:1368:ASP:OD1	4:E:21:LEU:HD23	1.93	0.69
2:C:317:LEU:HD13	2:C:322:LEU:HD21	1.75	0.69
3:D:1370:MET:CE	4:E:22:VAL:HG13	2.22	0.69
2:C:812:PHE:HD2	2:C:813:GLU:HG2	1.58	0.69
3:D:1221:LEU:HD11	3:D:1304:ARG:HB2	1.74	0.69
2:C:1045:GLY:HA3	2:C:1049:ILE:HD11	1.74	0.69
3:D:420:PRO:HA	3:D:439:PRO:HD3	1.75	0.69
1:B:83:LEU:HG	3:D:556:GLU:HG2	1.75	0.68
3:D:615:LYS:HG2	4:E:6:VAL:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:12:LYS:HB2	4:E:13:ILE:HD12	1.76	0.68
2:C:142:GLU:HB2	2:C:760:ASN:HD21	1.58	0.68
2:C:811:ASN:HA	2:C:815:SER:HB2	1.74	0.68
3:D:701:LEU:HD13	3:D:720:ASN:HD22	1.58	0.68
2:C:1138:VAL:HG12	2:C:1140:LYS:H	1.57	0.68
3:D:948:SER:CB	3:D:1022:PRO:HG3	2.24	0.68
4:E:46:THR:HG22	4:E:47:THR:H	1.58	0.68
3:D:84:ILE:HD13	3:D:84:ILE:H	1.59	0.68
3:D:384:LYS:HB3	3:D:411:ILE:HD11	1.76	0.68
4:E:37:PRO:HB3	4:E:58:LEU:HD23	1.75	0.68
4:E:41:GLU:HG3	4:E:42:GLU:H	1.56	0.68
1:A:61:ILE:HB	1:A:64:VAL:HB	1.75	0.67
3:D:211:GLU:HA	3:D:214:ARG:HG2	1.76	0.67
3:D:615:LYS:CG	4:E:6:VAL:N	2.55	0.67
3:D:482:ALA:HB2	4:E:3:ARG:NH1	2.08	0.67
1:A:6:THR:HG22	1:A:7:GLU:HG3	1.76	0.67
3:D:481:ARG:O	4:E:3:ARG:CD	2.41	0.67
2:C:1046:VAL:HG12	2:C:1047:LEU:HG	1.77	0.67
2:C:1291:LEU:HD12	3:D:345:LYS:HD3	1.76	0.67
3:D:41:PRO:HG3	3:D:273:ILE:HB	1.77	0.67
1:B:182:ARG:H	1:B:206:GLU:HB2	1.60	0.67
3:D:428:THR:HG23	3:D:433:GLY:HA3	1.77	0.67
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.76	0.67
3:D:482:ALA:HB2	4:E:3:ARG:HH12	1.60	0.66
2:C:616:ILE:HG12	2:C:652:TYR:HB2	1.77	0.66
3:D:93:THR:HG22	3:D:94:GLN:H	1.60	0.66
1:A:228:LEU:HB3	1:B:221:ALA:HB1	1.78	0.66
2:C:22:LEU:HG	2:C:603:ILE:HD13	1.77	0.66
4:E:76:GLU:O	4:E:80:LEU:HD23	1.95	0.66
3:D:746:LEU:HD13	3:D:754:ILE:HD11	1.78	0.65
3:D:1363:TYR:HD2	3:D:1365:TYR:H	1.43	0.65
2:C:1132:LEU:HG	2:C:1161:LEU:HD11	1.78	0.65
3:D:937:ILE:HG23	3:D:1135:THR:HG23	1.79	0.65
3:D:613:GLY:C	4:E:7:GLN:OE1	2.33	0.65
4:E:37:PRO:CB	4:E:58:LEU:HD23	2.25	0.65
2:C:230:PHE:HB2	2:C:333:ILE:HB	1.77	0.65
3:D:159:ILE:HD13	3:D:159:ILE:H	1.62	0.65
1:B:166:ARG:HB2	1:B:167:PRO:HD3	1.77	0.65
2:C:27:LEU:HB3	2:C:528:ARG:HD2	1.77	0.65
3:D:56:LEU:HB3	3:D:250:ARG:HH22	1.62	0.65
3:D:948:SER:HB3	3:D:1022:PRO:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:3:ARG:O	4:E:6:VAL:HG23	1.97	0.65
4:E:62:GLN:HG3	4:E:63:ILE:N	2.12	0.65
1:A:227:GLN:HE22	1:B:12:ARG:HE	1.45	0.65
4:E:39:VAL:HB	4:E:40:PRO:HD3	1.78	0.64
1:A:183:ILE:HG12	1:A:205:MET:HA	1.78	0.64
3:D:1194:ARG:H	3:D:1194:ARG:HD2	1.61	0.64
3:D:948:SER:OG	3:D:1022:PRO:HG3	1.98	0.64
2:C:120:GLN:HG2	2:C:121:GLU:H	1.63	0.64
3:D:504:GLN:HG3	3:D:505:ASP:H	1.62	0.64
3:D:1224:ARG:HD3	3:D:1228:ALA:HB2	1.80	0.64
4:E:81:GLN:O	4:E:84:THR:HG22	1.98	0.64
4:E:13:ILE:HG21	4:E:18:ASP:HB2	1.80	0.64
3:D:290:ILE:HD12	3:D:291:ILE:HG13	1.80	0.64
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.13	0.64
3:D:1005:LYS:HD2	3:D:1011:VAL:HG12	1.79	0.63
4:E:5:THR:HG21	4:E:55:GLU:CD	2.18	0.63
4:E:13:ILE:CG1	4:E:19:LEU:HG	2.26	0.63
1:A:111:THR:HG23	1:A:113:ALA:H	1.63	0.63
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.31	0.63
4:E:38:LEU:HD11	4:E:53:GLU:HG3	1.80	0.63
1:B:68:TYR:HB3	3:D:531:LYS:HB2	1.81	0.63
2:C:143:ARG:HH12	2:C:507:GLY:HA2	1.62	0.63
3:D:365:GLN:HG2	3:D:438:GLU:HB3	1.80	0.63
2:C:1287:LEU:HB3	3:D:1357:ILE:HD11	1.81	0.63
2:C:957:LYS:HA	2:C:1029:LEU:HD11	1.80	0.63
3:D:850:LYS:HB2	3:D:851:PRO:HD3	1.79	0.63
1:A:28:LEU:HD23	1:A:201:LEU:HD23	1.81	0.62
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	1.79	0.62
3:D:479:GLU:HB3	4:E:20:VAL:HG21	1.80	0.62
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.64	0.62
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.81	0.62
3:D:978:ARG:HB2	3:D:1199:PHE:HB3	1.81	0.62
4:E:38:LEU:HD12	4:E:38:LEU:N	2.14	0.62
4:E:41:GLU:HG3	4:E:42:GLU:N	2.15	0.62
2:C:42:ASP:HB3	2:C:43:PRO:HD3	1.82	0.62
3:D:1371:ARG:HE	3:D:1376:GLY:HA3	1.65	0.62
3:D:1261:LEU:HD11	3:D:1304:ARG:HD3	1.81	0.62
4:E:37:PRO:HB3	4:E:58:LEU:CD2	2.29	0.62
3:D:1372:ARG:HH21	4:E:84:THR:HG21	1.65	0.62
4:E:12:LYS:C	4:E:13:ILE:HD12	2.20	0.61
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:VAL:CA	4:E:19:LEU:HD21	2.30	0.61
3:D:615:LYS:HG3	4:E:7:GLN:H	1.65	0.61
3:D:1314:LEU:HD11	3:D:1327:GLU:HB2	1.82	0.61
3:D:587:LEU:HD12	3:D:588:PRO:HD2	1.83	0.61
3:D:1370:MET:SD	4:E:61:ASN:HB3	2.40	0.61
2:C:579:ALA:HB1	2:C:587:LEU:HD21	1.82	0.61
3:D:478:LEU:CD1	4:E:24:ALA:HA	2.28	0.61
3:D:960:LEU:HD12	3:D:1007:ASP:HB2	1.82	0.61
3:D:483:LEU:HG	4:E:16:ARG:HD3	1.83	0.61
2:C:635:THR:HB	2:C:637:ARG:HH12	1.65	0.61
3:D:245:LEU:HD22	3:D:246:PRO:HD2	1.83	0.61
3:D:587:LEU:HD11	3:D:616:PRO:HB3	1.82	0.61
2:C:1290:MET:HB3	2:C:1291:LEU:HD22	1.82	0.60
3:D:131:PRO:HB2	3:D:135:ILE:H	1.65	0.60
3:D:482:ALA:CB	4:E:3:ARG:HH12	2.14	0.60
4:E:3:ARG:HH21	4:E:51:LEU:HD22	1.66	0.60
3:D:74:LYS:HE2	3:D:87:LYS:HD3	1.82	0.60
3:D:1160:SER:HB2	3:D:1206:ARG:HB3	1.83	0.60
1:A:107:ILE:HD12	2:C:773:LEU:HD13	1.84	0.60
2:C:630:VAL:HG13	2:C:631:GLU:H	1.66	0.60
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	1.83	0.60
3:D:1371:ARG:NE	3:D:1376:GLY:HA3	2.16	0.60
1:B:71:LYS:HE2	1:B:71:LYS:HA	1.84	0.60
2:C:1246:ARG:HH21	2:C:1258:PRO:HB3	1.67	0.60
4:E:8:ASP:O	4:E:12:LYS:HG2	2.02	0.60
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.83	0.59
4:E:13:ILE:HD12	4:E:13:ILE:N	2.16	0.59
4:E:44:ASP:HB3	4:E:48:VAL:HG21	1.84	0.59
2:C:241:LEU:HD22	2:C:285:ILE:HD13	1.83	0.59
3:D:515:ARG:HE	3:D:515:ARG:HA	1.65	0.59
3:D:1373:ARG:CB	4:E:58:LEU:HD11	2.32	0.59
4:E:38:LEU:CD1	4:E:53:GLU:HG3	2.32	0.59
1:A:64:VAL:HG23	1:A:71:LYS:HD3	1.84	0.59
2:C:1155:VAL:HG12	2:C:1157:GLN:H	1.67	0.59
1:A:83:LEU:HD13	2:C:826:ASP:HB2	1.82	0.59
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.85	0.59
3:D:1370:MET:HB3	4:E:59:ILE:HD11	1.84	0.59
1:B:44:ARG:HA	1:B:183:ILE:HD12	1.84	0.59
4:E:86:ILE:HG23	4:E:87:ALA:N	2.17	0.59
3:D:1376:GLY:O	3:D:1379:PRO:HD2	2.03	0.59
2:C:862:LEU:HD23	2:C:865:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:431:ARG:HB3	3:D:921:GLN:HE22	1.67	0.58
3:D:694:SER:HB2	3:D:738:ARG:HG3	1.86	0.58
4:E:49:ILE:N	4:E:49:ILE:HD13	2.18	0.58
1:B:155:ALA:HB1	1:B:172:LEU:HB2	1.84	0.58
2:C:1276:TRP:HE1	3:D:1348:LYS:HE3	1.67	0.58
1:A:158:ARG:HH21	1:A:172:LEU:HD11	1.68	0.58
3:D:478:LEU:HD11	4:E:27:ALA:HB2	1.84	0.58
4:E:19:LEU:H	4:E:19:LEU:HD12	1.68	0.58
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.85	0.58
3:D:363:LEU:HD12	3:D:363:LEU:H	1.69	0.58
3:D:384:LYS:HD2	3:D:387:LEU:HD12	1.86	0.58
2:C:79:VAL:HG12	2:C:80:PHE:CD1	2.39	0.58
2:C:225:PHE:HE2	2:C:347:ILE:HB	1.69	0.58
3:D:430:HIS:HA	3:D:921:GLN:HB2	1.86	0.58
3:D:1371:ARG:HH21	3:D:1376:GLY:HA3	1.68	0.58
2:C:322:LEU:HD23	2:C:325:LEU:HD12	1.85	0.58
2:C:1339:LEU:H	2:C:1339:LEU:HD23	1.68	0.58
2:C:131:THR:HG22	2:C:132:ASP:H	1.69	0.58
2:C:406:ASN:HD22	2:C:414:ILE:HA	1.69	0.58
1:A:2:GLN:H	1:A:2:GLN:NE2	2.02	0.57
1:A:118:ASP:HB3	1:A:121:VAL:HB	1.86	0.57
3:D:803:VAL:HG21	3:D:1309:ILE:HB	1.86	0.57
4:E:63:ILE:HG23	4:E:64:LEU:N	2.18	0.57
3:D:504:GLN:HA	3:D:730:ALA:HA	1.86	0.57
3:D:1274:PHE:CD2	3:D:1275:LEU:HG	2.39	0.57
3:D:110:PRO:HG2	3:D:186:GLN:HE22	1.69	0.57
4:E:15:ASN:HB3	4:E:18:ASP:OD2	2.04	0.57
2:C:705:GLU:HB2	2:C:794:LEU:H	1.68	0.57
3:D:201:LEU:HD12	3:D:221:ILE:HD12	1.86	0.57
3:D:1169:THR:HG22	3:D:1171:GLY:H	1.70	0.57
1:A:35:PHE:HE2	1:B:227:GLN:HG3	1.69	0.57
2:C:1120:ALA:O	2:C:1124:ILE:HG13	2.05	0.57
3:D:128:LEU:HD22	3:D:130:MET:HG3	1.86	0.57
3:D:1261:LEU:HD21	3:D:1304:ARG:NH1	2.20	0.57
3:D:1371:ARG:NH2	3:D:1376:GLY:HA3	2.19	0.57
2:C:1123:GLY:HA3	2:C:1202:GLY:HA3	1.85	0.57
2:C:1282:GLY:HA2	4:E:17:PHE:HE2	1.67	0.57
3:D:1363:TYR:HD2	3:D:1365:TYR:CB	2.18	0.57
4:E:12:LYS:CB	4:E:13:ILE:HD12	2.35	0.57
4:E:49:ILE:HD13	4:E:49:ILE:H	1.69	0.57
3:D:1297:LYS:H	3:D:1297:LYS:HD3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1122:LYS:HE3	2:C:1203:ASP:HB2	1.86	0.56
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.87	0.56
2:C:979:LEU:HD21	2:C:1000:LEU:HD23	1.86	0.56
3:D:145:VAL:HA	3:D:180:MET:HB3	1.87	0.56
3:D:974:VAL:HG22	3:D:1002:VAL:HG22	1.85	0.56
2:C:1223:ARG:HB2	2:C:1223:ARG:HH11	1.70	0.56
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.88	0.56
2:C:813:GLU:HB2	3:D:461:PHE:HD1	1.71	0.56
2:C:890:LYS:HG2	2:C:914:LYS:HD3	1.87	0.56
3:D:222:LYS:HB2	3:D:222:LYS:NZ	2.20	0.56
2:C:1047:LEU:O	2:C:1048:LYS:HG2	2.05	0.56
3:D:614:LEU:CA	4:E:7:GLN:OE1	2.51	0.56
1:A:44:ARG:HH22	2:C:1093:PRO:HG3	1.71	0.56
3:D:64:PRO:HG2	3:D:92:VAL:HA	1.87	0.56
3:D:1347:LEU:HD21	3:D:1359:ALA:HB2	1.88	0.56
2:C:102:LEU:HD21	2:C:488:MET:HG3	1.87	0.56
2:C:561:ILE:HD11	2:C:680:LEU:HB2	1.87	0.56
3:D:420:PRO:HG2	3:D:481:ARG:HG2	1.88	0.56
3:D:547:ARG:HH11	3:D:547:ARG:HA	1.71	0.56
3:D:1371:ARG:HE	3:D:1376:GLY:CA	2.18	0.56
2:C:68:LEU:HD13	2:C:102:LEU:HD23	1.87	0.55
1:A:207:THR:HG22	1:A:209:GLY:H	1.71	0.55
2:C:1124:ILE:HG23	2:C:1198:LEU:HD13	1.88	0.55
2:C:41:GLN:HG3	2:C:75:LEU:HB3	1.88	0.55
2:C:120:GLN:H	2:C:120:GLN:NE2	2.04	0.55
1:B:118:ASP:HB3	1:B:121:VAL:HB	1.88	0.55
2:C:101:ARG:HG2	2:C:118:LYS:HG3	1.89	0.55
2:C:550:VAL:HG11	2:C:560:PRO:HB3	1.89	0.55
2:C:1204:LEU:H	2:C:1205:PRO:CD	2.20	0.55
3:D:121:PRO:HB2	3:D:123:ARG:HH12	1.70	0.55
1:A:221:ALA:HB1	1:B:228:LEU:HB3	1.88	0.55
2:C:1128:ILE:HA	2:C:1132:LEU:HD13	1.89	0.55
3:D:614:LEU:N	4:E:7:GLN:HG3	2.16	0.55
1:B:47:LEU:HB3	1:B:180:VAL:HG21	1.89	0.55
2:C:552:PRO:HA	3:D:773:PHE:CE1	2.41	0.55
2:C:1002:LEU:HD23	2:C:1003:THR:N	2.21	0.55
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.88	0.55
3:D:1090:ILE:HG13	3:D:1162:ILE:HD12	1.89	0.55
4:E:36:ASP:HB2	4:E:37:PRO:HD2	1.88	0.55
4:E:54:ILE:N	4:E:54:ILE:HD12	2.22	0.55
3:D:807:LEU:HD21	3:D:1259:GLN:HE21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1109:ILE:HD12	2:C:1112:ILE:HD12	1.89	0.54
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.43	0.54
3:D:1381:ALA:HB3	3:D:1382:PRO:CD	2.37	0.54
2:C:179:TYR:CD2	2:C:180:ARG:HG3	2.42	0.54
3:D:759:ILE:HD13	3:D:759:ILE:H	1.72	0.54
1:A:5:VAL:HG22	1:A:9:LEU:HD22	1.89	0.54
1:A:192:VAL:HG13	1:A:194:GLN:H	1.73	0.54
2:C:810:TYR:HB2	2:C:817:LEU:HD11	1.89	0.54
