



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 01:57 AM JST

PDB ID : 7CEC  
EMDB ID : EMD-30342  
Title : Structure of alpha6beta1 integrin in complex with laminin-511  
Authors : Arimori, T.; Miyazaki, N.; Takagi, J.  
Deposited on : 2020-06-22  
Resolution : 3.90 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

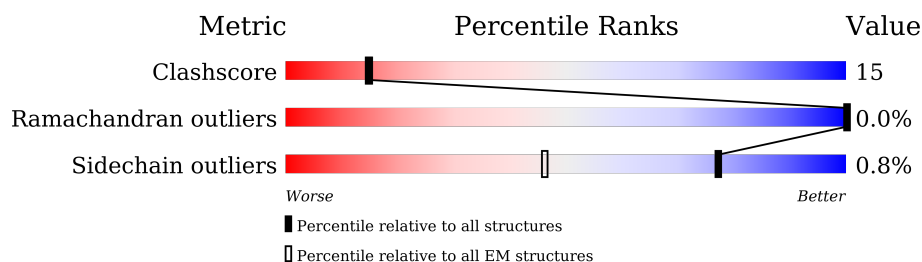
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	627	
2	B	454	
3	C	674	
4	D	74	
5	E	83	
6	F	172	
7	G	164	
8	H	174	

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Mol	Chain	Length	Quality of chain
9	I	159	<div><div></div><div>38%</div><div>61%</div><div>27%</div><div>12%</div></div>
10	J	2	<div><div></div><div>50%</div><div>100%</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17561 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 Integrin alpha-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	553	Total	C	N	O	S	0	0
			4308	2710	754	826	18		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	GLY	-	expression tag	UNP P23229
A	620	SER	-	expression tag	UNP P23229
A	621	LEU	-	expression tag	UNP P23229
A	622	GLU	-	expression tag	UNP P23229
A	623	ASN	-	expression tag	UNP P23229
A	624	LEU	-	expression tag	UNP P23229
A	625	TYR	-	expression tag	UNP P23229
A	626	PHE	-	expression tag	UNP P23229
A	627	GLN	-	expression tag	UNP P23229

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	427	Total	C	N	O	S	0	0
			3320	2079	562	655	24		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	446	GLY	-	expression tag	UNP P05556
B	447	GLY	-	expression tag	UNP P05556
B	448	LEU	-	expression tag	UNP P05556
B	449	GLU	-	expression tag	UNP P05556
B	450	ASN	-	expression tag	UNP P05556
B	451	LEU	-	expression tag	UNP P05556
B	452	TYR	-	expression tag	UNP P05556
B	453	PHE	-	expression tag	UNP P05556

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Chain	Residue	Modelled	Actual	Comment	Reference
B	454	GLN	-	expression tag	UNP P05556

- Molecule 3 is a protein called Laminin subunit alpha-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	574	Total	C	N	O	S	1	0
			4421	2808	773	822	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2654	GLY	-	expression tag	UNP O15230
C	2723	CYS	ILE	engineered mutation	UNP O15230

- Molecule 4 is a protein called Laminin subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	47	Total	C	N	O	S	0	0
			390	242	68	79	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1713	GLY	-	expression tag	UNP P07942

- Molecule 5 is a protein called Laminin subunit gamma-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	44	Total	C	N	O	S	0	0
			357	221	62	70	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1527	GLY	-	expression tag	UNP P11047
E	1585	CYS	ASP	engineered mutation	UNP P11047

- Molecule 6 is a protein called TS2/16 VH(S112C)-SARAH, TS2/16 VH(S112C)-SARAH.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	171	Total	C	N	O	S	1	0
			1360	858	224	269	9		

- Molecule 7 is a protein called TS2/16 VL-SARAH(S37C),TS2/16 VL-SARAH(S37C).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	160	Total	C	N	O	S	0	0
			1252	791	207	247	7		

- Molecule 8 is a protein called HUTS-4 VH(S112C)-SARAH,HUTS-4 VH(S112C)-SARAH.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	122	Total	C	N	O	S	0	0
			954	607	154	188	5		

- Molecule 9 is a protein called HUTS-4 VL(C87Y)-SARAH(S37C),HUTS-4 VL(C87Y)-SARAH(S37C).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	140	Total	C	N	O	S	0	0
			1080	681	184	208	7		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



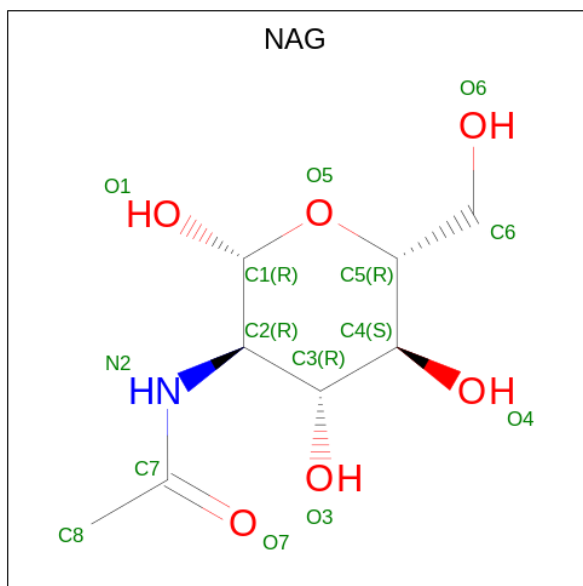
Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
11	A	3	Total	Ca	0
			3	3	
11	C	1	Total	Ca	0
			1	1	

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	C	1	Total	C	N	O	0
			14	8	1	5	

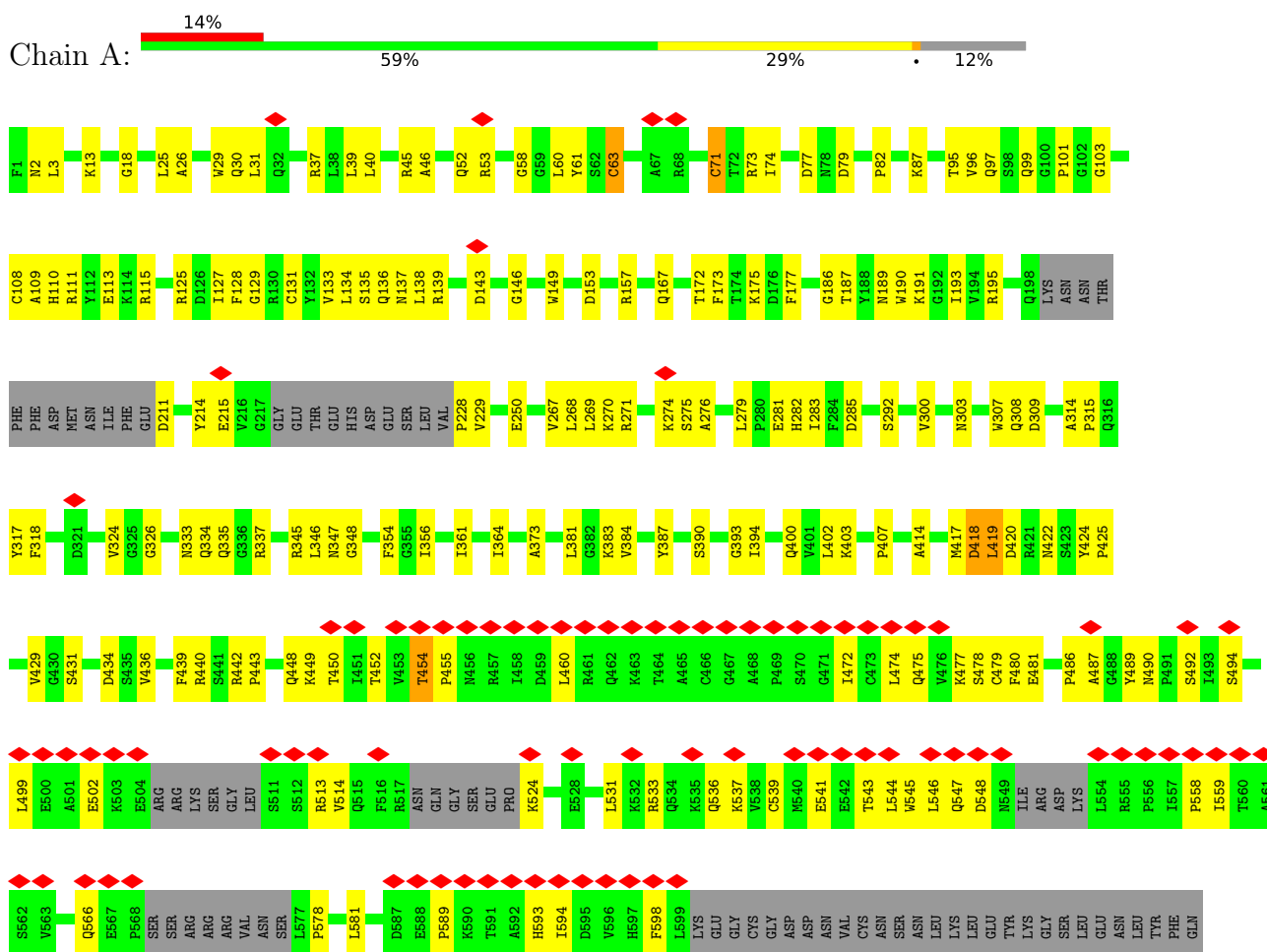
- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
13	B	3	Total	Mn	0
			3	3	

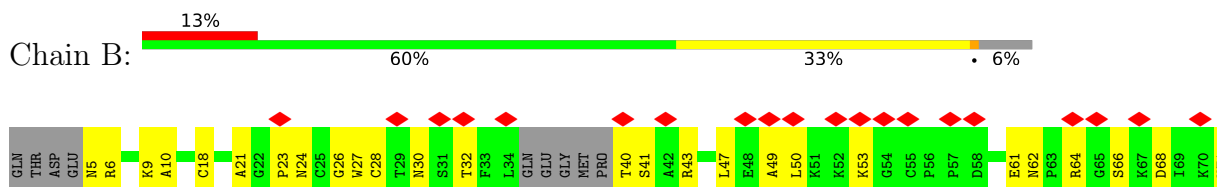
### 3 Residue-property plots

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.

