Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 11:56 AM JST

PDB ID	:	7WCD
EMDB ID	:	EMD-32421
Title	:	Cryo EM structure of SARS-CoV-2 spike in complex with TAU-2212 mAbs in conformation 4
Authors	:	Xiang, Y.; Ma, B.; Li, R.
Deposited on	:	2021-12-19
Resolution	:	3.30 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:

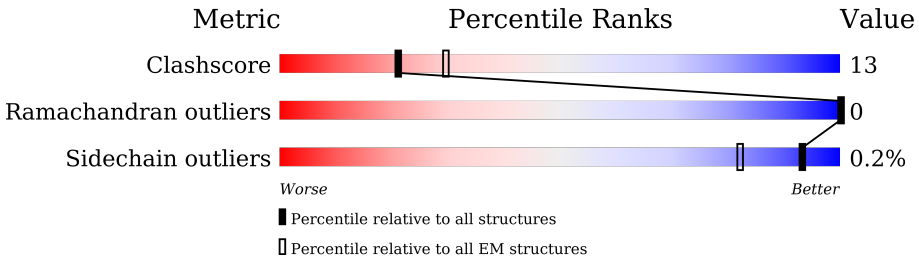
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	C	1237	9% 64% 16% 19%
1	H	1237	9% 64% 17% 19%
1	J	1237	9% 64% 16% 19%
2	A	238	71% 68% 22% 10%
2	E	238	71% 68% 22% 10%
2	G	238	71% 69% 21% 10%
3	B	214	89% 82% 18%
3	F	214	87% 82% 18%

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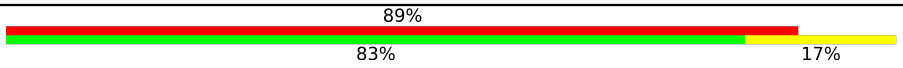
Mol	Chain	Length	Quality of chain
3	I	214	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33525 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	H	1000	Total	C	N	O	S	0	0
			7803	4982	1292	1494	35		
1	J	1000	Total	C	N	O	S	0	0
			7803	4982	1292	1494	35		
1	C	1000	Total	C	N	O	S	0	0
			7803	4982	1292	1494	35		

There are 102 discrepancies between the modelled and reference sequences:

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1236	PHE	-	expression tag	UNP P0DTC2
J	1237	LEU	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	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	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

- Molecule 2 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	214	Total	C	N	O	S	0	0
			1643	1047	272	316	8		

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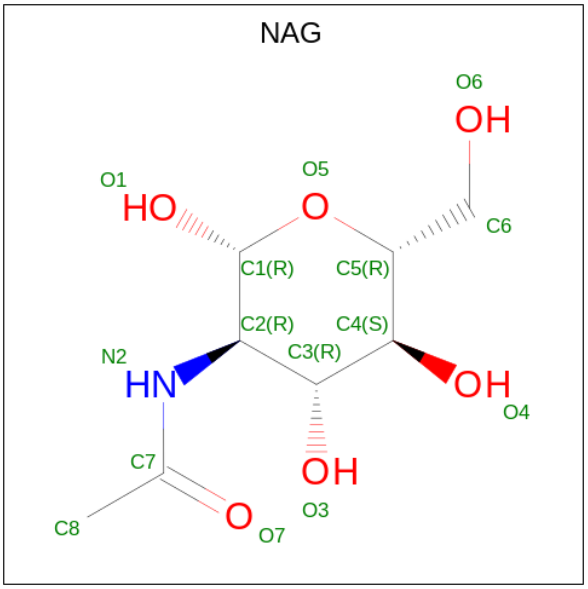
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	214	Total	C	N	O	S	0	0
			1643	1047	272	316	8		
2	A	214	Total	C	N	O	S	0	0
			1643	1047	272	316	8		

- Molecule 3 is a protein called Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	214	Total	C	N	O	S	0	0
			1575	982	263	324	6		
3	I	214	Total	C	N	O	S	0	0
			1575	982	263	324	6		
3	B	214	Total	C	N	O	S	0	0
			1575	982	263	324	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	H	1	Total	C	N	O	0
			154	88	11	55	
4	H	1	Total	C	N	O	0
			154	88	11	55	
4	H	1	Total	C	N	O	0
			154	88	11	55	
4	H	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms	AltConf
4	H	1	Total C N O 154 88 11 55	0
4	H	1	Total C N O 154 88 11 55	0
4	H	1	Total C N O 154 88 11 55	0
4	H	1	Total C N O 154 88 11 55	0
4	H	1	Total C N O 154 88 11 55	0
4	H	1	Total C N O 154 88 11 55	0
4	H	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	J	1	Total C N O 154 88 11 55	0
4	C	1	Total C N O 154 88 11 55	0
4	C	1	Total C N O 154 88 11 55	0
4	C	1	Total C N O 154 88 11 55	0

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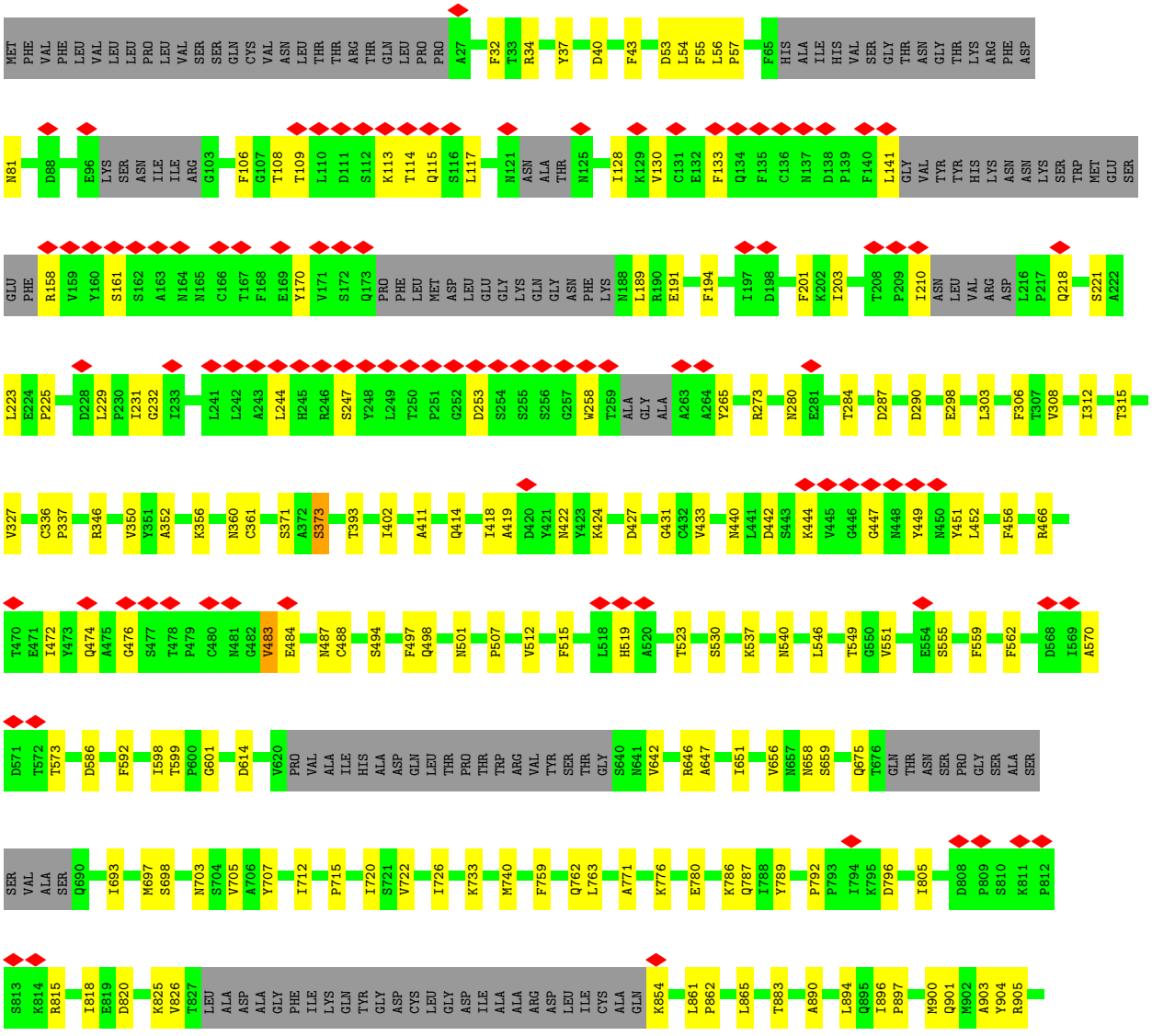
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0
4	C	1	Total 154	C 88	N 11	O 55	0

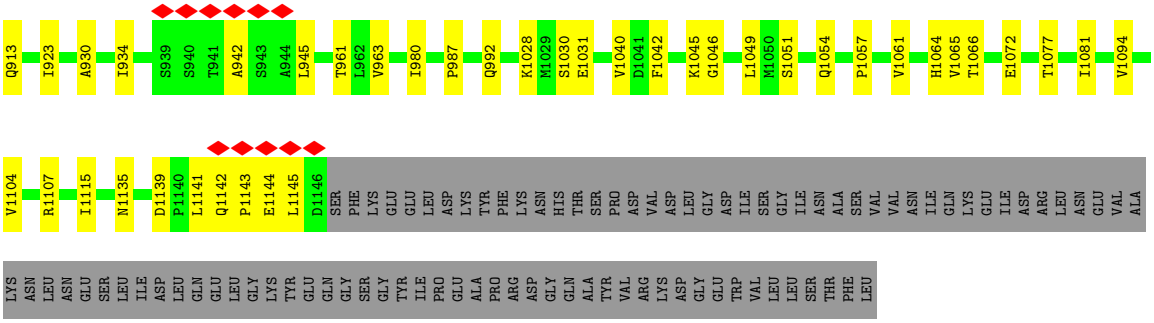
3 Residue-property plots (i)

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

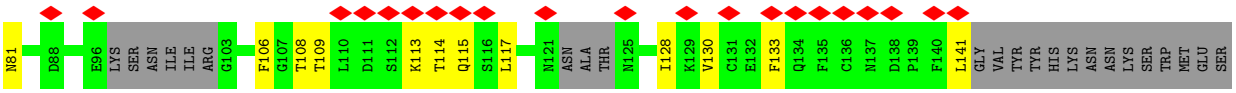
Chain H:

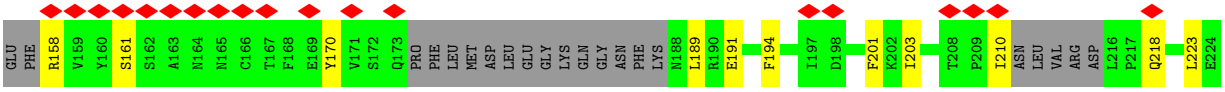


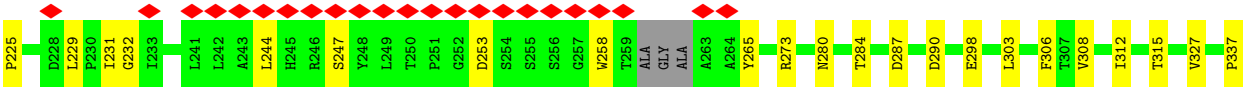


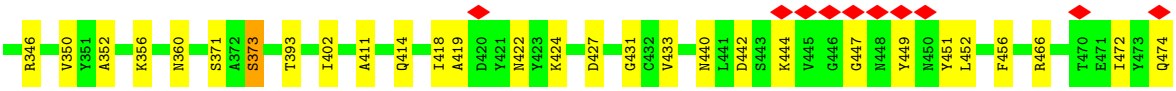
• Molecule 1: Spike glycoprotein

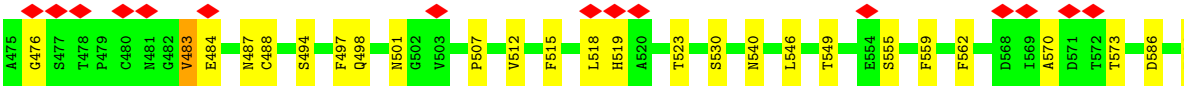
Chain J:

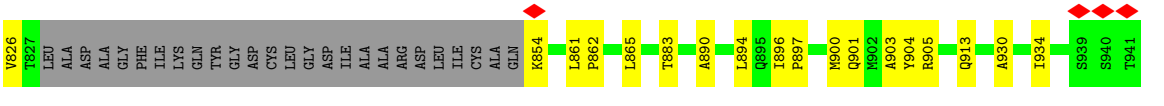


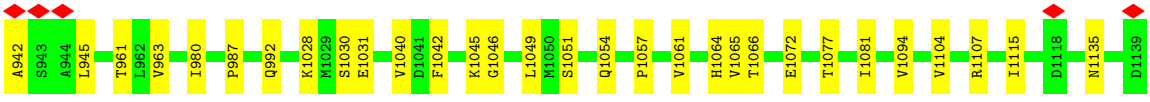


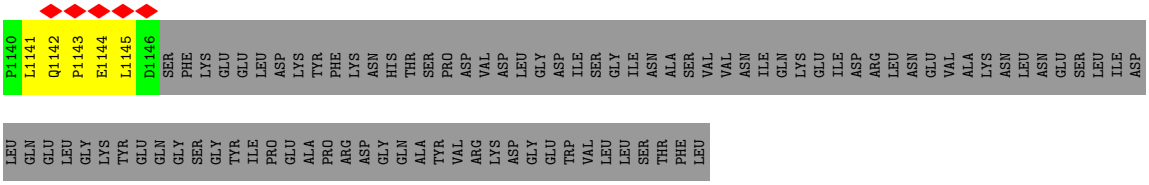






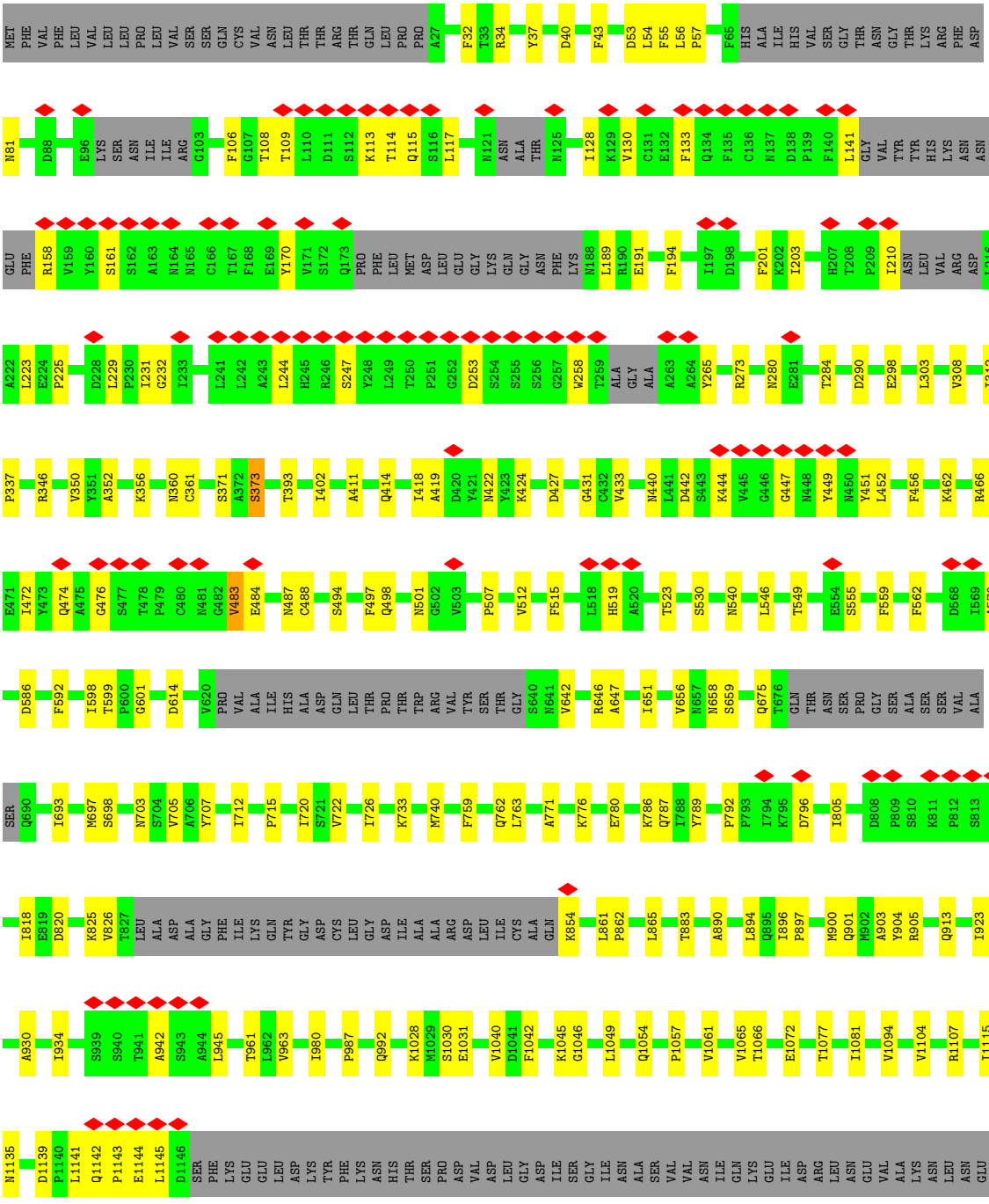






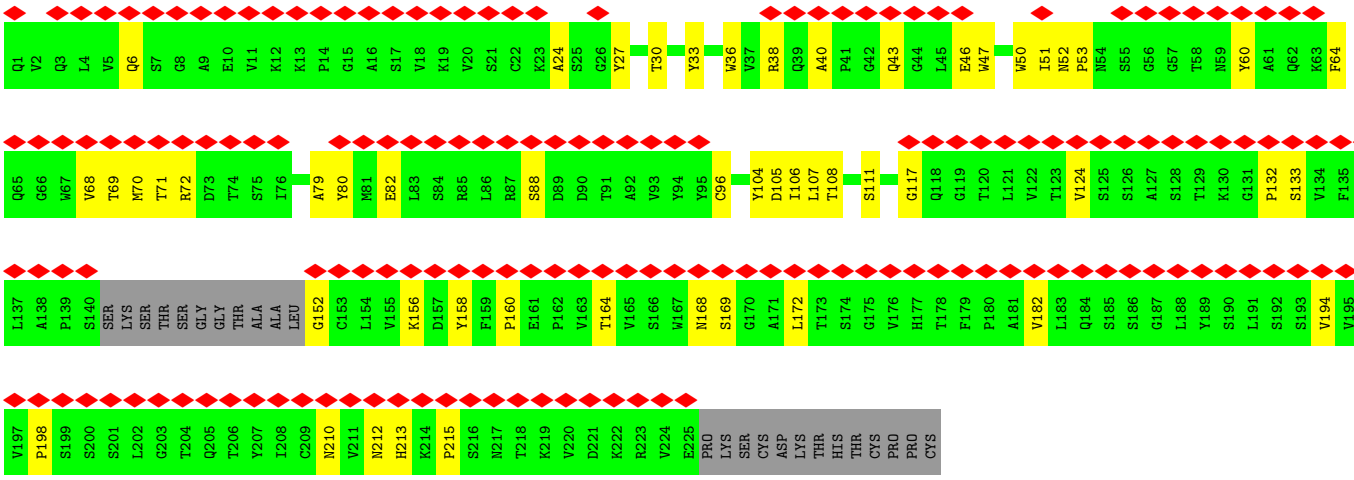
• Molecule 1: Spike glycoprotein

Chain C:



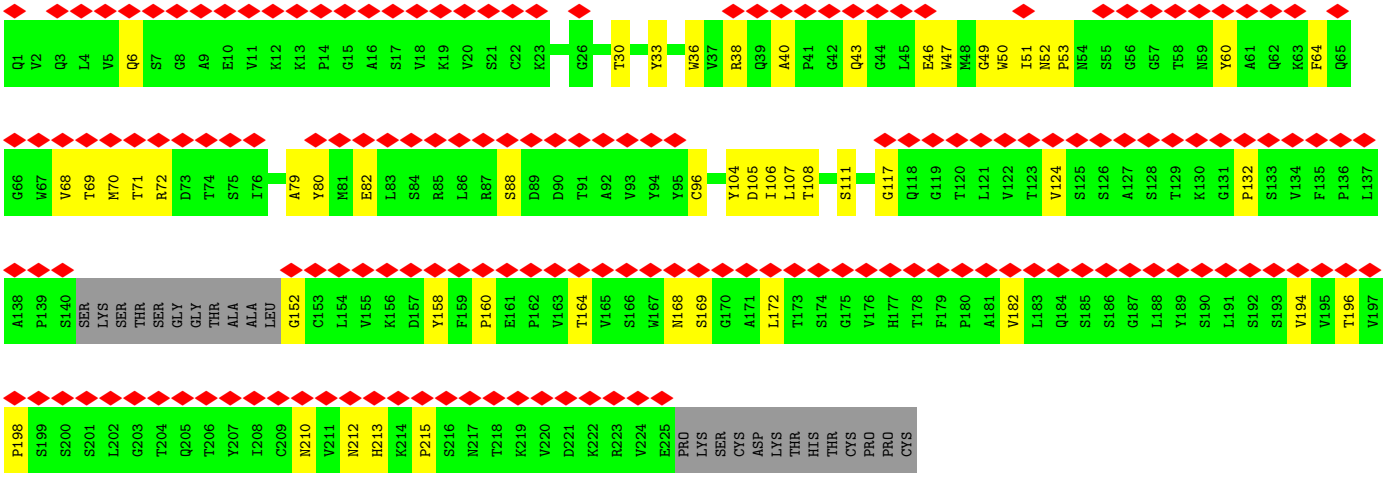
• Molecule 2: Heavy chain

Chain E:



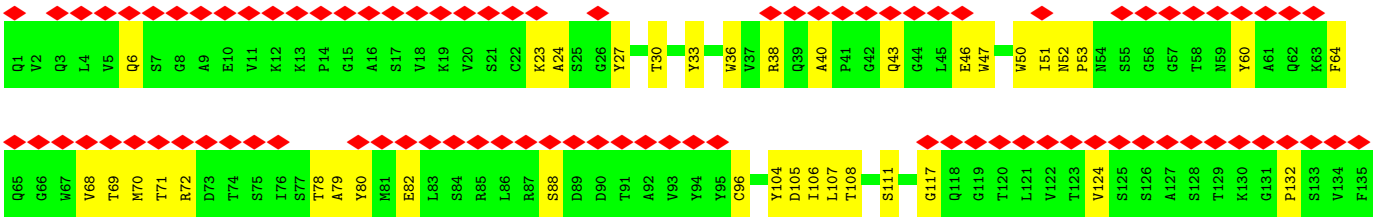
• Molecule 2: Heavy chain

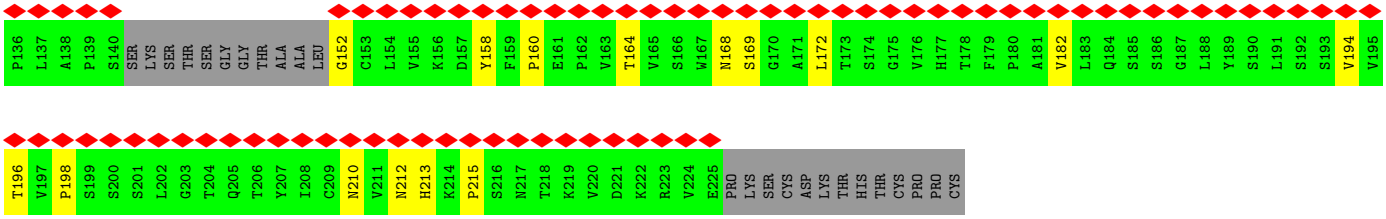
Chain G:



• Molecule 2: Heavy chain

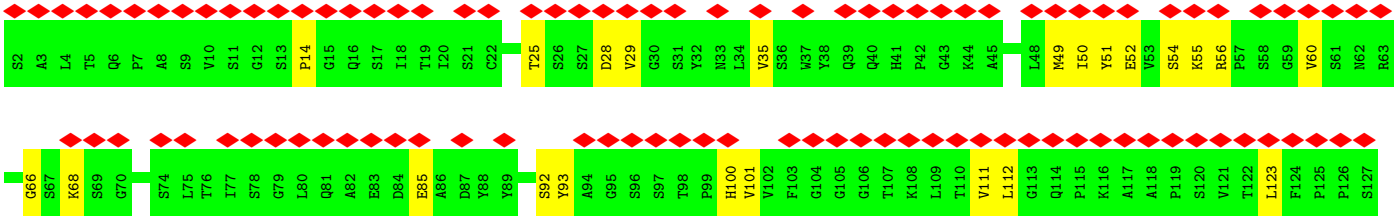
Chain A:





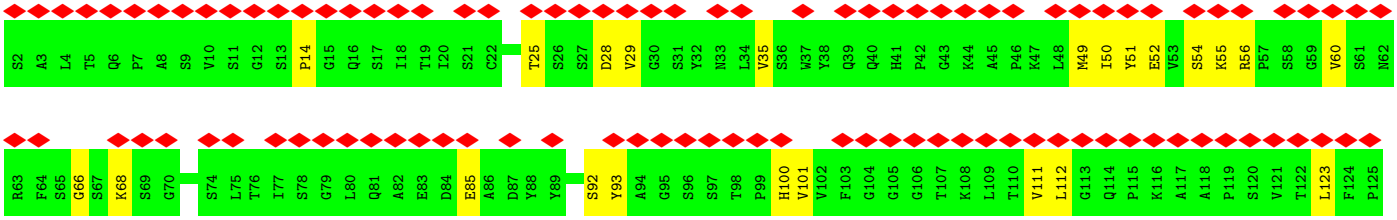
• Molecule 3: Light chain

Chain F:



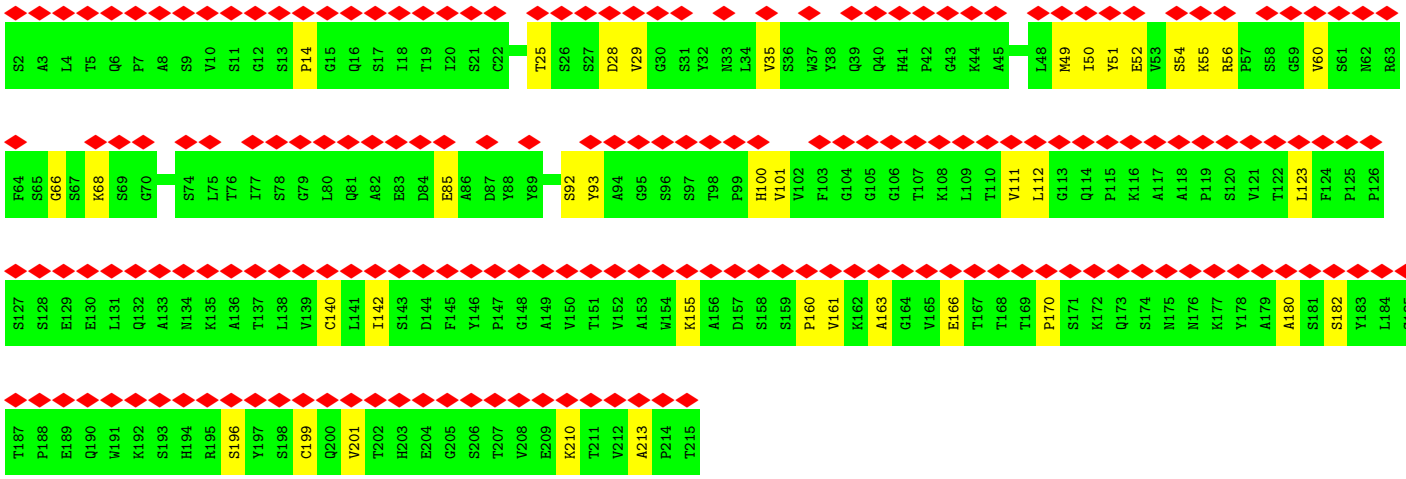
• Molecule 3: Light chain

Chain I:



• Molecule 3: Light chain

Chain B:


S2 A3 L4 T5 Q6 P7 A8 S9 V10 S11 G12 S13 P14 G15 Q16 S17 I18 T19 I20 S21 C22 T25 S26 S27 D28 V29 G30 S31 Y32 N33 L34 V35 S36 W37 Y38 Q39 Q40 H41 P42 G43 K44 A45 L48 M49 I50 Y51 E52 V53 S54 K55 R56 P57 S58 G59 V60 S61 N62 R63
F64 S65 G66 S67 K68 S69 G70 S74 L75 T76 I77 S78 G79 L80 Q81 A82 E83 D84 E85 A86 D87 Y88 Y89 S92 Y93 A94 G95 S96 S97 T98 P99 H100 V101 V102 F103 G104 G105 G106 T107 K108 L109 T110 V111 L112 G113 Q114 P115 K116 A117 A118 P119 S120 V121 T122 L123 F124 P125 P126
S127 S128 E129 E130 L131 Q132 A133 N134 K135 A136 T137 L138 V139 C140 L141 I142 S143 D144 F145 Y146 P147 G148 A149 V150 T151 V152 A153 W154 K155 A156 D157 S158 S159 P160 V161 K162 A163 G164 V165 E166 T167 T168 T169 P170 S171 K172 Q173 S174 N175 N176 K177 Y178 A179 A180 S181 S182 Y183 L184 S185 L186
T187 P188 E189 Q190 W191 K192 S193 H194 R195 S196 Y197 S198 C199 Q200 V201 T202 H203 E204 G205 S206 T207 V208 E209 K210 T211 V212 A213 P214 T215

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72056	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	310.40002, 310.40002, 310.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9700001, 0.9700001, 0.9700001	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.30	0/7978	0.49	0/10855
1	H	0.30	0/7978	0.49	0/10855
1	J	0.30	0/7978	0.49	0/10855
2	A	0.29	0/1689	0.50	0/2305
2	E	0.29	0/1689	0.50	0/2305
2	G	0.29	0/1689	0.50	0/2305
3	B	0.28	0/1613	0.45	0/2201
3	F	0.28	0/1613	0.45	0/2201
3	I	0.28	0/1613	0.45	0/2201
All	All	0.29	0/33840	0.48	0/46083

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	C	7803	0	7587	307	0
1	H	7803	0	7587	311	0
1	J	7803	0	7587	309	0
2	A	1643	0	1585	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1643	0	1585	64	0
2	G	1643	0	1585	64	0
3	B	1575	0	1528	23	0
3	F	1575	0	1528	25	0
3	I	1575	0	1528	22	0
4	C	154	0	143	0	0
4	H	154	0	143	0	0
4	J	154	0	143	0	0
All	All	33525	0	32529	873	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 13.

