Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 08:30 PM JST

PDB ID	:	7EY0
EMDB ID	:	EMD-31374
Title	:	Local CryoEM structure of the SARS-CoV-2 S6PV2 in complex with BD-813 Fab and BD-744 Fab
Authors	:	Du, S.; Xiao, J.
Deposited on	:	2021-05-29
Resolution	:	3.20 Å(reported)

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

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

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

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

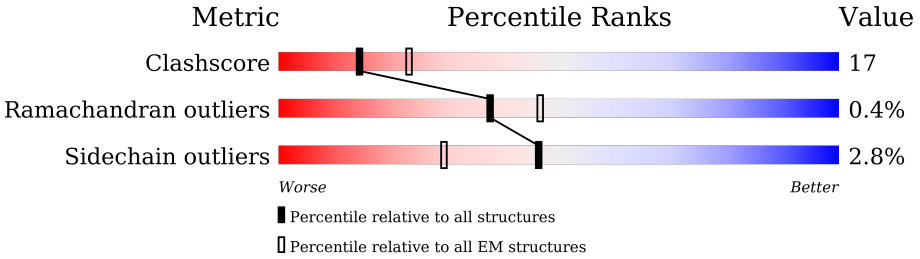
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	225	34% 18% 48%
2	H	223	30% 22% 48%
3	L	215	29% 17% 53%
4	N	1285	9% 87%
4	R	1285	10% 86%
5	B	213	14% 16% 66%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5963 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 BD-744H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	118	905	567	158	175	5	0	0

- Molecule 2 is a protein called BD-813H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	116	903	578	149	172	4	0	0

- Molecule 3 is a protein called BD-813L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	100	767	485	130	149	3	0	0

- Molecule 4 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	183	1465	941	243	274	7	0	0
4	N	165	1359	893	215	249	2	0	0

There are 202 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	21	PHE	LEU	conflict	UNP P0DTC2
R	83	ALA	ASP	conflict	UNP P0DTC2
R	218	GLY	ASP	conflict	UNP P0DTC2
R	?	-	LEU	deletion	UNP P0DTC2
R	?	-	LEU	deletion	UNP P0DTC2
R	?	-	ALA	deletion	UNP P0DTC2
R	417	ASN	LYS	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	484	LYS	GLU	conflict	UNP P0DTC2
R	501	TYR	ASN	conflict	UNP P0DTC2
R	614	GLY	ASP	conflict	UNP P0DTC2
R	682	GLY	ARG	conflict	UNP P0DTC2
R	683	SER	ARG	conflict	UNP P0DTC2
R	685	SER	ARG	conflict	UNP P0DTC2
R	701	VAL	ALA	conflict	UNP P0DTC2
R	817	PRO	PHE	conflict	UNP P0DTC2
R	892	PRO	ALA	conflict	UNP P0DTC2
R	899	PRO	ALA	conflict	UNP P0DTC2
R	942	PRO	ALA	conflict	UNP P0DTC2
R	986	PRO	LYS	conflict	UNP P0DTC2
R	987	PRO	VAL	conflict	UNP P0DTC2
R	1208	GLN	-	expression tag	UNP P0DTC2
R	1209	GLY	-	expression tag	UNP P0DTC2
R	1210	SER	-	expression tag	UNP P0DTC2
R	1211	GLY	-	expression tag	UNP P0DTC2
R	1212	TYR	-	expression tag	UNP P0DTC2
R	1213	ILE	-	expression tag	UNP P0DTC2
R	1214	PRO	-	expression tag	UNP P0DTC2
R	1215	GLU	-	expression tag	UNP P0DTC2
R	1216	ALA	-	expression tag	UNP P0DTC2
R	1217	PRO	-	expression tag	UNP P0DTC2
R	1218	ARG	-	expression tag	UNP P0DTC2
R	1219	ASP	-	expression tag	UNP P0DTC2
R	1220	GLY	-	expression tag	UNP P0DTC2
R	1221	GLN	-	expression tag	UNP P0DTC2
R	1222	ALA	-	expression tag	UNP P0DTC2
R	1223	TYR	-	expression tag	UNP P0DTC2
R	1224	VAL	-	expression tag	UNP P0DTC2
R	1225	ARG	-	expression tag	UNP P0DTC2
R	1226	LYS	-	expression tag	UNP P0DTC2
R	1227	ASP	-	expression tag	UNP P0DTC2
R	1228	GLY	-	expression tag	UNP P0DTC2
R	1229	GLU	-	expression tag	UNP P0DTC2
R	1230	TRP	-	expression tag	UNP P0DTC2
R	1231	VAL	-	expression tag	UNP P0DTC2
R	1232	LEU	-	expression tag	UNP P0DTC2
R	1233	LEU	-	expression tag	UNP P0DTC2
R	1234	SER	-	expression tag	UNP P0DTC2
R	1235	THR	-	expression tag	UNP P0DTC2
R	1236	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1237	LEU	-	expression tag	UNP P0DTC2
R	1238	GLY	-	expression tag	UNP P0DTC2
R	1239	ARG	-	expression tag	UNP P0DTC2
R	1240	SER	-	expression tag	UNP P0DTC2
R	1241	LEU	-	expression tag	UNP P0DTC2
R	1242	GLU	-	expression tag	UNP P0DTC2
R	1243	VAL	-	expression tag	UNP P0DTC2
R	1244	LEU	-	expression tag	UNP P0DTC2
R	1245	PHE	-	expression tag	UNP P0DTC2
R	1246	GLN	-	expression tag	UNP P0DTC2
R	1247	GLY	-	expression tag	UNP P0DTC2
R	1248	PRO	-	expression tag	UNP P0DTC2
R	1249	GLY	-	expression tag	UNP P0DTC2
R	1250	HIS	-	expression tag	UNP P0DTC2
R	1251	HIS	-	expression tag	UNP P0DTC2
R	1252	HIS	-	expression tag	UNP P0DTC2
R	1253	HIS	-	expression tag	UNP P0DTC2
R	1254	HIS	-	expression tag	UNP P0DTC2
R	1255	HIS	-	expression tag	UNP P0DTC2
R	1256	HIS	-	expression tag	UNP P0DTC2
R	1257	HIS	-	expression tag	UNP P0DTC2
R	1258	SER	-	expression tag	UNP P0DTC2
R	1259	ALA	-	expression tag	UNP P0DTC2
R	1260	TRP	-	expression tag	UNP P0DTC2
R	1261	SER	-	expression tag	UNP P0DTC2
R	1262	HIS	-	expression tag	UNP P0DTC2
R	1263	PRO	-	expression tag	UNP P0DTC2
R	1264	GLN	-	expression tag	UNP P0DTC2
R	1265	PHE	-	expression tag	UNP P0DTC2
R	1266	GLU	-	expression tag	UNP P0DTC2
R	1267	LYS	-	expression tag	UNP P0DTC2
R	1268	GLY	-	expression tag	UNP P0DTC2
R	1269	GLY	-	expression tag	UNP P0DTC2
R	1270	GLY	-	expression tag	UNP P0DTC2
R	1271	SER	-	expression tag	UNP P0DTC2
R	1272	GLY	-	expression tag	UNP P0DTC2
R	1273	GLY	-	expression tag	UNP P0DTC2
R	1274	GLY	-	expression tag	UNP P0DTC2
R	1275	GLY	-	expression tag	UNP P0DTC2
R	1276	SER	-	expression tag	UNP P0DTC2
R	1277	GLY	-	expression tag	UNP P0DTC2
R	1278	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1279	SER	-	expression tag	UNP P0DTC2
R	1280	ALA	-	expression tag	UNP P0DTC2
R	1281	TRP	-	expression tag	UNP P0DTC2
R	1282	SER	-	expression tag	UNP P0DTC2
R	1283	HIS	-	expression tag	UNP P0DTC2
R	1284	PRO	-	expression tag	UNP P0DTC2
R	1285	GLN	-	expression tag	UNP P0DTC2
R	1286	PHE	-	expression tag	UNP P0DTC2
R	1287	GLU	-	expression tag	UNP P0DTC2
R	1288	LYS	-	expression tag	UNP P0DTC2
N	18	PHE	LEU	conflict	UNP P0DTC2
N	80	ALA	ASP	conflict	UNP P0DTC2
N	215	GLY	ASP	conflict	UNP P0DTC2
N	?	-	LEU	deletion	UNP P0DTC2
N	?	-	LEU	deletion	UNP P0DTC2
N	?	-	ALA	deletion	UNP P0DTC2
N	417	ASN	LYS	conflict	UNP P0DTC2
N	484	LYS	GLU	conflict	UNP P0DTC2
N	501	TYR	ASN	conflict	UNP P0DTC2
N	614	GLY	ASP	conflict	UNP P0DTC2
N	682	GLY	ARG	conflict	UNP P0DTC2
N	683	SER	ARG	conflict	UNP P0DTC2
N	685	SER	ARG	conflict	UNP P0DTC2
N	701	VAL	ALA	conflict	UNP P0DTC2
N	817	PRO	PHE	conflict	UNP P0DTC2
N	892	PRO	ALA	conflict	UNP P0DTC2
N	899	PRO	ALA	conflict	UNP P0DTC2
N	942	PRO	ALA	conflict	UNP P0DTC2
N	986	PRO	LYS	conflict	UNP P0DTC2
N	987	PRO	VAL	conflict	UNP P0DTC2
N	1208	GLN	-	expression tag	UNP P0DTC2
N	1209	GLY	-	expression tag	UNP P0DTC2
N	1210	SER	-	expression tag	UNP P0DTC2
N	1211	GLY	-	expression tag	UNP P0DTC2
N	1212	TYR	-	expression tag	UNP P0DTC2
N	1213	ILE	-	expression tag	UNP P0DTC2
N	1214	PRO	-	expression tag	UNP P0DTC2
N	1215	GLU	-	expression tag	UNP P0DTC2
N	1216	ALA	-	expression tag	UNP P0DTC2
N	1217	PRO	-	expression tag	UNP P0DTC2
N	1218	ARG	-	expression tag	UNP P0DTC2
N	1219	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
N	1220	GLY	-	expression tag	UNP P0DTC2
N	1221	GLN	-	expression tag	UNP P0DTC2
N	1222	ALA	-	expression tag	UNP P0DTC2
N	1223	TYR	-	expression tag	UNP P0DTC2
N	1224	VAL	-	expression tag	UNP P0DTC2
N	1225	ARG	-	expression tag	UNP P0DTC2
N	1226	LYS	-	expression tag	UNP P0DTC2
N	1227	ASP	-	expression tag	UNP P0DTC2
N	1228	GLY	-	expression tag	UNP P0DTC2
N	1229	GLU	-	expression tag	UNP P0DTC2
N	1230	TRP	-	expression tag	UNP P0DTC2
N	1231	VAL	-	expression tag	UNP P0DTC2
N	1232	LEU	-	expression tag	UNP P0DTC2
N	1233	LEU	-	expression tag	UNP P0DTC2
N	1234	SER	-	expression tag	UNP P0DTC2
N	1235	THR	-	expression tag	UNP P0DTC2
N	1236	PHE	-	expression tag	UNP P0DTC2
N	1237	LEU	-	expression tag	UNP P0DTC2
N	1238	GLY	-	expression tag	UNP P0DTC2
N	1239	ARG	-	expression tag	UNP P0DTC2
N	1240	SER	-	expression tag	UNP P0DTC2
N	1241	LEU	-	expression tag	UNP P0DTC2
N	1242	GLU	-	expression tag	UNP P0DTC2
N	1243	VAL	-	expression tag	UNP P0DTC2
N	1244	LEU	-	expression tag	UNP P0DTC2
N	1245	PHE	-	expression tag	UNP P0DTC2
N	1246	GLN	-	expression tag	UNP P0DTC2
N	1247	GLY	-	expression tag	UNP P0DTC2
N	1248	PRO	-	expression tag	UNP P0DTC2
N	1249	GLY	-	expression tag	UNP P0DTC2
N	1250	HIS	-	expression tag	UNP P0DTC2
N	1251	HIS	-	expression tag	UNP P0DTC2
N	1252	HIS	-	expression tag	UNP P0DTC2
N	1253	HIS	-	expression tag	UNP P0DTC2
N	1254	HIS	-	expression tag	UNP P0DTC2
N	1255	HIS	-	expression tag	UNP P0DTC2
N	1256	HIS	-	expression tag	UNP P0DTC2
N	1257	HIS	-	expression tag	UNP P0DTC2
N	1258	SER	-	expression tag	UNP P0DTC2
N	1259	ALA	-	expression tag	UNP P0DTC2
N	1260	TRP	-	expression tag	UNP P0DTC2
N	1261	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
N	1262	HIS	-	expression tag	UNP P0DTC2
N	1263	PRO	-	expression tag	UNP P0DTC2
N	1264	GLN	-	expression tag	UNP P0DTC2
N	1265	PHE	-	expression tag	UNP P0DTC2
N	1266	GLU	-	expression tag	UNP P0DTC2
N	1267	LYS	-	expression tag	UNP P0DTC2
N	1268	GLY	-	expression tag	UNP P0DTC2
N	1269	GLY	-	expression tag	UNP P0DTC2
N	1270	GLY	-	expression tag	UNP P0DTC2
N	1271	SER	-	expression tag	UNP P0DTC2
N	1272	GLY	-	expression tag	UNP P0DTC2
N	1273	GLY	-	expression tag	UNP P0DTC2
N	1274	GLY	-	expression tag	UNP P0DTC2
N	1275	GLY	-	expression tag	UNP P0DTC2
N	1276	SER	-	expression tag	UNP P0DTC2
N	1277	GLY	-	expression tag	UNP P0DTC2
N	1278	GLY	-	expression tag	UNP P0DTC2
N	1279	SER	-	expression tag	UNP P0DTC2
N	1280	ALA	-	expression tag	UNP P0DTC2
N	1281	TRP	-	expression tag	UNP P0DTC2
N	1282	SER	-	expression tag	UNP P0DTC2
N	1283	HIS	-	expression tag	UNP P0DTC2
N	1284	PRO	-	expression tag	UNP P0DTC2
N	1285	GLN	-	expression tag	UNP P0DTC2
N	1286	PHE	-	expression tag	UNP P0DTC2
N	1287	GLU	-	expression tag	UNP P0DTC2
N	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 5 is a protein called BD-744L.

