



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 02:05 PM EDT

PDB ID : 9YB1 / pdb_00009yb1
EMDB ID : EMD-72745
Title : Localized reconstruction of the asymmetric unit of SINV/EEEV at pH 5.6.
Authors : Bandyopadhyay, A.; Klose, T.; Kuhn, R.J.
Deposited on : 2025-09-16
Resolution : 4.70 Å (reported)
Based on initial model : 6MX4

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

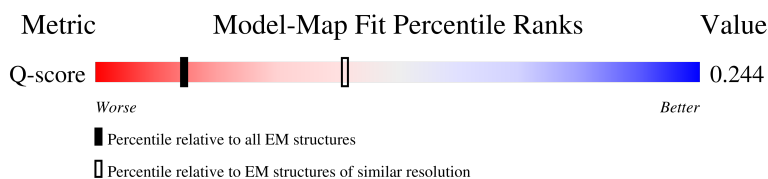
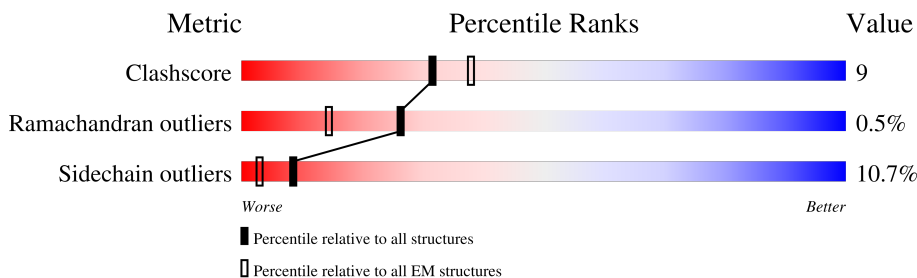
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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.





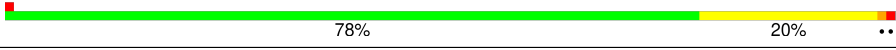



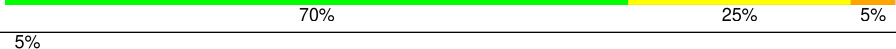




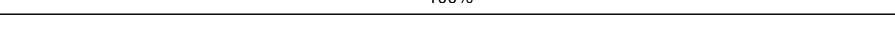
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	437	<div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	B	437	<div> <div>69%</div> <div>29%</div> <div>.</div> </div>
1	C	437	<div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	D	437	<div> <div>71%</div> <div>24%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	P	160	
2	Q	160	
2	R	160	
2	S	160	
3	a	420	
3	b	420	
3	c	420	
3	d	420	
4	E	3	
4	F	3	
4	G	3	
4	H	3	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31679 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 E1 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	437	Total	C	N	O	S	0	0
			3329	2121	551	637	20		
1	B	437	Total	C	N	O	S	0	0
			3329	2121	551	637	20		
1	C	437	Total	C	N	O	S	0	0
			3329	2121	551	637	20		
1	D	437	Total	C	N	O	S	0	0
			3329	2121	551	637	20		

- Molecule 2 is a protein called Capsid protein.

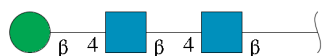
Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		
2	Q	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		
2	R	159	Total	C	N	O	S	0	0
			1230	773	219	231	7		
2	S	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		

- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	420	Total	C	N	O	S	0	0
			3301	2087	598	592	24		
3	b	420	Total	C	N	O	S	0	0
			3301	2087	598	592	24		
3	c	420	Total	C	N	O	S	0	0
			3301	2087	598	592	24		
3	d	420	Total	C	N	O	S	0	0
			3301	2087	598	592	24		

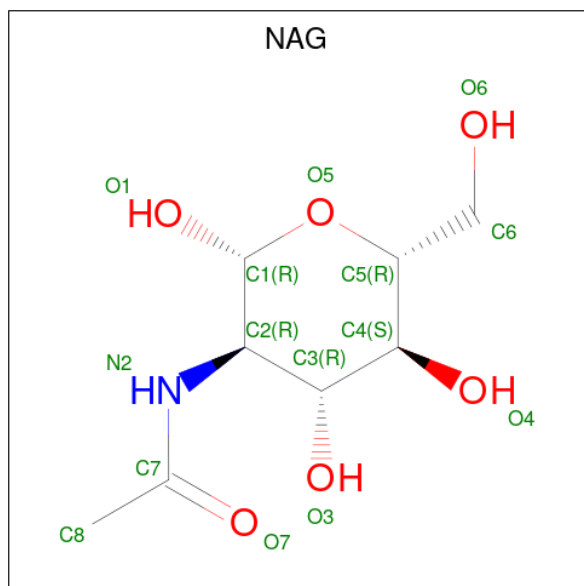
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	G	3	Total	C	N	O	0	0
			39	22	2	15		
4	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

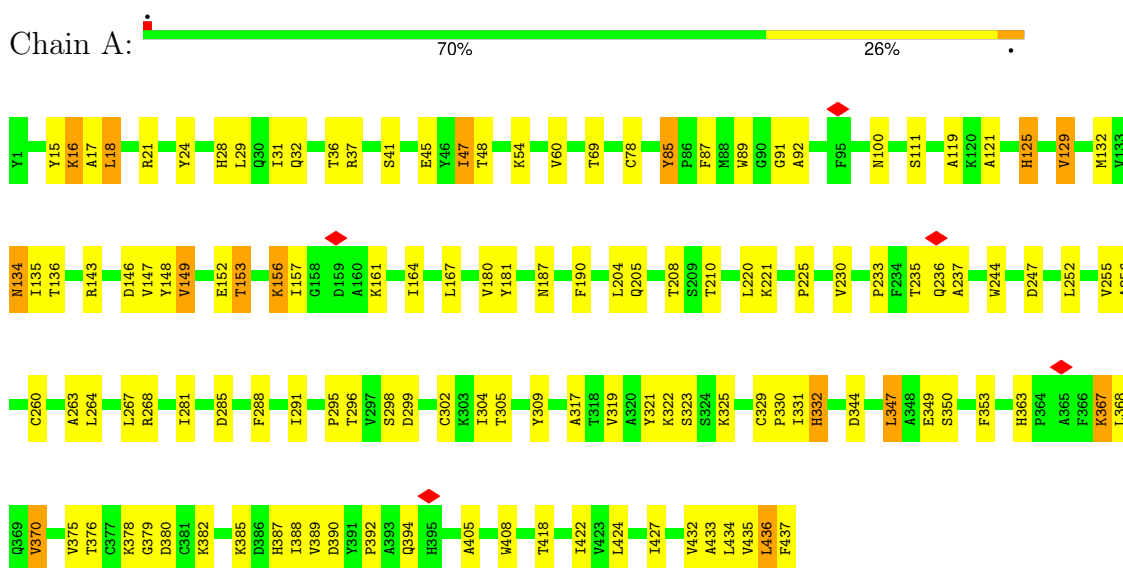


Mol	Chain	Residues	Atoms				AltConf
5	a	1	Total	C	N	O	0
			14	8	1	5	
5	b	1	Total	C	N	O	0
			14	8	1	5	
5	c	1	Total	C	N	O	0
			14	8	1	5	
5	d	1	Total	C	N	O	0
			14	8	1	5	

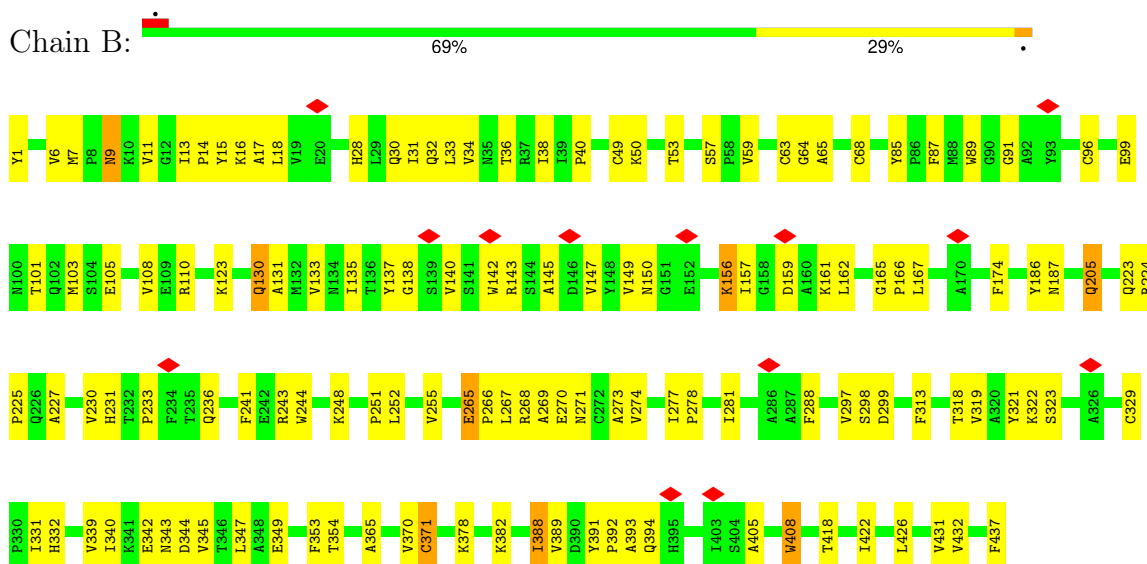
3 Residue-property plots

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.

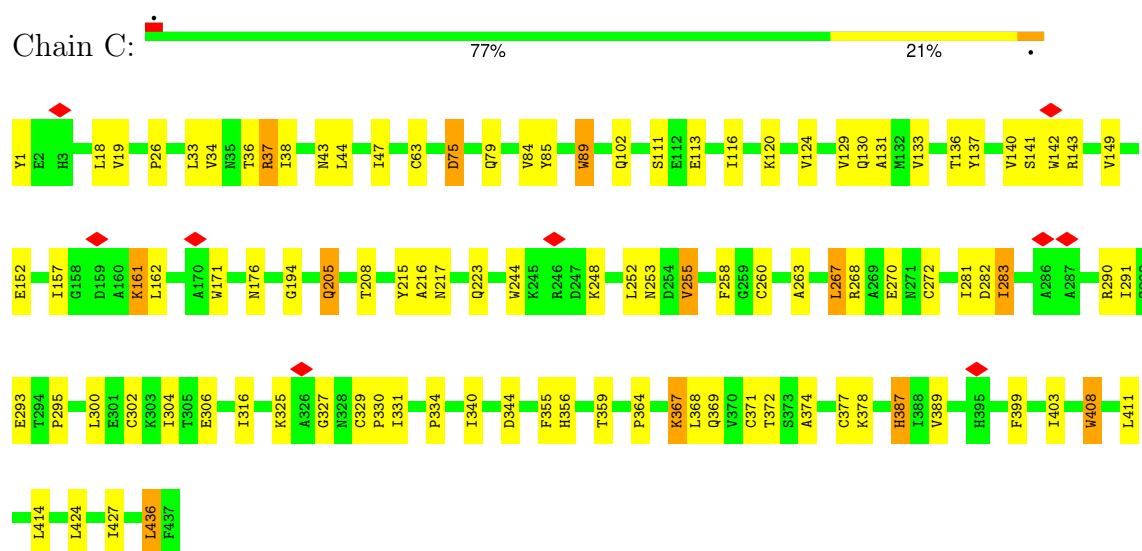
- Molecule 1: E1 glycoprotein



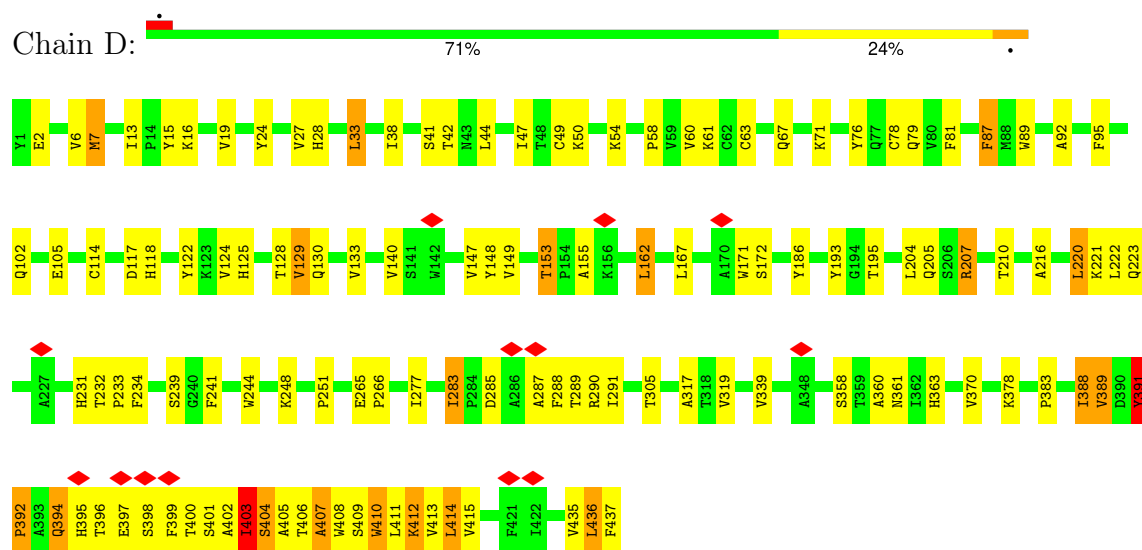
- Molecule 1: E1 glycoprotein



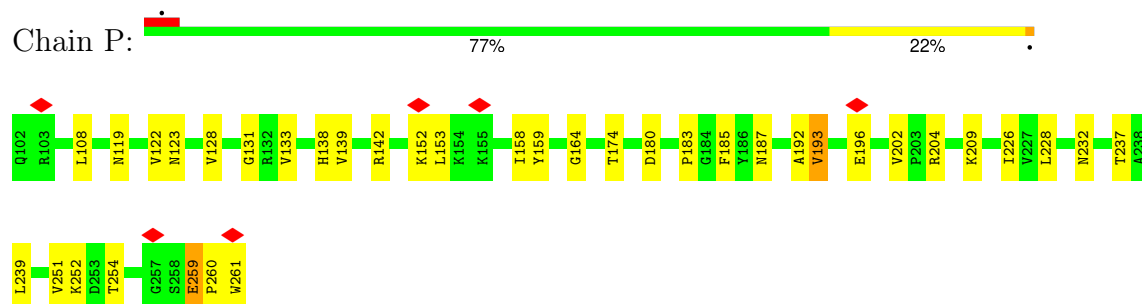
- Molecule 1: E1 glycoprotein



- Molecule 1: E1 glycoprotein

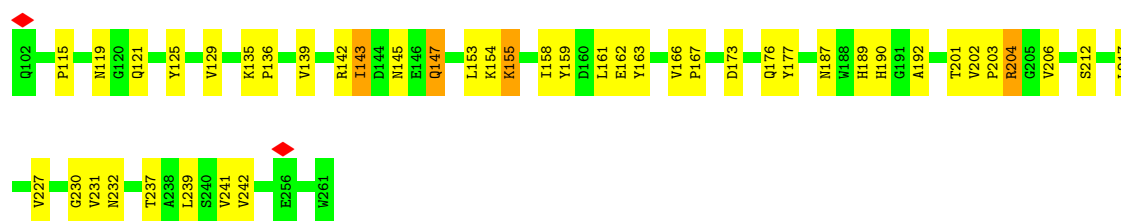


- Molecule 2: Capsid protein

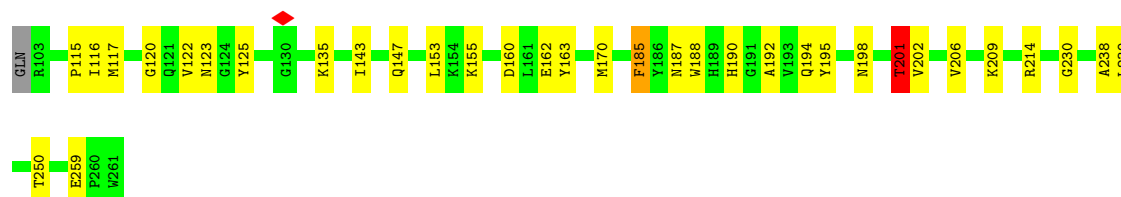
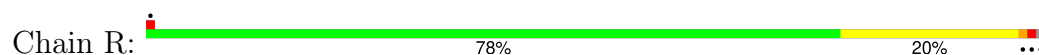


