Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 09:52 AM EST

PDB ID	:	6VSJ
EMDB ID	:	EMD-21377
Title	:	Cryo-electron microscopy structure of mouse coronavirus spike protein complexed with its murine receptor
Authors	:	Shang, J.; Wan, Y.S.; Liu, C.; Yount, B.; Gully, K.; Yang, Y.; Auerbach, A.; Peng, G.Q.; Baric, R.; Li, F.
Deposited on	:	2020-02-11
Resolution	:	3.94 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

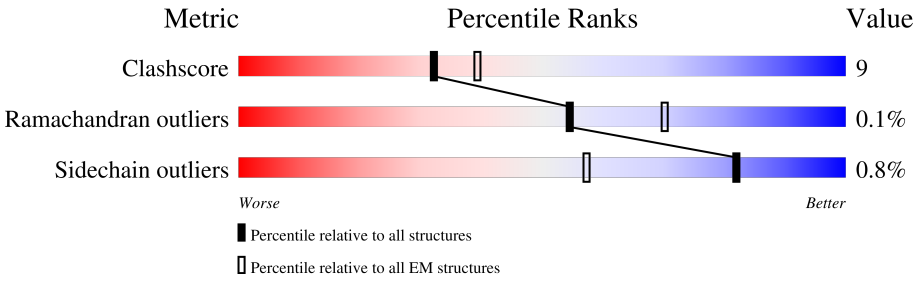
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

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 3.94 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	1275	68% 20% 12%
1	B	1275	68% 20% 12%
1	C	1275	67% 20% 12%
2	D	208	38% 13% 49%
2	E	208	39% 12% 49%
2	F	208	38% 13% 49%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28752 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	1122	Total	C	N	O	S	0	0
			8678	5491	1471	1667	49		
1	B	1122	Total	C	N	O	S	0	0
			8678	5491	1471	1667	49		
1	C	1122	Total	C	N	O	S	0	0
			8678	5491	1471	1667	49		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P11224
A	-5	LYS	-	expression tag	UNP P11224
A	-4	PHE	-	expression tag	UNP P11224
A	-3	LEU	-	expression tag	UNP P11224
A	-2	VAL	-	expression tag	UNP P11224
A	-1	ASN	-	expression tag	UNP P11224
A	0	VAL	-	expression tag	UNP P11224
A	1	ALA	-	expression tag	UNP P11224
A	2	LEU	-	expression tag	UNP P11224
A	3	VAL	-	expression tag	UNP P11224
A	4	PHE	-	expression tag	UNP P11224
A	5	MET	-	expression tag	UNP P11224
A	6	VAL	-	expression tag	UNP P11224
A	7	VAL	-	expression tag	UNP P11224
A	8	TYR	-	expression tag	UNP P11224
A	9	ILE	-	expression tag	UNP P11224
A	10	SER	-	expression tag	UNP P11224
A	11	TYR	-	expression tag	UNP P11224
A	12	ILE	-	expression tag	UNP P11224
A	13	TYR	-	expression tag	UNP P11224
A	14	ALA	-	expression tag	UNP P11224
A	478	PHE	TYR	conflict	UNP P11224
A	1229	ILE	-	expression tag	UNP P11224
A	1230	LYS	-	expression tag	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1231	ARG	-	expression tag	UNP P11224
A	1232	MET	-	expression tag	UNP P11224
A	1233	LYS	-	expression tag	UNP P11224
A	1234	GLN	-	expression tag	UNP P11224
A	1235	ILE	-	expression tag	UNP P11224
A	1236	GLU	-	expression tag	UNP P11224
A	1237	ASP	-	expression tag	UNP P11224
A	1238	LYS	-	expression tag	UNP P11224
A	1239	ILE	-	expression tag	UNP P11224
A	1240	GLU	-	expression tag	UNP P11224
A	1241	GLU	-	expression tag	UNP P11224
A	1242	ILE	-	expression tag	UNP P11224
A	1243	GLU	-	expression tag	UNP P11224
A	1244	SER	-	expression tag	UNP P11224
A	1245	LYS	-	expression tag	UNP P11224
A	1246	GLN	-	expression tag	UNP P11224
A	1247	LYS	-	expression tag	UNP P11224
A	1248	LYS	-	expression tag	UNP P11224
A	1249	ILE	-	expression tag	UNP P11224
A	1250	GLU	-	expression tag	UNP P11224
A	1251	ASN	-	expression tag	UNP P11224
A	1252	GLU	-	expression tag	UNP P11224
A	1253	ILE	-	expression tag	UNP P11224
A	1254	ALA	-	expression tag	UNP P11224
A	1255	ARG	-	expression tag	UNP P11224
A	1256	ILE	-	expression tag	UNP P11224
A	1257	LYS	-	expression tag	UNP P11224
A	1258	LYS	-	expression tag	UNP P11224
A	1259	ILE	-	expression tag	UNP P11224
A	1260	LYS	-	expression tag	UNP P11224
A	1261	HIS	-	expression tag	UNP P11224
A	1262	HIS	-	expression tag	UNP P11224
A	1263	HIS	-	expression tag	UNP P11224
A	1264	HIS	-	expression tag	UNP P11224
A	1265	HIS	-	expression tag	UNP P11224
A	1266	HIS	-	expression tag	UNP P11224
A	1267	HIS	-	expression tag	UNP P11224
A	1268	HIS	-	expression tag	UNP P11224
B	-6	MET	-	initiating methionine	UNP P11224
B	-5	LYS	-	expression tag	UNP P11224
B	-4	PHE	-	expression tag	UNP P11224
B	-3	LEU	-	expression tag	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	VAL	-	expression tag	UNP P11224
B	-1	ASN	-	expression tag	UNP P11224
B	0	VAL	-	expression tag	UNP P11224
B	1	ALA	-	expression tag	UNP P11224
B	2	LEU	-	expression tag	UNP P11224
B	3	VAL	-	expression tag	UNP P11224
B	4	PHE	-	expression tag	UNP P11224
B	5	MET	-	expression tag	UNP P11224
B	6	VAL	-	expression tag	UNP P11224
B	7	VAL	-	expression tag	UNP P11224
B	8	TYR	-	expression tag	UNP P11224
B	9	ILE	-	expression tag	UNP P11224
B	10	SER	-	expression tag	UNP P11224
B	11	TYR	-	expression tag	UNP P11224
B	12	ILE	-	expression tag	UNP P11224
B	13	TYR	-	expression tag	UNP P11224
B	14	ALA	-	expression tag	UNP P11224
B	478	PHE	TYR	conflict	UNP P11224
B	1229	ILE	-	expression tag	UNP P11224
B	1230	LYS	-	expression tag	UNP P11224
B	1231	ARG	-	expression tag	UNP P11224
B	1232	MET	-	expression tag	UNP P11224
B	1233	LYS	-	expression tag	UNP P11224
B	1234	GLN	-	expression tag	UNP P11224
B	1235	ILE	-	expression tag	UNP P11224
B	1236	GLU	-	expression tag	UNP P11224
B	1237	ASP	-	expression tag	UNP P11224
B	1238	LYS	-	expression tag	UNP P11224
B	1239	ILE	-	expression tag	UNP P11224
B	1240	GLU	-	expression tag	UNP P11224
B	1241	GLU	-	expression tag	UNP P11224
B	1242	ILE	-	expression tag	UNP P11224
B	1243	GLU	-	expression tag	UNP P11224
B	1244	SER	-	expression tag	UNP P11224
B	1245	LYS	-	expression tag	UNP P11224
B	1246	GLN	-	expression tag	UNP P11224
B	1247	LYS	-	expression tag	UNP P11224
B	1248	LYS	-	expression tag	UNP P11224
B	1249	ILE	-	expression tag	UNP P11224
B	1250	GLU	-	expression tag	UNP P11224
B	1251	ASN	-	expression tag	UNP P11224
B	1252	GLU	-	expression tag	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1253	ILE	-	expression tag	UNP P11224
B	1254	ALA	-	expression tag	UNP P11224
B	1255	ARG	-	expression tag	UNP P11224
B	1256	ILE	-	expression tag	UNP P11224
B	1257	LYS	-	expression tag	UNP P11224
B	1258	LYS	-	expression tag	UNP P11224
B	1259	ILE	-	expression tag	UNP P11224
B	1260	LYS	-	expression tag	UNP P11224
B	1261	HIS	-	expression tag	UNP P11224
B	1262	HIS	-	expression tag	UNP P11224
B	1263	HIS	-	expression tag	UNP P11224
B	1264	HIS	-	expression tag	UNP P11224
B	1265	HIS	-	expression tag	UNP P11224
B	1266	HIS	-	expression tag	UNP P11224
B	1267	HIS	-	expression tag	UNP P11224
B	1268	HIS	-	expression tag	UNP P11224
C	-6	MET	-	initiating methionine	UNP P11224
C	-5	LYS	-	expression tag	UNP P11224
C	-4	PHE	-	expression tag	UNP P11224
C	-3	LEU	-	expression tag	UNP P11224
C	-2	VAL	-	expression tag	UNP P11224
C	-1	ASN	-	expression tag	UNP P11224
C	0	VAL	-	expression tag	UNP P11224
C	1	ALA	-	expression tag	UNP P11224
C	2	LEU	-	expression tag	UNP P11224
C	3	VAL	-	expression tag	UNP P11224
C	4	PHE	-	expression tag	UNP P11224
C	5	MET	-	expression tag	UNP P11224
C	6	VAL	-	expression tag	UNP P11224
C	7	VAL	-	expression tag	UNP P11224
C	8	TYR	-	expression tag	UNP P11224
C	9	ILE	-	expression tag	UNP P11224
C	10	SER	-	expression tag	UNP P11224
C	11	TYR	-	expression tag	UNP P11224
C	12	ILE	-	expression tag	UNP P11224
C	13	TYR	-	expression tag	UNP P11224
C	14	ALA	-	expression tag	UNP P11224
C	478	PHE	TYR	conflict	UNP P11224
C	1229	ILE	-	expression tag	UNP P11224
C	1230	LYS	-	expression tag	UNP P11224
C	1231	ARG	-	expression tag	UNP P11224
C	1232	MET	-	expression tag	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1233	LYS	-	expression tag	UNP P11224
C	1234	GLN	-	expression tag	UNP P11224
C	1235	ILE	-	expression tag	UNP P11224
C	1236	GLU	-	expression tag	UNP P11224
C	1237	ASP	-	expression tag	UNP P11224
C	1238	LYS	-	expression tag	UNP P11224
C	1239	ILE	-	expression tag	UNP P11224
C	1240	GLU	-	expression tag	UNP P11224
C	1241	GLU	-	expression tag	UNP P11224
C	1242	ILE	-	expression tag	UNP P11224
C	1243	GLU	-	expression tag	UNP P11224
C	1244	SER	-	expression tag	UNP P11224
C	1245	LYS	-	expression tag	UNP P11224
C	1246	GLN	-	expression tag	UNP P11224
C	1247	LYS	-	expression tag	UNP P11224
C	1248	LYS	-	expression tag	UNP P11224
C	1249	ILE	-	expression tag	UNP P11224
C	1250	GLU	-	expression tag	UNP P11224
C	1251	ASN	-	expression tag	UNP P11224
C	1252	GLU	-	expression tag	UNP P11224
C	1253	ILE	-	expression tag	UNP P11224
C	1254	ALA	-	expression tag	UNP P11224
C	1255	ARG	-	expression tag	UNP P11224
C	1256	ILE	-	expression tag	UNP P11224
C	1257	LYS	-	expression tag	UNP P11224
C	1258	LYS	-	expression tag	UNP P11224
C	1259	ILE	-	expression tag	UNP P11224
C	1260	LYS	-	expression tag	UNP P11224
C	1261	HIS	-	expression tag	UNP P11224
C	1262	HIS	-	expression tag	UNP P11224
C	1263	HIS	-	expression tag	UNP P11224
C	1264	HIS	-	expression tag	UNP P11224
C	1265	HIS	-	expression tag	UNP P11224
C	1266	HIS	-	expression tag	UNP P11224
C	1267	HIS	-	expression tag	UNP P11224
C	1268	HIS	-	expression tag	UNP P11224

- Molecule 2 is a protein called Carcinoembryonic antigen-related cell adhesion molecule 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	107	Total	C	N	O	S	0	0
			850	540	145	160	5		

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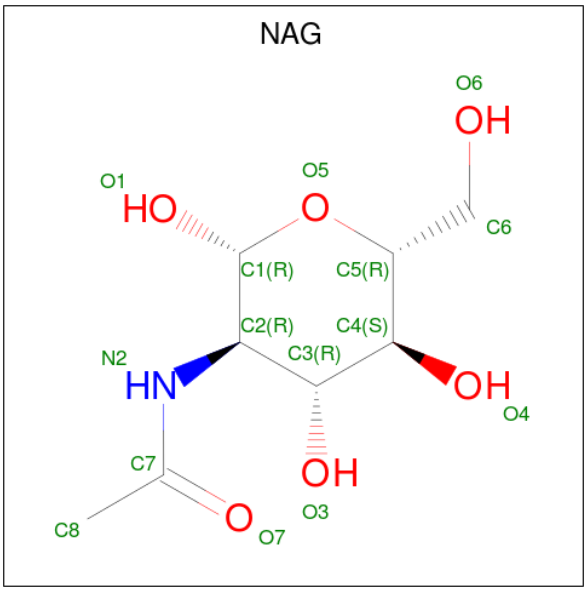
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			850	540	145	160	5		
2	F	107	Total	C	N	O	S	0	0
			850	540	145	160	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	237	HIS	-	expression tag	UNP P31809
D	238	HIS	-	expression tag	UNP P31809
D	239	HIS	-	expression tag	UNP P31809
D	240	HIS	-	expression tag	UNP P31809
D	241	HIS	-	expression tag	UNP P31809
D	242	HIS	-	expression tag	UNP P31809
E	237	HIS	-	expression tag	UNP P31809
E	238	HIS	-	expression tag	UNP P31809
E	239	HIS	-	expression tag	UNP P31809
E	240	HIS	-	expression tag	UNP P31809
E	241	HIS	-	expression tag	UNP P31809
E	242	HIS	-	expression tag	UNP P31809
F	237	HIS	-	expression tag	UNP P31809
F	238	HIS	-	expression tag	UNP P31809
F	239	HIS	-	expression tag	UNP P31809
F	240	HIS	-	expression tag	UNP P31809
F	241	HIS	-	expression tag	UNP P31809
F	242	HIS	-	expression tag	UNP P31809

