



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 07:00 PM EST

PDB ID : 8SKU  
EMDB ID : EMD-40567  
Title : Structure of human SIgA1 in complex with human CD89 (FcaR1)  
Authors : Liu, Q.; Stadtmueller, B.M.  
Deposited on : 2023-04-20  
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](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 : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

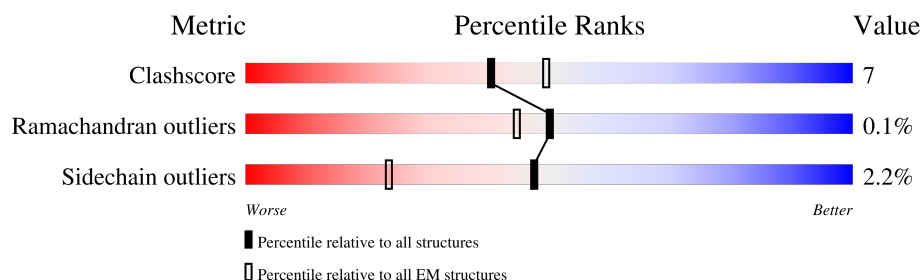
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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.




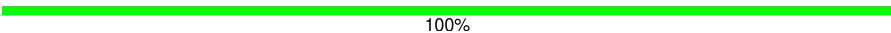
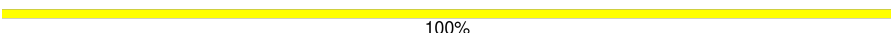

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	353	
1	B	353	
1	C	353	
1	D	353	
2	E	553	
3	R	207	
3	S	207	
4	J	137	

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Mol	Chain	Length	Quality of chain
5	H	2	 50%50%
5	I	2	 100%
5	K	2	 100%
5	L	2	 50%50%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28053 atoms, of which 13577 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 Immunoglobulin heavy constant alpha 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	222	Total	C	H	N	O	S	0	0
			2997	991	1438	267	293	8		
1	B	230	Total	C	H	N	O	S	0	0
			3104	1025	1483	277	310	9		
1	C	231	Total	C	H	N	O	S	0	0
			3144	1036	1512	280	306	10		
1	D	223	Total	C	H	N	O	S	0	0
			2978	990	1422	264	294	8		

- Molecule 2 is a protein called Secretory component.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	534	Total	C	H	N	O	S	0	0
			8097	2588	3988	709	792	20		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	548	HIS	-	expression tag	UNP P01833
E	549	HIS	-	expression tag	UNP P01833
E	550	HIS	-	expression tag	UNP P01833
E	551	HIS	-	expression tag	UNP P01833
E	552	HIS	-	expression tag	UNP P01833
E	553	HIS	-	expression tag	UNP P01833

- Molecule 3 is a protein called Immunoglobulin alpha Fc receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	R	190	Total	C	H	N	O	S	0	0
			2714	914	1300	239	255	6		
3	S	190	Total	C	H	N	O	S	0	0
			2714	914	1300	239	255	6		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	196	ALA	-	expression tag	UNP P24071
R	197	ILE	-	expression tag	UNP P24071
R	198	ASP	-	expression tag	UNP P24071
R	199	GLY	-	expression tag	UNP P24071
R	200	ARG	-	expression tag	UNP P24071
R	201	ALA	-	expression tag	UNP P24071
R	202	HIS	-	expression tag	UNP P24071
R	203	HIS	-	expression tag	UNP P24071
R	204	HIS	-	expression tag	UNP P24071
R	205	HIS	-	expression tag	UNP P24071
R	206	HIS	-	expression tag	UNP P24071
R	207	HIS	-	expression tag	UNP P24071
S	196	ALA	-	expression tag	UNP P24071
S	197	ILE	-	expression tag	UNP P24071
S	198	ASP	-	expression tag	UNP P24071
S	199	GLY	-	expression tag	UNP P24071
S	200	ARG	-	expression tag	UNP P24071
S	201	ALA	-	expression tag	UNP P24071
S	202	HIS	-	expression tag	UNP P24071
S	203	HIS	-	expression tag	UNP P24071
S	204	HIS	-	expression tag	UNP P24071
S	205	HIS	-	expression tag	UNP P24071
S	206	HIS	-	expression tag	UNP P24071
S	207	HIS	-	expression tag	UNP P24071

- Molecule 4 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	J	131	Total	C	H	N	O	S	0	0
			1985	622	982	179	193	9		

- Molecule 5 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
5	L	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
5	K	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
5	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

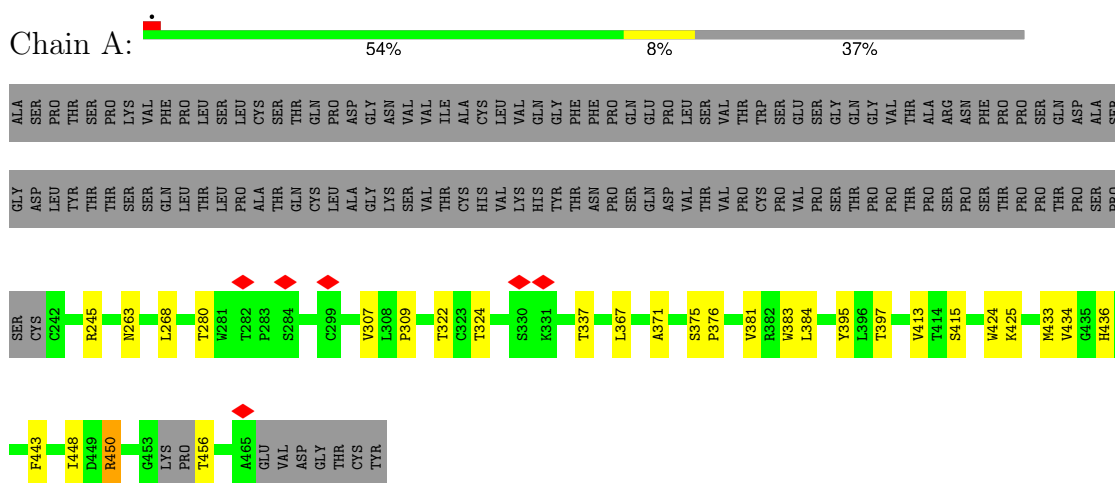


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
6	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
6	E	1	Total	C	H	N	O	0
			27	8	13	1	5	
6	E	1	Total	C	H	N	O	0
			27	8	13	1	5	

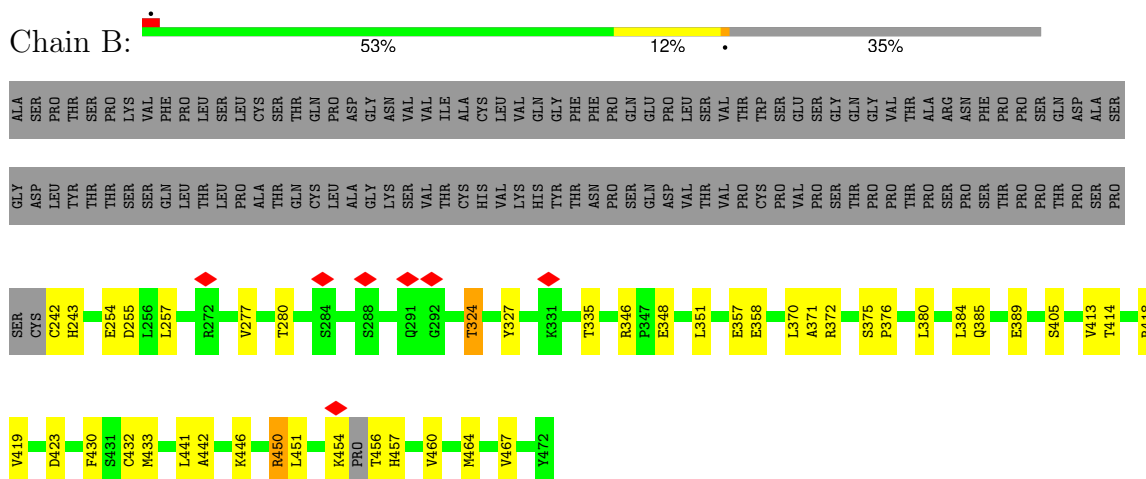
### 3 Residue-property plots

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.

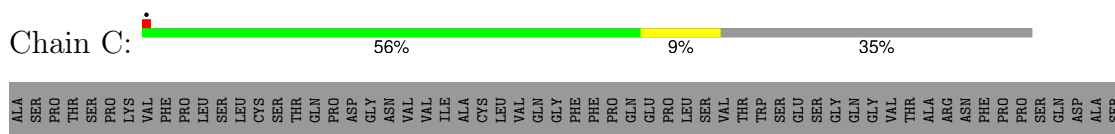
- Molecule 1: Immunoglobulin heavy constant alpha 1

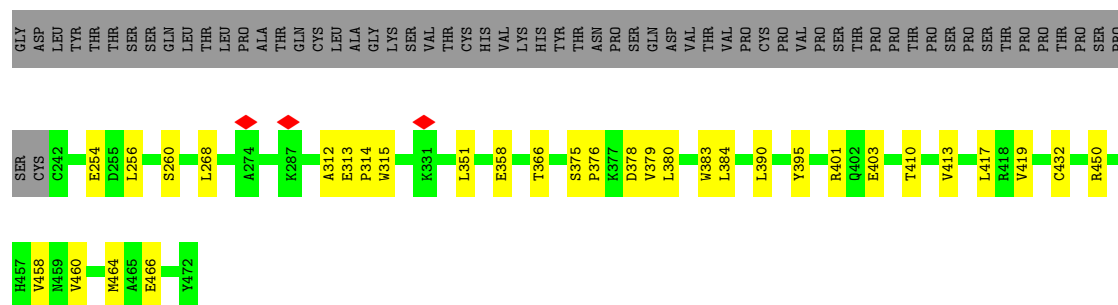


- Molecule 1: Immunoglobulin heavy constant alpha 1

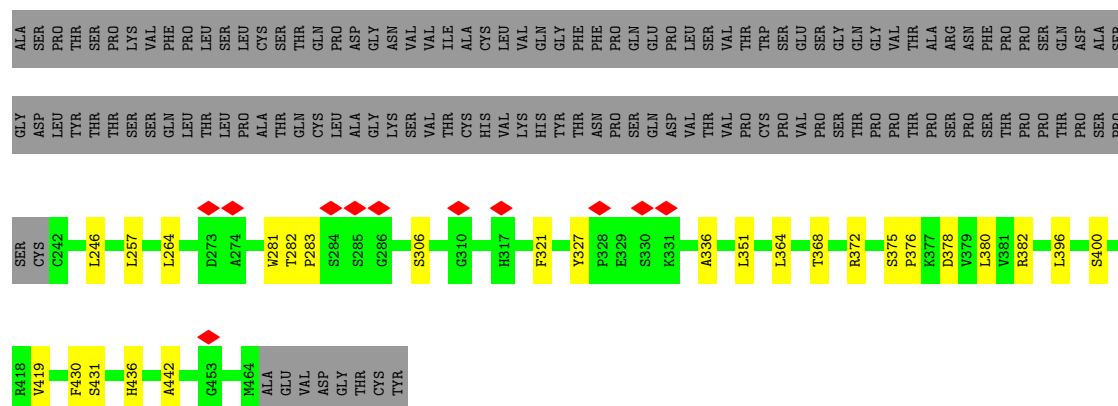


- Molecule 1: Immunoglobulin heavy constant alpha 1

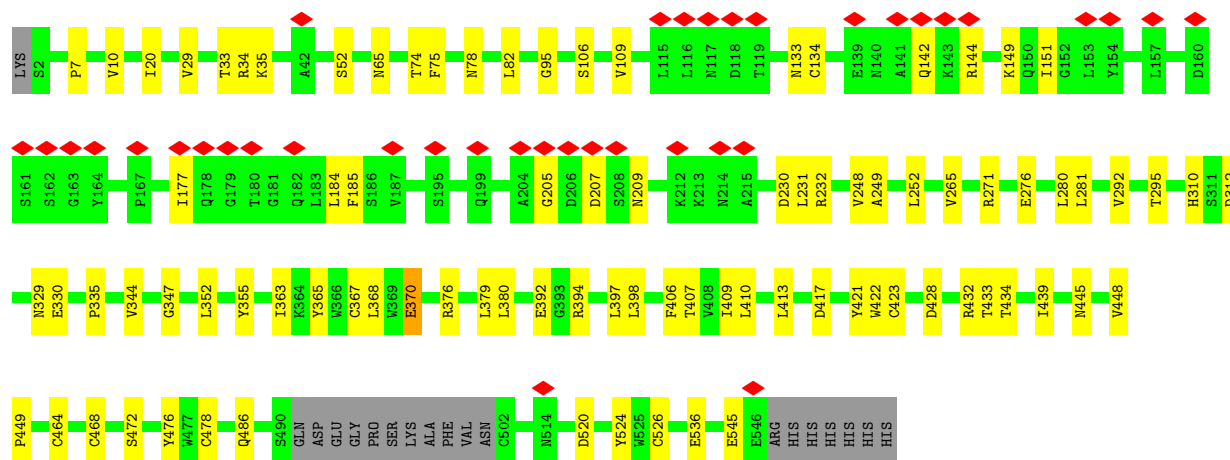
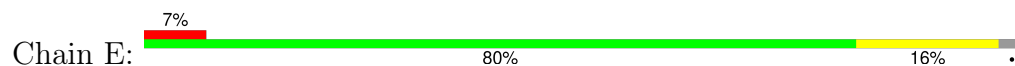




