Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:06 AM EST

PDB ID	:	7M6H
EMDB ID	:	EMD-23696
Title	:	Structure of the SARS-CoV-2 S 2P trimer in complex with the human neutralizing antibody Fab fragment, BG7-20
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2021-03-25
Resolution	:	4.00 Å(reported)
Based on initial model	:	6XKL

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:

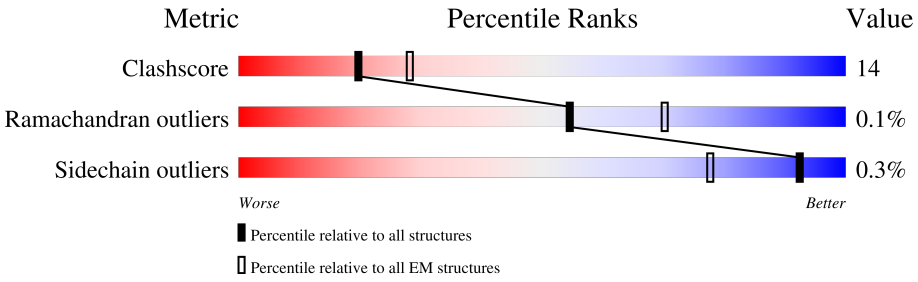
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	1259	7% 54% 25% 20%
1	B	1259	6% 57% 23% 20%
1	C	1259	21% 57% 22% . 20%
2	D	233	25% 38% 16% 46%
2	E	233	15% 37% 17% 46%
3	F	217	34% 29% 21% 50%
3	G	217	26% 32% 18% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		
1	B	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		
1	C	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	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
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	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
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	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

- Molecule 2 is a protein called BG7-20 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			953	592	165	187	9		

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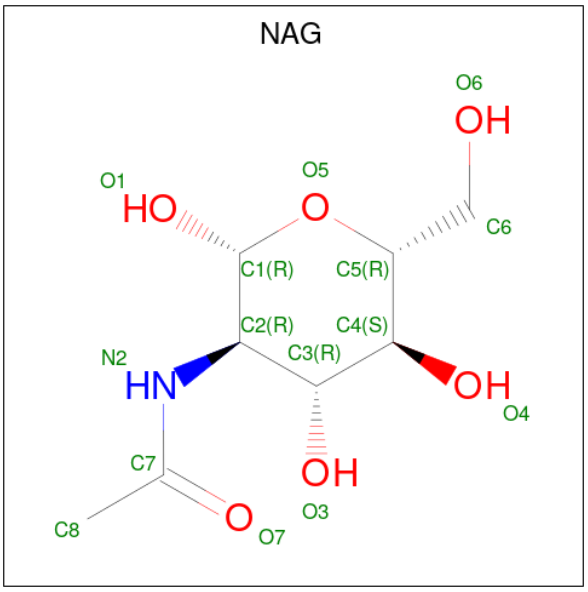
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	126	Total	C	N	O	S	0	0
			953	592	165	187	9		

- Molecule 3 is a protein called BG7-20 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	109	Total	C	N	O	S	0	0
			806	504	138	162	2		
3	G	109	Total	C	N	O	S	0	0
			806	504	138	162	2		

- 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	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	
4	A	1	Total	C	N	O	0
			140	80	10	50	

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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 140	C 80	N 10	O 50	0
4	A	1	Total 140	C 80	N 10	O 50	0
4	A	1	Total 140	C 80	N 10	O 50	0
4	A	1	Total 140	C 80	N 10	O 50	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 112	C 64	N 8	O 40	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0
4	C	1	Total 140	C 80	N 10	O 50	0

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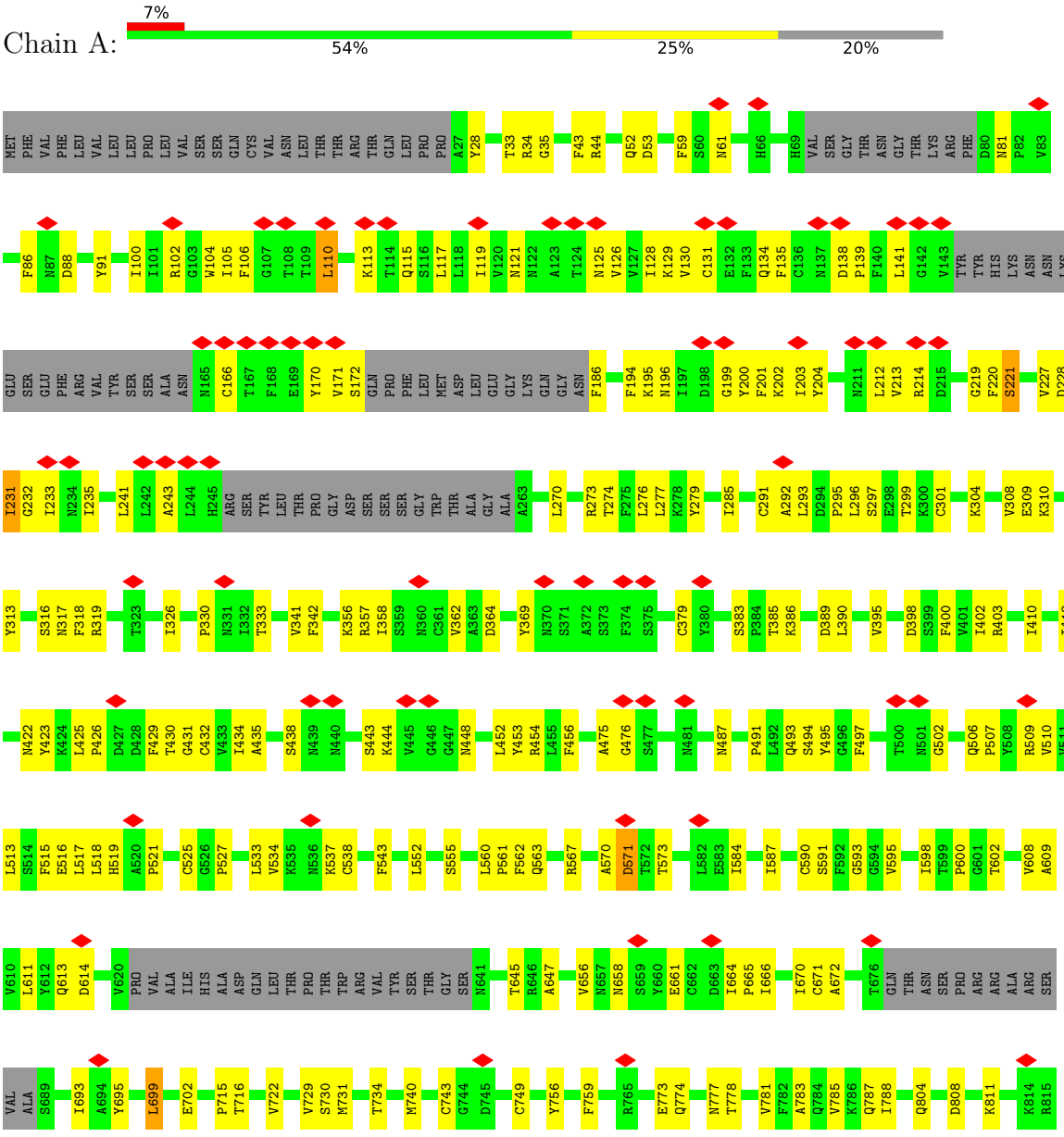
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			140	80	10	50	

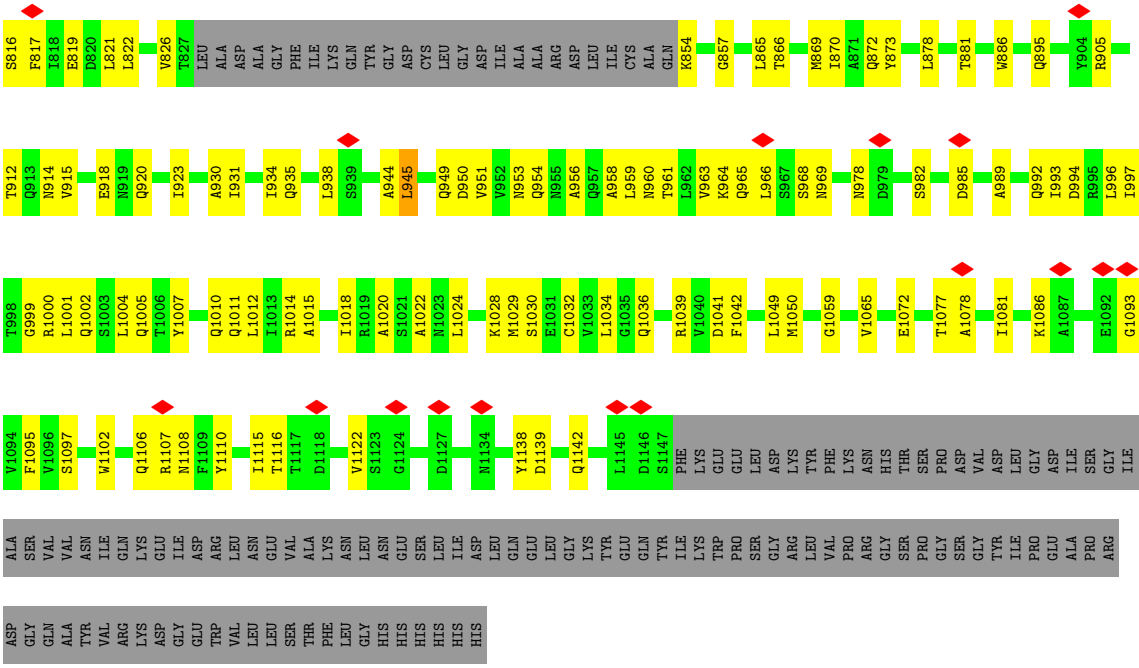
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

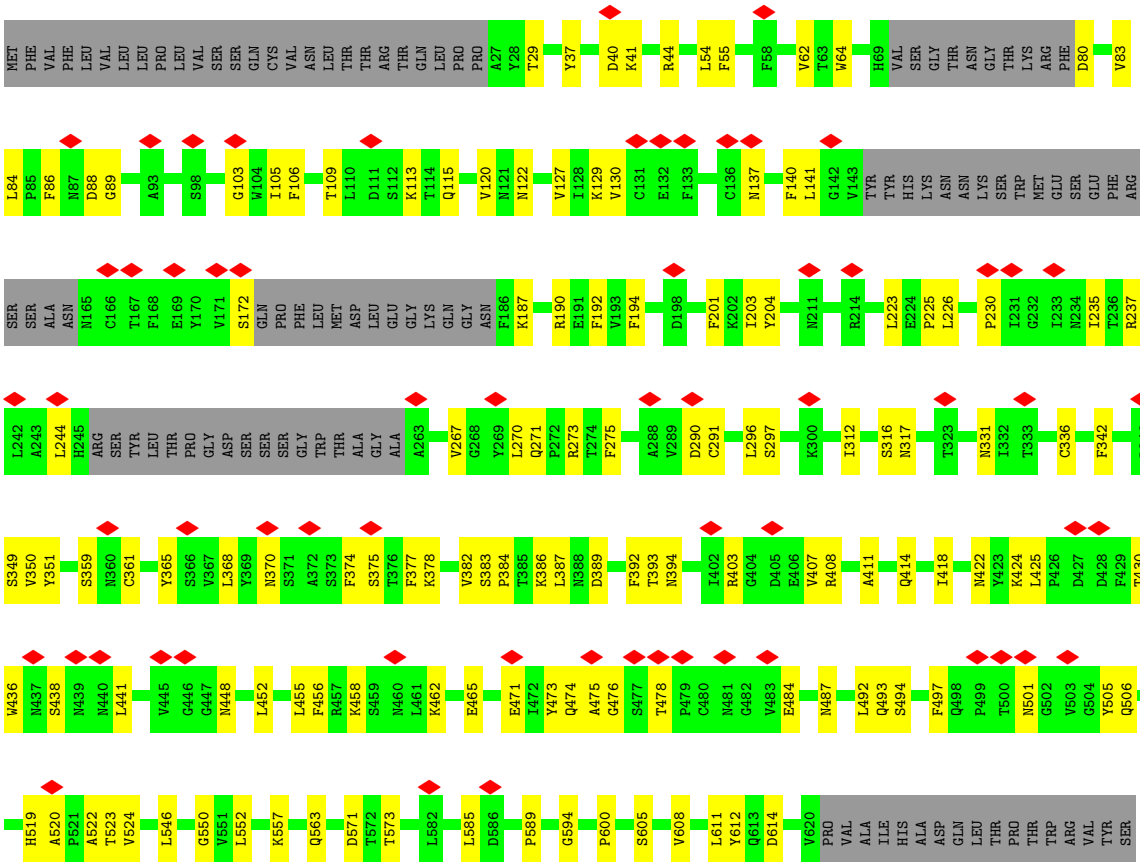
Chain A:

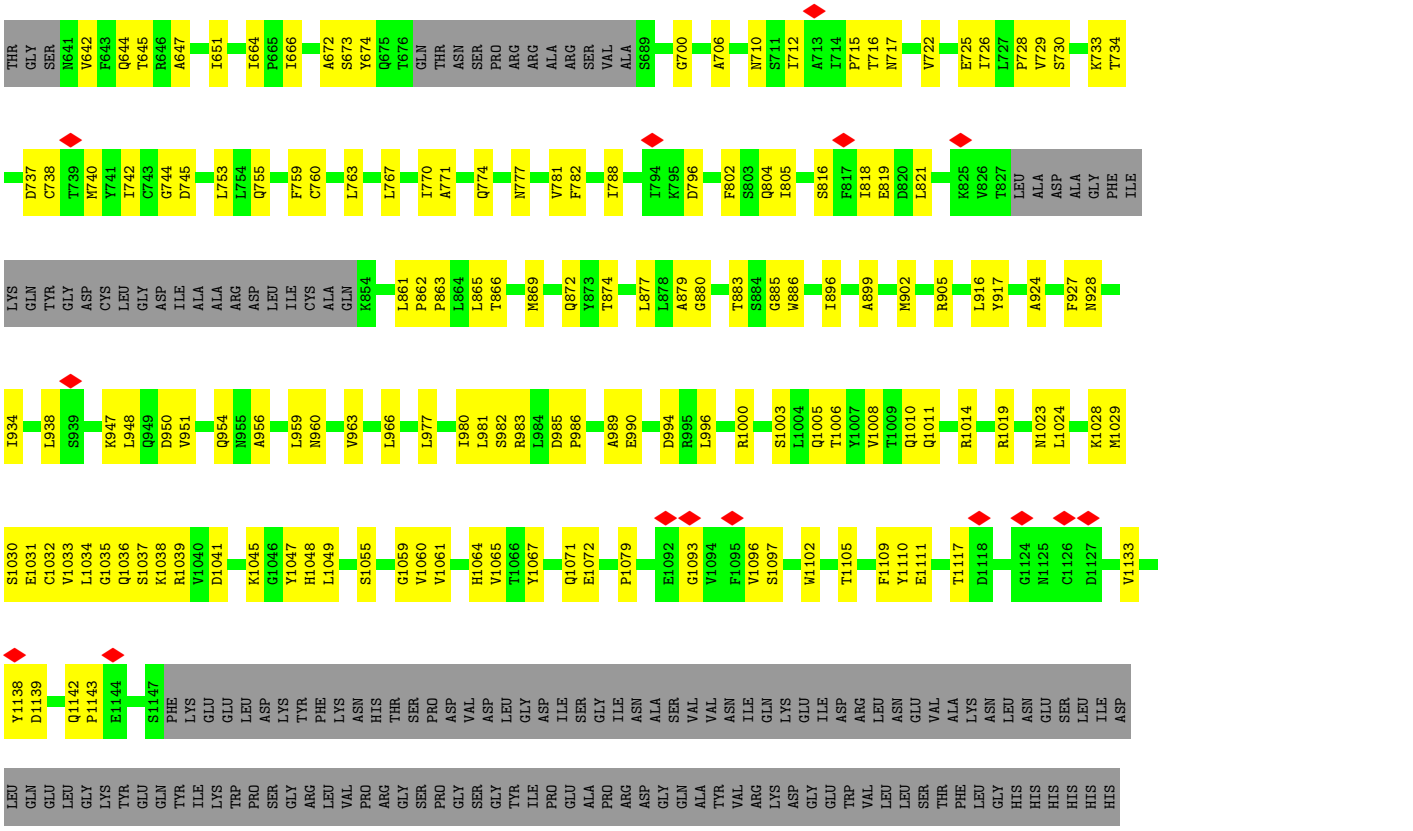




• Molecule 1: Spike glycoprotein

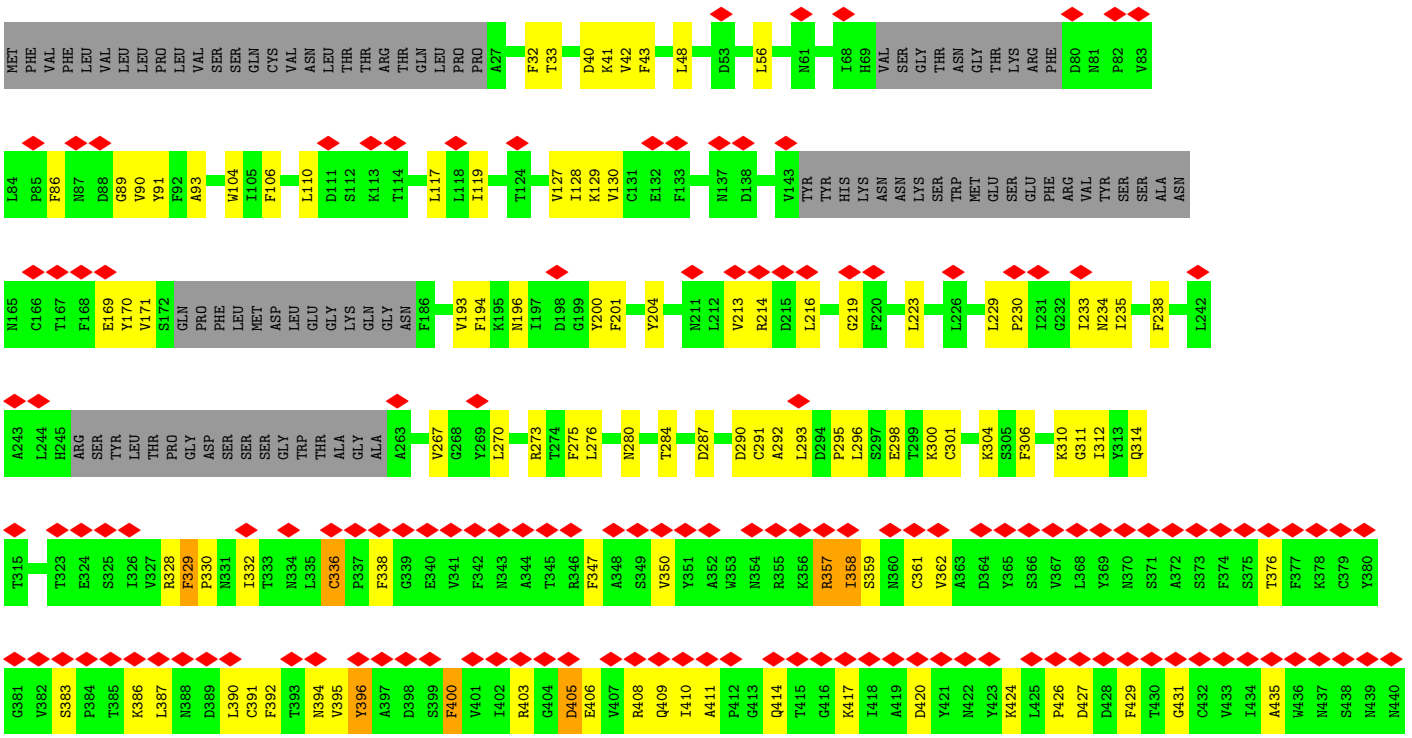
Chain B:

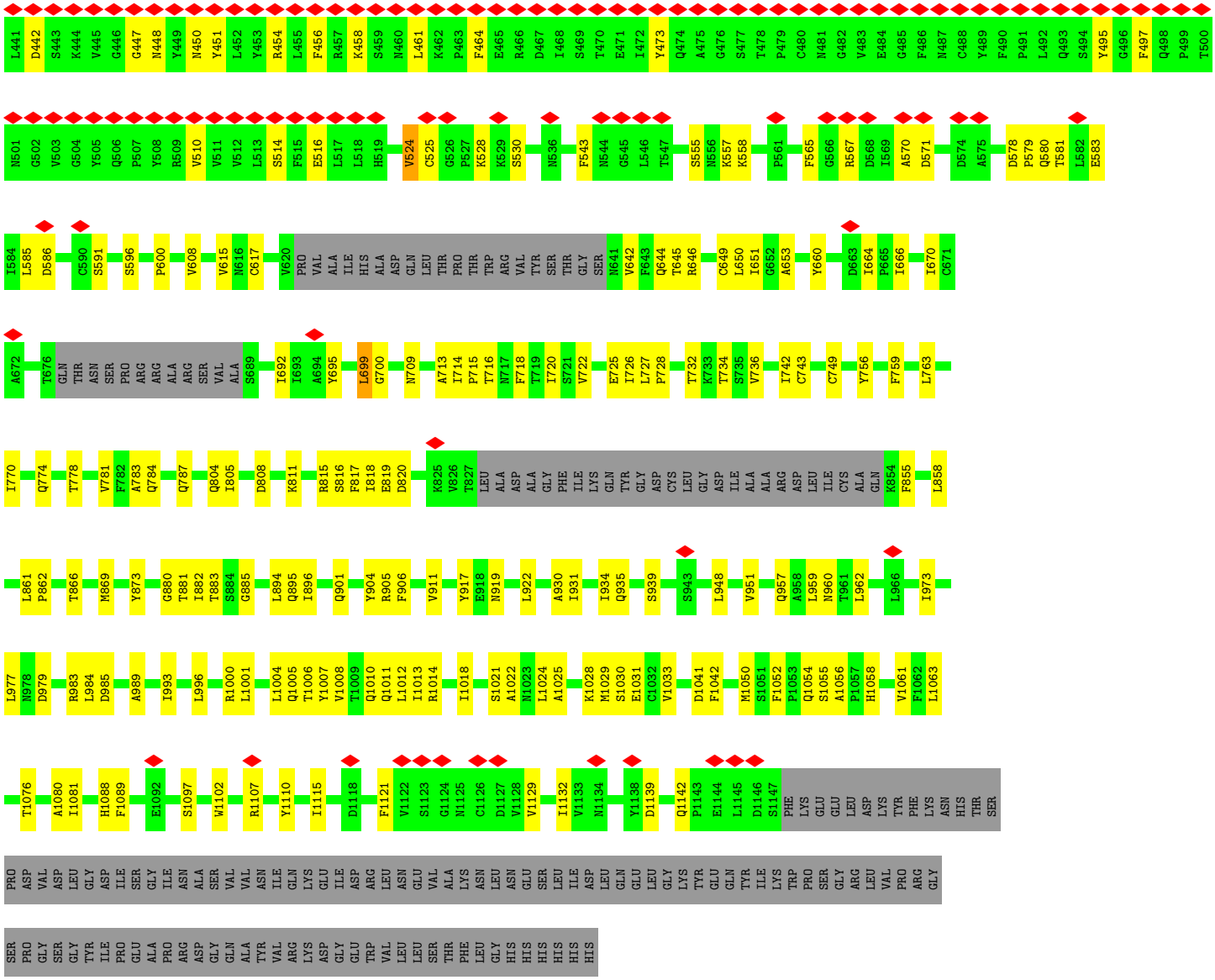




• Molecule 1: Spike glycoprotein

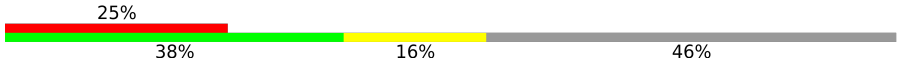
Chain C:

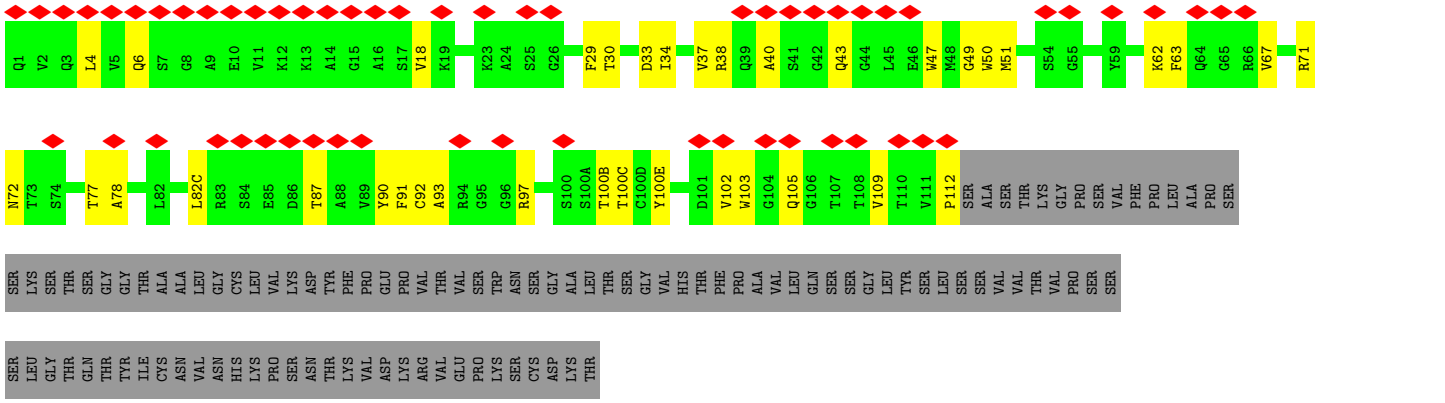




• Molecule 2: BG7-20 Fab Heavy Chain

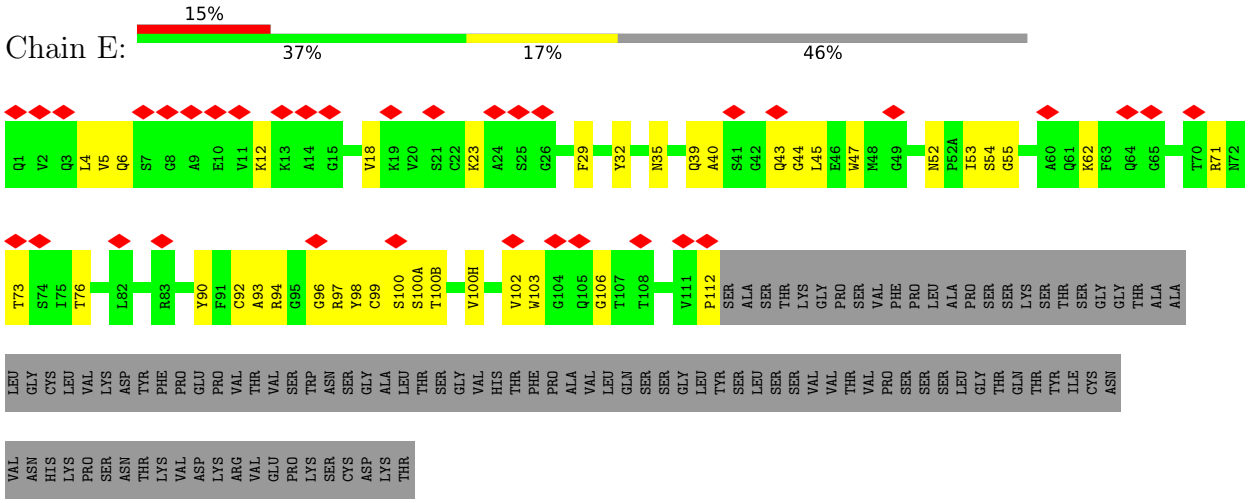
Chain D:





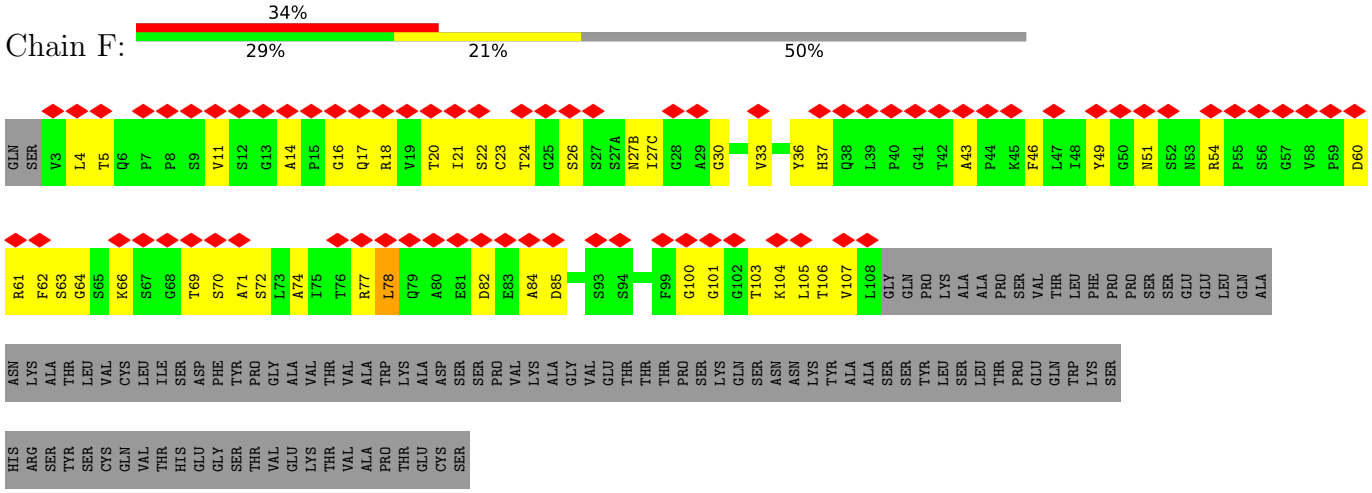
• Molecule 2: BG7-20 Fab Heavy Chain

Chain E:



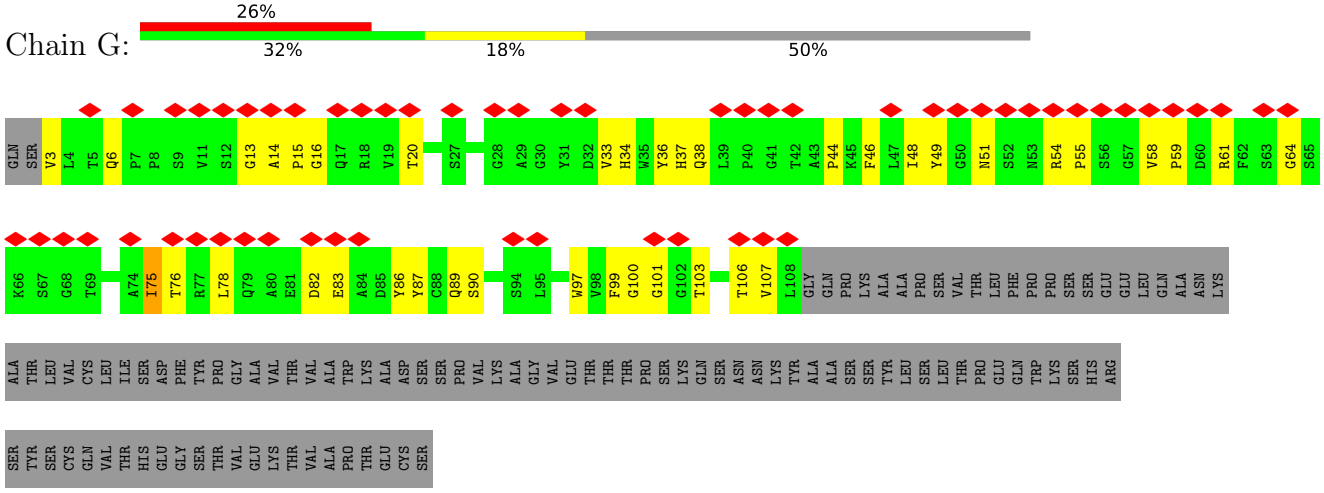
• Molecule 3: BG7-20 Fab Light Chain

Chain F:



• Molecule 3: BG7-20 Fab Light Chain

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.557	Depositor
Minimum map value	-0.243	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	375.40802, 375.40802, 375.40802	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	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	A	0.36	0/7999	0.65	6/10885 (0.1%)
1	B	0.35	0/7999	0.63	2/10885 (0.0%)
1	C	0.37	0/7999	0.66	5/10885 (0.0%)
2	D	0.31	0/972	0.67	1/1316 (0.1%)
2	E	0.33	0/972	0.72	1/1316 (0.1%)
3	F	0.32	0/827	0.71	1/1127 (0.1%)
3	G	0.35	0/827	0.70	1/1127 (0.1%)
All	All	0.36	0/27595	0.65	17/37541 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	699	LEU	CA-CB-CG	9.81	137.87	115.30
2	D	112	PRO	CA-N-CD	-8.57	99.50	111.50
2	E	112	PRO	CA-N-CD	-8.52	99.58	111.50
1	A	571	ASP	CB-CG-OD1	6.97	124.58	118.30
3	F	78	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	199	GLY	N-CA-C	5.55	126.98	113.10
1	C	699	LEU	C-N-CA	5.54	133.94	122.30
1	C	234	ASN	N-CA-CB	5.53	120.55	110.60
1	A	110	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	571	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	110	LEU	CA-CB-CG	5.47	127.89	115.30
3	G	75	ILE	CG1-CB-CG2	-5.43	99.46	111.40
1	A	301	CYS	CA-CB-SG	5.33	123.60	114.00
1	B	865	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	C	396	TYR	CA-CB-CG	5.24	123.36	113.40
1	C	571	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	945	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

There are no planarity outliers.