- Molecule 2: Capsid protein

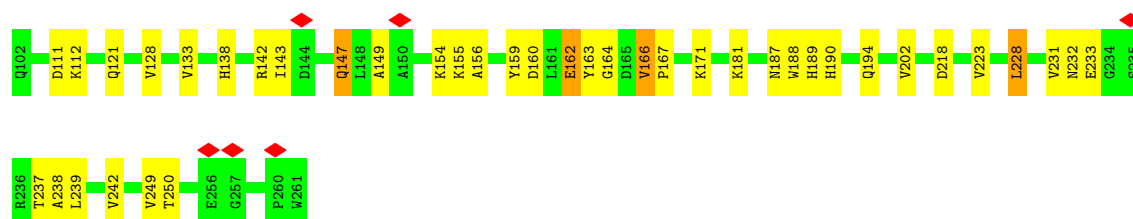
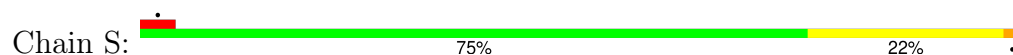




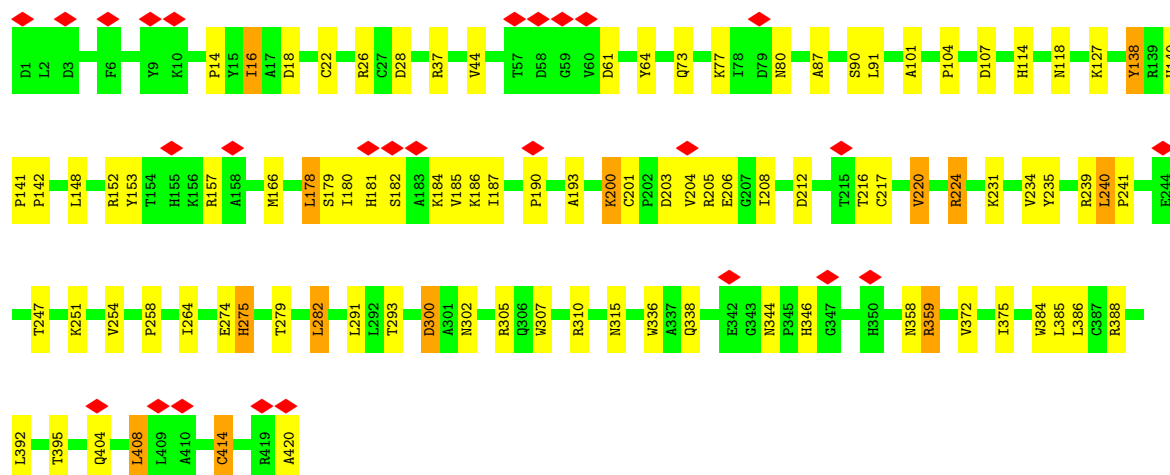
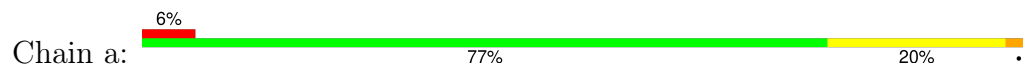
• Molecule 2: Capsid protein



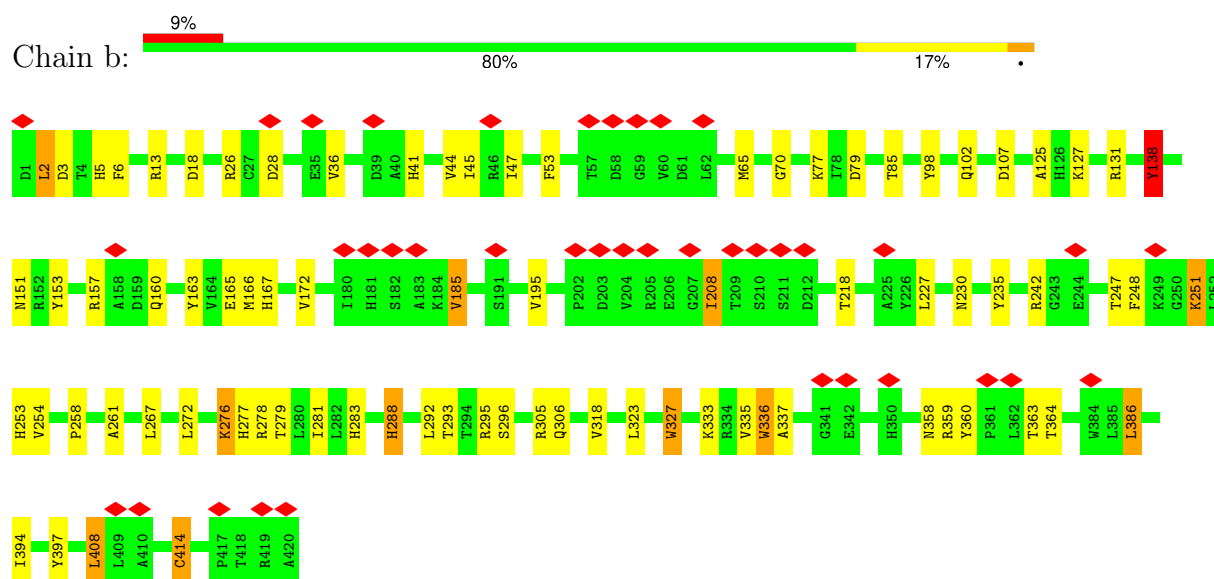
• Molecule 2: Capsid protein



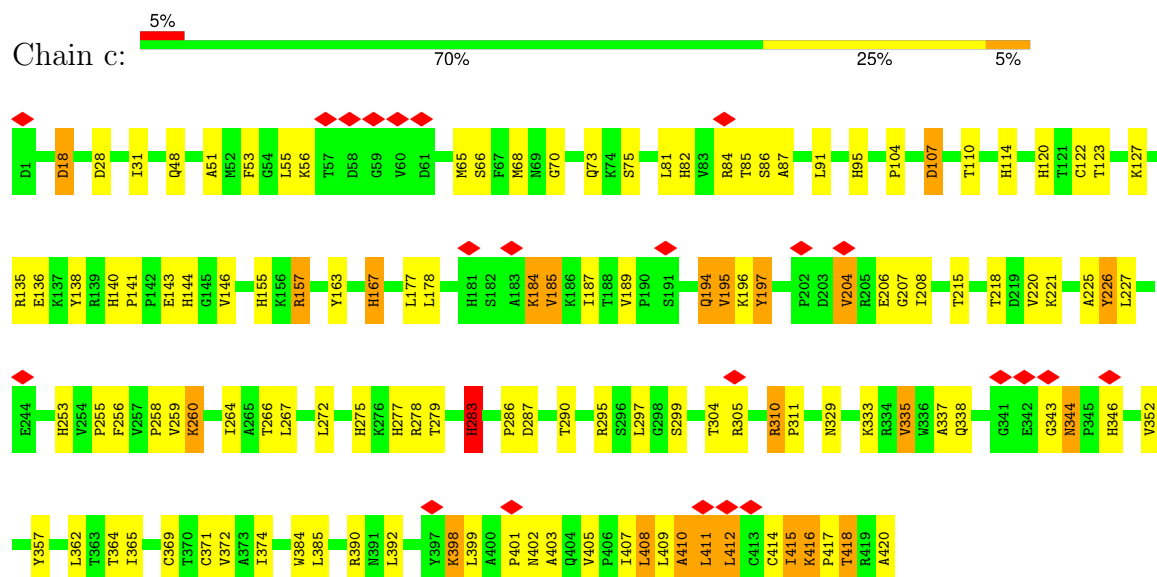
• Molecule 3: E2 glycoprotein



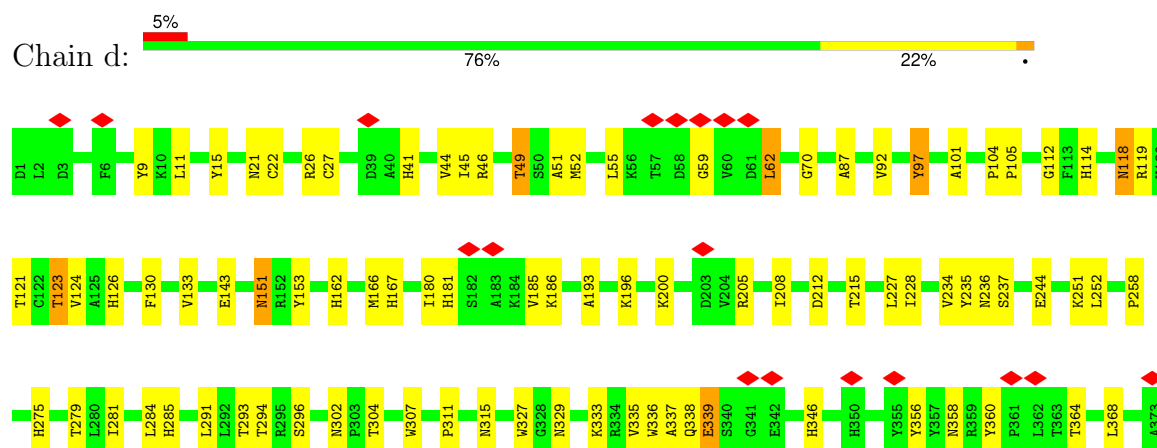
• Molecule 3: E2 glycoprotein



• Molecule 3: E2 glycoprotein



• Molecule 3: E2 glycoprotein





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



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



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



- Molecule 4: beta-D-mannopyranose-(1-4)-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	265738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36.2	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.354	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	279.30002, 279.30002, 279.30002	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.72	0/3419	1.03	0/4668
1	B	0.67	0/3419	0.93	0/4668
1	C	0.72	0/3419	1.07	3/4668 (0.1%)
1	D	0.71	0/3419	1.06	5/4668 (0.1%)
2	P	0.73	0/1266	1.08	0/1711
2	Q	0.69	0/1266	1.16	0/1711
2	R	0.72	0/1257	1.22	1/1699 (0.1%)
2	S	0.76	0/1266	1.23	0/1711
3	a	0.73	0/3396	1.12	8/4631 (0.2%)
3	b	0.79	0/3396	1.12	1/4631 (0.0%)
3	c	0.77	0/3396	1.16	9/4631 (0.2%)
3	d	0.79	0/3396	1.22	8/4631 (0.2%)
All	All	0.74	0/32315	1.10	35/44028 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
2	S	0	2
3	a	0	1
3	b	0	2
3	c	0	1
3	d	0	5
All	All	0	16