2:C:1203:ASP:HB3	2:C:1204:LEU:HB2	1.89	0.54
3:D:739:GLN:HB3	3:D:763:PHE:HE2	1.72	0.54
2:C:68:LEU:HD11	2:C:100:LEU:HB3	1.88	0.54
2:C:257:ALA:HB3	2:C:262:TYR:HE2	1.72	0.54
3:D:485:MET:HG2	3:D:487:THR:HG22	1.89	0.54
1:A:65:LEU:H	1:A:65:LEU:HD22	1.70	0.54
4:E:59:ILE:HG13	4:E:60:ASN:N	2.22	0.54
1:A:165:GLU:O	1:A:166:ARG:HB2	2.08	0.54
2:C:698:PRO:HG3	2:C:1231:TYR:CZ	2.43	0.54
3:D:857:LEU:HG	3:D:858:VAL:H	1.72	0.54
3:D:905:ARG:HG3	4:E:16:ARG:HH21	1.73	0.54
3:D:614:LEU:CB	4:E:7:GLN:HG2	2.37	0.54
2:C:1269:ARG:HB3	3:D:344:GLY:HA3	1.90	0.53
1:A:166:ARG:CB	1:A:167:PRO:HD3	2.31	0.53
4:E:5:THR:HG21	4:E:55:GLU:CG	2.39	0.53
3:D:370:LYS:HG2	3:D:441:LEU:HB3	1.90	0.53
3:D:903:LEU:HD22	3:D:910:ASN:H	1.73	0.53
4:E:5:THR:O	4:E:5:THR:HG23	2.08	0.53
2:C:724:VAL:HG21	2:C:771:VAL:HG11	1.89	0.53
3:D:767:LEU:HD12	3:D:772:TYR:HB2	1.90	0.53
3:D:1263:LYS:HD3	3:D:1307:LEU:HD13	1.90	0.53
3:D:1381:ALA:HB3	3:D:1382:PRO:HD3	1.89	0.53
2:C:183:TRP:H	2:C:199:ASP:HA	1.72	0.53
2:C:575:LEU:HD13	2:C:576:SER:N	2.23	0.53
3:D:615:LYS:HZ2	4:E:5:THR:HB	1.71	0.53
3:D:1263:LYS:NZ	3:D:1263:LYS:HB3	2.23	0.53
3:D:1279:GLN:HE22	3:D:1317:GLU:HB2	1.73	0.53
3:D:1360:GLY:O	3:D:1366:HIS:CD2	2.61	0.53
2:C:1313:HIS:CE1	4:E:28:ARG:NH1	2.76	0.53
3:D:377:PHE:O	3:D:381:ILE:HG13	2.08	0.53
3:D:1380:ALA:HA	3:D:1383:GLN:HG2	1.90	0.53
4:E:46:THR:HG22	4:E:47:THR:N	2.22	0.53
1:B:60:GLU:HB3	1:B:170:ARG:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.74	0.53
3:D:275:ARG:HH11	3:D:298:MET:HB3	1.74	0.53
3:D:1140:ARG:HH12	3:D:1214:PRO:HG3	1.74	0.53
4:E:56:GLU:HG2	4:E:57:GLY:N	2.23	0.53
2:C:49:LEU:HB3	2:C:53:PHE:CZ	2.44	0.53
3:D:110:PRO:HB3	3:D:240:THR:HA	1.91	0.53
3:D:1317:GLU:HG3	3:D:1340:LYS:HD3	1.91	0.53
2:C:148:GLN:HB3	2:C:454:ARG:HD3	1.91	0.52
3:D:217:LEU:HA	3:D:220:ARG:HG2	1.90	0.52
3:D:432:LEU:HD22	3:D:435:GLN:HE21	1.73	0.52
2:C:518:ASN:HD21	2:C:688:GLN:HA	1.73	0.52
2:C:681:MET:O	2:C:685:MET:HG2	2.10	0.52
3:D:108:ALA:HB1	3:D:283:LEU:HD11	1.91	0.52
3:D:1371:ARG:HB3	4:E:60:ASN:HB3	1.91	0.52
3:D:369:PRO:HD3	3:D:447:ILE:HG22	1.92	0.52
2:C:338:THR:HB	2:C:345:PRO:HG3	1.91	0.52
2:C:591:TYR:HB2	2:C:606:LEU:HD23	1.91	0.52
2:C:896:THR:O	2:C:900:LYS:HG3	2.10	0.52
3:D:113:HIS:CD2	3:D:307:LEU:HD22	2.44	0.52
3:D:482:ALA:CB	4:E:3:ARG:NH1	2.72	0.52
3:D:527:LEU:HD23	3:D:534:GLU:HA	1.91	0.52
4:E:13:ILE:HD13	4:E:19:LEU:CD2	2.39	0.52
1:B:68:TYR:CE1	3:D:535:ARG:HB2	2.45	0.52
2:C:74:ARG:HE	2:C:99:LYS:HE3	1.74	0.52
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.90	0.52
3:D:516:ASP:HA	3:D:572:THR:HG21	1.90	0.52
3:D:690:ASN:HB2	3:D:738:ARG:HD3	1.92	0.52
4:E:46:THR:CG2	4:E:47:THR:H	2.19	0.52
3:D:703:THR:HG23	3:D:704:GLU:HG2	1.91	0.52
3:D:825:VAL:HG13	3:D:826:ILE:HG13	1.92	0.52
1:A:161:SER:HB2	1:A:164:ASP:HB2	1.91	0.52
2:C:151:ARG:HE	2:C:177:ILE:HD12	1.75	0.52
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.44	0.52
2:C:689:ALA:HB2	2:C:1233:LEU:HD21	1.90	0.52
2:C:732:ILE:HG13	2:C:753:LEU:HD21	1.91	0.52
3:D:534:GLU:O	3:D:538:ARG:HB2	2.10	0.52
3:D:762:ASN:HD22	3:D:762:ASN:H	1.57	0.52
3:D:937:ILE:HD12	3:D:1151:LYS:H	1.76	0.51
3:D:960:LEU:HB3	3:D:963:VAL:HG11	1.92	0.51
2:C:40:GLU:HB3	2:C:43:PRO:HB2	1.92	0.51
3:D:733:SER:HB3	3:D:736:GLN:HG2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1348:LYS:HB2	3:D:1348:LYS:NZ	2.25	0.51
4:E:39:VAL:HB	4:E:40:PRO:CD	2.40	0.51
2:C:53:PHE:CD1	2:C:57:PHE:HE2	2.28	0.51
3:D:381:ILE:O	3:D:385:LEU:HG	2.11	0.51
3:D:393:THR:HG23	3:D:396:ALA:H	1.76	0.51
2:C:149:LEU:HD21	2:C:451:ARG:HB3	1.91	0.51
3:D:515:ARG:HA	3:D:515:ARG:NE	2.26	0.51
1:A:65:LEU:HD23	2:C:874:GLY:HA3	1.92	0.51
1:A:66:HIS:HB3	2:C:874:GLY:HA2	1.93	0.51
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.45	0.51
2:C:31:GLN:HE22	2:C:456:VAL:HG21	1.75	0.51
3:D:1191:PRO:HD2	3:D:1194:ARG:HD3	1.91	0.51
2:C:79:VAL:HG21	2:C:93:SER:H	1.76	0.51
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.93	0.51
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.91	0.51
3:D:647:PRO:HG3	3:D:697:MET:HB2	1.92	0.51
3:D:1369:ARG:NE	4:E:74:GLU:HB3	2.25	0.51
2:C:488:MET:HB2	2:C:489:PRO:HD3	1.93	0.51
2:C:840:SER:HB2	2:C:848:GLU:HB2	1.93	0.51
2:C:1127:LYS:HE2	2:C:1149:TYR:CD1	2.46	0.51
3:D:380:PHE:HB3	3:D:415:VAL:HG11	1.93	0.51
3:D:521:LYS:NZ	3:D:521:LYS:HB3	2.26	0.51
2:C:1065:LYS:HB3	2:C:1075:VAL:HG22	1.93	0.51
3:D:1165:PHE:HD1	3:D:1200:GLU:HG2	1.76	0.51
3:D:1190:ILE:HG21	3:D:1196:LEU:HD11	1.93	0.51
2:C:177:ILE:HG12	2:C:183:TRP:CZ3	2.46	0.51
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.93	0.51
2:C:50:GLU:HB2	2:C:73:TYR:HE1	1.76	0.50
3:D:425:ARG:CG	3:D:427:PRO:HD2	2.35	0.50
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.75	0.50
1:A:47:LEU:HD23	1:A:51:MET:HG3	1.93	0.50
1:B:69:SER:H	1:B:78:ILE:HD11	1.77	0.50
2:C:1185:PRO:HD2	2:C:1189:GLY:HA3	1.93	0.50
3:D:614:LEU:HD12	4:E:6:VAL:HB	1.92	0.50
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.93	0.50
1:A:234:LEU:H	1:A:234:LEU:CD1	2.21	0.50
2:C:694:ARG:HB2	2:C:798:GLN:NE2	2.27	0.50
2:C:1204:LEU:H	2:C:1205:PRO:HD2	1.77	0.50
3:D:1344:LEU:HD12	3:D:1355:ARG:HH11	1.76	0.50
3:D:1372:ARG:NH2	4:E:84:THR:HG21	2.25	0.50
2:C:451:ARG:HH21	2:C:554:HIS:CE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:718:ALA:HB2	2:C:783:LEU:HD21	1.93	0.50
3:D:1366:HIS:O	4:E:21:LEU:HD22	2.11	0.50
3:D:1373:ARG:HG3	3:D:1374:ALA:N	2.27	0.50
2:C:520:PRO:HG3	2:C:787:PRO:HG2	1.93	0.50
3:D:516:ASP:OD2	3:D:551:ARG:HG2	2.12	0.50
3:D:680:ASN:HD22	3:D:680:ASN:C	2.15	0.50
3:D:1193:TRP:HB2	3:D:1194:ARG:HH11	1.77	0.50
2:C:972:PHE:HB3	2:C:994:ARG:HH21	1.77	0.50
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.93	0.50
3:D:332:LYS:HB2	3:D:332:LYS:NZ	2.27	0.50
3:D:682:VAL:O	3:D:686:TRP:HD1	1.95	0.50
2:C:478:ARG:HA	2:C:481:LEU:HD23	1.93	0.50
2:C:572:ILE:N	2:C:572:ILE:HD12	2.27	0.50
3:D:296:LYS:HB2	3:D:296:LYS:NZ	2.27	0.50
3:D:481:ARG:HB3	4:E:3:ARG:HD2	1.94	0.50
1:B:83:LEU:HD12	1:B:86:LYS:HD2	1.94	0.50
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.46	0.50
2:C:557:ARG:HA	2:C:579:ALA:HB2	1.93	0.50
2:C:1336:ASN:HB2	3:D:25:ALA:HB2	1.92	0.50
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.93	0.49
2:C:31:GLN:NE2	2:C:456:VAL:HG21	2.26	0.49
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.93	0.49
2:C:1324:ASN:O	2:C:1328:LYS:HG2	2.12	0.49
3:D:521:LYS:HE3	3:D:551:ARG:NH2	2.27	0.49
3:D:1156:LEU:HD23	3:D:1223:LEU:HD11	1.93	0.49
2:C:680:LEU:HD13	3:D:783:LEU:HD22	1.94	0.49
2:C:821:ARG:HB2	2:C:1082:ILE:HD11	1.93	0.49
2:C:827:ARG:HG3	2:C:828:PHE:CD2	2.47	0.49
3:D:480:ALA:HA	3:D:484:MET:HB3	1.93	0.49
4:E:13:ILE:HG22	4:E:14:GLY:N	2.27	0.49
1:B:111:THR:HG23	1:B:113:ALA:H	1.76	0.49
2:C:169:LYS:HB2	2:C:169:LYS:NZ	2.27	0.49
3:D:233:LYS:HB3	3:D:235:GLU:OE1	2.13	0.49
3:D:378:LYS:N	3:D:379:PRO:CD	2.76	0.49
3:D:485:MET:HE1	4:E:3:ARG:HG3	1.94	0.49
3:D:500:ILE:O	3:D:500:ILE:HG12	2.12	0.49
3:D:843:VAL:O	3:D:882:VAL:HG23	2.11	0.49
4:E:12:LYS:HB2	4:E:13:ILE:CD1	2.42	0.49
3:D:430:HIS:HD2	3:D:432:LEU:H	1.61	0.49
1:B:173:VAL:HA	3:D:538:ARG:HH22	1.78	0.49
2:C:1141:LEU:O	2:C:1145:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:555:TYR:HE2	3:D:560:ASN:HB3	1.77	0.49
1:B:158:ARG:HE	1:B:158:ARG:HA	1.78	0.49
2:C:131:THR:HG22	2:C:132:ASP:N	2.26	0.49
3:D:558:ASP:HB3	3:D:577:ALA:HB1	1.94	0.49
3:D:1304:ARG:HE	3:D:1304:ARG:HA	1.77	0.49
2:C:1195:ILE:O	2:C:1199:LEU:HD13	2.12	0.49
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.94	0.49
2:C:891:GLY:O	2:C:895:LEU:HG	2.12	0.49
2:C:932:GLN:HG3	2:C:934:PHE:CE1	2.48	0.49
3:D:139:LEU:HD12	3:D:140:TYR:N	2.28	0.49
4:E:79:GLU:O	4:E:83:VAL:HG23	2.13	0.49
4:E:84:THR:HG23	4:E:85:ALA:N	2.28	0.49
3:D:1024:THR:HA	3:D:1124:ILE:O	2.12	0.49
2:C:735:LYS:NZ	2:C:735:LYS:HB3	2.27	0.48
3:D:864:LEU:O	3:D:867:GLN:HG2	2.13	0.48
3:D:1224:ARG:HH11	3:D:1228:ALA:HB2	1.77	0.48
1:A:71:LYS:NZ	1:A:71:LYS:HB3	2.28	0.48
2:C:598:VAL:HG13	2:C:627:GLY:HA2	1.94	0.48
3:D:114:ILE:HD13	3:D:311:ARG:HD3	1.96	0.48
3:D:138:VAL:O	3:D:142:GLU:HB2	2.13	0.48
2:C:404:LYS:NZ	2:C:452:ARG:HE	2.10	0.48
2:C:518:ASN:HD22	2:C:1236:ASN:ND2	2.11	0.48
3:D:858:VAL:HB	3:D:859:PRO:HD2	1.95	0.48
1:B:110:VAL:HG13	1:B:130:ILE:HG23	1.95	0.48
2:C:1034:ARG:O	2:C:1038:GLN:HB2	2.13	0.48
2:C:1204:LEU:HB3	2:C:1205:PRO:HD3	1.96	0.48
3:D:811:GLU:HG3	3:D:896:ALA:H	1.78	0.48
3:D:1206:ARG:HG3	3:D:1224:ARG:HA	1.95	0.48
1:A:159:ILE:HG23	1:A:159:ILE:O	2.12	0.48
2:C:519:ASN:HD21	2:C:796:LEU:HD22	1.79	0.48
3:D:325:LYS:NZ	3:D:325:LYS:HB3	2.28	0.48
3:D:385:LEU:HB3	3:D:391:ALA:HB3	1.95	0.48
3:D:881:LYS:HD2	3:D:881:LYS:N	2.28	0.48
3:D:926:PRO:HB3	3:D:1246:VAL:HG11	1.95	0.48
2:C:1103:VAL:HB	2:C:1104:PRO:HD3	1.95	0.48
3:D:378:LYS:HG3	3:D:379:PRO:HD3	1.95	0.48
3:D:1231:ARG:CZ	3:D:1231:ARG:HA	2.43	0.48
4:E:19:LEU:HD12	4:E:19:LEU:N	2.29	0.48
3:D:132:LEU:HD23	3:D:133:ARG:HG3	1.94	0.48
3:D:314:ARG:HD2	3:D:323:PRO:HG3	1.95	0.48
3:D:479:GLU:HB3	4:E:20:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:ALA:O	3:D:916:GLY:HA3	2.14	0.48
3:D:1142:ALA:O	3:D:1146:GLU:HB2	2.13	0.48
3:D:1210:ILE:HD13	3:D:1210:ILE:O	2.13	0.48
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.95	0.48
4:E:4:VAL:C	4:E:5:THR:HG22	2.33	0.48
2:C:1273:MET:HA	2:C:1276:TRP:CE3	2.48	0.48
3:D:184:ALA:O	3:D:188:LEU:HD13	2.14	0.48
1:A:102:LEU:HD12	1:A:142:MET:HG2	1.96	0.48
3:D:131:PRO:HB3	3:D:134:ASP:HB2	1.95	0.48
3:D:905:ARG:HD3	3:D:907:HIS:NE2	2.29	0.48
3:D:1263:LYS:HD2	3:D:1263:LYS:N	2.24	0.48
3:D:1360:GLY:N	3:D:1362:GLY:H	2.10	0.48
4:E:26:ARG:HH21	4:E:37:PRO:CD	2.27	0.48
4:E:63:ILE:CG1	4:E:64:LEU:HD12	2.38	0.48
1:A:86:LYS:HE3	2:C:826:ASP:OD2	2.14	0.47
2:C:1205:PRO:HG3	2:C:1210:ILE:HG13	1.96	0.47
3:D:275:ARG:NH1	3:D:298:MET:HB3	2.29	0.47
3:D:370:LYS:HB3	3:D:409:TRP:CZ3	2.49	0.47
3:D:421:VAL:HG22	3:D:439:PRO:HG3	1.95	0.47
3:D:1344:LEU:HD12	3:D:1355:ARG:NH1	2.28	0.47
1:A:102:LEU:HD23	1:A:115:ILE:HA	1.96	0.47
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	1.96	0.47
1:A:43:LEU:HD13	1:A:217:ILE:HD11	1.96	0.47
3:D:381:ILE:HG21	3:D:401:VAL:HG21	1.97	0.47
3:D:525:MET:HG2	3:D:537:TYR:CE1	2.49	0.47
3:D:1373:ARG:HB3	4:E:58:LEU:CD1	2.42	0.47
