Full wwPDB EM Validation Report

Nov 4, 2024 – 01:29 AM EST

PDB ID	:	8G7A
EMDB ID	:	EMD-29804
Title	:	SARS-CoV-2 spike/Nb3 complex with 2 RBDs up and 3 Nb3 (local refinement)
Authors	:	Ye, G.; Bu, F.; Liu, B.; Li, F.
Deposited on	:	2023-02-16
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:

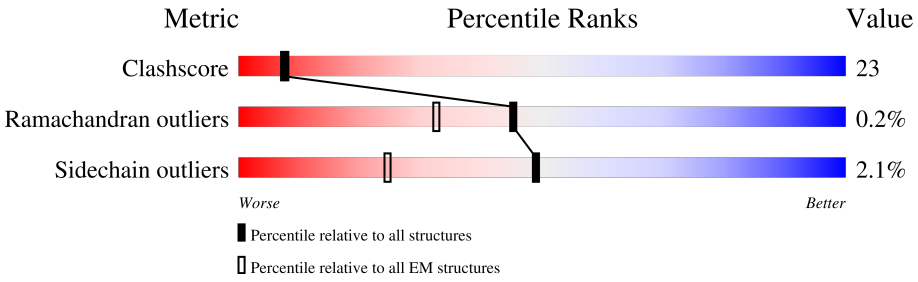
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	136	68% 56% 28% • 15%
1	E	136	79% 51% 32% • 15%
1	F	136	68% 45% 37% • 15%
2	A	1234	5% 33% 13% 54%
2	B	1234	9% 31% 14% • 54%
2	D	1234	8% 31% 14% 54%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16237 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 Nanosota-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	115	Total	C	N	O	S	0	0
			877	546	154	172	5		
1	C	115	Total	C	N	O	S	0	0
			877	546	154	172	5		
1	F	115	Total	C	N	O	S	0	0
			877	546	154	172	5		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	567	Total	C	N	O	S	0	0
			4526	2910	753	845	18		
2	B	567	Total	C	N	O	S	0	0
			4526	2910	753	845	18		
2	D	567	Total	C	N	O	S	0	0
			4526	2910	753	845	18		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	conflict	UNP P0DTC2
A	682	ALA	ARG	conflict	UNP P0DTC2
A	683	GLY	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLY	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	682	ALA	ARG	conflict	UNP P0DTC2
B	683	GLY	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLY	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
D	614	GLY	ASP	conflict	UNP P0DTC2
D	682	ALA	ARG	conflict	UNP P0DTC2
D	683	GLY	ARG	conflict	UNP P0DTC2
D	817	PRO	PHE	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2

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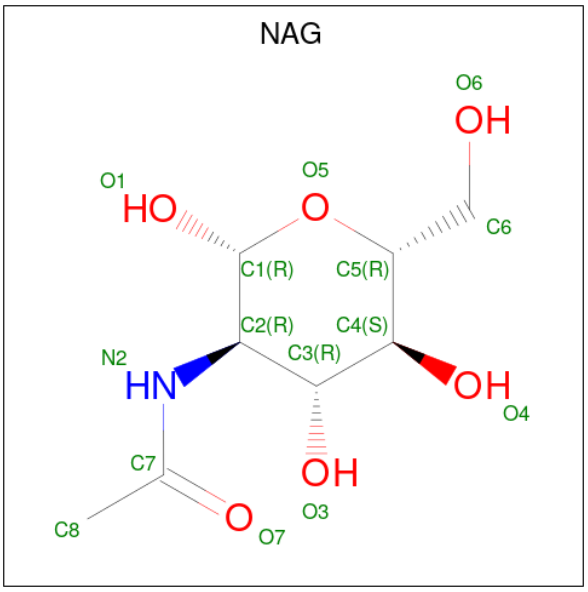
Chain	Residue	Modelled	Actual	Comment	Reference
D	986	PRO	LYS	conflict	UNP P0DTC2
D	987	PRO	VAL	conflict	UNP P0DTC2
D	1212	GLY	-	expression tag	UNP P0DTC2
D	1213	SER	-	expression tag	UNP P0DTC2
D	1214	GLY	-	expression tag	UNP P0DTC2
D	1215	TYR	-	expression tag	UNP P0DTC2
D	1216	ILE	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	GLU	-	expression tag	UNP P0DTC2
D	1219	ALA	-	expression tag	UNP P0DTC2
D	1220	PRO	-	expression tag	UNP P0DTC2
D	1221	ARG	-	expression tag	UNP P0DTC2
D	1222	ASP	-	expression tag	UNP P0DTC2
D	1223	GLY	-	expression tag	UNP P0DTC2
D	1224	GLN	-	expression tag	UNP P0DTC2
D	1225	ALA	-	expression tag	UNP P0DTC2
D	1226	TYR	-	expression tag	UNP P0DTC2
D	1227	VAL	-	expression tag	UNP P0DTC2
D	1228	ARG	-	expression tag	UNP P0DTC2
D	1229	LYS	-	expression tag	UNP P0DTC2
D	1230	ASP	-	expression tag	UNP P0DTC2
D	1231	GLY	-	expression tag	UNP P0DTC2
D	1232	GLU	-	expression tag	UNP P0DTC2
D	1233	TRP	-	expression tag	UNP P0DTC2
D	1234	VAL	-	expression tag	UNP P0DTC2
D	1235	LEU	-	expression tag	UNP P0DTC2
D	1236	LEU	-	expression tag	UNP P0DTC2
D	1237	SER	-	expression tag	UNP P0DTC2
D	1238	THR	-	expression tag	UNP P0DTC2
D	1239	PHE	-	expression tag	UNP P0DTC2
D	1240	LEU	-	expression tag	UNP P0DTC2
D	1241	GLY	-	expression tag	UNP P0DTC2
D	1242	HIS	-	expression tag	UNP P0DTC2
D	1243	HIS	-	expression tag	UNP P0DTC2
D	1244	HIS	-	expression tag	UNP P0DTC2
D	1245	HIS	-	expression tag	UNP P0DTC2
D	1246	HIS	-	expression tag	UNP P0DTC2
D	1247	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



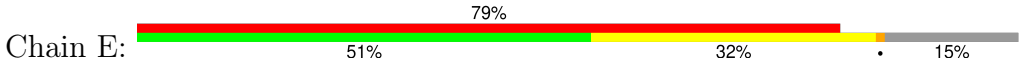
Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C N O 14 8 1 5	0
3	D	1	Total C N O 14 8 1 5	0

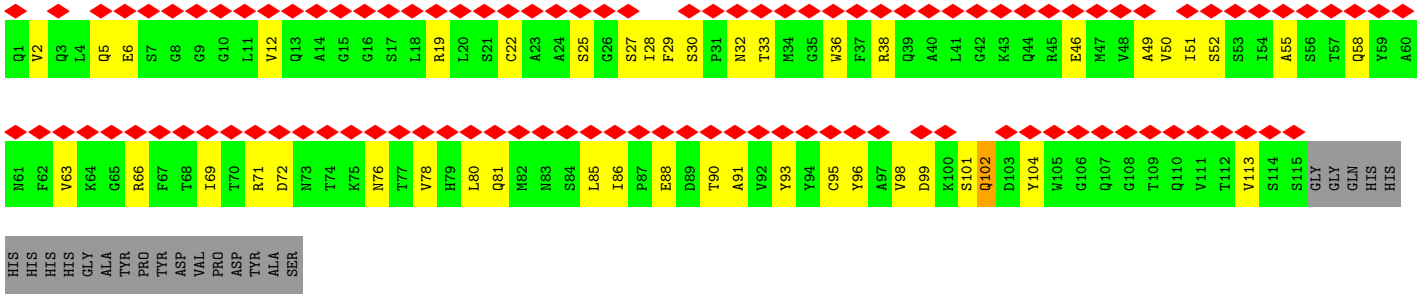
3 Residue-property plots (i)

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: Nanosota-3

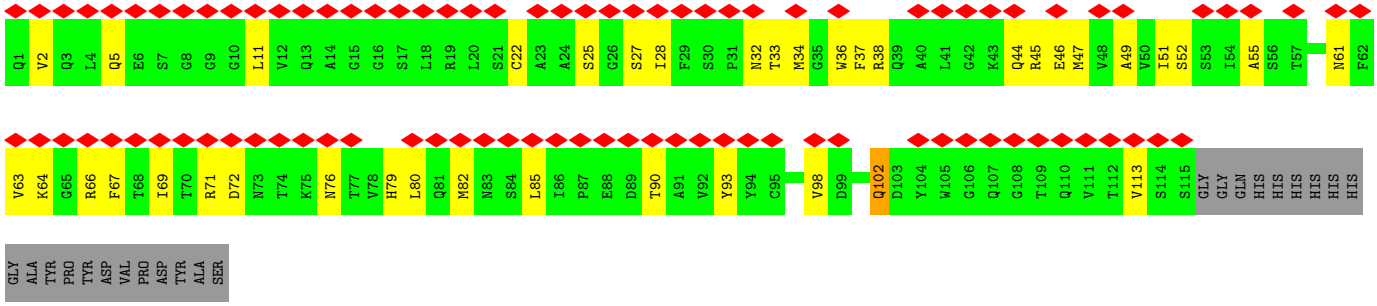
Chain E:





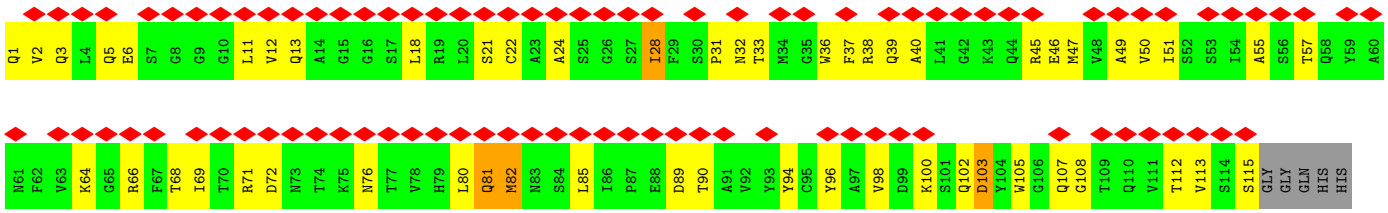
- Molecule 1: Nanosota-3

Chain C:



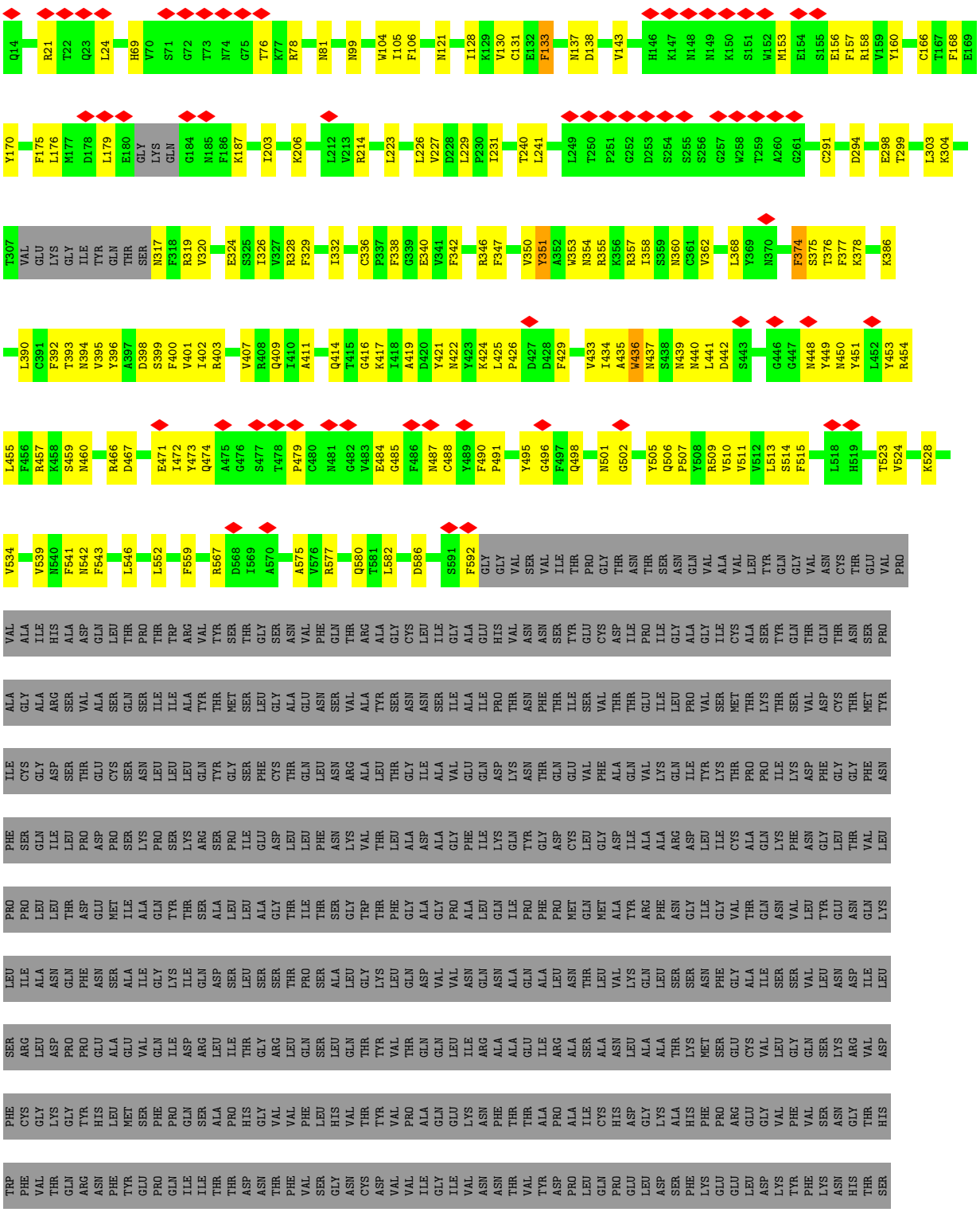
- Molecule 1: Nanosota-3

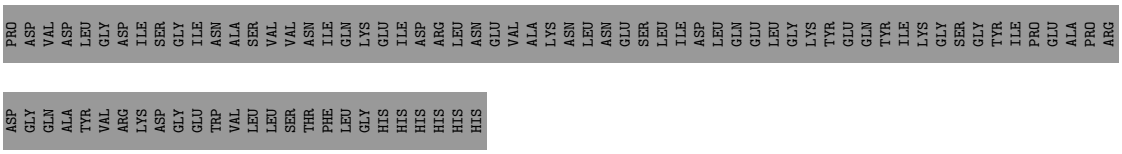
Chain F:



• Molecule 2: Spike glycoprotein

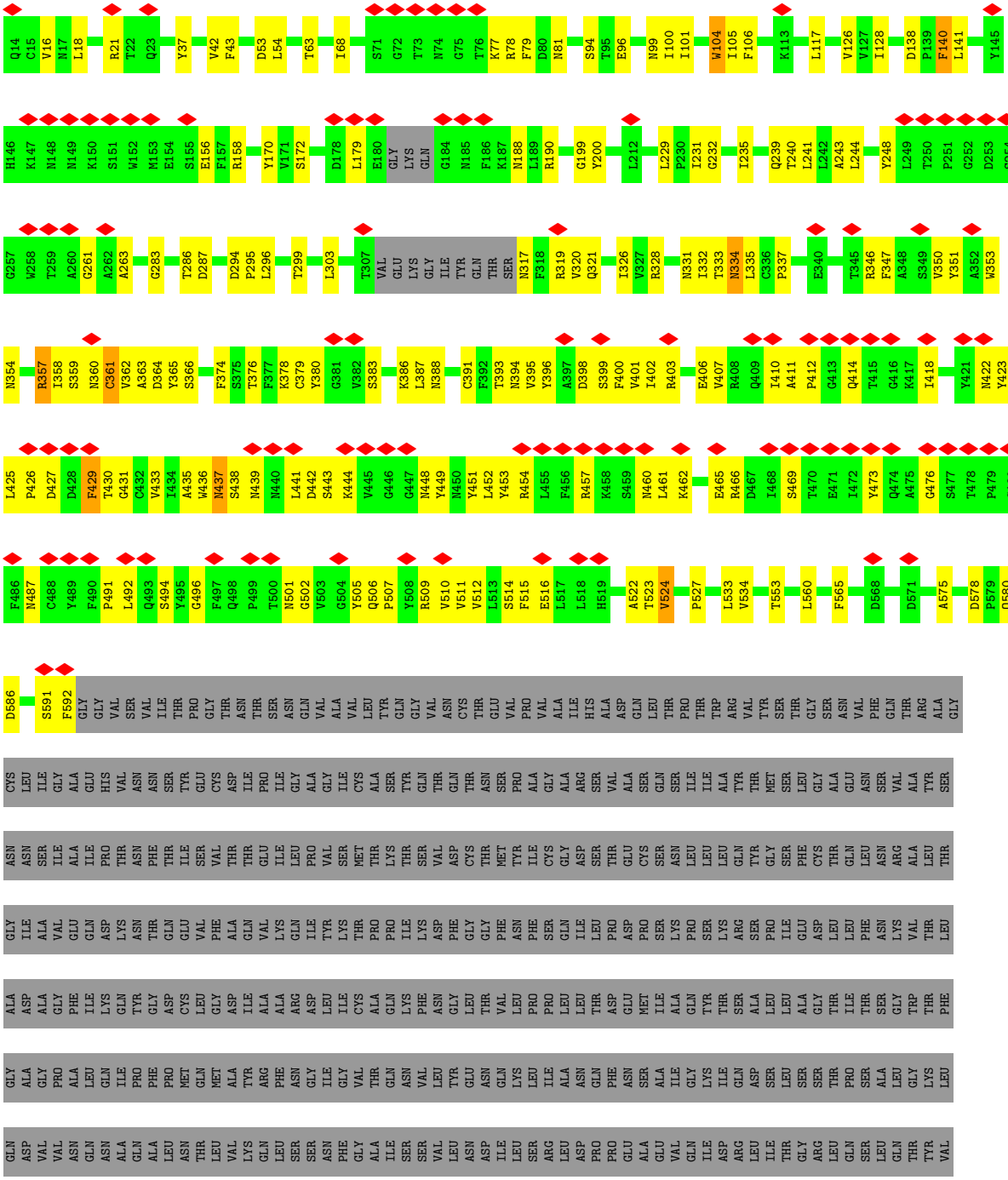
Chain A:

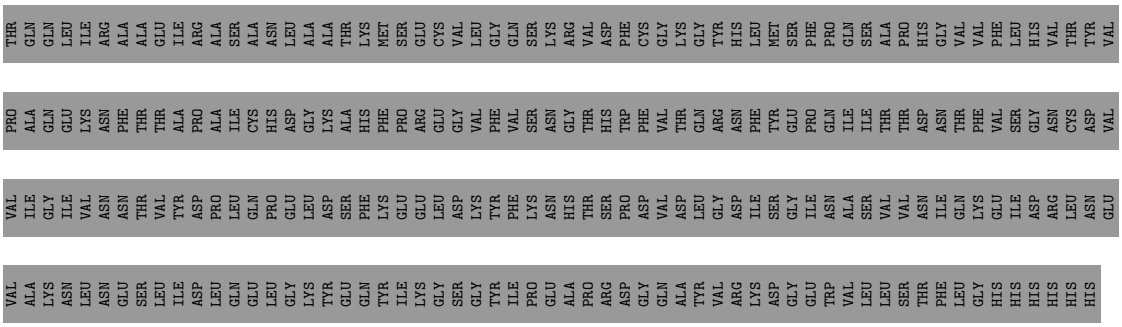




• Molecule 2: Spike glycoprotein

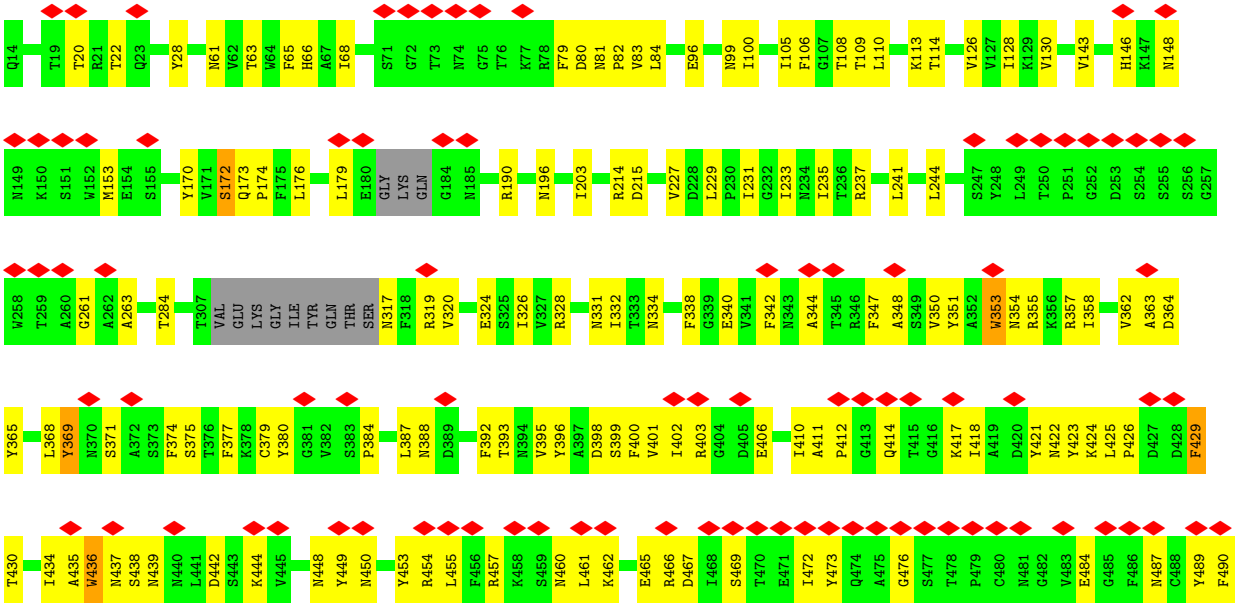
Chain B:

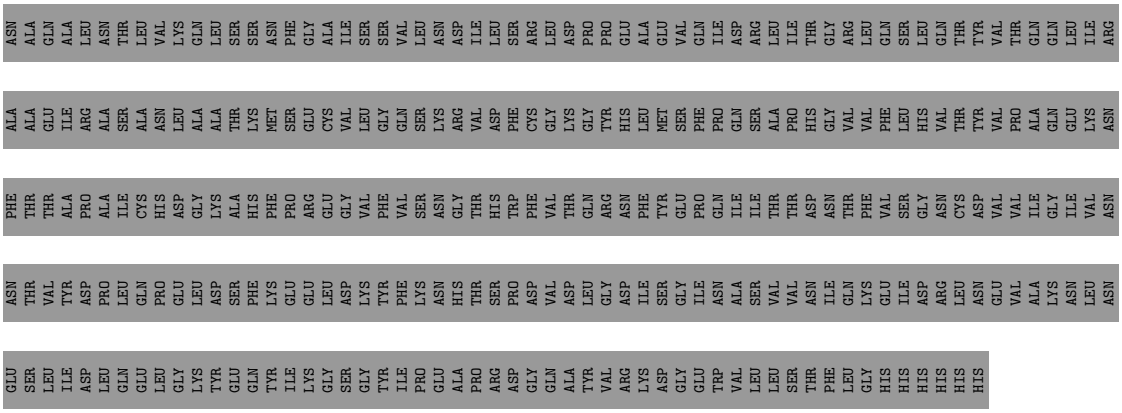




• Molecule 2: Spike glycoprotein

Chain D:




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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.041	Depositor
Minimum map value	-0.817	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0585	Depositor
Map size (Å)	335.80002, 335.80002, 335.80002	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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	0.29	0/892	0.60	0/1207
1	E	0.28	0/892	0.56	0/1207
1	F	0.30	0/892	0.61	0/1207
2	A	0.36	0/4649	0.56	0/6327
2	B	0.37	0/4649	0.57	0/6327
2	D	0.38	0/4649	0.57	0/6327
All	All	0.36	0/16623	0.57	0/22602

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	877	0	856	45	0
1	E	877	0	856	68	0
1	F	877	0	856	43	0
2	A	4526	0	4371	172	0
2	B	4526	0	4369	191	0
2	D	4526	0	4368	223	0
3	B	14	0	13	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	13	0	0
All	All	16237	0	15702	726	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 23.

