Full wwPDB EM Validation Report ⓘ

Sep 23, 2026 – 07:25 am BST

PDB ID	:	9TUC / pdb_00009tuc
EMDB ID	:	EMD-56256
Title	:	CryoEM structure of DruE:ATPgammaS:DNA from Druantia type III - dimer 5
Authors	:	Grass, L.M.; Himpich, S.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on	:	2026-01-08
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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

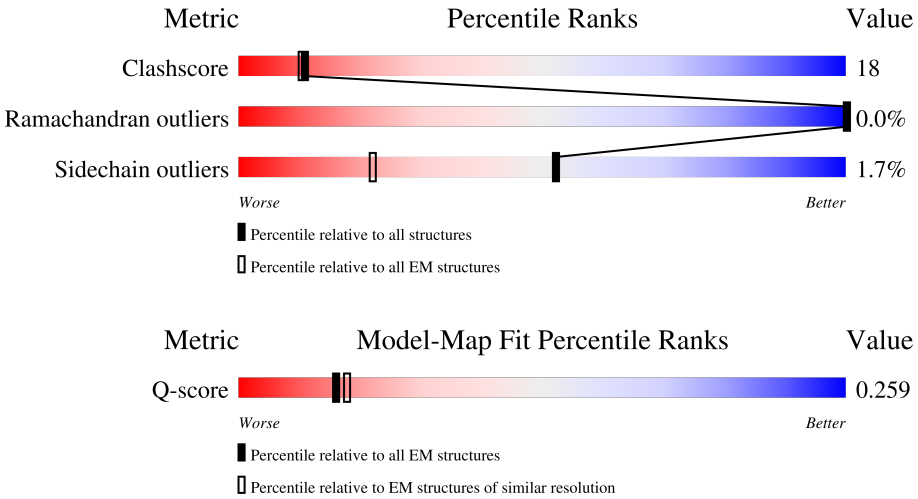
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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.



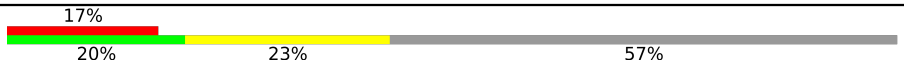
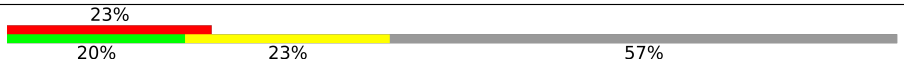
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	Y	2108	57% 40%
1	y	2108	10% 53% 33% 13%
2	I	30	23% 27% 50% 23%
2	i	30	43% 37% 50% 13%

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Mol	Chain	Length	Quality of chain
3	G	30	
3	g	30	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32402 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 DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	2049	Total	C	N	O	S	0	0
			16281	10268	2916	3025	72		
1	y	1833	Total	C	N	O	S	0	0
			14541	9165	2607	2702	67		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
Y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
Y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
Y	0	PHE	-	expression tag	UNP A0A4P8BDA5
y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
y	0	PHE	-	expression tag	UNP A0A4P8BDA5

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP *TP*CP*TP*AP*GP*GP*CP*TP*GP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	i	26	Total	C	N	O	P	0	0
			530	252	96	156	26		
2	I	23	Total	C	N	O	P	0	0
			471	224	85	139	23		

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*AP*GP*AP*CP*TP*AP*TP*CP *GP*AP*T)-3').

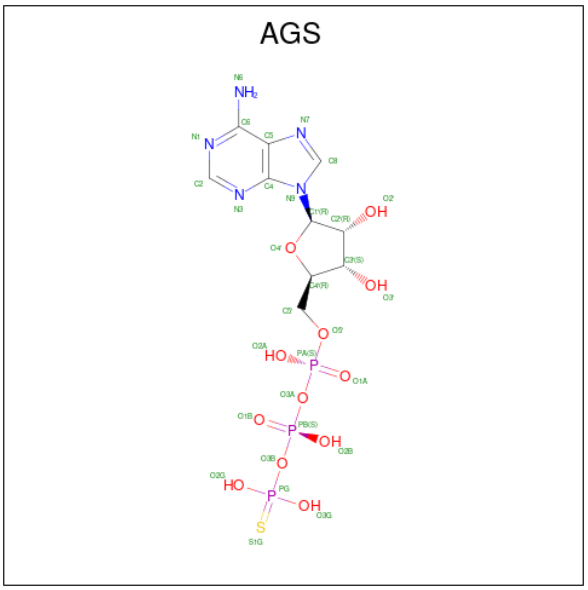
Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	13	Total	C	N	O	P	0	0
			269	128	52	76	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	13	Total	C	N	O	P	0	0
			269	128	52	76	13		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
4	Y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

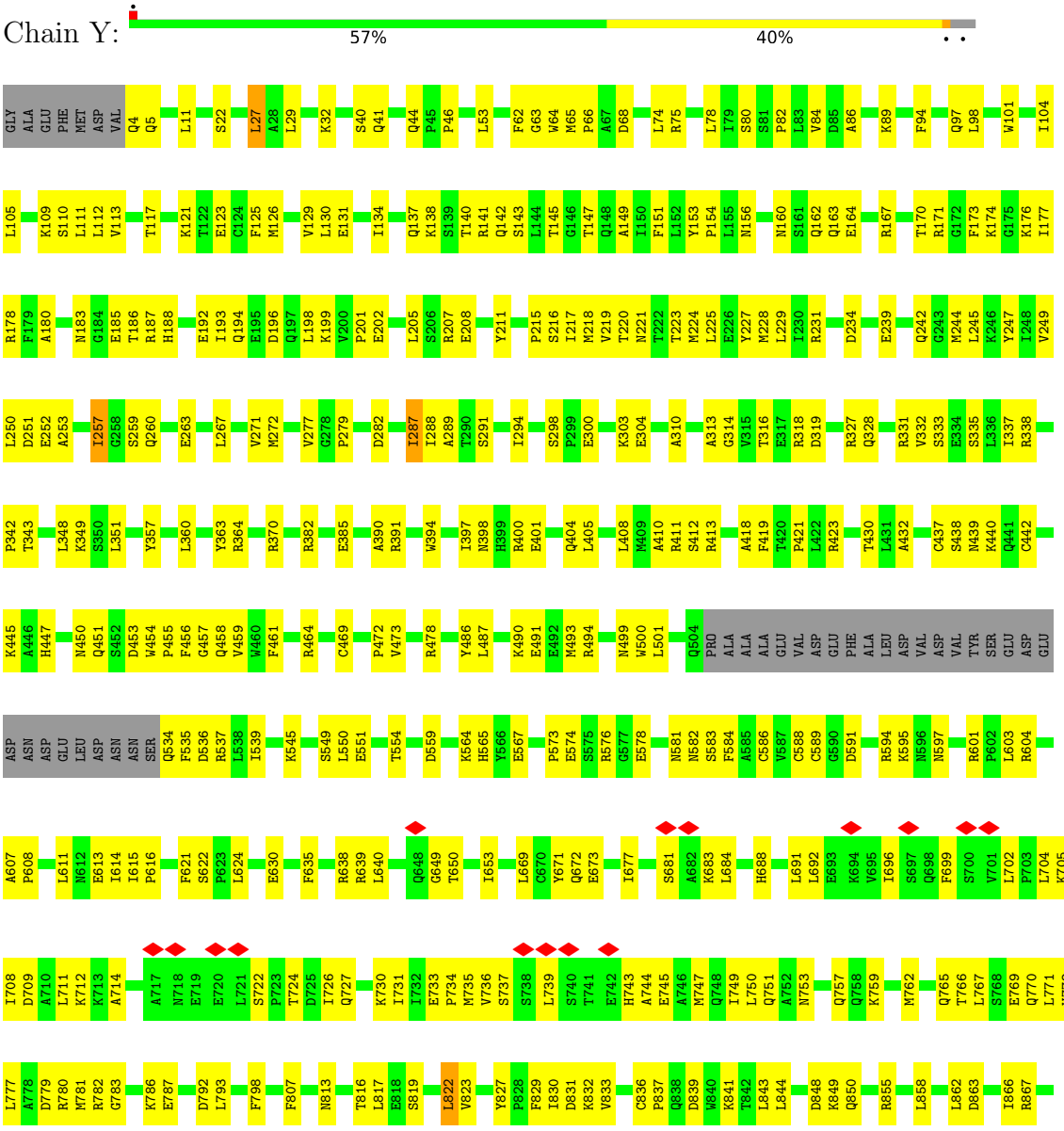
Mol	Chain	Residues	Atoms		AltConf
5	Y	5	Total	Zn	0
			5	5	
5	y	5	Total	Zn	0
			5	5	

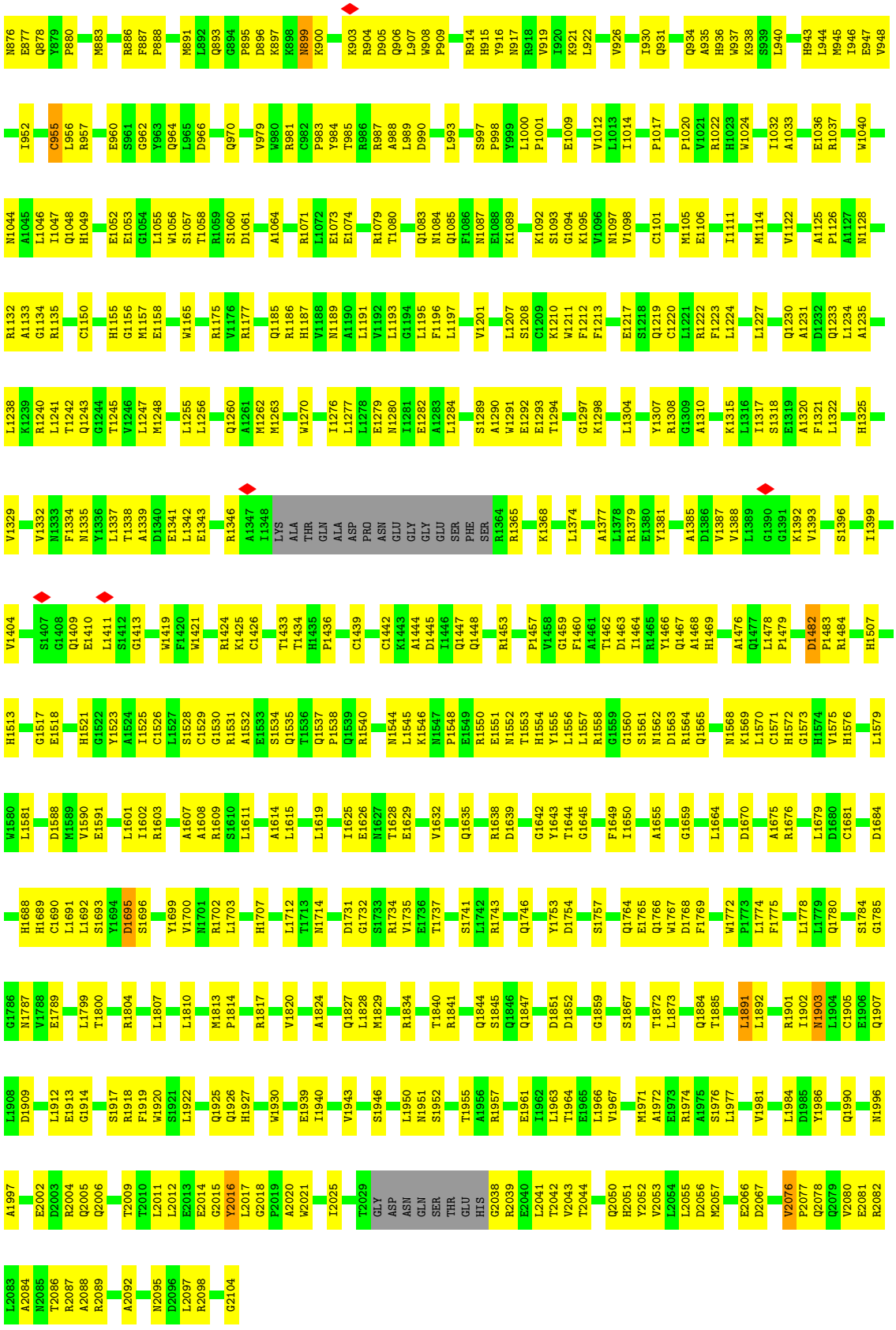
3 Residue-property plots (i)

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: DEAD/DEAH box helicase

Chain Y:

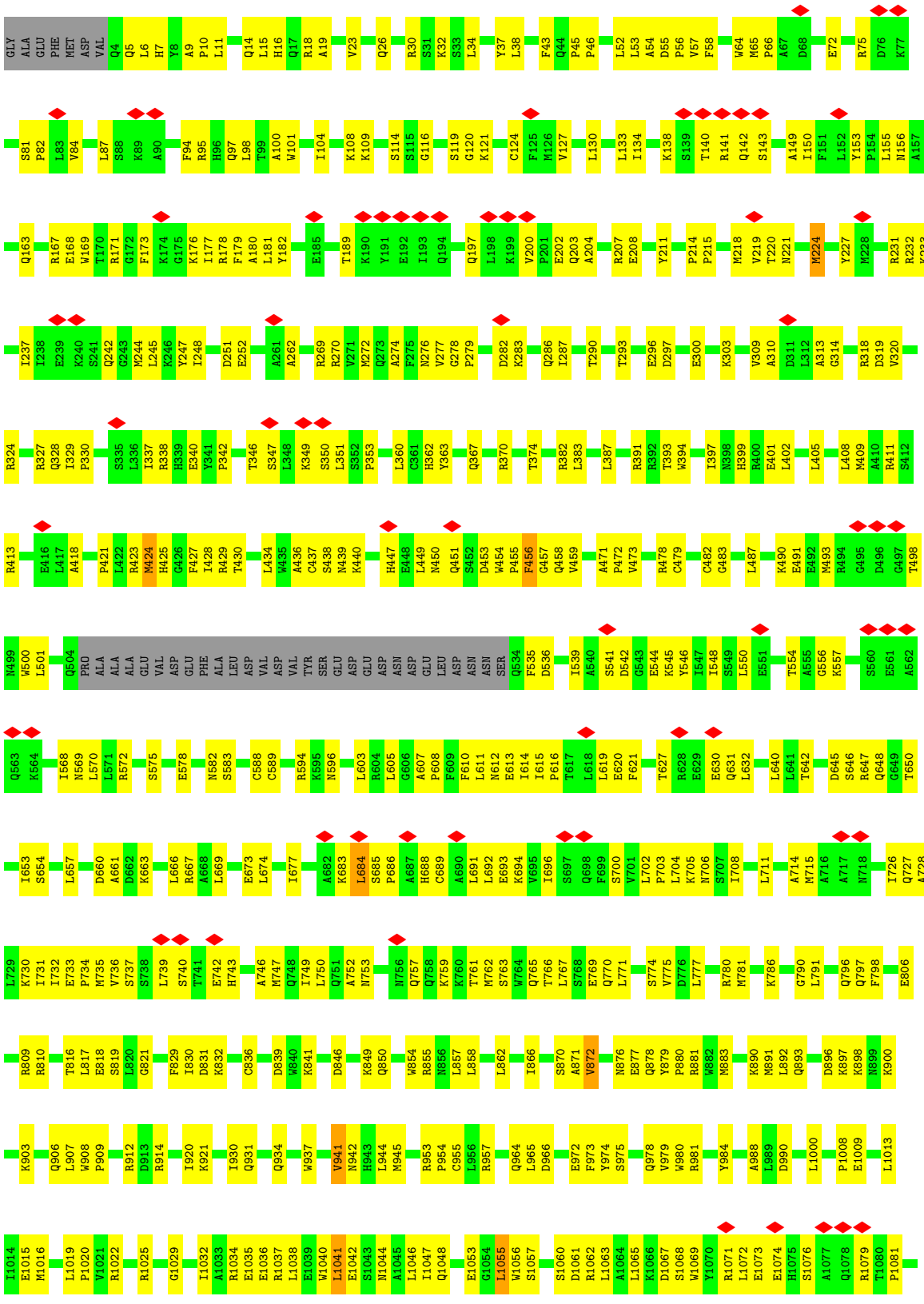


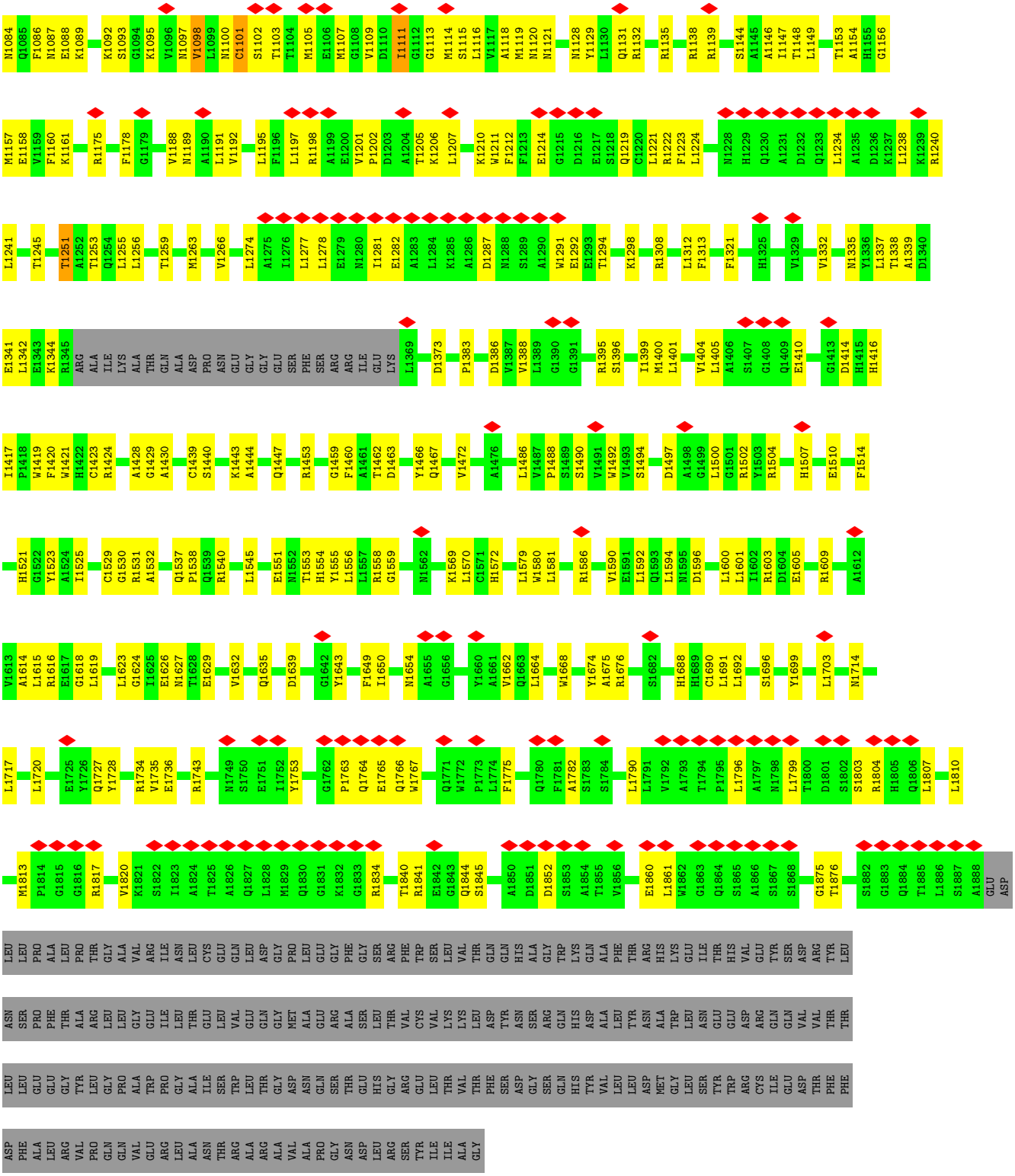


- Molecule 1: DEAD/DEAH box helicase

Chain y:

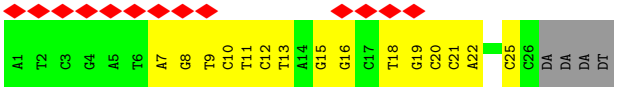

10%
53%
33%
13%


GLY ALA GLU PHE MET ASP VAL Q4 Q5 L6 H7 Y8 A9 P10 L11 Q14 L15 H16 Q17 R18 A19 V23 Q26 R30 S31 K32 S33 L34 Y37 L38 F43 Q44 P45 P46 L52 L53 A54 D55 P56 V57 F58 W64 M65 P66 A67 D68 E72 R75 D76 K77
S81 P82 L83 V84 L87 S88 K89 A90 F94 R95 H96 Q97 L98 T99 A100 W101 I104 K108 K109 S114 S115 G116 S119 G120 K121 C124 F125 M126 V127 L130 L133 I134 K138 S139 T140 R141 Q142 S143 A149 I150 F151 L152 Y153 P154 L155 N156 A157 L158
Q163 R167 E168 W169 T170 R171 G172 F173 K174 G175 K176 I177 R178 F179 A180 L181 Y182 E185 T189 K190 Y191 E192 I193 Q194 Q197 L198 K199 V200 P201 E202 Q203 A204 R207 E208 Y211 P214 P215 M218 V219 T220 N221 M224 Y227 M228 R231 R232 K233 D234
I237 T238 E239 K240 S241 Q242 G243 M244 L245 K246 Y247 I248 D251 E252 A261 A262 R269 R270 V271 M272 Q273 A274 F275 N276 V277 G278 P279 D282 K283 Q286 I287 T290 T293 E296 D297 E300 K303 V309 A310 D311 L312 A313 G314 R318 D319 V320
R324 R327 Q328 I329 P330 S335 L336 I337 R338 H339 E340 Y341 P342 T346 S347 L348 K349 S350 L351 S352 P353 L360 C361 H362 Y363 Q367 R370 T374 R382 L383 L387 R391 R392 T393 W394 I397 N398 H399 R400 E401 L402 L405 L408 M409 A410 R411 S412
R413 E416 L417 A418 P421 L422 R423 M424 H425 G426 F427 I428 R429 T430 L434 W435 A436 C437 S438 N439 K440 H447 E448 L449 N450 Q451 S452 D453 W454 P455 F456 G457 Q458 V459 A471 P472 V473 R478 C479 C482 G483 L487 K490 E491 E492 M493 R494 G495 D496 G497 T498
N499 W500 L501 Q504 PRO ALA ALA ALA GLU VAL ASP GLU PHE ALA LEU ASP VAL ASP VAL TYR SER GLU ASP GLU ASP ASN ASP GLU LEU ASP ASN ASN SER Q534 F535 D536 I539 A540 S541 D542 G543 E544 K545 Y546 I547 I548 S549 L550 E551 T554 A555 G556 K557 S560 E561 A562
Q563 K564 I568 N569 L570 L571 R572 S575 E578 N582 S583 C588 C589 R594 K595 N596 L603 R604 L605 G606 A607 P608 F609 F610 L611 N612 E613 I614 I615 P616 T617 L618 L619 E620 F621 T627 R628 E629 E630 Q631 L632 L640 L641 T642 D645 S646 R647 Q648 G649 T650
I653 S654 L657 D660 A661 D662 K663 L666 R667 A668 L669 E673 L674 I677 A682 K683 L684 S685 P686 A687 H688 C689 A690 L691 L692 E693 K694 V695 I696 S697 Q698 F699 S700 V701 L702 P703 L704 K705 N706 S707 I708 L711 A714 M715 A716 A717 N718 I726 Q727 A728
L729 K730 I731 I732 E733 P734 M735 V736 S737 S738 L739 S740 T741 E742 H743 A746 M747 Q748 I749 L750 Q751 A752 N753 N756 Q757 Q758 K759 K760 T761 M762 S763 W764 Q765 T766 L767 S768 E769 Q770 L771 S774 V775 D776 L777 R780 M781 K786 G790 L791 Q796 Q797 F798 E806
R809 R810 T816 L817 E818 S819 L820 G821 F829 I830 D831 K832 C836 D839 W840 K841 D846 K849 Q850 W854 R855 N856 L857 L858 L862 I866 S870 A871 V872 N876 E877 Q878 Y879 P880 R881 W882 M883 K890 M891 L892 Q893 D896 K897 K898 N899 K900
K903 Q906 L907 W908 P909 R912 D913 R914 I920 K921 I930 Q931 Q934 W937 V941 N942 H943 L944 N945 R953 P954 C955 L956 R957 Q964 L965 D966 E972 F973 Y974 S975 Q978 V979 W980 R981 Y984 A988 L989 D990 L1000 P1008 E1009 L1013
I1014 E1015 M1016 L1019 P1020 V1021 R1022 R1025 G1029 I1032 A1033 R1034 E1035 E1036 R1037 L1038 E1039 W1040 L1041 E1042 S1043 N1044 A1045 L1046 I1047 Q1048 E1053 G1054 L1055 W1056 S1057 S1060 D1061 R1062 L1063 A1064 L1065 K1066 D1067 S1068 W1069 Y1070 R1071 L1072 E1073 E1074 H1075 S1076 A1077 Q1078 R1079 T1080 P1081



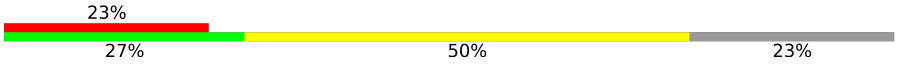
• Molecule 2: DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*CP*TP*GP*CP*CP*AP*G)-3')

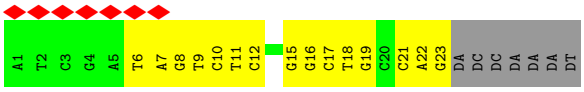




• Molecule 2: DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*CP*TP*GP*CP*CP*AP*G)-3')

Chain I:

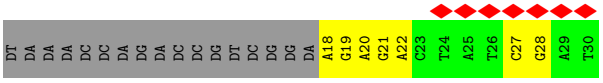




• Molecule 3: DNA (5'-D(P*AP*GP*AP*GP*AP*CP*TP*AP*TP*CP*GP*AP*T)-3')

Chain g:

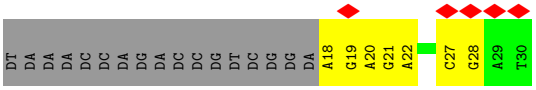




• Molecule 3: DNA (5'-D(P*AP*GP*AP*GP*AP*CP*TP*AP*TP*CP*GP*AP*T)-3')

Chain G:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21364	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.293	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1093334, 1.1093334, 1.1093334	Depositor

5 Model quality

5.1 Standard geometry

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

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	Y	0.13	0/16646	0.32	0/22561
1	y	0.11	0/14866	0.31	0/20143
2	I	0.17	0/527	0.36	0/811
2	i	0.19	0/593	0.36	0/912
3	G	0.15	0/302	0.34	0/464
3	g	0.13	0/302	0.29	0/464
All	All	0.12	0/33236	0.31	0/45355

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	Y	16281	0	16091	633	0
1	y	14541	0	14388	516	0
2	I	471	0	260	24	0
2	i	530	0	293	19	0
3	G	269	0	147	9	0
3	g	269	0	147	8	0
4	Y	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	5	0	0	0	0
5	y	5	0	0	0	0
All	All	32402	0	31338	1172	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 18.