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



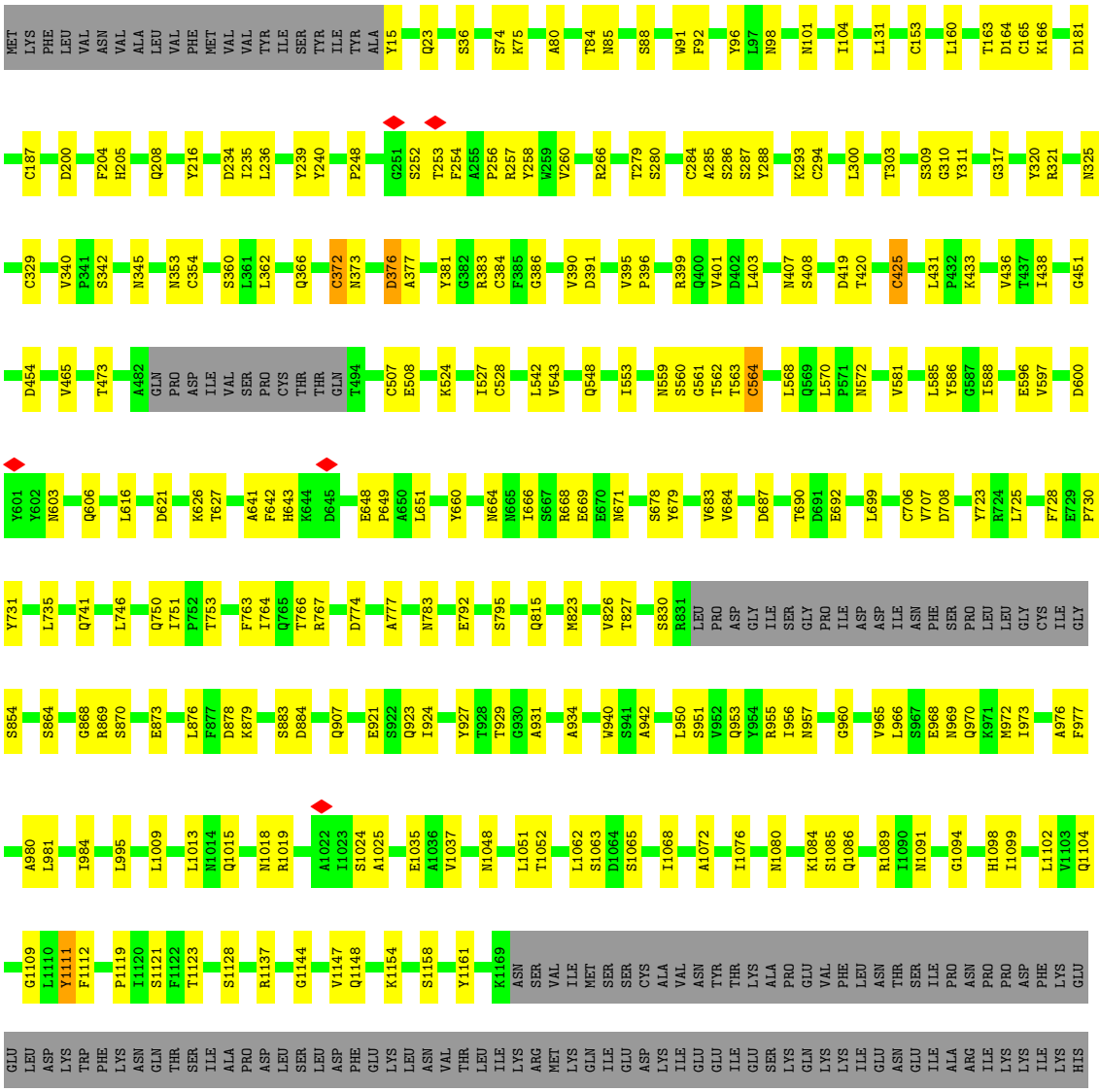
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			42	24	3	15	
3	A	1	Total	C	N	O	0
			42	24	3	15	
3	A	1	Total	C	N	O	0
			42	24	3	15	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			42	24	3	15	
3	B	1	Total	C	N	O	0
			42	24	3	15	
3	B	1	Total	C	N	O	0
			42	24	3	15	
3	E	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			42	24	3	15	
3	C	1	Total	C	N	O	0
			42	24	3	15	
3	C	1	Total	C	N	O	0
			42	24	3	15	
3	F	1	Total	C	N	O	0
			14	8	1	5	

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.

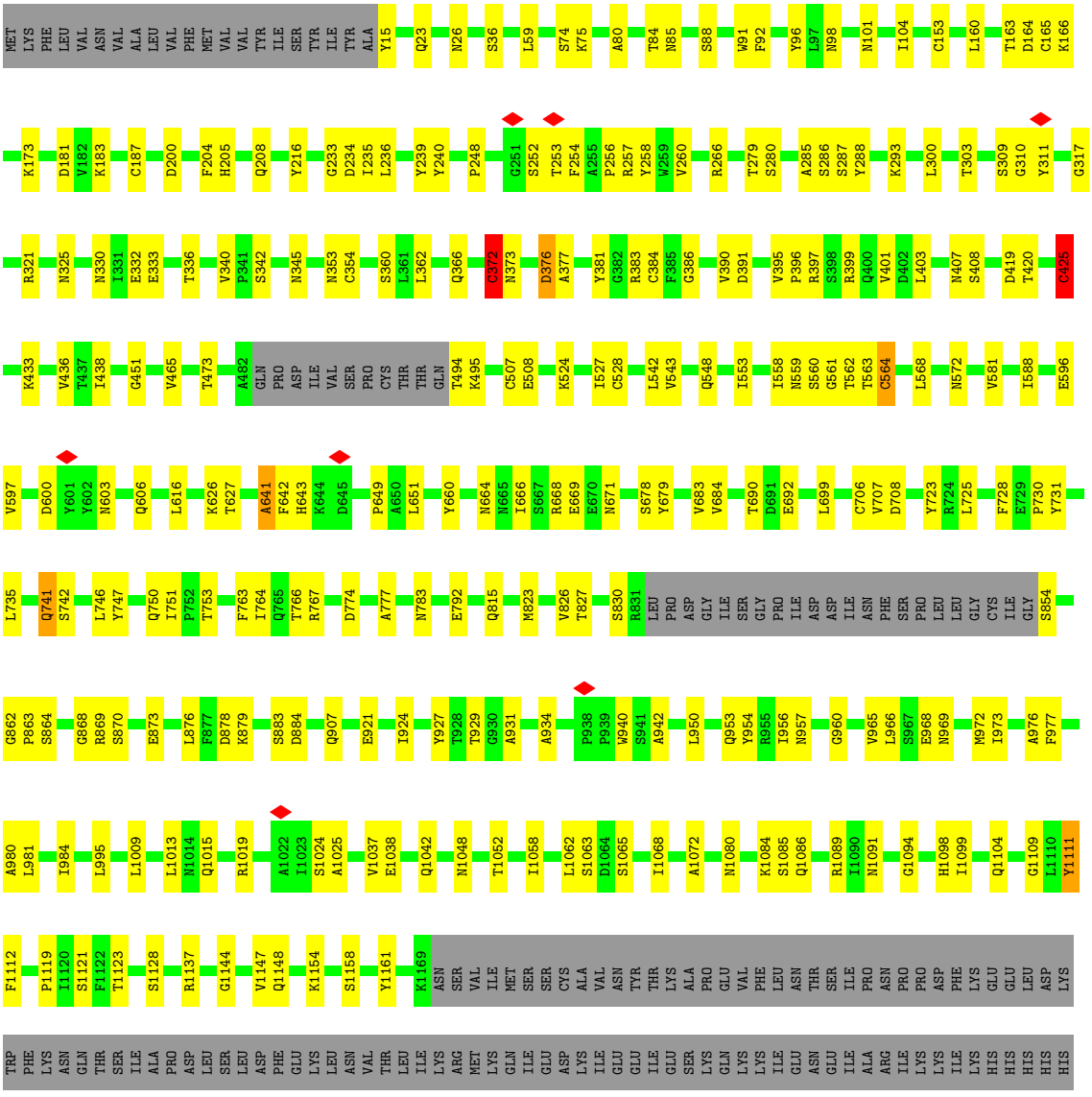
- Molecule 1: Spike glycoprotein

Chain A:



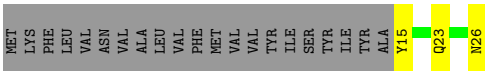
• Molecule 1: Spike glycoprotein

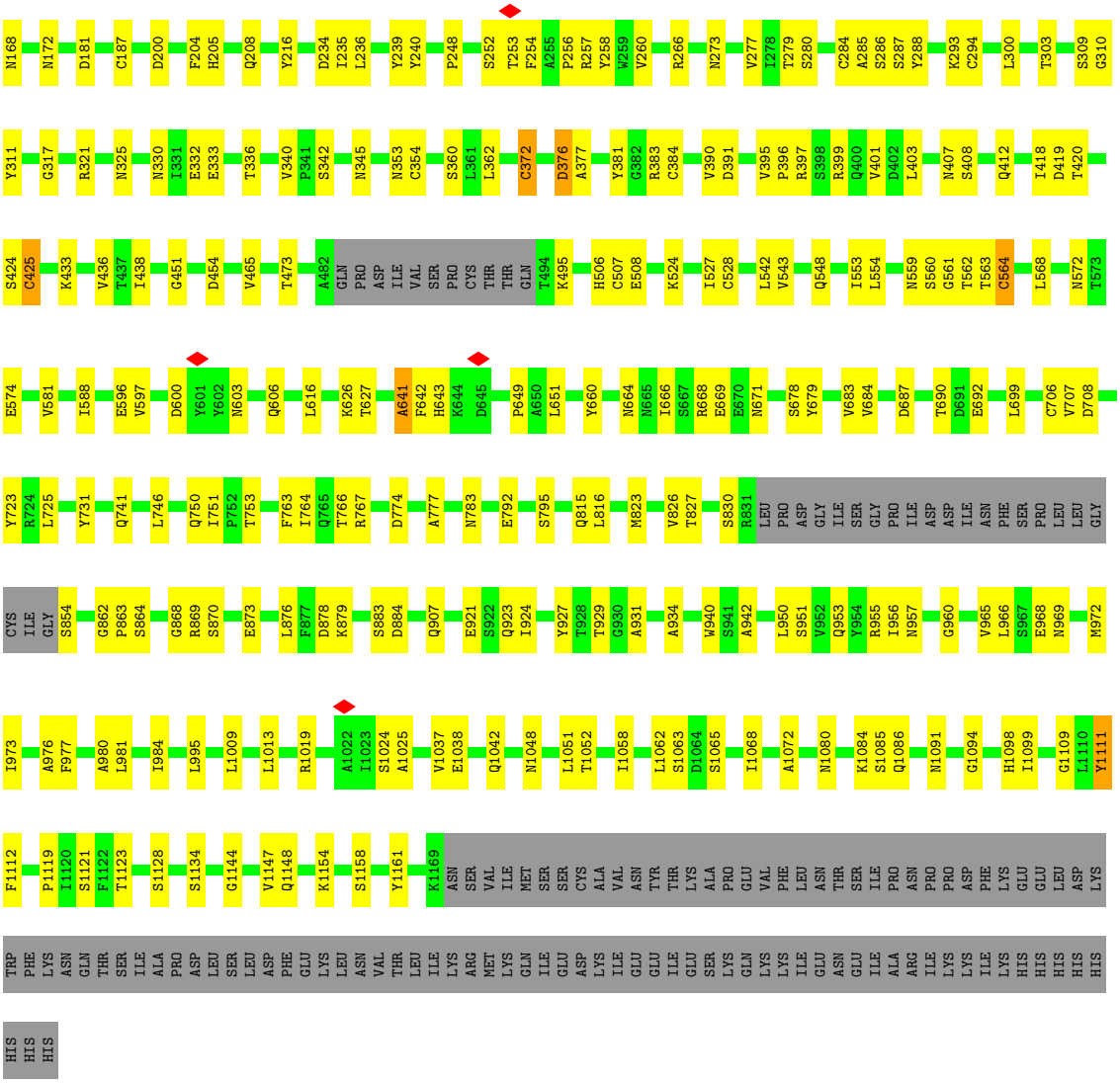
Chain B:



• Molecule 1: Spike glycoprotein

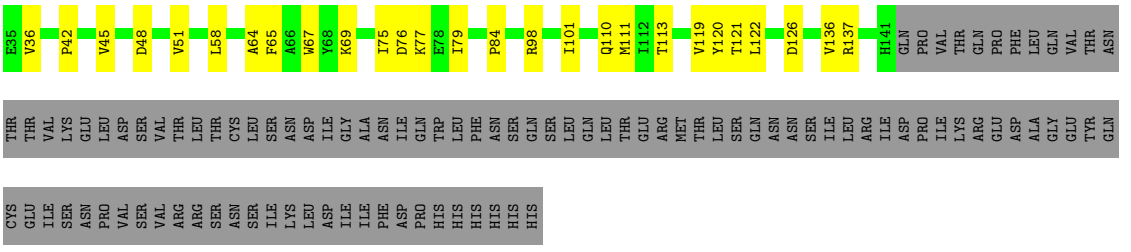
Chain C:





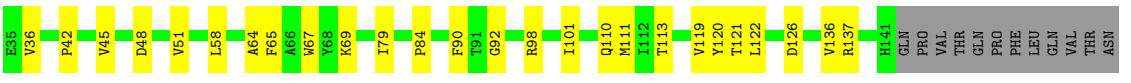
• Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 1

