Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 03:15 AM JST

PDB ID	:	7FB0
EMDB ID	:	EMD-31511
Title	:	SARS-CoV-2 spike protein in closed state
Authors	:	Zhu, Y.; Tai, L.H.; Sun, F.
Deposited on	:	2021-07-08
Resolution	:	3.40 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:

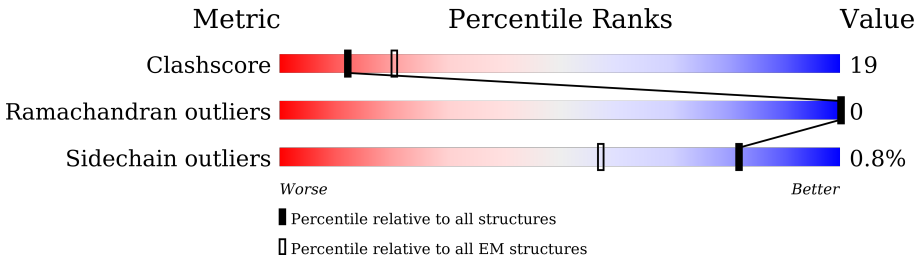
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1247	46% 32% 22%
1	B	1247	48% 30% 22%
1	C	1247	47% 30% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22876 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	976	Total	C	N	O	S	0	0
			7628	4876	1266	1453	33		
1	B	975	Total	C	N	O	S	0	0
			7624	4874	1265	1452	33		
1	C	975	Total	C	N	O	S	0	0
			7624	4874	1265	1452	33		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	ALA	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	LEU	-	expression tag	UNP P0DTC2
A	1210	VAL	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	ARG	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	TYR	-	expression tag	UNP P0DTC2
A	1217	ILE	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	GLU	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	ASP	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLN	-	expression tag	UNP P0DTC2
A	1226	ALA	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	LYS	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLU	-	expression tag	UNP P0DTC2
A	1234	TRP	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	THR	-	expression tag	UNP P0DTC2
A	1240	PHE	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	ALA	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	LEU	-	expression tag	UNP P0DTC2
B	1210	VAL	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	ARG	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	TYR	-	expression tag	UNP P0DTC2
B	1217	ILE	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	GLU	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	ASP	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	ALA	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	LYS	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLU	-	expression tag	UNP P0DTC2
B	1234	TRP	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	THR	-	expression tag	UNP P0DTC2
B	1240	PHE	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	ALA	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	LEU	-	expression tag	UNP P0DTC2
C	1210	VAL	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	ARG	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	TYR	-	expression tag	UNP P0DTC2
C	1217	ILE	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	GLU	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	ASP	-	expression tag	UNP P0DTC2

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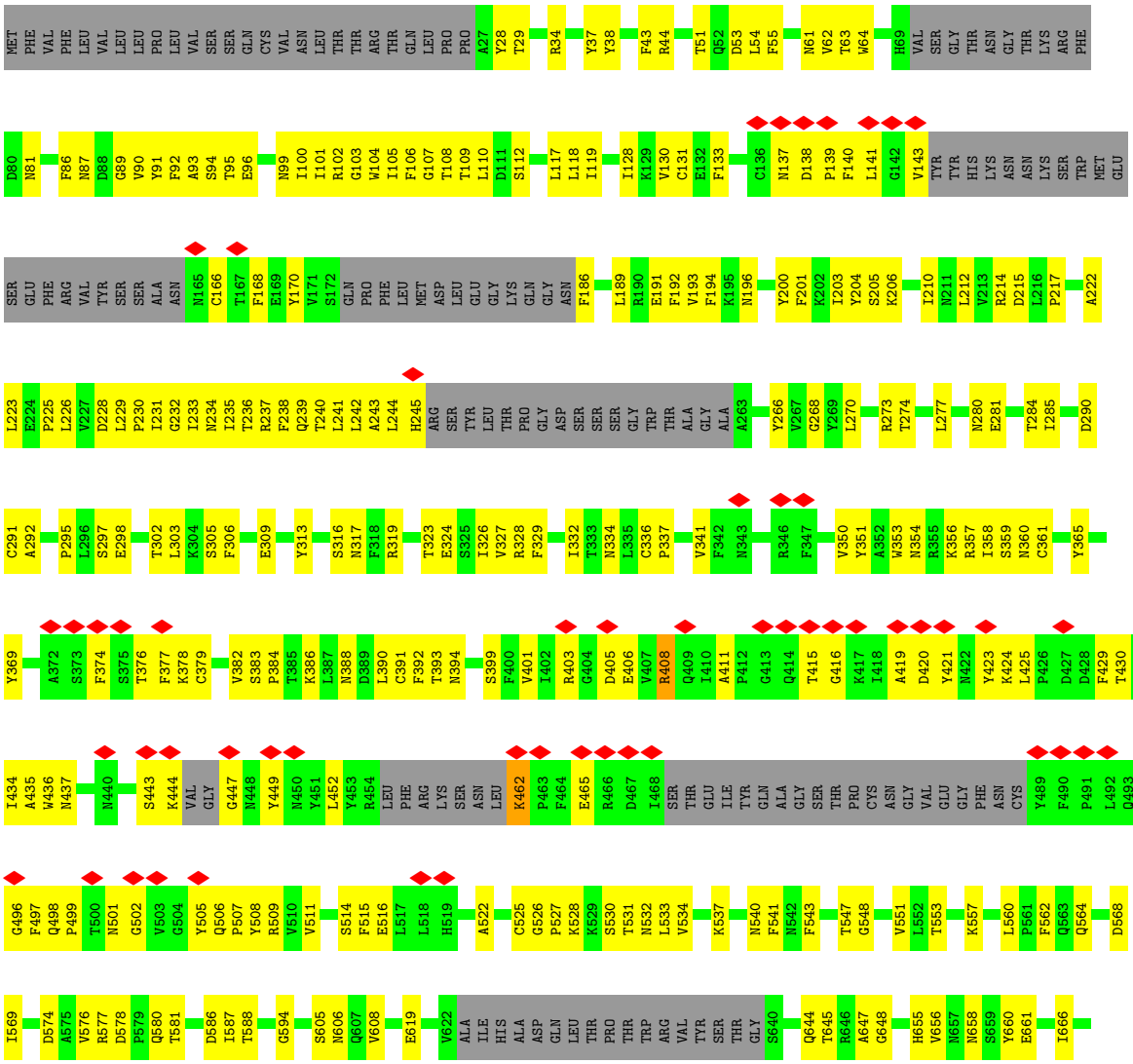
Chain	Residue	Modelled	Actual	Comment	Reference
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLN	-	expression tag	UNP P0DTC2
C	1226	ALA	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	LYS	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLU	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	THR	-	expression tag	UNP P0DTC2
C	1240	PHE	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2

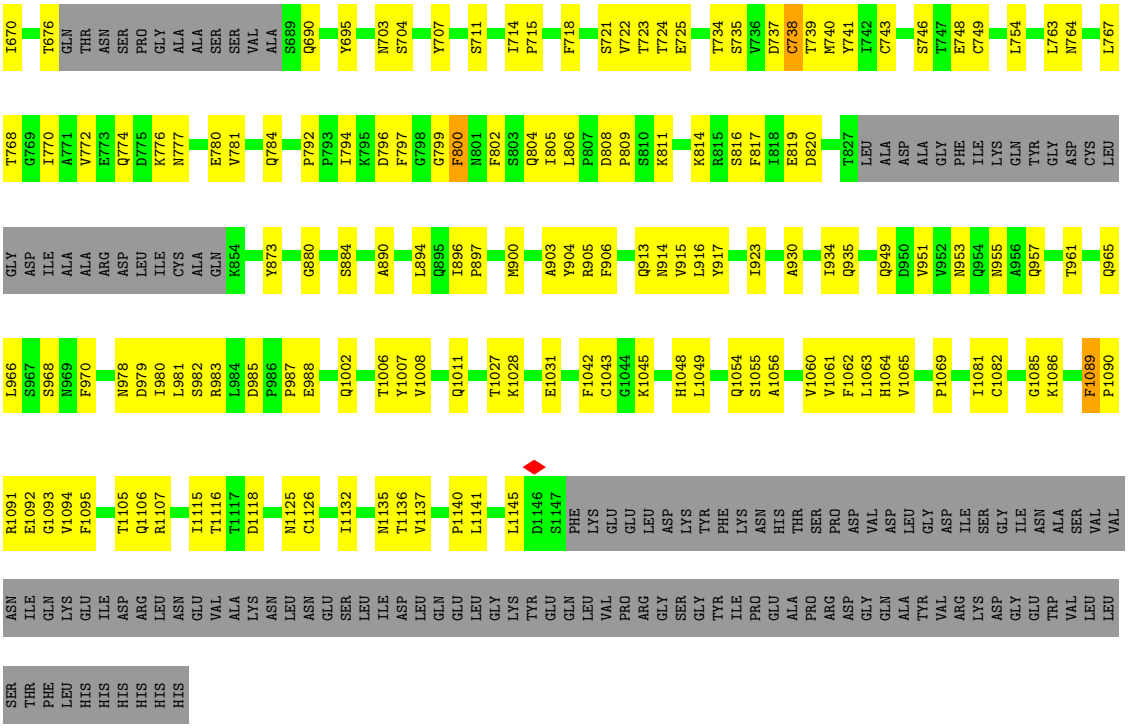
3 Residue-property plots (i)

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

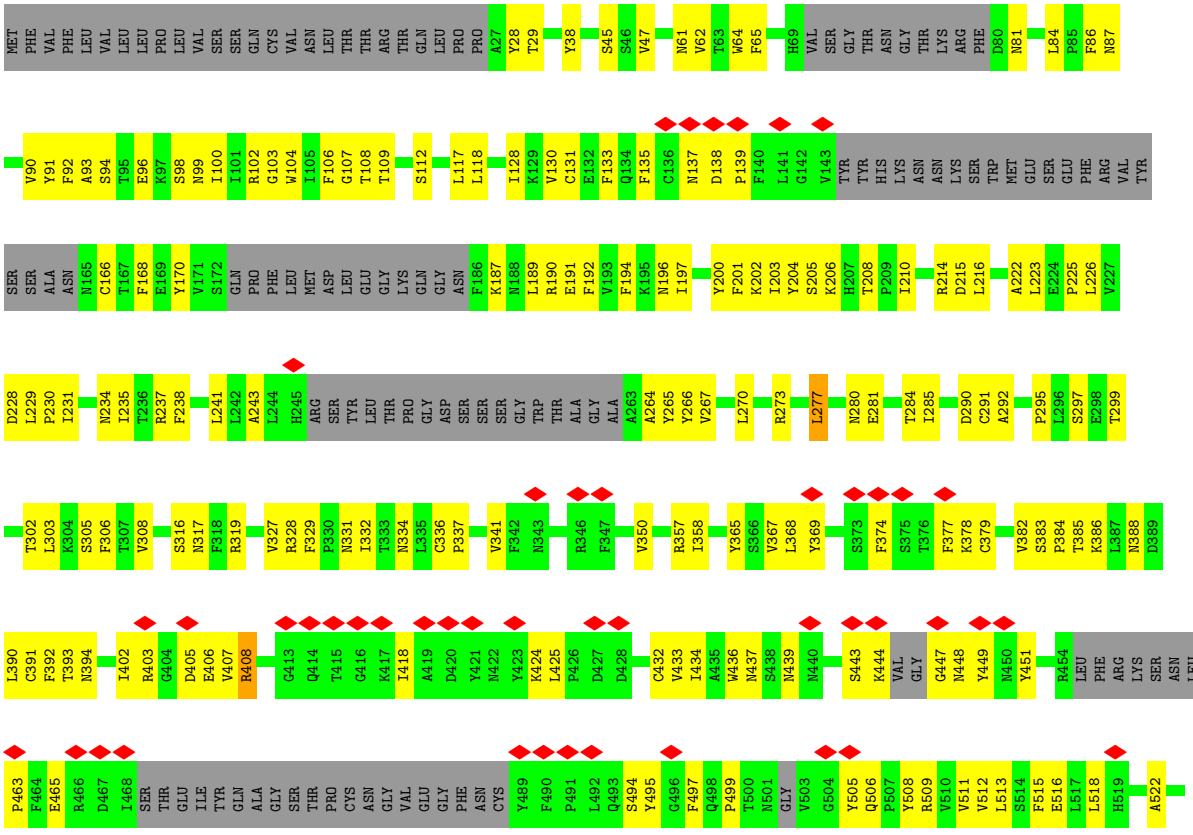
Chain A:

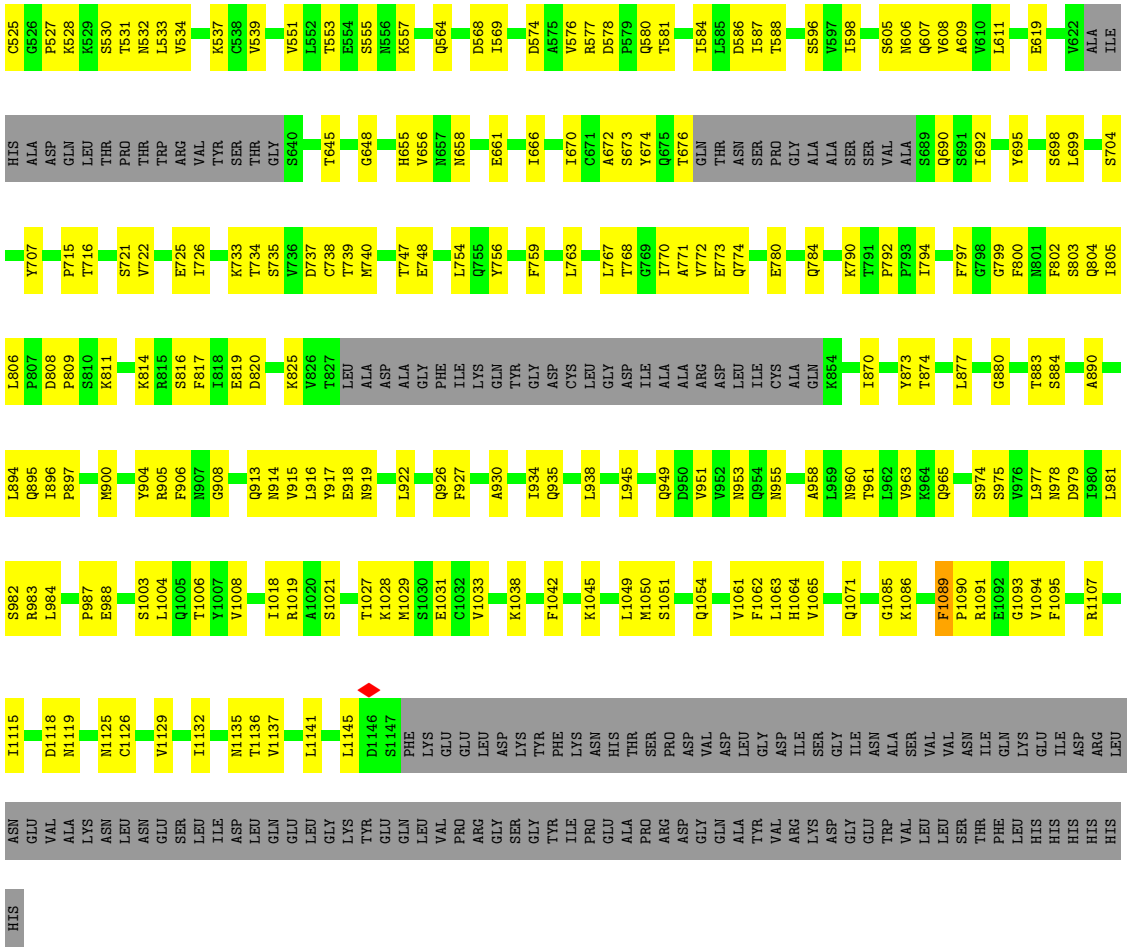




• Molecule 1: Spike glycoprotein

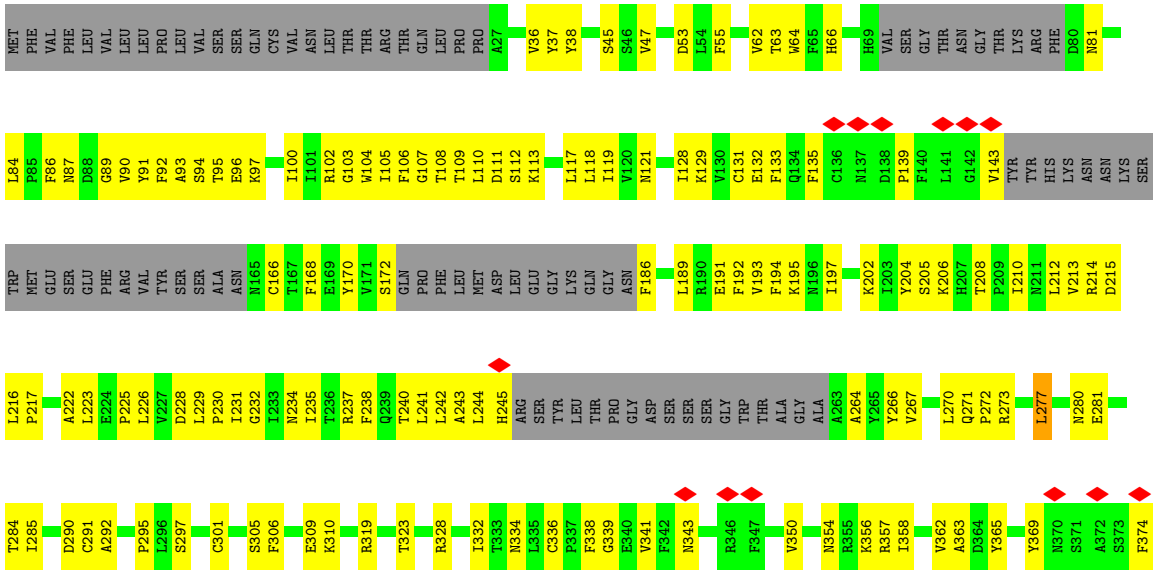
Chain B:

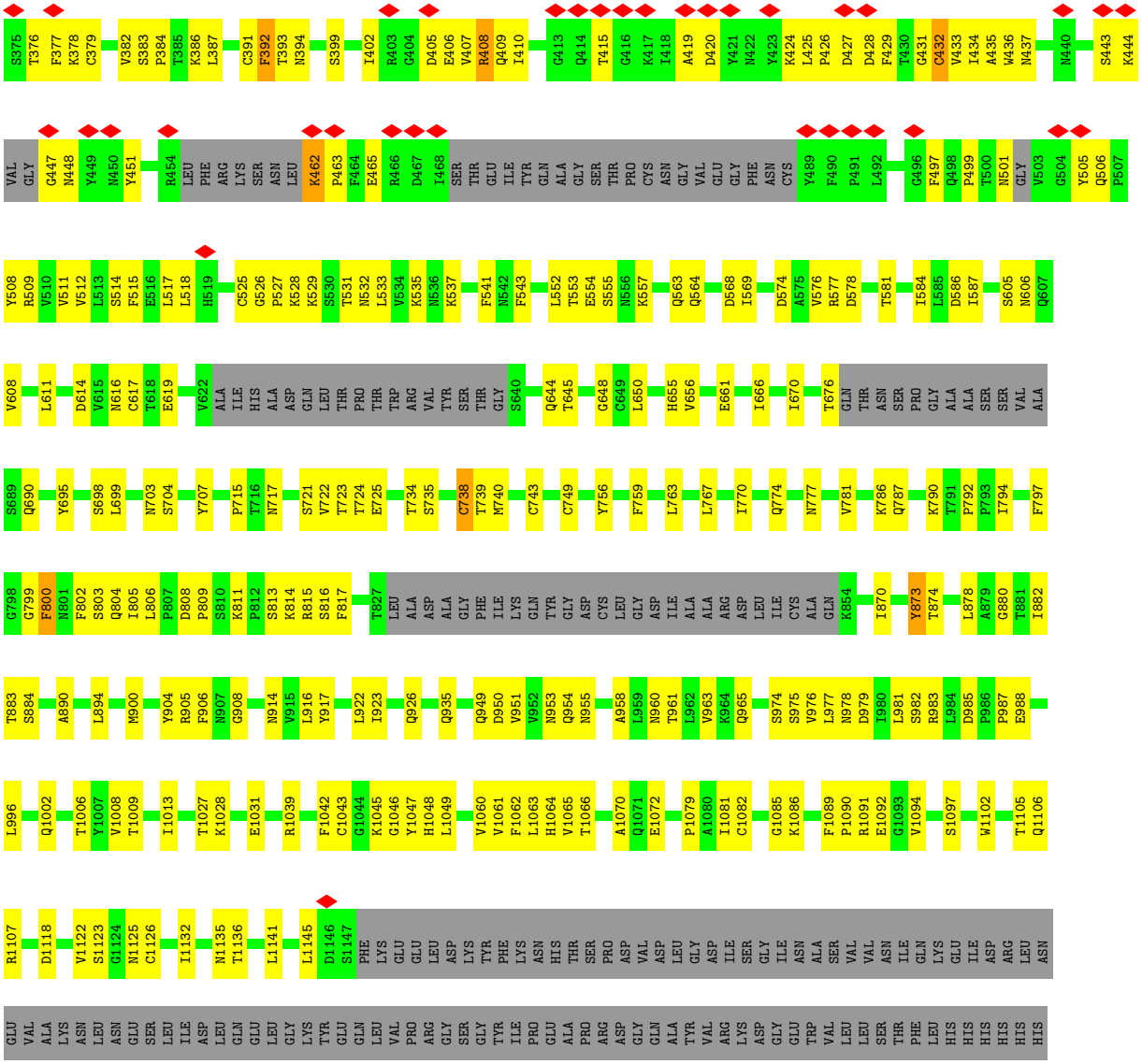




• Molecule 1: Spike glycoprotein

Chain C:




S375 T376 F377 K378 C379 V382 S383 P384 T385 K386 L387 C391 F392 T393 N394 S399 I402 R403 G404 D405 E406 V407 R408 Q409 I410 G413 Q414 T415 G416 K417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 I434 A435 W436 N437 N440 S443 K444
VAL GLY G447 N448 Y449 N450 Y451 R454 LEU PHE ARG LYS SER ASN LEU K462 P463 F464 E465 R466 D467 I468 SER THR GLU ILE TYR GLN ALA GLY SER THR PRO CYS ASN GLY VAL GLU GLY PHE ASN CYS Y489 F490 P491 L492 G496 F497 Q498 P499 T500 N501 GLY V503 G504 Y505 Q506 P507
Y508 R509 V510 V511 V512 L513 S514 F515 E516 L517 L518 H519 C525 G526 P527 K528 K529 S530 T531 N532 L533 V534 K535 N536 K537 F541 N542 F543 L552 T553 E554 S555 N556 K557 Q563 Q564 D568 I569 D574 A575 V576 R577 D578 T581 I584 L585 D586 I587 S605 N606 Q607
V608 L611 D614 V615 N616 C617 T618 E619 V622 ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER THR GLY S640 Q644 T645 G648 C649 L650 H655 V656 E661 I666 I670 T676 GLN THR ASN SER PRO GLY ALA ALA SER SER VAL ALA
S689 Q690 Y695 S698 L699 N703 S704 Y707 P715 T716 N717 S721 V722 T723 T724 E725 T734 S735 C738 T739 M740 C743 C749 Y756 F759 L763 L767 I770 Q774 N777 V781 K786 Q787 K790 T791 P792 P793 I794 F797
G798 G799 F800 N801 F802 S803 Q804 I805 L806 P807 D808 P809 S810 K811 P812 S813 K814 R815 S816 F817 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 I870 Y873 T874 L878 A879 G880 T881 I882
T883 S884 A890 L894 M900 Y904 R905 F906 N907 G908 N914 V915 L916 Y917 L922 I923 Q926 Q935 Q949 D950 V951 V952 N953 Q954 N955 A958 L959 N960 T961 L962 V963 K964 Q965 S974 S975 V976 L977 N978 D979 I980 L981 S982 R983 L984 D985 P986 P987 E988
L996 Q1002 T1006 Y1007 V1008 T1009 I1013 T1027 K1028 E1031 R1039 F1042 C1043 G1044 K1045 G1046 Y1047 H1048 L1049 V1060 V1061 F1062 L1063 H1064 V1065 T1066 A1070 Q1071 E1072 P1079 A1080 I1081 C1082 G1085 K1086 F1089 P1090 R1091 E1092 G1093 V1094 S1097 W1102 T1105 Q1106
R1107 D1118 V1122 S1123 G1124 N1125 C1126 I1132 N1135 T1136 L1141 L1145 D1146 S1147 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 LEU VAL PRO ARG GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55933	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 ($e^-/Å^2$)	3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.524	Depositor
Minimum map value	-1.742	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.53	0/7798	0.54	0/10610
1	B	0.52	0/7793	0.54	0/10602
1	C	0.52	0/7793	0.54	0/10602
All	All	0.52	0/23384	0.54	0/31814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7628	0	7455	317	0
1	B	7624	0	7451	304	0
1	C	7624	0	7451	301	0
All	All	22876	0	22357	870	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 19.