All (1172) 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:Y:1426:CYS:HB3	1:Y:1442:CYS:SG	1.98	1.03
1:y:942:ASN:HA	1:y:945:MET:HE2	1.47	0.96
3:G:21:DG:N2	2:I:10:DC:O2	2.02	0.92
1:Y:1526:CYS:SG	1:Y:1554:HIS:CE1	2.62	0.92
2:i:10:DC:O2	3:g:21:DG:N2	2.04	0.90
1:Y:1556:LEU:HB3	1:Y:1560:GLY:HA3	1.55	0.87
1:Y:573:PRO:HB2	1:Y:582:ASN:HB3	1.58	0.86
1:y:437:CYS:HB3	1:y:458:GLN:H	1.40	0.85
1:Y:111:LEU:HB3	1:Y:288:ILE:HG22	1.59	0.84
1:Y:904:ARG:NH1	3:G:18:DA:N7	2.27	0.81
1:y:487:LEU:HB2	1:y:539:ILE:HB	1.63	0.81
1:Y:174:LYS:HB3	1:Y:201:PRO:HG2	1.64	0.79
1:y:685:SER:HB2	1:y:688:HIS:HB2	1.63	0.79
1:Y:442:CYS:HB3	1:Y:469:CYS:SG	2.24	0.78
1:Y:66:PRO:HA	1:Y:94:PHE:HA	1.65	0.78
1:Y:880:PRO:HA	1:Y:883:MET:HE1	1.67	0.77
1:y:64:TRP:HA	1:y:327:ARG:HA	1.67	0.76
1:Y:1545:LEU:HA	1:Y:1554:HIS:HB3	1.68	0.75
1:Y:1329:VAL:HG12	1:Y:1655:ALA:HB1	1.68	0.75
1:Y:736:VAL:HA	1:Y:739:LEU:HG	1.68	0.75
3:G:21:DG:N1	2:I:10:DC:N3	2.29	0.75
2:I:18:DT:H2"	2:I:19:DG:H5"	1.69	0.73
1:y:545:LYS:HA	1:y:568:ILE:O	1.88	0.73
1:y:478:ARG:HE	1:y:483:GLY:HA2	1.54	0.72
3:G:19:DG:H2'	3:G:20:DA:C8	2.24	0.72
1:Y:578:GLU:OE1	1:Y:581:ASN:ND2	2.22	0.72
1:y:909:PRO:HB2	1:y:920:ILE:HD11	1.71	0.72
1:Y:1544:ASN:HA	1:Y:1550:ARG:HH22	1.54	0.71
1:y:615:ILE:HG13	1:y:616:PRO:HD3	1.72	0.71
1:Y:1332:VAL:HG21	1:Y:1374:LEU:HD13	1.72	0.70
1:y:224:MET:SD	1:y:224:MET:N	2.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:410:ALA:O	1:Y:413:ARG:NH2	2.25	0.70
1:Y:2009:THR:HA	1:Y:2025:ILE:HD11	1.74	0.70
1:Y:622:SER:HB2	1:Y:638:ARG:HB3	1.74	0.69
1:y:1688:HIS:HA	1:y:1692:LEU:HB2	1.74	0.69
1:Y:478:ARG:NH2	2:I:15:DG:O6	2.25	0.69
1:y:648:GLN:OE1	1:y:648:GLN:N	2.24	0.69
1:Y:1946:SER:HG	1:Y:2038:GLY:N	1.89	0.69
1:Y:101:TRP:HA	1:Y:104:ILE:HG22	1.74	0.69
1:y:272:MET:O	1:y:276:ASN:N	2.22	0.68
1:Y:844:LEU:O	1:Y:850:GLN:NE2	2.27	0.68
1:y:839:ASP:HB2	1:y:944:LEU:HD13	1.74	0.68
1:y:619:LEU:HD13	1:y:640:LEU:HD11	1.75	0.68
1:y:908:TRP:HE1	1:y:945:MET:HG3	1.57	0.68
1:Y:1537:GLN:HG3	1:Y:1540:ARG:HG2	1.75	0.68
1:Y:1807:LEU:HD21	1:Y:1820:VAL:HG21	1.76	0.68
1:Y:2042:THR:HA	1:Y:2052:TYR:HA	1.75	0.68
1:y:1175:ARG:HH11	1:y:1624:GLY:HA2	1.59	0.68
1:Y:1439:CYS:HB3	1:Y:1444:ALA:H	1.59	0.68
1:Y:259:SER:HB3	1:Y:1659:GLY:H	1.59	0.68
1:Y:733:GLU:HA	1:Y:747:MET:HE1	1.74	0.67
1:Y:1531:ARG:NH1	1:Y:1555:TYR:O	2.27	0.67
1:Y:40:SER:O	1:Y:44:GLN:NE2	2.27	0.67
1:y:279:PRO:O	1:y:1240:ARG:NH2	2.28	0.67
1:y:1601:LEU:O	1:y:1603:ARG:NH1	2.26	0.67
1:y:890:LYS:HG2	1:y:906:GLN:HB2	1.76	0.67
1:y:1109:VAL:O	1:y:1135:ARG:NH2	2.28	0.67
2:i:10:DC:N3	3:g:21:DG:N1	2.29	0.67
1:Y:635:PHE:H	1:Y:1097:ASN:HD21	1.40	0.67
1:Y:883:MET:HE2	1:Y:883:MET:H	1.60	0.67
1:Y:1466:TYR:HH	1:Y:1469:HIS:HE2	1.37	0.67
1:Y:65:MET:HA	1:Y:328:GLN:HB2	1.78	0.66
1:Y:749:ILE:O	1:Y:753:ASN:ND2	2.28	0.66
1:y:1810:LEU:HA	1:y:1813:MET:HE2	1.77	0.66
1:y:896:ASP:OD1	1:y:897:LYS:N	2.28	0.66
1:Y:1529:CYS:SG	1:Y:1554:HIS:CD2	2.88	0.66
1:Y:1551:GLU:HB2	1:Y:1570:LEU:HD13	1.77	0.66
1:Y:985:THR:O	1:Y:987:ARG:NH1	2.29	0.66
1:y:1840:THR:HG23	1:y:1845:SER:HB3	1.78	0.66
1:Y:1690:CYS:SG	1:Y:1691:LEU:N	2.68	0.66
1:y:197:GLN:NE2	1:y:203:GLN:O	2.29	0.66
1:y:227:TYR:O	1:y:231:ARG:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:762:MET:HE1	1:y:766:THR:HB	1.77	0.66
1:Y:224:MET:HG3	2:I:22:DA:H5"	1.77	0.66
1:Y:263:GLU:OE2	1:Y:1325:HIS:ND1	2.29	0.66
1:y:898:LYS:O	1:y:912:ARG:NH2	2.29	0.66
1:Y:1317:ILE:HG22	1:Y:1322:LEU:HB2	1.77	0.65
1:y:647:ARG:NH1	2:i:20:DC:OP2	2.30	0.65
1:y:245:LEU:O	1:y:283:LYS:NZ	2.29	0.65
1:y:353:PRO:HB2	1:y:413:ARG:HB2	1.78	0.65
1:Y:86:ALA:O	1:Y:89:LYS:NZ	2.28	0.65
1:Y:807:PHE:O	1:Y:867:ARG:NH1	2.30	0.65
1:Y:151:PHE:HB2	1:Y:219:VAL:HG12	1.79	0.65
1:Y:876:ASN:ND2	1:Y:878:GLN:OE1	2.27	0.65
1:Y:906:GLN:NE2	1:Y:907:LEU:O	2.29	0.65
1:y:1690:CYS:SG	1:y:1691:LEU:N	2.70	0.65
1:Y:418:ALA:HB3	1:Y:421:PRO:HG3	1.78	0.65
1:Y:1688:HIS:HA	1:Y:1692:LEU:HB2	1.78	0.65
1:Y:138:LYS:O	1:Y:141:ARG:NH1	2.27	0.65
1:Y:726:ILE:HG22	1:Y:730:LYS:HE3	1.77	0.65
2:I:6:DT:H2"	2:I:7:DA:H5"	1.79	0.65
1:Y:1903:ASN:O	1:Y:1907:GLN:NE2	2.30	0.65
1:y:329:ILE:HD12	1:y:374:THR:HB	1.79	0.65
1:y:1035:GLU:HA	1:y:1038:LEU:HD12	1.77	0.65
1:Y:639:ARG:NH2	1:Y:1092:LYS:O	2.30	0.64
2:I:10:DC:H3'	2:I:11:DT:H71	1.79	0.64
1:y:736:VAL:HB	1:y:747:MET:HE1	1.80	0.64
1:Y:279:PRO:O	1:Y:1240:ARG:NH1	2.28	0.64
1:y:1421:TRP:HZ3	1:y:1423:CYS:HB2	1.63	0.64
1:y:37:TYR:HB2	1:y:449:LEU:HD21	1.80	0.64
1:y:1763:PRO:HD2	1:y:1766:GLN:HE22	1.62	0.64
3:g:19:DG:H2'	3:g:20:DA:C8	2.32	0.64
1:y:66:PRO:HA	1:y:94:PHE:HA	1.79	0.64
1:Y:1563:ASP:HB2	1:Y:1568:ASN:HD22	1.62	0.64
1:y:114:SER:O	1:y:324:ARG:NH1	2.30	0.64
1:Y:454:TRP:NE1	1:Y:456:PHE:O	2.31	0.64
1:Y:348:LEU:HA	1:Y:351:LEU:HD12	1.80	0.64
1:Y:1457:PRO:HG3	1:Y:1581:LEU:HD13	1.80	0.64
1:Y:1044:ASN:HB3	1:Y:1047:ILE:HG12	1.80	0.63
1:Y:1189:ASN:ND2	1:Y:1262:MET:SD	2.71	0.63
1:y:479:CYS:HB3	1:y:482:CYS:SG	2.38	0.63
1:y:1507:HIS:O	1:y:1586:ARG:NH1	2.30	0.63
1:y:646:SER:HB3	2:i:18:DT:H5"	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:221:ASN:ND2	2:I:22:DA:OP1	2.29	0.63
1:Y:437:CYS:HB3	1:Y:458:GLN:H	1.63	0.63
1:Y:551:GLU:OE2	1:Y:554:THR:OG1	2.15	0.63
1:y:836:CYS:O	1:y:841:LYS:NZ	2.31	0.63
1:Y:1638:ARG:NH1	1:Y:1642:GLY:O	2.31	0.63
1:y:536:ASP:OD2	1:y:582:ASN:ND2	2.31	0.63
1:Y:594:ARG:HH21	1:Y:597:ASN:HD21	1.47	0.63
1:Y:1824:ALA:HB3	1:Y:1827:GLN:HG3	1.80	0.63
1:y:30:ARG:NH1	1:y:482:CYS:O	2.31	0.63
1:y:98:LEU:HA	1:y:101:TRP:CE2	2.34	0.63
1:y:575:SER:HA	1:y:583:SER:HB3	1.79	0.63
1:y:458:GLN:NE2	1:y:459:VAL:O	2.30	0.63
1:y:1153:THR:HG23	1:y:1156:GLY:H	1.64	0.63
1:Y:224:MET:HA	1:Y:227:TYR:HB2	1.80	0.63
1:y:1113:GLY:HA2	1:y:1138:ARG:HD3	1.81	0.63
1:Y:249:VAL:HG13	1:Y:288:ILE:HG13	1.80	0.63
1:Y:588:CYS:SG	1:Y:589:CYS:N	2.72	0.63
1:y:245:LEU:HB3	1:y:277:VAL:HG21	1.81	0.62
1:Y:145:THR:HA	1:Y:178:ARG:HH22	1.62	0.62
1:y:310:ALA:O	1:y:314:GLY:N	2.30	0.62
1:Y:64:TRP:HA	1:Y:327:ARG:HA	1.82	0.62
1:Y:1804:ARG:HD2	1:Y:1891:LEU:HB2	1.81	0.62
1:Y:1977:LEU:HB2	1:Y:2025:ILE:HG22	1.79	0.62
1:Y:683:LYS:HE2	1:Y:684:LEU:HB2	1.82	0.62
1:Y:1424:ARG:NH2	1:Y:1447:GLN:O	2.33	0.62
1:Y:1562:ASN:HB2	1:Y:1569:LYS:HA	1.81	0.62
1:y:957:ARG:HE	1:y:966:ASP:HB3	1.64	0.62
1:Y:1940:ILE:HG12	1:Y:1972:ALA:HB3	1.82	0.62
1:Y:934:GLN:HE22	1:Y:936:HIS:HB3	1.63	0.62
1:y:134:ILE:HG12	1:y:173:PHE:HZ	1.65	0.62
1:Y:699:PHE:HA	1:Y:702:LEU:HD12	1.81	0.61
1:y:143:SER:HA	1:y:176:LYS:HA	1.81	0.61
1:y:660:ASP:OD1	1:y:661:ALA:N	2.33	0.61
1:Y:952:ILE:HG13	1:Y:956:LEU:HD11	1.81	0.61
1:Y:1535:GLN:NE2	1:Y:1540:ARG:O	2.33	0.61
1:Y:1632:VAL:HG23	1:Y:1650:ILE:HG12	1.80	0.61
1:y:138:LYS:HA	1:y:141:ARG:HH11	1.64	0.61
1:y:1401:LEU:HB2	1:y:1404:VAL:HG22	1.82	0.61
1:Y:245:LEU:HB3	1:Y:277:VAL:HG21	1.83	0.61
1:Y:1245:THR:HG23	1:Y:1247:LEU:H	1.66	0.61
1:Y:779:ASP:OD1	1:Y:780:ARG:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1482:ASP:OD1	1:Y:1482:ASP:N	2.34	0.61
1:Y:1603:ARG:NH1	1:Y:1644:THR:O	2.34	0.61
1:Y:1764:GLN:NE2	1:Y:1764:GLN:O	2.30	0.61
1:y:817:LEU:O	1:y:821:GLY:N	2.33	0.61
1:y:1523:TYR:N	1:y:1579:LEU:O	2.24	0.61
1:Y:335:SER:O	1:Y:338:ARG:NH2	2.33	0.61
1:Y:1467:GLN:HE22	1:Y:1469:HIS:HD2	1.49	0.61
1:y:178:ARG:HG2	1:y:202:GLU:HA	1.82	0.61
1:y:1537:GLN:HG3	1:y:1540:ARG:HD2	1.83	0.61
1:Y:831:ASP:O	1:Y:855:ARG:NH2	2.34	0.60
1:Y:1951:ASN:HD21	1:Y:1984:LEU:HD12	1.66	0.60
1:Y:696:ILE:HD12	1:Y:708:ILE:HG23	1.83	0.60
1:y:1545:LEU:O	1:y:1554:HIS:ND1	2.29	0.60
1:Y:74:LEU:HD12	1:Y:78:LEU:HB3	1.83	0.60
1:Y:1056:TRP:HE1	1:Y:1061:ASP:HB3	1.66	0.60
1:y:232:ARG:H	1:y:232:ARG:HD3	1.67	0.60
1:y:767:LEU:HD12	1:y:973:PHE:HD2	1.66	0.60
3:g:27:DC:H2"	3:g:28:DG:C8	2.37	0.60
1:Y:221:ASN:OD1	1:Y:223:THR:OG1	2.14	0.60
1:Y:180:ALA:HB2	1:Y:215:PRO:HG3	1.83	0.60
1:Y:1298:LYS:HG3	1:Y:1346:ARG:HG3	1.83	0.60
1:Y:1984:LEU:HG	1:Y:1986:TYR:H	1.67	0.60
1:y:108:LYS:HD2	1:y:286:GLN:HE22	1.65	0.60
1:y:434:LEU:HB2	1:y:603:LEU:HD21	1.83	0.60
1:y:182:TYR:HB3	1:y:220:THR:HG23	1.83	0.60
1:Y:493:MET:HE3	1:Y:493:MET:HA	1.83	0.60
1:Y:573:PRO:O	1:Y:582:ASN:ND2	2.35	0.60
1:y:890:LYS:NZ	1:y:903:LYS:O	2.35	0.60
1:y:1626:GLU:HG2	1:y:1629:GLU:HG2	1.84	0.60
1:Y:731:ILE:HG12	1:y:734:PRO:HG2	1.83	0.60
1:y:500:TRP:HA	1:y:557:LYS:HA	1.83	0.60
1:Y:171:ARG:HD3	1:Y:174:LYS:HD3	1.84	0.59
1:Y:696:ILE:HD11	1:Y:711:LEU:HB3	1.83	0.59
1:Y:1212:PHE:HD2	1:Y:1220:CYS:HB3	1.67	0.59
1:Y:1799:LEU:HD11	1:Y:1804:ARG:HD3	1.83	0.59
1:y:439:ASN:HD22	1:y:471:ALA:HB2	1.65	0.59
1:Y:149:ALA:HA	1:Y:247:TYR:O	2.02	0.59
1:Y:1270:TRP:CD1	1:Y:1307:TYR:HH	2.20	0.59
2:I:10:DC:H2'	2:I:11:DT:C6	2.38	0.59
1:Y:442:CYS:CB	1:Y:469:CYS:SG	2.85	0.59
1:y:878:GLN:OE1	1:y:881:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1939:GLU:HA	1:Y:1972:ALA:HB2	1.83	0.59
1:y:906:GLN:NE2	1:y:907:LEU:O	2.30	0.59
1:y:979:VAL:HG11	1:y:988:ALA:HB1	1.83	0.59
1:Y:143:SER:O	1:Y:178:ARG:NH1	2.36	0.59
1:y:1056:TRP:HE1	1:y:1061:ASP:HB3	1.68	0.59
1:Y:1457:PRO:HD3	1:Y:1581:LEU:HD22	1.82	0.59
1:Y:163:GLN:NE2	1:Y:164:GLU:OE2	2.35	0.59
1:Y:1588:ASP:N	1:Y:1588:ASP:OD1	2.36	0.58
1:y:1424:ARG:NH2	1:y:1447:GLN:O	2.36	0.58
1:y:97:GLN:NE2	1:y:119:SER:O	2.35	0.58
1:Y:156:ASN:HD21	2:I:21:DC:H5'	1.68	0.58
1:Y:1270:TRP:CG	1:Y:1307:TYR:HH	2.21	0.58
1:Y:121:LYS:NZ	4:Y:2201:AGS:O3B	2.36	0.58
1:Y:1426:CYS:CB	1:Y:1442:CYS:SG	2.77	0.58
1:Y:1528:SER:HB2	1:Y:1573:GLY:HA3	1.86	0.58
1:y:1084:ASN:HA	1:y:1087:ASN:HD21	1.68	0.58
1:Y:1230:GLN:NE2	1:Y:1233:GLN:OE1	2.32	0.58
1:Y:253:ALA:N	1:Y:291:SER:OG	2.37	0.58
1:Y:736:VAL:HB	1:Y:743:HIS:HB3	1.84	0.58
1:Y:1230:GLN:HE22	1:Y:1234:LEU:HG	1.68	0.58
1:Y:62:PHE:O	1:Y:327:ARG:NH1	2.37	0.58
1:Y:440:LYS:HA	1:Y:457:GLY:H	1.68	0.58
1:Y:1210:LYS:HD3	1:Y:1308:ARG:HH11	1.69	0.58
1:Y:1392:LYS:HE3	1:Y:1468:ALA:HB1	1.85	0.58
1:Y:250:LEU:HD22	1:Y:287:ILE:HD11	1.86	0.58
1:Y:948:VAL:O	1:Y:952:ILE:HG22	2.03	0.58
1:y:1197:LEU:HD23	1:y:1201:VAL:HG21	1.85	0.58
1:Y:900:LYS:HD3	1:Y:904:ARG:HA	1.86	0.57
1:Y:1074:GLU:O	1:Y:1079:ARG:NH1	2.37	0.57
1:y:1775:PHE:HE1	1:y:1810:LEU:HD21	1.67	0.57
1:Y:390:ALA:O	1:Y:394:TRP:N	2.32	0.57
1:Y:1057:SER:OG	1:Y:1058:THR:N	2.36	0.57
1:Y:1787:ASN:HA	1:Y:1817:ARG:HB3	1.84	0.57
1:y:765:GLN:NE2	1:y:766:THR:OG1	2.37	0.57
3:G:27:DC:H2"	3:G:28:DG:C8	2.39	0.57
1:Y:1639:ASP:OD1	1:Y:1643:TYR:N	2.37	0.57
1:Y:1676:ARG:NH2	1:Y:1714:ASN:OD1	2.37	0.57
1:y:880:PRO:HA	1:y:883:MET:HE1	1.85	0.57
1:Y:196:ASP:HA	1:Y:199:LYS:HD2	1.86	0.57
1:Y:863:ASP:OD1	1:Y:867:ARG:NE	2.38	0.57
1:Y:2087:ARG:HB3	1:Y:2089:ARG:HH21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:990:ASP:N	1:y:990:ASP:OD1	2.37	0.57
1:y:1386:ASP:OD1	1:y:1395:ARG:NE	2.28	0.57
1:y:1807:LEU:HD22	1:y:1820:VAL:HG11	1.85	0.57
1:y:981:ARG:NH1	1:y:1053:GLU:O	2.35	0.57
1:Y:891:MET:O	1:Y:893:GLN:NE2	2.38	0.57
1:Y:1207:LEU:HD13	1:Y:1211:TRP:CD1	2.39	0.57
1:y:493:MET:SD	1:y:493:MET:N	2.78	0.57
1:y:546:TYR:OH	1:y:572:ARG:NH2	2.34	0.57
1:y:1219:GLN:OE1	1:y:1222:ARG:NH1	2.38	0.57
1:Y:357:TYR:HB2	1:Y:412:SER:HB2	1.86	0.57
1:y:116:GLY:O	1:y:121:LYS:NZ	2.33	0.57
1:y:761:THR:HB	1:y:972:GLU:HG3	1.86	0.57
1:y:1614:ALA:HB1	1:y:1675:ALA:HB1	1.86	0.57
1:Y:1557:LEU:HG	1:Y:1558:ARG:H	1.70	0.57
1:y:181:LEU:HA	1:y:219:VAL:HG23	1.86	0.57
1:y:930:ILE:HD13	1:y:937:TRP:HE3	1.68	0.57
1:y:1114:MET:SD	1:y:1115:SER:N	2.78	0.57
1:Y:1284:LEU:HD11	1:Y:1564:ARG:HH21	1.70	0.57
1:y:57:VAL:HB	1:y:425:HIS:HB2	1.86	0.57
1:y:1210:LYS:HA	1:y:1214:GLU:HB3	1.85	0.57
1:Y:486:TYR:OH	1:Y:586:CYS:SG	2.55	0.56
1:Y:1913:GLU:O	1:Y:1918:ARG:NH1	2.37	0.56
1:y:691:LEU:HD12	1:y:694:LYS:HD2	1.87	0.56
1:y:930:ILE:HD12	1:y:941:VAL:HG23	1.87	0.56
1:Y:188:HIS:H	1:Y:207:ARG:HG3	1.70	0.56
1:Y:737:SER:HA	1:Y:744:ALA:HB2	1.88	0.56
1:y:15:LEU:HD23	1:y:18:ARG:HD2	1.86	0.56
1:Y:955:CYS:O	1:Y:970:GLN:NE2	2.38	0.56
1:Y:1231:ALA:O	1:Y:1235:ALA:N	2.37	0.56
1:Y:2039:ARG:NH1	1:Y:2055:LEU:O	2.30	0.56
1:y:167:ARG:NH1	1:y:203:GLN:OE1	2.38	0.56
1:y:411:ARG:O	1:y:413:ARG:NH1	2.38	0.56
1:y:749:ILE:O	1:y:753:ASN:ND2	2.38	0.56
1:y:1105:MET:O	1:y:1135:ARG:NH1	2.39	0.56
1:Y:263:GLU:HG2	1:Y:1187:HIS:HE2	1.70	0.56
1:Y:957:ARG:NH1	1:Y:966:ASP:OD2	2.39	0.56
1:Y:1463:ASP:OD2	1:Y:1531:ARG:NH2	2.38	0.56
1:Y:1526:CYS:HA	1:Y:1575:VAL:HA	1.85	0.56
1:Y:1601:LEU:HD12	1:Y:1602:ILE:H	1.70	0.56
1:Y:1731:ASP:O	1:Y:1734:ARG:NH2	2.31	0.56
1:y:646:SER:O	1:y:650:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:711:LEU:O	1:Y:714:ALA:HB3	2.05	0.56
1:Y:1699:TYR:HB2	1:Y:1702:ARG:HD2	1.86	0.56
1:Y:2011:LEU:HD11	1:Y:2017:LEU:HD12	1.88	0.56
1:y:554:THR:HB	1:y:557:LYS:HB3	1.87	0.56
1:y:892:LEU:HA	1:y:906:GLN:HB3	1.88	0.56
1:Y:244:MET:SD	1:Y:244:MET:N	2.78	0.56
1:Y:673:GLU:HG2	1:Y:770:GLN:HE21	1.71	0.56
1:Y:1079:ARG:HE	1:Y:1083:GLN:HE21	1.53	0.56
1:Y:1186:ARG:HE	1:Y:1320:ALA:HB1	1.71	0.56
1:y:46:PRO:HG3	1:y:53:LEU:HD12	1.88	0.56
1:Y:735:MET:HE2	1:y:702:LEU:HD11	1.88	0.56
1:Y:1409:GLN:NE2	1:Y:1410:GLU:O	2.38	0.56
1:Y:1478:LEU:HD13	1:Y:1479:PRO:HD2	1.88	0.56
1:Y:1927:HIS:HB3	1:Y:1930:TRP:HB2	1.87	0.56
1:y:615:ILE:HG13	1:y:616:PRO:CD	2.35	0.56
1:y:702:LEU:HD12	1:y:703:PRO:HD2	1.86	0.56
1:y:1525:ILE:HG23	1:y:1532:ALA:HB2	1.86	0.56
1:Y:398:ASN:N	1:Y:401:GLU:OE1	2.39	0.56
1:Y:109:LYS:NZ	1:Y:318:ARG:O	2.33	0.56
1:Y:777:LEU:HA	1:Y:781:MET:SD	2.46	0.56
1:Y:207:ARG:NH2	2:I:23:DG:OP1	2.39	0.56
1:Y:1292:GLU:HG3	1:Y:1293:GLU:HG2	1.88	0.56
1:Y:1914:GLY:N	1:Y:1961:GLU:OE2	2.38	0.56
1:y:218:MET:HE3	1:y:218:MET:HA	1.87	0.56
1:y:454:TRP:NE1	1:y:456:PHE:O	2.39	0.56
1:y:883:MET:SD	1:y:883:MET:N	2.72	0.56
1:y:1205:THR:HG1	1:y:1211:TRP:CD1	2.24	0.55
1:y:1556:LEU:N	1:y:1569:LYS:O	2.39	0.55
1:Y:382:ARG:N	1:Y:385:GLU:OE2	2.35	0.55
2:I:7:DA:H2"	2:I:8:DG:H5"	1.87	0.55
1:Y:781:MET:SD	1:Y:781:MET:N	2.79	0.55
1:Y:1379:ARG:O	1:Y:1379:ARG:NH1	2.33	0.55
1:y:988:ALA:HB2	1:y:1055:LEU:HD11	1.88	0.55
1:y:1221:LEU:HA	1:y:1224:LEU:HD12	1.88	0.55
1:Y:1768:ASP:OD1	1:Y:1768:ASP:N	2.39	0.55
1:y:87:LEU:HD11	1:y:127:VAL:HG22	1.88	0.55
1:y:297:ASP:HB2	1:y:324:ARG:HH21	1.70	0.55
1:Y:564:LYS:NZ	1:Y:565:HIS:O	2.39	0.55
1:Y:630:GLU:HG3	1:Y:1094:GLY:HA3	1.88	0.55
1:Y:926:VAL:HG21	1:Y:993:LEU:HD23	1.89	0.55
1:Y:957:ARG:NH2	1:y:769:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:981:ARG:NH1	1:Y:1053:GLU:O	2.38	0.55
1:Y:1191:LEU:HD22	1:Y:1241:LEU:HD13	1.89	0.55
1:y:830:ILE:HG22	1:y:855:ARG:HD3	1.88	0.55
1:Y:702:LEU:HB3	1:Y:704:LEU:HD13	1.88	0.55
1:Y:945:MET:HA	1:Y:948:VAL:HG12	1.89	0.55
1:Y:1676:ARG:NH1	1:Y:1712:LEU:O	2.40	0.55
1:Y:360:LEU:HA	1:Y:363:TYR:CD2	2.42	0.55
1:Y:1946:SER:OG	1:Y:2039:ARG:N	2.39	0.55
1:y:1016:MET:SD	1:y:1016:MET:N	2.80	0.55
1:y:1736:GLU:OE2	1:y:1743:ARG:NE	2.36	0.55
1:Y:310:ALA:O	1:Y:314:GLY:N	2.21	0.55
1:Y:316:THR:O	1:Y:318:ARG:NH1	2.39	0.55
1:Y:75:ARG:HA	1:Y:84:VAL:HG21	1.89	0.55
1:Y:1125:ALA:HB3	1:Y:1128:ASN:HB2	1.89	0.55
1:y:908:TRP:CD2	1:y:909:PRO:HD2	2.42	0.55
1:Y:149:ALA:HB3	1:Y:217:ILE:HG12	1.87	0.54
1:Y:1217:GLU:N	1:Y:1217:GLU:OE2	2.38	0.54
1:Y:1277:LEU:HA	1:Y:1280:ASN:HD21	1.72	0.54
1:y:215:PRO:HD2	1:y:218:MET:HE1	1.89	0.54
1:y:1255:LEU:O	1:y:1259:THR:HG23	2.08	0.54
1:Y:669:LEU:HD12	1:Y:771:LEU:HD12	1.89	0.54
1:Y:734:PRO:HB3	1:y:727:GLN:HE22	1.71	0.54
1:Y:944:LEU:O	1:Y:947:GLU:HG2	2.06	0.54
1:y:490:LYS:HA	1:y:536:ASP:HA	1.88	0.54
1:y:1618:GLY:HA2	1:y:1674:TYR:CD2	2.42	0.54
1:Y:1884:GLN:NE2	1:Y:1885:THR:O	2.39	0.54
1:y:1559:GLY:O	1:y:1569:LYS:NZ	2.40	0.54
1:Y:117:THR:HG22	1:Y:1135:ARG:HH21	1.71	0.54
1:Y:673:GLU:O	1:Y:1022:ARG:NH1	2.41	0.54
1:y:696:ILE:HD12	1:y:711:LEU:HB3	1.88	0.54
1:y:711:LEU:HD22	1:y:732:ILE:HD12	1.89	0.54
1:y:714:ALA:HB1	1:y:750:LEU:HD13	1.88	0.54
2:i:16:DG:H2'	2:i:16:DG:N3	2.22	0.54
1:Y:1385:ALA:HA	1:Y:1476:ALA:HB3	1.89	0.54
1:y:97:GLN:HG2	1:y:124:CYS:HB2	1.89	0.54
1:y:627:THR:HB	1:y:630:GLU:HB2	1.89	0.54
1:y:1210:LYS:HB2	1:y:1308:ARG:HG2	1.89	0.54
1:Y:68:ASP:OD1	1:Y:68:ASP:N	2.39	0.54
1:Y:331:ARG:NH2	1:Y:332:VAL:O	2.37	0.54
1:Y:934:GLN:OE1	1:Y:937:TRP:N	2.39	0.54
1:Y:1092:LYS:HG2	1:Y:1111:ILE:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1093:SER:OG	1:y:1095:LYS:NZ	2.39	0.54
1:Y:1561:SER:HB3	1:Y:1564:ARG:HG3	1.89	0.54
1:Y:2006:GLN:HE22	1:Y:2076:VAL:HG22	1.73	0.54
1:Y:125:PHE:HB2	1:Y:288:ILE:HD12	1.89	0.54
1:Y:291:SER:HB3	1:Y:294:ILE:HD11	1.90	0.54
1:Y:111:LEU:O	1:Y:288:ILE:HA	2.08	0.53
1:y:777:LEU:HA	1:y:781:MET:HB2	1.90	0.53
1:Y:1548:PRO:HA	1:Y:1552:ASN:HA	1.89	0.53
1:Y:1903:ASN:OD1	1:Y:1903:ASN:N	2.41	0.53
1:y:231:ARG:HD2	1:y:233:LYS:HB3	1.90	0.53
1:Y:1234:LEU:O	1:Y:1238:LEU:HG	2.08	0.53
1:y:727:GLN:O	1:y:731:ILE:HG13	2.08	0.53
2:i:7:DA:H2"	2:i:8:DG:H5"	1.90	0.53
1:Y:447:HIS:O	1:Y:451:GLN:NE2	2.41	0.53
1:Y:550:LEU:HB3	1:Y:564:LYS:HG3	1.91	0.53
1:Y:1834:ARG:NH1	1:Y:1852:ASP:O	2.42	0.53
1:y:180:ALA:HB2	1:y:204:ALA:HB3	1.90	0.53
1:y:440:LYS:HA	1:y:457:GLY:H	1.73	0.53
1:Y:160:ASN:O	1:Y:163:GLN:HG3	2.09	0.53
1:Y:337:ILE:HB	1:Y:364:ARG:HG2	1.90	0.53
1:y:780:ARG:HD2	1:y:1069:TRP:HZ3	1.72	0.53
1:y:957:ARG:N	1:y:964:GLN:O	2.39	0.53
1:Y:783:GLY:O	1:Y:787:GLU:HG2	2.08	0.53
1:y:1102:SER:OG	2:i:20:DC:OP1	2.23	0.53
1:Y:1411:LEU:HG	1:Y:1413:GLY:H	1.74	0.53
1:y:109:LYS:NZ	1:y:318:ARG:O	2.41	0.53
1:y:330:PRO:O	1:y:370:ARG:NH2	2.42	0.53
1:y:1486:LEU:HB2	1:y:1510:GLU:HG2	1.91	0.53
1:Y:917:ASN:O	1:Y:921:LYS:NZ	2.42	0.53
1:Y:2050:GLN:HG3	1:Y:2052:TYR:HD2	1.74	0.53
1:y:1206:LYS:NZ	2:i:25:DC:OP1	2.42	0.53
1:Y:125:PHE:CD1	1:Y:249:VAL:HG11	2.44	0.53
1:Y:816:THR:N	1:Y:819:SER:OG	2.42	0.53
1:y:677:ILE:HD11	1:y:1022:ARG:HE	1.73	0.53
1:y:1154:ALA:O	1:y:1158:GLU:HB2	2.09	0.53