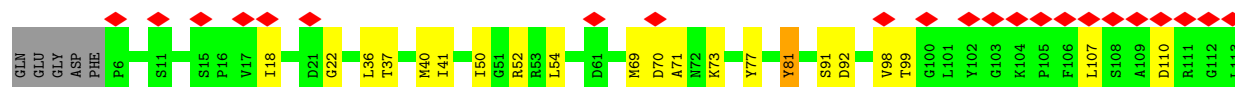
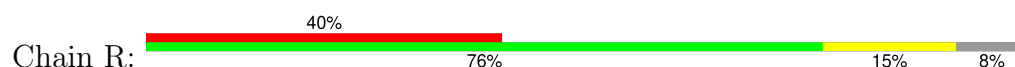
• Molecule 1: Immunoglobulin heavy constant alpha 1



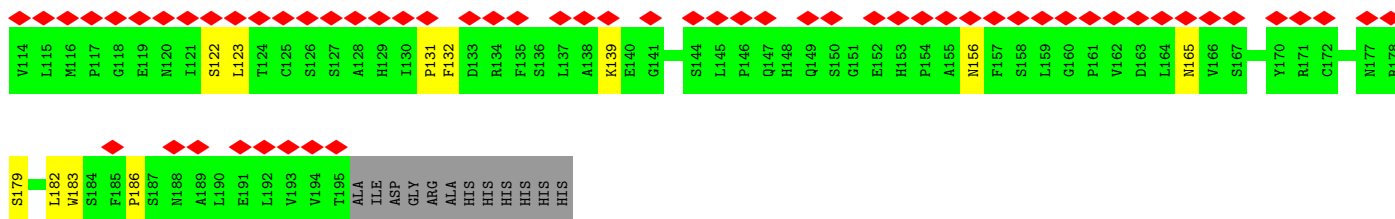
• Molecule 2: Secretory component



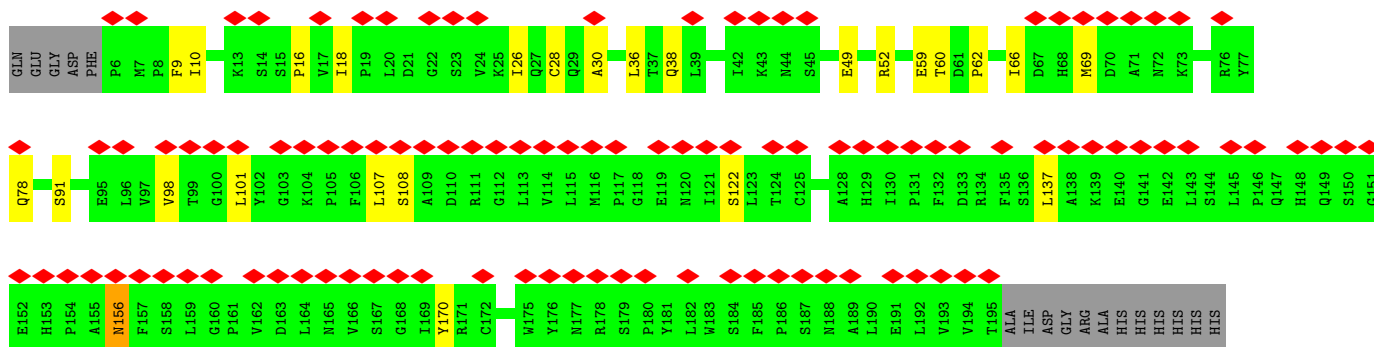
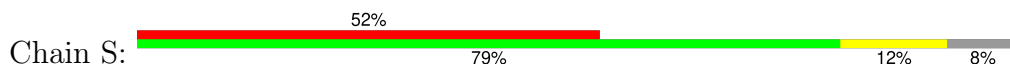
• Molecule 3: Immunoglobulin alpha Fc receptor







• Molecule 3: Immunoglobulin alpha Fc receptor



• Molecule 4: Immunoglobulin J chain



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249000	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 ( $e^-/\text{\AA}^2$ )	71.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.326	Depositor
Minimum map value	-0.867	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	361.68002, 361.68002, 361.68002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/1598	0.49	0/2204
1	B	0.26	0/1661	0.50	0/2291
1	C	0.28	0/1674	0.49	0/2308
1	D	0.26	0/1597	0.48	0/2208
2	E	0.28	0/4198	0.51	0/5708
3	R	0.26	0/1454	0.49	0/1989
3	S	0.25	0/1454	0.48	0/1989
4	J	0.29	0/1017	0.58	0/1387
All	All	0.27	0/14653	0.50	0/20084

