Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 01:39 AM JST

PDB ID	:	6ACJ
EMDB ID	:	EMD-9593
Title	:	Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-bound conformation 2
Authors	:	Gui, M.; Song, W.
Deposited on	:	2018-07-26
Resolution	:	4.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

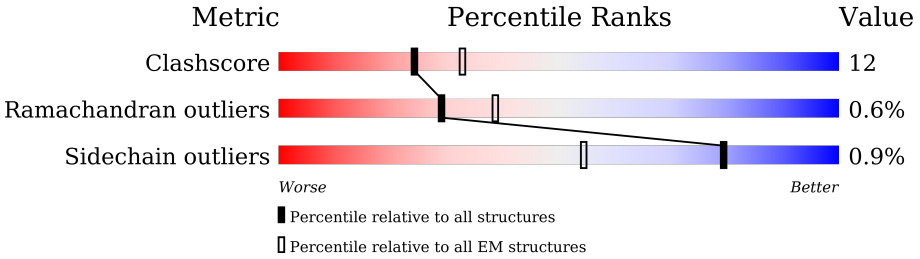
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1203	41% 63% 24% • 11%
1	B	1203	38% 62% 26% • 11%
1	C	1203	43% 60% 26% • 12%
2	D	603	99% 79% 20% •

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
			Total	C	N	O	S		
1	A	1065	8302	5304	1374	1579	45	0	0
1	B	1065	8302	5304	1374	1579	45	0	0
1	C	1057	8241	5264	1364	1568	45	0	0

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
			Total	C	N	O	S		
2	D	597	4870	3115	806	920	29	0	0

There are 6 discrepancies between the modelled and reference sequences:

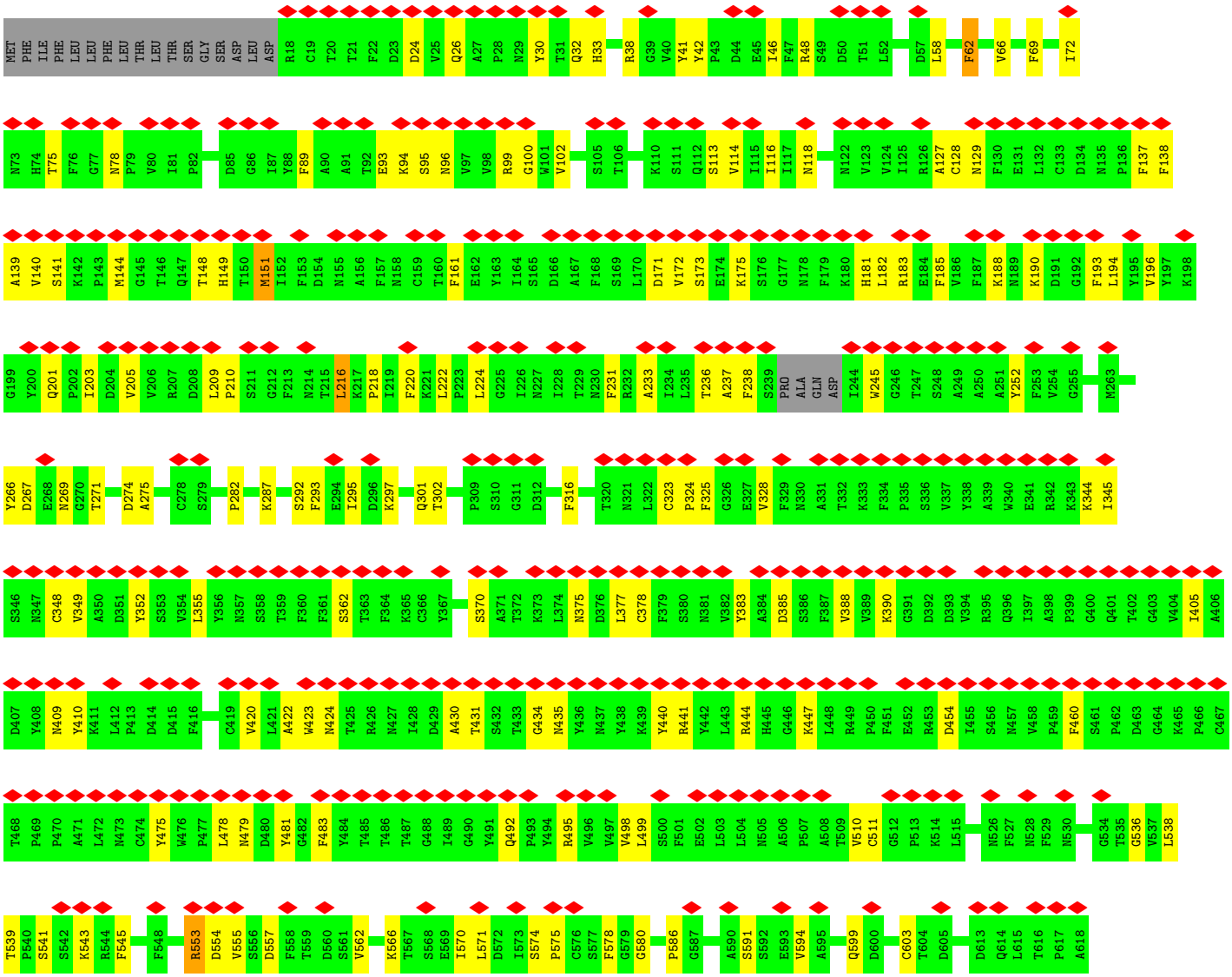
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1

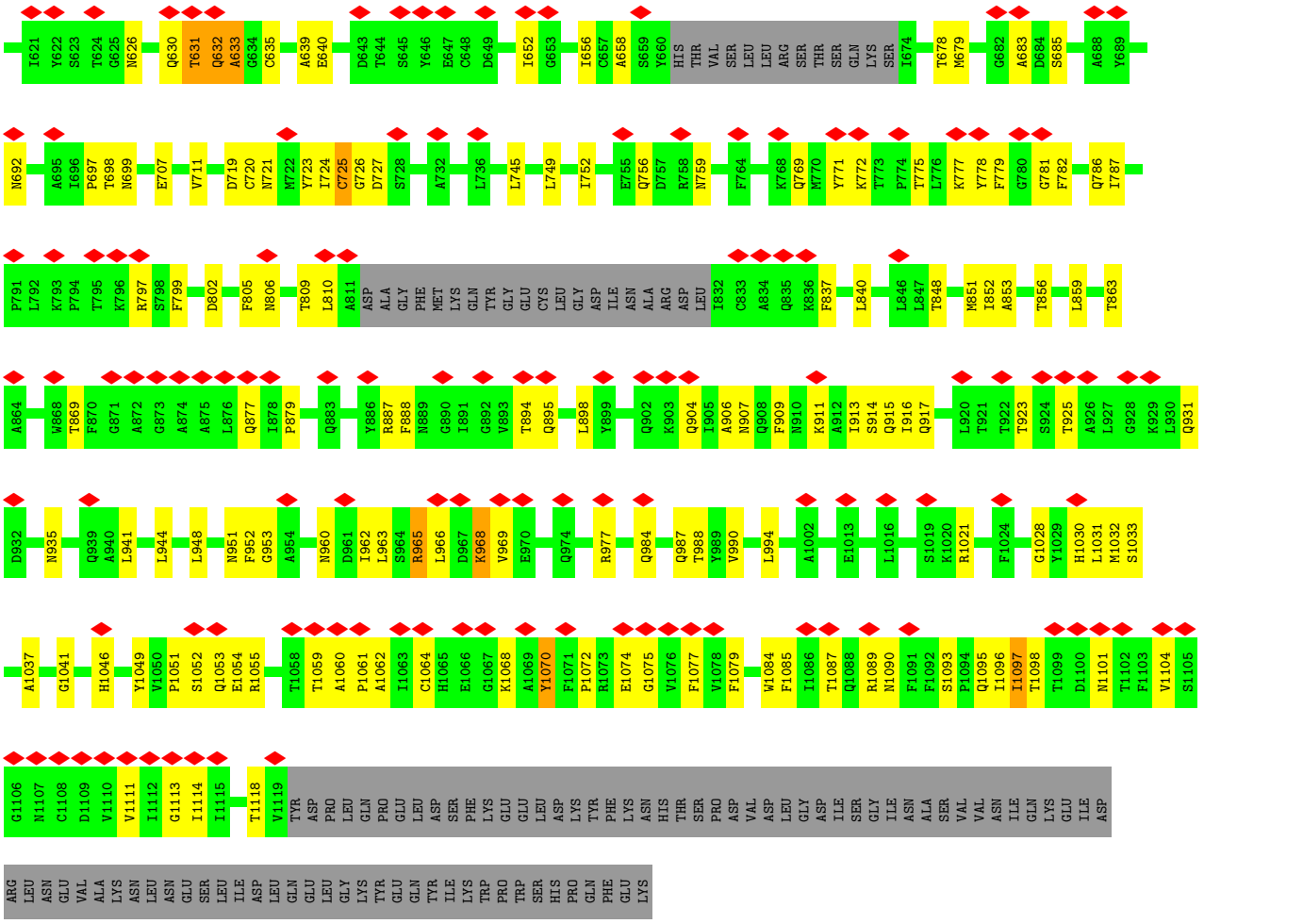
3 Residue-property plots (i)

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

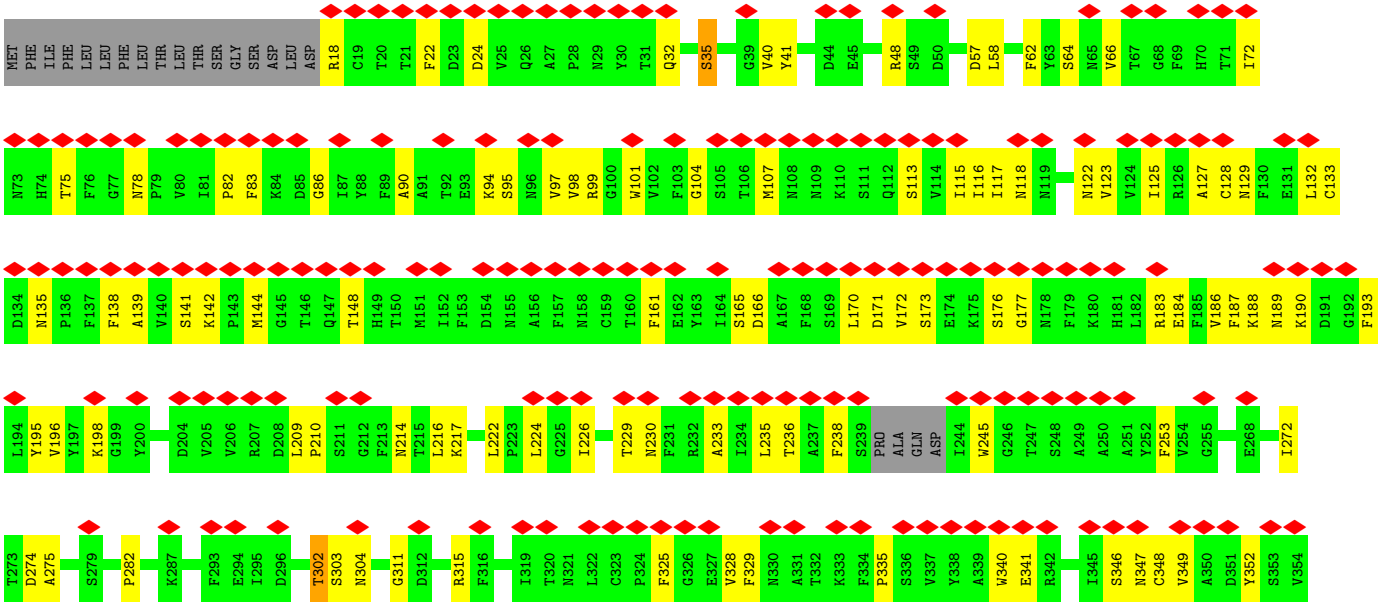
Chain A: 41% 63% 24% • 11%

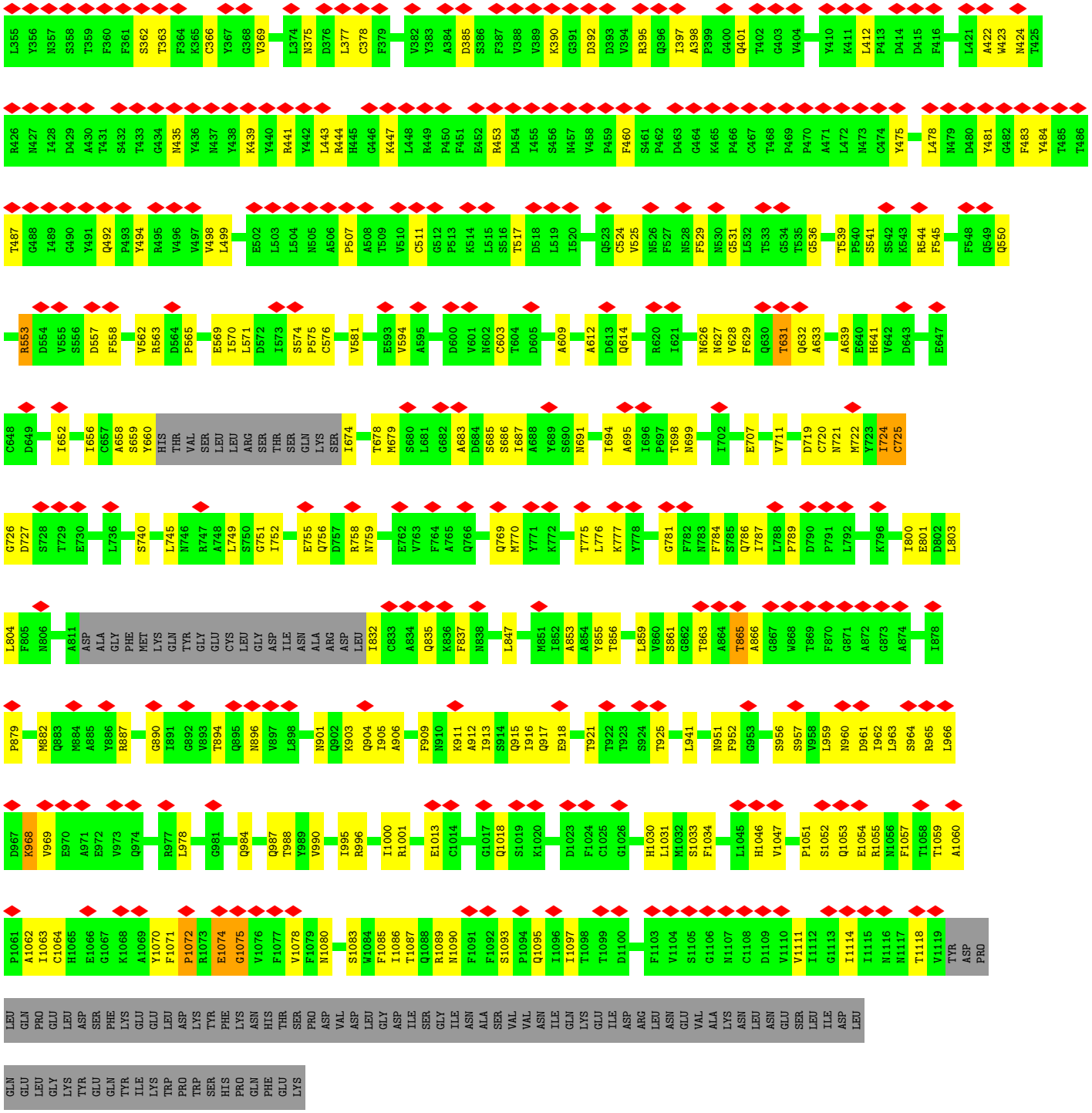




- Molecule 1: Spike glycoprotein

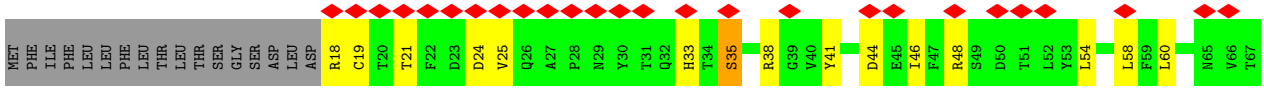
Chain B:

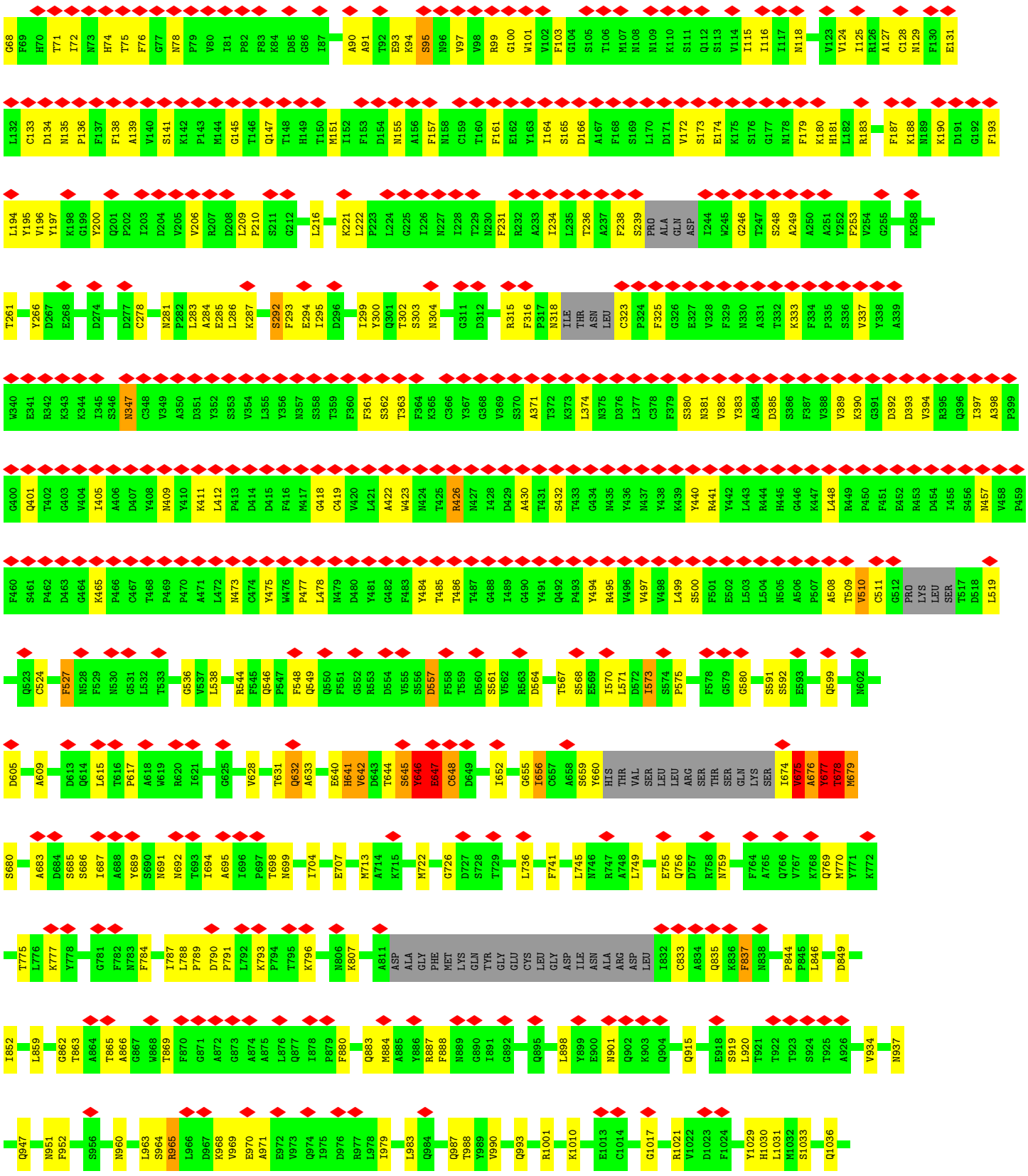




- Molecule 1: Spike glycoprotein

Chain C:




G68 F69 H70 T71 I72 N73 H74 T75 F76 G77 N78 P79 V80 I81 P82 F83 K84 D85 G86 I87 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 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 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 L216 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 K258
T261 Y266 D267 E268 D274 D277 C278 N281 P282 L283 A284 E285 L286 K287 S292 F293 E294 I295 D296 I299 Y300 Q301 T302 S303 N304 G311 D312 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 S358 T359 F360 F361 S362 T363 F364 K365 C366 Y367 G368 V369 S370 A371 T372 K373 L374 N375 D376 L377 C378 F379 S380 N381 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
Q523 C524 F527 N528 F529 N530 G531 L532 T533 G536 V537 L538 R544 F545 Q546 P547 F548 Q549 Q550 F551 G552 R553 D554 V555 S556 D557 F558 T559 D560 S561 V562 R563 D564 T567 S568 E569 I570 L571 D572 I573 S574 P575 F578 G579 G580 S591 S592 E593 Q599 N602
D605 A609 D613 Q614 L615 T616 P617 A618 W619 R620 I621 G625 V628 T631 Q632 A633 E640 H641 V642 D643 T644 S645 Y646 E647 C648 D649 I652 G655 I656 C657 A658 S659 Y660 HIS THR VAL SER LEU LEU ARG SER THR SER GLN LYS SER I674 V675 A676 Y677 T678 M679
S680 A683 D684 S685 S686 I687 A688 Y689 S690 N691 N692 T693 I694 A695 I696 P697 T698 N699 I704 E707 M713 A714 K715 M722 G726 D727 S728 T729 L736 F741 L745 W746 R747 A748 L749 E755 Q756 D757 R758 N759 F764 A765 Q766 V767 K768 Q769 M770 Y771 K772
T775 L776 K777 Y778 G781 F782 N783 F784 I787 L788 P789 D790 P791 L792 K793 P794 T795 K796 N806 K807 A811 ASP ALA GLY PHE MET LYS GLN TYR GLY GLU CYS LEU GLY ASP ILE ASN ALA ARG ASP LEU T832 C833 A834 Q835 K836 F837 N838 P844 P845 L846 D849
I852 L859 G862 T863 A864 T865 A866 G867 W868 T869 F870 G871 A872 G873 A874 A875 L876 Q877 I878 P879 F880 Q883 M884 A885 Y886 R887 F888 N889 G890 I891 G892 Q895 L898 Y899 E900 N901 Q902 K903 Q904 Q915 E918 S919 L920 T921 T922 T923 S924 T925 A926 V934 N937
Q947 N951 F952 S956 N960 L963 S964 R965 L966 D967 K968 V969 E970 A971 E972 V973 Q974 I975 D976 R977 L978 I979 L983 Q984 Q987 T988 Y989 V990 Q993 R1001 K1010 E1013 C1014 G1017 R1021 V1022 D1023 F1024 Y1029 H1030 L1031 M1032 S1033 Q1036

H1046 V1047 T1048 Y1049 S1052 Q1053 E1054 R1055 N1056 F1057 T1058 T1059 A1060 P1061 A1062 I1063 C1064 H1065 E1066 A1069 Y1070 F1071 P1072 R1073 E1074 G1075 V1076 F1077 V1078 F1079 N1080 S1083 W1084 F1085 I1086 T1087 Q1088 R1089 N1090 F1091 F1092 S1093 P1094 Q1095 I1096 I1097 T1098 T1099 D1100 N1101 T1102 F1103 V1104 S1105 G1106 N1107 C1108

D1109 V1110 V1111 I1112 G1113 I1114 I1115 N1116 N1117 T1118 V1119 TYR ASP PRO LEU GLN PRO GLU LEU ASP SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU

ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 2: Angiotensin-converting enzyme 2

Chain D: 99% 79% 20%

S19 T20 I21 E22 E23 Q24 A25 K26 T27 F28 L29 D30 K31 F32 N33 H34 E35 A36 E37 D38 L39 F40 Y41 Q42 S43 S44 L45 A46 S47 W48 N49 Y50 N51 T52 N53 I54 T55 E56 E57 N58 V59 Q60 N61 M62 N63 N64 A65 G66 D67 K68 W69 S70 A71 F72 L73 K74 E75 Q76 S77 T78

L79 A80 Q81 M82 Y83 P84 L85 Q86 E87 I88 Q89 N90 L91 T92 V93 K94 L95 Q96 L97 Q98 A99 L100 Q101 Q102 N103 G104 S105 S106 V107 L108 S109 E110 D111 K112 S113 K114 R115 L116 N117 T118 I119 L120 N121 T122 M123 S124 T125 I126 Y127 S128 T129 G130 K131 V132 C133 N134 P135 D136 N137 P138

Q139 E140 C141 L142 L143 L144 E145 P146 G147 L148 N149 E150 I151 M152 A153 N154 S155 L156 D157 Y158 N159 E160 R161 L162 W163 A164 W165 E166 S167 W168 R169 S170 E171 V172 G173 K174 Q175 L176 R177 P178 L179 Y180 E181 E182 Y183 V184 V185 L186 K187 N188 E189 M190 A191 R192 A193 N194 H195 Y196 E197 D198

Y199 G200 D201 Y202 W203 R204 G205 D206 Y207 E208 V209 N210 G211 V212 D213 G214 Y215 D216 Y217 S218 R219 G220 Q221 L222 I223 E224 D225 V226 E227 H228 T229 F230 E231 E232 I233 K234 P235 L236 Y237 E238 H239 L240 H241 A242 Y243 V244 R245 A246 K247 L248 M249 N250 A251 Y252 P253 S254 Y255 I256 S257 P258

I259 G260 C261 L262 P263 A264 H265 L266 L267 G268 D269 M270 W271 G272 R273 F274 W275 T276 N277 L278 Y279 S280 L281 T282 V283 P284 F285 G286 Q287 K288 P289 N290 I291 D292 V293 T294 D295 A296 M297 V298 D299 Q300 A301 W302 D303 A304 Q305 R306 I307 F308 K309 E310 A311 E312 K313 F314 F315 V316 S317 V318

G319 L320 P321 N322 N323 T324 Q325 G326 F327 W328 E329 N330 S331 M332 L333 T334 D335 P336 G337 N338 V339 Q340 K341 A342 V343 C344 H345 P346 T347 A348 W349 D350 L351 G352 K353 G354 D355 F356 R357 I358 L359 M360 C361 T362 K363 V364 T365 M366 D367 D368 F369 L370 T371 A372 H373 H374 E375 M376 G377 H378

I379 Q380 Y381 D382 M383 A384 Y385 A386 A387 Q388 P389 F390 L391 L392 R393 N394 G395 A396 N397 E398 G399 F400 H401 E402 A403 V404 G405 E406 I407 M408 S409 L410 S411 A412 A413 T414 P415 K416 H417 L418 K419 S420 I421 G422 L423 L424 S425 P426 D427 F428 Q429 E430 D431 N432 E433 T434 E435 I436 N437 F438

L439 L440 K441 Q442 A443 L444 T445 I446 V447 G448 T449 L450 P451 F452 T453 Y454 M455 L456 E457 K458 W459 R460 W461 M462 V463 F464 K465 G466 E467 I468 P469 K470 D471 Q472 W473 M474 K475 K476 W477 W478 E479 M480 K481 R482 E483 I484 V485 G486 V487 V488 E489 P490 V491 P492 H493 D494 E495 T496 Y497 C498

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	129462	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	33.479	Depositor
Minimum map value	-16.130	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.871	Depositor
Recommended contour level	8.0	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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.50	1/8499 (0.0%)	0.70	3/11568 (0.0%)
1	B	0.50	1/8499 (0.0%)	0.70	1/11568 (0.0%)
1	C	0.55	8/8435 (0.1%)	0.77	10/11477 (0.1%)
2	D	0.31	0/5007	0.56	1/6803 (0.0%)
All	All	0.49	10/30440 (0.0%)	0.70	15/41416 (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	14
1	B	0	19
1	C	0	21
2	D	0	1
All	All	0	55

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	677	TYR	CE2-CZ	-8.20	1.27	1.38
1	A	725	CYS	CB-SG	-6.94	1.70	1.82
1	C	678	THR	CA-C	-5.93	1.37	1.52
1	C	676	ALA	C-O	-5.67	1.12	1.23
1	C	646	TYR	CE1-CZ	-5.53	1.31	1.38
1	B	725	CYS	CB-SG	-5.40	1.73	1.81
1	C	642	VAL	N-CA	-5.33	1.35	1.46
1	C	677	TYR	CD2-CE2	-5.32	1.31	1.39
1	C	677	TYR	CA-C	-5.21	1.39	1.52
1	C	677	TYR	CA-CB	-5.18	1.42	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	642	VAL	CB-CA-C	-7.37	97.40	111.40
1	C	647	GLU	C-N-CA	-7.22	103.65	121.70
1	B	557	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	641	HIS	O-C-N	6.86	133.67	122.70
1	C	641	HIS	CA-C-N	-6.62	102.64	117.20
1	A	557	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	677	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	C	646	TYR	N-CA-C	5.95	127.06	111.00
2	D	558	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	787	ILE	C-N-CA	5.56	135.60	121.70
1	C	846	LEU	CA-CB-CG	-5.39	102.91	115.30
1	C	678	THR	C-N-CA	-5.30	108.46	121.70
1	C	557	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	675	VAL	C-N-CA	5.18	134.65	121.70
1	A	216	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	SER	Peptide
1	A	1074	GLU	Peptide
1	A	1077	PHE	Peptide
1	A	151	MET	Peptide
1	A	553	ARG	Peptide
1	A	62	PHE	Peptide
1	A	631	THR	Peptide
1	A	633	ALA	Peptide
1	A	724	ILE	Peptide
1	A	725	CYS	Peptide
1	A	726	GLY	Peptide
1	A	727	ASP	Peptide
1	A	923	THR	Peptide
1	A	968	LYS	Peptide
1	B	1052	SER	Peptide
1	B	1074	GLU	Peptide
1	B	1075	GLY	Peptide
1	B	35	SER	Peptide
1	B	507	PRO	Peptide
1	B	553	ARG	Peptide
1	B	558	PHE	Peptide
1	B	576	CYS	Peptide
1	B	62	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	629	PHE	Peptide
1	B	631	THR	Peptide
1	B	722	MET	Peptide
1	B	724	ILE	Peptide
1	B	726	GLY	Peptide
1	B	727	ASP	Peptide
1	B	776	LEU	Peptide
1	B	781	GLY	Peptide
1	B	837	PHE	Peptide
1	B	968	LYS	Peptide
1	C	1073	ARG	Peptide
1	C	1074	GLU	Peptide
1	C	1075	GLY	Peptide
1	C	1077	PHE	Peptide
1	C	151	MET	Peptide
1	C	206	VAL	Peptide
1	C	292	SER	Peptide
1	C	316	PHE	Peptide
1	C	347	ASN	Peptide
1	C	35	SER	Peptide
1	C	465	LYS	Peptide
1	C	511	CYS	Peptide
1	C	527	PHE	Peptide
1	C	54	LEU	Peptide
1	C	548	PHE	Peptide
1	C	567	THR	Peptide
1	C	573	ILE	Peptide
1	C	837	PHE	Peptide
1	C	865	THR	Peptide
1	C	95	SER	Peptide
1	C	97	VAL	Peptide
2	D	425	SER	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	200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8302	0	8082	210	0
1	C	8241	0	8011	259	0
2	D	4870	0	4643	73	0
All	All	29715	0	28818	697	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 12.