All (870) 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:379:CYS:HA	1:C:432:CYS:HB3	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.52	0.89
1:B:104:TRP:HB3	1:B:106:PHE:HE1	1.37	0.88
1:B:290:ASP:O	1:B:297:SER:OG	1.93	0.85
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.58	0.84
1:B:676:THR:HG22	1:B:690:GLN:HE21	1.43	0.84
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.11	0.83
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.62	0.81
1:A:676:THR:HG22	1:A:690:GLN:HE21	1.46	0.81
1:A:780:GLU:O	1:A:784:GLN:NE2	2.12	0.81
1:B:103:GLY:HA3	1:B:241:LEU:HB3	1.61	0.81
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.14	0.81
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.14	0.80
1:B:780:GLU:O	1:B:784:GLN:NE2	2.14	0.80
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.14	0.80
1:C:290:ASP:O	1:C:297:SER:OG	2.00	0.79
1:C:103:GLY:HA3	1:C:241:LEU:HB3	1.65	0.79
1:B:214:ARG:HE	1:B:215:ASP:HB2	1.49	0.78
1:A:328:ARG:NH1	1:A:578:ASP:OD2	2.17	0.78
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.16	0.78
1:C:1086:LYS:HA	1:C:1125:ASN:HA	1.67	0.77
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.01	0.77
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.16	0.77
1:C:424:LYS:HB2	1:C:463:PRO:HA	1.67	0.77
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.66	0.76
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.19	0.75
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.69	0.74
1:A:1086:LYS:HA	1:A:1125:ASN:HA	1.69	0.74
1:A:103:GLY:HA3	1:A:241:LEU:HB3	1.69	0.74
1:A:437:ASN:ND2	1:A:507:PRO:O	2.22	0.73
1:B:216:LEU:H	1:B:216:LEU:HD12	1.54	0.73
1:B:557:LYS:NZ	1:B:574:ASP:O	2.21	0.73
1:C:280:ASN:ND2	1:C:284:THR:OG1	2.21	0.72
1:B:802:PHE:HD2	1:B:805:ILE:HD11	1.54	0.72
1:A:327:VAL:HG11	1:A:528:LYS:HE3	1.71	0.72
1:A:644:GLN:NE2	1:A:645:THR:O	2.22	0.72
1:C:676:THR:HG22	1:C:690:GLN:HE21	1.54	0.72
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.53	0.72
1:B:369:TYR:HE2	1:B:384:PRO:HB2	1.52	0.72
1:A:81:ASN:O	1:A:239:GLN:NE2	2.21	0.72
1:B:424:LYS:HB2	1:B:463:PRO:HA	1.71	0.71
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.72	0.70
1:B:437:ASN:HA	1:B:508:TYR:HA	1.72	0.70
1:B:1045:LYS:NZ	1:C:890:ALA:O	2.24	0.70
1:A:95:THR:HG22	1:A:186:PHE:HB2	1.73	0.70
1:A:1091:ARG:NH1	1:A:1118:ASP:O	2.24	0.70
1:B:656:VAL:HG12	1:B:658:ASN:H	1.57	0.70
1:B:390:LEU:HD11	1:C:983:ARG:HG2	1.71	0.70
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.73	0.70
1:B:918:GLU:O	1:B:919:ASN:ND2	2.24	0.69
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.25	0.69
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.25	0.69
1:C:553:THR:HG23	1:C:586:ASP:HB3	1.73	0.69
1:A:740:MET:SD	1:C:319:ARG:NH1	2.59	0.69
1:A:564:GLN:OE1	1:A:577:ARG:NH2	2.25	0.69
1:B:319:ARG:NH1	1:C:740:MET:SD	2.57	0.69
1:C:557:LYS:NZ	1:C:574:ASP:OD2	2.24	0.69
1:B:379:CYS:HA	1:B:432:CYS:CB	2.23	0.69
1:C:108:THR:O	1:C:237:ARG:NH1	2.26	0.69
1:B:205:SER:OG	1:B:206:LYS:N	2.26	0.68
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.26	0.68
1:A:723:THR:HG22	1:A:724:THR:H	1.58	0.68
1:A:661:GLU:O	1:A:695:TYR:OH	2.09	0.68
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.26	0.68
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.27	0.68
1:C:214:ARG:HE	1:C:215:ASP:HB2	1.58	0.68
1:A:738:CYS:SG	1:A:739:THR:N	2.67	0.67
1:C:433:VAL:HA	1:C:512:VAL:HA	1.76	0.67
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.28	0.67
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.22	0.67
1:A:1045:LYS:NZ	1:B:890:ALA:O	2.27	0.66
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.76	0.66
1:B:290:ASP:OD1	1:B:291:CYS:N	2.28	0.66
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.77	0.66
1:C:402:ILE:HD12	1:C:406:GLU:HB2	1.78	0.66
1:B:402:ILE:HD12	1:B:406:GLU:HB2	1.76	0.66
1:B:108:THR:HG22	1:B:109:THR:HG23	1.77	0.66
1:C:661:GLU:O	1:C:695:TYR:OH	2.12	0.66
1:C:437:ASN:HA	1:C:508:TYR:HA	1.77	0.66
1:A:557:LYS:NZ	1:A:574:ASP:O	2.29	0.66
1:B:676:THR:HA	1:B:690:GLN:HG2	1.75	0.66
1:C:557:LYS:NZ	1:C:574:ASP:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:SER:OG	1:A:817:PHE:N	2.28	0.66
1:B:661:GLU:O	1:B:695:TYR:OH	2.14	0.66
1:A:390:LEU:HD11	1:B:983:ARG:HG2	1.77	0.65
1:B:99:ASN:OD1	1:B:190:ARG:NH1	2.28	0.65
1:A:1085:GLY:O	1:A:1126:CYS:N	2.28	0.65
1:C:1085:GLY:O	1:C:1126:CYS:N	2.29	0.65
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.29	0.65
1:C:290:ASP:OD1	1:C:291:CYS:N	2.30	0.65
1:A:189:LEU:HD21	1:A:191:GLU:HG2	1.79	0.64
1:C:444:LYS:O	1:C:447:GLY:N	2.30	0.64
1:B:382:VAL:HG12	1:C:983:ARG:HB3	1.79	0.64
1:A:711:SER:OG	1:B:895:GLN:NE2	2.21	0.64
1:C:564:GLN:OE1	1:C:577:ARG:NH2	2.30	0.64
1:A:108:THR:OG1	1:A:234:ASN:O	2.12	0.64
1:A:553:THR:O	1:A:586:ASP:N	2.29	0.64
1:B:86:PHE:HA	1:B:90:VAL:HG21	1.79	0.64
1:B:108:THR:O	1:B:237:ARG:NH1	2.30	0.64
1:B:444:LYS:O	1:B:447:GLY:N	2.30	0.64
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.79	0.64
1:A:619:GLU:OE1	1:A:619:GLU:N	2.32	0.63
1:B:96:GLU:HG3	1:B:98:SER:H	1.63	0.63
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.43	0.63
1:A:186:PHE:N	1:A:212:LEU:O	2.31	0.63
1:A:1093:GLY:HA2	1:A:1107:ARG:HG3	1.80	0.63
1:A:645:THR:HG23	1:A:647:ALA:H	1.62	0.63
1:A:1135:ASN:ND2	1:A:1136:THR:O	2.31	0.63
1:C:553:THR:O	1:C:586:ASP:N	2.31	0.63
1:C:723:THR:HG22	1:C:724:THR:H	1.63	0.63
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.79	0.63
1:C:229:LEU:HB3	1:C:231:ILE:HG23	1.81	0.63
1:A:444:LYS:O	1:A:447:GLY:N	2.32	0.63
1:B:96:GLU:HG2	1:B:100:ILE:H	1.64	0.63
1:B:619:GLU:N	1:B:619:GLU:OE1	2.32	0.63
1:A:605:SER:OG	1:A:606:ASN:N	2.32	0.62
1:A:951:VAL:O	1:A:955:ASN:ND2	2.32	0.62
1:A:985:ASP:OD1	1:A:985:ASP:N	2.32	0.62
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.80	0.62
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.32	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HG2	1.80	0.62
1:C:816:SER:OG	1:C:817:PHE:N	2.32	0.62
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:SER:N	1:A:819:GLU:OE1	2.21	0.62
1:B:564:GLN:OE1	1:B:577:ARG:NH2	2.33	0.62
1:C:448:ASN:HD21	1:C:451:TYR:HD2	1.48	0.62
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.82	0.61
1:A:192:PHE:O	1:A:193:VAL:HG23	1.99	0.61
1:A:305:SER:OG	1:A:306:PHE:N	2.33	0.61
1:B:131:CYS:HA	1:B:166:CYS:HB2	1.83	0.61
1:A:1007:TYR:OH	1:A:1011:GLN:NE2	2.33	0.61
1:C:323:THR:HG21	1:C:537:LYS:HD2	1.83	0.61
1:C:336:CYS:HB3	1:C:358:ILE:HG21	1.82	0.61
1:B:369:TYR:HH	1:B:385:THR:HG1	1.48	0.61
1:B:216:LEU:HG	1:B:266:TYR:HE2	1.66	0.60
1:B:816:SER:OG	1:B:817:PHE:N	2.34	0.60
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.34	0.60
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.32	0.60
1:C:377:PHE:H	1:C:378:LYS:HZ3	1.48	0.60
1:C:108:THR:HG22	1:C:109:THR:HG23	1.84	0.60
1:B:365:TYR:HH	1:B:392:PHE:HE2	1.48	0.59
1:C:216:LEU:HD12	1:C:216:LEU:H	1.67	0.59
1:B:1093:GLY:HA2	1:B:1107:ARG:HG3	1.83	0.59
1:C:192:PHE:O	1:C:193:VAL:HG23	2.01	0.59
1:C:767:LEU:HD23	1:C:770:ILE:HD12	1.85	0.59
1:A:189:LEU:HB2	1:A:210:ILE:HG12	1.83	0.59
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.85	0.59
1:C:95:THR:HG22	1:C:186:PHE:HB3	1.85	0.59
1:B:1094:VAL:HG13	1:B:1107:ARG:HG2	1.84	0.59
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.85	0.59
1:A:205:SER:OG	1:A:206:LYS:N	2.34	0.58
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.85	0.58
1:A:379:CYS:HA	1:A:432:CYS:HA	1.85	0.58
1:A:502:GLY:O	1:A:506:GLN:NE2	2.35	0.58
1:B:738:CYS:SG	1:B:739:THR:N	2.76	0.58
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.35	0.58
1:A:102:ARG:HB2	1:A:141:LEU:HD21	1.84	0.58
1:A:357:ARG:HH12	1:A:359:SER:HB3	1.69	0.58
1:C:676:THR:HA	1:C:690:GLN:HG2	1.85	0.58
1:A:374:PHE:HA	1:A:436:TRP:HB3	1.86	0.57
1:A:553:THR:HG23	1:A:586:ASP:HB2	1.87	0.57
1:A:1089:PHE:CE2	1:B:914:ASN:HA	2.39	0.57
1:B:316:SER:OG	1:B:317:ASN:N	2.36	0.57
1:A:214:ARG:HE	1:A:215:ASP:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLU:OE1	1:B:281:GLU:N	2.32	0.57
1:A:354:ASN:HD21	1:A:399:SER:HB3	1.69	0.57
1:A:576:VAL:HG12	1:A:577:ARG:H	1.69	0.57
1:A:281:GLU:N	1:A:281:GLU:OE1	2.37	0.57
1:A:462:LYS:HE3	1:A:465:GLU:HB2	1.87	0.57
1:C:645:THR:OG1	1:C:648:GLY:O	2.18	0.57
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.87	0.57
1:A:382:VAL:HG12	1:B:983:ARG:HB3	1.87	0.57
1:A:394:ASN:ND2	1:B:200:TYR:OH	2.37	0.57
1:B:802:PHE:CD2	1:B:805:ILE:HD11	2.37	0.57
1:C:205:SER:OG	1:C:206:LYS:N	2.38	0.57
1:B:1085:GLY:O	1:B:1126:CYS:N	2.36	0.57
1:C:961:THR:O	1:C:965:GLN:HG2	2.04	0.57
1:A:721:SER:OG	1:A:722:VAL:N	2.38	0.57
1:C:1135:ASN:ND2	1:C:1136:THR:O	2.37	0.56
1:C:100:ILE:HG22	1:C:242:LEU:HG	1.87	0.56
1:A:104:TRP:HB2	1:A:119:ILE:HB	1.88	0.56
1:A:130:VAL:HG12	1:A:168:PHE:O	2.05	0.56
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.40	0.56
1:A:214:ARG:NE	1:A:215:ASP:HB2	2.21	0.56
1:B:264:ALA:HB1	1:B:266:TYR:CE1	2.41	0.56
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.86	0.56
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.40	0.56
1:B:90:VAL:HG11	1:B:238:PHE:CE1	2.40	0.56
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.71	0.56
1:B:734:THR:OG1	1:B:735:SER:N	2.38	0.56
1:B:103:GLY:N	1:B:241:LEU:O	2.38	0.56
1:A:415:THR:HG22	1:A:416:GLY:H	1.70	0.56
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.04	0.56
1:B:531:THR:HG22	1:B:532:ASN:H	1.71	0.56
1:C:804:GLN:O	1:C:816:SER:OG	2.24	0.56
1:A:434:ILE:HB	1:A:511:VAL:HG23	1.86	0.56
1:A:890:ALA:O	1:C:1045:LYS:NZ	2.32	0.56
1:B:721:SER:OG	1:B:722:VAL:N	2.38	0.56
1:B:880:GLY:O	1:B:884:SER:OG	2.21	0.56
1:A:961:THR:O	1:A:965:GLN:HG2	2.06	0.56
1:A:131:CYS:HA	1:A:166:CYS:HB2	1.88	0.55
1:A:316:SER:OG	1:A:317:ASN:N	2.39	0.55
1:A:1049:LEU:HB2	1:A:1065:VAL:O	2.05	0.55
1:B:951:VAL:O	1:B:955:ASN:ND2	2.38	0.55
1:A:703:ASN:OD1	1:A:704:SER:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.89	0.55
1:B:596:SER:HB3	1:B:611:LEU:HB3	1.87	0.55
1:C:1141:LEU:HD23	1:C:1145:LEU:HD23	1.88	0.55
1:A:983:ARG:HB3	1:C:382:VAL:HG12	1.87	0.55
1:B:448:ASN:HD21	1:B:451:TYR:HD2	1.53	0.55
1:A:341:VAL:HG22	1:A:356:LYS:HZ1	1.72	0.55
1:A:979:ASP:HB3	1:A:983:ARG:HE	1.71	0.55
1:B:1141:LEU:HD23	1:B:1145:LEU:HD23	1.88	0.55
1:C:738:CYS:SG	1:C:739:THR:N	2.79	0.55
1:B:379:CYS:SG	1:B:384:PRO:HB3	2.46	0.55
1:C:434:ILE:HB	1:C:511:VAL:HG23	1.88	0.55
1:A:443:SER:HB3	1:A:499:PRO:HD3	1.88	0.55
1:C:800:PHE:N	1:C:800:PHE:CD1	2.75	0.55
1:B:958:ALA:O	1:B:961:THR:OG1	2.25	0.55
1:B:1049:LEU:HB2	1:B:1065:VAL:O	2.07	0.55
1:A:93:ALA:O	1:A:94:SER:OG	2.24	0.55
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.42	0.55
1:C:976:VAL:HB	1:C:979:ASP:OD2	2.06	0.55
1:A:904:TYR:OH	1:C:1094:VAL:HB	2.08	0.54
1:B:816:SER:N	1:B:819:GLU:OE1	2.34	0.54
1:A:86:PHE:H	1:A:237:ARG:HA	1.72	0.54
1:A:532:ASN:OD1	1:A:533:LEU:N	2.31	0.54
1:A:900:MET:HA	1:A:917:TYR:OH	2.07	0.54
1:C:281:GLU:N	1:C:281:GLU:OE1	2.40	0.54
1:C:131:CYS:HB3	1:C:133:PHE:CZ	2.41	0.54
1:C:974:SER:OG	1:C:975:SER:N	2.40	0.54
1:A:576:VAL:HG12	1:A:577:ARG:N	2.22	0.54
1:C:204:TYR:N	1:C:204:TYR:CD1	2.76	0.54
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.89	0.54
1:B:264:ALA:HB1	1:B:266:TYR:HE1	1.72	0.54
1:B:534:VAL:HG23	1:B:539:VAL:HG11	1.90	0.54
1:B:86:PHE:HE2	1:B:196:ASN:HD21	1.55	0.54
1:C:611:LEU:HD12	1:C:650:LEU:HD13	1.90	0.54
1:A:290:ASP:O	1:A:297:SER:HB2	2.07	0.54
1:C:212:LEU:HG	1:C:214:ARG:H	1.72	0.54
1:A:131:CYS:HB3	1:A:133:PHE:CE1	2.43	0.54
1:A:336:CYS:HB3	1:A:358:ILE:HG21	1.89	0.54
1:B:280:ASN:OD1	1:B:284:THR:N	2.34	0.54
1:C:605:SER:OG	1:C:606:ASN:N	2.41	0.54
1:C:803:SER:OG	1:C:804:GLN:NE2	2.40	0.54
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:PHE:HE2	1:B:914:ASN:HA	1.73	0.53
1:B:131:CYS:HB3	1:B:133:PHE:CZ	2.42	0.53
1:B:436:TRP:O	1:B:509:ARG:N	2.40	0.53
1:B:1118:ASP:OD1	1:B:1119:ASN:N	2.41	0.53
1:C:1043:CYS:HB2	1:C:1048:HIS:CD2	2.42	0.53
1:B:225:PRO:O	1:B:226:LEU:HD23	2.09	0.53
1:C:225:PRO:O	1:C:226:LEU:HD23	2.08	0.53
1:C:979:ASP:O	1:C:983:ARG:N	2.40	0.53
1:A:1141:LEU:HD23	1:A:1145:LEU:HD23	1.91	0.53
1:B:108:THR:OG1	1:B:234:ASN:O	2.17	0.53
1:B:192:PHE:HB3	1:B:194:PHE:CE1	2.43	0.53
1:C:102:ARG:HD2	1:C:243:ALA:HB2	1.90	0.53
1:A:64:TRP:HA	1:A:266:TYR:HD1	1.74	0.53
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.42	0.53
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.91	0.53
1:A:777:ASN:O	1:A:781:VAL:HG23	2.09	0.53
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.43	0.53
1:A:676:THR:HA	1:A:690:GLN:HG2	1.89	0.53
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.25	0.53
1:C:409:GLN:HB3	1:C:419:ALA:HB2	1.90	0.53
1:B:961:THR:O	1:B:965:GLN:HG2	2.08	0.53
1:C:721:SER:OG	1:C:722:VAL:N	2.42	0.53
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.91	0.53
1:C:81:ASN:ND2	1:C:139:PRO:O	2.41	0.53
1:C:586:ASP:OD1	1:C:587:ILE:N	2.41	0.53
1:C:644:GLN:HE21	1:C:645:THR:N	2.06	0.53
1:C:802:PHE:HD2	1:C:805:ILE:HD11	1.74	0.53
1:C:985:ASP:OD1	1:C:985:ASP:N	2.39	0.53
1:B:65:PHE:HD2	1:B:265:TYR:CZ	2.27	0.53
1:C:1043:CYS:HB2	1:C:1048:HIS:HD2	1.73	0.53
1:A:645:THR:HG22	1:A:648:GLY:O	2.08	0.53
1:B:38:TYR:CE1	1:B:285:ILE:HG13	2.44	0.53
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.92	0.53
1:A:86:PHE:N	1:A:237:ARG:HA	2.23	0.52
1:C:87:ASN:OD1	1:C:87:ASN:N	2.43	0.52
1:C:800:PHE:N	1:C:800:PHE:HD1	2.06	0.52
1:B:327:VAL:HG11	1:B:528:LYS:HZ2	1.74	0.52
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.35	0.52
1:C:949:GLN:O	1:C:953:ASN:ND2	2.41	0.52