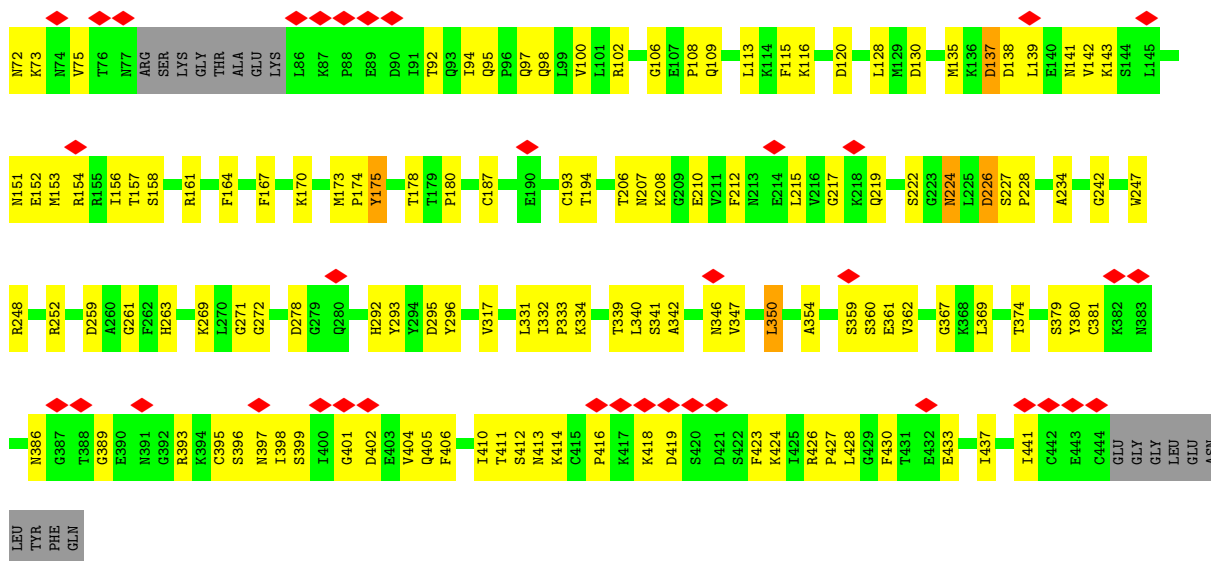
#### • Molecule 1: Integrin alpha-6



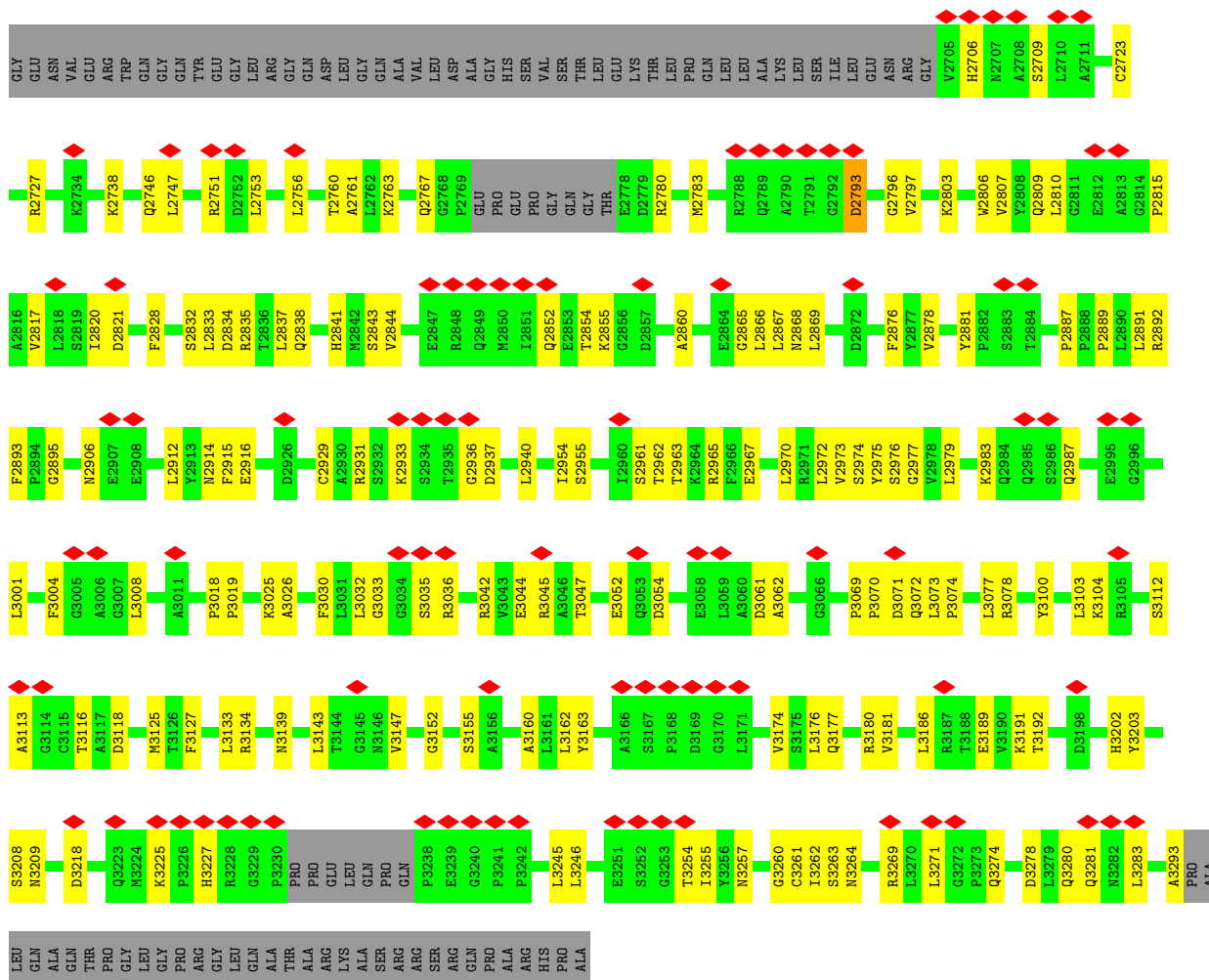
#### • Molecule 2: Integrin beta-1



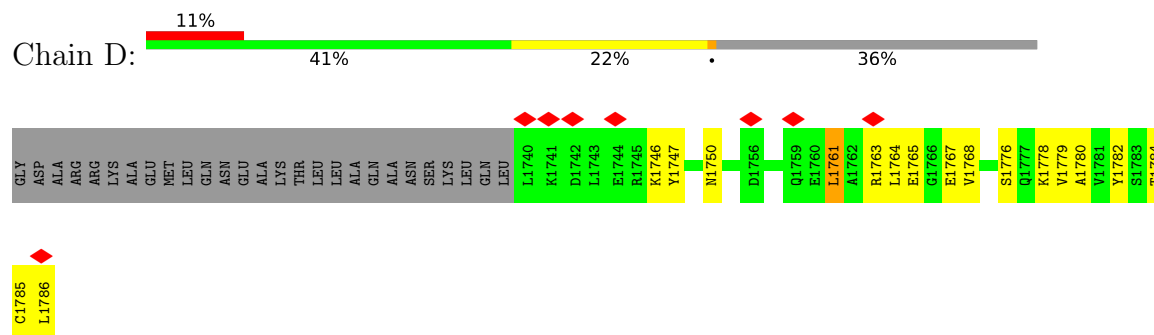




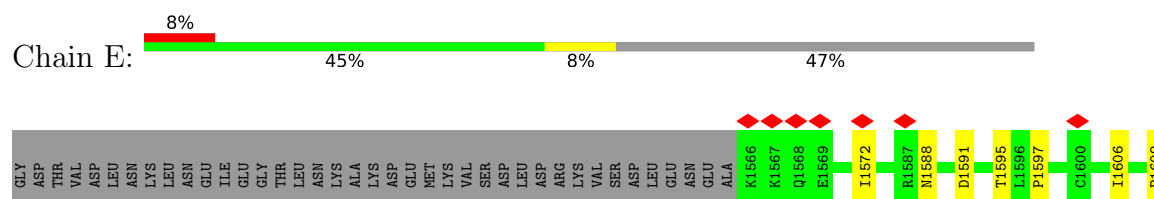
• Molecule 3: Laminin subunit alpha-5



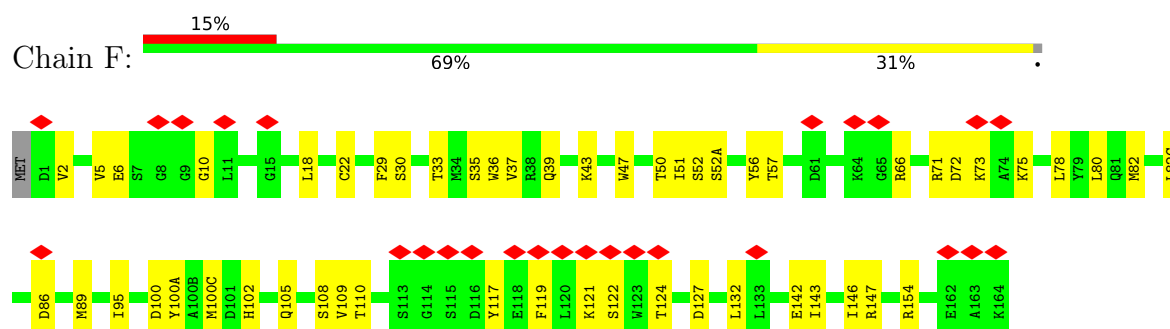
- Molecule 4: Laminin subunit beta-1



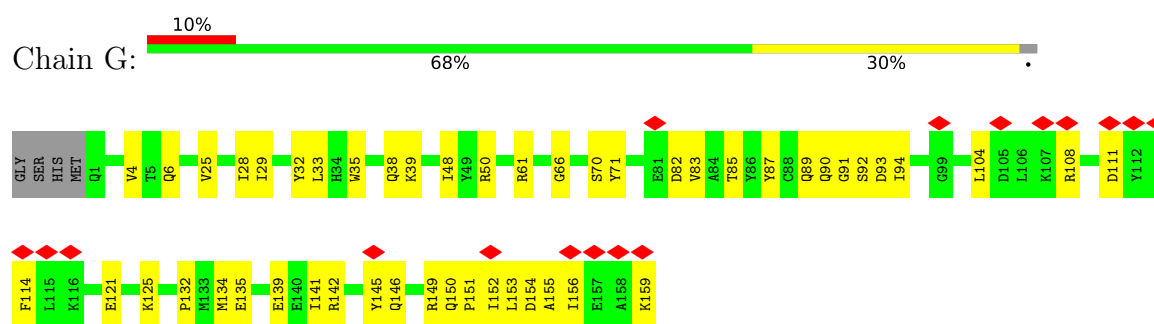
- Molecule 5: Laminin subunit gamma-1



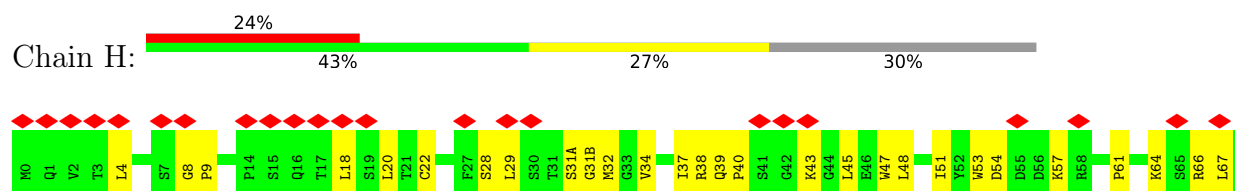
- Molecule 6: TS2/16 VH(S112C)-SARAH,TS2/16 VH(S112C)-SARAH

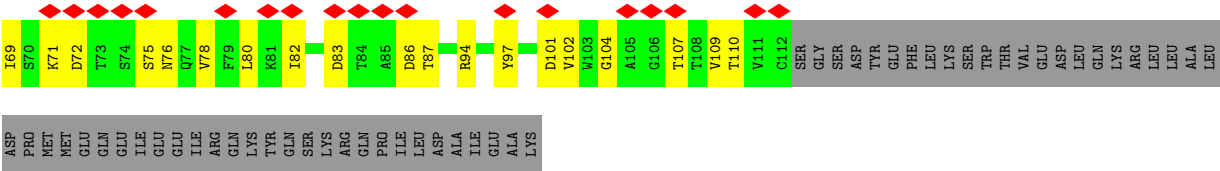


- Molecule 7: TS2/16 VL-SARAH(S37C),TS2/16 VL-SARAH(S37C)

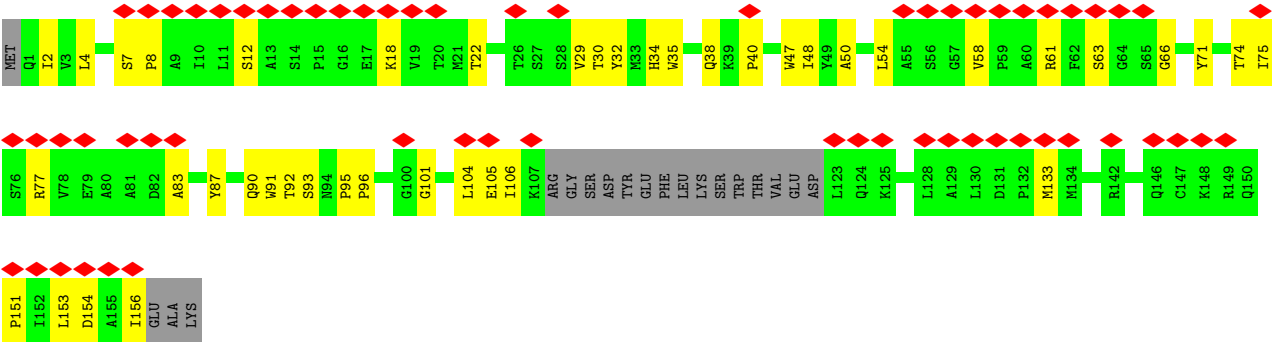


- Molecule 8: HUTS-4 VH(S112C)-SARAH,HUTS-4 VH(S112C)-SARAH





• Molecule 9: HUTS-4 VL(C87Y)-SARAH(S37C),HUTS-4 VL(C87Y)-SARAH(S37C)



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	429521	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	800	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	333.90002, 333.90002, 333.90002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.62	0/4400	0.69	2/5956 (0.0%)
2	B	0.56	0/3376	0.70	2/4557 (0.0%)
3	C	0.52	0/4517	0.65	0/6123
4	D	0.48	0/392	0.61	1/522 (0.2%)
5	E	0.44	0/361	0.60	0/481
6	F	0.58	0/1391	0.64	0/1875
7	G	0.57	0/1277	0.64	0/1727
8	H	0.43	0/979	0.65	0/1332
9	I	0.38	0/1104	0.58	1/1497 (0.1%)
All	All	0.55	0/17797	0.66	6/24070 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	CYS	CA-CB-SG	6.50	125.69	114.00
2	B	142	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	A	300	VAL	CG1-CB-CG2	-5.86	101.53	110.90
2	B	350	LEU	CA-CB-CG	5.60	128.18	115.30
9	I	38	GLN	C-N-CA	5.50	135.46	121.70
4	D	1761	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4308	0	4184	140	0
2	B	3320	0	3269	122	0
3	C	4421	0	4392	128	0
4	D	390	0	395	11	0
5	E	357	0	361	7	0
6	F	1360	0	1330	43	0
7	G	1252	0	1249	37	0
8	H	954	0	916	34	0
9	I	1080	0	1076	26	0
10	J	28	0	25	0	0
11	A	3	0	0	0	0
11	C	1	0	0	0	0
12	A	28	0	26	1	0
12	B	42	0	39	1	0
12	C	14	0	13	0	0
13	B	3	0	0	0	0
All	All	17561	0	17275	519	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 15.