All (697) 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	1.33	1.59
1:C:646:TYR:CB	1:C:677:TYR:CE2	1.90	1.53
1:C:647:GLU:O	1:C:648:CYS:CB	1.77	1.26
1:C:646:TYR:HB2	1:C:677:TYR:CD2	1.78	1.17
1:C:646:TYR:CA	1:C:677:TYR:CE2	2.28	1.16
1:C:646:TYR:CB	1:C:677:TYR:CZ	2.29	1.15
1:C:646:TYR:CA	1:C:677:TYR:HE2	1.57	1.14
1:C:646:TYR:HB2	1:C:677:TYR:CZ	1.85	1.12
1:C:678:THR:O	1:C:679:MET:HB2	1.40	1.08
1:C:647:GLU:O	1:C:648:CYS:HB3	1.49	1.07
1:C:647:GLU:OE1	1:C:680:SER:OG	1.73	1.06
1:C:656:ILE:HG12	1:C:677:TYR:O	1.57	1.04
1:C:655:GLY:O	1:C:678:THR:O	1.83	0.97
1:C:646:TYR:N	1:C:677:TYR:CE2	2.34	0.95
1:C:646:TYR:HB3	1:C:677:TYR:CZ	1.98	0.95
1:C:647:GLU:O	1:C:648:CYS:HB2	1.67	0.94
1:C:640:GLU:O	1:C:642:VAL:HG23	1.68	0.92
1:C:678:THR:O	1:C:679:MET:CB	2.16	0.92
1:C:678:THR:OG1	1:C:679:MET:N	2.03	0.87
2:D:346:PRO:HA	2:D:359:LEU:O	1.75	0.87
1:C:93:GLU:O	1:C:181:HIS:HB2	1.77	0.84
1:A:190:LYS:O	1:A:193:PHE:HB2	1.80	0.81
1:C:646:TYR:N	1:C:677:TYR:CD2	2.49	0.81
1:B:18:ARG:N	1:B:133:CYS:HG	1.78	0.80
1:B:113:SER:O	1:B:127:ALA:HA	1.81	0.80
1:C:647:GLU:N	1:C:677:TYR:OH	2.15	0.79
1:B:115:ILE:O	1:B:125:ILE:HA	1.82	0.79
1:B:190:LYS:O	1:B:193:PHE:HB2	1.82	0.79
1:C:418:GLY:HA3	1:C:499:LEU:O	1.84	0.78
1:C:1088:GLN:HE22	1:C:1093:SER:HB2	1.48	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:TYR:N	1:C:677:TYR:HE2	1.78	0.77
1:A:913:ILE:O	1:A:916:ILE:HB	1.85	0.77
1:B:909:PHE:O	1:B:912:ALA:HB3	1.85	0.77
2:D:566:TRP:O	2:D:570:LEU:HB2	1.85	0.76
1:C:564:ASP:HB3	1:C:568:SER:H	1.50	0.76
1:B:118:ASN:HB3	1:B:170:LEU:HD21	1.68	0.75
1:C:18:ARG:N	1:C:133:CYS:HG	1.85	0.75
1:C:646:TYR:HB3	1:C:677:TYR:OH	1.87	0.74
1:C:646:TYR:O	1:C:647:GLU:CG	2.36	0.73
1:C:648:CYS:N	1:C:677:TYR:OH	2.22	0.73
1:A:100:GLY:HA2	1:A:116:ILE:O	1.89	0.72
1:C:647:GLU:OE1	1:C:647:GLU:HA	1.90	0.71
1:C:677:TYR:HD1	1:C:677:TYR:H	1.38	0.71
1:A:348:CYS:SG	1:A:349:VAL:N	2.64	0.70
1:C:713:MET:HG2	1:C:756:GLN:HE22	1.55	0.70
1:A:895:GLN:HG3	1:B:1074:GLU:HG2	1.75	0.69
1:A:906:ALA:O	1:A:909:PHE:HB3	1.92	0.69
1:A:94:LYS:HB3	1:A:175:LYS:HB2	1.76	0.68
1:C:422:ALA:HA	1:C:495:ARG:O	1.94	0.68
1:B:835:GLN:NE2	1:C:575:PRO:O	2.26	0.68
1:C:1030:HIS:HE1	1:C:1033:SER:HB2	1.58	0.68
1:A:128:CYS:SG	1:A:129:ASN:N	2.67	0.67
1:C:707:GLU:OE1	1:C:1046:HIS:NE2	2.28	0.67
1:C:299:ILE:HD11	1:C:652:ILE:HG12	1.77	0.67
1:A:837:PHE:HB3	1:B:575:PRO:HD3	1.77	0.66
1:B:99:ARG:HH22	1:B:172:VAL:HA	1.60	0.66
1:A:1064:CYS:HB3	1:A:1114:ILE:HG23	1.77	0.66
1:A:1061:PRO:HD2	1:A:1113:GLY:H	1.61	0.65
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.29	0.65
1:A:149:HIS:NE2	1:A:151:MET:SD	2.69	0.65
1:C:1063:ILE:HB	1:C:1070:TYR:HB2	1.79	0.64
1:A:960:ASN:H	1:A:963:LEU:HD13	1.62	0.64
1:C:656:ILE:CG1	1:C:677:TYR:O	2.39	0.64
1:B:340:TRP:O	1:B:453:ARG:NH1	2.31	0.64
1:C:722:MET:HA	1:C:726:GLY:HA2	1.80	0.64
1:A:58:LEU:HB2	1:A:188:LYS:HE3	1.80	0.64
1:A:1096:ILE:O	1:A:1101:ASN:ND2	2.30	0.64
1:C:686:SER:OG	1:C:687:ILE:N	2.31	0.63
1:C:887:ARG:NH1	1:C:1031:LEU:O	2.29	0.63
2:D:406:GLU:HG3	2:D:518:ARG:HD3	1.80	0.63
1:B:1059:THR:O	1:B:1080:ASN:ND2	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ASN:H	1:C:509:THR:HB	1.62	0.63
1:C:1062:ALA:HB3	1:C:1111:VAL:HG13	1.81	0.63
1:A:887:ARG:NH1	1:A:1031:LEU:O	2.29	0.63
1:A:325:PHE:HA	1:A:328:VAL:HG12	1.80	0.63
1:A:1097:ILE:HD13	1:A:1118:THR:HA	1.81	0.63
1:B:107:MET:HA	1:B:132:LEU:HD12	1.80	0.62
1:B:348:CYS:SG	1:B:349:VAL:N	2.71	0.62
1:C:385:ASP:O	1:C:497:VAL:HA	1.98	0.62
1:A:869:THR:OG1	1:B:1089:ARG:NH1	2.32	0.62
1:A:632:GLN:NE2	1:C:833:CYS:SG	2.69	0.62
1:A:536:GLY:HA3	1:A:574:SER:HA	1.80	0.62
1:A:786:GLN:HB3	1:A:799:PHE:HB3	1.81	0.62
1:C:704:ILE:HG12	1:C:1047:VAL:HG22	1.82	0.62
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.33	0.62
1:C:1096:ILE:O	1:C:1101:ASN:ND2	2.27	0.62
1:C:361:PHE:HA	1:C:423:TRP:HB3	1.83	0.61
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.82	0.61
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.82	0.61
1:C:646:TYR:HB3	1:C:677:TYR:CE2	2.12	0.61
1:B:101:TRP:HB2	1:B:116:ILE:HB	1.82	0.61
1:A:96:ASN:OD1	1:A:183:ARG:NH1	2.34	0.60
1:A:779:PHE:HB2	1:A:782:PHE:HB2	1.82	0.60
1:B:541:SER:HA	1:B:571:LEU:HG	1.83	0.60
1:A:139:ALA:HB3	1:A:148:THR:HB	1.83	0.60
1:C:363:THR:HB	1:C:422:ALA:HB3	1.83	0.60
1:B:94:LYS:HD2	1:B:176:SER:HA	1.82	0.60
1:B:484:TYR:HB2	1:B:487:THR:HB	1.83	0.60
1:A:182:LEU:HD23	1:A:201:GLN:HB3	1.82	0.60
1:A:1030:HIS:HE1	1:A:1033:SER:HB2	1.67	0.60
1:A:1097:ILE:HB	1:A:1118:THR:HG23	1.83	0.60
1:B:835:GLN:NE2	1:C:573:ILE:O	2.35	0.60
1:B:302:THR:HG23	1:B:581:VAL:HG23	1.82	0.60
1:C:524:CYS:HA	1:C:536:GLY:O	2.02	0.60
1:C:646:TYR:O	1:C:647:GLU:OE1	2.20	0.60
1:A:756:GLN:HA	1:A:759:ASN:HD22	1.67	0.60
1:C:656:ILE:HG13	1:C:678:THR:HA	1.82	0.60
1:A:378:CYS:HA	1:A:511:CYS:HA	1.83	0.59
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.84	0.59
1:A:575:PRO:HD3	1:C:837:PHE:HB3	1.84	0.59
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.82	0.59
1:A:553:ARG:HE	1:C:46:ILE:HD13	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ASN:HB3	1:A:483:PHE:HB2	1.84	0.59
1:B:315:ARG:NH1	1:B:517:THR:O	2.34	0.59
1:B:41:TYR:HB3	1:B:216:LEU:HD12	1.85	0.58
1:A:1054:GLU:O	1:A:1055:ARG:NH1	2.35	0.58
1:A:541:SER:HB3	1:A:543:LYS:HG2	1.84	0.58
1:B:209:LEU:HB2	1:B:253:PHE:HE2	1.69	0.58
1:B:913:ILE:O	1:B:916:ILE:HB	2.03	0.58
1:A:95:SER:HB3	1:A:175:LYS:HE3	1.86	0.58
1:A:138:PHE:HB2	1:A:236:THR:HA	1.85	0.58
1:A:316:PHE:O	1:A:566:LYS:NZ	2.36	0.58
1:A:887:ARG:NH1	1:A:1032:MET:SD	2.77	0.58
1:A:30:TYR:O	1:A:32:GLN:NE2	2.34	0.58
1:B:117:ILE:O	1:B:123:VAL:HA	2.03	0.58
1:A:626:ASN:ND2	1:A:640:GLU:OE2	2.35	0.58
1:C:398:ALA:HB3	1:C:401:GLN:HG3	1.85	0.58
1:A:325:PHE:HE1	1:A:345:ILE:HD13	1.67	0.57
1:C:281:ASN:H	1:C:284:ALA:HB3	1.68	0.57
1:B:1064:CYS:HB3	1:B:1114:ILE:HG23	1.86	0.57
1:B:282:PRO:HB2	1:B:594:VAL:HG21	1.86	0.57
1:B:887:ARG:NH1	1:B:1031:LEU:O	2.36	0.57
1:C:124:VAL:HG22	1:C:164:ILE:HG12	1.85	0.57
1:C:646:TYR:O	1:C:647:GLU:HG2	2.03	0.57
1:C:677:TYR:N	1:C:677:TYR:CD1	2.70	0.57
1:C:25:VAL:HA	1:C:76:PHE:HB3	1.85	0.57
1:A:196:VAL:HB	1:A:220:PHE:HB2	1.87	0.57
1:B:777:LYS:NZ	1:B:789:PRO:O	2.37	0.57
1:A:99:ARG:HD3	1:A:118:ASN:HB2	1.85	0.57
1:C:381:ASN:H	1:C:509:THR:HG1	1.51	0.57
2:D:132:VAL:O	2:D:141:CYS:HA	2.05	0.57
1:C:383:TYR:HB2	1:C:500:SER:HB2	1.86	0.57
1:B:755:GLU:OE1	1:B:1001:ARG:NH2	2.38	0.57
1:B:756:GLN:HA	1:B:759:ASN:HD22	1.69	0.57
1:C:58:LEU:HB2	1:C:188:LYS:HE3	1.86	0.57
1:C:1029:TYR:HB2	1:C:1049:TYR:HB3	1.85	0.57
1:A:711:VAL:HG22	1:A:1041:GLY:HA2	1.87	0.56
1:B:424:ASN:ND2	1:B:492:GLN:OE1	2.38	0.56
1:B:678:THR:OG1	1:B:679:MET:N	2.34	0.56
1:B:720:CYS:SG	1:B:721:ASN:N	2.78	0.56
1:B:1060:ALA:HB2	1:B:1080:ASN:HD22	1.69	0.56
1:C:390:LYS:HE3	1:C:392:ASP:HB2	1.87	0.56
1:B:128:CYS:SG	1:B:129:ASN:N	2.77	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:THR:HG22	1:C:644:THR:O	2.05	0.56
1:C:1054:GLU:O	1:C:1055:ARG:NH1	2.37	0.56
2:D:245:ARG:NH2	2:D:605:GLY:O	2.36	0.56
2:D:278:LEU:O	2:D:282:THR:N	2.38	0.56
2:D:389:PRO:HG2	2:D:392:LEU:HB2	1.88	0.56
1:B:563:ARG:HG3	1:B:569:GLU:HG3	1.86	0.56
1:B:184:GLU:OE1	1:B:214:ASN:ND2	2.34	0.56
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.70	0.56
1:B:740:SER:OG	1:C:947:GLN:NE2	2.39	0.56
1:B:698:THR:OG1	1:B:1053:GLN:OE1	2.23	0.56
1:B:1030:HIS:CE1	1:B:1033:SER:HB2	2.41	0.56
1:B:1086:ILE:O	1:B:1095:GLN:NE2	2.38	0.56
1:C:642:VAL:HG21	1:C:675:VAL:CB	2.35	0.56
2:D:51:ASN:HB3	2:D:359:LEU:HG	1.87	0.56
1:A:720:CYS:SG	1:A:721:ASN:N	2.79	0.56
1:C:128:CYS:SG	1:C:129:ASN:N	2.79	0.56
1:B:536:GLY:HA3	1:B:574:SER:HA	1.87	0.55
1:B:719:ASP:OD1	1:C:304:ASN:ND2	2.39	0.55
1:A:41:TYR:OH	1:A:188:LYS:NZ	2.29	0.55
1:A:678:THR:OG1	1:A:679:MET:N	2.38	0.55
1:A:987:GLN:NE2	1:B:988:THR:OG1	2.39	0.55
1:B:423:TRP:O	1:B:494:TYR:HA	2.07	0.55
1:A:440:TYR:O	1:A:478:LEU:HA	2.05	0.55
1:C:642:VAL:HG21	1:C:675:VAL:HB	1.87	0.55
1:A:745:LEU:HD22	1:A:990:VAL:HG21	1.87	0.55
1:A:769:GLN:HE21	1:B:685:SER:HB2	1.71	0.55
1:A:1098:THR:OG1	1:A:1101:ASN:ND2	2.40	0.55
2:D:402:GLU:HG3	2:D:518:ARG:HG3	1.88	0.55
1:A:631:THR:O	1:A:633:ALA:N	2.40	0.55
1:A:699:ASN:H	1:A:1053:GLN:HB2	1.72	0.55
1:B:32:GLN:HA	1:B:66:VAL:O	2.07	0.55
1:B:99:ARG:HH12	1:B:172:VAL:HG13	1.71	0.55
1:C:777:LYS:HZ2	1:C:791:PRO:HD3	1.71	0.55
1:B:959:LEU:HD23	1:B:962:ILE:HD11	1.89	0.54
1:C:188:LYS:HB3	1:C:195:TYR:HB2	1.88	0.54
1:C:380:SER:HA	1:C:509:THR:H	1.71	0.54
1:B:866:ALA:HB2	1:C:689:TYR:HE1	1.72	0.54
1:A:1062:ALA:HB3	1:A:1111:VAL:HG13	1.89	0.54
1:A:1064:CYS:HB2	1:A:1111:VAL:HG11	1.88	0.54
1:B:186:VAL:O	1:B:196:VAL:HA	2.07	0.54
1:C:394:VAL:HG21	1:C:494:TYR:HD2	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:CYS:H	1:C:677:TYR:HH	1.53	0.54
2:D:524:GLN:HB3	2:D:574:VAL:HG11	1.90	0.54
1:B:879:PRO:HB3	1:C:691:ASN:HA	1.88	0.54
1:C:362:SER:N	1:C:422:ALA:O	2.37	0.54
1:B:1093:SER:O	1:B:1095:GLN:NE2	2.40	0.54
1:A:441:ARG:NH1	1:A:454:ASP:O	2.41	0.54
1:A:953:GLY:O	1:A:977:ARG:NH1	2.39	0.54
1:C:141:SER:HB3	1:C:145:GLY:H	1.72	0.54
1:C:646:TYR:O	1:C:680:SER:OG	2.26	0.54
1:C:698:THR:OG1	1:C:1055:ARG:NH2	2.41	0.54
1:B:99:ARG:NH2	1:B:171:ASP:O	2.41	0.54
1:B:325:PHE:HA	1:B:328:VAL:HG12	1.89	0.54
1:B:378:CYS:HA	1:B:511:CYS:HA	1.90	0.54
1:B:90:ALA:HA	1:B:183:ARG:O	2.08	0.54
1:C:960:ASN:H	1:C:963:LEU:HD13	1.73	0.54
1:B:524:CYS:HA	1:B:536:GLY:O	2.08	0.54
1:A:113:SER:O	1:A:127:ALA:HA	2.08	0.53
1:A:652:ILE:HD11	1:A:658:ALA:HB2	1.89	0.53
1:A:888:PHE:HE2	1:A:898:LEU:HB2	1.73	0.53
1:C:441:ARG:HG3	1:C:477:PRO:HB2	1.91	0.53
2:D:119:ILE:HD12	2:D:179:LEU:HD22	1.88	0.53
1:A:323:CYS:N	1:A:348:CYS:SG	2.82	0.53
1:A:420:VAL:HG22	1:A:498:VAL:HG22	1.90	0.53
2:D:378:HIS:HE1	2:D:402:GLU:HA	1.73	0.53
1:A:749:LEU:HD23	1:A:752:ILE:HD12	1.91	0.53
1:B:905:ILE:O	1:B:909:PHE:N	2.38	0.53
1:C:90:ALA:HB3	1:C:253:PHE:HB2	1.90	0.53
1:C:411:LYS:HB2	1:C:448:LEU:HB2	1.90	0.53
1:C:934:VAL:HA	1:C:937:ASN:HD22	1.74	0.53
1:A:431:THR:OG1	1:A:434:GLY:O	2.26	0.53
1:B:392:ASP:OD1	1:B:395:ARG:NH2	2.41	0.53
1:B:960:ASN:HA	1:B:963:LEU:HB2	1.90	0.53
1:B:1063:ILE:HD11	1:B:1078:VAL:HG11	1.91	0.53
1:B:1097:ILE:HD13	1:B:1118:THR:HA	1.91	0.53
1:C:538:LEU:HD22	1:C:570:ILE:HD12	1.90	0.53
1:C:100:GLY:HA3	1:C:234:ILE:HB	1.89	0.53
1:C:283:LEU:HD22	1:C:592:SER:HB2	1.89	0.53
2:D:439:LEU:HB3	2:D:591:LEU:HD22	1.91	0.53
1:A:1079:PHE:HB2	1:A:1087:THR:HG23	1.91	0.53