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	448	VAL	Peptide

## 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	1559	1438	1438	21	0
1	B	1621	1483	1483	26	0
1	C	1632	1512	1512	22	0
1	D	1556	1422	1422	14	0
2	E	4109	3988	3988	52	0
3	R	1414	1300	1300	19	0
3	S	1414	1300	1300	17	0
4	J	1003	982	982	31	0
5	H	28	25	25	1	0
5	I	28	25	25	0	0
5	K	28	25	25	1	0
5	L	28	25	25	2	0
6	A	14	13	13	1	0
6	B	14	13	13	0	0
6	E	28	26	26	0	0
All	All	14476	13577	13577	191	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 7.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:CYS:SG	2:E:433:THR:OG1	2.31	0.87
2:E:295:THR:OG1	2:E:432:ARG:O	1.94	0.83
1:B:280:THR:HG1	1:B:324:THR:HG1	1.19	0.83
2:E:368:LEU:HB2	2:E:380:LEU:HD11	1.61	0.83
1:C:390:LEU:HD12	1:C:417:LEU:HD11	1.60	0.81
2:E:394:ARG:NH2	2:E:417:ASP:OD1	2.16	0.78
1:B:351:LEU:HD21	1:B:432:CYS:HB3	1.65	0.78
1:B:357:GLU:N	1:B:357:GLU:OE2	2.19	0.76
1:A:383:TRP:HE1	1:A:415:SER:HG	1.32	0.75
1:C:450:ARG:NH1	4:J:32:ASP:OD2	2.20	0.74
3:R:110:ASP:OD2	3:R:122:SER:OG	2.05	0.72
1:A:456:THR:N	1:B:454:LYS:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:ARG:NH1	2:E:95:GLY:O	2.24	0.71
1:B:277:VAL:HG22	1:B:327:TYR:HB3	1.74	0.69
5:L:1:NAG:O7	5:L:1:NAG:O3	2.11	0.69
2:E:370:GLU:OE2	2:E:376:ARG:NH1	2.26	0.69
2:E:149:LYS:HG3	2:E:151:ILE:HG23	1.74	0.68
2:E:280:LEU:HD13	2:E:422:TRP:CH2	2.30	0.66
2:E:29:VAL:HG21	4:J:107:ASN:HA	1.77	0.66
2:E:363:ILE:HD11	2:E:365:TYR:OH	1.96	0.66
2:E:392:GLU:OE1	2:E:392:GLU:N	2.28	0.66
1:D:419:VAL:HG11	1:D:430:PHE:CE2	2.31	0.65
1:B:324:THR:HG22	1:B:335:THR:HG22	1.78	0.65
3:S:26:ILE:HD11	3:S:66:ILE:HD12	1.79	0.64
1:D:246:LEU:HD21	1:D:336:ALA:HB2	1.81	0.62
2:E:310:HIS:ND1	2:E:312:ASP:OD1	2.32	0.62
1:B:385:GLN:NE2	1:B:423:ASP:OD2	2.32	0.62
1:D:257:LEU:HD22	1:D:442:ALA:HB1	1.80	0.62
2:E:368:LEU:HD12	2:E:421:TYR:CZ	2.35	0.62
4:J:55:SER:O	4:J:57:LEU:N	2.33	0.62
5:H:1:NAG:H3	5:H:2:NAG:O5	1.98	0.61
1:B:257:LEU:HD22	1:B:442:ALA:HB1	1.82	0.61
1:B:419:VAL:HG21	1:B:430:PHE:CE1	2.36	0.61
1:D:264:LEU:HD22	1:D:321:PHE:CE2	2.36	0.60
1:A:371:ALA:HB2	1:A:434:VAL:HG21	1.83	0.60
3:S:59:GLU:HG3	3:S:60:THR:HG23	1.83	0.60
3:R:41:ILE:HD13	3:R:50:ILE:HG13	1.84	0.59
1:C:395:TYR:HB3	1:C:417:LEU:HD12	1.85	0.59
2:E:545:GLU:N	2:E:545:GLU:OE1	2.35	0.59
1:B:450:ARG:HG3	1:B:451:LEU:HD22	1.84	0.59
2:E:486:GLN:N	2:E:486:GLN:OE1	2.35	0.59
3:R:73:LYS:O	3:R:77:TYR:OH	2.12	0.59
4:J:81:ASN:OD1	4:J:81:ASN:O	2.20	0.59
2:E:207:ASP:OD2	2:E:209:ASN:ND2	2.36	0.57
1:A:384:LEU:HD11	1:A:433:MET:SD	2.45	0.57
1:D:380:LEU:HD12	1:D:382:ARG:HH21	1.70	0.57
3:S:30:ALA:HB2	3:S:62:PRO:HD3	1.86	0.57
2:E:520:ASP:O	2:E:524:TYR:OH	2.16	0.57
1:D:378:ASP:O	1:D:436:HIS:ND1	2.37	0.56
4:J:36:ARG:NH1	4:J:65:LEU:HD21	2.19	0.56
4:J:51:SER:OG	4:J:54:THR:OG1	2.24	0.56
1:A:307:VAL:HG12	1:A:309:PRO:HD3	1.88	0.55
2:E:410:LEU:HD21	2:E:417:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:38:GLN:NE2	3:S:49:GLU:OE1	2.33	0.55
1:B:456:THR:OG1	1:B:457:HIS:N	2.39	0.55
3:R:71:ALA:HA	3:R:98:VAL:HG21	1.89	0.55
3:R:179:SER:HB2	3:R:182:LEU:HD13	1.89	0.55
1:A:280:THR:O	1:A:324:THR:OG1	2.24	0.54
3:R:40:MET:HE3	3:R:40:MET:HA	1.90	0.54
1:C:379:VAL:HG11	1:C:413:VAL:HG11	1.89	0.54
4:J:87:THR:HG22	4:J:88:GLN:H	1.73	0.53
1:A:263:ASN:HB3	1:A:307:VAL:HG13	1.89	0.53
1:B:358:GLU:OE2	1:B:418:ARG:NH2	2.40	0.53
2:E:33:THR:O	2:E:35:LYS:NZ	2.39	0.53
1:C:401:ARG:HB2	1:D:396:LEU:HD11	1.91	0.53
2:E:367:CYS:SG	2:E:379:LEU:HD23	2.49	0.53
1:B:348:GLU:OE1	1:B:372:ARG:NH2	2.39	0.53
2:E:144:ARG:O	2:E:205:GLY:N	2.41	0.53
1:D:264:LEU:HD22	1:D:321:PHE:CD2	2.44	0.53
1:D:281:TRP:HZ2	1:D:306:SER:HG	1.57	0.53
1:C:403:GLU:OE2	1:C:410:THR:OG1	2.16	0.52
1:B:460:VAL:HG12	4:J:59:THR:HA	1.90	0.52
3:S:69:MET:HG3	3:S:98:VAL:HG12	1.92	0.52
1:B:254:GLU:HA	1:B:380:LEU:HD11	1.92	0.51
4:J:52:ASP:HB2	4:J:53:PRO:HD3	1.91	0.51
2:E:422:TRP:NE1	2:E:434:THR:OG1	2.43	0.51
1:B:242:CYS:SG	1:B:243:HIS:N	2.82	0.51
1:B:351:LEU:HD23	1:B:446:LYS:CB	2.40	0.51
1:D:375:SER:HB3	1:D:376:PRO:HD3	1.93	0.51
2:E:368:LEU:HD12	2:E:421:TYR:CE2	2.45	0.50
3:R:36:LEU:HD11	3:R:52:ARG:HG3	1.92	0.50
3:S:16:PRO:O	3:S:18:ILE:HD12	2.11	0.50
3:S:78:GLN:NE2	3:S:91:SER:O	2.40	0.50
2:E:428:ASP:OD1	2:E:428:ASP:N	2.39	0.50
1:C:384:LEU:HD21	4:J:77:VAL:HG13	1.93	0.49
2:E:445:ASN:ND2	2:E:536:GLU:OE2	2.44	0.49
3:R:69:MET:SD	3:R:70:ASP:N	2.85	0.49
4:J:48:GLU:O	4:J:58:ARG:NH1	2.45	0.49
1:A:322:THR:HG22	1:A:337:THR:HG22	1.93	0.49
1:A:397:THR:HG22	1:A:415:SER:HB2	1.94	0.49
3:R:36:LEU:HD12	3:R:37:THR:H	1.78	0.49
1:B:419:VAL:HG21	1:B:430:PHE:CZ	2.48	0.49
2:E:252:LEU:HD22	2:E:292:VAL:HG11	1.95	0.49
2:E:394:ARG:O	2:E:410:LEU:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:397:LEU:HD11	2:E:406:PHE:CE2	2.48	0.49
3:S:36:LEU:HD11	3:S:52:ARG:NH1	2.28	0.48
1:C:383:TRP:C	1:C:384:LEU:HD12	2.34	0.48
3:S:10:ILE:HD12	3:S:28:CYS:SG	2.53	0.48
1:D:282:THR:OG1	1:D:283:PRO:HD3	2.12	0.48
1:B:441:LEU:HD12	4:J:128:ALA:HB2	1.94	0.48
2:E:82:LEU:HD23	2:E:109:VAL:HG11	1.95	0.48
3:R:99:THR:HG22	3:R:183:TRP:HB2	1.94	0.48
1:D:364:LEU:HD23	1:D:419:VAL:C	2.34	0.48
1:A:367:LEU:HD21	1:A:424:TRP:CZ3	2.48	0.48
2:E:106:SER:O	2:E:106:SER:OG	2.31	0.48
2:E:281:LEU:HD12	2:E:292:VAL:HG22	1.96	0.48
1:A:367:LEU:HD22	1:A:448:ILE:HD11	1.95	0.47
2:E:133:ASN:HB3	2:E:184:LEU:HD21	1.96	0.47
4:J:73:ASP:O	4:J:88:GLN:NE2	2.45	0.47
1:C:466:GLU:HG3	4:J:44:LEU:HD12	1.95	0.47
2:E:271:ARG:NH1	2:E:276:GLU:OE1	2.47	0.47
1:A:376:PRO:HD2	1:A:436:HIS:NE2	2.30	0.47
1:B:346:ARG:NH2	4:J:132:ASP:OD1	2.47	0.47
1:A:381:VAL:HG22	1:A:434:VAL:HG22	1.96	0.47
3:S:122:SER:OG	3:S:156:ASN:OD1	2.32	0.47
2:E:7:PRO:HB2	2:E:10:VAL:HG22	1.96	0.47
3:R:98:VAL:O	3:R:183:TRP:N	2.37	0.46
3:S:9:PHE:O	3:S:10:ILE:HD13	2.15	0.46
1:C:254:GLU:HA	1:C:380:LEU:HD21	1.96	0.46
4:J:17:ARG:HE	4:J:39:ARG:HE	1.62	0.46
1:A:395:TYR:CE1	1:A:397:THR:HG23	2.50	0.46
3:R:18:ILE:HD11	3:R:22:GLY:HA3	1.98	0.46
1:D:351:LEU:HD12	1:D:368:THR:O	2.15	0.46
1:B:375:SER:HB3	1:B:376:PRO:HD3	1.97	0.46
1:C:384:LEU:HD21	4:J:77:VAL:CG1	2.46	0.46
2:E:177:ILE:HD11	2:E:185:PHE:HB3	1.97	0.46
1:C:464:MET:HG2	4:J:44:LEU:HD11	1.97	0.46
3:S:137:LEU:HD11	3:S:170:TYR:HB3	1.98	0.46
3:R:107:LEU:HD11	3:R:123:LEU:HB3	1.98	0.45
4:J:49:ASN:OD1	4:J:50:ILE:N	2.48	0.45
4:J:26:SER:O	4:J:26:SER:OG	2.30	0.45
1:C:351:LEU:HD13	1:C:432:CYS:HB3	1.99	0.45
3:R:69:MET:SD	3:R:98:VAL:HG22	2.57	0.45
4:J:79:LEU:HD11	4:J:84:VAL:HG21	1.98	0.45
1:C:358:GLU:OE2	1:C:366:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:VAL:HG21	2:E:20:ILE:HG12	1.98	0.45
4:J:53:PRO:O	4:J:54:THR:OG1	2.31	0.45
4:J:55:SER:O	4:J:56:PRO:C	2.55	0.45
2:E:397:LEU:HD11	2:E:406:PHE:HE2	1.82	0.44
2:E:248:VAL:HG12	2:E:249:ALA:N	2.32	0.44
3:R:81:TYR:CD1	3:R:81:TYR:N	2.85	0.44
2:E:74:THR:OG1	2:E:75:PHE:N	2.51	0.44
2:E:265:VAL:CG1	2:E:281:LEU:HD22	2.48	0.44
1:A:375:SER:HB3	1:A:376:PRO:HD3	1.99	0.44
1:D:417:LEU:HG	1:D:419:VAL:HG13	2.00	0.44
4:J:73:ASP:OD1	4:J:88:GLN:NE2	2.50	0.44
5:K:1:NAG:O4	5:K:2:NAG:O7	2.35	0.44
4:J:8:LEU:HD13	4:J:20:SER:OG	2.18	0.44
2:E:365:TYR:HB3	2:E:379:LEU:HD22	2.00	0.43
4:J:73:ASP:O	4:J:73:ASP:OD1	2.35	0.43
1:B:464:MET:SD	1:C:460:VAL:HG11	2.58	0.43
1:B:384:LEU:HD23	1:B:389:GLU:HA	1.99	0.43
3:S:98:VAL:HG23	3:S:101:LEU:HD11	2.01	0.43
1:C:456:THR:HG22	4:J:34:VAL:H	1.84	0.43
3:S:9:PHE:C	3:S:10:ILE:HD13	2.38	0.43
3:R:139:LYS:NZ	3:R:165:ASN:O	2.52	0.43
1:C:313:GLU:CB	1:C:314:PRO:HD3	2.48	0.43
4:J:32:ASP:OD1	4:J:33:ILE:N	2.52	0.43
2:E:329:ASN:O	2:E:330:GLU:HB2	2.19	0.42
3:R:91:SER:OG	3:R:92:ASP:N	2.51	0.42
1:B:467:VAL:HG12	1:C:458:VAL:HG21	2.00	0.42
3:S:18:ILE:HD12	3:S:18:ILE:H	1.84	0.42
1:B:370:LEU:HD13	1:B:414:THR:HG22	2.00	0.42
1:C:375:SER:HB3	1:C:376:PRO:HD3	2.01	0.42
1:A:371:ALA:HB3	1:A:413:VAL:HG12	2.01	0.42
1:A:436:HIS:HD2	1:A:438:ALA:HB3	1.85	0.42
1:C:417:LEU:HD23	1:C:419:VAL:HG23	2.02	0.42
1:B:371:ALA:HB3	1:B:413:VAL:HG12	2.01	0.41
4:J:54:THR:O	4:J:55:SER:C	2.59	0.41
1:A:263:ASN:OD1	6:A:501:NAG:N2	2.53	0.41
2:E:65:ASN:N	2:E:65:ASN:OD1	2.51	0.41
2:E:231:LEU:O	2:E:232:ARG:HG2	2.21	0.41
3:S:26:ILE:HD11	3:S:66:ILE:CD1	2.48	0.41
4:J:87:THR:HG22	4:J:88:GLN:N	2.35	0.41
2:E:344:VAL:HG23	2:E:347:GLY:HA3	2.01	0.41
5:L:1:NAG:HO3	5:L:1:NAG:C7	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:O	1:A:268:LEU:HD12	2.20	0.41
1:A:384:LEU:HD21	3:R:54:LEU:O	2.21	0.41
1:A:425:LYS:O	1:A:450:ARG:NH1	2.53	0.41
2:E:352:LEU:HD23	2:E:407:THR:HG22	2.03	0.41
2:E:413:LEU:HD13	2:E:439:ILE:CD1	2.51	0.41
3:R:131:PRO:O	3:R:132:PHE:C	2.59	0.41
4:J:11:ASN:O	4:J:15:CYS:N	2.53	0.41
2:E:281:LEU:CD1	2:E:292:VAL:HG22	2.51	0.41
2:E:476:TYR:CD2	2:E:478:CYS:HB2	2.56	0.41
1:C:256:LEU:HD21	1:C:315:TRP:CD1	2.55	0.41
1:C:260:SER:O	1:C:312:ALA:N	2.54	0.40
2:E:230:ASP:N	2:E:230:ASP:OD2	2.54	0.40
2:E:398:LEU:HD11	2:E:409:ILE:HD12	2.04	0.40
3:S:107:LEU:HD12	3:S:108:SER:H	1.86	0.40
2:E:65:ASN:OD1	2:E:78:ASN:HB2	2.21	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	218/353 (62%)	206 (94%)	12 (6%)	0	100	100
1	B	226/353 (64%)	214 (95%)	12 (5%)	0	100	100
1	C	229/353 (65%)	214 (93%)	15 (7%)	0	100	100
1	D	221/353 (63%)	206 (93%)	15 (7%)	0	100	100
2	E	530/553 (96%)	486 (92%)	43 (8%)	1 (0%)	44	75
3	R	188/207 (91%)	179 (95%)	9 (5%)	0	100	100
3	S	188/207 (91%)	179 (95%)	9 (5%)	0	100	100
4	J	127/137 (93%)	112 (88%)	14 (11%)	1 (1%)	16	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1927/2516 (77%)	1796 (93%)	129 (7%)	2 (0%)	50 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	449	PRO
4	J	56	PRO

### 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	153/307 (50%)	151 (99%)	2 (1%)	65 83
1	B	161/307 (52%)	156 (97%)	5 (3%)	35 66
1	C	162/307 (53%)	160 (99%)	2 (1%)	67 85
1	D	152/307 (50%)	148 (97%)	4 (3%)	41 70
2	E	450/472 (95%)	440 (98%)	10 (2%)	47 73
3	R	138/180 (77%)	135 (98%)	3 (2%)	47 73
3	S	138/180 (77%)	137 (99%)	1 (1%)	81 92
4	J	114/129 (88%)	109 (96%)	5 (4%)	24 57
All	All	1468/2189 (67%)	1436 (98%)	32 (2%)	47 73

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	PHE
1	A	450	ARG
1	B	255	ASP
1	B	324	THR
1	B	405	SER
1	B	433	MET
1	B	450	ARG
2	E	52	SER

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Mol	Chain	Res	Type
2	E	134	CYS
2	E	142	GLN
2	E	335	PRO
2	E	355	TYR
2	E	370	GLU
2	E	464	CYS
2	E	468	CYS
2	E	472	SER
2	E	526	CYS
3	R	81	TYR
3	R	156	ASN
3	R	186	PRO
1	C	268	LEU
1	C	378	ASP
3	S	156	ASN
1	D	327	TYR
1	D	372	ARG
1	D	400	SER
1	D	431	SER
4	J	13	CYS
4	J	37	ASN
4	J	46	ASN
4	J	89	SER
4	J	90	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

8 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	$\# Z  > 2$
5	NAG	H	1	5,2	14,14,15	0.92	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	H	2	5	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	I	1	5,1	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	I	2	5	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	K	1	5,4	14,14,15	0.16	0	17,19,21	0.52	0
5	NAG	K	2	5	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	L	1	5,2	14,14,15	0.31	0	17,19,21	0.44	0
5	NAG	L	2	5	14,14,15	0.17	0	17,19,21	0.45	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
5	NAG	H	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	K	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	NAG	L	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	O5-C1	-3.08	1.38	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C3-C4-C5	2.34	114.48	110.23

There are no chirality outliers.