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	7823	0	7630	246	0
1	B	7823	0	7632	223	0
1	C	7823	0	7631	209	0
2	D	953	0	919	35	0
2	E	953	0	919	28	0
3	F	806	0	765	31	0
3	G	806	0	765	35	0
4	A	140	0	130	2	0
4	B	112	0	104	1	0
4	C	140	0	129	3	0
All	All	27379	0	26624	748	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 14.

All (748) 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:D:71:ARG:NH1	2:D:78:ALA:HB2	1.58	1.17
1:C:291:CYS:SG	1:C:301:CYS:CB	2.42	1.08
2:D:71:ARG:HH11	2:D:78:ALA:HB2	1.13	0.94
1:A:996:LEU:O	1:A:1000:ARG:HB2	1.68	0.93
2:D:51:MET:HE2	2:D:71:ARG:HD2	1.52	0.90
1:A:1028:LYS:O	1:A:1032:CYS:HB2	1.70	0.89
1:A:44:ARG:NH2	1:A:279:TYR:HE1	1.72	0.87
1:A:44:ARG:NH2	1:A:279:TYR:CE1	2.43	0.86
1:C:1006:THR:O	1:C:1010:GLN:HB2	1.75	0.86
2:D:51:MET:CE	2:D:71:ARG:HD2	2.08	0.83
1:C:361:CYS:HB3	1:C:524:VAL:HG13	1.65	0.79
1:B:291:CYS:HA	1:B:297:SER:HB2	1.66	0.78
1:B:86:PHE:H	1:B:237:ARG:HA	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ARG:HE	1:A:1050:MET:HB3	1.48	0.77
1:B:730:SER:HB2	1:B:774:GLN:HE21	1.50	0.77
1:C:565:PHE:HB3	1:C:567:ARG:HH12	1.50	0.77
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.68	0.76
1:C:196:ASN:HD22	1:C:233:ILE:HG22	1.51	0.76
1:C:359:SER:HB2	1:C:394:ASN:O	1.87	0.74
2:E:96:GLY:H	2:E:100(H):VAL:H	1.34	0.74
1:C:1029:MET:O	1:C:1033:VAL:HB	1.88	0.74
1:B:317:ASN:HA	1:B:594:GLY:HA2	1.69	0.74
2:D:51:MET:HE2	2:D:71:ARG:CD	2.17	0.74
1:B:441:LEU:HB2	1:B:509:ARG:HD2	1.71	0.73
1:C:89:GLY:HA2	1:C:235:ILE:HG23	1.71	0.73
1:C:201:PHE:HB3	1:C:229:LEU:HB3	1.72	0.72
2:D:71:ARG:HG3	2:D:77:THR:O	1.90	0.72
1:B:1028:LYS:O	1:B:1032:CYS:HB3	1.91	0.71
1:B:393:THR:HA	1:B:522:ALA:HA	1.72	0.70
3:G:15:PRO:HG3	3:G:82:ASP:H	1.57	0.70
3:F:18:ARG:HA	3:F:77:ARG:H	1.57	0.70
1:A:702:GLU:HA	1:B:788:ILE:HB	1.74	0.69
1:A:808:ASP:HB3	1:A:811:LYS:HG3	1.74	0.69
1:B:1049:LEU:HB2	1:B:1065:VAL:HG23	1.74	0.69
1:C:448:ASN:OD1	1:C:450:ASN:ND2	2.24	0.69
1:B:866:THR:H	1:B:869:MET:HE2	1.57	0.69
1:A:1001:LEU:HA	1:A:1004:LEU:HB3	1.75	0.69
1:B:644:GLN:NE2	1:B:645:THR:O	2.26	0.69
1:B:777:ASN:HD21	1:B:1019:ARG:HG3	1.56	0.69
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.75	0.68
1:B:365:TYR:HA	1:B:368:LEU:HD13	1.76	0.68
1:C:117:LEU:HA	1:C:130:VAL:HA	1.76	0.68
1:C:291:CYS:SG	1:C:301:CYS:HB3	2.32	0.68
1:B:996:LEU:HD21	1:B:1000:ARG:HH21	1.58	0.68
1:C:1008:VAL:O	1:C:1012:LEU:HB2	1.93	0.68
1:B:342:PHE:O	1:B:509:ARG:NH2	2.26	0.68
3:F:54:ARG:HH12	3:F:60:ASP:HA	1.59	0.67
1:C:973:ILE:HD11	1:C:984:LEU:HD21	1.76	0.67
1:C:1011:GLN:HA	1:C:1014:ARG:HB2	1.77	0.66
2:D:37:VAL:HG12	2:D:93:ALA:HB2	1.75	0.66
1:C:447:GLY:H	1:C:497:PHE:HB2	1.60	0.66
1:A:131:CYS:SG	1:A:166:CYS:N	2.68	0.66
1:C:456:PHE:HB3	1:C:473:TYR:H	1.60	0.66
1:C:716:THR:HA	1:C:1110:TYR:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ILE:HG22	1:C:362:VAL:HG23	1.77	0.65
2:D:29:PHE:HD2	2:D:71:ARG:NH2	1.95	0.65
1:A:291:CYS:HA	1:A:297:SER:HB2	1.79	0.65
1:C:291:CYS:O	1:C:298:GLU:HG3	1.98	0.64
1:C:448:ASN:HB3	1:C:495:TYR:HB2	1.78	0.64
2:D:97:ARG:HE	2:D:100(E):TYR:HB3	1.61	0.64
1:B:403:ARG:NH1	1:B:505:TYR:O	2.30	0.64
3:F:37:HIS:ND1	3:F:46:PHE:O	2.29	0.64
1:B:84:LEU:HG	1:B:267:VAL:HG21	1.80	0.64
3:F:27(C):ILE:HG21	3:F:69:THR:HA	1.79	0.64
1:A:454:ARG:HG3	1:A:491:PRO:HB2	1.80	0.63
1:A:966:LEU:HD13	1:A:1000:ARG:HH22	1.62	0.63
2:D:51:MET:CE	2:D:71:ARG:CD	2.73	0.63
2:D:40:ALA:HB3	2:D:43:GLN:HB3	1.81	0.62
1:B:436:TRP:HD1	1:B:438:SER:HB3	1.64	0.62
3:F:85:ASP:HA	3:F:104:LYS:HA	1.81	0.62
1:A:509:ARG:NH1	1:A:510:VAL:O	2.33	0.62
1:A:1107:ARG:HG2	1:B:886:TRP:HZ2	1.64	0.62
1:A:276:LEU:HD11	1:A:304:LYS:HA	1.81	0.62
1:B:523:THR:HG23	1:B:524:VAL:HG13	1.82	0.62
1:C:1005:GLN:HA	1:C:1008:VAL:HG22	1.81	0.62
1:B:728:PRO:HB3	1:B:951:VAL:HG11	1.82	0.62
1:B:954:GLN:OE1	1:B:1014:ARG:NH1	2.32	0.62
1:C:376:THR:HB	1:C:435:ALA:HB3	1.79	0.62
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.30	0.62
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.81	0.62
3:G:51:ASN:HB3	3:G:64:GLY:HA3	1.82	0.61
1:C:644:GLN:NE2	1:C:645:THR:O	2.33	0.61
1:A:202:LYS:HD3	1:A:204:TYR:HE1	1.63	0.61
1:C:359:SER:HA	1:C:524:VAL:HG22	1.83	0.61
1:C:989:ALA:O	1:C:993:ILE:HB	2.00	0.61
2:D:33:ASP:OD2	2:D:97:ARG:NH1	2.33	0.61
1:A:804:GLN:O	1:A:816:SER:OG	2.19	0.61
1:B:753:LEU:HD11	1:B:760:CYS:HB3	1.82	0.61
1:C:330:PRO:HB3	1:C:579:PRO:HB2	1.82	0.60
1:B:375:SER:H	1:B:436:TRP:HA	1.65	0.60
1:A:104:TRP:HB2	1:A:119:ILE:HD13	1.83	0.60
1:B:966:LEU:HA	1:B:1000:ARG:HH12	1.63	0.60
3:G:3:VAL:HA	3:G:100:GLY:HA3	1.84	0.60
1:A:431:GLY:HA2	1:A:515:PHE:HB2	1.83	0.60
1:A:826:VAL:HG13	1:A:945:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:HG12	1:A:1065:VAL:HA	1.84	0.60
1:A:1012:LEU:HB3	1:C:1013:ILE:HG21	1.83	0.60
1:C:1001:LEU:O	1:C:1004:LEU:N	2.34	0.60
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.82	0.60
1:B:359:SER:HA	1:B:523:THR:HG21	1.83	0.60
1:C:93:ALA:HB3	1:C:267:VAL:HG22	1.83	0.60
3:F:54:ARG:NH2	3:F:62:PHE:O	2.33	0.60
1:A:202:LYS:NZ	1:A:228:ASP:OD1	2.35	0.59
1:A:945:LEU:HG	1:A:949:GLN:HB2	1.83	0.59
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.84	0.59
1:C:881:THR:O	1:C:901:GLN:NE2	2.34	0.59
3:G:34:HIS:NE2	3:G:89:GLN:OE1	2.35	0.59
2:E:35:ASN:HB2	2:E:93:ALA:HB3	1.84	0.59
3:F:26:SER:OG	3:F:27(B):ASN:ND2	2.32	0.59
1:B:438:SER:OG	1:B:509:ARG:N	2.34	0.59
1:B:1030:SER:HA	1:B:1034:LEU:HB2	1.83	0.59
1:C:32:PHE:H	1:C:216:LEU:HD11	1.67	0.59
1:C:213:VAL:HG23	1:C:214:ARG:HG3	1.84	0.59
1:A:86:PHE:HZ	1:A:194:PHE:HB2	1.68	0.59
1:A:400:PHE:O	1:A:509:ARG:NH1	2.36	0.59
1:B:880:GLY:O	1:B:885:GLY:N	2.36	0.59
1:A:1011:GLN:O	1:A:1015:ALA:CB	2.51	0.59
1:B:408:ARG:HH11	1:B:414:GLN:HE22	1.51	0.59
1:B:733:LYS:HE2	1:B:863:PRO:HA	1.85	0.59
1:C:396:TYR:OH	1:C:514:SER:N	2.34	0.58
2:D:47:TRP:O	2:D:62:LYS:NZ	2.33	0.58
3:G:83:GLU:HG2	3:G:106:THR:HA	1.85	0.58
1:B:977:LEU:HA	1:B:980:ILE:HG22	1.86	0.58
1:B:1045:LYS:NZ	1:C:784:GLN:O	2.37	0.58
1:C:127:VAL:HG22	1:C:171:VAL:HG23	1.85	0.58
1:C:424:LYS:HD3	1:C:461:LEU:HB2	1.85	0.58
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.37	0.58
1:C:1129:VAL:HB	1:C:1132:ILE:HD11	1.85	0.58
1:B:563:GLN:HB3	1:C:43:PHE:HB2	1.84	0.58
2:D:34:ILE:HB	2:D:51:MET:HB3	1.85	0.58
1:B:902:MET:HB3	1:B:916:LEU:HD11	1.85	0.58
1:B:394:ASN:ND2	1:C:200:TYR:OH	2.35	0.58
1:B:458:LYS:HE3	1:B:474:GLN:H	1.67	0.58
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.37	0.58
1:C:770:ILE:O	1:C:774:GLN:NE2	2.36	0.58
1:A:985:ASP:O	1:A:989:ALA:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:PHE:HE1	1:C:270:LEU:HB2	1.68	0.58
1:A:125:ASN:O	4:A:1302:NAG:O6	2.17	0.57
1:A:953:ASN:O	1:A:956:ALA:N	2.37	0.57
1:C:336:CYS:SG	1:C:338:PHE:CE2	2.97	0.57
1:B:1028:LYS:O	1:B:1032:CYS:CB	2.52	0.57
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.86	0.57
3:F:11:VAL:HG21	3:F:78:LEU:HD11	1.85	0.57
1:C:770:ILE:HG22	1:C:774:GLN:HE22	1.69	0.57
2:E:12:LYS:HE3	2:E:18:VAL:HB	1.87	0.57
1:A:202:LYS:H	1:A:231:ILE:HG12	1.68	0.57
1:A:326:ILE:HD11	1:A:533:LEU:HA	1.85	0.57
1:A:383:SER:N	1:B:983:ARG:O	2.38	0.57
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.85	0.57
1:B:54:LEU:HD13	1:B:88:ASP:HB2	1.86	0.57
2:E:39:GLN:HB3	2:E:45:LEU:HG	1.87	0.57
2:D:102:VAL:HB	3:F:43:ALA:HB1	1.86	0.57
1:A:905:ARG:O	1:A:1036:GLN:NE2	2.37	0.56
1:B:436:TRP:CD1	1:B:438:SER:HB3	2.40	0.56
1:A:316:SER:OG	1:A:317:ASN:N	2.39	0.56
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.23	0.56
1:C:357:ARG:O	1:C:395:VAL:HA	2.05	0.56
2:E:92:CYS:HB2	2:E:103:TRP:CD1	2.40	0.56
3:G:3:VAL:HG22	3:G:101:GLY:H	1.69	0.56
1:A:730:SER:OG	1:A:731:MET:N	2.39	0.56
1:A:778:THR:HA	1:A:781:VAL:HG12	1.88	0.56
1:C:119:ILE:HG22	1:C:128:ILE:HA	1.88	0.56
1:A:390:LEU:HD21	1:B:982:SER:HB2	1.87	0.56
2:D:87:THR:HG23	2:D:109:VAL:HG23	1.86	0.56
3:G:37:HIS:HE1	3:G:48:ILE:HB	1.71	0.56
1:A:453:TYR:O	1:A:493:GLN:N	2.33	0.56
2:D:71:ARG:CG	2:D:77:THR:O	2.53	0.56
2:D:97:ARG:NH2	2:D:100(C):THR:O	2.39	0.56
1:A:357:ARG:HE	1:B:230:PRO:HB3	1.71	0.56
1:C:311:GLY:HA2	1:C:664:ILE:HD12	1.87	0.56
1:C:1102:TRP:HB3	1:C:1115:ILE:HD11	1.87	0.56
1:A:81:ASN:ND2	1:A:138:ASP:OD2	2.38	0.56
1:C:129:LYS:HG2	1:C:169:GLU:HG3	1.86	0.56
1:C:193:VAL:HB	1:C:204:TYR:HD2	1.71	0.56
3:F:4:LEU:H	3:F:100:GLY:HA2	1.72	0.56
1:A:453:TYR:N	1:A:493:GLN:O	2.33	0.55
1:A:611:LEU:HD21	1:A:613:GLN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:GLY:O	1:C:904:TYR:OH	2.24	0.55
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.87	0.55
1:A:333:THR:HA	1:A:362:VAL:HG21	1.88	0.55
3:G:37:HIS:HD2	3:G:86:TYR:HA	1.70	0.55
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.88	0.55
1:C:86:PHE:CE1	1:C:270:LEU:HB2	2.41	0.55
1:A:567:ARG:NH1	1:A:571:ASP:O	2.35	0.55
1:A:128:ILE:HD11	1:A:170:TYR:HB3	1.88	0.55
1:B:725:GLU:HB2	1:B:1064:HIS:CD2	2.42	0.55
1:B:804:GLN:O	1:B:816:SER:OG	2.25	0.55
1:C:296:LEU:H	1:C:608:VAL:HG11	1.71	0.55
3:G:16:GLY:HA2	3:G:76:THR:O	2.06	0.55
3:F:22:SER:HA	3:F:72:SER:HA	1.88	0.55
1:A:822:LEU:HA	1:A:826:VAL:HB	1.88	0.55
1:B:129:LYS:NZ	1:B:172:SER:OG	2.36	0.55
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.88	0.55
1:A:1039:ARG:NE	1:B:1031:GLU:OE2	2.38	0.55
1:B:424:LYS:NZ	1:B:425:LEU:O	2.37	0.55
1:A:534:VAL:HG21	1:A:537:LYS:HE2	1.88	0.54
1:C:410:ILE:HD12	1:C:510:VAL:HB	1.89	0.54
1:C:804:GLN:O	1:C:816:SER:OG	2.25	0.54
1:A:969:ASN:HB3	1:B:755:GLN:HE22	1.71	0.54
1:B:611:LEU:HD11	1:B:666:ILE:HG23	1.88	0.54
1:B:1079:PRO:HB3	1:C:917:TYR:CZ	2.42	0.54
3:F:37:HIS:H	3:F:46:PHE:HA	1.72	0.54
1:A:1049:LEU:HD12	1:A:1065:VAL:HG12	1.89	0.54
1:C:880:GLY:O	1:C:885:GLY:N	2.40	0.54
1:A:295:PRO:HB2	1:A:608:VAL:HB	1.90	0.54
2:E:97:ARG:NH2	2:E:100(A):SER:O	2.38	0.54
1:A:456:PHE:HB2	1:A:491:PRO:HB3	1.90	0.54
1:C:357:ARG:HD3	1:C:516:GLU:HB2	1.89	0.54
1:C:778:THR:HA	1:C:781:VAL:HG12	1.90	0.54
1:C:882:ILE:HG13	1:C:883:THR:HG23	1.90	0.54
2:E:71:ARG:HE	2:E:73:THR:HG22	1.73	0.54
1:A:430:THR:HG23	1:A:516:GLU:HA	1.88	0.54
1:A:740:MET:HG3	1:A:857:GLY:HA2	1.89	0.54
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.90	0.53
1:A:756:TYR:HB3	1:A:759:PHE:HD2	1.73	0.53
1:A:1139:ASP:HB2	1:A:1142:GLN:HB2	1.89	0.53
1:C:391:CYS:SG	1:C:525:CYS:N	2.81	0.53
1:C:726:ILE:HG22	1:C:948:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:THR:OG1	1:A:219:GLY:O	2.25	0.53
1:A:203:ILE:HB	1:A:227:VAL:HB	1.90	0.53
1:B:40:ASP:OD2	1:B:44:ARG:NH2	2.41	0.53
1:C:117:LEU:HB3	1:C:130:VAL:HG12	1.90	0.53
1:A:341:VAL:HG23	1:A:342:PHE:HD1	1.74	0.53
1:A:398:ASP:HB2	1:A:512:VAL:HB	1.89	0.53
1:B:1041:ASP:HB3	1:C:1030:SER:HB2	1.89	0.53
1:C:962:LEU:HD11	1:C:1007:TYR:HB2	1.91	0.53
1:C:985:ASP:O	1:C:989:ALA:HB2	2.09	0.53
3:F:36:TYR:HA	3:F:46:PHE:HB3	1.91	0.53
1:A:403:ARG:HH21	1:A:507:PRO:HA	1.74	0.53
1:A:872:GLN:HB2	1:C:699:LEU:HD11	1.90	0.53
1:B:885:GLY:HA3	1:B:896:ILE:HD11	1.91	0.53
1:B:29:THR:HB	1:B:62:VAL:HG23	1.90	0.53
1:B:37:TYR:H	1:B:55:PHE:HE1	1.56	0.53
1:B:462:LYS:HB2	1:B:465:GLU:HG2	1.91	0.53
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.43	0.52
1:A:134:GLN:NE2	1:A:135:PHE:O	2.42	0.52
1:C:273:ARG:HG2	1:C:292:ALA:HB2	1.92	0.52
1:B:383:SER:N	1:C:983:ARG:O	2.42	0.52
1:B:722:VAL:HG12	1:B:1065:VAL:HG12	1.91	0.52
1:C:383:SER:HB3	1:C:386:LYS:HB2	1.90	0.52
2:E:52:ASN:O	2:E:71:ARG:NH1	2.42	0.52
1:B:475:ALA:HB1	2:D:100(B):THR:HB	1.91	0.52
1:B:934:ILE:O	1:B:938:LEU:HB2	2.10	0.52
1:A:590:CYS:SG	1:A:591:SER:N	2.83	0.52
1:B:706:ALA:H	1:C:895:GLN:HE21	1.57	0.52
1:C:40:ASP:OD1	1:C:41:LYS:N	2.34	0.52
1:C:578:ASP:HB2	1:C:585:LEU:HD23	1.90	0.52
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.73	0.52
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.92	0.52
1:C:591:SER:HB3	1:C:615:VAL:HG22	1.91	0.52
3:F:63:SER:HB3	3:F:74:ALA:HB3	1.91	0.52
1:A:519:HIS:CE1	1:B:41:LYS:H	2.28	0.52
1:B:55:PHE:HB2	1:B:275:PHE:CZ	2.45	0.52
1:C:48:LEU:HD13	1:C:276:LEU:HD21	1.92	0.52
1:C:403:ARG:HA	1:C:442:ASP:HB3	1.91	0.52
1:C:957:GLN:HA	1:C:960:ASN:HB2	1.92	0.52
1:C:90:VAL:HG13	1:C:235:ILE:HG12	1.91	0.52
1:C:530:SER:CB	1:C:580:GLN:HE22	2.23	0.52
1:A:773:GLU:O	1:A:777:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:LEU:HD11	1:A:935:GLN:HG2	1.91	0.52
1:C:996:LEU:HG	1:C:1000:ARG:HD3	1.92	0.52
1:A:645:THR:HG21	1:A:670:ILE:HG13	1.91	0.51
1:C:985:ASP:O	1:C:989:ALA:CB	2.58	0.51
1:A:318:PHE:HB3	1:A:595:VAL:HG22	1.91	0.51
1:B:106:PHE:CE2	1:B:194:PHE:HB2	2.46	0.51
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.92	0.51
1:A:105:ILE:HD12	1:A:110:LEU:HD22	1.92	0.51
1:A:593:GLY:HA3	1:A:613:GLN:HE21	1.75	0.51
1:A:931:ILE:HD13	1:A:934:ILE:HD11	1.93	0.51
1:B:109:THR:HG21	1:B:113:LYS:HD2	1.93	0.51
1:C:1008:VAL:O	1:C:1012:LEU:CB	2.58	0.51
1:A:231:ILE:HG22	1:A:233:ILE:H	1.75	0.51
1:A:560:LEU:O	1:A:563:GLN:HB3	2.10	0.51
1:C:33:THR:OG1	1:C:219:GLY:O	2.28	0.51
1:C:431:GLY:HA3	1:C:514:SER:HA	1.92	0.51
1:C:979:ASP:O	1:C:983:ARG:HB2	2.09	0.51
1:A:1093:GLY:HA2	1:A:1106:GLN:HA	1.91	0.51
1:B:767:LEU:HD23	1:B:770:ILE:HD12	1.91	0.51
1:B:1019:ARG:O	1:B:1023:ASN:ND2	2.43	0.51
1:B:1138:TYR:HE2	1:B:1143:PRO:HD3	1.76	0.51
1:A:961:THR:O	1:A:965:GLN:NE2	2.44	0.51
1:A:1001:LEU:O	1:A:1005:GLN:HB2	2.11	0.51
1:A:1081:ILE:HD11	1:A:1115:ILE:HG21	1.92	0.51
1:B:642:VAL:HG13	1:B:651:ILE:HG12	1.92	0.51
1:B:763:LEU:HD21	1:B:1005:GLN:HE22	1.76	0.51
1:C:392:PHE:H	1:C:524:VAL:HG23	1.76	0.51
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.92	0.51
3:F:14:ALA:O	3:F:77:ARG:NE	2.44	0.51
1:B:874:THR:HG21	1:B:1055:SER:HB3	1.92	0.51
1:A:34:ARG:HH12	1:A:221:SER:HB3	1.76	0.50
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.94	0.50
1:B:127:VAL:HG13	1:B:129:LYS:HZ3	1.76	0.50
1:B:802:PHE:HE1	1:B:927:PHE:HE2	1.59	0.50
1:A:119:ILE:HG13	1:A:128:ILE:HG22	1.93	0.50
1:B:203:ILE:HG23	1:B:226:LEU:HB2	1.92	0.50
1:A:330:PRO:HD2	1:A:525:CYS:SG	2.51	0.50
1:A:716:THR:HA	1:A:1110:TYR:HB3	1.93	0.50
1:A:1030:SER:HB3	1:C:1041:ASP:HB3	1.94	0.50
1:B:1011:GLN:HA	1:B:1014:ARG:HB3	1.94	0.50
1:B:1029:MET:O	1:B:1033:VAL:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:GLN:OE1	3:G:103:THR:OG1	2.24	0.50
1:A:200:TYR:O	1:A:231:ILE:HA	2.12	0.50
1:A:517:LEU:HD13	1:B:983:ARG:HH21	1.77	0.50
1:B:1105:THR:OG1	1:B:1111:GLU:N	2.40	0.50
1:C:296:LEU:O	1:C:300:LYS:HG3	2.11	0.50
3:F:24:THR:HA	3:F:70:SER:HA	1.93	0.50
1:A:1010:GLN:O	1:A:1014:ARG:CB	2.60	0.50
1:B:519:HIS:HE1	1:C:42:VAL:HG22	1.76	0.50
1:B:1139:ASP:HB3	1:B:1142:GLN:HG3	1.93	0.50
2:D:71:ARG:HG3	2:D:78:ALA:HA	1.93	0.50
1:A:44:ARG:HH21	1:A:279:TYR:HE1	1.51	0.50
1:A:1041:ASP:HB3	1:B:1030:SER:HB3	1.93	0.50
1:B:476:GLY:N	1:B:487:ASN:OD1	2.45	0.50
1:B:816:SER:HB3	1:B:819:GLU:HB2	1.94	0.50
1:C:815:ARG:HH21	1:C:820:ASP:HA	1.76	0.50
2:E:6:GLN:NE2	2:E:92:CYS:SG	2.84	0.50
1:B:478:THR:O	1:B:487:ASN:ND2	2.33	0.50
1:C:645:THR:OG1	1:C:646:ARG:N	2.45	0.50
2:E:102:VAL:HG11	3:G:44:PRO:HD2	1.94	0.49
1:A:886:TRP:HZ2	1:C:1107:ARG:HD3	1.77	0.49
1:A:1010:GLN:O	1:A:1014:ARG:HB3	2.13	0.49
3:F:61:ARG:NH1	3:F:82:ASP:OD2	2.44	0.49
1:A:277:LEU:HD12	1:A:285:ILE:HD13	1.93	0.49
1:B:990:GLU:O	1:B:994:ASP:HB2	2.13	0.49
1:C:709:ASN:HB3	4:C:1307:NAG:N2	2.27	0.49
1:A:1028:LYS:O	1:A:1032:CYS:CB	2.51	0.49
1:B:86:PHE:CZ	1:B:89:GLY:HA2	2.47	0.49
1:B:557:LYS:HE2	1:C:43:PHE:HE2	1.77	0.49
1:C:935:GLN:O	1:C:939:SER:OG	2.29	0.49
1:A:316:SER:O	1:A:595:VAL:N	2.40	0.49
1:A:985:ASP:O	1:A:989:ALA:CB	2.60	0.49
1:B:673:SER:OG	1:B:674:TYR:N	2.45	0.49
1:C:403:ARG:CZ	1:C:405:ASP:HB2	2.42	0.49
1:C:709:ASN:H	4:C:1307:NAG:H83	1.76	0.49
3:F:33:VAL:HG11	3:F:71:ALA:HB1	1.93	0.49
1:A:319:ARG:NH1	1:B:745:ASP:OD1	2.45	0.49
1:B:726:ILE:HD11	1:B:947:LYS:H	1.78	0.49
1:B:726:ILE:HG22	1:B:1061:VAL:HG13	1.95	0.49
1:B:948:LEU:HA	1:B:951:VAL:HG12	1.95	0.49
1:C:728:PRO:HG3	1:C:951:VAL:HG21	1.94	0.49
1:B:316:SER:OG	1:B:317:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:SER:OG	1:B:452:LEU:O	2.29	0.49
2:E:4:LEU:HD23	2:E:103:TRP:CD1	2.48	0.49
1:A:200:TYR:HB3	1:A:229:LEU:HB3	1.95	0.49
1:B:589:PRO:HG2	1:C:855:PHE:HB3	1.94	0.49
1:B:1032:CYS:HA	1:B:1048:HIS:CE1	2.48	0.49
1:B:1139:ASP:N	1:B:1142:GLN:OE1	2.46	0.49
1:C:756:TYR:HB3	1:C:759:PHE:HD2	1.77	0.49
3:G:33:VAL:HG12	3:G:90:SER:HA	1.94	0.49
3:G:89:GLN:NE2	3:G:97:TRP:O	2.45	0.49
1:B:382:VAL:HG11	1:B:387:LEU:HD13	1.95	0.49
1:C:91:TYR:HD1	1:C:193:VAL:HG22	1.78	0.49
1:C:1139:ASP:HB3	1:C:1142:GLN:HB2	1.94	0.49
1:A:521:PRO:HD3	1:A:562:PHE:CE2	2.48	0.48
1:A:521:PRO:HD3	1:A:562:PHE:HE2	1.78	0.48
1:B:351:TYR:HB2	1:B:492:LEU:HD11	1.94	0.48
1:B:956:ALA:O	1:B:960:ASN:HB2	2.13	0.48
1:C:347:PHE:HA	1:C:400:PHE:HB2	1.95	0.48
1:A:383:SER:HB2	1:B:985:ASP:N	2.28	0.48
1:B:80:ASP:N	1:B:80:ASP:OD1	2.46	0.48
1:B:733:LYS:HD2	1:B:771:ALA:HB1	1.95	0.48
1:B:194:PHE:HD1	1:B:201:PHE:HE2	1.61	0.48
1:C:280:ASN:OD1	1:C:284:THR:N	2.33	0.48
1:A:656:VAL:HG13	1:A:695:TYR:HB3	1.94	0.48
1:A:878:LEU:O	1:A:881:THR:OG1	2.28	0.48
3:G:54:ARG:HB2	3:G:58:VAL:HB	1.94	0.48
1:A:389:ASP:N	1:A:389:ASP:OD1	2.47	0.48
1:A:438:SER:HB2	1:A:509:ARG:HB2	1.96	0.48
1:B:378:LYS:NZ	1:B:407:VAL:O	2.47	0.48
1:B:475:ALA:N	1:B:487:ASN:OD1	2.47	0.48
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.96	0.48
1:A:435:ALA:HB2	1:A:510:VAL:HG23	1.95	0.48
1:B:740:MET:HA	1:B:744:GLY:HA2	1.94	0.48
1:C:104:TRP:HE1	1:C:119:ILE:HD11	1.78	0.48