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	383	PRO	N-CA-CB	5.95	106.52	103.19
1	C	387	HIS	CA-CB-CG	5.83	119.63	113.80
1	D	404	SER	N-CA-C	-5.78	106.00	113.16
3	a	80	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	D	412	LYS	N-CA-C	-5.53	105.35	111.71
3	c	412	LEU	N-CA-C	-5.49	107.13	113.88
3	a	37	ARG	NE-CZ-NH2	5.47	124.13	119.20
3	c	167	HIS	CB-CG-CD2	-5.41	124.17	131.20
3	c	48	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	D	392	PRO	N-CA-C	5.34	118.97	111.33
3	d	360	TYR	CA-C-N	5.31	125.39	119.87
3	d	360	TYR	C-N-CA	5.31	125.39	119.87
3	a	224	ARG	CD-NE-CZ	5.29	131.81	124.40
3	a	239	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	a	310	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	c	95	HIS	CB-CG-CD2	-5.28	124.33	131.20
3	d	339	GLU	CA-C-N	5.27	127.59	120.38
3	d	339	GLU	C-N-CA	5.27	127.59	120.38
3	a	138	TYR	N-CA-C	5.26	117.97	109.40
3	a	275	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	C	387	HIS	CB-CG-CD2	-5.19	124.45	131.20
3	d	302	ASN	CB-CA-C	5.18	115.51	111.00
3	c	410	ALA	N-CA-C	-5.15	106.96	114.12
3	c	283	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	C	223	GLN	OE1-CD-NE2	-5.12	117.48	122.60
3	c	135	ARG	NE-CZ-NH2	5.12	123.81	119.20
3	c	120	HIS	CB-CG-CD2	-5.12	124.55	131.20
3	d	114	HIS	CB-CG-CD2	-5.08	124.59	131.20
3	b	358	ASN	OD1-CG-ND2	-5.07	117.53	122.60
3	d	118	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	D	363	HIS	CB-CG-CD2	-5.05	124.64	131.20
3	a	346	HIS	CB-CG-CD2	-5.05	124.64	131.20
2	R	201	THR	CA-CB-CG2	5.03	119.05	110.50
3	d	162	HIS	CB-CG-CD2	-5.01	124.69	131.20
3	c	114	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	TYR	Sidechain
1	B	110	ARG	Sidechain
1	B	391	TYR	Sidechain
1	C	1	TYR	Sidechain
1	D	391	TYR	Sidechain
2	S	142	ARG	Sidechain
2	S	159	TYR	Sidechain
3	a	359	ARG	Sidechain
3	b	138	TYR	Sidechain
3	b	305	ARG	Sidechain
3	c	278	ARG	Sidechain
3	d	205	ARG	Sidechain
3	d	356	TYR	Sidechain
3	d	388	ARG	Sidechain
3	d	46	ARG	Sidechain
3	d	97	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3329	0	3239	72	0
1	B	3329	0	3239	74	0
1	C	3329	0	3239	50	0
1	D	3329	0	3239	98	0
2	P	1239	0	1225	18	0
2	Q	1239	0	1225	25	0
2	R	1230	0	1217	20	0
2	S	1239	0	1225	30	0
3	a	3301	0	3263	41	0
3	b	3301	0	3262	40	0
3	c	3301	0	3261	70	0
3	d	3301	0	3261	55	0
4	E	39	0	34	6	0
4	F	39	0	34	3	0
4	G	39	0	34	6	0
4	H	39	0	34	0	0
5	a	14	0	13	1	0
5	b	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	c	14	0	13	0	0
5	d	14	0	13	0	0
All	All	31679	0	31083	547	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (547) 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:S:156:ALA:HB2	3:d:398:LYS:NZ	1.36	1.35
1:A:32:GLN:NE2	4:E:1:NAG:HN2	1.26	1.33
1:A:134:ASN:OD1	4:E:1:NAG:C1	1.78	1.30
1:A:32:GLN:NE2	4:E:1:NAG:N2	1.89	1.17
3:d:397:TYR:HE2	3:d:403:ALA:O	1.34	1.08
2:S:154:LYS:HZ1	3:d:398:LYS:HE2	1.27	0.98
2:S:156:ALA:CB	3:d:398:LYS:NZ	2.27	0.97
2:S:156:ALA:HB2	3:d:398:LYS:HZ1	1.26	0.93
3:d:397:TYR:CE2	3:d:403:ALA:O	2.22	0.92
2:S:156:ALA:HB2	3:d:398:LYS:HZ2	1.08	0.89
1:D:397:GLU:HB3	1:D:401:SER:HB3	1.56	0.86
1:D:412:LYS:HA	1:D:415:VAL:HB	1.59	0.85
1:C:290:ARG:HB2	1:C:293:GLU:HG2	1.55	0.85
3:c:195:VAL:HG23	3:c:226:TYR:H	1.42	0.83
2:P:204:ARG:HH22	2:P:232:ASN:HD22	1.21	0.82
2:S:156:ALA:HA	3:d:398:LYS:HE3	1.62	0.82
1:A:437:PHE:HB2	2:P:251:VAL:HG11	1.60	0.81
3:c:408:LEU:HA	3:c:411:LEU:HB2	1.64	0.78
1:A:322:LYS:HA	1:A:350:SER:HA	1.67	0.77
1:D:79:GLN:HB2	1:D:222:LEU:HD12	1.65	0.76
1:A:330:PRO:HA	1:A:344:ASP:HB3	1.66	0.76
3:a:87:ALA:HB3	3:a:104:PRO:HG3	1.67	0.76
1:D:38:ILE:HA	1:D:129:VAL:HG12	1.70	0.73
3:a:179:SER:HB2	3:a:186:LYS:HB2	1.70	0.73
3:c:194:GLN:HB2	3:c:208:ILE:HA	1.71	0.73
2:S:156:ALA:HB2	3:d:398:LYS:CE	2.19	0.72
3:a:203:ASP:HB3	3:a:216:THR:HG21	1.72	0.72
2:S:154:LYS:HZ1	3:d:398:LYS:CE	2.01	0.72
1:A:331:ILE:HG23	1:A:370:VAL:HB	1.71	0.71
2:S:156:ALA:CB	3:d:398:LYS:HZ2	1.95	0.71
1:D:408:TRP:HB3	1:D:412:LYS:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:OE1	4:E:1:NAG:H82	1.91	0.71
1:C:34:VAL:CG1	4:G:1:NAG:H81	2.21	0.71
2:P:153:LEU:HD22	2:P:164:GLY:HA3	1.72	0.71
3:a:240:LEU:HD13	3:a:241:PRO:HD2	1.73	0.71
3:a:190:PRO:HD2	3:a:193:ALA:HB3	1.72	0.71
3:c:405:VAL:H	3:c:408:LEU:HD12	1.56	0.71
1:D:220:LEU:HD11	1:D:234:PHE:HD2	1.56	0.71
2:R:143:ILE:H	2:R:143:ILE:HD12	1.56	0.71
1:C:252:LEU:HA	1:C:255:VAL:HG12	1.72	0.70
1:A:367:LYS:HA	1:A:376:THR:HA	1.72	0.70
3:c:415:ILE:O	3:c:416:LYS:C	2.35	0.70
1:D:408:TRP:HA	1:D:411:LEU:HB2	1.74	0.69
1:D:410:TRP:CZ2	3:d:346:HIS:HB3	2.27	0.69
3:d:181:HIS:HB2	3:d:186:LYS:HB2	1.73	0.69
1:A:48:THR:HB	1:A:119:ALA:HB3	1.73	0.69
1:A:220:LEU:HD22	1:A:236:GLN:HA	1.75	0.68
1:C:263:ALA:HB3	1:C:268:ARG:HB3	1.75	0.67
2:S:156:ALA:CB	3:d:398:LYS:CE	2.71	0.67
3:c:407:ILE:HG13	3:c:411:LEU:HA	1.75	0.67
3:d:55:LEU:HD13	3:d:59:GLY:HA2	1.76	0.67
1:B:142:TRP:NE1	4:F:2:NAG:H81	2.08	0.67
1:D:285:ASP:HA	1:D:288:PHE:HD2	1.59	0.67
1:D:408:TRP:O	1:D:409:SER:C	2.37	0.67
1:D:361:ASN:HB3	1:D:403:ILE:HA	1.75	0.67
1:B:331:ILE:HD13	1:B:345:VAL:HG23	1.76	0.67
1:A:129:VAL:HG13	1:A:149:VAL:HG11	1.77	0.66
3:c:417:PRO:O	3:c:418:THR:C	2.38	0.66
1:B:143:ARG:HB3	1:B:157:ILE:HD11	1.78	0.66
2:P:158:ILE:HD12	2:P:158:ILE:H	1.61	0.66
1:B:388:ILE:HG13	3:b:335:VAL:HG13	1.77	0.66
1:C:18:LEU:HD11	1:C:26:PRO:HB2	1.77	0.66
3:a:178:LEU:HD13	3:a:220:VAL:HG23	1.78	0.65
1:B:59:VAL:HG22	3:b:242:ARG:HD2	1.79	0.64
1:B:223:GLN:HB2	1:B:233:PRO:HB2	1.79	0.64
1:C:295:PRO:HG3	1:C:327:GLY:HA3	1.80	0.64
3:c:178:LEU:HD22	3:c:220:VAL:HG13	1.80	0.63
1:D:61:LYS:HE2	1:D:63:CYS:H	1.64	0.62
3:b:292:LEU:HG	3:b:327:TRP:HB2	1.81	0.62
1:B:59:VAL:HB	1:B:103:MET:HB3	1.81	0.62
1:A:256:ALA:HB1	1:A:260:CYS:HB2	1.80	0.62
1:B:265:GLU:HB3	1:B:266:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD11	1:A:208:THR:HA	1.82	0.61
1:B:187:ASN:HB3	1:B:252:LEU:HD22	1.82	0.61
1:A:263:ALA:HB3	1:A:268:ARG:HB3	1.83	0.61
1:D:33:LEU:HA	1:D:133:VAL:HG12	1.83	0.61
1:A:302:CYS:HA	1:A:319:VAL:HG22	1.81	0.61
2:S:156:ALA:CA	3:d:398:LYS:HE3	2.30	0.61
1:C:34:VAL:HG13	4:G:1:NAG:H81	1.83	0.60
1:D:283:ILE:HD11	1:D:287:ALA:HB3	1.82	0.60
1:D:402:ALA:O	1:D:403:ILE:C	2.44	0.60
2:Q:129:VAL:HG21	2:Q:177:TYR:HB3	1.83	0.60
2:Q:129:VAL:HG23	2:Q:176:GLN:HA	1.83	0.60
1:A:32:GLN:NE2	4:E:1:NAG:C7	2.64	0.60
1:A:32:GLN:CD	4:E:1:NAG:H82	2.26	0.60
1:B:162:LEU:HG	1:B:281:ILE:HG12	1.84	0.60
1:C:359:THR:HG21	1:C:364:PRO:HG3	1.84	0.60
1:B:142:TRP:CD1	4:F:2:NAG:H81	2.37	0.59
1:C:424:LEU:HD13	1:C:427:ILE:HD11	1.83	0.59
3:a:61:ASP:HB3	3:a:64:TYR:HB2	1.83	0.59
3:c:87:ALA:HB3	3:c:104:PRO:HG3	1.84	0.59
3:c:196:LYS:HA	3:c:207:GLY:HA3	1.84	0.59
1:D:41:SER:HB3	1:D:125:HIS:HB3	1.84	0.59
3:a:293:THR:HG22	3:a:305:ARG:HA	1.85	0.59
1:B:9:ASN:HB2	1:B:273:ALA:HA	1.84	0.59
3:c:405:VAL:O	3:c:408:LEU:HB2	2.03	0.59
1:D:408:TRP:HA	1:D:412:LYS:N	2.17	0.59
1:C:194:GLY:H	1:C:205:GLN:HG2	1.68	0.58
1:A:132:MET:HA	1:A:146:ASP:HA	1.86	0.58
1:B:297:VAL:HA	1:B:323:SER:HA	1.85	0.58
1:B:331:ILE:HG22	1:B:370:VAL:HG13	1.85	0.58
1:D:95:PHE:CG	3:d:200:LYS:HG3	2.38	0.58
1:C:34:VAL:CG1	4:G:1:NAG:C8	2.81	0.58
1:C:34:VAL:HG11	4:G:1:NAG:C8	2.33	0.58
3:c:343:GLY:O	3:c:344:ASN:C	2.46	0.58
1:A:435:VAL:C	1:A:437:PHE:N	2.62	0.58
1:D:13:ILE:HD12	1:D:395:HIS:CD2	2.39	0.58
1:A:15:TYR:HE1	1:A:17:ALA:HB2	1.69	0.58
1:D:60:VAL:HG13	1:D:102:GLN:HG2	1.85	0.58
3:a:408:LEU:HB2	3:a:414:CYS:HB2	1.86	0.58
3:b:318:VAL:HG12	3:b:337:ALA:HB2	1.85	0.58
3:b:408:LEU:HB2	3:b:414:CYS:HB2	1.86	0.58
1:C:33:LEU:HA	1:C:133:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:SER:C	1:D:403:ILE:HG23	2.29	0.57
1:D:408:TRP:HA	1:D:411:LEU:CB	2.34	0.57
1:B:318:THR:HA	1:B:354:THR:HA	1.85	0.57
1:D:402:ALA:HB3	1:D:406:THR:HB	1.86	0.57
3:a:180:ILE:HA	3:a:185:VAL:HA	1.86	0.57
1:B:31:ILE:HD13	1:B:135:ILE:HB	1.87	0.57
1:D:148:TYR:HB2	1:D:153:THR:HG21	1.87	0.57
1:D:408:TRP:CA	1:D:412:LYS:H	2.18	0.57
2:S:228:LEU:HD21	2:S:242:VAL:HG23	1.87	0.57
1:A:432:VAL:O	1:A:433:ALA:C	2.48	0.57
3:c:31:ILE:HG22	3:c:51:ALA:HB2	1.86	0.56
3:d:407:ILE:HG22	3:d:410:ALA:HB3	1.87	0.56
1:D:402:ALA:O	1:D:406:THR:N	2.38	0.56
3:a:201:CYS:HB2	3:a:216:THR:HB	1.88	0.56
1:B:167:LEU:HA	1:B:277:ILE:HG22	1.88	0.56
3:b:167:HIS:HB3	3:b:247:THR:HG23	1.88	0.56
1:D:408:TRP:CA	1:D:411:LEU:HB2	2.36	0.56
3:a:107:ASP:HA	3:a:127:LYS:HA	1.87	0.56
3:b:107:ASP:HA	3:b:127:LYS:HA	1.86	0.56
3:c:408:LEU:O	3:c:409:LEU:C	2.47	0.56
3:c:68:MET:HA	3:c:73:GLN:HA	1.87	0.56
3:c:177:LEU:HD12	3:c:225:ALA:HB1	1.88	0.56
3:c:197:TYR:HE1	3:c:207:GLY:H	1.54	0.56
2:S:156:ALA:CB	3:d:398:LYS:HE3	2.36	0.56
1:A:220:LEU:HD22	1:A:237:ALA:H	1.71	0.55
1:D:79:GLN:HB3	1:D:81:PHE:CE2	2.41	0.55
1:A:187:ASN:H	1:A:252:LEU:HD21	1.70	0.55
1:C:34:VAL:HG11	4:G:1:NAG:H81	1.87	0.55
1:B:156:LYS:HA	1:B:161:LYS:HA	1.88	0.55
1:D:7:MET:HE2	1:D:15:TYR:HB3	1.87	0.55
2:Q:143:ILE:HG13	2:Q:145:ASN:H	1.70	0.55
3:c:310:ARG:HH21	3:c:310:ARG:N	2.04	0.55
1:D:406:THR:O	1:D:408:TRP:N	2.37	0.55
1:B:405:ALA:HA	1:B:408:TRP:HB2	1.89	0.55
1:D:204:LEU:HD23	1:D:216:ALA:HB2	1.89	0.55
1:D:360:ALA:O	1:D:403:ILE:HG22	2.06	0.55
1:B:33:LEU:HA	1:B:133:VAL:HA	1.89	0.55
3:c:85:THR:HG22	3:c:86:SER:H	1.72	0.54
3:a:315:ASN:HD21	5:a:501:NAG:C1	2.19	0.54
1:D:408:TRP:C	1:D:412:LYS:H	2.13	0.54
1:C:369:GLN:HA	1:C:374:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:147:GLN:CD	2:Q:147:GLN:H	2.16	0.54
3:a:291:LEU:HD13	3:a:307:TRP:CD1	2.42	0.54
3:d:87:ALA:HB3	3:d:104:PRO:HG3	1.90	0.54
1:B:64:GLY:H	1:B:99:GLU:HB3	1.73	0.54
1:C:387:HIS:HB3	3:c:337:ALA:HA	1.90	0.54
3:c:310:ARG:HH21	3:c:310:ARG:H	1.56	0.54
3:c:407:ILE:O	3:c:411:LEU:N	2.33	0.54
1:A:435:VAL:O	1:A:437:PHE:N	2.41	0.54
1:A:264:LEU:HD23	1:A:264:LEU:H	1.72	0.53
1:C:215:TYR:OH	1:C:217:ASN:HB2	2.07	0.53
1:D:47:ILE:HD11	1:D:118:HIS:CG	2.42	0.53
3:b:160:GLN:HB3	3:b:253:HIS:CE1	2.43	0.53
3:d:124:VAL:HG12	3:d:126:HIS:H	1.73	0.53
2:R:188:TRP:HE1	2:R:190:HIS:CG	2.25	0.53
3:c:407:ILE:O	3:c:408:LEU:C	2.51	0.53
1:D:95:PHE:CD1	3:d:200:LYS:HG3	2.43	0.53
1:D:412:LYS:CA	1:D:415:VAL:HB	2.37	0.53
2:R:188:TRP:HE1	2:R:190:HIS:CD2	2.26	0.53
3:a:344:ASN:HB2	3:a:359:ARG:HH22	1.73	0.53
1:A:432:VAL:HA	1:A:435:VAL:HB	1.89	0.53
2:Q:115:PRO:HA	2:Q:125:TYR:HA	1.90	0.53
2:P:183:PRO:HB3	2:P:196:GLU:HA	1.89	0.53
1:A:298:SER:O	1:A:322:LYS:HB3	2.08	0.53
2:P:228:LEU:HD12	2:P:261:TRP:HE1	1.74	0.53
1:B:321:TYR:HE2	1:B:353:PHE:HD2	1.56	0.53
1:B:370:VAL:HG12	1:B:371:CYS:SG	2.49	0.53
2:P:202:VAL:HG22	2:P:239:LEU:HD21	1.90	0.53
3:d:41:HIS:NE2	3:d:151:ASN:HB3	2.23	0.53
1:D:408:TRP:HA	1:D:412:LYS:H	1.74	0.52
1:C:408:TRP:HD1	1:C:411:LEU:HD21	1.74	0.52
2:Q:135:LYS:HE3	2:Q:162:GLU:CD	2.34	0.52
3:b:18:ASP:HA	3:b:28:ASP:HA	1.92	0.52
3:b:138:TYR:CE2	3:b:288:HIS:HB2	2.45	0.52
1:D:24:TYR:CE2	1:D:290:ARG:HG3	2.45	0.52
2:S:249:VAL:HG22	3:d:397:TYR:HE1	1.75	0.52
3:a:18:ASP:HA	3:a:28:ASP:HA	1.91	0.52
1:D:19:VAL:HG12	1:D:27:VAL:H	1.75	0.52
2:Q:204:ARG:H	2:Q:204:ARG:HD2	1.75	0.52
3:a:388:ARG:O	3:a:392:LEU:HG	2.10	0.52
1:A:29:LEU:HD13	1:A:281:ILE:HD11	1.92	0.52
2:Q:232:ASN:HB3	2:Q:237:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:HG3	1:C:131:ALA:HA	1.92	0.51
3:c:18:ASP:HA	3:c:28:ASP:HA	1.91	0.51
3:d:186:LYS:HA	3:d:215:THR:HG21	1.92	0.51
3:b:165:GLU:HA	3:b:251:LYS:HB2	1.91	0.51
1:B:143:ARG:HH22	1:B:159:ASP:H	1.58	0.51
1:D:78:CYS:HA	1:D:105:GLU:HA	1.92	0.51
3:c:414:CYS:SG	3:c:417:PRO:HD3	2.51	0.51
1:D:58:PRO:HB2	1:D:102:GLN:OE1	2.11	0.51
1:B:321:TYR:CE2	1:B:353:PHE:HD2	2.28	0.51
1:A:89:TRP:HE1	3:a:16:ILE:HD12	1.76	0.51
3:b:41:HIS:HA	3:b:131:ARG:HB2	1.93	0.51
3:c:204:VAL:HG13	3:c:206:GLU:H	1.76	0.51
3:c:357:TYR:HA	3:c:364:THR:HG21	1.91	0.51
1:A:148:TYR:HB2	1:A:153:THR:HG21	1.91	0.51
1:B:36:THR:HB	1:B:270:GLU:HA	1.93	0.51
1:D:414:LEU:O	1:D:415:VAL:C	2.54	0.51
2:R:188:TRP:HE1	2:R:190:HIS:CE1	2.29	0.51
1:D:339:VAL:HG21	1:D:395:HIS:CE1	2.46	0.50
2:R:250:THR:HG21	3:c:398:LYS:HB2	1.92	0.50
3:c:410:ALA:O	3:c:411:LEU:C	2.53	0.50
1:A:41:SER:HB2	1:A:125:HIS:HB2	1.94	0.50
1:C:129:VAL:HG23	1:C:149:VAL:HB	1.92	0.50
1:D:186:TYR:CE2	1:D:251:PRO:HA	2.46	0.50
2:R:201:THR:HG21	2:R:238:ALA:HA	1.93	0.50
3:a:291:LEU:HD11	3:a:305:ARG:HG3	1.93	0.50
1:B:145:ALA:HB2	1:B:157:ILE:HD12	1.94	0.50
1:D:408:TRP:O	1:D:412:LYS:N	2.38	0.50
3:c:53:PHE:CD2	3:c:65:MET:HE3	2.45	0.50
3:d:153:TYR:HA	3:d:258:PRO:HA	1.92	0.50
1:A:436:LEU:O	1:A:437:PHE:C	2.53	0.50
2:S:166:VAL:HG22	2:S:167:PRO:HD2	1.93	0.50
2:P:139:VAL:HG23	2:P:261:TRP:CE3	2.47	0.50
1:A:329:CYS:H	1:A:347:LEU:HD23	1.75	0.50
1:A:435:VAL:O	1:A:436:LEU:C	2.53	0.50
1:D:361:ASN:CB	1:D:403:ILE:HA	2.42	0.50
2:Q:189:HIS:CD2	2:Q:190:HIS:CE1	3.00	0.50
3:d:196:LYS:HA	3:d:208:ILE:HA	1.94	0.50
1:C:205:GLN:HB3	1:C:215:TYR:HB3	1.93	0.50
1:B:331:ILE:HD11	1:B:342:GLU:HB3	1.93	0.49
2:R:230:GLY:HA3	2:R:239:LEU:HD23	1.93	0.49
3:b:151:ASN:HA	3:b:261:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:180:ILE:HA	3:d:185:VAL:HA	1.94	0.49
1:D:285:ASP:HA	1:D:288:PHE:CD2	2.42	0.49
1:C:368:LEU:H	1:C:368:LEU:HD23	1.77	0.49
2:R:188:TRP:CD1	2:R:190:HIS:H	2.31	0.49
1:A:121:ALA:HB1	1:A:190:PHE:CZ	2.48	0.49
1:C:414:LEU:HD12	1:C:414:LEU:H	1.76	0.49
2:Q:212:SER:HA	2:Q:227:VAL:HG12	1.94	0.49
1:B:165:GLY:HA2	1:B:278:PRO:HD2	1.93	0.49
2:R:135:LYS:HB3	2:R:162:GLU:HB2	1.93	0.49
1:A:405:ALA:HA	1:A:408:TRP:HB2	1.93	0.49
3:b:36:VAL:HG22	3:b:47:ILE:HG12	1.95	0.49
1:D:394:GLN:O	1:D:396:THR:HG23	2.13	0.49
1:D:436:LEU:HD22	1:D:437:PHE:CE2	2.48	0.49
3:a:181:HIS:HB2	3:a:186:LYS:HE3	1.94	0.49
3:c:185:VAL:HG22	3:c:218:THR:HA	1.95	0.49
