Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 12:17 PM JST

PDB ID	:	7WDF
EMDB ID	:	EMD-32437
Title	:	SARS-CoV-2 Beta spike in complex with two S3H3 Fabs
Authors	:	Wang, Y.F.; Cong, Y.
Deposited on	:	2021-12-21
Resolution	:	3.90 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:

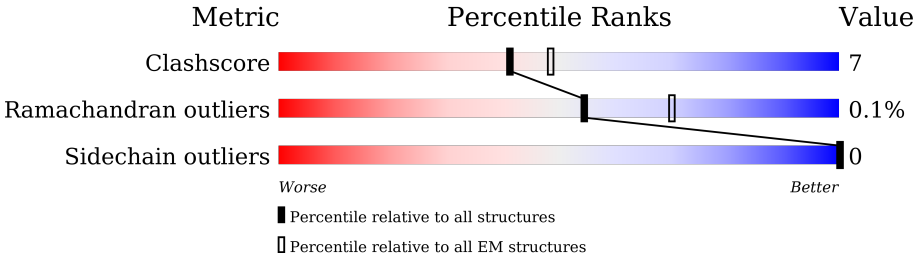
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.90 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	1258	25% 68% 18% 14%
1	B	1258	22% 69% 17% 14%
1	C	1258	19% 70% 16% 14%
2	D	217	34% 89% 11%
2	F	217	53% 83% 17%
3	E	215	23% 83% 17%
3	G	215	38% 79% 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31998 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	1079	8454	5399	1410	1606	39	0	0
1	B	1079	8454	5399	1410	1606	39	0	0
1	C	1079	8454	5399	1410	1606	39	0	0

There are 213 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	246	ILE	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	ASN	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	TYR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	TYR	-	expression tag	UNP P0DTC2
A	1247	LYS	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	ASP	-	expression tag	UNP P0DTC2
A	1251	ASP	-	expression tag	UNP P0DTC2
A	1252	LYS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	246	ILE	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	701	VAL	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	ASN	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	TYR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	TYR	-	expression tag	UNP P0DTC2
B	1247	LYS	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	ASP	-	expression tag	UNP P0DTC2
B	1251	ASP	-	expression tag	UNP P0DTC2
B	1252	LYS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	246	ILE	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	501	TYR	ASN	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	701	VAL	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLU	-	expression tag	UNP P0DTC2
C	1239	ASN	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1241	TYR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	TYR	-	expression tag	UNP P0DTC2
C	1247	LYS	-	expression tag	UNP P0DTC2
C	1248	ASP	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	ASP	-	expression tag	UNP P0DTC2
C	1251	ASP	-	expression tag	UNP P0DTC2
C	1252	LYS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of S3H3 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	217	1662	1055	274	325	8	0	0
2	F	217	1662	1055	274	325	8	0	0

- Molecule 3 is a protein called Light chain of S3H3 Fab.

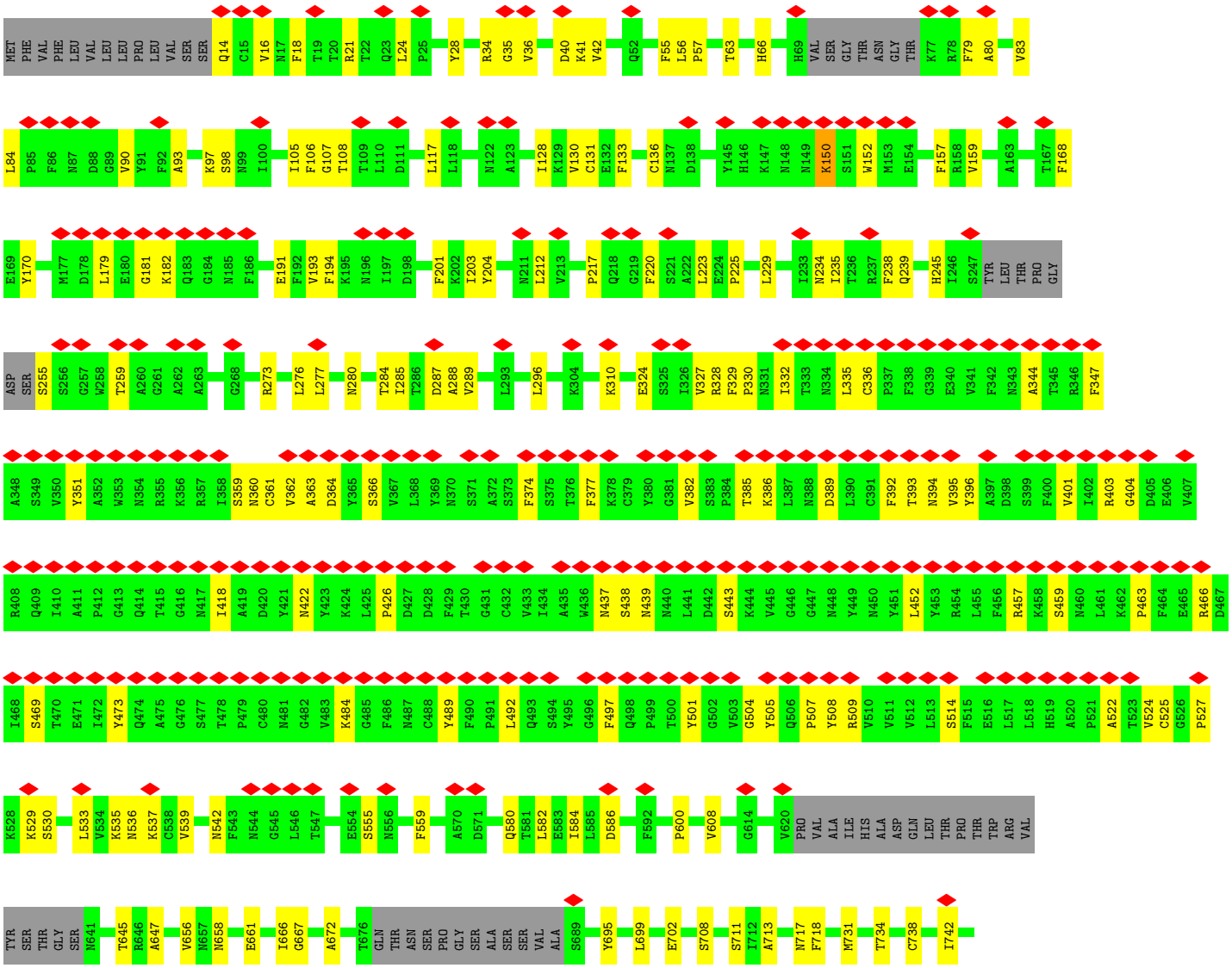
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	215	1656	1035	282	333	6	0	0
3	G	215	1656	1035	282	333	6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein

Chain A:



- Molecule 1: Spike glycoprotein

Chain B:

R646 A647 V656 N657 N658 I666 A672 T676 GLN THR ASN SER PRO GLY SER ALA SER SER VAL ALA S689 E702 S708 S711 I712 A713 N717 F718 V722 I726 M731 T734 C738 T739 M740 Y741 I742 C743 G744 D745 S746 T747 L754 F759

Q762 L763 N764 R765 V772 E773 Q774 D775 K776 F782 A783 Q784 V785 K786 Q787 I788 D796 F800 P807 P812 R815 S816 F817 F823 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG D848 L849 I850 C851 A852

F855 L858 L864 E868 Q872 L877 G885 W886 T887 F888 G889 A890 G891 A892 A893 L894 Q895 Y904 R905 T912 Q913 N914 A924 Q935 A942 S943 A944 L945 L959 L962 N978 D979 I980 L981 S982 R983 L984 D985 P986 P987 E988 A989 R1000 V1008

I1018 R1019 S1030 E1031 L1034 S1037 K1038 R1039 V1040 D1041 Y1047 H1048 L1049 M1050 S1051 A1056 P1057 V1061 V1065 T1066 Y1067 I1081 K1086 P1090 R1091 E1092 F1095 H1101 V1104 F1109 I1115 T1120 N1125 Y1138 D1139 Q1142 L1145 F1148

L1152 D1153 K1154 Y1155 F1156 K1157 N1158 S1161 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 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 GLU ASN LEU TYR PHE GLN GLY ASP TYR LYS ASP ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Spike glycoprotein

Chain C:

MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER Q14 N17 F18 T19 T20 R21 T22 Q23 L24 P25 P26 A27 Y28 G35 D40 K41 V42 F43 R44 L48 D53 L54 F55 L56 P57 F58 T63 W64 F65 H66 H69 VAL SER GLY THR ASN GLY THR K77 R78

F79 A80 L84 P85 F86 N87 D88 G89 V90 Y91 T95 E96 I100 I101 R102 I105 F106 G107 T108 T114 Q115 S116 L117 N122 V126 V127 I128 K129 V130 C131 N137 V143 Y144 Y145 H146 K147 N148 N149 K150 S151 W152 M153 E154 C166 T167 F168 E169 Y170 V171 S172