1:A:1086:LYS:HB3	1:A:1122:VAL:HG13	1.94	0.48
1:C:816:SER:OG	1:C:817:PHE:N	2.46	0.48
1:A:129:LYS:HE3	1:A:166:CYS:SG	2.54	0.48
1:B:37:TYR:HB3	1:B:223:LEU:HB3	1.96	0.48
1:B:106:PHE:HB3	1:B:235:ILE:HG12	1.96	0.48
1:B:1032:CYS:SG	1:B:1048:HIS:NE2	2.87	0.48
1:C:642:VAL:HG13	1:C:651:ILE:HB	1.95	0.48
2:D:47:TRP:HZ2	2:D:50:TRP:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:16:GLY:CA	3:G:78:LEU:HD23	2.43	0.48
1:A:516:GLU:HB3	1:A:518:LEU:HG	1.96	0.47
1:A:914:ASN:O	1:A:918:GLU:HG2	2.14	0.47
1:C:816:SER:O	1:C:820:ASP:HB2	2.14	0.47
1:A:308:VAL:HG12	1:A:602:THR:HG23	1.96	0.47
1:A:538:CYS:HB2	1:A:590:CYS:HB2	1.71	0.47
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.95	0.47
1:B:717:ASN:HB2	1:B:1071:GLN:HB2	1.96	0.47
3:G:46:PHE:HE2	3:G:49:TYR:HB3	1.78	0.47
1:A:296:LEU:O	1:A:299:THR:OG1	2.29	0.47
1:B:204:TYR:HB3	1:B:223:LEU:HG	1.95	0.47
1:B:519:HIS:CE1	1:C:42:VAL:HG22	2.50	0.47
1:B:905:ARG:O	1:B:1036:GLN:NE2	2.46	0.47
1:C:403:ARG:HH22	1:C:495:TYR:HD2	1.61	0.47
3:F:4:LEU:O	3:F:101:GLY:N	2.46	0.47
1:B:370:ASN:OD1	2:E:100(B):THR:OG1	2.23	0.47
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.96	0.47
1:B:1117:THR:OG1	1:B:1139:ASP:OD1	2.32	0.47
1:C:314:GLN:HA	1:C:596:SER:HA	1.95	0.47
1:C:1055:SER:OG	1:C:1056:ALA:N	2.47	0.47
1:A:115:GLN:HE21	1:A:130:VAL:HB	1.79	0.47
1:A:403:ARG:NH2	1:A:507:PRO:HA	2.29	0.47
1:A:598:ILE:HD11	1:A:666:ILE:HB	1.96	0.47
1:A:734:THR:HG21	1:A:959:LEU:HD11	1.97	0.47
1:C:387:LEU:HD23	1:C:390:LEU:HB2	1.97	0.47
1:C:743:CYS:HA	1:C:977:LEU:HD23	1.97	0.47
3:G:38:GLN:HA	3:G:44:PRO:HA	1.97	0.47
1:A:729:VAL:H	1:A:1059:GLY:HA2	1.79	0.47
1:A:788:ILE:HG13	1:C:699:LEU:HD23	1.96	0.47
1:A:1011:GLN:O	1:A:1015:ALA:HB2	2.15	0.47
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.50	0.47
2:E:29:PHE:CZ	2:E:76:THR:HG21	2.50	0.47
2:E:55:GLY:N	2:E:71:ARG:HH22	2.13	0.47
3:F:30:GLY:O	3:F:66:LYS:NZ	2.33	0.47
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.33	0.47
1:B:612:TYR:HE2	1:B:651:ILE:HD12	1.80	0.47
1:B:729:VAL:HG12	1:B:1059:GLY:HA2	1.95	0.47
1:B:886:TRP:HB3	1:B:1035:GLY:HA2	1.96	0.47
1:C:201:PHE:O	1:C:229:LEU:N	2.48	0.47
1:C:919:ASN:OD1	1:C:919:ASN:N	2.47	0.47
1:C:1081:ILE:O	1:C:1088:HIS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:PRO:HA	1:A:671:CYS:HB3	1.97	0.47
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.97	0.47
1:C:403:ARG:HD3	1:C:497:PHE:CD1	2.50	0.47
1:A:196:ASN:HA	1:A:232:GLY:H	1.80	0.46
1:A:494:SER:OG	1:A:495:TYR:N	2.48	0.46
1:B:83:VAL:HG21	1:B:237:ARG:HH11	1.78	0.46
1:C:406:GLU:O	1:C:410:ILE:HG12	2.15	0.46
2:E:32:TYR:CD2	2:E:94:ARG:HD3	2.50	0.46
3:G:14:ALA:HA	3:G:107:VAL:HG12	1.96	0.46
1:A:444:LYS:HE3	1:A:448:ASN:HA	1.96	0.46
1:A:1106:GLN:HG3	1:A:1108:ASN:H	1.79	0.46
1:B:430:THR:HB	1:C:983:ARG:HH22	1.79	0.46
1:B:600:PRO:HG2	1:B:605:SER:HB3	1.97	0.46
1:C:1018:ILE:O	1:C:1022:ALA:HB2	2.15	0.46
3:F:51:ASN:HB3	3:F:64:GLY:HA3	1.96	0.46
1:A:59:PHE:HB3	1:A:293:LEU:HD11	1.98	0.46
1:A:452:LEU:HD11	2:E:54:SER:HB3	1.98	0.46
1:C:420:ASP:OD1	1:C:454:ARG:N	2.48	0.46
2:D:29:PHE:HD2	2:D:71:ARG:HH22	1.62	0.46
1:A:126:VAL:HB	1:A:172:SER:H	1.80	0.46
1:A:395:VAL:HG12	1:A:515:PHE:HA	1.97	0.46
1:A:434:ILE:HD13	1:A:513:LEU:HD13	1.97	0.46
1:B:115:GLN:NE2	1:B:130:VAL:O	2.48	0.46
1:B:458:LYS:NZ	1:B:471:GLU:OE1	2.47	0.46
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.54	0.46
1:A:783:ALA:HB2	1:A:873:TYR:CE2	2.51	0.46
1:B:782:PHE:HA	1:B:877:LEU:HD11	1.97	0.46
1:C:386:LYS:HG3	1:C:390:LEU:HG	1.98	0.46
2:D:92:CYS:HB2	2:D:103:TRP:CD1	2.50	0.46
2:E:98:TYR:CE2	2:E:100:SER:HB3	2.50	0.46
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.96	0.46
3:G:37:HIS:CE1	3:G:48:ILE:HB	2.51	0.46
1:A:788:ILE:HG12	1:C:700:GLY:HA3	1.98	0.46
1:A:992:GLN:NE2	1:A:993:ILE:HG13	2.30	0.46
2:D:18:VAL:HG12	2:D:82(C):LEU:HD21	1.96	0.46
1:B:382:VAL:HG21	1:B:392:PHE:CZ	2.51	0.46
1:B:389:ASP:OD1	1:B:389:ASP:N	2.41	0.46
1:B:729:VAL:HG21	1:B:781:VAL:HG21	1.98	0.46
1:A:715:PRO:O	1:A:1110:TYR:N	2.47	0.46
1:A:756:TYR:HB3	1:A:759:PHE:CD2	2.51	0.46
1:B:710:ASN:OD1	1:B:710:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:SER:H	1:B:1048:HIS:CE1	2.34	0.46
1:C:666:ILE:HG12	1:C:670:ILE:O	2.16	0.46
1:A:102:ARG:HG2	1:A:141:LEU:HB2	1.98	0.46
1:B:712:ILE:HG21	1:B:1096:VAL:HG12	1.98	0.46
1:C:275:PHE:HE1	1:C:290:ASP:HB2	1.81	0.46
1:A:475:ALA:HB3	1:A:487:ASN:HA	1.98	0.45
1:A:598:ILE:HG13	1:A:666:ILE:HD13	1.97	0.45
1:A:997:ILE:O	1:A:1001:LEU:HB2	2.16	0.45
1:C:403:ARG:HD3	1:C:497:PHE:CE1	2.51	0.45
1:B:105:ILE:HD12	1:B:241:LEU:HB2	1.98	0.45
1:C:426:PRO:HG3	1:C:464:PHE:CZ	2.52	0.45
1:A:100:ILE:HD12	1:A:243:ALA:HB1	1.98	0.45
1:B:729:VAL:HG11	1:B:1060:VAL:HG23	1.98	0.45
1:C:90:VAL:HG11	1:C:238:PHE:HB3	1.99	0.45
1:C:329:PHE:HD1	1:C:330:PRO:HD2	1.80	0.45
1:C:709:ASN:HB3	4:C:1307:NAG:C7	2.47	0.45
3:G:15:PRO:HG3	3:G:82:ASP:HB2	1.98	0.45
3:G:15:PRO:CB	3:G:82:ASP:HB2	2.45	0.45
3:G:16:GLY:N	3:G:78:LEU:HD23	2.32	0.45
1:A:139:PRO:HB2	1:A:241:LEU:HD21	1.99	0.45
1:B:382:VAL:HG21	1:B:392:PHE:HZ	1.80	0.45
1:B:456:PHE:HB3	1:B:473:TYR:CG	2.52	0.45
1:C:458:LYS:HD3	1:C:473:TYR:HA	1.99	0.45
2:D:71:ARG:HH12	2:D:78:ALA:HB2	1.70	0.45
1:A:614:ASP:N	1:A:647:ALA:O	2.40	0.45
1:B:115:GLN:HG3	1:B:130:VAL:HB	1.97	0.45
1:B:455:LEU:HD22	1:B:493:GLN:HG3	1.98	0.45
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.81	0.45
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.98	0.45
1:A:912:THR:O	1:A:915:VAL:HG12	2.17	0.45
1:B:120:VAL:HG23	1:B:141:LEU:HD12	1.99	0.45
2:E:47:TRP:O	2:E:62:LYS:NZ	2.38	0.45
3:F:23:CYS:N	3:F:71:ALA:O	2.50	0.45
1:C:714:ILE:HG13	1:C:715:PRO:HD2	1.98	0.45
1:C:1021:SER:HA	1:C:1024:LEU:HB3	1.99	0.45
3:G:54:ARG:NH1	3:G:58:VAL:O	2.50	0.45
1:A:1018:ILE:O	1:A:1022:ALA:HB2	2.17	0.45
4:A:1306:NAG:O6	1:B:796:ASP:OD2	2.25	0.45
1:C:295:PRO:HA	1:C:298:GLU:HB2	1.98	0.45
1:C:408:ARG:NH1	3:F:21:ILE:O	2.49	0.45
1:A:364:ASP:HA	1:A:527:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:THR:H	1:A:869:MET:HB2	1.82	0.44
1:B:501:ASN:O	1:B:506:GLN:NE2	2.50	0.44
2:D:38:ARG:HD2	2:D:90:TYR:CD1	2.52	0.44
1:C:427:ASP:OD1	1:C:427:ASP:N	2.49	0.44
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.40	0.44
1:C:617:CYS:N	1:C:649:CYS:SG	2.91	0.44
1:A:386:LYS:NZ	1:B:981:LEU:O	2.35	0.44
1:A:543:PHE:HE2	1:A:552:LEU:HD11	1.81	0.44
1:C:56:LEU:HA	1:C:270:LEU:HD22	1.99	0.44
2:D:51:MET:HE1	2:D:71:ARG:CD	2.47	0.44
1:A:699:LEU:HD12	1:B:788:ILE:HA	1.98	0.44
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.00	0.44
1:B:737:ASP:HB2	1:B:740:MET:HB2	1.99	0.44
1:B:818:ILE:HA	1:B:821:LEU:HG	1.99	0.44
1:B:1024:LEU:O	1:B:1028:LYS:HB2	2.17	0.44
3:F:5:THR:OG1	3:F:24:THR:OG1	2.27	0.44
1:B:1038:LYS:HB2	1:B:1038:LYS:HE3	1.76	0.44
1:C:905:ARG:NE	1:C:1050:MET:HB3	2.32	0.44
2:E:5:VAL:HG23	2:E:23:LYS:HB3	2.00	0.44
2:E:90:TYR:N	2:E:106:GLY:O	2.47	0.44
1:A:357:ARG:HG3	1:B:230:PRO:HB3	1.99	0.44
1:A:570:ALA:HB2	1:B:963:VAL:HG13	1.99	0.44
1:A:656:VAL:HG22	1:A:658:ASN:H	1.82	0.44
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.70	0.44
1:B:88:ASP:OD1	1:B:88:ASP:N	2.49	0.44
1:B:271:GLN:HB2	1:B:273:ARG:HG3	2.00	0.44
1:C:229:LEU:HA	1:C:230:PRO:HD3	1.78	0.44
1:A:88:ASP:OD2	1:A:270:LEU:N	2.44	0.44
1:C:808:ASP:HB3	1:C:811:LYS:HG2	1.99	0.44
1:C:906:PHE:HB3	1:C:911:VAL:HG13	1.99	0.44
2:E:44:GLY:HA2	3:G:87:TYR:HE1	1.83	0.44
3:G:16:GLY:H	3:G:78:LEU:HD23	1.82	0.44
1:A:1007:TYR:O	1:A:1011:GLN:HG2	2.17	0.44
1:C:310:LYS:HG2	1:C:664:ILE:HD11	2.00	0.44
1:C:742:ILE:O	1:C:1000:ARG:NH2	2.51	0.44
2:D:72:ASN:HB2	2:D:77:THR:HB	1.99	0.44
1:C:725:GLU:OE1	1:C:1028:LYS:NZ	2.39	0.43
1:A:53:ASP:OD2	1:A:195:LYS:NZ	2.40	0.43
1:A:117:LEU:HA	1:A:130:VAL:HA	2.00	0.43
1:A:402:ILE:HD11	1:A:418:ILE:HG13	1.99	0.43
1:A:819:GLU:HA	1:A:822:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:THR:N	1:A:869:MET:HB2	2.32	0.43
1:B:612:TYR:CE2	1:B:651:ILE:HD12	2.53	0.43
1:B:700:GLY:HA3	1:C:787:GLN:HA	1.99	0.43
1:B:734:THR:HG21	1:B:959:LEU:HD21	2.00	0.43
3:G:78:LEU:HD23	3:G:78:LEU:HA	1.84	0.43
1:A:357:ARG:HH21	1:B:230:PRO:HA	1.83	0.43
1:C:722:VAL:HG21	1:C:934:ILE:HD11	2.00	0.43
1:A:598:ILE:HG23	1:A:664:ILE:HD13	1.99	0.43
1:A:954:GLN:O	1:A:958:ALA:HB2	2.19	0.43
1:A:978:ASN:O	1:A:982:SER:OG	2.30	0.43
1:B:804:GLN:HG2	1:B:805:ILE:HG23	1.99	0.43
1:B:861:LEU:HD12	1:B:862:PRO:HD2	2.00	0.43
1:A:126:VAL:HB	1:A:171:VAL:HA	2.00	0.43
1:A:356:LYS:NZ	1:A:357:ARG:O	2.44	0.43
1:A:364:ASP:OD1	1:A:364:ASP:N	2.52	0.43
1:A:567:ARG:HB3	1:A:571:ASP:HA	2.01	0.43
1:A:785:VAL:HG22	1:A:787:GLN:H	1.84	0.43
1:A:963:VAL:HG11	1:C:570:ALA:HB1	2.01	0.43
1:A:985:ASP:OD1	1:A:985:ASP:N	2.52	0.43
1:C:650:LEU:HD22	1:C:666:ILE:HD13	2.01	0.43
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.99	0.43
1:C:759:PHE:O	1:C:763:LEU:HB2	2.19	0.43
3:F:84:ALA:O	3:F:105:LEU:N	2.51	0.43
1:A:33:THR:HB	1:A:220:PHE:HD1	1.83	0.43
1:A:656:VAL:HG11	1:A:693:ILE:HD12	2.01	0.43
1:A:950:ASP:OD1	1:A:951:VAL:N	2.52	0.43
1:B:29:THR:N	1:B:62:VAL:O	2.50	0.43
1:C:660:TYR:HB2	1:C:695:TYR:CZ	2.54	0.43
1:C:1054:GLN:HB2	1:C:1061:VAL:HG13	2.01	0.43
1:A:369:TYR:CE1	1:A:385:THR:HA	2.53	0.43
1:A:895:GLN:HB2	1:C:713:ALA:H	1.83	0.43
1:A:1030:SER:HA	1:A:1034:LEU:HB2	2.01	0.43
1:B:336:CYS:HB2	1:B:361:CYS:HB3	1.83	0.43
1:B:879:ALA:O	1:B:883:THR:HG22	2.19	0.43
1:A:1116:THR:HG22	1:A:1138:TYR:HD2	1.84	0.43
1:B:296:LEU:HG	1:B:608:VAL:HG12	2.01	0.43
1:B:730:SER:HB2	1:B:774:GLN:NE2	2.27	0.43
1:A:497:PHE:HB3	1:A:507:PRO:HG3	2.01	0.43
1:A:555:SER:N	1:A:584:ILE:O	2.52	0.43
1:A:1000:ARG:O	1:A:1004:LEU:HB2	2.19	0.43
1:B:140:PHE:CG	1:B:244:LEU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:CYS:SG	1:C:362:VAL:N	2.92	0.43
2:D:63:PHE:CD2	2:D:67:VAL:HB	2.53	0.43
2:E:102:VAL:HG21	3:G:44:PRO:HB2	2.00	0.43
3:G:59:PRO:HB2	3:G:61:ARG:HG3	2.01	0.43
1:A:102:ARG:NH2	1:A:121:ASN:H	2.17	0.42
1:A:309:GLU:O	1:A:313:TYR:OH	2.34	0.42
1:A:443:SER:HB2	1:A:507:PRO:HG3	2.01	0.42
1:B:899:ALA:HB1	1:B:917:TYR:HE1	1.83	0.42
1:C:312:ILE:HG23	1:C:664:ILE:HG22	2.01	0.42
1:C:736:VAL:HG22	1:C:858:LEU:HB2	2.00	0.42
3:F:46:PHE:CE2	3:F:49:TYR:HB3	2.54	0.42
1:A:562:PHE:HE1	1:B:225:PRO:HB2	1.83	0.42
1:A:854:LYS:HD3	1:A:854:LYS:HA	1.87	0.42
1:A:938:LEU:HG	1:A:944:ALA:HB1	2.00	0.42
2:D:4:LEU:HD22	2:D:103:TRP:CE2	2.54	0.42
1:A:213:VAL:HG13	1:A:214:ARG:HD2	2.01	0.42
1:A:410:ILE:HG23	1:A:425:LEU:HD21	2.00	0.42
1:C:979:ASP:O	1:C:983:ARG:CB	2.68	0.42
1:C:1076:THR:N	1:C:1097:SER:O	2.46	0.42
2:D:91:PHE:HE1	2:D:105:GLN:HA	1.83	0.42
2:E:97:ARG:HH12	2:E:99:CYS:HA	1.83	0.42
1:B:546:LEU:HD11	1:B:573:THR:HG21	2.02	0.42
1:B:550:GLY:HA2	1:B:589:PRO:HA	2.01	0.42
1:B:869:MET:HA	1:B:872:GLN:HB2	2.00	0.42
1:C:555:SER:HB3	1:C:586:ASP:HB2	2.01	0.42
1:A:52:GLN:HB3	1:A:274:THR:HB	2.00	0.42
1:C:276:LEU:HD11	1:C:304:LYS:HA	2.02	0.42
1:C:732:THR:HG22	1:C:1058:HIS:CE1	2.54	0.42
2:E:32:TYR:CG	2:E:94:ARG:HD3	2.55	0.42
1:A:661:GLU:O	1:A:695:TYR:OH	2.36	0.42
3:G:36:TYR:HD1	3:G:99:PHE:HZ	1.66	0.42
1:A:996:LEU:O	1:A:1000:ARG:CB	2.54	0.42
1:B:377:PHE:HE2	1:B:384:PRO:HA	1.83	0.42
1:B:452:LEU:HB3	1:B:492:LEU:HG	2.00	0.42
1:C:448:ASN:HD22	1:C:495:TYR:HB2	1.85	0.42
1:C:458:LYS:HA	1:C:473:TYR:HD1	1.84	0.42
2:E:92:CYS:HB2	2:E:103:TRP:NE1	2.34	0.42
3:G:16:GLY:HA3	3:G:78:LEU:HA	2.01	0.42
1:A:186:PHE:N	1:A:212:LEU:O	2.52	0.42
1:A:989:ALA:HA	1:A:992:GLN:HG3	2.02	0.42
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLU:HB3	2:D:50:TRP:CE2	2.55	0.42
1:B:614:ASP:N	1:B:647:ALA:O	2.37	0.42
1:B:1109:PHE:HD2	1:B:1111:GLU:HG3	1.85	0.42
1:C:426:PRO:HG2	1:C:429:PHE:HB3	2.02	0.42
1:C:885:GLY:HA3	1:C:896:ILE:HD11	2.01	0.42
1:A:774:GLN:NE2	1:A:777:ASN:HD21	2.17	0.42
1:A:816:SER:OG	1:A:817:PHE:N	2.53	0.42
1:A:965:GLN:HA	1:A:968:SER:OG	2.20	0.42
1:A:1002:GLN:HB3	1:B:759:PHE:HZ	1.85	0.42
1:C:653:ALA:HB2	1:C:692:ILE:HG22	2.01	0.42
1:C:1006:THR:O	1:C:1010:GLN:CB	2.57	0.42
1:A:1011:GLN:O	1:A:1015:ALA:HB3	2.19	0.42
1:B:342:PHE:HE1	1:B:513:LEU:HD21	1.85	0.42
1:C:409:GLN:OE1	1:C:417:LYS:N	2.45	0.42
1:C:718:PHE:HE1	1:C:720:ILE:HG13	1.85	0.42
1:C:783:ALA:HB2	1:C:873:TYR:CE2	2.55	0.42
1:A:113:LYS:HB2	1:A:113:LYS:HE2	1.91	0.41
1:A:273:ARG:NH2	1:A:292:ALA:O	2.53	0.41
1:A:402:ILE:HG22	1:A:510:VAL:HG11	2.02	0.41
1:A:1029:MET:O	1:A:1034:LEU:N	2.32	0.41
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.54	0.41
1:B:374:PHE:HD1	1:B:436:TRP:HB3	1.85	0.41
1:B:950:ASP:OD1	1:B:951:VAL:N	2.53	0.41
1:B:1003:SER:O	1:B:1006:THR:OG1	2.35	0.41
1:C:106:PHE:HB3	1:C:235:ILE:HG13	2.02	0.41
1:C:557:LYS:NZ	1:C:558:LYS:O	2.46	0.41
1:C:1018:ILE:O	1:C:1022:ALA:CB	2.68	0.41
1:A:456:PHE:HE1	2:E:100(B):THR:HG22	1.85	0.41
1:A:729:VAL:HG21	1:A:781:VAL:HG11	2.02	0.41
1:A:865:LEU:HB3	1:A:870:ILE:HG13	2.02	0.41
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.85	0.41
1:B:738:CYS:HA	1:B:742:ILE:HD13	2.02	0.41
1:C:287:ASP:HB3	1:C:306:PHE:CE2	2.55	0.41
3:G:55:PRO:HD2	3:G:58:VAL:HG21	2.02	0.41
1:A:426:PRO:HG2	1:A:429:PHE:HB2	2.02	0.41
1:A:920:GLN:HA	1:A:923:ILE:HG22	2.02	0.41
1:A:960:ASN:O	1:A:964:LYS:HG2	2.21	0.41
1:A:1002:GLN:HB3	1:B:759:PHE:CZ	2.55	0.41
1:A:1014:ARG:O	1:A:1018:ILE:HG12	2.19	0.41
1:B:29:THR:OG1	1:B:64:TRP:HB2	2.19	0.41
1:B:331:ASN:HD21	4:B:1308:NAG:C7	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:SER:OG	1:B:350:VAL:N	2.53	0.41
1:B:924:ALA:O	1:B:928:ASN:ND2	2.53	0.41
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.53	0.41
1:B:374:PHE:HA	1:B:436:TRP:HA	2.02	0.41
1:B:393:THR:HB	1:B:520:ALA:HB3	2.02	0.41
1:B:706:ALA:H	1:C:895:GLN:NE2	2.18	0.41
1:C:815:ARG:HE	1:C:815:ARG:HB2	1.65	0.41
3:F:21:ILE:HD13	3:F:103:THR:HG21	2.03	0.41
1:A:295:PRO:HD2	1:A:608:VAL:HG21	2.03	0.41
1:A:402:ILE:HD12	1:A:402:ILE:HA	1.88	0.41
1:A:963:VAL:HA	1:A:966:LEU:HD23	2.03	0.41
1:B:438:SER:HB2	1:B:509:ARG:HD3	2.03	0.41
1:B:552:LEU:HB3	1:B:585:LEU:HD12	2.02	0.41
3:G:13:GLY:N	3:G:106:THR:O	2.54	0.41
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.56	0.41
1:B:312:ILE:HB	1:B:664:ILE:HG23	2.03	0.41
1:B:716:THR:HA	1:B:1110:TYR:HB3	2.03	0.41
1:C:919:ASN:HB2	1:C:922:LEU:HB2	2.03	0.41
1:A:100:ILE:HB	1:A:243:ALA:HA	2.03	0.41
1:A:905:ARG:NE	1:A:1050:MET:HB3	2.24	0.41
1:B:187:LYS:HA	1:B:187:LYS:HD3	1.95	0.41
1:C:805:ILE:HG22	1:C:818:ILE:HD12	2.01	0.41
1:C:1080:ALA:HB3	1:C:1132:ILE:HG12	2.02	0.41
2:D:47:TRP:NE1	2:D:49:GLY:O	2.52	0.41
1:A:561:PRO:O	1:A:562:PHE:HB3	2.21	0.41
1:A:999:GLY:HA2	1:A:1002:GLN:HB2	2.03	0.41
1:C:194:PHE:HB3	1:C:201:PHE:CZ	2.56	0.41
1:C:805:ILE:HD13	1:C:1052:PHE:CE2	2.56	0.41
3:F:16:GLY:N	3:F:77:ARG:HG2	2.35	0.41
3:G:75:ILE:HG22	3:G:76:THR:H	1.86	0.41
1:A:35:GLY:HA2	1:A:91:TYR:CG	2.56	0.41
1:A:43:PHE:CE1	1:C:557:LYS:HE3	2.55	0.41
1:A:106:PHE:HD2	1:A:117:LEU:HD23	1.85	0.41
1:A:318:PHE:N	1:A:593:GLY:O	2.54	0.41
1:A:476:GLY:H	1:A:487:ASN:HB3	1.86	0.41
1:A:493:GLN:HE22	2:E:53:ILE:HD13	1.86	0.41
1:A:573:THR:HG22	1:A:587:ILE:HD13	2.02	0.41
1:B:55:PHE:C	1:B:270:LEU:HD22	2.41	0.41
1:B:103:GLY:HA3	1:B:241:LEU:HD23	2.03	0.41
1:B:137:ASN:OD1	1:B:137:ASN:N	2.54	0.41
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:HG13	1:B:947:LYS:HB3	2.03	0.41
1:B:1030:SER:HA	1:B:1034:LEU:HD12	2.02	0.41
1:C:581:THR:O	1:C:583:GLU:N	2.52	0.41
1:A:28:TYR:HB3	1:A:61:ASN:HB3	2.02	0.41
1:A:502:GLY:O	1:A:506:GLN:N	2.54	0.41
1:C:1089:PHE:HB2	1:C:1121:PHE:CZ	2.56	0.41
3:G:36:TYR:CD1	3:G:99:PHE:HZ	2.39	0.41
1:A:666:ILE:HG22	1:A:670:ILE:O	2.21	0.40
1:B:494:SER:HB3	2:D:30:THR:HG21	2.02	0.40
1:C:358:ILE:HD13	1:C:358:ILE:HA	1.96	0.40
2:D:6:GLN:HG3	2:D:103:TRP:HB3	2.03	0.40
1:A:1000:ARG:O	1:A:1004:LEU:CB	2.69	0.40
1:B:122:ASN:OD1	1:B:122:ASN:N	2.53	0.40
1:B:1006:THR:O	1:B:1010:GLN:HB2	2.20	0.40
1:C:727:LEU:HD23	1:C:727:LEU:HA	1.94	0.40
1:A:1020:ALA:O	1:A:1024:LEU:HB2	2.21	0.40
1:B:86:PHE:CE2	1:B:89:GLY:HA2	2.56	0.40
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.88	0.40
1:B:883:THR:O	1:B:896:ILE:N	2.44	0.40
1:C:328:ARG:HB3	1:C:543:PHE:CE1	2.57	0.40
1:C:816:SER:HB3	1:C:819:GLU:H	1.86	0.40
3:G:89:GLN:NE2	3:G:97:TRP:HD1	2.19	0.40
1:A:672:ALA:HA	1:A:693:ILE:O	2.21	0.40
1:B:273:ARG:HE	1:B:290:ASP:CG	2.25	0.40
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG21	2.57	0.40
1:C:866:THR:HG22	1:C:869:MET:HG2	2.04	0.40
1:C:1025:ALA:HA	1:C:1028:LYS:HB2	2.02	0.40
3:F:17:GLN:N	3:F:77:ARG:HD3	2.36	0.40
3:F:106:THR:OG1	3:F:107:VAL:N	2.53	0.40
1:A:200:TYR:HB3	1:A:201:PHE:H	1.75	0.40
1:A:966:LEU:HA	1:A:1000:ARG:NH2	2.36	0.40
1:B:1005:GLN:HA	1:B:1008:VAL:HG22	2.04	0.40
1:C:350:VAL:HB	1:C:451:TYR:HE1	1.85	0.40
1:C:396:TYR:HH	1:C:514:SER:H	1.65	0.40
1:C:408:ARG:NH1	3:F:20:THR:HB	2.37	0.40
1:C:734:THR:HG21	1:C:959:LEU:HD11	2.02	0.40
1:C:861:LEU:HD12	1:C:862:PRO:HD2	2.02	0.40
1:C:931:ILE:HD13	1:C:934:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	986/1259 (78%)	928 (94%)	57 (6%)	1 (0%)	51 84
1	B	986/1259 (78%)	933 (95%)	53 (5%)	0	100 100
1	C	986/1259 (78%)	915 (93%)	69 (7%)	2 (0%)	47 79
2	D	124/233 (53%)	113 (91%)	11 (9%)	0	100 100
2	E	124/233 (53%)	110 (89%)	14 (11%)	0	100 100
3	F	107/217 (49%)	90 (84%)	17 (16%)	0	100 100
3	G	107/217 (49%)	87 (81%)	20 (19%)	0	100 100
All	All	3420/4677 (73%)	3176 (93%)	241 (7%)	3 (0%)	54 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ILE
1	C	405	ASP
1	C	524	VAL