1:C:367:LYS:HG2	1:C:374:ALA:HB1	1.95	0.49
2:S:188:TRP:CH2	2:S:190:HIS:HB2	2.48	0.49
3:d:105:PRO:HB3	3:d:130:PHE:H	1.78	0.49
1:A:323:SER:H	1:A:350:SER:H	1.60	0.49
1:B:87:PHE:CD1	1:B:91:GLY:HA2	2.48	0.48
3:c:362:LEU:HD23	3:c:362:LEU:H	1.78	0.48
1:B:224:ARG:HD3	1:B:225:PRO:HD2	1.95	0.48
2:P:202:VAL:HG13	2:P:239:LEU:HD11	1.94	0.48
2:S:238:ALA:C	2:S:239:LEU:HD22	2.39	0.48
1:C:408:TRP:CD1	1:C:411:LEU:HD21	2.48	0.48
3:a:22:CYS:H	3:a:26:ARG:HA	1.79	0.48
1:D:358:SER:HB2	1:D:394:GLN:OE1	2.13	0.48
1:D:408:TRP:C	1:D:411:LEU:H	2.21	0.48
2:Q:166:VAL:HG22	2:Q:167:PRO:O	2.14	0.48
2:Q:230:GLY:HA3	2:Q:239:LEU:HA	1.94	0.48
2:S:154:LYS:NZ	3:d:398:LYS:HE2	2.13	0.48
3:c:371:CYS:O	3:c:374:ILE:HG13	2.14	0.48
3:a:64:TYR:CZ	3:a:77:LYS:HG2	2.47	0.48
3:c:414:CYS:SG	3:c:415:ILE:O	2.71	0.48
1:D:49:CYS:HA	1:D:241:PHE:CZ	2.49	0.48
3:d:97:TYR:HE2	3:d:235:TYR:HB2	1.79	0.48
3:d:407:ILE:HB	3:d:411:LEU:HB2	1.95	0.48
1:B:297:VAL:HG21	1:B:371:CYS:SG	2.54	0.48
1:C:136:THR:HB	1:C:141:SER:O	2.14	0.48
1:D:193:TYR:HA	1:D:205:GLN:NE2	2.28	0.48
1:C:389:VAL:HA	3:c:335:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:232:ASN:HA	2:P:237:THR:HA	1.96	0.48
3:b:2:LEU:H	3:b:2:LEU:HD22	1.78	0.48
1:B:418:THR:O	1:B:422:ILE:HG12	2.14	0.48
3:d:9:TYR:CE2	3:d:55:LEU:HD11	2.49	0.48
1:B:30:GLN:H	1:B:137:TYR:HB2	1.79	0.47
1:B:205:GLN:N	1:B:205:GLN:HE21	2.12	0.47
1:A:321:TYR:HE2	1:A:353:PHE:HB3	1.79	0.47
3:b:163:TYR:HB3	3:b:253:HIS:CE1	2.50	0.47
3:b:167:HIS:HB2	3:b:247:THR:HA	1.96	0.47
3:c:136:GLU:CD	3:c:329:ASN:HD22	2.22	0.47
1:B:53:THR:HA	1:B:108:VAL:HG12	1.96	0.47
1:C:436:LEU:HD13	1:C:436:LEU:H	1.79	0.47
3:b:185:VAL:HG11	3:b:218:THR:HA	1.96	0.47
3:d:193:ALA:HB3	3:d:228:ILE:HB	1.97	0.47
1:C:34:VAL:HG13	4:G:1:NAG:C8	2.43	0.47
3:d:291:LEU:HA	3:d:307:TRP:HA	1.97	0.47
1:A:299:ASP:HB2	1:A:322:LYS:HB3	1.96	0.47
1:B:63:CYS:HA	1:B:99:GLU:HB3	1.95	0.47
1:C:295:PRO:HB3	1:C:325:LYS:HG3	1.97	0.47
3:a:404:GLN:HB2	3:a:420:ALA:HB3	1.95	0.47
3:c:81:LEU:HD13	3:c:82:HIS:N	2.28	0.47
1:B:96:CYS:HB3	1:B:99:GLU:HB2	1.96	0.47
1:C:116:ILE:HG13	3:c:260:LYS:HZ3	1.80	0.47
1:D:399:PHE:O	1:D:402:ALA:N	2.40	0.47
1:D:412:LYS:O	1:D:413:VAL:C	2.57	0.47
2:S:128:VAL:HG12	2:S:133:VAL:HA	1.97	0.47
3:b:292:LEU:HB2	3:b:306:GLN:HB2	1.97	0.47
2:P:159:TYR:HA	2:P:252:LYS:HE3	1.97	0.47
2:S:155:LYS:HA	2:S:162:GLU:HA	1.96	0.47
3:d:284:LEU:HD11	3:d:327:TRP:CE2	2.50	0.47
1:C:37:ARG:HE	1:C:130:GLN:HB3	1.80	0.47
1:A:225:PRO:HA	1:A:233:PRO:HG3	1.97	0.46
1:A:435:VAL:HA	1:A:437:PHE:CD2	2.49	0.46
1:D:67:GLN:CD	1:D:67:GLN:H	2.23	0.46
2:R:163:TYR:HB3	3:c:398:LYS:HE2	1.97	0.46
3:c:163:TYR:HA	3:c:253:HIS:HA	1.97	0.46
1:A:299:ASP:HB2	1:A:322:LYS:CB	2.45	0.46
1:D:89:TRP:CD2	3:d:70:GLY:HA3	2.50	0.46
2:Q:145:ASN:HB3	2:Q:147:GLN:OE1	2.14	0.46
3:a:180:ILE:HG12	3:a:182:SER:H	1.80	0.46
3:c:401:PRO:CB	3:c:420:ALA:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:O	1:A:349:GLU:HG3	2.16	0.46
1:C:334:PRO:CD	1:C:369:GLN:H	2.29	0.46
2:S:156:ALA:CB	3:d:398:LYS:HZ1	2.07	0.46
1:D:223:GLN:HB2	1:D:233:PRO:HB2	1.97	0.46
3:d:11:LEU:HD22	3:d:166:MET:HE3	1.98	0.46
1:A:156:LYS:HA	1:A:161:LYS:HA	1.97	0.46
1:B:13:ILE:HG22	1:B:393:ALA:HA	1.97	0.46
1:C:75:ASP:HB2	1:C:216:ALA:HB3	1.96	0.46
1:D:129:VAL:HG23	1:D:149:VAL:HB	1.98	0.46
1:B:130:GLN:HE21	1:B:131:ALA:N	2.14	0.46
1:D:47:ILE:HD11	1:D:118:HIS:ND1	2.30	0.46
2:S:188:TRP:CD1	2:S:189:HIS:H	2.33	0.46
1:B:186:TYR:CE2	1:B:251:PRO:HA	2.51	0.46
1:D:398:SER:O	1:D:403:ILE:HG23	2.16	0.46
2:Q:231:VAL:HG22	2:Q:232:ASN:H	1.81	0.46
3:a:282:LEU:N	3:a:282:LEU:HD22	2.30	0.46
3:c:369:CYS:HA	3:c:372:VAL:HG12	1.98	0.46
3:d:9:TYR:CD2	3:d:55:LEU:HD11	2.51	0.46
1:D:405:ALA:O	1:D:411:LEU:HG	2.15	0.46
1:A:418:THR:O	1:A:422:ILE:HG12	2.15	0.45
1:B:392:PRO:HG3	3:b:336:TRP:CZ3	2.51	0.45
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.77	0.45
1:B:299:ASP:HB2	1:B:322:LYS:HB2	1.98	0.45
1:C:136:THR:HG22	1:C:142:TRP:HA	1.97	0.45
1:D:397:GLU:HB3	1:D:401:SER:CB	2.38	0.45
3:a:384:TRP:CD1	3:a:385:LEU:HD23	2.51	0.45
1:C:161:LYS:HE3	1:C:282:ASP:H	1.82	0.45
2:R:185:PHE:HA	2:R:194:GLN:HB3	1.99	0.45
3:c:66:SER:HA	3:c:75:SER:HA	1.97	0.45
1:C:330:PRO:HA	1:C:344:ASP:HA	1.97	0.45
1:D:407:ALA:C	1:D:409:SER:N	2.73	0.45
1:A:87:PHE:CG	1:A:91:GLY:HA2	2.51	0.45
1:B:15:TYR:CE2	1:B:17:ALA:HB2	2.52	0.45
3:b:359:ARG:HB3	3:b:364:THR:HG21	1.97	0.45
1:D:49:CYS:HA	1:D:241:PHE:CE1	2.51	0.45
2:S:143:ILE:HB	2:S:149:ALA:HB2	1.98	0.45
3:b:166:MET:SD	3:b:235:TYR:HA	2.57	0.45
3:b:172:VAL:HB	3:b:227:LEU:HB2	1.99	0.45
3:d:26:ARG:H	3:d:26:ARG:HD3	1.82	0.45
1:D:244:TRP:CH2	1:D:248:LYS:HA	2.52	0.45
1:D:305:THR:H	1:D:317:ALA:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:142:ARG:HG2	2:Q:143:ILE:H	1.82	0.45
1:A:15:TYR:CE1	1:A:17:ALA:HB2	2.49	0.45
1:B:11:VAL:HA	1:B:33:LEU:HD21	1.99	0.45
1:D:220:LEU:HD11	1:D:234:PHE:CD2	2.45	0.45
2:Q:232:ASN:HA	2:Q:237:THR:HA	1.98	0.45
3:b:153:TYR:HA	3:b:258:PRO:HA	1.98	0.45
3:c:84:ARG:HB2	3:c:110:THR:HB	1.99	0.45
3:d:119:ARG:HB3	3:d:121:THR:HG23	1.98	0.45
1:A:147:VAL:HG21	1:A:164:ILE:HD12	1.98	0.44
1:B:140:VAL:HG11	1:B:143:ARG:NE	2.32	0.44
1:C:290:ARG:HE	1:C:290:ARG:HA	1.81	0.44
1:D:391:TYR:CG	1:D:392:PRO:HD2	2.52	0.44
1:A:18:LEU:HD22	1:A:332:HIS:HB3	1.99	0.44
1:A:331:ILE:HG22	1:A:368:LEU:HD11	1.99	0.44
1:B:225:PRO:HA	1:B:231:HIS:CE1	2.52	0.44
1:D:205:GLN:HE21	1:D:205:GLN:HB3	1.53	0.44
1:D:193:TYR:CZ	1:D:207:ARG:HD3	2.52	0.44
3:b:3:ASP:HA	3:b:6:PHE:HB3	1.99	0.44
3:c:178:LEU:HG	3:c:187:ILE:HD11	1.98	0.44
1:B:28:HIS:CD2	1:B:343:ASN:HB2	2.51	0.44
1:B:137:TYR:CG	1:B:138:GLY:N	2.85	0.44
1:D:60:VAL:HG22	1:D:102:GLN:HG2	1.98	0.44
1:A:424:LEU:HD12	1:A:427:ILE:HD11	1.99	0.44
2:Q:136:PRO:HB2	2:Q:139:VAL:HG12	2.00	0.44
2:Q:147:GLN:CD	2:Q:147:GLN:N	2.76	0.44
2:S:154:LYS:NZ	3:d:398:LYS:CE	2.78	0.44
1:B:227:ALA:HB3	3:b:26:ARG:HH22	1.83	0.44
3:c:277:HIS:O	3:c:279:THR:HG22	2.18	0.44
1:B:87:PHE:CG	1:B:91:GLY:HA2	2.52	0.44
1:D:130:GLN:HA	1:D:148:TYR:HA	2.00	0.44
2:Q:204:ARG:HA	2:Q:237:THR:HG21	1.99	0.44
3:b:408:LEU:HD13	3:b:414:CYS:HB2	2.00	0.44
1:A:295:PRO:HB3	1:A:325:LYS:H	1.82	0.44
1:D:239:SER:OG	1:D:241:PHE:HB3	2.17	0.44
3:a:300:ASP:OD2	3:a:302:ASN:HB2	2.18	0.44
3:b:277:HIS:ND1	3:b:278:ARG:HG3	2.33	0.44
3:c:184:LYS:HG2	3:c:185:VAL:O	2.18	0.44
3:d:62:LEU:C	3:d:62:LEU:HD22	2.43	0.44
1:A:309:TYR:H	1:A:382:LYS:C	2.26	0.43
1:D:44:LEU:HB3	1:D:122:TYR:CE2	2.52	0.43
3:a:408:LEU:HD13	3:a:414:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TRP:HE1	4:F:2:NAG:H81	1.81	0.43
1:C:124:VAL:HB	1:C:176:ASN:HA	1.99	0.43
1:D:44:LEU:HD23	1:D:44:LEU:H	1.83	0.43
2:S:188:TRP:CG	2:S:189:HIS:N	2.86	0.43
3:c:384:TRP:HE3	3:c:385:LEU:HD22	1.83	0.43
1:C:300:LEU:HD23	1:C:300:LEU:H	1.83	0.43
1:D:71:LYS:HD2	1:D:76:TYR:CE1	2.53	0.43
2:R:195:TYR:HD2	2:R:201:THR:HG23	1.83	0.43
2:Q:154:LYS:HB2	2:Q:163:TYR:HB2	1.99	0.43
3:c:195:VAL:HG23	3:c:226:TYR:N	2.23	0.43
1:B:365:ALA:HA	1:B:378:LYS:HA	2.00	0.43
1:D:391:TYR:CD2	1:D:392:PRO:HD2	2.53	0.43
3:c:405:VAL:HB	3:c:408:LEU:HB2	1.99	0.43
3:d:336:TRP:CG	3:d:337:ALA:N	2.86	0.43
1:C:140:VAL:HG11	1:C:143:ARG:HB2	2.01	0.43
1:D:407:ALA:O	1:D:410:TRP:N	2.44	0.43
2:P:187:ASN:HA	2:P:192:ALA:HA	2.00	0.43
1:C:38:ILE:HA	1:C:129:VAL:HG12	2.00	0.43
2:P:138:HIS:HB3	2:P:261:TRP:CE3	2.54	0.43
2:Q:202:VAL:HG11	2:Q:206:VAL:HG21	2.00	0.43
3:d:112:GLY:HA3	3:d:121:THR:HG22	2.00	0.43
1:B:89:TRP:CZ2	3:b:70:GLY:HA3	2.54	0.43
3:c:138:TYR:CD2	3:c:266:THR:HG21	2.54	0.43
2:R:187:ASN:HA	2:R:192:ALA:HA	2.00	0.43
3:b:125:ALA:HB2	3:c:140:HIS:ND1	2.34	0.43
1:A:21:ARG:HB3	1:A:24:TYR:HB2	2.00	0.43
3:b:360:TYR:HB2	3:b:363:THR:HB	2.01	0.43
1:A:85:TYR:CE1	1:A:92:ALA:HB1	2.54	0.42
3:a:201:CYS:HB2	3:a:217:CYS:H	1.83	0.42
1:A:37:ARG:HA	1:A:268:ARG:HG3	2.01	0.42
1:D:89:TRP:CE2	3:d:70:GLY:HA3	2.54	0.42
3:c:155:HIS:C	3:c:157:ARG:HH11	2.28	0.42
3:d:87:ALA:HB3	3:d:104:PRO:CG	2.49	0.42
3:c:390:ARG:NE	3:c:415:ILE:HG12	2.35	0.42
1:A:89:TRP:HE1	3:a:16:ILE:CD1	2.32	0.42
1:A:295:PRO:HG3	1:A:325:LYS:HB2	2.01	0.42
1:D:406:THR:C	1:D:408:TRP:N	2.77	0.42
3:a:153:TYR:HA	3:a:258:PRO:HA	2.02	0.42
3:a:372:VAL:O	3:a:375:ILE:HG12	2.19	0.42
1:A:363:HIS:HA	1:A:379:GLY:O	2.19	0.42
1:C:36:THR:HB	1:C:270:GLU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LYS:HA	1:D:61:LYS:HD2	1.79	0.42
2:Q:187:ASN:HA	2:Q:192:ALA:HA	2.01	0.42
3:a:166:MET:SD	3:a:235:TYR:HA	2.60	0.42
1:C:399:PHE:CE2	1:C:403:ILE:HA	2.54	0.42
1:D:403:ILE:HG13	1:D:404:SER:H	1.85	0.42
2:R:117:MET:HB3	2:R:122:VAL:HA	2.01	0.42
2:R:155:LYS:HA	2:R:162:GLU:HG2	2.01	0.42
3:b:296:SER:HA	3:b:323:LEU:HB3	2.02	0.42
1:A:389:VAL:HG12	1:A:390:ASP:N	2.35	0.42
1:B:36:THR:HB	1:B:271:ASN:N	2.35	0.42
1:B:298:SER:O	1:B:322:LYS:HB2	2.20	0.42
2:P:259:GLU:HG3	2:P:260:PRO:O	2.19	0.42
3:c:187:ILE:HD13	3:c:187:ILE:HA	1.80	0.42
3:c:402:ASN:O	3:c:403:ALA:C	2.63	0.42
1:B:332:HIS:HA	1:B:340:ILE:HD11	2.01	0.42
1:D:407:ALA:O	1:D:408:TRP:C	2.63	0.42
2:S:133:VAL:HB	2:S:164:GLY:HA3	2.00	0.42
2:S:154:LYS:HB3	2:S:163:TYR:HD2	1.84	0.42
3:b:53:PHE:HB2	3:b:65:MET:HA	2.02	0.42
1:B:14:PRO:HA	1:B:32:GLN:HB2	2.02	0.42
1:B:225:PRO:HA	1:B:233:PRO:HG3	2.02	0.42
1:C:283:ILE:HD12	1:C:283:ILE:H	1.85	0.42
1:D:399:PHE:CE2	3:d:364:THR:HG22	2.55	0.42
3:a:90:SER:O	3:a:101:ALA:HB1	2.20	0.42
3:a:142:PRO:HG2	3:a:264:ILE:HG13	2.01	0.42
1:A:392:PRO:HD3	3:a:336:TRP:CE3	2.55	0.42
1:C:89:TRP:CE2	3:c:70:GLY:HA2	2.55	0.42
1:C:113:GLU:HA	3:c:258:PRO:HG2	2.01	0.42
2:Q:227:VAL:HA	2:Q:241:VAL:HG12	2.00	0.42
3:b:44:VAL:HG12	3:b:102:GLN:HB2	2.00	0.42
3:b:276:LYS:HE2	3:b:276:LYS:HB3	1.87	0.42
1:D:16:LYS:HE3	1:D:28:HIS:NE2	2.35	0.41
1:D:87:PHE:HB3	1:D:92:ALA:HA	2.02	0.41
1:D:231:HIS:CG	1:D:232:THR:N	2.88	0.41
3:a:140:HIS:CG	3:a:141:PRO:HD2	2.55	0.41
1:A:296:THR:O	1:A:323:SER:HA	2.20	0.41
1:B:7:MET:HG2	1:B:15:TYR:CE1	2.54	0.41
2:P:128:VAL:HG12	2:P:133:VAL:HA	2.01	0.41
3:a:200:LYS:HE3	3:a:217:CYS:SG	2.60	0.41
3:a:204:VAL:HG22	3:a:206:GLU:H	1.85	0.41
1:A:16:LYS:HB2	1:A:332:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD22	1:B:332:HIS:HB3	2.01	0.41
1:B:65:ALA:HA	1:B:101:THR:HG21	2.02	0.41
1:D:155:ALA:HB3	1:D:162:LEU:HB2	2.01	0.41
2:S:232:ASN:HA	2:S:237:THR:HG22	2.03	0.41
3:c:418:THR:C	3:c:420:ALA:N	2.78	0.41
1:A:388:ILE:HG21	3:a:275:HIS:CG	2.55	0.41
1:A:435:VAL:C	1:A:437:PHE:H	2.27	0.41
1:B:57:SER:OG	3:b:242:ARG:HB2	2.19	0.41
1:B:321:TYR:O	1:B:322:LYS:HD2	2.21	0.41
1:C:267:LEU:HD22	1:C:267:LEU:HA	1.97	0.41
1:D:402:ALA:O	1:D:405:ALA:N	2.52	0.41
2:R:153:LEU:HB3	2:R:162:GLU:HB3	2.02	0.41
3:c:286:PRO:HD2	3:c:311:PRO:HA	2.02	0.41
1:A:285:ASP:HA	1:A:288:PHE:CE2	2.56	0.41
1:B:288:PHE:N	1:B:288:PHE:CD1	2.88	0.41
2:P:193:VAL:HB	2:P:202:VAL:HG12	2.03	0.41
3:d:385:LEU:HD13	3:d:385:LEU:HA	1.94	0.41
1:D:114:CYS:HA	1:D:117:ASP:O	2.21	0.41
3:a:14:PRO:HG2	3:a:73:GLN:HG3	2.01	0.41
3:c:255:PRO:HG2	3:c:256:PHE:CE2	2.56	0.41
3:c:272:LEU:HB3	3:c:283:HIS:HB2	2.02	0.41
3:d:92:VAL:HG23	3:d:101:ALA:HA	2.03	0.41
3:d:281:ILE:HG12	3:d:315:ASN:HB3	2.02	0.41
1:A:187:ASN:N	1:A:252:LEU:HD11	2.36	0.41
1:B:244:TRP:CZ3	1:B:248:LYS:HA	2.55	0.41
1:C:340:ILE:HB	1:C:355:PHE:CE2	2.56	0.41
1:D:399:PHE:C	1:D:402:ALA:H	2.25	0.41
2:R:115:PRO:HA	2:R:125:TYR:HA	2.02	0.41
2:R:117:MET:HA	2:R:122:VAL:HA	2.02	0.41
1:B:149:VAL:HG12	1:B:166:PRO:HA	2.03	0.41
1:B:150:ASN:HA	1:B:166:PRO:HB3	2.01	0.41
1:B:255:VAL:HA	3:b:295:ARG:HD3	2.03	0.41
1:D:265:GLU:CD	1:D:266:PRO:HD2	2.46	0.41
1:D:408:TRP:O	1:D:411:LEU:N	2.53	0.41
2:P:131:GLY:H	2:P:174:THR:HG21	1.85	0.41
2:P:183:PRO:CB	2:P:196:GLU:HA	2.50	0.41
2:Q:155:LYS:HE2	2:Q:155:LYS:HB3	1.88	0.41
2:R:116:ILE:HG12	2:R:143:ILE:HG23	2.03	0.41
3:c:53:PHE:HB3	3:c:65:MET:HG3	2.03	0.41
3:c:364:THR:HG23	3:c:365:ILE:N	2.36	0.41
3:d:21:ASN:HB2	3:d:123:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:C	1:B:142:TRP:H	2.29	0.41
1:D:220:LEU:HD13	1:D:220:LEU:HA	1.74	0.41
3:b:125:ALA:HB2	3:c:140:HIS:HD1	1.86	0.41
1:B:40:PRO:HD2	1:B:267:LEU:O	2.21	0.40
1:D:44:LEU:HA	1:D:122:TYR:HA	2.03	0.40
1:D:408:TRP:HA	1:D:411:LEU:CA	2.50	0.40
1:C:258:PHE:CE1	3:c:299:SER:HA	2.56	0.40
2:S:249:VAL:HG22	3:d:397:TYR:CE1	2.57	0.40
3:b:386:LEU:HA	3:b:386:LEU:HD22	1.88	0.40
3:c:107:ASP:HA	3:c:127:LYS:HA	2.03	0.40
1:A:143:ARG:HD3	1:A:157:ILE:C	2.46	0.40
1:B:174:PHE:HE1	1:B:269:ALA:HB2	1.86	0.40
2:R:120:GLY:HA3	2:S:147:GLN:HG2	2.02	0.40
3:c:55:LEU:H	3:c:55:LEU:HD22	1.85	0.40
3:c:146:VAL:HG23	3:c:267:LEU:HD21	2.03	0.40
1:A:305:THR:H	1:A:317:ALA:HA	1.87	0.40
1:B:49:CYS:HA	1:B:241:PHE:CE2	2.57	0.40
1:D:408:TRP:N	1:D:411:LEU:HB2	2.36	0.40
2:Q:158:ILE:HG23	2:Q:159:TYR:CD2	2.57	0.40
3:b:272:LEU:HB3	3:b:283:HIS:HB2	2.03	0.40
1:A:220:LEU:CD2	1:A:237:ALA:H	2.34	0.40
1:B:331:ILE:HG21	1:B:345:VAL:HG23	2.03	0.40
3:c:412:LEU:HD13	3:c:412:LEU:HA	1.95	0.40
3:d:49:THR:HG23	3:d:51:ALA:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	435/437 (100%)	398 (92%)	36 (8%)	1 (0%)	43 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	435/437 (100%)	403 (93%)	30 (7%)	2 (0%)	24	63
1	C	435/437 (100%)	399 (92%)	36 (8%)	0	100	100
1	D	435/437 (100%)	389 (89%)	41 (9%)	5 (1%)	11	45
2	P	158/160 (99%)	145 (92%)	13 (8%)	0	100	100
2	Q	158/160 (99%)	140 (89%)	17 (11%)	1 (1%)	21	59
2	R	157/160 (98%)	145 (92%)	12 (8%)	0	100	100
2	S	158/160 (99%)	144 (91%)	14 (9%)	0	100	100
3	a	418/420 (100%)	372 (89%)	46 (11%)	0	100	100
3	b	418/420 (100%)	373 (89%)	43 (10%)	2 (0%)	24	63
3	c	418/420 (100%)	370 (88%)	43 (10%)	5 (1%)	10	43
3	d	418/420 (100%)	369 (88%)	45 (11%)	4 (1%)	12	47
All	All	4043/4068 (99%)	3647 (90%)	376 (9%)	20 (0%)	26	63