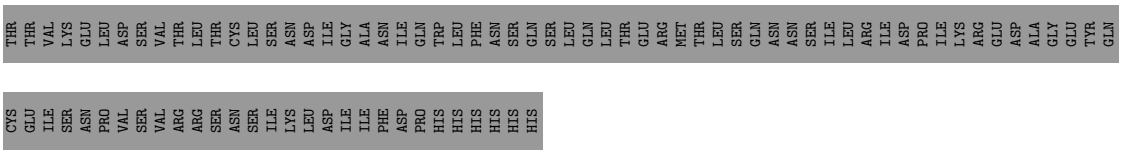
Chain D:



• Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 1

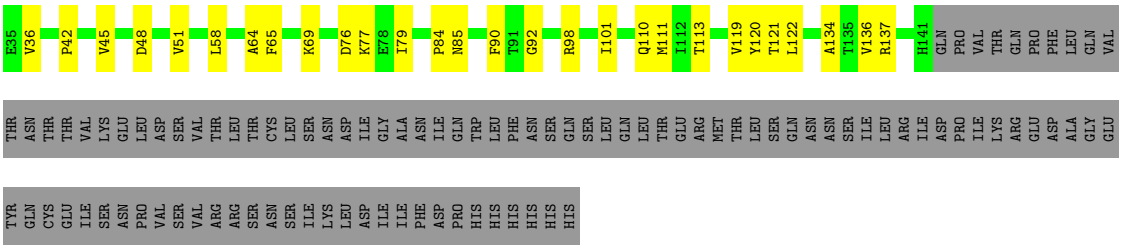
Chain E:





• Molecule 2: Carcinoembryonic antigen-related cell adhesion molecule 1

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	82923	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	77	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00869	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.47	0/8874	0.60	2/12088 (0.0%)
1	B	0.47	0/8874	0.60	2/12088 (0.0%)
1	C	0.47	0/8874	0.60	2/12088 (0.0%)
2	D	0.33	0/868	0.54	0/1180
2	E	0.33	0/868	0.54	0/1180
2	F	0.33	0/868	0.54	0/1180
All	All	0.46	0/29226	0.59	6/39804 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
All	All	0	9

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	425	CYS	CA-CB-SG	8.62	129.51	114.00
1	A	425	CYS	CA-CB-SG	8.59	129.46	114.00
1	C	425	CYS	CA-CB-SG	8.58	129.44	114.00
1	A	372	CYS	CA-CB-SG	5.24	123.44	114.00
1	C	372	CYS	CA-CB-SG	5.24	123.43	114.00
1	B	372	CYS	CA-CB-SG	5.23	123.41	114.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	641	ALA	Peptide
1	A	642	PHE	Peptide
1	A	966	LEU	Peptide
1	B	641	ALA	Peptide
1	B	642	PHE	Peptide
1	B	966	LEU	Peptide
1	C	641	ALA	Peptide
1	C	642	PHE	Peptide
1	C	966	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8678	0	8383	177	0
1	B	8678	0	8383	172	0
1	C	8678	0	8383	172	0
2	D	850	0	830	16	0
2	E	850	0	830	16	0
2	F	850	0	830	18	0
3	A	42	0	39	1	0
3	B	42	0	39	1	0
3	C	42	0	39	1	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	0	0
All	All	28752	0	27795	534	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 9.