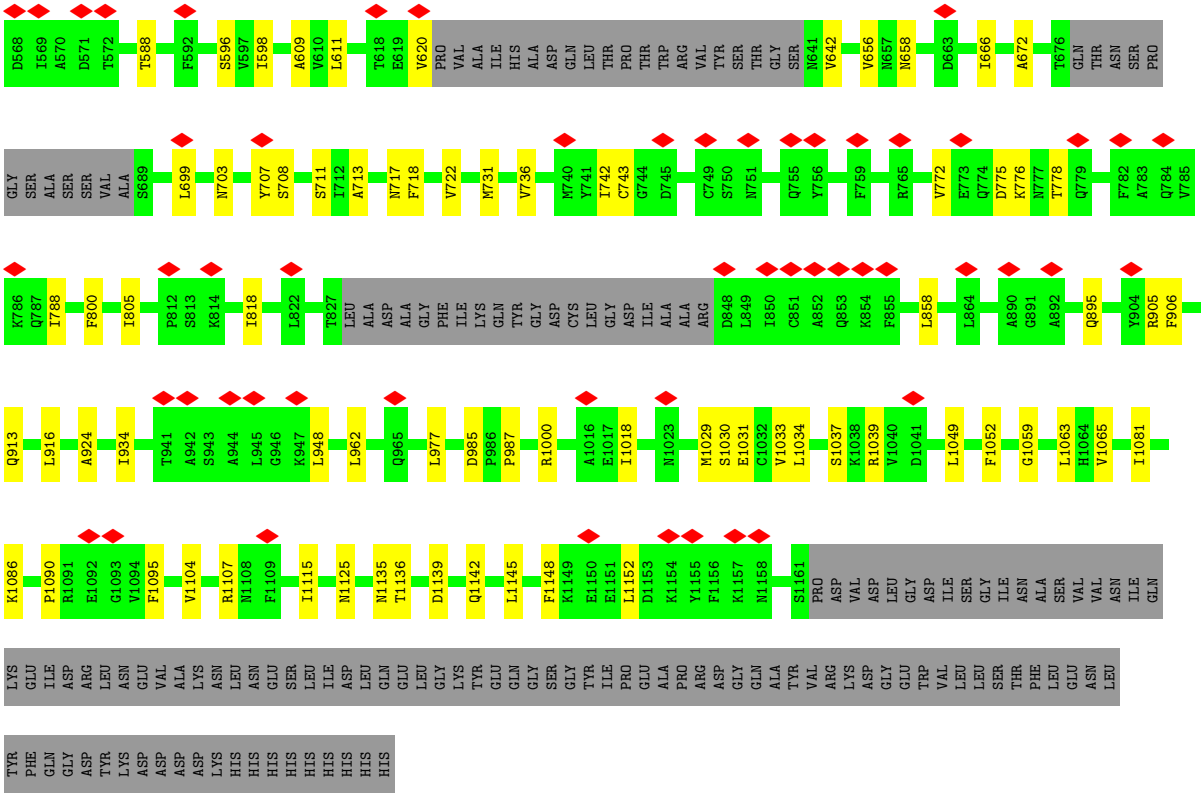
Q173 D178 L179 E180 G181 K182 Q183 G184 N185 E191 F192 V193 F194 K195 N196 I197 D198 I203 Y204 S205 K206 L212 P217 Q218 L223 E224 P225 N234 I235 T236 R237 F238 Q239 H245 I246 S247 TYR LEU THR PRO GLY ASP SER S255 S256 T259 A262 A263 Y266

Y269 L270 Q271 P272 R273 L276 L277 N280 T284 I285 T286 D287 A288 L293 E298 L303 N317 F318 R319 T323 I326 V327 R328 F329 P330 N331 I332 T333 N334 L335 C336 P337 F338 G339 F342 N343 A344 T345 R346 S349 A352 W353 N354 R355 K356 R357 I358

C361 V362 A363 D364 Y365 S366 V367 A372 S373 F374 S375 T376 F377 K378 C379 Y380 G381 V382 S383 P384 T385 K386 L387 N388 D389 L390 C391 F392 T393 N394 V395 V396 A397 D398 S399 F400 V401 I402 R403 G404 D405 E406 V407 R408 Q409 I410 A411 P412 G413 Q414 T415 I418 A419 D420 Y421 N422 Y423

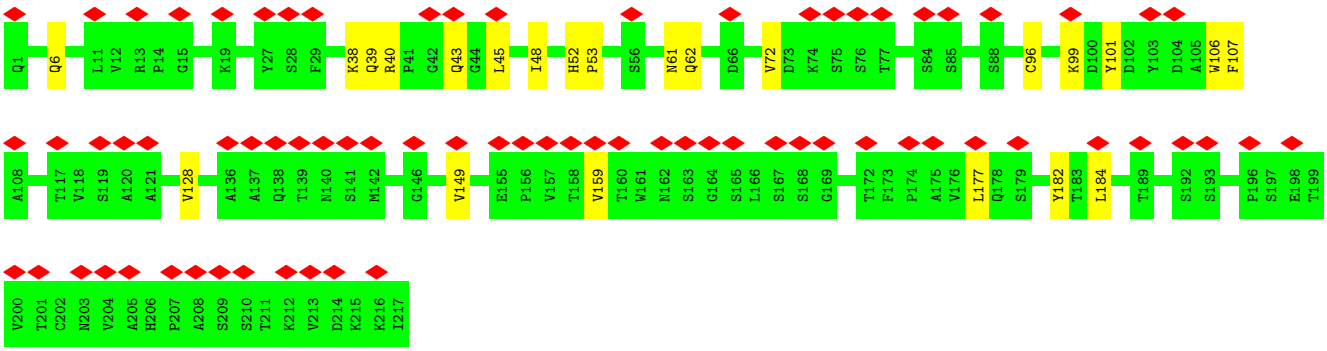
K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 N437 S438 N439 N440 L441 D442 S443 K444 V445 G446 G447 N448 Y449 N450 Y451 L452 L455 F456 R457 K458 S459 N460 L461 K462 P463 F464 E465 R466 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 S477 T478 P479 C480 N481 G482 V483 K484 N487

C488 Y489 F490 P491 L492 Q493 S494 Y495 G496 F497 Q498 P499 T500 Y501 G502 V503 G504 Y505 Q506 P507 Y508 R509 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 V524 C525 G526 P527 K528 K529 S530 T531 V534 N542 F543 N544 G545 L546 T547 G548 T549 G550 V551 F562 Q563



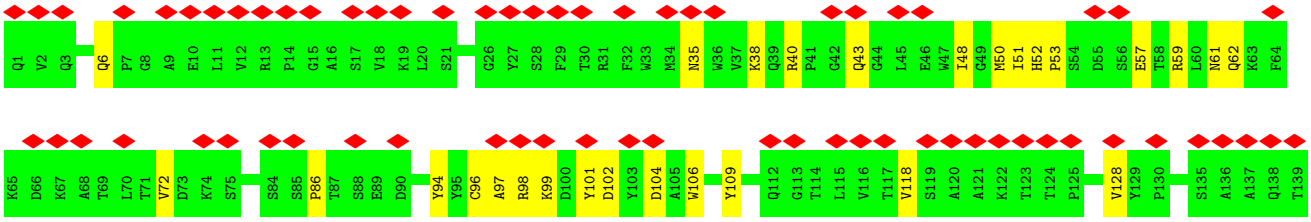
- Molecule 2: Heavy chain of S3H3 Fab

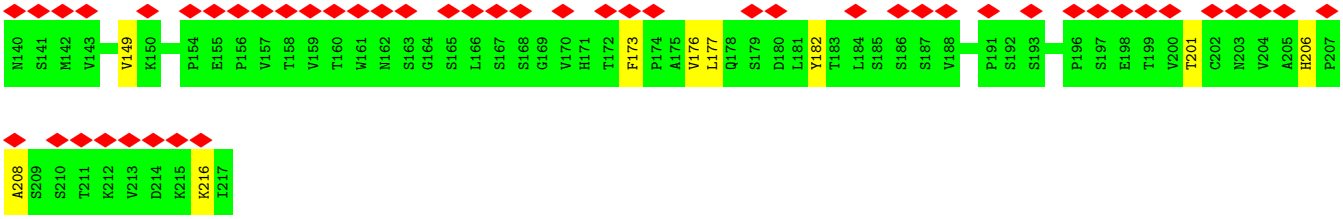
Chain D:



- Molecule 2: Heavy chain of S3H3 Fab

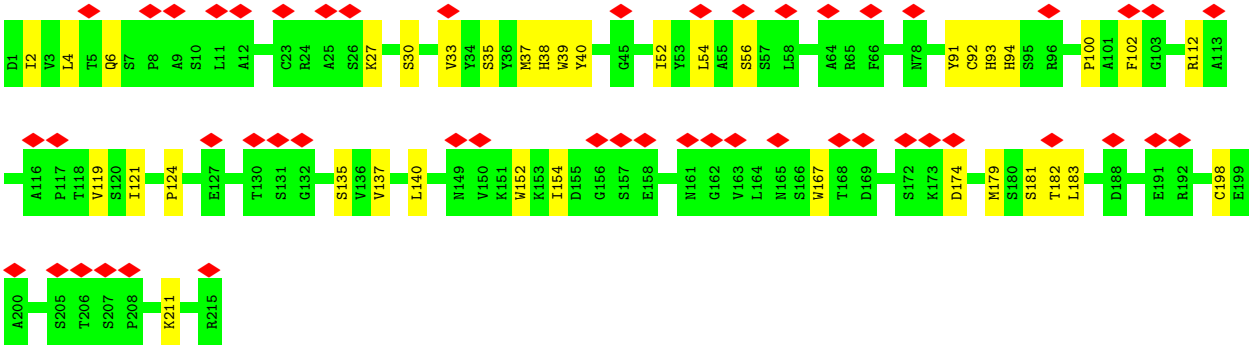
Chain F:





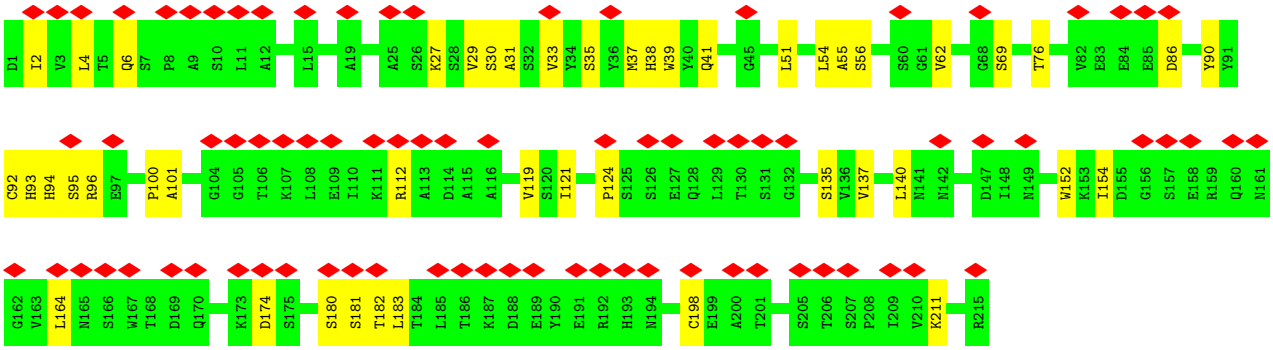
• Molecule 3: Light chain of S3H3 Fab

Chain E:



• Molecule 3: Light chain of S3H3 Fab

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53200	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)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.092	Depositor
Minimum map value	-2.430	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.124	Depositor
Recommended contour level	1.02	Depositor
Map size (Å)	393.48, 393.48, 393.48	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	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	0.26	1/8649 (0.0%)	0.42	0/11759
1	B	0.26	1/8649 (0.0%)	0.42	0/11759
1	C	0.25	0/8649	0.42	0/11759
2	D	0.24	0/1709	0.43	0/2336
2	F	0.24	0/1709	0.44	0/2336
3	E	0.24	0/1697	0.43	0/2306
3	G	0.24	0/1697	0.42	0/2306
All	All	0.25	2/32759 (0.0%)	0.42	0/44561

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	CYS	C-N	6.86	1.47	1.34
1	B	336	CYS	C-N	6.21	1.46	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	531	THR	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	8454	0	8245	147	0
1	B	8454	0	8245	140	0
1	C	8454	0	8245	130	0
2	D	1662	0	1619	13	0
2	F	1662	0	1619	26	0
3	E	1656	0	1595	22	0
3	G	1656	0	1595	29	0
All	All	31998	0	31163	466	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 7.