All (519) 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:A:424:TYR:CE1	1:A:443:PRO:HB3	1.92	1.03
2:B:224:ASN:H	2:B:224:ASN:ND2	1.55	1.00
2:B:224:ASN:HD22	2:B:224:ASN:N	1.61	0.98
1:A:37:ARG:HD3	1:A:419:LEU:HA	1.59	0.84
2:B:137:ASP:N	2:B:137:ASP:OD1	2.13	0.80
3:C:2866:LEU:HD11	3:C:3203:TYR:HB3	1.64	0.80
1:A:418:ASP:HB2	1:A:424:TYR:O	1.82	0.80
2:B:224:ASN:H	2:B:224:ASN:HD22	0.83	0.78
2:B:227:SER:HB3	2:B:228:PRO:HD3	1.66	0.78
1:A:422:ASN:HD21	1:A:424:TYR:HB2	1.48	0.77
2:B:130:ASP:HB3	2:B:135:MET:HE1	1.66	0.76
6:F:51:ILE:HG13	6:F:57:THR:HG22	1.68	0.74
1:A:30:GLN:HG2	1:A:136:GLN:HB2	1.69	0.73
1:A:480:PHE:O	1:A:537:LYS:HA	1.89	0.72
2:B:210:GLU:OE1	2:B:210:GLU:N	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:146:ILE:HD11	7:G:141:ILE:HD12	1.71	0.71
2:B:426:ARG:HB3	2:B:433:GLU:HB3	1.72	0.71
6:F:6:GLU:H	6:F:105[B]:GLN:HE22	1.37	0.71
6:F:121:LYS:HD2	7:G:159:LYS:HE2	1.71	0.71
1:A:417:MET:HA	1:A:417:MET:HE2	1.72	0.71
2:B:360:SER:HG	2:B:399:SER:HG	1.40	0.69
3:C:2767[A]:GLN:NE2	3:C:2929:CYS:SG	2.66	0.69
3:C:2767[B]:GLN:NE2	3:C:2929:CYS:SG	2.66	0.69
3:C:2837:LEU:HD13	3:C:2865:GLY:O	1.93	0.68
1:A:364:ILE:HG22	1:A:425:PRO:HG2	1.75	0.68
2:B:68:ASP:HB2	2:B:100:VAL:HB	1.74	0.68
1:A:37:ARG:HB3	1:A:419:LEU:HD23	1.73	0.68
3:C:2810:LEU:HD22	3:C:2867:LEU:HA	1.74	0.67
3:C:2807:VAL:HG22	3:C:2817:VAL:HG13	1.75	0.67
9:I:61:ARG:HD2	9:I:77:ARG:HB2	1.77	0.66
3:C:2793:ASP:OD1	3:C:2793:ASP:N	2.29	0.65
3:C:3133:LEU:HB3	3:C:3246:LEU:HB2	1.78	0.65
1:A:110:HIS:NE2	2:B:269:LYS:O	2.29	0.65
2:B:156:ILE:HG22	2:B:157:THR:HG23	1.78	0.65
2:B:340:LEU:HD12	2:B:347:VAL:HG12	1.80	0.64
6:F:95:ILE:HG12	6:F:100(C):MET:HG2	1.79	0.64
1:A:111:ARG:NH1	2:B:173:MET:O	2.31	0.64
6:F:22:CYS:HB3	6:F:78:LEU:HB3	1.79	0.64
7:G:66:GLY:HA3	7:G:71:TYR:HA	1.80	0.63
1:A:189:ASN:ND2	5:E:1609:PRO:O	2.32	0.63
8:H:87:THR:HA	8:H:109:VAL:O	1.99	0.63
1:A:195:ARG:NH1	1:A:215:GLU:OE1	2.32	0.62
6:F:29:PHE:O	6:F:71:ARG:NH2	2.32	0.62
1:A:115:ARG:HE	1:A:125:ARG:HD3	1.64	0.62
8:H:38:ARG:HB3	8:H:48:LEU:HD11	1.82	0.62
7:G:61:ARG:NH1	7:G:82:ASP:OD1	2.31	0.62
7:G:153:LEU:HA	7:G:156:ILE:HD12	1.82	0.62
1:A:422:ASN:ND2	1:A:424:TYR:HB2	2.15	0.62
3:C:2751:ARG:HH12	3:C:3293:ALA:HA	1.65	0.61
3:C:2793:ASP:HB3	3:C:2867:LEU:HD12	1.82	0.61
3:C:2780:ARG:NH2	3:C:2895:GLY:O	2.31	0.61
1:A:448:GLN:HE21	1:A:481:GLU:HG3	1.65	0.61
1:A:424:TYR:CZ	1:A:443:PRO:HB3	2.34	0.61
2:B:226:ASP:OD1	2:B:226:ASP:N	2.21	0.61
3:C:3070:PRO:HA	3:C:3073:LEU:HD12	1.82	0.61
6:F:39:GLN:HE21	6:F:43:LYS:HG3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3019:PRO:O	3:C:3025:LYS:NZ	2.33	0.61
9:I:63:SER:HG	9:I:74:THR:HG1	1.47	0.61
1:A:285:ASP:OD1	1:A:285:ASP:N	2.31	0.61
1:A:545:TRP:O	1:A:547:GLN:NE2	2.34	0.61
2:B:26:GLY:HA3	2:B:62:ASN:HB2	1.83	0.61
1:A:2:ASN:ND2	1:A:442:ARG:O	2.26	0.61
1:A:211:ASP:N	1:A:214:TYR:HH	1.99	0.61
3:C:3143:LEU:HB3	3:C:3186:LEU:HD11	1.83	0.60
3:C:3134:ARG:HG2	3:C:3283:LEU:HD12	1.84	0.60
1:A:474:LEU:HB2	1:A:544:LEU:HB3	1.84	0.60
7:G:108:ARG:HB3	7:G:111:ASP:HB2	1.83	0.60
3:C:3061:ASP:OD1	3:C:3061:ASP:N	2.32	0.60
8:H:51:ILE:HD12	8:H:57:LYS:HE2	1.83	0.60
2:B:66:SER:H	2:B:102:ARG:HB2	1.67	0.59
8:H:39:GLN:NE2	8:H:43:LYS:O	2.35	0.59
1:A:424:TYR:CE2	1:A:443:PRO:HA	2.38	0.59
2:B:135:MET:HG2	2:B:138:ASP:HB2	1.84	0.59
2:B:141:ASN:ND2	2:B:341:SER:OG	2.36	0.59
2:B:143:LYS:HE2	2:B:217:GLY:HA2	1.84	0.59
3:C:3269:ARG:O	3:C:3274:GLN:NE2	2.36	0.59
1:A:417:MET:HE2	1:A:417:MET:CA	2.33	0.59
1:A:449:LYS:NZ	1:A:589:PRO:O	2.35	0.59
8:H:4:LEU:HB3	8:H:104:GLY:HA2	1.85	0.59
1:A:133:VAL:HB	1:A:146:GLY:H	1.68	0.59
1:A:499:LEU:O	1:A:524:LYS:HA	2.03	0.58
3:C:2841:HIS:NE2	3:C:2843:SER:OG	2.36	0.58
3:C:3001:LEU:HB3	3:C:3008:LEU:HD11	1.84	0.58
1:A:270:LYS:HB3	1:A:279:LEU:HB2	1.85	0.58
6:F:6:GLU:OE1	6:F:105[B]:GLN:NE2	2.36	0.58
1:A:442:ARG:NH2	1:A:581:LEU:O	2.33	0.58
2:B:362:VAL:HG12	2:B:398:ILE:HG21	1.86	0.58
3:C:3202:HIS:ND1	3:C:3218:ASP:OD2	2.36	0.58
2:B:206:THR:OG1	2:B:207:ASN:N	2.37	0.57
3:C:2965:ARG:NH2	3:C:2967:GLU:OE2	2.36	0.57
4:D:1750:ASN:HA	5:E:1572:ILE:HD11	1.86	0.57
1:A:149:TRP:O	1:A:167:GLN:NE2	2.37	0.57
1:A:268:LEU:HB2	1:A:281:GLU:HB2	1.85	0.57
3:C:2706:HIS:HB2	3:C:2709:SER:H	1.68	0.57
3:C:3160:ALA:O	3:C:3176:LEU:N	2.32	0.57
1:A:548:ASP:OD1	1:A:548:ASP:N	2.37	0.57
3:C:3134:ARG:HB3	3:C:3283:LEU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:6:GLN:HE22	7:G:87:TYR:HA	1.69	0.57
3:C:2973:VAL:O	3:C:3280:GLN:NE2	2.38	0.57
6:F:10:GLY:H	6:F:109:VAL:HA	1.70	0.57
2:B:227:SER:N	2:B:228:PRO:CD	2.68	0.57
3:C:3112:SER:OG	3:C:3113:ALA:N	2.38	0.57
1:A:514:VAL:HB	1:A:544:LEU:HD11	1.86	0.57
2:B:116:LYS:NZ	2:B:401:GLY:O	2.38	0.57
2:B:340:LEU:HD11	2:B:346:ASN:HB3	1.87	0.57
3:C:3018:PRO:HB2	3:C:3025:LYS:HZ3	1.70	0.57
3:C:3070:PRO:O	3:C:3078:ARG:NH2	2.38	0.57
1:A:274:LYS:O	3:C:3045:ARG:NH2	2.38	0.56
9:I:18:LYS:HA	9:I:75:ILE:O	2.05	0.56
9:I:151:PRO:HA	9:I:154:ASP:HB2	1.87	0.56
6:F:82:MET:HB3	6:F:82(C):LEU:HD21	1.87	0.56
1:A:143:ASP:OD1	1:A:143:ASP:N	2.38	0.56
3:C:2866:LEU:CD1	3:C:3203:TYR:HB3	2.34	0.56
1:A:191:LYS:NZ	1:A:229:VAL:O	2.38	0.56
1:A:53:ARG:HE	1:A:82:PRO:HG3	1.70	0.56
7:G:35:TRP:HB2	7:G:48:ILE:HB	1.88	0.56
1:A:111:ARG:NH1	2:B:271:GLY:O	2.39	0.55
1:A:111:ARG:HA	1:A:127:ILE:HD11	1.88	0.55
3:C:3254:THR:HG23	3:C:3255:ILE:HG13	1.87	0.55
6:F:30:SER:HA	6:F:73:LYS:HD2	1.88	0.55
8:H:57:LYS:NZ	8:H:69:ILE:O	2.38	0.55
2:B:398:ILE:HD12	2:B:402:ASP:HB2	1.89	0.55
1:A:334:GLN:NE2	1:A:337:ARG:O	2.40	0.55
2:B:102:ARG:HB3	2:B:441:ILE:HD11	1.89	0.55
2:B:317:VAL:H	2:B:339:THR:HA	1.72	0.55
2:B:341:SER:OG	2:B:342:ALA:N	2.39	0.55
6:F:10:GLY:O	6:F:110:THR:N	2.34	0.55
2:B:227:SER:HB2	5:E:1609:PRO:HA	1.89	0.55
1:A:45:ARG:NH2	2:B:272:GLY:O	2.40	0.54
1:A:407:PRO:O	1:A:431:SER:OG	2.25	0.54
1:A:472:ILE:HB	1:A:546:LEU:HD23	1.88	0.54
3:C:2746:GLN:NE2	3:C:2916:GLU:OE2	2.39	0.54
8:H:32:MET:SD	8:H:94:ARG:NH1	2.81	0.54
1:A:475:GLN:HE22	1:A:543:THR:HB	1.72	0.54
9:I:90:GLN:OE1	9:I:92:THR:N	2.40	0.54
2:B:27:TRP:HB3	2:B:61:GLU:HB2	1.88	0.54
3:C:2837:LEU:CD1	3:C:2866:LEU:HD23	2.37	0.54
3:C:2976:SER:OG	3:C:2977:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:PRO:HD2	8:H:109:VAL:HG22	1.89	0.54
1:A:25:LEU:HD12	1:A:39:LEU:HD11	1.89	0.54
2:B:226:ASP:HB2	2:B:228:PRO:HD2	1.88	0.54
8:H:22:CYS:HB3	8:H:78:VAL:HG23	1.89	0.54
2:B:174:PRO:HD2	2:B:175:TYR:CE2	2.42	0.54
3:C:3209:ASN:O	3:C:3227:HIS:NE2	2.40	0.54
1:A:440:ARG:HH22	1:A:578:PRO:HD2	1.71	0.54
2:B:427:PRO:HG2	2:B:430:PHE:HB2	1.90	0.54
6:F:33:THR:HG22	6:F:52:SER:HA	1.90	0.54
1:A:125:ARG:NH1	2:B:178:THR:OG1	2.40	0.54
2:B:419:ASP:OD1	2:B:419:ASP:N	2.41	0.54
1:A:135:SER:OG	1:A:137:ASN:O	2.26	0.53
1:A:454:THR:HG23	1:A:455:PRO:HD3	1.90	0.53
3:C:2961:SER:OG	3:C:2963:THR:O	2.25	0.53
2:B:73:LYS:N	2:B:97:GLN:OE1	2.41	0.53
2:B:360:SER:O	2:B:397:ASN:N	2.42	0.53
6:F:72:ASP:OD2	6:F:75:LYS:NZ	2.39	0.53
8:H:72:ASP:OD1	8:H:75:SER:N	2.40	0.53
6:F:100:ASP:N	6:F:100:ASP:OD1	2.40	0.53
8:H:31(B):GLY:HA2	8:H:97:TYR:HB3	1.90	0.53
3:C:2760:THR:HB	3:C:2835:ARG:HG3	1.90	0.53
3:C:2955:SER:HA	3:C:3062:ALA:HA	1.90	0.53
7:G:150:GLN:HA	7:G:153:LEU:HD12	1.90	0.53
8:H:66:ARG:NH2	8:H:86:ASP:OD2	2.42	0.53
8:H:94:ARG:H	8:H:102:VAL:HG23	1.74	0.53
1:A:25:LEU:HA	1:A:40:LEU:O	2.09	0.53
3:C:2937:ASP:OD1	3:C:2940:LEU:N	2.42	0.53
4:D:1746:LYS:O	4:D:1750:ASN:ND2	2.42	0.53
2:B:30:ASN:ND2	2:B:32:THR:OG1	2.42	0.53
2:B:47:LEU:HA	2:B:50:LEU:HD12	1.90	0.53
3:C:2767[A]:GLN:HB3	3:C:2828:PHE:HA	1.91	0.53
3:C:2838:GLN:NE2	3:C:2860:ALA:O	2.42	0.53
2:B:414:LYS:HD3	2:B:416:PRO:HG3	1.91	0.52
3:C:2887:PRO:HB2	3:C:2892:ARG:HG2	1.92	0.52
4:D:1779:VAL:HA	4:D:1782:TYR:HB2	1.91	0.52
4:D:1780:ALA:O	4:D:1784:THR:OG1	2.26	0.52
1:A:99:GLN:HB3	1:A:103:GLY:HA3	1.91	0.52
3:C:2767[B]:GLN:HB3	3:C:2828:PHE:HA	1.92	0.52