2:i:11:DT:H2'	2:i:12:DC:C6	2.43	0.53
1:Y:611:LEU:HA	1:Y:614:ILE:HG12	1.90	0.52
1:Y:1753:TYR:HD1	1:Y:1841:ARG:HB2	1.74	0.52
1:Y:1903:ASN:HB3	1:Y:2098:ARG:HH11	1.74	0.52
1:Y:458:GLN:NE2	1:Y:459:VAL:O	2.41	0.52
1:y:846:ASP:OD2	1:y:849:LYS:NZ	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1071:ARG:NH2	1:y:1095:LYS:O	2.41	0.52
1:Y:536:ASP:O	1:Y:537:ARG:NH1	2.39	0.52
1:Y:583:SER:OG	1:Y:584:PHE:N	2.42	0.52
1:Y:739:LEU:HD23	1:y:704:LEU:HD22	1.91	0.52
1:y:155:LEU:HG	1:y:1107:MET:HE3	1.91	0.52
1:y:677:ILE:HG12	1:y:1022:ARG:HH21	1.74	0.52
1:y:696:ILE:O	1:y:700:SER:N	2.42	0.52
1:y:1188:VAL:HG13	1:y:1238:LEU:HD22	1.91	0.52
1:y:1529:CYS:SG	1:y:1530:GLY:N	2.83	0.52
1:Y:110:SER:N	1:Y:319:ASP:O	2.41	0.52
1:Y:1000:LEU:HD12	1:Y:1001:PRO:HD2	1.89	0.52
1:y:153:TYR:HB3	1:y:158:LEU:HD12	1.91	0.52
1:y:1691:LEU:HD13	1:y:1703:LEU:HD12	1.92	0.52
1:Y:1695:ASP:OD1	1:Y:1695:ASP:N	2.32	0.52
1:y:692:LEU:HD11	1:y:746:ALA:HB1	1.91	0.52
1:y:711:LEU:O	1:y:715:MET:HG2	2.10	0.52
1:Y:134:ILE:HD13	1:Y:177:ILE:HD12	1.91	0.52
1:Y:251:ASP:OD1	1:Y:252:GLU:N	2.36	0.52
1:Y:747:MET:O	1:Y:751:GLN:HG2	2.09	0.52
1:Y:899:ASN:N	1:Y:899:ASN:OD1	2.43	0.52
1:Y:1032:ILE:O	1:Y:1037:ARG:NH2	2.43	0.52
1:Y:1484:ARG:NE	1:Y:1635:GLN:OE1	2.39	0.52
1:y:158:LEU:HD11	1:y:1107:MET:HE1	1.92	0.52
1:Y:727:GLN:HA	1:Y:730:LYS:HD2	1.92	0.52
1:Y:1445:ASP:OD1	1:Y:1445:ASP:N	2.35	0.52
1:Y:1700:VAL:HA	1:Y:1703:LEU:HD12	1.90	0.52
1:Y:1951:ASN:OD1	1:Y:2004:ARG:NH1	2.43	0.52
1:y:953:ARG:O	1:y:953:ARG:NH1	2.41	0.52
1:Y:400:ARG:NH2	1:Y:404:GLN:OE1	2.38	0.52
1:Y:691:LEU:HB3	1:Y:743:HIS:CD2	2.45	0.52
1:Y:1828:LEU:HD12	1:Y:1834:ARG:HB2	1.91	0.52
1:Y:1914:GLY:O	1:Y:1917:SER:OG	2.26	0.52
1:y:34:LEU:O	1:y:38:LEU:HG	2.09	0.52
1:y:221:ASN:HB3	1:y:224:MET:SD	2.50	0.52
1:y:673:GLU:OE1	1:y:770:GLN:NE2	2.40	0.52
1:y:1292:GLU:O	1:y:1298:LYS:HG3	2.10	0.52
1:Y:112:LEU:HD13	1:Y:289:ALA:HB3	1.92	0.52
1:Y:437:CYS:HA	1:Y:473:VAL:HG12	1.90	0.52
1:Y:534:GLN:O	1:Y:537:ARG:NH1	2.26	0.52
1:y:338:ARG:HE	1:y:362:HIS:HB3	1.74	0.52
1:y:1074:GLU:O	1:y:1079:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1189:ASN:HB3	1:y:1321:PHE:CE1	2.45	0.52
1:y:1629:GLU:OE1	1:y:1654:ASN:ND2	2.40	0.52
1:y:607:ALA:HA	1:y:610:PHE:HD2	1.74	0.51
1:y:685:SER:O	1:y:689:CYS:N	2.42	0.51
1:y:1207:LEU:HD12	1:y:1312:LEU:HD23	1.92	0.51
2:I:22:DA:H2"	2:I:23:DG:C8	2.45	0.51
1:Y:671:TYR:CZ	1:Y:822:LEU:HD12	2.45	0.51
1:Y:1810:LEU:HD22	1:Y:2097:LEU:HD11	1.91	0.51
1:y:809:ARG:NH2	1:y:870:SER:OG	2.43	0.51
1:y:1129:TYR:O	1:y:1132:ARG:NH2	2.43	0.51
1:Y:342:PRO:HB2	1:Y:348:LEU:HD11	1.93	0.51
1:Y:762:MET:HE1	1:Y:767:LEU:HB2	1.91	0.51
1:y:455:PRO:HG2	1:y:456:PHE:CE2	2.45	0.51
1:y:544:GLU:N	1:y:570:LEU:O	2.34	0.51
1:y:1753:TYR:HD1	1:y:1841:ARG:HB2	1.74	0.51
1:Y:649:GLY:O	1:Y:653:ILE:HG12	2.10	0.51
1:Y:1388:VAL:HG22	1:Y:1393:VAL:HB	1.92	0.51
1:y:1092:LYS:HE3	1:y:1111:ILE:HA	1.93	0.51
1:Y:257:ILE:O	1:Y:260:GLN:NE2	2.42	0.51
1:Y:1106:GLU:OE2	1:Y:1132:ARG:NE	2.44	0.51
1:y:501:LEU:N	1:y:556:GLY:O	2.39	0.51
1:Y:684:LEU:HG	1:Y:753:ASN:HD21	1.76	0.51
1:y:7:HIS:H	1:y:621:PHE:HE2	1.59	0.51
1:y:337:ILE:HD11	1:y:367:GLN:HG3	1.93	0.51
1:y:705:LYS:HD3	1:y:708:ILE:HB	1.93	0.51
1:y:966:ASP:OD1	1:y:966:ASP:N	2.41	0.51
1:Y:229:LEU:HD21	1:Y:271:VAL:HG23	1.93	0.51
1:Y:762:MET:SD	1:Y:766:THR:HB	2.51	0.51
1:y:854:TRP:O	1:y:858:LEU:HG	2.10	0.51
1:Y:487:LEU:HB2	1:Y:539:ILE:HB	1.91	0.51
1:Y:916:TYR:CD1	2:I:10:DC:H4'	2.46	0.51
1:Y:931:GLN:HB2	1:Y:934:GLN:HB2	1.92	0.51
1:Y:1114:MET:HE2	1:Y:1114:MET:HA	1.92	0.51
1:y:227:TYR:HE1	1:y:1313:PHE:HB2	1.76	0.51
1:y:608:PRO:HA	1:y:611:LEU:HG	1.93	0.51
1:y:810:ARG:HG3	1:y:818:GLU:HG3	1.92	0.51
1:Y:170:THR:OG1	1:Y:202:GLU:OE1	2.28	0.51
1:Y:735:MET:HE1	1:y:704:LEU:HB2	1.93	0.51
1:Y:1175:ARG:HH22	1:Y:1177:ARG:HD2	1.75	0.51
1:Y:2011:LEU:HD12	1:Y:2015:GLY:HA3	1.93	0.51
1:y:293:THR:HA	1:y:324:ARG:HH12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:914:ARG:HA	1:y:920:ILE:HB	1.93	0.51
1:Y:80:SER:N	1:Y:131:GLU:OE1	2.42	0.51
1:Y:983:PRO:HD2	1:Y:997:SER:HB2	1.93	0.51
1:y:1086:PHE:O	1:y:1089:LYS:HG3	2.11	0.51
1:Y:1157:MET:N	1:Y:1157:MET:HE2	2.26	0.50
1:y:272:MET:SD	1:y:278:GLY:N	2.83	0.50
1:y:542:ASP:N	1:y:542:ASP:OD1	2.45	0.50
1:y:1844:GLN:HA	1:y:1876:THR:HA	1.92	0.50
1:Y:877:GLU:O	1:Y:880:PRO:HD2	2.12	0.50
1:Y:1840:THR:HG23	1:Y:1845:SER:HB3	1.91	0.50
1:y:58:PHE:HZ	1:y:383:LEU:HD12	1.76	0.50
1:Y:1529:CYS:HB2	1:Y:1556:LEU:HD23	1.93	0.50
1:y:1287:ASP:OD1	1:y:1287:ASP:N	2.41	0.50
1:Y:80:SER:OG	1:Y:82:PRO:HD2	2.12	0.50
1:Y:98:LEU:HA	1:Y:101:TRP:NE1	2.26	0.50
1:y:156:ASN:ND2	2:i:22:DA:OP1	2.44	0.50
1:Y:185:GLU:O	1:Y:187:ARG:NH1	2.39	0.50
1:Y:1892:LEU:HB3	1:Y:1901:ARG:HH22	1.77	0.50
1:y:32:LYS:N	1:y:453:ASP:OD2	2.44	0.50
1:y:130:LEU:HD11	1:y:169:TRP:HB3	1.93	0.50
1:Y:843:LEU:HD11	1:Y:930:ILE:HD11	1.93	0.50
1:Y:888:PRO:HD3	3:G:18:DA:N6	2.27	0.50
1:y:340:GLU:OE1	1:y:393:THR:OG1	2.26	0.50
1:y:439:ASN:HD21	1:y:550:LEU:HD11	1.77	0.50
1:Y:438:SER:OG	1:Y:472:PRO:O	2.25	0.50
1:Y:830:ILE:HB	1:Y:858:LEU:HD11	1.93	0.50
1:y:891:MET:O	1:y:906:GLN:N	2.36	0.50
1:y:1278:LEU:O	1:y:1282:GLU:HG3	2.12	0.50
2:I:8:DG:H2'	2:I:9:DT:H71	1.93	0.50
1:Y:827:TYR:HB2	1:Y:830:ILE:HG23	1.94	0.50
1:Y:1242:THR:O	1:Y:1248:MET:HE1	2.12	0.50
1:y:140:THR:HB	1:y:142:GLN:NE2	2.26	0.50
1:y:1062:ARG:NH1	1:y:1067:ASP:OD2	2.45	0.50
1:y:1439:CYS:HB3	1:y:1444:ALA:H	1.75	0.50
1:y:1796:LEU:HB3	1:y:1804:ARG:HH12	1.77	0.50
1:y:829:PHE:HA	1:y:832:LYS:HD2	1.92	0.49
1:y:1714:ASN:HA	1:y:1717:LEU:HD12	1.94	0.49
1:Y:303:LYS:NZ	1:Y:304:GLU:OE2	2.44	0.49
1:Y:445:LYS:HA	1:Y:458:GLN:HG3	1.92	0.49
1:Y:1033:ALA:N	1:Y:1036:GLU:OE2	2.44	0.49
1:Y:1219:GLN:HA	1:Y:1222:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1772:TRP:CD1	1:Y:1859:GLY:H	2.30	0.49
1:y:1072:LEU:HD11	1:y:1098:VAL:HB	1.93	0.49
1:y:1490:SER:HB2	1:y:1504:ARG:HD3	1.94	0.49
1:y:1834:ARG:HE	1:y:1852:ASP:HA	1.77	0.49
1:Y:1990:GLN:NE2	1:Y:1997:ALA:O	2.35	0.49
1:y:735:MET:SD	1:y:735:MET:N	2.86	0.49
1:y:1259:THR:O	1:y:1263:MET:HG2	2.13	0.49
1:Y:455:PRO:HG2	1:Y:456:PHE:CE2	2.47	0.49
1:Y:955:CYS:SG	1:Y:956:LEU:N	2.85	0.49
1:y:224:MET:HA	1:y:227:TYR:HB2	1.95	0.49
1:y:653:ILE:O	1:y:657:LEU:HG	2.12	0.49
1:Y:225:LEU:HA	1:Y:228:MET:HE3	1.95	0.49
1:Y:1963:LEU:HD23	1:Y:2012:LEU:HD22	1.93	0.49
1:y:342:PRO:HG3	1:y:363:TYR:CD2	2.47	0.49
1:y:1263:MET:HE1	1:y:1321:PHE:CE1	2.47	0.49
2:I:15:DG:H2"	2:I:16:DG:OP2	2.11	0.49
1:Y:1155:HIS:O	1:Y:1155:HIS:ND1	2.45	0.49
1:Y:1255:LEU:HD12	1:Y:1255:LEU:H	1.78	0.49
1:Y:1377:ALA:O	1:Y:1381:TYR:N	2.26	0.49
1:Y:1521:HIS:CE1	1:Y:1538:PRO:HD3	2.47	0.49
1:y:1596:ASP:OD2	1:y:1603:ARG:NH1	2.46	0.49
2:I:22:DA:H2"	2:I:23:DG:N7	2.27	0.49
1:Y:1224:LEU:O	1:Y:1227:LEU:HG	2.13	0.49
1:Y:1939:GLU:HB3	1:Y:1974:ARG:HH21	1.77	0.49
1:Y:765:GLN:NE2	1:Y:766:THR:OG1	2.45	0.49
1:y:46:PRO:HB2	1:y:56:PRO:HD3	1.94	0.49
1:y:214:PRO:HB3	1:y:237:ILE:HG23	1.95	0.49
1:y:232:ARG:NE	1:y:1202:PRO:O	2.46	0.49
1:y:702:LEU:HB3	1:y:708:ILE:HD11	1.94	0.49
1:y:1101:CYS:SG	1:y:1102:SER:N	2.85	0.49
1:y:1157:MET:O	1:y:1161:LYS:HG2	2.12	0.49
1:y:1615:LEU:O	1:y:1619:LEU:HG	2.13	0.49
1:Y:298:SER:OG	1:Y:300:GLU:OE1	2.30	0.49
1:Y:1828:LEU:HD12	1:Y:1828:LEU:O	2.13	0.49
1:y:588:CYS:SG	1:y:589:CYS:N	2.85	0.49
1:Y:672:GLN:NE2	1:Y:1064:ALA:O	2.46	0.49
1:Y:839:ASP:HB2	1:Y:940:LEU:HD11	1.94	0.49
1:Y:886:ARG:HH21	1:Y:887:PHE:C	2.21	0.49
1:Y:1930:TRP:CH2	1:Y:2051:HIS:HB3	2.48	0.49
1:y:1278:LEU:HA	1:y:1281:ILE:HG12	1.94	0.49
1:Y:692:LEU:HD21	1:Y:750:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:688:HIS:CE1	1:Y:745:GLU:HG3	2.49	0.48
1:Y:733:GLU:O	1:Y:747:MET:HE1	2.13	0.48
1:Y:817:LEU:HG	1:Y:823:VAL:HG12	1.94	0.48
1:Y:1196:PHE:CE2	1:Y:1223:PHE:HB2	2.48	0.48
1:Y:1294:THR:HG23	1:Y:1297:GLY:HA3	1.95	0.48
1:Y:1482:ASP:OD2	1:Y:1609:ARG:NH2	2.46	0.48
1:Y:1741:SER:HA	1:Y:1774:LEU:HD11	1.95	0.48
1:Y:1912:LEU:HD21	1:Y:1957:ARG:HE	1.78	0.48
1:Y:1912:LEU:H	1:Y:2089:ARG:NH2	2.10	0.48
1:y:728:ALA:O	1:y:732:ILE:HG12	2.13	0.48
1:y:866:ILE:HG23	1:y:871:ALA:HB3	1.95	0.48
1:y:1081:PRO:HA	1:y:1084:ASN:HD22	1.78	0.48
1:y:1291:TRP:O	1:y:1294:THR:OG1	2.27	0.48
1:y:1497:ASP:HB3	1:y:1500:LEU:HD23	1.95	0.48
1:y:1531:ARG:NH1	1:y:1555:TYR:O	2.32	0.48
2:I:16:DG:H2'	2:I:17:DC:C4	2.48	0.48
1:y:133:LEU:HB3	1:y:177:ILE:HD13	1.95	0.48
1:y:872:VAL:O	1:y:964:GLN:NE2	2.46	0.48
1:y:1042:GLU:O	1:y:1048:GLN:NE2	2.47	0.48
1:Y:173:PHE:HB3	1:Y:176:LYS:HB2	1.94	0.48
1:Y:1212:PHE:HB3	1:Y:1219:GLN:HB2	1.95	0.48
1:Y:1334:PHE:HA	1:Y:1460:PHE:O	2.11	0.48
1:Y:1396:SER:HA	1:Y:1462:THR:HG22	1.95	0.48
1:Y:1912:LEU:HD21	1:Y:1957:ARG:NE	2.28	0.48
1:y:296:GLU:N	1:y:296:GLU:OE1	2.46	0.48
1:y:829:PHE:CD2	1:y:955:CYS:HB2	2.48	0.48
1:Y:63:GLY:O	1:Y:328:GLN:N	2.42	0.48
1:Y:1227:LEU:HD13	1:Y:1256:LEU:HB3	1.95	0.48
1:Y:1335:ASN:N	1:Y:1335:ASN:OD1	2.46	0.48
1:y:611:LEU:HA	1:y:614:ILE:HG12	1.96	0.48
1:y:1619:LEU:O	1:y:1623:LEU:HG	2.13	0.48
1:Y:272:MET:HE1	1:Y:277:VAL:HG23	1.96	0.48
1:Y:705:LYS:O	1:Y:708:ILE:HB	2.12	0.48
1:Y:2017:LEU:HD21	1:Y:2084:ALA:HA	1.95	0.48
1:y:1071:ARG:NH1	1:y:1073:GLU:OE2	2.40	0.48
1:y:1650:ILE:HD12	1:y:1664:LEU:HD22	1.95	0.48
1:Y:1158:GLU:OE1	1:Y:1158:GLU:N	2.44	0.48
1:Y:2056:ASP:OD1	1:Y:2056:ASP:N	2.45	0.48
1:y:287:ILE:HD12	1:y:313:ALA:HB2	1.95	0.48
1:y:854:TRP:O	1:y:857:LEU:HG	2.14	0.48
1:Y:1785:GLY:O	1:Y:1817:ARG:NH1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:16:HIS:CE1	1:y:43:PHE:HA	2.49	0.48
1:y:251:ASP:OD1	1:y:290:THR:OG1	2.27	0.48
1:y:762:MET:CE	1:y:766:THR:HB	2.43	0.48
1:y:1084:ASN:O	1:y:1088:GLU:HG2	2.14	0.48
1:Y:147:THR:HA	1:Y:216:SER:HA	1.96	0.48
1:Y:154:PRO:HD3	1:Y:252:GLU:OE1	2.13	0.48
1:Y:370:ARG:HD2	1:Y:419:PHE:CZ	2.48	0.48
1:y:578:GLU:HG3	1:y:583:SER:HB2	1.96	0.48
1:y:1019:LEU:HD12	1:y:1020:PRO:HD2	1.96	0.48
1:y:1044:ASN:HD21	1:y:1046:LEU:HB2	1.79	0.48
1:Y:724:THR:O	1:Y:727:GLN:HG2	2.14	0.47
1:Y:1079:ARG:HB3	1:Y:1083:GLN:HE21	1.80	0.47
1:Y:1193:LEU:HD22	1:Y:1321:PHE:HE2	1.79	0.47
1:Y:1342:LEU:HD11	1:Y:1464:ILE:HG12	1.96	0.47
1:y:282:ASP:N	1:y:282:ASP:OD1	2.47	0.47
1:Y:640:LEU:HA	1:Y:1114:MET:HE1	1.94	0.47
1:Y:733:GLU:HB3	1:Y:734:PRO:HD3	1.96	0.47
1:Y:956:LEU:H	1:Y:956:LEU:HD12	1.79	0.47
1:Y:1156:GLY:C	1:Y:1157:MET:HE2	2.39	0.47
1:Y:1602:ILE:HG21	1:Y:1608:ALA:HB2	1.96	0.47
1:y:19:ALA:O	1:y:23:VAL:HG12	2.14	0.47
1:y:46:PRO:HB3	1:y:53:LEU:HB2	1.95	0.47
1:y:300:GLU:HA	1:y:303:LYS:HE3	1.95	0.47
1:y:387:LEU:HD13	1:y:402:LEU:HD22	1.95	0.47
1:Y:536:ASP:O	1:Y:573:PRO:HD3	2.14	0.47
1:Y:782:ARG:HG3	1:Y:798:PHE:CG	2.49	0.47
1:Y:1126:PRO:HG3	1:Y:1165:TRP:CZ3	2.49	0.47
1:y:762:MET:HE3	1:y:763:SER:N	2.29	0.47
1:y:1553:THR:HG21	1:y:1572:HIS:ND1	2.29	0.47
1:Y:4:GLN:HE21	1:Y:624:LEU:H	1.62	0.47
1:Y:917:ASN:HD21	1:Y:919:VAL:HG22	1.79	0.47
1:Y:935:ALA:HA	1:Y:938:LYS:HD2	1.95	0.47
1:Y:1338:THR:HG22	1:Y:1341:GLU:HG2	1.96	0.47
1:Y:1614:ALA:HB1	1:Y:1675:ALA:HB1	1.96	0.47
1:Y:1964:THR:HG21	1:Y:2018:GLY:HA3	1.96	0.47
1:y:397:ILE:HG13	1:y:401:GLU:HG3	1.96	0.47
1:y:747:MET:HA	1:y:750:LEU:HG	1.97	0.47
1:y:900:LYS:HB3	2:i:10:DC:OP1	2.15	0.47
1:y:1514:PHE:HB2	1:y:1580:TRP:HZ3	1.78	0.47
1:Y:836:CYS:O	1:Y:841:LYS:NZ	2.46	0.47
1:Y:1425:LYS:O	1:Y:1638:ARG:NE	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1546:LYS:HD3	1:Y:1553:THR:HA	1.95	0.47
1:y:262:ALA:HB1	1:y:1178:PHE:HB3	1.95	0.47
1:Y:183:ASN:C	1:Y:224:MET:HE1	2.40	0.47
1:Y:1550:ARG:HH11	1:Y:1554:HIS:HA	1.79	0.47
1:Y:1847:GLN:O	1:Y:1872:THR:OG1	2.31	0.47
1:y:214:PRO:HG3	1:y:237:ILE:HA	1.97	0.47
1:Y:734:PRO:HG2	1:y:731:ILE:HG12	1.96	0.47
1:Y:848:ASP:OD1	1:Y:849:LYS:N	2.47	0.47
1:Y:2057:MET:HE2	1:Y:2057:MET:O	2.15	0.47
1:y:616:PRO:O	1:y:620:GLU:HG2	2.15	0.47
1:y:640:LEU:HB2	1:y:1098:VAL:HG22	1.96	0.47
1:y:1084:ASN:HA	1:y:1087:ASN:ND2	2.30	0.47
1:y:1192:VAL:HG12	1:y:1223:PHE:HZ	1.79	0.47
1:y:1373:ASP:OD1	1:y:1373:ASP:N	2.37	0.47
2:i:10:DC:H2'	2:i:11:DT:C6	2.49	0.47
1:Y:1276:ILE:HD13	1:Y:1404:VAL:HG13	1.95	0.47
1:Y:1909:ASP:OD2	1:Y:2092:ALA:N	2.36	0.47
1:Y:1952:SER:HB3	1:Y:1955:THR:HG23	1.97	0.47
2:i:13:DT:O2	2:i:13:DT:H2'	2.15	0.47
1:Y:705:LYS:HA	1:Y:708:ILE:HB	1.97	0.47
1:Y:1248:MET:N	1:Y:1248:MET:HE2	2.29	0.47
1:Y:1892:LEU:HD22	1:Y:1901:ARG:HH12	1.80	0.47
1:Y:224:MET:HE3	2:I:22:DA:OP1	2.14	0.47
1:Y:640:LEU:O	1:Y:1098:VAL:HA	2.14	0.47
1:Y:1399:ILE:HD12	1:Y:1457:PRO:HB3	1.97	0.47
1:Y:1764:GLN:HA	1:Y:1767:TRP:CD1	2.50	0.47
1:y:163:GLN:OE1	1:y:167:ARG:NH2	2.48	0.47
1:y:613:GLU:O	1:y:616:PRO:HD2	2.15	0.47
1:y:777:LEU:HD22	1:y:781:MET:HG2	1.97	0.47
1:Y:1044:ASN:OD1	1:Y:1046:LEU:N	2.47	0.46
1:Y:1093:SER:O	1:Y:1095:LYS:NZ	2.48	0.46
1:Y:1343:GLU:OE2	1:Y:1346:ARG:NH1	2.34	0.46
1:Y:1813:MET:HE3	1:Y:1814:PRO:HD2	1.96	0.46
1:Y:1957:ARG:CZ	1:Y:2017:LEU:HD22	2.45	0.46
1:y:167:ARG:HH11	1:y:200:VAL:HG21	1.79	0.46
1:y:173:PHE:HB3	1:y:176:LYS:HB2	1.96	0.46
1:y:182:TYR:CE2	1:y:224:MET:HB2	2.50	0.46
1:y:244:MET:HA	1:y:283:LYS:HE2	1.97	0.46
1:y:1071:ARG:O	1:y:1097:ASN:ND2	2.42	0.46
1:Y:117:THR:O	4:Y:2201:AGS:O2B	2.33	0.46
1:Y:1518:GLU:OE1	1:Y:1534:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:65:MET:HA	1:y:328:GLN:HB2	1.97	0.46
1:y:405:LEU:O	1:y:409:MET:SD	2.73	0.46
1:Y:32:LYS:N	1:Y:453:ASP:OD2	2.48	0.46
1:Y:1433:THR:HG23	1:Y:1434:THR:HG23	1.98	0.46
1:Y:1607:ALA:HB2	1:Y:1707:HIS:HB3	1.97	0.46
1:y:252:GLU:N	1:y:290:THR:O	2.48	0.46
1:y:743:HIS:C	1:y:747:MET:HE3	2.40	0.46
1:y:1274:LEU:O	1:y:1278:LEU:HG	2.16	0.46
1:y:1277:LEU:O	1:y:1281:ILE:HG12	2.15	0.46
1:Y:174:LYS:HE3	1:Y:201:PRO:HD2	1.97	0.46
1:Y:464:ARG:HG3	1:Y:1684:ASP:HB2	1.97	0.46
1:Y:900:LYS:HZ2	1:Y:905:ASP:H	1.63	0.46
1:Y:1049:HIS:O	1:Y:1052:GLU:HG2	2.16	0.46
1:Y:1197:LEU:O	1:Y:1201:VAL:HG12	2.15	0.46
1:Y:1241:LEU:HD23	1:Y:1242:THR:HG23	1.98	0.46
1:Y:2082:ARG:HH12	1:Y:2086:THR:HB	1.80	0.46
1:y:1057:SER:H	1:y:1060:SER:HB2	1.81	0.46
1:y:1616:ARG:HD3	1:y:1632:VAL:HB	1.98	0.46
1:Y:391:ARG:NE	1:Y:397:ILE:O	2.44	0.46
1:Y:1079:ARG:NH2	1:Y:1087:ASN:OD1	2.47	0.46
1:Y:1689:HIS:N	1:Y:1689:HIS:CD2	2.84	0.46
1:Y:1769:PHE:HB3	1:Y:1775:PHE:CG	2.50	0.46
1:y:231:ARG:HG3	1:y:1313:PHE:HE2	1.79	0.46
1:y:693:GLU:HA	1:y:696:ILE:HG22	1.98	0.46
1:y:930:ILE:HD13	1:y:937:TRP:CE3	2.49	0.46
1:y:1072:LEU:HD12	1:y:1072:LEU:HA	1.55	0.46
1:Y:282:ASP:OD1	1:Y:282:ASP:N	2.49	0.46
1:Y:400:ARG:HH12	1:Y:404:GLN:HB2	1.81	0.46
1:Y:1780:GLN:O	1:Y:1784:SER:OG	2.34	0.46
1:y:500:TRP:CE2	1:y:557:LYS:HB2	2.51	0.46
1:Y:360:LEU:HA	1:Y:363:TYR:HD2	1.80	0.46
1:Y:491:GLU:N	1:Y:535:PHE:O	2.34	0.46
1:Y:1071:ARG:HG2	1:Y:1073:GLU:OE1	2.16	0.46
1:y:866:ILE:HG21	1:y:965:LEU:HD23	1.97	0.46
1:y:1338:THR:H	1:y:1341:GLU:HG2	1.81	0.46
1:y:1405:LEU:HD13	1:y:1410:GLU:HB3	1.96	0.46
1:y:1414:ASP:HB3	1:y:1416:HIS:NE2	2.31	0.46
1:y:1507:HIS:CE1	1:y:1662:VAL:HG21	2.50	0.46
1:y:1767:TRP:CD1	1:y:1803:SER:HB3	2.51	0.46
1:Y:1315:LYS:O	1:Y:1318:SER:OG	2.24	0.46
1:Y:1950:LEU:HD12	1:Y:1981:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:1212:PHE:CD1	1:y:1219:GLN:HB2	2.50	0.46
1:y:1763:PRO:HB2	1:y:1765:GLU:OE1	2.15	0.46
1:Y:1339:ALA:O	1:Y:1343:GLU:HG2	2.16	0.46
1:Y:1731:ASP:OD1	1:Y:1731:ASP:N	2.45	0.46
1:y:736:VAL:HG13	1:y:739:LEU:HD12	1.98	0.46
1:Y:98:LEU:HA	1:Y:101:TRP:CE2	2.51	0.46
1:Y:174:LYS:HA	1:Y:202:GLU:HB3	1.97	0.46
1:Y:545:LYS:HZ2	1:Y:567:GLU:CD	2.24	0.46
1:Y:979:VAL:HG11	1:Y:988:ALA:HB1	1.98	0.46
1:Y:1670:ASP:OD1	1:Y:1670:ASP:N	2.46	0.46
1:Y:1693:SER:H	1:Y:1696:SER:HB2	1.81	0.46
1:Y:1764:GLN:NE2	1:Y:1800:THR:OG1	2.49	0.46
1:y:660:ASP:HA	1:y:663:LYS:HG2	1.98	0.46
1:y:733:GLU:O	1:y:737:SER:OG	2.31	0.46
1:Y:349:LYS:HA	1:Y:411:ARG:HH22	1.81	0.45
1:Y:813:ASN:N	1:Y:813:ASN:OD1	2.48	0.45
1:Y:922:LEU:HD12	1:Y:998:PRO:HA	1.97	0.45
1:Y:1601:LEU:HG	1:Y:1645:GLY:HA3	1.98	0.45
1:Y:1626:GLU:HG2	1:Y:1628:THR:HG23	1.98	0.45
1:Y:1920:TRP:HE1	1:Y:1966:LEU:HB2	1.81	0.45
1:Y:1967:VAL:HG21	1:Y:2021:TRP:CD2	2.51	0.45
1:y:248:ILE:HB	1:y:287:ILE:HG12	1.98	0.45
1:y:491:GLU:N	1:y:535:PHE:O	2.47	0.45
1:y:816:THR:N	1:y:819:SER:OG	2.49	0.45
1:y:1103:THR:HG21	2:i:19:DG:N3	2.31	0.45
1:y:1494:SER:HA	1:y:1502:ARG:HA	1.98	0.45
1:Y:423:ARG:HH12	1:Y:1134:GLY:HA2	1.81	0.45
1:Y:709:ASP:HA	1:Y:712:LYS:HD2	1.98	0.45
1:Y:1681:CYS:SG	1:Y:1690:CYS:HB2	2.55	0.45
1:y:178:ARG:HB2	1:y:215:PRO:HB3	1.97	0.45
1:y:270:ARG:NE	1:y:1191:LEU:HA	2.32	0.45
1:y:1119:MET:N	1:y:1119:MET:SD	2.89	0.45
2:I:15:DG:H4'	2:I:16:DG:O5'	2.16	0.45
1:Y:447:HIS:HA	1:Y:450:ASN:ND2	2.32	0.45
1:Y:1619:LEU:HD22	1:Y:1664:LEU:HB2	1.97	0.45
1:Y:1696:SER:HA	1:Y:1699:TYR:CE1	2.52	0.45
1:y:786:LYS:NZ	1:y:790:GLY:O	2.50	0.45
1:Y:494:ARG:HD3	1:Y:500:TRP:HB2	1.99	0.45
1:Y:943:HIS:HA	1:Y:946:ILE:HG22	1.99	0.45
1:Y:1984:LEU:HB2	1:Y:2004:ARG:HH22	1.82	0.45
1:y:1845:SER:OG	1:y:1875:GLY:O	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:2066:GLU:O	1:Y:2088:ALA:HA	2.17	0.45
3:g:19:DG:H2'	3:g:20:DA:H8	1.79	0.45
1:Y:11:LEU:HA	1:Y:621:PHE:CE2	2.52	0.45
1:Y:187:ARG:HD3	1:Y:192:GLU:HB2	1.99	0.45
1:Y:862:LEU:O	1:Y:866:ILE:HG12	2.16	0.45
1:Y:1017:PRO:HB3	1:Y:1046:LEU:HB2	1.98	0.45
1:Y:1930:TRP:NE1	1:Y:2104:GLY:O	2.42	0.45
1:y:26:GLN:HG2	1:y:605:LEU:HD12	1.99	0.45
1:y:34:LEU:HD22	1:y:454:TRP:CZ3	2.51	0.45
1:y:349:LYS:HB3	1:y:408:LEU:HD21	1.97	0.45
1:y:427:PHE:C	1:y:428:ILE:HD13	2.42	0.45
1:y:726:ILE:O	1:y:730:LYS:HG3	2.17	0.45
1:y:1114:MET:SD	1:y:1116:LEU:N	2.90	0.45
1:Y:601:ARG:HD3	2:I:15:DG:C6	2.51	0.45
1:y:360:LEU:HD13	1:y:409:MET:HG3	1.99	0.45
1:y:781:MET:HB3	1:y:798:PHE:CE2	2.52	0.45
1:y:1763:PRO:O	1:y:1764:GLN:HG2	2.17	0.45