All (726) 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:353:TRP:CD1	2:A:400:PHE:HE1	1.18	1.60
2:A:353:TRP:HD1	2:A:400:PHE:CE1	1.23	1.55
2:B:331:ASN:HD21	3:B:1301:NAG:C1	1.21	1.53
1:E:51:ILE:CG2	1:E:71:ARG:HH21	1.22	1.46
2:B:436:TRP:CH2	2:B:509:ARG:HD2	1.53	1.44
2:D:403:ARG:HD2	2:D:495:TYR:CE2	1.51	1.44
2:A:474:GLN:NE2	2:A:479:PRO:HA	1.31	1.40
2:A:350:VAL:O	2:A:353:TRP:CZ2	1.78	1.34
1:E:51:ILE:HG22	1:E:71:ARG:CZ	1.56	1.34
2:B:331:ASN:ND2	3:B:1301:NAG:C1	1.91	1.32
2:D:403:ARG:CD	2:D:495:TYR:CE2	2.10	1.32
1:E:51:ILE:CG2	1:E:71:ARG:NH2	1.81	1.30
2:B:436:TRP:CH2	2:B:509:ARG:CD	2.15	1.29
2:D:435:ALA:CB	2:D:510:VAL:HG22	1.61	1.29
1:E:102:GLN:NE2	1:E:104:TYR:CE1	1.98	1.28
1:E:101:SER:HB2	2:A:354:ASN:OD1	1.16	1.25
1:C:55:ALA:HA	1:C:71:ARG:NH1	1.52	1.22
2:A:347:PHE:HD2	2:A:399:SER:OG	1.17	1.22
2:A:347:PHE:CD2	2:A:399:SER:OG	1.93	1.21
2:D:65:PHE:HB3	2:D:80:ASP:OD2	1.40	1.21
2:D:369:TYR:HA	2:D:377:PHE:CE2	1.74	1.20
2:A:353:TRP:CD1	2:A:400:PHE:CE1	2.08	1.19
2:D:392:PHE:CE1	2:D:515:PHE:HD2	1.58	1.19
1:E:51:ILE:HG22	1:E:71:ARG:NH2	0.86	1.18
1:E:101:SER:CB	2:A:354:ASN:OD1	1.92	1.16
1:C:55:ALA:HA	1:C:71:ARG:CZ	1.75	1.16
2:B:400:PHE:CE1	2:B:402:ILE:CD1	2.30	1.14
2:A:353:TRP:HZ2	2:A:422:ASN:HB3	1.00	1.13
1:E:102:GLN:HG2	1:E:104:TYR:CZ	1.84	1.12
1:C:52:SER:O	1:C:71:ARG:NH2	1.81	1.12
2:D:392:PHE:CE1	2:D:515:PHE:CD2	2.37	1.11
2:B:436:TRP:CZ3	2:B:509:ARG:HD2	1.84	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ILE:HG21	1:E:71:ARG:HE	1.14	1.09
2:B:400:PHE:HE1	2:B:402:ILE:HD12	1.07	1.08
2:B:400:PHE:HE1	2:B:402:ILE:CD1	1.65	1.07
2:B:353:TRP:CH2	2:B:400:PHE:CE2	2.43	1.07
2:D:400:PHE:CE1	2:D:402:ILE:HD12	1.90	1.07
2:A:474:GLN:NE2	2:A:479:PRO:CA	2.18	1.07
2:D:369:TYR:HA	2:D:377:PHE:CZ	1.90	1.06
2:D:403:ARG:CG	2:D:495:TYR:HE2	1.67	1.06
2:D:392:PHE:CZ	2:D:515:PHE:CD2	2.42	1.06
1:E:51:ILE:CG2	1:E:71:ARG:CZ	2.28	1.05
1:E:52:SER:O	1:E:71:ARG:NH2	1.89	1.05
2:D:403:ARG:NH2	2:D:505:TYR:CE1	2.24	1.04
2:A:350:VAL:O	2:A:353:TRP:CE2	2.10	1.04
1:E:51:ILE:HG21	1:E:71:ARG:NE	1.72	1.03
2:A:353:TRP:CZ2	2:A:422:ASN:HB3	1.92	1.03
2:D:435:ALA:HB1	2:D:510:VAL:HG22	1.38	1.03
1:E:55:ALA:HA	1:E:71:ARG:NH1	1.74	1.03
2:B:400:PHE:CE1	2:B:402:ILE:HD12	1.89	1.02
2:D:435:ALA:HB2	2:D:510:VAL:HG22	1.39	1.02
1:E:102:GLN:CG	1:E:104:TYR:CZ	2.43	1.02
1:E:51:ILE:CG2	1:E:71:ARG:NE	2.23	1.01
1:E:52:SER:O	1:E:71:ARG:CZ	2.08	1.01
1:E:51:ILE:CG2	1:E:71:ARG:HE	1.74	1.00
2:A:353:TRP:CZ2	2:A:422:ASN:O	2.13	1.00
1:C:51:ILE:HD12	1:C:71:ARG:HE	1.26	1.00
2:B:332:ILE:HG23	2:B:362:VAL:HG11	1.42	0.99
2:A:374:PHE:HA	2:A:436:TRP:HB3	1.02	0.99
2:D:400:PHE:CE1	2:D:402:ILE:CD1	2.45	0.99
2:B:346:ARG:HD2	1:C:102:GLN:HE21	1.25	0.99
2:D:353:TRP:CZ2	2:D:400:PHE:CE2	2.51	0.98
2:D:403:ARG:HG3	2:D:495:TYR:HE2	1.27	0.98
2:D:400:PHE:CE1	2:D:510:VAL:HB	1.98	0.98
2:D:369:TYR:CD1	2:D:377:PHE:CD2	2.51	0.98
1:C:55:ALA:CA	1:C:71:ARG:NH1	2.26	0.98
2:B:334:ASN:O	2:B:362:VAL:HG23	1.63	0.98
2:A:374:PHE:HA	2:A:436:TRP:CB	1.94	0.97
2:D:403:ARG:CD	2:D:495:TYR:HE2	1.61	0.97
2:A:353:TRP:HZ2	2:A:422:ASN:CB	1.75	0.97
2:A:376:THR:HB	2:A:435:ALA:HB3	1.42	0.97
2:B:436:TRP:HH2	2:B:509:ARG:HD2	1.17	0.96
2:D:403:ARG:NH2	2:D:505:TYR:CD1	2.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:474:GLN:HE21	2:A:479:PRO:CA	1.76	0.96
2:A:374:PHE:CA	2:A:436:TRP:HB3	1.94	0.95
2:D:392:PHE:CZ	2:D:515:PHE:HD2	1.83	0.93
2:B:353:TRP:CH2	2:B:400:PHE:CZ	2.58	0.93
1:E:102:GLN:HG2	1:E:104:TYR:OH	1.69	0.92
2:B:374:PHE:HA	2:B:436:TRP:HB3	1.52	0.92
2:D:388:ASN:O	2:D:526:GLY:HA3	1.68	0.92
2:A:376:THR:CB	2:A:435:ALA:HB3	2.00	0.92
2:A:351:TYR:HA	2:A:353:TRP:CH2	2.03	0.91
1:C:55:ALA:N	1:C:71:ARG:HH12	1.69	0.91
1:F:51:ILE:HG21	1:F:71:ARG:HD2	1.50	0.91
1:E:6:GLU:HG2	1:E:22:CYS:SG	2.11	0.90
2:A:484:GLU:HG2	2:A:488:CYS:O	1.72	0.90
2:D:403:ARG:CG	2:D:495:TYR:CE2	2.49	0.89
2:B:436:TRP:HH2	2:B:509:ARG:CD	1.66	0.89
2:D:66:HIS:O	2:D:80:ASP:HB3	1.73	0.88
2:D:403:ARG:HG3	2:D:495:TYR:CE2	2.09	0.88
2:B:442:ASP:O	2:B:448:ASN:ND2	2.07	0.88
2:D:328:ARG:NH1	2:D:578:ASP:OD1	2.07	0.88
2:A:400:PHE:HB2	2:A:510:VAL:HB	1.57	0.86
1:E:102:GLN:NE2	1:E:104:TYR:HE1	1.50	0.86
2:A:398:ASP:O	2:A:511:VAL:HA	1.75	0.86
2:A:353:TRP:CH2	2:A:422:ASN:O	2.29	0.86
2:B:334:ASN:O	2:B:362:VAL:N	2.09	0.85
2:A:375:SER:N	2:A:435:ALA:O	2.09	0.85
2:A:394:ASN:ND2	2:B:200:TYR:OH	2.10	0.85
2:D:375:SER:HB3	2:D:435:ALA:O	1.77	0.85
2:A:473:TYR:HE2	2:A:491:PRO:HB3	1.42	0.85
2:A:376:THR:HB	2:A:435:ALA:CB	2.08	0.84
2:B:400:PHE:CE1	2:B:402:ILE:HD11	2.10	0.84
2:D:403:ARG:HD2	2:D:495:TYR:CD2	2.12	0.84
2:A:484:GLU:CD	2:A:485:GLY:N	2.31	0.84
2:B:436:TRP:CH2	2:B:509:ARG:HD3	2.13	0.83
2:D:79:PHE:CZ	2:D:244:LEU:HD12	2.12	0.83
2:D:371:SER:OG	2:D:374:PHE:CD2	2.31	0.82
2:B:353:TRP:CZ2	2:B:400:PHE:CE2	2.67	0.82
2:A:417:LYS:NZ	2:A:495:TYR:OH	2.14	0.81
1:E:55:ALA:H	1:E:71:ARG:HH12	1.26	0.81
2:D:369:TYR:CA	2:D:377:PHE:CE2	2.63	0.81
2:D:435:ALA:CB	2:D:510:VAL:CG2	2.53	0.80
1:F:32:ASN:HD21	1:F:76:ASN:HD21	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ILE:CB	1:E:71:ARG:HH21	1.95	0.79
1:C:55:ALA:CA	1:C:71:ARG:HH12	1.92	0.79
2:D:368:LEU:O	2:D:377:PHE:HZ	1.65	0.79
2:B:473:TYR:HE2	2:B:491:PRO:HB3	1.45	0.79
2:D:363:ALA:O	2:D:527:PRO:HD3	1.82	0.78
2:A:353:TRP:CZ2	2:A:422:ASN:CB	2.59	0.78
2:A:442:ASP:O	2:A:448:ASN:ND2	2.12	0.78
2:A:426:PRO:HD2	2:A:429:PHE:HB2	1.66	0.78
2:A:474:GLN:HE21	2:A:479:PRO:HA	0.96	0.78
1:C:63:VAL:HG12	1:C:66:ARG:HB2	1.66	0.78
2:D:423:TYR:HE1	2:D:466:ARG:HG2	1.49	0.78
2:D:436:TRP:NE1	2:D:509:ARG:HB2	1.99	0.78
1:E:52:SER:O	1:E:71:ARG:NH1	2.17	0.78
2:D:398:ASP:O	2:D:511:VAL:HA	1.83	0.77
2:B:140:PHE:CE2	2:B:244:LEU:HD12	2.19	0.77
2:D:557:LYS:NZ	2:D:574:ASP:OD2	2.19	0.76
2:A:332:ILE:HG22	2:A:362:VAL:HG23	1.68	0.76
2:B:363:ALA:O	2:B:527:PRO:HD3	1.84	0.76
2:B:398:ASP:O	2:B:511:VAL:HA	1.85	0.76
2:D:79:PHE:HZ	2:D:244:LEU:HA	1.50	0.76
2:D:454:ARG:NH2	2:D:469:SER:O	2.17	0.76
2:A:353:TRP:CZ2	2:A:422:ASN:C	2.59	0.75
2:D:371:SER:OG	2:D:374:PHE:CE2	2.38	0.75
2:D:392:PHE:CZ	2:D:515:PHE:CE2	2.75	0.75
2:A:496:GLY:O	2:A:501:ASN:ND2	2.18	0.75
2:B:353:TRP:CZ3	2:B:400:PHE:CE2	2.75	0.75
2:B:436:TRP:HH2	2:B:509:ARG:HD3	1.49	0.75
2:D:423:TYR:CE1	2:D:466:ARG:HG2	2.22	0.75
2:B:454:ARG:NH2	2:B:469:SER:O	2.19	0.74
2:D:435:ALA:HB2	2:D:510:VAL:CG2	2.16	0.74
2:D:392:PHE:CD1	2:D:515:PHE:HB3	2.22	0.74
2:A:353:TRP:CZ2	2:A:422:ASN:CA	2.71	0.74
2:B:353:TRP:CZ2	2:B:400:PHE:CZ	2.75	0.74
2:A:376:THR:HG23	2:A:378:LYS:HG2	1.70	0.74
1:C:38:ARG:O	1:C:46:GLU:N	2.18	0.74
2:A:454:ARG:HH12	2:A:467:ASP:HB2	1.50	0.74
1:C:11:LEU:HD12	1:C:11:LEU:O	1.88	0.74
1:C:52:SER:O	1:C:71:ARG:CZ	2.36	0.73
2:D:328:ARG:NH2	2:D:580:GLN:HB2	2.02	0.73
2:D:403:ARG:HD3	2:D:495:TYR:CE2	2.23	0.73
2:D:364:ASP:HB3	2:D:527:PRO:HG2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLN:CG	1:E:104:TYR:CE1	2.71	0.73
2:A:121:ASN:HD21	2:A:175:PHE:HB2	1.54	0.72
2:A:351:TYR:HA	2:A:353:TRP:CZ3	2.23	0.72
2:D:435:ALA:HB1	2:D:510:VAL:CG2	2.17	0.72
2:D:401:VAL:HG22	2:D:509:ARG:HG2	1.70	0.72
2:A:353:TRP:CH2	2:A:422:ASN:HA	2.24	0.72
2:A:437:ASN:OD1	2:A:507:PRO:O	2.08	0.71
2:B:53:ASP:OD1	2:B:54:LEU:N	2.23	0.71
2:D:436:TRP:O	2:D:509:ARG:N	2.22	0.71
2:A:105:ILE:HG23	2:A:241:LEU:HD11	1.73	0.71
2:D:353:TRP:CH2	2:D:400:PHE:HE2	2.09	0.71
1:E:58:GLN:HE22	2:A:471:GLU:HA	1.54	0.71
2:B:334:ASN:HB3	2:B:361:CYS:HA	1.71	0.71
1:F:5:GLN:O	1:F:22:CYS:HA	1.91	0.71
1:F:69:ILE:HG12	1:F:80:LEU:HD21	1.72	0.71
1:E:102:GLN:CD	1:E:104:TYR:CE1	2.65	0.70
2:D:79:PHE:CE2	2:D:244:LEU:HD13	2.26	0.70
1:E:63:VAL:HG22	1:E:66:ARG:HB2	1.73	0.70
2:B:319:ARG:HG3	2:B:320:VAL:HG23	1.73	0.70
2:D:473:TYR:HE2	2:D:491:PRO:HB3	1.55	0.70
2:D:442:ASP:O	2:D:448:ASN:ND2	2.22	0.70
1:C:33:THR:HB	1:C:98:VAL:HB	1.73	0.70
1:F:6:GLU:HG3	1:F:22:CYS:SG	2.31	0.70
1:F:51:ILE:CG2	1:F:71:ARG:HD2	2.20	0.69
1:E:55:ALA:CA	1:E:71:ARG:NH1	2.53	0.69
2:B:436:TRP:CH2	2:B:509:ARG:CB	2.75	0.69
1:C:55:ALA:H	1:C:71:ARG:HH12	1.38	0.69
2:B:376:THR:HB	2:B:378:LYS:HE3	1.74	0.69
2:B:351:TYR:CE1	2:B:453:TYR:HA	2.28	0.69
2:A:473:TYR:CE2	2:A:491:PRO:HB3	2.27	0.69
2:A:421:TYR:HD1	2:A:457:ARG:HB2	1.57	0.69
2:B:346:ARG:HD2	1:C:102:GLN:NE2	2.04	0.69
2:D:353:TRP:CH2	2:D:400:PHE:CE2	2.80	0.68
1:F:55:ALA:HA	1:F:71:ARG:HH11	1.58	0.68
1:E:102:GLN:HG3	1:E:102:GLN:O	1.93	0.68
2:B:353:TRP:CZ3	2:B:400:PHE:HE2	2.10	0.68
2:A:436:TRP:CD1	2:A:509:ARG:O	2.46	0.68
2:D:79:PHE:CZ	2:D:244:LEU:CD1	2.76	0.68
2:D:371:SER:OG	2:D:374:PHE:HD2	1.77	0.68
2:A:317:ASN:HD22	2:A:592:PHE:H	1.41	0.67
2:A:350:VAL:HG12	2:A:422:ASN:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:354:ASN:O	2:A:398:ASP:HA	1.94	0.67
2:B:454:ARG:HG2	2:B:491:PRO:HB2	1.75	0.67
2:D:369:TYR:HD1	2:D:377:PHE:CD2	2.11	0.67
2:A:326:ILE:HD11	2:A:534:VAL:HG22	1.75	0.67
1:F:90:THR:HG22	1:F:113:VAL:H	1.59	0.67
2:A:340:GLU:OE1	2:A:340:GLU:N	2.23	0.67
2:B:99:ASN:H	2:B:179:LEU:HD12	1.57	0.67
1:E:55:ALA:N	1:E:71:ARG:HH12	1.91	0.67
2:B:100:ILE:HD11	2:B:263:ALA:HB3	1.77	0.67
2:B:286:THR:O	2:B:287:ASP:OD1	2.13	0.67
2:B:117:LEU:HD22	2:B:231:ILE:HD13	1.77	0.66
2:B:294:ASP:HB3	2:B:295:PRO:CD	2.24	0.66
1:F:36:TRP:CE3	1:F:80:LEU:HD12	2.30	0.66
2:D:355:ARG:HD3	2:D:398:ASP:OD1	1.95	0.66
1:C:2:VAL:HG22	1:C:27:SER:H	1.59	0.66
2:D:369:TYR:CA	2:D:377:PHE:CZ	2.76	0.66
2:B:366:SER:HB3	2:B:388:ASN:HD21	1.59	0.66
2:B:439:ASN:O	2:B:443:SER:OG	2.13	0.66
2:D:353:TRP:CE2	2:D:400:PHE:CD2	2.84	0.66
2:B:358:ILE:HG22	2:B:524:VAL:HG11	1.78	0.65
2:D:425:LEU:HB3	2:D:429:PHE:CE2	2.32	0.65
2:B:332:ILE:HG22	2:B:335:LEU:HD21	1.77	0.65
1:E:102:GLN:HE21	1:E:104:TYR:HE1	0.72	0.65
2:B:331:ASN:HD21	3:B:1301:NAG:C2	2.07	0.65
2:D:380:TYR:CE2	2:D:412:PRO:HD3	2.32	0.65
2:B:357:ARG:HH22	2:B:359:SER:HB2	1.62	0.65
2:D:368:LEU:O	2:D:377:PHE:CZ	2.49	0.65
1:E:102:GLN:HG3	1:E:104:TYR:CZ	2.29	0.65
2:B:156:GLU:OE1	2:B:158:ARG:NH2	2.30	0.65
1:E:28:ILE:O	1:E:28:ILE:HG13	1.97	0.65
1:C:51:ILE:HD12	1:C:71:ARG:NE	2.07	0.65
2:B:436:TRP:CZ2	2:B:509:ARG:CB	2.80	0.64
2:D:369:TYR:CD1	2:D:377:PHE:CE2	2.85	0.64
1:C:55:ALA:HA	1:C:71:ARG:NH2	2.12	0.64
2:D:351:TYR:CE1	2:D:453:TYR:HA	2.33	0.64
2:D:82:PRO:O	2:D:84:LEU:HG	1.97	0.64
1:E:5:GLN:O	1:E:22:CYS:HA	1.98	0.64
2:D:326:ILE:HD12	2:D:539:VAL:HG21	1.79	0.64
2:D:437:ASN:HA	2:D:508:TYR:HA	1.80	0.64
2:B:444:LYS:HG3	2:B:448:ASN:HD21	1.62	0.63
2:D:400:PHE:CZ	2:D:402:ILE:HD12	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:484:GLU:CD	2:A:485:GLY:H	2.02	0.63
2:B:401:VAL:HG22	2:B:509:ARG:HG2	1.81	0.63
2:D:317:ASN:ND2	2:D:592:PHE:H	1.97	0.63
2:B:452:LEU:HB3	2:B:492:LEU:HB3	1.79	0.63
2:B:400:PHE:CD1	2:B:402:ILE:HG13	2.34	0.62
2:D:436:TRP:CD1	2:D:509:ARG:HB2	2.35	0.62
2:D:473:TYR:CE2	2:D:491:PRO:HB3	2.35	0.62
1:E:52:SER:N	1:E:71:ARG:NH2	2.47	0.62
2:D:380:TYR:O	2:D:430:THR:HA	1.99	0.62
2:D:513:LEU:HB3	2:D:515:PHE:HE1	1.63	0.62
2:B:406:GLU:HB3	2:B:418:ILE:HD12	1.80	0.62
2:B:401:VAL:HB	2:B:451:TYR:HE2	1.64	0.62
2:D:403:ARG:HH21	2:D:505:TYR:HD1	1.42	0.62
2:A:378:LYS:HB2	2:A:433:VAL:CG1	2.30	0.62
1:C:85:LEU:HB3	1:C:113:VAL:HG21	1.81	0.62
2:D:109:THR:OG1	2:D:114:THR:OG1	2.12	0.62
2:D:340:GLU:OE1	2:D:340:GLU:N	2.27	0.61
2:A:76:THR:OG1	2:A:78:ARG:NH1	2.33	0.61
2:A:421:TYR:CD1	2:A:457:ARG:HB2	2.35	0.61
2:A:395:VAL:HG23	2:A:524:VAL:HG11	1.81	0.61
2:D:355:ARG:HB2	2:D:466:ARG:HH22	1.66	0.61
2:A:472:ILE:HD11	2:A:490:PHE:CE1	2.36	0.61
2:B:436:TRP:CZ2	2:B:509:ARG:HB3	2.35	0.61
1:F:3:GLN:OE1	1:F:3:GLN:N	2.34	0.61
2:B:436:TRP:CH2	2:B:509:ARG:HB2	2.37	0.60
1:E:6:GLU:OE2	1:E:95:CYS:HB2	2.01	0.60
2:A:317:ASN:ND2	2:A:592:PHE:H	1.99	0.60
2:A:353:TRP:CH2	2:A:422:ASN:CA	2.83	0.60
2:A:353:TRP:O	2:A:466:ARG:NH1	2.34	0.60
2:D:332:ILE:O	2:D:332:ILE:HG22	1.99	0.60
2:D:403:ARG:HD2	2:D:495:TYR:CZ	2.28	0.60
2:D:425:LEU:HB3	2:D:429:PHE:HE2	1.66	0.60
2:A:346:ARG:NH2	2:A:347:PHE:O	2.34	0.60
2:B:436:TRP:CH2	2:B:509:ARG:CG	2.84	0.60
2:B:294:ASP:HB3	2:B:295:PRO:HD2	1.82	0.60
2:B:436:TRP:CZ3	2:B:509:ARG:HB2	2.36	0.60
2:D:100:ILE:HD11	2:D:263:ALA:HB3	1.82	0.60
2:B:436:TRP:CZ3	2:B:509:ARG:CD	2.70	0.60
2:A:319:ARG:HG3	2:A:320:VAL:HG23	1.84	0.60
2:A:357:ARG:NH2	2:A:396:TYR:OH	2.34	0.60
2:D:400:PHE:CZ	2:D:402:ILE:CD1	2.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:353:TRP:CE2	2:A:422:ASN:O	2.56	0.59
2:B:81:ASN:ND2	2:B:240:THR:O	2.35	0.59
2:A:400:PHE:N	2:A:510:VAL:O	2.35	0.59
2:B:400:PHE:CE1	2:B:402:ILE:CG1	2.85	0.59
2:B:128:ILE:HG21	2:B:229:LEU:HD21	1.84	0.59
2:A:376:THR:CG2	2:A:378:LYS:HG2	2.32	0.59
2:B:332:ILE:HG23	2:B:362:VAL:CG1	2.28	0.59
2:A:99:ASN:H	2:A:179:LEU:HD12	1.66	0.59
2:B:424:LYS:HE3	2:B:460:ASN:HB3	1.85	0.59
2:D:355:ARG:HB2	2:D:466:ARG:NH2	2.18	0.59
2:A:374:PHE:HD2	2:A:377:PHE:CE1	2.21	0.59
2:D:406:GLU:HB3	2:D:418:ILE:HD12	1.84	0.59
2:B:351:TYR:HE1	2:B:453:TYR:HA	1.68	0.58
2:D:400:PHE:HE1	2:D:402:ILE:HD12	1.61	0.58
2:B:473:TYR:CE2	2:B:491:PRO:HB3	2.33	0.58
2:D:354:ASN:O	2:D:398:ASP:HA	2.02	0.58
2:D:450:ASN:OD1	1:F:45:ARG:NH2	2.35	0.58
2:A:130:VAL:HG21	2:A:231:ILE:HD12	1.85	0.58
2:A:342:PHE:HZ	2:A:513:LEU:HD21	1.69	0.58
2:B:412:PRO:HB2	2:B:427:ASP:HA	1.84	0.58
2:D:400:PHE:CE1	2:D:402:ILE:HD11	2.38	0.58
2:D:79:PHE:CE2	2:D:244:LEU:CD1	2.87	0.58
2:A:128:ILE:HB	2:A:170:TYR:HB3	1.85	0.58
1:E:85:LEU:HB3	1:E:113:VAL:HG21	1.85	0.58
1:F:6:GLU:HA	1:F:21:SER:O	2.04	0.58
1:F:39:GLN:NE2	1:F:40:ALA:O	2.37	0.57
2:D:403:ARG:CD	2:D:495:TYR:CZ	2.83	0.57
2:D:400:PHE:CD1	2:D:402:ILE:HG13	2.39	0.57
2:D:172:SER:OG	2:D:173:GLN:N	2.37	0.57
2:B:21:ARG:NH1	2:B:81:ASN:O	2.38	0.57
2:D:484:GLU:OE2	2:D:490:PHE:N	2.33	0.57
1:E:86:ILE:HG12	1:E:88:GLU:H	1.69	0.57
2:B:331:ASN:ND2	3:B:1301:NAG:C2	2.67	0.57
2:B:333:THR:O	2:B:335:LEU:HG	2.05	0.57
2:D:438:SER:HB3	2:D:509:ARG:HG3	1.87	0.57
2:A:156:GLU:OE1	2:A:158:ARG:NH2	2.38	0.57
2:B:366:SER:HB3	2:B:388:ASN:ND2	2.20	0.56
2:B:433:VAL:HG22	2:B:512:VAL:HG22	1.86	0.56
2:D:511:VAL:HG12	2:D:513:LEU:HD22	1.86	0.56
2:B:78:ARG:NH1	2:B:79:PHE:O	2.37	0.56
2:D:332:ILE:HD12	2:D:332:ILE:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:424:LYS:HE3	2:D:460:ASN:HB3	1.86	0.56
2:A:355:ARG:HD2	2:A:396:TYR:CD1	2.40	0.56
2:A:376:THR:OG1	2:A:435:ALA:HB3	2.03	0.56
1:F:85:LEU:HB3	1:F:113:VAL:HG21	1.88	0.56
2:B:393:THR:HA	2:B:522:ALA:HA	1.87	0.56
2:B:396:TYR:HB2	2:B:514:SER:OG	2.06	0.56
2:A:168:PHE:HE1	2:A:170:TYR:HB2	1.69	0.56
2:A:137:ASN:OD1	2:A:138:ASP:N	2.38	0.56
1:C:55:ALA:CA	1:C:71:ARG:CZ	2.66	0.56
1:F:45:ARG:NH1	1:F:94:TYR:HD2	2.03	0.56
2:D:128:ILE:HB	2:D:170:TYR:HB3	1.87	0.56
2:B:317:ASN:ND2	2:B:592:PHE:H	2.04	0.55
2:B:350:VAL:HG21	2:B:453:TYR:CZ	2.41	0.55
2:B:418:ILE:HG12	2:B:422:ASN:ND2	2.20	0.55
1:C:38:ARG:HB3	1:C:46:GLU:HB2	1.88	0.55
2:A:99:ASN:OD1	2:A:179:LEU:N	2.37	0.55
2:D:96:GLU:N	2:D:96:GLU:OE1	2.39	0.55
2:D:110:LEU:HD12	2:D:237:ARG:HH12	1.70	0.55
2:A:332:ILE:HG22	2:A:362:VAL:CG2	2.35	0.55
1:C:5:GLN:O	1:C:22:CYS:HA	2.05	0.55
1:C:49:ALA:HB3	1:C:69:ILE:HD11	1.87	0.55
2:B:229:LEU:HB3	2:B:231:ILE:HG23	1.89	0.55
2:D:342:PHE:HZ	2:D:513:LEU:HD21	1.71	0.55
2:B:37:TYR:OH	2:B:53:ASP:OD1	2.25	0.55
2:B:401:VAL:HB	2:B:451:TYR:CE2	2.41	0.55
2:D:379:CYS:SG	2:D:384:PRO:HB3	2.47	0.55
1:C:38:ARG:N	1:C:46:GLU:O	2.30	0.54
2:D:130:VAL:HG21	2:D:231:ILE:HD12	1.89	0.54
2:D:368:LEU:C	2:D:377:PHE:HZ	2.09	0.54
2:A:329:PHE:CE2	2:A:528:LYS:HD3	2.42	0.54
2:D:106:PHE:HB3	2:D:235:ILE:HD13	1.88	0.54
1:F:72:ASP:O	1:F:76:ASN:N	2.39	0.54
2:B:350:VAL:O	2:B:423:TYR:HE2	1.91	0.54
2:A:374:PHE:HD2	2:A:377:PHE:CZ	2.25	0.54
2:B:423:TYR:HE1	2:B:466:ARG:HD3	1.73	0.54
1:E:36:TRP:HE1	1:E:78:VAL:HG11	1.73	0.54
1:E:90:THR:HG22	1:E:113:VAL:H	1.71	0.54
2:A:454:ARG:HG2	2:A:491:PRO:HB2	1.90	0.54
2:D:105:ILE:HG23	2:D:241:LEU:HD11	1.89	0.54
2:D:328:ARG:HG3	2:D:328:ARG:HH11	1.72	0.54
2:D:454:ARG:NH1	2:D:467:ASP:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:TYR:OH	2:A:450:ASN:O	2.24	0.54
1:C:36:TRP:CG	1:C:80:LEU:HD11	2.43	0.54
2:D:358:ILE:HB	2:D:395:VAL:O	2.07	0.54
2:D:365:TYR:HB2	2:D:388:ASN:OD1	2.06	0.54
2:B:347:PHE:HB3	2:B:400:PHE:HA	1.90	0.54
1:C:90:THR:HG22	1:C:113:VAL:H	1.72	0.54
2:D:79:PHE:CZ	2:D:244:LEU:HA	2.38	0.54