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	GLU
1	D	388	ILE
1	D	403	ILE
3	b	208	ILE
1	A	436	LEU
3	c	411	LEU
1	D	389	VAL
3	b	230	ASN
3	c	344	ASN
3	c	418	THR
3	d	339	GLU
1	D	391	TYR
1	D	407	ALA
3	d	403	ALA
1	B	389	VAL
3	c	141	PRO
2	Q	203	PRO
3	d	415	ILE
3	d	311	PRO
3	c	416	LYS

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	366/366 (100%)	318 (87%)	48 (13%)	4	16
1	B	366/366 (100%)	330 (90%)	36 (10%)	7	24
1	C	366/366 (100%)	320 (87%)	46 (13%)	4	17
1	D	366/366 (100%)	327 (89%)	39 (11%)	6	22
2	P	134/134 (100%)	121 (90%)	13 (10%)	8	25
2	Q	134/134 (100%)	122 (91%)	12 (9%)	9	28
2	R	133/134 (99%)	121 (91%)	12 (9%)	9	28
2	S	134/134 (100%)	115 (86%)	19 (14%)	3	15
3	a	367/367 (100%)	333 (91%)	34 (9%)	8	27
3	b	367/367 (100%)	337 (92%)	30 (8%)	10	31
3	c	367/367 (100%)	324 (88%)	43 (12%)	5	19
3	d	367/367 (100%)	328 (89%)	39 (11%)	6	22
All	All	3467/3468 (100%)	3096 (89%)	371 (11%)	8	22

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	18	LEU
1	A	28	HIS
1	A	31	ILE
1	A	36	THR
1	A	45	GLU
1	A	47	ILE
1	A	54	LYS
1	A	60	VAL
1	A	69	THR
1	A	78	CYS
1	A	85	TYR
1	A	100	ASN
1	A	111	SER

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Mol	Chain	Res	Type
1	A	125	HIS
1	A	129	VAL
1	A	134	ASN
1	A	135	ILE
1	A	136	THR
1	A	149	VAL
1	A	152	GLU
1	A	153	THR
1	A	156	LYS
1	A	167	LEU
1	A	180	VAL
1	A	204	LEU
1	A	205	GLN
1	A	210	THR
1	A	221	LYS
1	A	230	VAL
1	A	235	THR
1	A	244	TRP
1	A	247	ASP
1	A	255	VAL
1	A	267	LEU
1	A	291	ILE
1	A	304	ILE
1	A	332	HIS
1	A	347	LEU
1	A	367	LYS
1	A	370	VAL
1	A	375	VAL
1	A	378	LYS
1	A	380	ASP
1	A	385	LYS
1	A	387	HIS
1	A	394	GLN
1	A	434	LEU
1	B	1	TYR
1	B	6	VAL
1	B	9	ASN
1	B	16	LYS
1	B	34	VAL
1	B	38	ILE
1	B	50	LYS
1	B	68	CYS

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Mol	Chain	Res	Type
1	B	85	TYR
1	B	105	GLU
1	B	123	LYS
1	B	130	GLN
1	B	147	VAL
1	B	156	LYS
1	B	205	GLN
1	B	230	VAL
1	B	236	GLN
1	B	243	ARG
1	B	268	ARG
1	B	274	VAL
1	B	313	PHE
1	B	319	VAL
1	B	329	CYS
1	B	339	VAL
1	B	344	ASP
1	B	347	LEU
1	B	349	GLU
1	B	371	CYS
1	B	382	LYS
1	B	388	ILE
1	B	394	GLN
1	B	408	TRP
1	B	426	LEU
1	B	431	VAL
1	B	432	VAL
1	B	437	PHE
1	C	19	VAL
1	C	37	ARG
1	C	43	ASN
1	C	44	LEU
1	C	47	ILE
1	C	63	CYS
1	C	75	ASP
1	C	79	GLN
1	C	84	VAL
1	C	85	TYR
1	C	89	TRP
1	C	102	GLN
1	C	111	SER
1	C	120	LYS

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Mol	Chain	Res	Type
1	C	137	TYR
1	C	152	GLU
1	C	157	ILE
1	C	161	LYS
1	C	162	LEU
1	C	171	TRP
1	C	205	GLN
1	C	208	THR
1	C	244	TRP
1	C	248	LYS
1	C	253	ASN
1	C	255	VAL
1	C	260	CYS
1	C	267	LEU
1	C	272	CYS
1	C	281	ILE
1	C	283	ILE
1	C	291	ILE
1	C	302	CYS
1	C	304	ILE
1	C	306	GLU
1	C	316	ILE
1	C	329	CYS
1	C	331	ILE
1	C	356	HIS
1	C	367	LYS
1	C	371	CYS
1	C	372	THR
1	C	377	CYS
1	C	378	LYS
1	C	408	TRP
1	C	436	LEU
1	D	2	GLU
1	D	6	VAL
1	D	7	MET
1	D	33	LEU
1	D	42	THR
1	D	50	LYS
1	D	54	LYS
1	D	87	PHE
1	D	124	VAL
1	D	128	THR

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Mol	Chain	Res	Type
1	D	129	VAL
1	D	140	VAL
1	D	147	VAL
1	D	153	THR
1	D	162	LEU
1	D	167	LEU
1	D	171	TRP
1	D	172	SER
1	D	195	THR
1	D	207	ARG
1	D	210	THR
1	D	220	LEU
1	D	221	LYS
1	D	277	ILE
1	D	283	ILE
1	D	289	THR
1	D	291	ILE
1	D	319	VAL
1	D	370	VAL
1	D	378	LYS
1	D	388	ILE
1	D	389	VAL
1	D	394	GLN
1	D	400	THR
1	D	403	ILE
1	D	410	TRP
1	D	414	LEU
1	D	435	VAL
1	D	436	LEU
2	P	108	LEU
2	P	119	ASN
2	P	122	VAL
2	P	123	ASN
2	P	142	ARG
2	P	152	LYS
2	P	180	ASP
2	P	185	PHE
2	P	193	VAL
2	P	209	LYS
2	P	226	ILE
2	P	254	THR
2	P	259	GLU

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Mol	Chain	Res	Type
2	Q	119	ASN
2	Q	121	GLN
2	Q	143	ILE
2	Q	147	GLN
2	Q	153	LEU
2	Q	155	LYS
2	Q	161	LEU
2	Q	173	ASP
2	Q	201	THR
2	Q	204	ARG
2	Q	217	LEU
2	Q	242	VAL
2	R	123	ASN
2	R	147	GLN
2	R	160	ASP
2	R	170	MET
2	R	185	PHE
2	R	198	ASN
2	R	201	THR
2	R	202	VAL
2	R	206	VAL
2	R	209	LYS
2	R	214	ARG
2	R	259	GLU
2	S	111	ASP
2	S	112	LYS
2	S	121	GLN
2	S	138	HIS
2	S	147	GLN
2	S	160	ASP
2	S	162	GLU
2	S	166	VAL
2	S	171	LYS
2	S	181	LYS
2	S	187	ASN
2	S	194	GLN
2	S	202	VAL
2	S	218	ASP
2	S	223	VAL
2	S	228	LEU
2	S	231	VAL
2	S	233	GLU