2:C:150:HIS:CD2	2:C:454:ARG:HD2	2.49	0.47
2:C:975:ILE:HD11	2:C:997:TRP:HE3	1.78	0.47
3:D:1266:ILE:HD13	3:D:1266:ILE:H	1.79	0.47
3:D:1371:ARG:CZ	3:D:1376:GLY:HA3	2.44	0.47
2:C:333:ILE:N	2:C:333:ILE:HD12	2.30	0.47
2:C:867:GLU:HB2	2:C:947:GLU:OE1	2.13	0.47
3:D:38:VAL:HG13	3:D:55:GLY:HA2	1.96	0.47
3:D:1369:ARG:HE	4:E:74:GLU:HB3	1.78	0.47
4:E:10:VAL:HA	4:E:19:LEU:HD22	1.94	0.47
2:C:88:ARG:HA	2:C:932:GLN:HE22	1.80	0.47
2:C:1190:ALA:HB1	2:C:1195:ILE:HD11	1.97	0.47
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.97	0.47
3:D:423:LEU:HD13	3:D:437:PHE:HD2	1.78	0.47
3:D:801:VAL:O	3:D:805:GLN:HB3	2.15	0.47
3:D:1163:VAL:HG21	3:D:1198:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:43:ASN:CG	4:E:44:ASP:H	2.18	0.47
4:E:54:ILE:HD12	4:E:54:ILE:H	1.78	0.47
4:E:63:ILE:HG12	4:E:64:LEU:HD11	1.93	0.47
1:A:224:LEU:HD23	1:B:228:LEU:HD21	1.96	0.47
1:B:123:ILE:HG22	1:B:125:LYS:H	1.80	0.47
2:C:30:ILE:N	2:C:30:ILE:HD12	2.30	0.47
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.50	0.47
2:C:145:ILE:N	2:C:145:ILE:HD12	2.29	0.47
2:C:153:PRO:HB3	2:C:397:LEU:HD22	1.97	0.47
2:C:551:HIS:CD2	2:C:553:THR:H	2.33	0.47
2:C:559:CYS:SG	2:C:562:GLU:HG2	2.55	0.47
2:C:870:ILE:HD12	2:C:870:ILE:N	2.30	0.47
2:C:1108:ASN:O	2:C:1111:GLN:HG2	2.15	0.47
2:C:1135:GLN:HB2	2:C:1142:ARG:HA	1.95	0.47
3:D:118:LYS:HG2	3:D:311:ARG:HH21	1.80	0.47
3:D:598:LYS:HG3	3:D:599:LYS:HD3	1.96	0.47
3:D:848:VAL:HB	3:D:856:ILE:HD11	1.95	0.47
3:D:885:VAL:HG11	3:D:1255:VAL:HG12	1.96	0.47
4:E:64:LEU:HD12	4:E:64:LEU:N	2.29	0.47
2:C:22:LEU:HD13	2:C:23:ASP:O	2.13	0.47
4:E:36:ASP:HB2	4:E:37:PRO:CD	2.45	0.47
1:A:47:LEU:HB3	1:A:180:VAL:HG21	1.97	0.47
1:B:69:SER:N	1:B:78:ILE:HD11	2.30	0.47
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.80	0.47
1:B:102:LEU:HD12	1:B:115:ILE:HG12	1.97	0.47
2:C:99:LYS:HA	2:C:120:GLN:O	2.14	0.47
2:C:161:LYS:HE3	2:C:175:ARG:HH21	1.80	0.47
2:C:552:PRO:HA	3:D:773:PHE:HE1	1.79	0.47
2:C:810:TYR:CD2	3:D:359:PRO:HG2	2.50	0.47
2:C:1216:ARG:HH22	3:D:633:ALA:HB3	1.79	0.47
2:C:403:MET:HG2	2:C:407:ARG:HH12	1.80	0.46
2:C:562:GLU:HG3	2:C:662:SER:HB2	1.97	0.46
2:C:672:GLU:HB2	3:D:767:LEU:HB3	1.98	0.46
2:C:1182:ILE:HD12	2:C:1183:ALA:N	2.30	0.46
3:D:614:LEU:HB2	4:E:7:GLN:OE1	2.16	0.46
3:D:1234:VAL:HG11	3:D:1254:GLU:HG2	1.97	0.46
1:B:88:LEU:HB2	1:B:128:HIS:CE1	2.49	0.46
3:D:41:PRO:HG2	3:D:274:ASN:ND2	2.29	0.46
3:D:378:LYS:CG	3:D:379:PRO:HD3	2.44	0.46
3:D:430:HIS:CD2	3:D:432:LEU:H	2.33	0.46
2:C:176:ILE:O	2:C:178:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:201:LEU:HD22	3:D:217:LEU:HD23	1.97	0.46
3:D:1234:VAL:HG12	3:D:1253:ILE:HG22	1.98	0.46
3:D:1322:ALA:HB3	3:D:1331:VAL:HG11	1.96	0.46
2:C:1128:ILE:O	2:C:1132:LEU:HB2	2.15	0.46
3:D:30:ILE:HA	3:D:33:TRP:CZ3	2.49	0.46
3:D:160:LEU:N	3:D:160:LEU:HD13	2.31	0.46
1:A:74:VAL:HG22	1:A:76:GLU:H	1.80	0.46
2:C:29:SER:HB2	2:C:580:GLN:NE2	2.31	0.46
2:C:142:GLU:HG3	2:C:517:GLN:OE1	2.15	0.46
2:C:453:ILE:HD11	2:C:587:LEU:HD12	1.98	0.46
3:D:614:LEU:CB	4:E:7:GLN:OE1	2.64	0.46
4:E:53:GLU:O	4:E:56:GLU:HB3	2.15	0.46
2:C:434:ASP:HB3	2:C:439:LYS:HG3	1.98	0.46
2:C:630:VAL:HG13	2:C:631:GLU:N	2.29	0.46
2:C:932:GLN:HG3	2:C:934:PHE:HE1	1.81	0.46
2:C:932:GLN:CB	2:C:1051:LYS:H	2.28	0.46
3:D:557:LYS:HG3	3:D:560:ASN:H	1.80	0.46
4:E:31:GLN:HA	4:E:31:GLN:NE2	2.26	0.46
2:C:472:GLU:HG2	2:C:476:LYS:NZ	2.31	0.46
2:C:810:TYR:HB3	2:C:817:LEU:HD21	1.97	0.46
3:D:51:PRO:HD2	3:D:71:LEU:HD11	1.98	0.46
3:D:500:ILE:H	3:D:500:ILE:CD1	2.26	0.46
3:D:759:ILE:HD13	3:D:759:ILE:N	2.31	0.46
4:E:31:GLN:HE21	4:E:31:GLN:CA	2.24	0.46
4:E:68:GLU:HG2	4:E:69:ARG:N	2.31	0.46
1:B:207:THR:HG21	1:B:211:ILE:O	2.16	0.46
2:C:138:ILE:HD12	2:C:138:ILE:N	2.31	0.46
2:C:1187:PHE:CD1	3:D:769:VAL:HG12	2.51	0.46
3:D:114:ILE:H	3:D:307:LEU:HD13	1.81	0.46
3:D:148:GLU:HB3	3:D:187:ALA:HB3	1.96	0.46
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.79	0.46
3:D:623:GLN:O	3:D:627:THR:HG22	2.16	0.46
1:A:2:GLN:HB2	1:A:9:LEU:HD11	1.99	0.45
2:C:151:ARG:HB3	2:C:156:PHE:CZ	2.51	0.45
3:D:77:ARG:NE	3:D:77:ARG:HA	2.31	0.45
3:D:804:ALA:HB1	3:D:807:LEU:HD23	1.98	0.45
1:A:29:GLU:OE1	1:A:200:LYS:HE2	2.16	0.45
1:B:10:LYS:HB3	1:B:10:LYS:NZ	2.31	0.45
1:B:222:THR:O	1:B:226:GLU:HG3	2.16	0.45
2:C:448:LEU:HD11	2:C:554:HIS:CG	2.51	0.45
2:C:519:ASN:HB3	2:C:522:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:121:PRO:HB2	3:D:123:ARG:NH1	2.31	0.45
3:D:1380:ALA:CA	3:D:1383:GLN:HG2	2.46	0.45
4:E:39:VAL:HG12	4:E:40:PRO:N	2.30	0.45
1:A:82:LEU:O	1:A:86:LYS:HG3	2.16	0.45
2:C:528:ARG:NH2	2:C:577:VAL:HA	2.31	0.45
3:D:77:ARG:HA	3:D:77:ARG:HE	1.81	0.45
3:D:527:LEU:HD12	3:D:527:LEU:N	2.31	0.45
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.99	0.45
2:C:212:ALA:HA	2:C:359:ARG:HG3	1.98	0.45
3:D:113:HIS:O	3:D:117:LEU:HD13	2.15	0.45
3:D:232:ASN:HD22	3:D:232:ASN:N	2.13	0.45
3:D:566:LYS:HB2	3:D:566:LYS:NZ	2.31	0.45
3:D:615:LYS:CE	4:E:5:THR:CA	2.33	0.45
3:D:762:ASN:HD21	3:D:765:GLU:H	1.64	0.45
3:D:823:THR:HB	3:D:880:VAL:HB	1.98	0.45
3:D:1041:ILE:N	3:D:1041:ILE:HD12	2.32	0.45
1:A:130:ILE:N	1:A:130:ILE:HD12	2.32	0.45
1:A:166:ARG:HB2	1:A:167:PRO:CD	2.36	0.45
2:C:478:ARG:NH1	2:C:494:ASN:HB2	2.31	0.45
2:C:518:ASN:O	2:C:691:PRO:HD3	2.17	0.45
3:D:113:HIS:HB3	3:D:116:PHE:HD2	1.81	0.45
3:D:1025:MET:HB2	3:D:1124:ILE:HD12	1.99	0.45
3:D:1238:GLN:NE2	3:D:1242:ARG:HH21	2.15	0.45
3:D:1371:ARG:HD2	4:E:65:ASP:OD2	2.16	0.45
1:B:46:ILE:HG23	1:B:50:SER:HB2	1.98	0.45
2:C:68:LEU:HA	2:C:102:LEU:HB3	1.98	0.45
2:C:233:ARG:O	2:C:236:LYS:HG2	2.16	0.45
2:C:551:HIS:HD2	2:C:553:THR:H	1.65	0.45
3:D:94:GLN:O	3:D:97:VAL:HG22	2.16	0.45
3:D:1253:ILE:O	3:D:1257:VAL:HG23	2.16	0.45
2:C:138:ILE:HG12	2:C:506:PHE:HB3	1.99	0.45
2:C:827:ARG:HG3	2:C:828:PHE:HD2	1.82	0.45
2:C:1121:ALA:O	2:C:1126:ASP:HB3	2.17	0.45
2:C:1325:VAL:HG22	3:D:249:LEU:HD11	1.99	0.45
3:D:87:LYS:N	3:D:87:LYS:HD2	2.32	0.45
3:D:339:ARG:O	3:D:343:LEU:HB2	2.17	0.45
3:D:850:LYS:H	3:D:851:PRO:CD	2.30	0.45
1:A:56:VAL:HG11	1:A:86:LYS:HA	1.99	0.45
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.52	0.45
2:C:1103:VAL:H	2:C:1104:PRO:CD	2.30	0.45
3:D:227:PHE:CZ	3:D:1337:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:565:ALA:HB2	3:D:574:VAL:HG21	1.99	0.45
1:A:83:LEU:HD22	2:C:693:LEU:HD13	1.99	0.44
1:B:191:ARG:HH21	3:D:417:ARG:HD3	1.82	0.44
3:D:135:ILE:HG13	3:D:139:LEU:HD23	1.99	0.44
3:D:1348:LYS:HB2	3:D:1348:LYS:HZ2	1.81	0.44
4:E:47:THR:C	4:E:48:VAL:HG13	2.37	0.44
1:A:152:TYR:CZ	2:C:823:VAL:HG22	2.53	0.44
2:C:188:PHE:CE1	2:C:194:LEU:HB2	2.52	0.44
2:C:673:HIS:HB3	2:C:1109:ILE:HG23	1.98	0.44
2:C:705:GLU:CD	2:C:705:GLU:H	2.20	0.44
2:C:932:GLN:HB3	2:C:1051:LYS:H	1.82	0.44
3:D:69:GLU:HG2	3:D:76:LYS:HB3	1.99	0.44
3:D:71:LEU:H	3:D:71:LEU:HD22	1.82	0.44
3:D:644:MET:HA	3:D:644:MET:HE3	2.00	0.44
3:D:983:LYS:HD3	3:D:991:THR:HG23	1.98	0.44
1:A:58:GLU:H	1:A:145:LYS:HB3	1.83	0.44
1:A:165:GLU:O	1:A:166:ARG:CB	2.65	0.44
2:C:400:VAL:HG22	2:C:584:TYR:HD1	1.83	0.44
2:C:517:GLN:HA	2:C:523:GLU:HG2	2.00	0.44
2:C:1327:LEU:HG	2:C:1337:ILE:HG23	2.00	0.44
3:D:525:MET:HG2	3:D:537:TYR:CD1	2.52	0.44
3:D:1263:LYS:HB3	3:D:1263:LYS:HZ2	1.82	0.44
3:D:1373:ARG:NH1	4:E:58:LEU:HD22	2.32	0.44
4:E:9:ALA:O	4:E:19:LEU:HD21	2.17	0.44
2:C:1304:MET:HG3	3:D:472:LEU:HD13	1.99	0.44
3:D:799:ARG:HA	3:D:799:ARG:NE	2.32	0.44
4:E:7:GLN:HE21	4:E:7:GLN:HB3	1.44	0.44
1:A:61:ILE:N	1:A:61:ILE:HD12	2.33	0.44
2:C:155:VAL:HG11	2:C:428:VAL:HG21	2.00	0.44
2:C:464:PHE:O	2:C:468:LEU:HG	2.17	0.44
2:C:496:LYS:H	2:C:497:PRO:CD	2.30	0.44
2:C:549:ASP:OD2	3:D:750:PRO:HB3	2.16	0.44
2:C:577:VAL:HG11	2:C:658:GLN:OE1	2.18	0.44
2:C:588:GLU:HG2	2:C:607:SER:HA	2.00	0.44
2:C:1128:ILE:HG23	2:C:1132:LEU:HD22	2.00	0.44
2:C:1135:GLN:HB3	2:C:1145:ILE:HG13	1.99	0.44
2:C:1270:PHE:CE1	2:C:1290:MET:HE2	2.53	0.44
3:D:950:ILE:HB	3:D:1018:ALA:HB3	2.00	0.44
3:D:1297:LYS:HD3	3:D:1297:LYS:N	2.30	0.44
2:C:446:ASP:HB3	2:C:551:HIS:HB2	2.00	0.44
3:D:583:VAL:N	3:D:584:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:815:GLY:HA2	3:D:883:ARG:NH1	2.32	0.44
3:D:894:VAL:HG22	3:D:1258:ARG:HH22	1.82	0.44
4:E:67:ARG:HG3	4:E:68:GLU:N	2.32	0.44
2:C:463:GLN:HG3	2:C:505:PHE:CG	2.52	0.44
2:C:557:ARG:HB3	2:C:587:LEU:HD13	2.00	0.44
3:D:1095:MET:HE2	3:D:1162:ILE:H	1.83	0.44
1:A:83:LEU:HD12	1:A:86:LYS:HD2	2.00	0.44
2:C:87:ILE:HG12	2:C:88:ARG:NH2	2.33	0.44
2:C:636:CYS:HB2	2:C:645:PHE:HD1	1.83	0.44
2:C:1073:LYS:HE2	3:D:462:ASP:O	2.17	0.44
2:C:1325:VAL:O	2:C:1329:GLU:HG3	2.18	0.44
3:D:485:MET:HB3	3:D:488:ASN:ND2	2.33	0.44
1:A:192:VAL:HG22	1:A:193:GLU:N	2.33	0.44
1:B:215:GLU:HA	1:B:218:ARG:HG2	2.00	0.44
2:C:819:SER:O	2:C:822:VAL:HG12	2.18	0.44
2:C:1106:ARG:HD2	2:C:1106:ARG:N	2.33	0.44
2:C:1328:LYS:HG3	3:D:246:PRO:HG2	2.00	0.44
3:D:168:ALA:H	3:D:176:PHE:HZ	1.64	0.44
3:D:416:ILE:HG21	3:D:439:PRO:HB2	1.99	0.44
3:D:479:GLU:HA	4:E:20:VAL:CG2	2.48	0.44
3:D:1095:MET:HE2	3:D:1161:GLY:HA3	2.00	0.44
1:A:110:VAL:HG21	1:A:140:ILE:HD11	2.00	0.43
1:A:168:ILE:HD13	1:A:168:ILE:N	2.32	0.43
3:D:1203:ARG:HB3	3:D:1203:ARG:NH1	2.33	0.43
3:D:1220:ILE:HD13	3:D:1220:ILE:O	2.17	0.43
4:E:15:ASN:O	4:E:19:LEU:HD12	2.18	0.43
1:A:60:GLU:HB3	1:A:143:ARG:HB2	2.00	0.43
1:A:168:ILE:HD13	1:A:168:ILE:H	1.83	0.43
2:C:218:GLU:HG2	2:C:299:LYS:HA	2.01	0.43
2:C:517:GLN:HE21	2:C:759:SER:HB3	1.82	0.43
2:C:1203:ASP:HA	2:C:1204:LEU:HA	1.59	0.43
3:D:288:PRO:O	3:D:292:VAL:HG22	2.17	0.43
1:B:30:PRO:C	1:B:31:LEU:HD22	2.39	0.43
2:C:788:SER:HB3	2:C:795:ALA:O	2.18	0.43
3:D:334:LYS:HD3	3:D:334:LYS:C	2.39	0.43
3:D:845:ALA:HB3	3:D:881:LYS:HB3	2.00	0.43
3:D:1290:ARG:O	3:D:1297:LYS:HA	2.18	0.43
3:D:1379:PRO:CD	3:D:1380:ALA:H	2.31	0.43
4:E:13:ILE:CG2	4:E:14:GLY:N	2.81	0.43
1:A:171:LEU:N	1:A:171:LEU:HD13	2.34	0.43
2:C:87:ILE:HG23	2:C:88:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:939:VAL:O	2:C:939:VAL:HG12	2.18	0.43
2:C:1309:VAL:HG12	3:D:382:TYR:HB2	2.00	0.43
1:B:29:GLU:HB2	1:B:30:PRO:HA	2.01	0.43
2:C:488:MET:H	2:C:489:PRO:CD	2.31	0.43
2:C:1274:GLU:HB3	3:D:434:ILE:HD11	1.99	0.43
3:D:136:GLU:O	3:D:140:TYR:HD1	2.00	0.43
3:D:190:LYS:HG2	3:D:235:GLU:HG2	1.99	0.43