All (466) 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:14:GLN:N	1:C:255:SER:HG	1.75	0.85
3:E:152:TRP:HE1	3:E:181:SER:HG	1.25	0.81
3:G:152:TRP:HE1	3:G:181:SER:HG	1.26	0.80
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.68	0.75
1:B:1152:LEU:HD13	1:C:1152:LEU:HD11	1.70	0.74
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.72	0.72
1:C:331:ASN:HA	1:C:529:LYS:HE2	1.71	0.71
1:A:362:VAL:H	1:A:524:VAL:HG11	1.56	0.70
1:C:337:PRO:HD3	1:C:358:ILE:HB	1.73	0.70
1:A:193:VAL:HB	1:A:204:TYR:HB2	1.74	0.70
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.24	0.69
3:E:93:HIS:HE1	3:E:100:PRO:HB2	1.55	0.69
3:G:31:ALA:HB2	3:G:96:ARG:HH12	1.58	0.69
1:C:361:CYS:HB3	1:C:392:PHE:H	1.57	0.69
2:D:6:GLN:NE2	2:D:96:CYS:SG	2.66	0.69
3:G:6:GLN:NE2	3:G:92:CYS:SG	2.66	0.69
1:C:193:VAL:HB	1:C:204:TYR:HB2	1.75	0.68
1:B:193:VAL:HB	1:B:204:TYR:HB2	1.75	0.67
1:A:332:ILE:HG22	1:A:525:CYS:H	1.59	0.66
1:A:466:ARG:HH21	1:B:167:THR:HG22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:GLN:NE2	2:F:96:CYS:SG	2.70	0.65
3:E:93:HIS:CE1	3:E:100:PRO:HB2	2.32	0.64
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.80	0.64
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.30	0.64
1:B:335:LEU:HD23	1:B:364:ASP:HA	1.80	0.64
3:E:2:ILE:HG12	3:E:27:LYS:HB2	1.81	0.63
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.63	0.63
1:A:559:PHE:HB3	1:A:584:ILE:HD11	1.80	0.63
1:B:245:HIS:N	1:B:259:THR:O	2.31	0.63
1:B:337:PRO:HD3	1:B:358:ILE:HB	1.79	0.63
1:C:335:LEU:HD23	1:C:364:ASP:HA	1.80	0.63
1:A:1123:SER:OG	1:B:914:ASN:ND2	2.32	0.62
3:E:6:GLN:NE2	3:E:92:CYS:SG	2.71	0.62
3:G:29:VAL:HA	3:G:96:ARG:HD2	1.81	0.62
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	1.81	0.62
1:A:1148:PHE:HE2	1:C:1145:LEU:HD23	1.64	0.62
1:A:484:LYS:HE3	1:A:489:TYR:HA	1.81	0.61
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.82	0.61
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.63	0.61
3:E:121:ILE:HD12	3:E:198:CYS:HB2	1.83	0.61
3:G:93:HIS:CE1	3:G:100:PRO:HB2	2.36	0.61
1:B:738:CYS:SG	1:B:764:ASN:ND2	2.74	0.61
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.82	0.60
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.32	0.60
3:E:112:ARG:NH1	3:E:174:ASP:O	2.34	0.60
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.34	0.60
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.33	0.60
1:B:912:THR:HG22	1:B:914:ASN:H	1.67	0.60
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.82	0.60
1:B:331:ASN:HA	1:B:529:LYS:HD3	1.84	0.60
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.32	0.60
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.83	0.60
1:C:35:GLY:HA3	1:C:56:LEU:HB3	1.84	0.60
1:C:334:ASN:OD1	1:C:335:LEU:N	2.30	0.59
3:E:30:SER:HA	3:E:35:SER:HA	1.84	0.59
1:A:335:LEU:HD23	1:A:364:ASP:HA	1.85	0.59
1:B:328:ARG:NH2	2:F:102:ASP:OD1	2.36	0.59
1:A:105:ILE:HB	1:A:239:GLN:HB2	1.85	0.59
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.84	0.58
1:A:277:LEU:HD22	1:A:285:ILE:HD13	1.85	0.58
1:A:439:ASN:O	1:A:443:SER:OG	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLY:HA3	1:B:56:LEU:HB3	1.85	0.58
2:F:98:ARG:HD3	2:F:109:TYR:HD2	1.68	0.58
3:G:2:ILE:O	3:G:94:HIS:NE2	2.35	0.58
1:C:277:LEU:HD22	1:C:285:ILE:HD13	1.84	0.58
1:A:245:HIS:N	1:A:259:THR:O	2.36	0.58
1:C:452:LEU:HB3	1:C:492:LEU:HD11	1.86	0.58
1:A:393:THR:HG22	1:A:522:ALA:HB2	1.86	0.57
1:B:484:LYS:HE3	1:B:489:TYR:HA	1.86	0.57
1:A:55:PHE:HB2	1:A:273:ARG:HB2	1.86	0.57
1:B:334:ASN:OD1	1:B:335:LEU:N	2.30	0.57
1:C:327:VAL:HG13	1:C:542:ASN:HB3	1.85	0.57
1:B:14:GLN:N	1:B:255:SER:HG	2.03	0.57
1:C:452:LEU:HD13	1:C:492:LEU:HD21	1.86	0.57
1:C:332:ILE:HA	1:C:524:VAL:HG12	1.86	0.57
3:E:2:ILE:O	3:E:94:HIS:NE2	2.37	0.57
1:B:1056:ALA:HB2	1:B:1061:VAL:HG23	1.87	0.57
3:G:124:PRO:HB3	3:G:135:SER:H	1.68	0.57
1:A:351:TYR:HE2	1:A:452:LEU:HB2	1.69	0.56
1:B:551:VAL:HB	1:B:588:THR:HB	1.86	0.56
1:C:858:LEU:HD21	1:C:962:LEU:HD23	1.87	0.56
1:A:533:LEU:O	1:A:535:LYS:HB3	2.06	0.56
1:C:128:ILE:HD13	1:C:170:TYR:HD2	1.71	0.56
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.69	0.56
1:C:484:LYS:HE3	1:C:489:TYR:HA	1.87	0.56
1:A:536:ASN:OD1	1:A:537:LYS:N	2.34	0.56
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.88	0.56
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.87	0.56
2:F:57:GLU:OE2	2:F:59:ARG:NH2	2.37	0.56
3:G:121:ILE:HD12	3:G:198:CYS:HB2	1.86	0.56
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.87	0.56
1:A:895:GLN:H	1:C:713:ALA:HB3	1.71	0.56
1:B:362:VAL:H	1:B:524:VAL:HG11	1.71	0.56
3:G:30:SER:HA	3:G:35:SER:HA	1.87	0.56
1:A:452:LEU:HD13	1:A:492:LEU:HD21	1.88	0.56
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.87	0.56
1:C:457:ARG:NH1	1:C:459:SER:OG	2.38	0.56
3:G:86:ASP:O	3:G:90:TYR:OH	2.21	0.56
1:B:361:CYS:HB3	1:B:392:PHE:HB2	1.88	0.55
1:A:42:VAL:O	1:C:563:GLN:NE2	2.39	0.55
1:B:102:ARG:NH1	1:B:141:LEU:O	2.39	0.55
1:A:717:ASN:OD1	1:A:718:PHE:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LEU:HB3	1:B:492:LEU:HD11	1.88	0.55
1:A:822:LEU:HA	1:A:945:LEU:HD21	1.89	0.55
1:C:105:ILE:HB	1:C:239:GLN:HB2	1.89	0.55
2:F:35:ASN:ND2	2:F:99:LYS:HB2	2.21	0.55
2:D:40:ARG:NH2	2:D:43:GLN:OE1	2.40	0.55
3:G:112:ARG:NH1	3:G:174:ASP:O	2.40	0.55
1:C:245:HIS:N	1:C:259:THR:O	2.40	0.55
1:C:736:VAL:HG22	1:C:858:LEU:HG	1.89	0.55
1:A:738:CYS:SG	1:A:764:ASN:ND2	2.80	0.55
1:B:277:LEU:HD22	1:B:285:ILE:HD13	1.88	0.55
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.89	0.54
1:B:566:GLY:HA2	1:C:43:PHE:H	1.73	0.54
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.88	0.54
1:B:800:PHE:HE1	1:B:924:ALA:HA	1.73	0.54
1:B:717:ASN:OD1	1:B:718:PHE:N	2.40	0.54
1:C:95:THR:HG21	1:C:212:LEU:HD23	1.89	0.54
2:F:106:TRP:HB3	3:G:38:HIS:CE1	2.42	0.54
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.89	0.54
1:A:1148:PHE:CE2	1:C:1145:LEU:HD23	2.43	0.54
1:B:332:ILE:HG13	1:B:529:LYS:HE3	1.89	0.54
1:B:55:PHE:O	1:B:271:GLN:N	2.33	0.54
1:C:329:PHE:HD2	1:C:525:CYS:HB2	1.73	0.54
1:C:717:ASN:OD1	1:C:718:PHE:N	2.40	0.54
1:C:362:VAL:H	1:C:524:VAL:HG21	1.73	0.53
1:B:559:PHE:HB3	1:B:584:ILE:HD11	1.89	0.53
1:B:276:LEU:HB2	1:B:289:VAL:HB	1.90	0.53
2:F:61:ASN:OD1	2:F:62:GLN:N	2.41	0.53
1:B:452:LEU:HD13	1:B:492:LEU:HD21	1.90	0.53
1:B:979:ASP:O	1:B:983:ARG:NE	2.41	0.53
3:G:69:SER:OG	3:G:76:THR:OG1	2.27	0.53
1:B:430:THR:H	1:B:515:PHE:HD2	1.56	0.52
3:G:137:VAL:HG22	3:G:182:THR:HG23	1.90	0.52
1:B:1031:GLU:HB3	1:B:1037:SER:HB2	1.91	0.52
1:C:56:LEU:HD12	1:C:57:PRO:HD2	1.91	0.52
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.91	0.52
2:D:61:ASN:OD1	2:D:62:GLN:N	2.41	0.52
1:C:1081:ILE:HG13	1:C:1115:ILE:HD13	1.91	0.52
1:A:823:PHE:HD1	1:A:1057:PRO:HD3	1.75	0.52
1:C:206:LYS:HB2	1:C:223:LEU:HA	1.92	0.52
1:B:537:LYS:NZ	2:F:57:GLU:OE1	2.42	0.52
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:HB2	1:A:133:PHE:CE1	2.44	0.52
3:G:39:TRP:HZ3	3:G:51:LEU:HD22	1.75	0.52
1:B:1090:PRO:HD2	1:C:913:GLN:HE22	1.75	0.51
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.92	0.51
1:C:349:SER:HB2	1:C:452:LEU:O	2.09	0.51
2:F:38:LYS:HB2	2:F:48:ILE:HD11	1.92	0.51
1:B:193:VAL:HG23	1:B:223:LEU:HD22	1.93	0.51
1:C:1139:ASP:HB3	1:C:1142:GLN:HB2	1.90	0.51
3:E:154:ILE:HD11	3:E:183:LEU:HD21	1.92	0.51
1:B:18:PHE:HB2	1:B:21:ARG:HB2	1.91	0.51
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.92	0.51
1:A:787:GLN:HE21	1:C:703:ASN:HB3	1.74	0.51
2:F:50:MET:HG2	2:F:59:ARG:HB2	1.93	0.51
1:B:81:ASN:ND2	1:B:240:THR:O	2.40	0.51
1:B:194:PHE:HE1	1:B:203:ILE:HG23	1.76	0.51
1:B:212:LEU:HD22	1:B:217:PRO:HD3	1.92	0.51
1:B:543:PHE:HD2	1:B:576:VAL:HG21	1.76	0.51
1:B:328:ARG:HH11	1:B:533:LEU:HD13	1.76	0.51
1:A:327:VAL:HA	1:A:542:ASN:HB3	1.93	0.51
1:B:33:THR:OG1	1:B:219:GLY:O	2.17	0.51
1:A:1086:LYS:HA	1:A:1125:ASN:HA	1.92	0.51
1:C:21:ARG:HA	1:C:79:PHE:HB3	1.92	0.51
1:C:24:LEU:HD12	1:C:80:ALA:HB2	1.92	0.51
1:A:152:TRP:HB3	1:A:179:LEU:HD12	1.93	0.51
1:A:825:LYS:HB2	1:A:945:LEU:HD22	1.92	0.51
1:C:287:ASP:OD1	1:C:288:ALA:N	2.44	0.50
1:B:784:GLN:HB3	1:B:877:LEU:HD21	1.93	0.50
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.93	0.50
1:C:731:MET:HG3	1:C:1018:ILE:HG12	1.94	0.50
1:A:212:LEU:HD22	1:A:217:PRO:HD3	1.94	0.50
1:A:396:TYR:O	1:A:514:SER:N	2.36	0.50
2:F:176:VAL:HG11	3:G:164:LEU:HD22	1.94	0.50
3:G:41:GLN:HG3	3:G:90:TYR:HE1	1.77	0.50
1:C:102:ARG:NE	1:C:154:GLU:OE2	2.35	0.50
1:C:1086:LYS:HA	1:C:1125:ASN:HA	1.92	0.50
2:F:53:PRO:HA	2:F:72:VAL:HG21	1.94	0.50
1:C:24:LEU:HD13	1:C:66:HIS:CE1	2.47	0.50
2:F:35:ASN:HD21	2:F:99:LYS:HD2	1.76	0.50
1:C:64:TRP:CD1	1:C:266:TYR:HE1	2.30	0.49
1:C:280:ASN:OD1	1:C:284:THR:N	2.45	0.49
1:C:430:THR:H	1:C:515:PHE:HD2	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:TRP:HB3	3:E:38:HIS:CE1	2.47	0.49
1:A:1041:ASP:HB3	1:B:1030:SER:HB3	1.93	0.49
1:B:287:ASP:OD1	1:B:288:ALA:N	2.45	0.49
1:C:336:CYS:H	1:C:363:ALA:HA	1.78	0.49
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.94	0.49
1:A:28:TYR:HD1	1:A:63:THR:HA	1.77	0.49
1:B:55:PHE:HB2	1:B:273:ARG:HB2	1.93	0.49
2:D:128:VAL:HG22	2:D:149:VAL:HG22	1.94	0.49
2:F:52:HIS:HD2	2:F:53:PRO:HD2	1.76	0.49
1:B:713:ALA:HB3	1:C:895:GLN:H	1.76	0.49
3:G:119:VAL:HG22	3:G:140:LEU:HG	1.94	0.49
1:A:734:THR:HG21	1:A:959:LEU:HD21	1.93	0.49
3:G:4:LEU:HG	3:G:94:HIS:HD2	1.77	0.49
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.94	0.49
1:A:287:ASP:OD1	1:A:288:ALA:N	2.46	0.49
1:B:823:PHE:HD1	1:B:1057:PRO:HD3	1.77	0.49
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.93	0.49
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.44	0.49
1:B:280:ASN:OD1	1:B:284:THR:N	2.46	0.49
1:B:128:ILE:HD13	1:B:170:TYR:HD2	1.77	0.49
1:A:332:ILE:HG12	1:A:529:LYS:HE2	1.95	0.49
1:B:19:THR:HG23	1:B:256:SER:HB2	1.95	0.49
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.94	0.48
2:F:38:LYS:HG3	2:F:94:TYR:HE1	1.78	0.48
2:F:51:ILE:HD13	2:F:72:VAL:HG13	1.93	0.48
2:F:206:HIS:CE1	2:F:208:ALA:HB3	2.47	0.48
1:B:329:PHE:CD2	1:B:525:CYS:HB2	2.48	0.48
1:C:484:LYS:HD2	1:C:490:PHE:HB2	1.95	0.48
3:E:4:LEU:HG	3:E:94:HIS:HD2	1.79	0.48
3:E:137:VAL:HG22	3:E:182:THR:HG23	1.95	0.48
1:A:34:ARG:NE	1:A:191:GLU:OE2	2.46	0.48
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.93	0.48
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.94	0.48
1:A:16:VAL:O	1:A:255:SER:OG	2.30	0.48
1:B:800:PHE:CE1	1:B:924:ALA:HA	2.48	0.48
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.94	0.48
1:C:934:ILE:HD13	1:C:1063:LEU:HD22	1.96	0.48
3:E:119:VAL:HG22	3:E:140:LEU:HG	1.96	0.48
2:F:201:THR:HG22	2:F:216:LYS:HG2	1.96	0.48
1:A:437:ASN:HA	1:A:508:TYR:HD1	1.79	0.47
1:B:1048:HIS:HE1	1:B:1051:SER:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HB3	1:A:492:LEU:HD11	1.95	0.47
1:A:979:ASP:O	1:A:983:ARG:NE	2.44	0.47
1:B:58:PHE:HB2	1:B:293:LEU:HD22	1.96	0.47
1:C:96:GLU:HG2	1:C:263:ALA:HB1	1.97	0.47
1:C:194:PHE:HE1	1:C:203:ILE:HG23	1.78	0.47
1:A:108:THR:OG1	1:A:234:ASN:O	2.28	0.47
1:A:276:LEU:HB2	1:A:289:VAL:HB	1.96	0.47
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.97	0.47
1:A:1104:VAL:HG23	1:A:1115:ILE:HG12	1.95	0.47