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Mol	Chain	Res	Type
2	S	250	THR
3	a	16	ILE
3	a	44	VAL
3	a	91	LEU
3	a	114	HIS
3	a	118	ASN
3	a	138	TYR
3	a	148	LEU
3	a	152	ARG
3	a	157	ARG
3	a	178	LEU
3	a	184	LYS
3	a	187	ILE
3	a	200	LYS
3	a	205	ARG
3	a	208	ILE
3	a	212	ASP
3	a	220	VAL
3	a	224	ARG
3	a	231	LYS
3	a	234	VAL
3	a	240	LEU
3	a	247	THR
3	a	251	LYS
3	a	254	VAL
3	a	274	GLU
3	a	279	THR
3	a	282	LEU
3	a	300	ASP
3	a	338	GLN
3	a	358	ASN
3	a	386	LEU
3	a	395	THR
3	a	408	LEU
3	a	414	CYS
3	b	2	LEU
3	b	5	HIS
3	b	13	ARG
3	b	45	ILE
3	b	77	LYS
3	b	79	ASP
3	b	85	THR

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Mol	Chain	Res	Type
3	b	98	TYR
3	b	138	TYR
3	b	157	ARG
3	b	185	VAL
3	b	195	VAL
3	b	208	ILE
3	b	248	PHE
3	b	251	LYS
3	b	254	VAL
3	b	267	LEU
3	b	276	LYS
3	b	279	THR
3	b	281	ILE
3	b	288	HIS
3	b	293	THR
3	b	327	TRP
3	b	333	LYS
3	b	336	TRP
3	b	386	LEU
3	b	394	ILE
3	b	397	TYR
3	b	408	LEU
3	b	414	CYS
3	c	18	ASP
3	c	56	LYS
3	c	91	LEU
3	c	107	ASP
3	c	122	CYS
3	c	123	THR
3	c	143	GLU
3	c	144	HIS
3	c	157	ARG
3	c	167	HIS
3	c	184	LYS
3	c	185	VAL
3	c	189	VAL
3	c	194	GLN
3	c	195	VAL
3	c	197	TYR
3	c	204	VAL
3	c	215	THR
3	c	221	LYS

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Mol	Chain	Res	Type
3	c	226	TYR
3	c	227	LEU
3	c	259	VAL
3	c	260	LYS
3	c	264	ILE
3	c	275	HIS
3	c	283	HIS
3	c	287	ASP
3	c	290	THR
3	c	295	ARG
3	c	297	LEU
3	c	304	THR
3	c	305	ARG
3	c	310	ARG
3	c	333	LYS
3	c	335	VAL
3	c	338	GLN
3	c	346	HIS
3	c	352	VAL
3	c	392	LEU
3	c	398	LYS
3	c	399	LEU
3	c	408	LEU
3	c	415	ILE
3	d	15	TYR
3	d	22	CYS
3	d	27	CYS
3	d	44	VAL
3	d	45	ILE
3	d	49	THR
3	d	52	MET
3	d	62	LEU
3	d	118	ASN
3	d	123	THR
3	d	133	VAL
3	d	143	GLU
3	d	151	ASN
3	d	167	HIS
3	d	212	ASP
3	d	227	LEU
3	d	234	VAL
3	d	236	ASN

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Mol	Chain	Res	Type
3	d	237	SER
3	d	244	GLU
3	d	251	LYS
3	d	252	LEU
3	d	275	HIS
3	d	279	THR
3	d	285	HIS
3	d	293	THR
3	d	294	THR
3	d	296	SER
3	d	304	THR
3	d	329	ASN
3	d	333	LYS
3	d	335	VAL
3	d	338	GLN
3	d	358	ASN
3	d	368	LEU
3	d	394	ILE
3	d	399	LEU
3	d	411	LEU
3	d	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	28	HIS
1	A	32	GLN
1	A	102	GLN
1	A	130	GLN
1	A	219	ASN
1	A	223	GLN
1	A	332	HIS
1	A	369	GLN
1	B	35	ASN
1	B	130	GLN
1	B	150	ASN
1	B	271	ASN
1	D	30	GLN
1	D	43	ASN
1	D	125	HIS
1	D	134	ASN

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Mol	Chain	Res	Type
1	D	205	GLN
1	D	343	ASN
1	D	395	HIS
2	P	147	GLN
2	P	189	HIS
2	P	232	ASN
2	Q	145	ASN
2	Q	187	ASN
2	Q	189	HIS
2	Q	190	HIS
2	R	194	GLN
2	S	119	ASN
2	S	121	GLN
2	S	123	ASN
3	a	82	HIS
3	a	118	ASN
3	a	302	ASN
3	b	120	HIS
3	b	253	HIS
3	b	350	HIS
3	b	391	ASN
3	c	114	HIS
3	c	118	ASN
3	c	126	HIS
3	c	275	HIS
3	c	277	HIS
3	c	329	ASN
3	d	95	HIS
3	d	118	ASN
3	d	162	HIS
3	d	344	ASN
3	d	346	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	$\# Z > 2$
4	NAG	E	1	4	14,14,15	0.39	0	17,19,21	0.55	0
4	NAG	E	2	4	14,14,15	0.39	0	17,19,21	0.39	0
4	BMA	E	3	4	11,11,12	0.17	0	15,15,17	0.48	0
4	NAG	F	1	4	14,14,15	0.38	0	17,19,21	0.55	0
4	NAG	F	2	4	14,14,15	0.40	0	17,19,21	0.39	0
4	BMA	F	3	4	11,11,12	0.17	0	15,15,17	0.49	0
4	NAG	G	1	4	14,14,15	0.40	0	17,19,21	0.54	0
4	NAG	G	2	4	14,14,15	0.39	0	17,19,21	0.39	0
4	BMA	G	3	4	11,11,12	0.17	0	15,15,17	0.48	0
4	NAG	H	1	4	14,14,15	0.41	0	17,19,21	0.55	0
4	NAG	H	2	4	14,14,15	0.38	0	17,19,21	0.38	0
4	BMA	H	3	4	11,11,12	0.17	0	15,15,17	0.49	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
4	NAG	E	1	4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	NAG	F	1	4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	NAG	H	1	4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

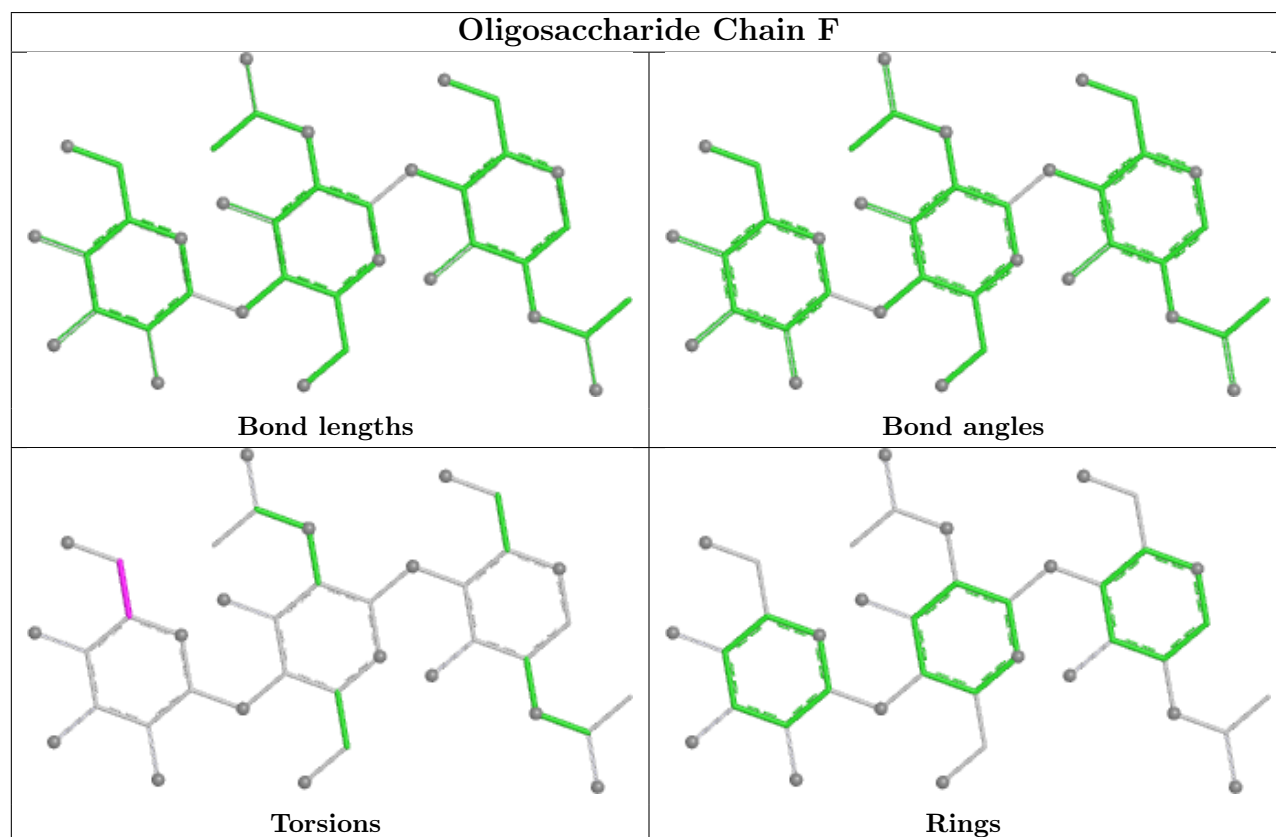
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6

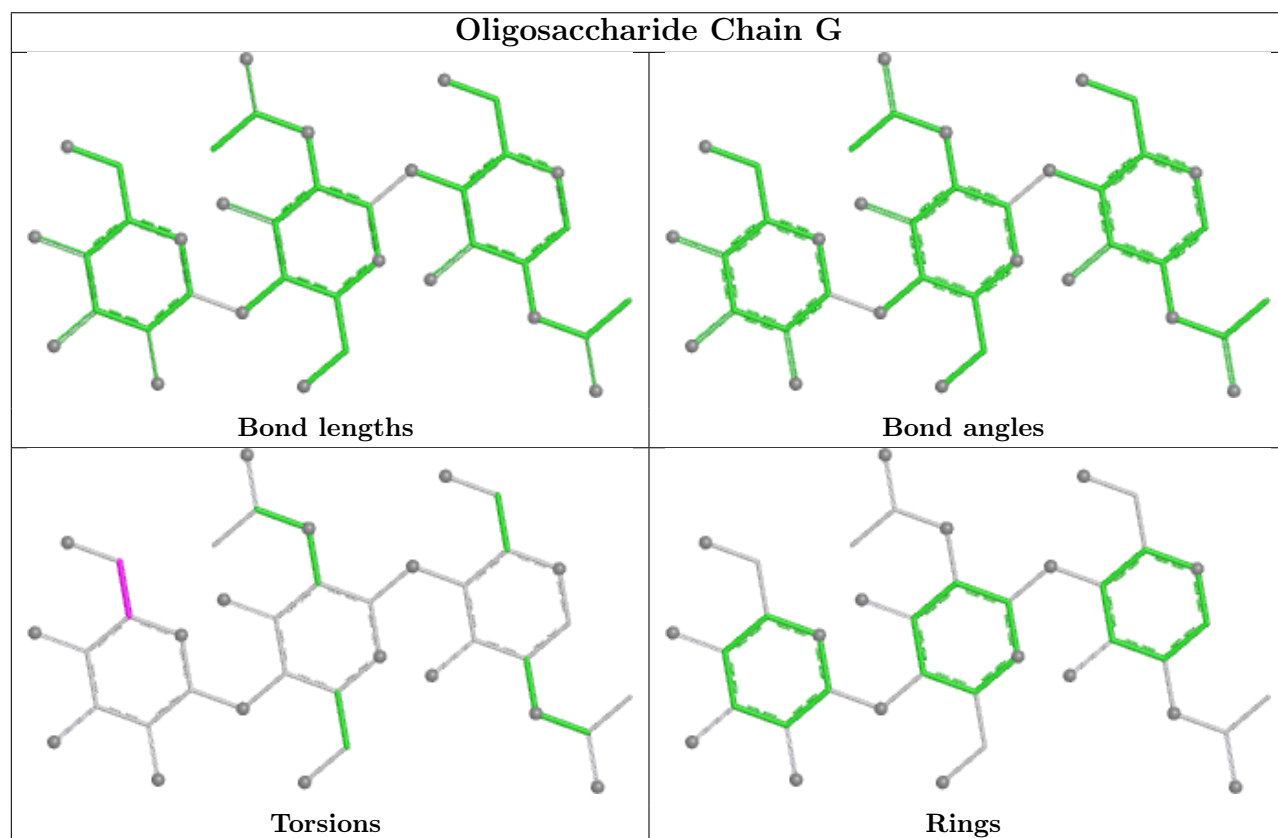
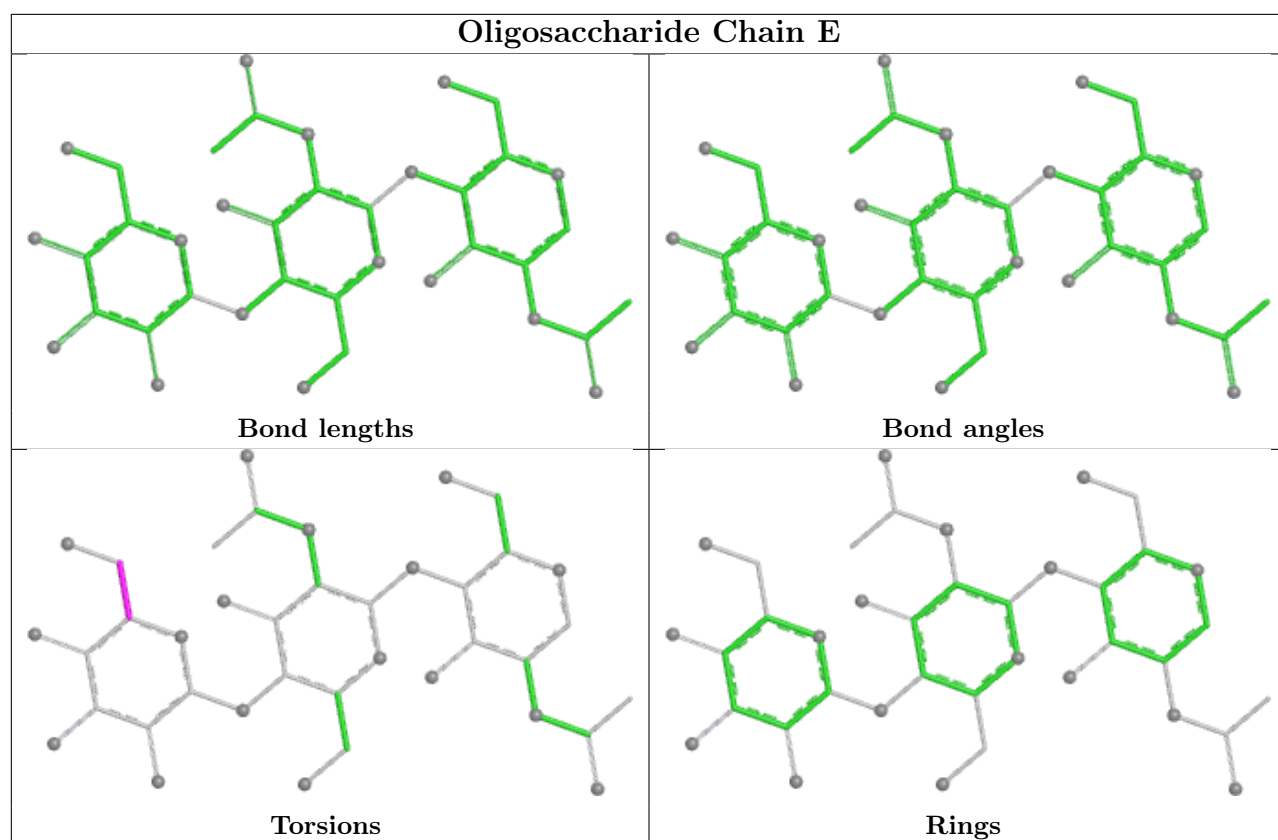
There are no ring outliers.

