Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 01:01 PM JST

PDB ID	:	6ACK
EMDB ID	:	EMD-9594
Title	:	Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-bound conformation 3
Authors	:	Gui, M.; Song, W.
Deposited on	:	2018-07-26
Resolution	:	4.50 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:

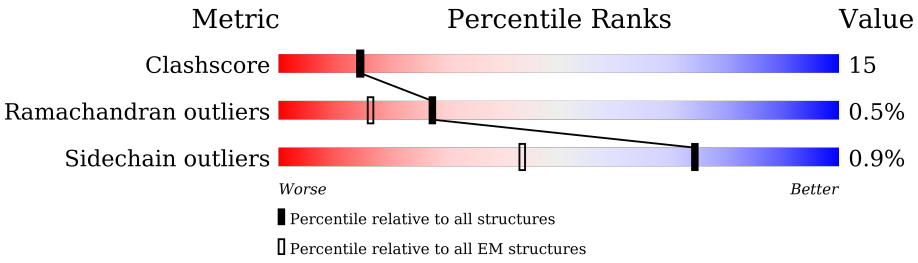
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1203	39% 54% 33% · 11%
1	B	1203	37% 57% 30% · 11%
1	C	1203	41% 55% 31% · 12%
2	D	603	99% 72% 27% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29715 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	B	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	C	1057	Total	C	N	O	S	0	0
			8241	5264	1364	1568	45		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 6 discrepancies between the modelled and reference sequences:

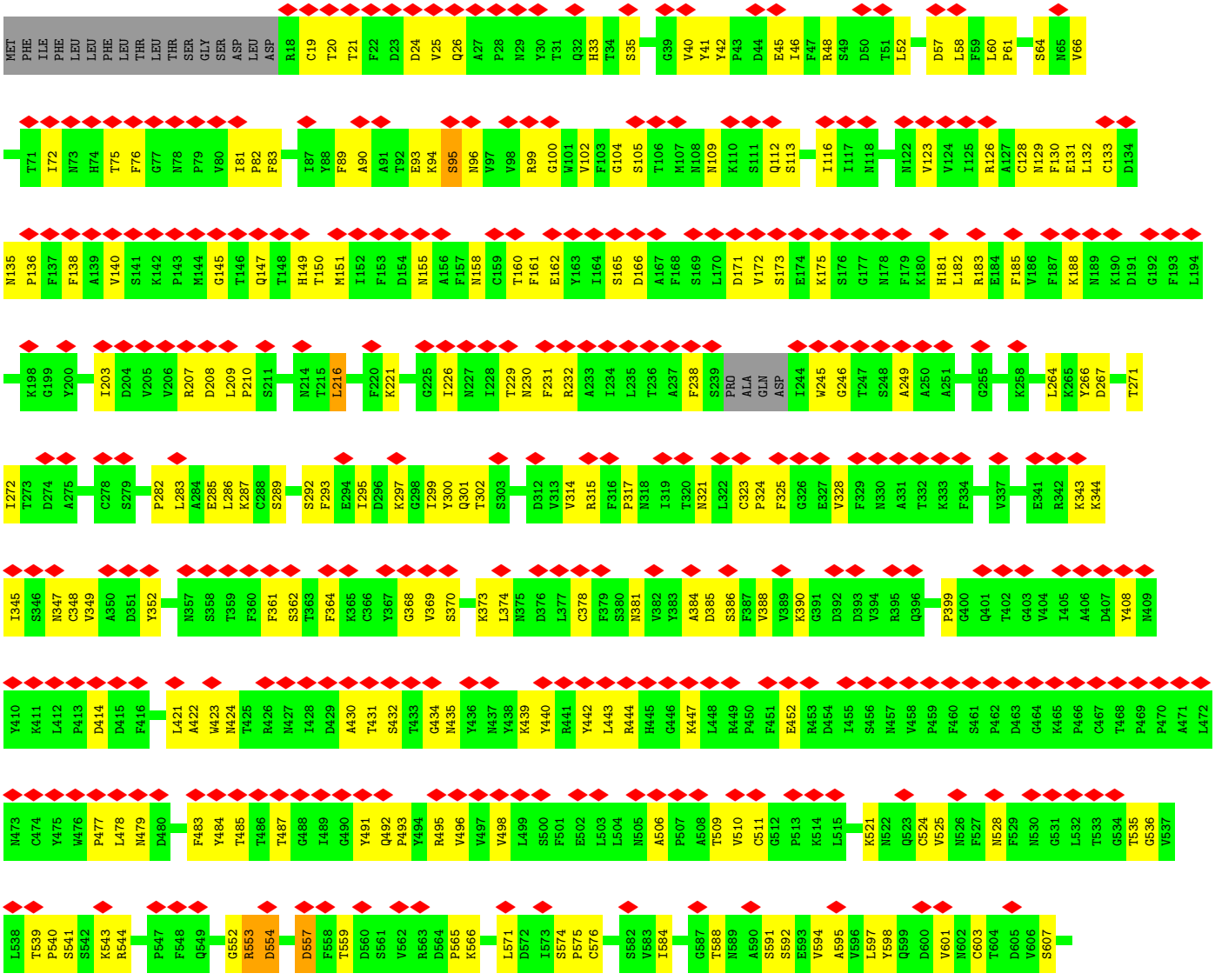
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1

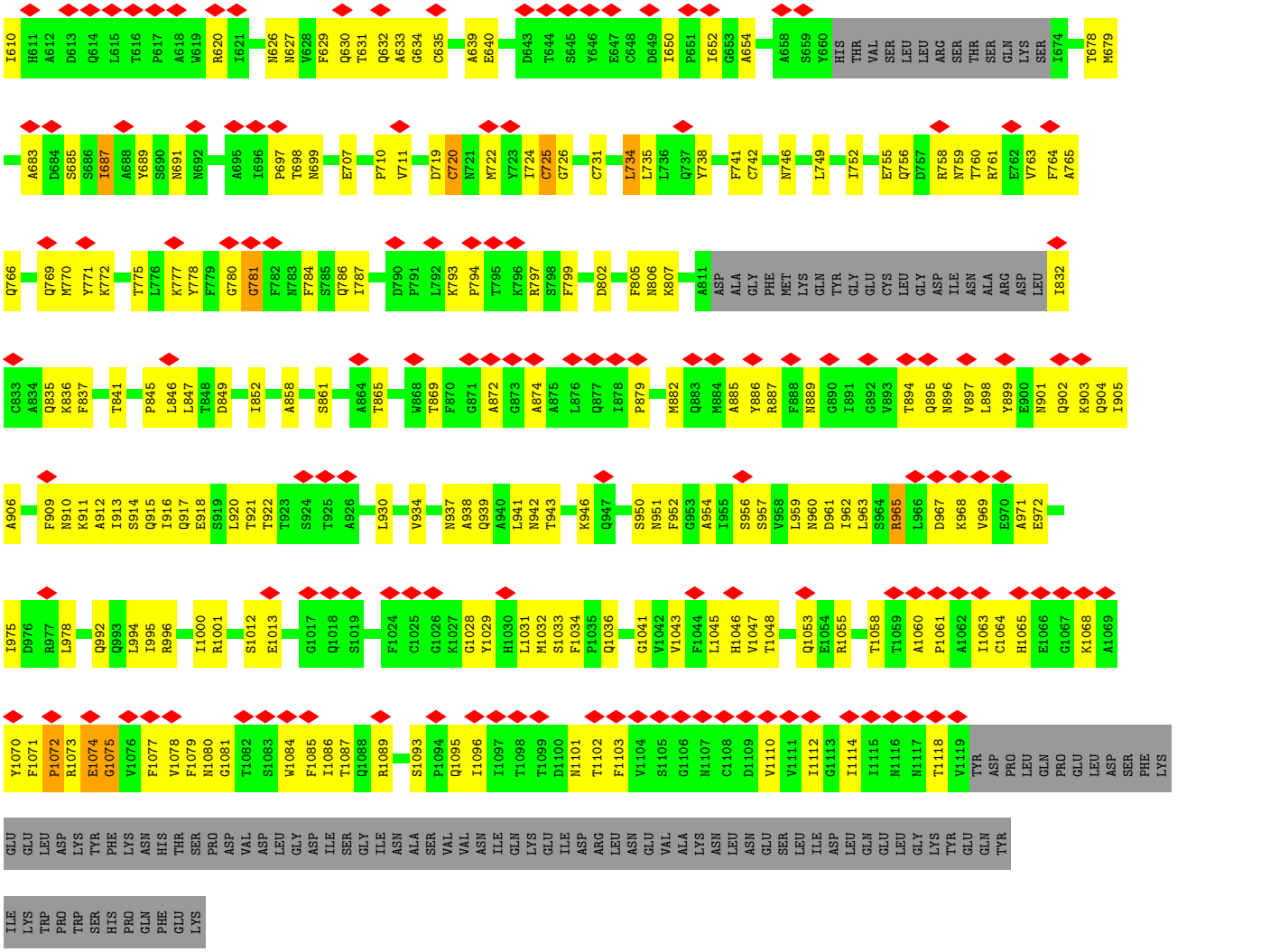
3 Residue-property plots (i)

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: Spike glycoprotein

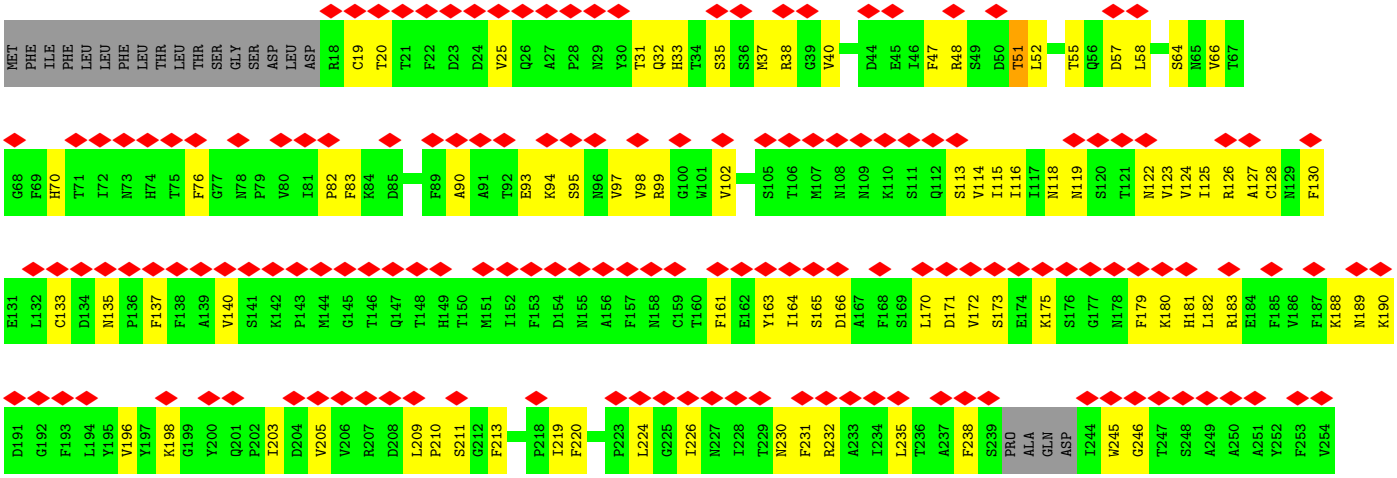
Chain A:

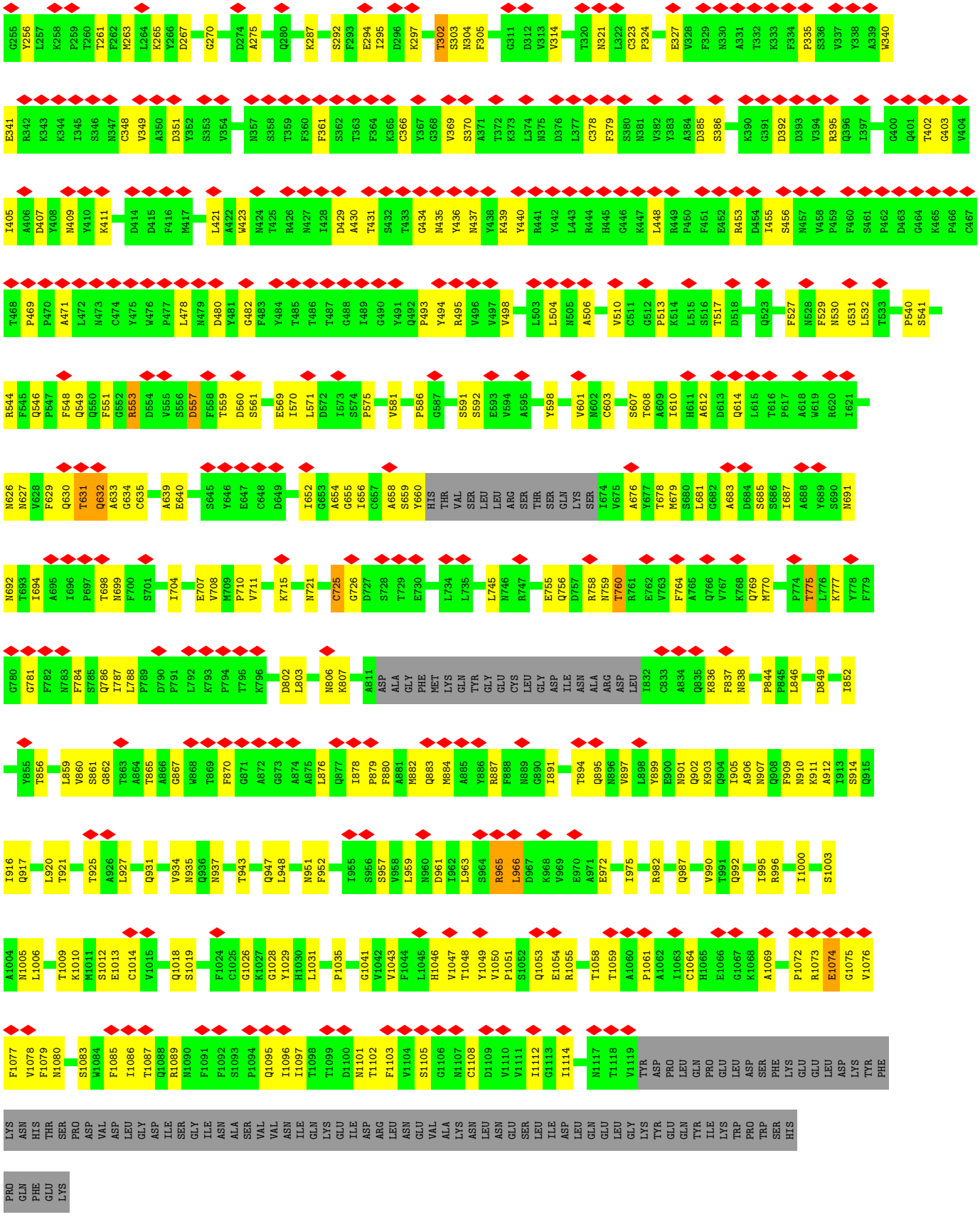




• Molecule 1: Spike glycoprotein

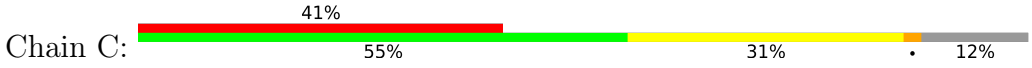
Chain B:

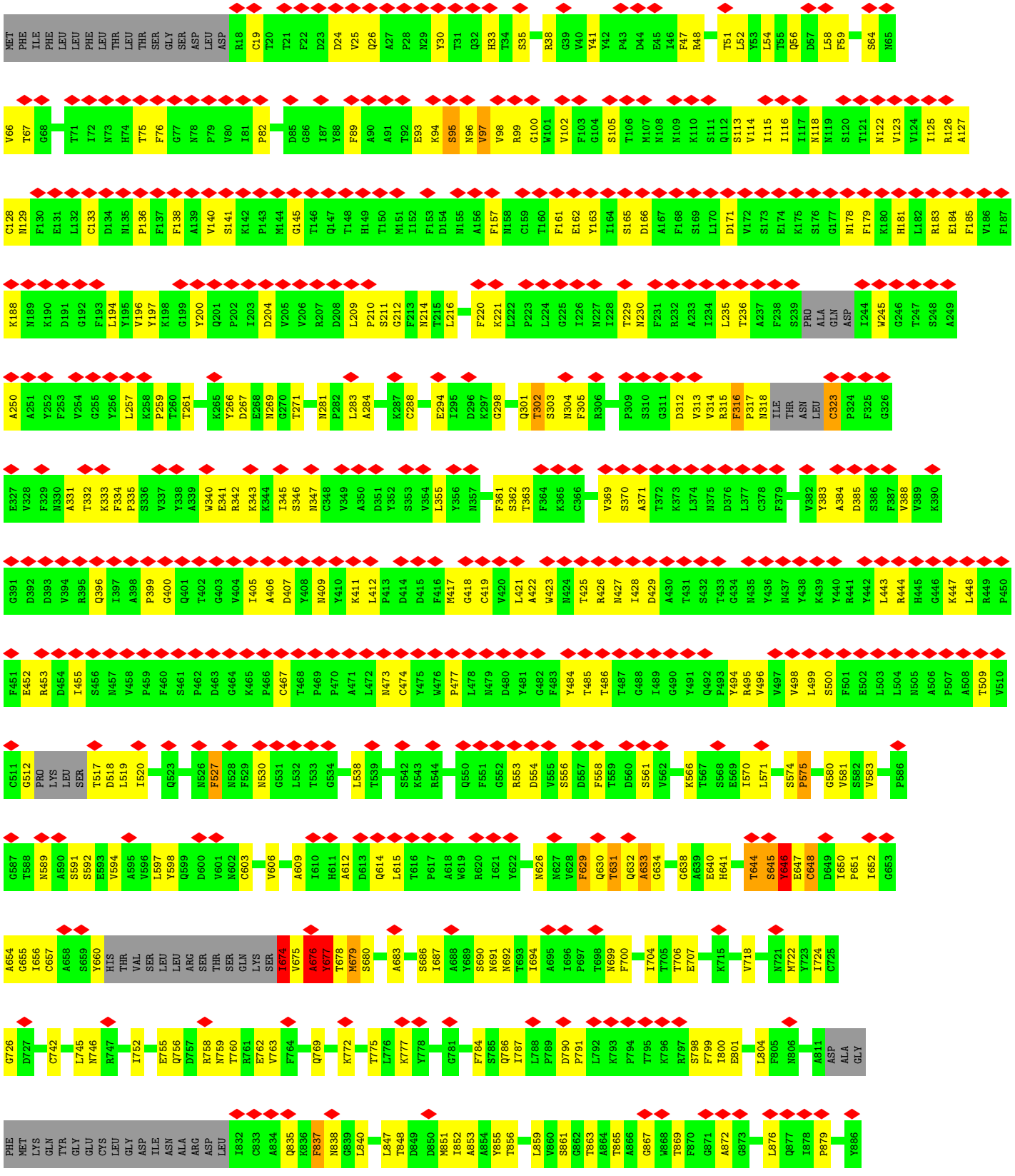


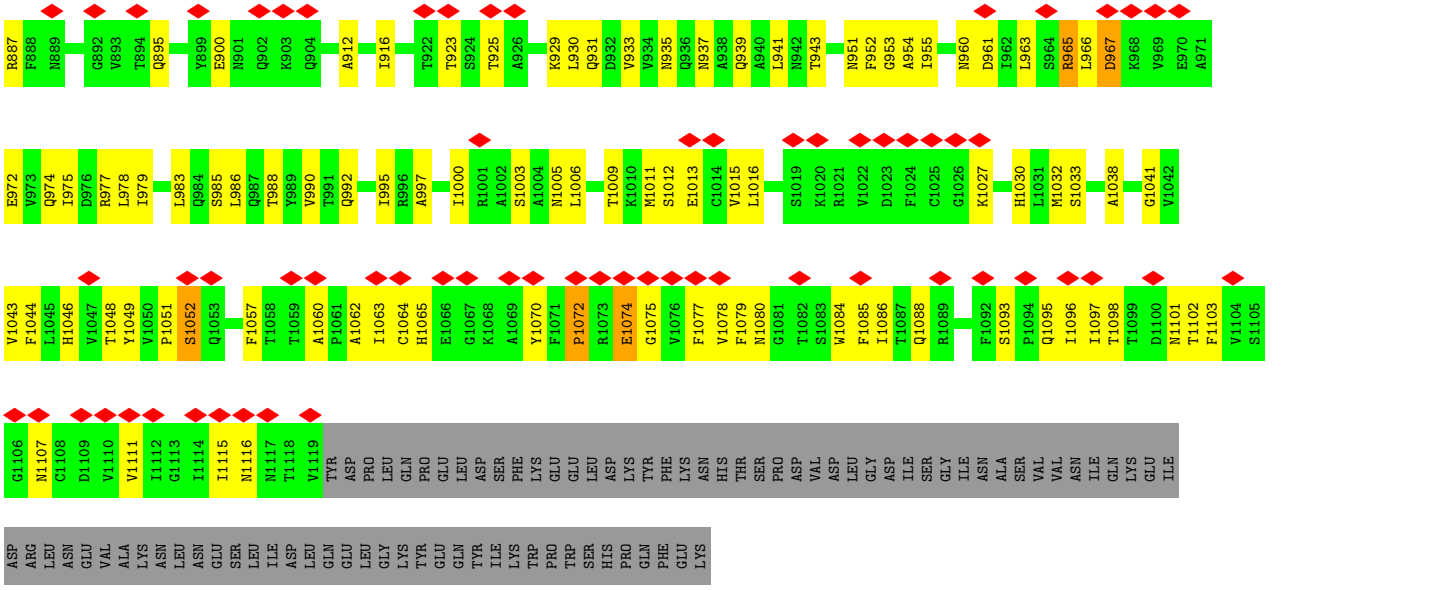


• Molecule 1: Spike glycoprotein

Chain C:

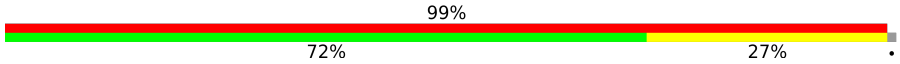

41%
55%
31%
12%

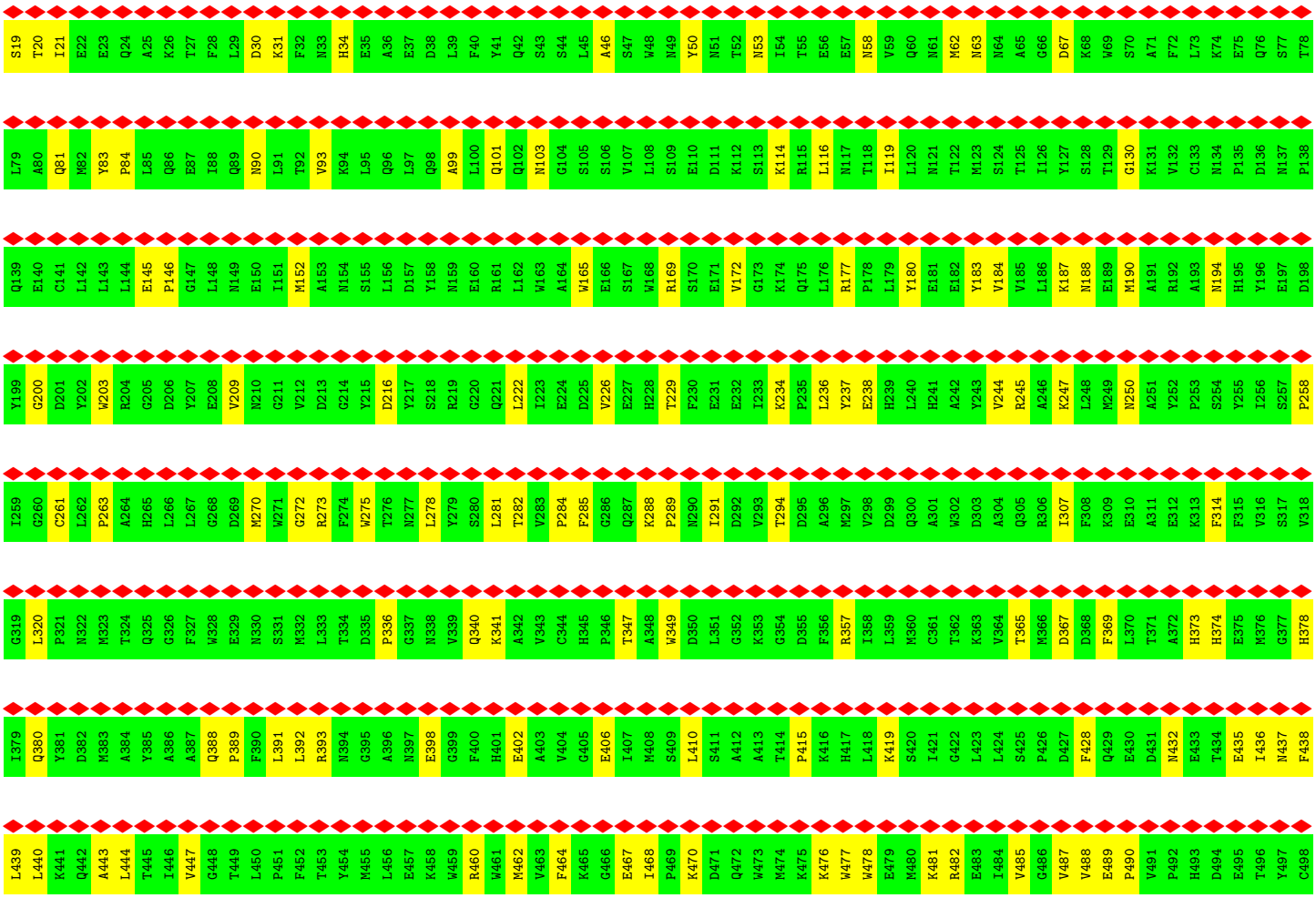

MET PHE ILE PHE LEU LEU PHE LEU THR LEU THR SER GLY SER ASP LEU ASP R18 C19 T20 T21 F22 D23 D24 V25 Q26 A27 P28 N29 Y30 T31 Q32 H33 T34 S35 R38 G39 V40 Y41 Y42 P43 D44 E45 I46 F47 R48 T51 L52 Y53 L54 T55 Q56 D57 L58 F59 S64 N65
V66 T67 G68 T71 I72 N73 H74 T75 F76 G77 N78 P79 V80 I81 P82 D85 G86 I87 Y88 F89 A90 A91 T92 E93 K94 S95 N96 V97 V98 R99 G100 W101 V102 F103 G104 S105 T106 M107 N108 N109 K110 S111 Q112 S113 V114 I115 I116 I117 N118 N119 S120 T121 N122 V123 V124 I125 R126 A127
C128 N129 F130 E131 L132 C133 D134 N135 P136 F137 F138 A139 V140 S141 K142 P143 M144 G145 T146 Q147 T148 H149 T150 M151 I152 F153 D154 N155 A156 F157 N158 C159 T160 F161 E162 Y163 I164 S165 D166 A167 F168 S169 L170 D171 V172 S173 E174 K175 S176 G177 N178 F179 K180 H181 L182 R183 E184 F185 V186 F187
K188 N189 K190 D191 G192 F193 L194 Y195 V196 Y197 K198 G199 Y200 Q201 P202 I203 D204 V205 V206 R207 D208 L209 P210 S211 G212 F213 N214 T215 L216 F220 K221 L222 P223 L224 G225 I226 N227 I228 T229 N230 F231 R232 A233 I234 L235 T236 A237 F238 S239 PRO ALA GLN ASP I244 W245 G246 T247 S248 A249
A250 A251 Y252 F253 V254 G255 Y256 L257 K258 P259 T260 T261 K265 Y266 D267 E268 N269 G270 T271 N281 P282 L283 A284 K287 C288 E294 I295 D296 K297 G298 Q301 T302 S303 N304 F305 R306 P309 S310 G311 D312 V313 V314 R315 F316 P317 N318 ILE THR ASN LEU C323 P324 F325 G326
E327 V328 F329 N330 A331 T332 K333 F334 P335 S336 V337 Y338 A339 W340 E341 R342 K343 K344 I345 S346 N347 C348 V349 A350 D351 Y352 S353 V354 L355 Y356 N357 F361 S362 T363 F364 K365 C366 V369 S370 A371 T372 K373 L374 N375 D376 L377 C378 F379 V382 Y383 A384 D385 S386 F387 V388 V389 K390
G391 D392 D393 V394 R395 Q396 I397 A398 P399 G400 Q401 T402 G403 V404 I405 A406 D407 Y408 N409 Y410 K411 L412 P413 D414 D415 F416 M417 G418 C419 V420 L421 A422 W423 N424 T425 R426 N427 I428 D429 A430 T431 S432 T433 G434 N435 Y436 N437 Y438 K439 Y440 R441 Y442 L443 R444 H445 G446 K447 L448 R449 P450
F451 E452 R453 D454 I455 S456 N457 V458 P459 F460 S461 P462 D463 G464 K465 P466 C467 T468 P469 P470 A471 L472 N473 C474 Y475 W476 P477 L478 N479 D480 Y481 G482 F483 Y484 T485 T486 T487 G488 I489 G490 Y491 Q492 P493 Y494 R495 V496 V497 V498 L499 S500 F501 E502 L503 L504 N505 A506 P507 A508 T509 V510
C511 G512 PRO LYS LEU SER T517 D518 L519 I520 Q523 N526 F527 N528 F529 N530 G531 L532 T533 G534 L538 T539 S542 K543 R544 Q550 F551 G552 R553 D554 V555 S556 D557 F558 T559 D560 S561 V562 K566 T567 S568 E569 I570 L571 S574 P575 G580 V581 S582 V583 P586
G587 T588 N589 A590 S591 S592 E593 V594 A595 V596 L597 Y598 Q599 D600 V601 N602 C603 V606 A609 I610 H611 A612 D613 Q614 L615 T616 P617 A618 W619 R620 I621 Y622 N626 N627 V628 F629 Q630 T631 Q632 A633 G634 G638 A639 E640 H641 T644 S645 Y646 E647 C648 D649 I650 P651 I652 G653
A654 G655 I656 C657 A658 S659 Y660 HIS THR VAL SER LEU LEU LEU ARG SER THR SER GLN LYS SER I674 V675 A676 Y677 T678 M679 S680 A683 S686 I687 A688 Y689 S690 N691 N692 T693 I694 A696 I696 P697 T698 N699 F700 I704 T705 T706 E707 K715 V718 N721 M722 Y723 I724 C725
G726 D727 C742 L745 N746 R747 I752 E755 Q756 D757 R758 N759 T760 R761 E762 V763 F764 Q769 K772 T775 L776 K777 Y778 G781 F784 S785 Q786 I787 L788 P789 D790 P791 L792 K793 P794 T795 K796 R797 S798 F799 I800 E801 L804 F805 N806 A811 ASP ALA GLY
PHE MET LYS GLN TYR GLY GLU CYS LEU GLY ASP ILE ASN ALA ARG ASP LEU I832 C833 A834 Q835 K836 F837 N838 G839 L840 L847 T848 D849 D850 M851 I852 A853 A854 Y855 T856 L859 V860 S861 G862 T863 A864 T865 A866 G867 W868 T869 F870 G871 A872 G873 L876 Q877 I878 P879 Y886

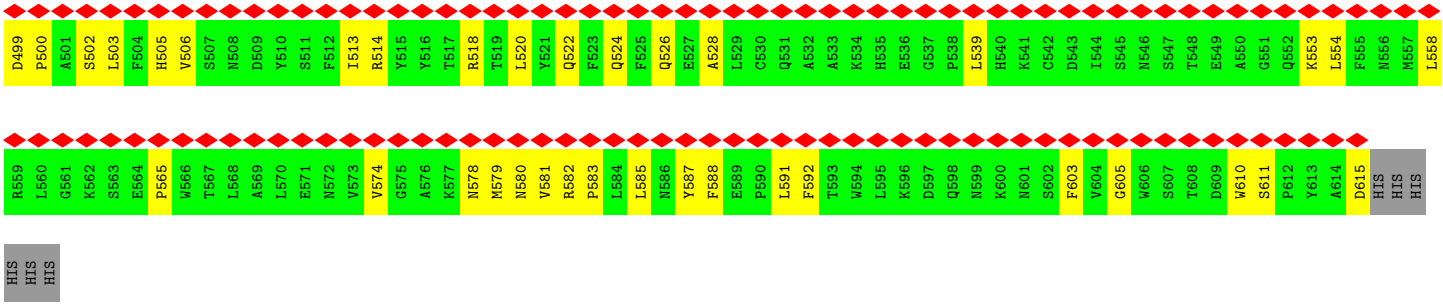


- Molecule 2: Angiotensin-converting enzyme 2

Chain D:






D499 P500 A501 S502 L503 F504 H505 V506 S507 N508 D509 Y510 S511 F512 I513 R514 Y515 Y516 T517 R518 T519 L520 Y521 Q522 F523 Q524 F525 Q526 E527 A528 L529 C530 Q531 A532 A533 K534 H535 E536 G537 P538 L539 H540 K541 C542 D543 I544 S545 N546 S547 T548 E549 A550 G551 Q552 K553 L554 F555 N556 M557 L558
R559 L560 G561 K562 S563 E564 P565 W566 T567 L568 A569 L570 E571 N572 V573 V574 G575 A576 K577 N578 M579 N580 V581 R582 P583 L584 L585 N586 Y587 F588 E589 P590 L591 F592 T593 W594 L595 K596 D597 Q598 N599 K600 N601 S602 F603 V604 G605 W606 S607 T608 D609 W610 S611 P612 Y613 A614 D615 HIS HIS HIS
HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.588	Depositor
Minimum map value	-14.552	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.908	Depositor
Recommended contour level	8	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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	0.54	2/8499 (0.0%)	0.73	5/11568 (0.0%)
1	B	0.53	1/8499 (0.0%)	0.73	2/11568 (0.0%)
1	C	0.59	5/8435 (0.1%)	0.76	7/11477 (0.1%)
2	D	0.34	0/5007	0.58	0/6803
All	All	0.53	8/30440 (0.0%)	0.72	14/41416 (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
1	A	0	13
1	B	0	14
1	C	0	18
All	All	0	45

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	CYS	CB-SG	-9.21	1.66	1.82
1	A	731	CYS	CB-SG	-8.50	1.67	1.82
1	C	677	TYR	CE2-CZ	-8.19	1.27	1.38
1	B	725	CYS	CB-SG	-6.59	1.71	1.82
1	C	676	ALA	C-O	-6.38	1.11	1.23
1	C	677	TYR	CB-CG	-5.41	1.43	1.51
1	C	677	TYR	CD2-CE2	-5.39	1.31	1.39
1	C	677	TYR	CA-CB	-5.28	1.42	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	677	TYR	CB-CG-CD2	-6.45	117.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	674	ILE	CB-CA-C	-6.36	98.89	111.60
1	B	557	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	644	THR	O-C-N	5.97	132.25	122.70
1	C	644	THR	CA-C-N	-5.78	104.49	117.20
1	B	966	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	734	LEU	CA-CB-CG	-5.37	102.96	115.30
1	A	557	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	512	GLY	N-CA-C	5.28	126.31	113.10
1	A	553	ARG	C-N-CA	5.27	134.88	121.70
1	C	648	CYS	CA-CB-SG	-5.19	104.66	114.00
1	A	216	LEU	CA-CB-CG	-5.13	103.51	115.30
1	C	646	TYR	C-N-CA	-5.06	109.06	121.70
1	A	554	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1074	GLU	Peptide
1	A	1075	GLY	Peptide
1	A	506	ALA	Peptide
1	A	629	PHE	Peptide
1	A	632	GLN	Peptide
1	A	633	ALA	Peptide
1	A	726	GLY	Peptide
1	A	781	GLY	Peptide
1	A	836	LYS	Peptide
1	A	845	PRO	Peptide
1	A	865	THR	Peptide
1	A	922	THR	Peptide
1	A	95	SER	Peptide
1	B	1074	GLU	Peptide
1	B	1075	GLY	Peptide
1	B	1077	PHE	Peptide
1	B	506	ALA	Peptide
1	B	51	THR	Peptide
1	B	527	PHE	Peptide
1	B	548	PHE	Peptide
1	B	553	ARG	Peptide
1	B	629	PHE	Peptide
1	B	631	THR	Peptide
1	B	726	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	775	THR	Peptide
1	B	870	PHE	Peptide
1	B	884	MET	Peptide
1	C	1052	SER	Peptide
1	C	1074	GLU	Peptide
1	C	1077	PHE	Peptide
1	C	323	CYS	Peptide
1	C	370	SER	Peptide
1	C	527	PHE	Peptide
1	C	556	SER	Peptide
1	C	574	SER	Peptide
1	C	575	PRO	Peptide
1	C	629	PHE	Peptide
1	C	631	THR	Peptide
1	C	633	ALA	Peptide
1	C	724	ILE	Peptide
1	C	837	PHE	Peptide
1	C	923	THR	Peptide
1	C	95	SER	Peptide
1	C	967	ASP	Peptide
1	C	97	VAL	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	8302	0	8082	286	0
1	B	8302	0	8082	259	0
1	C	8241	0	8009	293	0
2	D	4870	0	4643	99	0
All	All	29715	0	28816	884	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 15.