3:D:430:HIS:NE2	3:D:432:LEU:HB2	2.33	0.43
3:D:901:ARG:H	3:D:1251:LYS:NZ	2.17	0.43
3:D:1184:ASP:HB2	3:D:1185:PRO:HD3	2.01	0.43
1:B:47:LEU:HD21	1:B:220:ALA:HB2	2.01	0.43
3:D:68:TYR:HA	3:D:92:VAL:HG21	1.99	0.43
3:D:137:ARG:HB3	3:D:312:ARG:HH22	1.83	0.43
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.99	0.43
3:D:978:ARG:HG2	3:D:979:ASN:H	1.83	0.43
4:E:63:ILE:HG23	4:E:64:LEU:CD1	2.47	0.43
1:A:192:VAL:HG22	1:A:193:GLU:H	1.84	0.43
1:B:12:ARG:HD2	1:B:12:ARG:N	2.34	0.43
1:B:68:TYR:HE1	3:D:535:ARG:HB2	1.82	0.43
2:C:155:VAL:HG11	2:C:428:VAL:HG11	2.01	0.43
2:C:489:PRO:HB2	2:C:490:GLN:H	1.57	0.43
2:C:753:LEU:N	2:C:753:LEU:HD22	2.34	0.43
2:C:806:PRO:HD3	2:C:1100:PRO:HG2	2.01	0.43
2:C:1125:GLY:HA3	2:C:1182:ILE:HG22	2.01	0.43
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.43
3:D:66:LYS:HG2	3:D:67:ASP:H	1.82	0.43
3:D:296:LYS:HD3	3:D:296:LYS:H	1.84	0.43
3:D:406:ALA:HA	3:D:409:TRP:CD1	2.54	0.43
3:D:473:THR:HG23	3:D:476:ALA:H	1.84	0.43
3:D:501:VAL:HG23	3:D:502:PRO:HD2	2.00	0.43
4:E:4:VAL:HG13	4:E:5:THR:HG22	1.99	0.43
1:A:77:ASP:O	1:A:81:ILE:HG13	2.19	0.43
1:A:133:LEU:HD11	1:A:140:ILE:HD13	2.01	0.43
2:C:949:GLU:O	2:C:953:LEU:HD23	2.19	0.43
2:C:1065:LYS:HG2	2:C:1235:LEU:HB2	2.00	0.43
2:C:1329:GLU:HG2	3:D:327:LEU:HD22	2.00	0.43
3:D:875:ASN:N	3:D:875:ASN:HD22	2.16	0.43
3:D:1075:ARG:NH1	3:D:1184:ASP:HB3	2.34	0.43
3:D:1163:VAL:HG23	3:D:1175:LEU:HD11	2.01	0.43
1:A:60:GLU:HB2	1:A:170:ARG:NE	2.34	0.43
1:B:73:GLY:HA3	1:B:138:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HA	1:B:158:ARG:NE	2.34	0.43
2:C:1080:ASN:HA	2:C:1081:PRO:HD3	1.93	0.43
4:E:37:PRO:HG2	4:E:53:GLU:OE2	2.19	0.43
2:C:540:ARG:HD2	2:C:540:ARG:N	2.34	0.42
2:C:820:GLU:HB2	2:C:1081:PRO:HA	2.00	0.42
3:D:222:LYS:CD	3:D:223:LEU:HG	2.46	0.42
3:D:245:LEU:HB3	3:D:250:ARG:HE	1.83	0.42
3:D:373:ALA:HA	3:D:377:PHE:HD2	1.84	0.42
3:D:490:ILE:HA	3:D:500:ILE:HD11	2.00	0.42
3:D:510:LEU:HD21	3:D:627:THR:HG23	2.01	0.42
3:D:667:GLN:HG2	3:D:672:LEU:HD22	2.00	0.42
3:D:1328:THR:O	3:D:1332:LEU:HD23	2.19	0.42
1:B:74:VAL:HG11	1:B:81:ILE:HD11	2.01	0.42
3:D:99:ARG:HH21	3:D:248:ASP:HB3	1.85	0.42
3:D:587:LEU:HD22	3:D:620:PHE:HB2	2.01	0.42
2:C:448:LEU:HD13	2:C:553:THR:HG22	2.02	0.42
3:D:416:ILE:O	3:D:416:ILE:HG22	2.19	0.42
3:D:1370:MET:CE	4:E:22:VAL:CG1	2.95	0.42
3:D:1376:GLY:C	3:D:1379:PRO:HD2	2.40	0.42
4:E:41:GLU:CG	4:E:42:GLU:N	2.82	0.42
1:B:61:ILE:HB	1:B:64:VAL:HB	2.00	0.42
1:A:65:LEU:HD13	1:A:65:LEU:N	2.34	0.42
1:B:65:LEU:O	1:B:171:LEU:HD21	2.19	0.42
1:B:135:ASP:CG	1:B:136:GLU:H	2.21	0.42
2:C:120:GLN:H	2:C:120:GLN:CD	2.22	0.42
2:C:152:SER:HA	2:C:153:PRO:HD3	1.91	0.42
2:C:1270:PHE:CE1	2:C:1274:GLU:HB3	2.54	0.42
3:D:762:ASN:ND2	3:D:765:GLU:H	2.17	0.42
2:C:143:ARG:NH1	2:C:507:GLY:HA2	2.32	0.42
3:D:218:THR:OG1	3:D:1275:LEU:HB2	2.20	0.42
3:D:478:LEU:HD11	4:E:27:ALA:HB3	2.01	0.42
3:D:812:ASP:O	3:D:813:ASP:C	2.57	0.42
3:D:1370:MET:SD	4:E:61:ASN:CB	3.07	0.42
4:E:50:ALA:O	4:E:54:ILE:HD13	2.20	0.42
2:C:1064:ASP:O	2:C:1076:ILE:HG22	2.20	0.42
2:C:1072:ASN:ND2	2:C:1098:LEU:HD23	2.34	0.42
2:C:1223:ARG:HB2	2:C:1223:ARG:NH1	2.32	0.42
3:D:98:ARG:HG2	3:D:247:PRO:HG2	2.01	0.42
3:D:227:PHE:CG	3:D:234:PRO:HG3	2.54	0.42
3:D:485:MET:HE2	4:E:3:ARG:HD3	2.02	0.42
3:D:923:ILE:HD13	3:D:1248:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1289:ASN:O	3:D:1293:GLU:HB2	2.19	0.42
4:E:13:ILE:CD1	4:E:13:ILE:N	2.82	0.42
4:E:13:ILE:HG22	4:E:15:ASN:N	2.26	0.42
1:A:70:THR:HG21	2:C:755:LYS:HE2	2.01	0.42
2:C:221:LEU:HD22	2:C:336:LEU:HD11	2.00	0.42
2:C:344:GLY:HA2	2:C:345:PRO:HD3	1.85	0.42
3:D:482:ALA:HA	4:E:3:ARG:NH1	2.35	0.42
3:D:1306:LEU:C	3:D:1307:LEU:HD12	2.40	0.42
3:D:1347:LEU:N	3:D:1347:LEU:HD12	2.34	0.42
2:C:97:ARG:HD2	2:C:121:GLU:HB3	2.02	0.42
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.55	0.42
2:C:865:LEU:HD23	2:C:871:VAL:HB	2.02	0.42
2:C:936:ARG:HA	2:C:1042:LEU:HD11	2.02	0.42
2:C:1164:PHE:HD2	2:C:1168:GLU:HB3	1.83	0.42
3:D:491:LEU:HD12	3:D:905:ARG:O	2.19	0.42
3:D:680:ASN:HD22	3:D:681:LYS:N	2.18	0.42
3:D:1095:MET:HG3	3:D:1162:ILE:H	1.85	0.42
3:D:1282:TYR:O	3:D:1286:LYS:HG3	2.20	0.42
1:A:79:LEU:HG	2:C:831:ILE:HD11	2.02	0.42
2:C:384:LEU:O	2:C:388:LEU:HG	2.19	0.42
2:C:496:LYS:HD3	2:C:496:LYS:C	2.40	0.42
2:C:587:LEU:HD23	2:C:588:GLU:N	2.35	0.42
2:C:706:ARG:HA	2:C:793:GLU:HA	2.02	0.42
2:C:1103:VAL:HG22	2:C:1111:GLN:HE21	1.83	0.42
3:D:587:LEU:HA	3:D:588:PRO:HD3	1.92	0.42
3:D:756:GLU:O	3:D:758:PRO:HD3	2.19	0.42
3:D:1131:THR:HG22	3:D:1132:LYS:HG3	2.02	0.42
4:E:13:ILE:HG21	4:E:18:ASP:CB	2.49	0.42
1:A:45:ARG:HG2	1:B:38:THR:HB	2.02	0.41
2:C:409:LEU:HD21	2:C:428:VAL:HG22	2.02	0.41
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.41
3:D:271:ARG:O	3:D:275:ARG:HG2	2.20	0.41
3:D:381:ILE:HD13	3:D:408:VAL:HG21	2.02	0.41
3:D:685:ILE:HG13	3:D:686:TRP:CD1	2.55	0.41
3:D:762:ASN:H	3:D:762:ASN:ND2	2.18	0.41
3:D:1372:ARG:HG2	3:D:1375:ALA:HB2	2.01	0.41
4:E:20:VAL:HG13	4:E:21:LEU:N	2.34	0.41
4:E:56:GLU:CG	4:E:57:GLY:N	2.83	0.41
4:E:86:ILE:CG2	4:E:87:ALA:N	2.83	0.41
1:A:185:TYR:HB2	1:A:201:LEU:HD11	2.02	0.41
2:C:150:HIS:NE2	2:C:454:ARG:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:ILE:HG22	2:C:430:LYS:HE3	2.01	0.41
3:D:26:SER:O	3:D:30:ILE:HG13	2.20	0.41
3:D:118:LYS:HZ1	3:D:118:LYS:HA	1.85	0.41
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.95	0.41
3:D:481:ARG:O	3:D:485:MET:HE2	2.20	0.41
1:A:30:PRO:C	1:A:31:LEU:HD22	2.41	0.41
1:B:10:LYS:HD2	1:B:30:PRO:HG2	2.01	0.41
2:C:698:PRO:HG3	2:C:1231:TYR:CE1	2.55	0.41
2:C:1246:ARG:HD2	2:C:1265:PHE:O	2.21	0.41
3:D:118:LYS:HA	3:D:118:LYS:NZ	2.35	0.41
3:D:1263:LYS:O	3:D:1305:ASP:HB3	2.20	0.41
4:E:20:VAL:CG1	4:E:21:LEU:N	2.83	0.41
4:E:71:GLU:HG2	4:E:72:GLN:N	2.35	0.41
2:C:93:SER:OG	2:C:126:GLU:HB3	2.19	0.41
2:C:125:GLY:H	2:C:495:ALA:HB1	1.86	0.41
3:D:506:VAL:HB	3:D:629:PHE:CZ	2.55	0.41
1:A:90:VAL:HG21	1:A:146:VAL:HG21	2.02	0.41
1:A:188:GLU:OE2	1:A:200:LYS:HD2	2.20	0.41
2:C:316:GLU:HG3	2:C:352:ARG:NH2	2.35	0.41
2:C:1339:LEU:H	2:C:1339:LEU:CD2	2.34	0.41
3:D:905:ARG:HG3	4:E:16:ARG:NH2	2.34	0.41
3:D:1126:GLN:OE1	3:D:1170:LYS:HE3	2.21	0.41
4:E:30:MET:HE3	4:E:50:ALA:HB2	2.01	0.41
1:A:168:ILE:HG21	2:C:864:LYS:NZ	2.35	0.41
2:C:820:GLU:O	2:C:823:VAL:HG12	2.21	0.41
3:D:128:LEU:HD11	3:D:188:LEU:HB3	2.02	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.85	0.41
3:D:292:VAL:HB	3:D:296:LYS:HE3	2.02	0.41
3:D:1199:PHE:HE2	3:D:1202:GLU:O	2.02	0.41
3:D:1229:VAL:O	3:D:1233:ILE:HG22	2.21	0.41
2:C:519:ASN:ND2	2:C:796:LEU:HD22	2.36	0.41
2:C:843:THR:HG22	2:C:844:LYS:N	2.36	0.41
2:C:1205:PRO:HB3	2:C:1210:ILE:HB	2.02	0.41
2:C:1276:TRP:HA	2:C:1279:GLU:HB3	2.01	0.41
3:D:978:ARG:HG2	3:D:979:ASN:N	2.35	0.41
3:D:1163:VAL:CG2	3:D:1175:LEU:HD11	2.50	0.41
1:A:64:VAL:HG13	1:A:69:SER:HB2	2.02	0.41
2:C:161:LYS:C	2:C:161:LYS:HD2	2.41	0.41
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.92	0.41
2:C:519:ASN:O	2:C:523:GLU:HG3	2.21	0.41
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:374:LEU:HD11	3:D:409:TRP:CH2	2.55	0.41
3:D:926:PRO:HB2	3:D:1241:TYR:CE2	2.56	0.41
3:D:978:ARG:CB	3:D:1199:PHE:HB3	2.50	0.41
3:D:1021:ASP:HA	3:D:1022:PRO:HD3	1.80	0.41
4:E:38:LEU:N	4:E:38:LEU:CD1	2.83	0.41
1:A:71:LYS:HG2	1:A:78:ILE:HD11	2.02	0.41
1:A:159:ILE:HA	1:A:172:LEU:HD22	2.02	0.41
1:B:172:LEU:H	1:B:172:LEU:CD1	2.23	0.41
1:B:198:LEU:N	1:B:198:LEU:HD22	2.36	0.41
2:C:807:TRP:HE1	2:C:1086:PRO:HD3	1.86	0.41
2:C:854:ILE:HD13	2:C:917:SER:HB3	2.03	0.41
2:C:870:ILE:HD13	2:C:944:ARG:HD3	2.03	0.41
2:C:1117:LEU:HD21	2:C:1182:ILE:HD11	2.03	0.41
3:D:27:PRO:HG3	3:D:240:THR:OG1	2.20	0.41
3:D:279:LEU:O	3:D:279:LEU:HD23	2.21	0.41
3:D:381:ILE:HG23	3:D:411:ILE:HD12	2.03	0.41
3:D:401:VAL:O	3:D:401:VAL:HG22	2.21	0.41
4:E:54:ILE:H	4:E:54:ILE:CD1	2.33	0.41
2:C:11:ILE:O	2:C:13:LYS:HG3	2.21	0.41
2:C:216:THR:O	2:C:220:ILE:HG13	2.21	0.41
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.36	0.41
2:C:447:HIS:CD2	2:C:553:THR:HG21	2.56	0.41
2:C:1212:LEU:HB3	2:C:1213:TYR:H	1.77	0.41
3:D:482:ALA:C	3:D:483:LEU:HD12	2.41	0.41
3:D:555:TYR:CE1	3:D:564:VAL:HG21	2.56	0.41
3:D:663:GLU:O	3:D:667:GLN:HG3	2.21	0.41
1:A:10:LYS:HE2	1:A:30:PRO:HB2	2.03	0.40
1:A:44:ARG:HE	1:A:48:LEU:HD11	1.86	0.40
1:A:228:LEU:HG	1:B:224:LEU:HD23	2.02	0.40
1:B:59:VAL:HG22	1:B:144:ILE:HG13	2.03	0.40
3:D:362:ARG:HH21	3:D:365:GLN:HE21	1.69	0.40
3:D:719:PHE:HA	3:D:724:MET:SD	2.62	0.40
3:D:761:ALA:H	3:D:771:GLN:HE22	1.68	0.40
3:D:1318:SER:HB3	3:D:1320:ILE:HD13	2.02	0.40
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.21	0.40
4:E:4:VAL:O	4:E:5:THR:HG22	2.21	0.40
4:E:63:ILE:CG2	4:E:64:LEU:N	2.82	0.40
1:B:109:PRO:HG3	1:B:132:HIS:CE1	2.57	0.40
2:C:849:GLU:O	2:C:887:VAL:HG12	2.20	0.40
2:C:967:LEU:O	2:C:971:LEU:HD13	2.21	0.40
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:119:SER:OG	3:D:121:PRO:HD2	2.21	0.40
3:D:126:LEU:HD22	3:D:223:LEU:HD12	2.03	0.40
3:D:1323:ALA:HA	3:D:1328:THR:HG22	2.03	0.40
4:E:63:ILE:O	4:E:64:LEU:HD12	2.21	0.40
3:D:148:GLU:HB3	3:D:187:ALA:CB	2.51	0.40
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.93	0.40
3:D:720:ASN:HB3	3:D:723:TYR:HB3	2.03	0.40
2:C:84:GLU:O	2:C:88:ARG:HB2	2.22	0.40
3:D:71:LEU:HD22	3:D:71:LEU:N	2.36	0.40
3:D:405:GLU:HG2	3:D:407:VAL:H	1.87	0.40
3:D:697:MET:HE3	3:D:701:LEU:HD11	2.03	0.40
3:D:1077:ALA:HB2	3:D:1100:PHE:CD1	2.57	0.40
3:D:1184:ASP:N	3:D:1185:PRO:CD	2.84	0.40
3:D:1320:ILE:H	3:D:1320:ILE:CD1	2.29	0.40
2:C:511:LEU:HD13	2:C:533:LEU:O	2.22	0.40
2:C:864:LYS:HE2	2:C:864:LYS:N	2.37	0.40
2:C:1064:ASP:OD2	2:C:1234:LYS:HE3	2.21	0.40
2:C:1131:MET:HB3	2:C:1145:ILE:HD12	2.02	0.40
3:D:388:ARG:HB3	3:D:389:GLY:H	1.80	0.40
3:D:429:LEU:HB3	3:D:925:GLU:HB2	2.04	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	233/329 (71%)	196 (84%)	31 (13%)	6 (3%)	5 31
1	B	233/329 (71%)	197 (84%)	28 (12%)	8 (3%)	3 26
2	C	1333/1342 (99%)	1109 (83%)	190 (14%)	34 (3%)	5 31
3	D	1362/1407 (97%)	1124 (82%)	198 (14%)	40 (3%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	E	87/91 (96%)	74 (85%)	10 (12%)	3 (3%)	3 26
All	All	3248/3498 (93%)	2700 (83%)	457 (14%)	91 (3%)	8 30