1:A:645:THR:HG23	1:A:647:ALA:H	1.79	0.47
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.95	0.47
1:B:1081:ILE:HG13	1:B:1115:ILE:HD13	1.97	0.47
1:B:1139:ASP:HB3	1:B:1142:GLN:HB2	1.96	0.47
1:C:152:TRP:HB3	1:C:179:LEU:HD12	1.97	0.47
2:D:52:HIS:HD2	2:D:53:PRO:HD2	1.78	0.47
1:A:90:VAL:HG11	1:A:238:PHE:CE2	2.50	0.47
1:A:361:CYS:SG	1:A:362:VAL:HA	2.55	0.47
1:A:713:ALA:HB3	1:B:895:GLN:H	1.79	0.47
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.96	0.47
1:B:374:PHE:HB2	1:B:377:PHE:CE1	2.50	0.47
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.96	0.47
1:C:90:VAL:HG11	1:C:238:PHE:CE2	2.50	0.47
1:B:361:CYS:HA	1:B:362:VAL:C	2.35	0.47
1:B:645:THR:HG23	1:B:647:ALA:H	1.79	0.47
1:A:360:ASN:HB3	1:A:524:VAL:HG23	1.97	0.47
1:B:90:VAL:HG11	1:B:238:PHE:CE2	2.49	0.47
1:B:708:SER:HB3	1:B:711:SER:HB2	1.97	0.47
1:C:58:PHE:HB2	1:C:293:LEU:HD22	1.97	0.47
3:G:93:HIS:ND1	3:G:101:ALA:O	2.48	0.47
1:A:374:PHE:HB2	1:A:377:PHE:CE1	2.49	0.47
1:B:212:LEU:HD21	1:B:215:GLY:O	2.14	0.46
1:B:564:GLN:HG3	1:C:41:LYS:HD3	1.95	0.46
1:A:21:ARG:HA	1:A:79:PHE:HB3	1.97	0.46
1:A:280:ASN:OD1	1:A:284:THR:N	2.48	0.46
3:E:40:TYR:HB2	3:E:91:TYR:HB2	1.98	0.46
1:B:1047:TYR:HD2	1:B:1067:TYR:HD2	1.62	0.46
1:C:1031:GLU:HB3	1:C:1037:SER:HB2	1.97	0.46
1:A:731:MET:HG3	1:A:1018:ILE:HG12	1.97	0.46
1:B:858:LEU:HD21	1:B:962:LEU:HD23	1.97	0.46
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.98	0.46
1:A:24:LEU:HD13	1:A:66:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:CZ	1:A:159:VAL:HB	2.51	0.46
1:A:194:PHE:HE1	1:A:203:ILE:HG23	1.80	0.46
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.98	0.46
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.46	0.46
2:F:40:ARG:HH11	2:F:43:GLN:HG2	1.81	0.46
1:A:886:TRP:HZ2	1:C:1107:ARG:HD3	1.81	0.46
1:A:24:LEU:HD12	1:A:80:ALA:HB2	1.98	0.46
1:C:620:VAL:HG11	1:C:642:VAL:HG11	1.97	0.45
1:C:743:CYS:HB2	1:C:977:LEU:HD22	1.97	0.45
2:F:128:VAL:HG22	2:F:149:VAL:HG22	1.98	0.45
1:A:858:LEU:HD21	1:A:962:LEU:HD23	1.98	0.45
1:B:734:THR:HG21	1:B:959:LEU:HD21	1.98	0.45
1:A:457:ARG:NH1	1:A:459:SER:OG	2.49	0.45
1:B:532:ASN:ND2	2:F:101:TYR:HB2	2.32	0.45
1:B:731:MET:HG3	1:B:1018:ILE:HG12	1.97	0.45
1:C:131:CYS:HA	1:C:166:CYS:HA	1.98	0.45
1:C:551:VAL:HB	1:C:588:THR:HB	1.97	0.45
1:B:454:ARG:NH1	1:B:467:ASP:OD2	2.50	0.45
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.98	0.45
3:E:124:PRO:HB3	3:E:135:SER:H	1.82	0.45
1:A:661:GLU:O	1:A:695:TYR:OH	2.26	0.45
1:C:28:TYR:HD1	1:C:63:THR:HA	1.82	0.45
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.99	0.45
3:G:54:LEU:C	3:G:56:SER:H	2.19	0.45
1:A:772:VAL:HG12	1:A:776:LYS:HE3	1.99	0.45
1:B:332:ILE:HG12	1:B:524:VAL:HG13	1.98	0.45
1:B:741:TYR:CE2	1:B:1000:ARG:HB3	2.52	0.45
1:C:19:THR:HG23	1:C:256:SER:HB2	1.98	0.45
1:C:424:LYS:HZ1	1:C:463:PRO:HD3	1.82	0.45
1:C:656:VAL:HG12	1:C:658:ASN:H	1.81	0.45
1:C:1030:SER:HA	1:C:1034:LEU:HD12	1.99	0.45
1:A:792:PRO:HB3	1:C:707:TYR:CD2	2.52	0.45
1:A:97:LYS:HB3	1:A:182:LYS:HB2	1.98	0.45
1:A:385:THR:OG1	1:C:487:ASN:ND2	2.50	0.45
1:C:497:PHE:CD2	1:C:507:PRO:HB3	2.52	0.45
3:E:39:TRP:CD1	3:E:52:ILE:HB	2.52	0.45
1:B:469:SER:HB3	1:B:473:TYR:HE2	1.82	0.45
1:C:708:SER:HB3	1:C:711:SER:HB2	1.98	0.45
1:B:21:ARG:HA	1:B:79:PHE:HB3	1.98	0.44
1:A:699:LEU:HD13	1:B:872:GLN:HG2	1.99	0.44
1:A:1047:TYR:HD2	1:A:1067:TYR:HD2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:VAL:HG12	1:C:776:LYS:HE3	2.00	0.44
1:C:800:PHE:CE1	1:C:924:ALA:HA	2.52	0.44
1:A:497:PHE:HA	1:A:505:TYR:O	2.17	0.44
1:C:126:VAL:HB	1:C:172:SER:HB3	1.99	0.44
1:C:805:ILE:HG22	1:C:818:ILE:HD12	2.00	0.44
2:D:53:PRO:HA	2:D:72:VAL:HG21	1.98	0.44
1:A:330:PRO:HA	1:A:580:GLN:HG2	2.00	0.44
1:A:888:PHE:CE1	1:A:1034:LEU:HG	2.53	0.44
1:A:150:LYS:C	1:A:152:TRP:H	2.21	0.44
1:A:201:PHE:HB2	1:A:229:LEU:HB2	2.00	0.44
1:A:361:CYS:HB3	1:A:392:PHE:HB2	2.00	0.44
1:A:14:GLN:NE2	1:A:136:CYS:SG	2.76	0.44
1:A:107:GLY:H	1:A:235:ILE:HG23	1.83	0.44
1:C:64:TRP:HD1	1:C:266:TYR:HE1	1.65	0.44
1:B:823:PHE:CD1	1:B:1057:PRO:HD3	2.53	0.43
1:C:362:VAL:N	1:C:524:VAL:HG21	2.33	0.43
1:A:797:PHE:CD2	1:A:802:PHE:HD2	2.36	0.43
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.34	0.43
2:F:104:ASP:OD1	3:G:95:SER:HB2	2.18	0.43
1:A:559:PHE:HZ	1:A:582:LEU:HB3	1.82	0.43
1:B:107:GLY:HA2	1:B:235:ILE:HG12	2.01	0.43
1:B:620:VAL:HG11	1:B:642:VAL:HG11	2.00	0.43
1:B:887:THR:HG21	1:B:894:LEU:HB2	2.00	0.43
1:C:143:VAL:HG22	1:C:154:GLU:HA	2.01	0.43
1:C:361:CYS:HA	1:C:362:VAL:C	2.38	0.43
1:B:372:ALA:H	1:B:377:PHE:HE2	1.66	0.43
1:B:150:LYS:C	1:B:152:TRP:H	2.21	0.43
1:A:403:ARG:HB2	1:A:504:GLY:O	2.18	0.43
1:A:708:SER:HB3	1:A:711:SER:HB2	2.00	0.43
1:B:598:ILE:HB	1:B:609:ALA:HB3	2.00	0.43
1:C:374:PHE:HB2	1:C:377:PHE:CZ	2.53	0.43
2:D:38:LYS:HB2	2:D:48:ILE:HD11	2.00	0.43
1:A:40:ASP:OD1	1:A:41:LYS:N	2.48	0.43
1:B:189:LEU:HB2	1:B:210:ILE:HD13	2.00	0.43
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.00	0.43
1:C:362:VAL:HG13	1:C:388:ASN:HA	2.00	0.43
3:G:121:ILE:HG22	3:G:211:LYS:HG3	2.01	0.43
1:B:48:LEU:HD11	1:B:276:LEU:HB3	2.00	0.43
1:C:411:ALA:HB3	1:C:414:GLN:HB2	2.00	0.43
1:C:800:PHE:HE1	1:C:924:ALA:HA	1.83	0.43
3:G:154:ILE:HD11	3:G:183:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PRO:HA	1:A:463:PRO:HB2	2.00	0.43
2:D:99:LYS:HD2	2:D:101:TYR:CZ	2.54	0.43
1:A:152:TRP:CD2	1:A:179:LEU:HB2	2.54	0.42
1:A:362:VAL:HG12	1:A:363:ALA:O	2.19	0.42
1:A:667:GLY:HA2	1:B:864:LEU:HA	2.01	0.42
1:A:853:GLN:NE2	1:A:960:ASN:OD1	2.51	0.42
1:B:437:ASN:HA	1:B:508:TYR:HD1	1.84	0.42
3:E:54:LEU:C	3:E:56:SER:H	2.22	0.42
3:E:121:ILE:HG22	3:E:211:LYS:HG3	2.01	0.42
1:A:1029:MET:O	1:A:1033:VAL:HB	2.19	0.42
1:B:425:LEU:HD11	1:B:512:VAL:HG21	2.01	0.42
1:B:437:ASN:HA	1:B:508:TYR:CD1	2.54	0.42
1:C:362:VAL:HG12	1:C:363:ALA:O	2.19	0.42
1:A:328:ARG:NH1	1:A:530:SER:HB2	2.34	0.42
1:A:559:PHE:CZ	1:A:582:LEU:HB3	2.55	0.42
1:B:457:ARG:NH1	1:B:459:SER:OG	2.52	0.42
1:B:772:VAL:HG12	1:B:776:LYS:HE3	2.00	0.42
1:A:93:ALA:HA	1:A:191:GLU:HG2	2.02	0.42
1:A:702:GLU:HA	1:B:788:ILE:HB	2.01	0.42
1:C:474:GLN:HG3	1:C:479:PRO:HA	2.02	0.42
1:A:324:GLU:HB2	1:A:539:VAL:HG12	2.02	0.42
3:E:37:MET:SD	3:E:92:CYS:HB2	2.59	0.42
1:A:469:SER:HB3	1:A:473:TYR:HE2	1.83	0.42
1:B:106:PHE:O	1:B:117:LEU:N	2.52	0.42
1:C:48:LEU:HD11	1:C:276:LEU:HB3	2.01	0.42
1:A:913:GLN:NE2	1:C:1090:PRO:HD2	2.34	0.42
1:B:497:PHE:CE2	1:B:507:PRO:HB3	2.55	0.42
2:D:159:VAL:HG21	2:D:184:LEU:HD11	2.01	0.42
1:B:1041:ASP:HB3	1:C:1030:SER:HB3	2.01	0.42
1:C:384:PRO:HA	1:C:387:LEU:HG	2.01	0.42
2:D:107:PHE:HE2	3:E:102:PHE:HZ	1.67	0.42
3:G:51:LEU:HD23	3:G:62:VAL:HG13	2.01	0.42
1:A:1039:ARG:NE	1:B:1031:GLU:OE2	2.41	0.42
1:B:702:GLU:HA	1:C:788:ILE:HB	2.01	0.42
1:B:1030:SER:O	1:B:1034:LEU:HB3	2.20	0.42
1:C:775:ASP:O	1:C:778:THR:OG1	2.33	0.42
1:A:404:GLY:HA3	1:A:504:GLY:HA2	2.01	0.42
1:A:555:SER:HB2	1:A:586:ASP:HB2	2.02	0.42
1:B:382:VAL:HB	1:B:386:LYS:HB2	2.02	0.42
1:B:1091:ARG:NE	1:B:1120:THR:O	2.53	0.42
1:A:872:GLN:HG2	1:C:699:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HB2	1:B:238:PHE:CZ	2.55	0.41
1:B:403:ARG:HB3	1:B:504:GLY:O	2.20	0.41
2:F:173:PHE:CE2	3:G:180:SER:HB2	2.56	0.41
1:B:131:CYS:HA	1:B:166:CYS:HA	2.02	0.41
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.55	0.41
1:A:501:TYR:HB3	1:A:505:TYR:HD2	1.85	0.41
1:C:985:ASP:HB3	1:C:987:PRO:HD2	2.02	0.41
2:F:35:ASN:HB2	2:F:97:ALA:HB3	2.02	0.41
1:A:359:SER:HB2	1:A:394:ASN:HA	2.01	0.41
1:A:1031:GLU:OE2	1:C:1039:ARG:NE	2.30	0.41
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.55	0.41
1:B:807:PRO:HA	1:B:816:SER:HA	2.01	0.41
1:C:108:THR:OG1	1:C:234:ASN:O	2.31	0.41
1:C:501:TYR:HB3	1:C:505:TYR:HD2	1.85	0.41
3:E:167:TRP:NE1	3:E:179:MET:SD	2.94	0.41
1:A:1090:PRO:HD2	1:B:913:GLN:NE2	2.36	0.41
1:C:91:TYR:HD1	1:C:193:VAL:HG22	1.86	0.41
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.85	0.41
1:A:329:PHE:HB2	1:A:525:CYS:CB	2.51	0.41
1:B:422:ASN:HD21	1:B:454:ARG:H	1.69	0.41
1:B:743:CYS:SG	1:B:746:SER:HB3	2.60	0.41
1:B:1081:ILE:HG12	1:B:1095:PHE:CE2	2.55	0.41
1:C:437:ASN:HA	1:C:508:TYR:HD1	1.85	0.41
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.55	0.41
1:A:823:PHE:CD1	1:A:1057:PRO:HD3	2.55	0.41
1:B:106:PHE:HD2	1:B:117:LEU:HD23	1.85	0.41
1:B:362:VAL:HG12	1:B:363:ALA:O	2.21	0.41
1:B:763:LEU:HB3	1:B:1008:VAL:HG21	2.02	0.41
1:C:55:PHE:O	1:C:271:GLN:N	2.38	0.41
1:C:419:ALA:O	1:C:424:LYS:HG3	2.20	0.41
1:C:1029:MET:O	1:C:1033:VAL:HB	2.20	0.41
1:A:364:ASP:OD1	1:A:366:SER:OG	2.33	0.41
1:A:934:ILE:HD13	1:A:1063:LEU:HD22	2.02	0.41
1:B:405:ASP:H	1:B:504:GLY:HA2	1.85	0.41
1:B:542:ASN:HA	1:B:546:LEU:O	2.21	0.41
1:A:83:VAL:HG22	1:A:239:GLN:HG2	2.03	0.41
1:A:84:LEU:HB2	1:A:238:PHE:CZ	2.55	0.41
1:A:329:PHE:HB3	1:A:330:PRO:HD2	2.02	0.41
1:A:359:SER:HA	1:A:395:VAL:H	1.86	0.41
1:A:1056:ALA:HB2	1:A:1061:VAL:HG23	2.03	0.41
1:A:1090:PRO:HD2	1:B:913:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:OG1	1:B:234:ASN:O	2.34	0.41
1:B:332:ILE:HA	1:B:524:VAL:HG22	2.03	0.41
1:B:656:VAL:HG12	1:B:658:ASN:H	1.85	0.41
1:B:1156:PHE:HZ	1:C:1152:LEU:HG	1.86	0.41
1:C:107:GLY:H	1:C:235:ILE:HG23	1.86	0.41
1:C:212:LEU:HD13	1:C:217:PRO:HD3	2.02	0.41
2:F:86:PRO:HB2	2:F:118:VAL:HG21	2.02	0.41
2:F:177:LEU:HD13	2:F:182:TYR:CE1	2.56	0.41
3:G:37:MET:SD	3:G:92:CYS:HB2	2.60	0.41
1:A:555:SER:HB3	1:A:584:ILE:HG22	2.03	0.41
1:C:596:SER:HB2	1:C:611:LEU:HB3	2.03	0.41
2:D:177:LEU:HD13	2:D:182:TYR:CE1	2.56	0.41
3:G:2:ILE:HG12	3:G:27:LYS:HB2	2.03	0.41
1:B:327:VAL:HG13	1:B:542:ASN:HB3	2.02	0.40
1:C:65:PHE:CZ	1:C:84:LEU:HD11	2.57	0.40
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.85	0.40
1:A:438:SER:OG	1:A:509:ARG:HG3	2.21	0.40
1:B:484:LYS:HD2	1:B:490:PHE:HB2	2.03	0.40
1:B:1145:LEU:HD13	1:C:1148:PHE:HE2	1.86	0.40
1:A:98:SER:HB3	1:A:181:GLY:HA2	2.04	0.40
1:A:374:PHE:HB2	1:A:377:PHE:HE1	1.85	0.40
1:A:389:ASP:HA	1:A:527:PRO:HD3	2.02	0.40
1:A:913:GLN:HE22	1:C:1090:PRO:HD2	1.86	0.40
1:B:126:VAL:HB	1:B:172:SER:HB3	2.02	0.40
1:C:150:LYS:C	1:C:152:TRP:H	2.23	0.40
3:G:94:HIS:ND1	3:G:94:HIS:O	2.54	0.40
1:A:18:PHE:HB2	1:A:21:ARG:HB2	2.04	0.40
1:A:36:VAL:HG21	1:A:220:PHE:HE1	1.85	0.40
1:A:347:PHE:HB2	1:A:401:VAL:HG23	2.02	0.40
1:A:1081:ILE:HG13	1:A:1115:ILE:HD13	2.03	0.40
1:B:423:TYR:HD1	1:B:466:ARG:HB3	1.87	0.40
1:B:985:ASP:HB3	1:B:987:PRO:HD2	2.03	0.40
1:A:382:VAL:HB	1:A:386:LYS:HB2	2.03	0.40
1:A:656:VAL:HG12	1:A:658:ASN:H	1.86	0.40
1:B:327:VAL:HG22	1:B:542:ASN:HB3	2.02	0.40
1:C:906:PHE:CE2	1:C:916:LEU:HB2	2.57	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	1064/1258 (85%)	1011 (95%)	52 (5%)	1 (0%)	51	84
1	B	1064/1258 (85%)	1016 (96%)	47 (4%)	1 (0%)	51	84
1	C	1064/1258 (85%)	1014 (95%)	50 (5%)	0	100	100
2	D	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
2	F	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
3	E	213/215 (99%)	206 (97%)	6 (3%)	1 (0%)	29	67
3	G	213/215 (99%)	205 (96%)	6 (3%)	2 (1%)	17	54
All	All	4048/4638 (87%)	3870 (96%)	173 (4%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	33	VAL
3	G	33	VAL
1	A	150	LYS
1	B	150	LYS
3	G	55	ALA