1:A:140:PHE:HB2	1:A:244:LEU:HD13	1.91	0.52
1:A:880:GLY:O	1:A:884:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.91	0.52
1:C:1002:GLN:O	1:C:1006:THR:HG23	2.10	0.52
1:B:62:VAL:CG1	1:B:266:TYR:HB3	2.40	0.52
1:C:84:LEU:HD22	1:C:267:VAL:HG21	1.91	0.52
1:A:981:LEU:O	1:C:386:LYS:NZ	2.42	0.52
1:B:336:CYS:HB3	1:B:358:ILE:HG21	1.92	0.52
1:B:65:PHE:HE2	1:B:84:LEU:HD21	1.74	0.52
1:B:661:GLU:N	1:B:661:GLU:OE1	2.43	0.52
1:B:825:LYS:HE3	1:B:938:LEU:O	2.09	0.52
1:C:543:PHE:CD1	1:C:576:VAL:HG21	2.44	0.52
1:B:388:ASN:HD21	1:B:527:PRO:HG2	1.74	0.52
1:C:365:TYR:O	1:C:369:TYR:HB2	2.09	0.52
1:A:1055:SER:OG	1:A:1056:ALA:N	2.42	0.52
1:B:568:ASP:OD1	1:B:569:ILE:N	2.39	0.52
1:C:666:ILE:HB	1:C:670:ILE:O	2.09	0.52
1:C:1092:GLU:OE2	1:C:1092:GLU:N	2.43	0.52
1:A:391:CYS:CB	1:A:525:CYS:HA	2.38	0.51
1:A:917:TYR:HD2	1:C:1089:PHE:CE2	2.28	0.51
1:B:117:LEU:HD23	1:B:118:LEU:N	2.25	0.51
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.11	0.51
1:A:91:TYR:HB2	1:A:270:LEU:HD21	1.92	0.51
1:A:100:ILE:O	1:A:243:ALA:N	2.39	0.51
1:A:388:ASN:HD21	1:A:527:PRO:HG2	1.76	0.51
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.26	0.51
1:A:767:LEU:HD23	1:A:770:ILE:HD12	1.92	0.51
1:B:65:PHE:HD2	1:B:265:TYR:HH	1.58	0.51
1:C:108:THR:OG1	1:C:234:ASN:O	2.16	0.51
1:C:703:ASN:OD1	1:C:704:SER:N	2.43	0.51
1:C:354:ASN:HD21	1:C:399:SER:HG	1.58	0.51
1:A:43:PHE:O	1:A:44:ARG:HG3	2.10	0.51
1:A:108:THR:HG22	1:A:109:THR:HG23	1.91	0.51
1:A:421:TYR:O	1:A:424:LYS:NZ	2.39	0.51
1:A:1081:ILE:HD12	1:A:1095:PHE:HE2	1.76	0.51
1:C:809:PRO:HA	1:C:814:LYS:HE2	1.91	0.51
1:C:189:LEU:HB2	1:C:210:ILE:HG12	1.92	0.51
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.41	0.51
1:C:222:ALA:O	1:C:223:LEU:HD12	2.11	0.51
1:A:105:ILE:HG22	1:A:110:LEU:HG	1.92	0.51
1:B:329:PHE:O	1:B:580:GLN:HG3	2.10	0.51
1:B:448:ASN:HD22	1:B:497:PHE:HD2	1.57	0.51
1:B:984:LEU:HD12	1:B:988:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG11	1:A:245:HIS:CG	2.46	0.51
1:A:290:ASP:OD1	1:A:292:ALA:N	2.44	0.51
1:A:291:CYS:O	1:A:298:GLU:HG3	2.10	0.51
1:A:1089:PHE:N	1:A:1089:PHE:CD1	2.79	0.51
1:B:707:TYR:CD2	1:C:883:THR:HG22	2.46	0.51
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.11	0.51
1:C:808:ASP:HB3	1:C:811:LYS:HG2	1.93	0.51
1:A:96:GLU:HG3	1:A:99:ASN:H	1.74	0.51
1:A:704:SER:HB3	1:B:790:LYS:HE2	1.93	0.51
1:B:329:PHE:HE2	1:B:528:LYS:HB3	1.76	0.51
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.93	0.50
1:A:980:ILE:HD12	1:A:980:ILE:H	1.76	0.50
1:C:133:PHE:HB2	1:C:135:PHE:CZ	2.45	0.50
1:C:922:LEU:O	1:C:926:GLN:HG3	2.11	0.50
1:B:62:VAL:HG12	1:B:266:TYR:HB3	1.93	0.50
1:B:532:ASN:OD1	1:B:533:LEU:N	2.32	0.50
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.76	0.50
1:B:197:ILE:HB	1:B:202:LYS:NZ	2.26	0.50
1:A:103:GLY:CA	1:A:241:LEU:HB3	2.39	0.50
1:A:291:CYS:HA	1:A:297:SER:OG	2.12	0.50
1:C:950:ASP:OD2	1:C:954:GLN:NE2	2.45	0.50
1:A:105:ILE:HD12	1:A:139:PRO:HB3	1.93	0.50
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.47	0.50
1:A:222:ALA:O	1:A:223:LEU:HD12	2.12	0.50
1:A:1093:GLY:HA2	1:A:1107:ARG:HE	1.76	0.50
1:C:103:GLY:CA	1:C:241:LEU:HB3	2.38	0.50
1:C:978:ASN:O	1:C:982:SER:N	2.44	0.50
1:A:117:LEU:HD23	1:A:118:LEU:N	2.26	0.50
1:A:405:ASP:HA	1:A:408:ARG:HH12	1.76	0.50
1:C:661:GLU:OE1	1:C:661:GLU:N	2.45	0.50
1:C:880:GLY:O	1:C:884:SER:OG	2.26	0.50
1:A:377:PHE:H	1:A:378:LYS:NZ	2.09	0.50
1:B:443:SER:HB3	1:B:499:PRO:HD3	1.93	0.50
1:C:436:TRP:O	1:C:509:ARG:N	2.45	0.50
1:C:655:HIS:CD2	1:C:656:VAL:H	2.29	0.50
1:A:130:VAL:HG23	1:A:233:ILE:HD11	1.94	0.50
1:A:1105:THR:HG23	1:A:1106:GLN:O	2.12	0.50
1:B:204:TYR:N	1:B:204:TYR:CD1	2.80	0.50
1:C:206:LYS:HD3	1:C:208:THR:HG21	1.93	0.50
1:C:568:ASP:OD1	1:C:569:ILE:N	2.42	0.50
1:B:506:GLN:HB2	1:B:508:TYR:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:SER:OG	1:B:606:ASN:N	2.42	0.49
1:B:698:SER:OG	1:B:699:LEU:N	2.45	0.49
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.93	0.49
1:C:443:SER:HB3	1:C:499:PRO:HD3	1.93	0.49
1:A:379:CYS:SG	1:A:384:PRO:HB3	2.52	0.49
1:B:45:SER:O	1:B:47:VAL:HG13	2.12	0.49
1:B:305:SER:OG	1:B:306:PHE:N	2.42	0.49
1:B:551:VAL:HG12	1:B:588:THR:O	2.13	0.49
1:B:979:ASP:O	1:B:983:ARG:N	2.45	0.49
1:C:107:GLY:HA2	1:C:235:ILE:HG12	1.94	0.49
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.93	0.49
1:A:498:GLN:H	1:A:501:ASN:HD21	1.61	0.49
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.94	0.49
1:B:1062:PHE:O	1:B:1063:LEU:HD23	2.13	0.49
1:A:764:ASN:O	1:A:768:THR:HG23	2.12	0.49
1:B:130:VAL:HG22	1:B:168:PHE:O	2.13	0.49
1:B:201:PHE:N	1:B:229:LEU:O	2.46	0.49
1:B:393:THR:HA	1:B:522:ALA:HA	1.94	0.49
1:C:189:LEU:HD12	1:C:210:ILE:HD13	1.94	0.49
1:A:734:THR:OG1	1:A:735:SER:N	2.46	0.49
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.76	0.49
1:B:434:ILE:HB	1:B:511:VAL:HG23	1.94	0.49
1:B:704:SER:HB3	1:C:790:LYS:HE2	1.95	0.49
1:B:1004:LEU:O	1:B:1008:VAL:HG23	2.13	0.49
1:C:309:GLU:OE1	1:C:310:LYS:N	2.45	0.49
1:A:914:ASN:HD22	1:C:1123:SER:CB	2.25	0.49
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.48	0.49
1:B:273:ARG:NH1	1:B:292:ALA:HB3	2.28	0.49
1:B:656:VAL:HG12	1:B:658:ASN:N	2.24	0.49
1:B:1089:PHE:CE2	1:C:914:ASN:HA	2.48	0.49
1:C:112:SER:HB2	1:C:133:PHE:C	2.33	0.49
1:A:201:PHE:HE2	1:A:203:ILE:HG13	1.76	0.49
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.95	0.49
1:B:978:ASN:O	1:B:982:SER:N	2.46	0.49
1:A:62:VAL:HG12	1:A:266:TYR:HB3	1.95	0.48
1:A:191:GLU:HB3	1:A:223:LEU:HD21	1.95	0.48
1:A:978:ASN:O	1:A:982:SER:N	2.46	0.48
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.36	0.48
1:B:645:THR:OG1	1:B:648:GLY:O	2.21	0.48
1:B:797:PHE:O	1:B:799:GLY:N	2.45	0.48
1:B:803:SER:OG	1:B:804:GLN:NE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.48	0.48
1:C:951:VAL:O	1:C:955:ASN:ND2	2.46	0.48
1:A:800:PHE:CD1	1:A:800:PHE:N	2.80	0.48
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.95	0.48
1:C:619:GLU:OE1	1:C:619:GLU:N	2.37	0.48
1:C:813:SER:O	1:C:815:ARG:N	2.41	0.48
1:A:405:ASP:OD1	1:A:406:GLU:HG3	2.13	0.48
1:B:666:ILE:HD12	1:B:670:ILE:HG22	1.94	0.48
1:C:117:LEU:HD23	1:C:118:LEU:N	2.28	0.48
1:C:305:SER:OG	1:C:306:PHE:N	2.46	0.48
1:B:870:ILE:O	1:B:874:THR:HG23	2.14	0.48
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.49	0.48
1:A:809:PRO:HA	1:A:814:LYS:HE2	1.95	0.48
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.13	0.48
1:C:202:LYS:HB3	1:C:204:TYR:HE1	1.78	0.48
1:A:707:TYR:CD2	1:B:883:THR:HG22	2.48	0.48
1:B:87:ASN:N	1:B:87:ASN:OD1	2.46	0.48
1:B:405:ASP:HA	1:B:408:ARG:HH12	1.79	0.48
1:C:1081:ILE:HG23	1:C:1135:ASN:HB3	1.96	0.48
1:A:376:THR:HG22	1:A:435:ALA:HB3	1.95	0.48
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.46	0.48
1:C:291:CYS:HA	1:C:297:SER:OG	2.13	0.48
1:C:462:LYS:HE3	1:C:465:GLU:HB2	1.96	0.48
1:C:870:ILE:O	1:C:874:THR:HG23	2.14	0.48
1:A:204:TYR:N	1:A:204:TYR:CD1	2.79	0.48
1:A:230:PRO:HG3	1:C:357:ARG:NH1	2.28	0.48
1:A:399:SER:HB2	1:A:511:VAL:HG12	1.96	0.48
1:A:797:PHE:O	1:A:799:GLY:N	2.46	0.48
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.96	0.48
1:B:806:LEU:HD23	1:B:806:LEU:HA	1.59	0.48
1:B:808:ASP:HB3	1:B:811:LYS:HG2	1.96	0.48
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.47	0.48
1:C:38:TYR:CE1	1:C:285:ILE:HG13	2.49	0.48
1:A:365:TYR:OH	1:A:392:PHE:HE2	1.97	0.48
1:A:746:SER:OG	1:A:748:GLU:OE1	2.32	0.48
1:B:809:PRO:HA	1:B:814:LYS:HE2	1.96	0.48
1:C:339:GLY:O	1:C:343:ASN:N	2.37	0.48
1:C:431:GLY:HA2	1:C:515:PHE:HD2	1.78	0.48
1:B:107:GLY:HA2	1:B:235:ILE:HG12	1.95	0.48
1:B:586:ASP:O	1:B:587:ILE:HG13	2.14	0.48
1:B:930:ALA:O	1:B:934:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLU:HG2	1:C:97:LYS:H	1.78	0.48
1:C:531:THR:HG22	1:C:532:ASN:H	1.78	0.48
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.14	0.48
1:A:329:PHE:O	1:A:580:GLN:HG3	2.12	0.47
1:A:578:ASP:HB3	1:A:581:THR:O	2.13	0.47
1:B:107:GLY:N	1:B:235:ILE:HG23	2.29	0.47
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.96	0.47
1:B:726:ILE:HD13	1:B:945:LEU:HD13	1.96	0.47
1:C:379:CYS:SG	1:C:384:PRO:HB3	2.54	0.47
1:C:410:ILE:HG23	1:C:425:LEU:HD11	1.96	0.47
1:A:103:GLY:HA3	1:A:241:LEU:HD22	1.96	0.47
1:A:189:LEU:HD12	1:A:210:ILE:HD13	1.95	0.47
1:A:365:TYR:O	1:A:369:TYR:HB2	2.14	0.47
1:B:327:VAL:HG21	1:B:528:LYS:HZ1	1.79	0.47
1:B:433:VAL:O	1:B:434:ILE:HD13	2.14	0.47
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.13	0.47
1:B:768:THR:O	1:B:772:VAL:HG12	2.15	0.47
1:B:974:SER:OG	1:B:975:SER:N	2.48	0.47
1:B:1089:PHE:N	1:B:1089:PHE:CD1	2.82	0.47
1:A:62:VAL:HG13	1:A:268:GLY:N	2.30	0.47
1:A:280:ASN:OD1	1:A:284:THR:N	2.29	0.47
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.49	0.47
1:C:698:SER:OG	1:C:699:LEU:N	2.47	0.47
1:A:29:THR:HG22	1:A:62:VAL:O	2.14	0.47
1:A:229:LEU:HB3	1:A:231:ILE:HG23	1.97	0.47
1:A:540:ASN:OD1	1:A:540:ASN:N	2.47	0.47
1:B:107:GLY:H	1:B:235:ILE:HG23	1.80	0.47
1:B:133:PHE:HB2	1:B:135:PHE:CZ	2.50	0.47
1:A:501:ASN:ND2	1:A:505:TYR:O	2.47	0.47
1:A:979:ASP:HB3	1:A:983:ARG:HH21	1.80	0.47
1:A:1090:PRO:HB3	1:A:1095:PHE:CE1	2.50	0.47
1:B:299:THR:HG22	1:B:308:VAL:HG21	1.97	0.47
1:C:131:CYS:SG	1:C:132:GLU:N	2.87	0.47
1:C:802:PHE:CD2	1:C:805:ILE:HD11	2.50	0.47
1:A:91:TYR:HD2	1:A:268:GLY:H	1.62	0.47
1:A:1089:PHE:N	1:A:1089:PHE:HD1	2.12	0.47
1:B:29:THR:HG22	1:B:62:VAL:O	2.15	0.47
1:B:228:ASP:OD1	1:B:229:LEU:N	2.48	0.47
1:C:92:PHE:HZ	1:C:240:THR:HB	1.79	0.47
1:C:143:VAL:HG12	1:C:243:ALA:HB1	1.97	0.47
1:C:392:PHE:HB3	1:C:517:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:ASN:HB3	1:C:505:TYR:HB2	1.97	0.47
1:A:43:PHE:HD1	1:C:563:GLN:NE2	2.13	0.47
1:A:660:TYR:H	1:A:695:TYR:HE2	1.59	0.47
1:B:773:GLU:OE2	1:B:1019:ARG:HD3	2.14	0.47
1:C:977:LEU:HG	1:C:981:LEU:HD12	1.97	0.47
1:A:394:ASN:ND2	1:A:516:GLU:OE2	2.33	0.47
1:A:913:GLN:O	1:A:916:LEU:N	2.48	0.47
1:B:609:ALA:HB2	1:B:692:ILE:HD12	1.96	0.47
1:B:896:ILE:HG13	1:B:897:PRO:HD2	1.96	0.47
1:A:86:PHE:HA	1:A:90:VAL:CG2	2.45	0.46
1:C:228:ASP:OD1	1:C:229:LEU:N	2.48	0.46
1:A:894:LEU:HD13	1:C:715:PRO:HD3	1.98	0.46
1:A:968:SER:HB2	1:A:970:PHE:CE1	2.50	0.46
1:B:394:ASN:HB3	1:B:516:GLU:OE2	2.15	0.46
1:B:1094:VAL:HG12	1:C:904:TYR:OH	2.14	0.46
1:C:36:VAL:O	1:C:222:ALA:HA	2.16	0.46
1:C:172:SER:O	1:C:172:SER:OG	2.30	0.46
1:C:376:THR:HG22	1:C:435:ALA:HB3	1.96	0.46
1:C:377:PHE:CD1	1:C:434:ILE:HD12	2.51	0.46
1:C:794:ILE:HG13	1:C:794:ILE:O	2.15	0.46
1:A:449:TYR:O	1:A:494:SER:OG	2.27	0.46
1:B:187:LYS:O	1:B:210:ILE:N	2.33	0.46
1:B:578:ASP:HB3	1:B:581:THR:O	2.15	0.46
1:C:86:PHE:HA	1:C:90:VAL:HG21	1.96	0.46
1:A:498:GLN:H	1:A:501:ASN:ND2	2.13	0.46
1:B:93:ALA:O	1:B:94:SER:OG	2.29	0.46
1:B:978:ASN:HA	1:B:981:LEU:HB2	1.96	0.46
1:A:38:TYR:CE1	1:A:285:ILE:HG13	2.51	0.46
1:A:930:ALA:O	1:A:934:ILE:HG12	2.15	0.46
1:B:655:HIS:CD2	1:B:656:VAL:H	2.34	0.46
1:B:747:THR:OG1	1:B:748:GLU:N	2.48	0.46
1:B:794:ILE:HG13	1:B:794:ILE:O	2.16	0.46
1:C:119:ILE:HG12	1:C:128:ILE:HD12	1.97	0.46
1:A:231:ILE:HG13	1:A:232:GLY:N	2.31	0.46
1:A:666:ILE:HB	1:A:670:ILE:O	2.15	0.46
1:C:131:CYS:HB2	1:C:166:CYS:HB3	1.68	0.46
1:C:429:PHE:HE1	1:C:514:SER:HA	1.80	0.46
1:C:734:THR:OG1	1:C:735:SER:N	2.48	0.46
1:A:337:PRO:O	1:A:341:VAL:HG23	2.16	0.46
1:C:86:PHE:H	1:C:237:ARG:HA	1.81	0.46
1:C:104:TRP:CD1	1:C:194:PHE:HE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:THR:HG22	1:A:532:ASN:H	1.81	0.46
1:A:655:HIS:CD2	1:A:656:VAL:H	2.33	0.46
1:A:794:ILE:O	1:A:794:ILE:HG13	2.16	0.46
1:A:804:GLN:O	1:A:816:SER:OG	2.34	0.46
1:C:960:ASN:HA	1:C:963:VAL:HG12	1.98	0.46
1:C:1049:LEU:HB2	1:C:1065:VAL:O	2.14	0.46
1:A:714:ILE:HD11	1:A:1094:VAL:HG21	1.96	0.46
1:C:89:GLY:C	1:C:270:LEU:HD12	2.35	0.46
1:C:949:GLN:HG3	1:C:953:ASN:ND2	2.31	0.46
1:A:393:THR:HA	1:A:522:ALA:HA	1.97	0.46
1:A:530:SER:OG	1:A:580:GLN:NE2	2.49	0.46
1:C:92:PHE:HE2	1:C:238:PHE:HE2	1.62	0.46
1:C:212:LEU:HD22	1:C:217:PRO:HB3	1.98	0.46
1:B:302:THR:HG23	1:B:303:LEU:HD23	1.98	0.45
1:C:797:PHE:O	1:C:799:GLY:N	2.49	0.45
1:A:92:PHE:HZ	1:A:240:THR:HB	1.81	0.45
1:A:770:ILE:O	1:A:774:GLN:HG2	2.16	0.45
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.17	0.45
1:B:201:PHE:HE2	1:B:203:ILE:HG13	1.81	0.45
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.96	0.45
1:C:332:ILE:HD12	1:C:332:ILE:HA	1.81	0.45
1:C:532:ASN:OD1	1:C:533:LEU:N	2.34	0.45
1:C:770:ILE:O	1:C:774:GLN:HG2	2.16	0.45
1:C:1060:VAL:HG22	1:C:1061:VAL:H	1.80	0.45
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.50	0.45
1:A:754:LEU:HD23	1:A:754:LEU:HA	1.83	0.45
1:B:530:SER:OG	1:B:580:GLN:NE2	2.49	0.45
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.97	0.45
1:A:1082:CYS:HB2	1:A:1126:CYS:HB2	1.93	0.45
1:A:1093:GLY:H	1:A:1107:ARG:NH2	2.15	0.45
1:B:337:PRO:O	1:B:341:VAL:HG23	2.16	0.45
1:C:405:ASP:HA	1:C:408:ARG:HH22	1.82	0.45
1:A:949:GLN:HE21	1:A:953:ASN:HD21	1.63	0.45
1:B:86:PHE:H	1:B:237:ARG:HA	1.81	0.45
1:B:200:TYR:CD2	1:B:230:PRO:HB3	2.52	0.45
1:C:63:THR:O	1:C:63:THR:OG1	2.17	0.45
1:C:118:LEU:HB3	1:C:129:LYS:HB2	1.99	0.45
1:A:107:GLY:HA2	1:A:235:ILE:HG12	1.97	0.45
1:A:403:ARG:HD3	1:A:505:TYR:HA	1.99	0.45
1:A:715:PRO:HD3	1:B:894:LEU:HD13	1.99	0.45
1:B:391:CYS:CB	1:B:525:CYS:HA	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.99	0.45
1:C:407:VAL:HG22	1:C:408:ARG:HH11	1.82	0.45
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.67	0.45
1:B:357:ARG:CZ	1:C:230:PRO:HG3	2.46	0.45
1:B:357:ARG:NH1	1:C:230:PRO:HG3	2.31	0.45
1:B:433:VAL:HG23	1:B:512:VAL:HG22	1.99	0.45
1:C:189:LEU:HD23	1:C:191:GLU:H	1.81	0.45