2:D:79:PHE:HZ	2:D:244:LEU:HD12	1.71	0.54
2:D:332:ILE:HG23	2:D:362:VAL:HG11	1.88	0.54
2:D:351:TYR:CE2	2:D:454:ARG:HB2	2.43	0.54
1:E:6:GLU:OE2	1:E:95:CYS:N	2.39	0.54
2:A:187:LYS:HD2	2:A:214:ARG:HH12	1.73	0.54
1:E:102:GLN:NE2	1:E:104:TYR:CD1	2.68	0.54
1:E:101:SER:OG	2:A:354:ASN:OD1	2.26	0.53
2:B:105:ILE:HG23	2:B:241:LEU:HD11	1.89	0.53
2:D:353:TRP:CZ2	2:D:400:PHE:CD2	2.95	0.53
2:B:358:ILE:HB	2:B:395:VAL:HB	1.89	0.53
2:A:393:THR:O	2:A:523:THR:OG1	2.21	0.53
2:A:559:PHE:HB2	2:A:577:ARG:NH2	2.23	0.53
1:C:72:ASP:O	1:C:76:ASN:N	2.41	0.53
2:A:401:VAL:HG11	2:A:451:TYR:CE2	2.44	0.53
2:A:502:GLY:O	2:A:506:GLN:HG3	2.07	0.53
1:F:69:ILE:HG12	1:F:80:LEU:CD2	2.38	0.53
2:A:392:PHE:CD2	2:A:515:PHE:HB3	2.43	0.53
2:B:502:GLY:O	2:B:506:GLN:HG3	2.09	0.53
2:A:143:VAL:HG13	2:A:153:MET:HB3	1.90	0.52
2:B:391:CYS:SG	2:B:522:ALA:HB1	2.50	0.52
1:C:55:ALA:N	1:C:71:ARG:NH1	2.45	0.52
2:D:81:ASN:N	2:D:81:ASN:OD1	2.43	0.52
2:A:353:TRP:HH2	2:A:422:ASN:HA	1.71	0.52
2:A:355:ARG:HB2	2:A:466:ARG:HH22	1.73	0.52
2:B:400:PHE:CE1	2:B:402:ILE:HG13	2.45	0.52
2:D:344:ALA:HB3	2:D:347:PHE:HE1	1.74	0.52
2:B:337:PRO:HD2	2:B:358:ILE:HD12	1.91	0.52
2:D:417:LYS:HD3	2:D:455:LEU:HD22	1.90	0.52
2:A:360:ASN:H	2:A:523:THR:HB	1.72	0.52
2:D:435:ALA:HA	2:D:509:ARG:O	2.10	0.52
1:F:96:TYR:HB2	1:F:105:TRP:CZ3	2.44	0.52
2:B:188:ASN:HB2	2:B:190:ARG:HH22	1.75	0.52
2:B:438:SER:O	2:B:507:PRO:HG2	2.08	0.52
2:D:454:ARG:HA	2:D:491:PRO:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:454:ARG:HG2	2:D:491:PRO:HB2	1.91	0.52
2:A:501:ASN:HB3	2:A:505:TYR:HB2	1.92	0.52
2:D:350:VAL:HA	2:D:353:TRP:HE1	1.75	0.52
1:E:102:GLN:HG3	1:E:104:TYR:CE2	2.45	0.52
2:B:346:ARG:HD3	2:B:347:PHE:N	2.25	0.52
2:D:348:ALA:HB2	1:F:102:GLN:NE2	2.25	0.52
2:A:474:GLN:NE2	2:A:479:PRO:CB	2.73	0.51
1:E:49:ALA:HB3	1:E:69:ILE:HD11	1.92	0.51
2:B:441:LEU:HD13	2:B:509:ARG:NH1	2.25	0.51
2:D:126:VAL:HG23	2:D:174:PRO:HA	1.92	0.51
2:B:141:LEU:O	2:B:243:ALA:HA	2.09	0.51
2:D:328:ARG:HH21	2:D:580:GLN:CD	2.13	0.51
1:F:103:ASP:OD1	1:F:103:ASP:N	2.38	0.51
2:B:437:ASN:N	2:B:437:ASN:OD1	2.44	0.51
1:C:69:ILE:HG12	1:C:80:LEU:HD22	1.91	0.51
2:D:83:VAL:HG11	2:D:237:ARG:NH1	2.26	0.51
2:D:350:VAL:O	2:D:423:TYR:HE2	1.94	0.51
2:A:347:PHE:CE1	2:A:509:ARG:HD3	2.46	0.51
2:A:567:ARG:HD3	2:B:42:VAL:HG11	1.93	0.51
1:C:55:ALA:CA	1:C:71:ARG:NH2	2.73	0.51
2:D:99:ASN:OD1	2:D:179:LEU:N	2.42	0.51
2:D:332:ILE:HG12	2:D:527:PRO:HB3	1.92	0.51
2:A:81:ASN:ND2	2:A:240:THR:O	2.44	0.51
2:B:436:TRP:CE3	2:B:509:ARG:HB2	2.46	0.51
2:A:436:TRP:CD1	2:A:436:TRP:N	2.78	0.51
2:D:402:ILE:HG22	2:D:403:ARG:N	2.25	0.50
2:D:435:ALA:HB2	2:D:510:VAL:HG13	1.93	0.50
2:B:199:GLY:HA2	2:B:232:GLY:HA2	1.93	0.50
2:B:332:ILE:HD13	2:B:527:PRO:CA	2.42	0.50
2:B:364:ASP:OD1	2:B:527:PRO:HG2	2.11	0.50
2:D:351:TYR:OH	2:D:422:ASN:OD1	2.22	0.50
2:D:502:GLY:O	2:D:506:GLN:HG3	2.11	0.50
1:E:72:ASP:O	1:E:76:ASN:N	2.45	0.50
2:B:335:LEU:HD23	2:B:362:VAL:HB	1.94	0.50
2:A:229:LEU:HB2	2:A:231:ILE:HG12	1.94	0.50
2:B:328:ARG:NH1	2:B:533:LEU:HB2	2.26	0.50
2:B:353:TRP:CE2	2:B:423:TYR:CD2	3.00	0.50
2:D:369:TYR:CE1	2:D:377:PHE:CD2	2.99	0.50
2:D:575:ALA:HA	2:D:586:ASP:HA	1.94	0.50
2:A:403:ARG:HG3	2:A:495:TYR:HE2	1.75	0.50
2:B:436:TRP:CZ2	2:B:509:ARG:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:ARG:HA	2:B:491:PRO:O	2.12	0.50
2:A:575:ALA:HA	2:A:586:ASP:HA	1.94	0.49
2:B:334:ASN:O	2:B:362:VAL:CG2	2.49	0.49
2:D:196:ASN:HD22	2:D:235:ILE:HB	1.78	0.49
2:D:400:PHE:CE1	2:D:510:VAL:CB	2.84	0.49
2:A:449:TYR:HE1	2:A:496:GLY:HA2	1.77	0.49
2:B:435:ALA:HB2	2:B:510:VAL:HG22	1.95	0.49
2:D:400:PHE:CD1	2:D:400:PHE:C	2.86	0.49
2:B:347:PHE:CE1	2:B:509:ARG:HD3	2.48	0.49
1:F:38:ARG:NH1	1:F:89:ASP:HA	2.26	0.49
2:B:496:GLY:O	2:B:501:ASN:ND2	2.43	0.49
2:D:176:LEU:HD23	2:D:190:ARG:NH1	2.28	0.49
2:B:380:TYR:O	2:B:430:THR:HA	2.13	0.49
2:D:369:TYR:HD1	2:D:377:PHE:CE2	2.26	0.49
2:B:104:TRP:HB2	2:B:106:PHE:CE1	2.47	0.49
2:B:553:THR:OG1	2:B:586:ASP:OD1	2.20	0.49
2:A:368:LEU:O	2:A:374:PHE:HE2	1.96	0.49
2:A:417:LYS:HE3	2:A:455:LEU:HD23	1.95	0.49
2:A:484:GLU:CG	2:A:485:GLY:N	2.76	0.49
2:D:435:ALA:HB2	2:D:510:VAL:CB	2.42	0.49
1:C:37:PHE:CE2	1:C:47:MET:HG2	2.48	0.49
2:D:83:VAL:HG11	2:D:237:ARG:HH11	1.78	0.49
2:D:410:ILE:HG23	2:D:425:LEU:HD11	1.95	0.49
2:D:454:ARG:HH11	2:D:457:ARG:NH2	2.10	0.49
2:A:358:ILE:HB	2:A:395:VAL:HB	1.95	0.49
2:A:376:THR:N	2:A:435:ALA:O	2.36	0.49
2:B:360:ASN:H	2:B:523:THR:HB	1.78	0.49
2:D:354:ASN:HB3	2:D:399:SER:OG	2.13	0.48
1:E:91:ALA:HB3	1:E:93:TYR:HE1	1.78	0.48
2:A:291:CYS:O	2:A:298:GLU:HG3	2.13	0.48
2:A:350:VAL:HB	2:A:453:TYR:CD2	2.48	0.48
1:E:55:ALA:HA	1:E:71:ARG:CZ	2.39	0.48
2:D:371:SER:OG	2:D:374:PHE:HE2	1.93	0.48
2:B:357:ARG:NH2	2:B:358:ILE:O	2.46	0.48
2:D:328:ARG:HH22	2:D:580:GLN:HB2	1.74	0.48
2:B:77:LYS:NZ	2:B:255:SER:H	2.11	0.48
2:D:435:ALA:CB	2:D:510:VAL:HA	2.44	0.48
2:B:438:SER:HB3	2:B:509:ARG:HG3	1.95	0.48
2:A:203:ILE:HB	2:A:227:VAL:HG22	1.96	0.48
2:D:355:ARG:HD2	2:D:396:TYR:HB3	1.96	0.48
2:D:411:ALA:HB3	2:D:414:GLN:CD	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:498:GLN:H	2:A:501:ASN:ND2	2.11	0.48
2:B:425:LEU:HB3	2:B:429:PHE:CE2	2.49	0.48
2:D:319:ARG:HG3	2:D:320:VAL:HG23	1.95	0.48
1:E:2:VAL:HA	1:E:25:SER:O	2.14	0.48
2:D:364:ASP:HB3	2:D:527:PRO:CG	2.41	0.48
2:A:457:ARG:NH2	2:A:459:SER:O	2.45	0.48
2:B:575:ALA:HA	2:B:586:ASP:HA	1.96	0.48
1:C:38:ARG:HG3	1:C:93:TYR:HE1	1.80	0.47
1:C:44:GLN:HG3	1:C:45:ARG:N	2.29	0.47
2:D:537:LYS:O	2:D:539:VAL:HG13	2.14	0.47
1:F:82:MET:HB3	1:F:85:LEU:HD21	1.96	0.47
2:B:96:GLU:HG3	2:B:190:ARG:HH21	1.78	0.47
2:A:449:TYR:CE1	2:A:496:GLY:HA2	2.50	0.47
1:C:32:ASN:ND2	1:C:76:ASN:HD21	2.12	0.47
2:B:353:TRP:CD1	2:B:423:TYR:CE2	3.02	0.47
2:D:402:ILE:HG22	2:D:403:ARG:H	1.79	0.47
2:A:353:TRP:HB2	2:A:466:ARG:NE	2.29	0.47
2:D:553:THR:OG1	2:D:586:ASP:OD1	2.26	0.47
2:A:133:PHE:HE1	2:A:160:TYR:CD1	2.32	0.47
2:B:354:ASN:O	2:B:398:ASP:HA	2.15	0.47
1:C:36:TRP:CD1	1:C:80:LEU:HD21	2.50	0.47
1:C:64:LYS:O	1:C:66:ARG:HG3	2.15	0.47
1:F:49:ALA:HB3	1:F:69:ILE:HD11	1.96	0.47
1:F:107:GLN:NE2	1:F:108:GLY:O	2.48	0.47
1:E:50:VAL:C	1:E:51:ILE:HD13	2.35	0.47
2:A:402:ILE:HG22	2:A:403:ARG:N	2.29	0.47
2:A:304:LYS:HE2	2:A:304:LYS:HB2	1.76	0.47
2:B:328:ARG:HH21	2:B:580:GLN:HB2	1.80	0.47
2:D:203:ILE:HB	2:D:227:VAL:HG22	1.96	0.47
2:B:350:VAL:HA	2:B:353:TRP:HE1	1.80	0.47
2:B:354:ASN:HB3	2:B:399:SER:OG	2.14	0.47
1:C:11:LEU:HD12	1:C:11:LEU:C	2.34	0.47
2:B:317:ASN:HB3	2:B:591:SER:HB2	1.97	0.46
2:B:358:ILE:HG22	2:B:524:VAL:CG1	2.45	0.46
1:C:80:LEU:HB3	1:C:82:MET:SD	2.54	0.46
2:B:364:ASP:CG	2:B:527:PRO:HG2	2.35	0.46
2:B:449:TYR:HB3	2:B:494:SER:HB2	1.97	0.46
2:B:454:ARG:HH11	2:B:457:ARG:CZ	2.29	0.46
2:D:143:VAL:HG13	2:D:153:MET:HB3	1.97	0.46
2:D:324:GLU:N	2:D:324:GLU:OE1	2.47	0.46
2:A:166:CYS:O	2:D:357:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:411:ALA:HB3	2:A:414:GLN:CD	2.36	0.46
2:B:395:VAL:HG23	2:B:524:VAL:HG21	1.98	0.46
2:D:400:PHE:HE1	2:D:510:VAL:HB	1.70	0.46
1:E:51:ILE:HD11	1:E:69:ILE:HD12	1.97	0.46
2:B:436:TRP:CE2	2:B:509:ARG:HB2	2.51	0.46
2:A:378:LYS:HB2	2:A:433:VAL:HG13	1.98	0.46
2:B:299:THR:O	2:B:303:LEU:HG	2.15	0.46
2:B:332:ILE:CG2	2:B:362:VAL:HG11	2.29	0.46
2:D:423:TYR:HE1	2:D:466:ARG:CG	2.23	0.46
2:B:383:SER:OG	2:B:386:LYS:HG2	2.15	0.46
1:C:32:ASN:HD21	1:C:76:ASN:HD21	1.63	0.46
2:A:396:TYR:HB2	2:A:514:SER:OG	2.16	0.45
2:A:346:ARG:NH1	2:A:347:PHE:H	2.14	0.45
2:D:396:TYR:HB2	2:D:514:SER:OG	2.17	0.45
2:A:474:GLN:HE22	2:A:479:PRO:HB3	1.80	0.45
2:A:577:ARG:NH1	2:A:582:LEU:O	2.49	0.45
1:C:36:TRP:CE2	1:C:80:LEU:HG	2.50	0.45
2:D:400:PHE:CZ	2:D:402:ILE:HD11	2.51	0.45
2:D:435:ALA:HB2	2:D:510:VAL:HA	1.99	0.45
1:F:11:LEU:HD12	1:F:112:THR:HB	1.98	0.45
2:B:43:PHE:CE1	2:B:283:GLY:HA3	2.52	0.45
2:B:94:SER:HB3	2:B:101:ILE:HD13	1.99	0.45
2:D:436:TRP:N	2:D:509:ARG:O	2.44	0.45
2:D:426:PRO:HD2	2:D:429:PHE:CE2	2.52	0.45
2:B:68:ILE:O	2:B:261:GLY:HA3	2.16	0.45
2:B:411:ALA:HB3	2:B:414:GLN:CD	2.36	0.45
1:E:51:ILE:CA	1:E:71:ARG:HH21	2.30	0.45
2:D:369:TYR:CE2	2:D:384:PRO:HB2	2.51	0.45
2:A:21:ARG:NH1	2:A:81:ASN:O	2.50	0.45
2:B:81:ASN:OD1	2:B:239:GLN:NE2	2.49	0.45
2:A:299:THR:O	2:A:303:LEU:HG	2.16	0.45
2:A:324:GLU:N	2:A:324:GLU:OE1	2.49	0.45
2:A:484:GLU:CG	2:A:485:GLY:H	2.30	0.45
2:D:28:TYR:HD2	2:D:61:ASN:HB3	1.81	0.45
1:F:12:VAL:O	1:F:113:VAL:HA	2.17	0.45
1:E:12:VAL:O	1:E:113:VAL:HA	2.17	0.45
2:B:328:ARG:NH2	2:B:580:GLN:HB2	2.32	0.45
1:E:36:TRP:CD2	1:E:80:LEU:HD12	2.52	0.44
2:B:332:ILE:HD13	2:B:527:PRO:HA	1.99	0.44
1:E:19:ARG:HG2	1:E:81:GLN:HG2	1.98	0.44
2:B:328:ARG:HH11	2:B:533:LEU:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:TRP:CD2	2:B:509:ARG:HB2	2.52	0.44
1:C:55:ALA:H	1:C:71:ARG:NH1	2.12	0.44
2:D:351:TYR:CD2	2:D:454:ARG:HD2	2.52	0.44
2:D:377:PHE:HA	2:D:434:ILE:HG12	1.99	0.44
2:A:336:CYS:HB2	2:A:338:PHE:CE2	2.52	0.44
2:A:403:ARG:NE	2:A:495:TYR:CE2	2.84	0.44
2:A:439:ASN:OD1	2:A:506:GLN:HB3	2.17	0.44
2:D:20:THR:HG22	2:D:22:THR:H	1.82	0.44
1:E:29:PHE:N	1:E:99:ASP:OD1	2.51	0.44
1:E:55:ALA:CA	1:E:71:ARG:HH12	2.23	0.44
2:B:410:ILE:HG22	2:B:433:VAL:HG21	1.99	0.44
2:A:376:THR:O	2:A:434:ILE:HA	2.17	0.44
2:B:379:CYS:C	2:B:380:TYR:HD1	2.20	0.44
2:B:439:ASN:OD1	2:B:507:PRO:HD2	2.18	0.44
2:B:485:GLY:HA2	1:C:61:ASN:ND2	2.32	0.44
2:D:363:ALA:O	2:D:526:GLY:HA2	2.17	0.44
2:D:436:TRP:HD1	2:D:509:ARG:O	2.01	0.44
1:F:47:MET:SD	1:F:50:VAL:HG23	2.58	0.44
1:E:58:GLN:NE2	2:A:471:GLU:HA	2.26	0.44
2:A:206:LYS:HB3	2:A:223:LEU:HD23	2.00	0.44
2:A:346:ARG:NH1	2:A:346:ARG:HA	2.33	0.44
2:B:403:ARG:O	2:B:407:VAL:HG23	2.17	0.44
2:A:121:ASN:HD22	2:A:176:LEU:HG	1.83	0.44
2:A:403:ARG:O	2:A:407:VAL:HG23	2.17	0.44
2:B:435:ALA:CB	2:B:510:VAL:HG22	2.48	0.44
2:D:400:PHE:CE1	2:D:402:ILE:CG1	3.01	0.44
2:D:65:PHE:CB	2:D:80:ASP:OD2	2.35	0.43
1:E:38:ARG:O	1:E:46:GLU:N	2.39	0.43
2:B:439:ASN:OD1	2:B:506:GLN:HB3	2.18	0.43
2:D:392:PHE:CD1	2:D:515:PHE:CD2	3.02	0.43
2:D:515:PHE:N	2:D:515:PHE:CD1	2.85	0.43
1:F:13:GLN:HE21	1:F:115:SER:HB3	1.82	0.43
2:A:78:ARG:HH11	2:A:78:ARG:HG3	1.83	0.43
2:A:338:PHE:HB3	2:A:342:PHE:CD2	2.53	0.43
2:A:231:ILE:HD13	2:A:231:ILE:HA	1.83	0.43
2:A:324:GLU:HG2	2:A:539:VAL:HG23	2.01	0.43
2:B:378:LYS:HB3	2:B:380:TYR:CE1	2.53	0.43
2:D:350:VAL:HA	2:D:353:TRP:NE1	2.33	0.43
2:D:498:GLN:H	2:D:501:ASN:ND2	2.16	0.43
1:F:50:VAL:O	1:F:51:ILE:HD13	2.18	0.43
1:E:33:THR:HB	1:E:98:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:424:LYS:NZ	2:A:460:ASN:HB3	2.34	0.43
1:F:31:PRO:HB2	1:F:100:LYS:HD3	2.00	0.43
1:F:37:PHE:CZ	1:F:47:MET:HG2	2.53	0.43
2:B:365:TYR:CD2	2:B:387:LEU:HB3	2.53	0.43
2:D:387:LEU:HD23	2:D:387:LEU:HA	1.72	0.43
2:A:409:GLN:NE2	2:A:416:GLY:HA3	2.33	0.43
2:B:326:ILE:HD13	2:B:534:VAL:H	1.84	0.43
2:D:418:ILE:HG12	2:D:422:ASN:ND2	2.33	0.43
2:D:582:LEU:HD23	2:D:582:LEU:HA	1.84	0.43
2:B:431:GLY:HA2	2:B:515:PHE:HD2	1.84	0.43
2:D:214:ARG:HG3	2:D:215:ASP:N	2.33	0.43
2:D:231:ILE:HG22	2:D:233:ILE:HG23	2.00	0.43
2:D:338:PHE:HB3	2:D:342:PHE:CD2	2.54	0.43
2:B:229:LEU:HB3	2:B:231:ILE:CG2	2.49	0.42
2:D:401:VAL:HG21	2:D:442:ASP:OD2	2.18	0.42
2:A:355:ARG:CB	2:A:466:ARG:HH12	2.31	0.42
2:B:476:GLY:N	2:B:487:ASN:HB3	2.33	0.42
2:B:560:LEU:HD11	2:D:284:THR:HG22	2.00	0.42
2:D:424:LYS:HD2	2:D:461:LEU:O	2.19	0.42
1:F:55:ALA:HA	1:F:71:ARG:NH1	2.30	0.42
1:F:72:ASP:O	1:F:76:ASN:CA	2.67	0.42
2:B:426:PRO:HD2	2:B:429:PHE:CE2	2.54	0.42
2:B:462:LYS:HB2	2:B:465:GLU:CD	2.40	0.42
1:C:34:MET:SD	1:C:34:MET:N	2.91	0.42
2:D:68:ILE:O	2:D:261:GLY:HA3	2.18	0.42
2:D:444:LYS:HG3	2:D:448:ASN:HD21	1.84	0.42
2:B:438:SER:OG	2:B:507:PRO:HB2	2.19	0.42
2:B:457:ARG:NH1	2:B:461:LEU:HD21	2.35	0.42
2:D:368:LEU:C	2:D:377:PHE:CZ	2.92	0.42
2:D:476:GLY:N	2:D:487:ASN:HB3	2.34	0.42
1:F:68:THR:OG1	1:F:81:GLN:OE1	2.19	0.42
2:A:350:VAL:HG12	2:A:422:ASN:ND2	2.30	0.42
2:B:106:PHE:HB3	2:B:235:ILE:HD13	2.01	0.42
2:B:422:ASN:HB3	2:B:423:TYR:CD2	2.54	0.42
2:D:439:ASN:OD1	2:D:507:PRO:HD2	2.19	0.42
1:E:32:ASN:OD1	1:E:32:ASN:N	2.52	0.42
2:A:419:ALA:O	2:A:424:LYS:HG2	2.19	0.42
2:B:418:ILE:HA	2:B:422:ASN:CG	2.40	0.42
2:D:332:ILE:N	2:D:332:ILE:CD1	2.83	0.42
2:D:338:PHE:CD1	2:D:342:PHE:HE2	2.37	0.42
1:E:69:ILE:HG12	1:E:80:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:SER:HA	2:B:524:VAL:HG13	2.02	0.42
1:E:36:TRP:HE1	1:E:78:VAL:CG1	2.32	0.42
2:A:328:ARG:NH2	2:A:580:GLN:HB2	2.34	0.42
2:A:386:LYS:O	2:A:390:LEU:HG	2.20	0.42
2:D:317:ASN:HB3	2:D:591:SER:HB2	2.01	0.42
2:D:457:ARG:NH1	2:D:461:LEU:HD21	2.35	0.42
2:A:226:LEU:HG	2:A:227:VAL:HG13	2.01	0.42
2:A:541:PHE:HB2	2:A:543:PHE:HE1	1.85	0.42
2:B:332:ILE:HD13	2:B:527:PRO:HB3	2.02	0.42
2:D:340:GLU:O	2:D:344:ALA:HB2	2.20	0.42
2:D:472:ILE:HG23	2:D:489:TYR:O	2.20	0.42
1:F:1:GLN:NE2	1:F:2:VAL:O	2.53	0.42
2:B:326:ILE:HD11	2:B:534:VAL:HB	2.01	0.42
2:A:346:ARG:CZ	2:A:347:PHE:H	2.33	0.41
2:A:425:LEU:HD23	2:A:425:LEU:HA	1.65	0.41
2:D:417:LYS:O	2:D:421:TYR:HB2	2.20	0.41
2:B:425:LEU:HB3	2:B:429:PHE:CD2	2.55	0.41
2:A:294:ASP:OD1	2:A:294:ASP:N	2.53	0.41
2:A:355:ARG:HB2	2:A:466:ARG:NH2	2.35	0.41
2:B:126:VAL:HG22	2:B:172:SER:H	1.85	0.41
2:B:376:THR:OG1	2:B:435:ALA:N	2.48	0.41
2:D:334:ASN:HB2	2:D:362:VAL:HG23	2.02	0.41
2:D:350:VAL:O	2:D:350:VAL:HG12	2.21	0.41
2:A:542:ASN:HA	2:A:546:LEU:O	2.20	0.41
2:A:543:PHE:CZ	2:A:552:LEU:HD21	2.55	0.41
2:B:18:LEU:HB2	2:B:138:ASP:OD2	2.20	0.41
2:D:438:SER:CB	2:D:509:ARG:HG3	2.50	0.41
1:F:64:LYS:O	1:F:66:ARG:HG3	2.20	0.41
2:A:350:VAL:HG21	2:A:402:ILE:HG12	2.02	0.41
2:B:96:GLU:OE1	2:B:101:ILE:HD12	2.20	0.41
1:C:63:VAL:HG11	1:C:67:PHE:CE2	2.55	0.41
2:D:363:ALA:C	2:D:527:PRO:HD3	2.40	0.41
2:D:392:PHE:CE2	2:D:515:PHE:CE2	3.09	0.41
2:B:441:LEU:HB3	2:B:509:ARG:NH2	2.35	0.41
2:D:108:THR:O	2:D:237:ARG:NH2	2.54	0.41
2:A:104:TRP:HB2	2:A:106:PHE:CE1	2.56	0.41
2:A:411:ALA:HB3	2:A:414:GLN:OE1	2.21	0.41
2:B:364:ASP:HA	2:B:527:PRO:CG	2.50	0.41
2:D:392:PHE:N	2:D:524:VAL:O	2.52	0.41
1:F:51:ILE:HG21	1:F:71:ARG:CD	2.37	0.41
1:E:50:VAL:O	1:E:51:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:SER:N	1:E:71:ARG:HH22	2.16	0.41
2:A:131:CYS:HB2	2:A:133:PHE:CD2	2.56	0.41
2:A:338:PHE:HB3	2:A:342:PHE:HD2	1.85	0.41
2:D:128:ILE:HD13	2:D:229:LEU:HD11	2.03	0.41
2:D:317:ASN:HB2	2:D:592:PHE:O	2.20	0.41
2:D:358:ILE:HA	2:D:358:ILE:HD13	1.85	0.41
2:D:363:ALA:O	2:D:527:PRO:CD	2.61	0.41
1:E:28:ILE:HD11	1:E:32:ASN:HD22	1.85	0.41
2:B:454:ARG:HH22	2:B:469:SER:N	2.19	0.41
2:D:146:HIS:CE1	2:D:148:ASN:HB2	2.56	0.41
2:D:457:ARG:HA	2:D:473:TYR:CE1	2.55	0.41
1:F:12:VAL:HG21	1:F:18:LEU:HG	2.01	0.41
2:A:332:ILE:HD13	2:A:332:ILE:HA	2.00	0.41
2:B:16:VAL:HG11	2:B:248:TYR:CD1	2.56	0.41
2:B:364:ASP:CB	2:B:527:PRO:HG3	2.51	0.41
2:B:394:ASN:HB2	2:B:516:GLU:OE1	2.20	0.41
1:F:38:ARG:HG3	1:F:39:GLN:N	2.35	0.41
2:A:347:PHE:CE2	2:A:399:SER:OG	2.60	0.40
2:B:444:LYS:HG3	2:B:448:ASN:ND2	2.31	0.40
2:D:400:PHE:HZ	2:D:410:ILE:HD13	1.85	0.40
2:A:24:LEU:HD21	2:A:69:HIS:CE1	2.57	0.40
2:B:426:PRO:HD2	2:B:429:PHE:CD2	2.57	0.40
2:D:348:ALA:HB2	1:F:102:GLN:HE22	1.84	0.40
2:D:462:LYS:HB2	2:D:465:GLU:CD	2.41	0.40
2:A:121:ASN:ND2	2:A:175:PHE:HB2	2.29	0.40
2:B:317:ASN:HB2	2:B:592:PHE:O	2.21	0.40
2:D:393:THR:HA	2:D:522:ALA:HA	2.03	0.40
1:F:24:ALA:HB1	1:F:28:ILE:HG21	2.03	0.40
2:A:440:ASN:OD1	2:A:441:LEU:HG	2.22	0.40
1:C:63:VAL:HG11	1:C:67:PHE:CD2	2.56	0.40
1:F:51:ILE:HD12	1:F:57:THR:HG22	2.03	0.40
1:E:63:VAL:HG13	1:E:63:VAL:O	2.21	0.40
2:B:332:ILE:HD11	2:B:527:PRO:C	2.40	0.40
2:B:402:ILE:HG22	2:B:403:ARG:N	2.36	0.40
2:B:424:LYS:CE	2:B:460:ASN:HB3	2.50	0.40
2:D:449:TYR:HB3	2:D:494:SER:HB2	2.03	0.40
2:D:564:GLN:HB2	2:D:565:PHE:CE2	2.56	0.40
1:F:33:THR:O	1:F:98:VAL:HG23	2.21	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	113/136 (83%)	103 (91%)	8 (7%)	2 (2%)	7 30
1	E	113/136 (83%)	106 (94%)	7 (6%)	0	100 100
1	F	113/136 (83%)	108 (96%)	4 (4%)	1 (1%)	14 44
2	A	561/1234 (46%)	540 (96%)	21 (4%)	0	100 100
2	B	561/1234 (46%)	536 (96%)	24 (4%)	1 (0%)	44 71
2	D	561/1234 (46%)	542 (97%)	18 (3%)	1 (0%)	44 71
All	All	2022/4110 (49%)	1935 (96%)	82 (4%)	5 (0%)	45 71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	334	ASN
1	C	102	GLN
2	D	527	PRO
1	C	28	ILE
1	F	28	ILE