All (534) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:826:VAL:HG12	1:C:827:THR:H	1.36	0.91
1:A:826:VAL:HG12	1:A:827:THR:H	1.36	0.90
1:B:826:VAL:HG12	1:B:827:THR:H	1.36	0.89
1:C:826:VAL:HG12	1:C:827:THR:N	1.97	0.79
1:B:826:VAL:HG12	1:B:827:THR:N	1.97	0.79
1:A:826:VAL:HG12	1:A:827:THR:N	1.97	0.79
1:C:826:VAL:CG1	1:C:827:THR:H	2.07	0.67
1:C:376:ASP:OD1	1:C:376:ASP:N	2.30	0.65
1:B:826:VAL:CG1	1:B:827:THR:H	2.07	0.65
1:A:826:VAL:CG1	1:A:827:THR:H	2.07	0.65
1:C:766:THR:HG22	1:C:1109:GLY:HA2	1.79	0.65
1:A:377:ALA:HB3	1:B:408:SER:H	1.62	0.64
1:B:1065:SER:HA	1:B:1068:ILE:HD12	1.81	0.63
1:B:766:THR:HG22	1:B:1109:GLY:HA2	1.79	0.63
1:A:766:THR:HG22	1:A:1109:GLY:HA2	1.79	0.63
1:B:303:THR:HG22	1:B:643:HIS:HA	1.81	0.63
1:A:1065:SER:HA	1:A:1068:ILE:HD12	1.81	0.62
1:B:376:ASP:OD1	1:B:376:ASP:N	2.30	0.62
1:C:285:ALA:O	1:C:668:ARG:NH2	2.33	0.62
1:C:383:ARG:NH1	1:C:559:ASN:OD1	2.32	0.62
1:B:383:ARG:NH1	1:B:559:ASN:OD1	2.32	0.62
1:C:1065:SER:HA	1:C:1068:ILE:HD12	1.81	0.61
1:A:383:ARG:NH1	1:A:559:ASN:OD1	2.32	0.61
1:A:690:THR:HG22	1:A:692:GLU:H	1.65	0.61
1:C:706:CYS:SG	1:C:707:VAL:N	2.74	0.61
1:B:934:ALA:HB1	1:B:942:ALA:HB3	1.83	0.61
1:B:690:THR:HG22	1:B:692:GLU:H	1.65	0.60
1:C:690:THR:HG22	1:C:692:GLU:H	1.65	0.60
1:A:303:THR:HG22	1:A:643:HIS:HA	1.81	0.60
1:A:376:ASP:OD1	1:A:376:ASP:N	2.30	0.60
1:B:395:VAL:HG21	1:B:403:LEU:HD11	1.83	0.60
1:C:303:THR:HG22	1:C:643:HIS:HA	1.81	0.60
1:A:256:PRO:O	1:A:257:ARG:NH1	2.35	0.60
1:B:706:CYS:SG	1:B:707:VAL:N	2.74	0.60
1:A:706:CYS:SG	1:A:707:VAL:N	2.74	0.60
1:A:285:ALA:O	1:A:668:ARG:NH2	2.33	0.60
1:B:256:PRO:O	1:B:257:ARG:NH1	2.35	0.60
1:A:934:ALA:HB1	1:A:942:ALA:HB3	1.83	0.59
1:C:395:VAL:HG21	1:C:403:LEU:HD11	1.83	0.59
1:B:285:ALA:O	1:B:668:ARG:NH2	2.33	0.59
1:C:934:ALA:HB1	1:C:942:ALA:HB3	1.83	0.59
1:B:1085:SER:OG	1:B:1086:GLN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:HG21	1:A:403:LEU:HD11	1.83	0.58
1:C:205:HIS:HB2	1:C:216:TYR:HB2	1.86	0.58
1:B:660:TYR:O	1:B:664:ASN:ND2	2.34	0.58
1:A:1019:ARG:NH2	1:C:792:GLU:OE2	2.36	0.58
1:B:208:GLN:NE2	1:B:236:LEU:O	2.37	0.58
1:B:205:HIS:HB2	1:B:216:TYR:HB2	1.86	0.58
1:A:362:LEU:O	1:B:399:ARG:NH2	2.37	0.58
1:C:208:GLN:NE2	1:C:236:LEU:O	2.37	0.58
1:A:208:GLN:NE2	1:A:236:LEU:O	2.37	0.57
1:A:956:ILE:HG12	1:A:1099:ILE:HD12	1.86	0.57
1:B:767:ARG:NH1	1:B:921:GLU:OE2	2.37	0.57
1:B:869:ARG:HD2	1:B:929:THR:HG23	1.86	0.57
1:C:767:ARG:NH1	1:C:921:GLU:OE2	2.37	0.57
1:A:205:HIS:HB2	1:A:216:TYR:HB2	1.86	0.57
1:B:407:ASN:OD1	1:B:407:ASN:N	2.37	0.57
1:B:883:SER:OG	1:B:884:ASP:N	2.38	0.57
1:A:600:ASP:OD1	1:A:600:ASP:N	2.38	0.57
1:B:360:SER:HB3	3:B:1303:NAG:H83	1.86	0.57
1:B:956:ILE:HG12	1:B:1099:ILE:HD12	1.85	0.57
1:A:883:SER:OG	1:A:884:ASP:N	2.38	0.57
1:C:26:ASN:HA	2:F:90:PHE:HB3	1.85	0.57
1:C:869:ARG:HD2	1:C:929:THR:HG23	1.86	0.57
1:B:864:SER:O	1:B:868:GLY:N	2.35	0.57
1:C:956:ILE:HG12	1:C:1099:ILE:HD12	1.86	0.57
1:C:1085:SER:OG	1:C:1086:GLN:N	2.36	0.57
1:A:660:TYR:O	1:A:664:ASN:ND2	2.34	0.57
1:C:256:PRO:O	1:C:257:ARG:NH1	2.35	0.57
1:A:767:ARG:NH1	1:A:921:GLU:OE2	2.37	0.57
1:C:15:TYR:N	1:C:92:PHE:O	2.38	0.57
1:A:708:ASP:OD1	1:A:708:ASP:N	2.38	0.56
1:A:869:ARG:HD2	1:A:929:THR:HG23	1.86	0.56
1:A:1085:SER:OG	1:A:1086:GLN:N	2.36	0.56
1:B:15:TYR:N	1:B:92:PHE:O	2.38	0.56
1:C:407:ASN:N	1:C:407:ASN:OD1	2.37	0.56
1:C:969:ASN:O	1:C:973:ILE:N	2.36	0.56
1:A:15:TYR:N	1:A:92:PHE:O	2.38	0.56
1:A:360:SER:HB3	3:A:1303:NAG:H83	1.87	0.56
1:B:976:ALA:O	1:B:980:ALA:N	2.38	0.56
1:B:969:ASN:O	1:B:973:ILE:N	2.36	0.56
1:C:678:SER:OG	1:C:679:TYR:N	2.39	0.56
1:C:360:SER:HB3	3:C:1303:NAG:H83	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:ASP:OD1	1:C:600:ASP:N	2.38	0.56
1:A:976:ALA:O	1:A:980:ALA:N	2.38	0.56
1:B:708:ASP:OD1	1:B:708:ASP:N	2.38	0.56
1:A:678:SER:OG	1:A:679:TYR:N	2.39	0.56
1:C:976:ALA:O	1:C:980:ALA:N	2.38	0.56
1:C:708:ASP:N	1:C:708:ASP:OD1	2.38	0.56
1:A:407:ASN:OD1	1:A:407:ASN:N	2.37	0.56
1:C:883:SER:OG	1:C:884:ASP:N	2.38	0.56
1:B:600:ASP:OD1	1:B:600:ASP:N	2.38	0.55
1:B:678:SER:OG	1:B:679:TYR:N	2.39	0.55
1:B:321:ARG:HD3	1:B:572:ASN:HD21	1.72	0.55
1:C:165:CYS:SG	1:C:166:LYS:N	2.79	0.55
1:B:165:CYS:SG	1:B:166:LYS:N	2.79	0.55
1:C:1024:SER:OG	1:C:1025:ALA:N	2.39	0.55
1:C:1158:SER:O	1:C:1158:SER:OG	2.24	0.55
1:B:204:PHE:O	1:B:205:HIS:ND1	2.40	0.55
1:C:953:GLN:O	1:C:957:ASN:ND2	2.40	0.55
1:A:953:GLN:O	1:A:957:ASN:ND2	2.40	0.55
1:B:377:ALA:HB3	1:C:408:SER:H	1.72	0.55
1:B:420:THR:HB	1:C:1037:VAL:HG22	1.89	0.55
1:A:165:CYS:SG	1:A:166:LYS:N	2.80	0.55
1:C:321:ARG:HD3	1:C:572:ASN:HD21	1.72	0.55
1:A:878:ASP:OD2	1:A:879:LYS:NZ	2.38	0.54
1:C:401:VAL:O	1:C:407:ASN:ND2	2.40	0.54
1:A:321:ARG:HD3	1:A:572:ASN:HD21	1.72	0.54
1:B:953:GLN:O	1:B:957:ASN:ND2	2.40	0.54
1:B:433:LYS:HE2	1:B:542:LEU:HD11	1.90	0.54
1:C:204:PHE:O	1:C:205:HIS:ND1	2.40	0.54
1:B:401:VAL:O	1:B:407:ASN:ND2	2.40	0.54
1:B:792:GLU:OE2	1:C:1019:ARG:NH2	2.40	0.54
1:B:1024:SER:OG	1:B:1025:ALA:N	2.39	0.54
1:A:763:PHE:HA	1:A:1111:TYR:HB2	1.90	0.54
1:A:1024:SER:OG	1:A:1025:ALA:N	2.39	0.54
1:C:660:TYR:O	1:C:664:ASN:ND2	2.34	0.54
1:A:401:VAL:O	1:A:407:ASN:ND2	2.40	0.54
1:A:433:LYS:HE2	1:A:542:LEU:HD11	1.90	0.54
1:C:433:LYS:HE2	1:C:542:LEU:HD11	1.89	0.54
1:A:864:SER:O	1:A:868:GLY:N	2.35	0.53
1:C:783:ASN:OD1	1:C:783:ASN:N	2.40	0.53
1:A:1158:SER:O	1:A:1158:SER:OG	2.24	0.53
1:A:204:PHE:O	1:A:205:HIS:ND1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASP:N	1:B:181:ASP:OD1	2.41	0.53
1:C:560:SER:OG	1:C:561:GLY:N	2.41	0.53
1:C:763:PHE:HA	1:C:1111:TYR:HB2	1.89	0.53
1:C:864:SER:O	1:C:868:GLY:N	2.35	0.53
1:A:181:ASP:OD1	1:A:181:ASP:N	2.41	0.53
1:B:560:SER:OG	1:B:561:GLY:N	2.41	0.53
1:B:878:ASP:OD2	1:B:879:LYS:NZ	2.38	0.53
1:B:1158:SER:O	1:B:1158:SER:OG	2.24	0.53
1:C:311:TYR:OH	1:C:668:ARG:NH1	2.42	0.53
1:B:524:LYS:HD2	1:B:527:ILE:HD11	1.90	0.53
1:B:783:ASN:OD1	1:B:783:ASN:N	2.40	0.53
1:C:524:LYS:HD2	1:C:527:ILE:HD11	1.90	0.53
1:A:311:TYR:OH	1:A:668:ARG:NH1	2.42	0.53
1:A:950:LEU:HD21	1:B:1144:GLY:HA2	1.89	0.53
1:B:603:ASN:H	1:B:606:GLN:HE21	1.57	0.53
1:C:340:VAL:HG21	1:C:436:VAL:HG23	1.91	0.53
1:A:408:SER:H	1:C:377:ALA:HB3	1.74	0.53
1:C:473:THR:HB	1:C:508:GLU:HG3	1.91	0.53
1:A:420:THR:HB	1:B:1037:VAL:HG22	1.91	0.53
1:A:560:SER:OG	1:A:561:GLY:N	2.41	0.53
1:A:473:THR:HB	1:A:508:GLU:HG3	1.91	0.52
1:B:311:TYR:OH	1:B:668:ARG:NH1	2.42	0.52
1:B:763:PHE:HA	1:B:1111:TYR:HB2	1.90	0.52
2:E:64:ALA:HA	2:E:84:PRO:HD3	1.91	0.52
1:B:266:ARG:HD2	1:B:285:ALA:HB3	1.92	0.52
1:B:340:VAL:HG21	1:B:436:VAL:HG23	1.91	0.52
1:C:597:VAL:O	1:C:627:THR:OG1	2.25	0.52
1:A:266:ARG:HD2	1:A:285:ALA:HB3	1.92	0.52
2:D:64:ALA:HA	2:D:84:PRO:HD3	1.91	0.52
1:B:751:ILE:HG21	1:B:1119:PRO:HB2	1.91	0.52
1:A:524:LYS:HD2	1:A:527:ILE:HD11	1.90	0.52
1:C:603:ASN:H	1:C:606:GLN:HE21	1.57	0.52
1:A:751:ILE:HG21	1:A:1119:PRO:HB2	1.91	0.52
1:C:266:ARG:HD2	1:C:285:ALA:HB3	1.92	0.52
1:A:340:VAL:HG21	1:A:436:VAL:HG23	1.91	0.52
1:A:286:SER:OG	1:A:287:SER:N	2.43	0.51
1:B:597:VAL:O	1:B:627:THR:OG1	2.25	0.51
1:C:973:ILE:O	1:C:977:PHE:N	2.42	0.51
1:A:603:ASN:H	1:A:606:GLN:HE21	1.57	0.51
1:C:286:SER:OG	1:C:287:SER:N	2.43	0.51
1:B:473:THR:HB	1:B:508:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:SER:OG	1:C:253:THR:N	2.43	0.51
1:C:751:ILE:HG21	1:C:1119:PRO:HB2	1.91	0.51
2:F:64:ALA:HA	2:F:84:PRO:HD3	1.91	0.51
1:A:792:GLU:OE2	1:B:1019:ARG:NH2	2.44	0.51
2:F:65:PHE:HE2	2:F:101:ILE:HD11	1.76	0.51
2:D:65:PHE:HE2	2:D:101:ILE:HD11	1.76	0.51
1:B:252:SER:OG	1:B:253:THR:N	2.43	0.51
1:C:181:ASP:OD1	1:C:181:ASP:N	2.41	0.51
1:A:252:SER:OG	1:A:253:THR:N	2.43	0.51
1:C:878:ASP:OD2	1:C:879:LYS:NZ	2.38	0.51
1:C:750:GLN:O	1:C:1123:THR:OG1	2.29	0.51
2:E:65:PHE:HE2	2:E:101:ILE:HD11	1.76	0.51
1:A:342:SER:OG	1:A:345:ASN:OD1	2.28	0.50
1:A:783:ASN:N	1:A:783:ASN:OD1	2.40	0.50
1:B:366:GLN:OE1	1:C:397:ARG:NH1	2.42	0.50
1:A:965:VAL:O	1:A:968:GLU:N	2.45	0.50
2:D:98:ARG:NH2	2:D:113:THR:OG1	2.45	0.50
1:A:750:GLN:O	1:A:1123:THR:OG1	2.29	0.50
1:B:286:SER:OG	1:B:287:SER:N	2.43	0.50
1:B:965:VAL:O	1:B:968:GLU:N	2.45	0.50
2:E:98:ARG:NH2	2:E:113:THR:OG1	2.45	0.50
1:C:965:VAL:O	1:C:968:GLU:N	2.45	0.50
1:A:366:GLN:OE1	1:B:397:ARG:NH1	2.45	0.50
1:B:927:TYR:O	1:B:931:ALA:N	2.45	0.49
1:A:969:ASN:O	1:A:973:ILE:N	2.36	0.49
1:C:342:SER:OG	1:C:345:ASN:OD1	2.28	0.49
1:B:956:ILE:O	1:B:960:GLY:N	2.45	0.49
1:A:309:SER:OG	1:A:310:GLY:N	2.46	0.49
1:A:596:GLU:OE2	1:A:626:LYS:NZ	2.44	0.49
1:B:309:SER:OG	1:B:310:GLY:N	2.46	0.49
2:F:98:ARG:NH2	2:F:113:THR:OG1	2.45	0.49
1:A:956:ILE:O	1:A:960:GLY:N	2.45	0.49
1:B:750:GLN:O	1:B:1123:THR:OG1	2.29	0.49
2:F:79:ILE:O	2:F:92:GLY:N	2.41	0.49
1:B:973:ILE:O	1:B:977:PHE:N	2.42	0.49
1:C:454:ASP:OD1	1:C:454:ASP:N	2.43	0.49
1:A:731:TYR:HB2	1:C:823:MET:HG2	1.95	0.48
1:C:750:GLN:HB3	1:C:1161:TYR:HB2	1.95	0.48
1:B:764:ILE:HD12	1:B:1112:PHE:HE2	1.77	0.48
1:B:870:SER:OG	1:B:873:GLU:OE1	2.28	0.48
1:A:973:ILE:O	1:A:977:PHE:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:120:TYR:N	2:E:136:VAL:O	2.42	0.48
1:C:309:SER:OG	1:C:310:GLY:N	2.46	0.48
1:B:588:ILE:HG21	1:B:616:LEU:HD13	1.96	0.48
1:C:303:THR:HB	1:C:699:LEU:HD11	1.96	0.48
1:C:764:ILE:HD12	1:C:1112:PHE:HE2	1.77	0.48
1:C:956:ILE:O	1:C:960:GLY:N	2.45	0.48
1:A:23:GLN:NE2	1:A:160:LEU:O	2.47	0.48
2:E:79:ILE:O	2:E:92:GLY:N	2.41	0.48
1:A:248:PRO:HG3	1:A:254:PHE:HB2	1.96	0.48
1:A:764:ILE:HD12	1:A:1112:PHE:HE2	1.77	0.48
1:C:596:GLU:OE2	1:C:626:LYS:NZ	2.44	0.48
1:B:23:GLN:NE2	1:B:160:LEU:O	2.47	0.48
1:C:23:GLN:NE2	1:C:160:LEU:O	2.47	0.48
1:B:164:ASP:OD1	1:B:166:LYS:N	2.47	0.48
1:C:391:ASP:N	1:C:391:ASP:OD1	2.47	0.48
1:A:750:GLN:HB3	1:A:1161:TYR:HB2	1.95	0.48
1:B:342:SER:OG	1:B:345:ASN:OD1	2.28	0.48
1:B:750:GLN:HB3	1:B:1161:TYR:HB2	1.95	0.48
1:C:1148:GLN:HG3	1:C:1154:LYS:HB2	1.96	0.48
1:B:303:THR:HB	1:B:699:LEU:HD11	1.96	0.47
1:B:345:ASN:OD1	1:B:345:ASN:N	2.47	0.47
1:C:248:PRO:HG3	1:C:254:PHE:HB2	1.96	0.47
2:D:48:ASP:HA	2:D:111:MET:HG2	1.96	0.47
1:C:588:ILE:HG21	1:C:616:LEU:HD13	1.96	0.47
1:B:362:LEU:O	1:C:399:ARG:NH2	2.47	0.47
1:B:950:LEU:HD21	1:C:1144:GLY:HA2	1.95	0.47
1:C:164:ASP:OD1	1:C:166:LYS:N	2.47	0.47
1:A:1128:SER:H	1:A:1147:VAL:HB	1.80	0.47
1:B:248:PRO:HG3	1:B:254:PHE:HB2	1.96	0.47
1:A:823:MET:HG2	1:B:731:TYR:HB2	1.96	0.47
1:A:1148:GLN:HG3	1:A:1154:LYS:HB2	1.96	0.47
1:B:1148:GLN:HG3	1:B:1154:LYS:HB2	1.97	0.47
1:A:1144:GLY:HA2	1:C:950:LEU:HD21	1.95	0.47
1:A:588:ILE:HG21	1:A:616:LEU:HD13	1.96	0.47
1:B:325:ASN:OD1	1:B:325:ASN:N	2.48	0.47
1:B:384:CYS:HA	1:B:564:CYS:HB3	1.97	0.47
1:C:325:ASN:N	1:C:325:ASN:OD1	2.48	0.47
1:C:980:ALA:O	1:C:984:ILE:N	2.44	0.47
2:D:119:VAL:HG12	2:D:137:ARG:HB2	1.97	0.47
2:F:119:VAL:HG12	2:F:137:ARG:HB2	1.97	0.47
1:A:774:ASP:OD2	1:A:777:ALA:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:VAL:CG1	1:A:827:THR:N	2.67	0.47
1:B:391:ASP:OD1	1:B:391:ASP:N	2.47	0.47
1:C:753:THR:HB	1:C:1121:SER:H	1.80	0.47
1:A:325:ASN:N	1:A:325:ASN:OD1	2.48	0.46
1:A:664:ASN:HB2	1:A:666:ILE:HG12	1.97	0.46
1:C:870:SER:OG	1:C:870:SER:O	2.33	0.46
1:A:345:ASN:OD1	1:A:345:ASN:N	2.47	0.46
1:B:257:ARG:HA	1:B:257:ARG:HD3	1.72	0.46
1:A:98:ASN:ND2	1:A:239:TYR:OH	2.49	0.46
1:A:753:THR:HB	1:A:1121:SER:H	1.81	0.46
2:E:48:ASP:HA	2:E:111:MET:HG2	1.97	0.46
2:E:119:VAL:HG12	2:E:137:ARG:HB2	1.97	0.46
1:C:384:CYS:HA	1:C:564:CYS:HB3	1.97	0.46
1:C:927:TYR:O	1:C:931:ALA:N	2.45	0.46
1:B:419:ASP:OD1	1:B:419:ASP:N	2.42	0.46
1:C:36:SER:O	1:C:36:SER:OG	2.32	0.46
1:B:651:LEU:HB2	1:B:684:VAL:HB	1.98	0.46
1:C:288:TYR:HB2	1:C:649:PRO:HG3	1.97	0.46
1:C:353:ASN:ND2	1:C:562:THR:OG1	2.48	0.46
1:C:1128:SER:H	1:C:1147:VAL:HB	1.80	0.46
2:F:48:ASP:HA	2:F:111:MET:HG2	1.97	0.46
1:A:303:THR:HB	1:A:699:LEU:HD11	1.96	0.46
1:A:869:ARG:O	1:A:1104:GLN:NE2	2.44	0.46
1:B:664:ASN:HB2	1:B:666:ILE:HG12	1.97	0.46
1:B:869:ARG:O	1:B:1104:GLN:NE2	2.44	0.46
1:B:1128:SER:H	1:B:1147:VAL:HB	1.80	0.46
1:C:651:LEU:HB2	1:C:684:VAL:HB	1.98	0.46