1:C:506:GLN:HB2	1:C:508:TYR:HE1	1.81	0.45
1:A:137:ASN:OD1	1:A:138:ASP:N	2.49	0.45
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.73	0.45
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.99	0.45
1:A:914:ASN:OD1	1:A:915:VAL:N	2.49	0.45
1:C:94:SER:OG	1:C:95:THR:N	2.50	0.45
1:C:906:PHE:O	1:C:908:GLY:N	2.49	0.45
1:A:351:TYR:CE1	1:A:452:LEU:HB2	2.52	0.45
1:B:91:TYR:HB2	1:B:270:LEU:HD21	1.98	0.45
1:B:273:ARG:HD3	1:B:273:ARG:HA	1.75	0.45
1:B:392:PHE:CD1	1:B:515:PHE:HB3	2.52	0.45
1:B:402:ILE:HD11	1:B:407:VAL:HG12	1.98	0.45
1:B:673:SER:OG	1:B:674:TYR:N	2.50	0.45
1:C:197:ILE:HB	1:C:202:LYS:NZ	2.31	0.45
1:C:231:ILE:HG13	1:C:232:GLY:N	2.31	0.45
1:C:958:ALA:O	1:C:961:THR:OG1	2.31	0.45
1:A:34:ARG:NH1	1:A:189:LEU:HD11	2.32	0.45
1:B:214:ARG:NE	1:B:215:ASP:HB2	2.25	0.45
1:B:979:ASP:HB3	1:B:983:ARG:HE	1.81	0.45
1:C:271:GLN:HB2	1:C:272:PRO:HD2	1.98	0.45
1:B:403:ARG:HH21	1:B:495:TYR:HD1	1.64	0.44
1:B:949:GLN:HG3	1:B:953:ASN:HD21	1.83	0.44
1:B:979:ASP:HB3	1:B:983:ARG:NE	2.32	0.44
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.76	0.44
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.75	0.44
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.52	0.44
1:A:419:ALA:HA	1:A:423:TYR:O	2.17	0.44
1:B:222:ALA:C	1:B:223:LEU:HD12	2.37	0.44
1:C:379:CYS:HB2	1:C:384:PRO:HD3	1.99	0.44
1:A:64:TRP:C	1:A:64:TRP:CD1	2.90	0.44
1:A:189:LEU:HB2	1:A:210:ILE:CG1	2.47	0.44
1:A:273:ARG:NH1	1:A:292:ALA:HB3	2.33	0.44
1:A:737:ASP:OD2	1:C:319:ARG:NH2	2.51	0.44
1:B:189:LEU:O	1:B:189:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TYR:CE2	1:B:230:PRO:HB3	2.52	0.44
1:B:222:ALA:O	1:B:223:LEU:HD12	2.17	0.44
1:C:66:HIS:ND1	1:C:66:HIS:O	2.51	0.44
1:A:568:ASP:OD1	1:A:569:ILE:N	2.44	0.44
1:B:106:PHE:HZ	1:B:194:PHE:CE2	2.35	0.44
1:B:449:TYR:O	1:B:494:SER:OG	2.27	0.44
1:B:1089:PHE:N	1:B:1089:PHE:HD1	2.15	0.44
1:B:1129:VAL:CG2	1:C:917:TYR:HB3	2.48	0.44
1:C:341:VAL:HG22	1:C:356:LYS:HE3	1.99	0.44
1:C:949:GLN:HG3	1:C:953:ASN:HD21	1.81	0.44
1:A:212:LEU:HD22	1:A:217:PRO:HB3	1.99	0.44
1:A:411:ALA:N	1:A:425:LEU:HD12	2.33	0.44
1:B:191:GLU:HB3	1:B:223:LEU:HD21	1.99	0.44
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.99	0.44
1:C:979:ASP:HB3	1:C:983:ARG:NE	2.32	0.44
1:C:1009:THR:O	1:C:1013:ILE:HG13	2.17	0.44
1:C:121:ASN:OD1	1:C:121:ASN:N	2.51	0.44
1:A:92:PHE:CZ	1:A:240:THR:HB	2.52	0.44
1:A:277:LEU:H	1:A:277:LEU:HG	1.65	0.44
1:A:498:GLN:CD	1:A:499:PRO:HD2	2.38	0.44
1:A:768:THR:O	1:A:772:VAL:HG12	2.18	0.44
1:B:277:LEU:H	1:B:277:LEU:HG	1.49	0.44
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.85	0.44
1:B:1090:PRO:HB3	1:B:1095:PHE:CE1	2.52	0.44
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.26	0.44
1:C:1062:PHE:O	1:C:1063:LEU:HD23	2.17	0.44
1:A:383:SER:OG	1:B:983:ARG:O	2.27	0.44
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.53	0.44
1:B:379:CYS:HA	1:B:432:CYS:HB2	1.99	0.44
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.53	0.44
1:A:748:GLU:OE1	1:A:748:GLU:N	2.36	0.44
1:B:137:ASN:OD1	1:B:138:ASP:N	2.51	0.44
1:A:51:THR:O	1:A:274:THR:HG23	2.18	0.43
1:A:201:PHE:CE2	1:A:203:ILE:HG13	2.52	0.43
1:A:228:ASP:OD1	1:A:229:LEU:N	2.51	0.43
1:B:383:SER:HB3	1:C:985:ASP:H	1.82	0.43
1:C:277:LEU:HD12	1:C:277:LEU:O	2.18	0.43
1:C:756:TYR:N	1:C:756:TYR:CD1	2.86	0.43
1:A:526:GLY:O	1:A:528:LYS:N	2.50	0.43
1:A:913:GLN:NE2	1:C:1090:PRO:HD2	2.34	0.43
1:C:45:SER:O	1:C:47:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:PRO:HA	1:C:387:LEU:HG	2.00	0.43
1:A:443:SER:OG	1:A:497:PHE:HB3	2.18	0.43
1:B:350:VAL:HG12	1:B:402:ILE:HG22	2.00	0.43
1:B:383:SER:N	1:C:983:ARG:O	2.30	0.43
1:B:770:ILE:O	1:B:774:GLN:HG2	2.18	0.43
1:B:103:GLY:CA	1:B:241:LEU:HB3	2.41	0.43
1:B:229:LEU:HB3	1:B:231:ILE:HG12	2.00	0.43
1:B:405:ASP:OD1	1:B:406:GLU:HG3	2.18	0.43
1:B:800:PHE:H	1:B:800:PHE:HD1	1.64	0.43
1:B:1003:SER:O	1:B:1006:THR:OG1	2.33	0.43
1:C:105:ILE:HD12	1:C:139:PRO:HB3	2.01	0.43
1:C:806:LEU:HA	1:C:806:LEU:HD23	1.62	0.43
1:A:420:ASP:C	1:A:424:LYS:HD2	2.39	0.43
1:B:332:ILE:HG12	1:B:334:ASN:H	1.82	0.43
1:B:568:ASP:CG	1:B:569:ILE:H	2.21	0.43
1:B:737:ASP:OD1	1:B:737:ASP:N	2.51	0.43
1:C:202:LYS:HB3	1:C:204:TYR:CE1	2.53	0.43
1:C:900:MET:HA	1:C:917:TYR:OH	2.18	0.43
1:A:323:THR:HG22	1:A:324:GLU:HG2	2.01	0.43
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.53	0.43
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.54	0.43
1:A:1089:PHE:HB3	1:A:1090:PRO:HD2	2.00	0.43
1:A:1090:PRO:HD2	1:B:913:GLN:NE2	2.34	0.43
1:B:62:VAL:HG13	1:B:267:VAL:C	2.38	0.43
1:B:189:LEU:HB3	1:B:208:THR:HG23	2.00	0.43
1:B:914:ASN:OD1	1:B:915:VAL:N	2.51	0.43
1:C:90:VAL:HG11	1:C:238:PHE:CZ	2.53	0.43
1:C:365:TYR:HH	1:C:392:PHE:HZ	1.66	0.43
1:A:107:GLY:N	1:A:235:ILE:HG23	2.33	0.43
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.99	0.43
1:B:555:SER:OG	1:B:584:ILE:HG22	2.18	0.43
1:B:576:VAL:HG12	1:B:577:ARG:H	1.83	0.43
1:C:215:ASP:HA	1:C:266:TYR:OH	2.18	0.43
1:A:89:GLY:O	1:A:270:LEU:HD12	2.19	0.43
1:A:110:LEU:HD22	1:A:237:ARG:HH12	1.84	0.43
1:A:429:PHE:HE1	1:A:514:SER:HA	1.82	0.43
1:B:64:TRP:CD1	1:B:64:TRP:C	2.91	0.43
1:B:607:GLN:O	1:B:692:ILE:HD11	2.19	0.43
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.53	0.43
1:C:526:GLY:O	1:C:528:LYS:N	2.50	0.43
1:A:81:ASN:OD1	1:A:81:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:HG13	1:A:534:VAL:HG22	2.01	0.43
1:A:403:ARG:HH21	1:A:495:TYR:HD1	1.65	0.43
1:B:393:THR:HG22	1:B:516:GLU:O	2.19	0.43
1:C:354:ASN:ND2	1:C:399:SER:OG	2.32	0.43
1:C:870:ILE:H	1:C:870:ILE:HG12	1.67	0.43
1:A:204:TYR:N	1:A:204:TYR:HD1	2.16	0.43
1:A:776:LYS:O	1:A:780:GLU:HG3	2.19	0.43
1:A:903:ALA:HB1	1:A:913:GLN:HB2	2.00	0.43
1:C:64:TRP:HD1	1:C:266:TYR:CE1	2.37	0.43
1:C:105:ILE:HG22	1:C:110:LEU:HG	2.01	0.43
1:C:291:CYS:HB3	1:C:301:CYS:HB2	1.40	0.43
1:C:426:PRO:HB2	1:C:429:PHE:HB2	2.00	0.43
1:C:777:ASN:O	1:C:781:VAL:HG23	2.19	0.43
1:A:107:GLY:O	1:A:236:THR:N	2.47	0.42
1:A:551:VAL:HG22	1:A:588:THR:O	2.19	0.42
1:A:1031:GLU:OE2	1:C:1039:ARG:HB3	2.19	0.42
1:B:576:VAL:HG12	1:B:577:ARG:N	2.34	0.42
1:B:756:TYR:CD1	1:B:756:TYR:N	2.87	0.42
1:B:756:TYR:HB3	1:B:759:PHE:HD2	1.84	0.42
1:A:103:GLY:N	1:A:241:LEU:O	2.51	0.42
1:A:104:TRP:CD1	1:A:194:PHE:HE2	2.37	0.42
1:A:290:ASP:OD1	1:A:291:CYS:N	2.52	0.42
1:B:870:ILE:H	1:B:870:ILE:HG12	1.70	0.42
1:C:878:LEU:HD12	1:C:882:ILE:HD11	2.00	0.42
1:C:1047:TYR:O	1:C:1066:THR:OG1	2.21	0.42
1:A:86:PHE:HA	1:A:90:VAL:HG23	2.01	0.42
1:A:87:ASN:OD1	1:A:87:ASN:N	2.51	0.42
1:A:332:ILE:HG12	1:A:334:ASN:H	1.85	0.42
1:A:718:PHE:HA	1:A:1069:PRO:HA	2.02	0.42
1:A:917:TYR:CE2	1:C:1079:PRO:HB2	2.54	0.42
1:B:112:SER:HB2	1:B:133:PHE:C	2.39	0.42
1:B:418:ILE:HD11	1:B:495:TYR:OH	2.19	0.42
1:B:1107:ARG:HD3	1:C:904:TYR:CE2	2.55	0.42
1:C:186:PHE:HB2	1:C:213:VAL:HA	2.01	0.42
1:A:28:TYR:HD2	1:A:61:ASN:HB3	1.84	0.42
1:A:63:THR:O	1:A:63:THR:OG1	2.35	0.42
1:A:86:PHE:HE2	1:A:196:ASN:HD21	1.66	0.42
1:A:104:TRP:HD1	1:A:106:PHE:CZ	2.37	0.42
1:A:386:LYS:NZ	1:B:982:SER:HA	2.35	0.42
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.85	0.42
1:B:977:LEU:HG	1:B:981:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:PHE:CZ	1:C:240:THR:HB	2.54	0.42
1:C:222:ALA:C	1:C:223:LEU:HD12	2.40	0.42
1:C:264:ALA:HB1	1:C:266:TYR:CE1	2.54	0.42
1:A:106:PHE:CD1	1:A:106:PHE:N	2.87	0.42
1:A:547:THR:HG22	1:A:548:GLY:N	2.35	0.42
1:A:1043:CYS:HB3	1:A:1048:HIS:HD2	1.83	0.42
1:C:113:LYS:HA	1:C:113:LYS:HD2	1.83	0.42
1:B:277:LEU:HD12	1:B:277:LEU:O	2.20	0.42
1:B:805:ILE:HB	1:B:1054:GLN:HE22	1.83	0.42
1:B:1029:MET:HA	1:B:1033:VAL:HG23	2.02	0.42
1:C:91:TYR:HE2	1:C:93:ALA:HB2	1.84	0.42
1:C:334:ASN:O	1:C:362:VAL:HG22	2.19	0.42
1:C:415:THR:HG1	1:C:420:ASP:CG	2.20	0.42
1:A:1093:GLY:H	1:A:1107:ARG:HH21	1.65	0.42
1:B:92:PHE:HE1	1:B:238:PHE:HE2	1.67	0.42
1:C:616:ASN:OD1	1:C:617:CYS:N	2.52	0.42
1:A:112:SER:HB2	1:A:133:PHE:C	2.39	0.42
1:A:225:PRO:O	1:A:226:LEU:HD22	2.19	0.42
1:A:334:ASN:HB3	1:A:361:CYS:HA	2.02	0.42
1:A:916:LEU:HD12	1:A:923:ILE:HD12	2.01	0.42
1:A:957:GLN:O	1:A:961:THR:HG22	2.20	0.42
1:A:985:ASP:H	1:C:383:SER:HB3	1.85	0.42
1:B:102:ARG:HD2	1:B:243:ALA:HB2	2.02	0.42
1:B:403:ARG:HD3	1:B:505:TYR:HA	2.01	0.42
1:B:512:VAL:O	1:B:513:LEU:HD23	2.19	0.42
1:C:62:VAL:HG13	1:C:267:VAL:C	2.41	0.42
1:C:90:VAL:HG11	1:C:238:PHE:CE1	2.54	0.42
1:C:578:ASP:HB3	1:C:581:THR:O	2.19	0.42
1:C:979:ASP:O	1:C:982:SER:N	2.51	0.42
1:A:890:ALA:HA	1:C:1046:GLY:HA2	2.01	0.42
1:A:1060:VAL:HG22	1:A:1061:VAL:H	1.83	0.42
1:A:1062:PHE:O	1:A:1063:LEU:HD23	2.20	0.42
1:B:86:PHE:HB2	1:B:238:PHE:HD1	1.85	0.42
1:B:987:PRO:HB2	1:B:988:GLU:OE1	2.19	0.42
1:C:143:VAL:HG11	1:C:245:HIS:CE1	2.54	0.42
1:A:319:ARG:HH12	1:B:740:MET:HB2	1.85	0.42
1:A:506:GLN:HB2	1:A:508:TYR:HE1	1.84	0.42
1:A:560:LEU:O	1:A:562:PHE:N	2.53	0.42
1:A:1094:VAL:HG12	1:B:904:TYR:OH	2.18	0.42
1:B:537:LYS:O	1:B:539:VAL:HG13	2.20	0.42
1:B:800:PHE:CD1	1:B:800:PHE:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:ASN:HA	1:B:963:VAL:HG12	2.00	0.42
1:C:204:TYR:N	1:C:204:TYR:HD1	2.17	0.42
1:C:266:TYR:CD1	1:C:266:TYR:N	2.85	0.42
1:C:273:ARG:NH1	1:C:292:ALA:HB3	2.34	0.42
1:C:584:ILE:HD13	1:C:584:ILE:HA	1.83	0.42
1:C:614:ASP:N	1:C:614:ASP:OD1	2.52	0.42
1:A:323:THR:HG21	1:A:537:LYS:HD2	2.02	0.41
1:A:350:VAL:O	1:A:353:TRP:HD1	2.03	0.41
1:A:430:THR:O	1:A:430:THR:OG1	2.37	0.41
1:A:725:GLU:CD	1:A:1028:LYS:HZ1	2.22	0.41
1:A:979:ASP:O	1:A:983:ARG:N	2.53	0.41
1:C:332:ILE:HG13	1:C:334:ASN:HD22	1.85	0.41
1:C:873:TYR:HD1	1:C:873:TYR:HA	1.73	0.41
1:B:437:ASN:HD22	1:B:439:ASN:H	1.68	0.41
1:B:598:ILE:HB	1:B:609:ALA:HB3	2.02	0.41
1:C:191:GLU:OE1	1:C:223:LEU:HD11	2.19	0.41
1:C:350:VAL:HG12	1:C:402:ILE:HG22	2.01	0.41
1:A:37:TYR:OH	1:A:54:LEU:O	2.26	0.41
1:A:101:ILE:HG12	1:A:242:LEU:HD11	2.02	0.41
1:A:403:ARG:HH22	1:A:496:GLY:H	1.68	0.41
1:A:913:GLN:HE21	1:C:1090:PRO:HD2	1.84	0.41
1:A:949:GLN:O	1:A:953:ASN:ND2	2.44	0.41
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.84	0.41
1:B:462:LYS:HE3	1:B:465:GLU:OE1	2.20	0.41
1:C:336:CYS:O	1:C:338:PHE:N	2.53	0.41
1:C:541:PHE:HB3	1:C:552:LEU:HD11	2.02	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:HA	2.01	0.41
1:A:143:VAL:HG11	1:A:245:HIS:CD2	2.55	0.41
1:C:427:ASP:OD1	1:C:428:ASP:N	2.52	0.41
1:C:443:SER:OG	1:C:497:PHE:HB3	2.20	0.41
1:A:796:ASP:OD1	1:A:796:ASP:N	2.52	0.41
1:A:802:PHE:CD2	1:A:805:ILE:HD11	2.44	0.41
1:A:805:ILE:HB	1:A:1054:GLN:NE2	2.35	0.41
1:B:804:GLN:O	1:B:816:SER:OG	2.39	0.41
1:B:949:GLN:HG3	1:B:953:ASN:ND2	2.35	0.41
1:A:1049:LEU:HD23	1:A:1049:LEU:HA	1.77	0.41
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.30	0.41
1:C:462:LYS:HE3	1:C:465:GLU:OE2	2.20	0.41
1:A:543:PHE:CD1	1:A:576:VAL:HG11	2.56	0.41
1:B:131:CYS:HA	1:B:166:CYS:CB	2.49	0.41
1:B:328:ARG:HH11	1:B:533:LEU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:906:PHE:O	1:B:908:GLY:N	2.52	0.41
1:C:434:ILE:N	1:C:511:VAL:O	2.28	0.41
1:B:81:ASN:ND2	1:B:139:PRO:O	2.53	0.41
1:B:716:THR:N	1:B:1071:GLN:O	2.45	0.41
1:B:1018:ILE:O	1:B:1021:SER:OG	2.32	0.41
1:C:399:SER:HB3	1:C:511:VAL:HG12	2.03	0.41
1:C:717:ASN:O	1:C:1070:ALA:N	2.52	0.41
1:A:987:PRO:HB2	1:A:988:GLU:OE1	2.21	0.41
1:A:1116:THR:HB	1:A:1140:PRO:HG3	2.02	0.41
1:B:28:TYR:HD2	1:B:61:ASN:HB3	1.86	0.41
1:B:117:LEU:HD23	1:B:118:LEU:H	1.86	0.41
1:B:266:TYR:N	1:B:266:TYR:CD1	2.89	0.41
1:B:386:LYS:NZ	1:C:982:SER:HA	2.36	0.41
1:B:443:SER:OG	1:B:497:PHE:HB3	2.21	0.41
1:B:733:LYS:HE3	1:B:771:ALA:HB1	2.03	0.41
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.51	0.41
1:B:1050:MET:O	1:B:1051:SER:OG	2.35	0.41
1:C:242:LEU:HB3	1:C:244:LEU:HD22	2.03	0.41
1:C:328:ARG:HH11	1:C:533:LEU:HB2	1.86	0.41
1:C:763:LEU:HA	1:C:763:LEU:HD23	1.75	0.41
1:C:996:LEU:HA	1:C:996:LEU:HD23	1.78	0.41
1:C:1105:THR:HG23	1:C:1106:GLN:O	2.21	0.41
1:B:377:PHE:C	1:B:378:LYS:HD2	2.41	0.41
1:B:754:LEU:HD23	1:B:754:LEU:HA	1.84	0.41
1:C:104:TRP:HB2	1:C:119:ILE:HB	2.03	0.41
1:C:106:PHE:CD1	1:C:106:PHE:N	2.88	0.41
1:C:363:ALA:O	1:C:527:PRO:HD3	2.21	0.41
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	2.02	0.41
1:A:302:THR:HG23	1:A:303:LEU:HD23	2.03	0.40
1:A:309:GLU:O	1:A:313:TYR:OH	2.29	0.40
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.87	0.40
1:A:1092:GLU:OE1	1:A:1092:GLU:N	2.54	0.40
1:B:331:ASN:HD22	1:B:580:GLN:HG2	1.86	0.40
1:B:900:MET:HA	1:B:917:TYR:OH	2.21	0.40
1:B:922:LEU:CD2	1:B:926:GLN:HE21	2.34	0.40
1:B:1038:LYS:HE2	1:B:1038:LYS:HB3	1.79	0.40
1:C:189:LEU:HB2	1:C:210:ILE:CG1	2.51	0.40
1:C:916:LEU:HD12	1:C:923:ILE:HD13	2.03	0.40
1:C:1082:CYS:HB2	1:C:1126:CYS:HB2	2.03	0.40
1:A:359:SER:OG	1:A:360:ASN:ND2	2.55	0.40
1:C:393:THR:HG21	1:C:518:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.83	0.40
1:C:978:ASN:HA	1:C:981:LEU:HB2	2.03	0.40
1:C:377:PHE:H	1:C:378:LYS:NZ	2.16	0.40
1:C:402:ILE:HD11	1:C:407:VAL:HG12	2.03	0.40
1:C:987:PRO:HB2	1:C:988:GLU:OE1	2.20	0.40
1:A:748:GLU:H	1:A:748:GLU:CD	2.21	0.40
1:B:327:VAL:HG21	1:B:528:LYS:NZ	2.37	0.40
1:B:393:THR:HG21	1:B:518:LEU:HD12	2.03	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	954/1247 (76%)	849 (89%)	105 (11%)	0	100	100
1	B	951/1247 (76%)	845 (89%)	106 (11%)	0	100	100
1	C	951/1247 (76%)	834 (88%)	117 (12%)	0	100	100
All	All	2856/3741 (76%)	2528 (88%)	328 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	855/1085 (79%)	849 (99%)	6 (1%)	84 92
1	B	855/1085 (79%)	850 (99%)	5 (1%)	86 94
1	C	855/1085 (79%)	845 (99%)	10 (1%)	71 85
All	All	2565/3255 (79%)	2544 (99%)	21 (1%)	82 91