All (18) torsion outliers are listed below:

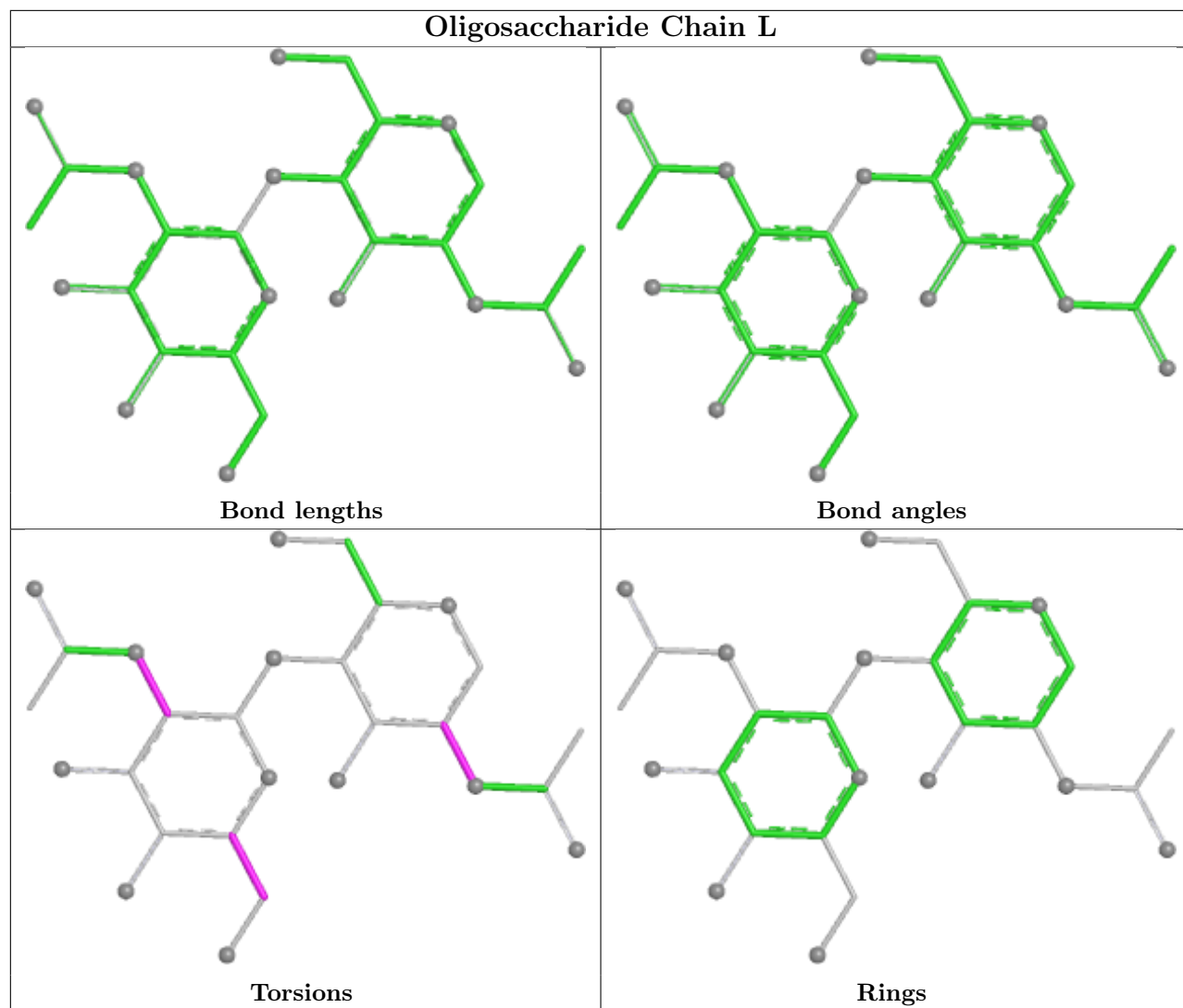
Mol	Chain	Res	Type	Atoms
5	L	2	NAG	C1-C2-N2-C7
5	K	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	L	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	L	1	NAG	C1-C2-N2-C7
5	L	1	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
5	K	1	NAG	C1-C2-N2-C7

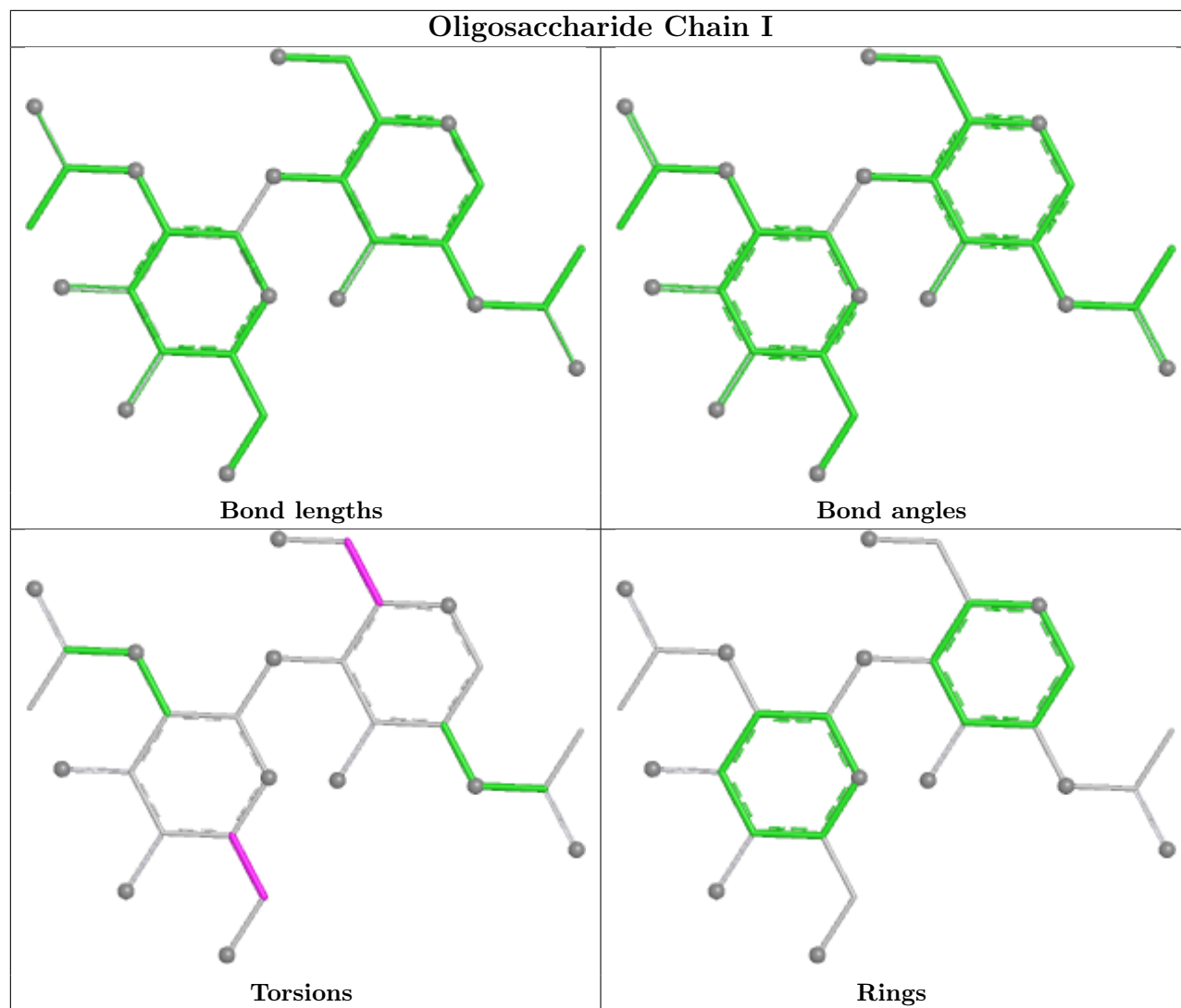
There are no ring outliers.

5 monomers are involved in 4 short contacts:

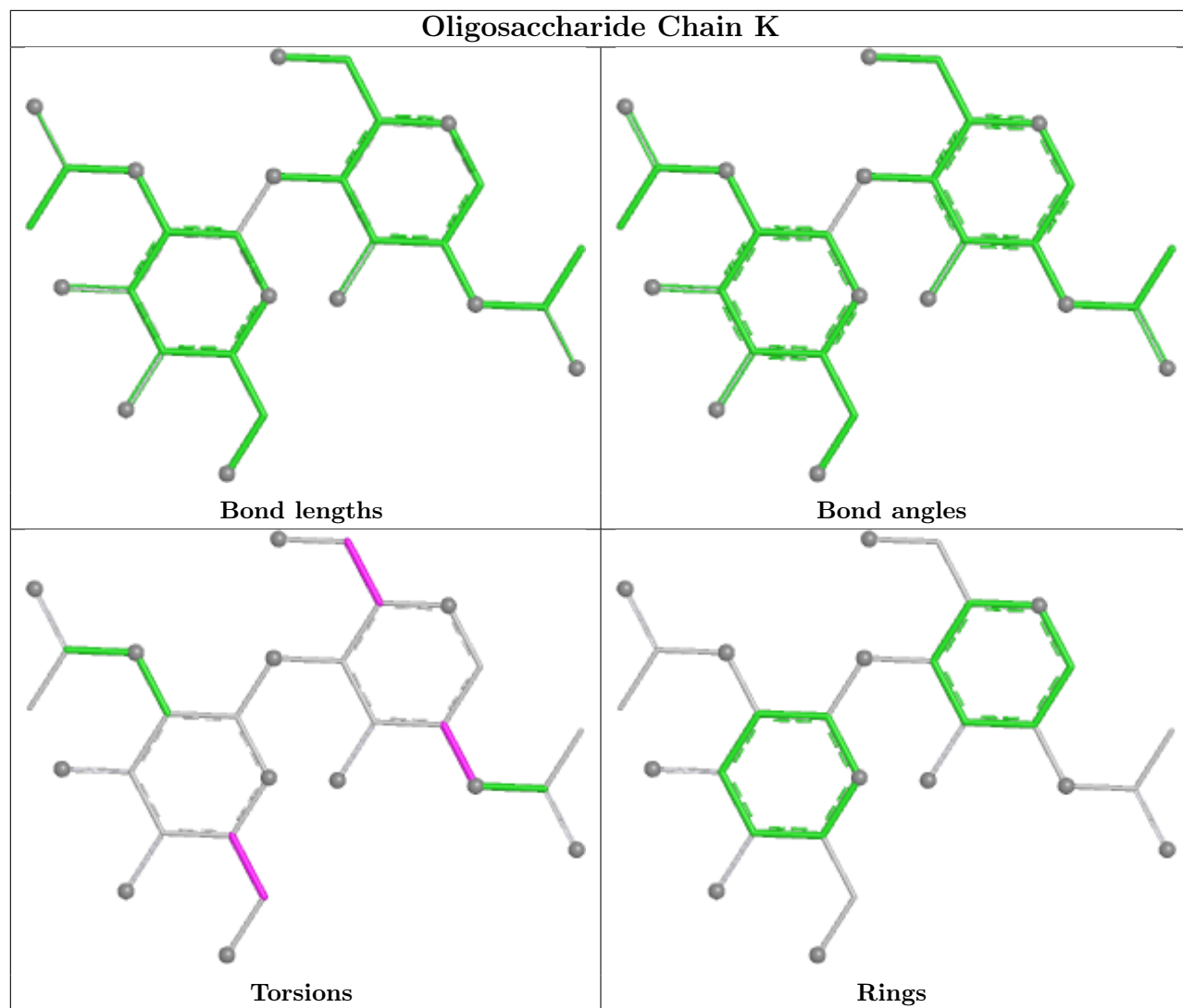
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2	NAG	1	0
5	L	1	NAG	2	0
5	H	2	NAG	1	0
5	H	1	NAG	1	0
5	K	1	NAG	1	0