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	876/1096 (80%)	874 (100%)	2 (0%)	93 96
1	B	876/1096 (80%)	876 (100%)	0	100 100
1	C	876/1096 (80%)	869 (99%)	7 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	102/195 (52%)	102 (100%)	0	100 100
2	E	102/195 (52%)	102 (100%)	0	100 100
3	F	88/181 (49%)	88 (100%)	0	100 100
3	G	88/181 (49%)	87 (99%)	1 (1%)	73 85
All	All	3008/4040 (74%)	2998 (100%)	10 (0%)	92 95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	SER
1	A	235	ILE
1	C	293	LEU
1	C	329	PHE
1	C	336	CYS
1	C	357	ARG
1	C	358	ILE
1	C	400	PHE
1	C	528	LYS
3	G	20	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	777	ASN
1	A	992	GLN
1	B	414	GLN
1	B	644	GLN
1	B	777	ASN
1	B	1005	GLN
1	B	1108	ASN
1	C	774	GLN
3	G	17	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 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	B	1306	1	14,14,15	0.25	0	17,19,21	0.31	0
4	NAG	A	1306	1	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	B	1307	1	14,14,15	0.66	0	17,19,21	1.95	2 (11%)
4	NAG	A	1303	1	14,14,15	0.75	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	C	1305	1	14,14,15	0.45	0	17,19,21	0.84	1 (5%)
4	NAG	A	1308	1	14,14,15	0.37	0	17,19,21	0.85	1 (5%)
4	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.34	0
4	NAG	C	1310	1	14,14,15	0.28	0	17,19,21	0.98	1 (5%)
4	NAG	B	1305	1	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	A	1304	1	14,14,15	0.62	0	17,19,21	0.65	0
4	NAG	B	1304	1	14,14,15	0.45	0	17,19,21	0.44	0
4	NAG	A	1309	1	14,14,15	0.31	0	17,19,21	1.10	2 (11%)
4	NAG	A	1310	-	14,14,15	0.37	0	17,19,21	0.79	1 (5%)
4	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1308	1	14,14,15	0.42	0	17,19,21	0.57	0
4	NAG	A	1307	1	14,14,15	0.53	0	17,19,21	0.95	2 (11%)
4	NAG	C	1301	1	14,14,15	0.32	0	17,19,21	0.91	1 (5%)
4	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	C	1307	1	14,14,15	0.93	1 (7%)	17,19,21	1.00	2 (11%)
4	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1304	1	14,14,15	0.53	0	17,19,21	0.98	2 (11%)
4	NAG	A	1302	1	14,14,15	0.40	0	17,19,21	0.82	1 (5%)
4	NAG	A	1305	1	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
4	NAG	C	1303	1	14,14,15	0.93	1 (7%)	17,19,21	1.39	1 (5%)
4	NAG	B	1302	1	14,14,15	0.98	1 (7%)	17,19,21	2.07	3 (17%)
4	NAG	C	1309	1	14,14,15	0.82	1 (7%)	17,19,21	1.97	2 (11%)
4	NAG	C	1308	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
4	NAG	C	1302	1	14,14,15	0.69	1 (7%)	17,19,21	1.43	3 (17%)