All (884) 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:C:646:TYR:HB2	1:C:677:TYR:CE2	1.47	1.48
1:C:646:TYR:CB	1:C:677:TYR:CE2	2.02	1.41
1:C:646:TYR:O	1:C:680:SER:OG	1.62	1.15
1:C:646:TYR:HB2	1:C:677:TYR:CD2	1.84	1.11
1:C:646:TYR:CA	1:C:677:TYR:CE2	2.36	1.07
1:C:646:TYR:CA	1:C:677:TYR:HE2	1.68	1.05
1:C:646:TYR:CB	1:C:677:TYR:CZ	2.41	1.03
1:C:418:GLY:HA3	1:C:499:LEU:O	1.60	1.00
1:C:646:TYR:N	1:C:677:TYR:CE2	2.32	0.98
1:B:93:GLU:O	1:B:181:HIS:HB2	1.63	0.98
1:C:100:GLY:HA2	1:C:116:ILE:O	1.63	0.98
1:C:646:TYR:HB2	1:C:677:TYR:CZ	1.99	0.98
1:B:102:VAL:O	1:B:231:PHE:HA	1.66	0.95
1:B:704:ILE:HA	1:B:1046:HIS:O	1.64	0.94
1:A:93:GLU:O	1:A:181:HIS:HB2	1.69	0.93
1:A:100:GLY:HA2	1:A:116:ILE:O	1.70	0.91
1:A:140:VAL:O	1:A:238:PHE:HA	1.71	0.90
2:D:415:PRO:O	2:D:419:LYS:HB2	1.74	0.87
1:C:646:TYR:HB3	1:C:677:TYR:CZ	2.09	0.87
1:A:760:THR:O	1:A:764:PHE:HB2	1.73	0.86
1:C:646:TYR:N	1:C:677:TYR:HE2	1.72	0.86
1:B:90:ALA:HA	1:B:183:ARG:O	1.77	0.85
1:C:422:ALA:HA	1:C:495:ARG:O	1.77	0.85
1:C:598:TYR:O	1:C:634:GLY:HA3	1.77	0.84
1:B:760:THR:O	1:B:764:PHE:HB2	1.77	0.84
1:A:909:PHE:O	1:A:912:ALA:HB3	1.79	0.83
1:C:93:GLU:O	1:C:181:HIS:HB2	1.79	0.83
1:B:914:SER:O	1:B:917:GLN:HB2	1.80	0.81
1:A:913:ILE:O	1:A:916:ILE:HB	1.82	0.78
1:C:646:TYR:N	1:C:677:TYR:CD2	2.53	0.76
1:C:678:THR:OG1	1:C:679:MET:N	2.14	0.74
2:D:406:GLU:HG3	2:D:518:ARG:HD3	1.70	0.73
1:C:323:CYS:HB2	1:C:345:ILE:HG23	1.69	0.72
1:C:655:GLY:O	1:C:678:THR:O	2.08	0.71
1:C:674:ILE:HD12	1:C:674:ILE:N	2.05	0.71
1:C:677:TYR:HD1	1:C:677:TYR:H	1.39	0.71
1:A:1079:PHE:HB2	1:A:1087:THR:HG23	1.74	0.69
1:C:194:LEU:O	1:C:221:LYS:HA	1.92	0.69
1:B:906:ALA:O	1:B:909:PHE:HB3	1.93	0.69
1:C:25:VAL:HA	1:C:76:PHE:HB3	1.73	0.69
1:A:889:ASN:HD21	1:A:895:GLN:HE21	1.40	0.69
1:B:887:ARG:NH1	1:B:1031:LEU:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:HA	1:A:131:GLU:HA	1.76	0.68
1:C:1063:ILE:HB	1:C:1070:TYR:HB2	1.75	0.68
1:B:996:ARG:O	1:B:1000:ILE:HB	1.92	0.68
1:A:536:GLY:HA3	1:A:574:SER:HA	1.74	0.68
1:B:135:ASN:HA	1:B:232:ARG:HH22	1.59	0.68
1:A:584:ILE:HB	1:A:595:ALA:HB3	1.75	0.67
1:C:644:THR:O	1:C:645:SER:O	2.12	0.67
1:C:704:ILE:HA	1:C:1046:HIS:O	1.94	0.67
1:A:759:ASN:O	1:A:763:VAL:HB	1.94	0.67
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.28	0.66
1:A:385:ASP:HB2	1:A:498:VAL:HB	1.77	0.66
1:A:484:TYR:HB2	1:A:487:THR:HB	1.76	0.66
1:A:378:CYS:HA	1:A:511:CYS:HA	1.77	0.66
1:B:348:CYS:SG	1:B:349:VAL:N	2.69	0.66
1:B:626:ASN:ND2	1:B:640:GLU:OE2	2.25	0.66
1:C:99:ARG:NH2	1:C:171:ASP:O	2.27	0.66
1:A:140:VAL:HG13	1:A:145:GLY:HA2	1.78	0.66
1:B:1086:ILE:O	1:B:1095:GLN:NE2	2.29	0.66
2:D:524:GLN:HG2	2:D:583:PRO:HG2	1.76	0.66
1:B:1079:PHE:H	1:B:1086:ILE:HA	1.61	0.65
1:C:937:ASN:O	1:C:941:LEU:HB2	1.96	0.65
2:D:50:TYR:HA	2:D:58:ASN:HB3	1.78	0.65
1:C:133:CYS:HB2	1:C:136:PRO:HD3	1.78	0.65
1:A:102:VAL:O	1:A:231:PHE:HA	1.95	0.65
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.78	0.65
1:B:784:PHE:HA	1:B:787:ILE:HD12	1.77	0.65
1:A:95:SER:H	1:A:181:HIS:HD2	1.45	0.65
1:C:1096:ILE:O	1:C:1101:ASN:ND2	2.30	0.65
1:C:388:VAL:HG22	1:C:495:ARG:HG2	1.78	0.65
1:C:1063:ILE:HG23	1:C:1115:ILE:HB	1.78	0.65
1:A:96:ASN:HA	1:A:183:ARG:HH12	1.61	0.64
1:B:659:SER:OG	1:B:660:TYR:N	2.31	0.64
1:A:887:ARG:NH1	1:A:1031:LEU:O	2.29	0.64
2:D:347:THR:HG1	2:D:349:TRP:HE1	1.46	0.64
1:C:113:SER:O	1:C:127:ALA:HA	1.98	0.64
1:C:421:LEU:O	1:C:496:VAL:HA	1.98	0.64
1:A:901:ASN:O	1:A:904:GLN:HB3	1.98	0.64
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.79	0.64
1:C:38:ARG:NH1	1:C:184:GLU:OE2	2.31	0.64
1:C:341:GLU:O	1:C:385:ASP:HA	1.97	0.64
1:C:383:TYR:HB2	1:C:500:SER:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.81	0.63
1:A:128:CYS:SG	1:A:129:ASN:N	2.72	0.63
1:A:959:LEU:HD23	1:A:962:ILE:HD11	1.80	0.63
1:C:626:ASN:ND2	1:C:640:GLU:OE2	2.31	0.63
1:C:953:GLY:O	1:C:977:ARG:NH1	2.30	0.63
1:C:784:PHE:HA	1:C:787:ILE:HD12	1.80	0.63
1:B:786:GLN:OE1	1:B:917:GLN:NE2	2.32	0.63
1:C:686:SER:OG	1:C:687:ILE:N	2.32	0.63
1:C:58:LEU:HB2	1:C:188:LYS:HE3	1.80	0.63
2:D:30:ASP:O	2:D:34:HIS:ND1	2.32	0.63
1:C:554:ASP:OD1	1:C:554:ASP:N	2.31	0.63
1:A:575:PRO:HD3	1:C:837:PHE:HB3	1.81	0.63
2:D:177:ARG:NH1	2:D:470:LYS:O	2.32	0.63
1:A:786:GLN:HB3	1:A:799:PHE:HB3	1.81	0.63
1:B:123:VAL:HB	1:B:165:SER:HB3	1.81	0.63
2:D:261:CYS:HB2	2:D:488:VAL:HG13	1.81	0.63
1:B:99:ARG:HH12	1:B:172:VAL:HA	1.64	0.62
1:B:188:LYS:HG2	1:B:190:LYS:HB2	1.81	0.62
1:B:721:ASN:HD22	1:C:304:ASN:HD22	1.47	0.62
1:C:56:GLN:NE2	1:C:259:PRO:O	2.32	0.62
2:D:580:ASN:HD21	2:D:582:ARG:HH11	1.47	0.62
1:A:575:PRO:O	1:C:835:GLN:NE2	2.32	0.62
1:B:94:LYS:HB3	1:B:175:LYS:HB2	1.81	0.62
1:B:711:VAL:H	1:B:1041:GLY:HA2	1.64	0.62
1:A:992:GLN:HA	1:A:995:ILE:HD12	1.81	0.62
2:D:244:VAL:HG11	2:D:444:LEU:HD11	1.82	0.62
2:D:320:LEU:HD13	2:D:380:GLN:HG2	1.80	0.62
1:B:38:ARG:NH2	1:B:210:PRO:O	2.28	0.62
1:B:423:TRP:O	1:B:494:TYR:HA	2.00	0.62
1:A:90:ALA:HA	1:A:183:ARG:O	1.99	0.62
1:C:315:ARG:HE	1:C:519:LEU:HG	1.64	0.62
1:C:141:SER:HB3	1:C:145:GLY:H	1.65	0.61
1:C:651:PRO:HA	1:C:657:CYS:HA	1.81	0.61
1:A:960:ASN:HA	1:A:963:LEU:HB2	1.82	0.61
1:A:1073:ARG:NH2	1:A:1101:ASN:O	2.33	0.61
1:A:1093:SER:O	1:A:1095:GLN:NE2	2.33	0.61
1:A:35:SER:HB2	1:A:60:LEU:HD21	1.83	0.61
1:C:301:GLN:NE2	1:C:302:THR:O	2.34	0.61
1:B:710:PRO:HB2	1:B:1000:ILE:HD11	1.82	0.61
1:C:304:ASN:HA	1:C:580:GLY:HA2	1.81	0.61
1:A:626:ASN:ND2	1:A:640:GLU:OE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:LYS:O	1:A:906:ALA:HB3	2.00	0.61
1:B:366:CYS:HB3	1:B:369:VAL:HG23	1.81	0.61
1:C:422:ALA:HB1	1:C:494:TYR:HB3	1.82	0.61
1:C:335:PRO:HG3	1:C:341:GLU:HG2	1.83	0.61
1:B:867:GLY:HA3	1:B:876:LEU:H	1.66	0.61
2:D:209:VAL:HG21	2:D:565:PRO:HB3	1.82	0.60
1:B:882:MET:SD	1:B:899:TYR:OH	2.59	0.60
1:C:30:TYR:HB3	1:C:67:THR:HG23	1.84	0.60
1:A:1077:PHE:O	1:A:1087:THR:OG1	2.19	0.60
1:B:544:ARG:O	1:B:546:GLN:NE2	2.34	0.60
1:C:54:LEU:HD21	1:C:288:CYS:HB2	1.82	0.60
1:C:128:CYS:SG	1:C:129:ASN:N	2.74	0.60
1:A:369:VAL:HA	1:C:965:ARG:HG3	1.83	0.60
1:A:996:ARG:O	1:A:1000:ILE:HB	2.02	0.60
1:B:323:CYS:N	1:B:348:CYS:SG	2.74	0.60
1:B:1097:ILE:HA	1:B:1101:ASN:HD22	1.66	0.60
1:C:867:GLY:HA3	1:C:876:LEU:HB2	1.81	0.60
1:B:907:ASN:HB3	1:B:911:LYS:HE3	1.84	0.60
1:B:1096:ILE:O	1:B:1101:ASN:ND2	2.35	0.60
1:A:835:GLN:NE2	1:B:575:PRO:O	2.35	0.59
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.83	0.59
1:A:761:ARG:O	1:A:765:ALA:N	2.29	0.59
1:A:24:ASP:HB3	1:A:245:TRP:HE1	1.65	0.59
1:B:411:LYS:NZ	1:B:448:LEU:O	2.34	0.59
1:C:960:ASN:HA	1:C:963:LEU:HB2	1.84	0.59
1:A:82:PRO:HA	1:A:230:ASN:HA	1.84	0.59
1:B:540:PRO:HA	1:B:570:ILE:HA	1.85	0.59
1:B:987:GLN:NE2	1:C:988:THR:OG1	2.36	0.59
1:C:396:GLN:HB3	1:C:406:ALA:HB2	1.85	0.59
1:B:302:THR:OG1	1:B:303:SER:N	2.35	0.59
1:B:867:GLY:HA2	1:B:878:ILE:HG12	1.84	0.59
1:C:473:ASN:ND2	2:D:83:TYR:OH	2.34	0.59
1:A:99:ARG:HH22	1:A:172:VAL:HA	1.66	0.59
1:A:872:ALA:HB2	1:B:1028:GLY:HA2	1.85	0.59
1:B:198:LYS:HD3	1:B:219:ILE:HG13	1.85	0.58
1:C:992:GLN:HA	1:C:995:ILE:HD12	1.84	0.58
1:A:46:ILE:HD13	1:B:553:ARG:HE	1.67	0.58
1:B:302:THR:HG23	1:B:581:VAL:HG23	1.85	0.58
1:C:340:TRP:O	1:C:453:ARG:NE	2.33	0.58
2:D:462:MET:O	2:D:467:GLU:N	2.37	0.58
1:A:123:VAL:HB	1:A:165:SER:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:SER:HB2	1:C:769:GLN:HE21	1.68	0.58
1:A:720:CYS:SG	1:A:746:ASN:ND2	2.77	0.58
1:C:315:ARG:NH2	1:C:518:ASP:OD1	2.37	0.58
2:D:245:ARG:NH1	2:D:603:PHE:O	2.37	0.58
1:C:756:GLN:HA	1:C:759:ASN:HD22	1.68	0.58
1:B:626:ASN:ND2	1:B:639:ALA:O	2.37	0.58
2:D:236:LEU:HD21	2:D:588:PHE:HD2	1.68	0.58
1:A:348:CYS:SG	1:A:349:VAL:N	2.77	0.58
1:B:961:ASP:OD1	1:B:965:ARG:NH2	2.37	0.58
1:C:99:ARG:HD3	1:C:118:ASN:HB2	1.84	0.58
1:C:1003:SER:HA	1:C:1006:LEU:HD12	1.86	0.58
1:C:444:ARG:NH1	1:C:447:LYS:O	2.37	0.58
1:A:541:SER:HA	1:A:571:LEU:HG	1.86	0.57
1:A:698:THR:H	1:A:1053:GLN:HB2	1.69	0.57
1:A:711:VAL:HG22	1:A:1041:GLY:HA2	1.86	0.57
1:A:975:ILE:HA	1:A:978:LEU:HD12	1.86	0.57
1:B:341:GLU:HB3	1:B:386:SER:HB3	1.85	0.57
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.37	0.57
2:D:90:ASN:HB3	2:D:93:VAL:HG22	1.85	0.57
2:D:152:MET:HE1	2:D:165:TRP:HD1	1.68	0.57
1:B:692:ASN:HA	1:B:1059:THR:HG22	1.86	0.57
1:C:1086:ILE:O	1:C:1095:GLN:N	2.31	0.57
1:A:149:HIS:NE2	1:A:151:MET:SD	2.77	0.57
1:A:301:GLN:NE2	1:A:302:THR:O	2.37	0.57
1:C:707:GLU:OE1	1:C:1046:HIS:NE2	2.37	0.57
1:A:45:GLU:OE2	1:A:221:LYS:NZ	2.35	0.57
1:B:504:LEU:HD22	1:B:531:GLY:HA3	1.87	0.57
1:A:21:THR:HA	1:A:135:ASN:HB3	1.86	0.57
1:B:867:GLY:O	1:B:883:GLN:NE2	2.37	0.57
1:C:609:ALA:HA	1:C:614:GLN:HB2	1.87	0.57
1:C:647:GLU:N	1:C:677:TYR:OH	2.37	0.57
1:B:546:GLN:HB2	1:B:549:GLN:HB2	1.86	0.57
1:B:861:SER:O	1:B:865:THR:OG1	2.23	0.57
1:B:957:SER:O	1:B:982:ARG:NH2	2.38	0.57
1:C:775:THR:HA	1:C:777:LYS:HE3	1.85	0.57
2:D:439:LEU:HB3	2:D:591:LEU:HD22	1.86	0.57
1:A:41:TYR:OH	1:A:188:LYS:NZ	2.33	0.56
1:B:1078:VAL:HA	1:B:1086:ILE:HG23	1.86	0.56
1:C:763:VAL:HG12	1:C:1011:MET:HE3	1.86	0.56
1:C:89:PHE:HB3	1:C:185:PHE:HB2	1.87	0.56
1:A:631:THR:O	1:A:634:GLY:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ILE:HD11	1:C:772:LYS:H	1.70	0.56
1:B:1029:TYR:H	1:B:1049:TYR:H	1.53	0.56
1:C:758:ARG:NH2	1:C:762:GLU:OE2	2.39	0.56
1:C:1060:ALA:HB3	1:C:1080:ASN:HD22	1.70	0.56
1:A:539:THR:HG23	1:A:571:LEU:HB2	1.87	0.56
1:A:894:THR:OG1	1:A:895:GLN:N	2.38	0.56
1:B:51:THR:OG1	1:B:52:LEU:N	2.39	0.56
1:C:1012:SER:HA	1:C:1016:LEU:HD12	1.88	0.56
1:A:885:ALA:HB2	1:A:898:LEU:HD22	1.88	0.56
1:A:784:PHE:HA	1:A:787:ILE:HD12	1.88	0.56
1:B:31:THR:HG21	1:B:70:HIS:HD2	1.69	0.56
1:B:402:THR:HB	1:B:407:ASP:HB2	1.87	0.56
1:B:1078:VAL:HG13	1:B:1086:ILE:HG12	1.88	0.56
2:D:190:MET:SD	2:D:194:ASN:ND2	2.79	0.56
1:A:348:CYS:H	1:A:510:VAL:HG22	1.71	0.56
1:A:424:ASN:ND2	1:A:492:GLN:OE1	2.37	0.56
1:B:115:ILE:O	1:B:125:ILE:HA	2.06	0.56
1:C:646:TYR:HB3	1:C:677:TYR:OH	2.05	0.56
1:A:444:ARG:NH2	1:A:452:GLU:OE2	2.39	0.55
1:B:392:ASP:OD1	1:B:395:ARG:NH2	2.40	0.55
1:B:903:LYS:O	1:B:906:ALA:HB3	2.06	0.55
1:C:527:PHE:HZ	1:C:538:LEU:HD21	1.71	0.55
1:C:1098:THR:H	1:C:1101:ASN:HB2	1.71	0.55
1:B:303:SER:OG	1:B:304:ASN:N	2.39	0.55
1:A:435:ASN:HB3	1:A:483:PHE:HB2	1.87	0.55
1:A:1058:THR:OG1	1:A:1080:ASN:O	2.19	0.55
1:C:979:ILE:O	1:C:983:LEU:HB2	2.07	0.55
1:A:315:ARG:HH22	1:A:566:LYS:HD2	1.71	0.55
1:A:553:ARG:HD3	1:A:559:THR:HA	1.88	0.55
1:B:114:VAL:HA	1:B:126:ARG:O	2.07	0.55
1:C:700:PHE:HA	1:C:1052:SER:H	1.69	0.55
2:D:46:ALA:HB1	2:D:62:MET:HA	1.88	0.55
2:D:588:PHE:O	2:D:592:PHE:N	2.39	0.55
1:A:19:CYS:HA	1:A:133:CYS:HB3	1.87	0.55
1:A:756:GLN:HA	1:A:759:ASN:HD22	1.71	0.55
1:B:1005:ASN:O	1:B:1009:THR:OG1	2.21	0.55
1:B:802:ASP:O	1:B:806:ASN:ND2	2.40	0.55
1:C:631:THR:O	1:C:633:ALA:N	2.38	0.55
1:B:118:ASN:HB3	1:B:170:LEU:HD21	1.89	0.55
1:C:126:ARG:NH2	1:C:162:GLU:OE2	2.39	0.55
1:C:331:ALA:O	1:C:495:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:O	1:A:478:LEU:HA	2.07	0.55
1:A:678:THR:OG1	1:A:679:MET:N	2.40	0.55
1:A:691:ASN:HA	1:C:879:PRO:HB3	1.87	0.55
1:B:756:GLN:O	1:B:760:THR:OG1	2.24	0.55
1:B:631:THR:O	1:B:633:ALA:N	2.40	0.55
1:C:838:ASN:HB3	1:C:840:LEU:HG	1.87	0.55
1:A:105:SER:O	1:A:229:THR:OG1	2.23	0.55
1:B:48:ARG:HB3	1:C:553:ARG:HB2	1.88	0.55
1:B:992:GLN:HA	1:B:995:ILE:HD12	1.89	0.55
1:C:26:GLN:HB2	1:C:75:THR:HA	1.89	0.55
2:D:499:ASP:HA	2:D:502:SER:HB3	1.89	0.55
1:C:56:GLN:OE1	1:C:261:THR:OG1	2.24	0.54
1:C:706:THR:OG1	1:C:707:GLU:N	2.40	0.54
1:A:131:GLU:HB2	1:A:155:ASN:HD22	1.72	0.54
1:B:435:ASN:OD1	1:B:437:ASN:ND2	2.40	0.54
1:C:1078:VAL:HA	1:C:1086:ILE:HG12	1.90	0.54
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.87	0.54
1:B:856:THR:HA	1:B:859:LEU:HD12	1.89	0.54
1:C:798:SER:N	1:C:801:GLU:OE1	2.40	0.54
1:A:328:VAL:HA	1:A:343:LYS:HE3	1.90	0.54
1:A:911:LYS:O	1:A:915:GLN:N	2.39	0.54
1:A:48:ARG:HB2	1:A:266:TYR:HD2	1.71	0.54
1:A:209:LEU:HD12	1:A:210:PRO:HD2	1.90	0.54
1:A:283:LEU:HD21	1:A:588:THR:HG22	1.90	0.54
1:B:1031:LEU:N	1:B:1047:VAL:O	2.39	0.54
1:B:114:VAL:HG11	1:B:224:LEU:HD13	1.88	0.54
1:C:951:ASN:ND2	1:C:954:ALA:O	2.40	0.54
1:C:24:ASP:HB3	1:C:245:TRP:HE1	1.73	0.54
1:C:59:PHE:O	1:C:257:LEU:HA	2.08	0.54
1:C:305:PHE:HB2	1:C:615:LEU:HD22	1.90	0.54
1:C:859:LEU:O	1:C:863:THR:OG1	2.19	0.54
1:A:104:GLY:HA2	1:A:113:SER:HA	1.89	0.54
1:B:1003:SER:HA	1:B:1006:LEU:HD12	1.90	0.54
1:C:1085:PHE:HD1	1:C:1096:ILE:HA	1.72	0.54
1:A:525:VAL:O	1:A:535:THR:HA	2.08	0.53
1:B:553:ARG:HA	1:B:559:THR:H	1.73	0.53
1:B:770:MET:N	1:C:683:ALA:O	2.41	0.53
1:B:1058:THR:OG1	1:B:1080:ASN:O	2.20	0.53
2:D:245:ARG:NE	2:D:258:PRO:O	2.41	0.53
1:A:105:SER:O	1:A:230:ASN:ND2	2.41	0.53
1:A:314:VAL:HA	1:A:528:ASN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:ASN:O	1:A:941:LEU:HB2	2.07	0.53
1:B:1085:PHE:HB3	1:B:1095:GLN:H	1.74	0.53
1:C:281:ASN:H	1:C:284:ALA:HB3	1.74	0.53
1:C:848:THR:HB	1:C:851:MET:HB2	1.90	0.53
2:D:263:PRO:HB3	2:D:490:PRO:HG3	1.89	0.53
1:A:165:SER:OG	1:A:166:ASP:N	2.39	0.53
1:B:561:SER:HB3	1:B:571:LEU:HD23	1.89	0.53
1:C:303:SER:OG	1:C:304:ASN:N	2.41	0.53
2:D:285:PHE:H	2:D:437:ASN:HD21	1.56	0.53
1:B:715:LYS:HZ1	1:B:846:LEU:HB2	1.73	0.53