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	A	166	ARG
1	B	124	VAL
2	C	489	PRO
2	C	582	ASN
2	C	1182	ILE
3	D	903	LEU
4	E	39	VAL
4	E	46	THR
4	E	48	VAL
2	C	483	ASP
2	C	807	TRP
3	D	741	ALA
3	D	745	GLY
3	D	839	VAL
3	D	857	LEU
3	D	937	ILE
3	D	1134	ILE
3	D	1179	PRO
3	D	1224	ARG
3	D	1293	GLU
3	D	1296	GLY
1	A	62	ASP
1	A	137	ASN
1	B	49	SER
1	B	93	GLN
1	B	165	GLU
1	B	194	GLN
2	C	64	GLY
2	C	81	ASP
2	C	140	GLY
2	C	544	GLY
2	C	812	PHE
2	C	813	GLU
2	C	1048	LYS
2	C	1204	LEU

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Mol	Chain	Res	Type
3	D	66	LYS
3	D	229	GLN
3	D	285	LEU
3	D	359	PRO
3	D	594	GLN
3	D	612	LEU
3	D	813	ASP
3	D	899	TYR
1	A	194	GLN
2	C	44	GLU
2	C	92	TYR
2	C	134	GLY
2	C	398	SER
2	C	492	MET
2	C	496	LYS
2	C	573	ASN
2	C	940	GLU
2	C	1123	GLY
2	C	1185	PRO
3	D	153	ASN
3	D	494	ALA
3	D	728	SER
3	D	850	LYS
3	D	1131	THR
1	A	179	PRO
1	B	21	SER
1	B	159	ILE
2	C	13	LYS
2	C	746	ALA
2	C	1223	ARG
2	C	1296	ASP
3	D	64	PRO
3	D	463	GLY
3	D	588	PRO
3	D	671	GLY
3	D	675	ALA
3	D	729	GLY
3	D	1183	SER
3	D	1344	LEU
1	B	69	SER
2	C	1103	VAL
2	C	1341	ASP