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	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1307	NAG	C1-C2	3.12	1.57	1.52
4	B	1302	NAG	C1-C2	3.08	1.56	1.52
4	C	1303	NAG	O5-C1	2.55	1.47	1.43
4	C	1309	NAG	C1-C2	2.54	1.56	1.52
4	A	1303	NAG	C1-C2	-2.17	1.49	1.52
4	C	1302	NAG	O5-C1	2.13	1.47	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1307	NAG	C2-N2-C7	6.89	132.71	122.90
4	C	1309	NAG	C2-N2-C7	6.88	132.71	122.90
4	B	1302	NAG	C2-N2-C7	6.74	132.50	122.90
4	C	1303	NAG	C1-O5-C5	5.30	119.38	112.19
4	C	1302	NAG	C2-N2-C7	3.99	128.59	122.90
4	B	1302	NAG	C1-O5-C5	3.49	116.92	112.19
4	B	1307	NAG	C1-C2-N2	3.20	115.95	110.49
4	A	1302	NAG	C1-O5-C5	3.09	116.38	112.19
4	C	1309	NAG	C1-C2-N2	3.08	115.76	110.49
4	A	1309	NAG	C1-O5-C5	3.00	116.25	112.19
4	A	1305	NAG	C1-O5-C5	2.98	116.23	112.19
4	C	1301	NAG	C2-N2-C7	2.85	126.96	122.90
4	B	1302	NAG	C1-C2-N2	2.85	115.35	110.49
4	C	1307	NAG	C1-O5-C5	2.80	115.99	112.19
4	A	1303	NAG	C3-C4-C5	2.78	115.19	110.24
4	C	1310	NAG	C2-N2-C7	2.69	126.73	122.90
4	C	1302	NAG	C1-O5-C5	2.59	115.71	112.19
4	C	1304	NAG	C1-O5-C5	2.49	115.57	112.19
4	A	1309	NAG	C2-N2-C7	2.48	126.44	122.90
4	C	1308	NAG	C2-N2-C7	2.44	126.38	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1310	NAG	C2-N2-C7	2.42	126.36	122.90
4	A	1307	NAG	C1-O5-C5	2.42	115.47	112.19
4	A	1307	NAG	C2-N2-C7	2.37	126.28	122.90
4	C	1305	NAG	C2-N2-C7	2.31	126.19	122.90
4	A	1308	NAG	C2-N2-C7	2.30	126.18	122.90
4	C	1302	NAG	C1-C2-N2	2.17	114.19	110.49
4	C	1307	NAG	C2-N2-C7	2.15	125.96	122.90
4	C	1304	NAG	C2-N2-C7	2.11	125.91	122.90