1:B:78:ASN:ND2	1:B:233:ALA:O	2.36	0.53
1:B:377:LEU:HD22	1:B:531:GLY:HA2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:VAL:HG22	1:C:389:VAL:HG12	1.91	0.53
1:B:626:ASN:ND2	1:B:639:ALA:O	2.42	0.52
1:C:432:SER:HA	1:C:484:TYR:HB3	1.91	0.52
1:C:646:TYR:O	1:C:647:GLU:CB	2.53	0.52
1:C:1078:VAL:HG22	1:C:1086:ILE:HG12	1.91	0.52
1:A:1051:PRO:HB3	1:A:1090:ASN:HD21	1.74	0.52
1:C:99:ARG:HE	1:C:118:ASN:HD22	1.58	0.52
2:D:233:ILE:HD11	2:D:581:VAL:HG21	1.91	0.52
1:A:543:LYS:HB3	1:A:545:PHE:HB2	1.91	0.52
1:B:444:ARG:NH1	1:B:447:LYS:O	2.42	0.52
1:C:94:LYS:NZ	1:C:249:ALA:O	2.40	0.52
2:D:351:LEU:HB2	2:D:355:ASP:O	2.09	0.52
1:A:352:TYR:HD1	1:A:355:LEU:HD12	1.74	0.52
1:B:99:ARG:HE	1:B:118:ASN:HD22	1.58	0.52
2:D:37:GLU:OE1	2:D:393:ARG:NH1	2.43	0.52
1:C:101:TRP:HB2	1:C:116:ILE:HB	1.91	0.52
1:C:486:THR:O	2:D:330:ASN:ND2	2.42	0.52
2:D:134:ASN:ND2	2:D:140:GLU:OE1	2.43	0.52
1:A:538:LEU:HD22	1:A:570:ILE:HD12	1.91	0.52
1:A:769:GLN:NE2	1:B:683:ALA:O	2.42	0.52
1:B:302:THR:OG1	1:B:303:SER:N	2.43	0.52
1:C:473:ASN:ND2	1:C:475:TYR:OH	2.42	0.52
2:D:75:GLU:O	2:D:78:THR:OG1	2.26	0.52
1:A:370:SER:OG	1:C:965:ARG:O	2.28	0.52
1:A:430:ALA:HA	1:A:435:ASN:HB2	1.92	0.52
1:B:35:SER:OG	1:B:64:SER:N	2.42	0.52
1:C:99:ARG:HD2	1:C:147:GLN:HE22	1.74	0.52
1:C:193:PHE:HA	1:C:222:LEU:O	2.10	0.52
1:B:397:ILE:HG23	1:B:412:LEU:HD11	1.92	0.51
1:C:292:SER:OG	1:C:293:PHE:N	2.43	0.51
1:A:301:GLN:NE2	1:A:302:THR:O	2.43	0.51
1:A:771:TYR:HD1	1:B:687:ILE:HG12	1.74	0.51
1:B:987:GLN:NE2	1:C:988:THR:OG1	2.42	0.51
1:C:238:PHE:HB2	1:C:246:GLY:H	1.74	0.51
1:A:1093:SER:O	1:A:1095:GLN:NE2	2.42	0.51
1:B:439:LYS:HD3	1:B:478:LEU:HB3	1.92	0.51
1:B:539:THR:HG23	1:B:571:LEU:HB2	1.91	0.51
1:C:302:THR:OG1	1:C:303:SER:N	2.42	0.51
1:B:116:ILE:HG13	1:B:125:ILE:HG12	1.92	0.51
1:B:303:SER:OG	1:B:304:ASN:N	2.43	0.51
1:C:646:TYR:H	1:C:677:TYR:HD2	1.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.51
1:A:988:THR:OG1	1:C:987:GLN:NE2	2.43	0.51
1:C:645:SER:HB3	1:C:680:SER:N	2.26	0.51
1:C:755:GLU:OE1	1:C:1001:ARG:NH2	2.44	0.51
2:D:148:LEU:HG	2:D:164:ALA:HB1	1.93	0.51
1:B:956:SER:OG	1:B:957:SER:N	2.41	0.51
1:C:440:TYR:O	1:C:478:LEU:HA	2.11	0.51
1:C:1063:ILE:H	1:C:1070:TYR:H	1.59	0.51
1:A:69:PHE:HB2	1:A:252:TYR:O	2.11	0.51
1:B:1063:ILE:HB	1:B:1070:TYR:HB2	1.91	0.51
1:A:26:GLN:HB2	1:A:75:THR:HA	1.93	0.50
1:C:138:PHE:HB2	1:C:236:THR:HG22	1.92	0.50
1:C:419:CYS:HB2	1:C:499:LEU:HD12	1.91	0.50
1:C:1086:ILE:O	1:C:1095:GLN:NE2	2.44	0.50
2:D:554:LEU:O	2:D:558:LEU:HB2	2.11	0.50
1:A:78:ASN:ND2	1:A:233:ALA:O	2.42	0.50
1:A:580:GLY:H	1:A:599:GLN:HB2	1.76	0.50
1:B:562:VAL:HG23	1:B:570:ILE:HG13	1.92	0.50
1:C:968:LYS:O	1:C:971:ALA:N	2.39	0.50
1:A:267:ASP:OD1	1:A:271:THR:N	2.40	0.50
1:B:1030:HIS:HE1	1:B:1033:SER:HB2	1.76	0.50
2:D:330:ASN:HB3	2:D:357:ARG:HE	1.76	0.50
1:A:1089:ARG:NH1	1:C:869:THR:OG1	2.44	0.50
1:C:174:GLU:HG3	1:C:248:SER:HB3	1.93	0.50
2:D:245:ARG:NH1	2:D:603:PHE:O	2.44	0.50
1:A:33:HIS:HB2	1:A:66:VAL:HB	1.93	0.50
1:C:1031:LEU:N	1:C:1047:VAL:O	2.45	0.50
1:C:1083:SER:HB3	1:C:1115:ILE:HG23	1.94	0.50
2:D:80:ALA:O	2:D:101:GLN:NE2	2.38	0.50
2:D:529:LEU:HD21	2:D:554:LEU:HD22	1.93	0.50
1:B:165:SER:OG	1:B:166:ASP:N	2.45	0.50
1:B:694:ILE:O	1:B:1057:PHE:N	2.39	0.50
1:C:591:SER:OG	1:C:592:SER:N	2.45	0.50
1:A:89:PHE:HB3	1:A:185:PHE:O	2.12	0.50
1:A:99:ARG:NH2	1:A:171:ASP:O	2.44	0.50
1:A:848:THR:O	1:A:852:ILE:N	2.36	0.50
1:C:190:LYS:O	1:C:193:PHE:HB2	2.12	0.50
1:C:380:SER:HB2	1:C:508:ALA:HA	1.94	0.50
1:A:656:ILE:HA	1:A:678:THR:HA	1.94	0.49
1:A:685:SER:HB2	1:C:769:GLN:HE21	1.76	0.49
1:B:612:ALA:O	1:B:614:GLN:NE2	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:LEU:HD13	1:B:921:THR:HG22	1.93	0.49
2:D:237:TYR:OH	2:D:485:VAL:O	2.20	0.49
1:B:962:ILE:HG13	1:B:963:LEU:HD12	1.94	0.49
1:C:145:GLY:HA3	1:C:173:SER:HB3	1.94	0.49
1:C:887:ARG:NH2	1:C:1017:GLY:O	2.45	0.49
2:D:275:TRP:HB3	2:D:444:LEU:HD12	1.94	0.49
1:C:527:PHE:HE1	1:C:538:LEU:HD11	1.77	0.49
1:A:362:SER:N	1:A:422:ALA:O	2.44	0.49
1:B:125:ILE:HD13	1:B:222:LEU:HD11	1.93	0.49
1:B:529:PHE:HE2	1:B:562:VAL:HG21	1.78	0.49
1:B:1031:LEU:N	1:B:1047:VAL:O	2.46	0.49
1:C:640:GLU:O	1:C:642:VAL:CG2	2.52	0.49
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.94	0.49
1:A:127:ALA:HB3	1:A:161:PHE:HB3	1.93	0.49
1:B:962:ILE:O	1:B:966:LEU:N	2.46	0.49
1:A:140:VAL:O	1:A:238:PHE:HA	2.13	0.49
1:B:960:ASN:O	1:B:964:SER:N	2.41	0.49
1:C:103:PHE:CD1	1:C:231:PHE:HB2	2.48	0.49
1:C:580:GLY:H	1:C:599:GLN:HB2	1.78	0.49
1:C:631:THR:O	1:C:631:THR:OG1	2.30	0.49
1:C:775:THR:HA	1:C:777:LYS:HE3	1.94	0.49
2:D:281:LEU:HD12	2:D:282:THR:HG23	1.94	0.49
2:D:435:GLU:OE2	2:D:540:HIS:NE2	2.46	0.49
1:B:609:ALA:HA	1:B:614:GLN:HB2	1.94	0.49
1:C:99:ARG:HE	1:C:118:ASN:HB2	1.77	0.49
1:B:903:LYS:O	1:B:906:ALA:HB3	2.13	0.49
1:C:285:GLU:OE2	1:C:302:THR:OG1	2.31	0.49
1:A:405:ILE:O	1:A:409:ASN:N	2.46	0.48
1:B:859:LEU:O	1:B:863:THR:OG1	2.21	0.48
2:D:588:PHE:O	2:D:592:PHE:N	2.46	0.48
1:A:292:SER:OG	1:A:293:PHE:N	2.45	0.48
1:A:960:ASN:HA	1:A:963:LEU:HD22	1.95	0.48
1:A:352:TYR:HD2	1:A:375:ASN:HB3	1.78	0.48
1:A:994:LEU:HG	1:B:995:ILE:HG21	1.95	0.48
1:A:1097:ILE:H	1:A:1097:ILE:HG13	1.45	0.48
2:D:365:THR:HG22	2:D:367:ASP:H	1.78	0.48
1:A:46:ILE:HD13	1:B:553:ARG:HE	1.78	0.48
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.94	0.48
1:A:41:TYR:HB3	1:A:216:LEU:HB2	1.94	0.48
1:A:692:ASN:HA	1:A:1059:THR:HG22	1.95	0.48
1:C:21:THR:HA	1:C:135:ASN:HD22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ALA:HB1	1:C:239:SER:HB2	1.95	0.48
1:C:381:ASN:N	1:C:509:THR:HG1	2.12	0.48
2:D:482:ARG:NH2	2:D:613:TYR:OH	2.47	0.48
1:B:82:PRO:HA	1:B:230:ASN:HA	1.95	0.48
1:B:188:LYS:HB3	1:B:195:TYR:HB2	1.94	0.48
1:C:129:ASN:ND2	1:C:157:PHE:O	2.47	0.48
1:C:605:ASP:O	1:C:609:ALA:HB2	2.13	0.48
1:C:968:LYS:HG3	1:C:969:VAL:HG23	1.96	0.48
1:B:894:THR:HG23	1:B:896:ASN:H	1.79	0.48
1:B:912:ALA:O	1:B:916:ILE:N	2.35	0.48
1:B:1064:CYS:HB2	1:B:1111:VAL:HG21	1.95	0.48
1:C:898:LEU:O	1:C:901:ASN:N	2.35	0.48
1:A:222:LEU:HB3	1:A:224:LEU:HG	1.96	0.48
1:A:772:LYS:HB2	1:B:686:SER:HA	1.96	0.48
1:A:914:SER:O	1:A:917:GLN:HB2	2.14	0.48
1:A:444:ARG:NH1	1:A:447:LYS:O	2.46	0.48
1:C:115:ILE:O	1:C:125:ILE:HA	2.13	0.48
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.96	0.48
2:D:503:LEU:HD23	2:D:505:HIS:H	1.79	0.48
1:A:539:THR:HG23	1:A:571:LEU:HB2	1.95	0.48
1:A:887:ARG:HH12	1:A:1032:MET:HA	1.78	0.48
1:C:694:ILE:N	1:C:1057:PHE:O	2.45	0.48
1:A:141:SER:HB3	1:A:144:MET:HB2	1.96	0.47
1:A:203:ILE:HD13	1:A:210:PRO:HG3	1.94	0.47
1:C:646:TYR:O	1:C:647:GLU:CD	2.53	0.47
2:D:247:LYS:HD2	2:D:250:ASN:HD22	1.79	0.47
1:A:203:ILE:HD12	1:A:205:VAL:HG23	1.96	0.47
1:A:859:LEU:O	1:A:863:THR:OG1	2.27	0.47
1:A:879:PRO:HB3	1:B:691:ASN:HA	1.97	0.47
1:A:984:GLN:HE21	1:B:984:GLN:HE22	1.62	0.47
1:B:1062:ALA:HB3	1:B:1111:VAL:HG13	1.95	0.47
2:D:198:ASP:OD1	2:D:201:ASP:N	2.46	0.47
1:B:139:ALA:HB3	1:B:148:THR:HB	1.96	0.47
1:B:188:LYS:HE2	1:B:190:LYS:HB2	1.96	0.47
1:B:652:ILE:HB	1:B:656:ILE:HG22	1.96	0.47
1:C:315:ARG:HH22	1:C:519:LEU:HB3	1.80	0.47
1:C:745:LEU:HD22	1:C:990:VAL:HG21	1.96	0.47
1:C:968:LYS:HG3	1:C:969:VAL:H	1.79	0.47
1:A:697:PRO:HB3	1:A:1053:GLN:H	1.80	0.47
1:A:1060:ALA:HA	1:A:1113:GLY:HA3	1.96	0.47
1:B:86:GLY:CA	1:B:187:PHE:O	2.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:HIS:HB3	1:C:1070:TYR:HE2	1.79	0.47
2:D:344:CYS:HB3	2:D:361:CYS:HB2	1.76	0.47
1:A:575:PRO:HG2	1:C:835:GLN:HG2	1.95	0.47
1:B:329:PHE:HZ	1:B:499:LEU:HD11	1.79	0.47
1:B:390:LYS:HE2	1:B:481:TYR:HA	1.95	0.47
1:C:605:ASP:O	1:C:609:ALA:CB	2.63	0.47
1:C:628:VAL:HG13	1:C:641:HIS:CE1	2.49	0.47
1:C:628:VAL:HG13	1:C:641:HIS:NE2	2.30	0.47
1:C:777:LYS:NZ	1:C:789:PRO:O	2.44	0.47
1:C:784:PHE:O	1:C:788:LEU:N	2.42	0.47
2:D:184:VAL:HG12	2:D:464:PHE:HE1	1.80	0.47
1:A:698:THR:OG1	1:A:1053:GLN:OE1	2.19	0.47
1:B:24:ASP:O	1:B:245:TRP:NE1	2.40	0.47
1:B:628:VAL:HG22	1:B:641:HIS:CE1	2.49	0.47
1:C:646:TYR:C	1:C:680:SER:OG	2.53	0.47
1:C:1060:ALA:HB3	1:C:1080:ASN:HD22	1.80	0.47
1:A:377:LEU:HD11	1:C:964:SER:HB2	1.96	0.47
1:B:22:PHE:H	1:B:135:ASN:HD22	1.61	0.47
1:B:770:MET:N	1:C:683:ALA:O	2.48	0.47
1:C:165:SER:OG	1:C:166:ASP:N	2.46	0.47
1:C:418:GLY:CA	1:C:499:LEU:O	2.60	0.47
1:C:713:MET:SD	1:C:993:GLN:NE2	2.88	0.47
1:C:790:ASP:HB2	1:C:793:LYS:HG2	1.96	0.47
1:A:460:PHE:N	1:A:475:TYR:O	2.48	0.47
1:A:633:ALA:HB2	1:C:844:PRO:HG3	1.97	0.47
1:C:131:GLU:OE1	1:C:155:ASN:ND2	2.48	0.47
1:C:979:ILE:O	1:C:983:LEU:HB2	2.15	0.47
1:A:114:VAL:HG23	1:A:127:ALA:HB2	1.96	0.47
1:A:424:ASN:ND2	1:A:492:GLN:OE1	2.43	0.47
1:B:97:VAL:HG12	1:B:98:VAL:HG13	1.98	0.47
2:D:116:LEU:HD13	2:D:186:LEU:HB2	1.97	0.47
1:B:1013:GLU:OE2	1:C:1021:ARG:NE	2.46	0.46
1:B:769:GLN:HE22	1:C:685:SER:HB3	1.81	0.46
1:B:861:SER:O	1:B:865:THR:OG1	2.32	0.46
1:B:960:ASN:H	1:B:963:LEU:HD13	1.80	0.46
1:C:194:LEU:O	1:C:221:LYS:HA	2.14	0.46
1:C:849:ASP:HA	1:C:852:ILE:HD12	1.96	0.46
1:C:180:LYS:O	1:C:200:TYR:OH	2.31	0.46
1:A:99:ARG:HH12	1:A:172:VAL:HG13	1.81	0.46
1:B:784:PHE:HA	1:B:787:ILE:HD12	1.97	0.46
1:C:24:ASP:OD2	1:C:74:HIS:ND1	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:SER:HB3	1:C:680:SER:CA	2.45	0.46
1:C:787:ILE:HG23	1:C:1036:GLN:HE22	1.81	0.46
1:B:198:LYS:O	1:B:217:LYS:N	2.34	0.46
1:B:911:LYS:O	1:B:915:GLN:N	2.42	0.46
1:C:41:TYR:OH	1:C:188:LYS:NZ	2.43	0.46
1:C:91:ALA:HB3	1:C:183:ARG:HB2	1.98	0.46
1:A:370:SER:OG	1:C:970:GLU:OE2	2.25	0.46
1:B:603:CYS:HB3	1:B:627:ASN:HD21	1.79	0.46
1:C:95:SER:H	1:C:181:HIS:CD2	2.34	0.46
1:C:646:TYR:N	1:C:677:TYR:HD2	2.07	0.46
1:A:575:PRO:O	1:C:835:GLN:NE2	2.36	0.46
1:C:286:LEU:HD11	1:C:300:TYR:HD2	1.81	0.46
1:C:287:LYS:HA	1:C:295:ILE:HD11	1.98	0.46
1:C:381:ASN:N	1:C:509:THR:OG1	2.43	0.46
1:A:93:GLU:HG3	1:A:183:ARG:HH22	1.81	0.46
1:A:626:ASN:ND2	1:A:639:ALA:O	2.48	0.46
2:D:453:THR:HG21	2:D:516:TYR:HB2	1.98	0.46
1:B:104:GLY:O	1:B:229:THR:N	2.41	0.46
1:B:346:SER:OG	1:B:347:ASN:N	2.48	0.46
1:A:775:THR:HA	1:A:777:LYS:HG3	1.97	0.46
1:C:116:ILE:HA	1:C:125:ILE:HG12	1.98	0.46
1:B:340:TRP:CE2	1:B:453:ARG:HD3	2.51	0.45
1:B:398:ALA:HB3	1:B:401:GLN:HG3	1.98	0.45
1:A:274:ASP:OD1	1:A:275:ALA:N	2.48	0.45
1:C:807:LYS:NZ	1:C:920:LEU:O	2.38	0.45
1:A:809:THR:OG1	1:A:810:LEU:N	2.50	0.45
2:D:539:LEU:HD23	2:D:587:TYR:HB2	1.97	0.45
1:A:324:PRO:O	1:A:328:VAL:N	2.39	0.45
1:A:440:TYR:HB3	1:A:481:TYR:HE1	1.82	0.45