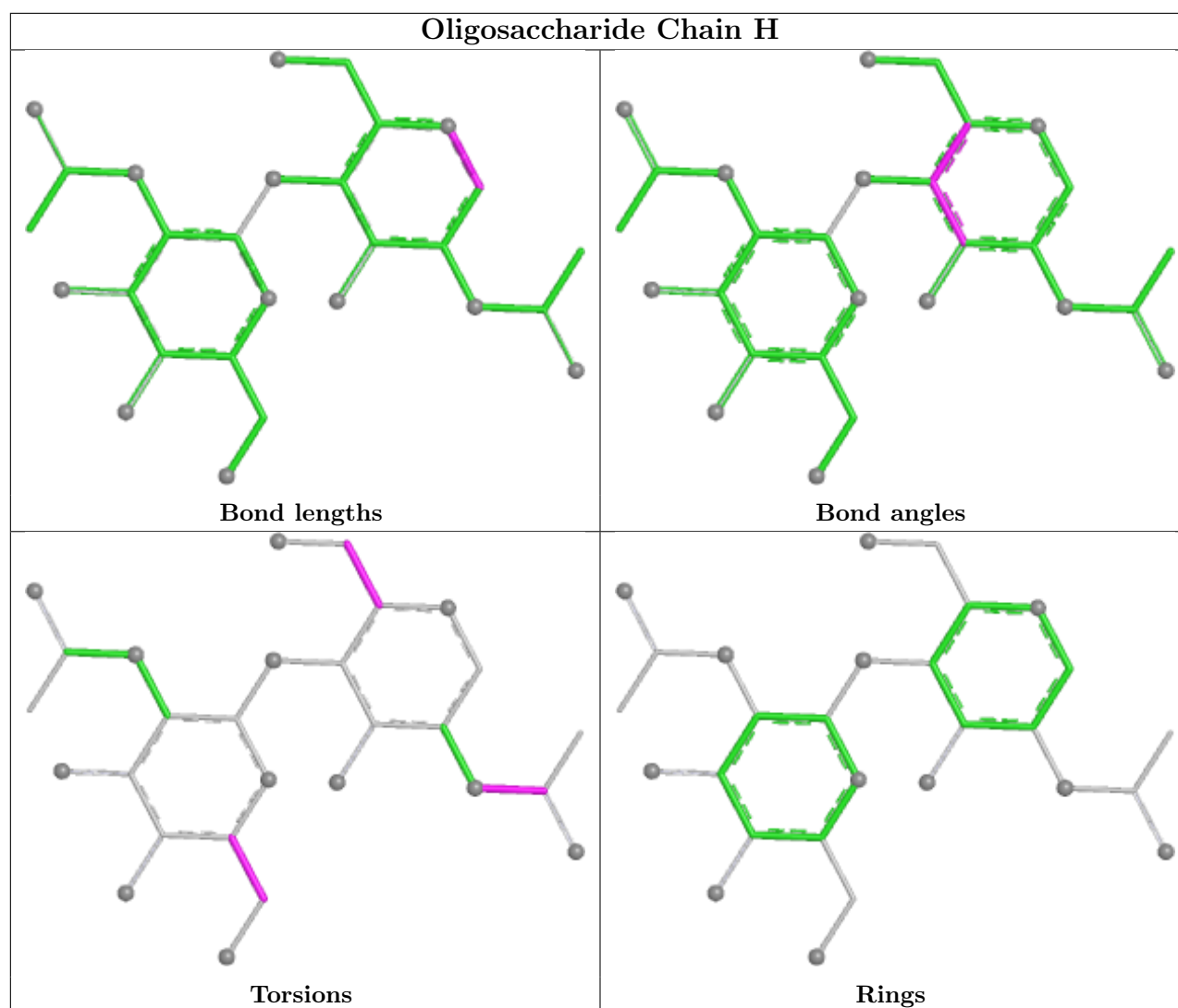
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	B	501	1	14,14,15	0.23	0	17,19,21	0.53	0
6	NAG	E	602	2	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	E	601	2	14,14,15	0.17	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	501	1	14,14,15	0.43	0	17,19,21	0.64	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	501	1	-	2/6/23/26	0/1/1/1
6	NAG	E	602	2	-	2/6/23/26	0/1/1/1
6	NAG	E	601	2	-	2/6/23/26	0/1/1/1
6	NAG	A	501	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	601	NAG	O5-C5-C6-O6
6	E	602	NAG	C4-C5-C6-O6
6	E	601	NAG	C4-C5-C6-O6
6	E	602	NAG	O5-C5-C6-O6
6	B	501	NAG	C8-C7-N2-C2
6	B	501	NAG	O7-C7-N2-C2
6	A	501	NAG	O5-C5-C6-O6
6	A	501	NAG	C4-C5-C6-O6
6	A	501	NAG	C3-C2-N2-C7
6	A	501	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	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.

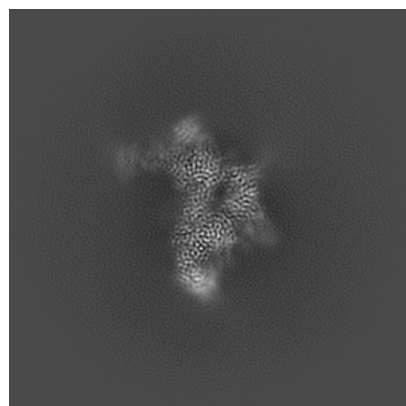
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40567. These allow visual inspection of the internal detail of the map and identification of artifacts.

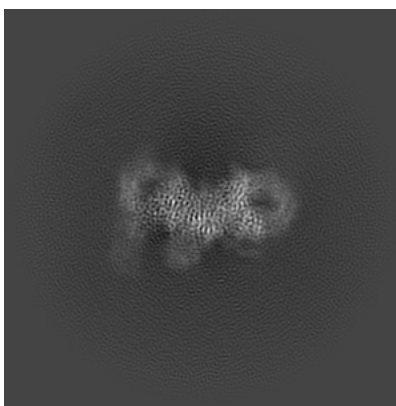
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

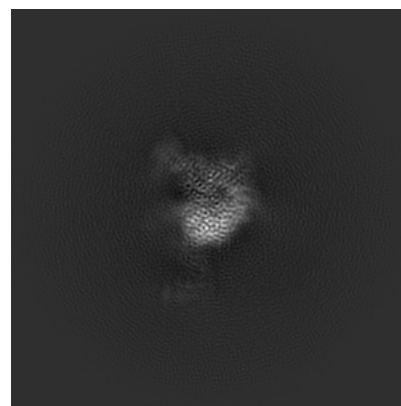
#### 6.1.1 Primary map



X

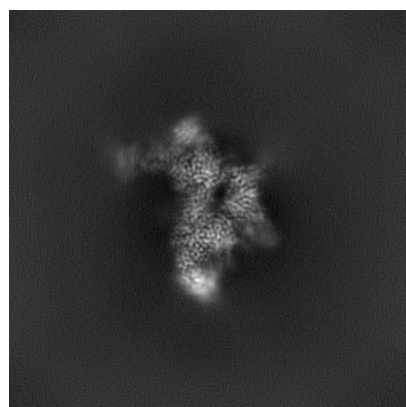


Y

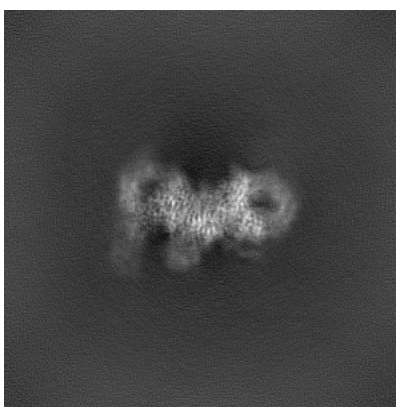


Z

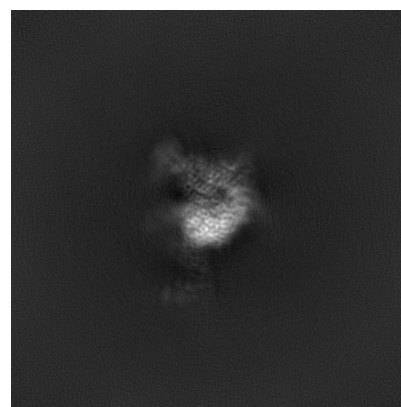
#### 6.1.2 Raw map



X



Y

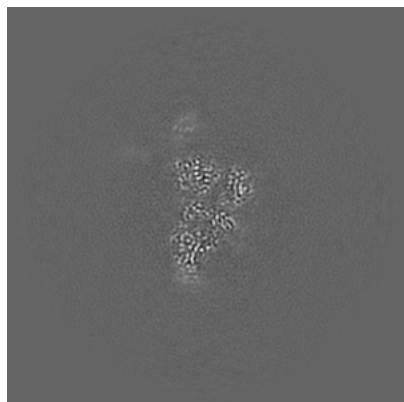


Z

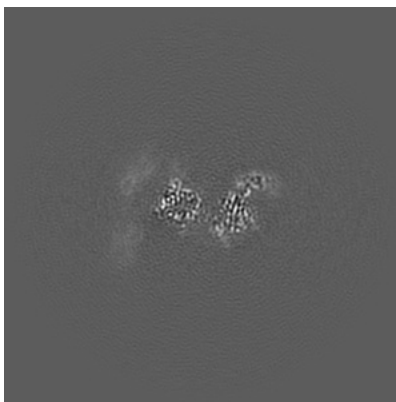
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