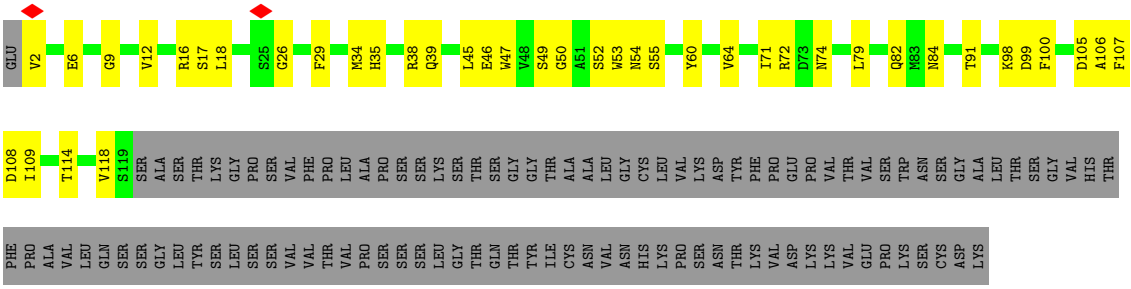
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	73	564	360	99	102	3	0	0

3 Residue-property plots (i)

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

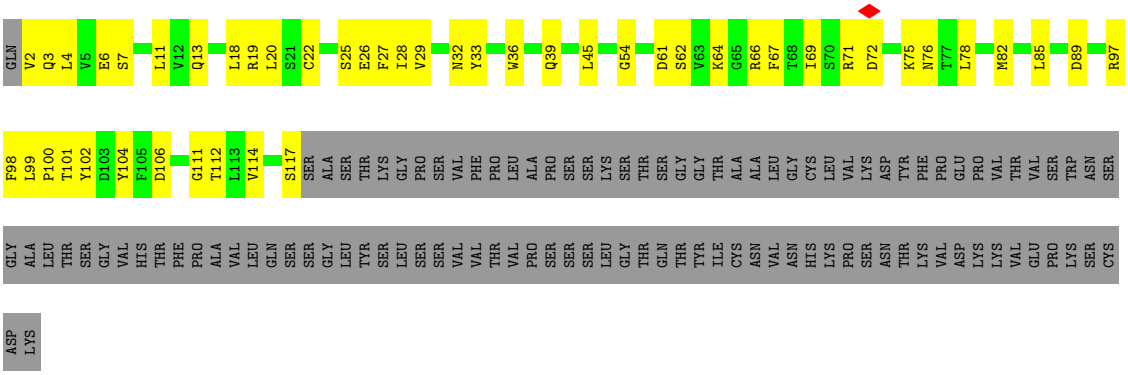
- Molecule 1: BD-744H

Chain A:



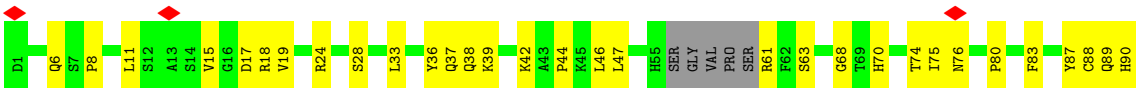
- Molecule 2: BD-813H

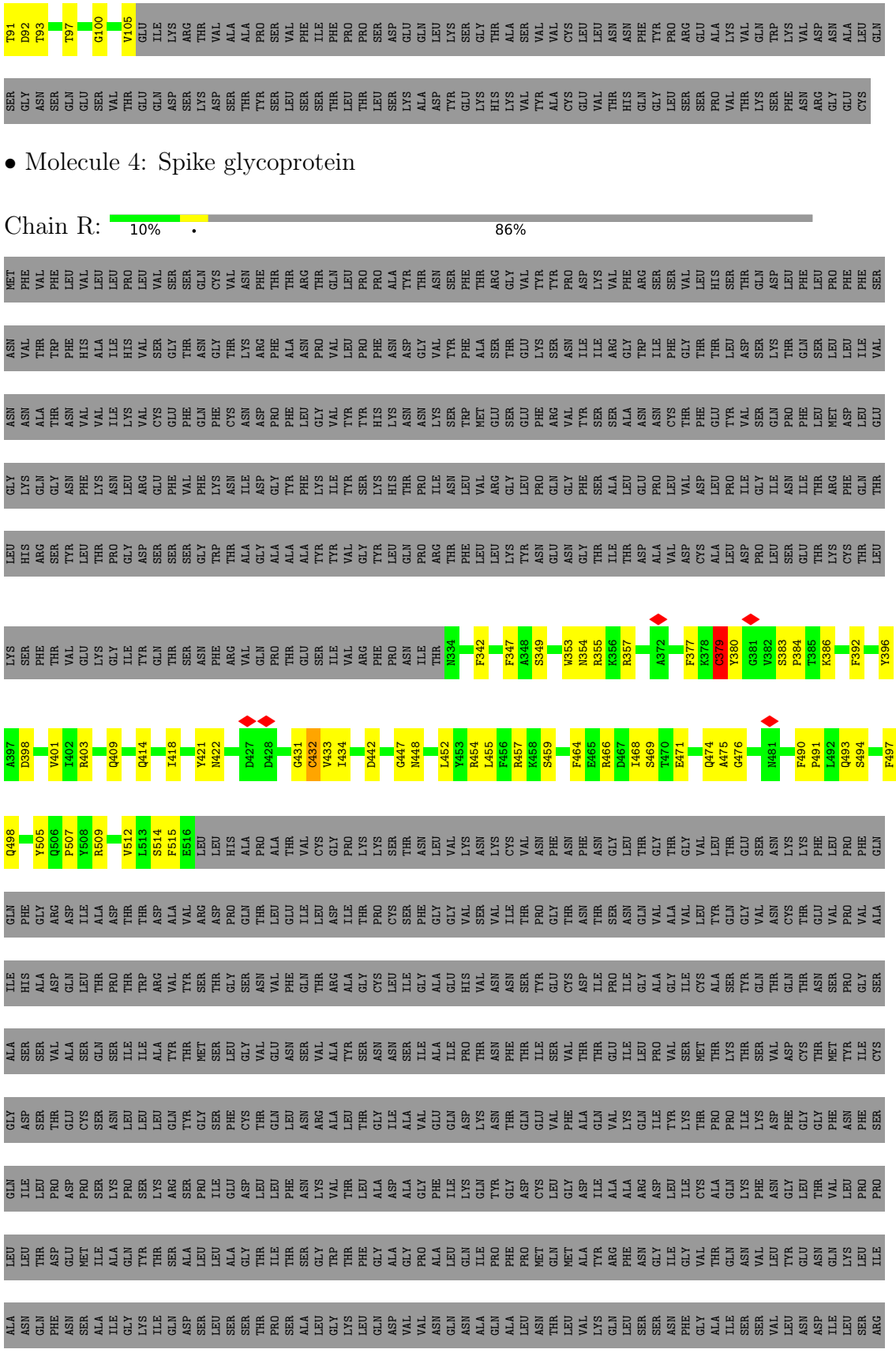
Chain H:

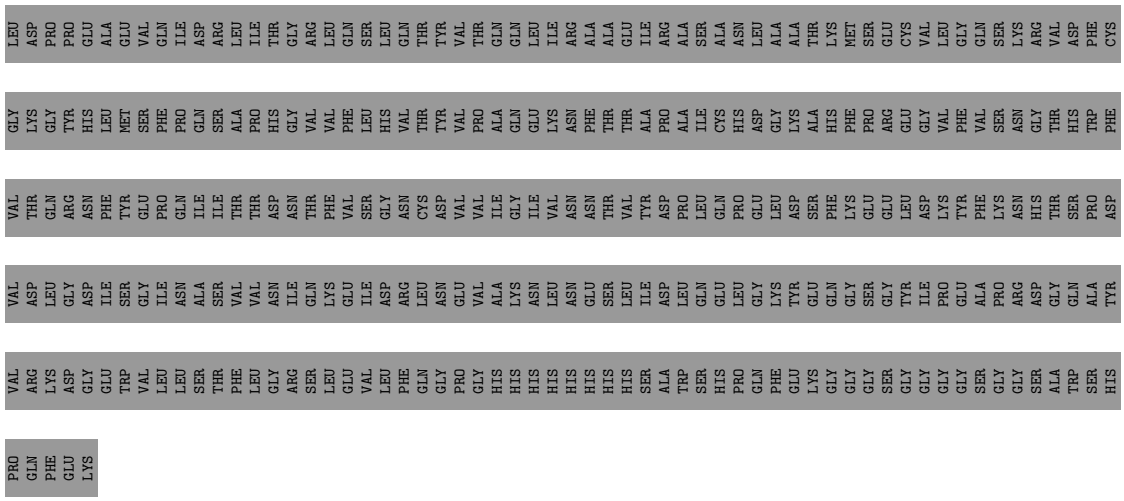


- Molecule 3: BD-813L

Chain L:

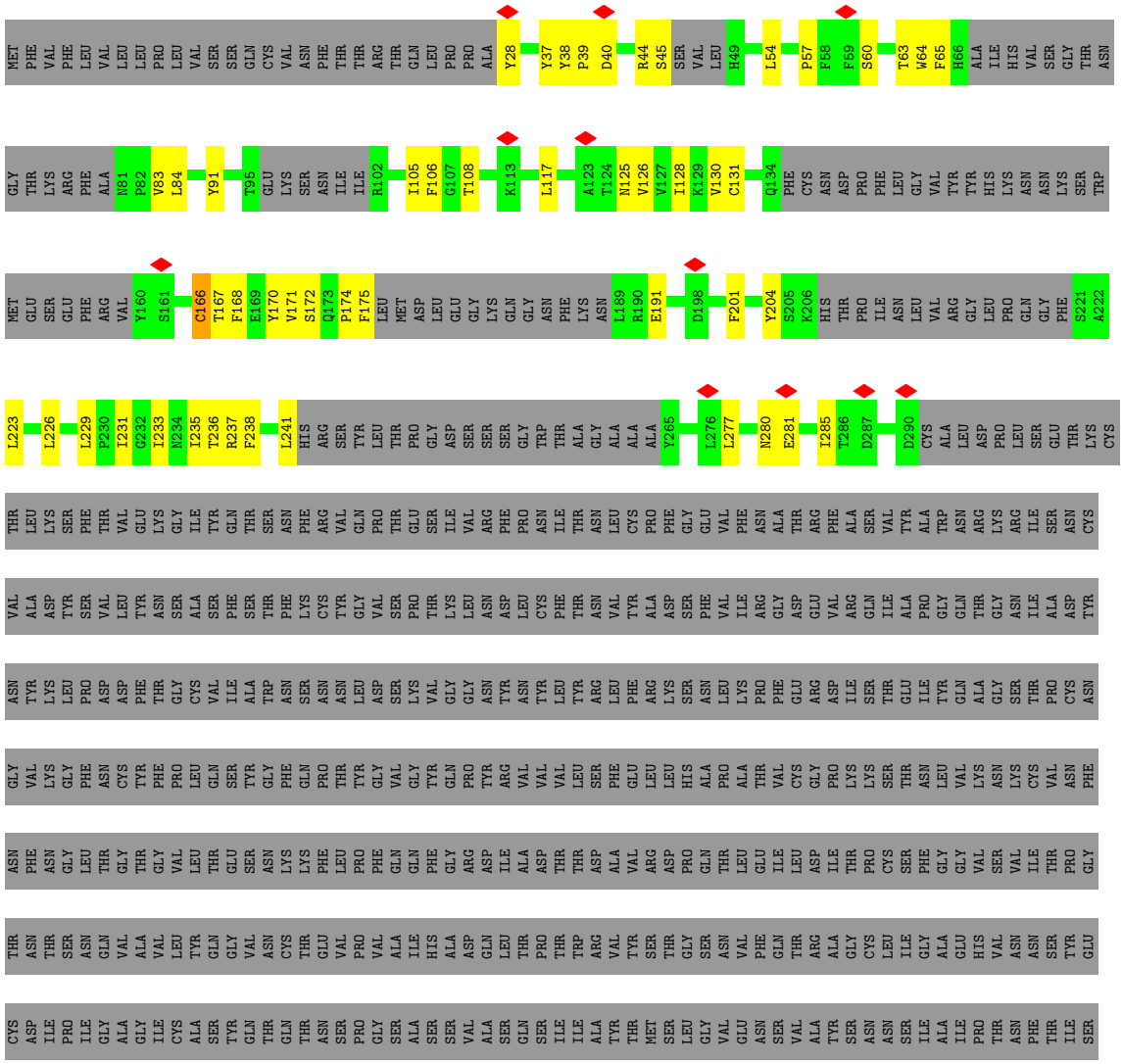


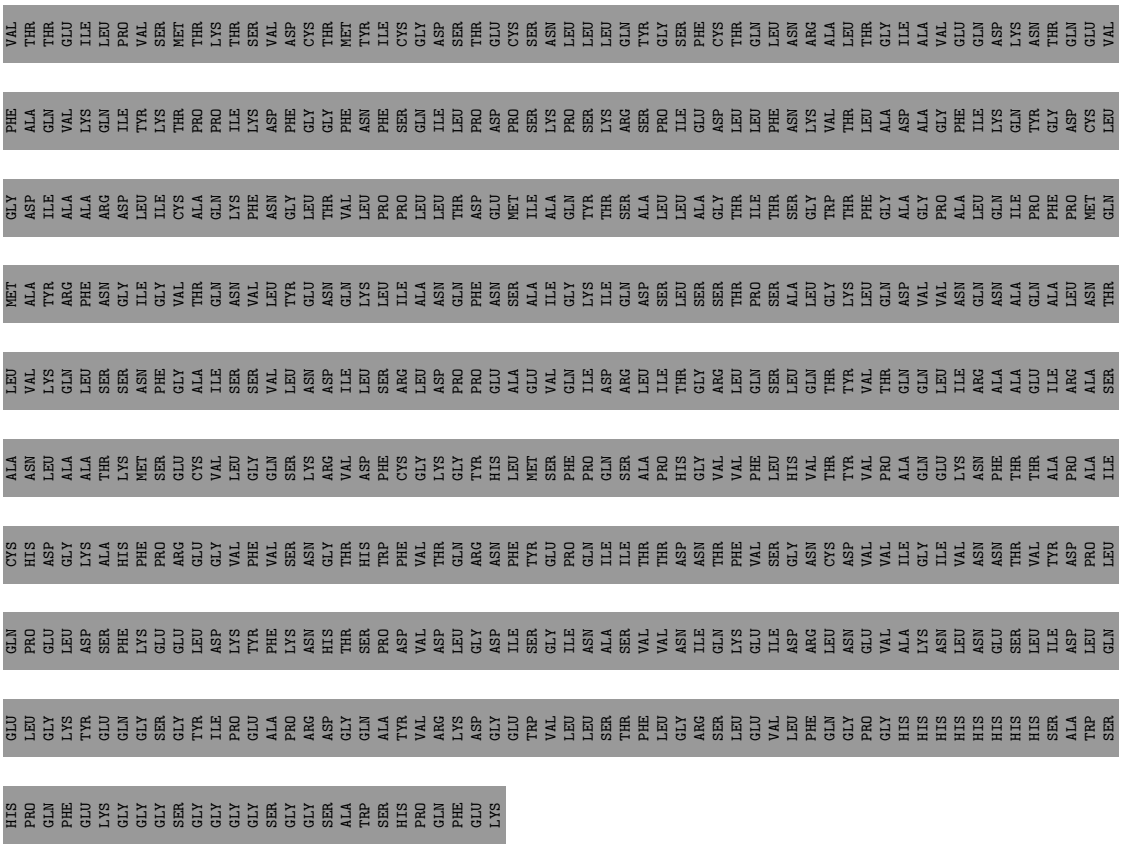

T91 D92 T93 T97 G100 V105
• Molecule 4: Spike glycoprotein
Chain R:
10%
86%
N334 F342 F347 A348 S349 W353 N354 R355 K356 R357 A372 F377 K378 C379 Y380 G381 V382 S383 P384 T385 K386 F392 Y396
A397 D398 V401 I402 R403 Q409 Q414 I418 Y421 N422 D427 D428 G431 C432 V433 I434 D442 G447 N448 L452 Y453 R454 L455 F456 R457 K458 S459 F464 E465 R466 D467 I468 S469 T470 E471 Q474 A475 G476 N481 F490 P491 L492 Q493 S494 F497
Q498 Y505 Q506 P507 Y508 R509 V512 L513 S514 F515 E516