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	95/111 (86%)	93 (98%)	2 (2%)	48 70
1	E	95/111 (86%)	92 (97%)	3 (3%)	34 61
1	F	95/111 (86%)	91 (96%)	4 (4%)	25 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	505/1073 (47%)	499 (99%)	6 (1%)	67 80
2	B	505/1073 (47%)	491 (97%)	14 (3%)	38 64
2	D	505/1073 (47%)	496 (98%)	9 (2%)	54 74
All	All	1800/3552 (51%)	1762 (98%)	38 (2%)	49 70

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	27	SER
1	E	30	SER
1	E	102	GLN
2	A	133	PHE
2	A	157	PHE
2	A	351	TYR
2	A	374	PHE
2	A	436	TRP
2	A	487	ASN
2	B	63	THR
2	B	104	TRP
2	B	140	PHE
2	B	170	TYR
2	B	296	LEU
2	B	321	GLN
2	B	357	ARG
2	B	361	CYS
2	B	429	PHE
2	B	437	ASN
2	B	505	TYR
2	B	524	VAL
2	B	565	PHE
2	B	578	ASP
1	C	25	SER
1	C	79	HIS
2	D	63	THR
2	D	113	LYS
2	D	172	SER
2	D	331	ASN
2	D	353	TRP
2	D	369	TYR
2	D	429	PHE
2	D	436	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	546	LEU
1	F	46	GLU
1	F	81	GLN
1	F	82	MET
1	F	103	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	58	GLN
2	A	66	HIS
2	A	69	HIS
2	A	188	ASN
2	A	207	HIS
2	A	317	ASN
2	A	394	ASN
2	A	422	ASN
2	A	474	GLN
2	B	66	HIS
2	B	188	ASN
2	B	207	HIS
2	B	211	ASN
2	B	317	ASN
2	B	331	ASN
1	C	32	ASN
1	C	102	GLN
2	D	66	HIS
2	D	188	ASN
2	D	196	ASN
2	D	207	HIS
2	D	317	ASN
1	F	13	GLN
1	F	44	GLN
1	F	76	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	NAG	D	1301	2	14,14,15	0.23	0	17,19,21	0.59	0
3	NAG	B	1301	-	14,14,15	0.37	0	17,19,21	0.72	1 (5%)