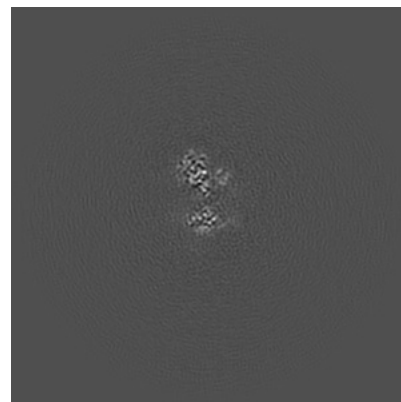
### 6.2.1 Primary map



X Index: 220

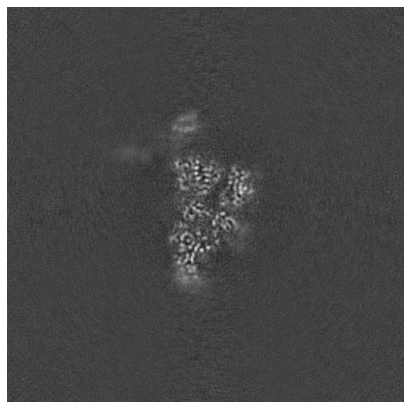


Y Index: 220

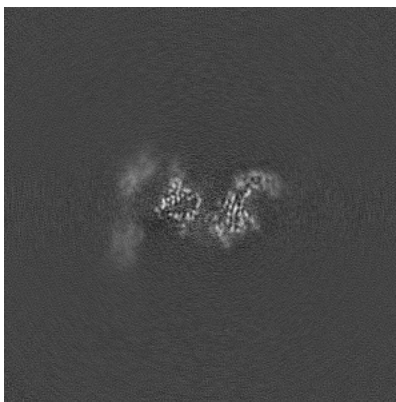


Z Index: 220

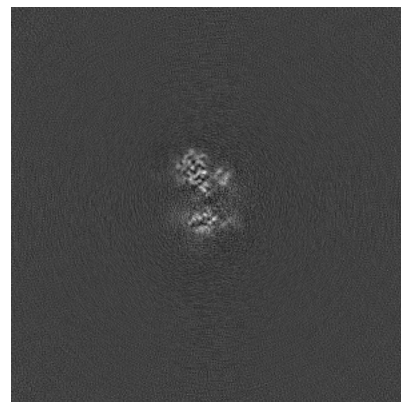
### 6.2.2 Raw map



X Index: 220



Y Index: 220

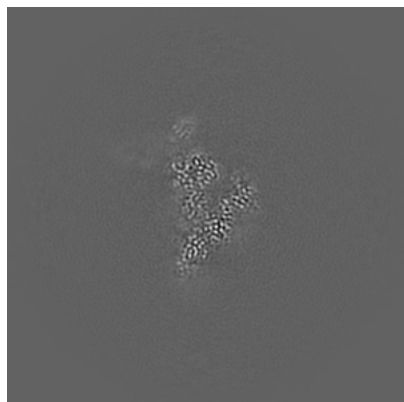


Z Index: 220

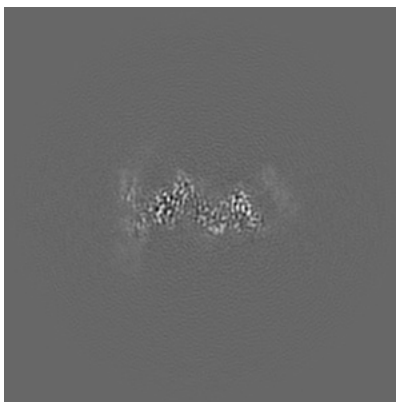
The images above show central slices of the map in three orthogonal directions.

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

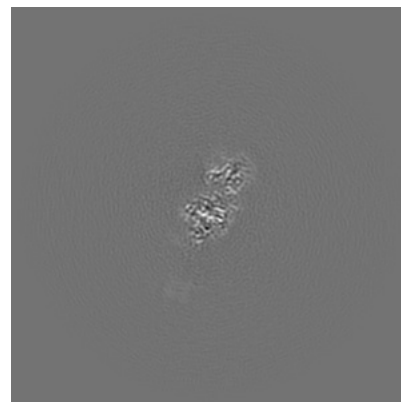
### 6.3.1 Primary map



X Index: 213

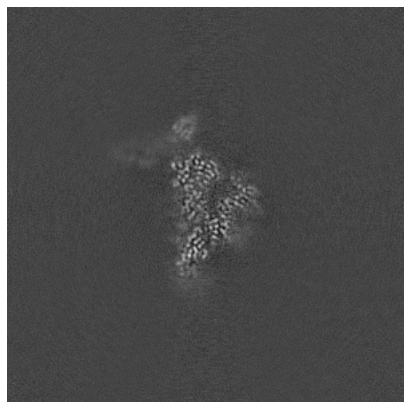


Y Index: 208

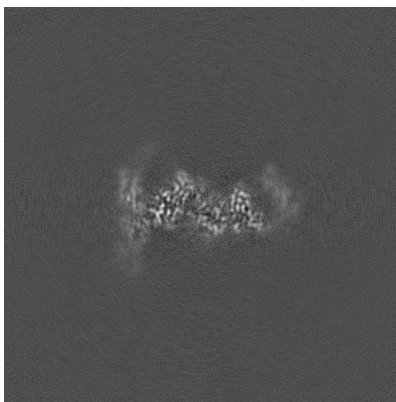


Z Index: 257

### 6.3.2 Raw map



X Index: 214



Y Index: 207



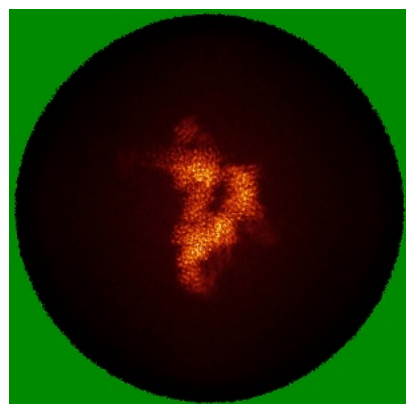
Z Index: 186

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

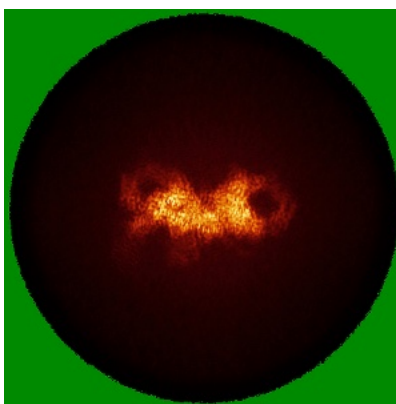


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

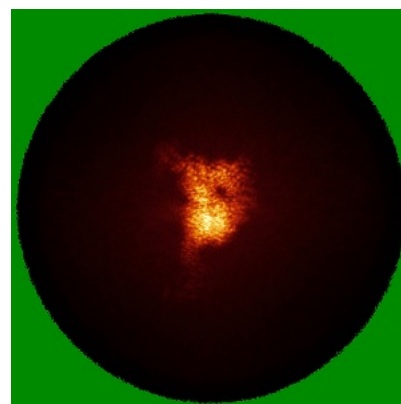
### 6.4.1 Primary map



X

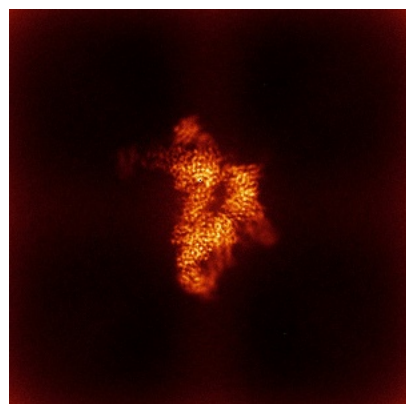


Y

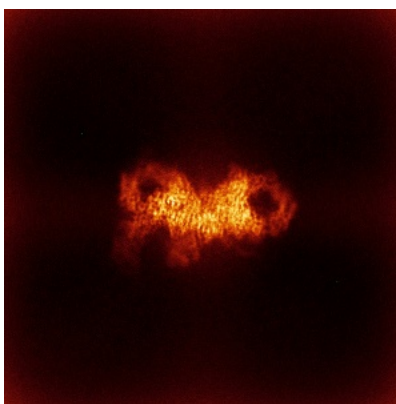


Z

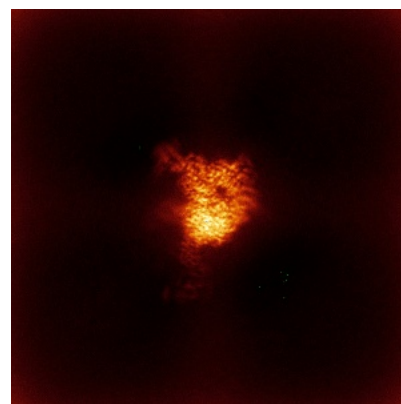
### 6.4.2 Raw map



X



Y



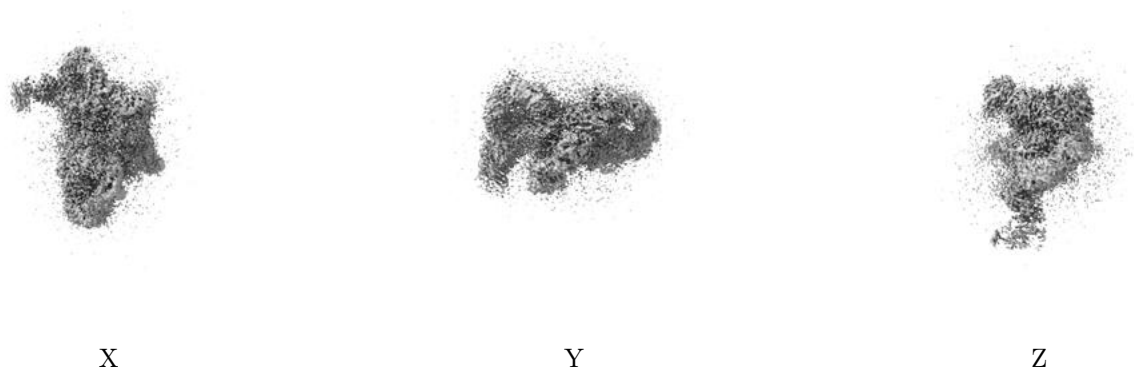
Z

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



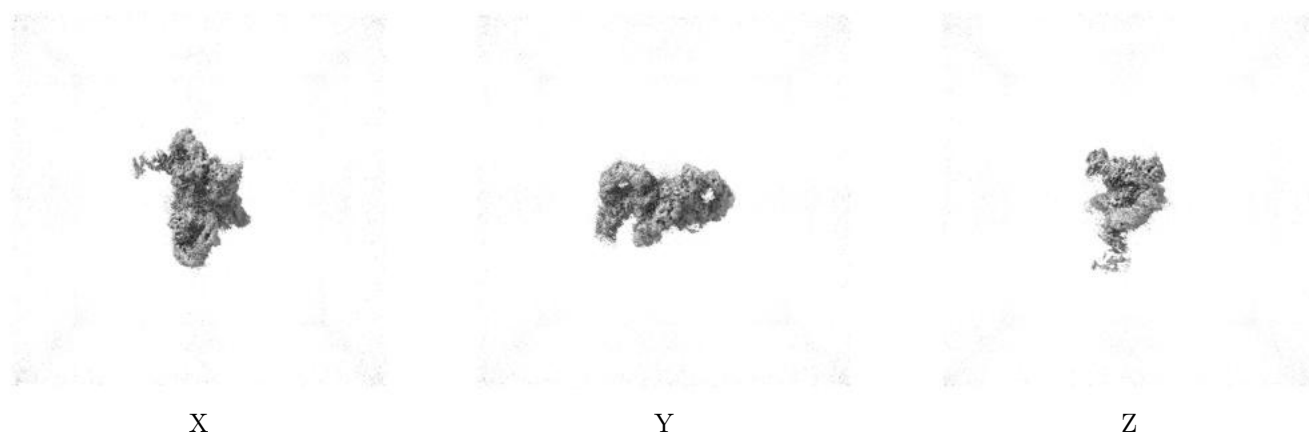
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