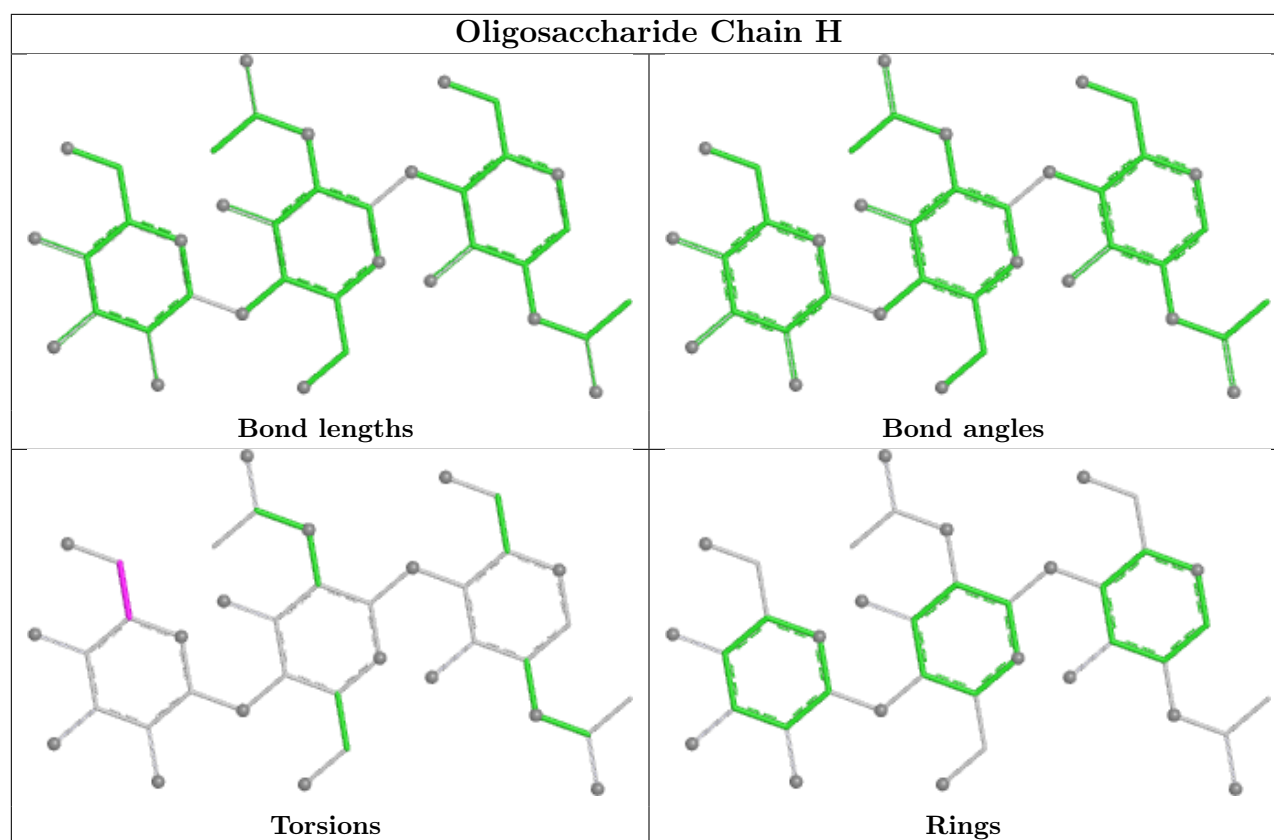
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	3	0
4	E	1	NAG	6	0
4	G	1	NAG	6	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	$\# Z > 2$
5	NAG	b	501	3	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	d	501	3	14,14,15	0.37	0	17,19,21	0.74	0
5	NAG	a	501	-	14,14,15	0.73	0	17,19,21	1.57	3 (17%)
5	NAG	c	501	3	14,14,15	0.39	0	17,19,21	1.16	2 (11%)

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	b	501	3	-	2/6/23/26	0/1/1/1
5	NAG	d	501	3	-	3/6/23/26	0/1/1/1
5	NAG	a	501	-	-	4/6/23/26	0/1/1/1
5	NAG	c	501	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	501	NAG	C1-C2-N2	3.41	115.80	110.43
5	a	501	NAG	C1-O5-C5	-3.32	107.73	112.19
5	a	501	NAG	C4-C3-C2	-3.14	106.42	111.02
5	c	501	NAG	C2-N2-C7	2.68	126.49	122.90
5	a	501	NAG	C1-C2-N2	2.33	114.10	110.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	501	NAG	C1-C2-N2-C7
5	c	501	NAG	C3-C2-N2-C7
5	d	501	NAG	C8-C7-N2-C2
5	d	501	NAG	O7-C7-N2-C2
5	a	501	NAG	O5-C5-C6-O6
5	b	501	NAG	C8-C7-N2-C2
5	b	501	NAG	O7-C7-N2-C2
5	a	501	NAG	C4-C5-C6-O6
5	c	501	NAG	C8-C7-N2-C2
5	d	501	NAG	C3-C2-N2-C7
5	c	501	NAG	O7-C7-N2-C2
5	c	501	NAG	C1-C2-N2-C7
5	a	501	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	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.

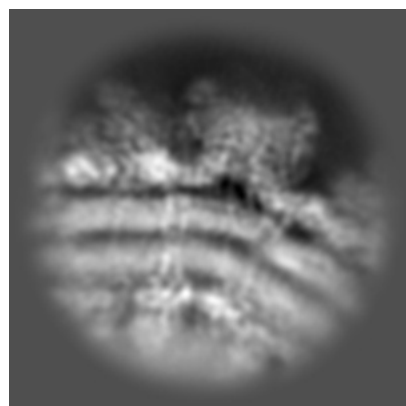
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72745. These allow visual inspection of the internal detail of the map and identification of artifacts.

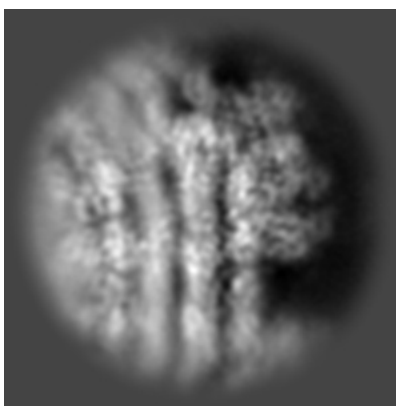
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

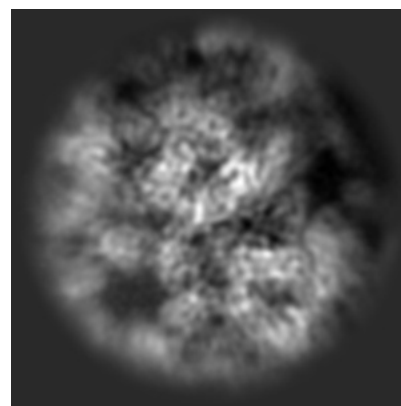
6.1.1 Primary map



X

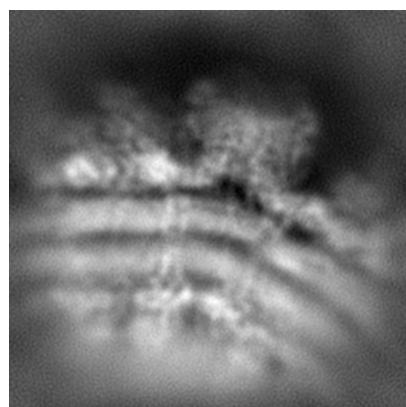


Y

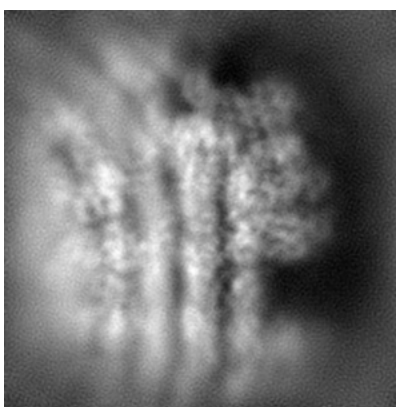


Z

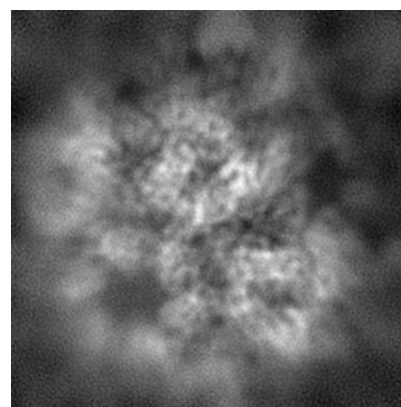
6.1.2 Raw map



X



Y

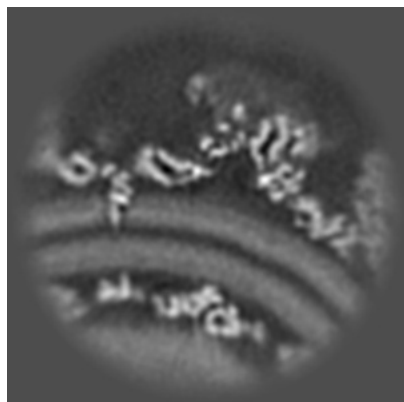


Z

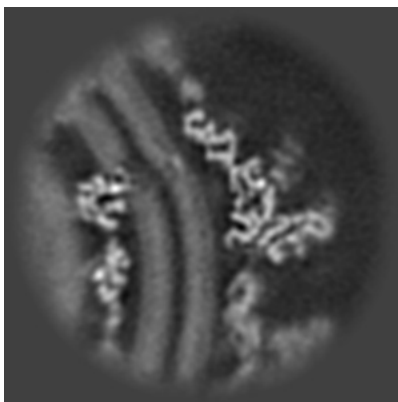
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

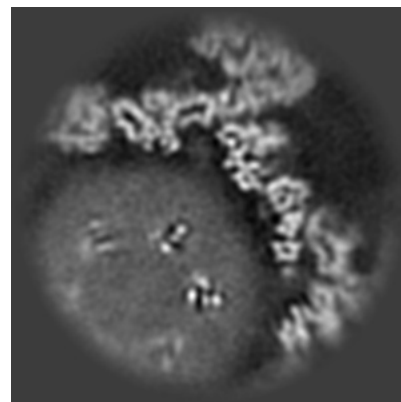
6.2.1 Primary map



X Index: 105



Y Index: 105

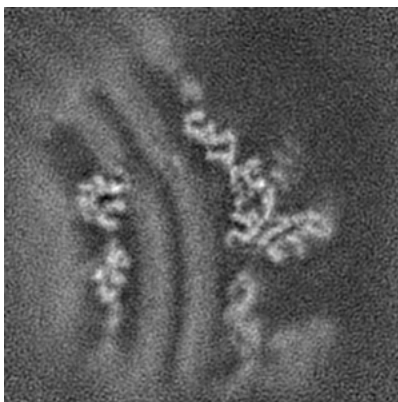


Z Index: 105

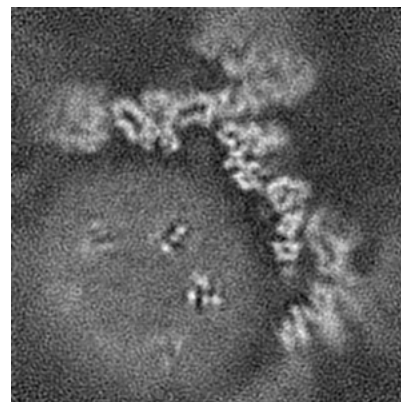
6.2.2 Raw map



X Index: 105



Y Index: 105

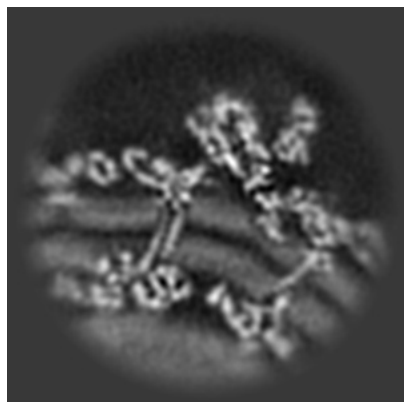


Z Index: 105

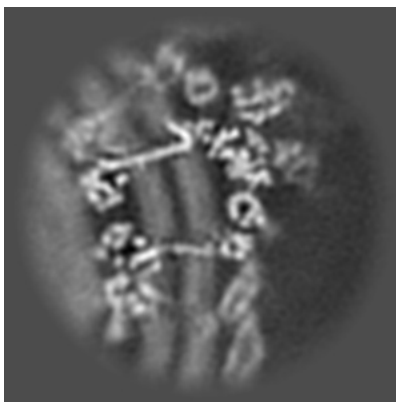
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

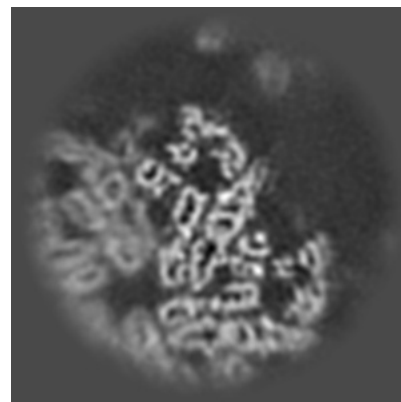
6.3.1 Primary map



X Index: 85

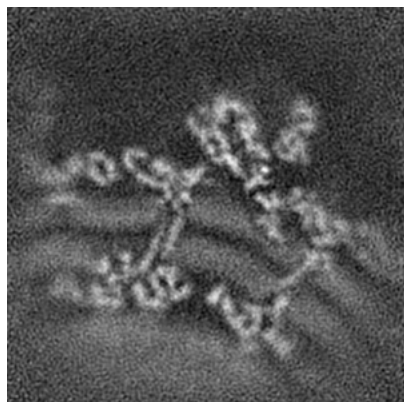


Y Index: 81

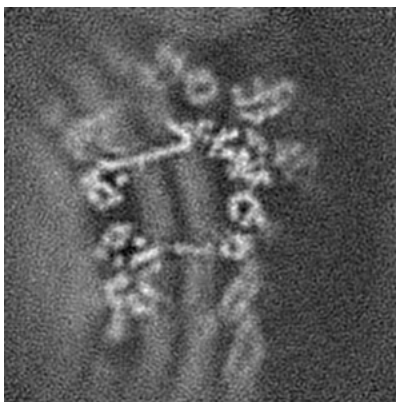


Z Index: 125

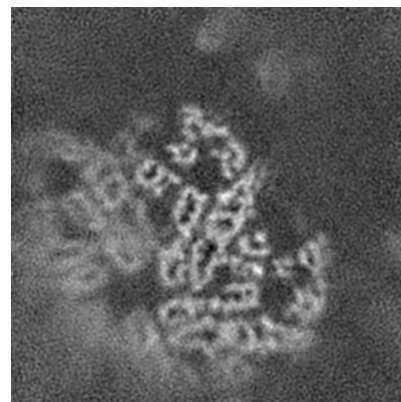
6.3.2 Raw map



X Index: 85



Y Index: 81

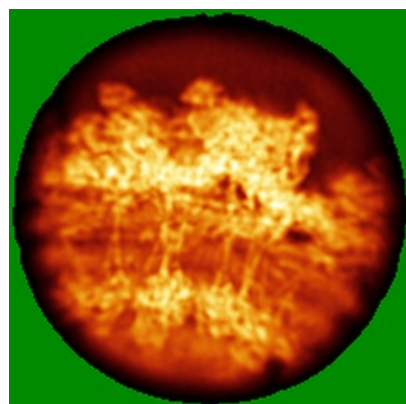


Z Index: 125

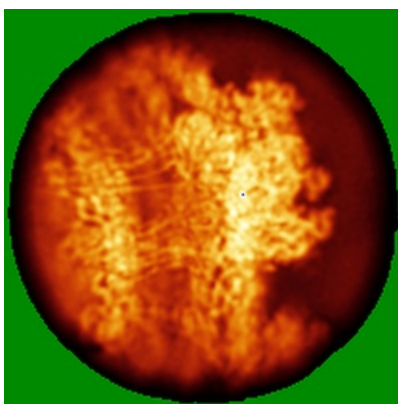
The images above show the largest variance slices of the map in three orthogonal directions.