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
3	NAG	D	1301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1301	NAG	C2-N2-C7	2.09	125.71	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

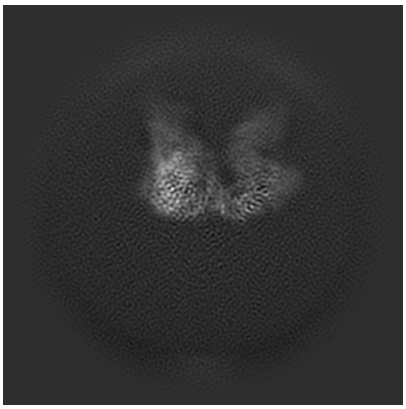
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29804. These allow visual inspection of the internal detail of the map and identification of artifacts.

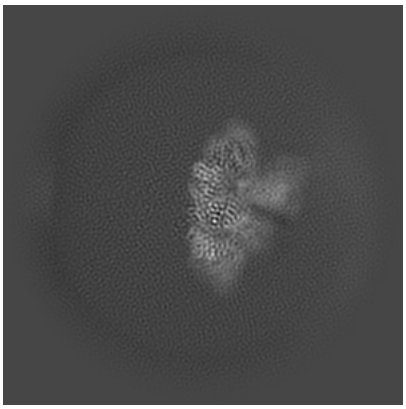
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

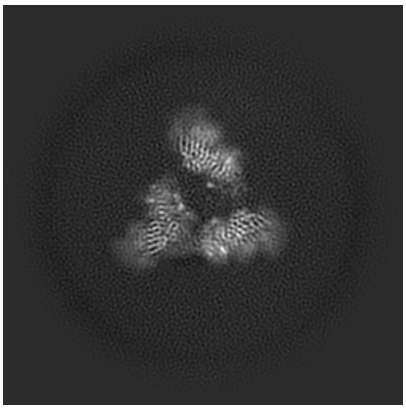
6.1.1 Primary map



X

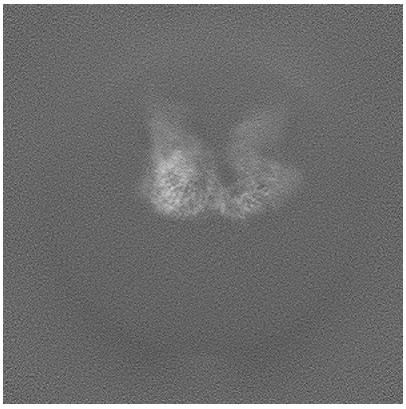


Y

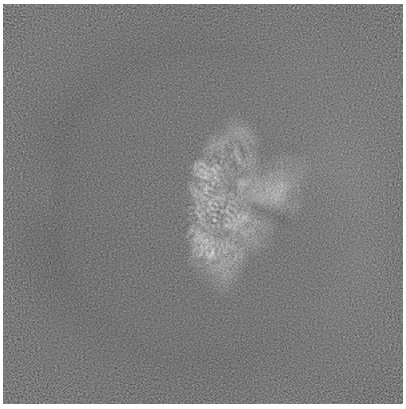


Z

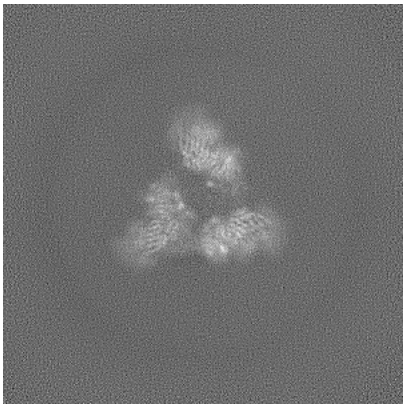
6.1.2 Raw map



X



Y

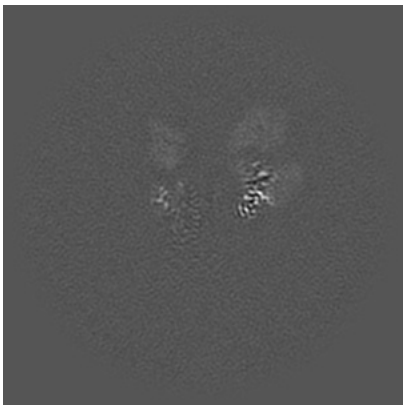


Z

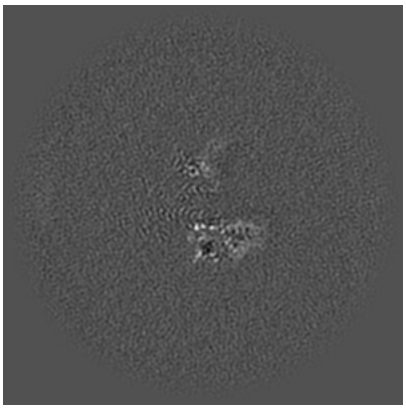
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

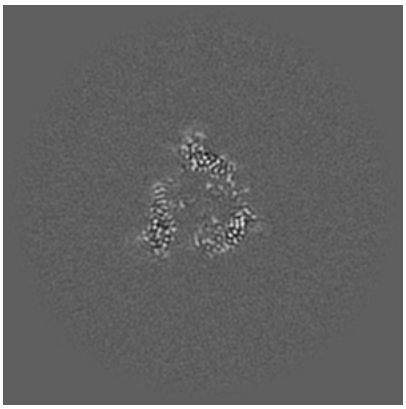
6.2.1 Primary map



X Index: 230

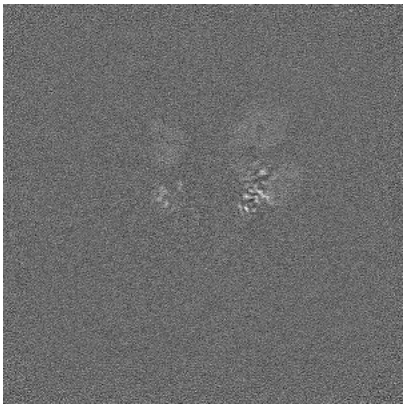


Y Index: 230

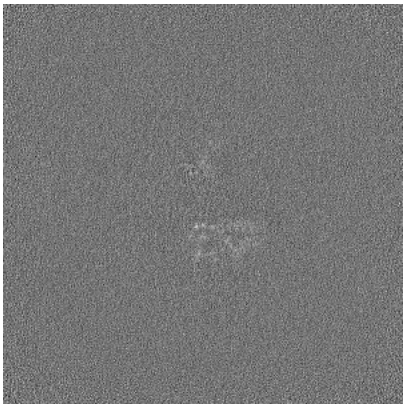


Z Index: 230

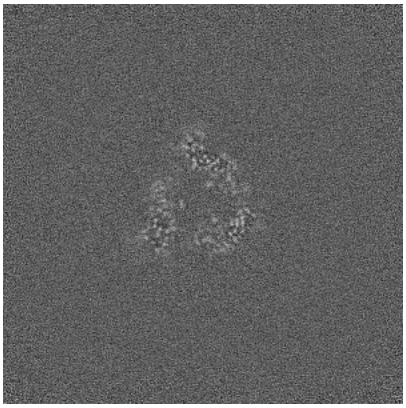
6.2.2 Raw map



X Index: 230



Y Index: 230

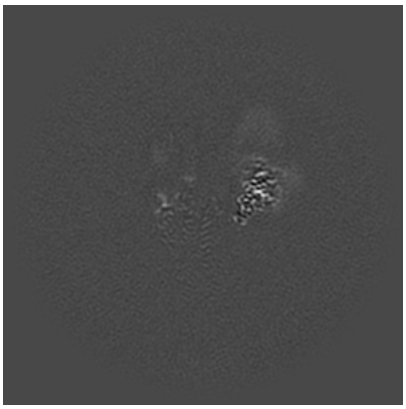


Z Index: 230

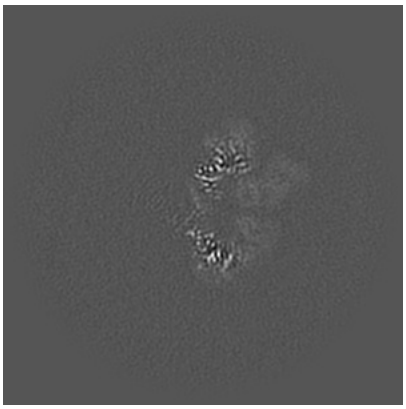
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