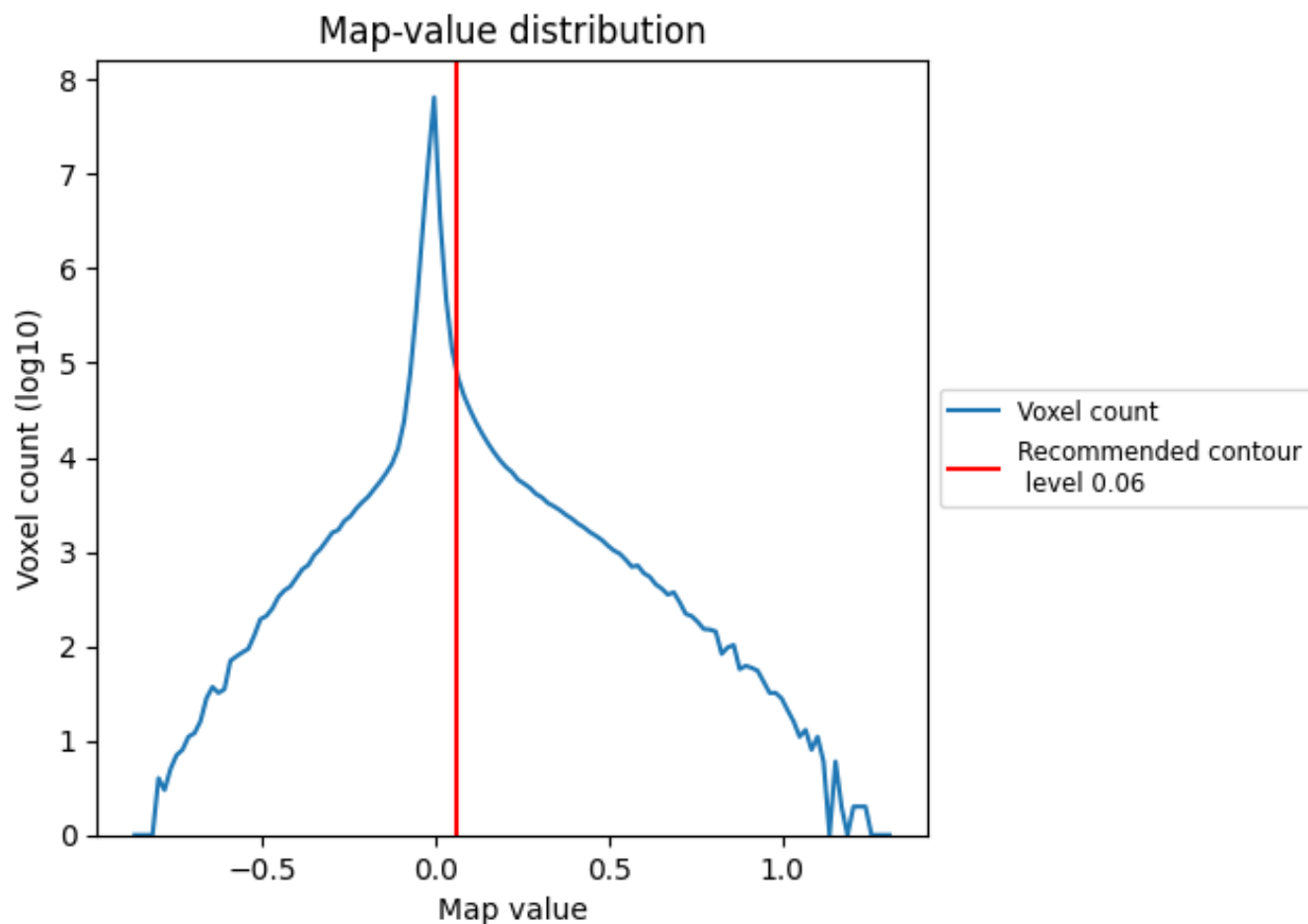
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

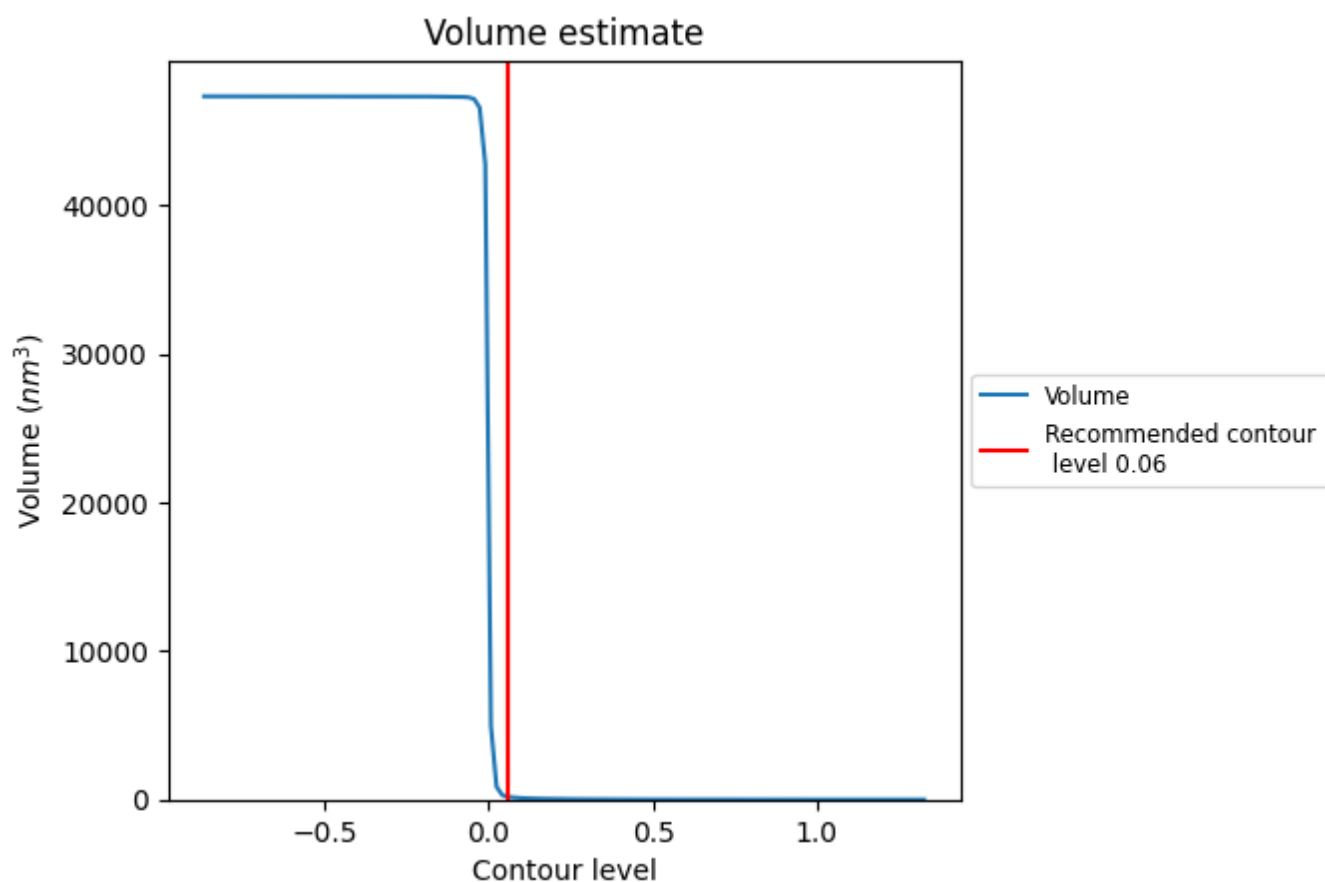
This section contains the results of statistical analysis of the map.

### 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.

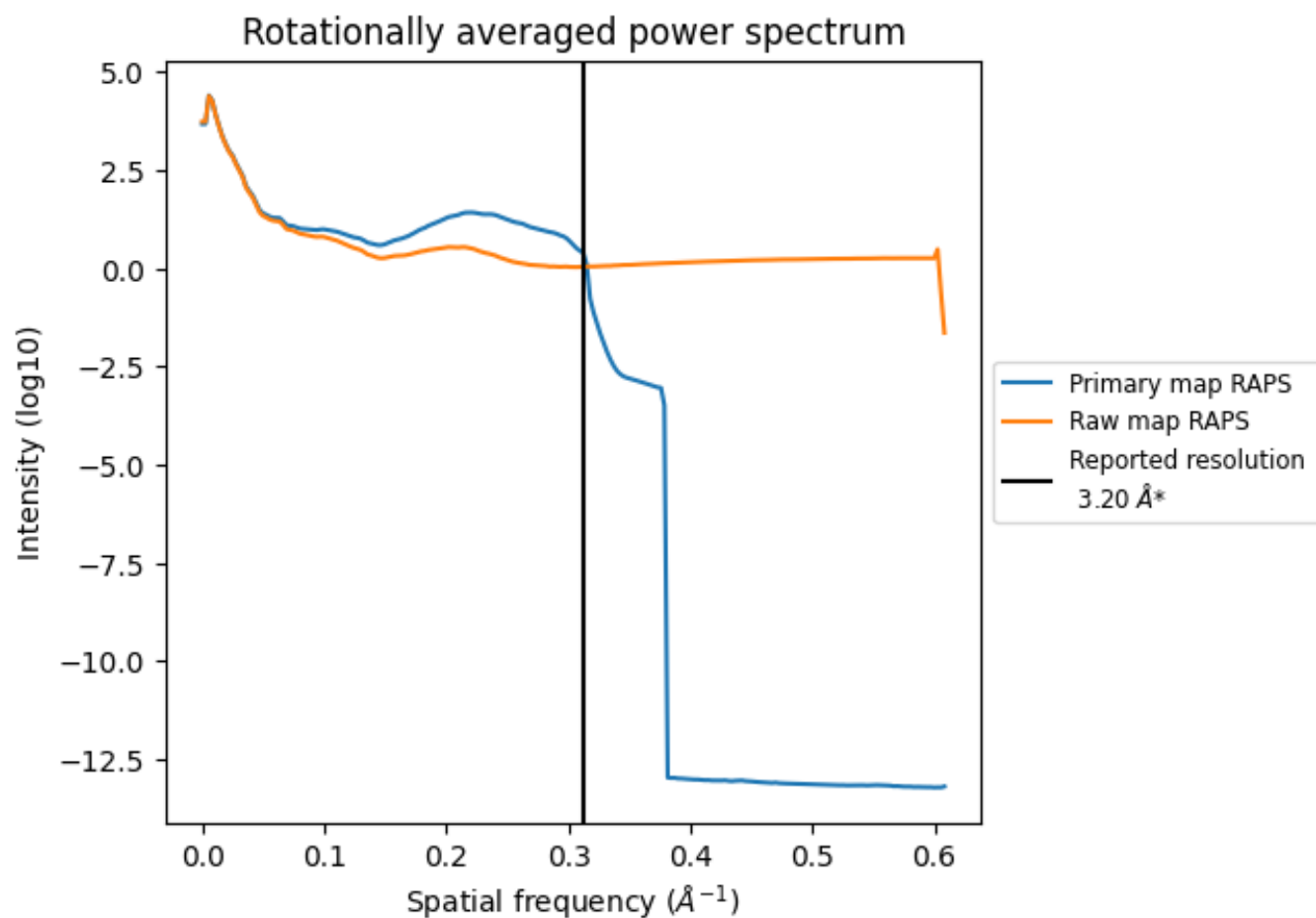
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182  $\text{nm}^3$ ; this corresponds to an approximate mass of 165 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 ⓘ