1:B:311:GLY:H	1:B:525:VAL:HG12	1.80	0.45
1:B:631:THR:O	1:B:633:ALA:N	2.40	0.45
1:C:371:ALA:HA	1:C:374:LEU:HD22	1.98	0.45
1:A:72:ILE:H	1:A:75:THR:HB	1.82	0.45
1:C:698:THR:OG1	1:C:1053:GLN:OE1	2.20	0.45
2:D:32:PHE:O	2:D:36:ALA:CB	2.64	0.45
1:A:802:ASP:O	1:A:806:ASN:ND2	2.49	0.45
1:B:362:SER:N	1:B:422:ALA:O	2.47	0.45
1:B:366:CYS:HB3	1:B:369:VAL:HG23	1.99	0.45
1:B:660:TYR:HB2	1:B:674:ILE:HA	1.98	0.45
1:B:721:ASN:HD22	1:C:304:ASN:HD22	1.65	0.45
2:D:81:GLN:NE2	2:D:103:ASN:OD1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASP:OD1	1:A:555:VAL:N	2.49	0.45
1:B:138:PHE:HB2	1:B:236:THR:HG22	1.98	0.45
1:B:224:LEU:HB3	1:B:226:ILE:HG12	1.98	0.45
1:B:363:THR:HB	1:B:422:ALA:HB3	1.97	0.45
1:A:269:ASN:OD1	1:B:544:ARG:NE	2.49	0.45
1:A:344:LYS:HG3	1:A:383:TYR:HE1	1.81	0.45
1:B:435:ASN:HB3	1:B:483:PHE:HB2	1.99	0.45
1:B:563:ARG:NE	1:B:569:GLU:OE2	2.49	0.45
1:C:646:TYR:C	1:C:677:TYR:HE2	2.17	0.45
1:C:951:ASN:OD1	1:C:952:PHE:N	2.49	0.45
2:D:518:ARG:O	2:D:522:GLN:HB2	2.16	0.45
1:A:948:LEU:HD23	1:A:948:LEU:HA	1.75	0.45
1:C:642:VAL:HG21	1:C:675:VAL:CA	2.46	0.45
2:D:247:LYS:HA	2:D:250:ASN:HD22	1.81	0.45
2:D:370:LEU:HB3	2:D:409:SER:HB2	1.99	0.44
1:A:848:THR:HB	1:A:851:MET:HB2	1.98	0.44
1:B:775:THR:HA	1:B:777:LYS:HE3	1.99	0.44
1:C:209:LEU:HD12	1:C:210:PRO:HD2	1.99	0.44
1:C:397:ILE:HA	1:C:412:LEU:HD21	1.98	0.44
1:C:426:ARG:HA	1:C:430:ALA:HB3	1.99	0.44
1:C:674:ILE:HD12	1:C:675:VAL:O	2.17	0.44
1:B:95:SER:OG	1:B:173:SER:O	2.27	0.44
1:B:951:ASN:OD1	1:B:952:PHE:N	2.50	0.44
1:A:24:ASP:HB3	1:A:245:TRP:HE1	1.83	0.44
1:A:352:TYR:HA	1:A:355:LEU:HD12	1.99	0.44
1:A:405:ILE:HG23	1:A:409:ASN:HD22	1.82	0.44
1:B:978:LEU:HD23	1:B:978:LEU:HA	1.85	0.44
1:C:35:SER:HB2	1:C:60:LEU:HD21	1.98	0.44
1:A:951:ASN:OD1	1:A:952:PHE:N	2.48	0.44
1:B:1080:ASN:HA	1:B:1083:SER:HA	2.00	0.44
1:C:187:PHE:HE1	1:C:196:VAL:HG13	1.81	0.44
1:A:282:PRO:HB2	1:A:594:VAL:HG21	2.00	0.44
1:A:385:ASP:OD2	1:A:410:TYR:OH	2.33	0.44
1:C:19:CYS:HB3	1:C:134:ASP:HB2	1.99	0.44
1:C:441:ARG:HH22	1:C:457:ASN:HA	1.82	0.44
1:C:615:LEU:HB3	1:C:617:PRO:HD2	2.00	0.44
1:B:86:GLY:HA3	1:B:187:PHE:O	2.17	0.44
1:B:335:PRO:HG3	1:B:341:GLU:HB2	1.98	0.44
1:C:38:ARG:NH2	1:C:210:PRO:O	2.40	0.44
2:D:237:TYR:HD1	2:D:447:VAL:HG12	1.82	0.44
2:D:566:TRP:O	2:D:570:LEU:CB	2.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD12	1:A:210:PRO:HD2	2.00	0.44
1:B:352:TYR:HD2	1:B:375:ASN:HB3	1.81	0.44
1:B:1051:PRO:HG3	1:B:1090:ASN:HD21	1.83	0.44
1:C:561:SER:HB3	1:C:571:LEU:HD23	1.99	0.44
1:A:1079:PHE:CE2	1:A:1084:TRP:HB2	2.53	0.44
1:B:78:ASN:HB2	1:B:235:LEU:HD13	1.99	0.44
1:B:1031:LEU:HD12	1:B:1031:LEU:HA	1.85	0.44
1:C:323:CYS:O	1:C:325:PHE:N	2.50	0.44
1:B:460:PHE:N	1:B:475:TYR:O	2.51	0.43
1:C:631:THR:O	1:C:633:ALA:N	2.52	0.43
1:A:96:ASN:HA	1:A:183:ARG:HH12	1.83	0.43
1:A:698:THR:H	1:A:1053:GLN:HB2	1.84	0.43
1:A:778:TYR:CZ	1:A:781:GLY:HA2	2.53	0.43
1:C:884:MET:HE3	1:C:1031:LEU:HD21	2.00	0.43
1:C:1102:THR:OG1	1:C:1103:PHE:N	2.50	0.43
2:D:33:ASN:ND2	2:D:390:PHE:H	2.16	0.43
2:D:482:ARG:NH2	2:D:611:SER:OG	2.51	0.43
1:C:72:ILE:H	1:C:75:THR:HB	1.82	0.43
1:A:370:SER:H	1:C:965:ARG:HB2	1.83	0.43
1:A:968:LYS:HD3	1:A:968:LYS:HA	1.91	0.43
1:C:99:ARG:NE	1:C:118:ASN:HB2	2.33	0.43
1:A:1070:TYR:HE1	1:A:1104:VAL:HA	1.84	0.43
1:B:224:LEU:HD13	1:B:226:ILE:HD11	2.01	0.43
2:D:152:MET:HE2	2:D:270:MET:HA	2.00	0.43
1:A:390:LYS:HG2	1:A:483:PHE:HZ	1.83	0.43
1:B:656:ILE:HG12	1:B:678:THR:HA	2.00	0.43
1:B:915:GLN:O	1:B:918:GLU:HB2	2.17	0.43
1:C:546:GLN:HB2	1:C:549:GLN:OE1	2.19	0.43
1:A:390:LYS:HG2	1:A:483:PHE:CZ	2.53	0.43
1:A:575:PRO:HB3	1:A:578:PHE:HE1	1.84	0.43
1:A:856:THR:HG21	1:A:1037:ALA:HB2	2.00	0.43
1:A:348:CYS:HB3	1:A:510:VAL:HG22	2.01	0.43
1:A:895:GLN:HB2	1:B:1071:PHE:CD2	2.53	0.43
1:A:1021:ARG:H	1:A:1021:ARG:HG2	1.71	0.43
1:B:72:ILE:H	1:B:75:THR:HB	1.84	0.43
1:A:287:LYS:HA	1:A:295:ILE:HD11	2.01	0.43
1:A:965:ARG:HB2	1:B:369:VAL:HA	2.01	0.43
1:C:1030:HIS:CE1	1:C:1033:SER:HB2	2.46	0.43
1:A:95:SER:OG	1:A:173:SER:O	2.37	0.43
1:A:1028:GLY:HA3	1:A:1049:TYR:H	1.82	0.43
1:B:274:ASP:OD1	1:B:275:ALA:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:LEU:O	1:B:961:ASP:N	2.52	0.43
1:C:71:THR:OG1	1:C:75:THR:O	2.28	0.43
1:C:99:ARG:HH22	1:C:172:VAL:HG22	1.84	0.43
1:C:261:THR:HB	1:C:278:CYS:HB2	2.01	0.43
1:C:315:ARG:HH12	1:C:519:LEU:HB3	1.83	0.43
1:C:544:ARG:O	1:C:546:GLN:NE2	2.52	0.43
1:C:862:GLY:HA2	1:C:866:ALA:HB3	2.01	0.43
1:A:840:LEU:HD13	1:A:941:LEU:HD11	2.01	0.42
1:A:1079:PHE:HE2	1:A:1084:TRP:HB2	1.84	0.42
1:C:659:SER:OG	1:C:660:TYR:N	2.52	0.42
2:D:375:GLU:HA	2:D:378:HIS:HD2	1.84	0.42
1:A:137:PHE:HB2	1:A:237:ALA:HB2	2.00	0.42
1:A:562:VAL:HG23	1:A:570:ILE:HG13	2.00	0.42
1:C:197:TYR:HB3	1:C:216:LEU:HB3	2.01	0.42
1:C:640:GLU:O	1:C:642:VAL:N	2.46	0.42
2:D:209:VAL:HG11	2:D:565:PRO:HB3	2.00	0.42
1:B:142:LYS:HB2	1:B:238:PHE:HB3	2.01	0.42
1:B:176:SER:OG	1:B:177:GLY:N	2.50	0.42
1:B:721:ASN:ND2	1:C:304:ASN:HD22	2.17	0.42
1:B:724:ILE:HG22	1:B:725:CYS:HB2	2.01	0.42
1:B:1072:PRO:HB3	1:B:1078:VAL:HG22	1.99	0.42
2:D:205:GLY:HA2	2:D:208:GLU:HB2	2.00	0.42
1:C:292:SER:OG	1:C:294:GLU:N	2.52	0.42
1:B:209:LEU:HD12	1:B:210:PRO:HD2	2.01	0.42
1:B:853:ALA:O	1:B:856:THR:OG1	2.30	0.42
1:B:1054:GLU:O	1:B:1055:ARG:NH1	2.52	0.42
1:C:756:GLN:HA	1:C:759:ASN:HD22	1.84	0.42
2:D:247:LYS:HB2	2:D:282:THR:HG22	2.00	0.42
1:A:362:SER:H	1:A:423:TRP:HA	1.84	0.42
1:B:122:ASN:OD1	1:B:123:VAL:N	2.52	0.42
1:B:996:ARG:O	1:B:1000:ILE:HB	2.20	0.42
1:C:382:VAL:H	1:C:510:VAL:HG11	1.84	0.42
1:C:1098:THR:H	1:C:1101:ASN:ND2	2.18	0.42
2:D:362:THR:HG23	2:D:368:ASP:HB3	2.01	0.42
1:B:138:PHE:HB2	1:B:236:THR:HA	2.01	0.42
1:C:78:ASN:HD21	1:C:136:PRO:HG2	1.85	0.42
2:D:461:TRP:O	2:D:465:LYS:CB	2.68	0.42
1:A:603:CYS:N	1:A:635:CYS:SG	2.92	0.42
1:A:1079:PHE:HB3	1:A:1085:PHE:C	2.39	0.42
1:B:40:VAL:HG11	1:B:272:ILE:HG21	2.00	0.42
1:B:751:GLY:O	1:B:755:GLU:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ALA:H	1:C:412:LEU:HG	1.84	0.42
1:A:95:SER:H	1:A:181:HIS:CD2	2.37	0.42
1:A:911:LYS:O	1:A:915:GLN:N	2.46	0.42
1:B:749:LEU:HD23	1:B:749:LEU:HA	1.86	0.42
1:B:1097:ILE:H	1:B:1097:ILE:HG13	1.52	0.42
1:C:707:GLU:OE2	1:C:1010:LYS:NZ	2.35	0.42
1:C:960:ASN:HA	1:C:963:LEU:HD22	2.02	0.42
2:D:320:LEU:HD13	2:D:380:GLN:HG2	2.02	0.42
1:B:786:GLN:OE1	1:B:917:GLN:NE2	2.53	0.42
1:C:33:HIS:HD2	1:C:68:GLY:HA3	1.84	0.42
1:C:880:PHE:HA	1:C:883:GLN:HB2	2.02	0.42
2:D:56:GLU:HA	2:D:59:VAL:HG12	2.01	0.42
2:D:557:MET:HA	2:D:560:LEU:HD13	2.02	0.42
1:A:38:ARG:NH2	1:A:210:PRO:O	2.42	0.41
1:A:42:TYR:HB2	1:A:218:PRO:HD3	2.01	0.41
1:A:630:GLN:HG2	1:A:631:THR:H	1.84	0.41
1:B:801:GLU:HA	1:B:804:LEU:HD12	2.01	0.41
1:B:916:ILE:HD13	1:B:916:ILE:HA	1.88	0.41
2:D:581:VAL:HG13	2:D:585:LEU:HD23	2.02	0.41
1:B:83:PHE:HE2	1:B:189:ASN:HB2	1.86	0.41
1:B:968:LYS:HD3	1:B:968:LYS:HA	1.83	0.41
1:A:683:ALA:O	1:C:770:MET:N	2.53	0.41
1:A:904:GLN:HA	1:A:907:ASN:HD22	1.85	0.41
1:B:961:ASP:OD1	1:B:965:ARG:NH1	2.38	0.41
1:B:1060:ALA:HB2	1:B:1080:ASN:ND2	2.34	0.41
1:C:78:ASN:ND2	1:C:136:PRO:HG2	2.35	0.41
1:C:645:SER:CB	1:C:680:SER:HB3	2.50	0.41
1:A:1068:LYS:NZ	1:A:1104:VAL:HG13	2.35	0.41
1:C:48:ARG:HB2	1:C:266:TYR:CE2	2.55	0.41
2:D:198:ASP:OD1	2:D:204:ARG:NH2	2.53	0.41
1:A:853:ALA:O	1:A:856:THR:OG1	2.32	0.41
1:A:877:GLN:HE21	1:B:695:ALA:HB3	1.85	0.41
1:B:832:ILE:O	1:C:632:GLN:NE2	2.53	0.41
1:C:432:SER:HB3	1:C:485:THR:HB	2.03	0.41
2:D:326:GLY:O	2:D:330:ASN:HB2	2.20	0.41
1:A:719:ASP:OD1	1:A:721:ASN:N	2.50	0.41
1:B:141:SER:HB3	1:B:144:MET:HB2	2.02	0.41
1:B:659:SER:OG	1:B:660:TYR:N	2.49	0.41
1:A:102:VAL:O	1:A:231:PHE:HA	2.20	0.41
1:B:1085:PHE:HB3	1:B:1095:GLN:H	1.85	0.41
1:C:131:GLU:HB2	1:C:155:ASN:HD22	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:915:GLN:O	1:C:919:SER:OG	2.30	0.41
1:A:89:PHE:HD2	1:A:185:PHE:HB2	1.86	0.41
1:A:499:LEU:HA	1:A:499:LEU:HD23	1.90	0.41
1:A:692:ASN:HD22	1:A:1059:THR:HG22	1.85	0.41
1:B:545:PHE:HZ	1:B:550:GLN:HA	1.84	0.41
1:B:800:ILE:O	1:B:804:LEU:HG	2.21	0.41
1:C:136:PRO:HB2	1:C:234:ILE:HG12	2.01	0.41
2:D:581:VAL:HG22	2:D:584:LEU:HB3	2.02	0.41
1:A:48:ARG:HB2	1:A:266:TYR:CD2	2.56	0.41
1:A:440:TYR:OH	1:A:479:ASN:ND2	2.54	0.41
1:A:962:ILE:O	1:A:966:LEU:N	2.54	0.41
1:B:835:GLN:HE21	1:C:575:PRO:HG2	1.85	0.41
1:B:890:GLY:O	1:B:1018:GLN:NE2	2.54	0.41
1:C:44:ASP:OD2	1:C:48:ARG:NH1	2.54	0.41
1:C:695:ALA:HB1	1:C:1055:ARG:H	1.86	0.41
1:C:741:PHE:CD2	1:C:983:LEU:HD21	2.56	0.41
2:D:32:PHE:O	2:D:36:ALA:HB3	2.20	0.41
2:D:41:TYR:CG	2:D:353:LYS:HD2	2.56	0.41
2:D:149:ASN:HA	2:D:152:MET:HB2	2.03	0.41
2:D:406:GLU:HG3	2:D:518:ARG:HH21	1.86	0.41
2:D:418:LEU:HD13	2:D:418:LEU:HA	1.91	0.41
1:A:931:GLN:O	1:A:935:ASN:ND2	2.54	0.41
1:B:315:ARG:HB3	1:B:565:PRO:HD2	2.03	0.41
1:C:389:VAL:HB	1:C:393:ASP:HB2	2.02	0.41
1:C:736:LEU:HD23	1:C:736:LEU:HA	1.85	0.41
1:A:586:PRO:HG2	1:A:591:SER:HB3	2.03	0.40
1:A:723:TYR:CE1	1:A:944:LEU:HG	2.56	0.40
1:A:1068:LYS:HB2	1:A:1068:LYS:HE3	1.87	0.40
1:B:18:ARG:N	1:B:133:CYS:SG	2.88	0.40
1:B:758:ARG:CZ	1:B:1001:ARG:HH12	2.34	0.40
1:B:909:PHE:HZ	1:B:1034:PHE:HE2	1.69	0.40
1:C:94:LYS:HA	1:C:181:HIS:CD2	2.56	0.40
1:C:382:VAL:HG22	1:C:510:VAL:HG11	2.03	0.40
1:C:749:LEU:HD23	1:C:749:LEU:HA	1.90	0.40
1:A:297:LYS:HG3	1:A:586:PRO:HA	2.03	0.40
1:C:859:LEU:O	1:C:863:THR:OG1	2.28	0.40
1:C:888:PHE:CZ	1:C:898:LEU:HB2	2.56	0.40
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.77	0.40
1:B:441:ARG:NH2	1:B:443:LEU:O	2.53	0.40
1:B:847:LEU:HD11	1:B:855:TYR:HE2	1.86	0.40
1:B:1063:ILE:HG21	1:B:1118:THR:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LYS:HD2	1:C:179:PHE:HA	2.04	0.40
2:D:560:LEU:HD23	2:D:564:GLU:HB2	2.02	0.40
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.91	0.40
1:A:797:ARG:HD2	1:A:805:PHE:CE2	2.56	0.40
1:B:57:ASP:OD1	1:B:58:LEU:N	2.54	0.40
2:D:130:GLY:HA3	2:D:172:VAL:HG11	2.03	0.40
2:D:261:CYS:HB2	2:D:488:VAL:HG13	2.03	0.40
1:B:749:LEU:HD23	1:B:752:ILE:HD12	2.03	0.40
1:B:901:ASN:O	1:B:904:GLN:HB3	2.22	0.40
1:B:941:LEU:HA	1:B:941:LEU:HD12	1.83	0.40
1:C:95:SER:H	1:C:181:HIS:CG	2.40	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%)	853 (81%)	199 (19%)	5 (0%)	29	68
1	B	1057/1203 (88%)	848 (80%)	204 (19%)	5 (0%)	29	68
1	C	1045/1203 (87%)	840 (80%)	193 (18%)	12 (1%)	14	52
2	D	595/603 (99%)	562 (94%)	33 (6%)	0	100	100
All	All	3754/4212 (89%)	3103 (83%)	629 (17%)	22 (1%)	29	64