All (873) 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)
2:A:51:ILE:HG13	2:A:72:ARG:NH2	1.41	1.35
2:E:51:ILE:HG13	2:E:72:ARG:NH2	1.41	1.32
2:G:51:ILE:HG13	2:G:72:ARG:NH2	1.41	1.31
2:E:51:ILE:HG13	2:E:72:ARG:CZ	1.62	1.30
2:G:51:ILE:HG13	2:G:72:ARG:CZ	1.62	1.29
2:A:51:ILE:HG13	2:A:72:ARG:CZ	1.62	1.28
1:H:705:VAL:CG1	1:J:883:THR:HG21	1.67	1.25
1:H:1040:VAL:HG11	1:J:1030:SER:O	1.38	1.24
1:H:1030:SER:O	1:C:1040:VAL:HG11	1.37	1.23
1:J:705:VAL:CG1	1:C:883:THR:HG21	1.68	1.23
1:H:883:THR:HG21	1:C:705:VAL:CG1	1.68	1.21
1:C:484:GLU:O	1:C:488:CYS:HB2	1.41	1.21
1:J:484:GLU:O	1:J:488:CYS:HB2	1.41	1.19
1:H:1072:GLU:HG2	1:J:894:LEU:CD2	1.73	1.18
1:H:894:LEU:CD2	1:C:1072:GLU:HG2	1.73	1.18
1:J:1040:VAL:HG11	1:C:1030:SER:O	1.38	1.18
1:J:1072:GLU:HG2	1:C:894:LEU:CD2	1.74	1.17
1:H:484:GLU:O	1:H:488:CYS:HB2	1.41	1.17
1:H:1077:THR:HG21	1:J:900:MET:HE3	1.20	1.16
1:H:900:MET:HE3	1:C:1077:THR:HG21	1.23	1.13
1:H:1141:LEU:HD21	1:J:1144:GLU:HG2	1.32	1.11
1:J:1077:THR:HG21	1:C:900:MET:HE3	1.23	1.11
1:J:1072:GLU:HG2	1:C:894:LEU:HD21	1.31	1.10
1:J:705:VAL:HG11	1:C:883:THR:HG21	1.33	1.10
1:H:1144:GLU:HG2	1:C:1141:LEU:HD21	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:72:ARG:HG2	2:A:79:ALA:CA	1.82	1.10
1:J:1141:LEU:HD21	1:C:1144:GLU:HG2	1.33	1.09
1:H:894:LEU:HD21	1:C:1072:GLU:HG2	1.32	1.09
2:G:72:ARG:HG2	2:G:79:ALA:CA	1.82	1.08
2:E:72:ARG:HG2	2:E:79:ALA:CA	1.82	1.08
2:A:71:THR:O	2:A:72:ARG:HG3	1.55	1.07
2:E:71:THR:O	2:E:72:ARG:HG3	1.55	1.06
1:H:900:MET:CE	1:C:1077:THR:HG21	1.86	1.06
2:G:71:THR:O	2:G:72:ARG:HG3	1.55	1.06
1:H:1077:THR:HG21	1:J:900:MET:CE	1.85	1.06
2:G:51:ILE:CG1	2:G:72:ARG:CZ	2.34	1.06
1:H:883:THR:HG21	1:C:705:VAL:HG11	1.33	1.05
1:H:1077:THR:CG2	1:J:900:MET:CE	2.33	1.05
2:E:51:ILE:CG1	2:E:72:ARG:CZ	2.34	1.05
1:J:1077:THR:HG21	1:C:900:MET:CE	1.86	1.05
2:A:72:ARG:HG2	2:A:79:ALA:HA	1.06	1.05
2:G:72:ARG:HG2	2:G:79:ALA:HA	1.06	1.05
1:H:900:MET:CE	1:C:1077:THR:CG2	2.34	1.05
1:H:705:VAL:HG11	1:J:883:THR:HG21	1.33	1.05
2:E:72:ARG:HG2	2:E:79:ALA:HA	1.06	1.04
1:J:1077:THR:CG2	1:C:900:MET:CE	2.34	1.04
1:H:894:LEU:HD21	1:C:1072:GLU:CG	1.88	1.04
1:H:1072:GLU:HG2	1:J:894:LEU:HD21	1.31	1.03
1:H:1072:GLU:CG	1:J:894:LEU:HD21	1.87	1.03
2:A:51:ILE:CG1	2:A:72:ARG:CZ	2.34	1.03
1:H:904:TYR:CZ	1:C:1107:ARG:HD3	1.93	1.03
1:J:1045:LYS:HE2	1:C:786:LYS:HZ2	1.19	1.02
1:J:1072:GLU:CG	1:C:894:LEU:HD21	1.88	1.02
2:A:52:ASN:C	2:A:72:ARG:HH22	1.63	1.01
1:J:1107:ARG:HD3	1:C:904:TYR:CZ	1.95	1.01
1:H:1107:ARG:HD3	1:J:904:TYR:CZ	1.94	1.00
1:J:570:ALA:HB1	1:C:963:VAL:HG12	1.41	1.00
2:E:52:ASN:C	2:E:72:ARG:HH22	1.63	0.99
2:G:52:ASN:C	2:G:72:ARG:HH22	1.63	0.99
1:H:963:VAL:HG12	1:C:570:ALA:HB1	1.42	0.99
1:H:1077:THR:CG2	1:J:900:MET:HE3	1.92	0.98
1:H:570:ALA:HB1	1:J:963:VAL:HG12	1.42	0.98
2:G:72:ARG:CG	2:G:79:ALA:HA	1.95	0.97
1:H:987:PRO:HB3	1:J:427:ASP:OD1	1.65	0.97
1:J:1045:LYS:HE2	1:C:786:LYS:NZ	1.80	0.97
2:A:51:ILE:HG12	2:A:72:ARG:NE	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:72:ARG:CG	2:A:79:ALA:HA	1.95	0.96
2:E:72:ARG:CG	2:E:79:ALA:HA	1.95	0.96
1:H:786:LYS:NZ	1:C:1045:LYS:HE2	1.81	0.95
1:H:1144:GLU:HG2	1:C:1141:LEU:CD2	1.96	0.95
1:H:1045:LYS:HE2	1:J:786:LYS:NZ	1.81	0.95
2:E:51:ILE:HG12	2:E:72:ARG:NE	1.81	0.95
2:G:51:ILE:HG12	2:G:72:ARG:NE	1.81	0.94
1:H:427:ASP:OD1	1:C:987:PRO:HB3	1.66	0.94
1:H:1141:LEU:CD2	1:J:1144:GLU:HG2	1.96	0.94
1:J:987:PRO:HB3	1:C:427:ASP:OD1	1.66	0.94
1:H:1045:LYS:HE2	1:J:786:LYS:HZ2	1.31	0.94
1:J:1141:LEU:CD2	1:C:1144:GLU:HG2	1.97	0.94
1:H:559:PHE:HE1	1:J:43:PHE:CD2	1.86	0.93
1:J:484:GLU:O	1:J:488:CYS:CB	2.16	0.93
1:C:484:GLU:O	1:C:488:CYS:CB	2.16	0.93
2:G:51:ILE:CG1	2:G:72:ARG:NE	2.32	0.93
2:A:51:ILE:CG1	2:A:72:ARG:NE	2.32	0.93
1:H:43:PHE:CD2	1:C:559:PHE:HE1	1.86	0.93
1:H:705:VAL:HG11	1:J:883:THR:CG2	1.99	0.92
2:E:51:ILE:CG1	2:E:72:ARG:NE	2.32	0.92
1:H:484:GLU:O	1:H:488:CYS:CB	2.16	0.92
1:J:559:PHE:HE1	1:C:43:PHE:CD2	1.86	0.92
1:H:883:THR:CG2	1:C:705:VAL:HG11	2.00	0.92
1:H:1031:GLU:HA	1:C:1040:VAL:CG1	2.00	0.92
3:F:50:ILE:HG22	3:F:52:GLU:O	1.70	0.91
1:H:705:VAL:HG13	1:J:883:THR:HG21	1.51	0.91
1:J:705:VAL:HG11	1:C:883:THR:CG2	2.00	0.91
1:J:705:VAL:HG13	1:C:883:THR:HG21	1.51	0.91
1:H:786:LYS:HZ2	1:C:1045:LYS:HE2	1.34	0.91
1:H:1040:VAL:CG1	1:J:1031:GLU:HA	2.00	0.91
1:H:712:ILE:CG2	1:J:896:ILE:HD12	2.00	0.91
1:J:712:ILE:CG2	1:C:896:ILE:HD12	2.00	0.90
1:J:1040:VAL:CG1	1:C:1031:GLU:HA	2.01	0.90
1:H:896:ILE:HD12	1:C:712:ILE:CG2	2.00	0.90
3:I:50:ILE:HG22	3:I:52:GLU:O	1.70	0.90
3:B:50:ILE:HG22	3:B:52:GLU:O	1.70	0.90
1:J:570:ALA:CB	1:C:963:VAL:HG12	2.02	0.89
1:H:883:THR:HG21	1:C:705:VAL:HG13	1.52	0.89
1:H:570:ALA:CB	1:J:963:VAL:HG12	2.02	0.88
1:J:1077:THR:CG2	1:C:900:MET:HE3	2.01	0.88
1:C:210:ILE:HG22	1:C:210:ILE:O	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:51:ILE:HG23	2:G:72:ARG:NH1	1.90	0.87
1:J:210:ILE:HG22	1:J:210:ILE:O	1.74	0.87
1:J:1077:THR:CG2	1:C:900:MET:HE1	2.03	0.87
1:H:963:VAL:HG12	1:C:570:ALA:CB	2.03	0.87
1:H:900:MET:HE3	1:C:1077:THR:CG2	1.99	0.86
2:E:51:ILE:HG23	2:E:72:ARG:NH1	1.90	0.86
1:H:210:ILE:HG22	1:H:210:ILE:O	1.74	0.86
2:A:51:ILE:HG23	2:A:72:ARG:NH1	1.90	0.86
1:H:900:MET:HE1	1:C:1077:THR:CG2	2.05	0.85
1:H:1040:VAL:CG1	1:J:1030:SER:O	2.23	0.85
1:H:1030:SER:O	1:C:1040:VAL:CG1	2.22	0.85
1:H:1107:ARG:HD2	1:J:904:TYR:CE2	2.13	0.84
1:H:904:TYR:CE2	1:C:1107:ARG:HD2	2.12	0.84
1:J:1107:ARG:HD2	1:C:904:TYR:CE2	2.13	0.84
1:H:904:TYR:CZ	1:C:1107:ARG:CD	2.63	0.82
2:E:52:ASN:C	2:E:72:ARG:NH2	2.33	0.82
2:A:52:ASN:C	2:A:72:ARG:NH2	2.33	0.82
1:H:1144:GLU:CG	1:C:1141:LEU:HD21	2.09	0.82
1:J:1040:VAL:CG1	1:C:1030:SER:O	2.23	0.82
1:J:1141:LEU:HD21	1:C:1144:GLU:CG	2.10	0.81
1:H:1072:GLU:HG2	1:J:894:LEU:HD23	1.62	0.81
1:H:1040:VAL:HG12	1:J:1031:GLU:HA	1.63	0.81
1:H:1141:LEU:HD21	1:J:1144:GLU:CG	2.10	0.81
1:J:1072:GLU:HG2	1:C:894:LEU:HD23	1.63	0.81
1:H:1072:GLU:CG	1:J:894:LEU:CD2	2.52	0.81
2:A:53:PRO:N	2:A:72:ARG:HH22	1.79	0.81
1:H:894:LEU:HD23	1:C:1072:GLU:HG2	1.62	0.80
1:H:1107:ARG:CD	1:J:904:TYR:CZ	2.63	0.80
1:J:1040:VAL:HG12	1:C:1031:GLU:HA	1.63	0.80
2:G:52:ASN:C	2:G:72:ARG:NH2	2.33	0.80
2:G:53:PRO:N	2:G:72:ARG:HH22	1.79	0.80
2:E:53:PRO:N	2:E:72:ARG:HH22	1.79	0.80
1:J:1107:ARG:CD	1:C:904:TYR:CZ	2.64	0.80
1:H:1077:THR:CG2	1:J:900:MET:HE1	2.12	0.80
1:H:559:PHE:CE1	1:J:43:PHE:CD2	2.70	0.80
1:H:1145:LEU:HD21	1:J:1145:LEU:HD21	1.63	0.79
1:H:614:ASP:HB3	1:J:854:LYS:NZ	1.98	0.79
1:H:43:PHE:CD2	1:C:559:PHE:CE1	2.71	0.79
2:G:51:ILE:HG13	2:G:72:ARG:HH21	1.48	0.79
1:J:712:ILE:HG21	1:C:896:ILE:HD12	1.65	0.79
1:H:1145:LEU:HD21	1:C:1145:LEU:HD21	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:712:ILE:HG22	1:J:896:ILE:HD12	1.65	0.78
1:H:854:LYS:NZ	1:C:614:ASP:HB3	1.98	0.78
1:H:712:ILE:HG21	1:J:896:ILE:HD12	1.64	0.78
1:J:1145:LEU:HD21	1:C:1145:LEU:HD21	1.64	0.78
2:E:53:PRO:N	2:E:72:ARG:NH2	2.32	0.78
2:A:53:PRO:N	2:A:72:ARG:NH2	2.32	0.78
1:H:1031:GLU:HA	1:C:1040:VAL:HG12	1.62	0.78
2:G:53:PRO:N	2:G:72:ARG:NH2	2.32	0.78
1:J:614:ASP:HB3	1:C:854:LYS:NZ	1.99	0.77
1:J:559:PHE:CE1	1:C:43:PHE:CD2	2.70	0.77
1:H:570:ALA:CB	1:J:963:VAL:CG1	2.63	0.77
1:H:963:VAL:CG1	1:C:570:ALA:CB	2.63	0.77
1:H:1031:GLU:HA	1:C:1040:VAL:HG11	1.67	0.77
2:G:51:ILE:CG1	2:G:72:ARG:NH2	2.38	0.77
1:J:570:ALA:CB	1:C:963:VAL:CG1	2.62	0.77
1:J:712:ILE:HG22	1:C:896:ILE:HD12	1.66	0.77
1:H:896:ILE:HD12	1:C:712:ILE:HG21	1.65	0.76
1:H:1077:THR:HG23	1:J:900:MET:HE1	1.68	0.76
1:H:900:MET:HE1	1:C:1077:THR:HG23	1.67	0.76
2:E:51:ILE:HG21	2:E:72:ARG:HD3	1.68	0.75
1:H:904:TYR:CE2	1:C:1107:ARG:CD	2.69	0.75
2:E:51:ILE:HG13	2:E:72:ARG:HH21	1.48	0.75
1:J:1077:THR:HG23	1:C:900:MET:HE1	1.66	0.75
1:J:987:PRO:CB	1:C:427:ASP:OD1	2.35	0.75
1:H:1040:VAL:HG11	1:J:1031:GLU:HA	1.66	0.75
1:H:427:ASP:OD1	1:C:987:PRO:CB	2.35	0.75
1:J:1107:ARG:CD	1:C:904:TYR:CE2	2.70	0.75
1:H:447:GLY:HA3	1:H:497:PHE:HB2	1.68	0.74
1:C:447:GLY:HA3	1:C:497:PHE:HB2	1.68	0.74
2:G:51:ILE:HG21	2:G:72:ARG:HD3	1.68	0.74
1:H:896:ILE:HD12	1:C:712:ILE:HG22	1.66	0.74
1:H:987:PRO:CB	1:J:427:ASP:OD1	2.34	0.74
1:J:599:THR:HG22	1:J:601:GLY:H	1.53	0.74
2:A:51:ILE:HG21	2:A:72:ARG:HD3	1.68	0.74
1:J:1040:VAL:HG11	1:C:1031:GLU:HA	1.67	0.74
2:G:71:THR:O	2:G:72:ARG:CG	2.34	0.74
2:A:51:ILE:CG1	2:A:72:ARG:NH2	2.38	0.74
2:A:71:THR:O	2:A:72:ARG:CG	2.34	0.74
1:H:1107:ARG:CD	1:J:904:TYR:CE2	2.70	0.73
1:H:1145:LEU:HD21	1:J:1145:LEU:CD2	2.18	0.73
1:J:447:GLY:HA3	1:J:497:PHE:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1107:ARG:HD3	1:C:904:TYR:CE1	2.23	0.73
1:H:904:TYR:CE1	1:C:1107:ARG:HD3	2.22	0.73
2:E:71:THR:O	2:E:72:ARG:CG	2.34	0.73
1:H:1077:THR:HG23	1:J:900:MET:CE	2.17	0.73
1:C:599:THR:HG22	1:C:601:GLY:H	1.53	0.73
1:J:1145:LEU:HD21	1:C:1145:LEU:CD2	2.19	0.73
1:J:1072:GLU:CG	1:C:894:LEU:CD2	2.53	0.73
1:H:1107:ARG:HD3	1:J:904:TYR:CE1	2.23	0.72
1:H:1145:LEU:CD2	1:C:1145:LEU:HD21	2.19	0.72
1:H:599:THR:HG22	1:H:601:GLY:H	1.53	0.72
1:J:189:LEU:HB2	1:J:210:ILE:HD12	1.72	0.72
1:H:894:LEU:CD2	1:C:1072:GLU:CG	2.53	0.72
1:H:1072:GLU:HG3	1:J:894:LEU:HD21	1.72	0.72
1:C:189:LEU:HB2	1:C:210:ILE:HD12	1.72	0.72
1:H:189:LEU:HB2	1:H:210:ILE:HD12	1.72	0.72
1:J:411:ALA:HB3	1:J:414:GLN:HG2	1.72	0.71
1:C:411:ALA:HB3	1:C:414:GLN:HG2	1.72	0.71
1:J:642:VAL:HG12	1:J:651:ILE:HG12	1.72	0.71
1:H:411:ALA:HB3	1:H:414:GLN:HG2	1.72	0.71
1:H:642:VAL:HG12	1:H:651:ILE:HG12	1.72	0.71
1:C:642:VAL:HG12	1:C:651:ILE:HG12	1.72	0.71
1:J:189:LEU:HD22	1:J:210:ILE:CD1	2.21	0.71
1:H:189:LEU:HD22	1:H:210:ILE:CD1	2.21	0.70
1:H:894:LEU:HD21	1:C:1072:GLU:HG3	1.72	0.70
1:C:189:LEU:HD22	1:C:210:ILE:CD1	2.21	0.70
2:E:51:ILE:CG1	2:E:72:ARG:NH2	2.37	0.70
1:J:707:TYR:HB2	1:C:883:THR:HG23	1.73	0.70
2:A:51:ILE:HG13	2:A:72:ARG:HH21	1.48	0.70
1:J:703:ASN:ND2	1:C:787:GLN:OE1	2.24	0.69
1:H:883:THR:HG23	1:C:707:TYR:HB2	1.74	0.69
3:F:56:ARG:HD3	3:F:60:VAL:HG12	1.75	0.69
1:J:1077:THR:HG23	1:C:900:MET:CE	2.18	0.69
1:H:787:GLN:OE1	1:C:703:ASN:ND2	2.25	0.69
1:H:897:PRO:HD2	1:C:712:ILE:HG22	1.75	0.69
1:H:712:ILE:HG22	1:J:897:PRO:HD2	1.75	0.69
3:I:56:ARG:HD3	3:I:60:VAL:HG12	1.75	0.68
1:J:1072:GLU:HG3	1:C:894:LEU:HD21	1.73	0.68
2:A:6:GLN:HE22	2:A:117:GLY:HA3	1.58	0.68
1:H:1145:LEU:CD2	1:J:1145:LEU:CD2	2.71	0.68
1:H:707:TYR:HB2	1:J:883:THR:HG23	1.73	0.68
3:B:56:ARG:HD3	3:B:60:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:712:ILE:HG22	1:C:897:PRO:HD2	1.76	0.68
1:H:697:MET:CE	1:J:865:LEU:HD23	2.24	0.67
1:H:1145:LEU:CD2	1:C:1145:LEU:CD2	2.72	0.67
2:E:53:PRO:HD3	2:E:72:ARG:HH12	1.59	0.67
2:G:53:PRO:HD3	2:G:72:ARG:HH12	1.59	0.67
1:H:703:ASN:ND2	1:J:787:GLN:OE1	2.24	0.67
1:H:865:LEU:HD23	1:C:697:MET:CE	2.24	0.67
2:E:6:GLN:HE22	2:E:117:GLY:HA3	1.58	0.67
1:J:697:MET:CE	1:C:865:LEU:HD23	2.25	0.67
2:A:53:PRO:HD3	2:A:72:ARG:HH12	1.59	0.67
1:H:900:MET:CE	1:C:1077:THR:HG23	2.18	0.66
1:H:312:ILE:HG12	1:H:598:ILE:HG12	1.77	0.66
1:J:1145:LEU:CD2	1:C:1145:LEU:CD2	2.72	0.66
1:H:792:PRO:HG3	1:C:707:TYR:HB3	1.77	0.66
2:G:6:GLN:HE22	2:G:117:GLY:HA3	1.58	0.66
1:H:707:TYR:HB3	1:J:792:PRO:HG3	1.78	0.66
2:A:51:ILE:HG12	2:A:72:ARG:HE	1.61	0.66
2:E:51:ILE:HG12	2:E:72:ARG:HE	1.61	0.66
2:A:72:ARG:HG2	2:A:79:ALA:CB	2.26	0.66
2:G:72:ARG:HG2	2:G:79:ALA:CB	2.26	0.66
1:J:352:ALA:HA	1:J:466:ARG:HD3	1.78	0.65
1:J:707:TYR:HB3	1:C:792:PRO:HG3	1.78	0.65