2:i:15:DG:H2"	2:i:16:DG:C5	2.51	0.45
1:Y:331:ARG:HE	1:Y:332:VAL:N	2.15	0.45
1:Y:333:SER:HG	1:Y:335:SER:HG	1.62	0.45
1:Y:1057:SER:N	1:Y:1060:SER:OG	2.50	0.45
1:Y:2002:GLU:HA	1:Y:2005:GLN:HG2	1.98	0.45
1:y:642:THR:HA	1:y:1118:ALA:O	2.17	0.45
1:y:1590:VAL:HG11	1:y:1664:LEU:HD23	1.98	0.45
1:Y:140:THR:HG23	1:Y:142:GLN:H	1.81	0.45
1:Y:2011:LEU:HA	1:Y:2015:GLY:HA3	1.98	0.45
1:Y:1291:TRP:CE3	1:Y:1292:GLU:HB2	2.52	0.45
1:Y:1764:GLN:HA	1:Y:1767:TRP:NE1	2.32	0.45
1:y:980:TRP:CE2	1:y:1013:LEU:HD13	2.51	0.45
1:y:1074:GLU:HA	1:y:1100:ASN:OD1	2.17	0.45
1:y:1400:MET:SD	1:y:1400:MET:N	2.89	0.45
1:Y:27:LEU:HB3	1:Y:29:LEU:HD23	1.99	0.44
1:Y:27:LEU:HD11	1:Y:603:LEU:HG	1.99	0.44
1:Y:1157:MET:HG3	1:Y:1689:HIS:CG	2.51	0.44
1:Y:1626:GLU:HG2	1:Y:1628:THR:H	1.81	0.44
1:y:242:GLN:NE2	1:y:274:ALA:O	2.24	0.44
1:y:548:ILE:HD11	1:y:568:ILE:HG21	1.98	0.44
1:y:645:ASP:H	1:y:1121:ASN:HD21	1.65	0.44
1:y:740:SER:HB3	1:y:743:HIS:ND1	2.32	0.44
1:Y:490:LYS:HG3	1:Y:535:PHE:HB3	1.98	0.44
1:Y:766:THR:HG22	1:Y:770:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:962:GLY:N	1:y:1025:ARG:HH22	2.15	0.44
1:Y:1101:CYS:HB2	1:Y:1105:MET:CG	2.48	0.44
1:Y:1381:TYR:CD1	1:Y:1387:VAL:HG11	2.52	0.44
1:Y:1419:TRP:NE1	1:Y:1453:ARG:HE	2.16	0.44
1:Y:1591:GLU:HG3	1:Y:1649:PHE:CE2	2.52	0.44
1:Y:2044:THR:OG1	1:Y:2050:GLN:NE2	2.51	0.44
1:y:666:LEU:HD21	1:y:777:LEU:HD11	2.00	0.44
1:y:1600:LEU:HB2	1:y:1603:ARG:NH1	2.32	0.44
1:y:1796:LEU:HD13	1:y:1799:LEU:HD21	1.99	0.44
1:Y:757:GLN:O	1:Y:759:LYS:NZ	2.40	0.44
1:Y:1079:ARG:HE	1:Y:1083:GLN:NE2	2.15	0.44
1:Y:1290:ALA:HB1	1:Y:1294:THR:HG21	1.99	0.44
1:Y:1732:GLY:HA3	1:Y:1873:LEU:HD13	2.00	0.44
1:Y:1775:PHE:CZ	1:Y:1810:LEU:HD21	2.52	0.44
1:Y:2067:ASP:OD1	1:Y:2082:ARG:NH2	2.50	0.44
1:y:100:ALA:O	1:y:104:ILE:HG22	2.17	0.44
1:y:447:HIS:HA	1:y:450:ASN:HD21	1.82	0.44
1:y:1639:ASP:OD1	1:y:1643:TYR:N	2.46	0.44
1:Y:1105:MET:SD	1:Y:1106:GLU:N	2.90	0.44
1:Y:1195:LEU:HD23	1:Y:1195:LEU:HA	1.86	0.44
1:Y:1294:THR:N	1:Y:1346:ARG:HD2	2.32	0.44
1:y:759:LYS:HD2	1:y:974:TYR:CD2	2.53	0.44
1:Y:251:ASP:HB3	1:Y:252:GLU:OE1	2.16	0.44
1:Y:578:GLU:HG3	3:G:22:DA:H5"	1.99	0.44
1:Y:839:ASP:OD1	1:Y:839:ASP:N	2.45	0.44
1:Y:1392:LYS:HA	1:Y:1392:LYS:HD2	1.81	0.44
1:y:55:ASP:HB2	1:y:382:ARG:HH21	1.82	0.44
1:y:180:ALA:HB3	1:y:218:MET:HE1	2.00	0.44
1:y:660:ASP:OD1	1:y:660:ASP:C	2.61	0.44
1:y:781:MET:HE1	1:y:1069:TRP:CE3	2.52	0.44
1:y:791:LEU:HD21	1:y:878:GLN:HE21	1.82	0.44
1:y:854:TRP:CE2	1:y:858:LEU:HD21	2.52	0.44
1:Y:987:ARG:HA	1:Y:987:ARG:HD3	1.84	0.44
1:Y:1085:GLN:O	1:Y:1089:LYS:HG2	2.18	0.44
1:Y:1212:PHE:CD2	1:Y:1220:CYS:HB3	2.50	0.44
1:y:309:VAL:CG1	1:y:320:VAL:HG21	2.48	0.44
1:y:438:SER:OG	1:y:472:PRO:O	2.31	0.44
1:y:796:GLN:OE1	1:y:796:GLN:N	2.47	0.44
1:y:1332:VAL:HB	1:y:1459:GLY:HA2	1.98	0.44
1:y:1488:PRO:O	1:y:1504:ARG:NH1	2.49	0.44
2:i:20:DC:H2"	2:i:21:DC:C5	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:DT:H2'	2:I:12:DC:C6	2.53	0.44
1:Y:672:GLN:HE22	1:Y:1024:TRP:CD1	2.35	0.44
1:Y:696:ILE:HG12	1:Y:711:LEU:HD23	1.98	0.44
1:Y:896:ASP:CG	1:y:1029:GLY:HA2	2.42	0.44
1:Y:1047:ILE:HG13	1:Y:1048:GLN:N	2.33	0.44
1:Y:1829:MET:HA	1:Y:1829:MET:HE3	1.99	0.44
1:y:181:LEU:HD13	1:y:203:GLN:HE21	1.81	0.44
1:y:418:ALA:HB3	1:y:421:PRO:HG3	2.00	0.44
1:y:582:ASN:OD1	1:y:582:ASN:N	2.49	0.44
1:Y:398:ASN:ND2	1:Y:401:GLU:OE2	2.51	0.44
1:Y:891:MET:HE1	1:Y:964:GLN:HB2	1.99	0.44
1:Y:1080:THR:O	1:Y:1083:GLN:HG2	2.18	0.44
1:Y:1224:LEU:HD13	1:Y:1260:GLN:HG3	2.00	0.44
1:Y:1562:ASN:ND2	1:Y:1570:LEU:O	2.49	0.44
1:Y:1765:GLU:CD	1:Y:1766:GLN:HG3	2.42	0.44
1:y:75:ARG:HD2	1:y:84:VAL:HG11	2.00	0.44
1:y:1020:PRO:HD3	1:y:1040:TRP:CZ2	2.53	0.44
1:y:1668:TRP:HB3	1:y:1720:LEU:HD21	1.98	0.44
1:Y:750:LEU:HA	1:Y:753:ASN:HD21	1.83	0.44
1:Y:1157:MET:HG3	1:Y:1689:HIS:CD2	2.53	0.44
1:Y:1332:VAL:HG13	1:Y:1459:GLY:HA2	1.99	0.44
1:y:1696:SER:HA	1:y:1699:TYR:CZ	2.53	0.44
1:Y:545:LYS:HG3	1:Y:567:GLU:OE2	2.18	0.43
1:Y:886:ARG:HE	1:Y:887:PHE:N	2.16	0.43
1:Y:1185:GLN:NE2	1:Y:1189:ASN:OD1	2.51	0.43
1:Y:1754:ASP:OD1	1:Y:1754:ASP:N	2.51	0.43
1:Y:1757:SER:HA	1:Y:1789:GLU:O	2.18	0.43
1:Y:2095:ASN:HB2	1:Y:2097:LEU:HD23	2.00	0.43
1:y:667:ARG:HG2	1:y:817:LEU:HG	2.00	0.43
1:y:877:GLU:O	1:y:880:PRO:HD2	2.18	0.43
1:y:1463:ASP:HB3	1:y:1466:TYR:HB2	2.00	0.43
1:Y:178:ARG:HG2	1:Y:215:PRO:HB3	2.00	0.43
1:Y:574:GLU:OE2	1:Y:576:ARG:HB2	2.17	0.43
1:Y:684:LEU:HG	1:Y:753:ASN:ND2	2.32	0.43
1:Y:1017:PRO:HG3	1:Y:1047:ILE:HG22	1.99	0.43
1:Y:1381:TYR:HD1	1:Y:1387:VAL:HG11	1.83	0.43
1:Y:1507:HIS:HA	1:Y:1588:ASP:HB3	1.99	0.43
1:y:423:ARG:HB2	1:y:1144:SER:HB2	2.00	0.43
1:y:428:ILE:HB	1:y:1149:LEU:HD12	1.99	0.43
1:y:541:SER:O	1:y:569:ASN:ND2	2.51	0.43
1:y:612:ASN:OD1	1:y:612:ASN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:693:GLU:HG2	1:y:715:MET:SD	2.58	0.43
1:y:893:GLN:N	1:y:906:GLN:O	2.47	0.43
1:y:1337:LEU:O	1:y:1558:ARG:NH1	2.51	0.43
1:y:1727:GLN:HG2	1:y:1734:ARG:HA	2.00	0.43
2:i:8:DG:H2'	2:i:9:DT:H71	1.99	0.43
1:Y:405:LEU:O	1:Y:408:LEU:HG	2.18	0.43
1:y:501:LEU:HD23	1:y:501:LEU:HA	1.81	0.43
1:Y:792:ASP:OD1	1:Y:793:LEU:N	2.51	0.43
1:Y:904:ARG:HH22	2:I:12:DC:H42	1.65	0.43
1:Y:1291:TRP:HE3	1:Y:1292:GLU:HB2	1.83	0.43
3:G:18:DA:H2"	3:G:19:DG:C8	2.54	0.43
1:Y:4:GLN:NE2	1:Y:624:LEU:H	2.16	0.43
1:Y:432:ALA:HA	1:Y:604:ARG:HG3	2.00	0.43
1:Y:888:PRO:HD3	3:G:18:DA:H62	1.84	0.43
1:y:11:LEU:O	1:y:14:GLN:HG2	2.19	0.43
1:y:232:ARG:HH12	1:y:1207:LEU:HD11	1.81	0.43
1:y:1146:ALA:C	1:y:1147:ILE:HD13	2.44	0.43
1:y:1263:MET:HA	1:y:1266:VAL:HG12	1.99	0.43
1:y:1635:GLN:HB2	1:y:1649:PHE:CE2	2.53	0.43
1:Y:218:MET:SD	1:Y:220:THR:OG1	2.77	0.43
1:Y:1421:TRP:HB3	1:Y:1436:PRO:HG3	1.99	0.43
1:Y:1971:MET:N	1:Y:1971:MET:HE2	2.34	0.43
1:y:674:LEU:HD21	1:y:974:TYR:C	2.43	0.43
1:y:674:LEU:HD23	1:y:975:SER:HB2	1.99	0.43
1:y:1551:GLU:O	1:y:1553:THR:HG23	2.19	0.43
3:g:21:DG:H2"	3:g:22:DA:C8	2.54	0.43
1:Y:1517:GLY:HA2	1:Y:1523:TYR:CZ	2.53	0.43
1:Y:1902:ILE:HG21	1:Y:1926:GLN:CD	2.44	0.43
1:Y:2078:GLN:O	1:Y:2081:GLU:HG3	2.18	0.43
1:y:1417:ILE:HG21	1:y:1579:LEU:HD21	2.01	0.43
3:g:18:DA:H2"	3:g:19:DG:C8	2.53	0.43
1:Y:97:GLN:NE2	1:Y:123:GLU:OE2	2.52	0.43
1:Y:153:TYR:CE2	1:Y:162:GLN:HG3	2.53	0.43
1:Y:167:ARG:O	1:Y:171:ARG:NH2	2.50	0.43
1:Y:193:ILE:HD11	1:Y:205:LEU:HB3	2.01	0.43
1:Y:287:ILE:HG21	1:Y:313:ALA:HB2	2.00	0.43
1:y:666:LEU:HD22	1:y:777:LEU:HD21	2.00	0.43
1:y:686:PRO:HA	1:y:689:CYS:HB2	2.01	0.43
1:y:1139:ARG:HD2	1:y:1139:ARG:HA	1.77	0.43
1:y:1339:ALA:O	1:y:1342:LEU:HG	2.18	0.43
1:Y:46:PRO:HB3	1:Y:53:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:227:TYR:O	1:Y:231:ARG:N	2.34	0.43
1:Y:702:LEU:HD11	1:y:702:LEU:HA	2.00	0.43
1:Y:880:PRO:CA	1:Y:883:MET:HE1	2.42	0.43
1:Y:893:GLN:NE2	1:Y:905:ASP:HB3	2.34	0.43
4:Y:2201:AGS:O3A	4:Y:2201:AGS:O2G	2.37	0.43
1:y:182:TYR:HE1	1:y:207:ARG:HG2	1.83	0.43
1:y:424:MET:SD	1:y:424:MET:N	2.91	0.43
1:y:1423:CYS:N	1:y:1428:ALA:O	2.33	0.43
1:y:1782:ALA:O	1:y:1817:ARG:NH2	2.49	0.43
1:Y:5:GLN:HE22	1:Y:411:ARG:HA	1.83	0.43
1:Y:1020:PRO:HD3	1:Y:1040:TRP:CZ2	2.54	0.43
1:Y:1943:VAL:HG13	1:Y:2043:VAL:HG12	2.01	0.43
1:y:9:ALA:HB3	1:y:10:PRO:HD3	2.01	0.43
1:y:881:ARG:NH2	1:y:1467:GLN:HB3	2.33	0.43
1:y:1105:MET:SD	1:y:1105:MET:N	2.92	0.43
1:Y:1530:GLY:C	1:Y:1557:LEU:HD22	2.43	0.42
1:Y:2082:ARG:O	1:Y:2082:ARG:NH1	2.52	0.42
1:y:54:ALA:HB3	1:y:427:PHE:HB2	2.01	0.42
1:y:696:ILE:HD11	1:y:708:ILE:HG23	2.00	0.42
1:y:727:GLN:HA	1:y:730:LYS:HD2	2.01	0.42
1:y:797:GLN:H	1:y:797:GLN:HG3	1.69	0.42
1:y:900:LYS:HB2	1:y:907:LEU:HG	2.01	0.42
1:y:1419:TRP:CD1	1:y:1453:ARG:HG2	2.54	0.42
1:y:1421:TRP:CZ3	1:y:1429:GLY:HA2	2.54	0.42
1:Y:722:SER:O	1:Y:726:ILE:HG13	2.19	0.42
1:Y:1990:GLN:HA	1:Y:1996:ASN:ND2	2.34	0.42
1:y:684:LEU:HD12	1:y:684:LEU:H	1.84	0.42
1:y:1105:MET:HA	1:y:1109:VAL:HG21	2.01	0.42
1:y:1211:TRP:CZ2	1:y:1219:GLN:HG3	2.54	0.42
1:Y:786:LYS:HD3	1:Y:792:ASP:HB2	2.01	0.42
1:Y:1263:MET:HE2	1:Y:1263:MET:HA	2.00	0.42
1:Y:1337:LEU:HB3	1:Y:1342:LEU:HD21	2.00	0.42
1:Y:1558:ARG:HA	1:Y:1558:ARG:HD2	1.68	0.42
1:Y:1764:GLN:OE1	1:Y:1799:LEU:HA	2.19	0.42
1:Y:1892:LEU:HD22	1:Y:1901:ARG:HH22	1.85	0.42
1:Y:1927:HIS:CD2	1:Y:1930:TRP:H	2.37	0.42
1:y:5:GLN:OE1	1:y:6:LEU:N	2.52	0.42
1:y:447:HIS:HA	1:y:450:ASN:ND2	2.34	0.42
1:y:1195:LEU:HD13	1:y:1234:LEU:HD22	2.01	0.42
1:y:1396:SER:HA	1:y:1462:THR:HG22	2.01	0.42
1:y:1627:ASN:OD1	1:y:1627:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1012:VAL:HG23	1:Y:1014:ILE:HD11	2.01	0.42
1:Y:1518:GLU:OE1	1:Y:1518:GLU:N	2.49	0.42
1:Y:1554:HIS:CE1	1:Y:1571:CYS:SG	3.11	0.42
1:Y:1851:ASP:OD2	1:Y:1867:SER:OG	2.38	0.42
1:y:429:ARG:HB2	1:y:1160:PHE:CZ	2.54	0.42
1:y:647:ARG:HD2	1:y:1076:SER:HB2	2.01	0.42
1:y:667:ARG:HB3	1:y:1063:LEU:HD11	2.01	0.42
1:y:829:PHE:CE1	1:y:954:PRO:HB2	2.54	0.42
1:y:908:TRP:CE3	1:y:909:PRO:HD2	2.54	0.42
1:Y:1095:LYS:HA	1:Y:1095:LYS:HD3	1.75	0.42
1:Y:1230:GLN:HE22	1:Y:1234:LEU:H	1.66	0.42
1:Y:1529:CYS:HB2	1:Y:1557:LEU:H	1.85	0.42
1:Y:1557:LEU:HG	1:Y:1558:ARG:N	2.33	0.42
1:y:269:ARG:NH1	1:y:1241:LEU:O	2.53	0.42
1:y:1032:ILE:O	1:y:1037:ARG:NH2	2.44	0.42
1:y:1421:TRP:NE1	1:y:1430:ALA:HB3	2.35	0.42
2:i:18:DT:H6	2:i:18:DT:H2'	1.70	0.42
1:Y:183:ASN:O	1:Y:186:THR:HG23	2.20	0.42
1:Y:607:ALA:N	1:Y:608:PRO:HD2	2.35	0.42
1:Y:769:GLU:HA	1:Y:772:VAL:HB	2.02	0.42
1:Y:1240:ARG:O	1:Y:1243:GLN:HG2	2.19	0.42
1:Y:1922:LEU:O	1:Y:1925:GLN:HG3	2.19	0.42
1:Y:2077:PRO:HA	1:Y:2080:VAL:HG22	2.02	0.42
1:y:149:ALA:C	1:y:150:ILE:HD13	2.44	0.42
1:y:436:ALA:HA	1:y:459:VAL:HA	2.02	0.42
1:y:791:LEU:HD11	1:y:878:GLN:HE21	1.84	0.42
1:y:1157:MET:C	1:y:1157:MET:HE2	2.45	0.42
1:y:1399:ILE:O	1:y:1530:GLY:HA3	2.20	0.42
1:Y:549:SER:HB3	1:Y:559:ASP:HB3	2.01	0.42
1:Y:934:GLN:NE2	1:Y:936:HIS:HB3	2.32	0.42
1:Y:1425:LYS:HE3	1:Y:1448:GLN:HE22	1.83	0.42
1:Y:1626:GLU:OE1	1:Y:1629:GLU:N	2.52	0.42
1:y:1420:PHE:HE1	1:y:1486:LEU:HD11	1.84	0.42
1:y:1472:VAL:O	1:y:1472:VAL:HG22	2.19	0.42
1:Y:829:PHE:HA	1:Y:832:LYS:HG2	2.01	0.42
1:Y:1603:ARG:HH22	1:Y:1643:TYR:HB3	1.84	0.42
1:Y:1907:GLN:OE1	1:Y:1907:GLN:N	2.42	0.42
1:y:391:ARG:HA	1:y:394:TRP:O	2.20	0.42
1:Y:267:LEU:HD12	1:Y:267:LEU:HA	1.93	0.42
1:Y:591:ASP:HB3	1:Y:594:ARG:HH22	1.85	0.42
1:Y:635:PHE:H	1:Y:1097:ASN:ND2	2.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1074:GLU:HB3	1:Y:1079:ARG:HH11	1.85	0.42
1:Y:1208:SER:HB2	1:Y:1310:ALA:O	2.19	0.42
1:Y:1483:PRO:HB3	1:Y:1513:HIS:HA	2.02	0.42
1:Y:1753:TYR:HE1	1:Y:1844:GLN:HE21	1.67	0.42
1:y:451:GLN:N	1:y:451:GLN:OE1	2.51	0.42
1:y:763:SER:OG	1:y:765:GLN:OE1	2.38	0.42
1:y:781:MET:HB3	1:y:798:PHE:HE2	1.84	0.42
1:y:781:MET:N	1:y:781:MET:HE2	2.34	0.42
1:y:1035:GLU:HG2	1:y:1036:GLU:OE2	2.19	0.42
1:Y:208:GLU:HA	1:Y:211:TYR:HB2	2.01	0.42
1:Y:855:ARG:O	1:Y:858:LEU:HG	2.19	0.42
1:Y:1365:ARG:HB3	1:Y:1368:LYS:NZ	2.35	0.42
1:Y:1526:CYS:SG	1:Y:1575:VAL:HG22	2.59	0.42
1:Y:1905:CYS:N	1:Y:1907:GLN:OE1	2.52	0.42
1:y:72:GLU:HA	1:y:75:ARG:HB2	2.02	0.42
1:y:247:TYR:C	1:y:248:ILE:HD13	2.45	0.42
1:y:683:LYS:HZ1	1:y:750:LEU:HA	1.85	0.42
1:y:688:HIS:HB3	1:y:742:GLU:OE1	2.20	0.42
1:y:1592:LEU:HD21	1:y:1594:LEU:HG	2.01	0.42
1:Y:41:GLN:HG2	1:Y:461:PHE:CZ	2.55	0.41
1:Y:145:THR:HA	1:Y:178:ARG:NH2	2.31	0.41
1:Y:491:GLU:HG2	1:Y:499:ASN:OD1	2.20	0.41
1:Y:650:THR:O	1:Y:653:ILE:HG13	2.20	0.41
1:Y:681:SER:O	1:Y:681:SER:OG	2.32	0.41
1:Y:1080:THR:O	1:Y:1084:ASN:ND2	2.53	0.41
1:y:45:PRO:HG3	1:y:399:HIS:CD2	2.54	0.41
1:y:97:GLN:NE2	1:y:120:GLY:O	2.53	0.41
1:y:189:THR:HA	1:y:208:GLU:HG2	2.02	0.41
1:y:594:ARG:HB2	1:y:596:ASN:OD1	2.20	0.41
1:y:726:ILE:HG22	1:y:730:LYS:HE3	2.02	0.41
1:y:846:ASP:O	1:y:850:GLN:HG3	2.20	0.41
1:y:980:TRP:CZ3	1:y:1013:LEU:HB2	2.55	0.41
2:I:17:DC:H6	2:I:17:DC:H2'	1.74	0.41
1:Y:105:LEU:HD23	1:Y:105:LEU:HA	1.92	0.41
1:Y:229:LEU:HD11	1:Y:271:VAL:HA	2.00	0.41
1:Y:897:LYS:HB2	1:Y:897:LYS:HE2	1.87	0.41
1:Y:988:ALA:HB2	1:Y:1055:LEU:HD11	2.02	0.41
1:y:309:VAL:HG11	1:y:320:VAL:HG21	2.01	0.41
1:y:1128:ASN:O	1:y:1131:GLN:NE2	2.51	0.41
1:y:1753:TYR:CD1	1:y:1841:ARG:HB2	2.53	0.41
1:Y:423:ARG:NH1	1:Y:1133:ALA:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:439:ASN:HB3	1:Y:442:CYS:SG	2.60	0.41
1:Y:957:ARG:HB3	1:Y:964:GLN:O	2.20	0.41
1:y:752:ALA:O	1:y:757:GLN:NE2	2.53	0.41
1:y:903:LYS:NZ	2:i:11:DT:OP2	2.49	0.41
1:y:1000:LEU:HD22	1:y:1008:PRO:HB3	2.03	0.41
1:y:1344:LYS:O	1:y:1344:LYS:NZ	2.41	0.41
1:y:1521:HIS:ND1	1:y:1538:PRO:HD3	2.35	0.41
1:Y:130:LEU:HD13	1:Y:130:LEU:HA	1.93	0.41
1:Y:837:PRO:O	1:Y:841:LYS:HG3	2.21	0.41
1:Y:1554:HIS:HD1	1:Y:1554:HIS:H	1.68	0.41
1:Y:1609:ARG:HA	1:Y:1609:ARG:HD3	1.77	0.41
1:y:56:PRO:HG2	1:y:383:LEU:HD13	2.02	0.41
1:y:1223:PHE:HE2	1:y:1263:MET:HE2	1.85	0.41
1:y:1251:THR:OG1	1:y:1253:THR:OG1	2.30	0.41
1:Y:101:TRP:O	1:Y:105:LEU:HB2	2.21	0.41
1:Y:1289:SER:O	1:Y:1289:SER:OG	2.33	0.41
1:y:1041:LEU:HD11	1:y:1061:ASP:HB2	2.03	0.41
1:y:1074:GLU:OE1	1:y:1074:GLU:N	2.53	0.41
1:y:1531:ARG:HB3	1:y:1545:LEU:HD21	2.02	0.41
1:Y:595:LYS:HA	1:Y:595:LYS:HD2	1.82	0.41
1:Y:731:ILE:HG12	1:y:735:MET:HE3	2.01	0.41
1:Y:903:LYS:HD2	1:Y:904:ARG:HB2	2.02	0.41
1:Y:909:PRO:HG2	1:Y:945:MET:HE1	2.02	0.41
1:Y:1576:HIS:ND1	1:Y:1579:LEU:HG	2.36	0.41
1:y:704:LEU:C	1:y:706:ASN:H	2.27	0.41
1:y:934:GLN:HB2	1:y:937:TRP:HD1	1.85	0.41
1:y:1841:ARG:HE	1:y:1844:GLN:HG2	1.86	0.41
1:y:1860:GLU:HG2	1:y:1861:LEU:HG	2.01	0.41
1:Y:137:GLN:O	1:Y:141:ARG:N	2.35	0.41
1:Y:501:LEU:HD13	1:Y:501:LEU:HA	1.93	0.41
1:Y:1277:LEU:HA	1:Y:1280:ASN:ND2	2.34	0.41
1:Y:1699:TYR:HB3	1:Y:1702:ARG:HH11	1.86	0.41
1:Y:1743:ARG:HD3	1:Y:1746:GLN:HE21	1.85	0.41
1:y:437:CYS:HA	1:y:473:VAL:HG12	2.03	0.41
1:y:627:THR:O	1:y:631:GLN:N	2.49	0.41
1:y:667:ARG:HD2	1:y:806:GLU:OE1	2.21	0.41
1:y:854:TRP:HE3	1:y:857:LEU:HD21	1.85	0.41
1:y:1207:LEU:HG	1:y:1313:PHE:CE2	2.56	0.41
1:y:1492:TRP:NE1	1:y:1504:ARG:HH21	2.19	0.41
1:Y:1775:PHE:O	1:Y:1778:LEU:HG	2.21	0.41
1:y:498:THR:OG1	1:y:500:TRP:NE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:733:GLU:H	1:y:733:GLU:HG3	1.69	0.41
1:y:734:PRO:HD2	1:y:735:MET:HE1	2.02	0.41
1:y:978:GLN:HB3	1:y:1015:GLU:OE1	2.21	0.41
1:y:1044:ASN:OD1	1:y:1047:ILE:N	2.53	0.41
1:y:1178:PHE:HE1	1:y:1245:THR:HA	1.86	0.41
1:y:1256:LEU:O	1:y:1259:THR:OG1	2.30	0.41
1:Y:112:LEU:HD12	1:Y:113:VAL:N	2.35	0.41
1:Y:194:GLN:O	1:Y:198:LEU:HG	2.21	0.41
1:Y:239:GLU:HA	1:Y:242:GLN:CD	2.45	0.41
1:Y:342:PRO:HB3	1:Y:363:TYR:CE2	2.55	0.41
1:Y:451:GLN:OE1	1:Y:451:GLN:N	2.53	0.41
1:Y:615:ILE:HG22	1:Y:616:PRO:HD3	2.03	0.41
1:Y:673:GLU:HG2	1:Y:770:GLN:NE2	2.34	0.41
1:Y:960:GLU:OE2	1:y:774:SER:HA	2.20	0.41
1:Y:984:TYR:OH	1:Y:1009:GLU:OE1	2.23	0.41
1:Y:1525:ILE:HD13	1:Y:1532:ALA:HB2	2.02	0.41
1:y:15:LEU:O	1:y:18:ARG:HG2	2.21	0.41
1:y:81:SER:OG	1:y:82:PRO:HD3	2.21	0.41
1:y:168:GLU:HG3	1:y:171:ARG:HE	1.86	0.41
1:y:347:SER:O	1:y:351:LEU:HG	2.21	0.41
1:y:430:THR:HG23	1:y:610:PHE:HE2	1.85	0.41
1:y:862:LEU:HD11	1:y:965:LEU:HD22	2.03	0.41
1:y:876:ASN:HB3	1:y:879:TYR:CG	2.56	0.41
1:y:1632:VAL:HG23	1:y:1650:ILE:HG12	2.02	0.41
1:Y:126:MET:HG3	1:Y:130:LEU:HD23	2.03	0.41
1:Y:447:HIS:HA	1:Y:450:ASN:HD21	1.85	0.41
1:Y:608:PRO:O	1:Y:611:LEU:HG	2.21	0.41
1:Y:759:LYS:H	1:Y:759:LYS:HG2	1.62	0.41
1:Y:895:PRO:HA	1:Y:908:TRP:HB3	2.03	0.41
1:Y:1967:VAL:HG11	1:Y:2021:TRP:HB2	2.02	0.41
1:Y:2014:GLU:HA	1:Y:2020:ALA:HB1	2.02	0.41
1:y:931:GLN:H	1:y:937:TRP:CG	2.38	0.41
1:y:1068:SER:OG	1:y:1069:TRP:N	2.54	0.41
1:y:1462:THR:H	1:y:1558:ARG:NH2	2.18	0.41
1:y:1553:THR:OG1	1:y:1570:LEU:HB3	2.20	0.41
1:y:1676:ARG:HH12	1:y:1714:ASN:N	2.19	0.41
1:Y:117:THR:OG1	1:Y:1134:GLY:HA3	2.21	0.40
1:Y:733:GLU:CA	1:Y:747:MET:HE1	2.46	0.40
1:Y:1233:GLN:H	1:Y:1233:GLN:CD	2.27	0.40
1:Y:1529:CYS:O	1:Y:1557:LEU:HB3	2.21	0.40
1:Y:1903:ASN:HD22	1:Y:2098:ARG:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1976:SER:O	1:Y:1977:LEU:HD23	2.22	0.40
1:y:65:MET:CE	1:y:95:ARG:HG2	2.51	0.40
1:y:654:SER:HB2	1:y:1074:GLU:OE2	2.21	0.40
1:y:1383:PRO:HG3	1:y:1460:PHE:HE2	1.86	0.40
1:Y:1611:LEU:HD12	1:Y:1615:LEU:HD23	2.02	0.40
1:y:270:ARG:HH22	1:y:1198:ARG:NH2	2.18	0.40
1:y:1440:SER:O	1:y:1443:LYS:NZ	2.43	0.40
1:y:1605:GLU:OE2	1:y:1609:ARG:NH2	2.54	0.40
1:y:1790:LEU:HD12	1:y:1820:VAL:HG22	2.03	0.40
1:Y:22:SER:HB3	1:Y:613:GLU:HG3	2.03	0.40
1:Y:677:ILE:HG12	1:Y:1022:ARG:HH21	1.86	0.40
1:Y:989:LEU:HD13	1:Y:989:LEU:HA	1.87	0.40
1:Y:1304:LEU:HD21	1:Y:1308:ARG:HH21	1.86	0.40
1:Y:2041:LEU:O	1:Y:2053:VAL:N	2.37	0.40
1:y:179:PHE:O	1:y:203:GLN:HA	2.21	0.40
1:y:914:ARG:O	1:y:921:LYS:HG3	2.21	0.40
1:y:1219:GLN:HA	1:y:1222:ARG:HD3	2.03	0.40
1:y:1421:TRP:HE1	1:y:1430:ALA:HB3	1.86	0.40
1:Y:1217:GLU:HA	1:Y:1222:ARG:HH21	1.86	0.40
1:Y:1279:GLU:O	1:Y:1282:GLU:HG3	2.21	0.40
1:Y:1927:HIS:HD2	1:Y:1930:TRP:H	1.70	0.40
1:y:689:CYS:HA	1:y:692:LEU:HD12	2.03	0.40
1:y:736:VAL:O	1:y:739:LEU:HB2	2.21	0.40
1:y:1114:MET:HE2	1:y:1114:MET:HA	2.02	0.40
1:y:1211:TRP:CE2	1:y:1219:GLN:HG3	2.55	0.40
1:Y:430:THR:HG22	1:Y:1150:CYS:O	2.22	0.40
1:Y:2016:TYR:CE2	1:Y:2080:VAL:HG23	2.56	0.40
1:y:130:LEU:HA	1:y:130:LEU:HD23	1.82	0.40
1:y:208:GLU:HA	1:y:211:TYR:CD2	2.56	0.40
1:y:347:SER:O	1:y:350:SER:OG	2.32	0.40
1:y:578:GLU:H	3:g:21:DG:P	2.44	0.40
1:y:984:TYR:OH	1:y:1009:GLU:N	2.45	0.40
1:y:1034:ARG:HG3	1:y:1065:LEU:HD21	2.03	0.40
1:y:1335:ASN:O	1:y:1558:ARG:NH2	2.54	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	Y	2041/2108 (97%)	1932 (95%)	108 (5%)	1 (0%)	100	100
1	y	1827/2108 (87%)	1766 (97%)	61 (3%)	0	100	100
All	All	3868/4216 (92%)	3698 (96%)	169 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	343	THR