3:C:3116:THR:OG1	3:C:3118:ASP:OD1	2.28	0.52
1:A:492:SER:HA	1:A:531:LEU:O	2.09	0.52
2:B:108:PRO:O	2:B:109:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3180:ARG:NE	3:C:3192:THR:O	2.33	0.52
1:A:308:GLN:O	1:A:333:ASN:ND2	2.42	0.52
1:A:502:GLU:OE2	1:A:513:ARG:N	2.42	0.51
1:A:384:VAL:HB	1:A:402:LEU:HB2	1.91	0.51
8:H:61:PRO:HA	8:H:64:LYS:HB2	1.91	0.51
1:A:13:LYS:HB2	1:A:436:VAL:HB	1.93	0.51
7:G:4:VAL:HG22	7:G:25:VAL:HG13	1.93	0.51
1:A:79:ASP:O	1:A:87:LYS:NZ	2.40	0.51
8:H:101:ASP:OD1	8:H:101:ASP:N	2.43	0.51
2:B:154:ARG:HH12	2:B:158:SER:HA	1.76	0.51
5:E:1591:ASP:O	5:E:1595:THR:OG1	2.23	0.51
3:C:3035:SER:OG	3:C:3036:ARG:N	2.44	0.51
1:A:137:ASN:OD1	1:A:137:ASN:N	2.44	0.51
1:A:275:SER:OG	1:A:276:ALA:N	2.44	0.51
2:B:224:ASN:ND2	2:B:224:ASN:N	2.29	0.50
3:C:3162:LEU:HD22	3:C:3262:ILE:HD11	1.93	0.50
8:H:72:ASP:O	8:H:76:ASN:N	2.44	0.50
2:B:227:SER:CB	2:B:228:PRO:HD3	2.39	0.50
1:A:460:LEU:HG	1:A:598:PHE:HE2	1.76	0.50
3:C:2954:ILE:HD11	3:C:3103:LEU:HD21	1.92	0.50
6:F:117:TYR:HB2	7:G:151:PRO:HB2	1.94	0.50
2:B:5:ASN:OD1	2:B:9:LYS:N	2.38	0.50
3:C:3133:LEU:HD23	3:C:3246:LEU:HD12	1.92	0.50
6:F:100:ASP:OD2	7:G:50:ARG:NE	2.45	0.50
9:I:153:LEU:HA	9:I:156:ILE:HG12	1.92	0.50
3:C:2931:ARG:O	3:C:2933:LYS:NZ	2.38	0.50
3:C:3160:ALA:H	3:C:3176:LEU:HB2	1.76	0.50
6:F:56:TYR:CD2	6:F:56:TYR:C	2.86	0.50
2:B:350:LEU:O	2:B:354:ALA:HB2	2.12	0.49
3:C:3036:ARG:NH2	3:C:3054:ASP:OD1	2.45	0.49
1:A:417:MET:HA	1:A:417:MET:CE	2.30	0.49
3:C:3177:GLN:OE1	3:C:3191:LYS:NZ	2.32	0.49
9:I:66:GLY:HA3	9:I:71:TYR:HA	1.93	0.49
9:I:40:PRO:HB2	9:I:133:MET:HG2	1.94	0.49
7:G:38:GLN:HB3	7:G:85:THR:HG23	1.95	0.49
8:H:87:THR:HG23	8:H:110:THR:HA	1.95	0.49
1:A:267:VAL:HG22	1:A:283:ILE:HG23	1.93	0.49
2:B:120:ASP:HB3	2:B:157:THR:HG22	1.94	0.49
2:B:164:PHE:HB2	2:B:212:PHE:HE1	1.78	0.49
8:H:83:ASP:OD1	8:H:83:ASP:N	2.44	0.49
1:A:345:ARG:HH11	1:A:347:ASN:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:SER:N	2:B:228:PRO:HD2	2.27	0.49
9:I:2:ILE:HD11	9:I:93:SER:HB2	1.94	0.49
3:C:3125:MET:O	3:C:3261:CYS:HA	2.12	0.49
4:D:1776:SER:HA	4:D:1779:VAL:HG22	1.94	0.49
7:G:142:ARG:O	7:G:149:ARG:NH2	2.46	0.49
1:A:250:GLU:OE2	1:A:271:ARG:NE	2.46	0.49
4:D:1763:ARG:NH1	4:D:1767:GLU:OE2	2.46	0.49
9:I:29:VAL:O	9:I:71:TYR:OH	2.30	0.49
2:B:27:TRP:HH2	2:B:41:SER:HA	1.78	0.48
3:C:3030:PHE:HD2	3:C:3032:LEU:HD21	1.78	0.48
8:H:40:PRO:HD2	8:H:43:LYS:HD3	1.96	0.48
2:B:194:THR:HG23	2:B:222:SER:HB2	1.95	0.48
9:I:34:HIS:CE1	9:I:50:ALA:H	2.30	0.48
1:A:172:THR:OG1	1:A:173:PHE:N	2.47	0.48
2:B:248:ARG:O	2:B:252:ARG:NH2	2.46	0.48
7:G:111:ASP:HB3	7:G:114:PHE:HB2	1.94	0.48
1:A:364:ILE:CG2	1:A:425:PRO:HG2	2.44	0.48
2:B:128:LEU:HD21	2:B:234:ALA:HB1	1.96	0.48
3:C:2820:ILE:HD12	3:C:2854:THR:HG22	1.94	0.48
6:F:124:THR:HG23	6:F:127:ASP:H	1.77	0.48
9:I:30:THR:OG1	9:I:32:TYR:N	2.47	0.48
1:A:533:ARG:HD2	1:A:536:GLN:HE22	1.79	0.48
3:C:2809:GLN:HB2	3:C:2815:PRO:HB3	1.96	0.48
9:I:7:SER:N	9:I:22:THR:O	2.46	0.48
2:B:71:LYS:HD3	2:B:73:LYS:HE3	1.95	0.47
3:C:2867:LEU:HG	3:C:2869:LEU:HG	1.95	0.47
8:H:20:LEU:HD12	8:H:80:LEU:HD23	1.95	0.47
9:I:61:ARG:NH1	9:I:77:ARG:O	2.47	0.47
2:B:106:GLY:N	2:B:412:SER:O	2.36	0.47
6:F:2:VAL:HG11	6:F:102:HIS:CG	2.49	0.47
3:C:2820:ILE:HG21	3:C:2844:VAL:HB	1.96	0.47
3:C:3147:VAL:HB	3:C:3208:SER:HB3	1.96	0.47
1:A:486:PRO:HD2	1:A:489:TYR:HB3	1.95	0.47
3:C:3152:GLY:HA2	3:C:3203:TYR:HA	1.97	0.47
3:C:3163:TYR:HB3	3:C:3174:VAL:HB	1.95	0.47
1:A:3:LEU:O	1:A:400:GLN:NE2	2.47	0.47
1:A:186:GLY:HA2	1:A:190:TRP:CD1	2.49	0.47
1:A:422:ASN:HD22	1:A:443:PRO:HG3	1.79	0.47
2:B:100:VAL:HG22	2:B:437:ILE:HD12	1.95	0.47
3:C:2760:THR:O	3:C:2834:ASP:HA	2.14	0.47
1:A:125:ARG:HH21	2:B:180:PRO:HD3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:GLU:HA	2:B:396:SER:HA	1.96	0.47
3:C:2868:ASN:N	3:C:2868:ASN:ND2	2.60	0.47
3:C:2970:LEU:HD21	3:C:2979:LEU:HD22	1.96	0.47
6:F:119:PHE:O	6:F:122:SER:OG	2.33	0.47
7:G:89:GLN:NE2	7:G:90:GLN:O	2.47	0.47
2:B:23:PRO:O	2:B:64:ARG:NH2	2.46	0.47
2:B:215:LEU:O	2:B:219:GLN:NE2	2.40	0.47
3:C:3139:ASN:OD1	3:C:3271:LEU:N	2.48	0.47
7:G:135:GLU:O	7:G:139:GLU:HB2	2.15	0.47
2:B:381:CYS:HB3	2:B:404:VAL:HG12	1.96	0.47
3:C:3042:ARG:HG2	3:C:3047:THR:HA	1.96	0.47
7:G:146:GLN:HA	7:G:149:ARG:HE	1.80	0.47
1:A:109:ALA:O	1:A:129:GLY:HA2	2.14	0.47
1:A:318:PHE:HD2	2:B:331:LEU:HD13	1.80	0.47
2:B:40:THR:OG1	2:B:43:ARG:NE	2.46	0.47
3:C:3278:ASP:OD2	3:C:3281:GLN:N	2.48	0.47
2:B:367:GLY:N	2:B:424:LYS:O	2.47	0.46
3:C:2796:GLY:HA3	3:C:2891:LEU:HD11	1.97	0.46
6:F:37:VAL:HG22	6:F:47:TRP:HA	1.95	0.46
9:I:83:ALA:HA	9:I:104:LEU:HB3	1.97	0.46
1:A:60:LEU:HB3	1:A:74:ILE:HD12	1.97	0.46
1:A:424:TYR:CZ	1:A:443:PRO:HA	2.51	0.46
1:A:494:SER:OG	1:A:566:GLN:NE2	2.48	0.46
3:C:3203:TYR:HE2	3:C:3264:ASN:HB3	1.80	0.46
3:C:2881:TYR:OH	3:C:2893:PHE:O	2.28	0.46
1:A:108:CYS:HA	1:A:131:CYS:HA	1.98	0.46
1:A:46:ALA:H	1:A:58:GLY:HA2	1.81	0.46
1:A:487:ALA:O	1:A:490:ASN:ND2	2.47	0.46
2:B:49:ALA:HB1	2:B:53:LYS:HE3	1.98	0.46
1:A:314:ALA:O	1:A:326:GLY:HA2	2.15	0.46
1:A:324:VAL:HG23	1:A:348:GLY:H	1.81	0.46
3:C:3074:PRO:HG2	3:C:3077:LEU:HB2	1.97	0.46
6:F:36:TRP:CG	6:F:80:LEU:HD22	2.50	0.46
8:H:39:GLN:HB2	8:H:45:LEU:HG	1.98	0.46
8:H:18:LEU:HD22	8:H:82:ILE:HD12	1.96	0.46
3:C:2761:ALA:HB3	3:C:2906:ASN:HA	1.98	0.46
3:C:2763:LYS:HG2	3:C:2832:SER:HA	1.98	0.46
3:C:2962:THR:O	3:C:3033:GLY:N	2.37	0.46
3:C:2738:LYS:HE3	3:C:2738:LYS:HB2	1.76	0.46
1:A:307:TRP:CD2	1:A:335:GLN:HA	2.51	0.45
2:B:135:MET:CG	2:B:138:ASP:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:SER:HB3	2:B:398:ILE:N	2.30	0.45
3:C:2753:LEU:HA	3:C:2753:LEU:HD23	1.83	0.45
7:G:83:VAL:HA	7:G:104:LEU:O	2.15	0.45
2:B:66:SER:O	2:B:102:ARG:N	2.49	0.45
2:B:98:GLN:HE21	2:B:437:ILE:HD11	1.81	0.45
2:B:411:THR:O	2:B:413:ASN:ND2	2.48	0.45
1:A:187:THR:HG21	1:A:193:ILE:HD13	1.98	0.45
2:B:187:CYS:HB2	2:B:193:CYS:HB2	1.76	0.45
3:C:2807:VAL:HG13	3:C:2817:VAL:HG22	1.99	0.45
12:B:1004:NAG:H82	7:G:28:ILE:HD11	1.99	0.45
6:F:66:ARG:NH2	6:F:86:ASP:OD2	2.50	0.45
7:G:70:SER:O	7:G:70:SER:OG	2.31	0.45
4:D:1765:GLU:HA	4:D:1768:VAL:HG22	1.99	0.45
9:I:106:ILE:HD13	9:I:106:ILE:HA	1.76	0.45
1:A:268:LEU:HD12	1:A:282:HIS:HB3	1.98	0.45
1:A:317:TYR:H	1:A:326:GLY:HA2	1.82	0.45
2:B:359:SER:OG	2:B:360:SER:N	2.49	0.45
4:D:1761:LEU:HA	4:D:1764:LEU:HB2	1.98	0.45
1:A:303:ASN:OD1	1:A:303:ASN:N	2.44	0.45
1:A:364:ILE:HA	1:A:425:PRO:HD2	1.97	0.45
2:B:374:THR:O	2:B:410:ILE:HA	2.17	0.45
2:B:210:GLU:HB3	6:F:56:TYR:CD1	2.51	0.44
3:C:2955:SER:OG	3:C:3061:ASP:O	2.28	0.44
6:F:56:TYR:CD2	6:F:56:TYR:O	2.70	0.44
8:H:34:VAL:HG11	8:H:78:VAL:HG11	1.99	0.44
2:B:228:PRO:HB2	2:B:263:HIS:NE2	2.32	0.44
6:F:5:VAL:HA	6:F:105[A]:GLN:HE22	1.82	0.44
1:A:228:PRO:HB2	1:A:229:VAL:H	1.60	0.44
1:A:346:LEU:H	1:A:346:LEU:HG	1.59	0.44
9:I:12:SER:HA	9:I:105:GLU:HB2	1.99	0.44
9:I:54:LEU:HB3	9:I:58:VAL:HB	2.00	0.44
1:A:345:ARG:NH1	12:A:1005:NAG:H83	2.32	0.44
1:A:364:ILE:HA	1:A:425:PRO:HG2	1.98	0.44
2:B:72:ASN:O	2:B:95:GLN:NE2	2.51	0.44
3:C:2747:LEU:HD23	3:C:2915:PHE:HB3	1.99	0.44
3:C:2866:LEU:HB2	3:C:2868:ASN:HD21	1.82	0.44
3:C:3036:ARG:NH1	3:C:3052:GLU:O	2.51	0.44
7:G:155:ALA:O	7:G:159:LYS:N	2.39	0.44
2:B:208:LYS:HD2	6:F:100(A):TYR:CE2	2.53	0.44
7:G:150:GLN:NE2	7:G:154:ASP:OD1	2.45	0.44
1:A:29:TRP:HB3	1:A:101:PRO:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:HG3	4:D:1786:LEU:HD21	2.00	0.44
2:B:75:VAL:HG23	2:B:92:THR:HG22	2.00	0.44
2:B:334:LYS:HD2	2:B:334:LYS:HA	1.72	0.44
6:F:143:ILE:O	6:F:147:ARG:HG3	2.18	0.44
7:G:39:LYS:HD3	7:G:39:LYS:HA	1.79	0.44
8:H:8:GLY:H	8:H:107:THR:HB	1.83	0.44
1:A:403:LYS:HE2	1:A:403:LYS:HB2	1.83	0.44
1:A:474:LEU:HD12	1:A:544:LEU:HD23	2.00	0.44
1:A:558:PRO:HA	1:A:594:ILE:O	2.17	0.44
1:A:559:ILE:O	1:A:593:HIS:HA	2.17	0.44
3:C:3263:SER:OG	3:C:3264:ASN:N	2.50	0.44