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Mol	Chain	Res	Type
3	D	859	PRO
2	C	577	VAL
3	D	742	GLY
2	C	700	VAL
3	D	247	PRO
3	D	828	GLY
2	C	178	PRO
2	C	488	MET
2	C	1124	ILE
3	D	752	GLY
3	D	1191	PRO
3	D	1201	GLY
3	D	1360	GLY

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	202/286 (71%)	195 (96%)	7 (4%)	36	59
1	B	202/286 (71%)	199 (98%)	3 (2%)	65	80
2	C	1150/1157 (99%)	1139 (99%)	11 (1%)	76	86
3	D	1129/1168 (97%)	1091 (97%)	38 (3%)	37	60
4	E	73/75 (97%)	71 (97%)	2 (3%)	44	65
All	All	2756/2972 (93%)	2695 (98%)	61 (2%)	54	71

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	65	LEU
1	A	148	ARG
1	A	159	ILE
1	A	168	ILE
1	A	171	LEU

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Mol	Chain	Res	Type
1	A	234	LEU
1	B	71	LYS
1	B	124	VAL
1	B	172	LEU
2	C	17	LYS
2	C	59	ILE
2	C	120	GLN
2	C	169	LYS
2	C	647	ARG
2	C	864	LYS
2	C	1065	LYS
2	C	1108	ASN
2	C	1176	LEU
2	C	1210	ILE
2	C	1314	GLN
3	D	33	TRP
3	D	84	ILE
3	D	118	LYS
3	D	132	LEU
3	D	159	ILE
3	D	160	LEU
3	D	201	LEU
3	D	222	LYS
3	D	232	ASN
3	D	255	LEU
3	D	296	LYS
3	D	332	LYS
3	D	411	ILE
3	D	500	ILE
3	D	549	LYS
3	D	556	GLU
3	D	566	LYS
3	D	591	ILE
3	D	641	ILE
3	D	644	MET
3	D	674	THR
3	D	678	ARG
3	D	680	ASN
3	D	759	ILE
3	D	762	ASN
3	D	767	LEU
3	D	875	ASN

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Mol	Chain	Res	Type
3	D	881	LYS
3	D	911	LYS
3	D	1156	LEU
3	D	1210	ILE
3	D	1220	ILE
3	D	1231	ARG
3	D	1263	LYS
3	D	1266	ILE
3	D	1297	LYS
3	D	1304	ARG
3	D	1320	ILE
4	E	31	GLN
4	E	49	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	18	GLN
1	A	84	ASN
1	A	93	GLN
1	A	227	GLN
1	B	18	GLN
1	B	93	GLN
1	B	127	GLN
1	B	160	HIS
2	C	31	GLN
2	C	41	GLN
2	C	83	GLN
2	C	120	GLN
2	C	258	ASN
2	C	330	HIS
2	C	343	HIS
2	C	437	ASN
2	C	462	ASN
2	C	463	GLN
2	C	490	GLN
2	C	510	GLN
2	C	517	GLN
2	C	551	HIS
2	C	604	HIS
2	C	613	ASN

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Mol	Chain	Res	Type
2	C	618	GLN
2	C	649	GLN
2	C	688	GLN
2	C	737	ASN
2	C	798	GLN
2	C	799	ASN
2	C	932	GLN
2	C	955	GLN
2	C	1013	GLN
2	C	1023	HIS
2	C	1080	ASN
2	C	1090	ASN
2	C	1108	ASN
2	C	1209	GLN
2	C	1220	GLN
2	C	1236	ASN
2	C	1256	GLN
2	C	1299	ASN
2	C	1313	HIS
3	D	158	GLN
3	D	164	GLN
3	D	186	GLN
3	D	232	ASN
3	D	274	ASN
3	D	294	ASN
3	D	300	GLN
3	D	340	GLN
3	D	430	HIS
3	D	489	ASN
3	D	593	ASN
3	D	594	GLN
3	D	665	GLN
3	D	680	ASN
3	D	720	ASN
3	D	762	ASN
3	D	777	HIS
3	D	792	ASN
3	D	867	GLN
3	D	875	ASN
3	D	910	ASN
3	D	921	GLN
3	D	951	GLN

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Mol	Chain	Res	Type
3	D	954	ASN
3	D	1019	ASN
3	D	1114	GLN
3	D	1197	ASN
3	D	1238	GLN
3	D	1259	GLN
3	D	1295	ASN
3	D	1366	HIS
3	D	1383	GLN
4	E	31	GLN
4	E	62	GLN
4	E	73	GLN
4	E	75	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

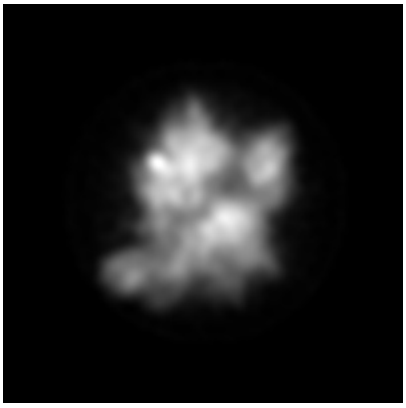
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5169. These allow visual inspection of the internal detail of the map and identification of artifacts.