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	632	GLN
1	C	648	CYS
1	C	676	ALA
1	A	632	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1072	PRO
1	B	1072	PRO
1	C	647	GLU
1	C	679	MET
1	C	1072	PRO
1	B	925	THR
1	C	632	GLN
1	C	645	SER
1	C	1076	VAL
1	A	925	THR
1	B	969	VAL
1	C	675	VAL
1	C	692	ASN
1	A	969	VAL
1	C	557	ASP
1	B	1075	GLY
1	C	1075	GLY
1	A	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%)	917 (100%)	5 (0%)	88 93
1	B	922/1048 (88%)	915 (99%)	7 (1%)	81 89
1	C	914/1048 (87%)	902 (99%)	12 (1%)	69 82
2	D	527/533 (99%)	521 (99%)	6 (1%)	73 84
All	All	3285/3677 (89%)	3255 (99%)	30 (1%)	79 87

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	PHE
1	A	894	THR
1	A	965	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1070	TYR
1	A	1097	ILE
1	B	48	ARG
1	B	302	THR
1	B	699	ASN
1	B	711	VAL
1	B	865	THR
1	B	882	MET
1	B	1087	THR
1	C	318	ASN
1	C	333	LYS
1	C	426	ARG
1	C	510	VAL
1	C	646	TYR
1	C	647	GLU
1	C	656	ILE
1	C	677	TYR
1	C	678	THR
1	C	699	ASN
1	C	796	LYS
1	C	965	ARG
2	D	53	ASN
2	D	114	LYS
2	D	273	ARG
2	D	288	LYS
2	D	341	LYS
2	D	455	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	301	GLN
1	A	479	ASN
1	A	589	ASN
1	A	632	GLN
1	A	692	ASN
1	A	759	ASN
1	A	769	GLN
1	A	806	ASN
1	A	877	GLN
1	A	889	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	907	ASN
1	A	935	ASN
1	A	937	ASN
1	A	987	GLN
1	A	993	GLN
1	A	1005	ASN
1	A	1090	ASN
1	A	1101	ASN
1	B	70	HIS
1	B	118	ASN
1	B	135	ASN
1	B	699	ASN
1	B	733	ASN
1	B	759	ASN
1	B	766	GLN
1	B	769	GLN
1	B	806	ASN
1	B	835	GLN
1	B	904	GLN
1	B	984	GLN
1	B	987	GLN
1	B	1101	ASN
1	C	112	GLN
1	C	129	ASN
1	C	135	ASN
1	C	147	GLN
1	C	155	ASN
1	C	181	HIS
1	C	214	ASN
1	C	304	ASN
1	C	318	ASN
1	C	473	ASN
1	C	479	ASN
1	C	523	GLN
1	C	632	GLN
1	C	699	ASN
1	C	759	ASN
1	C	769	GLN
1	C	947	GLN
1	C	987	GLN
1	C	993	GLN
1	C	1030	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1088	GLN
2	D	53	ASN
2	D	210	ASN
2	D	239	HIS
2	D	250	ASN
2	D	437	ASN
2	D	526	GLN
2	D	552	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