1:A:29:TRP:HE1	1:A:31:LEU:HD13	1.82	0.44
1:A:137:ASN:HB2	1:A:139:ARG:HH11	1.82	0.44
1:A:361:ILE:HD13	1:A:373:ALA:HB2	2.00	0.44
2:B:18:CYS:HA	2:B:21:ALA:HB3	1.99	0.44
2:B:94:ILE:HD11	2:B:113:LEU:HD11	2.00	0.44
3:C:2793:ASP:CB	3:C:2867:LEU:HD12	2.48	0.44
3:C:2852:GLN:NE2	3:C:2854:THR:OG1	2.37	0.44
2:B:130:ASP:CB	2:B:135:MET:HE1	2.41	0.43
3:C:3071:ASP:OD1	3:C:3071:ASP:N	2.50	0.43
2:B:94:ILE:HB	2:B:115:PHE:HD1	1.83	0.43
2:B:151:ASN:OD1	2:B:152:GLU:N	2.50	0.43
3:C:2841:HIS:CE1	3:C:2855:LYS:HD3	2.53	0.43
1:A:113:GLU:HA	1:A:127:ILE:HA	2.01	0.43
2:B:6:ARG:O	2:B:10:ALA:N	2.51	0.43
2:B:170:LYS:HD3	2:B:296:TYR:CZ	2.53	0.43
2:B:295:ASP:OD1	2:B:296:TYR:N	2.52	0.43
2:B:389:GLY:O	2:B:393:ARG:N	2.52	0.43
2:B:428:LEU:HD23	2:B:428:LEU:HA	1.83	0.43
3:C:3269:ARG:N	3:C:3274:GLN:OE1	2.49	0.43
1:A:61:TYR:HE1	1:A:73:ARG:HG2	1.84	0.43
3:C:2747:LEU:HD21	3:C:2912:LEU:HA	2.00	0.43
3:C:2806:TRP:CG	3:C:2833:LEU:HD13	2.54	0.43
1:A:74:ILE:HD13	1:A:138:LEU:HD13	2.00	0.43
2:B:278:ASP:OD1	2:B:278:ASP:N	2.51	0.43
3:C:2974:SER:OG	3:C:2975:TYR:N	2.51	0.43
3:C:3143:LEU:HA	3:C:3143:LEU:HD23	1.83	0.43
1:A:478:SER:O	1:A:539:CYS:HA	2.18	0.43
2:B:242:GLY:HA2	2:B:247:TRP:HD1	1.83	0.43
9:I:35:TRP:HB2	9:I:48:ILE:HB	2.01	0.43
1:A:153:ASP:O	3:C:3100:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:OG1	1:A:173:PHE:O	2.37	0.43
2:B:130:ASP:HB2	2:B:167:PHE:CZ	2.53	0.43
3:C:2912:LEU:HA	3:C:2912:LEU:HD23	1.88	0.43
3:C:3026:ALA:N	3:C:3044:GLU:OE2	2.52	0.43
3:C:3103:LEU:HA	3:C:3103:LEU:HD23	1.80	0.43
3:C:3104:LYS:HE3	3:C:3104:LYS:HB2	1.82	0.43
8:H:37:ILE:HA	8:H:47:TRP:HA	1.99	0.43
1:A:384:VAL:HG21	1:A:429:VAL:HG11	2.01	0.43
2:B:215:LEU:HD12	2:B:215:LEU:HA	1.81	0.43
7:G:90:GLN:OE1	7:G:92:SER:N	2.51	0.43
8:H:38:ARG:HG2	8:H:48:LEU:HD21	2.00	0.43
9:I:90:GLN:NE2	9:I:95:PRO:O	2.52	0.43
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.85	0.43
2:B:380:TYR:HB2	2:B:405:GLN:HB3	2.00	0.43
6:F:89:MET:HA	6:F:108:SER:HA	2.00	0.43
3:C:2868:ASN:N	3:C:2868:ASN:HD22	2.17	0.42
7:G:121:GLU:HG2	7:G:125:LYS:HZ2	1.84	0.42
1:A:348:GLY:HA3	1:A:354:PHE:CG	2.54	0.42
2:B:28:CYS:HA	2:B:61:GLU:HG3	2.02	0.42
2:B:369:LEU:O	9:I:32:TYR:OH	2.28	0.42
3:C:2915:PHE:O	5:E:1588:ASN:ND2	2.41	0.42
1:A:95:THR:OG1	1:A:96:VAL:N	2.52	0.42
1:A:99:GLN:NE2	1:A:177:PHE:HA	2.34	0.42
2:B:113:LEU:HD12	2:B:113:LEU:HA	1.82	0.42
3:C:2972:LEU:HD12	3:C:2972:LEU:HA	1.87	0.42
7:G:33:LEU:HD12	7:G:90:GLN:HA	2.00	0.42
9:I:91:TRP:CG	9:I:96:PRO:HB3	2.53	0.42
1:A:450:THR:OG1	1:A:479:CYS:N	2.46	0.42
3:C:2706:HIS:HD2	3:C:2709:SER:HB3	1.84	0.42
7:G:94:ILE:HD13	7:G:94:ILE:HA	1.84	0.42
1:A:29:TRP:HE3	1:A:417:MET:HE1	1.85	0.42
1:A:315:PRO:HG3	1:A:356:ILE:HG13	2.01	0.42
1:A:361:ILE:HD12	1:A:364:ILE:HD13	2.02	0.42
1:A:418:ASP:HB2	1:A:424:TYR:C	2.38	0.42
2:B:6:ARG:HA	2:B:9:LYS:HB2	2.01	0.42
3:C:2747:LEU:HB2	3:C:2876:PHE:HD2	1.84	0.42
3:C:2803:LYS:HD3	3:C:2821:ASP:HA	2.00	0.42
8:H:67:LEU:HD23	8:H:82:ILE:HG12	2.01	0.42
3:C:2889:PRO:HA	3:C:2892:ARG:HG3	1.99	0.42
6:F:36:TRP:NE1	6:F:80:LEU:HB2	2.35	0.42
6:F:18:LEU:HD23	6:F:18:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.82	0.42
1:A:390:SER:N	1:A:393:GLY:O	2.53	0.42
2:B:367:GLY:HA3	2:B:423:PHE:HB2	2.01	0.42
3:C:2756:LEU:HA	3:C:2756:LEU:HD23	1.80	0.42
3:C:3139:ASN:HD21	3:C:3271:LEU:HB3	1.84	0.42
3:C:3155:SER:OG	3:C:3260:GLY:HA3	2.19	0.42
8:H:32:MET:HB3	8:H:94:ARG:HD3	2.00	0.42
1:A:477:LYS:HG3	1:A:541:GLU:HB2	2.02	0.42
3:C:2841:HIS:HE1	3:C:2855:LYS:HB3	1.85	0.42
4:D:1778:LYS:NZ	5:E:1597:PRO:O	2.41	0.42
9:I:4:LEU:HD21	9:I:90:GLN:HG2	2.01	0.42
3:C:2936:GLY:HA3	3:C:2940:LEU:HD23	2.02	0.42
3:C:3069:PRO:HG2	3:C:3072:GLN:HB2	2.02	0.42
3:C:3245:LEU:HD13	3:C:3245:LEU:HA	1.89	0.42
6:F:35:SER:OG	6:F:36:TRP:N	2.53	0.42
7:G:132:PRO:HA	7:G:135:GLU:HG2	2.02	0.42
8:H:38:ARG:HG3	8:H:40:PRO:HD3	2.02	0.42
9:I:87:TYR:HA	9:I:101:GLY:HA2	2.02	0.42
1:A:309:ASP:OD1	1:A:333:ASN:N	2.46	0.41
2:B:210:GLU:HB3	6:F:56:TYR:CE1	2.55	0.41
3:C:3176:LEU:HD23	3:C:3176:LEU:HA	1.77	0.41
2:B:332:ILE:HA	2:B:333:PRO:HD3	1.93	0.41
6:F:154:ARG:NH1	7:G:134:MET:SD	2.78	0.41
1:A:18:GLY:N	1:A:434:ASP:OD2	2.49	0.41
1:A:134:LEU:HD13	1:A:138:LEU:HB3	2.02	0.41
2:B:228:PRO:HA	2:B:261:GLY:C	2.41	0.41
6:F:6:GLU:OE1	6:F:6:GLU:N	2.53	0.41
6:F:132:LEU:HB2	7:G:152:ILE:HG21	2.02	0.41
7:G:121:GLU:HG2	7:G:125:LYS:NZ	2.35	0.41
1:A:63:CYS:HB3	1:A:71:CYS:HB3	1.47	0.41
1:A:175:LYS:HD3	1:A:175:LYS:HA	1.89	0.41
1:A:346:LEU:HD22	1:A:387:TYR:HE2	1.85	0.41
7:G:32:TYR:O	7:G:91:GLY:N	2.53	0.41
1:A:2:ASN:OD1	1:A:2:ASN:N	2.29	0.41
1:A:26:ALA:HA	1:A:414:ALA:HB1	2.03	0.41
1:A:61:TYR:CE1	1:A:73:ARG:HG2	2.56	0.41
1:A:424:TYR:CE1	1:A:443:PRO:CB	2.84	0.41
3:C:2756:LEU:O	3:C:2867:LEU:HB3	2.21	0.41
3:C:2837:LEU:O	3:C:2865:GLY:HA2	2.21	0.41
4:D:1747:TYR:HA	4:D:1750:ASN:HD22	1.86	0.41
8:H:29:LEU:HD13	8:H:71:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:SER:HB3	2:B:398:ILE:H	1.85	0.41
6:F:52(A):SER:HA	6:F:71:ARG:NH1	2.36	0.41
2:B:153:MET:HA	2:B:156:ILE:HD12	2.01	0.41
3:C:2756:LEU:O	3:C:2867:LEU:HD23	2.21	0.41
3:C:2783:MET:HG3	3:C:2797:VAL:HB	2.01	0.41
3:C:2837:LEU:HD13	3:C:2866:LEU:HD23	2.01	0.41
1:A:394:ILE:HD12	1:A:394:ILE:HA	1.84	0.41
2:B:208:LYS:NZ	6:F:100(A):TYR:CD2	2.87	0.41
2:B:418:LYS:HA	2:B:418:LYS:HD2	1.87	0.41
3:C:2837:LEU:CD1	3:C:2865:GLY:O	2.67	0.41
1:A:292:SER:O	1:A:292:SER:OG	2.34	0.41
1:A:402:LEU:HD13	1:A:439:PHE:CE2	2.56	0.41
2:B:113:LEU:HB3	2:B:406:PHE:HB2	2.02	0.41
2:B:227:SER:CB	5:E:1609:PRO:HA	2.49	0.41
2:B:292:HIS:CE1	2:B:293:TYR:HB2	2.55	0.41
3:C:2878:VAL:HG11	3:C:2912:LEU:HD21	2.03	0.41
3:C:2983:LYS:HE3	3:C:2983:LYS:HB2	1.73	0.41
3:C:2987:GLN:HB3	3:C:3004:PHE:HA	2.02	0.41
3:C:3069:PRO:HA	3:C:3070:PRO:HD3	1.84	0.41
3:C:3189:GLU:O	3:C:3225:LYS:NZ	2.35	0.41
6:F:142:GLU:OE2	7:G:145:TYR:OH	2.28	0.41
8:H:28:SER:HA	8:H:76:ASN:HD21	1.86	0.41
2:B:75:VAL:HA	2:B:92:THR:HB	2.03	0.41
2:B:379:SER:O	2:B:386:ASN:HA	2.21	0.41
7:G:146:GLN:HA	7:G:149:ARG:HB2	2.02	0.41
1:A:97:GLN:HG3	1:A:172:THR:HA	2.04	0.40
1:A:128:PHE:O	1:A:167:GLN:N	2.41	0.40
2:B:100:VAL:HA	2:B:437:ILE:HB	2.04	0.40
8:H:31(A):SER:HA	8:H:53:TRP:CG	2.56	0.40
2:B:161:ARG:HH12	7:G:29:ILE:HA	1.86	0.40
2:B:227:SER:CB	2:B:228:PRO:CD	2.99	0.40
2:B:242:GLY:HA2	2:B:247:TRP:CD1	2.56	0.40
3:C:3127:PHE:N	3:C:3260:GLY:O	2.54	0.40
6:F:80:LEU:HD12	6:F:80:LEU:HA	1.82	0.40
9:I:7:SER:HA	9:I:8:PRO:HA	1.97	0.40
1:A:52:GLN:NE2	1:A:77:ASP:O	2.47	0.40
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.86	0.40
1:A:419:LEU:H	1:A:419:LEU:HG	1.60	0.40
1:A:452:THR:OG1	1:A:477:LYS:O	2.37	0.40
2:B:27:TRP:CZ2	2:B:43:ARG:HD2	2.57	0.40
3:C:2727:ARG:O	3:C:2914:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3163:TYR:HA	3:C:3246:LEU:HD23	2.03	0.40
3:C:3181:VAL:N	3:C:3192:THR:OG1	2.46	0.40
6:F:142:GLU:O	6:F:146:ILE:HG13	2.21	0.40
9:I:47:TRP:HA	9:I:58:VAL:HG21	2.02	0.40
1:A:383:LYS:HA	1:A:402:LEU:O	2.21	0.40
2:B:24:ASN:N	2:B:24:ASN:OD1	2.48	0.40
2:B:128:LEU:HD12	2:B:128:LEU:HA	1.92	0.40
2:B:350:LEU:O	2:B:354:ALA:CB	2.70	0.40
3:C:2723:CYS:HB3	3:C:2727:ARG:HH12	1.86	0.40
7:G:92:SER:OG	7:G:93:ASP:OD1	2.36	0.40
8:H:31(B):GLY:O	8:H:97:TYR:N	2.45	0.40
8:H:54:ASP:OD1	8:H:54:ASP:N	2.49	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	539/627 (86%)	481 (89%)	58 (11%)	0	100	100
2	B	421/454 (93%)	372 (88%)	49 (12%)	0	100	100
3	C	569/674 (84%)	525 (92%)	44 (8%)	0	100	100
4	D	45/74 (61%)	44 (98%)	1 (2%)	0	100	100
5	E	42/83 (51%)	39 (93%)	2 (5%)	1 (2%)	5	30
6	F	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
7	G	158/164 (96%)	148 (94%)	10 (6%)	0	100	100
8	H	120/174 (69%)	108 (90%)	12 (10%)	0	100	100
9	I	136/159 (86%)	126 (93%)	10 (7%)	0	100	100
All	All	2200/2581 (85%)	2008 (91%)	191 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	1606	ILE