1:C:105:SER:O	1:C:229:THR:OG1	2.24	0.53
1:C:197:TYR:HB3	1:C:216:LEU:HB3	1.89	0.53
1:C:1093:SER:O	1:C:1095:GLN:NE2	2.38	0.53
1:A:292:SER:OG	1:A:293:PHE:N	2.42	0.53
1:A:323:CYS:N	1:A:348:CYS:SG	2.81	0.53
1:A:1028:GLY:HA2	1:C:872:ALA:HB2	1.90	0.53
1:B:379:PHE:O	1:B:510:VAL:N	2.38	0.53
1:C:777:LYS:NZ	1:C:790:ASP:OD1	2.35	0.53
1:C:96:ASN:HB3	1:C:183:ARG:HH22	1.74	0.53
2:D:247:LYS:HD3	2:D:250:ASN:HD22	1.73	0.53
1:B:631:THR:HB	1:B:654:ALA:HB3	1.91	0.53
1:B:775:THR:HA	1:B:777:LYS:HE3	1.90	0.53
1:C:294:GLU:HG3	1:C:589:ASN:HD21	1.73	0.53
1:A:541:SER:HB3	1:A:543:LYS:HG2	1.91	0.53
1:A:956:SER:HB3	1:A:962:ILE:HG23	1.91	0.53
1:B:601:VAL:HG23	1:B:634:GLY:HA3	1.90	0.53
1:B:1013:GLU:HB3	1:B:1019:SER:HB2	1.89	0.53
1:C:19:CYS:HA	1:C:133:CYS:HB3	1.91	0.53
2:D:365:THR:HG22	2:D:367:ASP:H	1.74	0.53
1:A:432:SER:HA	1:A:485:THR:H	1.73	0.53
1:A:914:SER:O	1:A:918:GLU:N	2.41	0.53
1:C:200:TYR:O	1:C:214:ASN:ND2	2.41	0.53
1:A:399:PRO:HB3	1:A:414:ASP:HA	1.90	0.52
1:A:735:LEU:HD21	1:A:742:CYS:HB2	1.89	0.52
1:A:1063:ILE:HD11	1:A:1078:VAL:HG11	1.92	0.52
1:A:1096:ILE:O	1:A:1101:ASN:ND2	2.28	0.52
1:C:399:PRO:HD3	1:C:417:MET:HG2	1.92	0.52
1:A:872:ALA:HB1	1:B:1050:VAL:HA	1.90	0.52
1:A:951:ASN:ND2	1:A:954:ALA:O	2.30	0.52
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.92	0.52
2:D:539:LEU:HB3	2:D:587:TYR:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ILE:O	1:B:632:GLN:NE2	2.31	0.52
1:C:102:VAL:HA	1:C:114:VAL:O	2.09	0.52
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.74	0.52
2:D:503:LEU:HD22	2:D:506:VAL:HG23	1.92	0.52
1:A:81:ILE:O	1:A:231:PHE:N	2.36	0.52
1:A:207:ARG:NH1	1:A:208:ASP:OD1	2.43	0.52
1:B:559:THR:O	1:B:561:SER:N	2.42	0.52
1:B:603:CYS:HB3	1:B:627:ASN:HD21	1.74	0.52
1:C:125:ILE:HB	1:C:163:TYR:HB3	1.90	0.52
1:C:645:SER:HB3	1:C:680:SER:CA	2.40	0.52
1:C:848:THR:O	1:C:852:ILE:N	2.34	0.52
1:A:1063:ILE:HB	1:A:1070:TYR:HB2	1.92	0.52
1:C:412:LEU:HD11	1:C:498:VAL:HG11	1.90	0.52
1:C:652:ILE:N	1:C:656:ILE:O	2.43	0.52
1:B:99:ARG:NH2	1:B:171:ASP:O	2.34	0.52
1:B:897:VAL:O	1:B:901:ASN:ND2	2.39	0.52
1:B:35:SER:OG	1:B:64:SER:N	2.41	0.52
1:B:321:ASN:HB3	1:B:348:CYS:HA	1.92	0.52
1:B:1061:PRO:HG2	1:B:1112:ILE:HD12	1.91	0.52
1:C:407:ASP:HB3	1:C:447:LYS:HA	1.91	0.52
1:C:1038:ALA:HB2	1:C:1043:VAL:HG23	1.91	0.52
2:D:81:GLN:NE2	2:D:103:ASN:OD1	2.43	0.52
1:A:1033:SER:HA	1:A:1045:LEU:O	2.09	0.52
1:B:340:TRP:O	1:B:453:ARG:NH1	2.43	0.52
1:C:315:ARG:HD2	1:C:566:LYS:HD2	1.90	0.52
1:C:853:ALA:O	1:C:856:THR:OG1	2.21	0.52
1:B:83:PHE:HE2	1:B:189:ASN:HB2	1.75	0.52
1:B:140:VAL:O	1:B:238:PHE:HA	2.09	0.52
1:B:607:SER:HA	1:B:610:ILE:HD12	1.91	0.52
1:B:948:LEU:O	1:B:957:SER:OG	2.27	0.52
2:D:482:ARG:NH2	2:D:611:SER:OG	2.43	0.52
1:B:32:GLN:HA	1:B:66:VAL:O	2.10	0.51
1:B:125:ILE:HD12	1:B:163:TYR:HD2	1.75	0.51
1:B:469:PRO:HA	1:B:471:ALA:H	1.75	0.51
2:D:184:VAL:O	2:D:188:ASN:ND2	2.42	0.51
1:C:95:SER:H	1:C:181:HIS:CD2	2.28	0.51
1:B:1064:CYS:HB3	1:B:1114:ILE:HA	1.92	0.51
1:C:363:THR:O	1:C:421:LEU:HA	2.11	0.51
1:A:683:ALA:O	1:C:769:GLN:NE2	2.43	0.51
1:A:896:ASN:OD1	1:B:1105:SER:OG	2.26	0.51
1:A:112:GLN:HE22	1:B:456:SER:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:SER:HA	1:A:496:VAL:O	2.10	0.51
1:A:1078:VAL:HG13	1:A:1086:ILE:HG12	1.93	0.51
1:B:94:LYS:HD2	1:B:179:PHE:HA	1.93	0.51
1:B:608:THR:O	1:B:612:ALA:N	2.41	0.51
1:B:678:THR:OG1	1:B:679:MET:N	2.42	0.51
1:B:849:ASP:HA	1:B:852:ILE:HD12	1.92	0.51
1:C:425:THR:HB	1:C:428:ILE:HB	1.93	0.51
1:C:961:ASP:O	1:C:965:ARG:NE	2.43	0.51
2:D:247:LYS:HB2	2:D:282:THR:HG22	1.92	0.51
2:D:284:PRO:HD3	2:D:440:LEU:HD12	1.93	0.51
2:D:443:ALA:O	2:D:447:VAL:HB	2.10	0.51
1:A:94:LYS:NZ	1:A:249:ALA:O	2.38	0.51
1:C:267:ASP:OD1	1:C:271:THR:N	2.43	0.51
1:C:400:GLY:O	1:C:411:LYS:NZ	2.33	0.51
1:A:99:ARG:NH2	1:A:171:ASP:O	2.43	0.51
1:A:1028:GLY:HA3	1:A:1048:THR:HB	1.93	0.51
1:B:348:CYS:H	1:B:510:VAL:HG22	1.75	0.51
2:D:99:ALA:HB1	2:D:391:LEU:HD22	1.92	0.51
1:A:755:GLU:OE1	1:A:1001:ARG:NH2	2.44	0.51
1:A:1073:ARG:HH22	1:A:1101:ASN:HB3	1.75	0.51
1:C:114:VAL:HA	1:C:126:ARG:O	2.11	0.51
1:A:749:LEU:HA	1:A:752:ILE:HD12	1.92	0.51
1:C:1072:PRO:HA	1:C:1102:THR:HA	1.91	0.51
1:A:897:VAL:O	1:A:901:ASN:ND2	2.43	0.51
1:B:598:TYR:HB2	1:B:635:CYS:HB2	1.92	0.51
1:C:677:TYR:N	1:C:677:TYR:CD1	2.71	0.51
2:D:294:THR:HG23	2:D:365:THR:HA	1.93	0.51
2:D:610:TRP:NE1	2:D:615:ASP:OD2	2.44	0.51
1:A:229:THR:OG1	1:A:230:ASN:N	2.45	0.50
1:A:879:PRO:HB3	1:B:691:ASN:HA	1.93	0.50
1:A:1029:TYR:OH	1:A:1089:ARG:NH2	2.43	0.50
1:B:436:TYR:HE1	1:B:482:GLY:HA2	1.76	0.50
1:C:211:SER:OG	1:C:212:GLY:N	2.44	0.50
1:A:915:GLN:O	1:A:918:GLU:HB2	2.10	0.50
1:B:934:VAL:HA	1:B:937:ASN:HD22	1.77	0.50
1:C:302:THR:OG1	1:C:303:SER:N	2.45	0.50
1:C:1102:THR:OG1	1:C:1103:PHE:N	2.44	0.50
1:A:443:LEU:HB2	1:A:477:PRO:HB3	1.94	0.50
1:B:755:GLU:OE2	1:B:758:ARG:NH1	2.45	0.50
1:B:1073:ARG:HE	1:B:1101:ASN:HA	1.77	0.50
1:C:630:GLN:HB3	1:C:631:THR:HG23	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:HE1	1:A:447:LYS:HG2	1.77	0.50
1:A:442:TYR:HE1	1:A:479:ASN:HB2	1.77	0.50
1:A:1074:GLU:HG2	1:C:895:GLN:HG3	1.94	0.50
1:B:37:MET:SD	1:B:211:SER:OG	2.69	0.50
1:B:423:TRP:HE1	1:B:495:ARG:HD2	1.77	0.50
1:A:40:VAL:HG11	1:A:272:ILE:HG21	1.94	0.50
1:B:708:VAL:HG22	1:B:1043:VAL:HG22	1.92	0.50
1:C:419:CYS:HB2	1:C:499:LEU:HB2	1.93	0.50
2:D:169:ARG:NH1	2:D:270:MET:O	2.39	0.50
1:A:286:LEU:HD21	1:A:300:TYR:HD2	1.76	0.50
1:A:362:SER:N	1:A:422:ALA:O	2.36	0.50
1:B:182:LEU:HD22	1:B:203:ILE:HD13	1.92	0.50
1:B:894:THR:OG1	1:C:1074:GLU:OE2	2.23	0.50
1:C:1062:ALA:HB3	1:C:1111:VAL:HG13	1.93	0.50
1:A:793:LYS:HE3	1:A:794:PRO:HD2	1.93	0.50
1:A:849:ASP:HA	1:A:852:ILE:HD12	1.92	0.50
1:B:931:GLN:O	1:B:935:ASN:HB2	2.12	0.50
1:C:612:ALA:O	1:C:614:GLN:NE2	2.33	0.50
1:B:40:VAL:HB	1:B:213:PHE:HB2	1.94	0.49
1:B:124:VAL:HG22	1:B:164:ILE:HG12	1.94	0.49
1:C:644:THR:C	1:C:645:SER:O	2.49	0.49
2:D:116:LEU:HD11	2:D:187:LYS:HE2	1.93	0.49
1:A:778:TYR:CZ	1:A:781:GLY:HA2	2.47	0.49
1:B:238:PHE:HB2	1:B:246:GLY:HA3	1.94	0.49
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.93	0.49
1:C:347:ASN:H	1:C:509:THR:HB	1.77	0.49
1:C:486:THR:HB	2:D:357:ARG:HH12	1.77	0.49
1:C:755:GLU:OE2	1:C:758:ARG:NH1	2.45	0.49
1:A:837:PHE:HB3	1:B:575:PRO:HD3	1.94	0.49
1:B:972:GLU:HA	1:B:975:ILE:HD12	1.94	0.49
1:C:178:ASN:HB2	1:C:204:ASP:HA	1.94	0.49
1:C:660:TYR:HB2	1:C:674:ILE:HA	1.95	0.49
1:A:287:LYS:HA	1:A:295:ILE:HD11	1.94	0.49
1:A:1036:GLN:HG2	1:A:1045:LEU:HD11	1.95	0.49
1:C:887:ARG:NH1	1:C:1032:MET:SD	2.85	0.49
2:D:291:ILE:HG13	2:D:438:PHE:HB2	1.94	0.49
1:A:364:PHE:HD1	1:A:421:LEU:HD13	1.76	0.49
1:A:698:THR:OG1	1:A:1053:GLN:OE1	2.24	0.49
1:A:1086:ILE:H	1:A:1095:GLN:H	1.58	0.49
1:B:1031:LEU:HB3	1:B:1047:VAL:HG12	1.95	0.49
1:C:332:THR:O	1:C:495:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1015:VAL:HA	1:C:1033:SER:HB3	1.94	0.49
1:A:882:MET:SD	1:A:899:TYR:OH	2.70	0.49
1:B:324:PRO:O	1:B:327:GLU:HB3	2.13	0.49
1:A:719:ASP:HB3	1:A:722:MET:HB2	1.95	0.49
1:C:538:LEU:HD22	1:C:570:ILE:HD12	1.95	0.49
1:A:297:LYS:HG2	1:A:650:ILE:HD11	1.93	0.49
1:A:626:ASN:ND2	1:A:639:ALA:O	2.46	0.49
1:B:1054:GLU:O	1:B:1055:ARG:NH1	2.45	0.49
1:C:972:GLU:HA	1:C:975:ILE:HD12	1.94	0.49
1:A:902:GLN:O	1:A:905:ILE:HB	2.13	0.49
1:A:603:CYS:HB3	1:A:627:ASN:HD21	1.78	0.48
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.78	0.48
1:C:448:LEU:HB3	1:C:452:GLU:HB3	1.94	0.48
1:C:937:ASN:O	1:C:941:LEU:CB	2.60	0.48
1:C:1030:HIS:CE1	1:C:1033:SER:HB2	2.47	0.48
2:D:272:GLY:HA2	2:D:275:TRP:HE1	1.76	0.48
2:D:388:GLN:O	2:D:393:ARG:NE	2.47	0.48
1:A:544:ARG:NE	1:C:269:ASN:OD1	2.46	0.48
1:B:656:ILE:HA	1:B:678:THR:HA	1.95	0.48
1:A:299:ILE:HG12	1:A:584:ILE:HG13	1.94	0.48
1:C:138:PHE:HB3	1:C:140:VAL:HG23	1.95	0.48
1:B:351:ASP:HA	1:B:513:PRO:HD3	1.94	0.48
1:B:439:LYS:HD3	1:B:478:LEU:HB3	1.96	0.48
1:B:891:ILE:HB	1:B:1018:GLN:HE22	1.79	0.48
2:D:226:VAL:HG21	2:D:513:ILE:HD11	1.95	0.48
1:A:33:HIS:HB2	1:A:66:VAL:HB	1.96	0.48
1:A:138:PHE:HB3	1:A:140:VAL:HG23	1.96	0.48
1:B:102:VAL:HA	1:B:115:ILE:HG12	1.93	0.48
2:D:63:ASN:O	2:D:67:ASP:N	2.46	0.48
1:A:368:GLY:O	1:C:965:ARG:NH1	2.46	0.48
1:B:267:ASP:OD1	1:B:270:GLY:N	2.47	0.48
1:A:94:LYS:HB3	1:A:175:LYS:HB2	1.95	0.48
1:A:1032:MET:HB2	1:A:1047:VAL:HB	1.96	0.48
1:B:25:VAL:HG22	1:B:76:PHE:HB3	1.94	0.48
1:B:378:CYS:N	1:B:530:ASN:O	2.44	0.48
1:A:769:GLN:HG2	1:A:874:ALA:HB1	1.95	0.48
1:C:82:PRO:HA	1:C:230:ASN:HA	1.96	0.48
2:D:460:ARG:HD2	2:D:506:VAL:HG22	1.95	0.48
1:A:769:GLN:HA	1:B:683:ALA:HB3	1.95	0.47
1:A:1072:PRO:HB3	1:A:1086:ILE:HD13	1.96	0.47
1:B:98:VAL:HG12	1:B:235:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ASP:O	1:B:435:ASN:ND2	2.46	0.47
1:B:846:LEU:HD11	1:C:651:PRO:HB2	1.96	0.47
1:C:165:SER:OG	1:C:166:ASP:N	2.47	0.47
1:C:298:GLY:HA2	1:C:650:ILE:HG21	1.95	0.47
2:D:58:ASN:O	2:D:62:MET:HB2	2.14	0.47
1:A:807:LYS:NZ	1:A:920:LEU:O	2.42	0.47
1:B:758:ARG:HH22	1:C:929:LYS:HE2	1.78	0.47
1:C:363:THR:HB	1:C:422:ALA:H	1.79	0.47
2:D:169:ARG:NH2	2:D:270:MET:SD	2.86	0.47
1:B:756:GLN:HA	1:B:759:ASN:HD22	1.78	0.47
1:C:48:ARG:HB2	1:C:266:TYR:CD2	2.49	0.47
2:D:468:ILE:HG12	2:D:476:LYS:HG2	1.97	0.47
1:A:147:GLN:HB3	1:A:150:THR:HB	1.95	0.47
1:A:939:GLN:O	1:A:943:THR:OG1	2.25	0.47
1:A:521:LYS:HD3	1:A:540:PRO:HD3	1.97	0.47
1:B:541:SER:HA	1:B:571:LEU:HG	1.96	0.47
1:B:781:GLY:O	1:B:910:ASN:ND2	2.41	0.47
1:C:51:THR:OG1	1:C:52:LEU:N	2.48	0.47
1:A:129:ASN:HD22	1:A:158:ASN:HB2	1.79	0.47
1:A:906:ALA:O	1:A:910:ASN:N	2.44	0.47
1:A:968:LYS:HG3	1:A:969:VAL:HG23	1.96	0.47
1:B:122:ASN:OD1	1:B:123:VAL:N	2.48	0.47
1:B:314:VAL:O	1:B:517:THR:N	2.42	0.47
1:B:837:PHE:HB3	1:C:575:PRO:HG3	1.96	0.47
1:B:879:PRO:HG3	1:C:691:ASN:HA	1.96	0.47
1:C:930:LEU:HD22	1:C:1041:GLY:HA3	1.97	0.47
2:D:245:ARG:NH2	2:D:605:GLY:O	2.48	0.47
2:D:462:MET:HB3	2:D:468:ILE:HG13	1.95	0.47
1:A:324:PRO:O	1:A:328:VAL:N	2.35	0.47
1:B:694:ILE:HD12	1:B:1059:THR:HB	1.97	0.47
1:A:267:ASP:OD1	1:A:271:THR:N	2.39	0.47
1:A:325:PHE:HA	1:A:328:VAL:HG12	1.96	0.47
1:A:390:LYS:HB3	1:A:491:TYR:HA	1.97	0.47
1:C:313:VAL:HG22	1:C:520:ILE:H	1.80	0.47
1:C:453:ARG:HG2	1:C:455:ILE:HD11	1.96	0.47
1:A:373:LYS:NZ	1:C:966:LEU:O	2.39	0.47
1:C:94:LYS:HB2	1:C:94:LYS:HE2	1.72	0.47
1:C:694:ILE:N	1:C:1057:PHE:O	2.44	0.47
2:D:432:ASN:HA	2:D:435:GLU:HB3	1.96	0.47
1:B:113:SER:O	1:B:127:ALA:HA	2.15	0.46
1:C:975:ILE:HA	1:C:978:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1063:ILE:H	1:C:1070:TYR:H	1.61	0.46
1:A:591:SER:OG	1:A:592:SER:N	2.48	0.46
1:C:646:TYR:O	1:C:680:SER:CB	2.59	0.46
2:D:314:PHE:HB3	2:D:373:HIS:HE1	1.79	0.46
1:A:83:PHE:N	1:A:229:THR:O	2.47	0.46
1:A:99:ARG:HH12	1:A:172:VAL:HG13	1.79	0.46
1:A:135:ASN:HA	1:A:232:ARG:HH12	1.79	0.46
1:B:431:THR:OG1	1:B:434:GLY:O	2.33	0.46
1:C:129:ASN:ND2	1:C:157:PHE:O	2.49	0.46
1:C:939:GLN:O	1:C:943:THR:OG1	2.21	0.46
2:D:180:TYR:HA	2:D:183:TYR:HB3	1.97	0.46
1:A:128:CYS:HB3	1:A:130:PHE:CE1	2.51	0.46
1:B:865:THR:O	1:B:883:GLN:NE2	2.48	0.46
1:B:903:LYS:O	1:B:907:ASN:N	2.41	0.46
2:D:278:LEU:O	2:D:282:THR:N	2.48	0.46
1:A:430:ALA:O	1:A:485:THR:OG1	2.27	0.46
1:A:1061:PRO:HG2	1:A:1112:ILE:HB	1.97	0.46
1:B:931:GLN:O	1:B:935:ASN:ND2	2.49	0.46
1:C:869:THR:HB	1:C:876:LEU:HD21	1.97	0.46
2:D:389:PRO:HG2	2:D:392:LEU:HD13	1.98	0.46
1:A:52:LEU:HA	1:A:264:LEU:O	2.15	0.46
1:B:99:ARG:HD3	1:B:118:ASN:HB2	1.98	0.46
1:C:426:ARG:HB2	1:C:485:THR:HG23	1.98	0.46
1:A:711:VAL:HG11	1:A:763:VAL:HG11	1.97	0.46
1:B:612:ALA:O	1:B:614:GLN:NE2	2.44	0.46
2:D:281:LEU:HD12	2:D:282:THR:HG23	1.97	0.46
1:A:786:GLN:OE1	1:A:917:GLN:NE2	2.49	0.46
1:C:209:LEU:HD12	1:C:210:PRO:HD2	1.98	0.46
2:D:419:LYS:HE3	2:D:428:PHE:HB3	1.98	0.46
2:D:520:LEU:HD22	2:D:579:MET:HB2	1.97	0.46
1:A:317:PRO:HG3	1:A:565:PRO:HB3	1.97	0.46
1:A:835:GLN:HE21	1:B:575:PRO:HB2	1.81	0.46
1:A:1064:CYS:HB3	1:A:1114:ILE:HG23	1.98	0.46
1:B:83:PHE:HD1	1:B:231:PHE:HB3	1.80	0.46
1:A:35:SER:N	1:A:64:SER:O	2.46	0.46
1:A:886:TYR:HA	1:A:889:ASN:ND2	2.30	0.46
1:B:361:PHE:CG	1:B:421:LEU:HD11	2.51	0.46
1:C:678:THR:O	1:C:679:MET:HB2	2.16	0.46
1:C:931:GLN:O	1:C:935:ASN:ND2	2.48	0.46
1:A:100:GLY:CA	1:A:116:ILE:O	2.55	0.45
1:A:344:LYS:HE3	1:A:381:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:GLN:HB2	1:A:1043:VAL:O	2.16	0.45
1:B:1026:GLY:HA3	1:B:1048:THR:HG22	1.98	0.45
1:B:1080:ASN:HA	1:B:1083:SER:HA	1.98	0.45
1:C:93:GLU:OE1	1:C:97:VAL:N	2.45	0.45
1:C:99:ARG:HG3	1:C:138:PHE:HE2	1.81	0.45
1:C:801:GLU:HA	1:C:804:LEU:HD12	1.98	0.45
1:A:42:TYR:HE1	1:A:272:ILE:HG13	1.81	0.45
1:B:784:PHE:HB3	1:B:788:LEU:HG	1.98	0.45
1:C:722:MET:HA	1:C:726:GLY:HA2	1.98	0.45
1:B:561:SER:HA	1:B:571:LEU:HA	1.98	0.45
1:C:869:THR:H	1:C:876:LEU:HD11	1.81	0.45
2:D:229:THR:HG21	2:D:579:MET:HE2	1.98	0.45
1:A:46:ILE:HG12	1:B:551:PHE:HB2	1.98	0.45
1:A:158:ASN:HB3	1:B:455:ILE:HG21	1.98	0.45
1:A:285:GLU:O	1:A:289:SER:OG	2.26	0.45
1:A:607:SER:HA	1:A:610:ILE:HD12	1.97	0.45
1:A:1031:LEU:HB3	1:A:1047:VAL:HG12	1.98	0.45
1:C:33:HIS:HB2	1:C:66:VAL:HB	1.97	0.45
1:C:346:SER:HA	1:C:509:THR:HB	1.98	0.45
1:C:426:ARG:O	1:C:485:THR:OG1	2.27	0.45