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1310	NAG	C8-C7-N2-C2
4	C	1310	NAG	O7-C7-N2-C2
4	B	1303	NAG	C4-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	C	1310	NAG	C1-C2-N2-C7
4	A	1301	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	A	1310	NAG	C4-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	O5-C5-C6-O6
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1307	NAG	C8-C7-N2-C2
4	B	1307	NAG	O7-C7-N2-C2
4	C	1309	NAG	C8-C7-N2-C2
4	C	1309	NAG	O7-C7-N2-C2
4	A	1307	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	A	1308	NAG	C3-C2-N2-C7
4	A	1309	NAG	C3-C2-N2-C7
4	B	1302	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	C	1304	NAG	C3-C2-N2-C7
4	C	1305	NAG	C3-C2-N2-C7
4	C	1307	NAG	C3-C2-N2-C7
4	C	1309	NAG	C3-C2-N2-C7
4	C	1310	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1310	NAG	O5-C5-C6-O6
4	A	1307	NAG	C3-C2-N2-C7
4	A	1310	NAG	C3-C2-N2-C7
4	C	1301	NAG	C3-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7
4	C	1308	NAG	C3-C2-N2-C7
4	B	1304	NAG	O5-C5-C6-O6
4	C	1301	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1306	NAG	1	0
4	B	1308	NAG	1	0
4	C	1307	NAG	3	0
4	A	1302	NAG	1	0

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.

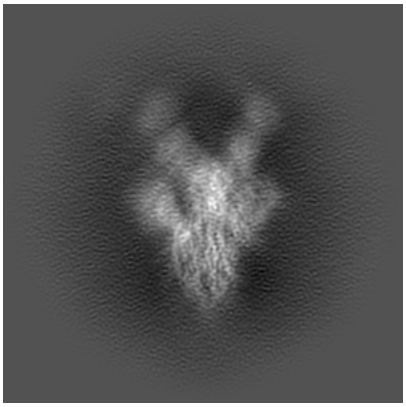
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23696. These allow visual inspection of the internal detail of the map and identification of artifacts.

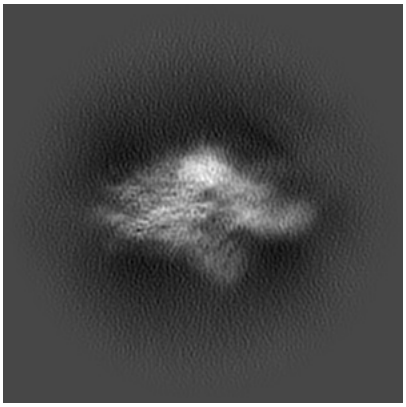
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

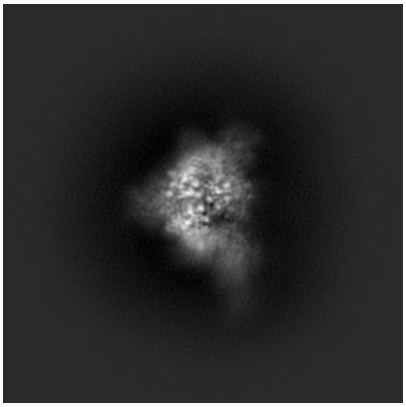
6.1.1 Primary map



X



Y

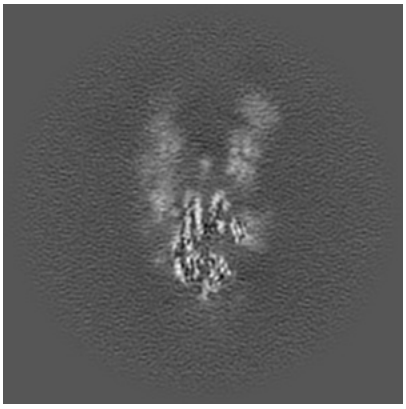


Z

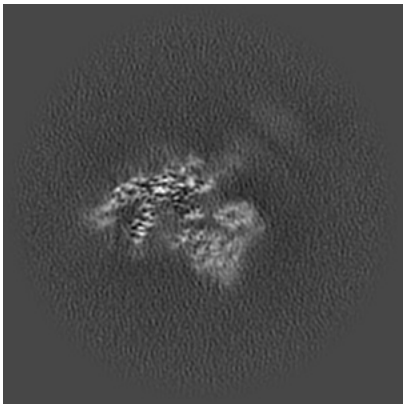
The images above show the map projected in three orthogonal directions.

6.2 Central slices

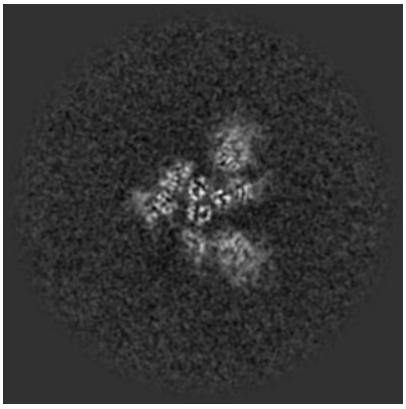
6.2.1 Primary map



X Index: 216



Y Index: 216

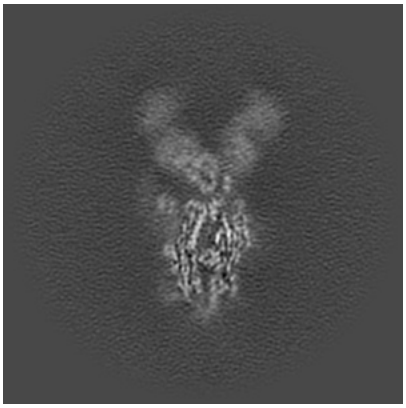


Z Index: 216

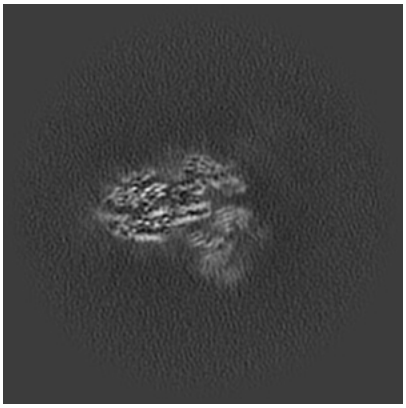
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

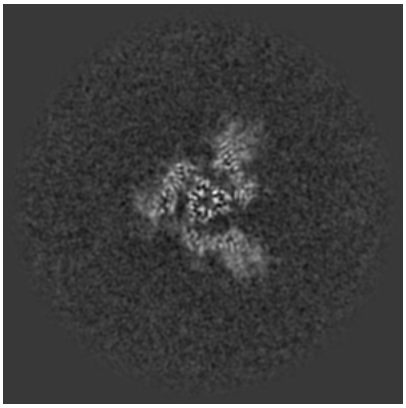
6.3.1 Primary map



X Index: 202



Y Index: 227



Z Index: 212

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

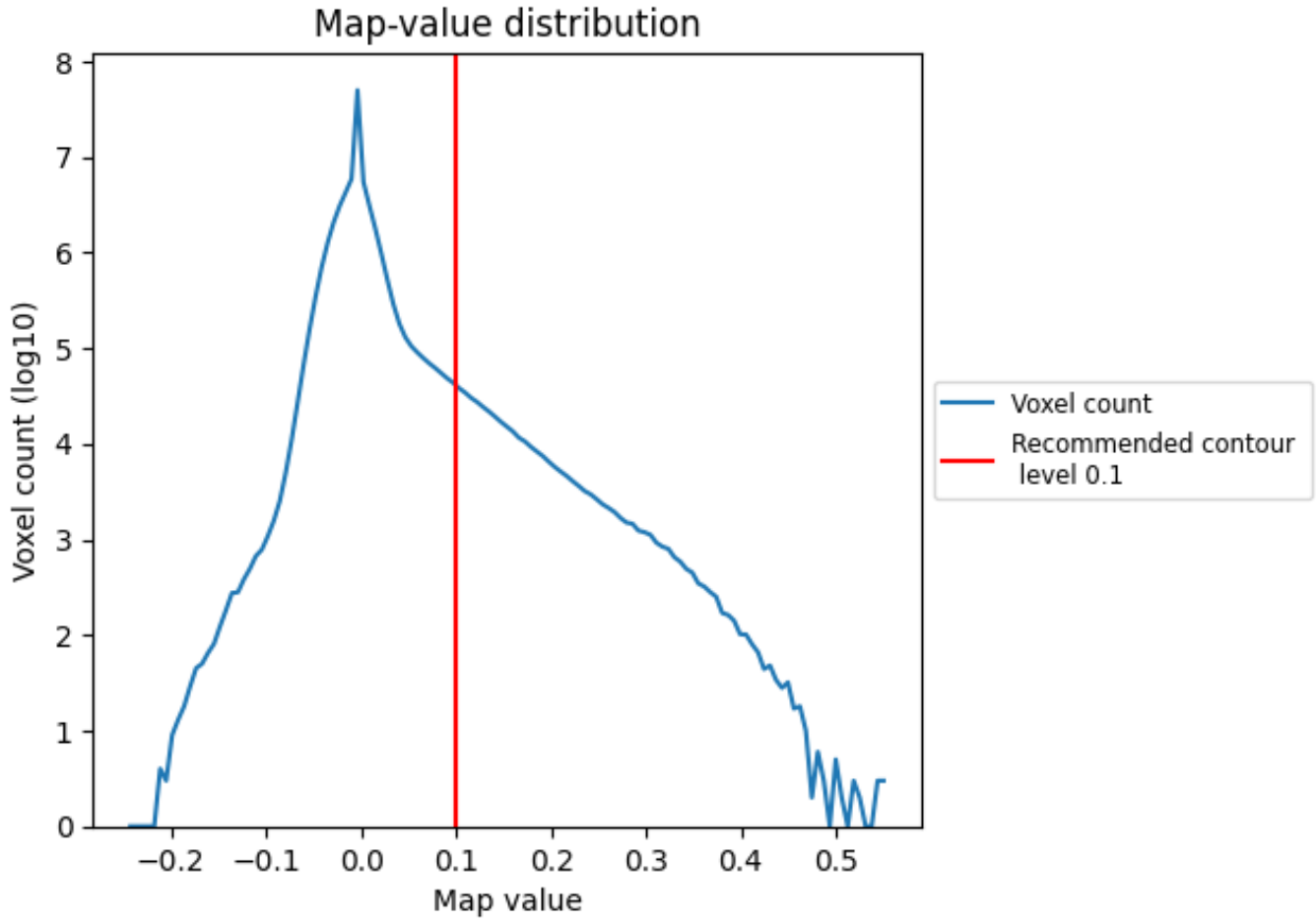
6.5 Mask visualisation (i)

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

7 Map analysis

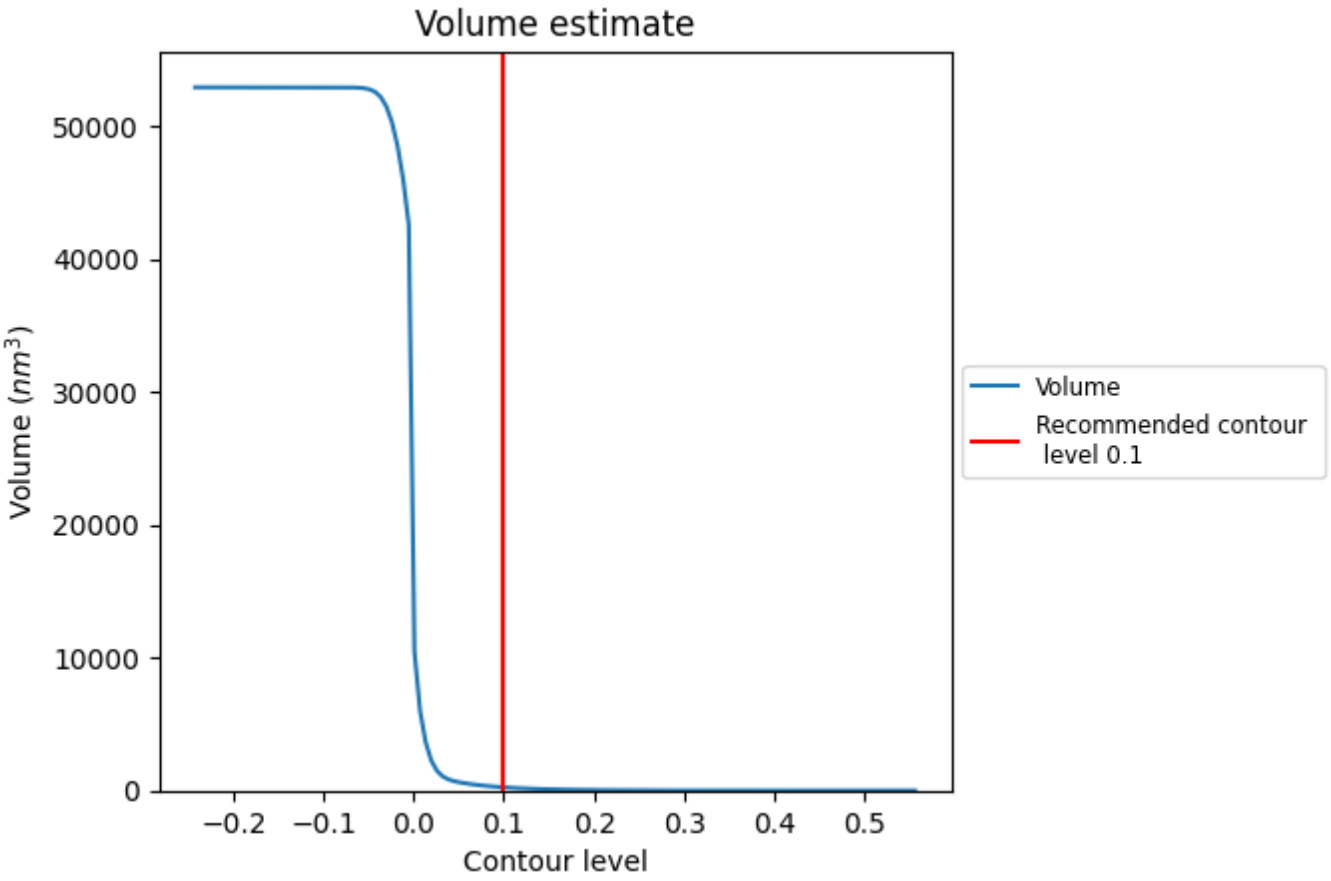
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