- Molecule 4: Spike glycoprotein

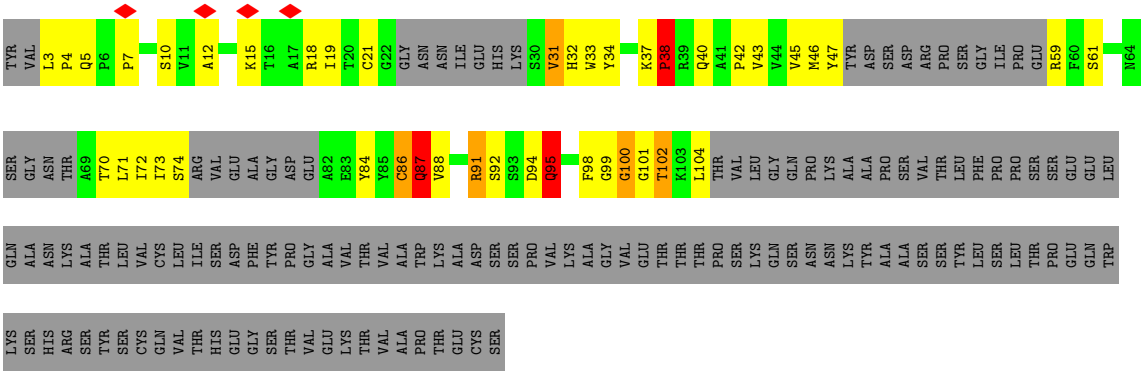
Chain N:





- Molecule 5: BD-744L

Chain B: 14% 16% 66%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	425831	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 ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.766	Depositor
Minimum map value	-6.340	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.405	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/925	0.52	0/1250
2	H	0.44	0/925	0.54	0/1256
3	L	0.39	0/786	0.52	0/1067
4	N	0.31	0/1394	0.54	1/1890 (0.1%)
4	R	0.41	0/1507	0.57	2/2049 (0.1%)
5	B	0.65	0/577	1.00	3/781 (0.4%)
All	All	0.42	0/6114	0.60	6/8293 (0.1%)

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
2	H	0	1
4	R	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	379	CYS	CA-CB-SG	8.81	129.86	114.00
4	R	432	CYS	CA-CB-SG	8.27	128.88	114.00
4	N	166	CYS	CA-CB-SG	6.61	125.89	114.00
5	B	98	PHE	CB-CA-C	-6.56	97.27	110.40
5	B	87	GLN	CB-CA-C	-5.42	99.57	110.40
5	B	95	GLN	CB-CA-C	-5.21	99.97	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	101	THR	Peptide
4	R	379	CYS	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	905	0	858	30	0
2	H	903	0	868	37	0
3	L	767	0	743	25	0
4	N	1359	0	1301	40	0
4	R	1465	0	1381	47	0
5	B	564	0	550	38	0
All	All	5963	0	5701	201	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 17.