1:J:776:LYS:NZ	1:J:780:GLU:OE2	2.26	0.65
1:H:963:VAL:CG1	1:C:570:ALA:HB1	2.22	0.65
1:J:312:ILE:HG12	1:J:598:ILE:HG12	1.77	0.65
1:H:352:ALA:HA	1:H:466:ARG:HD3	1.78	0.65
1:J:555:SER:HB3	1:J:586:ASP:HB2	1.79	0.65
1:H:1040:VAL:HG11	1:J:1030:SER:C	2.16	0.65
2:G:51:ILE:HG13	2:G:72:ARG:NE	2.04	0.65
1:C:312:ILE:HG12	1:C:598:ILE:HG12	1.77	0.64
1:J:210:ILE:O	1:J:210:ILE:CG2	2.45	0.64
1:C:210:ILE:O	1:C:210:ILE:CG2	2.45	0.64
1:H:555:SER:HB3	1:H:586:ASP:HB2	1.79	0.64
2:E:72:ARG:HG2	2:E:79:ALA:CB	2.26	0.64
1:H:1030:SER:C	1:C:1040:VAL:HG11	2.16	0.64
2:G:6:GLN:NE2	2:G:96:CYS:SG	2.71	0.64
1:J:1077:THR:OG1	1:C:900:MET:HE1	1.97	0.64
2:G:51:ILE:HG12	2:G:72:ARG:HE	1.61	0.64
1:C:352:ALA:HA	1:C:466:ARG:HD3	1.78	0.63
2:E:6:GLN:NE2	2:E:96:CYS:SG	2.71	0.63
1:H:776:LYS:NZ	1:H:780:GLU:OE2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:189:LEU:CD2	1:J:210:ILE:CD1	2.76	0.63
2:A:52:ASN:CA	2:A:72:ARG:HH22	2.12	0.63
1:C:337:PRO:HG2	1:C:356:LYS:HZ1	1.64	0.63
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.79	0.63
2:A:6:GLN:NE2	2:A:96:CYS:SG	2.71	0.63
1:H:133:PHE:HB2	1:H:161:SER:HB3	1.81	0.63
2:G:52:ASN:CA	2:G:72:ARG:HH22	2.12	0.63
1:H:189:LEU:CD2	1:H:210:ILE:CD1	2.77	0.62
1:J:133:PHE:HB2	1:J:161:SER:HB3	1.81	0.62
2:E:52:ASN:CA	2:E:72:ARG:HH22	2.12	0.62
1:H:427:ASP:OD1	1:C:987:PRO:CG	2.48	0.62
1:J:1040:VAL:HG11	1:C:1030:SER:C	2.16	0.62
3:F:54:SER:HB3	3:F:66:GLY:O	2.00	0.62
1:C:189:LEU:CD2	1:C:210:ILE:CD1	2.77	0.62
3:I:54:SER:HB3	3:I:66:GLY:O	2.00	0.62
1:H:472:ILE:HG13	1:H:483:VAL:HA	1.81	0.62
1:H:900:MET:HE1	1:C:1077:THR:OG1	1.99	0.62
3:B:54:SER:HB3	3:B:66:GLY:O	2.00	0.62
1:C:472:ILE:HG13	1:C:483:VAL:HA	1.81	0.61
1:H:656:VAL:HG12	1:H:658:ASN:H	1.66	0.61
1:J:472:ILE:HG21	1:J:484:GLU:H	1.66	0.61
1:C:133:PHE:HB2	1:C:161:SER:HB3	1.81	0.61
1:C:472:ILE:HG21	1:C:484:GLU:H	1.66	0.61
1:H:987:PRO:CG	1:J:427:ASP:OD1	2.48	0.61
1:J:472:ILE:HG13	1:J:483:VAL:HA	1.81	0.61
1:J:656:VAL:HG12	1:J:658:ASN:H	1.66	0.61
1:H:472:ILE:HG21	1:H:484:GLU:H	1.66	0.60
1:J:570:ALA:HB1	1:C:963:VAL:CG1	2.21	0.60
1:C:656:VAL:HG12	1:C:658:ASN:H	1.66	0.60
1:H:427:ASP:OD1	1:C:987:PRO:HG3	2.02	0.60
1:J:987:PRO:CG	1:C:427:ASP:OD1	2.48	0.60
1:H:210:ILE:O	1:H:210:ILE:CG2	2.45	0.60
1:H:987:PRO:HG3	1:J:427:ASP:OD1	2.02	0.59
2:A:60:TYR:HE1	2:A:70:MET:HG2	1.67	0.59
1:H:712:ILE:HG21	1:J:896:ILE:CD1	2.30	0.59
1:C:776:LYS:NZ	1:C:780:GLU:OE2	2.26	0.59
1:H:896:ILE:CD1	1:C:712:ILE:HG21	2.31	0.59
2:A:132:PRO:HB3	2:A:158:TYR:HB3	1.85	0.59
3:F:29:VAL:O	3:F:68:LYS:NZ	2.30	0.59
1:H:883:THR:CG2	1:C:705:VAL:CG1	2.58	0.59
1:J:712:ILE:HG21	1:C:896:ILE:CD1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:51:ILE:HG23	2:G:72:ARG:CZ	2.33	0.58
2:A:51:ILE:HG23	2:A:72:ARG:CZ	2.33	0.58
2:G:132:PRO:HB3	2:G:158:TYR:HB3	1.85	0.58
1:H:327:VAL:HG13	1:H:530:SER:HA	1.86	0.58
1:C:327:VAL:HG13	1:C:530:SER:HA	1.86	0.58
2:E:60:TYR:HE1	2:E:70:MET:HG2	1.68	0.58
1:J:987:PRO:HG3	1:C:427:ASP:OD1	2.03	0.58
2:E:132:PRO:HB3	2:E:158:TYR:HB3	1.85	0.58
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.86	0.57
1:J:449:TYR:HB2	1:J:451:TYR:CE2	2.39	0.57
2:G:60:TYR:HE1	2:G:70:MET:HG2	1.67	0.57
1:H:449:TYR:HB2	1:H:451:TYR:CE2	2.39	0.57
1:J:327:VAL:HG13	1:J:530:SER:HA	1.86	0.57
1:H:789:TYR:HA	1:C:703:ASN:O	2.05	0.57
1:H:703:ASN:O	1:J:789:TYR:HA	2.04	0.57
1:J:337:PRO:HG2	1:J:356:LYS:HZ1	1.69	0.57
2:A:52:ASN:N	2:A:72:ARG:HH22	2.02	0.57
2:G:40:ALA:HB3	2:G:43:GLN:HB2	1.86	0.57
2:A:40:ALA:HB3	2:A:43:GLN:HB2	1.86	0.57
1:H:646:ARG:NH1	1:J:862:PRO:HB3	2.20	0.57
2:E:51:ILE:HG23	2:E:72:ARG:CZ	2.33	0.57
1:J:37:TYR:OH	1:J:54:LEU:O	2.20	0.56
2:E:52:ASN:N	2:E:72:ARG:HH22	2.02	0.56
1:J:273:ARG:NH1	1:J:290:ASP:OD2	2.38	0.56
1:C:449:TYR:HB2	1:C:451:TYR:CE2	2.39	0.56
1:H:273:ARG:NH1	1:H:290:ASP:OD2	2.38	0.56
1:J:280:ASN:HD21	1:J:284:THR:HB	1.70	0.56
1:J:703:ASN:O	1:C:789:TYR:HA	2.05	0.56
2:G:52:ASN:N	2:G:72:ARG:HH22	2.02	0.56
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.38	0.56
3:F:51:TYR:OH	3:F:55:LYS:HB3	2.06	0.56
1:J:189:LEU:HD23	1:J:210:ILE:HD11	1.88	0.56
3:F:155:LYS:HA	3:F:160:PRO:HA	1.88	0.56
1:J:646:ARG:NH1	1:C:862:PRO:HB3	2.20	0.56
1:H:189:LEU:HD23	1:H:210:ILE:HD11	1.88	0.56
1:H:280:ASN:HD21	1:H:284:THR:HB	1.70	0.55
1:C:280:ASN:HD21	1:C:284:THR:HB	1.70	0.55
1:H:37:TYR:OH	1:H:54:LEU:O	2.20	0.55
1:H:570:ALA:HB1	1:J:963:VAL:CG1	2.22	0.55
1:H:862:PRO:HB3	1:C:646:ARG:NH1	2.21	0.55
1:C:37:TYR:OH	1:C:54:LEU:O	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:484:GLU:OE2	2:G:33:TYR:OH	2.19	0.55
3:I:155:LYS:HA	3:I:160:PRO:HA	1.88	0.55
3:F:49:MET:HG3	3:F:50:ILE:HG12	1.89	0.55
1:H:712:ILE:CG2	1:J:897:PRO:HD2	2.37	0.55
1:J:350:VAL:HG22	1:J:402:ILE:HG22	1.89	0.55
3:B:51:TYR:OH	3:B:55:LYS:HB3	2.06	0.55
1:H:570:ALA:HB2	1:J:963:VAL:CG1	2.37	0.55
1:H:883:THR:CB	1:C:705:VAL:HG11	2.37	0.54
1:J:484:GLU:OE1	2:G:52:ASN:ND2	2.41	0.54
3:B:155:LYS:HA	3:B:160:PRO:HA	1.88	0.54
1:H:484:GLU:OE1	2:E:52:ASN:ND2	2.41	0.54
1:H:1077:THR:OG1	1:J:900:MET:CE	2.56	0.54
1:C:189:LEU:HD23	1:C:210:ILE:HD11	1.88	0.54
1:H:337:PRO:HG2	1:H:356:LYS:HZ1	1.71	0.54
1:H:705:VAL:HG11	1:J:883:THR:CB	2.36	0.54
1:J:570:ALA:HB2	1:C:963:VAL:CG1	2.36	0.54
1:C:447:GLY:CA	1:C:497:PHE:HB2	2.37	0.54
3:B:49:MET:HG3	3:B:50:ILE:HG12	1.89	0.54
1:J:726:ILE:HG23	1:J:1061:VAL:HG12	1.88	0.54
1:C:726:ILE:HG23	1:C:1061:VAL:HG12	1.88	0.54
1:H:350:VAL:HG22	1:H:402:ILE:HG22	1.89	0.54
1:H:447:GLY:CA	1:H:497:PHE:HB2	2.37	0.54
1:J:1077:THR:OG1	1:C:900:MET:CE	2.56	0.54
3:I:49:MET:HG3	3:I:50:ILE:HG12	1.89	0.54
1:H:442:ASP:HB3	1:H:451:TYR:CE2	2.43	0.54
1:J:646:ARG:HH12	1:C:862:PRO:HB3	1.73	0.54
3:I:51:TYR:OH	3:I:55:LYS:HB3	2.06	0.54
3:B:29:VAL:O	3:B:68:LYS:NZ	2.30	0.54
1:H:726:ILE:HG23	1:H:1061:VAL:HG12	1.88	0.54
1:J:712:ILE:CG2	1:C:897:PRO:HD2	2.38	0.54
1:C:393:THR:HG21	1:C:519:HIS:HB2	1.90	0.54
1:H:705:VAL:CG1	1:J:883:THR:CG2	2.58	0.54
1:J:705:VAL:HG11	1:C:883:THR:CB	2.37	0.54
1:H:722:VAL:HG22	1:H:1065:VAL:HG22	1.90	0.53
1:C:484:GLU:OE1	2:A:52:ASN:ND2	2.41	0.53
2:A:52:ASN:N	2:A:72:ARG:NH2	2.56	0.53
1:H:897:PRO:HD2	1:C:712:ILE:CG2	2.37	0.53
1:H:963:VAL:CG1	1:C:570:ALA:HB2	2.37	0.53
1:J:442:ASP:HB3	1:J:451:TYR:CE2	2.43	0.53
2:G:52:ASN:N	2:G:72:ARG:NH2	2.56	0.53
1:C:350:VAL:HG22	1:C:402:ILE:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:646:ARG:HH12	1:J:862:PRO:HB3	1.73	0.53
1:H:862:PRO:HB3	1:C:646:ARG:HH12	1.74	0.53
1:J:189:LEU:HD22	1:J:210:ILE:HD12	1.91	0.53
3:I:29:VAL:O	3:I:68:LYS:NZ	2.30	0.53
1:C:442:ASP:HB3	1:C:451:TYR:CE2	2.43	0.53
1:H:1104:VAL:HG23	1:H:1115:ILE:HG12	1.91	0.53
2:E:71:THR:C	2:E:72:ARG:HG3	2.27	0.53
1:H:900:MET:CE	1:C:1077:THR:OG1	2.56	0.53
1:H:961:THR:HG21	1:J:762:GLN:NE2	2.23	0.53
1:J:298:GLU:HG2	1:J:315:THR:HB	1.90	0.53
1:J:896:ILE:HD12	1:J:897:PRO:HD2	1.91	0.53
1:H:298:GLU:HG2	1:H:315:THR:HB	1.90	0.53
1:H:484:GLU:OE2	2:E:33:TYR:OH	2.19	0.53
1:H:762:GLN:NE2	1:C:961:THR:CG2	2.72	0.53
2:E:52:ASN:N	2:E:72:ARG:NH2	2.56	0.53
3:I:142:ILE:HG12	3:I:201:VAL:HG21	1.90	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.90	0.53
1:H:896:ILE:HD12	1:H:897:PRO:HD2	1.91	0.53
1:J:393:THR:HG21	1:J:519:HIS:HB2	1.90	0.53
1:C:189:LEU:CB	1:C:210:ILE:HD12	2.39	0.53
2:A:71:THR:C	2:A:72:ARG:HG3	2.27	0.53
1:C:189:LEU:CD2	1:C:210:ILE:HD11	2.39	0.53
1:H:762:GLN:NE2	1:C:961:THR:HG21	2.24	0.52
1:J:697:MET:HE1	1:C:865:LEU:HD23	1.90	0.52
1:J:1104:VAL:HG23	1:J:1115:ILE:HG12	1.91	0.52
1:H:697:MET:HE1	1:J:865:LEU:HD23	1.89	0.52
1:H:961:THR:CG2	1:J:762:GLN:NE2	2.72	0.52
3:F:123:LEU:HD21	3:F:199:CYS:HB3	1.91	0.52
1:J:189:LEU:CD2	1:J:210:ILE:HD11	2.39	0.52
1:J:961:THR:CG2	1:C:762:GLN:NE2	2.72	0.52
1:H:189:LEU:HD22	1:H:210:ILE:HD12	1.91	0.52
1:H:393:THR:HG21	1:H:519:HIS:HB2	1.90	0.52
1:H:1040:VAL:HG12	1:J:1031:GLU:CG	2.40	0.52
1:H:865:LEU:HD23	1:C:697:MET:HE1	1.91	0.52
3:F:142:ILE:HG12	3:F:201:VAL:HG21	1.90	0.52
1:C:298:GLU:HG2	1:C:315:THR:HB	1.90	0.52
1:C:896:ILE:HD12	1:C:897:PRO:HD2	1.91	0.52
3:B:142:ILE:HG12	3:B:201:VAL:HG21	1.90	0.52
1:H:1028:LYS:NZ	1:H:1042:PHE:O	2.43	0.52
1:J:722:VAL:HG22	1:J:1065:VAL:HG22	1.90	0.52
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:231:ILE:HG23	1:J:232:GLY:H	1.75	0.52
2:E:105:ASP:HB3	2:E:108:THR:OG1	2.10	0.52
2:A:105:ASP:HB3	2:A:108:THR:OG1	2.10	0.52
3:B:123:LEU:HD21	3:B:199:CYS:HB3	1.92	0.52
3:F:140:CYS:HB3	3:F:182:SER:HB3	1.92	0.52
1:J:189:LEU:CB	1:J:210:ILE:HD12	2.38	0.52
1:H:189:LEU:CD2	1:H:210:ILE:HD11	2.39	0.51
1:H:786:LYS:CE	1:C:1045:LYS:HE2	2.40	0.51
1:H:231:ILE:HG23	1:H:232:GLY:H	1.75	0.51
2:G:105:ASP:HB3	2:G:108:THR:OG1	2.10	0.51
3:I:123:LEU:HD21	3:I:199:CYS:HB3	1.92	0.51
3:B:140:CYS:HB3	3:B:182:SER:HB3	1.92	0.51
1:H:894:LEU:HD13	1:C:715:PRO:HD3	1.92	0.51
1:J:447:GLY:CA	1:J:497:PHE:HB2	2.37	0.51
1:J:961:THR:HG21	1:C:762:GLN:NE2	2.24	0.51
1:C:231:ILE:HG23	1:C:232:GLY:H	1.75	0.51
1:J:1028:LYS:NZ	1:J:1042:PHE:O	2.43	0.51
1:J:1040:VAL:HG12	1:C:1031:GLU:CG	2.40	0.51
2:G:71:THR:C	2:G:72:ARG:HG3	2.27	0.51
3:I:140:CYS:HB3	3:I:182:SER:HB3	1.92	0.51
1:H:201:PHE:HB3	1:H:229:LEU:HD22	1.93	0.51
1:H:715:PRO:HD3	1:J:894:LEU:HD13	1.93	0.51
2:E:106:ILE:HG23	2:E:107:LEU:HD22	1.92	0.51
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.43	0.51
1:J:715:PRO:HD3	1:C:894:LEU:HD13	1.93	0.51
1:J:201:PHE:HB3	1:J:229:LEU:HD22	1.93	0.51
1:C:201:PHE:HB3	1:C:229:LEU:HD22	1.93	0.51
1:H:1040:VAL:HG12	1:J:1031:GLU:CA	2.37	0.51
3:I:170:PRO:HG3	3:I:180:ALA:HB2	1.93	0.51
1:C:546:LEU:HD11	1:C:573:THR:HG21	1.93	0.51
1:C:733:LYS:O	1:C:861:LEU:N	2.40	0.51
1:H:1031:GLU:CG	1:C:1040:VAL:HG12	2.41	0.50
1:H:189:LEU:CB	1:H:210:ILE:HD12	2.39	0.50
1:J:1040:VAL:HG12	1:C:1031:GLU:CA	2.38	0.50
1:J:1045:LYS:HE2	1:C:786:LYS:CE	2.40	0.50
2:G:106:ILE:HG23	2:G:107:LEU:HD22	1.92	0.50
1:H:303:LEU:HD12	1:H:308:VAL:HG22	1.93	0.50
1:H:705:VAL:CG2	1:J:883:THR:HG21	2.42	0.50
1:H:1045:LYS:HE2	1:J:786:LYS:CE	2.41	0.50
2:A:51:ILE:CG2	2:A:72:ARG:HD3	2.41	0.50
1:H:498:GLN:O	1:H:501:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:81:ASN:OD1	1:J:265:TYR:OH	2.28	0.50
1:J:106:PHE:N	1:J:117:LEU:O	2.45	0.50
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.93	0.50
1:H:350:VAL:HG12	1:H:422:ASN:HB3	1.94	0.50
3:F:93:TYR:HA	3:F:101:VAL:HG12	1.93	0.50
1:J:303:LEU:HD12	1:J:308:VAL:HG22	1.93	0.50
1:J:350:VAL:HG12	1:J:422:ASN:HB3	1.94	0.50
1:C:189:LEU:HD22	1:C:210:ILE:HD12	1.91	0.50
1:H:540:ASN:OD1	1:H:549:THR:OG1	2.25	0.50
1:H:559:PHE:CE1	1:J:43:PHE:CG	3.00	0.50
1:C:350:VAL:HG12	1:C:422:ASN:HB3	1.94	0.50
1:C:901:GLN:O	1:C:905:ARG:HG3	2.12	0.50
1:H:106:PHE:N	1:H:117:LEU:O	2.45	0.49
1:C:81:ASN:OD1	1:C:265:TYR:OH	2.28	0.49
1:C:106:PHE:N	1:C:117:LEU:O	2.45	0.49
1:J:546:LEU:HD11	1:J:573:THR:HG21	1.93	0.49
3:I:93:TYR:HA	3:I:101:VAL:HG12	1.93	0.49
2:A:106:ILE:HG23	2:A:107:LEU:HD22	1.92	0.49
1:H:740:MET:SD	1:C:592:PHE:CE2	3.06	0.49
3:B:93:TYR:HA	3:B:101:VAL:HG12	1.93	0.49
1:H:472:ILE:HG21	1:H:484:GLU:N	2.28	0.49
1:H:890:ALA:HB1	1:C:1046:GLY:HA2	1.95	0.49
1:H:901:GLN:O	1:H:905:ARG:HG3	2.12	0.49
1:H:1145:LEU:HD22	1:J:1145:LEU:CD2	2.42	0.49
2:E:51:ILE:CG2	2:E:72:ARG:HD3	2.41	0.49
1:C:498:GLN:O	1:C:501:ASN:ND2	2.45	0.49
1:J:705:VAL:CG2	1:C:883:THR:HG21	2.43	0.49
1:J:646:ARG:NH1	1:C:862:PRO:CB	2.75	0.49
1:C:484:GLU:OE2	2:A:33:TYR:OH	2.19	0.49