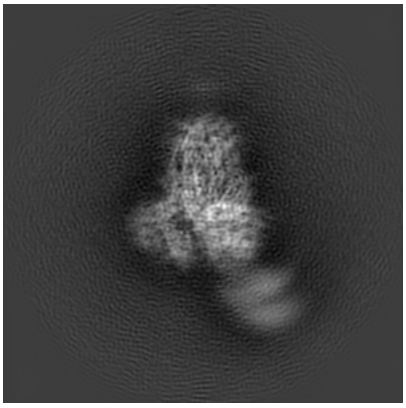
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9593. These allow visual inspection of the internal detail of the map and identification of artifacts.

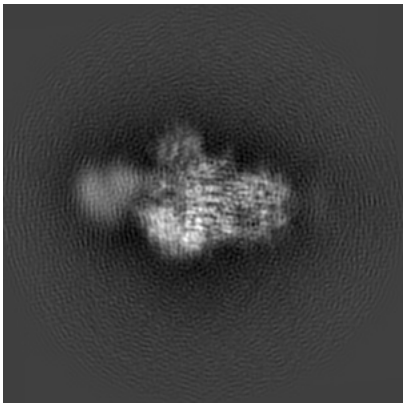
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

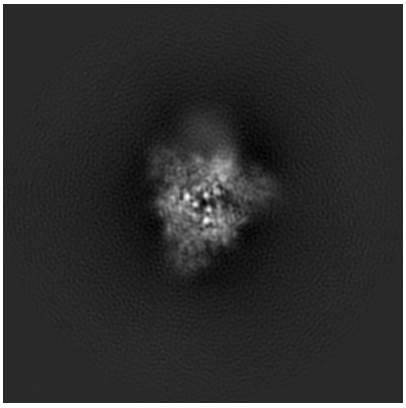
6.1.1 Primary map



X



Y

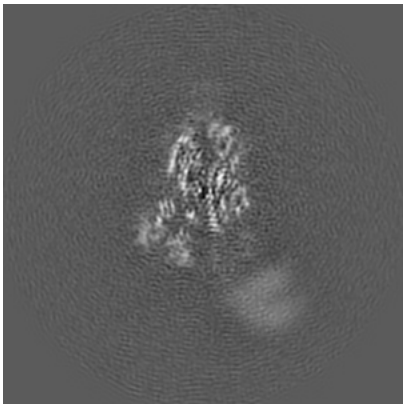


Z

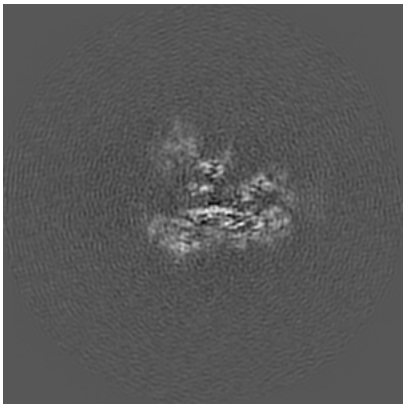
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

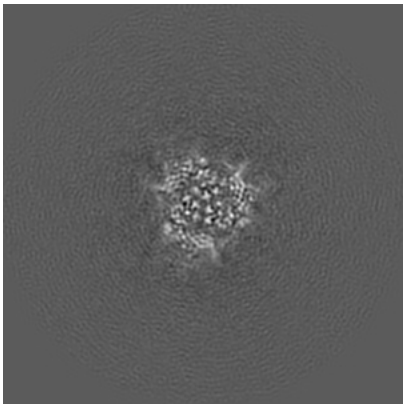
6.2.1 Primary map



X Index: 144



Y Index: 144

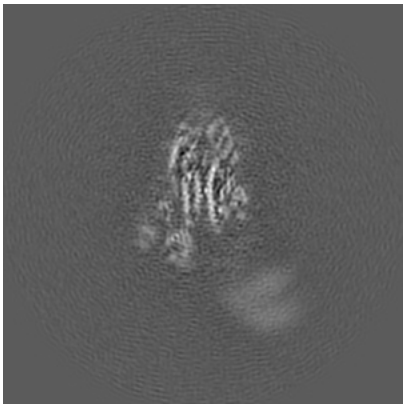


Z Index: 144

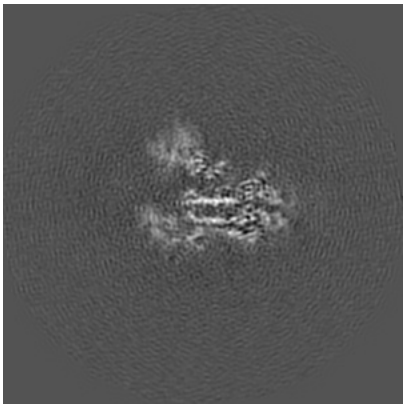
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

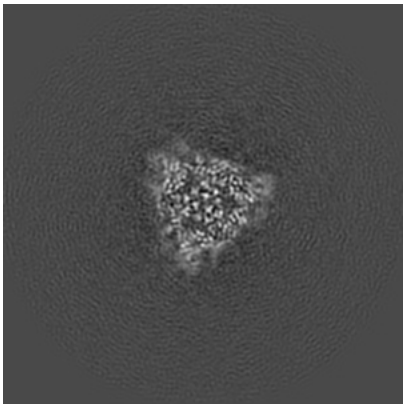
6.3.1 Primary map



X Index: 146



Y Index: 149



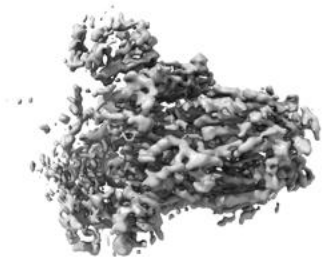
Z Index: 141

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

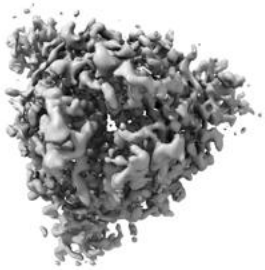
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

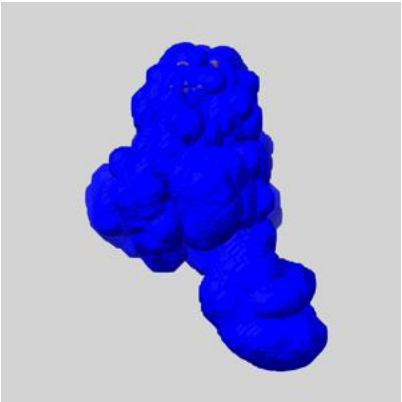
6.5 Mask visualisation (i)

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

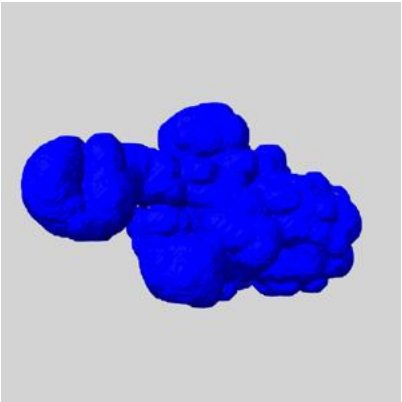
A mask typically either:

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

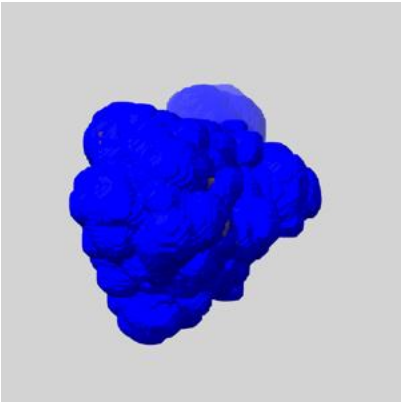
6.5.1 emd_9593_msk_1.map (i)



X



Y

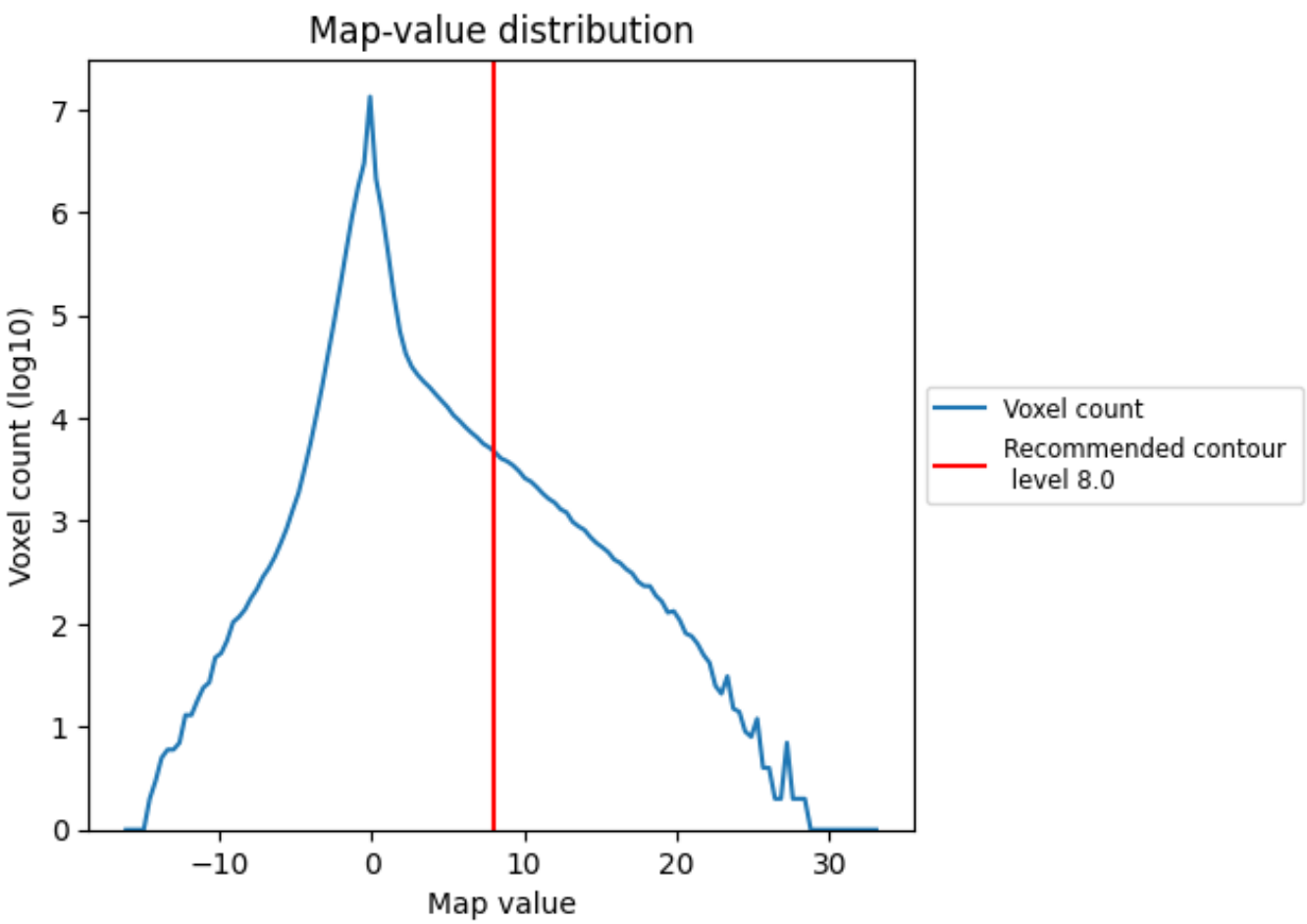


Z

7 Map analysis (i)

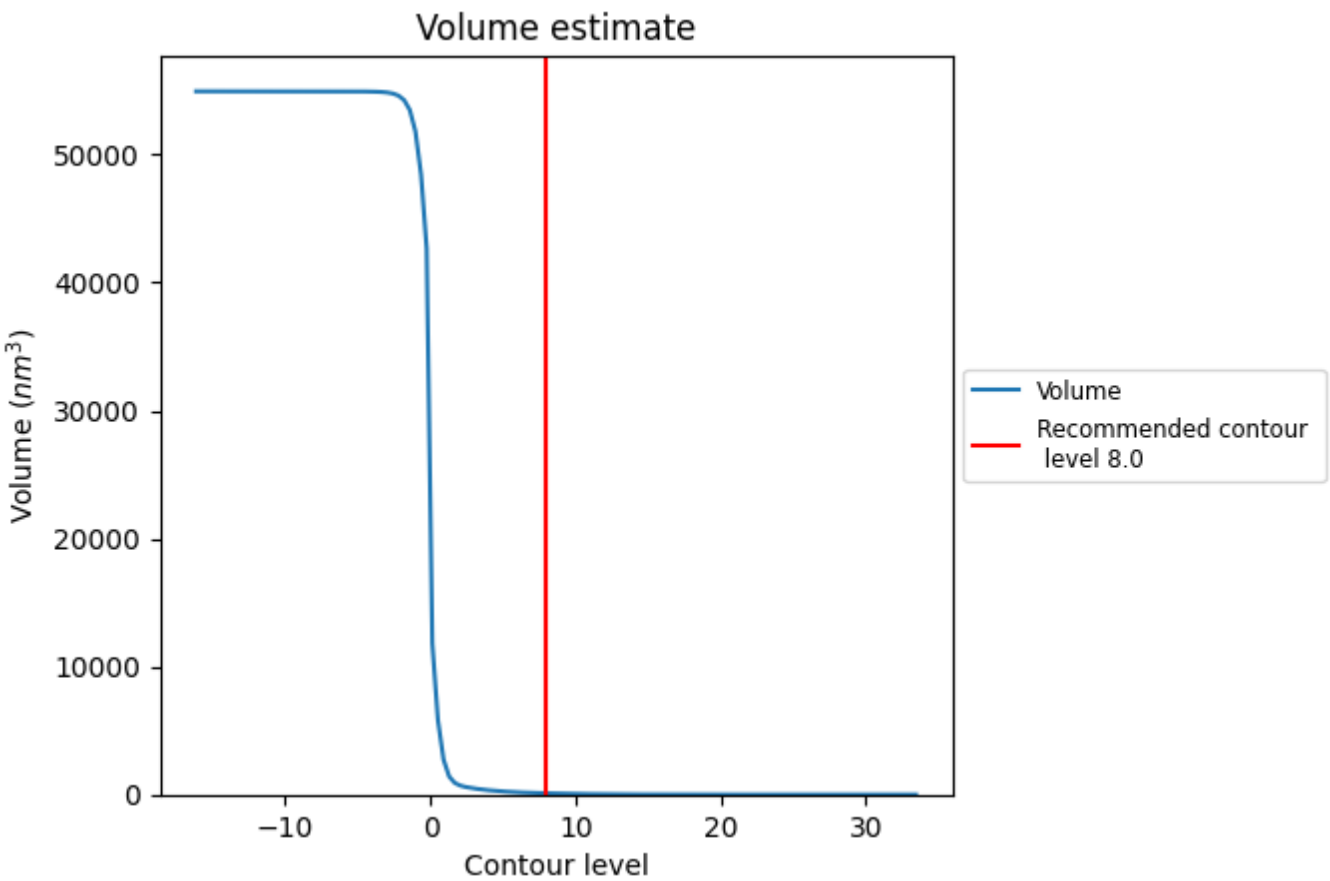
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