1:B:870:SER:OG	1:B:870:SER:O	2.34	0.46
1:C:419:ASP:N	1:C:419:ASP:OD1	2.42	0.46
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.83	0.46
1:B:753:THR:HB	1:B:1121:SER:H	1.81	0.46
1:A:651:LEU:HB2	1:A:684:VAL:HB	1.98	0.46
1:A:1062:LEU:HD23	1:A:1062:LEU:HA	1.82	0.46
1:B:288:TYR:HB2	1:B:649:PRO:HG3	1.98	0.46
1:B:373:ASN:OD1	1:B:373:ASN:N	2.43	0.46
1:A:927:TYR:O	1:A:931:ALA:N	2.45	0.46
1:A:1068:ILE:O	1:A:1072:ALA:N	2.42	0.46
1:A:153:CYS:HA	1:A:187:CYS:HB3	1.97	0.45
1:B:1062:LEU:HD23	1:B:1062:LEU:HA	1.82	0.45
2:E:98:ARG:HB2	2:E:110:GLN:HB2	1.98	0.45
1:C:1094:GLY:HA3	1:C:1098:HIS:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:HA	1:B:735:LEU:HD21	1.98	0.45
1:B:98:ASN:ND2	1:B:239:TYR:OH	2.49	0.45
1:A:74:SER:OG	1:A:75:LYS:N	2.49	0.45
1:A:384:CYS:HA	1:A:564:CYS:HB3	1.97	0.45
2:D:45:VAL:HG21	2:D:51:VAL:HB	1.98	0.45
1:B:153:CYS:HA	1:B:187:CYS:HB3	1.98	0.45
1:B:332:GLU:O	1:B:336:THR:OG1	2.34	0.45
1:B:830:SER:O	1:B:854:SER:N	2.50	0.45
1:A:36:SER:O	1:A:36:SER:OG	2.32	0.45
1:B:980:ALA:O	1:B:984:ILE:N	2.44	0.45
1:A:160:LEU:HD11	2:D:75:ILE:HD13	1.98	0.45
1:A:419:ASP:OD1	1:A:419:ASP:N	2.42	0.45
1:A:870:SER:OG	1:A:870:SER:O	2.33	0.45
1:A:1015:GLN:NE2	1:C:795:SER:OG	2.49	0.45
1:C:74:SER:OG	1:C:75:LYS:N	2.49	0.45
1:C:664:ASN:HB2	1:C:666:ILE:HG12	1.97	0.45
1:C:830:SER:O	1:C:854:SER:N	2.50	0.45
1:C:288:TYR:HE2	1:C:669:GLU:HB2	1.82	0.45
1:C:907:GLN:HG2	1:C:1013:LEU:HD22	1.98	0.45
1:A:279:THR:OG1	1:A:280:SER:N	2.49	0.45
1:A:288:TYR:HE2	1:A:669:GLU:HB2	1.82	0.45
1:A:1089:ARG:H	1:A:1089:ARG:HG2	1.60	0.45
1:B:80:ALA:HB2	1:B:258:TYR:HB2	1.99	0.45
1:B:596:GLU:OE2	1:B:626:LYS:NZ	2.44	0.45
1:B:1068:ILE:O	1:B:1072:ALA:N	2.42	0.45
1:C:98:ASN:ND2	1:C:239:TYR:OH	2.49	0.45
1:C:153:CYS:HA	1:C:187:CYS:HB3	1.97	0.45
1:B:279:THR:OG1	1:B:280:SER:N	2.50	0.45
1:B:396:PRO:HD3	1:B:465:VAL:HG11	1.99	0.45
1:C:257:ARG:HD3	1:C:257:ARG:HA	1.72	0.45
1:A:396:PRO:HD3	1:A:465:VAL:HG11	1.99	0.45
1:A:907:GLN:HG2	1:A:1013:LEU:HD22	1.98	0.45
1:A:1080:ASN:OD1	1:B:1091:ASN:ND2	2.50	0.45
1:B:74:SER:OG	1:B:75:LYS:N	2.49	0.45
1:B:1094:GLY:HA3	1:B:1098:HIS:HE1	1.81	0.45
1:C:279:THR:OG1	1:C:280:SER:N	2.49	0.45
1:B:1048:ASN:O	1:B:1052:THR:OG1	2.26	0.45
1:C:317:GLY:H	1:C:581:VAL:HG23	1.82	0.45
1:A:288:TYR:HB2	1:A:649:PRO:HG3	1.98	0.44
1:A:597:VAL:O	1:A:627:THR:OG1	2.25	0.44
1:C:172:ASN:HD21	2:F:85:ASN:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:CYS:H	1:C:563:THR:HG22	1.81	0.44
1:C:396:PRO:HD3	1:C:465:VAL:HG11	1.99	0.44
1:A:354:CYS:H	1:A:563:THR:HG22	1.82	0.44
1:A:830:SER:O	1:A:854:SER:N	2.50	0.44
1:A:735:LEU:HD21	1:C:827:THR:HA	2.00	0.44
1:A:1037:VAL:HG22	1:C:420:THR:HB	1.99	0.44
2:D:120:TYR:N	2:D:136:VAL:O	2.42	0.44
1:C:345:ASN:OD1	1:C:345:ASN:N	2.47	0.44
1:C:870:SER:OG	1:C:873:GLU:OE1	2.28	0.44
1:A:1094:GLY:HA3	1:A:1098:HIS:HE1	1.81	0.44
2:E:45:VAL:HG21	2:E:51:VAL:HB	1.98	0.44
1:C:80:ALA:HB2	1:C:258:TYR:HB2	1.99	0.44
1:C:273:ASN:OD1	1:C:277:VAL:N	2.37	0.44
1:C:815:GLN:HE21	1:C:924:ILE:HD11	1.83	0.44
1:A:293:LYS:HE2	1:A:300:LEU:H	1.83	0.44
1:A:879:LYS:HG3	1:A:995:LEU:HD11	2.00	0.44
1:B:26:ASN:HA	2:E:90:PHE:HB3	2.00	0.44
1:B:84:THR:OG1	1:B:85:ASN:N	2.50	0.44
2:F:69:LYS:HG2	2:F:79:ILE:HD11	1.99	0.44
2:D:69:LYS:HG2	2:D:79:ILE:HD11	1.99	0.44
1:B:288:TYR:HE2	1:B:669:GLU:HB2	1.82	0.44
1:B:354:CYS:H	1:B:563:THR:HG22	1.82	0.44
1:C:332:GLU:O	1:C:336:THR:OG1	2.34	0.44
1:B:879:LYS:HG3	1:B:995:LEU:HD11	2.00	0.44
1:A:84:THR:OG1	1:A:85:ASN:N	2.50	0.44
1:A:687:ASP:N	1:A:723:TYR:O	2.47	0.44
1:B:317:GLY:H	1:B:581:VAL:HG23	1.81	0.44
1:B:954:TYR:HD1	1:B:954:TYR:HA	1.72	0.44
1:C:774:ASP:OD2	1:C:777:ALA:N	2.42	0.44
1:C:862:GLY:HA2	1:C:863:PRO:HD3	1.85	0.44
1:A:80:ALA:HB2	1:A:258:TYR:HB2	1.99	0.44
1:A:164:ASP:OD1	1:A:166:LYS:N	2.47	0.44
1:A:317:GLY:H	1:A:581:VAL:HG23	1.82	0.44
1:A:353:ASN:ND2	1:A:562:THR:OG1	2.48	0.44
1:A:815:GLN:HE21	1:A:924:ILE:HD11	1.83	0.44
1:C:84:THR:OG1	1:C:85:ASN:N	2.50	0.44
2:F:120:TYR:N	2:F:136:VAL:O	2.42	0.44
1:A:257:ARG:HA	1:A:257:ARG:HD3	1.72	0.43
2:D:98:ARG:HB2	2:D:110:GLN:HB2	1.98	0.43
2:F:98:ARG:HB2	2:F:110:GLN:HB2	1.98	0.43
1:A:1048:ASN:O	1:A:1052:THR:OG1	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:GLN:HE21	1:B:924:ILE:HD11	1.83	0.43
1:B:879:LYS:HA	1:B:879:LYS:HD3	1.87	0.43
1:B:1009:LEU:O	1:B:1013:LEU:N	2.51	0.43
1:C:293:LYS:HE2	1:C:300:LEU:H	1.83	0.43
1:A:795:SER:OG	1:B:1015:GLN:NE2	2.51	0.43
1:A:1018:ASN:HD21	1:C:795:SER:H	1.66	0.43
1:B:200:ASP:OD1	1:B:200:ASP:N	2.51	0.43
1:A:234:ASP:OD1	1:A:235:ILE:N	2.51	0.43
1:A:1137:ARG:HA	1:A:1137:ARG:HD2	1.73	0.43
1:B:438:ILE:HD13	1:B:438:ILE:HA	1.86	0.43
1:B:907:GLN:HG2	1:B:1013:LEU:HD22	1.98	0.43
1:B:969:ASN:HA	1:B:972:MET:HB2	2.01	0.43
2:F:45:VAL:HG21	2:F:51:VAL:HB	1.98	0.43
2:F:120:TYR:O	2:F:136:VAL:N	2.48	0.43
1:A:438:ILE:HD13	1:A:438:ILE:HA	1.86	0.43
1:A:730:PRO:HB2	1:C:823:MET:HE1	2.00	0.43
1:A:969:ASN:HA	1:A:972:MET:HB2	2.01	0.43
1:B:774:ASP:OD2	1:B:777:ALA:N	2.42	0.43
1:C:746:LEU:HD23	1:C:746:LEU:HA	1.85	0.43
1:C:879:LYS:HG3	1:C:995:LEU:HD11	2.00	0.43
2:E:69:LYS:HG2	2:E:79:ILE:HD11	1.99	0.43
1:C:200:ASP:OD1	1:C:200:ASP:N	2.51	0.43
1:A:200:ASP:OD1	1:A:200:ASP:N	2.51	0.43
1:A:870:SER:OG	1:A:873:GLU:OE1	2.28	0.43
1:B:823:MET:HG2	1:C:731:TYR:HB2	2.01	0.43
1:C:495:LYS:HA	1:C:495:LYS:HD2	1.78	0.43
2:F:36:VAL:HG12	2:F:58:LEU:HA	2.01	0.43
1:A:648:GLU:O	1:A:723:TYR:OH	2.37	0.43
1:A:1051:LEU:HD23	1:A:1051:LEU:HA	1.90	0.43
1:B:88:SER:HB3	1:B:91:TRP:CE2	2.54	0.43
1:B:234:ASP:OD1	1:B:235:ILE:N	2.51	0.43
1:C:969:ASN:HA	1:C:972:MET:HB2	2.01	0.43
1:B:1080:ASN:OD1	1:C:1091:ASN:ND2	2.52	0.43
1:C:687:ASP:N	1:C:723:TYR:O	2.47	0.43
1:A:381:TYR:HB3	1:A:568:LEU:HD13	2.01	0.42
1:B:293:LYS:HE2	1:B:300:LEU:H	1.83	0.42
2:D:42:PRO:HG2	2:D:45:VAL:HG22	2.01	0.42
1:B:353:ASN:ND2	1:B:562:THR:OG1	2.48	0.42
1:B:827:THR:HG22	1:B:940:TRP:NE1	2.35	0.42
1:B:862:GLY:HA2	1:B:863:PRO:HD3	1.85	0.42
1:C:234:ASP:OD1	1:C:235:ILE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:827:THR:HG22	1:C:940:TRP:NE1	2.34	0.42
1:A:88:SER:HB3	1:A:91:TRP:CE2	2.54	0.42
1:A:284:CYS:HB2	1:A:294:CYS:HB2	1.34	0.42
1:A:399:ARG:NH2	1:C:362:LEU:O	2.52	0.42
1:A:585:LEU:HA	1:A:585:LEU:HD23	1.81	0.42
1:B:683:VAL:HG11	1:B:725:LEU:HD11	2.01	0.42
1:B:1089:ARG:H	1:B:1089:ARG:HG2	1.60	0.42
1:C:101:ASN:OD1	1:C:101:ASN:N	2.53	0.42
2:F:77:LYS:HA	2:F:77:LYS:HD3	1.92	0.42
1:A:1084:LYS:HD2	1:A:1084:LYS:HA	1.86	0.42
1:C:88:SER:HB3	1:C:91:TRP:CE2	2.54	0.42
2:F:42:PRO:HG2	2:F:45:VAL:HG22	2.01	0.42
1:A:390:VAL:HG12	1:A:553:ILE:HG12	2.02	0.42
1:A:728:PHE:O	1:C:923:GLN:NE2	2.53	0.42
1:C:381:TYR:HB3	1:C:568:LEU:HD13	2.01	0.42
1:A:391:ASP:OD1	1:A:391:ASP:N	2.47	0.42
1:B:36:SER:O	1:B:36:SER:OG	2.32	0.42
1:B:942:ALA:O	1:B:1084:LYS:NZ	2.39	0.42
1:A:101:ASN:OD1	1:A:101:ASN:N	2.53	0.42
1:A:586:TYR:OH	1:A:621:ASP:OD1	2.35	0.42
1:A:823:MET:HE1	1:B:730:PRO:HB2	2.02	0.42
2:E:42:PRO:HG2	2:E:45:VAL:HG22	2.01	0.42
1:C:543:VAL:HG21	1:C:548:GLN:HE21	1.85	0.42
1:A:1035:GLU:H	1:A:1035:GLU:HG3	1.74	0.42
1:A:543:VAL:HG21	1:A:548:GLN:HE21	1.85	0.42
1:A:827:THR:HG22	1:A:940:TRP:NE1	2.35	0.42
1:A:1009:LEU:O	1:A:1013:LEU:N	2.51	0.42
1:A:1076:ILE:HD13	1:A:1076:ILE:HA	1.92	0.42
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.93	0.42
1:B:233:GLY:HA3	1:C:506:HIS:CE1	2.55	0.42
1:B:390:VAL:HG12	1:B:553:ILE:HG12	2.01	0.42
1:B:1038:GLU:O	1:B:1042:GLN:N	2.52	0.41
1:C:683:VAL:HG11	1:C:725:LEU:HD11	2.01	0.41
1:A:879:LYS:HA	1:A:879:LYS:HD3	1.87	0.41
1:A:980:ALA:O	1:A:984:ILE:N	2.44	0.41
1:B:101:ASN:OD1	1:B:101:ASN:N	2.53	0.41
1:A:88:SER:HB3	1:A:91:TRP:CD2	2.55	0.41
1:A:104:ILE:HG23	1:A:260:VAL:HG13	2.02	0.41
1:A:163:THR:OG1	1:A:164:ASP:N	2.53	0.41
2:D:36:VAL:HG12	2:D:58:LEU:HA	2.01	0.41
1:C:451:GLY:HA3	1:C:528:CYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:816:LEU:HD23	1:C:816:LEU:HA	1.89	0.41
1:A:320:TYR:OH	1:A:570:LEU:O	2.35	0.41
1:A:451:GLY:HA3	1:A:528:CYS:H	1.86	0.41
1:A:923:GLN:NE2	1:B:728:PHE:O	2.53	0.41
1:B:163:THR:OG1	1:B:164:ASP:N	2.53	0.41
1:C:96:TYR:HB3	1:C:240:TYR:HE1	1.85	0.41
1:C:1009:LEU:O	1:C:1013:LEU:N	2.51	0.41
1:C:1038:GLU:O	1:C:1042:GLN:N	2.52	0.41
1:C:1084:LYS:HD2	1:C:1084:LYS:HA	1.86	0.41
1:A:454:ASP:OD1	1:A:454:ASP:N	2.43	0.41
1:B:381:TYR:HB3	1:B:568:LEU:HD13	2.01	0.41
1:B:451:GLY:HA3	1:B:528:CYS:H	1.86	0.41
1:C:438:ILE:HD13	1:C:438:ILE:HA	1.86	0.41
1:C:1058:ILE:O	1:C:1062:LEU:N	2.49	0.41
1:A:373:ASN:OD1	1:A:373:ASN:N	2.43	0.41
1:A:431:LEU:HD23	1:A:431:LEU:HA	1.80	0.41
1:B:1058:ILE:O	1:B:1062:LEU:N	2.49	0.41
2:E:36:VAL:HG12	2:E:58:LEU:HA	2.01	0.41
1:C:671:ASN:OD1	1:C:671:ASN:N	2.54	0.41
1:C:981:LEU:HA	1:C:984:ILE:HB	2.03	0.41
1:C:1051:LEU:HD23	1:C:1051:LEU:HA	1.90	0.41
1:B:494:THR:OG1	1:B:495:LYS:N	2.53	0.41
1:C:390:VAL:HG12	1:C:553:ILE:HG12	2.01	0.41
1:C:1068:ILE:O	1:C:1072:ALA:N	2.42	0.41
2:F:122:LEU:N	2:F:134:ALA:O	2.41	0.41
1:B:641:ALA:O	1:B:723:TYR:OH	2.39	0.41
1:B:876:LEU:HD11	1:B:1111:TYR:HE1	1.86	0.41
1:B:981:LEU:HA	1:B:984:ILE:HB	2.03	0.41
1:C:88:SER:HB3	1:C:91:TRP:CD2	2.55	0.41
1:A:96:TYR:HB3	1:A:240:TYR:HE1	1.85	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.90	0.41
1:A:671:ASN:OD1	1:A:671:ASN:N	2.54	0.41
1:A:683:VAL:HG11	1:A:725:LEU:HD11	2.01	0.41
1:A:746:LEU:HD23	1:A:746:LEU:HA	1.85	0.41
1:A:970:GLN:HA	1:A:973:ILE:HG22	2.03	0.41
2:D:76:ASP:OD2	2:D:77:LYS:NZ	2.54	0.41
1:B:104:ILE:HG23	1:B:260:VAL:HG13	2.02	0.41
1:B:330:ASN:HB3	1:B:333:GLU:HG3	2.03	0.41
1:B:372:CYS:HB3	1:B:425:CYS:HB3	1.04	0.41
1:A:329:CYS:HB3	1:A:354:CYS:HB3	1.98	0.41
1:A:981:LEU:HA	1:A:984:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:LEU:HD23	1:A:1102:LEU:HA	1.94	0.41
2:D:67:TRP:CE2	2:D:122:LEU:HD13	2.56	0.41
2:D:126:ASP:N	2:D:126:ASP:OD1	2.54	0.41
1:B:383:ARG:HH11	1:B:558:ILE:HG12	1.86	0.41
2:E:67:TRP:CE2	2:E:122:LEU:HD13	2.56	0.41
1:C:163:THR:OG1	1:C:164:ASP:N	2.53	0.41
1:C:412:GLN:HE22	1:C:418:ILE:HG13	1.86	0.41
1:C:1048:ASN:O	1:C:1052:THR:OG1	2.26	0.41
1:A:876:LEU:HD11	1:A:1111:TYR:HE1	1.86	0.40
1:B:543:VAL:HG21	1:B:548:GLN:HE21	1.85	0.40
1:C:104:ILE:HG23	1:C:260:VAL:HG13	2.02	0.40
1:C:284:CYS:HB2	1:C:294:CYS:HB2	1.35	0.40
1:C:876:LEU:HD11	1:C:1111:TYR:HE1	1.86	0.40
2:F:76:ASP:OD2	2:F:77:LYS:NZ	2.54	0.40
1:B:747:TYR:HD1	1:B:747:TYR:HA	1.76	0.40
1:B:981:LEU:HA	1:B:981:LEU:HD23	1.86	0.40
2:E:126:ASP:N	2:E:126:ASP:OD1	2.54	0.40
1:C:641:ALA:O	1:C:723:TYR:OH	2.39	0.40
1:C:1134:SER:O	1:C:1134:SER:OG	2.30	0.40
1:A:386:GLY:HA2	1:A:561:GLY:HA3	2.03	0.40
2:D:77:LYS:HA	2:D:77:LYS:HD3	1.92	0.40
1:B:96:TYR:HB3	1:B:240:TYR:HE1	1.85	0.40
1:B:173:LYS:HE2	1:B:173:LYS:HB2	1.92	0.40
1:B:1137:ARG:HA	1:B:1137:ARG:HD2	1.73	0.40
1:C:321:ARG:HH11	1:C:574:GLU:HA	1.87	0.40
1:C:330:ASN:HB3	1:C:333:GLU:HG3	2.03	0.40
1:C:554:LEU:HD23	1:C:554:LEU:HA	1.95	0.40
1:C:951:SER:OG	1:C:955:ARG:NH1	2.55	0.40
1:A:1091:ASN:ND2	1:C:1080:ASN:OD1	2.54	0.40
1:B:183:LYS:HE3	1:B:183:LYS:HB3	1.91	0.40
1:B:386:GLY:HA2	1:B:561:GLY:HA3	2.04	0.40
1:B:671:ASN:OD1	1:B:671:ASN:N	2.54	0.40
1:B:741:GLN:HB2	1:B:742:SER:H	1.69	0.40
1:B:746:LEU:HD23	1:B:746:LEU:HA	1.85	0.40
1:C:35:PRO:HB3	1:C:96:TYR:HE1	1.87	0.40
1:C:879:LYS:HA	1:C:879:LYS:HD3	1.86	0.40
1:A:951:SER:OG	1:A:955:ARG:NH1	2.55	0.40
1:B:88:SER:HB3	1:B:91:TRP:CD2	2.55	0.40
2:E:120:TYR:O	2:E:136:VAL:N	2.48	0.40
1:C:168:ASN:OD1	1:C:168:ASN:N	2.55	0.40
1:C:424:SER:HB3	1:C:554:LEU:HD23	2.04	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	1116/1275 (88%)	1003 (90%)	112 (10%)	1 (0%)	51 83
1	B	1116/1275 (88%)	1003 (90%)	112 (10%)	1 (0%)	51 83
1	C	1116/1275 (88%)	1004 (90%)	111 (10%)	1 (0%)	51 83
2	D	105/208 (50%)	99 (94%)	6 (6%)	0	100 100
2	E	105/208 (50%)	99 (94%)	6 (6%)	0	100 100
2	F	105/208 (50%)	99 (94%)	6 (6%)	0	100 100
All	All	3663/4449 (82%)	3307 (90%)	353 (10%)	3 (0%)	54 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	741	GLN
1	B	741	GLN
1	C	741	GLN