All (201) 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)
4:R:357:ARG:NH1	4:N:167:THR:HB	1.61	1.15
5:B:5:GLN:NE2	5:B:21:CYS:SG	2.20	1.14
5:B:5:GLN:CD	5:B:21:CYS:HA	1.82	1.00
5:B:5:GLN:NE2	5:B:21:CYS:HA	1.75	0.99
5:B:5:GLN:HE22	5:B:21:CYS:CA	1.75	0.98
5:B:5:GLN:OE1	5:B:21:CYS:HA	1.63	0.96
5:B:5:GLN:HE22	5:B:21:CYS:CB	1.80	0.94
5:B:5:GLN:HG3	5:B:101:GLY:HA2	1.54	0.89
4:N:131:CYS:HA	4:N:166:CYS:HB3	1.56	0.86
4:R:357:ARG:NH1	4:N:167:THR:CB	2.40	0.84
1:A:91:THR:HG22	1:A:118:VAL:H	1.43	0.84
5:B:34:TYR:HE1	5:B:87:GLN:HB2	1.42	0.84
3:L:91:THR:HG22	3:L:97:THR:HG22	1.60	0.83
5:B:4:PRO:O	5:B:5:GLN:HG2	1.81	0.81
4:N:28:TYR:HB2	4:N:64:TRP:HB3	1.63	0.81
5:B:18:ARG:HD2	5:B:70:THR:HG21	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:GLU:OE2	2:H:111:GLY:N	2.11	0.78
5:B:5:GLN:NE2	5:B:21:CYS:CA	2.40	0.77
4:R:377:PHE:HD1	4:R:434:ILE:HG22	1.53	0.73
5:B:5:GLN:NE2	5:B:86:CYS:SG	2.62	0.72
4:N:83:VAL:HG11	4:N:237:ARG:HE	1.55	0.71
4:R:383:SER:HB3	4:R:386:LYS:HG2	1.70	0.71
3:L:38:GLN:NE2	3:L:42:LYS:O	2.25	0.69
5:B:5:GLN:CG	5:B:101:GLY:HA2	2.23	0.69
2:H:28:ILE:HA	2:H:76:ASN:HD21	1.59	0.68
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.76	0.67
3:L:6:GLN:HE21	3:L:100:GLY:HA3	1.58	0.67
4:R:357:ARG:HH12	4:N:167:THR:HB	1.52	0.67
1:A:108:ASP:OD1	1:A:109:ILE:N	2.28	0.67
4:N:106:PHE:HB3	4:N:235:ILE:HD12	1.76	0.67
4:N:106:PHE:CD1	4:N:238:PHE:HB2	2.31	0.66
2:H:20:LEU:HD21	2:H:114:VAL:HG21	1.78	0.66
1:A:54:ASN:OD1	1:A:74:ASN:ND2	2.28	0.65
2:H:11:LEU:HD11	2:H:117:SER:HB3	1.77	0.65
3:L:92:ASP:OD1	3:L:93:THR:N	2.30	0.64
1:A:29:PHE:O	1:A:72:ARG:NH2	2.31	0.63
4:N:126:VAL:HB	4:N:174:PRO:HA	1.81	0.63
1:A:35:HIS:CG	1:A:107:PHE:HE1	2.17	0.62
5:B:34:TYR:CE1	5:B:87:GLN:HB2	2.31	0.62
5:B:18:ARG:HH11	5:B:72:ILE:HD13	1.64	0.62
5:B:31:VAL:HG23	5:B:86:CYS:HB3	1.81	0.62
2:H:66:ARG:NH2	2:H:89:ASP:OD2	2.32	0.62
4:R:474:GLN:NE2	4:R:476:GLY:O	2.30	0.62
1:A:100:PHE:CE1	1:A:108:ASP:HB3	2.35	0.61
1:A:106:ALA:HB2	5:B:32:HIS:CG	2.36	0.61
4:R:469:SER:OG	4:R:471:GLU:OE1	2.17	0.60
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.66	0.60
3:L:89:GLN:HG2	3:L:90:HIS:N	2.17	0.60
4:N:57:PRO:HB2	4:N:60:SER:HB2	1.84	0.60
3:L:61:ARG:O	3:L:76:ASN:ND2	2.35	0.59
4:N:37:TYR:OH	4:N:54:LEU:O	2.15	0.59
5:B:4:PRO:O	5:B:5:GLN:CG	2.50	0.59
4:R:403:ARG:HD3	4:R:505:TYR:HD1	1.68	0.58
4:R:433:VAL:HG22	4:R:512:VAL:HG22	1.85	0.58
5:B:84:TYR:O	5:B:101:GLY:HA3	2.04	0.58
5:B:19:ILE:H	5:B:70:THR:HG23	1.67	0.57
5:B:19:ILE:HD12	5:B:102:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:5:GLN:CB	5:B:101:GLY:HA2	2.34	0.57
3:L:36:TYR:HB3	3:L:44:PRO:HB3	1.85	0.57
3:L:63:SER:OG	3:L:74:THR:OG1	2.20	0.57
2:H:72:ASP:OD1	2:H:75:LYS:NZ	2.37	0.57
5:B:3:LEU:HB3	5:B:99:GLY:HA3	1.85	0.57
2:H:61:ASP:HA	2:H:64:LYS:HZ3	1.69	0.56
2:H:61:ASP:OD1	2:H:62:SER:N	2.38	0.56
1:A:12:VAL:HG21	1:A:18:LEU:HD22	1.88	0.56
4:R:355:ARG:HG3	4:R:355:ARG:HH11	1.70	0.55
5:B:5:GLN:OE1	5:B:21:CYS:CA	2.47	0.55
4:R:354:ASN:OD1	4:R:355:ARG:N	2.39	0.55
4:N:131:CYS:CA	4:N:166:CYS:HB3	2.30	0.55
4:R:464:PHE:HZ	4:R:514:SER:HG	1.55	0.55
4:N:280:ASN:O	4:N:281:GLU:HG2	2.06	0.55
1:A:99:ASP:N	1:A:99:ASP:OD1	2.39	0.54
4:R:409:GLN:HA	4:R:414:GLN:HG2	1.89	0.54
4:R:455:LEU:HD22	4:R:493:GLN:HB2	1.89	0.54
2:H:33:TYR:CE2	2:H:100:PRO:HB3	2.43	0.54
3:L:37:GLN:HE22	3:L:39:LYS:HE2	1.73	0.54
1:A:82:GLN:NE2	1:A:84:ASN:OD1	2.41	0.53
4:N:91:TYR:OH	4:N:191:GLU:OE1	2.22	0.53
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.91	0.53
4:N:105:ILE:HD11	4:N:241:LEU:HD12	1.90	0.53
2:H:61:ASP:HA	2:H:64:LYS:NZ	2.25	0.52
5:B:5:GLN:NE2	5:B:21:CYS:CB	2.59	0.52
4:N:277:LEU:HD13	4:N:285:ILE:HD13	1.91	0.52
4:R:418:ILE:HA	4:R:422:ASN:HD22	1.74	0.52
4:N:231:ILE:HG22	4:N:233:ILE:HG12	1.92	0.51
2:H:4:LEU:HD11	2:H:27:PHE:CD2	2.45	0.51
3:L:8:PRO:HG2	3:L:11:LEU:HD11	1.91	0.51
4:N:38:TYR:O	4:N:40:ASP:N	2.37	0.51
1:A:38:ARG:NE	1:A:46:GLU:OE1	2.43	0.51
2:H:32:ASN:ND2	4:R:475:ALA:O	2.44	0.51
4:N:168:PHE:CE2	4:N:229:LEU:HD23	2.46	0.51
1:A:54:ASN:O	4:R:354:ASN:ND2	2.44	0.50
1:A:106:ALA:HA	5:B:87:GLN:OE1	2.10	0.50
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.92	0.50
1:A:54:ASN:HB3	4:R:354:ASN:ND2	2.27	0.50
2:H:18:LEU:HD13	2:H:114:VAL:HG13	1.94	0.50
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.77	0.50
4:N:83:VAL:CG1	4:N:237:ARG:HE	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:130:VAL:HG13	4:N:130:VAL:O	2.12	0.49
3:L:83:PHE:HD1	3:L:105:VAL:HG12	1.76	0.49
4:R:401:VAL:HG22	4:R:509:ARG:HG2	1.95	0.49
1:A:105:ASP:OD1	1:A:106:ALA:N	2.44	0.49
3:L:63:SER:HG	3:L:74:THR:HG1	1.56	0.49
2:H:2:VAL:HG22	2:H:26:GLU:HB3	1.94	0.49
4:R:379:CYS:HA	4:R:380:TYR:CD2	2.48	0.49
4:N:168:PHE:HE2	4:N:229:LEU:HD23	1.76	0.49
3:L:33:LEU:HA	3:L:89:GLN:O	2.13	0.49
2:H:18:LEU:HD23	2:H:19:ARG:N	2.27	0.48
4:N:106:PHE:HB2	4:N:117:LEU:HB3	1.96	0.48
4:R:403:ARG:HD3	4:R:505:TYR:CD1	2.48	0.48
3:L:24:ARG:HH11	3:L:70:HIS:HB2	1.78	0.48
4:R:355:ARG:HG3	4:R:355:ARG:NH1	2.29	0.48
2:H:102:TYR:O	2:H:104:TYR:HD1	1.96	0.48
4:R:431:GLY:HA2	4:R:515:PHE:CE2	2.49	0.47
4:R:342:PHE:CD2	4:R:434:ILE:HD11	2.49	0.47
4:R:342:PHE:CE2	4:R:434:ILE:HD11	2.49	0.47
2:H:3:GLN:H	2:H:25:SER:HB2	1.80	0.47
4:R:392:PHE:CG	4:R:515:PHE:HB3	2.49	0.47
4:R:355:ARG:HG3	4:R:398:ASP:OD1	2.15	0.47
5:B:33:TRP:HD1	5:B:46:MET:HE3	1.80	0.47
5:B:91:ARG:HE	5:B:91:ARG:HB2	1.40	0.47
4:R:457:ARG:NH1	4:R:459:SER:O	2.36	0.47
2:H:13:GLN:NE2	2:H:117:SER:O	2.32	0.47
4:R:357:ARG:HG3	4:R:396:TYR:CE1	2.50	0.47
4:N:125:ASN:HD21	4:N:171:VAL:HG13	1.78	0.46
4:N:84:LEU:HB2	4:N:238:PHE:CE1	2.51	0.46
2:H:67:PHE:CD1	2:H:82:MET:HA	2.51	0.46
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.96	0.46
4:R:379:CYS:HB2	4:R:432:CYS:HB3	1.37	0.46
4:N:40:ASP:OD1	4:N:204:TYR:OH	2.20	0.46
4:N:83:VAL:HG11	4:N:237:ARG:HH21	1.80	0.46
1:A:54:ASN:HB3	4:R:354:ASN:HD21	1.81	0.46
1:A:2:VAL:HA	1:A:26:GLY:HA3	1.98	0.46
1:A:16:ARG:HD3	1:A:17:SER:H	1.80	0.46
1:A:9:GLY:HA3	1:A:114:THR:HB	1.98	0.46
4:R:452:LEU:HD23	4:R:494:SER:HA	1.98	0.45
4:R:454:ARG:NH2	4:R:469:SER:O	2.47	0.45
4:R:377:PHE:HE2	4:R:384:PRO:HB3	1.82	0.45
5:B:4:PRO:C	5:B:5:GLN:HG2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:28:SER:HA	3:L:68:GLY:O	2.17	0.45
4:R:447:GLY:N	4:R:498:GLN:OE1	2.50	0.45
1:A:98:LYS:NZ	1:A:108:ASP:OD2	2.41	0.45
1:A:53:TRP:CE3	1:A:54:ASN:HB2	2.51	0.45
5:B:99:GLY:O	5:B:100:GLY:C	2.55	0.45
4:N:44:ARG:HG2	4:N:45:SER:N	2.32	0.45
1:A:2:VAL:HG11	1:A:109:ILE:HD13	1.99	0.44
2:H:106:ASP:HA	3:L:46:LEU:HD22	1.99	0.44
2:H:6:GLU:HG2	2:H:112:THR:HG23	2.00	0.44
2:H:28:ILE:O	2:H:28:ILE:HG13	2.17	0.44
3:L:19:VAL:HB	3:L:75:ILE:HB	1.99	0.44
4:R:347:PHE:HB2	4:R:401:VAL:HG23	2.00	0.44
1:A:71:ILE:HG21	4:R:468:ILE:HG21	1.99	0.44
2:H:22:CYS:HB3	2:H:78:LEU:HB3	2.00	0.44
4:R:349:SER:HB2	4:R:452:LEU:H	1.83	0.43
1:A:47:TRP:CZ3	5:B:95:GLN:HB3	2.53	0.43
1:A:52:SER:HB3	1:A:55:SER:HB2	1.99	0.43
5:B:12:ALA:HB3	5:B:15:LYS:HE2	2.00	0.43
2:H:99:LEU:HD12	2:H:106:ASP:HB2	2.00	0.43
2:H:104:TYR:CE2	3:L:46:LEU:HD21	2.54	0.43
4:R:497:PHE:CE2	4:R:507:PRO:HB3	2.53	0.43
4:N:175:PHE:CD2	4:N:226:LEU:HD21	2.53	0.43
4:R:357:ARG:HH11	4:N:167:THR:HA	1.82	0.43
4:N:126:VAL:HG12	4:N:172:SER:O	2.19	0.43
1:A:49:SER:OG	1:A:50:GLY:N	2.52	0.43
3:L:17:ASP:OD1	3:L:18:ARG:N	2.51	0.42
4:R:490:PHE:CD1	4:R:491:PRO:HD2	2.53	0.42
2:H:32:ASN:OD1	2:H:97:ARG:HD3	2.19	0.42
5:B:3:LEU:HB3	5:B:99:GLY:CA	2.48	0.42
3:L:63:SER:O	3:L:74:THR:OG1	2.37	0.42
5:B:4:PRO:O	5:B:5:GLN:NE2	2.52	0.42
5:B:37:LYS:O	5:B:38:PRO:C	2.57	0.42
1:A:60:TYR:HA	1:A:64:VAL:HG23	2.01	0.42
4:R:431:GLY:HA3	4:R:514:SER:HA	2.00	0.42
4:N:106:PHE:CE1	4:N:238:PHE:HB2	2.54	0.42
1:A:6:GLU:N	1:A:6:GLU:OE2	2.52	0.42
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.02	0.42
3:L:15:VAL:HG23	3:L:80:PRO:HD3	2.02	0.42
5:B:73:ILE:HD13	5:B:104:LEU:HD22	2.02	0.42
2:H:28:ILE:HA	2:H:76:ASN:ND2	2.31	0.42
4:R:379:CYS:HB3	4:R:432:CYS:HB2	1.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:108:THR:HG22	4:N:236:THR:HG23	2.01	0.42
2:H:6:GLU:HA	2:H:22:CYS:HA	2.02	0.41
4:R:442:ASP:O	4:R:448:ASN:ND2	2.53	0.41
2:H:29:VAL:O	2:H:71:ARG:NH1	2.53	0.41
4:N:65:PHE:CE2	4:N:84:LEU:HD11	2.56	0.41
4:N:128:ILE:HB	4:N:170:TYR:HB3	2.03	0.41
2:H:7:SER:HA	2:H:112:THR:HG21	2.03	0.41
3:L:6:GLN:NE2	3:L:88:CYS:H	2.19	0.41
4:R:353:TRP:CE2	4:R:466:ARG:HB3	2.56	0.41
2:H:3:GLN:N	2:H:3:GLN:OE1	2.54	0.41
4:R:357:ARG:CZ	4:N:167:THR:HB	2.39	0.41
5:B:19:ILE:HD12	5:B:102:THR:CG2	2.50	0.41
5:B:45:VAL:HG21	5:B:71:LEU:CD2	2.51	0.41
4:N:38:TYR:HA	4:N:39:PRO:HD3	1.91	0.40
4:N:191:GLU:OE2	4:N:223:LEU:HD21	2.22	0.40
2:H:54:GLY:N	4:R:421:TYR:OH	2.40	0.40
3:L:11:LEU:HD23	3:L:19:VAL:HG13	2.02	0.40
4:N:106:PHE:HE2	4:N:201:PHE:CZ	2.40	0.40
2:H:33:TYR:HD2	2:H:98:PHE:CD2	2.39	0.40
2:H:33:TYR:HD2	2:H:98:PHE:HD2	1.69	0.40
4:N:63:THR:HG1	4:N:65:PHE:HE2	1.65	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	116/225 (52%)	95 (82%)	21 (18%)	0	100	100
2	H	114/223 (51%)	103 (90%)	11 (10%)	0	100	100
3	L	96/215 (45%)	80 (83%)	16 (17%)	0	100	100
4	N	149/1285 (12%)	133 (89%)	16 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	181/1285 (14%)	169 (93%)	12 (7%)	0	100	100
5	B	63/213 (30%)	48 (76%)	12 (19%)	3 (5%)	2	17
All	All	719/3446 (21%)	628 (87%)	88 (12%)	3 (0%)	38	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	100	GLY
5	B	38	PRO
5	B	7	PRO