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	ARG
1	A	462	LYS
1	A	738	CYS
1	A	800	PHE
1	A	873	TYR
1	A	1089	PHE
1	B	277	LEU
1	B	408	ARG
1	B	462	LYS
1	B	873	TYR
1	B	1089	PHE
1	C	277	LEU
1	C	392	PHE
1	C	408	ARG
1	C	432	CYS
1	C	462	LYS
1	C	529	LYS
1	C	738	CYS
1	C	800	PHE
1	C	873	TYR
1	C	1107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	354	ASN
1	A	360	ASN
1	A	388	ASN
1	A	394	ASN
1	A	501	ASN
1	A	655	HIS
1	A	658	ASN

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Mol	Chain	Res	Type
1	A	675	GLN
1	A	690	GLN
1	A	926	GLN
1	A	928	ASN
1	A	949	GLN
1	A	955	ASN
1	A	965	GLN
1	A	1005	GLN
1	A	1011	GLN
1	A	1088	HIS
1	A	1142	GLN
1	B	196	ASN
1	B	331	ASN
1	B	388	ASN
1	B	437	ASN
1	B	439	ASN
1	B	448	ASN
1	B	501	ASN
1	B	655	HIS
1	B	658	ASN
1	B	675	GLN
1	B	690	GLN
1	B	919	ASN
1	B	926	GLN
1	B	953	ASN
1	B	955	ASN
1	B	965	GLN
1	B	1088	HIS
1	C	334	ASN
1	C	394	ASN
1	C	439	ASN
1	C	448	ASN
1	C	644	GLN
1	C	655	HIS
1	C	690	GLN