### 5.3.2 Protein sidechains ⓘ

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	467/535 (87%)	462 (99%)	5 (1%)	70	79
2	B	380/402 (94%)	373 (98%)	7 (2%)	54	71
3	C	473/550 (86%)	471 (100%)	2 (0%)	89	91
4	D	43/64 (67%)	42 (98%)	1 (2%)	45	64
5	E	41/76 (54%)	41 (100%)	0	100	100
6	F	149/149 (100%)	148 (99%)	1 (1%)	81	86
7	G	141/144 (98%)	141 (100%)	0	100	100
8	H	107/155 (69%)	107 (100%)	0	100	100
9	I	119/136 (88%)	119 (100%)	0	100	100
All	All	1920/2211 (87%)	1904 (99%)	16 (1%)	77	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	CYS
1	A	418	ASP
1	A	419	LEU
1	A	420	ASP
1	A	454	THR
2	B	137	ASP
2	B	139	LEU
2	B	175	TYR
2	B	224	ASN
2	B	226	ASP
2	B	259	ASP
2	B	395	CYS

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Mol	Chain	Res	Type
3	C	2793	ASP
3	C	3257	ASN
4	D	1785	CYS
6	F	50	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	HIS
1	A	308	GLN
1	A	388	HIS
1	A	448	GLN
1	A	475	GLN
1	A	485	ASN
1	A	547	GLN
1	A	566	GLN
2	B	30	ASN
2	B	77	ASN
2	B	109	GLN
2	B	141	ASN
2	B	292	HIS
2	B	309	ASN
2	B	310	ASN
2	B	413	ASN
3	C	2706	HIS
3	C	2725	GLN
3	C	2805	HIS
3	C	2852	GLN
3	C	2868	ASN
3	C	2984	GLN
3	C	2994	GLN
3	C	3220	GLN
5	E	1602	ASN
6	F	39	GLN
6	F	76	ASN
7	G	6	GLN
7	G	38	GLN
8	H	76	ASN

### 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 ⓘ

2 monosaccharides 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	$\# Z  > 2$
10	NAG	J	1	10,3	14,14,15	0.57	0	17,19,21	0.54	0
10	NAG	J	2	10	14,14,15	0.51	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	J	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

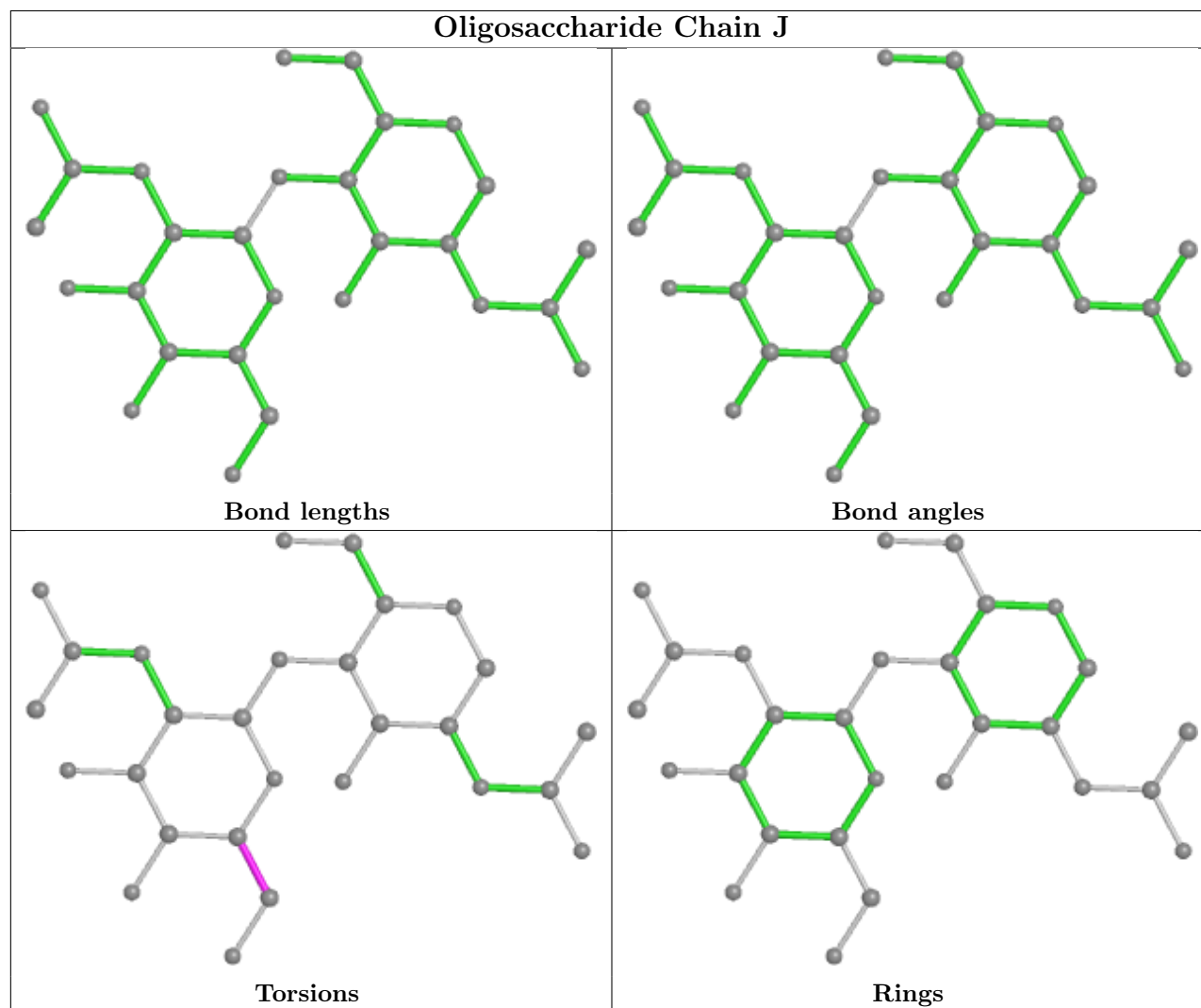
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	2	NAG	O5-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

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
12	NAG	C	3402	3	14,14,15	0.43	0	17,19,21	0.99	1 (5%)
12	NAG	A	1004	1	14,14,15	0.31	0	17,19,21	0.73	1 (5%)
12	NAG	A	1005	1	14,14,15	0.72	0	17,19,21	0.84	1 (5%)
12	NAG	B	1006	2	14,14,15	0.38	0	17,19,21	0.45	0
12	NAG	B	1004	2	14,14,15	0.23	0	17,19,21	0.45	0
12	NAG	B	1005	2	14,14,15	0.74	1 (7%)	17,19,21	2.36	4 (23%)

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
12	NAG	C	3402	3	-	2/6/23/26	0/1/1/1
12	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
12	NAG	A	1005	1	-	3/6/23/26	0/1/1/1
12	NAG	B	1006	2	-	1/6/23/26	0/1/1/1
12	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
12	NAG	B	1005	2	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1005	NAG	C1-C2	2.27	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1005	NAG	C2-N2-C7	7.75	133.93	122.90
12	B	1005	NAG	C1-C2-N2	3.76	116.90	110.49
12	B	1005	NAG	C1-O5-C5	3.43	116.84	112.19
12	C	3402	NAG	C1-O5-C5	3.26	116.61	112.19
12	A	1004	NAG	C1-O5-C5	2.56	115.66	112.19
12	A	1005	NAG	C2-N2-C7	2.50	126.46	122.90
12	B	1005	NAG	C8-C7-N2	2.10	119.65	116.10

There are no chirality outliers.

All (13) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
12	A	1004	NAG	O5-C5-C6-O6
12	A	1004	NAG	C4-C5-C6-O6
12	A	1005	NAG	C8-C7-N2-C2
12	A	1005	NAG	O7-C7-N2-C2
12	B	1005	NAG	C8-C7-N2-C2
12	B	1005	NAG	O7-C7-N2-C2
12	B	1005	NAG	O5-C5-C6-O6
12	B	1005	NAG	C4-C5-C6-O6
12	B	1006	NAG	O5-C5-C6-O6
12	A	1005	NAG	O5-C5-C6-O6
12	C	3402	NAG	C4-C5-C6-O6
12	C	3402	NAG	O5-C5-C6-O6
12	B	1005	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1005	NAG	1	0
12	B	1004	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.

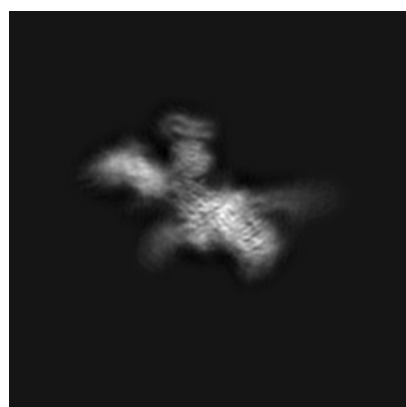
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30342. These allow visual inspection of the internal detail of the map and identification of artifacts.