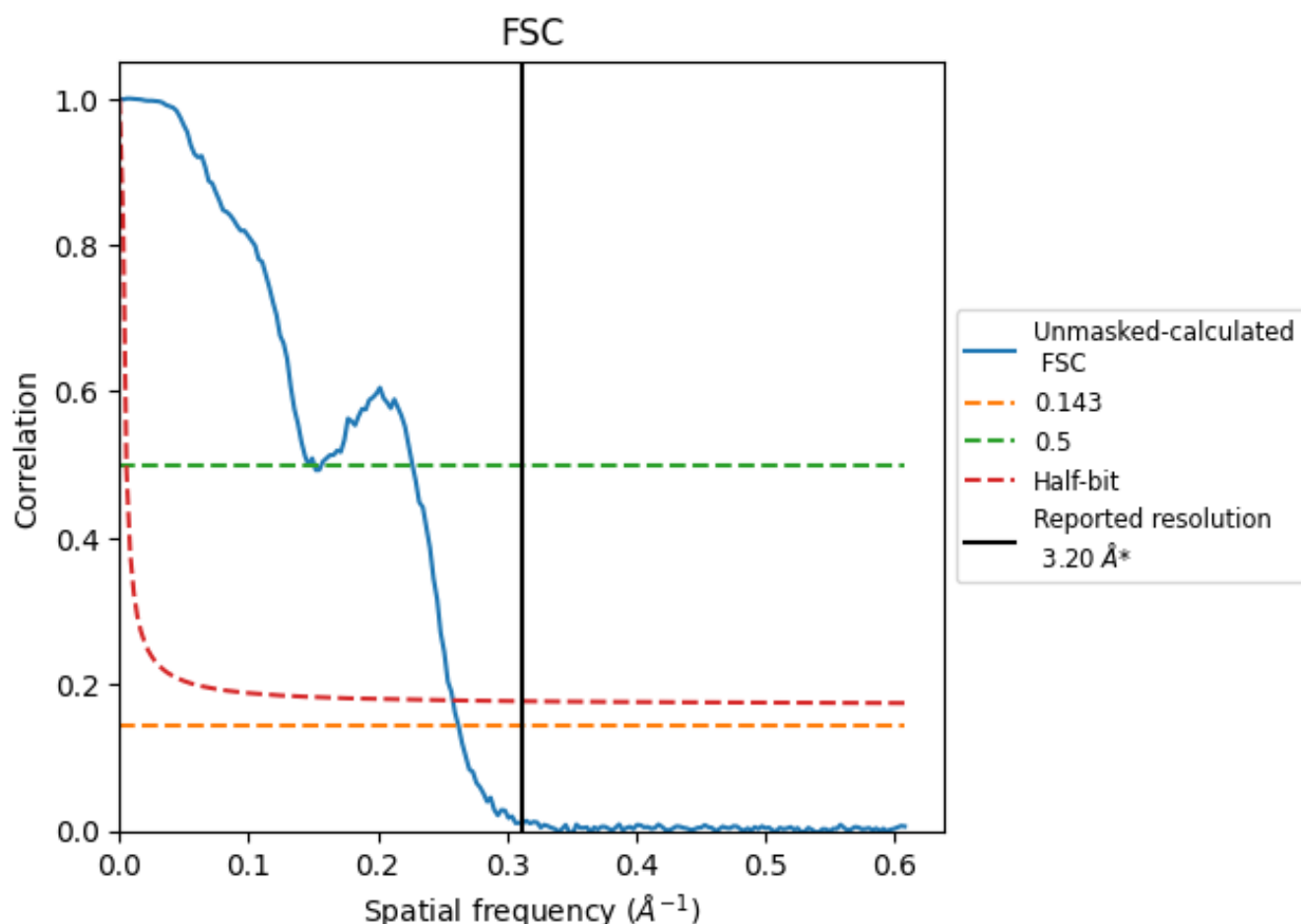


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

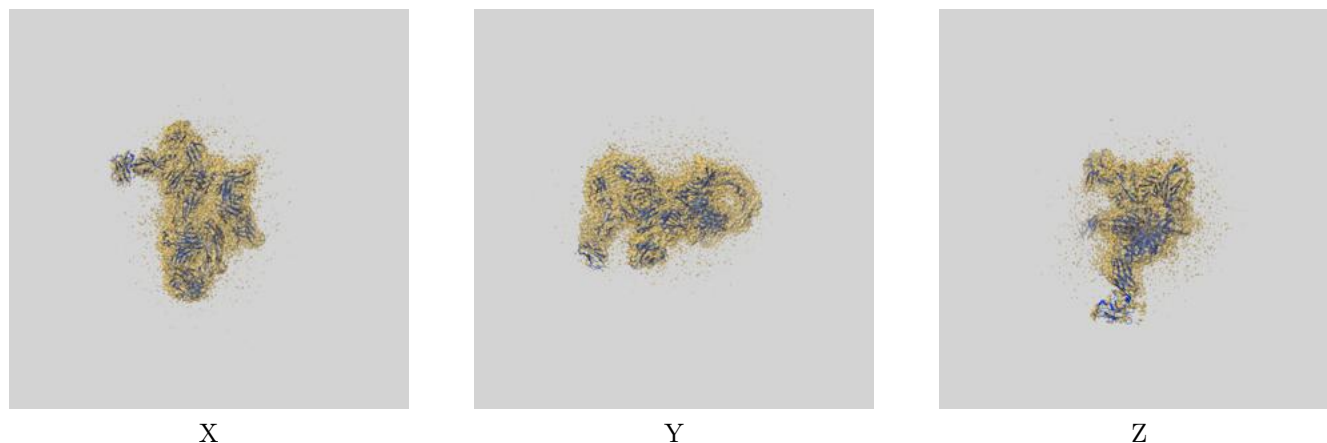
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	6.84	3.87

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.81 differs from the reported value 3.2 by more than 10 %

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

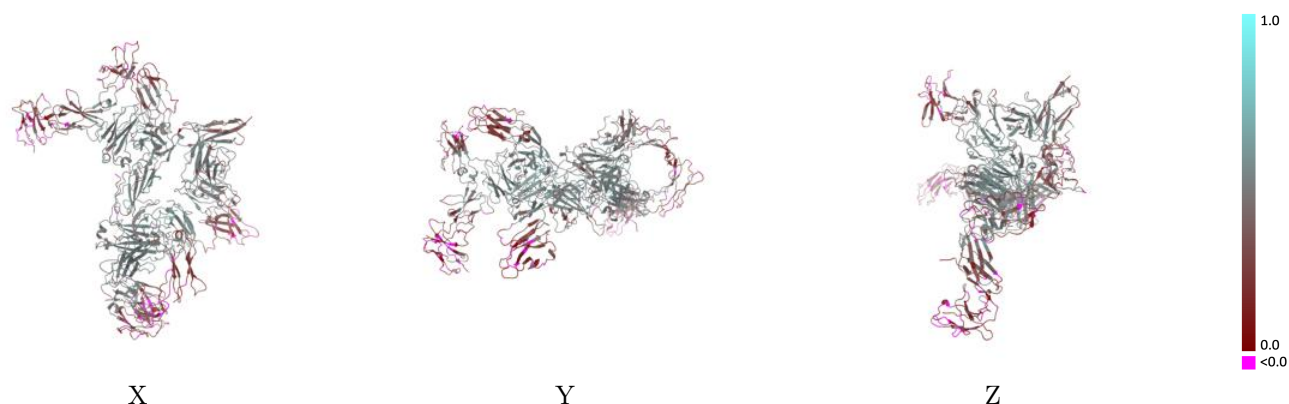
This section contains information regarding the fit between EMDB map EMD-40567 and PDB model 8SKU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



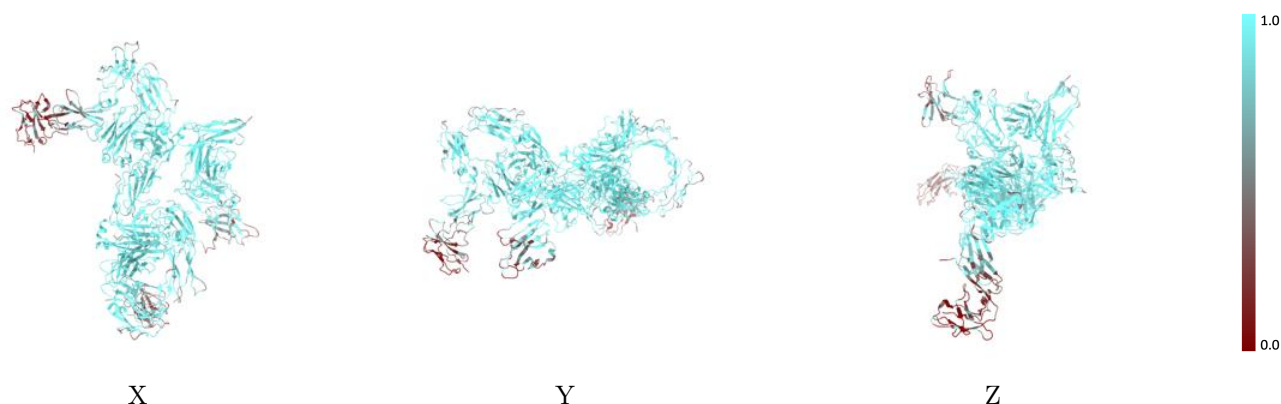
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

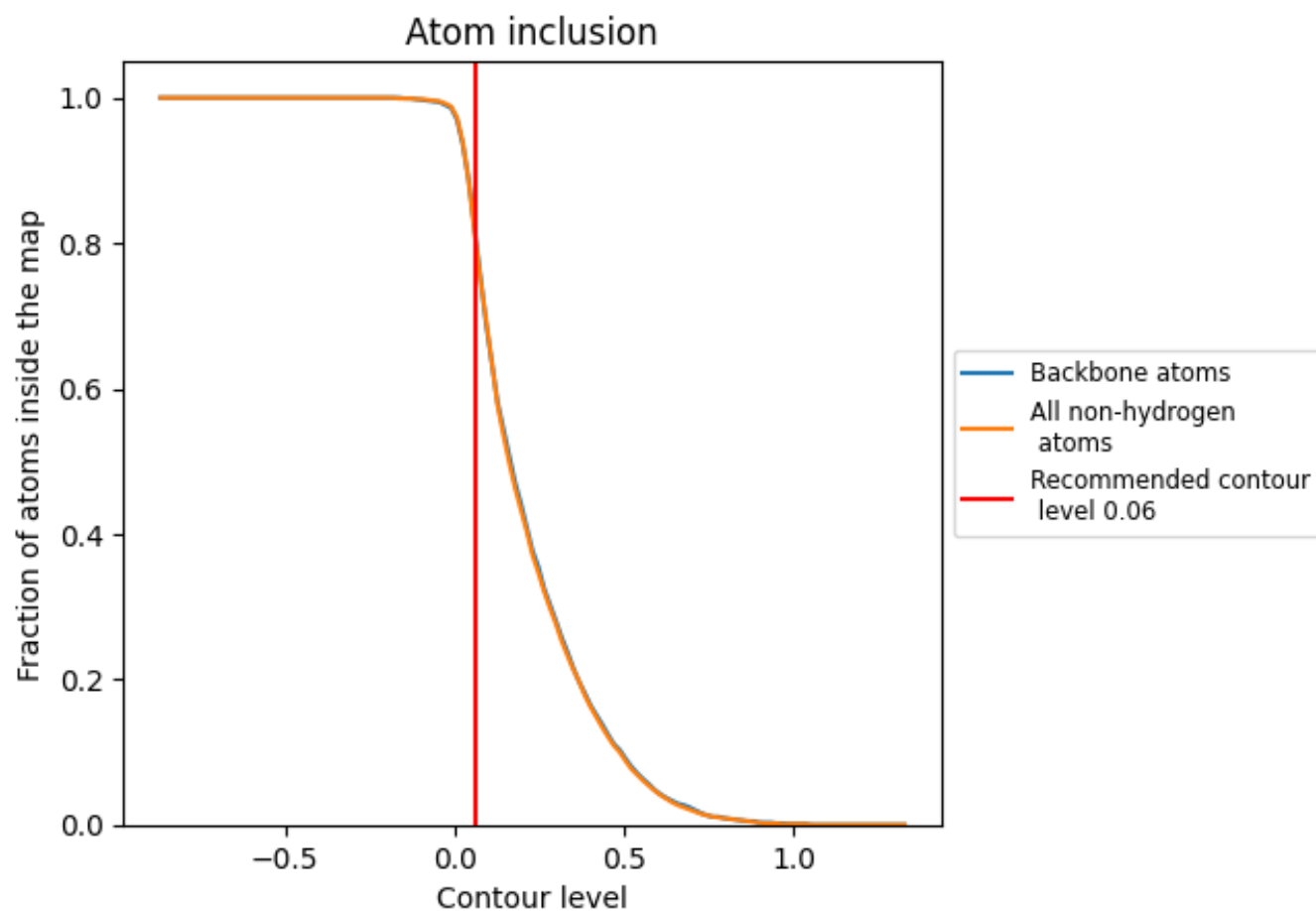
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.06).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8110	<div></div> 0.4000
A	<div></div> 0.9110	<div></div> 0.4270
B	<div></div> 0.9040	<div></div> 0.4170
C	<div></div> 0.9190	<div></div> 0.4630
D	<div></div> 0.9020	<div></div> 0.4030
E	<div></div> 0.8550	<div></div> 0.4270
H	<div></div> 0.6430	<div></div> 0.2190
I	<div></div> 0.8930	<div></div> 0.4020
J	<div></div> 0.9230	<div></div> 0.4950
K	<div></div> 0.9290	<div></div> 0.3870
L	<div></div> 0.8930	<div></div> 0.3720
R	<div></div> 0.5230	<div></div> 0.2680
S	<div></div> 0.4220	<div></div> 0.2660