5.3.3 RNA

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.

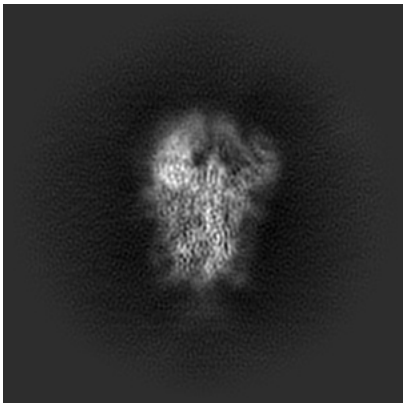
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31511. These allow visual inspection of the internal detail of the map and identification of artifacts.

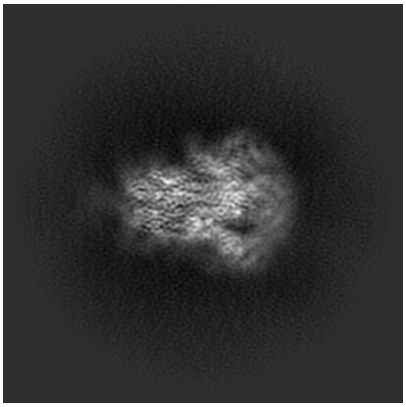
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

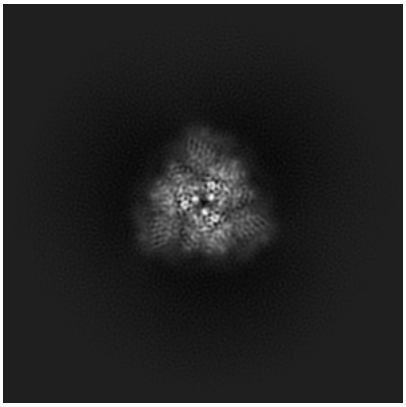
6.1.1 Primary map



X



Y

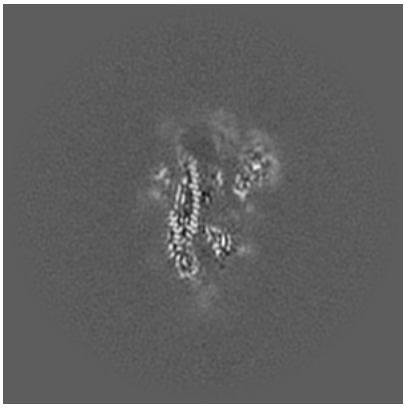


Z

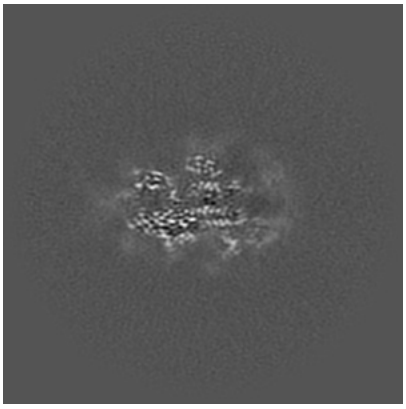
The images above show the map projected in three orthogonal directions.

6.2 Central slices

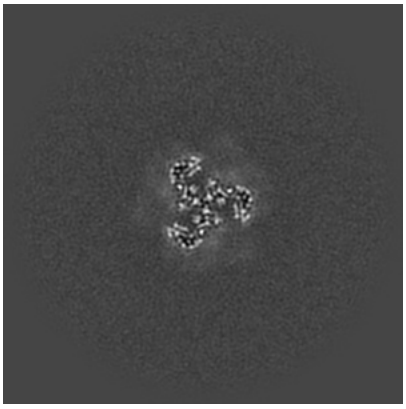
6.2.1 Primary map



X Index: 128



Y Index: 128

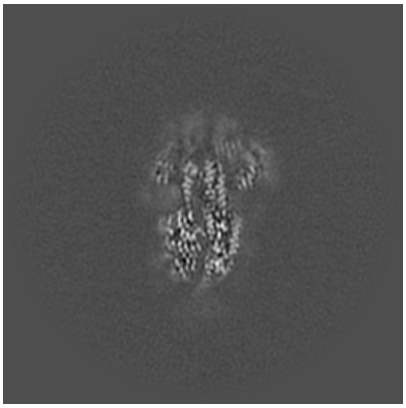


Z Index: 128

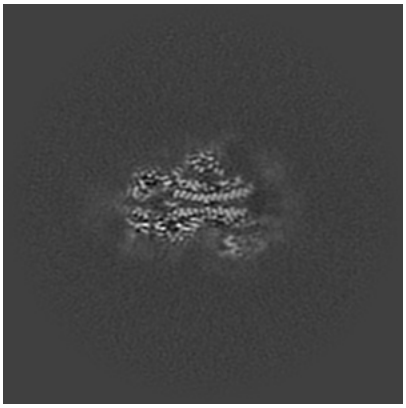
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

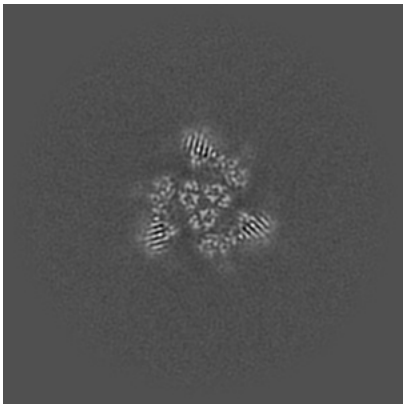
6.3.1 Primary map



X Index: 134



Y Index: 131



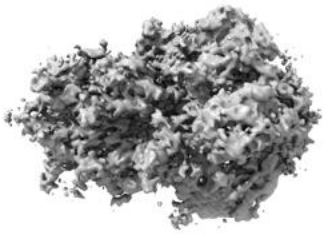
Z Index: 150

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

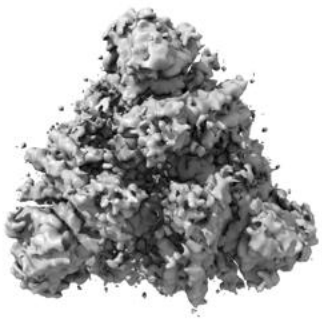
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

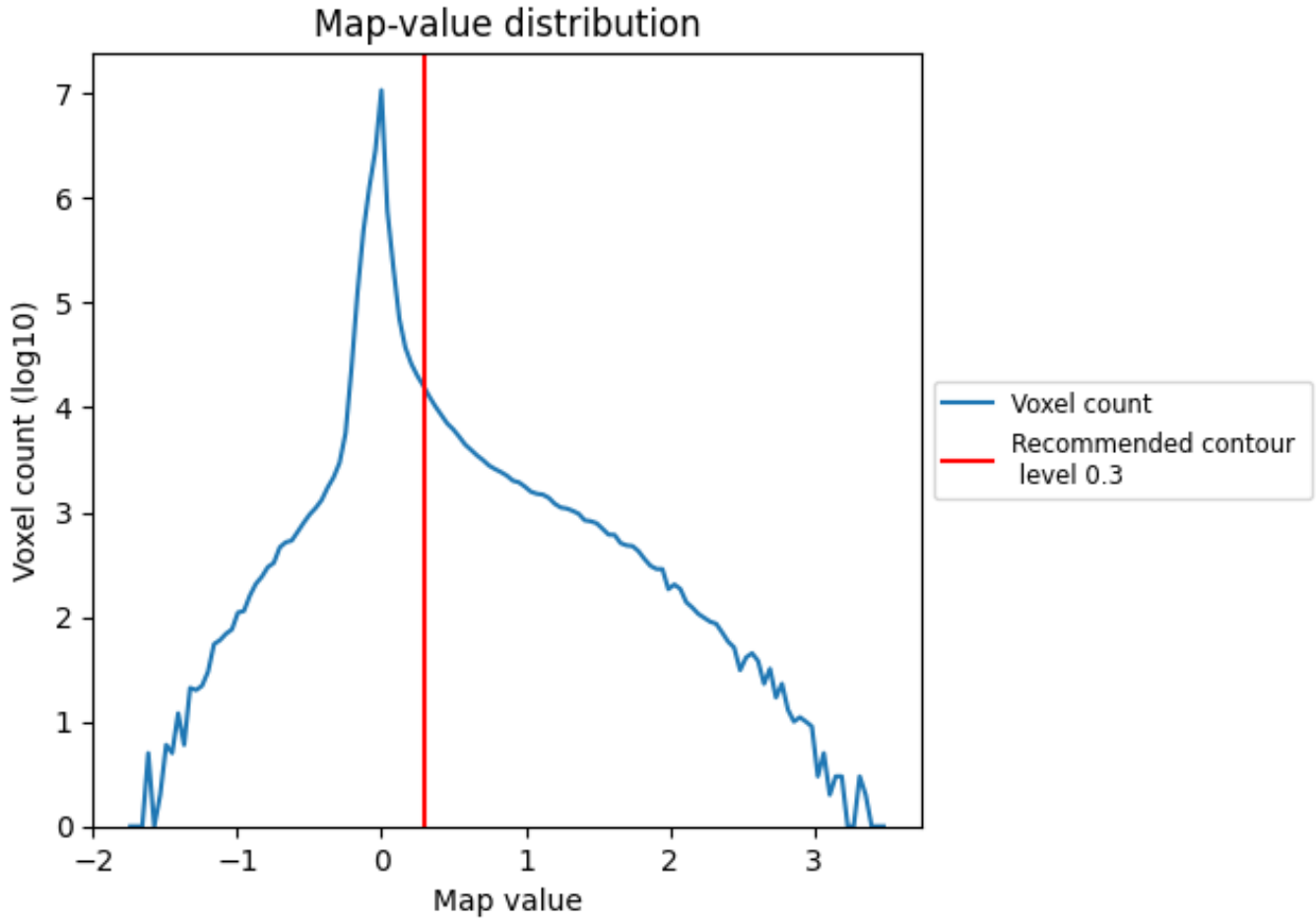
6.5 Mask visualisation (i)

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

7 Map analysis

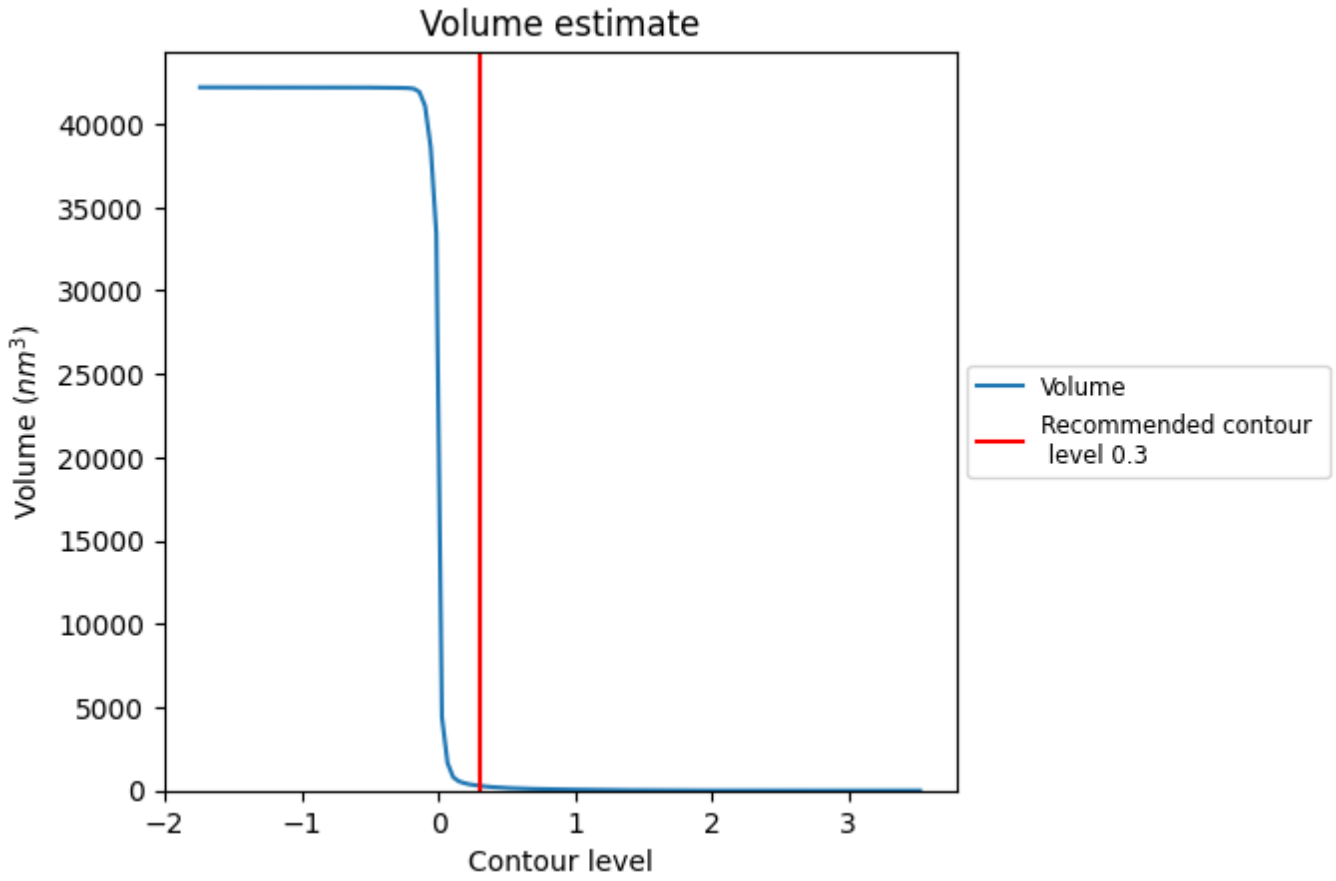
This section contains the results of statistical analysis of the map.

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.