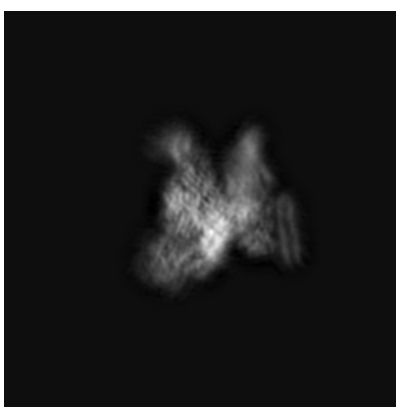
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

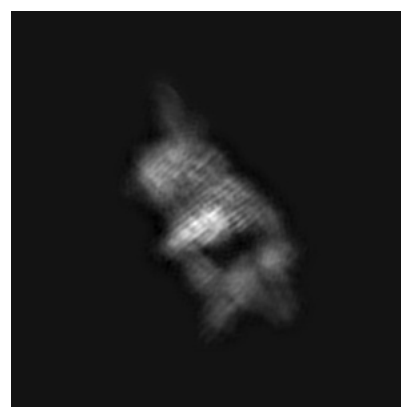
#### 6.1.1 Primary map



X



Y

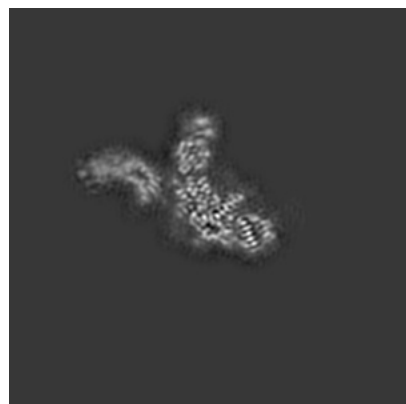


Z

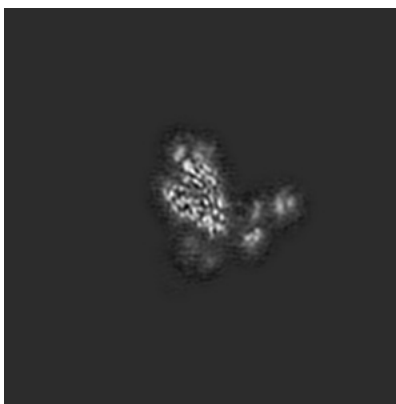
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

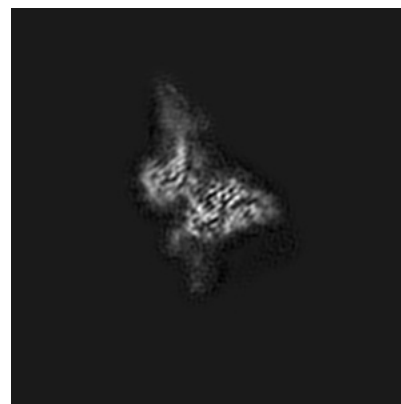
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

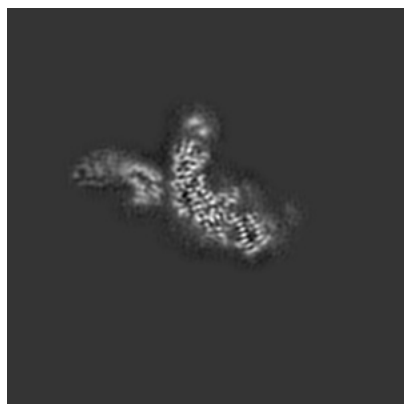


Z Index: 150

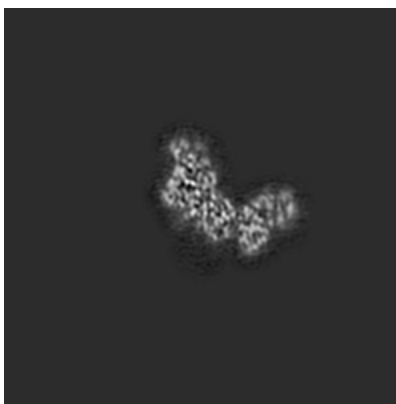
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

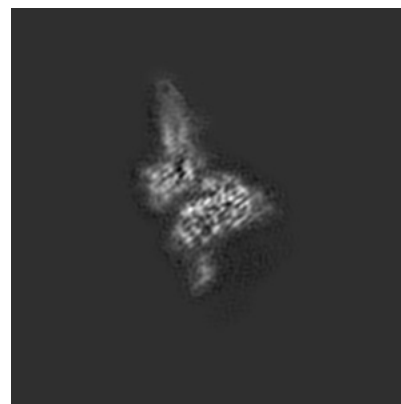
### 6.3.1 Primary map



X Index: 146



Y Index: 143

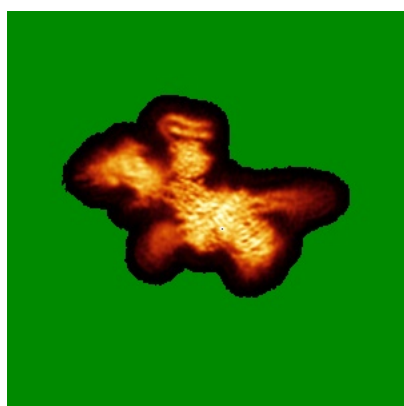


Z Index: 154

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

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X



Y

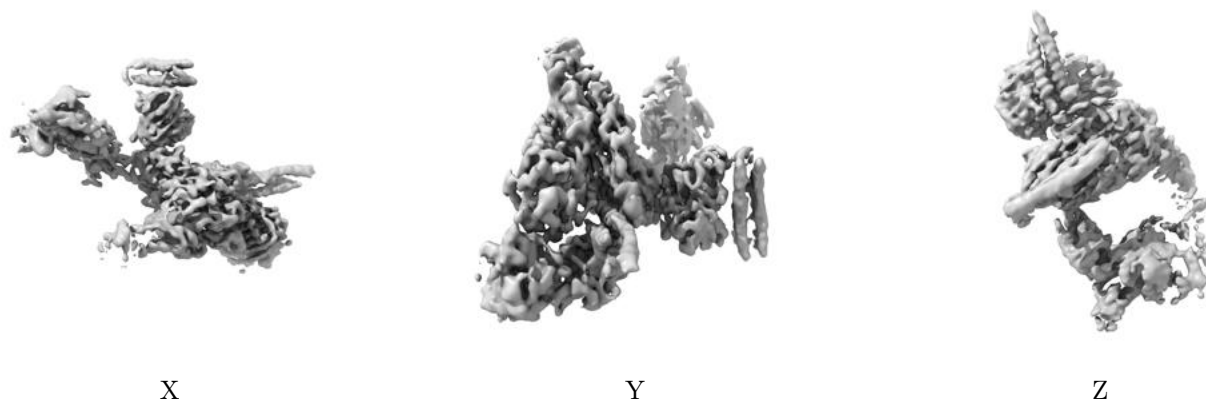


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

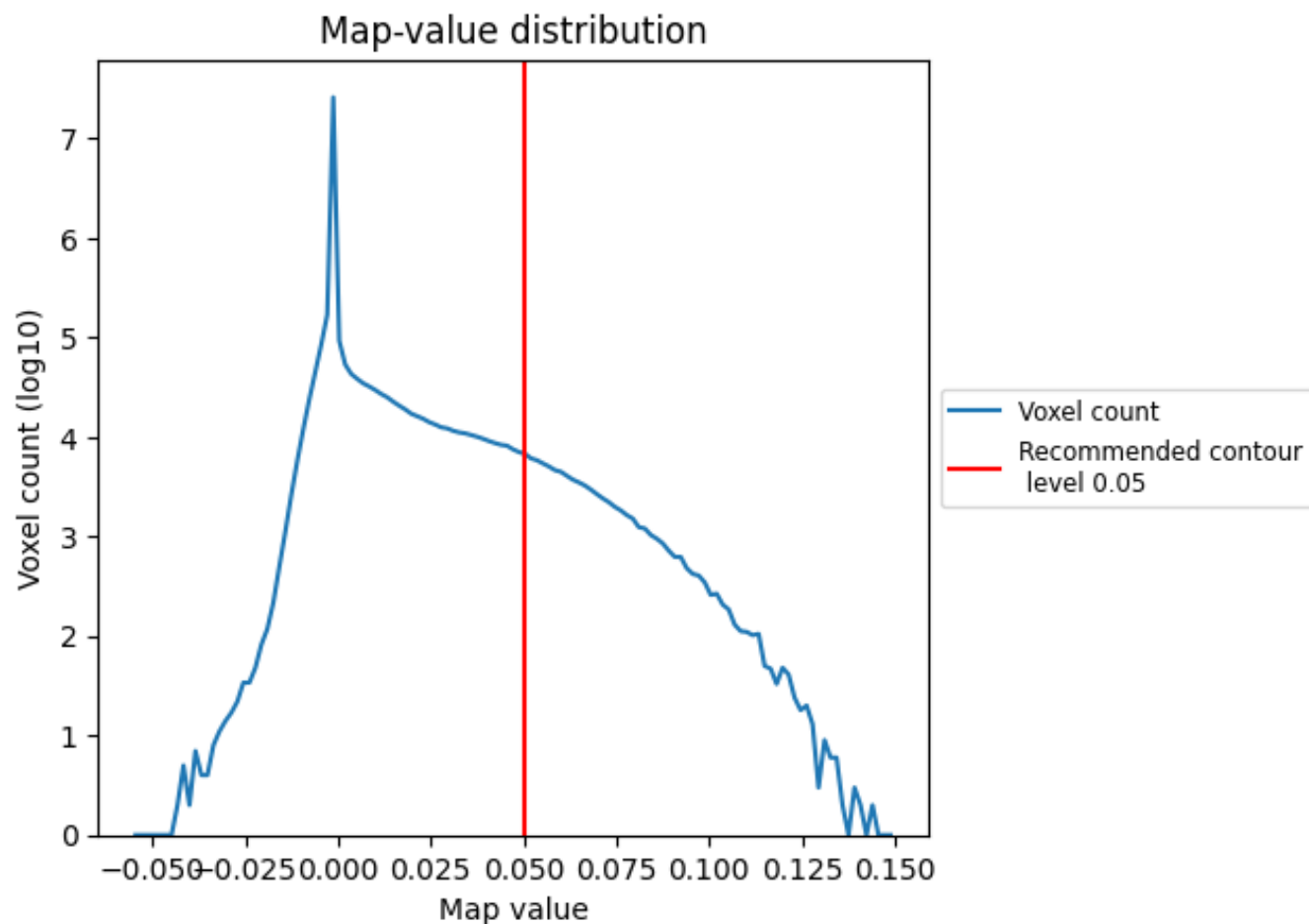
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

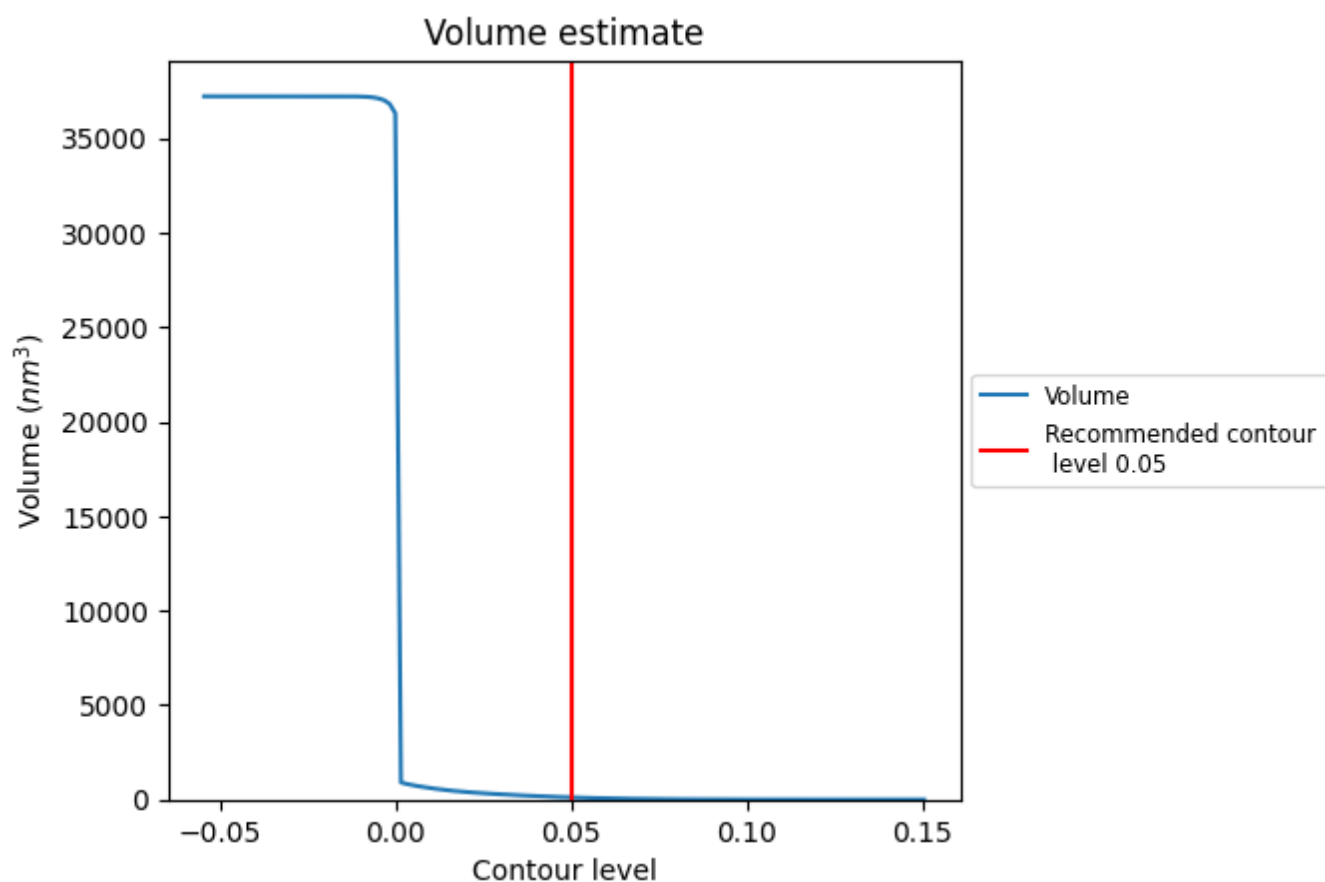
This section contains the results of statistical analysis of the map.