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	Y	1747/1795 (97%)	1719 (98%)	28 (2%)	55	69
1	y	1564/1795 (87%)	1537 (98%)	27 (2%)	53	68
All	All	3311/3590 (92%)	3256 (98%)	55 (2%)	52	68

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	27	LEU
1	Y	129	VAL
1	Y	234	ASP
1	Y	257	ILE
1	Y	287	ILE

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Mol	Chain	Res	Type
1	Y	822	LEU
1	Y	833	VAL
1	Y	899	ASN
1	Y	914	ARG
1	Y	915	HIS
1	Y	955	CYS
1	Y	990	ASP
1	Y	1122	VAL
1	Y	1213	PHE
1	Y	1482	ASP
1	Y	1565	GLN
1	Y	1572	HIS
1	Y	1590	VAL
1	Y	1625	ILE
1	Y	1679	LEU
1	Y	1695	ASP
1	Y	1735	VAL
1	Y	1737	THR
1	Y	1891	LEU
1	Y	1903	ASN
1	Y	1919	PHE
1	Y	2016	TYR
1	Y	2076	VAL
1	y	52	LEU
1	y	224	MET
1	y	234	ASP
1	y	319	ASP
1	y	346	THR
1	y	424	MET
1	y	456	PHE
1	y	632	LEU
1	y	669	LEU
1	y	684	LEU
1	y	771	LEU
1	y	775	VAL
1	y	831	ASP
1	y	872	VAL
1	y	941	VAL
1	y	1041	LEU
1	y	1055	LEU
1	y	1098	VAL
1	y	1101	CYS

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Mol	Chain	Res	Type
1	y	1111	ILE
1	y	1120	ASN
1	y	1148	THR
1	y	1251	THR
1	y	1388	VAL
1	y	1581	LEU
1	y	1728	TYR
1	y	1735	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	4	GLN
1	Y	7	HIS
1	Y	14	GLN
1	Y	26	GLN
1	Y	197	GLN
1	Y	286	GLN
1	Y	636	ASN
1	Y	753	ASN
1	Y	838	GLN
1	Y	1083	GLN
1	Y	1185	GLN
1	Y	1230	GLN
1	Y	1280	ASN
1	Y	1409	GLN
1	Y	1448	GLN
1	Y	1467	GLN
1	Y	1521	HIS
1	Y	1535	GLN
1	Y	1568	ASN
1	Y	1689	HIS
1	Y	1749	ASN
1	Y	1764	GLN
1	Y	1819	GLN
1	Y	1932	GLN
1	y	14	GLN
1	y	41	GLN
1	y	48	GLN
1	y	97	GLN
1	y	136	GLN
1	y	148	GLN

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Mol	Chain	Res	Type
1	y	286	GLN
1	y	404	GLN
1	y	439	ASN
1	y	444	HIS
1	y	450	ASN
1	y	751	GLN
1	y	765	GLN
1	y	813	ASN
1	y	838	GLN
1	y	1075	HIS
1	y	1120	ASN
1	y	1229	HIS
1	y	1641	ASN
1	y	1727	GLN
1	y	1749	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\|>2$
4	AGS	Y	2201	-	29,33,33	0.47	1 (3%)	39,52,52	0.68	1 (2%)