1:H:43:PHE:CG	1:C:559:PHE:CE1	3.01	0.49
1:H:862:PRO:CB	1:C:646:ARG:NH1	2.76	0.49
2:E:51:ILE:CG2	2:E:72:ARG:CZ	2.91	0.49
3:F:170:PRO:HG3	3:F:180:ALA:HB2	1.93	0.49
3:B:170:PRO:HG3	3:B:180:ALA:HB2	1.93	0.49
1:H:592:PHE:CE2	1:J:740:MET:SD	3.05	0.49
1:J:498:GLN:O	1:J:501:ASN:ND2	2.45	0.49
1:J:592:PHE:CE2	1:C:740:MET:SD	3.05	0.49
2:A:51:ILE:CG2	2:A:72:ARG:CZ	2.91	0.49
1:H:646:ARG:NH1	1:J:862:PRO:CB	2.76	0.48
1:H:883:THR:HG21	1:C:705:VAL:CG2	2.42	0.48
1:H:1031:GLU:CA	1:C:1040:VAL:HG12	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:901:GLN:O	1:J:905:ARG:HG3	2.12	0.48
1:H:546:LEU:HD11	1:H:573:THR:HG21	1.93	0.48
1:H:433:VAL:HG22	1:H:512:VAL:HG23	1.96	0.48
1:H:786:LYS:NZ	1:C:1045:LYS:CE	2.67	0.48
1:H:1040:VAL:HG12	1:J:1031:GLU:HG2	1.95	0.48
2:E:69:THR:HB	2:E:82:GLU:HB3	1.95	0.48
1:J:559:PHE:CE1	1:C:43:PHE:CG	3.01	0.48
2:G:51:ILE:CG2	2:G:72:ARG:CZ	2.91	0.48
1:C:930:ALA:O	1:C:934:ILE:HG12	2.13	0.48
1:J:433:VAL:HG22	1:J:512:VAL:HG23	1.96	0.48
1:J:1145:LEU:HD22	1:C:1145:LEU:CD2	2.42	0.48
1:J:1040:VAL:HG12	1:C:1031:GLU:HG2	1.95	0.48
1:H:1145:LEU:CD2	1:C:1145:LEU:HD22	2.42	0.48
1:C:472:ILE:HG21	1:C:484:GLU:N	2.28	0.48
1:H:703:ASN:CB	1:J:787:GLN:OE1	2.62	0.48
1:J:659:SER:HB3	1:J:698:SER:HB2	1.96	0.48
1:C:433:VAL:HG22	1:C:512:VAL:HG23	1.96	0.48
1:C:659:SER:HB3	1:C:698:SER:HB2	1.96	0.48
2:A:53:PRO:CA	2:A:72:ARG:NH2	2.77	0.48
1:H:225:PRO:HG2	1:C:562:PHE:CD2	2.49	0.47
1:J:456:PHE:HZ	2:G:104:TYR:H	1.62	0.47
1:J:562:PHE:CD2	1:C:225:PRO:HG2	2.49	0.47
1:J:703:ASN:CB	1:C:787:GLN:OE1	2.62	0.47
1:C:189:LEU:CD2	1:C:210:ILE:HD12	2.45	0.47
2:E:51:ILE:HG13	2:E:72:ARG:NE	2.04	0.47
1:J:1046:GLY:HA2	1:C:890:ALA:HB1	1.96	0.47
1:J:826:VAL:HG11	1:J:1057:PRO:HG2	1.97	0.47
2:G:69:THR:HB	2:G:82:GLU:HB3	1.95	0.47
1:H:1077:THR:OG1	1:J:900:MET:HE1	2.14	0.47
1:J:128:ILE:HB	1:J:170:TYR:HB3	1.96	0.47
1:J:930:ALA:O	1:J:934:ILE:HG12	2.14	0.47
2:G:53:PRO:CA	2:G:72:ARG:NH2	2.77	0.47
1:H:733:LYS:O	1:H:861:LEU:N	2.40	0.47
1:H:1031:GLU:CA	1:C:1040:VAL:CG1	2.85	0.47
1:C:109:THR:HB	1:C:113:LYS:HB3	1.96	0.47
1:C:456:PHE:HZ	2:A:104:TYR:H	1.62	0.47
2:A:38:ARG:HG3	2:A:46:GLU:HB3	1.97	0.47
2:A:69:THR:HB	2:A:82:GLU:HB3	1.95	0.47
1:H:371:SER:OG	2:A:106:ILE:HG22	2.15	0.47
1:J:905:ARG:HD3	1:J:1049:LEU:O	2.15	0.47
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:562:PHE:CD2	1:J:225:PRO:HG2	2.49	0.47
1:H:930:ALA:O	1:H:934:ILE:HG12	2.13	0.47
1:H:1030:SER:C	1:C:1040:VAL:CG1	2.80	0.47
1:H:1046:GLY:HA2	1:J:890:ALA:HB1	1.95	0.47
2:E:53:PRO:CA	2:E:72:ARG:NH2	2.77	0.47
1:J:34:ARG:NH2	1:J:191:GLU:OE2	2.48	0.47
2:G:36:TRP:CZ3	2:G:96:CYS:HB3	2.50	0.47
1:C:826:VAL:HG11	1:C:1057:PRO:HG2	1.97	0.47
2:A:36:TRP:CZ3	2:A:96:CYS:HB3	2.50	0.47
1:H:905:ARG:HD3	1:H:1049:LEU:O	2.15	0.47
2:G:51:ILE:CG2	2:G:72:ARG:HD3	2.41	0.47
1:H:614:ASP:HB3	1:J:854:LYS:HZ1	1.80	0.47
1:H:659:SER:HB3	1:H:698:SER:HB2	1.96	0.47
1:H:1031:GLU:HG2	1:C:1040:VAL:HG12	1.96	0.47
2:E:106:ILE:HG22	1:J:371:SER:OG	2.15	0.47
1:J:189:LEU:CD2	1:J:210:ILE:HD12	2.44	0.47
1:H:280:ASN:ND2	1:H:284:THR:O	2.48	0.47
2:G:105:ASP:OD2	1:C:373:SER:OG	2.33	0.47
1:C:34:ARG:NH2	1:C:191:GLU:OE2	2.48	0.47
3:B:25:THR:OG1	3:B:28:ASP:OD2	2.31	0.47
1:J:614:ASP:HB3	1:C:854:LYS:HZ1	1.80	0.46
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.97	0.46
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.15	0.46
1:H:726:ILE:HD13	1:H:945:LEU:HD23	1.97	0.46
2:E:107:LEU:HD23	1:J:373:SER:HB2	1.97	0.46
1:J:540:ASN:OD1	1:J:549:THR:OG1	2.25	0.46
1:H:712:ILE:HG22	1:J:896:ILE:HA	1.97	0.46
1:H:963:VAL:HG11	1:C:570:ALA:CB	2.45	0.46
1:J:1077:THR:CB	1:C:900:MET:HE1	2.44	0.46
2:G:38:ARG:HG3	2:G:46:GLU:HB3	1.97	0.46
1:H:189:LEU:CD2	1:H:210:ILE:HD12	2.45	0.46
2:G:213:HIS:CD2	2:G:215:PRO:HD2	2.51	0.46
1:H:34:ARG:NH2	1:H:191:GLU:OE2	2.48	0.46
1:H:373:SER:HB2	2:A:107:LEU:HD23	1.96	0.46
1:H:787:GLN:OE1	1:C:703:ASN:CB	2.63	0.46
1:H:826:VAL:HG11	1:H:1057:PRO:HG2	1.97	0.46
1:J:109:THR:HB	1:J:113:LYS:HB3	1.96	0.46
1:C:360:ASN:H	1:C:523:THR:HB	1.81	0.46
2:A:213:HIS:CD2	2:A:215:PRO:HD2	2.51	0.46
1:J:452:LEU:HG	1:J:494:SER:HA	1.98	0.46
1:J:646:ARG:HH12	1:C:862:PRO:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:712:ILE:HG22	1:C:896:ILE:HA	1.97	0.46
1:C:280:ASN:ND2	1:C:284:THR:O	2.48	0.46
1:J:726:ILE:HD13	1:J:945:LEU:HD23	1.98	0.46
2:G:64:PHE:HB3	2:G:68:VAL:HG21	1.98	0.46
2:G:107:LEU:HD23	1:C:373:SER:HB2	1.96	0.46
2:A:164:THR:HB	2:A:212:ASN:HB3	1.98	0.46
1:H:128:ILE:HB	1:H:170:TYR:HB3	1.97	0.46
1:H:456:PHE:HZ	2:E:104:TYR:H	1.62	0.46
2:E:38:ARG:HG3	2:E:46:GLU:HB3	1.97	0.46
3:F:14:PRO:HD3	3:F:112:LEU:HB2	1.98	0.46
3:I:25:THR:OG1	3:I:28:ASP:OD2	2.31	0.46
2:E:152:GLY:HA2	2:E:194:VAL:HA	1.98	0.46
3:F:35:VAL:HG12	3:F:92:SER:HB2	1.98	0.46
1:J:472:ILE:HG21	1:J:484:GLU:N	2.28	0.46
2:G:106:ILE:HG22	1:C:371:SER:OG	2.15	0.46
2:G:164:THR:HB	2:G:212:ASN:HB3	1.98	0.46
3:I:35:VAL:HG12	3:I:92:SER:HB2	1.98	0.46
1:C:980:ILE:HD13	1:C:992:GLN:HB3	1.98	0.46
1:H:109:THR:HB	1:H:113:LYS:HB3	1.96	0.46
1:H:360:ASN:H	1:H:523:THR:HB	1.81	0.46
1:H:703:ASN:HB2	1:J:787:GLN:OE1	2.16	0.46
2:E:36:TRP:CZ3	2:E:96:CYS:HB3	2.50	0.46
1:C:56:LEU:HD12	1:C:57:PRO:HD2	1.98	0.46
2:A:30:THR:HA	2:A:53:PRO:HG2	1.98	0.46
2:A:152:GLY:HA2	2:A:194:VAL:HA	1.98	0.46
3:B:85:GLU:HB3	3:B:111:VAL:HG12	1.98	0.46
2:E:182:VAL:HG11	3:F:166:GLU:HB3	1.98	0.45
2:A:64:PHE:HB3	2:A:68:VAL:HG21	1.98	0.45
3:B:14:PRO:HD3	3:B:112:LEU:HB2	1.98	0.45
1:H:452:LEU:HG	1:H:494:SER:HA	1.98	0.45
1:H:1045:LYS:O	1:H:1066:THR:HG21	2.16	0.45
1:H:1051:SER:OG	1:H:1064:HIS:ND1	2.29	0.45
1:J:346:ARG:NH2	1:J:449:TYR:HB3	2.31	0.45
1:J:360:ASN:H	1:J:523:THR:HB	1.81	0.45
1:J:980:ILE:HD13	1:J:992:GLN:HB3	1.98	0.45
2:G:182:VAL:HG11	3:I:166:GLU:HB3	1.98	0.45
1:C:1045:LYS:O	1:C:1066:THR:HG21	2.16	0.45
1:H:1094:VAL:HB	1:J:904:TYR:OH	2.17	0.45
2:E:30:THR:HA	2:E:53:PRO:HG2	1.98	0.45
2:E:213:HIS:CD2	2:E:215:PRO:HD2	2.51	0.45
1:J:280:ASN:ND2	1:J:284:THR:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:THR:HA	2:G:53:PRO:HG2	1.98	0.45
3:I:85:GLU:HB3	3:I:111:VAL:HG12	1.98	0.45
1:H:346:ARG:NH2	1:H:449:TYR:HB3	2.31	0.45
1:H:980:ILE:HD13	1:H:992:GLN:HB3	1.98	0.45
1:H:1040:VAL:CG1	1:J:1030:SER:C	2.81	0.45
1:J:56:LEU:HD12	1:J:57:PRO:HD2	1.98	0.45
1:J:476:GLY:HA3	1:J:487:ASN:HB3	1.98	0.45
1:H:336:CYS:HB3	1:H:361:CYS:HB3	1.74	0.45
1:J:570:ALA:HB2	1:C:963:VAL:HG11	1.99	0.45
1:H:646:ARG:HH12	1:J:862:PRO:CB	2.29	0.45
1:C:113:LYS:HD3	1:C:114:THR:N	2.32	0.45
2:E:105:ASP:OD2	1:J:373:SER:OG	2.34	0.45
1:J:759:PHE:O	1:J:763:LEU:HG	2.16	0.45
1:C:141:LEU:O	1:C:158:ARG:N	2.50	0.45
1:C:476:GLY:HA3	1:C:487:ASN:HB3	1.98	0.45
1:H:141:LEU:O	1:H:158:ARG:N	2.50	0.45
1:H:697:MET:CE	1:J:865:LEU:CD2	2.93	0.45
1:H:787:GLN:OE1	1:C:703:ASN:HB2	2.17	0.45
1:H:862:PRO:CB	1:C:646:ARG:HH12	2.29	0.45
1:H:865:LEU:CD2	1:C:697:MET:CE	2.94	0.45
1:J:1141:LEU:HD23	1:C:1144:GLU:HG2	1.91	0.45
1:H:759:PHE:O	1:H:763:LEU:HG	2.16	0.45
2:E:64:PHE:HB3	2:E:68:VAL:HG21	1.98	0.45
1:J:308:VAL:H	1:J:602:THR:HG1	1.59	0.45
3:F:85:GLU:HB3	3:F:111:VAL:HG12	1.98	0.45
1:J:675:GLN:HG3	1:J:693:ILE:HD11	1.99	0.45
1:J:1045:LYS:O	1:J:1066:THR:HG21	2.16	0.45
3:B:161:VAL:HG22	3:B:163:ALA:H	1.83	0.45
1:H:373:SER:OG	2:A:105:ASP:OD2	2.34	0.44
1:J:141:LEU:O	1:J:158:ARG:N	2.50	0.44
3:I:161:VAL:HG22	3:I:163:ALA:H	1.83	0.44
1:H:113:LYS:HD3	1:H:114:THR:N	2.32	0.44
1:H:900:MET:HE1	1:C:1077:THR:CB	2.47	0.44
1:J:244:LEU:HD13	1:J:258:TRP:HD1	1.83	0.44
1:J:703:ASN:HB2	1:C:787:GLN:OE1	2.16	0.44
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.74	0.44
1:C:675:GLN:HG3	1:C:693:ILE:HD11	1.99	0.44
2:A:182:VAL:HG11	3:B:166:GLU:HB3	1.98	0.44
3:B:35:VAL:HG12	3:B:92:SER:HB2	1.98	0.44
1:H:109:THR:HG21	1:H:114:THR:OG1	2.18	0.44
1:H:476:GLY:HA3	1:H:487:ASN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:896:ILE:HA	1:C:712:ILE:HG22	1.97	0.44
1:J:113:LYS:HD3	1:J:114:THR:N	2.32	0.44
1:J:474:GLN:NE2	1:J:476:GLY:O	2.51	0.44
3:I:14:PRO:HD3	3:I:112:LEU:HB2	1.98	0.44
1:C:346:ARG:NH2	1:C:449:TYR:HB3	2.31	0.44
1:C:759:PHE:O	1:C:763:LEU:HG	2.16	0.44
1:H:56:LEU:HD12	1:H:57:PRO:HD2	1.98	0.44
1:H:904:TYR:OH	1:C:1094:VAL:HB	2.17	0.44
1:H:1081:ILE:HG23	1:H:1135:ASN:HB3	2.00	0.44
1:C:452:LEU:HG	1:C:494:SER:HA	1.98	0.44
1:J:37:TYR:HB3	1:J:223:LEU:HB2	2.00	0.44
2:G:152:GLY:HA2	2:G:194:VAL:HA	1.98	0.44
1:C:540:ASN:OD1	1:C:549:THR:OG1	2.25	0.44
2:A:88:SER:HA	2:A:124:VAL:HG13	2.00	0.44
1:H:37:TYR:HB3	1:H:223:LEU:HB2	2.00	0.44
1:H:247:SER:HB2	1:H:258:TRP:HE1	1.83	0.44
1:H:896:ILE:CD1	1:C:712:ILE:CG2	2.86	0.44
2:E:164:THR:HB	2:E:212:ASN:HB3	1.98	0.44
1:J:109:THR:HG21	1:J:114:THR:OG1	2.18	0.44
1:J:419:ALA:O	1:J:424:LYS:HD3	2.18	0.44
1:J:1081:ILE:HG23	1:J:1135:ASN:HB3	1.99	0.44
1:J:1094:VAL:HB	1:C:904:TYR:OH	2.17	0.44
1:H:194:PHE:HD1	1:H:203:ILE:HG12	1.82	0.44
1:H:675:GLN:HG3	1:H:693:ILE:HD11	1.99	0.44
2:E:47:TRP:CZ3	3:F:100:HIS:HB2	2.53	0.44
1:J:570:ALA:CB	1:C:963:VAL:HG11	2.45	0.44
2:G:88:SER:HA	2:G:124:VAL:HG13	2.00	0.44
1:C:37:TYR:HB3	1:C:223:LEU:HB2	2.00	0.44
1:H:81:ASN:OD1	1:H:265:TYR:OH	2.28	0.44
1:H:570:ALA:CB	1:J:963:VAL:HG11	2.45	0.44
1:H:762:GLN:HE21	1:C:961:THR:CG2	2.30	0.44
1:H:1141:LEU:HD23	1:J:1144:GLU:HG2	1.91	0.44
2:A:169:SER:N	2:A:210:ASN:OD1	2.45	0.44
1:H:474:GLN:NE2	1:H:476:GLY:O	2.51	0.44
1:H:854:LYS:HZ1	1:C:614:ASP:HB3	1.80	0.44
2:E:111:SER:HA	3:F:51:TYR:HB2	2.00	0.44
1:J:194:PHE:HD1	1:J:203:ILE:HG12	1.82	0.44
1:C:244:LEU:HD13	1:C:258:TRP:HD1	1.83	0.44
1:C:247:SER:HB2	1:C:258:TRP:HE1	1.83	0.44
1:C:462:LYS:HA	1:C:462:LYS:HD3	1.83	0.44
2:A:47:TRP:CZ3	3:B:100:HIS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:TYR:HB2	2:E:213:HIS:CE1	2.53	0.43
3:F:161:VAL:HG22	3:F:163:ALA:H	1.83	0.43
1:C:109:THR:HG21	1:C:114:THR:OG1	2.18	0.43
1:C:194:PHE:HD1	1:C:203:ILE:HG12	1.82	0.43
2:A:196:THR:HG22	2:A:198:PRO:HD3	2.00	0.43
1:J:697:MET:CE	1:C:865:LEU:CD2	2.94	0.43
2:G:47:TRP:CZ3	3:I:100:HIS:HB2	2.53	0.43
1:H:40:ASP:N	1:H:40:ASP:OD1	2.51	0.43
1:H:570:ALA:HB2	1:J:963:VAL:HG11	2.00	0.43
1:J:733:LYS:O	1:J:861:LEU:N	2.40	0.43
1:J:1040:VAL:CG1	1:C:1030:SER:C	2.81	0.43
1:H:497:PHE:CG	1:H:507:PRO:HG3	2.54	0.43
1:H:805:ILE:HG22	1:H:818:ILE:HD12	2.01	0.43
1:J:247:SER:HB2	1:J:258:TRP:HE1	1.83	0.43
1:J:733:LYS:HE3	1:J:771:ALA:HB1	2.01	0.43
1:C:419:ALA:O	1:C:424:LYS:HD3	2.18	0.43
1:H:419:ALA:O	1:H:424:LYS:HD3	2.18	0.43
1:H:697:MET:HE1	1:J:865:LEU:CD2	2.49	0.43
1:J:440:ASN:O	1:J:444:LYS:HD3	2.19	0.43
1:J:961:THR:CG2	1:C:762:GLN:HE21	2.31	0.43
1:C:253:ASP:OD1	1:C:253:ASP:N	2.51	0.43
1:C:474:GLN:NE2	1:C:476:GLY:O	2.51	0.43
1:C:1139:ASP:OD1	1:C:1139:ASP:N	2.48	0.43
2:A:158:TYR:HB2	2:A:213:HIS:CE1	2.53	0.43
1:H:440:ASN:O	1:H:444:LYS:HD3	2.19	0.43
1:H:963:VAL:HG11	1:C:570:ALA:HB2	2.00	0.43
2:G:158:TYR:HB2	2:G:213:HIS:CE1	2.53	0.43
1:C:1081:ILE:HG23	1:C:1135:ASN:HB3	2.00	0.43
1:H:447:GLY:HA3	1:H:497:PHE:CB	2.45	0.43
3:F:25:THR:OG1	3:F:28:ASP:OD2	2.32	0.43
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.54	0.43
1:H:733:LYS:HE3	1:H:771:ALA:HB1	2.01	0.43
1:J:447:GLY:HA3	1:J:497:PHE:CB	2.45	0.43
1:H:34:ARG:NH2	1:H:221:SER:OG	2.49	0.43
1:H:722:VAL:O	1:H:934:ILE:HD11	2.19	0.43
1:C:114:THR:HG22	1:C:115:GLN:N	2.34	0.43
1:C:497:PHE:CD2	1:C:507:PRO:HG3	2.54	0.43
1:C:825:LYS:HD2	1:C:942:ALA:HA	2.01	0.43