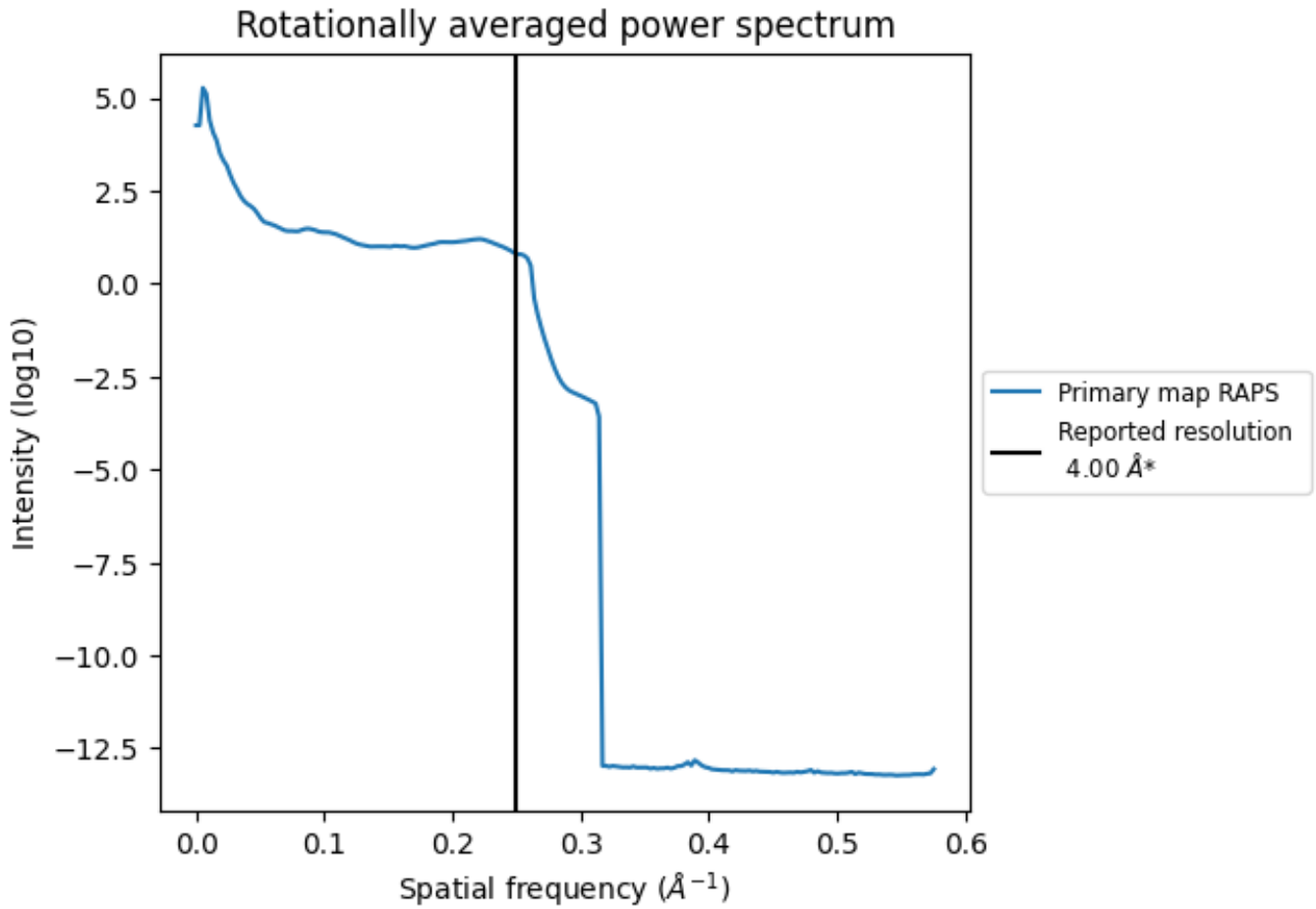
7.2 Volume estimate



The volume at the recommended contour level is 243 nm^3; this corresponds to an approximate mass of 219 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)

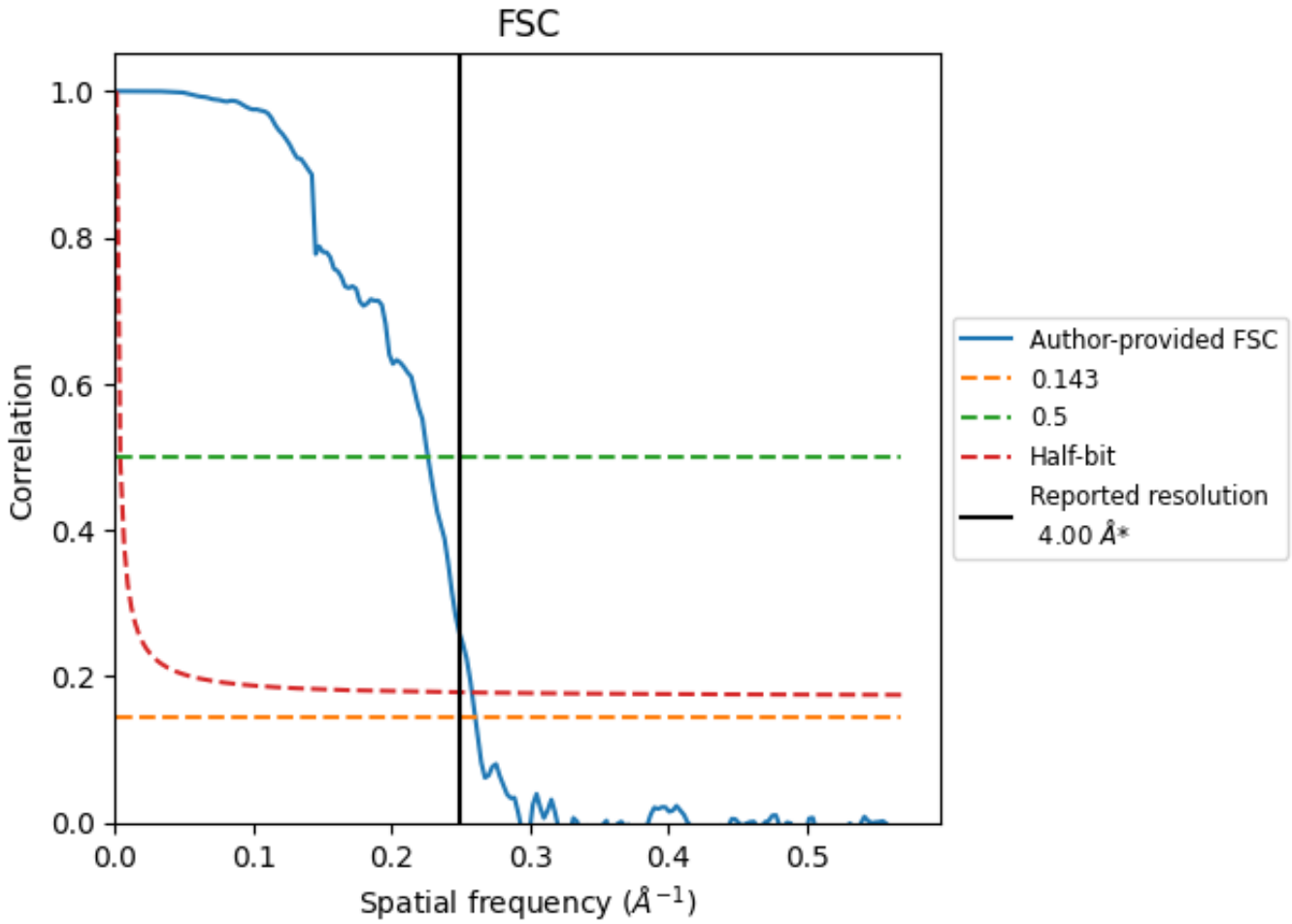


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

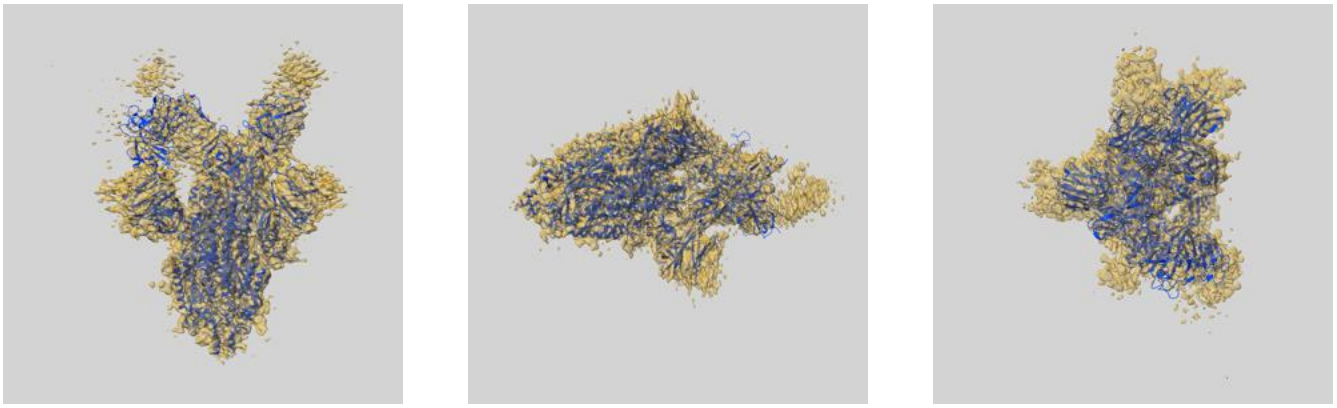
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.83	4.42	3.87
Unmasked-calculated*	-	-	-

*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-23696 and PDB model 7M6H. Per-residue inclusion information can be found in section 3 on page 10.

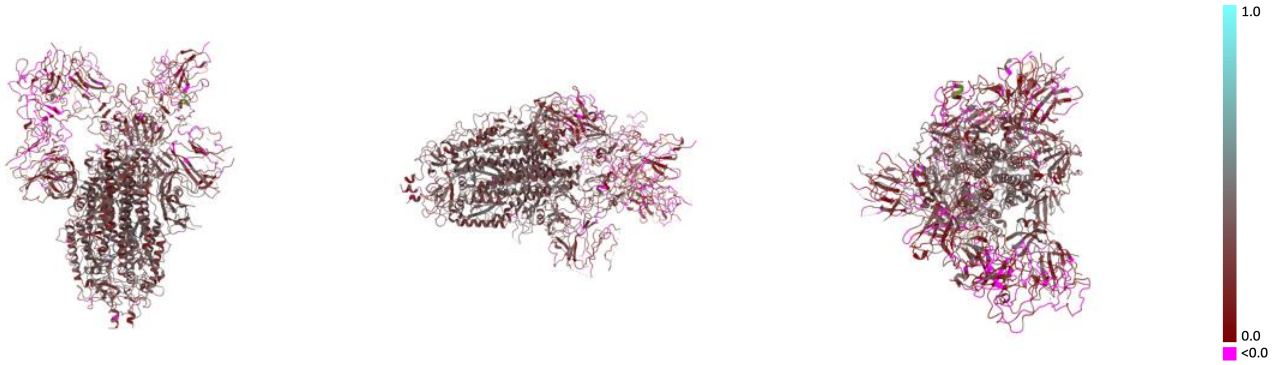
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

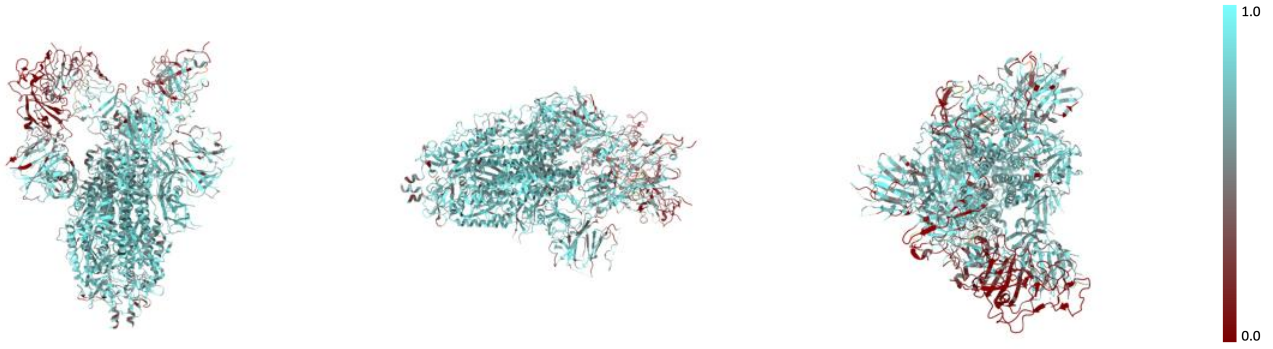
9.2 Q-score mapped to coordinate model (i)



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.

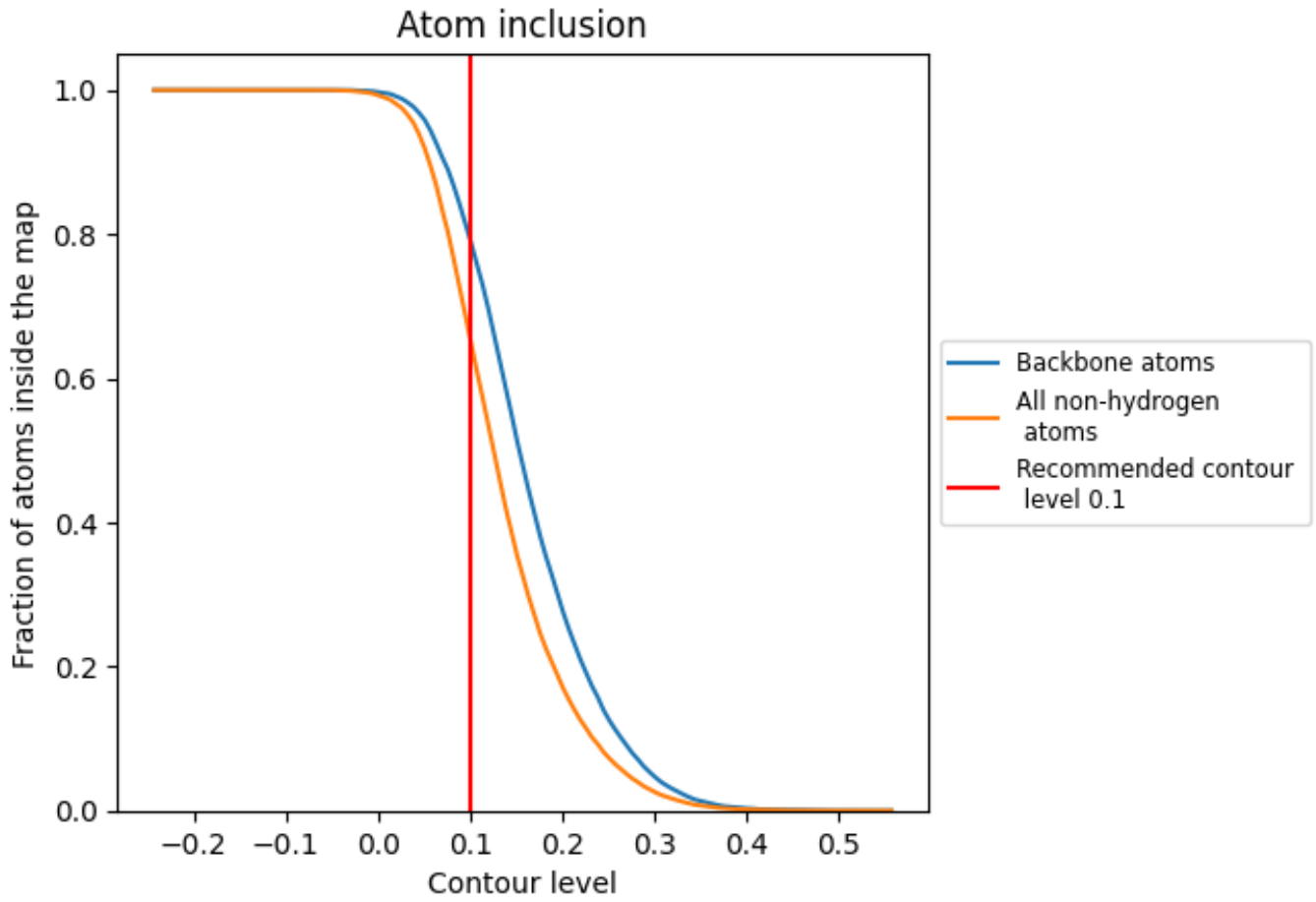
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 65% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6533	0.2540
A	0.7224	0.2790
B	0.7325	0.2890
C	0.6013	0.2490
D	0.4473	0.1500
E	0.5774	0.1590
F	0.3025	0.1110
G	0.3810	0.0980