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	958/1104 (87%)	951 (99%)	7 (1%)	84 90
1	B	958/1104 (87%)	951 (99%)	7 (1%)	84 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	958/1104 (87%)	951 (99%)	7 (1%)	84 90
2	D	92/189 (49%)	91 (99%)	1 (1%)	73 84
2	E	92/189 (49%)	91 (99%)	1 (1%)	73 84
2	F	92/189 (49%)	91 (99%)	1 (1%)	73 84
All	All	3150/3879 (81%)	3126 (99%)	24 (1%)	82 88

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	CYS
1	A	376	ASP
1	A	425	CYS
1	A	507	CYS
1	A	564	CYS
1	A	1063	SER
1	A	1111	TYR
2	D	121	THR
1	B	372	CYS
1	B	376	ASP
1	B	425	CYS
1	B	507	CYS
1	B	564	CYS
1	B	1063	SER
1	B	1111	TYR
2	E	121	THR
1	C	372	CYS
1	C	376	ASP
1	C	425	CYS
1	C	507	CYS
1	C	564	CYS
1	C	1063	SER
1	C	1111	TYR
2	F	121	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	154	GLN
1	A	172	ASN

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Mol	Chain	Res	Type
1	A	353	ASN
1	A	374	ASN
1	A	400	GLN
1	A	412	GLN
1	A	447	ASN
1	A	469	GLN
1	A	530	ASN
1	A	544	ASN
1	A	548	GLN
1	A	606	GLN
1	A	688	ASN
1	A	815	GLN
1	A	1011	ASN
1	A	1015	GLN
1	A	1018	ASN
1	A	1091	ASN
1	A	1114	HIS
2	D	93	GLN
2	D	128	ASN
2	D	141	HIS
1	B	98	ASN
1	B	154	GLN
1	B	172	ASN
1	B	353	ASN
1	B	400	GLN
1	B	412	GLN
1	B	447	ASN
1	B	469	GLN
1	B	530	ASN
1	B	544	ASN
1	B	548	GLN
1	B	606	GLN
1	B	688	ASN
1	B	759	HIS
1	B	815	GLN
1	B	1011	ASN
1	B	1015	GLN
1	B	1018	ASN
1	B	1091	ASN
1	B	1114	HIS
2	E	93	GLN
2	E	128	ASN

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Mol	Chain	Res	Type
2	E	141	HIS
1	C	98	ASN
1	C	154	GLN
1	C	172	ASN
1	C	353	ASN
1	C	400	GLN
1	C	412	GLN
1	C	447	ASN
1	C	469	GLN
1	C	530	ASN
1	C	544	ASN
1	C	548	GLN
1	C	606	GLN
1	C	688	ASN
1	C	759	HIS
1	C	815	GLN
1	C	1011	ASN
1	C	1015	GLN
1	C	1018	ASN
1	C	1091	ASN
1	C	1114	HIS
2	F	93	GLN
2	F	128	ASN
2	F	141	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 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	A	1301	1	14,14,15	0.32	0	17,19,21	1.03	1 (5%)
3	NAG	A	1303	-	14,14,15	0.39	0	17,19,21	0.93	1 (5%)
3	NAG	C	1303	-	14,14,15	0.39	0	17,19,21	0.93	1 (5%)
3	NAG	E	301	2	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	F	301	2	14,14,15	0.33	0	17,19,21	0.48	0
3	NAG	B	1302	1	14,14,15	0.36	0	17,19,21	0.41	0
3	NAG	B	1303	-	14,14,15	0.40	0	17,19,21	0.94	1 (5%)
3	NAG	C	1302	1	14,14,15	0.37	0	17,19,21	0.40	0
3	NAG	A	1302	1	14,14,15	0.36	0	17,19,21	0.41	0
3	NAG	D	301	2	14,14,15	0.31	0	17,19,21	0.48	0
3	NAG	B	1301	1	14,14,15	0.34	0	17,19,21	1.03	1 (5%)
3	NAG	C	1301	1	14,14,15	0.34	0	17,19,21	1.03	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	A	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1303	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1303	-	-	3/6/23/26	0/1/1/1
3	NAG	E	301	2	-	0/6/23/26	0/1/1/1
3	NAG	F	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	D	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1301	NAG	C2-N2-C7	3.03	127.21	122.90
3	B	1301	NAG	C2-N2-C7	3.02	127.20	122.90
3	C	1301	NAG	C2-N2-C7	3.02	127.20	122.90
3	B	1303	NAG	C2-N2-C7	2.92	127.06	122.90
3	A	1303	NAG	C2-N2-C7	2.87	126.99	122.90
3	C	1303	NAG	C2-N2-C7	2.84	126.95	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	C3-C2-N2-C7
3	A	1303	NAG	C3-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	B	1303	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7
3	C	1303	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1303	NAG	1	0
3	C	1303	NAG	1	0
3	B	1303	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.

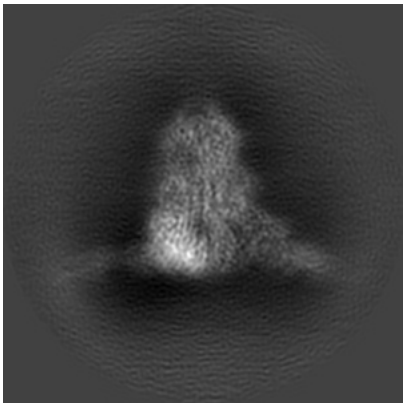
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21377. These allow visual inspection of the internal detail of the map and identification of artifacts.

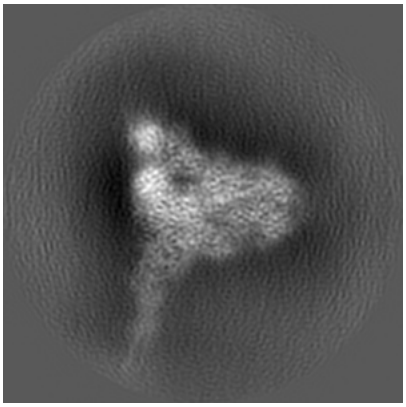
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

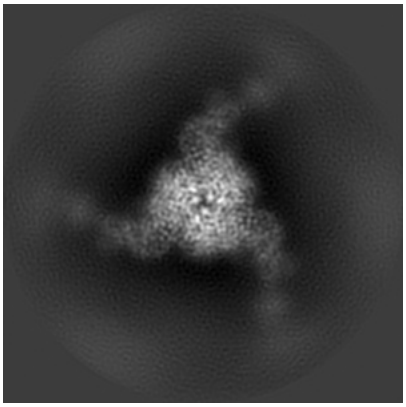
6.1.1 Primary map



X



Y

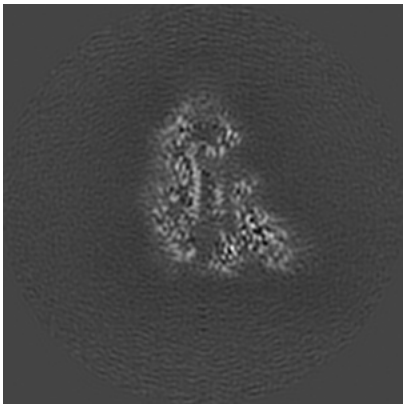


Z

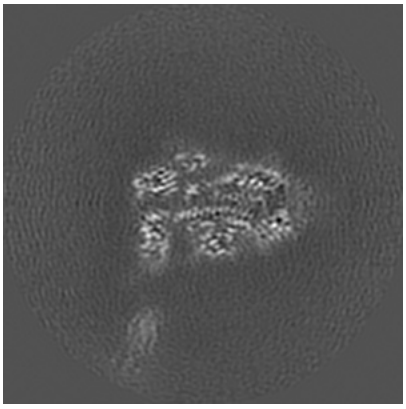
The images above show the map projected in three orthogonal directions.