1:C:955:ILE:HG21	1:C:965:ARG:HH12	1.82	0.45
1:C:1044:PHE:HB3	1:C:1046:HIS:CE1	2.51	0.45
1:A:886:TYR:HD1	1:B:1076:VAL:HG13	1.82	0.45
1:A:946:LYS:O	1:A:950:SER:N	2.49	0.45
1:A:1034:PHE:HB2	1:A:1045:LEU:HD12	1.97	0.45
1:A:1065:HIS:HB2	1:A:1118:THR:HB	1.99	0.45
1:C:425:THR:O	1:C:429:ASP:N	2.40	0.45
1:C:443:LEU:HB2	1:C:477:PRO:HA	1.98	0.45
1:B:55:THR:O	1:B:261:THR:HA	2.17	0.45
1:B:895:GLN:HG3	1:C:1074:GLU:HG2	1.98	0.45
1:C:138:PHE:HD2	1:C:236:THR:HG22	1.82	0.45
1:C:467:CYS:HB3	1:C:474:CYS:HB3	1.76	0.45
1:C:648:CYS:N	1:C:677:TYR:OH	2.47	0.45
1:A:858:ALA:O	1:A:861:SER:OG	2.32	0.45
1:B:94:LYS:HG3	1:B:180:LYS:HB3	1.98	0.45
1:A:26:GLN:HB2	1:A:75:THR:HA	1.98	0.45
1:A:749:LEU:HD23	1:A:752:ILE:HD12	1.99	0.45
1:A:1072:PRO:HG3	1:A:1078:VAL:HG22	1.98	0.45
1:C:979:ILE:O	1:C:983:LEU:CB	2.65	0.45
2:D:410:LEU:HD23	2:D:526:GLN:HE21	1.82	0.45
1:B:335:PRO:HG3	1:B:341:GLU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:756:GLN:HA	1:B:759:ASN:ND2	2.32	0.45
1:C:847:LEU:HD11	1:C:855:TYR:HE2	1.82	0.45
2:D:209:VAL:HG23	2:D:216:ASP:HA	1.99	0.45
2:D:518:ARG:O	2:D:522:GLN:HB2	2.17	0.45
1:A:57:ASP:OD1	1:A:58:LEU:N	2.50	0.44
1:A:687:ILE:HB	1:A:689:TYR:CE2	2.51	0.44
1:A:760:THR:HG22	1:A:847:LEU:HD23	1.99	0.44
1:B:1095:GLN:HB3	1:B:1101:ASN:HD21	1.82	0.44
1:C:94:LYS:HZ3	1:C:250:ALA:HB2	1.82	0.44
1:C:369:VAL:HG23	1:C:371:ALA:H	1.82	0.44
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.75	0.44
1:B:19:CYS:HA	1:B:133:CYS:HB3	1.98	0.44
1:B:405:ILE:HG23	1:B:409:ASN:HD22	1.82	0.44
2:D:234:LYS:O	2:D:238:GLU:HB2	2.18	0.44
1:A:72:ILE:HG13	1:A:75:THR:H	1.83	0.44
1:A:1084:TRP:HB3	1:A:1085:PHE:CD2	2.52	0.44
1:B:880:PHE:HA	1:B:883:GLN:HB2	1.99	0.44
1:C:302:THR:HG23	1:C:581:VAL:HG23	1.99	0.44
1:C:1084:TRP:HB3	1:C:1085:PHE:CD2	2.52	0.44
1:A:343:LYS:HB2	1:A:384:ALA:HB3	2.00	0.44
1:A:597:LEU:HD22	1:A:652:ILE:HG23	1.99	0.44
1:A:951:ASN:OD1	1:A:952:PHE:N	2.50	0.44
1:A:1055:ARG:HA	1:A:1055:ARG:HD3	1.70	0.44
1:B:860:VAL:HG22	1:B:1035:PRO:HD2	1.99	0.44
1:C:343:LYS:HB3	1:C:384:ALA:HB3	2.00	0.44
1:C:1012:SER:OG	1:C:1013:GLU:N	2.51	0.44
1:A:802:ASP:O	1:A:806:ASN:ND2	2.51	0.44
1:B:82:PRO:O	1:B:256:TYR:OH	2.23	0.44
1:C:98:VAL:HG12	1:C:235:LEU:HG	1.99	0.44
1:C:997:ALA:HA	1:C:1000:ILE:HG22	1.99	0.44
1:C:1088:GLN:HG2	1:C:1093:SER:HB2	1.99	0.44
2:D:222:LEU:HD21	2:D:513:ILE:HG21	1.99	0.44
1:A:238:PHE:HB2	1:A:246:GLY:HA3	2.00	0.44
1:A:370:SER:HB3	1:C:967:ASP:HB2	1.99	0.44
1:B:82:PRO:HA	1:B:230:ASN:HA	1.99	0.44
1:B:305:PHE:HB3	1:B:581:VAL:HG13	2.00	0.44
1:B:430:ALA:HB2	1:B:493:PRO:HG3	1.99	0.44
1:A:112:GLN:HB3	1:A:226:ILE:HD12	1.99	0.44
1:A:771:TYR:HB3	1:B:687:ILE:HG12	2.00	0.44
1:B:287:LYS:HA	1:B:295:ILE:HD11	1.99	0.44
1:C:646:TYR:H	1:C:677:TYR:HE2	1.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:ALA:O	1:A:942:ASN:ND2	2.51	0.44
1:B:1049:TYR:CE2	1:B:1051:PRO:HG3	2.53	0.44
1:C:316:PHE:CD1	1:C:317:PRO:HD2	2.53	0.44
1:C:334:PHE:HB2	1:C:388:VAL:HG23	1.99	0.44
2:D:554:LEU:O	2:D:558:LEU:HB2	2.18	0.44
2:D:554:LEU:HG	2:D:558:LEU:HD13	2.00	0.44
1:A:89:PHE:HB3	1:A:185:PHE:HB2	1.99	0.44
1:A:770:MET:N	1:B:683:ALA:O	2.51	0.44
1:B:803:LEU:HD22	1:B:921:THR:HG22	1.99	0.44
1:C:362:SER:H	1:C:423:TRP:HA	1.82	0.44
1:C:638:GLY:O	1:C:674:ILE:HD13	2.18	0.44
1:C:690:SER:OG	1:C:691:ASN:N	2.51	0.44
1:C:1064:CYS:HB2	1:C:1111:VAL:HG11	2.00	0.44
2:D:374:HIS:HE1	2:D:406:GLU:HG2	1.83	0.44
1:A:64:SER:HA	1:A:620:ARG:CZ	2.48	0.43
1:A:797:ARG:HD2	1:A:805:PHE:HE2	1.83	0.43
1:A:869:THR:OG1	1:B:1089:ARG:NH1	2.51	0.43
1:B:630:GLN:HG2	1:B:631:THR:H	1.82	0.43
1:C:94:LYS:HZ2	1:C:179:PHE:HE1	1.64	0.43
2:D:21:ILE:HD13	2:D:84:PRO:HG2	2.00	0.43
1:A:390:LYS:HG2	1:A:483:PHE:HE1	1.84	0.43
1:A:724:ILE:HG22	1:A:725:CYS:HB2	2.00	0.43
1:A:1065:HIS:HB3	1:A:1070:TYR:HE2	1.82	0.43
1:B:33:HIS:HB2	1:B:66:VAL:HB	1.99	0.43
1:B:963:LEU:HA	1:B:966:LEU:HB3	2.00	0.43
1:C:933:VAL:O	1:C:937:ASN:ND2	2.51	0.43
2:D:19:SER:OG	2:D:20:THR:N	2.52	0.43
1:A:41:TYR:HB3	1:A:216:LEU:HB2	2.01	0.43
1:A:968:LYS:HD3	1:A:968:LYS:HA	1.83	0.43
1:B:943:THR:O	1:B:947:GLN:HG2	2.18	0.43
1:C:530:ASN:OD1	1:C:530:ASN:N	2.50	0.43
1:C:951:ASN:OD1	1:C:952:PHE:N	2.49	0.43
1:C:974:GLN:OE1	1:C:977:ARG:NH1	2.50	0.43
1:A:95:SER:OG	1:A:173:SER:O	2.35	0.43
1:A:282:PRO:HB2	1:A:594:VAL:HG11	1.99	0.43
1:A:431:THR:OG1	1:A:434:GLY:O	2.37	0.43
1:A:710:PRO:HA	1:A:930:LEU:HD21	1.99	0.43
1:A:1102:THR:OG1	1:A:1103:PHE:N	2.51	0.43
1:C:631:THR:HB	1:C:654:ALA:HB3	2.00	0.43
2:D:188:ASN:HD21	2:D:464:PHE:HA	1.83	0.43
1:A:361:PHE:HA	1:A:423:TRP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:HD3	1:A:478:LEU:HD13	1.99	0.43
1:A:630:GLN:HG2	1:A:631:THR:H	1.84	0.43
1:A:1060:ALA:HB2	1:A:1080:ASN:HD22	1.82	0.43
1:B:681:LEU:HD13	1:B:681:LEU:HA	1.87	0.43
2:D:200:GLY:HA2	2:D:203:TRP:CE3	2.53	0.43
1:A:126:ARG:NH2	1:A:162:GLU:OE2	2.51	0.43
1:A:780:GLY:O	1:A:903:LYS:NZ	2.52	0.43
1:A:1071:PHE:HB2	1:A:1103:PHE:CZ	2.54	0.43
1:B:861:SER:OG	1:B:862:GLY:N	2.51	0.43
1:C:427:ASN:OD1	1:C:427:ASN:N	2.42	0.43
2:D:130:GLY:HA3	2:D:172:VAL:HG11	2.00	0.43
2:D:581:VAL:HG22	2:D:585:LEU:HD23	2.00	0.43
1:B:1069:ALA:HB2	1:B:1108:CYS:HA	2.00	0.43
1:C:742:CYS:O	1:C:746:ASN:ND2	2.52	0.43
1:C:756:GLN:O	1:C:760:THR:OG1	2.28	0.43
2:D:528:ALA:HB1	2:D:553:LYS:HE3	2.01	0.43
1:B:1079:PHE:HB2	1:B:1087:THR:HG23	2.00	0.43
1:C:56:GLN:HB2	1:C:261:THR:HG23	2.00	0.43
1:C:283:LEU:H	1:C:594:VAL:HG11	1.84	0.43
1:C:597:LEU:HD22	1:C:652:ILE:HG23	2.01	0.43
1:C:603:CYS:HA	1:C:606:VAL:HB	2.01	0.43
1:C:745:LEU:HD22	1:C:990:VAL:HG21	2.01	0.43
1:A:48:ARG:HB2	1:A:266:TYR:CD2	2.53	0.43
1:A:524:CYS:HB2	1:A:576:CYS:HB3	1.92	0.43
1:B:47:PHE:HE1	1:B:270:GLY:HA3	1.83	0.43
1:B:631:THR:HG21	1:B:656:ILE:HG13	2.01	0.43
1:C:281:ASN:HB3	1:C:283:LEU:HB3	2.01	0.43
1:C:312:ASP:H	1:C:520:ILE:HD13	1.84	0.43
1:C:861:SER:O	1:C:865:THR:N	2.37	0.43
2:D:307:ILE:HG23	2:D:369:PHE:HD1	1.84	0.43
1:A:626:ASN:OD1	1:A:626:ASN:N	2.51	0.43
1:B:57:ASP:OD1	1:B:58:LEU:N	2.51	0.43
1:C:553:ARG:HA	1:C:558:PHE:O	2.19	0.43
1:C:752:ILE:O	1:C:756:GLN:HG3	2.18	0.43
1:A:959:LEU:HA	1:A:962:ILE:HD11	2.00	0.42
1:B:1031:LEU:HD12	1:B:1031:LEU:HA	1.85	0.42
1:C:302:THR:HG21	1:C:583:VAL:HG23	2.00	0.42
2:D:503:LEU:HD23	2:D:505:HIS:H	1.84	0.42
1:A:352:TYR:CE2	1:A:374:LEU:HG	2.54	0.42
1:A:772:LYS:N	1:B:685:SER:O	2.53	0.42
2:D:237:TYR:OH	2:D:485:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:524:GLN:HB3	2:D:574:VAL:HG11	2.00	0.42
2:D:578:ASN:OD1	2:D:579:MET:N	2.52	0.42
1:B:529:PHE:HB2	1:B:532:LEU:HB3	2.00	0.42
1:C:122:ASN:OD1	1:C:123:VAL:N	2.52	0.42
1:C:140:VAL:HB	1:C:236:THR:HB	2.00	0.42
1:C:629:PHE:H	1:C:641:HIS:CE1	2.37	0.42
1:C:1005:ASN:O	1:C:1009:THR:OG1	2.21	0.42
1:B:93:GLU:O	1:B:181:HIS:CB	2.51	0.42
1:B:836:LYS:HD3	1:B:838:ASN:HD22	1.85	0.42
2:D:152:MET:HE1	2:D:165:TRP:CD1	2.52	0.42
2:D:288:LYS:HD3	2:D:288:LYS:HA	1.88	0.42
1:A:598:TYR:HB2	1:A:635:CYS:HB2	2.01	0.42
1:B:205:VAL:HG11	1:B:210:PRO:HD3	2.01	0.42
1:B:807:LYS:NZ	1:B:920:LEU:O	2.42	0.42
1:B:1009:THR:O	1:B:1012:SER:OG	2.29	0.42
1:A:972:GLU:HA	1:A:975:ILE:HB	2.02	0.42
1:A:1064:CYS:SG	1:A:1068:LYS:N	2.92	0.42
1:A:1110:VAL:HG11	1:C:900:GLU:HA	2.01	0.42
1:B:931:GLN:H	1:B:931:GLN:HG3	1.67	0.42
1:C:196:VAL:HB	1:C:220:PHE:HB2	2.00	0.42
1:C:676:ALA:O	1:C:677:TYR:O	2.38	0.42
1:C:786:GLN:HB3	1:C:799:PHE:HB3	2.01	0.42
2:D:489:GLU:HA	2:D:490:PRO:HD3	1.89	0.42
1:A:160:THR:OG1	1:A:161:PHE:N	2.53	0.42
1:A:1012:SER:OG	1:A:1013:GLU:N	2.52	0.42
1:B:541:SER:HB2	1:B:569:GLU:HB3	2.01	0.42
1:B:1010:LYS:O	1:B:1014:CYS:N	2.46	0.42
1:C:115:ILE:O	1:C:125:ILE:HA	2.19	0.42
1:C:340:TRP:HH2	1:C:342:ARG:HH21	1.68	0.42
1:C:674:ILE:O	1:C:674:ILE:CD1	2.68	0.42
1:C:718:VAL:HG21	1:C:986:LEU:HD11	2.02	0.42
2:D:145:GLU:HA	2:D:146:PRO:HA	1.94	0.42
1:A:95:SER:H	1:A:181:HIS:CD2	2.31	0.42
1:A:552:GLY:HA2	1:C:47:PHE:HB3	2.01	0.42
1:A:631:THR:HB	1:A:654:ALA:HB3	2.01	0.42
1:B:97:VAL:N	1:B:183:ARG:HH12	2.18	0.42
1:B:715:LYS:NZ	1:B:844:PRO:O	2.46	0.42
1:B:894:THR:OG1	1:B:895:GLN:N	2.53	0.42
1:C:1027:LYS:H	1:C:1048:THR:HG21	1.85	0.42
1:C:1049:TYR:CE2	1:C:1051:PRO:HG3	2.55	0.42
2:D:477:TRP:HD1	2:D:478:TRP:CD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:TYR:HB3	1:A:601:VAL:HG11	2.02	0.42
1:A:738:TYR:HB3	1:A:741:PHE:CE2	2.55	0.42
1:A:994:LEU:HG	1:B:995:ILE:HG21	2.01	0.42
1:B:292:SER:OG	1:B:294:GLU:O	2.29	0.42
1:B:439:LYS:NZ	1:B:480:ASP:OD1	2.39	0.42
1:B:844:PRO:HG3	1:C:633:ALA:HB2	2.01	0.42
1:B:951:ASN:OD1	1:B:952:PHE:N	2.52	0.42
1:C:48:ARG:HB2	1:C:266:TYR:HD2	1.85	0.42
1:C:629:PHE:H	1:C:641:HIS:HE1	1.66	0.42
1:C:646:TYR:C	1:C:677:TYR:HE2	2.19	0.42
1:C:912:ALA:O	1:C:916:ILE:HG12	2.20	0.42
1:C:1107:ASN:OD1	1:C:1107:ASN:N	2.42	0.42
2:D:398:GLU:HG3	2:D:514:ARG:HB3	2.02	0.42
1:A:321:ASN:HB3	1:A:348:CYS:HA	2.02	0.41
1:A:934:VAL:HA	1:A:937:ASN:HD22	1.84	0.41
1:B:658:ALA:HA	1:B:676:ALA:HA	2.02	0.41
1:B:775:THR:HA	1:B:777:LYS:HG3	2.01	0.41
1:B:902:GLN:O	1:B:905:ILE:HB	2.20	0.41
1:B:1055:ARG:HD3	1:B:1055:ARG:HA	1.84	0.41
2:D:526:GLN:HG3	2:D:539:LEU:HD11	2.01	0.41
1:A:24:ASP:O	1:A:245:TRP:NE1	2.53	0.41
1:A:896:ASN:HD21	1:B:1103:PHE:HE2	1.66	0.41
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	2.02	0.41
1:C:122:ASN:ND2	1:C:165:SER:O	2.45	0.41
1:C:603:CYS:SG	1:C:629:PHE:HB2	2.59	0.41
1:C:1065:HIS:HA	1:C:1116:ASN:HA	2.01	0.41
2:D:81:GLN:HG2	2:D:101:GLN:HG2	2.02	0.41
2:D:238:GLU:HG3	2:D:605:GLY:HA2	2.02	0.41
1:B:95:SER:OG	1:B:173:SER:O	2.37	0.41
1:B:119:ASN:OD1	1:B:122:ASN:N	2.53	0.41
1:B:912:ALA:O	1:B:916:ILE:HG12	2.21	0.41
1:C:645:SER:HB3	1:C:680:SER:HA	2.02	0.41
2:D:336:PRO:HB2	2:D:340:GLN:HB3	2.03	0.41
2:D:477:TRP:CE2	2:D:500:PRO:HD3	2.55	0.41
1:A:60:LEU:HD12	1:A:61:PRO:HD2	2.02	0.41
1:C:96:ASN:O	1:C:99:ARG:NH2	2.53	0.41
1:A:967:ASP:HB2	1:B:370:SER:HB3	2.01	0.41
1:B:114:VAL:HG12	1:B:226:ILE:HD11	2.02	0.41
1:B:128:CYS:HB3	1:B:130:PHE:CE1	2.56	0.41
1:B:165:SER:OG	1:B:166:ASP:N	2.52	0.41
1:B:725:CYS:HA	1:B:959:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:O	1:C:181:HIS:CB	2.61	0.41
1:C:361:PHE:HA	1:C:423:TRP:HB3	2.02	0.41
2:D:481:LYS:O	2:D:487:VAL:N	2.42	0.41
1:A:758:ARG:NH1	1:A:1001:ARG:HH12	2.17	0.41
1:B:20:THR:HB	1:B:137:PHE:HE1	1.86	0.41
1:B:591:SER:OG	1:B:592:SER:N	2.54	0.41
1:C:41:TYR:HB3	1:C:216:LEU:HB2	2.01	0.41
1:C:638:GLY:O	1:C:674:ILE:CD1	2.68	0.41
1:A:895:GLN:HG3	1:B:1074:GLU:HG2	2.01	0.41
1:C:527:PHE:HE1	1:C:538:LEU:HD11	1.85	0.41
1:A:347:ASN:H	1:A:509:THR:HB	1.86	0.41
1:A:846:LEU:HD12	1:B:655:GLY:H	1.86	0.41
1:B:769:GLN:HA	1:C:683:ALA:HB3	2.02	0.41
1:B:1086:ILE:HD12	1:B:1101:ASN:HB3	2.02	0.41
1:A:133:CYS:HB2	1:A:136:PRO:HD3	2.02	0.41
1:A:182:LEU:HD22	1:A:203:ILE:HD13	2.02	0.41
1:A:775:THR:HA	1:A:777:LYS:HG3	2.03	0.41
1:B:76:PHE:HB2	1:B:245:TRP:CE2	2.56	0.41
1:B:196:VAL:HB	1:B:220:PHE:HB2	2.03	0.41
1:B:263:MET:O	1:B:275:ALA:HA	2.20	0.41
1:B:402:THR:OG1	1:B:403:GLY:N	2.54	0.41
1:B:409:ASN:HD21	1:B:440:TYR:HB2	1.86	0.41
1:B:1102:THR:OG1	1:B:1103:PHE:N	2.54	0.41
1:C:35:SER:OG	1:C:64:SER:N	2.40	0.41
1:C:591:SER:OG	1:C:592:SER:N	2.54	0.41
1:C:852:ILE:O	1:C:856:THR:HG23	2.21	0.41
2:D:184:VAL:HG12	2:D:464:PHE:HE1	1.86	0.41
2:D:440:LEU:HA	2:D:443:ALA:HB3	2.03	0.41
1:A:57:ASP:OD2	1:A:188:LYS:NZ	2.47	0.41
1:A:112:GLN:HE21	1:B:455:ILE:H	1.69	0.41
1:A:793:LYS:HA	1:A:793:LYS:HD2	1.79	0.41
1:A:1079:PHE:CZ	1:A:1081:GLY:HA3	2.56	0.41
1:B:911:LYS:O	1:B:914:SER:HB2	2.20	0.41
1:B:927:LEU:HD12	1:B:927:LEU:HA	1.90	0.41
1:B:553:ARG:HD3	1:B:557:ASP:HA	2.02	0.40
2:D:119:ILE:HD13	2:D:119:ILE:HA	1.97	0.40
2:D:289:PRO:HG2	2:D:428:PHE:HE1	1.86	0.40
1:A:553:ARG:HD2	1:A:557:ASP:HA	2.03	0.40
1:A:734:LEU:HA	1:A:734:LEU:HD23	1.85	0.40
1:A:961:ASP:O	1:A:965:ARG:NE	2.53	0.40
1:C:561:SER:HB3	1:C:571:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:LYS:HZ2	1:C:791:PRO:HD3	1.85	0.40
1:C:1009:THR:O	1:C:1013:GLU:HB2	2.22	0.40
1:A:20:THR:HG21	1:A:149:HIS:HE1	1.86	0.40
1:A:483:PHE:CE2	1:A:493:PRO:HB3	2.57	0.40
1:A:536:GLY:HA2	1:A:576:CYS:SG	2.62	0.40
1:A:956:SER:OG	1:A:957:SER:N	2.54	0.40
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.90	0.40
1:B:297:LYS:HG3	1:B:586:PRO:HA	2.03	0.40
1:B:698:THR:H	1:B:1053:GLN:HB2	1.86	0.40
1:C:141:SER:H	1:C:145:GLY:HA2	1.86	0.40
1:C:314:VAL:HB	1:C:517:THR:HB	2.03	0.40
1:C:385:ASP:HB2	1:C:498:VAL:HB	2.02	0.40
1:C:800:ILE:O	1:C:804:LEU:HG	2.21	0.40
1:A:324:PRO:HD2	1:A:345:ILE:HG12	2.02	0.40
1:A:697:PRO:HB3	1:A:1053:GLN:H	1.86	0.40
1:A:968:LYS:O	1:A:971:ALA:N	2.36	0.40
1:C:355:LEU:HB3	1:C:421:LEU:HD21	2.03	0.40
1:A:25:VAL:HA	1:A:76:PHE:HB3	2.04	0.40
1:A:72:ILE:HG12	1:A:75:THR:HB	2.02	0.40
1:A:763:VAL:O	1:A:766:GLN:NE2	2.54	0.40
1:C:985:SER:OG	1:C:986:LEU:N	2.55	0.40
1:C:1079:PHE:N	1:C:1085:PHE:O	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	A	1057/1203 (88%)	874 (83%)	180 (17%)	3 (0%)	37	72
1	B	1057/1203 (88%)	852 (81%)	201 (19%)	4 (0%)	30	68
1	C	1045/1203 (87%)	843 (81%)	192 (18%)	10 (1%)	13	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	595/603 (99%)	564 (95%)	31 (5%)	0	100 100
All	All	3754/4212 (89%)	3133 (84%)	604 (16%)	17 (0%)	27 64