### 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.

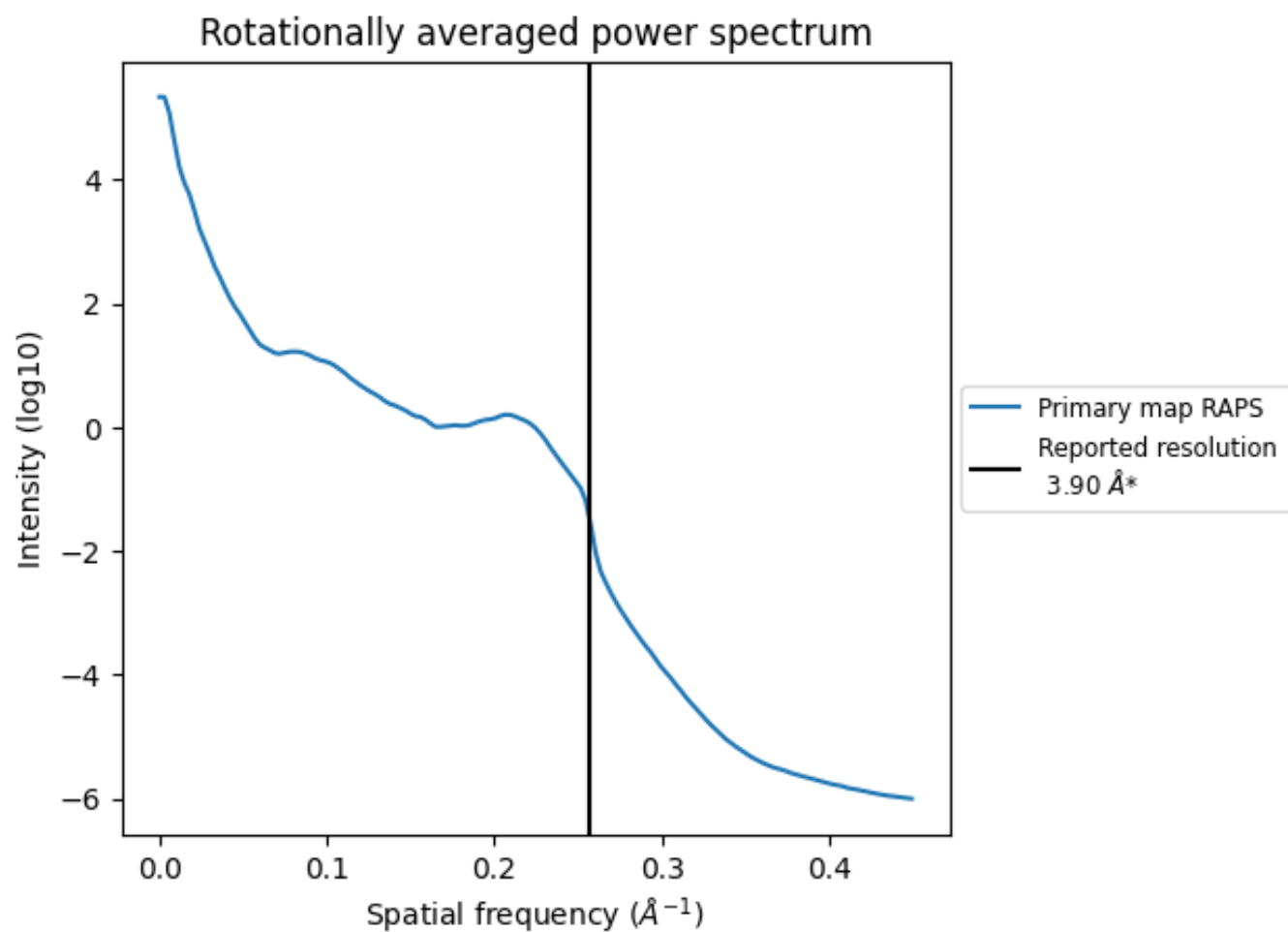
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm<sup>3</sup>; this corresponds to an approximate mass of 103 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

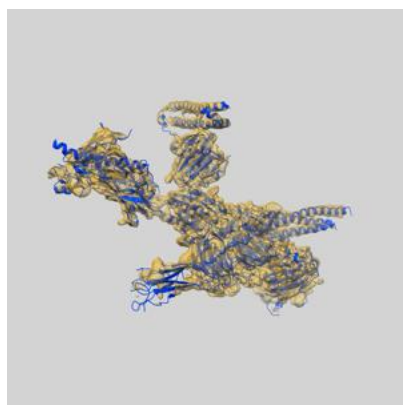
This section was not generated. No FSC curve or half-maps provided.



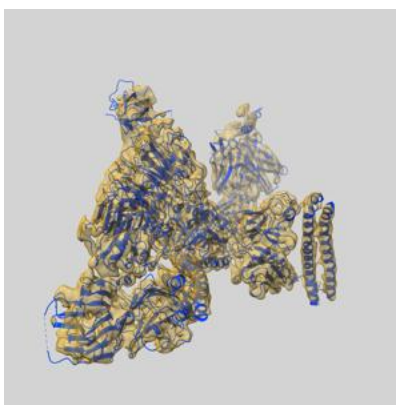
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30342 and PDB model 7CEC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

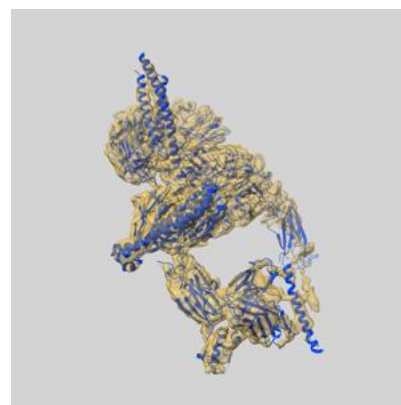
### 9.1 Map-model overlay [i](#)



X



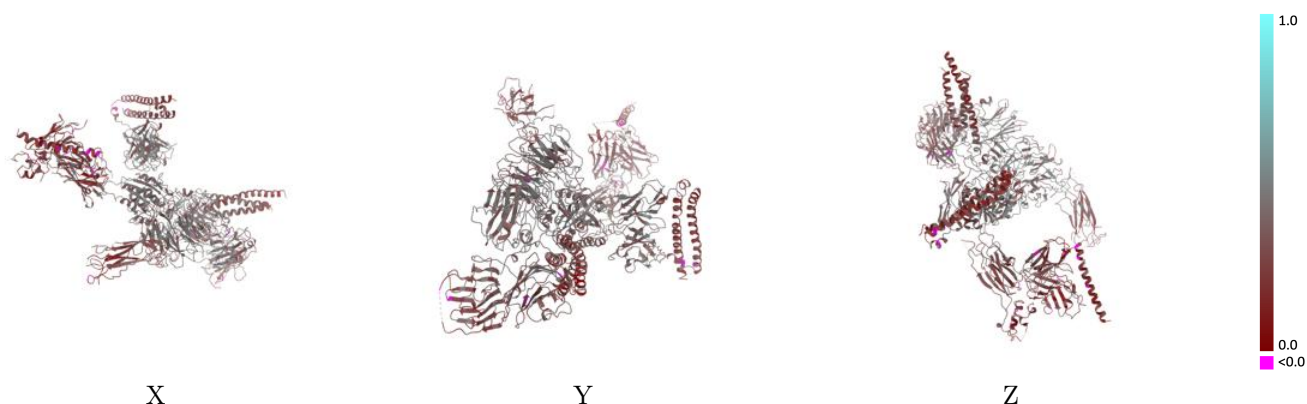
Y



Z

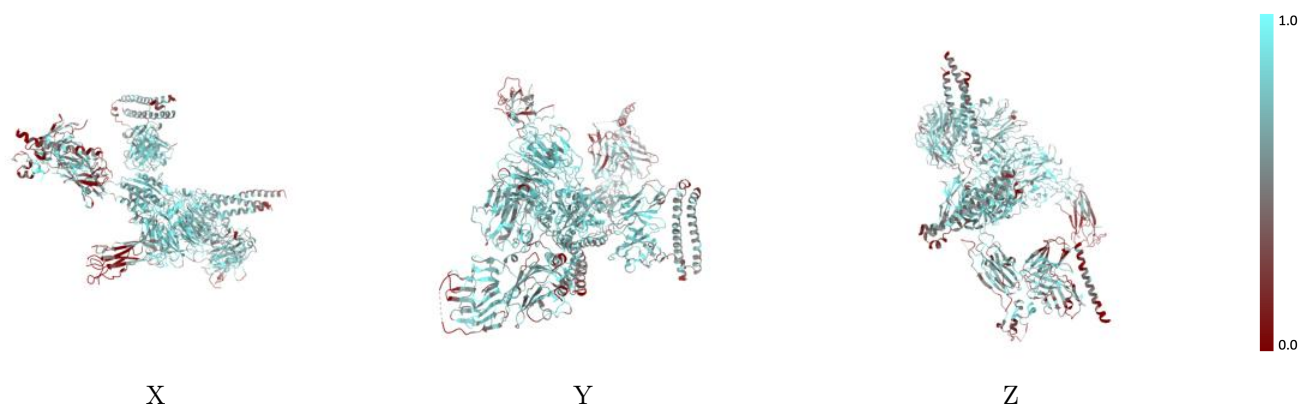
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



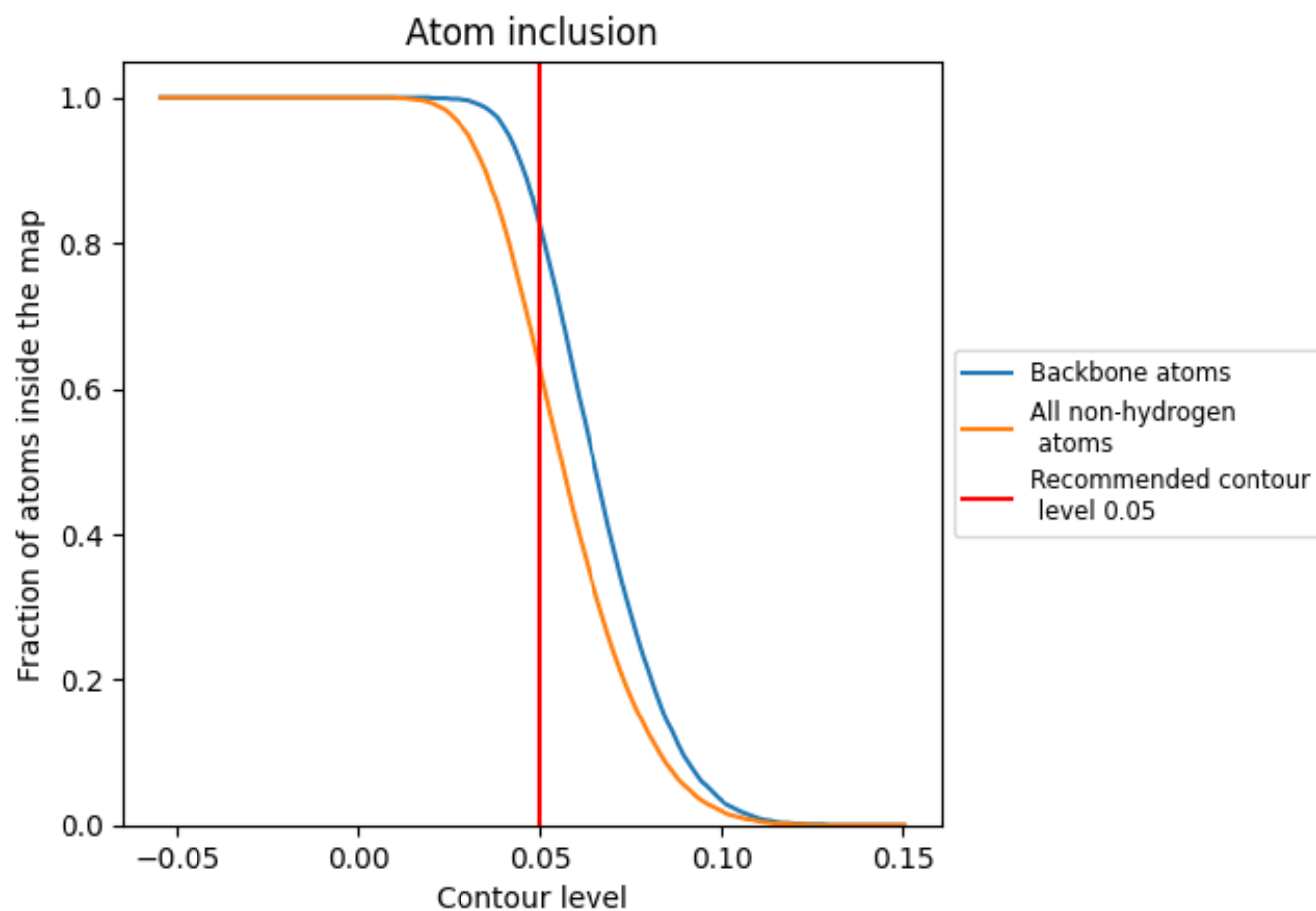
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 62% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6250	<div></div> 0.3470
A	<div></div> 0.6630	<div></div> 0.3850
B	<div></div> 0.6530	<div></div> 0.3600
C	<div></div> 0.6340	<div></div> 0.3590
D	<div></div> 0.5170	<div></div> 0.2350
E	<div></div> 0.5660	<div></div> 0.3080
F	<div></div> 0.6470	<div></div> 0.3420
G	<div></div> 0.6590	<div></div> 0.3510
H	<div></div> 0.5020	<div></div> 0.2590
I	<div></div> 0.4530	<div></div> 0.2410
J	<div></div> 0.3570	<div></div> 0.2650

1.0

0.0

<0.0