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
4	AGS	Y	2201	-	-	10/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	2201	AGS	PG-S1G	2.15	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	2201	AGS	PA-O3A-PB	-3.52	120.74	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	2201	AGS	C5'-O5'-PA-O1A
4	Y	2201	AGS	C2'-C1'-N9-C8
4	Y	2201	AGS	C5'-O5'-PA-O3A
4	Y	2201	AGS	C5'-O5'-PA-O2A
4	Y	2201	AGS	O4'-C4'-C5'-O5'
4	Y	2201	AGS	C2'-C1'-N9-C4
4	Y	2201	AGS	O4'-C1'-N9-C8
4	Y	2201	AGS	PG-O3B-PB-O2B
4	Y	2201	AGS	C4'-C5'-O5'-PA
4	Y	2201	AGS	PG-O3B-PB-O3A

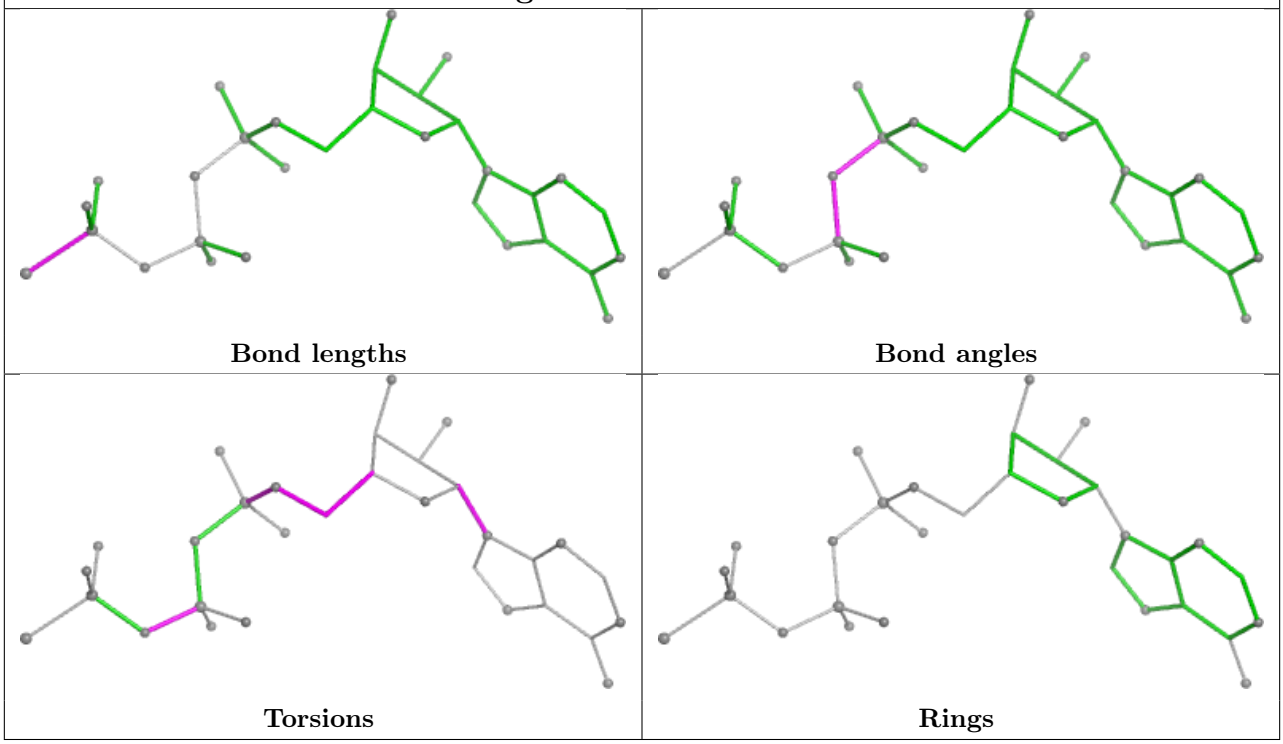
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	2201	AGS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AGS Y 2201



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.

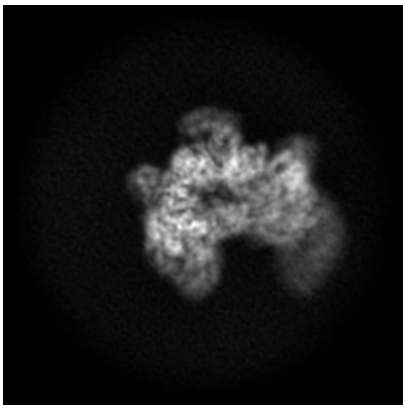
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56256. These allow visual inspection of the internal detail of the map and identification of artifacts.

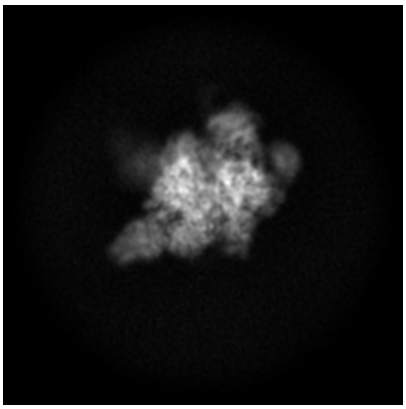
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

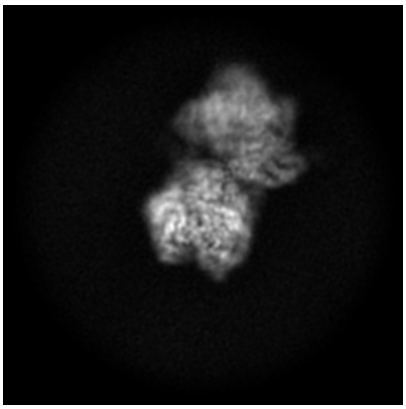
6.1.1 Primary map



X

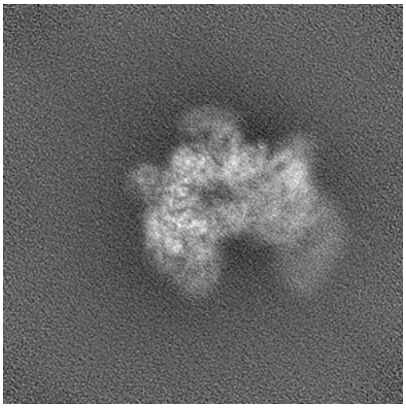


Y

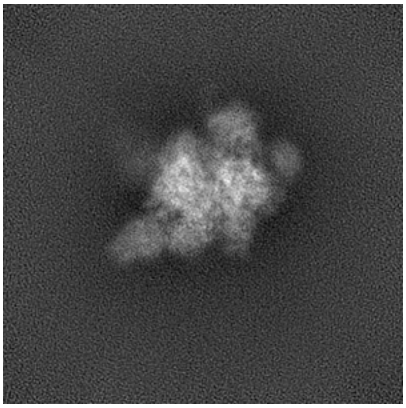


Z

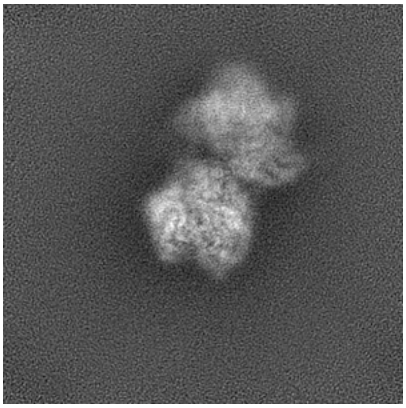
6.1.2 Raw map



X



Y

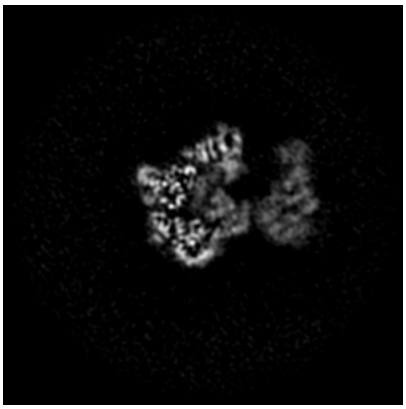


Z

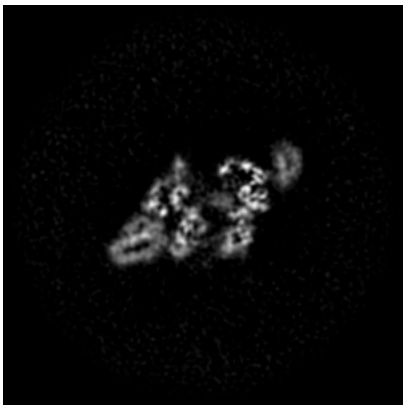
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

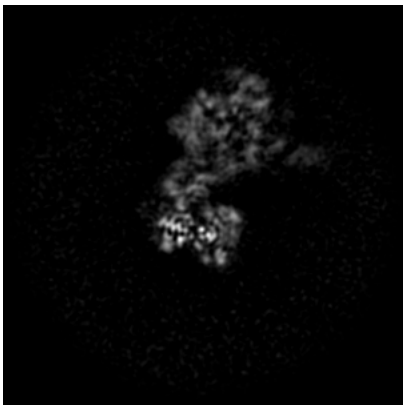
6.2.1 Primary map



X Index: 144

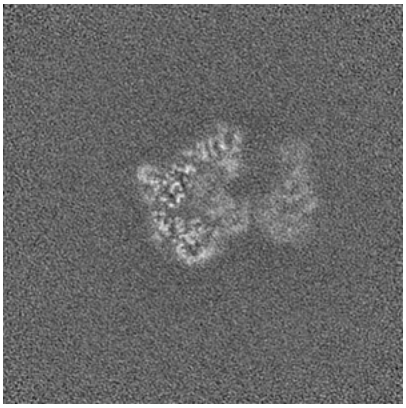


Y Index: 144

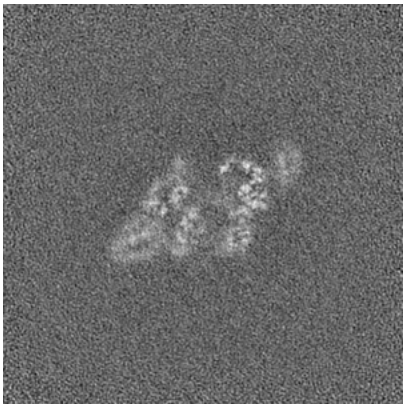


Z Index: 144

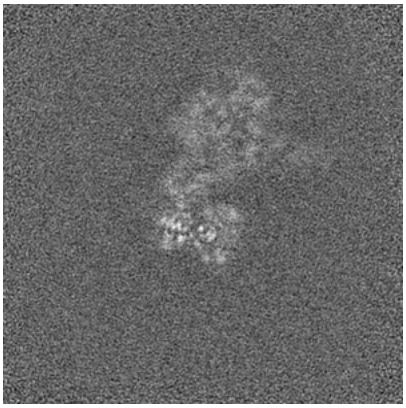
6.2.2 Raw map



X Index: 144



Y Index: 144

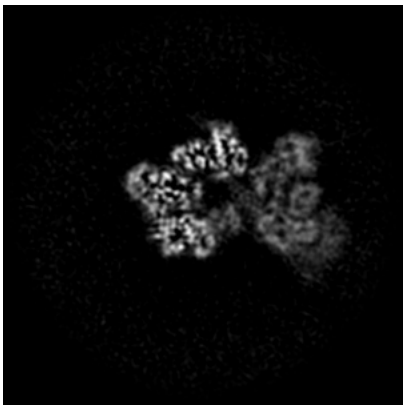


Z Index: 144

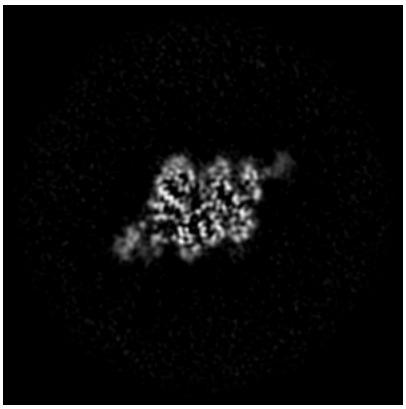
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

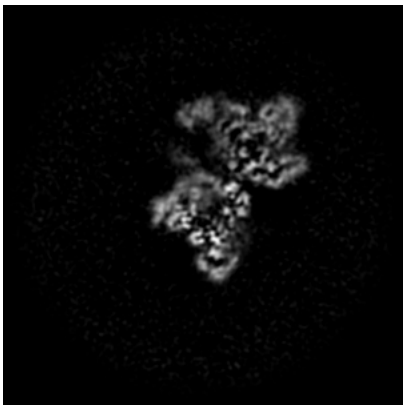
6.3.1 Primary map



X Index: 154

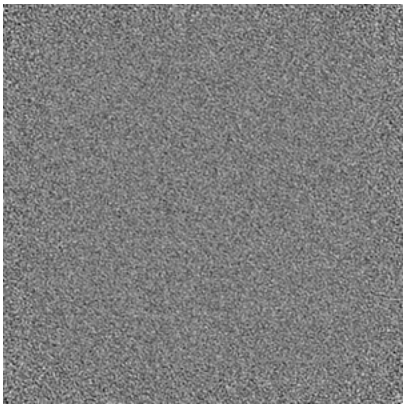


Y Index: 127

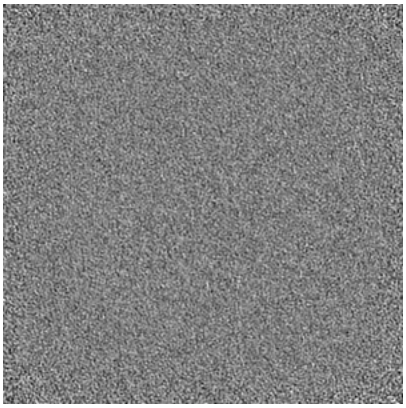


Z Index: 164

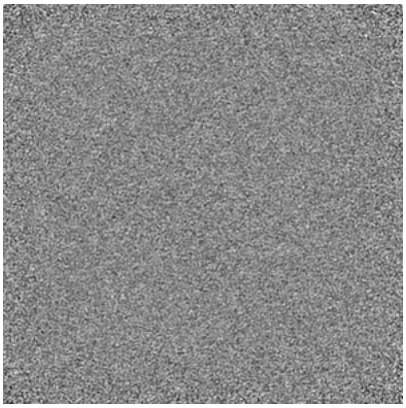
6.3.2 Raw map



X Index: 0



Y Index: 0

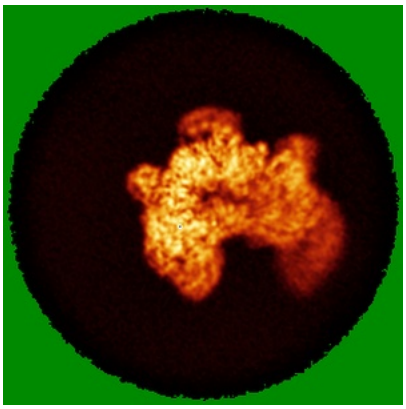


Z Index: 287

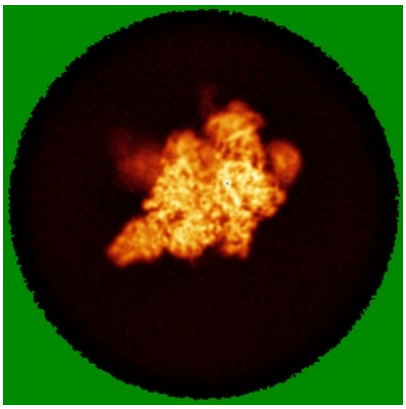
The images above show the largest variance slices of the map in three orthogonal directions.

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

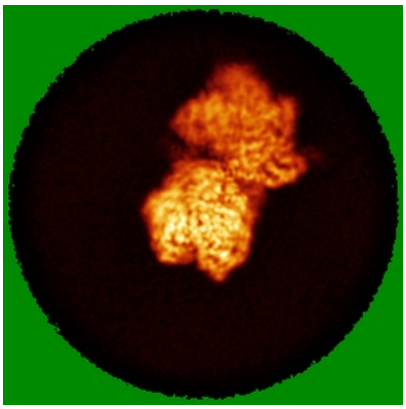
6.4.1 Primary map



X

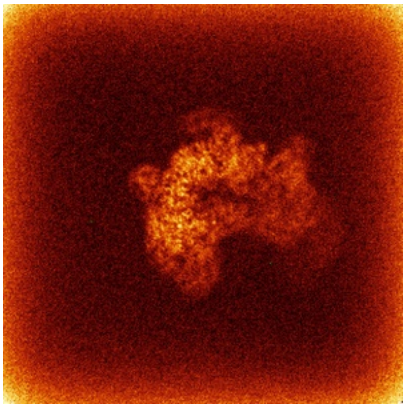


Y

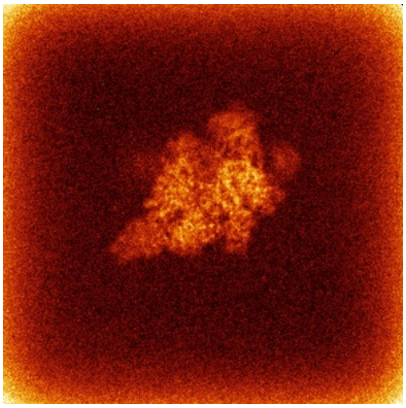


Z

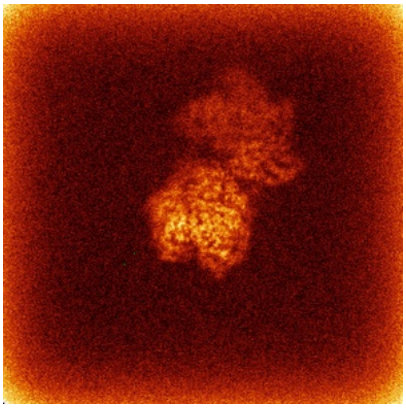
6.4.2 Raw map



X



Y

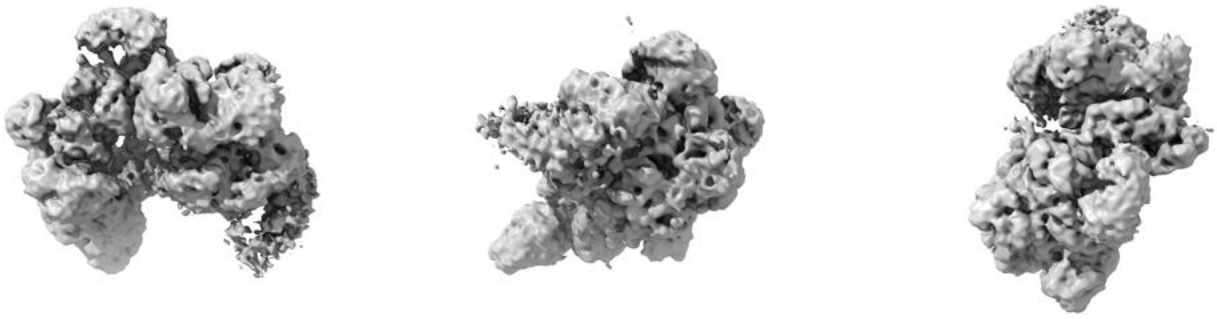


Z

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

6.5 Orthogonal surface views (i)

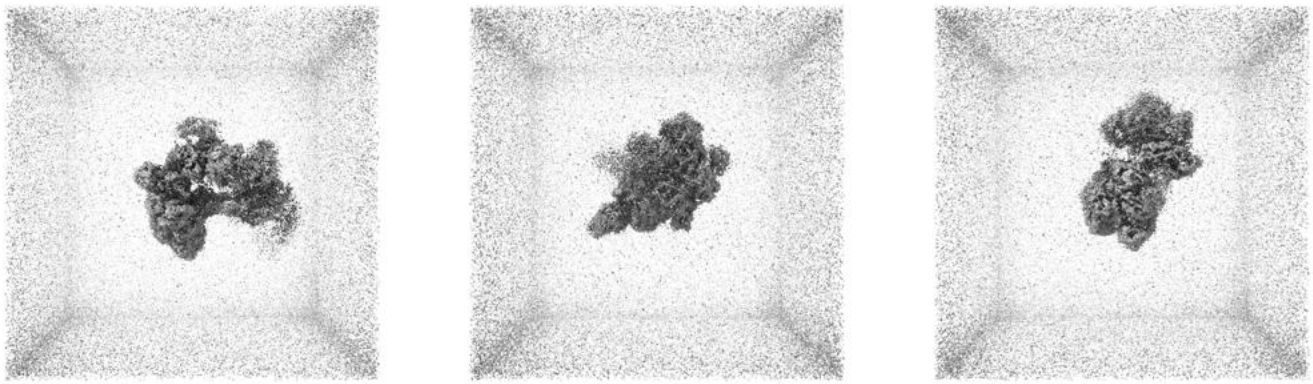
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