1:H:244:LEU:HD13	1:H:258:TRP:HD1	1.83	0.42
1:H:961:THR:CG2	1:J:762:GLN:HE21	2.30	0.42
2:E:88:SER:HA	2:E:124:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:497:PHE:CD2	1:J:507:PRO:HG3	2.54	0.42
1:J:805:ILE:HG22	1:J:818:ILE:HD12	2.01	0.42
2:G:111:SER:HA	3:I:51:TYR:HB2	2.00	0.42
1:H:497:PHE:CD2	1:H:507:PRO:HG3	2.54	0.42
1:J:722:VAL:O	1:J:934:ILE:HD11	2.19	0.42
1:C:865:LEU:HD23	1:C:865:LEU:HA	1.91	0.42
1:J:253:ASP:OD1	1:J:253:ASP:N	2.51	0.42
1:J:825:LYS:HD2	1:J:942:ALA:HA	2.01	0.42
1:C:440:ASN:O	1:C:444:LYS:HD3	2.19	0.42
2:A:111:SER:HA	3:B:51:TYR:HB2	2.00	0.42
1:H:53:ASP:HB3	1:H:55:PHE:CE2	2.54	0.42
1:J:350:VAL:HG11	1:J:418:ILE:HD12	2.02	0.42
2:G:196:THR:HG22	2:G:198:PRO:HD3	2.00	0.42
1:C:40:ASP:N	1:C:40:ASP:OD1	2.51	0.42
1:C:733:LYS:HE3	1:C:771:ALA:HB1	2.01	0.42
2:A:71:THR:OG1	2:A:80:TYR:HB2	2.20	0.42
2:E:196:THR:HG22	2:E:198:PRO:HD3	2.00	0.42
1:J:497:PHE:CG	1:J:507:PRO:HG3	2.54	0.42
1:J:697:MET:HE1	1:C:865:LEU:CD2	2.49	0.42
1:J:815:ARG:HG2	1:J:820:ASP:OD1	2.19	0.42
2:G:71:THR:OG1	2:G:80:TYR:HB2	2.20	0.42
2:G:168:ASN:HD22	2:G:172:LEU:HB2	1.85	0.42
1:C:805:ILE:HG22	1:C:818:ILE:HD12	2.01	0.42
2:E:169:SER:N	2:E:210:ASN:OD1	2.45	0.42
1:H:253:ASP:N	1:H:253:ASP:OD1	2.51	0.42
1:H:431:GLY:HA2	1:H:515:PHE:CD2	2.55	0.42
2:E:168:ASN:HD22	2:E:172:LEU:HB2	1.85	0.42
1:J:40:ASP:N	1:J:40:ASP:OD1	2.51	0.42
1:J:53:ASP:HB3	1:J:55:PHE:CE2	2.54	0.42
1:J:130:VAL:O	1:J:130:VAL:HG13	2.19	0.42
1:C:34:ARG:NH2	1:C:221:SER:OG	2.49	0.42
1:H:130:VAL:O	1:H:130:VAL:HG13	2.19	0.42
1:H:903:ALA:HB1	1:H:913:GLN:HB2	2.02	0.42
1:H:1139:ASP:OD1	1:H:1139:ASP:N	2.48	0.42
2:E:71:THR:OG1	2:E:80:TYR:HB2	2.20	0.42
1:C:722:VAL:O	1:C:934:ILE:HD11	2.19	0.42
1:J:114:THR:HG22	1:J:115:GLN:N	2.34	0.42
1:J:518:LEU:HD23	1:J:518:LEU:HA	1.87	0.42
3:I:51:TYR:CD2	3:I:52:GLU:HG2	2.55	0.42
1:C:815:ARG:HG2	1:C:820:ASP:OD1	2.19	0.42
1:H:32:PHE:CE1	1:H:218:GLN:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:815:ARG:HG2	1:H:820:ASP:OD1	2.19	0.41
1:H:1045:LYS:CE	1:J:786:LYS:NZ	2.68	0.41
1:H:1054:GLN:HB2	1:H:1061:VAL:CG2	2.50	0.41
2:E:160:PRO:HD2	2:E:213:HIS:HE1	1.85	0.41
3:F:123:LEU:HD23	3:F:210:LYS:HB2	2.02	0.41
1:J:1045:LYS:CE	1:C:786:LYS:NZ	2.67	0.41
1:C:32:PHE:CE1	1:C:218:GLN:HG3	2.55	0.41
1:C:350:VAL:HG11	1:C:418:ILE:HD12	2.02	0.41
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.55	0.41
1:H:114:THR:HG22	1:H:115:GLN:N	2.34	0.41
1:H:1142:GLN:HB2	1:H:1143:PRO:HD3	2.02	0.41
2:E:47:TRP:HZ2	2:E:50:TRP:CD1	2.38	0.41
1:J:442:ASP:HB3	1:J:451:TYR:HE2	1.84	0.41
1:J:903:ALA:HB1	1:J:913:GLN:HB2	2.02	0.41
3:I:123:LEU:HD23	3:I:210:LYS:HB2	2.02	0.41
1:C:1142:GLN:HB2	1:C:1143:PRO:HD3	2.02	0.41
1:H:106:PHE:O	1:H:117:LEU:HB3	2.21	0.41
1:H:796:ASP:N	1:H:796:ASP:OD1	2.52	0.41
1:H:825:LYS:HD2	1:H:942:ALA:HA	2.01	0.41
1:H:1077:THR:CB	1:J:900:MET:HE3	2.50	0.41
3:F:51:TYR:CD2	3:F:52:GLU:HG2	2.55	0.41
1:J:32:PHE:CE1	1:J:218:GLN:HG3	2.55	0.41
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.54	0.41
1:C:130:VAL:O	1:C:130:VAL:HG13	2.19	0.41
3:B:123:LEU:HD23	3:B:210:LYS:HB2	2.02	0.41
1:J:1107:ARG:HD3	1:C:904:TYR:CE2	2.40	0.41
2:G:47:TRP:HZ2	2:G:50:TRP:CD1	2.38	0.41
2:A:47:TRP:HZ2	2:A:50:TRP:CD1	2.38	0.41
2:A:160:PRO:HD2	2:A:213:HIS:HE1	1.85	0.41
1:J:865:LEU:HD23	1:J:865:LEU:HA	1.91	0.41
3:B:196:SER:HA	3:B:213:ALA:HA	2.03	0.41
1:H:900:MET:CE	1:C:1077:THR:CB	2.98	0.41
1:J:796:ASP:OD1	1:J:796:ASP:N	2.52	0.41
1:J:1051:SER:OG	1:J:1064:HIS:ND1	2.30	0.41
1:C:1054:GLN:HB2	1:C:1061:VAL:CG2	2.50	0.41
1:H:720:ILE:HD13	1:H:923:ILE:HG23	2.02	0.41
3:F:56:ARG:HD3	3:F:60:VAL:CG1	2.49	0.41
2:G:47:TRP:CZ2	2:G:49:GLY:HA2	2.56	0.41
1:H:442:ASP:HB3	1:H:451:TYR:HE2	1.84	0.41
1:J:108:THR:HG23	1:J:109:THR:HG23	2.03	0.41
1:J:287:ASP:HB3	1:J:306:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:431:GLY:HA2	1:J:515:PHE:CD2	2.55	0.41
1:C:108:THR:HG23	1:C:109:THR:HG23	2.03	0.41
1:C:796:ASP:OD1	1:C:796:ASP:N	2.52	0.41
1:C:903:ALA:HB1	1:C:913:GLN:HB2	2.02	0.41
2:A:168:ASN:HD22	2:A:172:LEU:HB2	1.85	0.41
3:B:51:TYR:CD2	3:B:52:GLU:HG2	2.55	0.41
2:G:160:PRO:HD2	2:G:213:HIS:HE1	1.85	0.41
1:C:106:PHE:O	1:C:117:LEU:HB3	2.21	0.41
1:C:720:ILE:HD13	1:C:923:ILE:HG23	2.02	0.41
2:A:23:LYS:HB2	2:A:78:THR:HG22	2.04	0.40
1:H:108:THR:HG23	1:H:109:THR:HG23	2.03	0.40
2:G:169:SER:N	2:G:210:ASN:OD1	2.45	0.40
2:A:24:ALA:HB1	2:A:27:TYR:HE1	1.86	0.40
1:H:350:VAL:HG11	1:H:418:ILE:HD12	2.02	0.40
1:H:862:PRO:HG3	1:C:647:ALA:HB2	2.03	0.40
1:J:106:PHE:O	1:J:117:LEU:HB3	2.21	0.40
1:J:109:THR:HB	1:J:113:LYS:HD2	2.03	0.40
1:J:1054:GLN:HB2	1:J:1061:VAL:CG2	2.51	0.40
1:H:287:ASP:HB3	1:H:306:PHE:HE2	1.86	0.40
1:H:537:LYS:N	1:H:551:VAL:HG23	2.37	0.40
1:H:647:ALA:HB2	1:J:862:PRO:HG3	2.03	0.40
2:E:24:ALA:HB1	2:E:27:TYR:HE1	1.86	0.40
2:E:133:SER:O	2:E:156:LYS:N	2.49	0.40
3:F:50:ILE:CG2	3:F:52:GLU:O	2.57	0.40
3:F:196:SER:HA	3:F:213:ALA:HA	2.03	0.40
1:J:1054:GLN:HB2	1:J:1061:VAL:HG22	2.04	0.40
1:J:1142:GLN:HB2	1:J:1143:PRO:HD3	2.02	0.40
2:G:51:ILE:CG1	2:G:72:ARG:HE	2.22	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	C	978/1237 (79%)	930 (95%)	48 (5%)	0	100	100
1	H	978/1237 (79%)	930 (95%)	48 (5%)	0	100	100
1	J	978/1237 (79%)	930 (95%)	48 (5%)	0	100	100
2	A	210/238 (88%)	201 (96%)	9 (4%)	0	100	100
2	E	210/238 (88%)	201 (96%)	9 (4%)	0	100	100
2	G	210/238 (88%)	201 (96%)	9 (4%)	0	100	100
3	B	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	F	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	I	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
All	All	4200/5067 (83%)	3996 (95%)	204 (5%)	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	C	874/1076 (81%)	872 (100%)	2 (0%)	93	97
1	H	874/1076 (81%)	872 (100%)	2 (0%)	93	97
1	J	874/1076 (81%)	872 (100%)	2 (0%)	93	97
2	A	181/201 (90%)	181 (100%)	0	100	100
2	E	181/201 (90%)	181 (100%)	0	100	100
2	G	181/201 (90%)	181 (100%)	0	100	100
3	B	179/179 (100%)	179 (100%)	0	100	100
3	F	179/179 (100%)	179 (100%)	0	100	100
3	I	179/179 (100%)	179 (100%)	0	100	100
All	All	3702/4368 (85%)	3696 (100%)	6 (0%)	93	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	373	SER
1	H	483	VAL
1	J	373	SER
1	J	483	VAL
1	C	373	SER
1	C	483	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	394	ASN
1	H	501	ASN
1	H	762	GLN
1	H	1002	GLN
2	E	6	GLN
1	J	394	ASN
1	J	501	ASN
1	J	762	GLN
1	J	1002	GLN
1	J	1005	GLN
2	G	6	GLN
1	C	394	ASN
1	C	501	ASN
1	C	762	GLN
1	C	1005	GLN
2	A	6	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	H	1305	1	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	C	1303	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	H	1302	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	J	1301	1	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	H	1308	1	14,14,15	0.19	0	17,19,21	0.41	0
4	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	J	1303	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	H	1310	1	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	J	1308	1	14,14,15	0.19	0	17,19,21	0.41	0
4	NAG	H	1304	1	14,14,15	0.35	0	17,19,21	0.39	0
4	NAG	J	1311	1	14,14,15	0.41	0	17,19,21	0.36	0
4	NAG	J	1309	1	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	H	1307	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	H	1306	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	J	1302	1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	C	1309	1	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	C	1306	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	H	1301	1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	C	1304	1	14,14,15	0.35	0	17,19,21	0.39	0
4	NAG	J	1310	1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	C	1310	1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	J	1304	1	14,14,15	0.35	0	17,19,21	0.39	0
4	NAG	J	1305	1	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	C	1308	1	14,14,15	0.19	0	17,19,21	0.41	0
4	NAG	C	1302	1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	H	1311	1	14,14,15	0.41	0	17,19,21	0.36	0
4	NAG	C	1311	1	14,14,15	0.40	0	17,19,21	0.36	0
4	NAG	J	1306	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	H	1309	1	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	H	1303	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	J	1307	1	14,14,15	0.21	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1307	1	14,14,15	0.20	0	17,19,21	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	H	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	J	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	H	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	J	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	H	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	H	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	J	1311	1	-	4/6/23/26	0/1/1/1
4	NAG	J	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	H	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	H	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	H	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	J	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	J	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	H	1311	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	4/6/23/26	0/1/1/1
4	NAG	J	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	H	1309	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	J	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1307	NAG	O5-C5-C6-O6
4	J	1307	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	H	1310	NAG	O5-C5-C6-O6
4	J	1310	NAG	O5-C5-C6-O6
4	C	1310	NAG	O5-C5-C6-O6
4	H	1303	NAG	O5-C5-C6-O6
4	H	1306	NAG	O5-C5-C6-O6
4	J	1303	NAG	O5-C5-C6-O6
4	J	1306	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	H	1305	NAG	O5-C5-C6-O6
4	J	1305	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	H	1306	NAG	C4-C5-C6-O6
4	H	1307	NAG	C4-C5-C6-O6
4	J	1306	NAG	C4-C5-C6-O6
4	J	1307	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	H	1304	NAG	C4-C5-C6-O6
4	J	1304	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	H	1310	NAG	C4-C5-C6-O6
4	J	1310	NAG	C4-C5-C6-O6
4	C	1310	NAG	C4-C5-C6-O6
4	H	1302	NAG	C8-C7-N2-C2
4	H	1302	NAG	O7-C7-N2-C2
4	H	1304	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	H	1304	NAG	O7-C7-N2-C2
4	H	1311	NAG	C8-C7-N2-C2
4	H	1311	NAG	O7-C7-N2-C2
4	J	1302	NAG	C8-C7-N2-C2
4	J	1302	NAG	O7-C7-N2-C2
4	J	1304	NAG	C8-C7-N2-C2
4	J	1304	NAG	O7-C7-N2-C2
4	J	1311	NAG	C8-C7-N2-C2
4	J	1311	NAG	O7-C7-N2-C2
4	C	1302	NAG	C8-C7-N2-C2
4	C	1302	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1311	NAG	C8-C7-N2-C2
4	C	1311	NAG	O7-C7-N2-C2
4	H	1304	NAG	O5-C5-C6-O6
4	J	1304	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	H	1303	NAG	C4-C5-C6-O6
4	J	1303	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	H	1302	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	J	1302	NAG	O5-C5-C6-O6
4	H	1311	NAG	O5-C5-C6-O6
4	J	1311	NAG	O5-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	H	1305	NAG	C4-C5-C6-O6
4	J	1305	NAG	C4-C5-C6-O6
4	J	1301	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	H	1301	NAG	O5-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	H	1311	NAG	C4-C5-C6-O6
4	J	1311	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