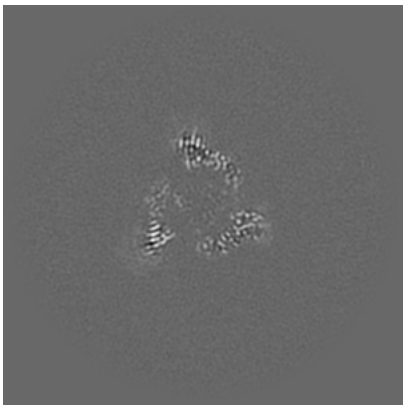
6.3.1 Primary map



X Index: 223

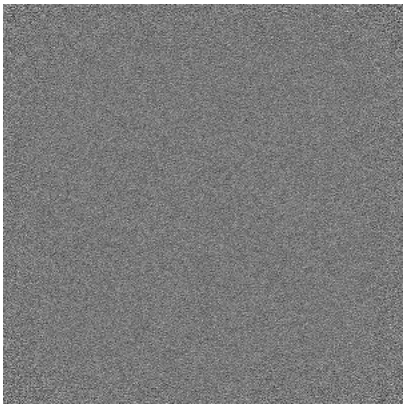


Y Index: 195

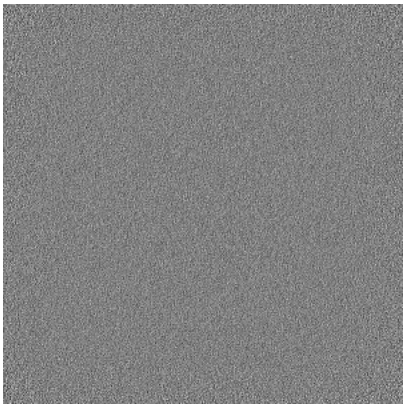


Z Index: 241

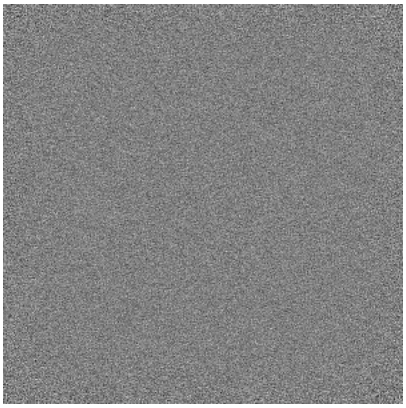
6.3.2 Raw map



X Index: 0



Y Index: 0

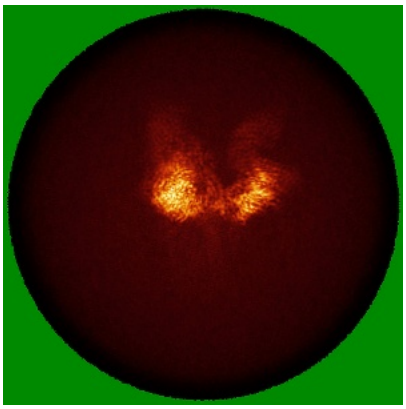


Z Index: 0

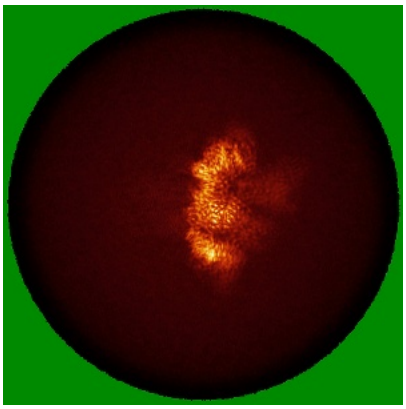
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

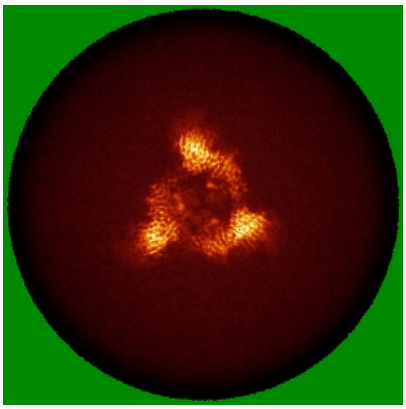
6.4.1 Primary map



X

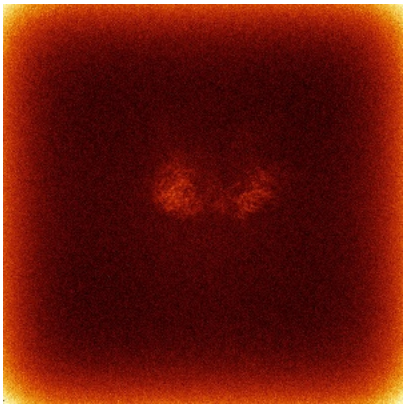


Y

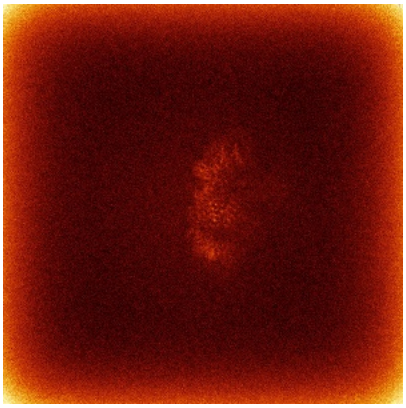


Z

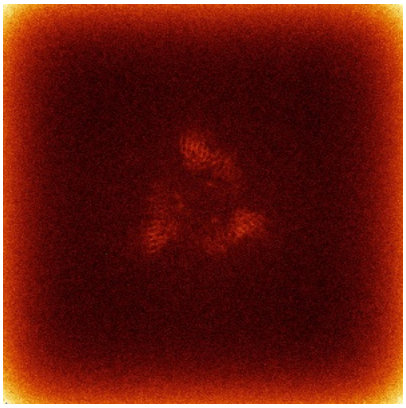
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

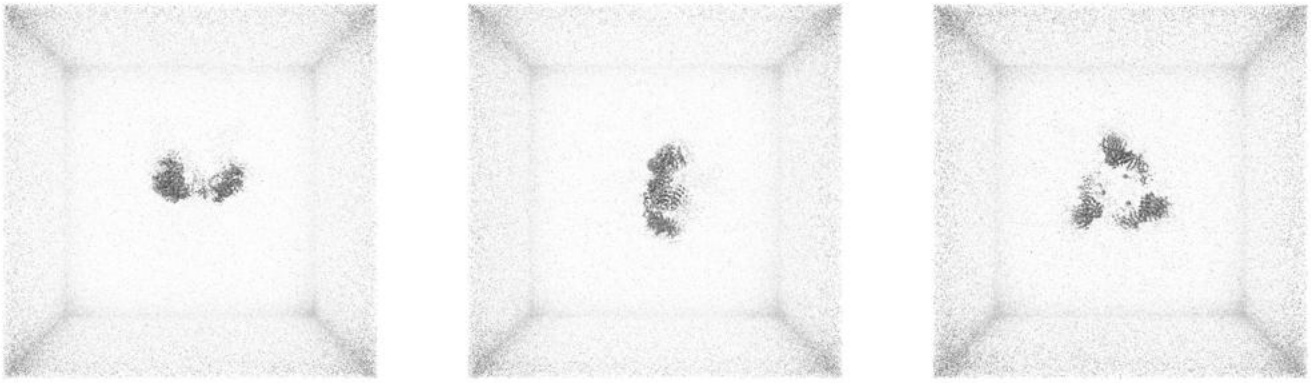
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0585. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

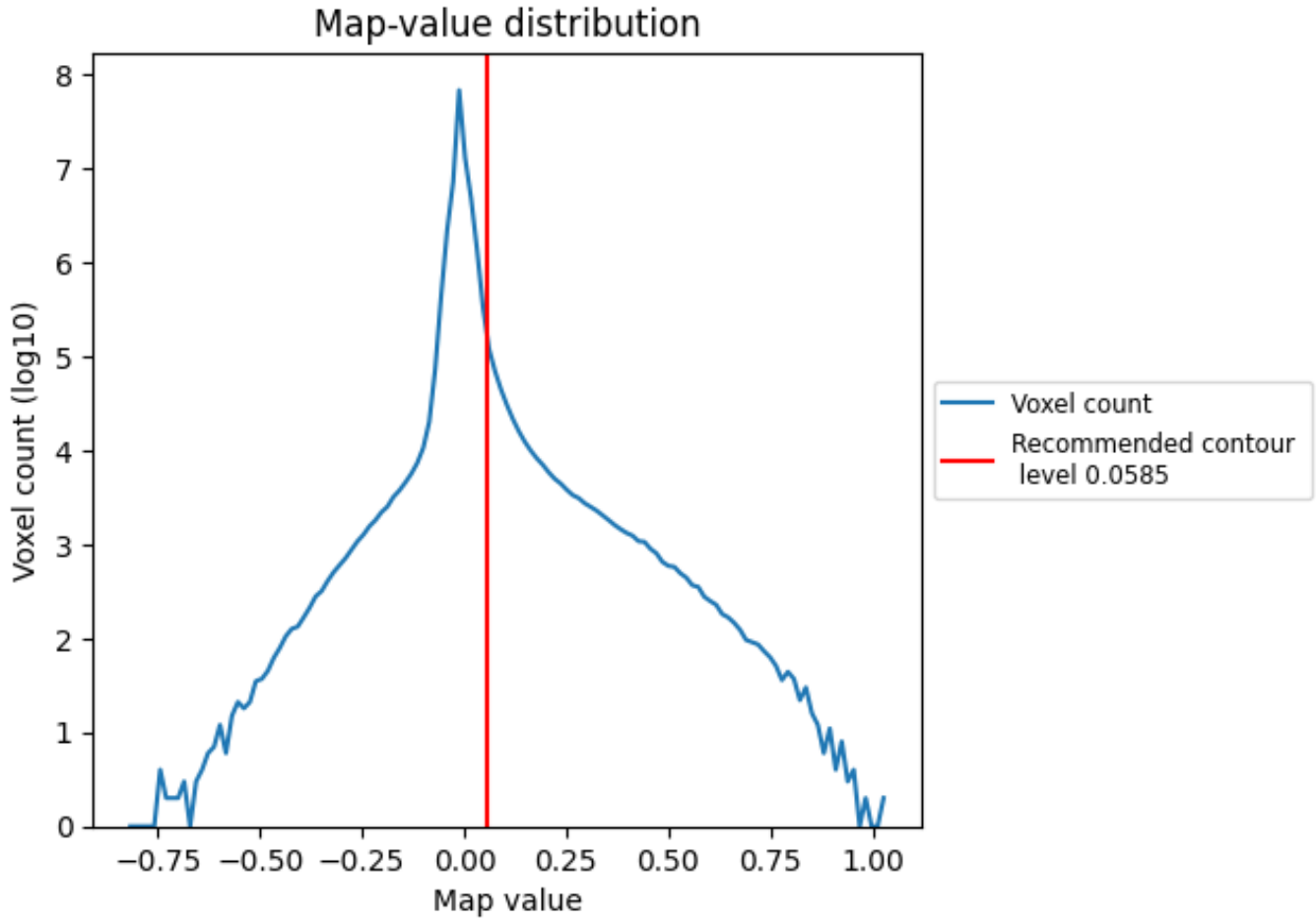
6.6 Mask visualisation (i)

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

7 Map analysis

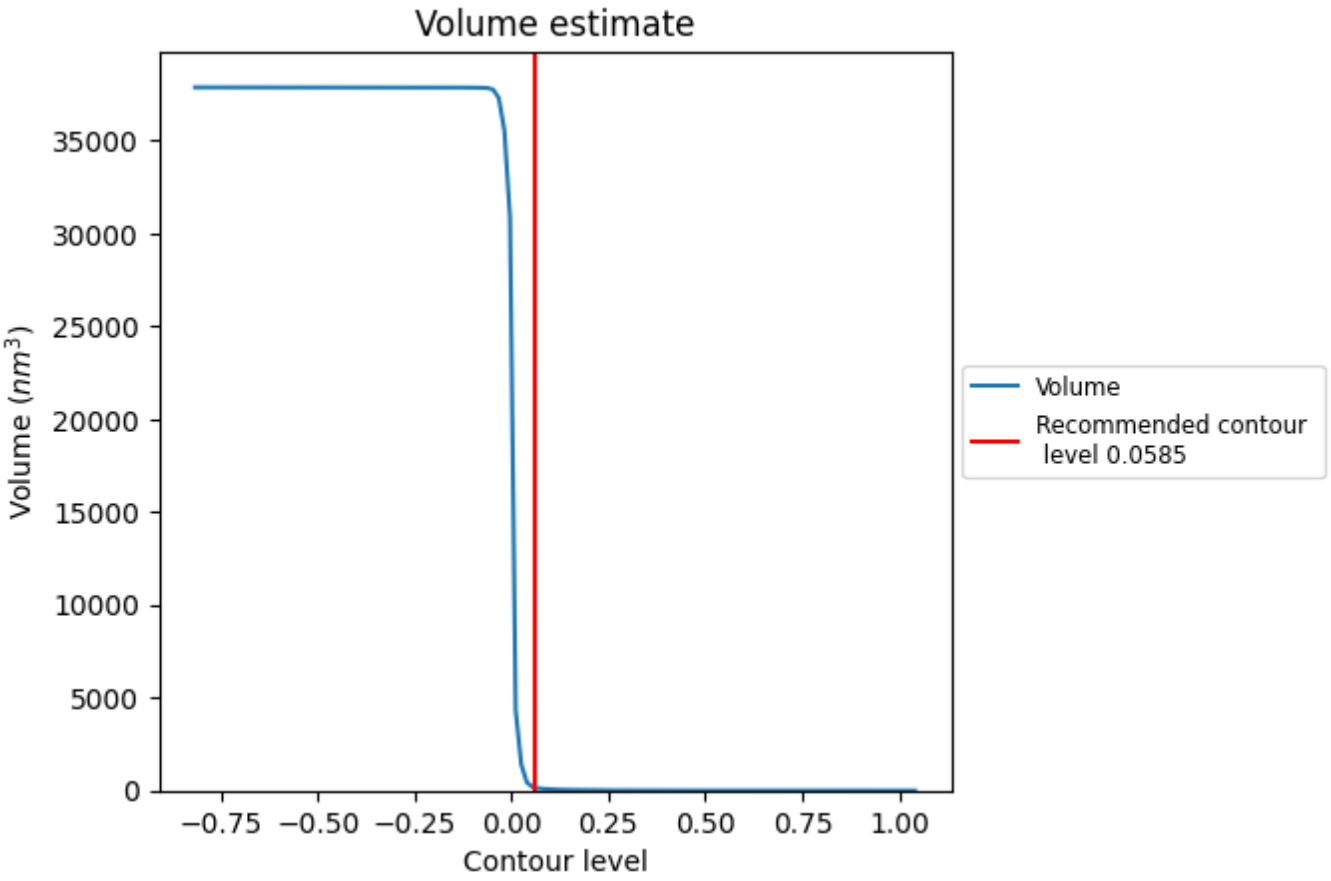
This section contains the results of statistical analysis of the map.

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.