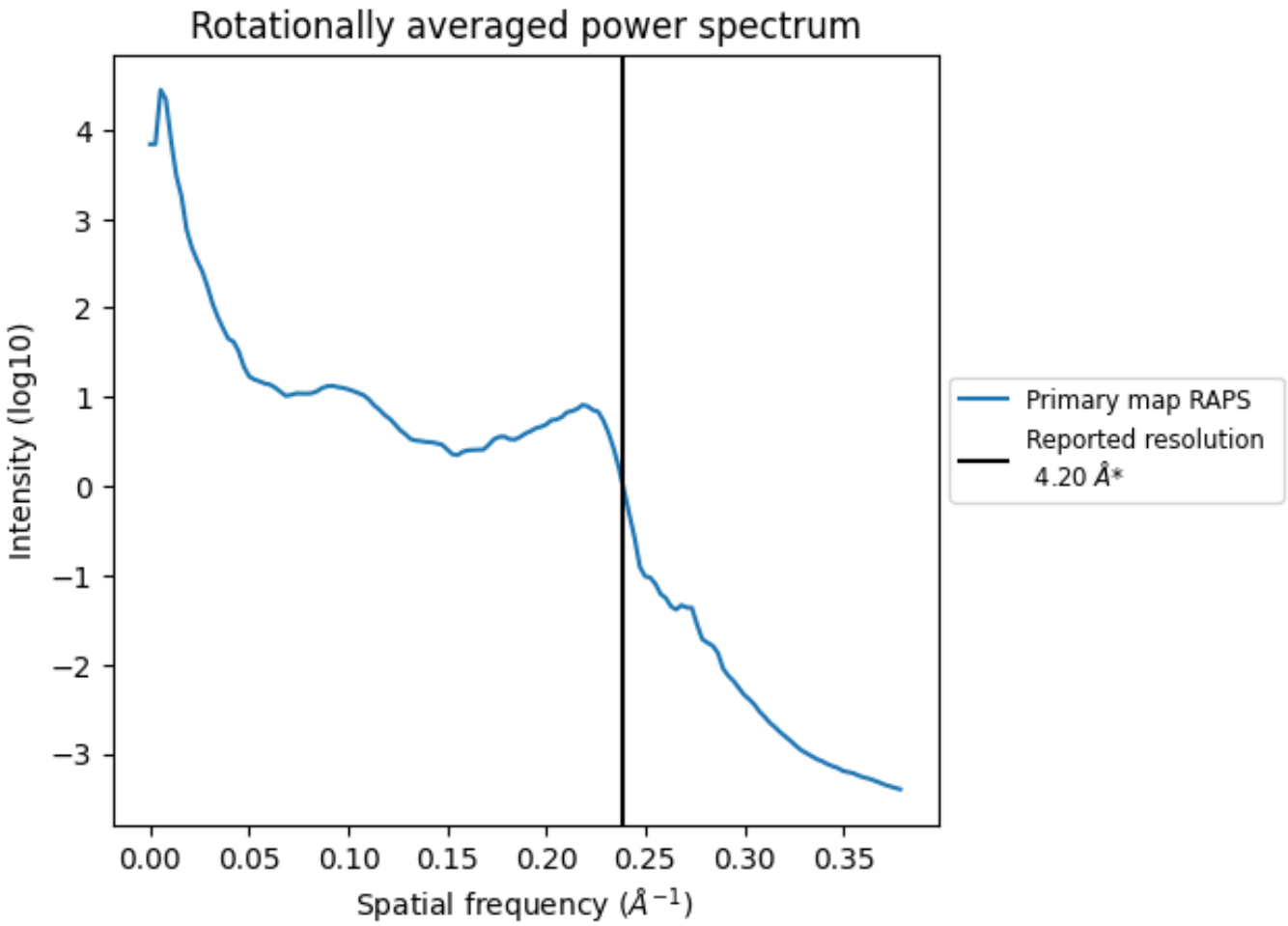
7.2 Volume estimate (i)



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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)

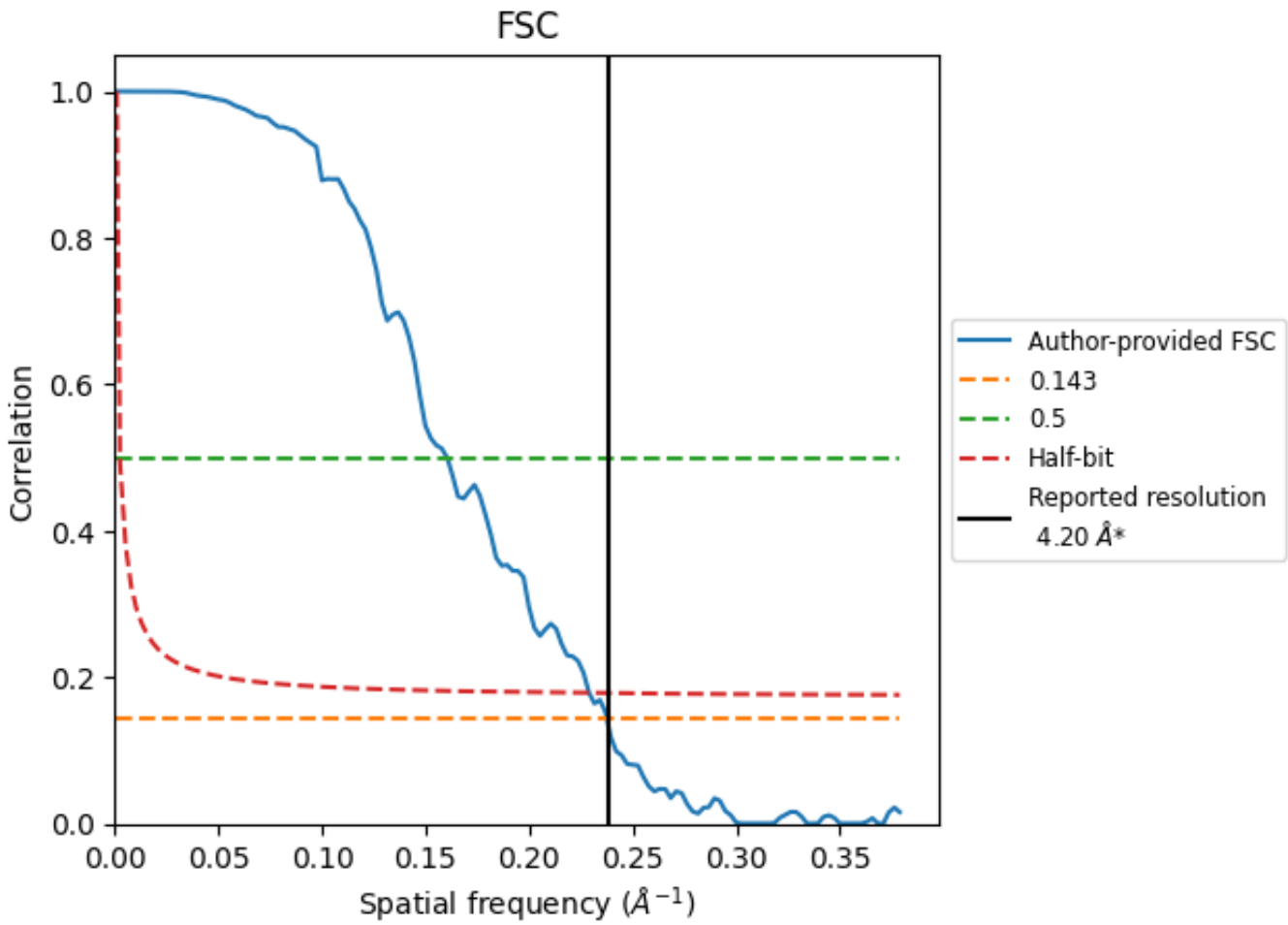


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

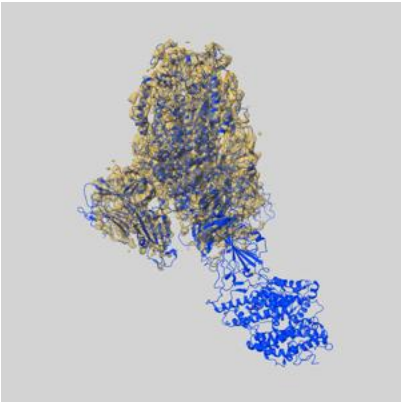
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.21	6.24	4.37
Unmasked-calculated*	-	-	-

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

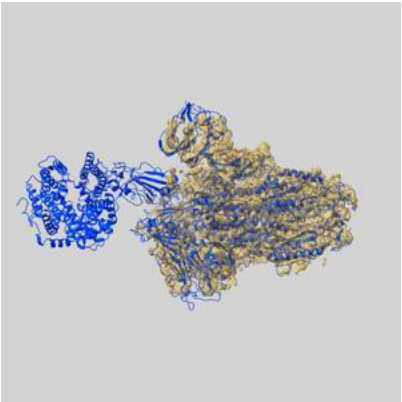
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9593 and PDB model 6ACJ. Per-residue inclusion information can be found in section 3 on page 5.

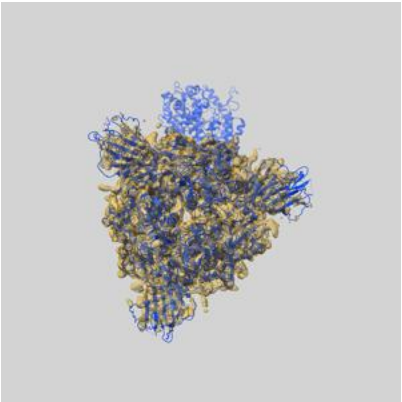
9.1 Map-model overlay (i)



X



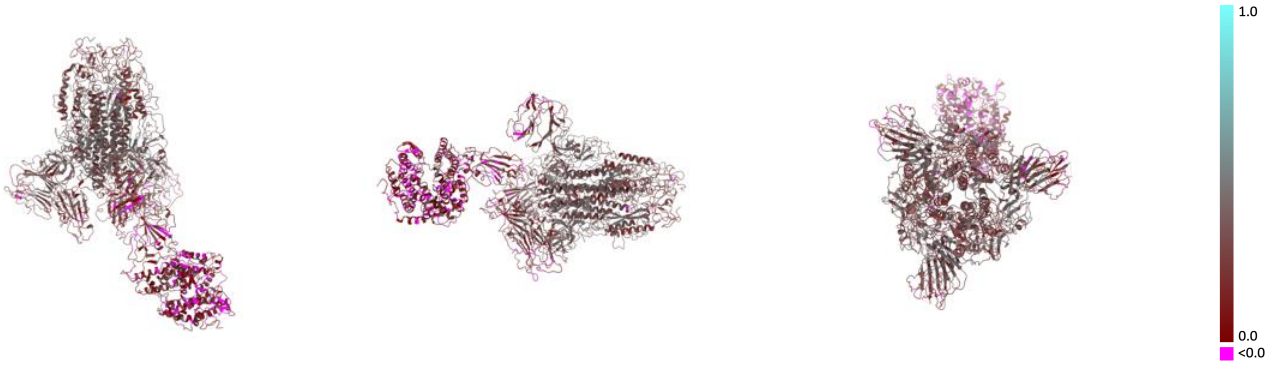
Y



Z

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

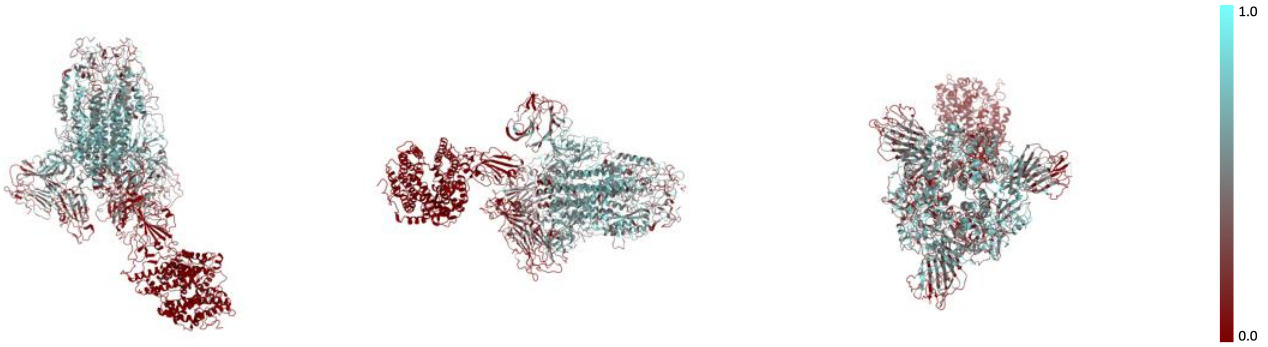
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

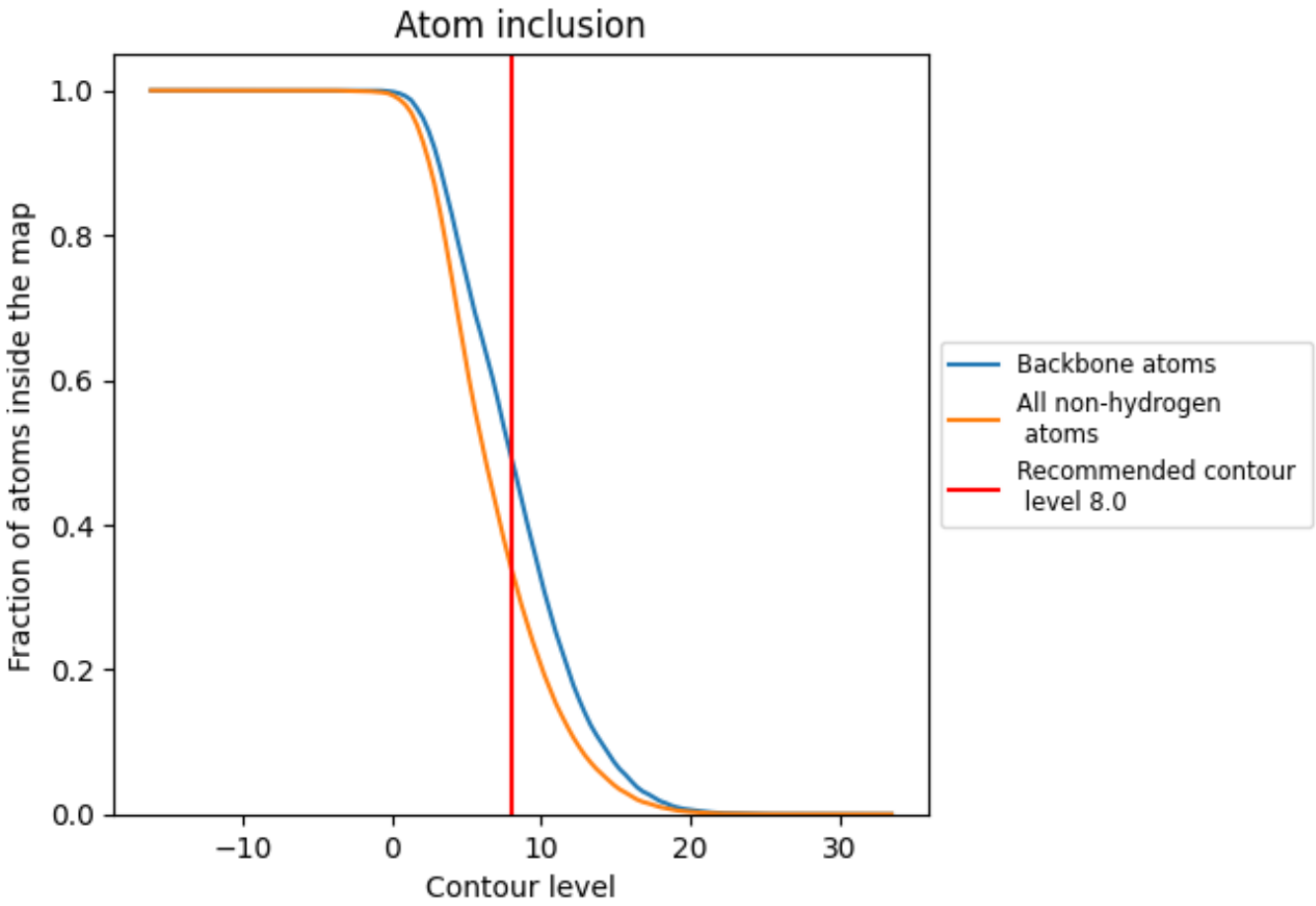
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.0).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3399	0.2770
A	0.4188	0.3200
B	0.4253	0.3080
C	0.3748	0.2960
D	0.0000	0.1150