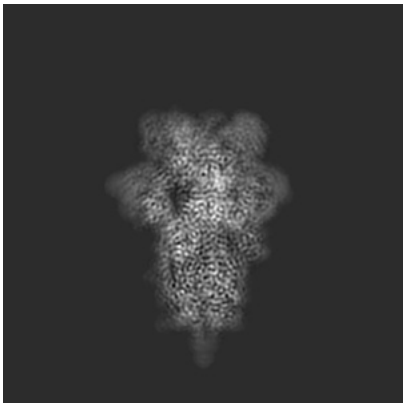
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32421. These allow visual inspection of the internal detail of the map and identification of artifacts.

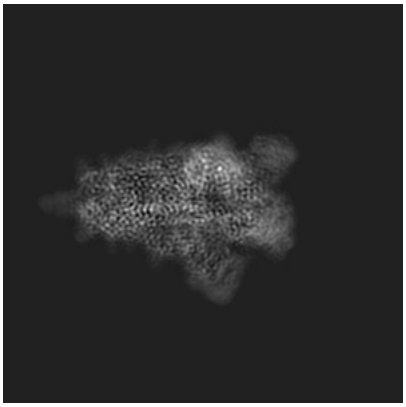
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

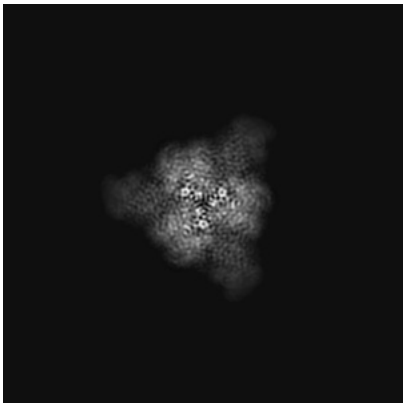
6.1.1 Primary map



X



Y

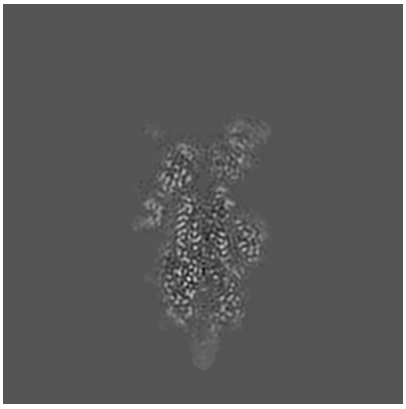


Z

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

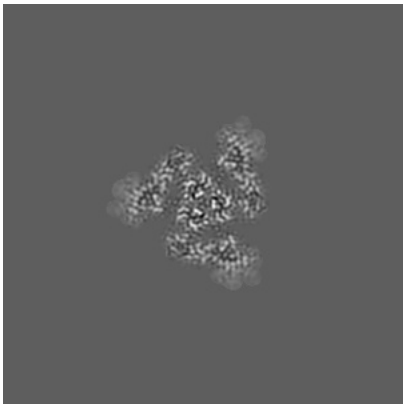
6.2 Central slices

6.2.1 Primary map



X Index: 160

Y Index: 160

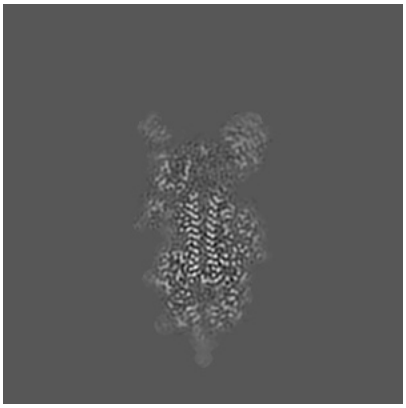


Z Index: 160

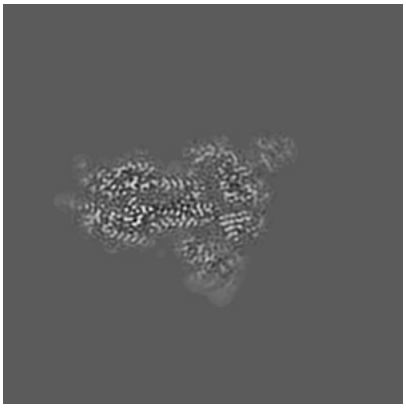
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

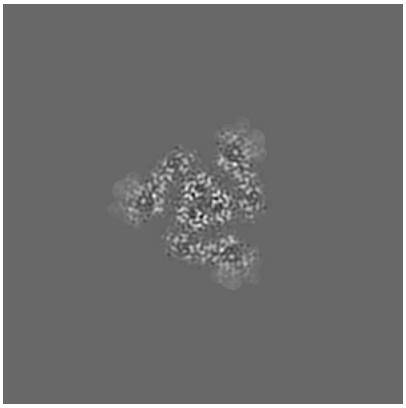
6.3.1 Primary map



X Index: 155



Y Index: 170

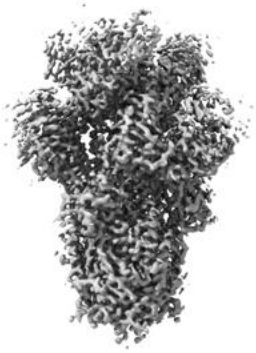


Z Index: 159

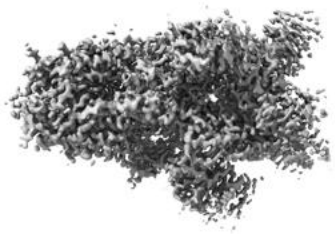
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

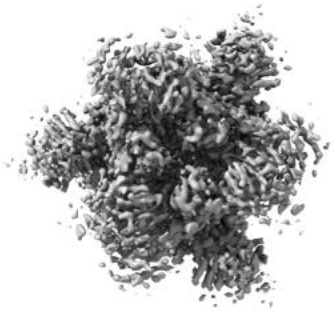
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

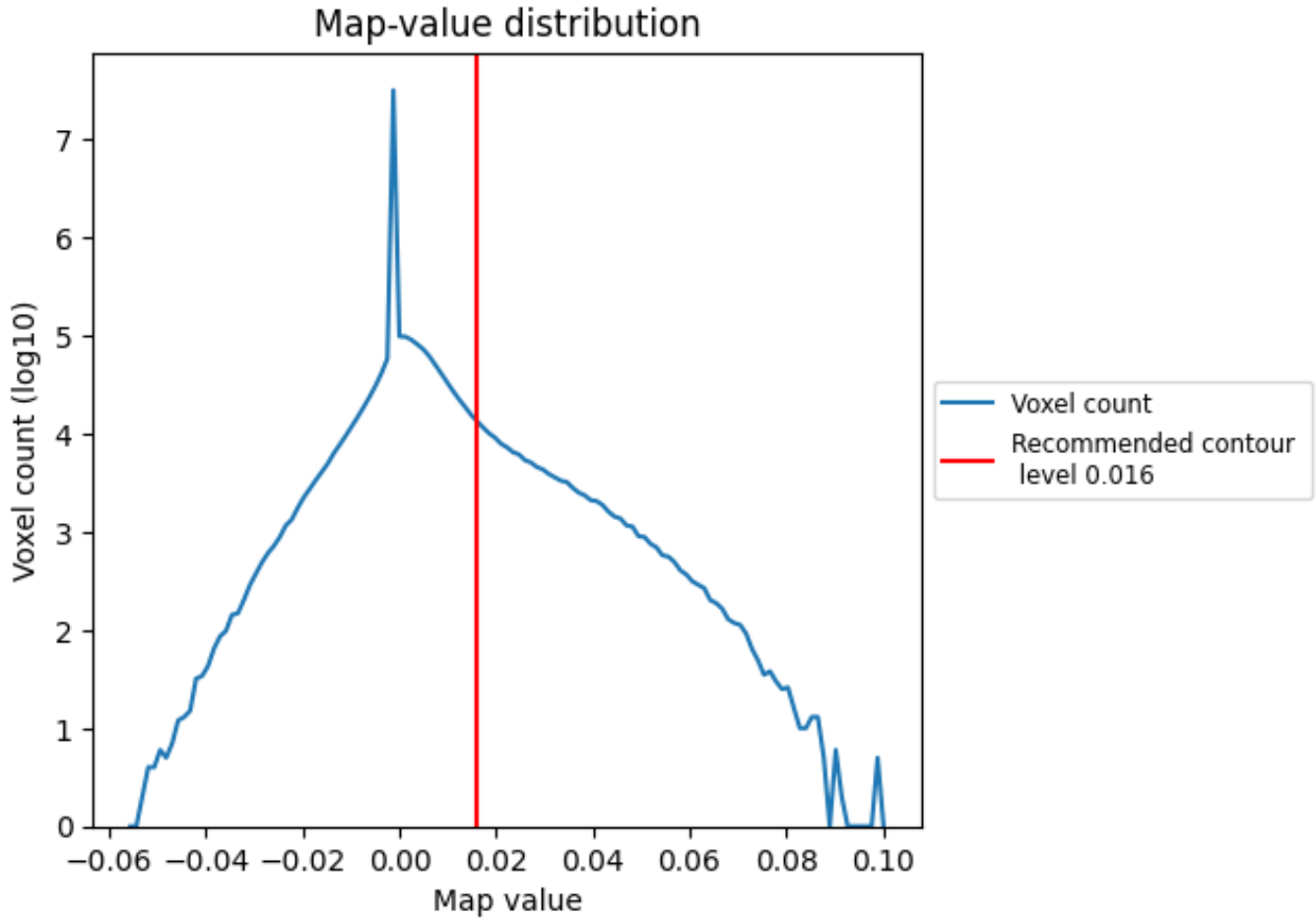
6.5 Mask visualisation (i)

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

7 Map analysis

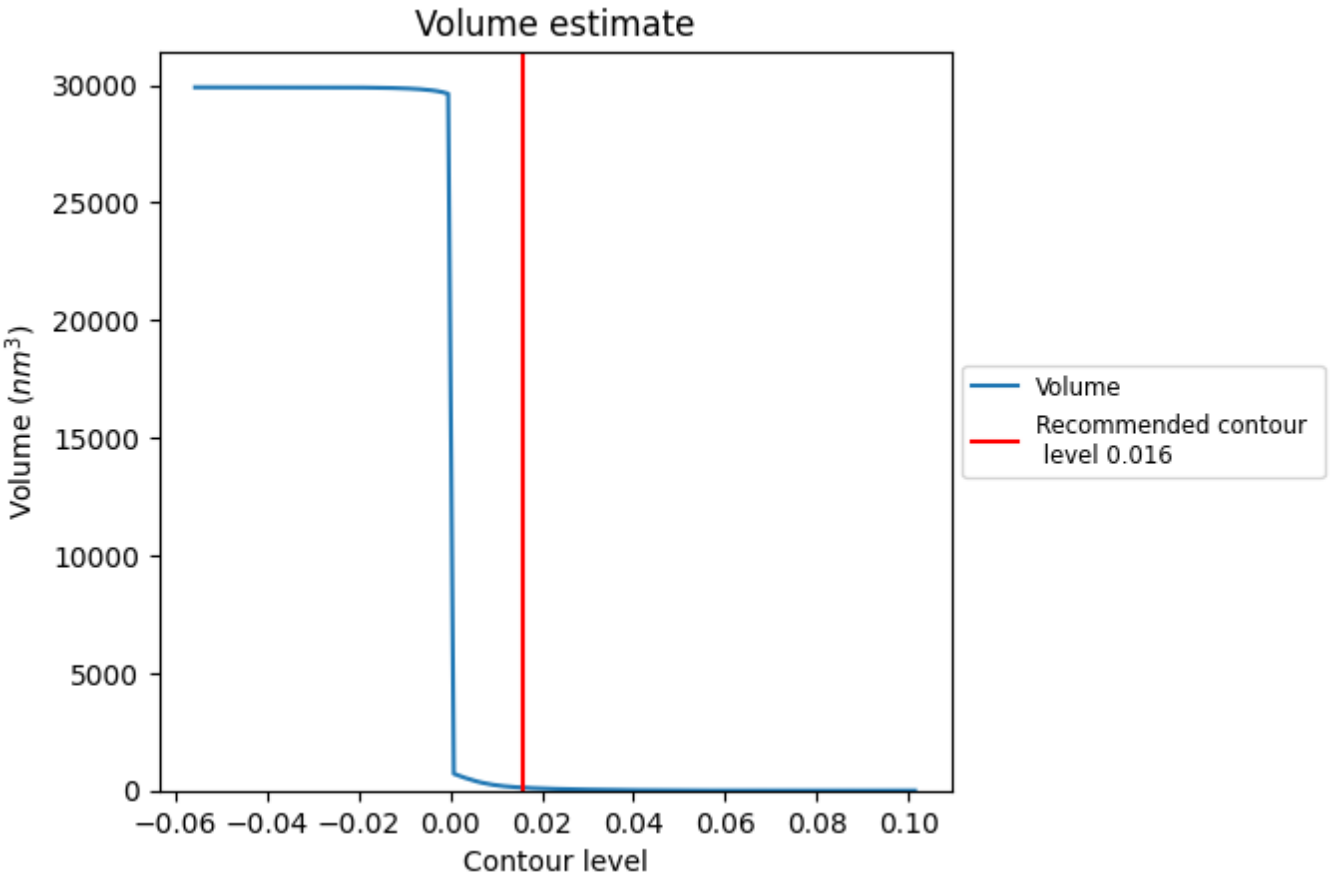
This section contains the results of statistical analysis of the map.