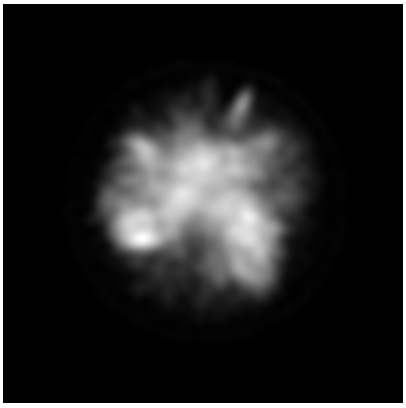
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

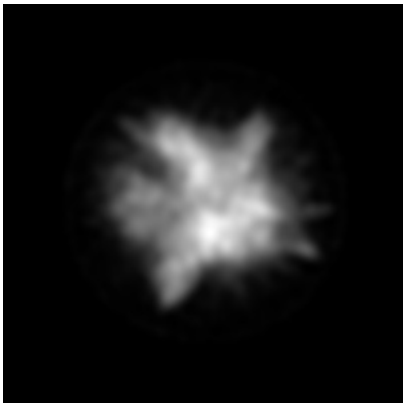
6.1.1 Primary map



X



Y

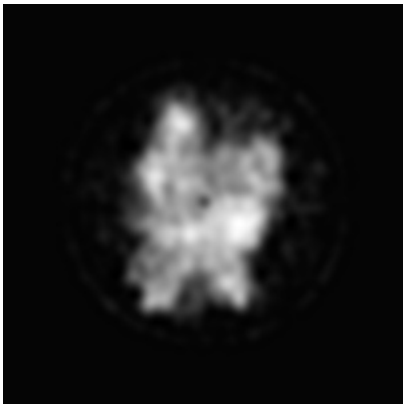


Z

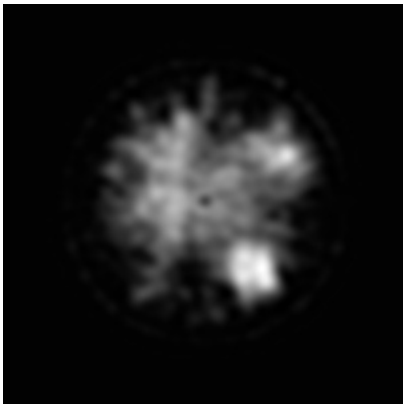
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

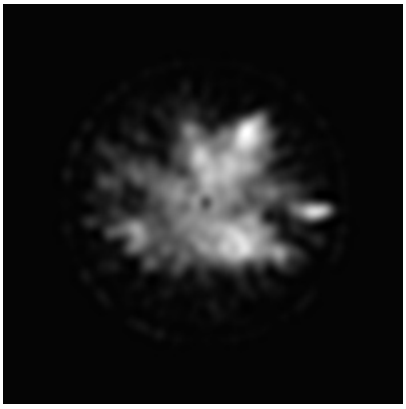
6.2.1 Primary map



X Index: 45



Y Index: 45

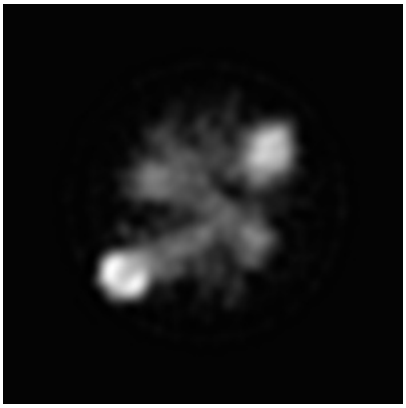


Z Index: 45

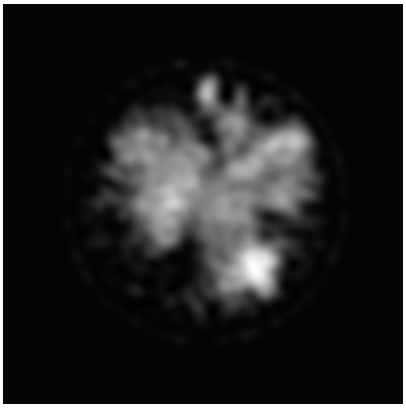
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

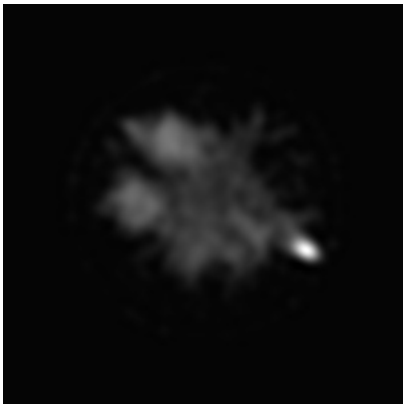
6.3.1 Primary map



X Index: 38



Y Index: 42

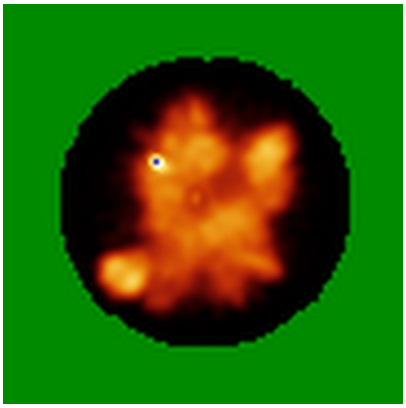


Z Index: 54

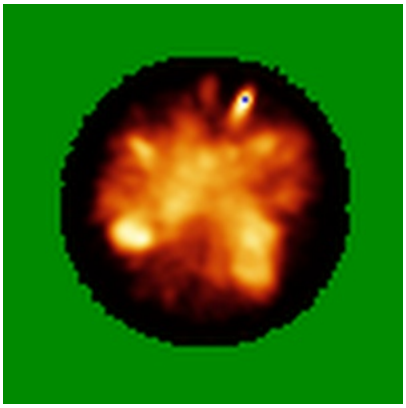
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

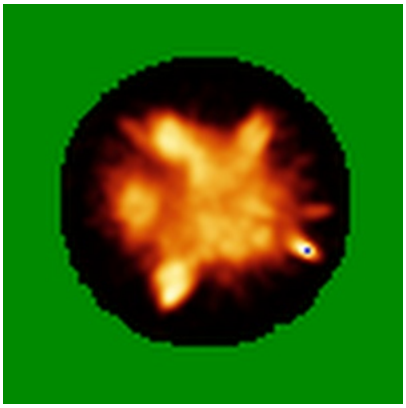
6.4.1 Primary map



X



Y

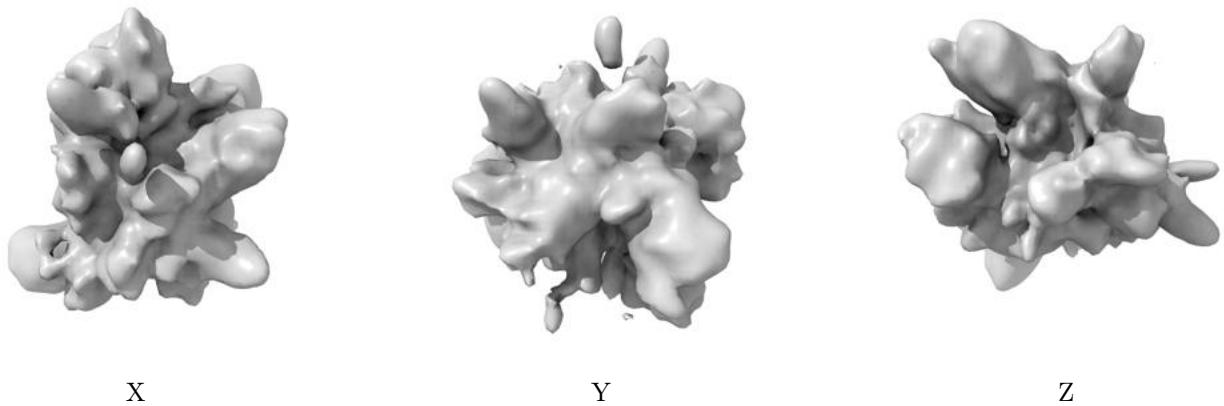


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 11.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

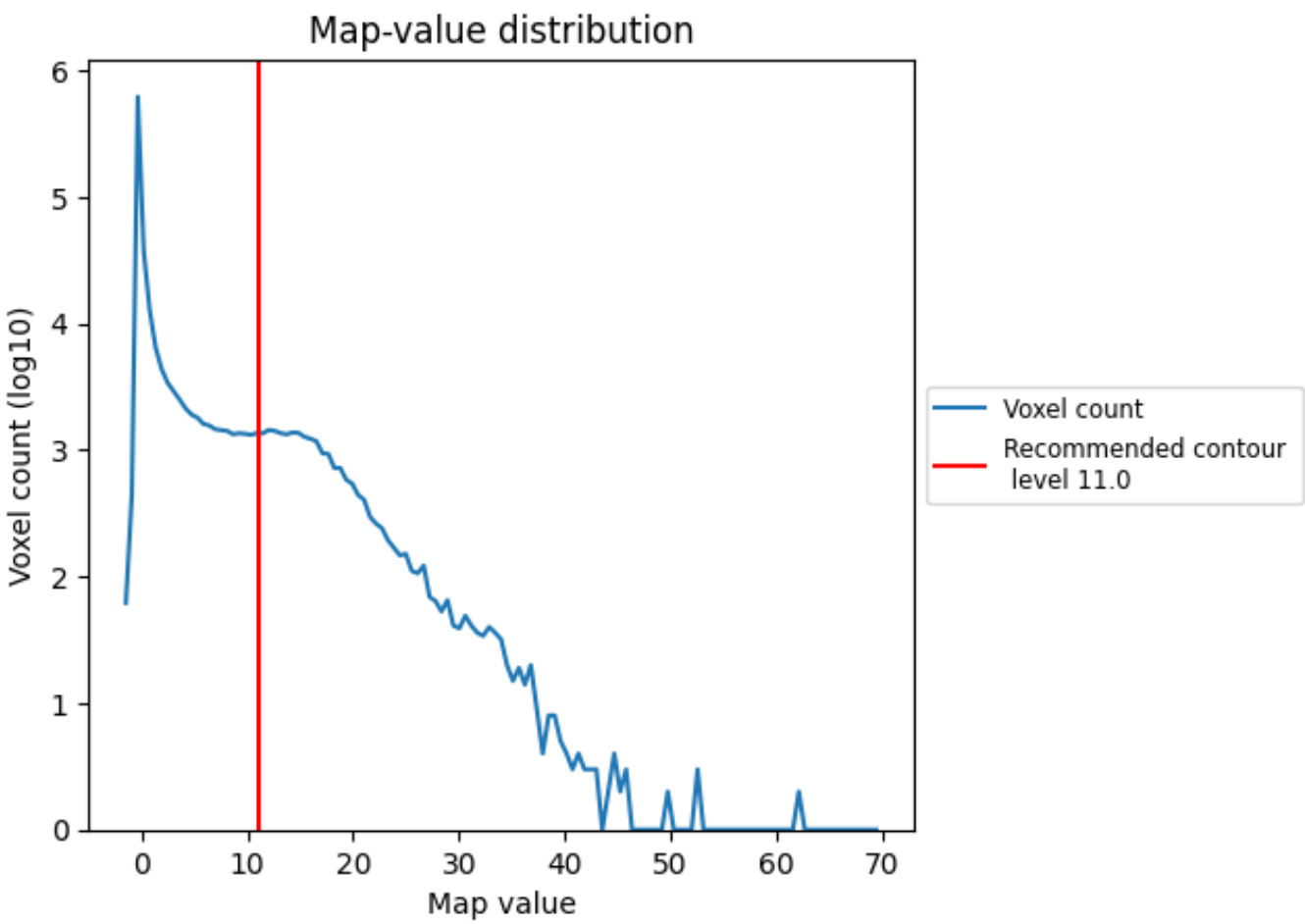
6.6 Mask visualisation (i)

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

7 Map analysis (i)

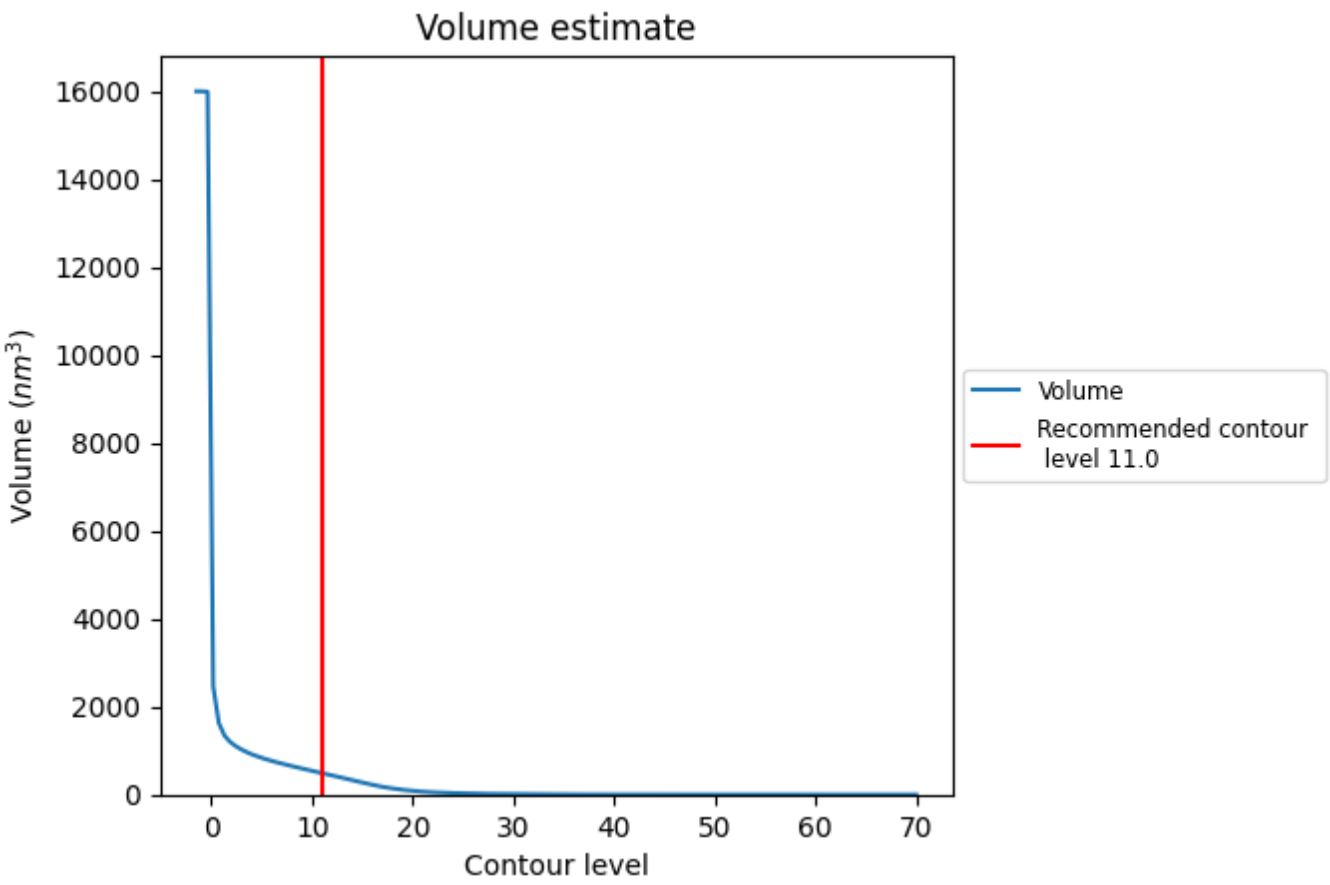
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