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	94/187 (50%)	94 (100%)	0	100	100
2	H	97/190 (51%)	97 (100%)	0	100	100
3	L	86/189 (46%)	86 (100%)	0	100	100
4	N	152/1112 (14%)	152 (100%)	0	100	100
4	R	159/1112 (14%)	159 (100%)	0	100	100
5	B	62/182 (34%)	44 (71%)	18 (29%)	0	1
All	All	650/2972 (22%)	632 (97%)	18 (3%)	46	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	10	SER
5	B	31	VAL
5	B	38	PRO
5	B	40	GLN
5	B	42	PRO
5	B	43	VAL
5	B	47	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	59	ARG
5	B	61	SER
5	B	74	SER
5	B	86	CYS
5	B	87	GLN
5	B	88	VAL
5	B	91	ARG
5	B	92	SER
5	B	94	ASP
5	B	95	GLN
5	B	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	76	ASN
3	L	6	GLN
5	B	5	GLN
4	N	165	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

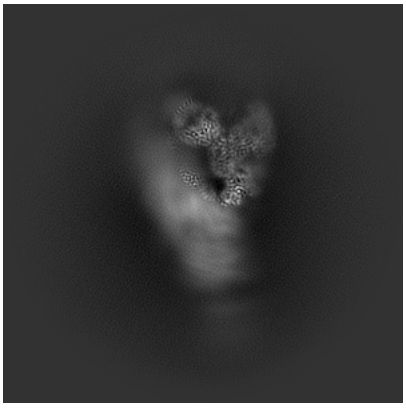
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31374. These allow visual inspection of the internal detail of the map and identification of artifacts.

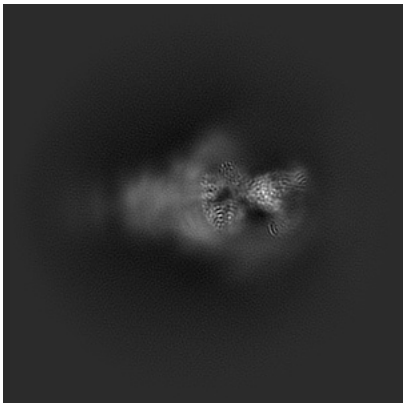
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

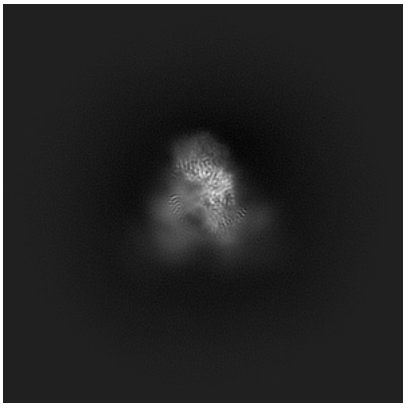
6.1.1 Primary map



X



Y



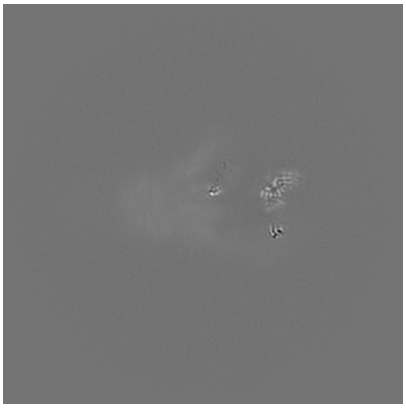
Z

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

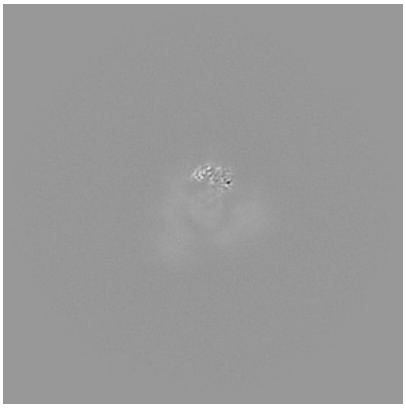
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200



Y Index: 200

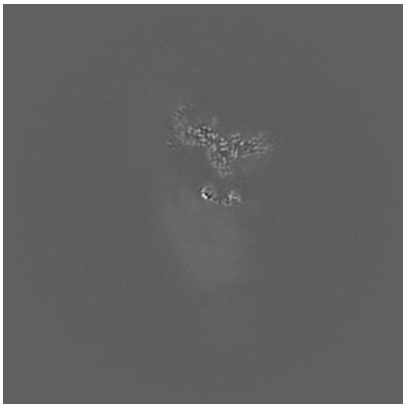


Z Index: 200

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: 210

Y Index: 229

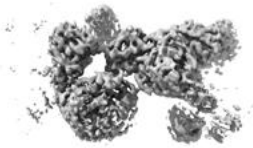
Z Index: 215

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

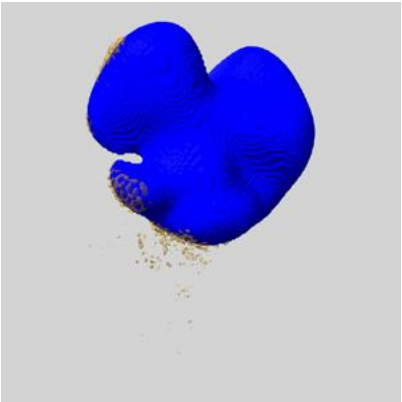
6.5 Mask visualisation (i)

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

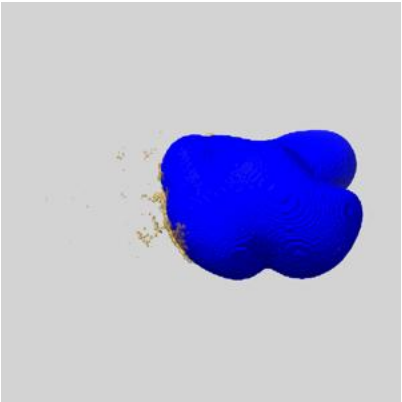
A mask typically either:

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

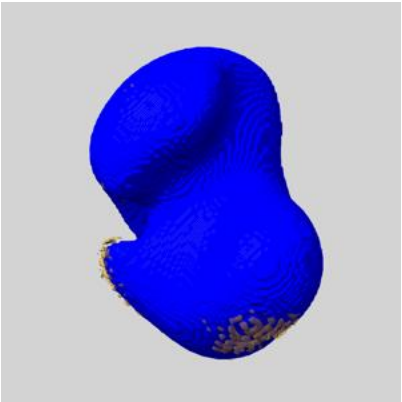
6.5.1 emd_31374_msk_1.map (i)