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	ASP
1	B	560	ASP
1	B	1072	PRO
1	C	645	SER
1	B	632	GLN
1	C	632	GLN
1	C	675	VAL
1	C	1072	PRO
1	A	1072	PRO
1	C	677	TYR
1	C	692	ASN
1	C	925	THR
1	C	679	MET
1	B	925	THR
1	A	1075	GLY
1	C	676	ALA
1	C	1075	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	922/1048 (88%)	916 (99%)	6 (1%)	81 87
1	B	922/1048 (88%)	917 (100%)	5 (0%)	86 89
1	C	914/1048 (87%)	903 (99%)	11 (1%)	67 79
2	D	527/533 (99%)	521 (99%)	6 (1%)	70 80
All	All	3285/3677 (89%)	3257 (99%)	28 (1%)	74 83

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	687	ILE
1	A	699	ASN
1	A	720	CYS
1	A	841	THR
1	A	921	THR
1	A	965	ARG
1	B	265	LYS
1	B	302	THR
1	B	699	ASN
1	B	760	THR
1	B	965	ARG
1	C	302	THR
1	C	316	PHE
1	C	318	ASN
1	C	333	LYS
1	C	484	TYR
1	C	646	TYR
1	C	674	ILE
1	C	677	TYR
1	C	699	ASN
1	C	965	ARG
1	C	1097	ILE
2	D	31	LYS
2	D	53	ASN
2	D	114	LYS
2	D	273	ARG
2	D	341	LYS
2	D	436	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	155	ASN
1	A	181	HIS
1	A	230	ASN
1	A	437	ASN
1	A	445	HIS
1	A	627	ASN
1	A	691	ASN
1	A	699	ASN