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	944/1095 (86%)	944 (100%)	0	100	100
1	B	944/1095 (86%)	944 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	944/1095 (86%)	944 (100%)	0	100	100
2	D	187/187 (100%)	187 (100%)	0	100	100
2	F	187/187 (100%)	187 (100%)	0	100	100
3	E	187/187 (100%)	187 (100%)	0	100	100
3	G	187/187 (100%)	187 (100%)	0	100	100
All	All	3580/4033 (89%)	3580 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	563	GLN
1	A	613	GLN
1	A	787	GLN
1	A	913	GLN
1	A	1005	GLN
1	A	1010	GLN
1	B	532	ASN
1	B	913	GLN
1	B	914	ASN
1	C	207	HIS
1	C	417	ASN
1	C	487	ASN
1	C	563	GLN
1	C	913	GLN
1	C	1002	GLN
1	C	1010	GLN
1	C	1106	GLN
1	C	1159	HIS
2	D	52	HIS
2	F	35	ASN
2	F	52	HIS

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	C	3
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	241:LEU	C	245:HIS	N	10.67
1	C	241:LEU	C	245:HIS	N	10.24
1	B	241:LEU	C	245:HIS	N	10.23
1	A	246:ILE	C	247:SER	N	7.08
1	B	246:ILE	C	247:SER	N	6.86
1	C	246:ILE	C	247:SER	N	6.68
1	A	245:HIS	C	246:ILE	N	4.11
1	B	245:HIS	C	246:ILE	N	3.85
1	C	245:HIS	C	246:ILE	N	3.75