6.2 Central slices

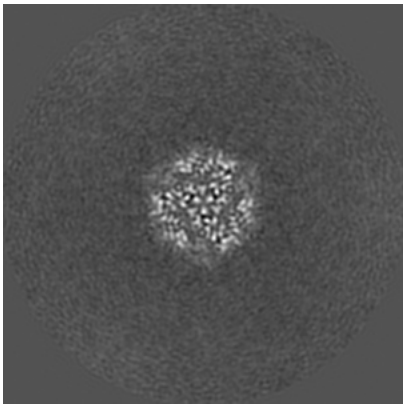
6.2.1 Primary map



X Index: 160



Y Index: 160

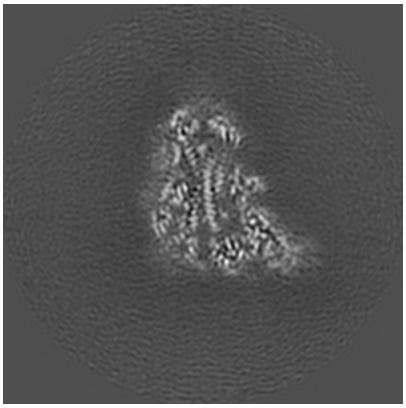


Z Index: 160

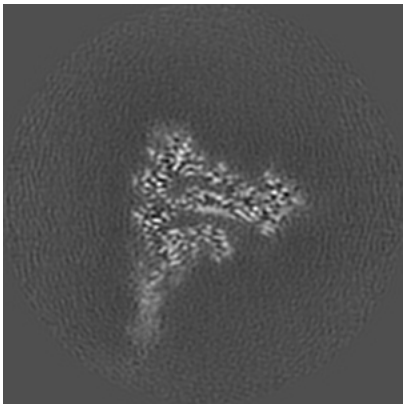
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

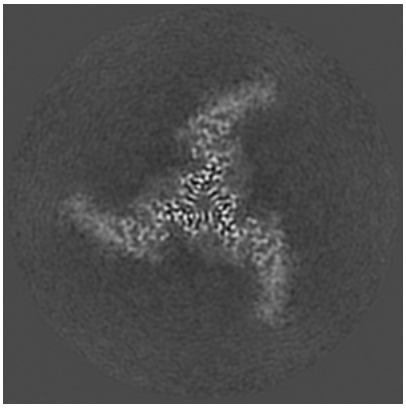
6.3.1 Primary map



X Index: 164



Y Index: 145



Z Index: 120

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 0.00869. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

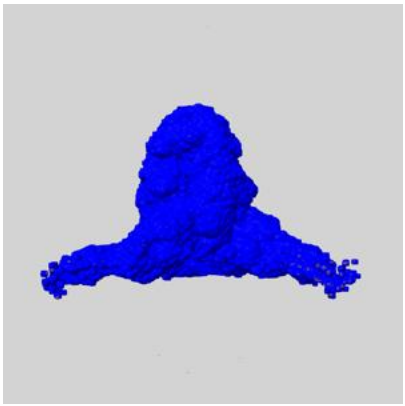
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

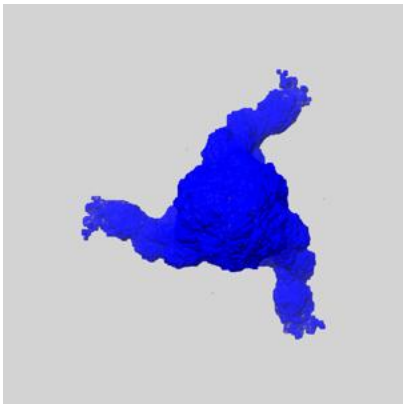
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_21377_msk_1.map



X

Y

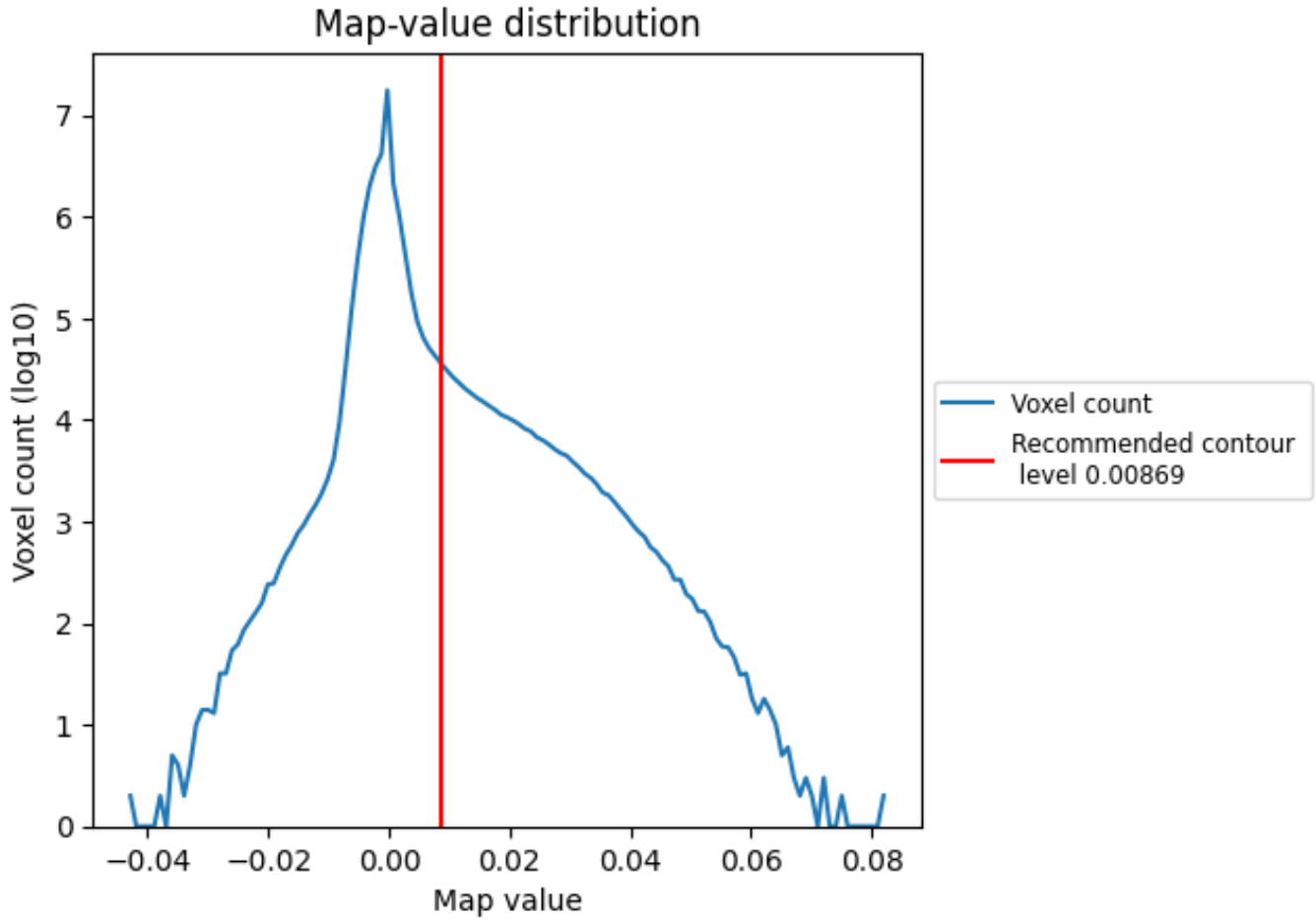


Z

7 Map analysis

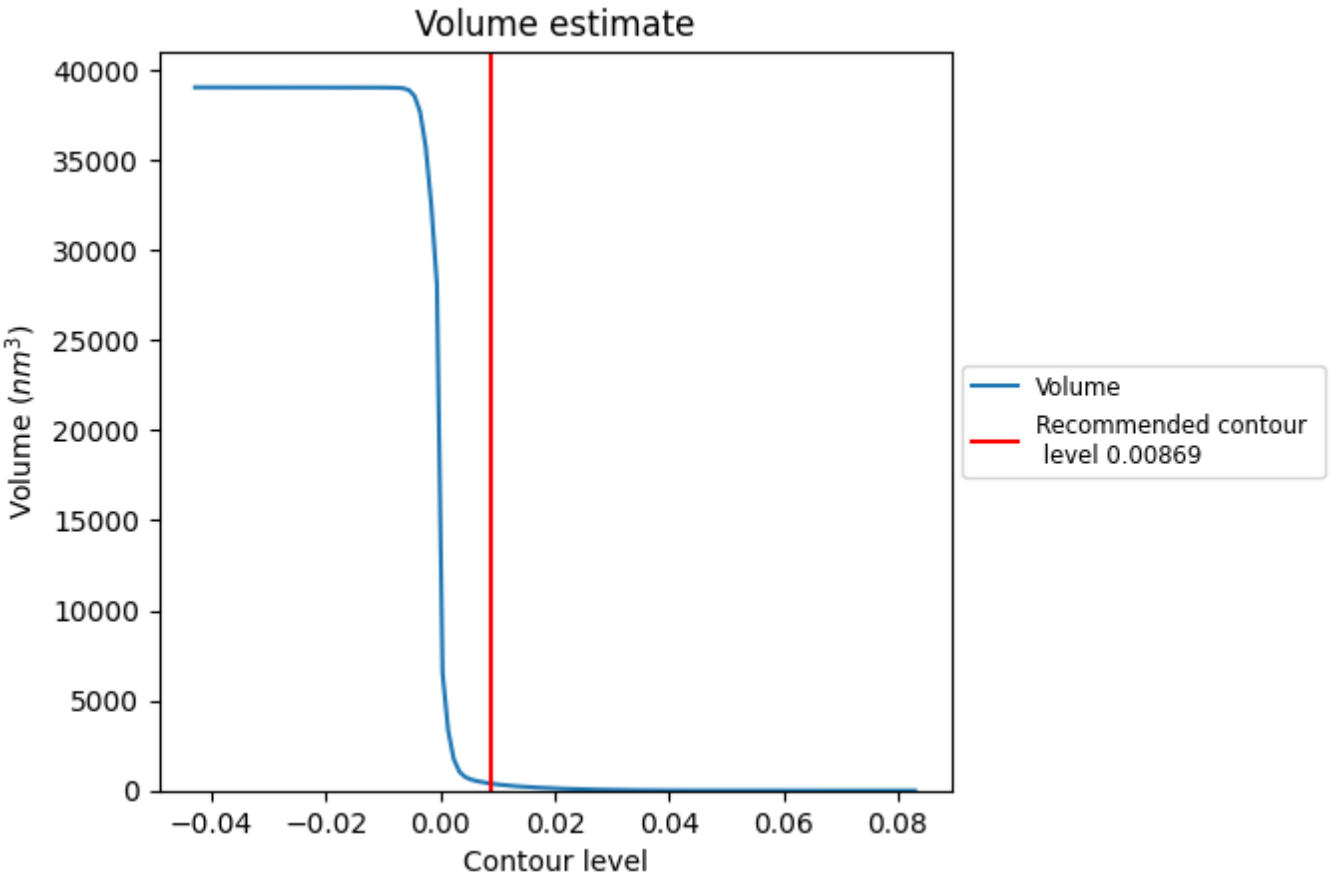
This section contains the results of statistical analysis of the map.

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.

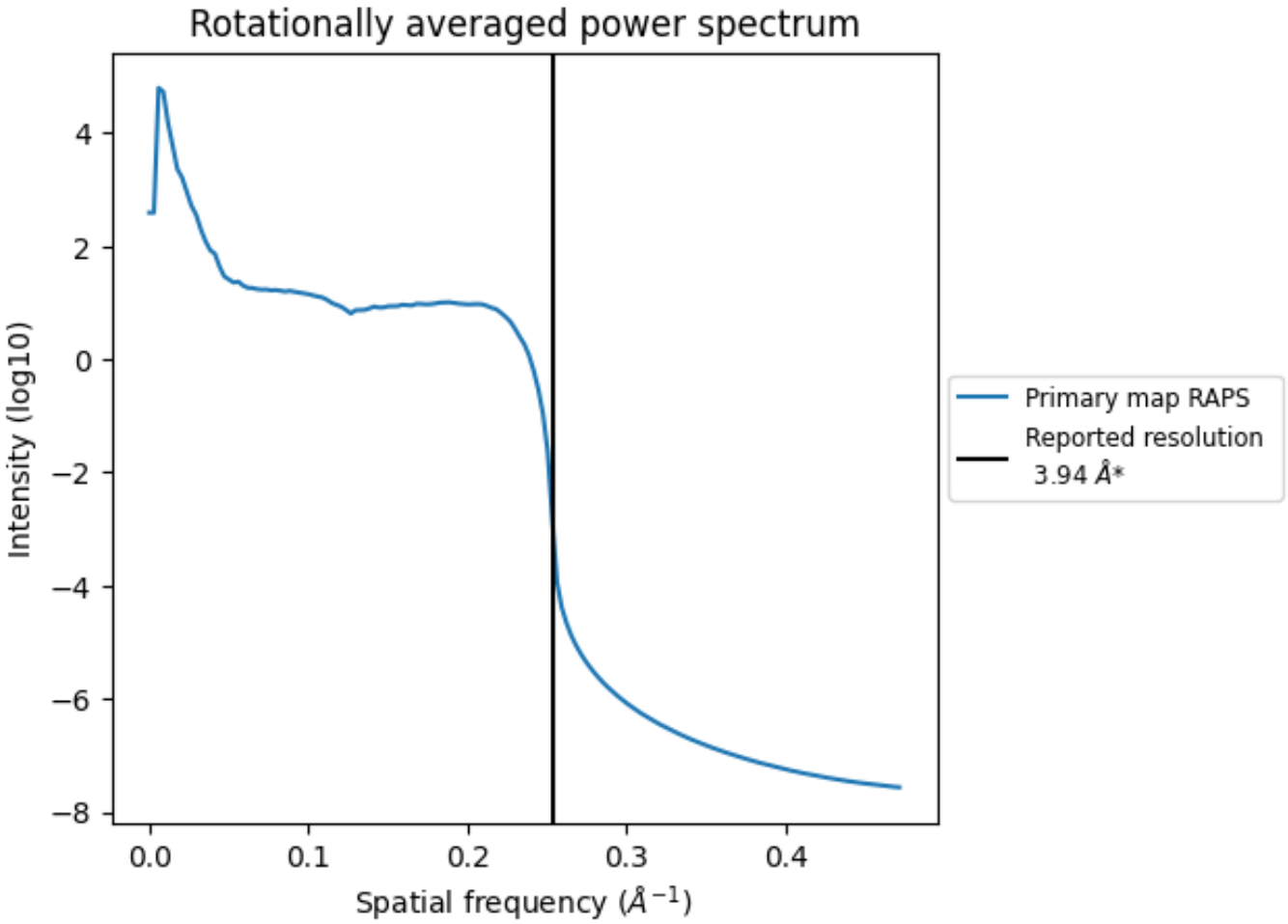
7.2 Volume estimate



The volume at the recommended contour level is 395 nm^3; this corresponds to an approximate mass of 357 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)