X



Y

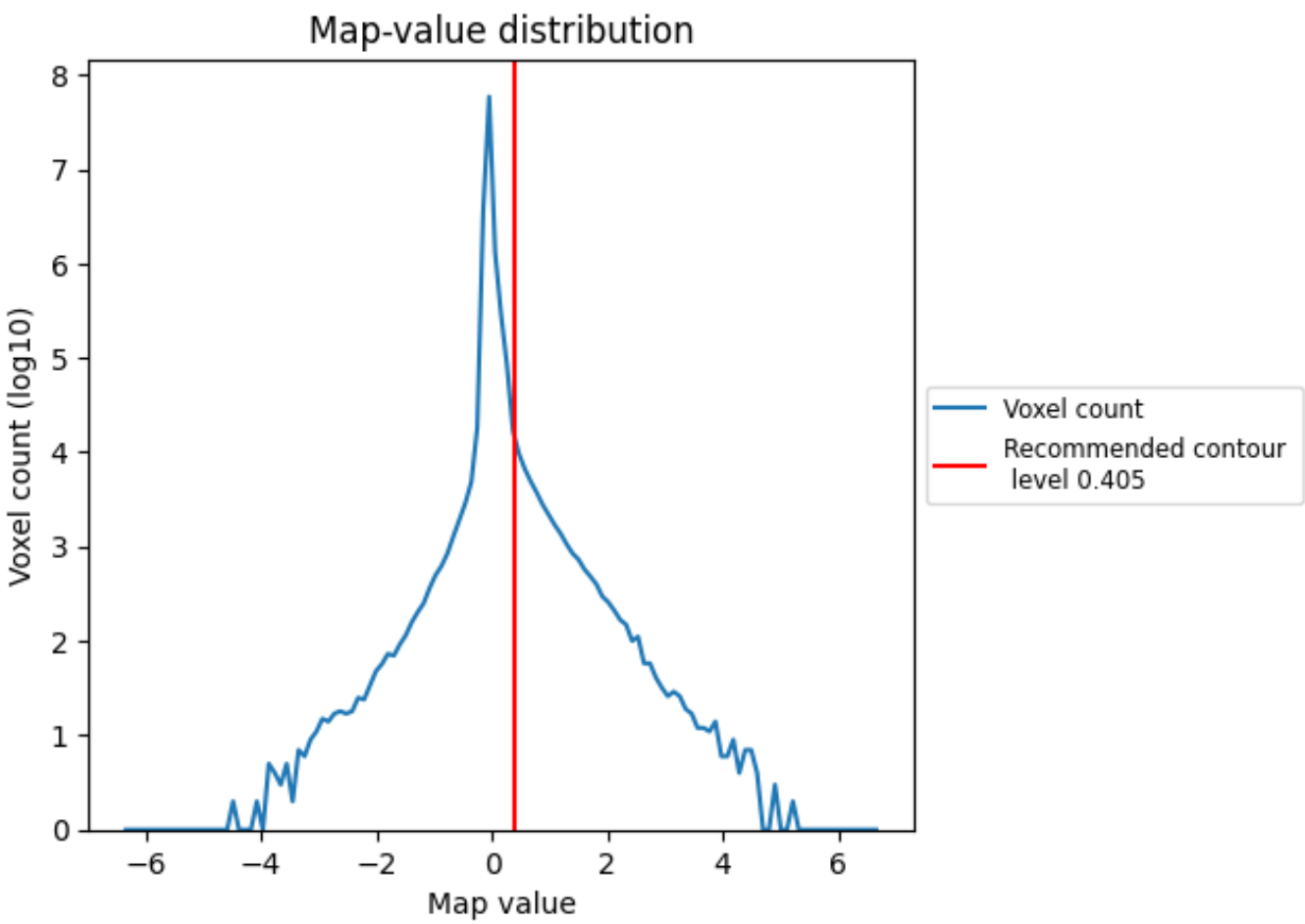


Z

7 Map analysis (i)

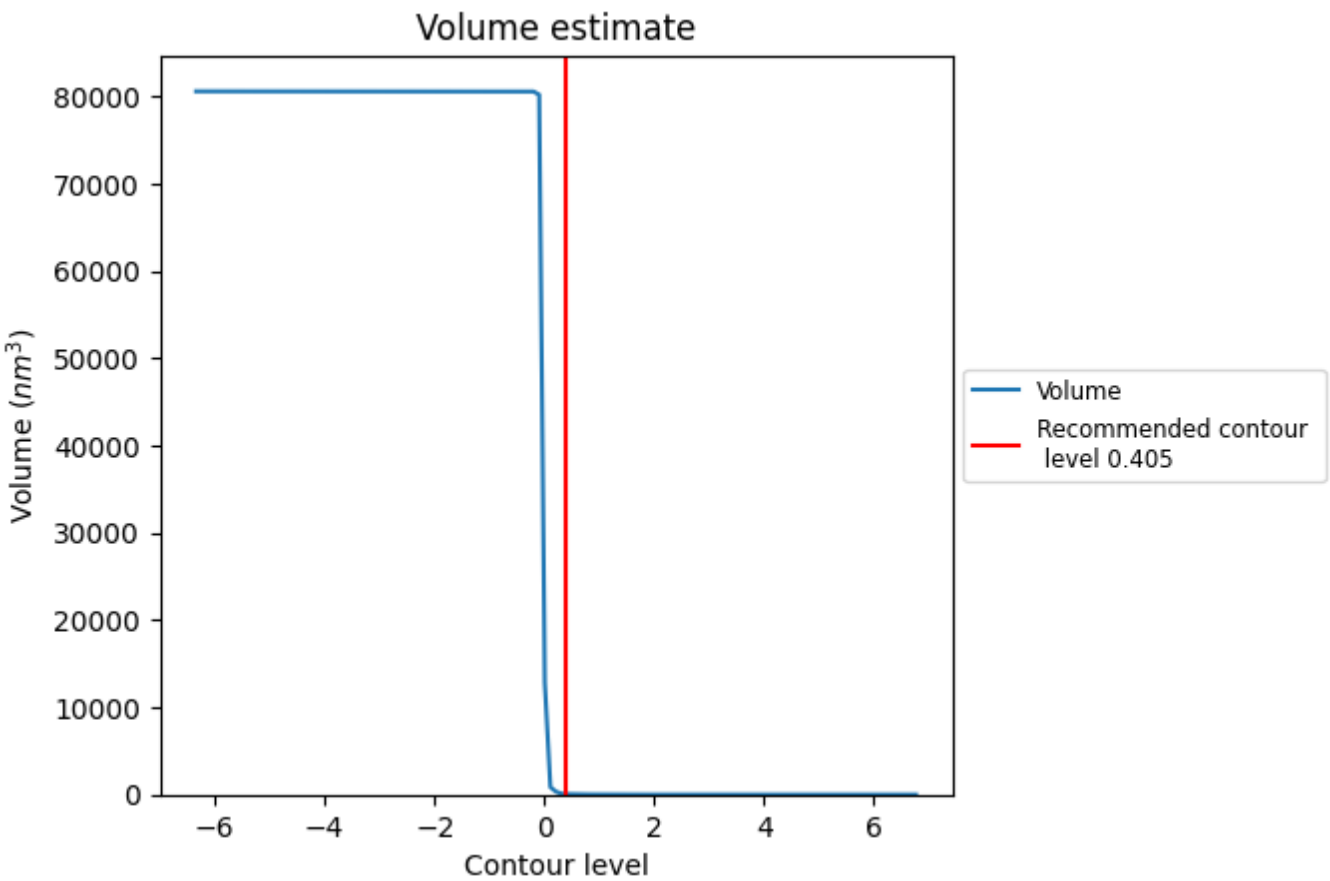
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

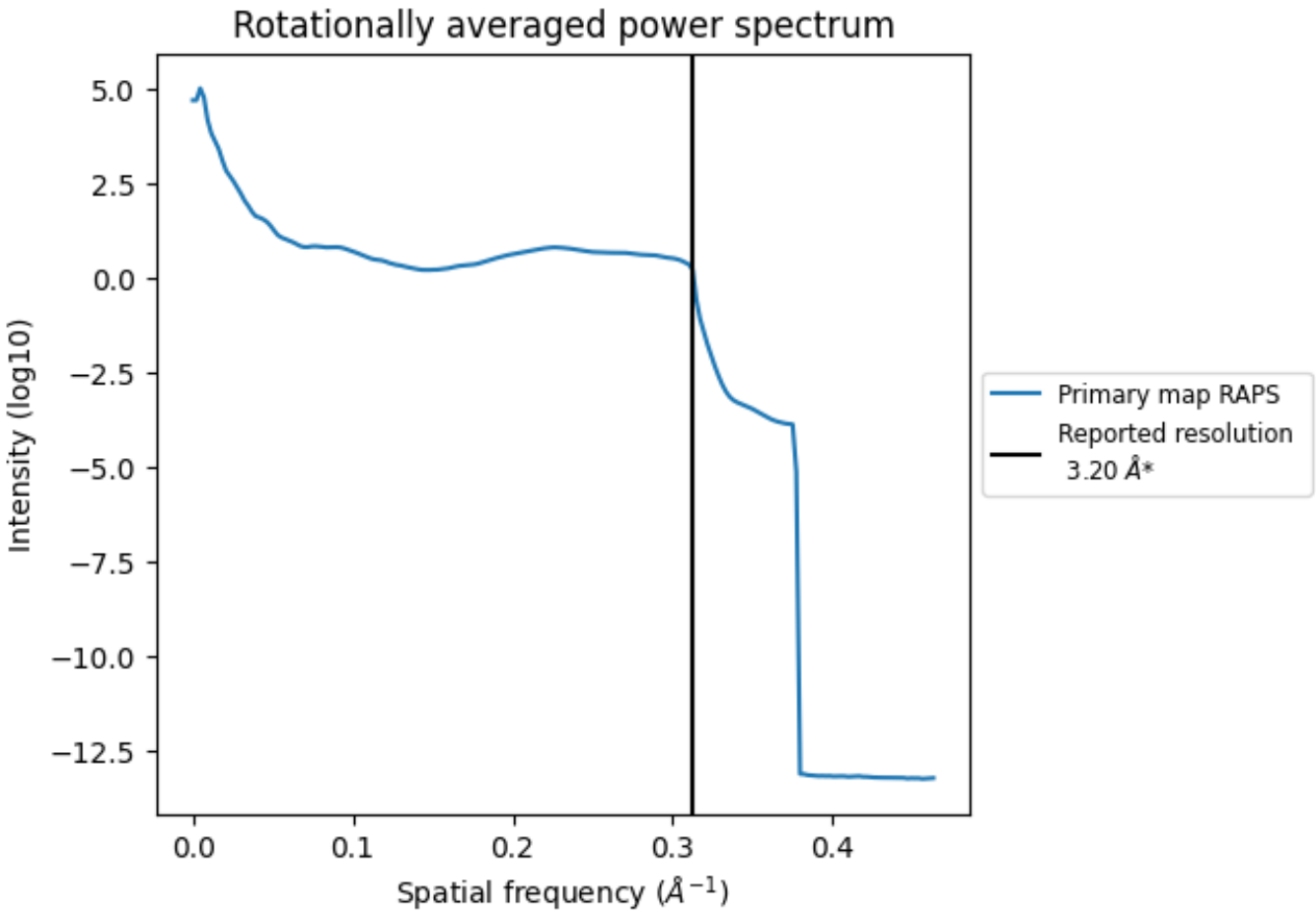
7.2 Volume estimate (i)