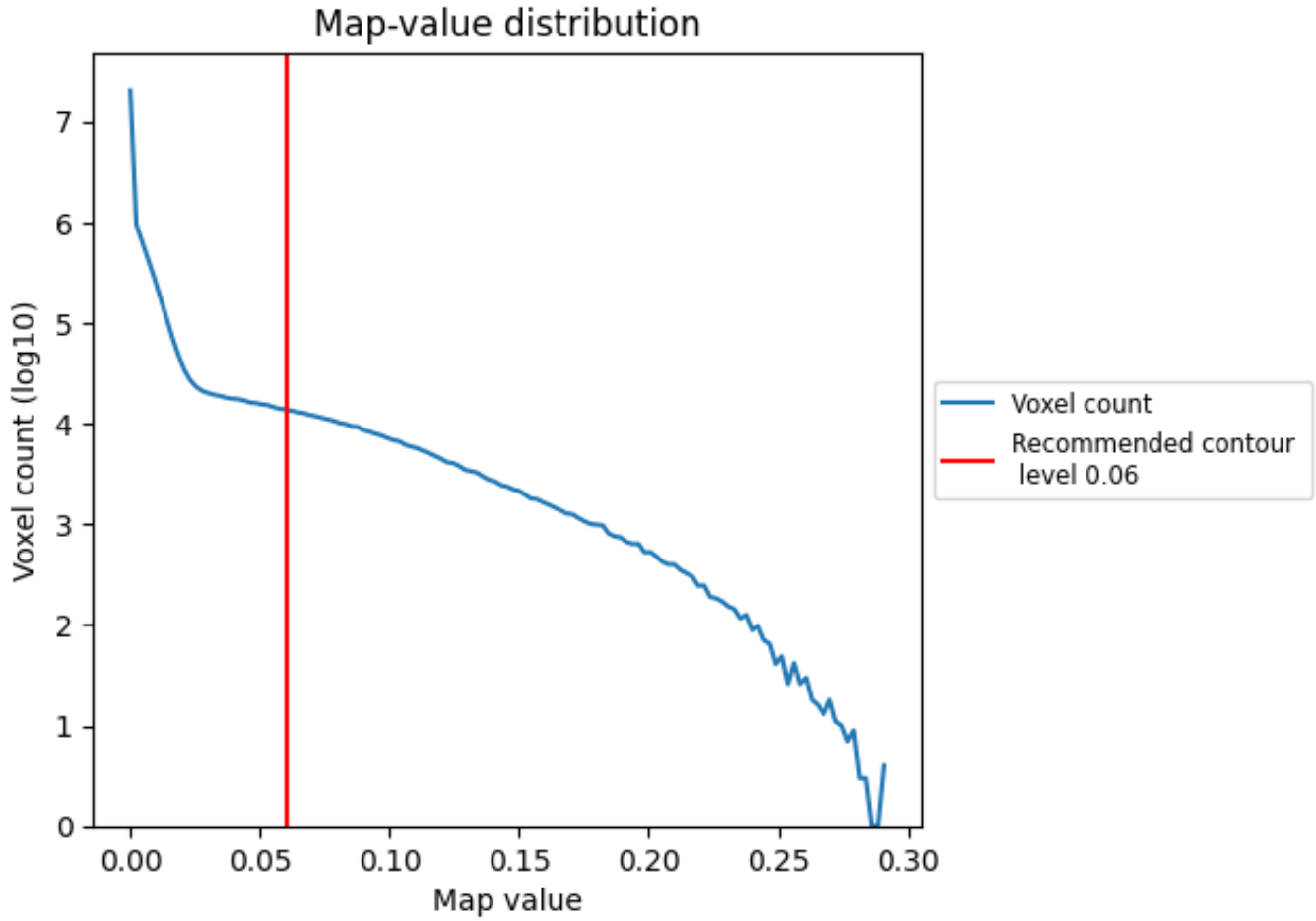
6.6 Mask visualisation (i)

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

7 Map analysis

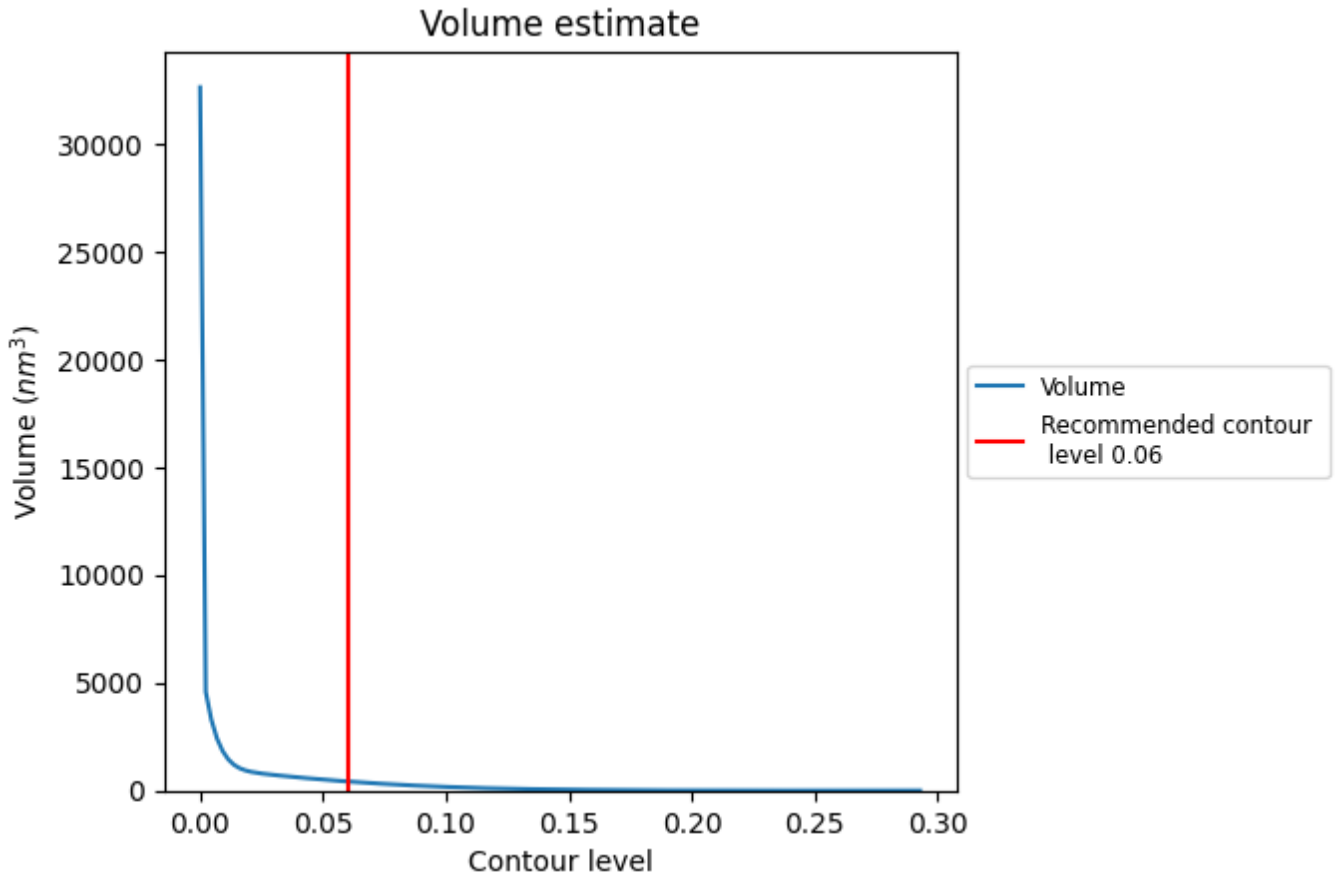
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

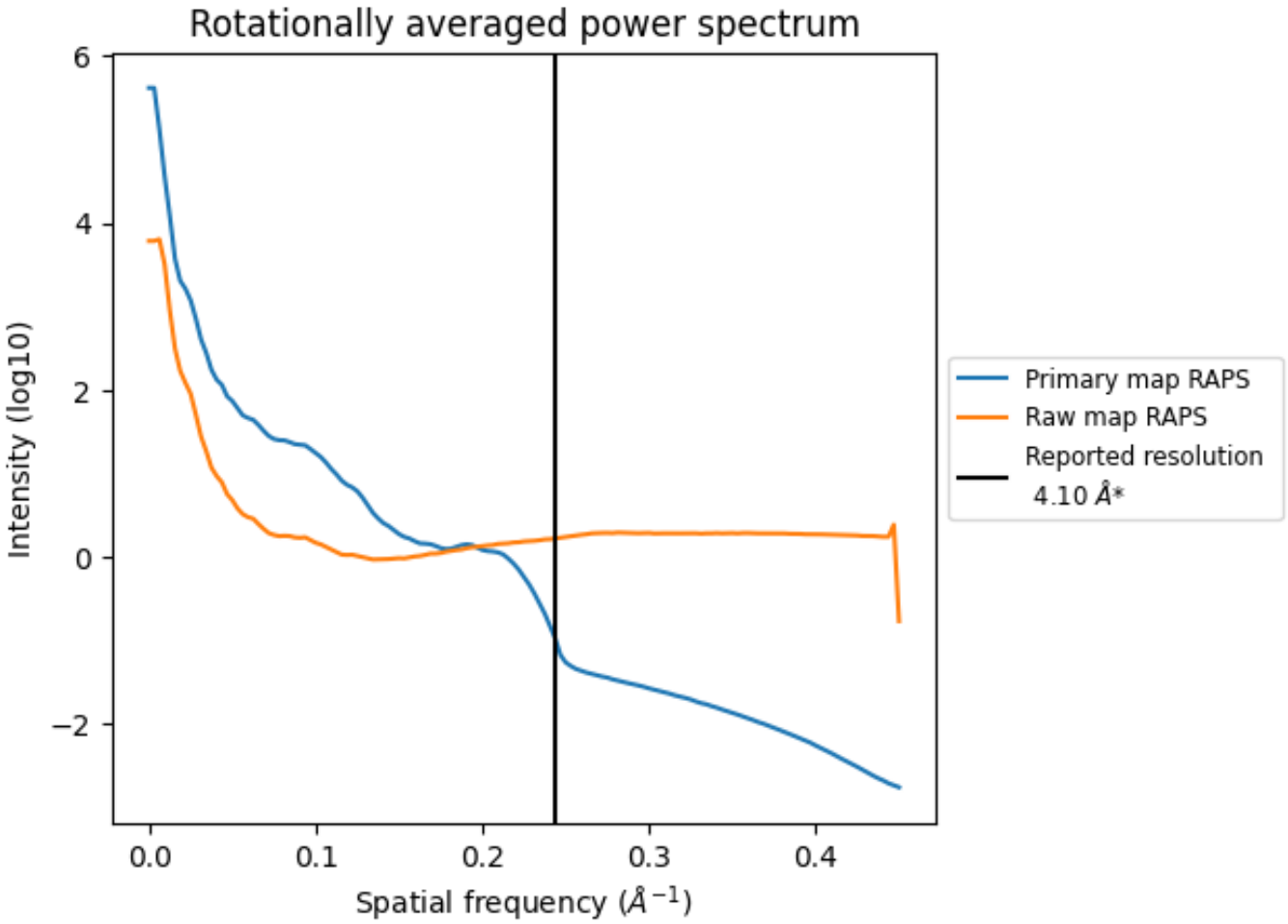
7.2 Volume estimate



The volume at the recommended contour level is 421 nm^3; this corresponds to an approximate mass of 381 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)

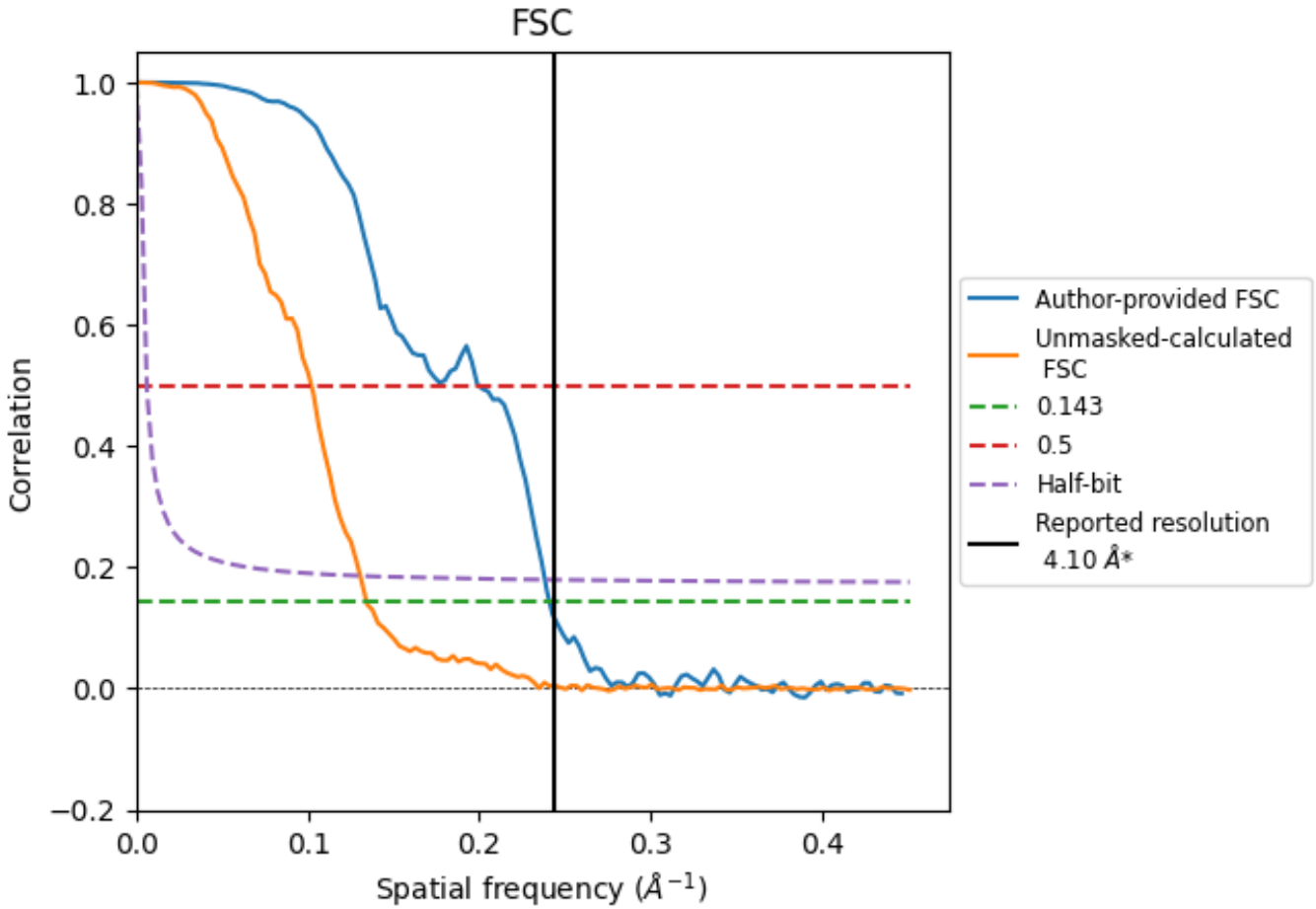


*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

8.2 Resolution estimates (i)

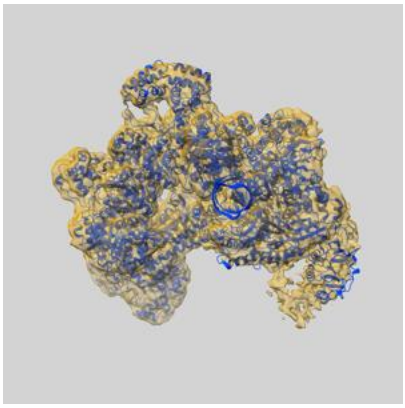
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.15	5.01	4.20
Unmasked-calculated*	7.45	9.79	7.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.45 differs from the reported value 4.1 by more than 10 %

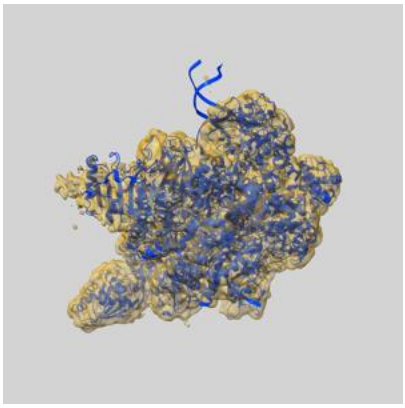
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56256 and PDB model 9TUC. Per-residue inclusion information can be found in section 3 on page 6.

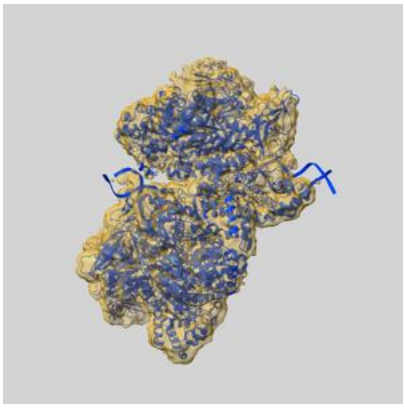
9.1 Map-model overlay



X



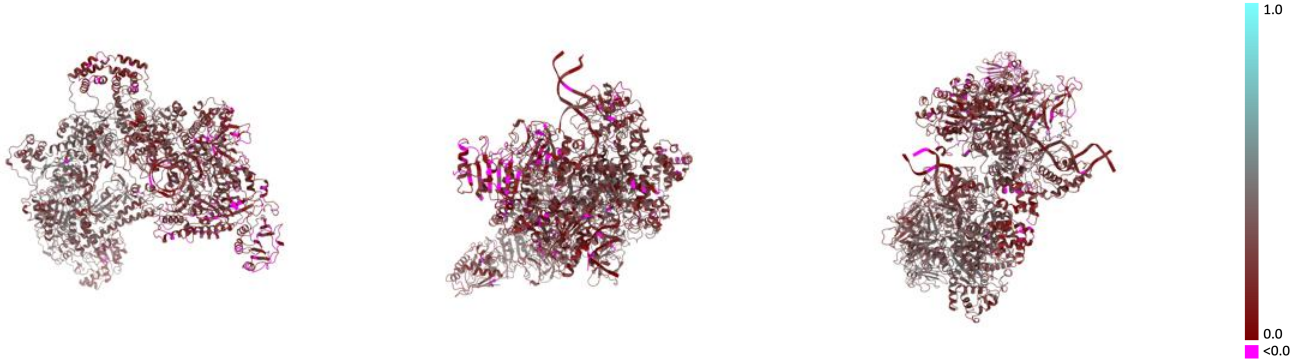
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

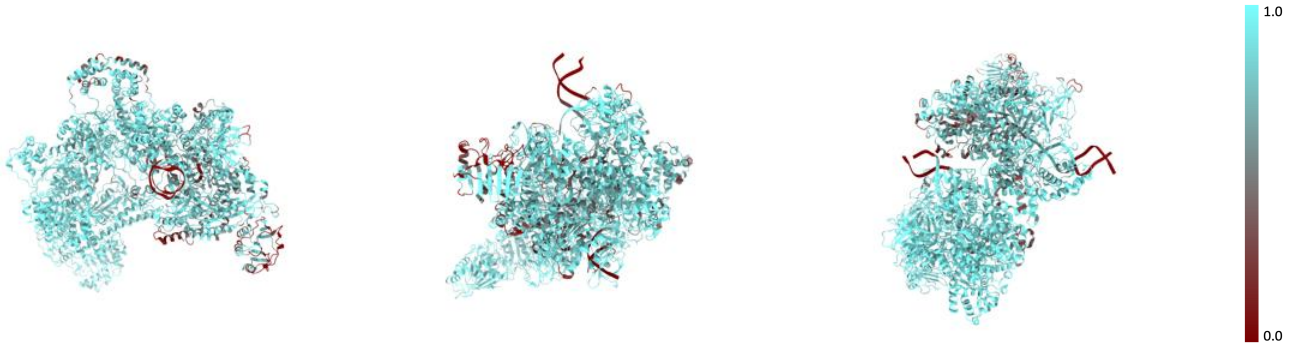
9.2 Q-score mapped to coordinate model



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.

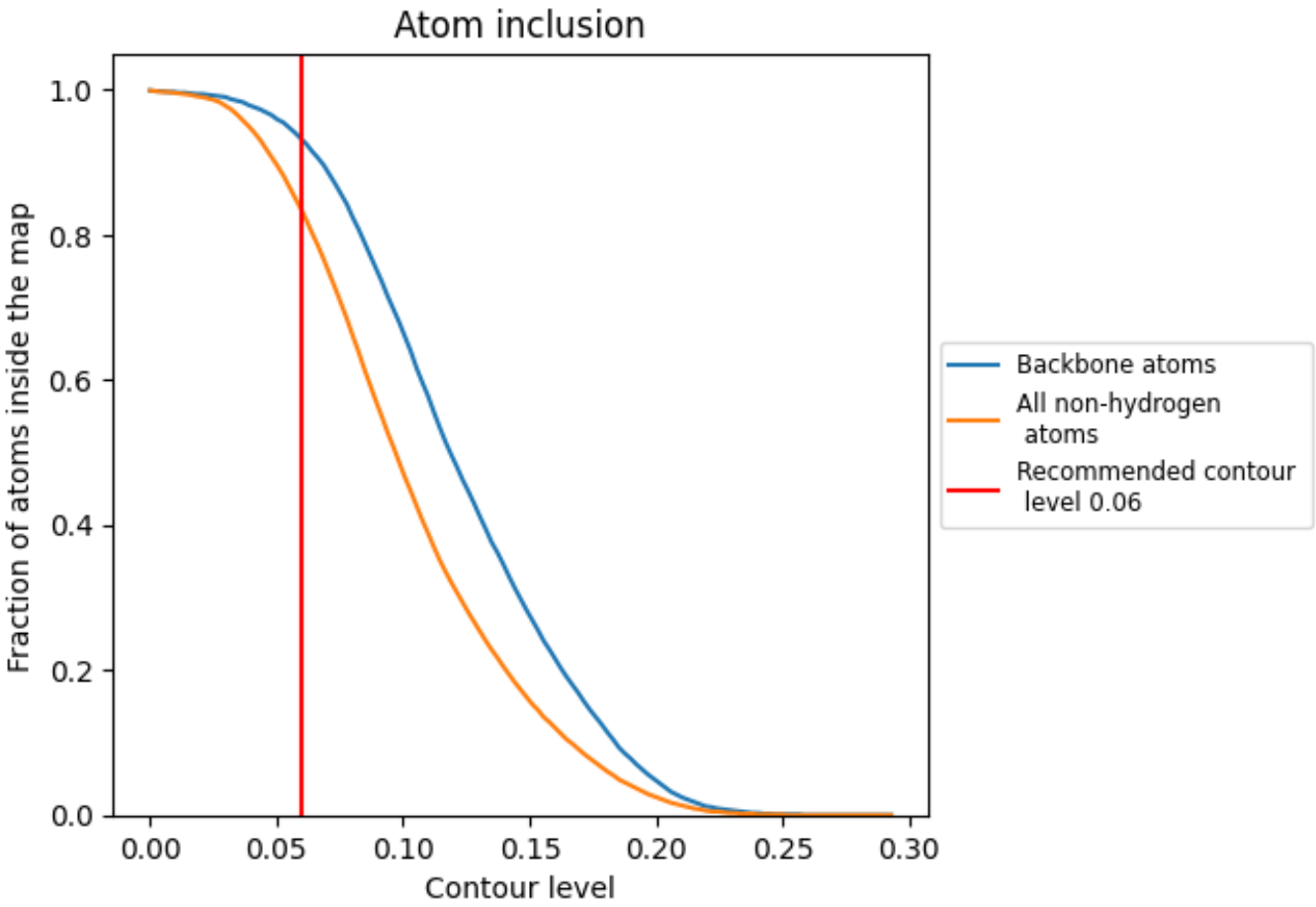
9.3 Atom inclusion mapped to coordinate model



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.2590
G	0.5540	0.1140
I	0.5690	0.1540
Y	0.9270	0.3110
g	0.4130	0.1840
i	0.4770	0.1950
y	0.7620	0.2100