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Mol	Chain	Res	Type
1	A	759	ASN
1	A	806	ASN
1	A	835	GLN
1	A	883	GLN
1	A	895	GLN
1	A	937	ASN
1	A	993	GLN
1	B	70	HIS
1	B	129	ASN
1	B	155	ASN
1	B	437	ASN
1	B	445	HIS
1	B	479	ASN
1	B	546	GLN
1	B	692	ASN
1	B	699	ASN
1	B	721	ASN
1	B	733	ASN
1	B	759	ASN
1	B	806	ASN
1	B	835	GLN
1	B	838	ASN
1	B	904	GLN
1	B	917	GLN
1	B	937	ASN
1	B	984	GLN
1	B	987	GLN
1	B	993	GLN
1	B	1005	ASN
1	B	1018	GLN
1	B	1030	HIS
1	B	1095	GLN
1	C	149	HIS
1	C	318	ASN
1	C	347	ASN
1	C	473	ASN
1	C	479	ASN
1	C	523	GLN
1	C	589	ASN
1	C	692	ASN
1	C	699	ASN
1	C	733	ASN

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Mol	Chain	Res	Type
1	C	759	ASN
1	C	769	GLN
1	C	935	ASN
1	C	937	ASN
1	C	987	GLN
1	C	993	GLN
1	C	1005	ASN
1	C	1101	ASN
2	D	33	ASN
2	D	53	ASN
2	D	250	ASN
2	D	526	GLN
2	D	572	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

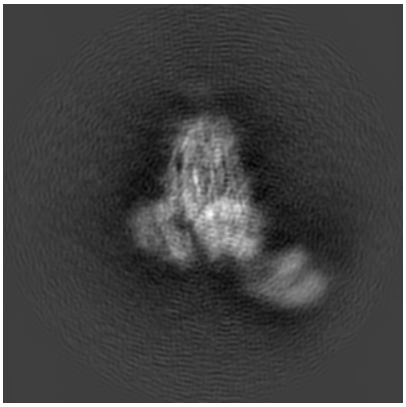
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9594. These allow visual inspection of the internal detail of the map and identification of artifacts.

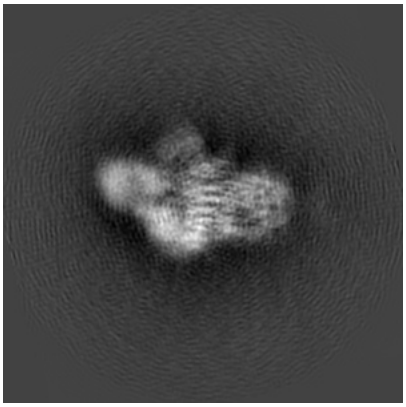
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

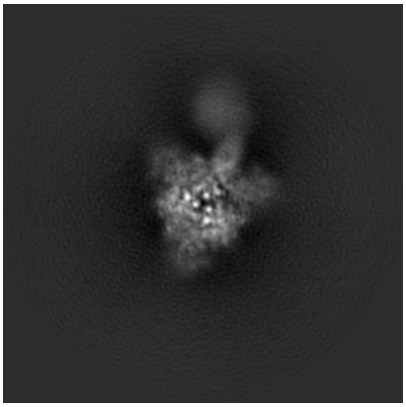
6.1.1 Primary map



X



Y

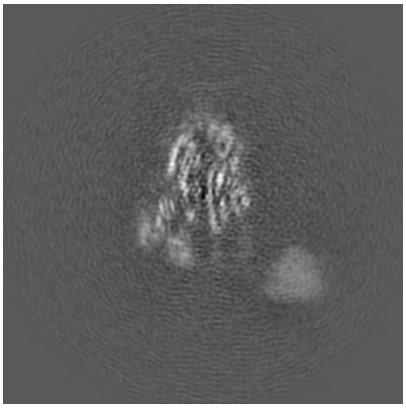


Z

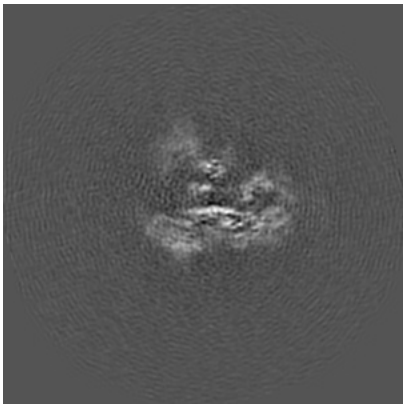
The images above show the map projected in three orthogonal directions.

6.2 Central slices

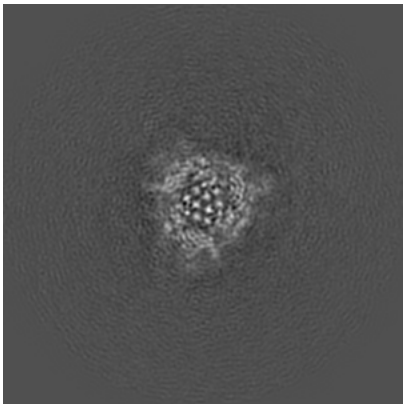
6.2.1 Primary map



X Index: 144



Y Index: 144

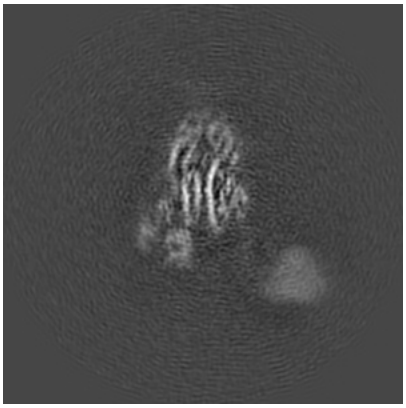


Z Index: 144

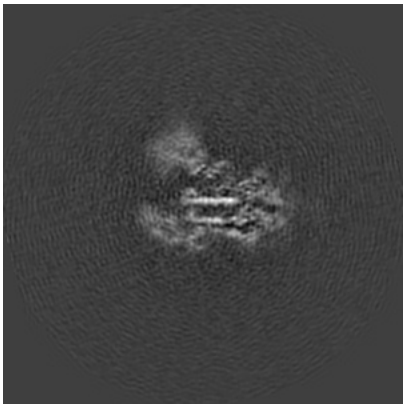
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

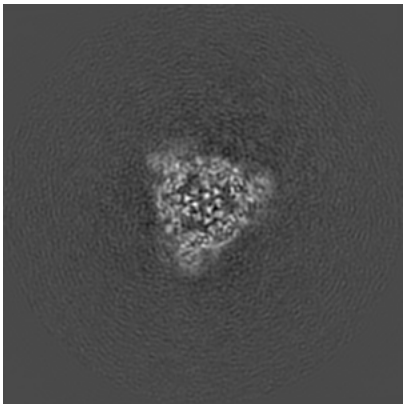
6.3.1 Primary map



X Index: 146



Y Index: 149

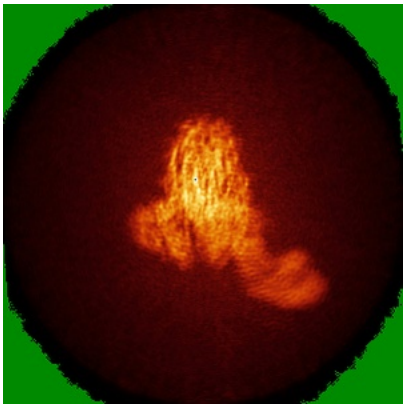


Z Index: 141

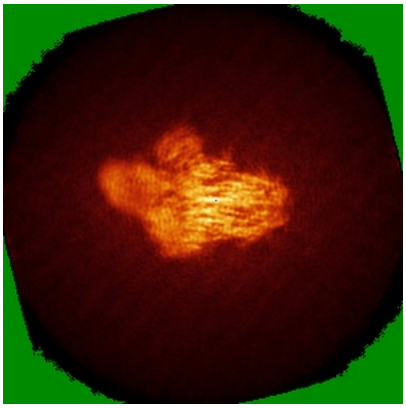
The images above show the largest variance slices of the map in three orthogonal directions.

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

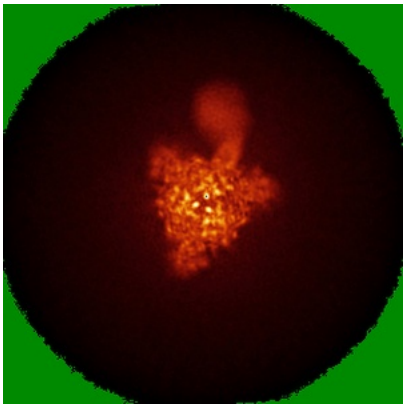
6.4.1 Primary map



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

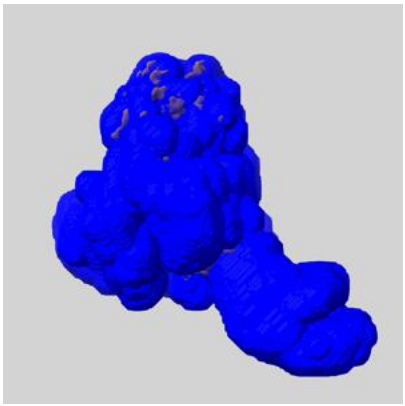
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

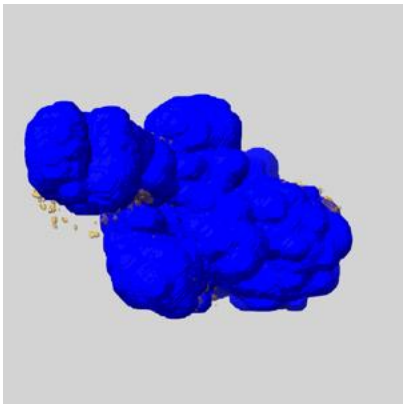
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

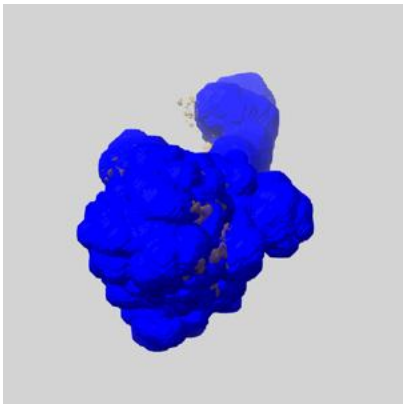
6.6.1 emd_9594_msk_1.map



X



Y

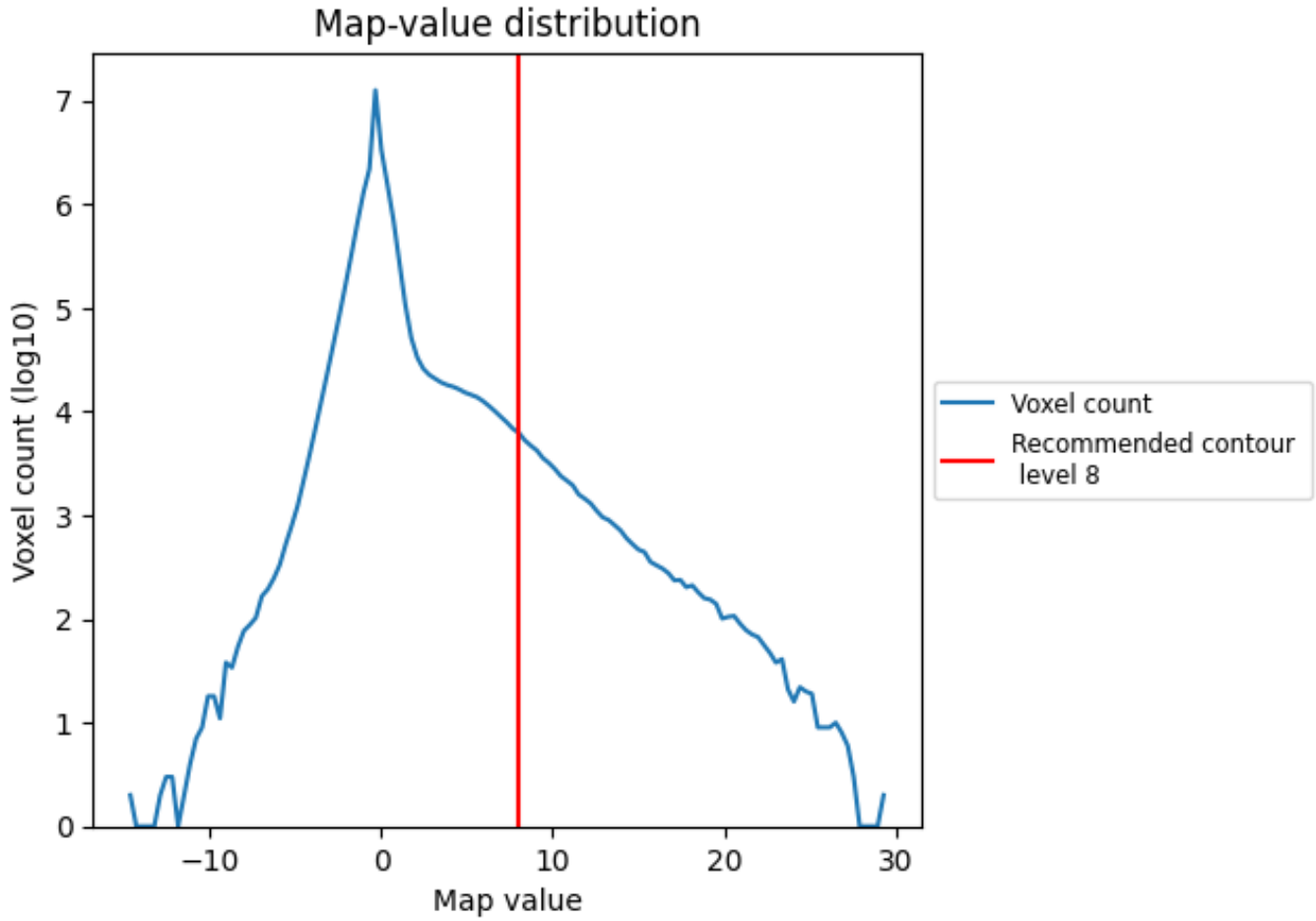


Z

7 Map analysis

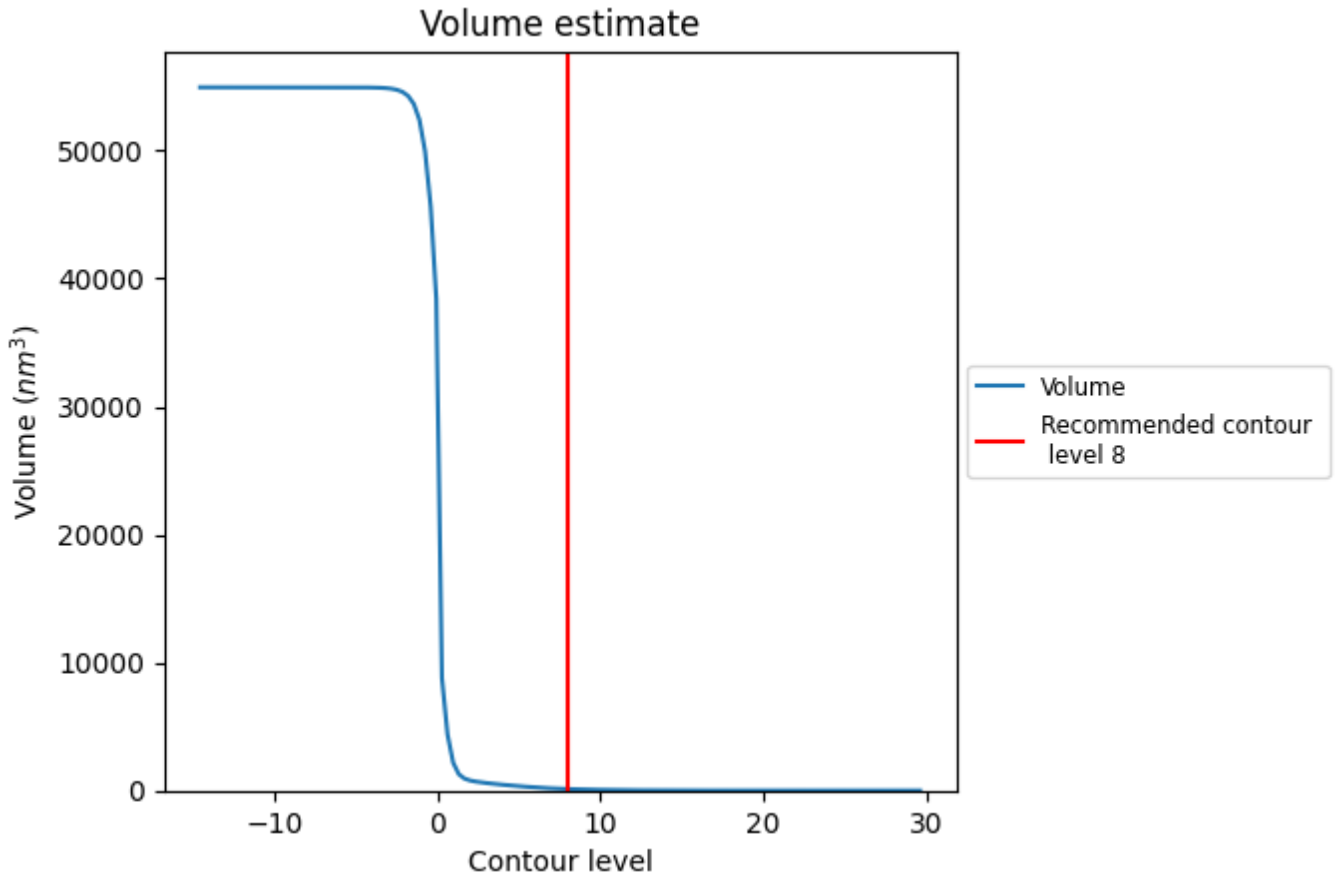
This section contains the results of statistical analysis of the map.