The volume at the recommended contour level is 63 nm^3; this corresponds to an approximate mass of 57 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 0.312 Å^{-1}

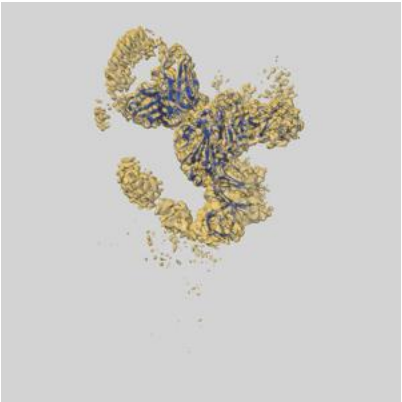
8 Fourier-Shell correlation (i)

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

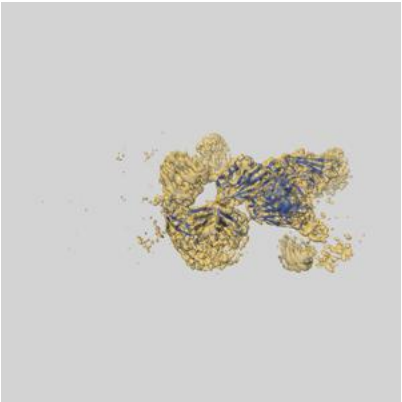
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31374 and PDB model 7EY0. Per-residue inclusion information can be found in section 3 on page 9.

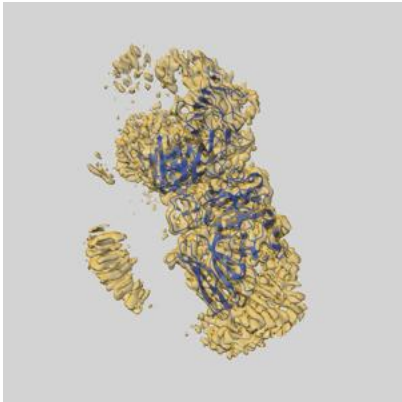
9.1 Map-model overlay (i)



X



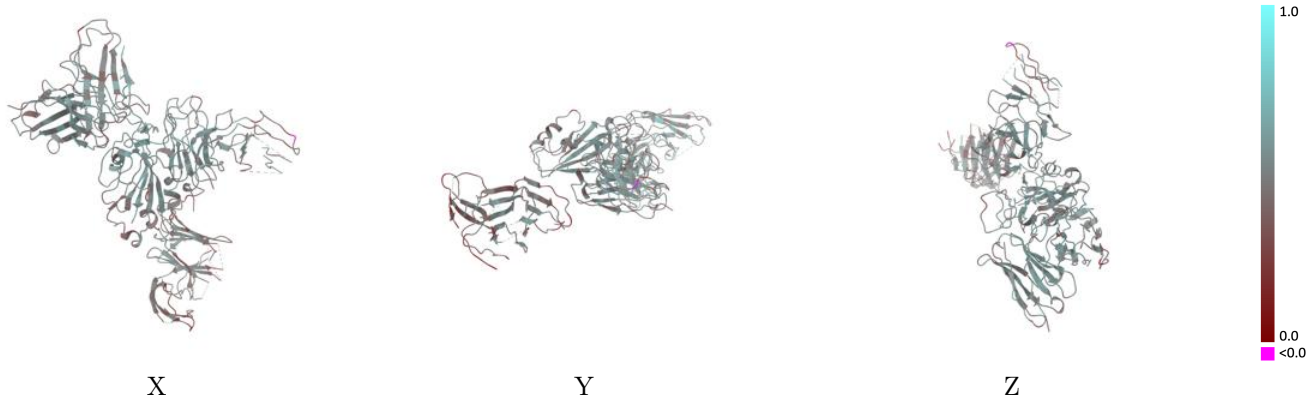
Y



Z

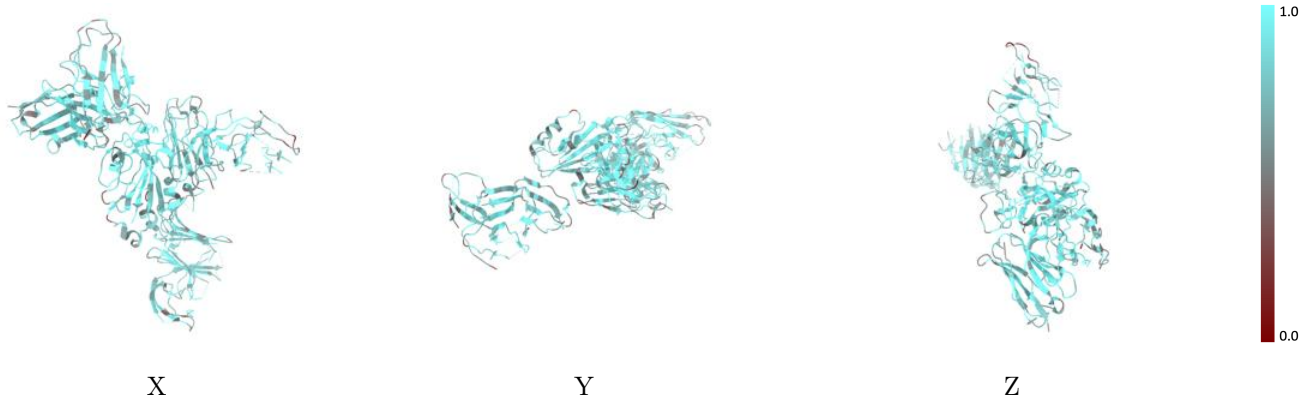
The images above show the 3D surface view of the map at the recommended contour level 0.405 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



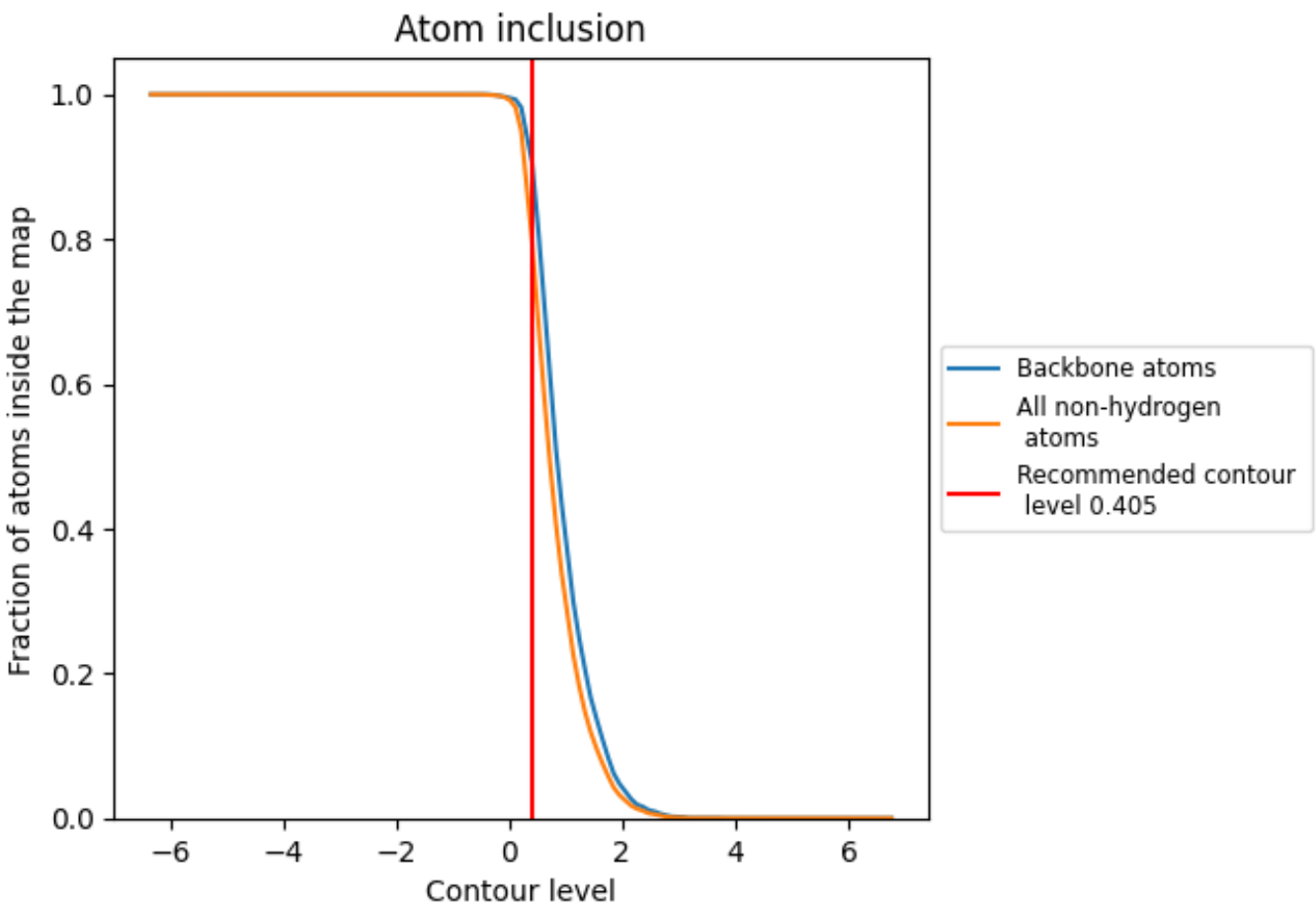
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.405).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.405) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7965	0.4860
A	0.8005	0.5170
B	0.7400	0.4700
H	0.8193	0.5130
L	0.7854	0.5060
N	0.7629	0.4090
R	0.8390	0.5190