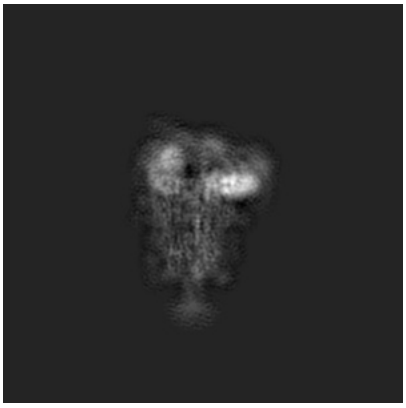
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32437. These allow visual inspection of the internal detail of the map and identification of artifacts.

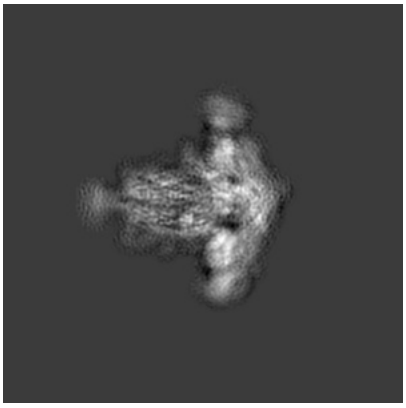
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

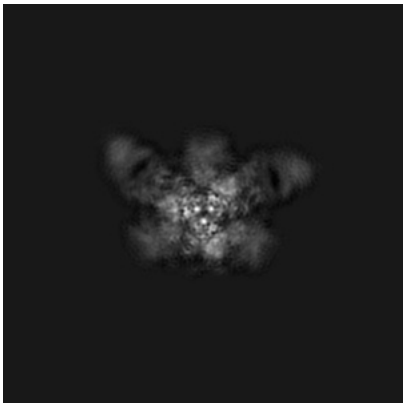
6.1.1 Primary map



X



Y



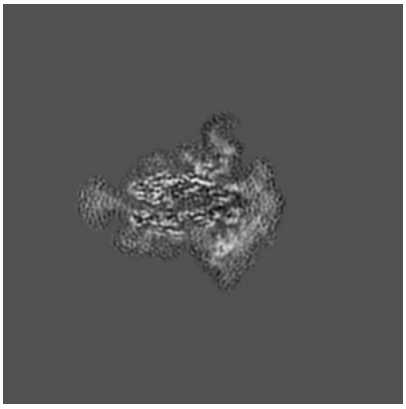
Z

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

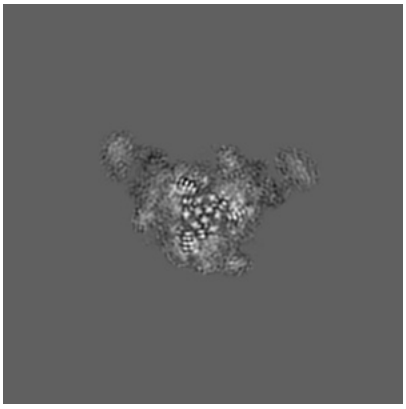
6.2 Central slices (i)