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.

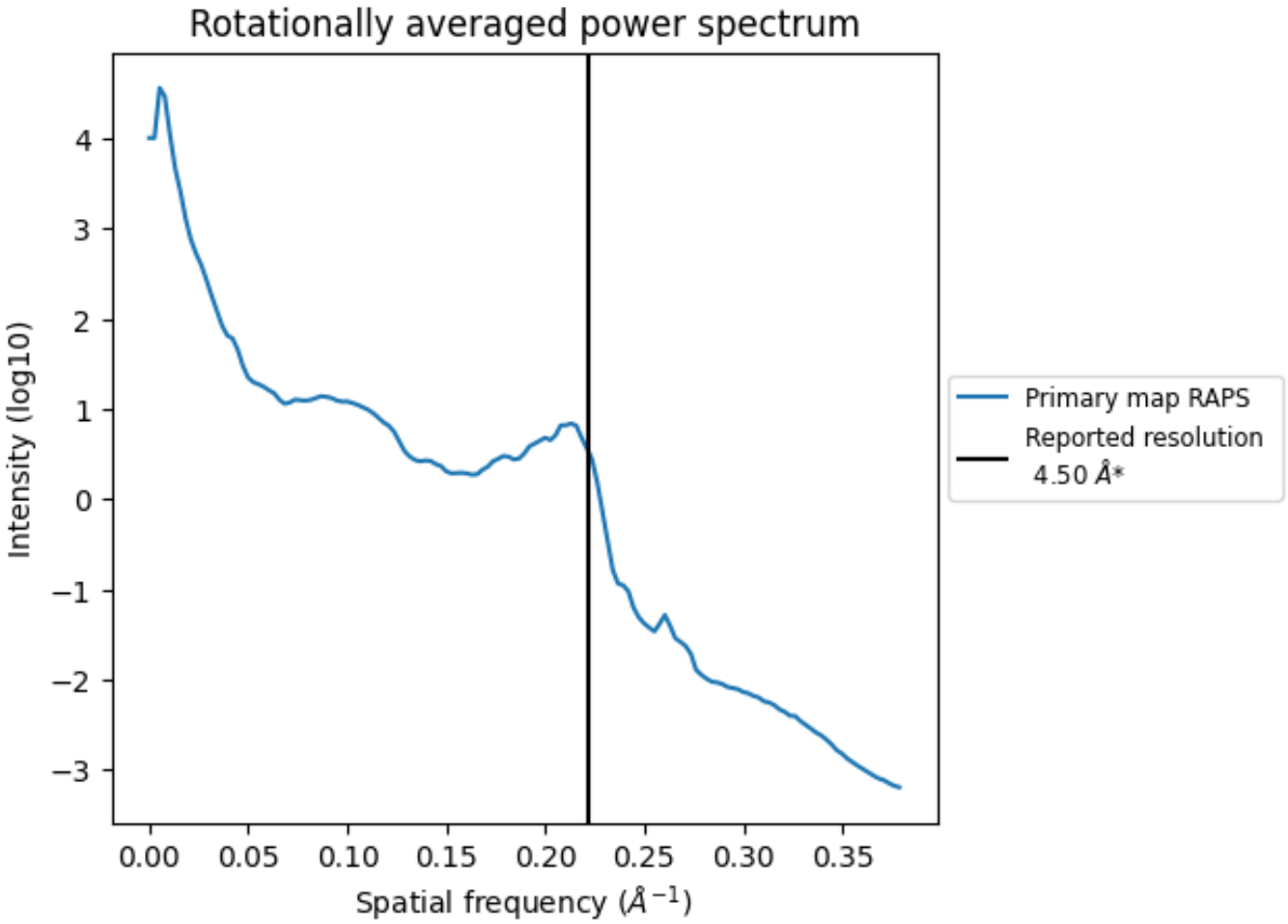
7.2 Volume estimate



The volume at the recommended contour level is 119 nm^3; this corresponds to an approximate mass of 108 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)

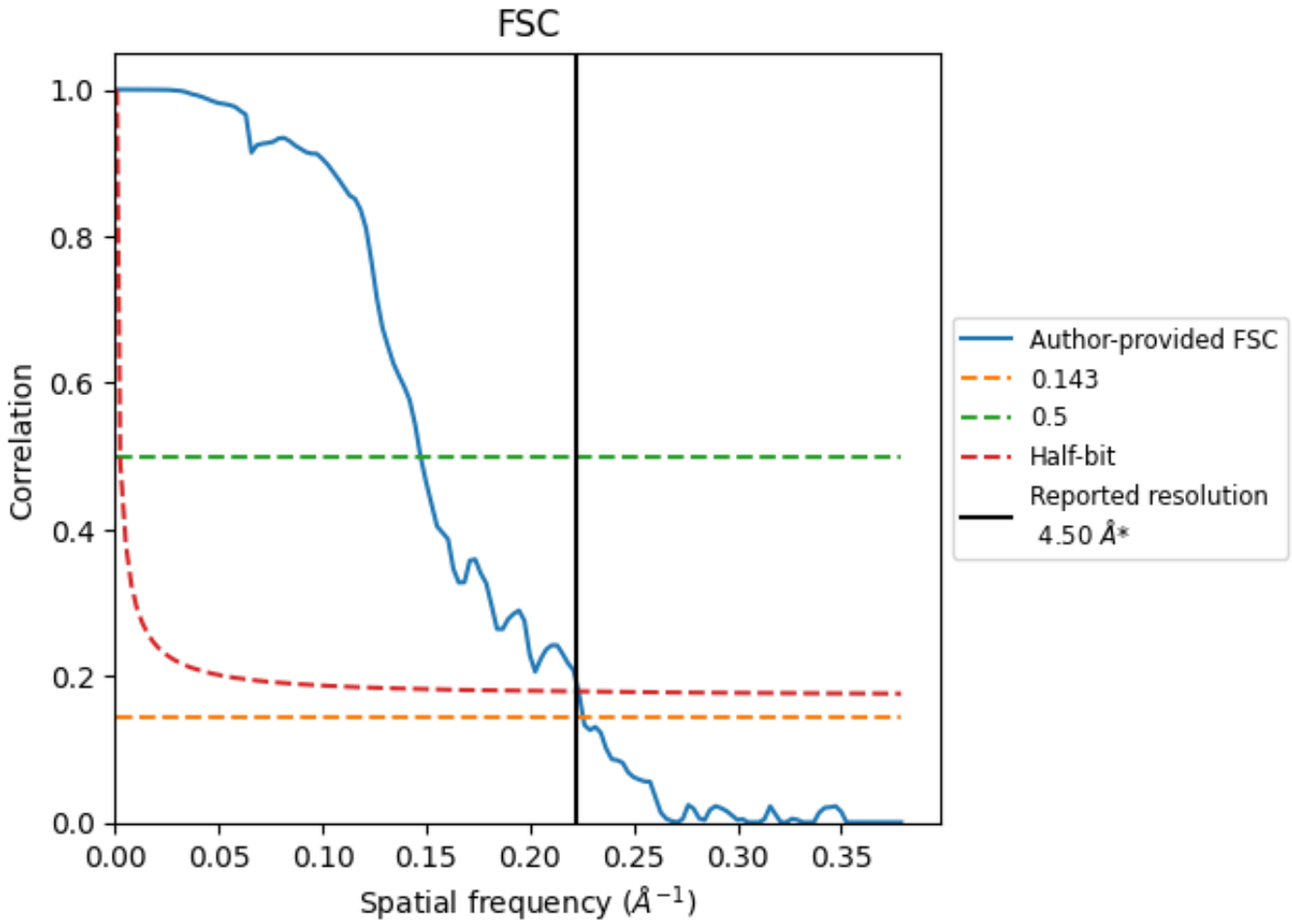


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

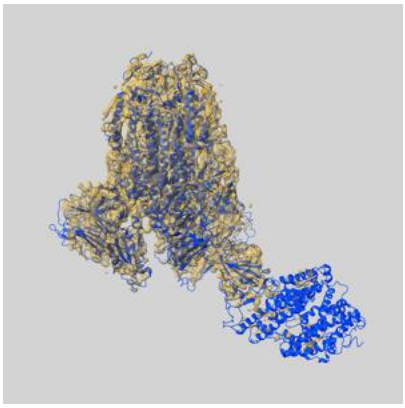
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.43	6.79	4.48
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

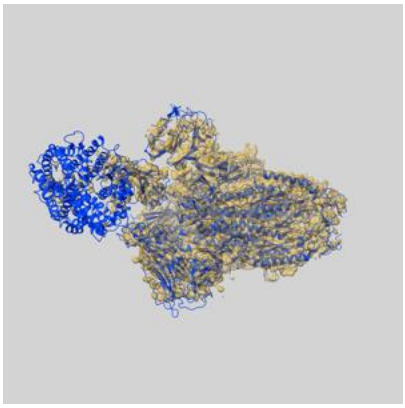
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9594 and PDB model 6ACK. Per-residue inclusion information can be found in section 3 on page 5.

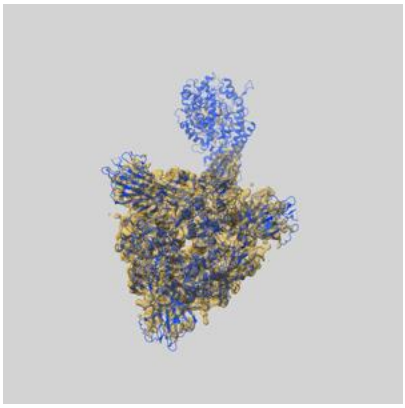
9.1 Map-model overlay



X



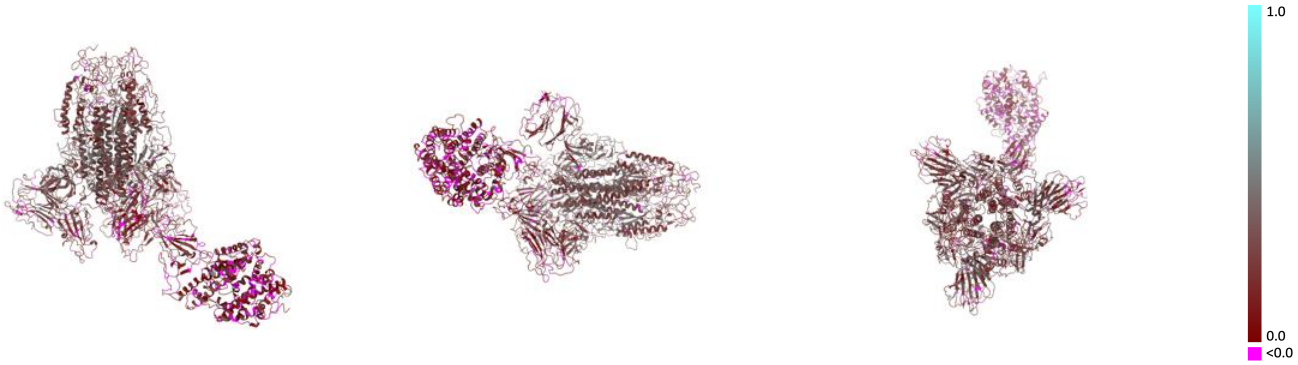
Y



Z

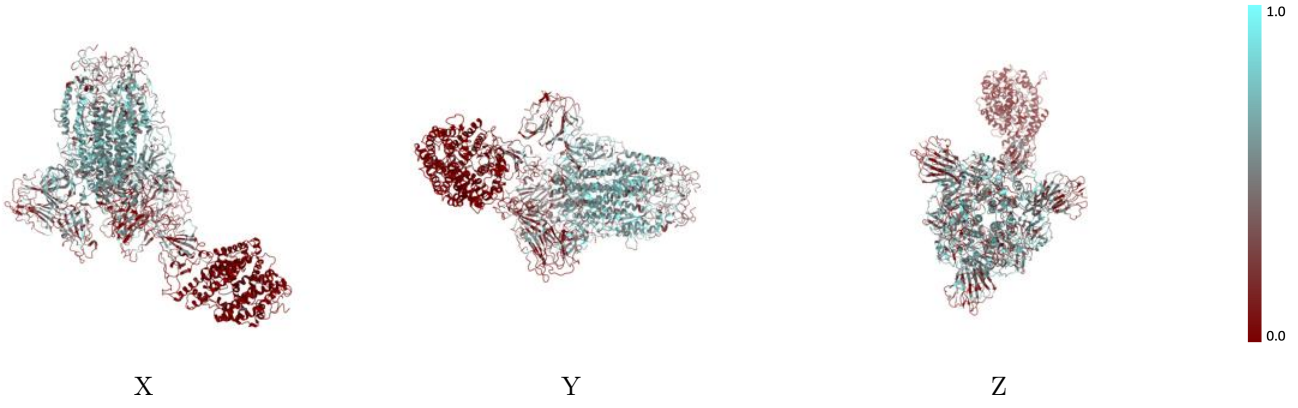
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



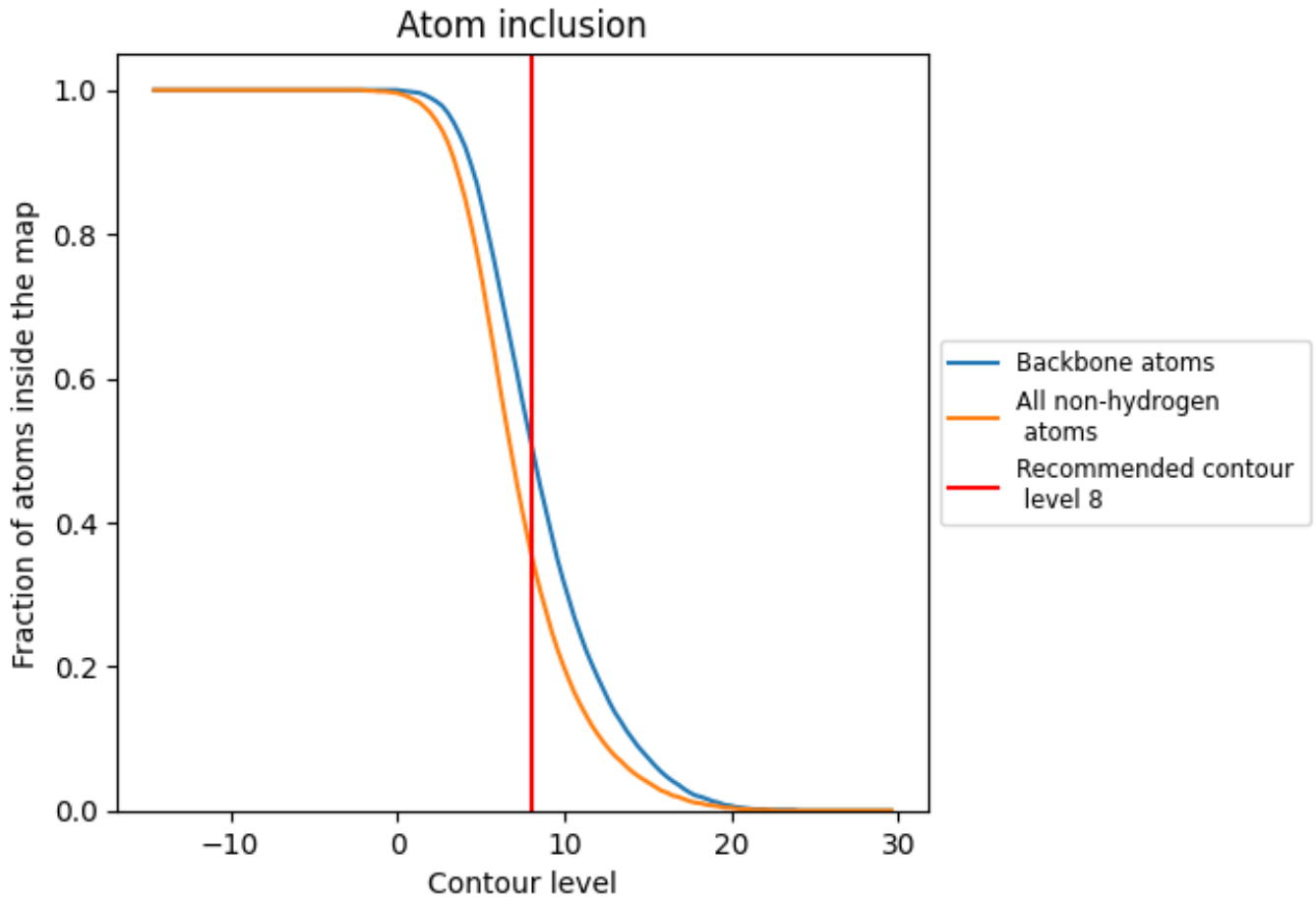
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (8).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 36% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3590	0.2390
A	0.4340	0.2750
B	0.4370	0.2630
C	0.4110	0.2560
D	0.0110	0.1050