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.

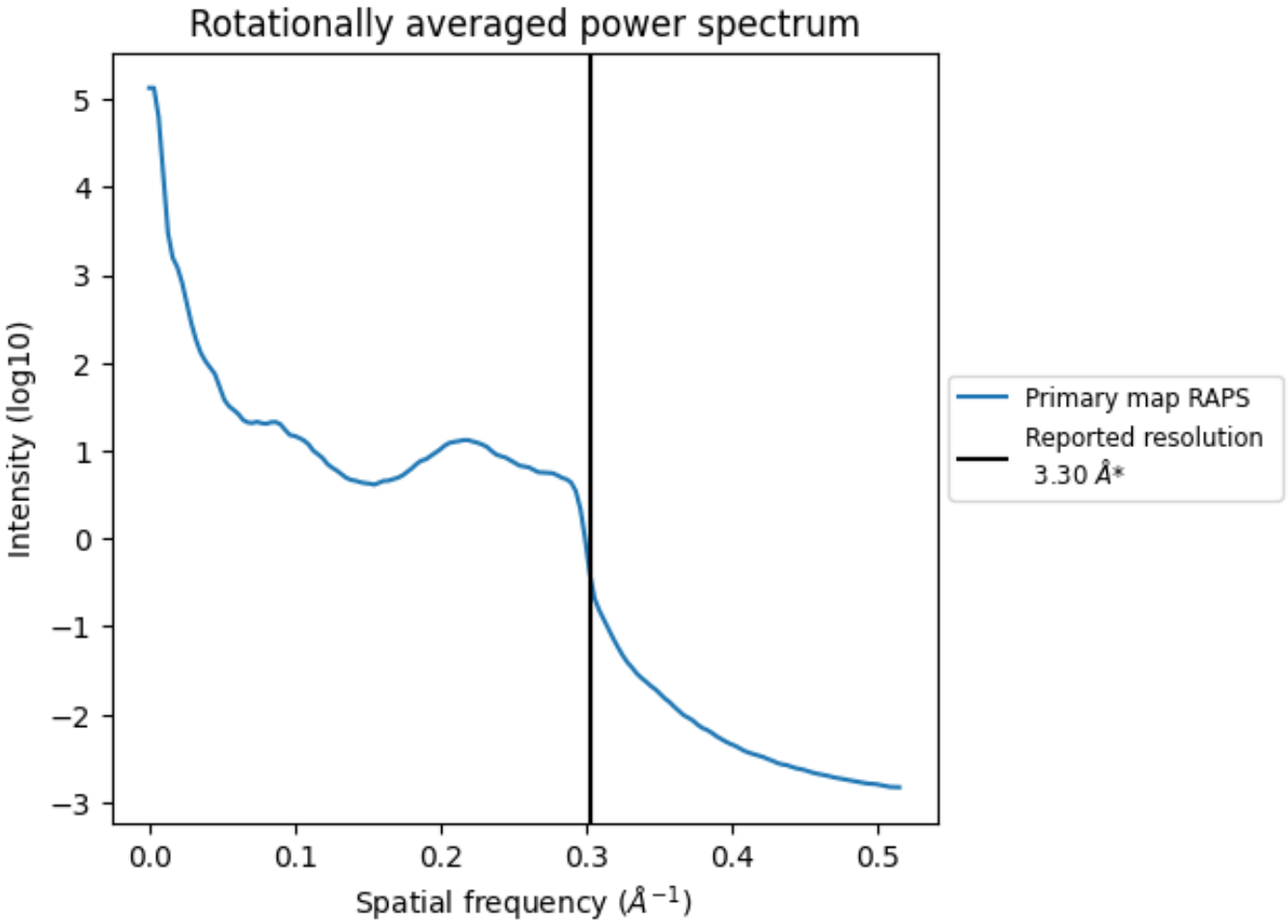
7.2 Volume estimate (i)



The volume at the recommended contour level is 123 nm^3; this corresponds to an approximate mass of 111 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)

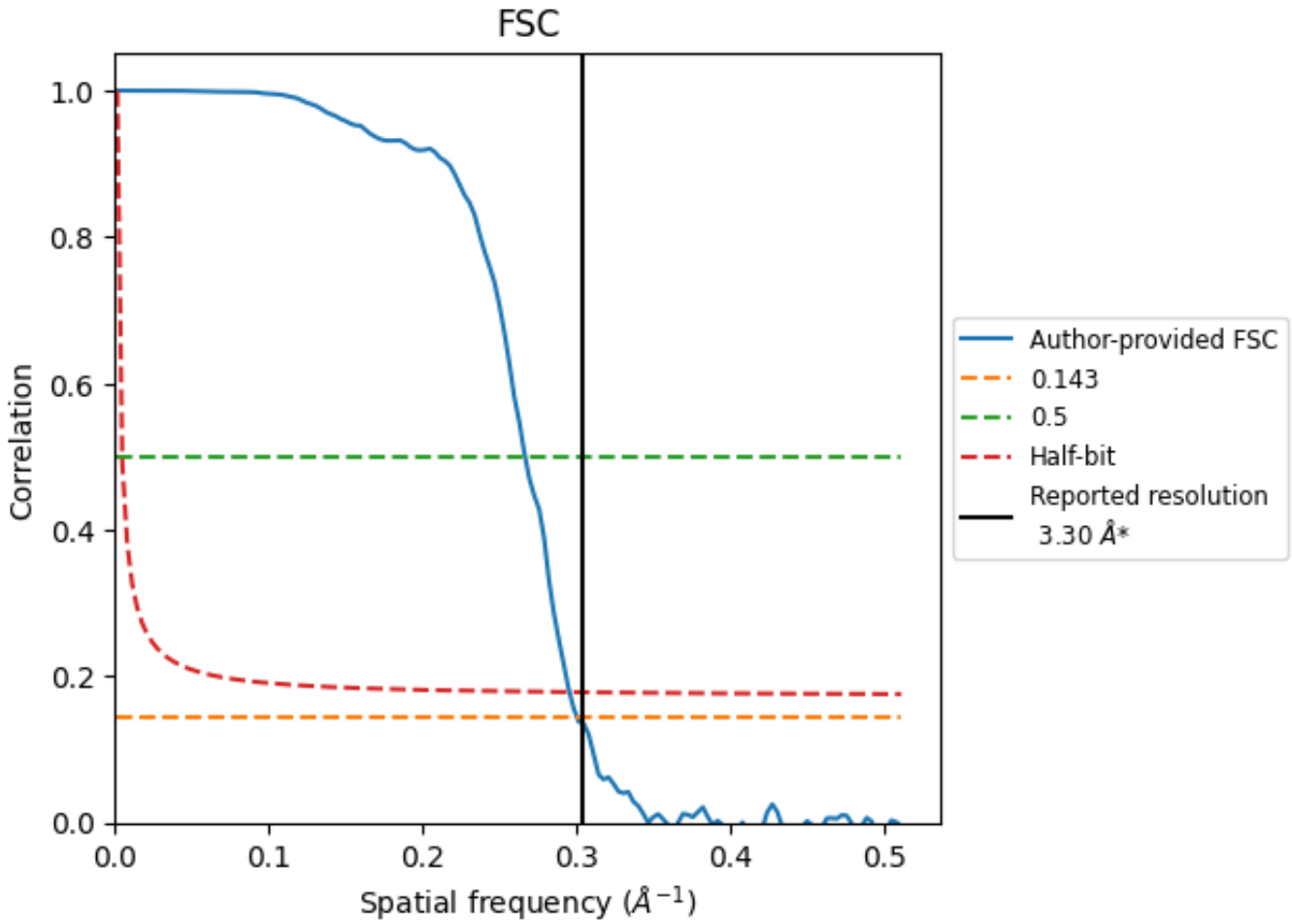


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

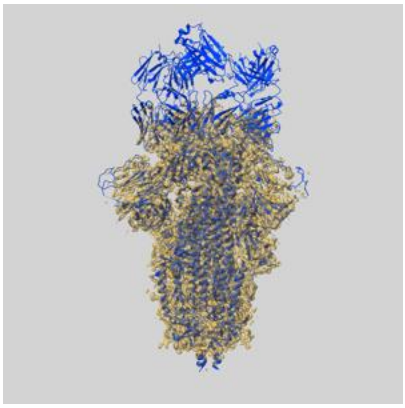
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.75	3.39
Unmasked-calculated*	-	-	-

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

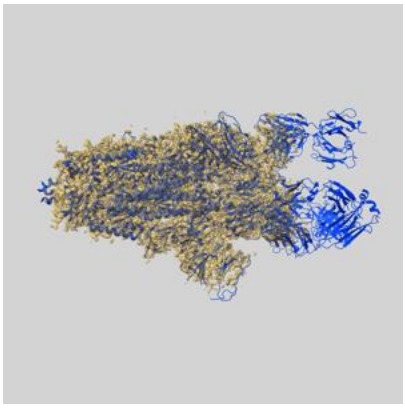
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32421 and PDB model 7WCD. Per-residue inclusion information can be found in section 3 on page 10.

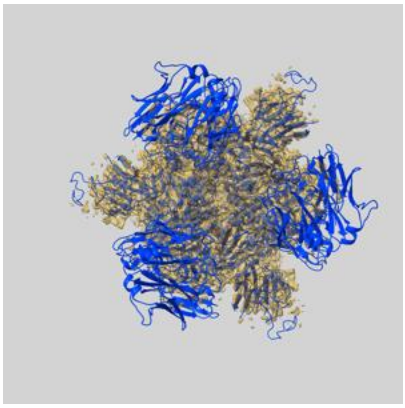
9.1 Map-model overlay



X



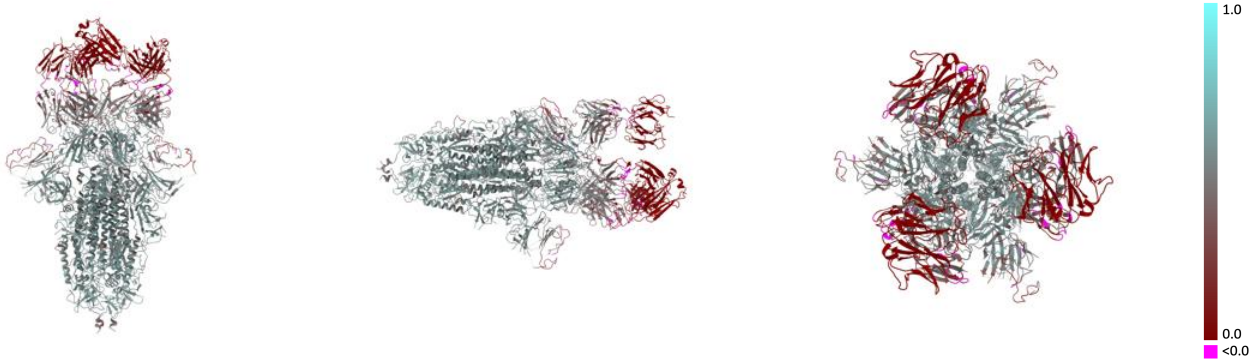
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

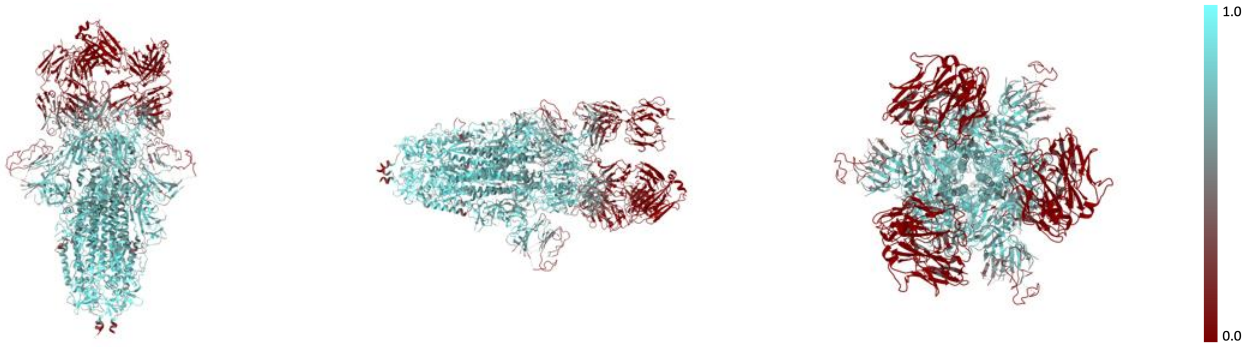
9.2 Q-score mapped to coordinate model (i)



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.

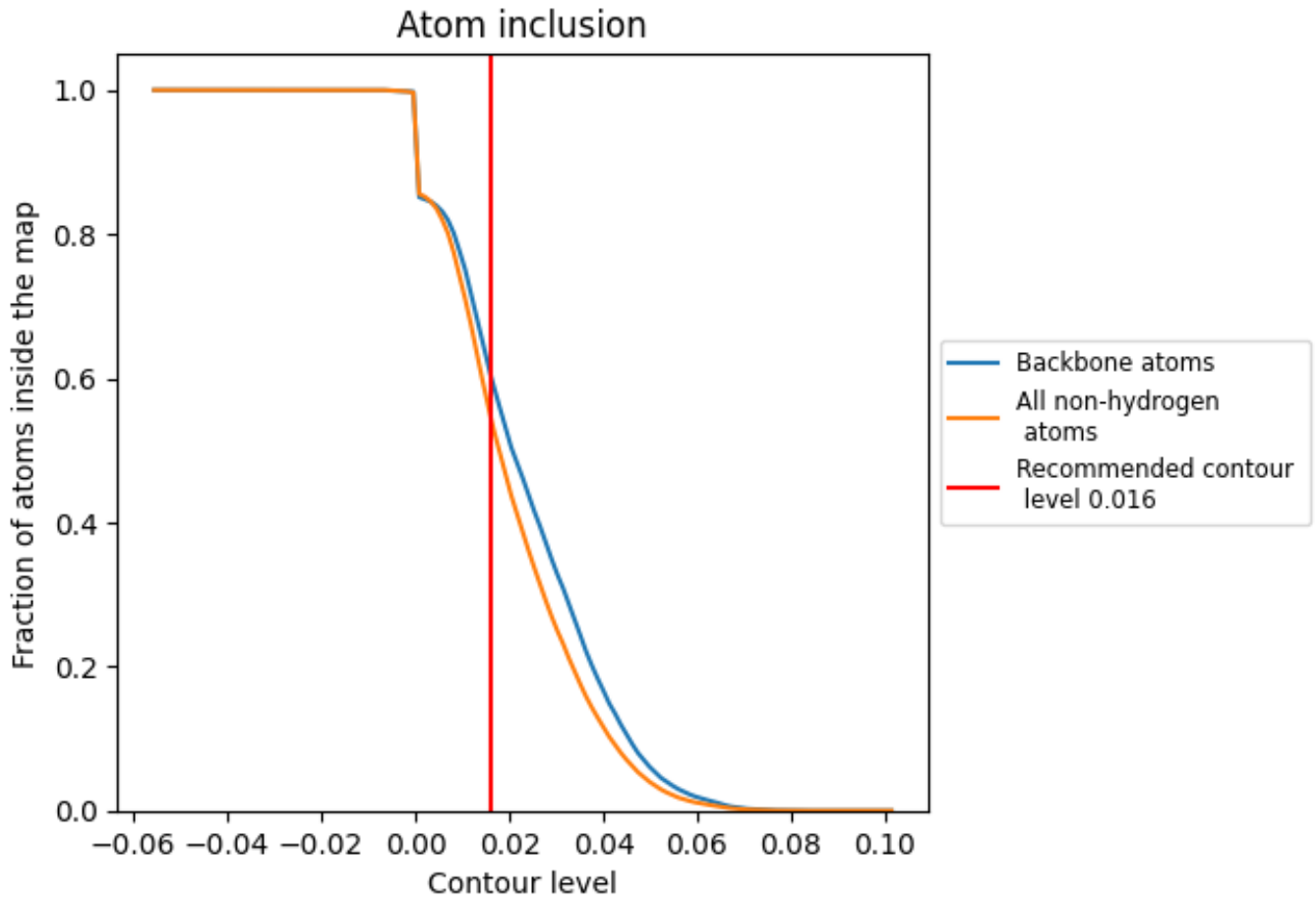
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 55% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5471	0.4280
A	0.1851	0.2210
B	0.1189	0.1890
C	0.7077	0.5180
E	0.1845	0.2200
F	0.1189	0.1890
G	0.1832	0.2320
H	0.7065	0.5160
I	0.1163	0.1900
J	0.7059	0.5170