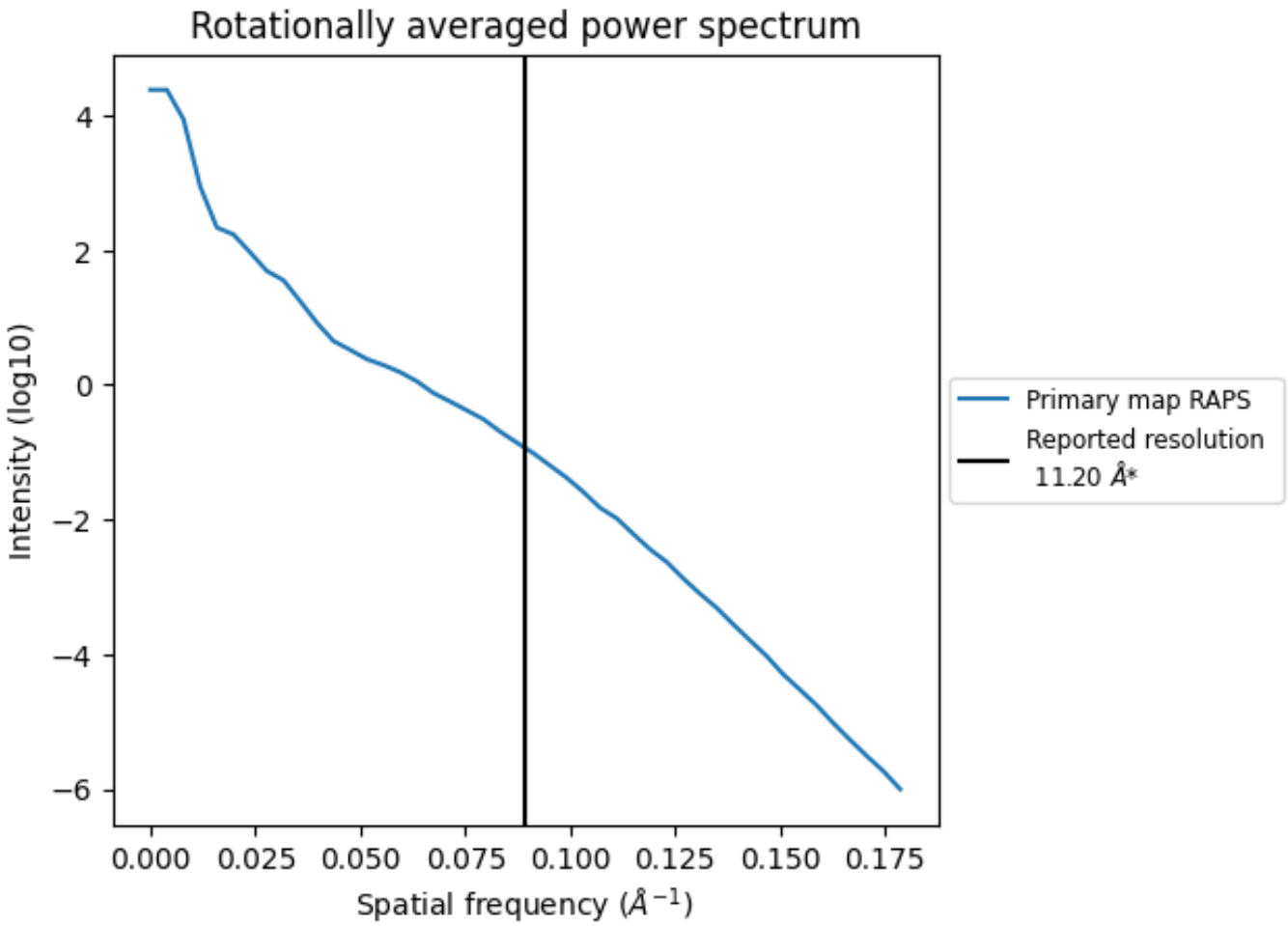
7.2 Volume estimate (i)



The volume at the recommended contour level is 488 nm^3; this corresponds to an approximate mass of 441 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.089 Å^{-1}

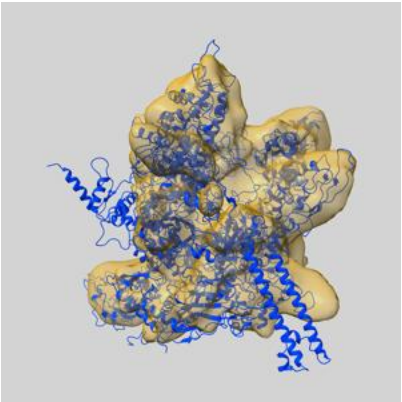
8 Fourier-Shell correlation (i)

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

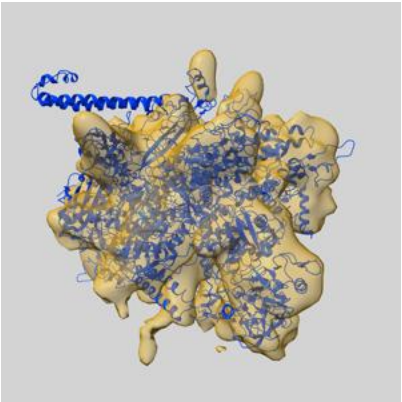
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5169 and PDB model 3LU0. Per-residue inclusion information can be found in section 3 on page 5.

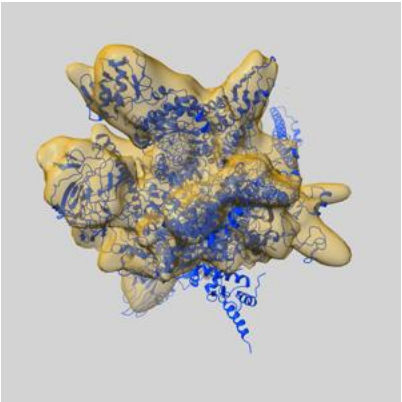
9.1 Map-model overlay (i)



X



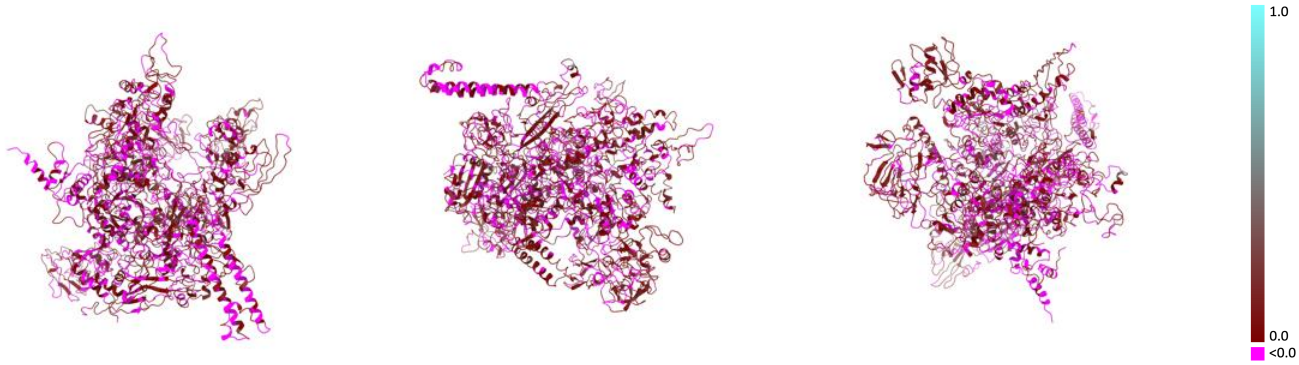
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 11.0 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.

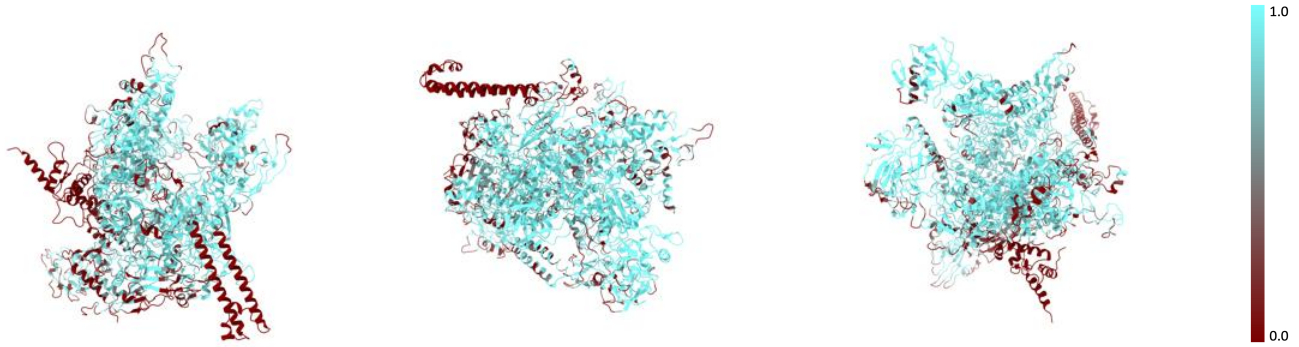
9.2 Q-score mapped to coordinate model (i)



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.

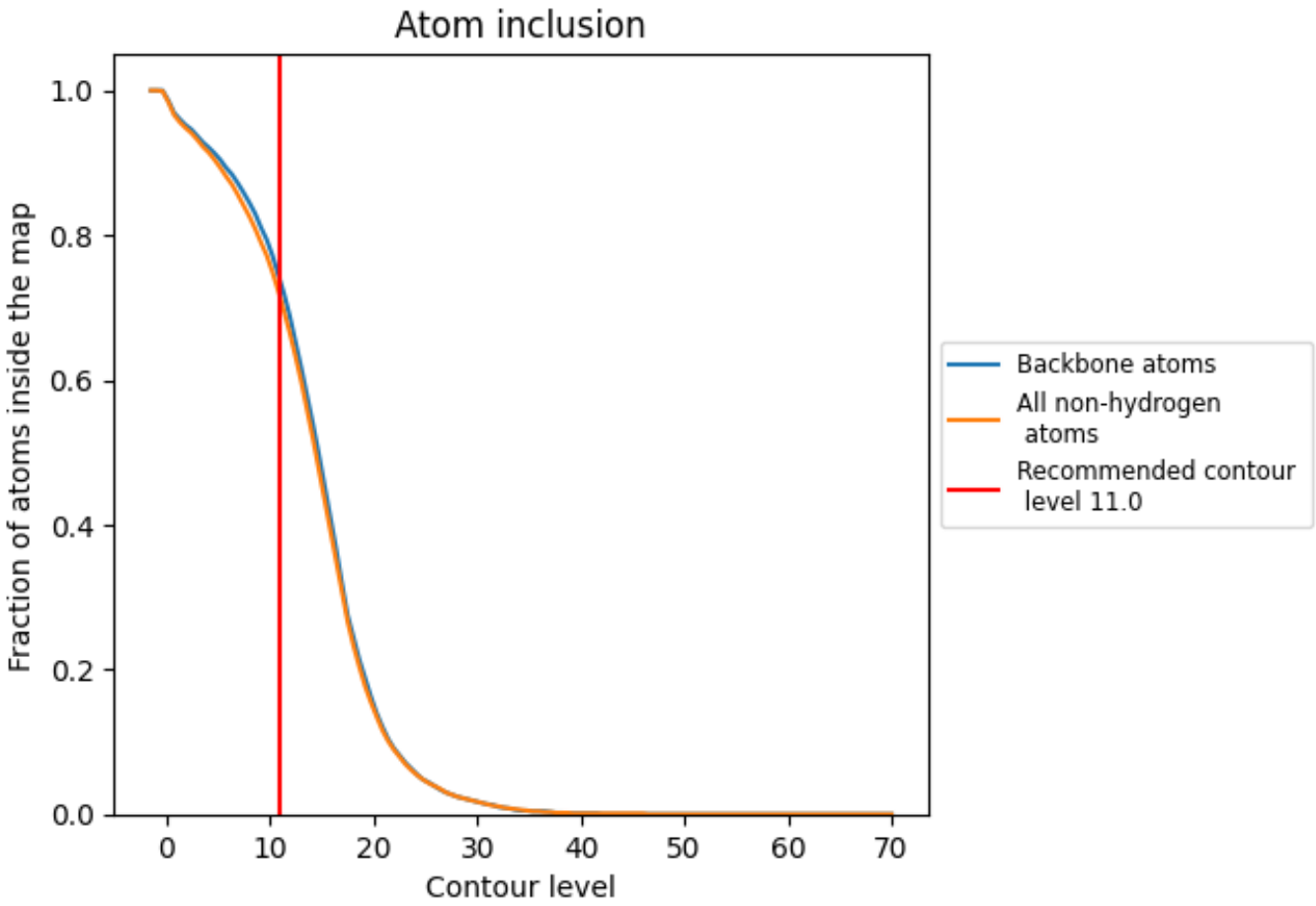
9.3 Atom inclusion mapped to coordinate model (i)



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 (11.0).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 71% 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 (11.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.0350
A	0.5290	0.0420
B	0.5290	0.0160
C	0.7860	0.0390
D	0.7530	0.0370
E	0.0030	-0.0260