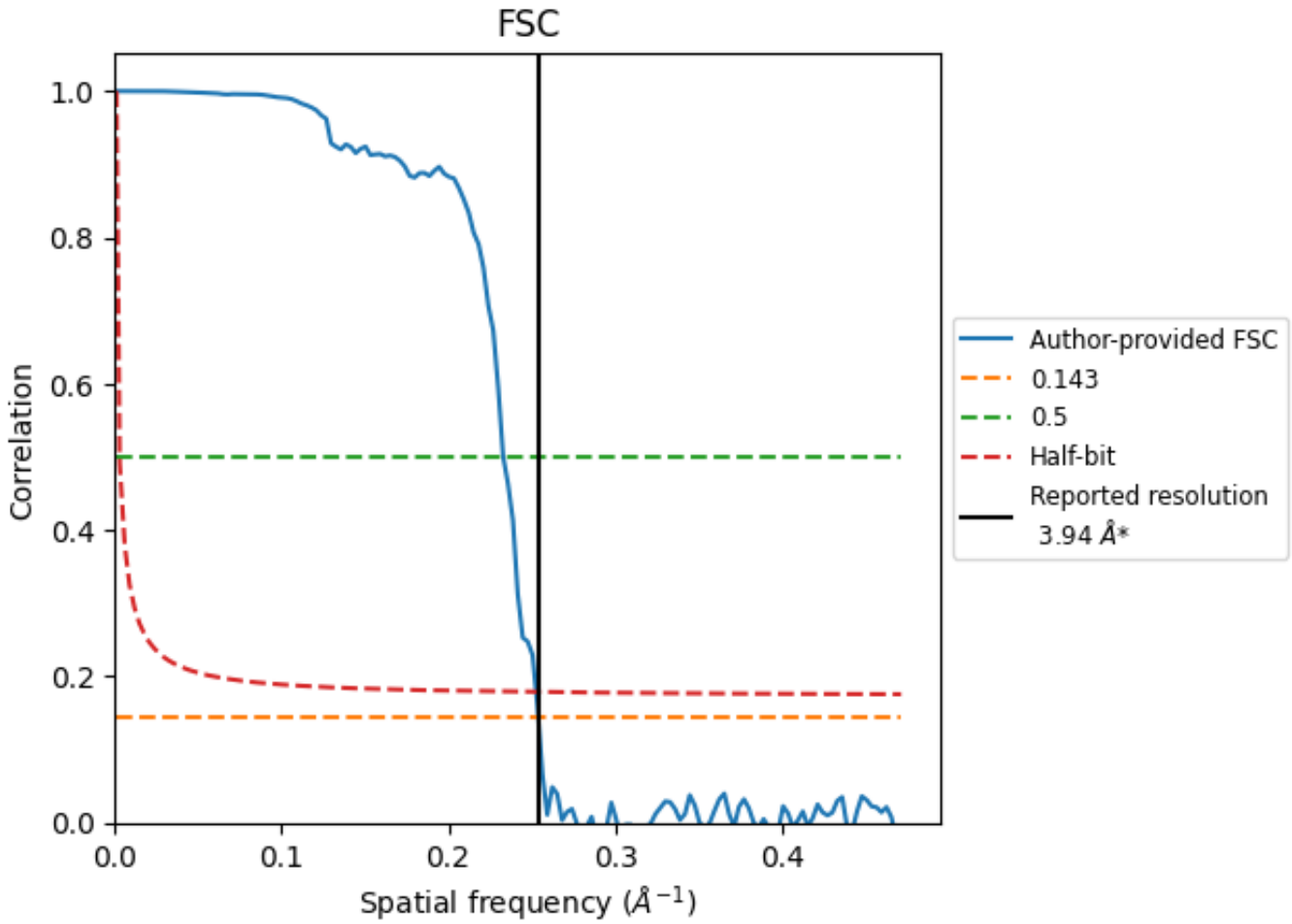


*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

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 0.254 Å^{-1}

8.2 Resolution estimates (i)

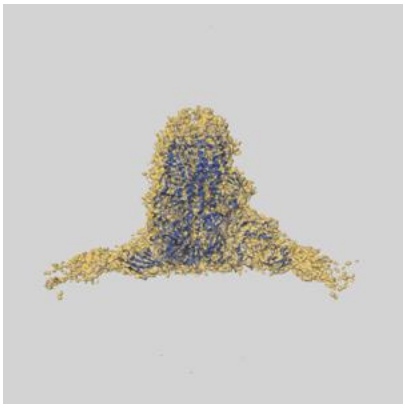
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	3.94	4.29	3.96
Unmasked-calculated*	-	-	-

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

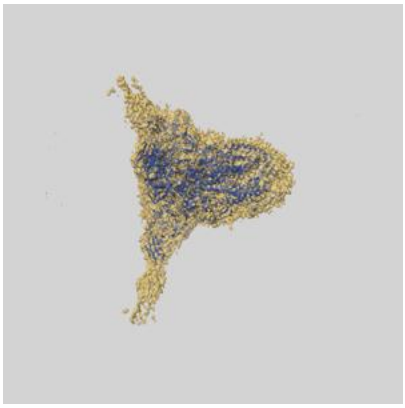
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21377 and PDB model 6VSJ. Per-residue inclusion information can be found in section 3 on page 10.

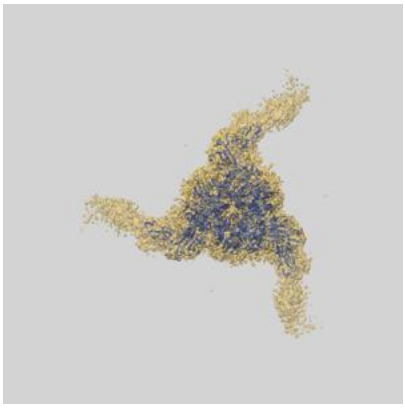
9.1 Map-model overlay



X



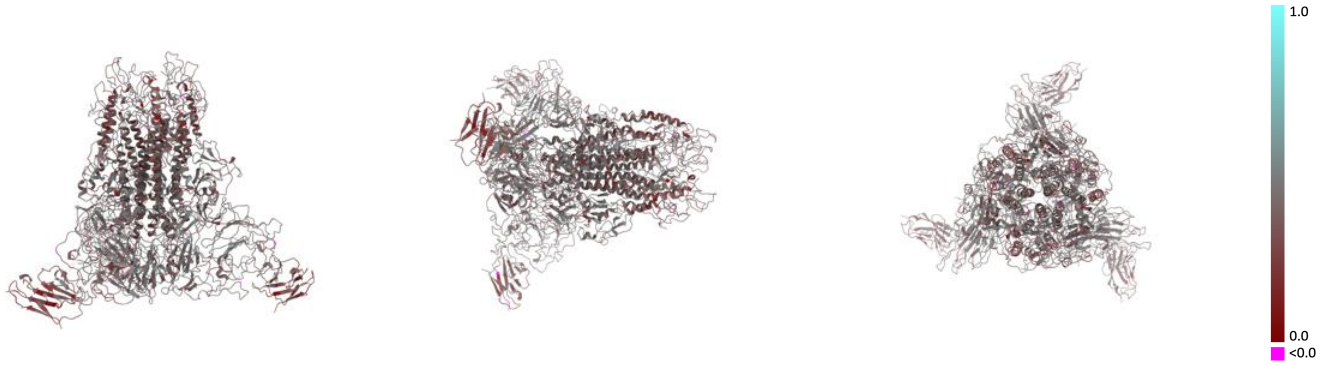
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00869 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.

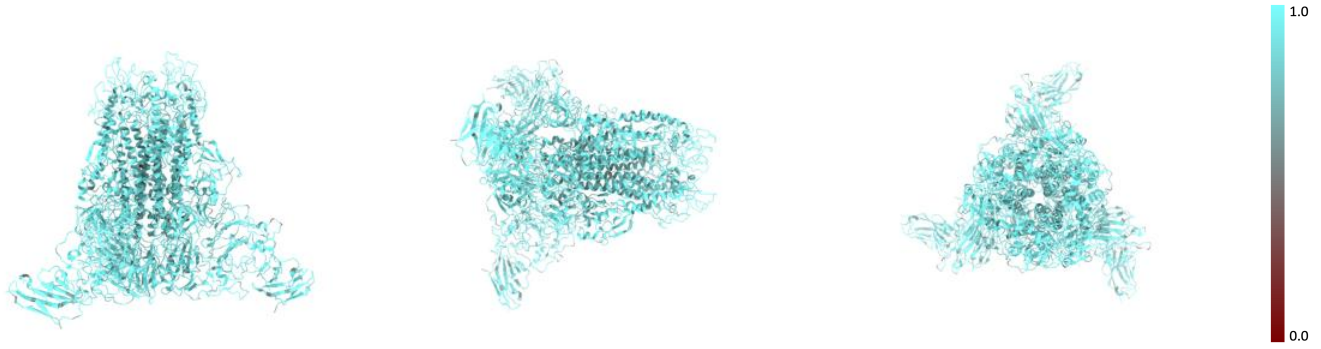
9.2 Q-score mapped to coordinate model (i)



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.

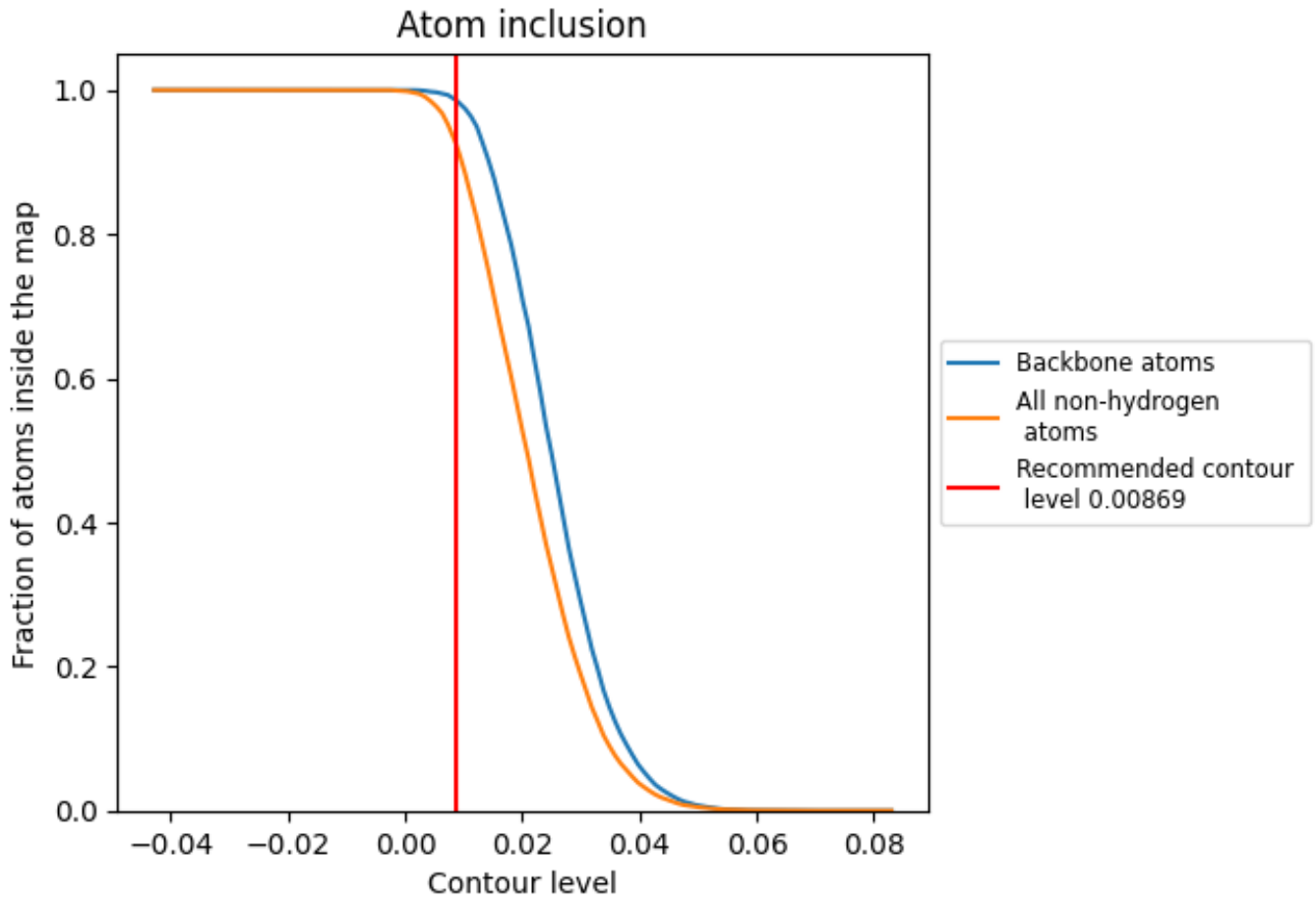
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00869).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.00869) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9248	0.4010
A	0.9252	0.4080
B	0.9247	0.4090
C	0.9253	0.4090
D	0.9210	0.3240
E	0.9222	0.3200
F	0.9233	0.3160