6.2.1 Primary map

X Index: 180



Y Index: 180



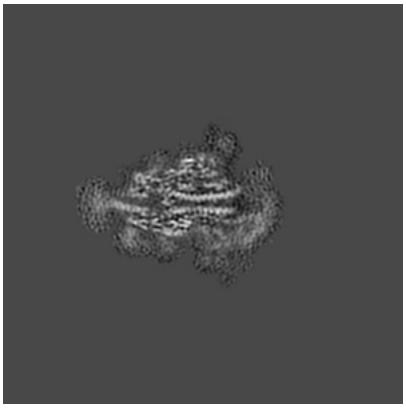
Z Index: 180

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

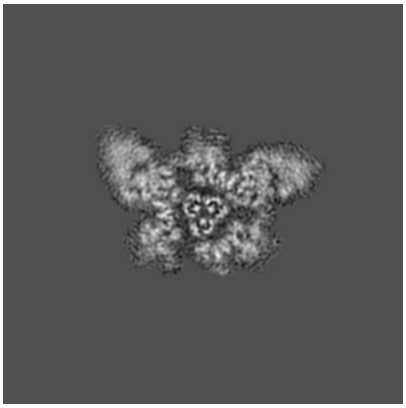
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 187



Y Index: 175



Z Index: 200

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

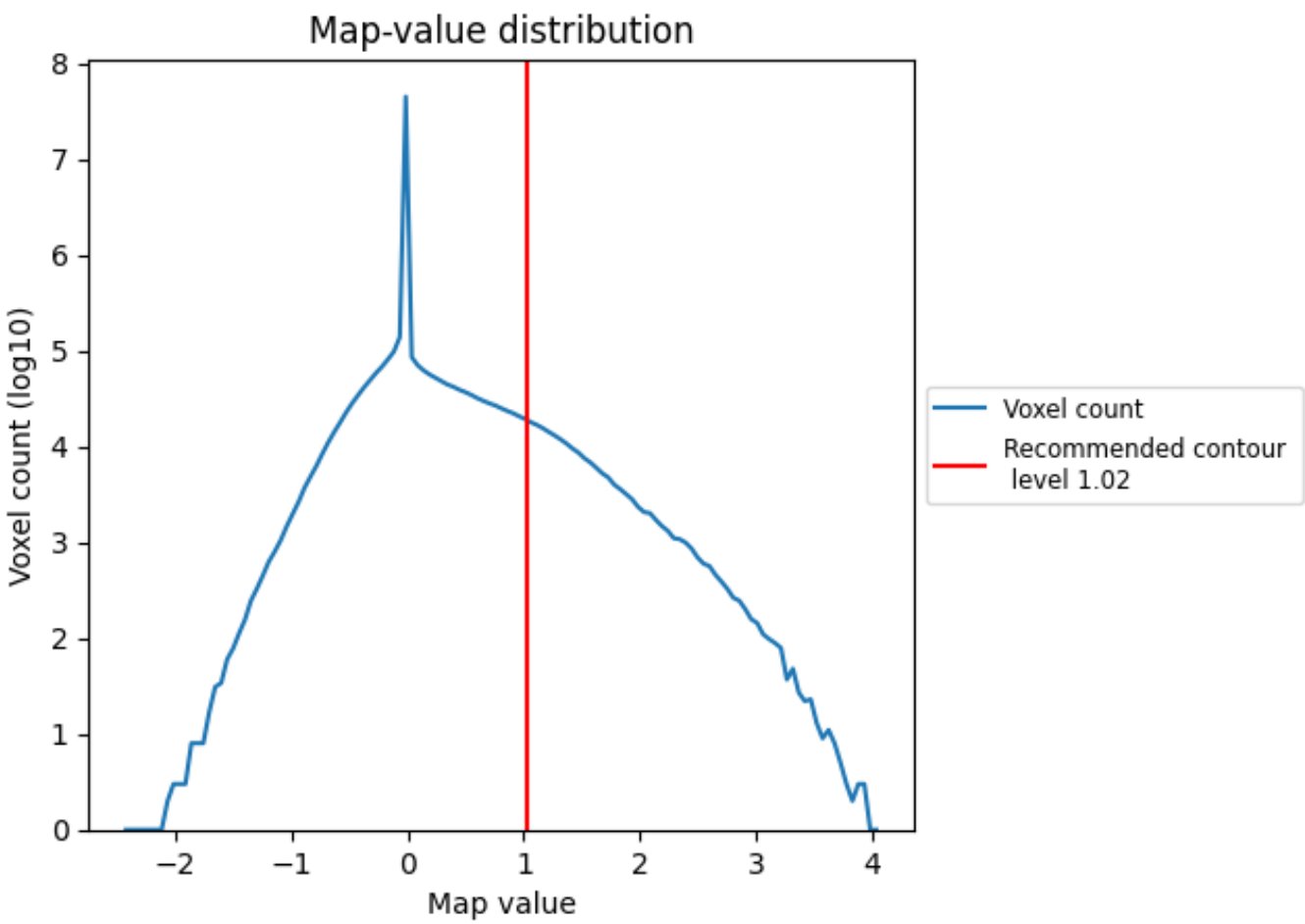
6.5 Mask visualisation (i)

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

7 Map analysis (i)

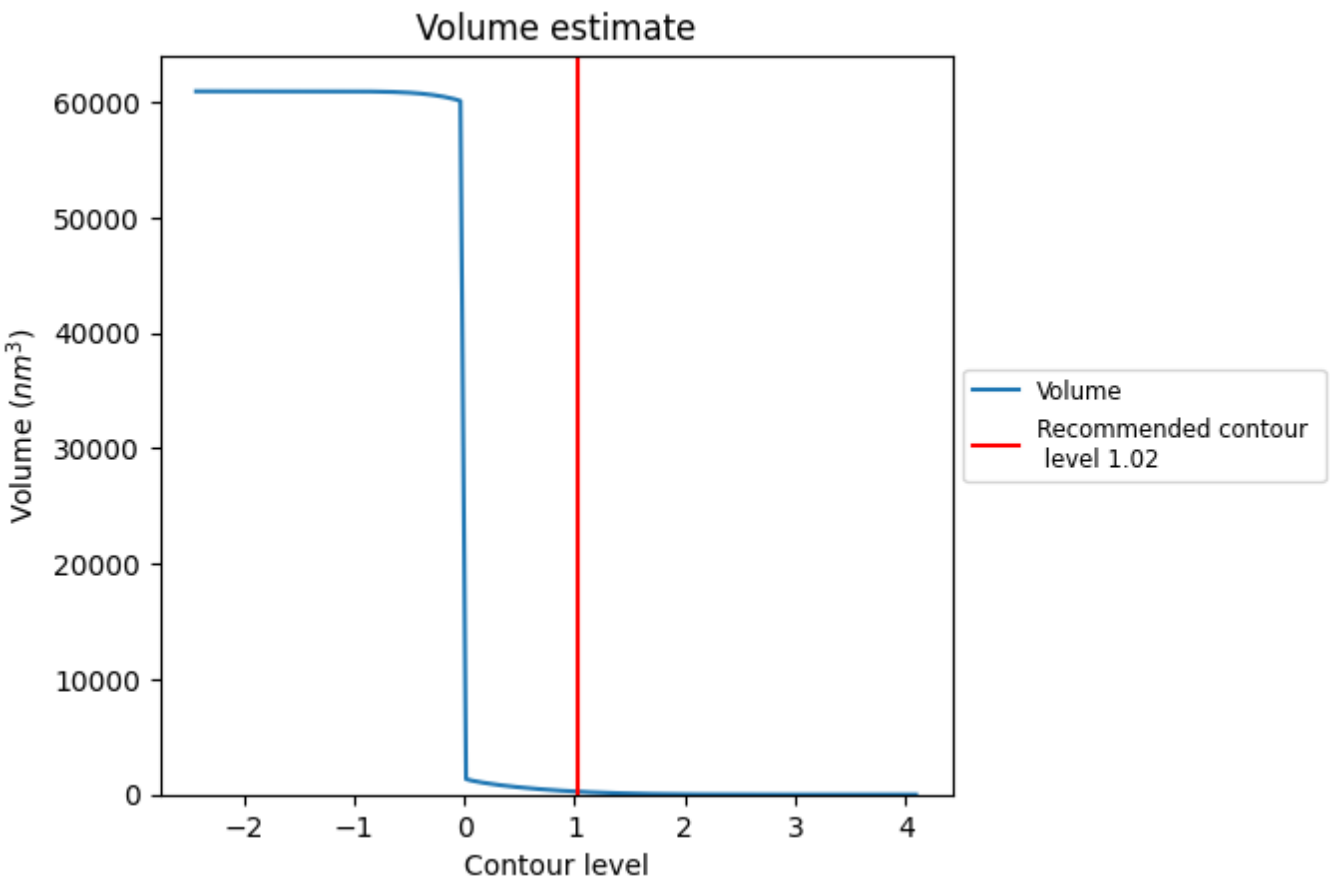
This section contains the results of statistical analysis of the map.

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.