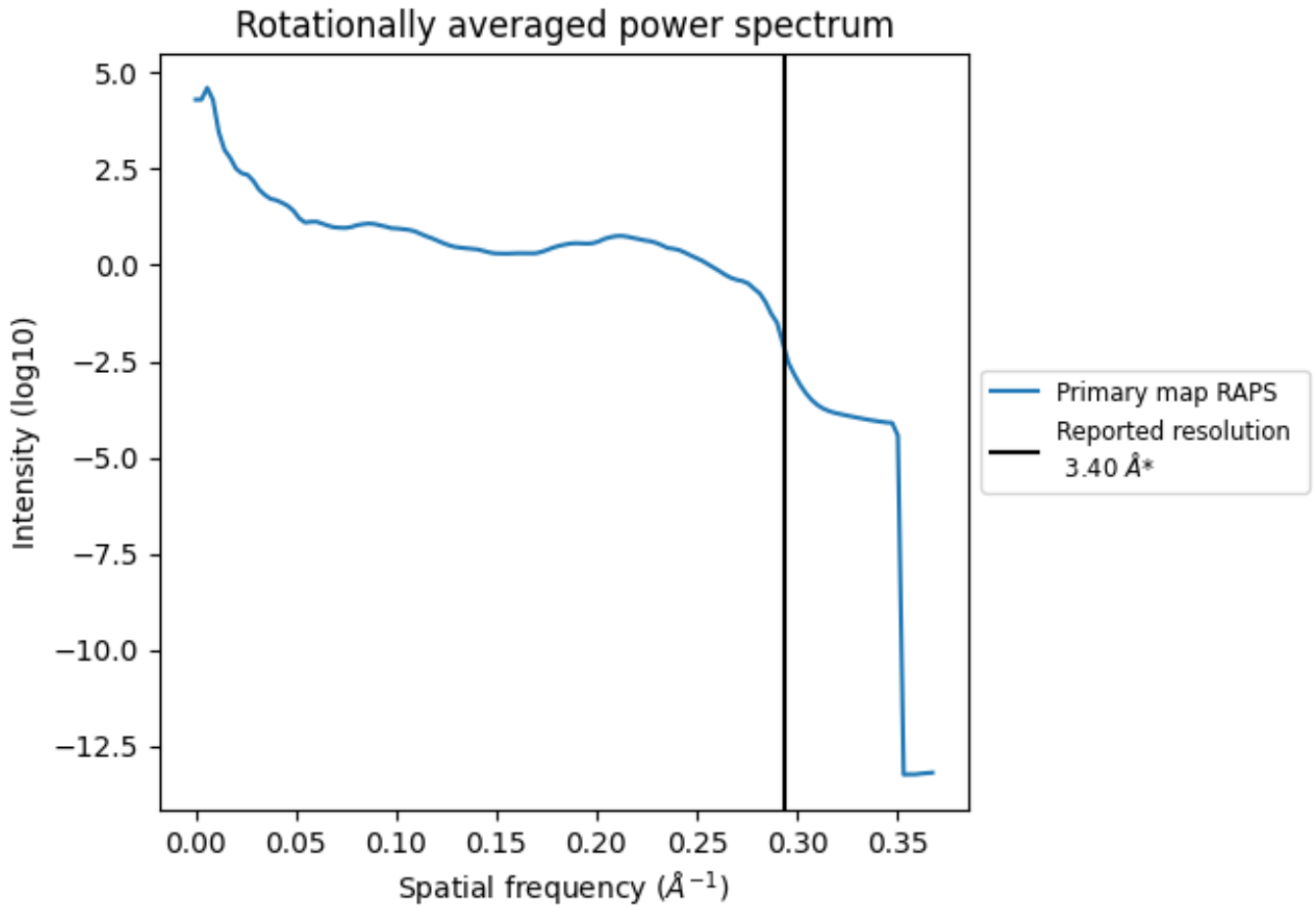
7.2 Volume estimate



The volume at the recommended contour level is 285 nm^3; this corresponds to an approximate mass of 258 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)

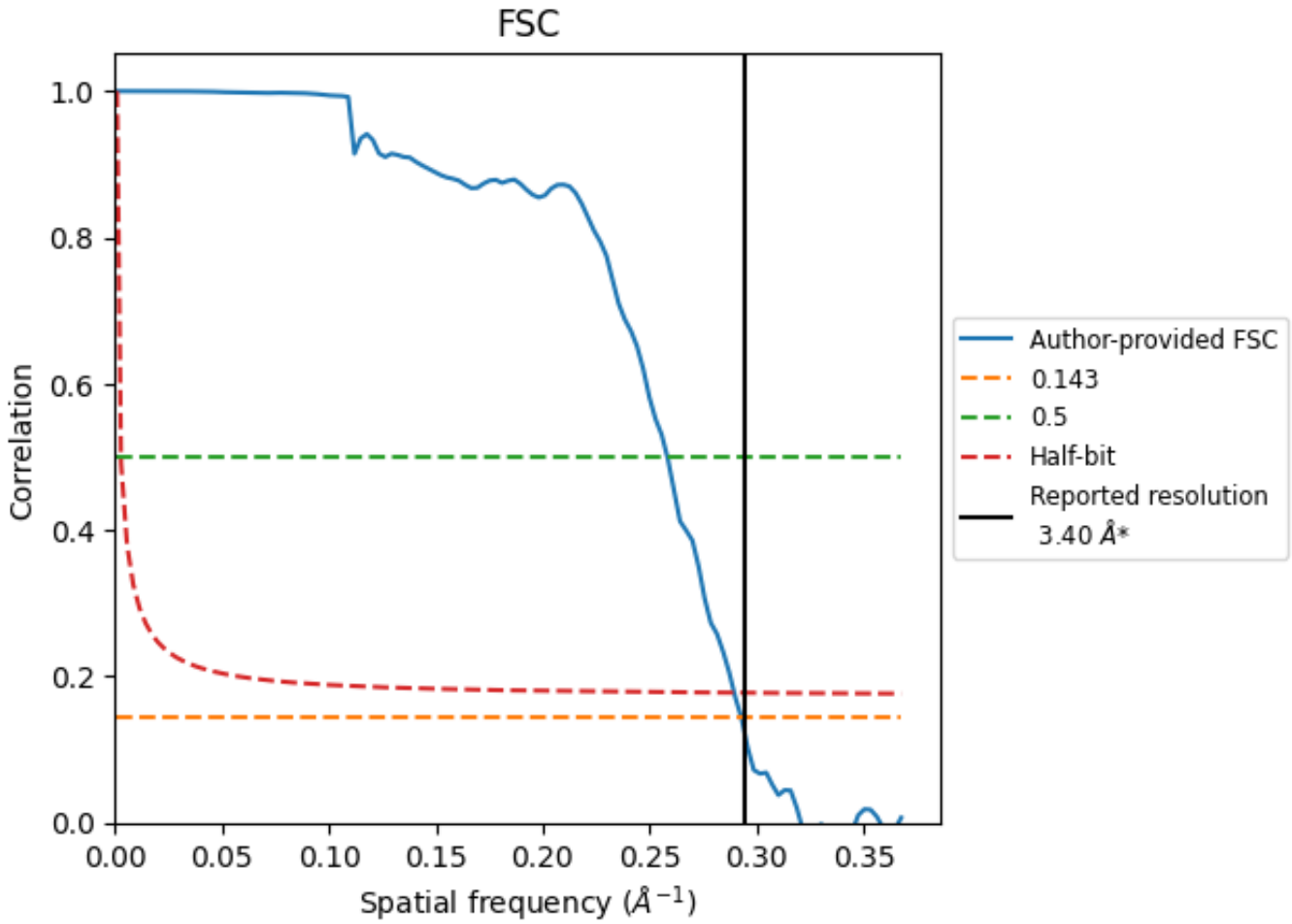


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

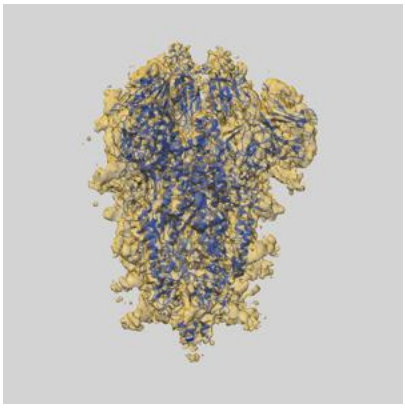
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	3.87	3.45
Unmasked-calculated*	-	-	-

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

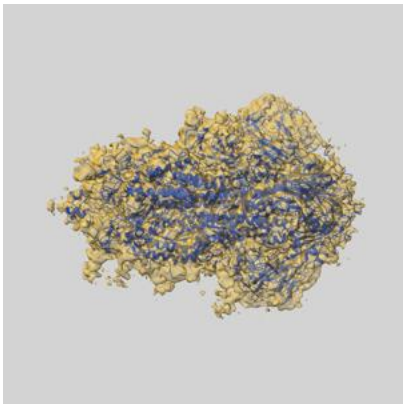
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31511 and PDB model 7FB0. Per-residue inclusion information can be found in section 3 on page 7.

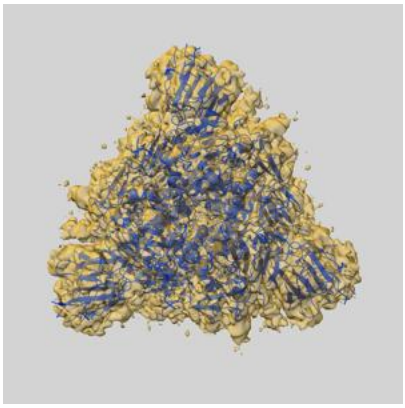
9.1 Map-model overlay



X



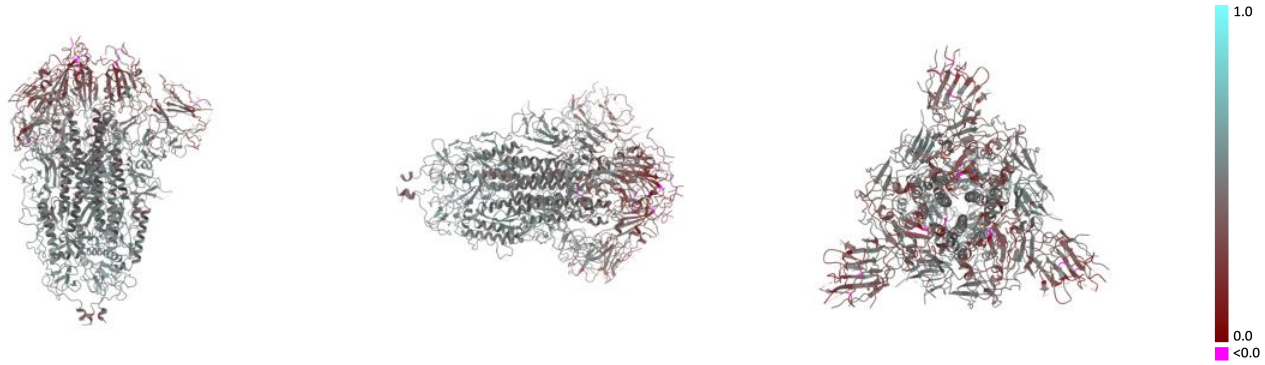
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

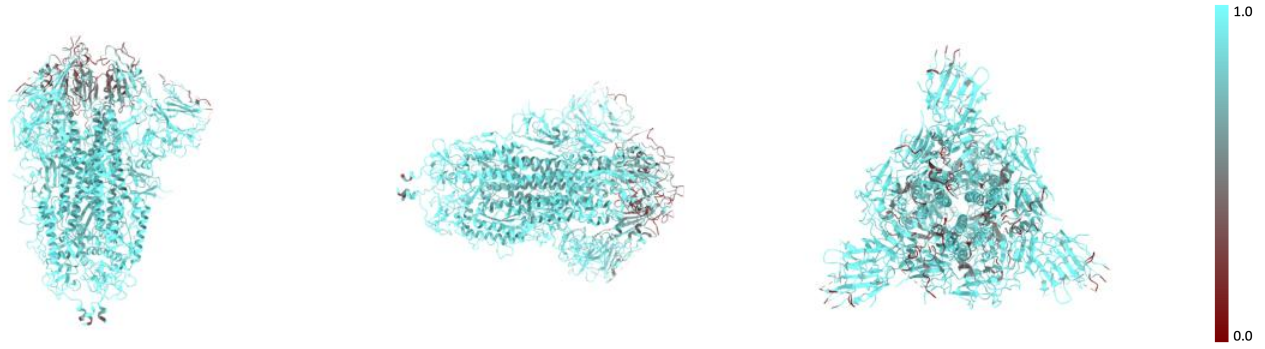
9.2 Q-score mapped to coordinate model



X Y Z

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

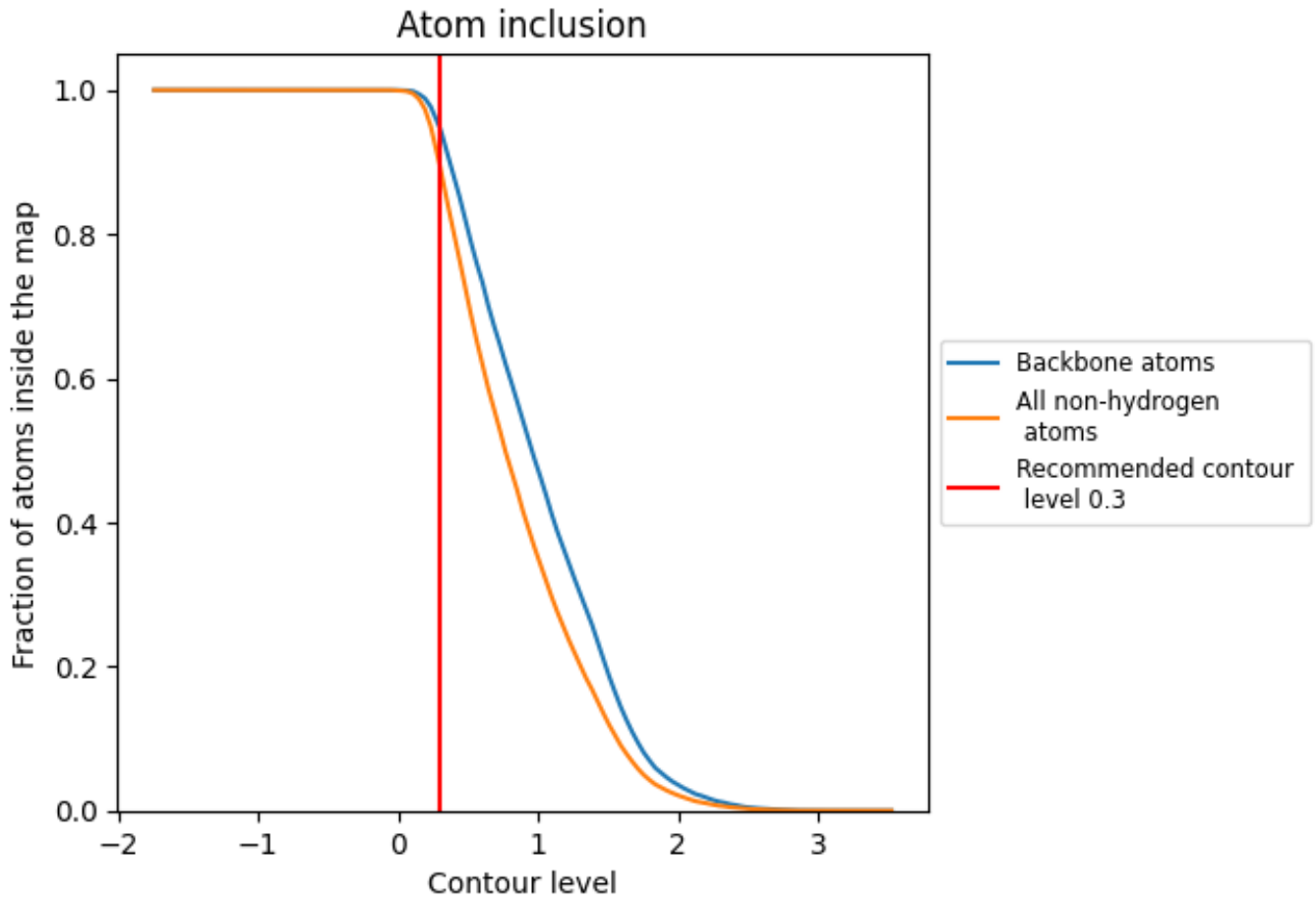
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8935	0.4360
A	0.8927	0.4350
B	0.8931	0.4360
C	0.8946	0.4360