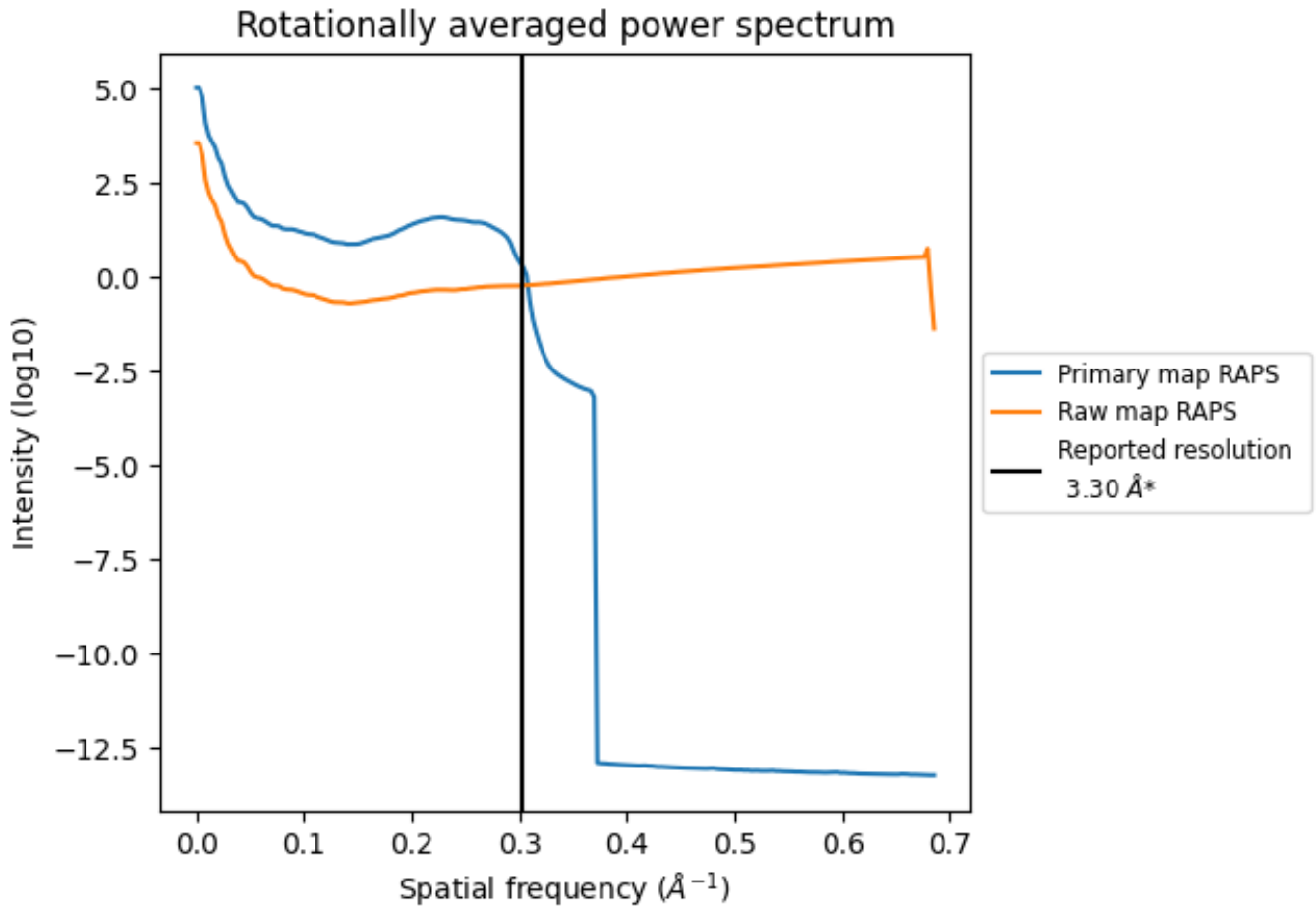
7.2 Volume estimate



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 156 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)

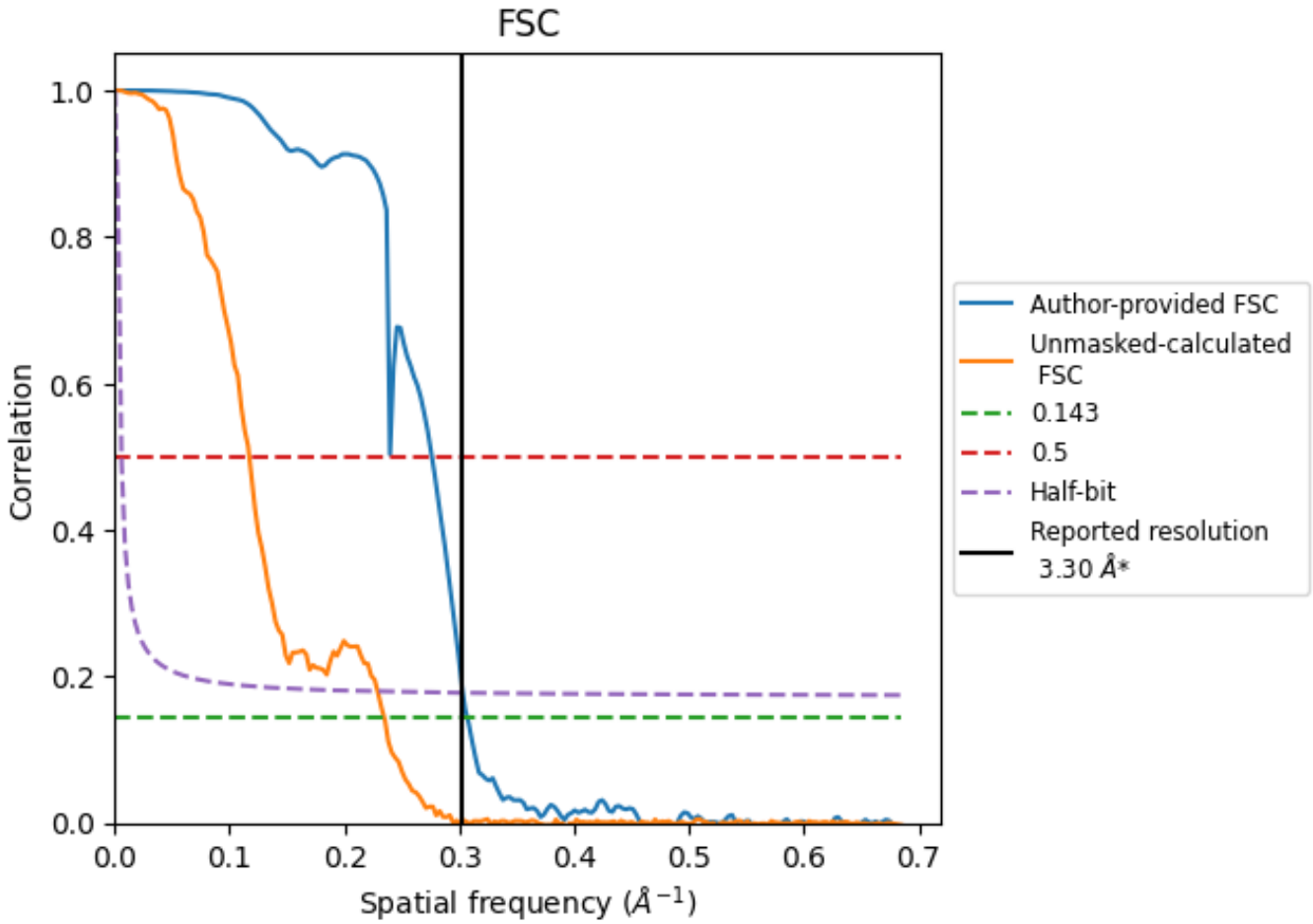


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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)

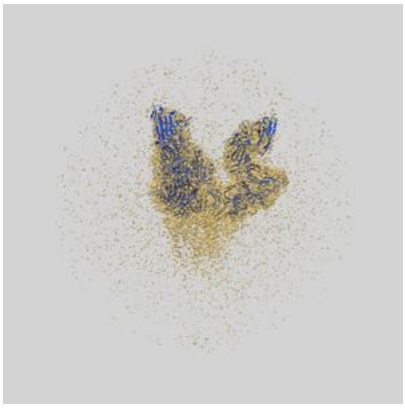
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.62	3.30
Unmasked-calculated*	4.26	8.53	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.3 by more than 10 %

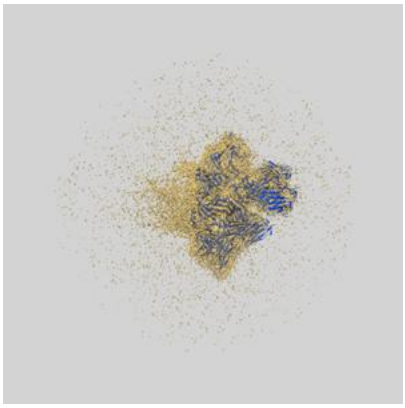
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29804 and PDB model 8G7A. Per-residue inclusion information can be found in section 3 on page 8.

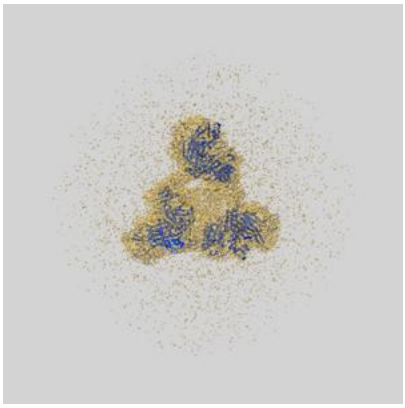
9.1 Map-model overlay



X



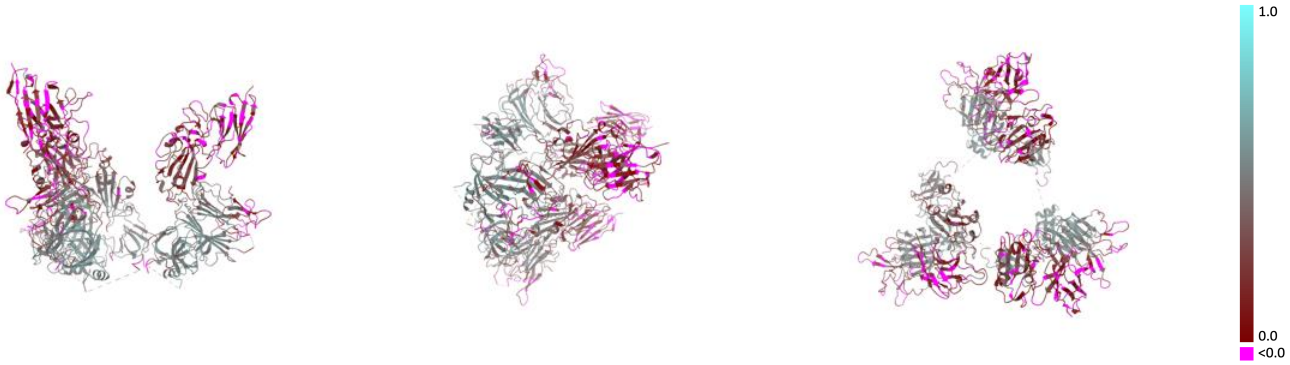
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0585 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

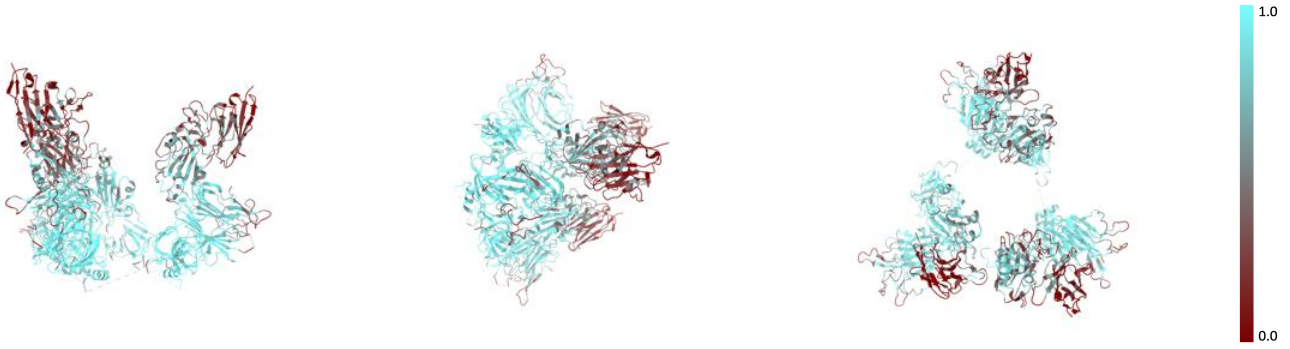
9.2 Q-score mapped to coordinate model



X Y Z

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

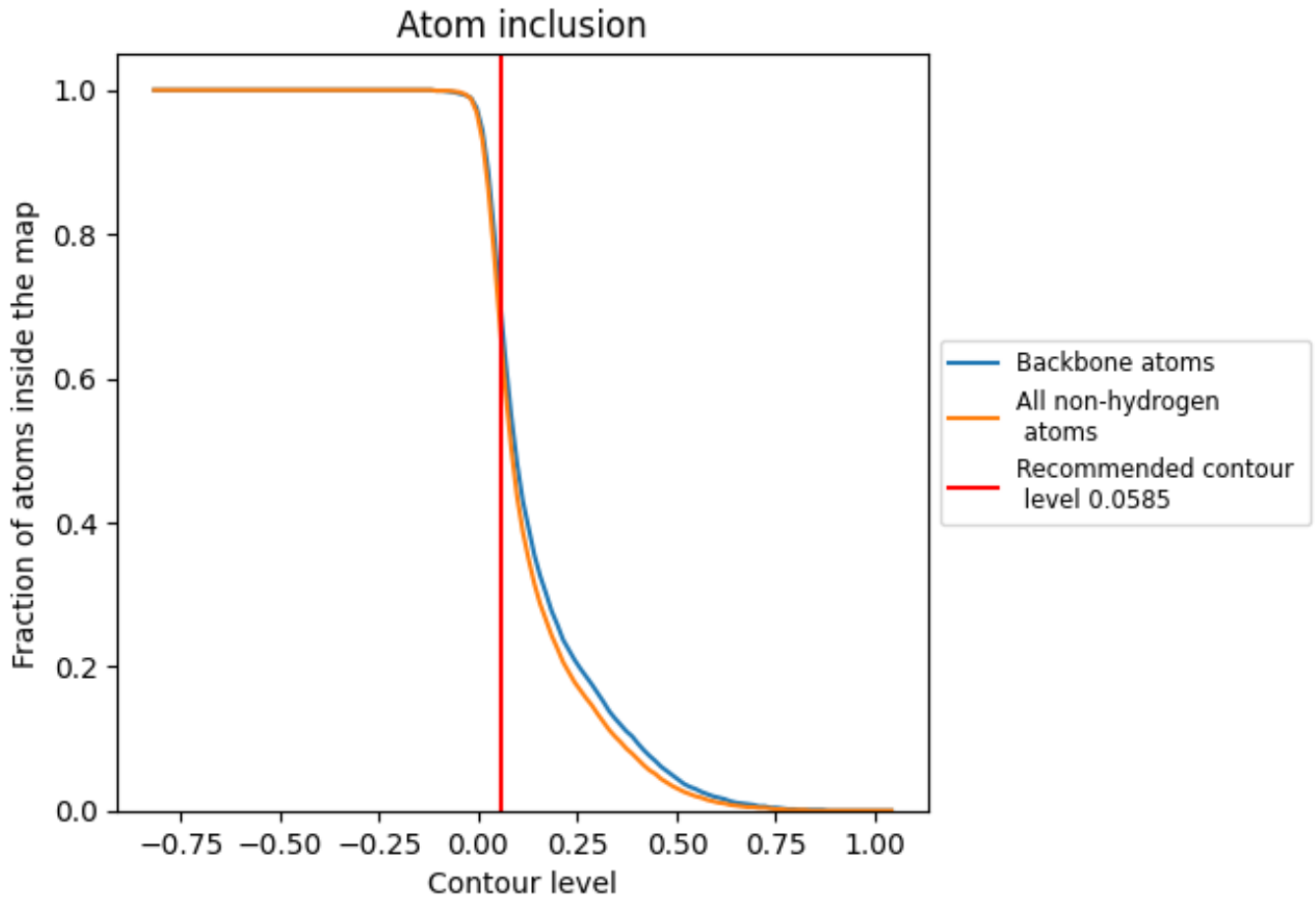
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0585).

9.4 Atom inclusion (i)



At the recommended contour level, 68% 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 (0.0585) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6460	0.2930
A	0.7820	0.3700
B	0.6970	0.3160
C	0.2170	0.0640
D	0.7220	0.3190
E	0.1350	0.0810
F	0.2280	0.0850