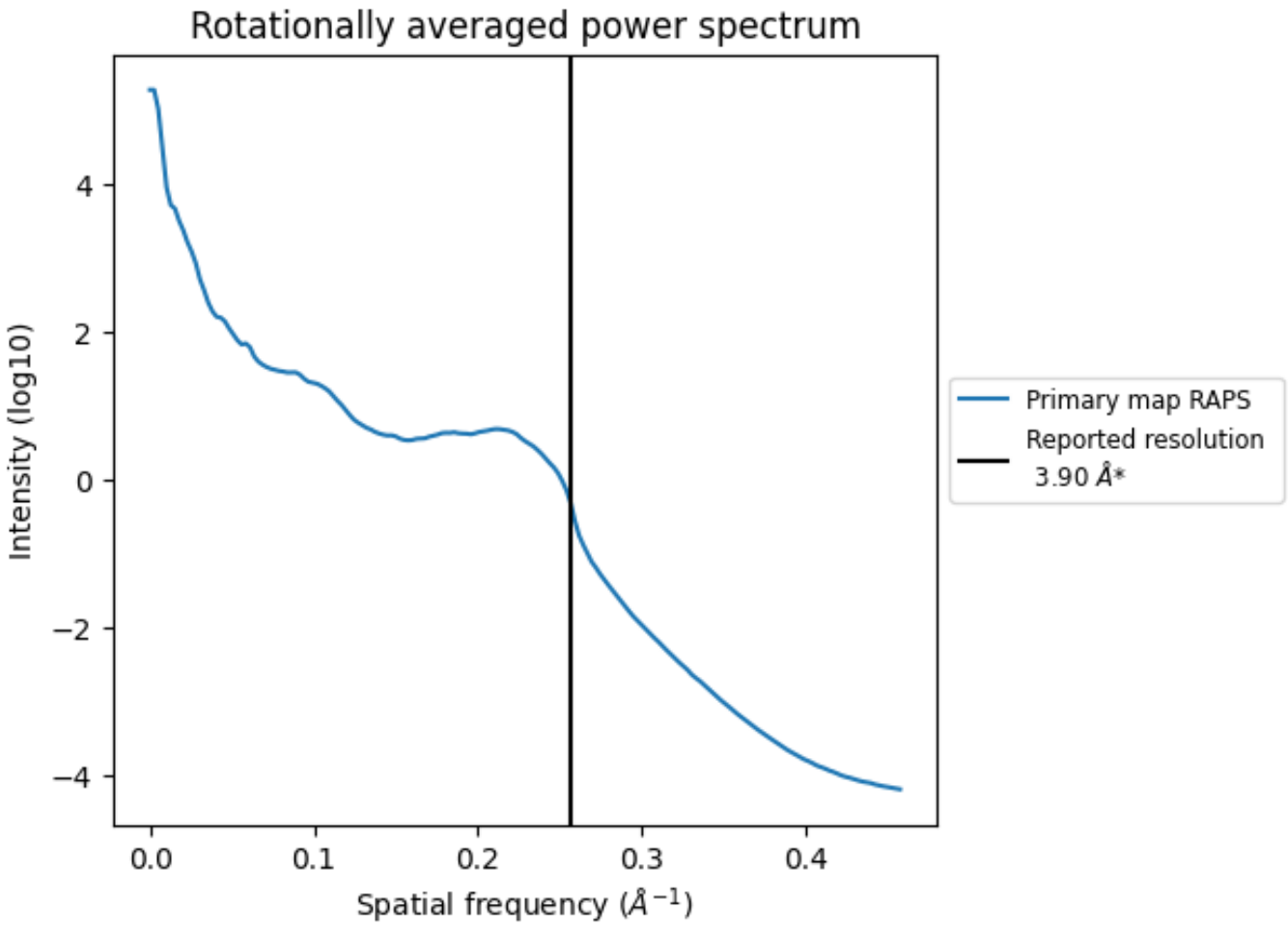
7.2 Volume estimate (i)



The volume at the recommended contour level is 259 nm^3; this corresponds to an approximate mass of 234 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 0.256 Å^{-1}

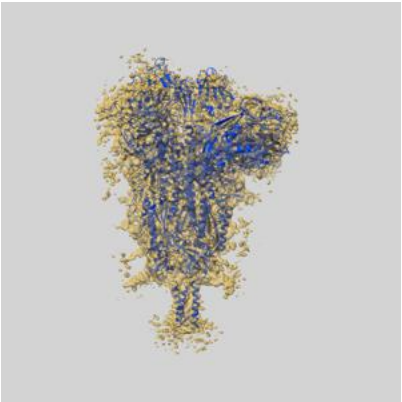
8 Fourier-Shell correlation (i)

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

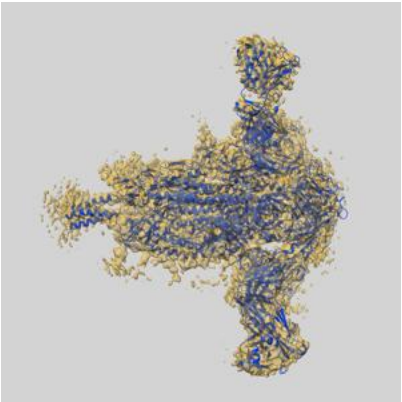
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32437 and PDB model 7WDF. Per-residue inclusion information can be found in section 3 on page 9.

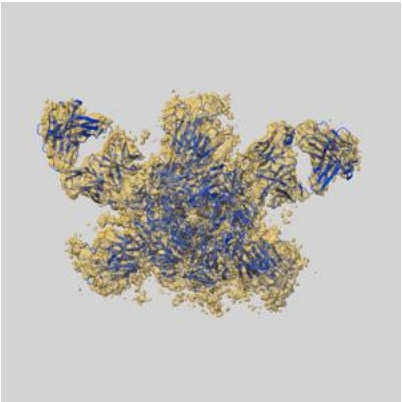
9.1 Map-model overlay (i)



X



Y



Z

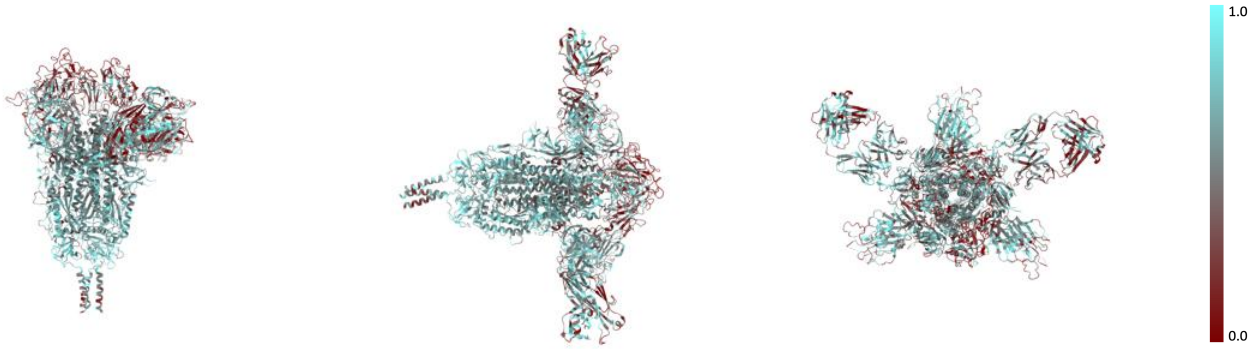
The images above show the 3D surface view of the map at the recommended contour level 1.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

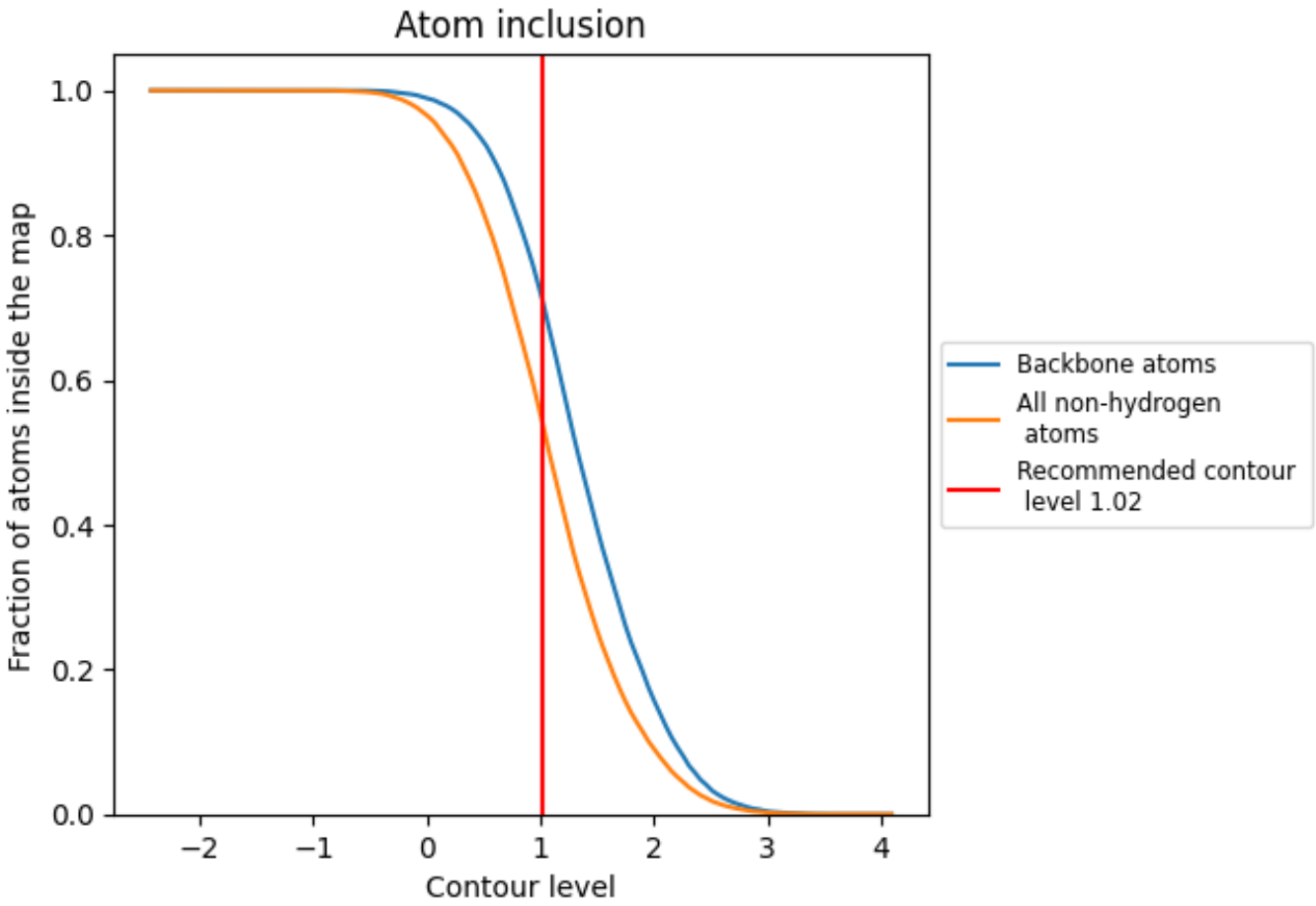
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.02).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 54% 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 (1.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5396	0.1880
A	0.5258	0.2110
B	0.5465	0.2020
C	0.5686	0.2110
D	0.5113	0.1270
E	0.6423	0.1200
F	0.3988	0.1080
G	0.4935	0.0870