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

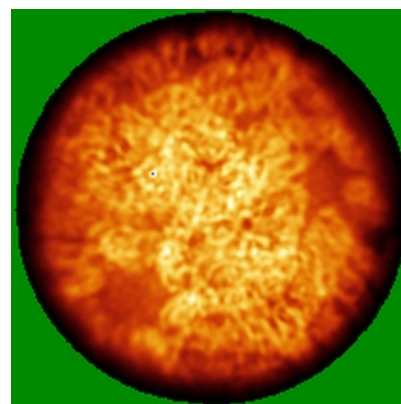
6.4.1 Primary map



X

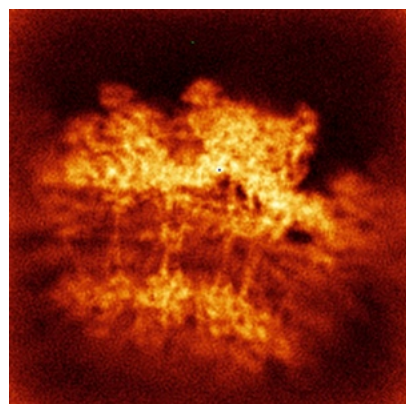


Y

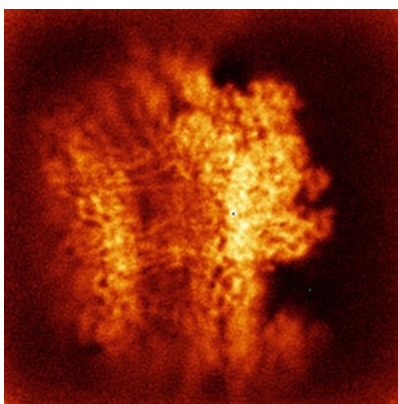


Z

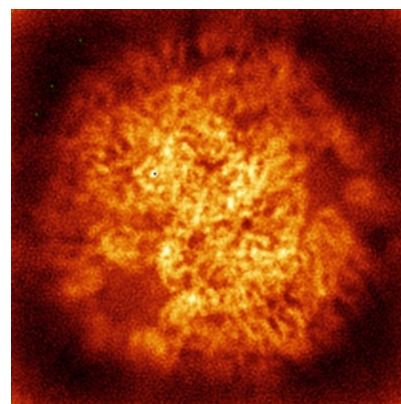
6.4.2 Raw map



X



Y

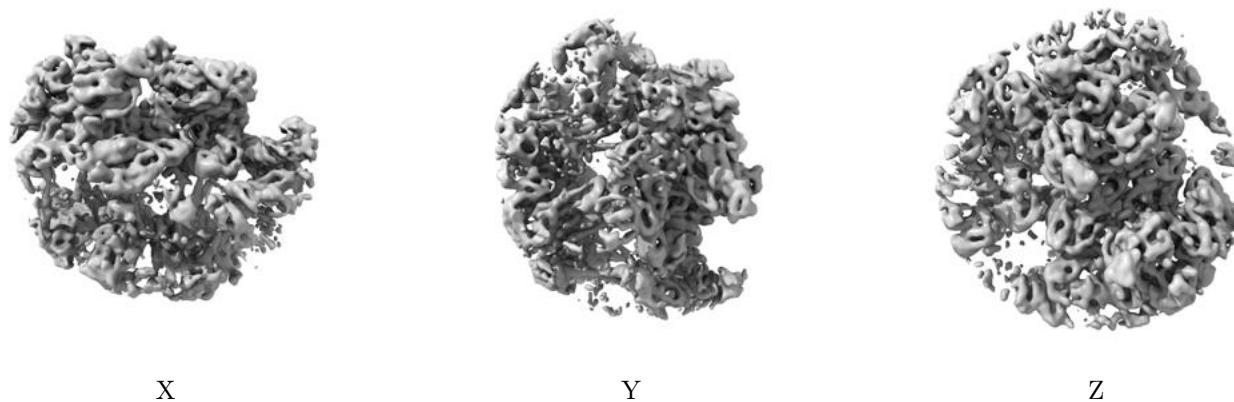


Z

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.

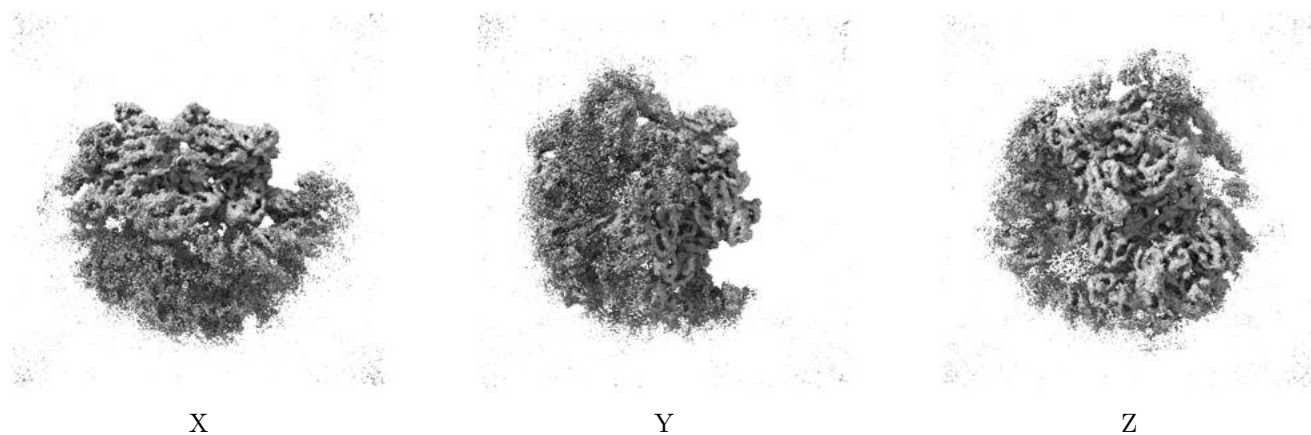
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

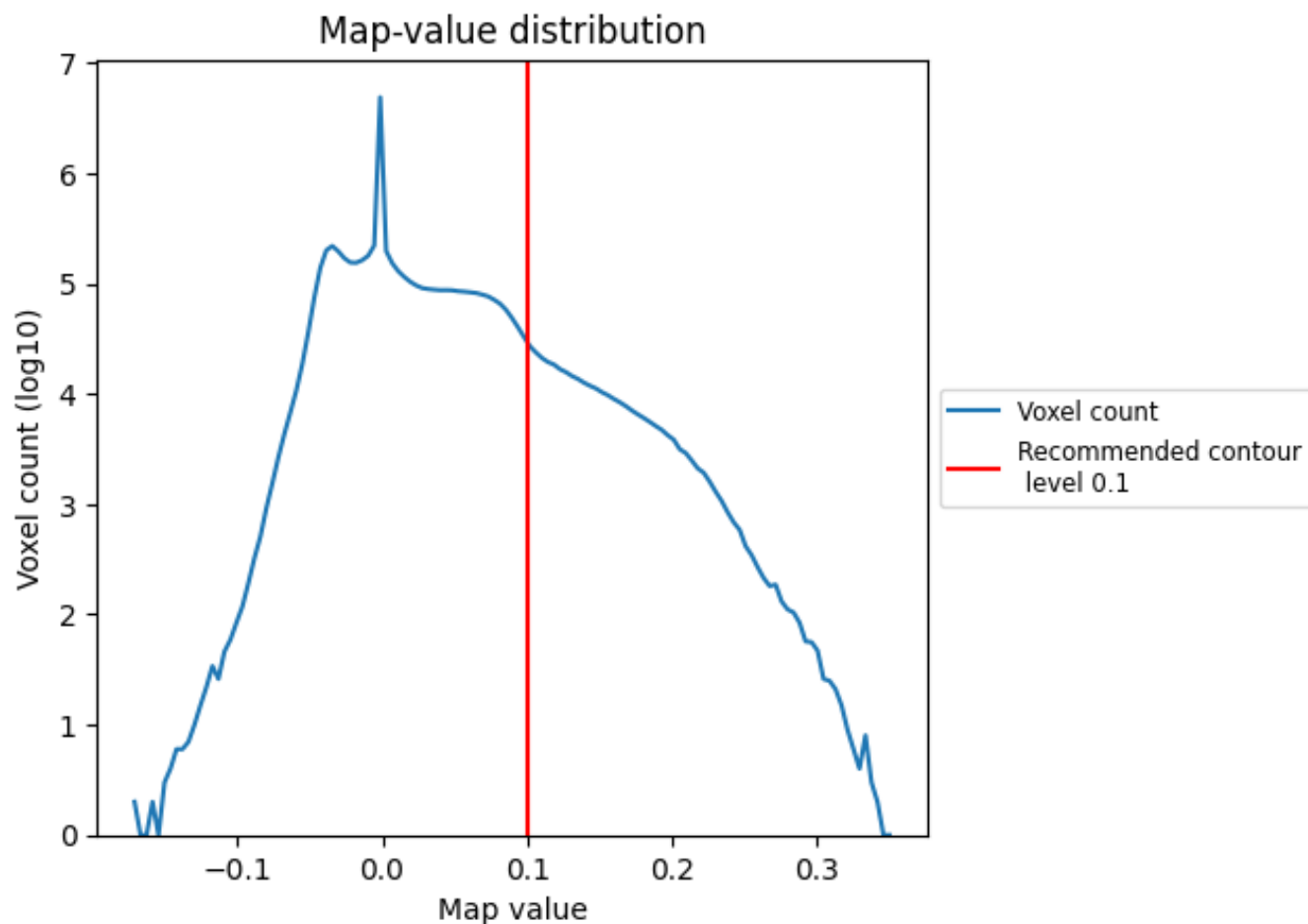
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

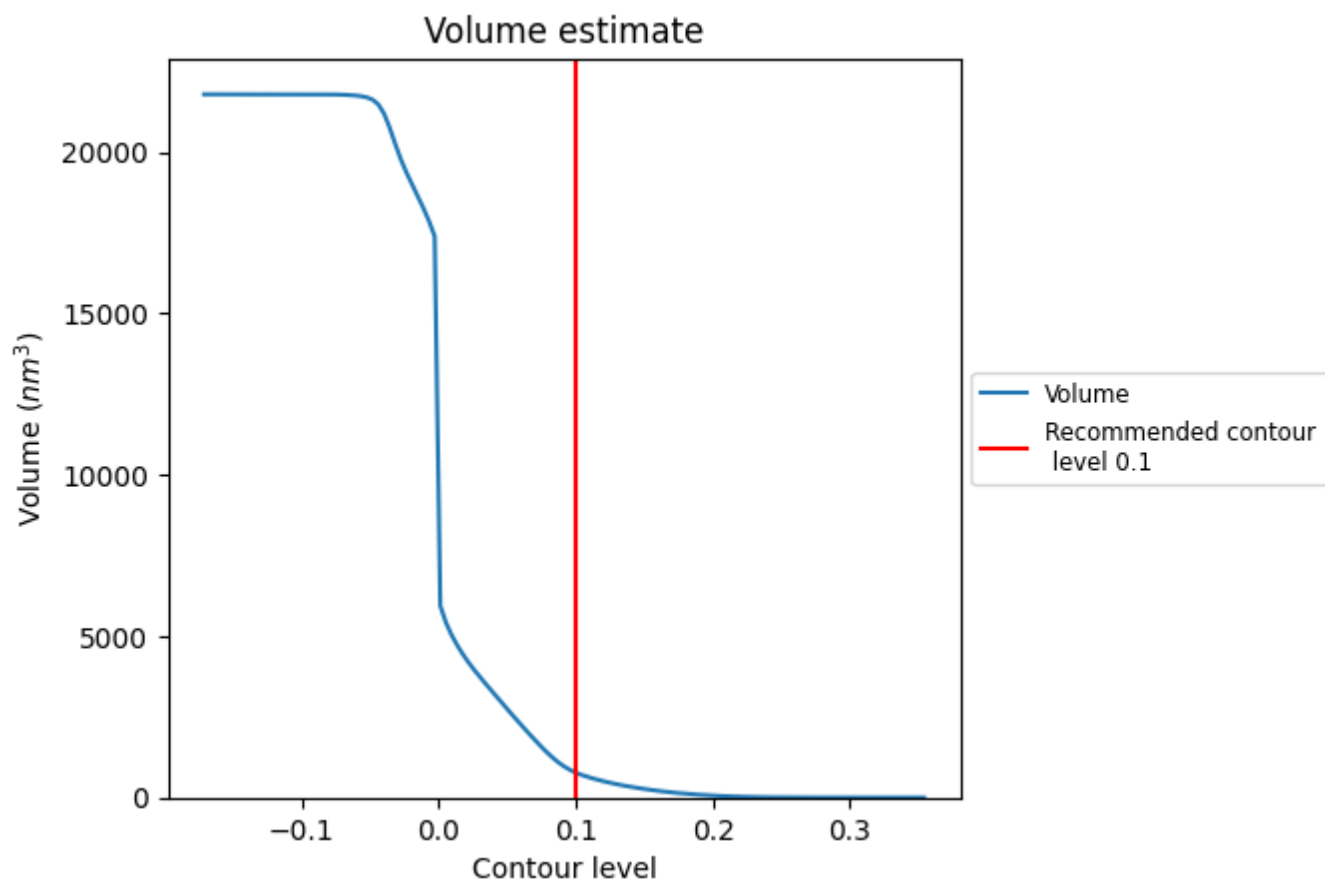
This section contains the results of statistical analysis of the map.

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.

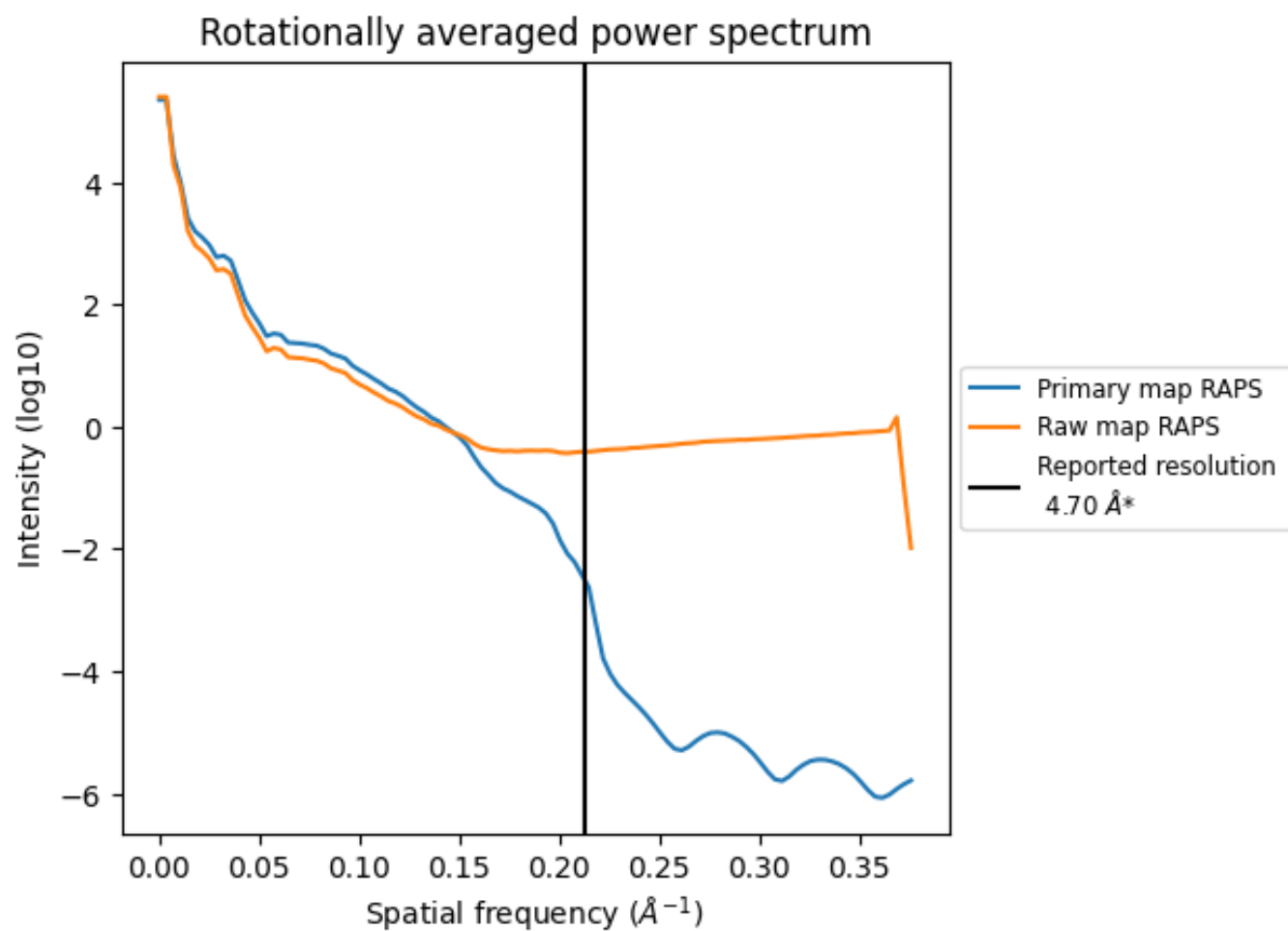
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 775 nm³; this corresponds to an approximate mass of 700 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 ⓘ

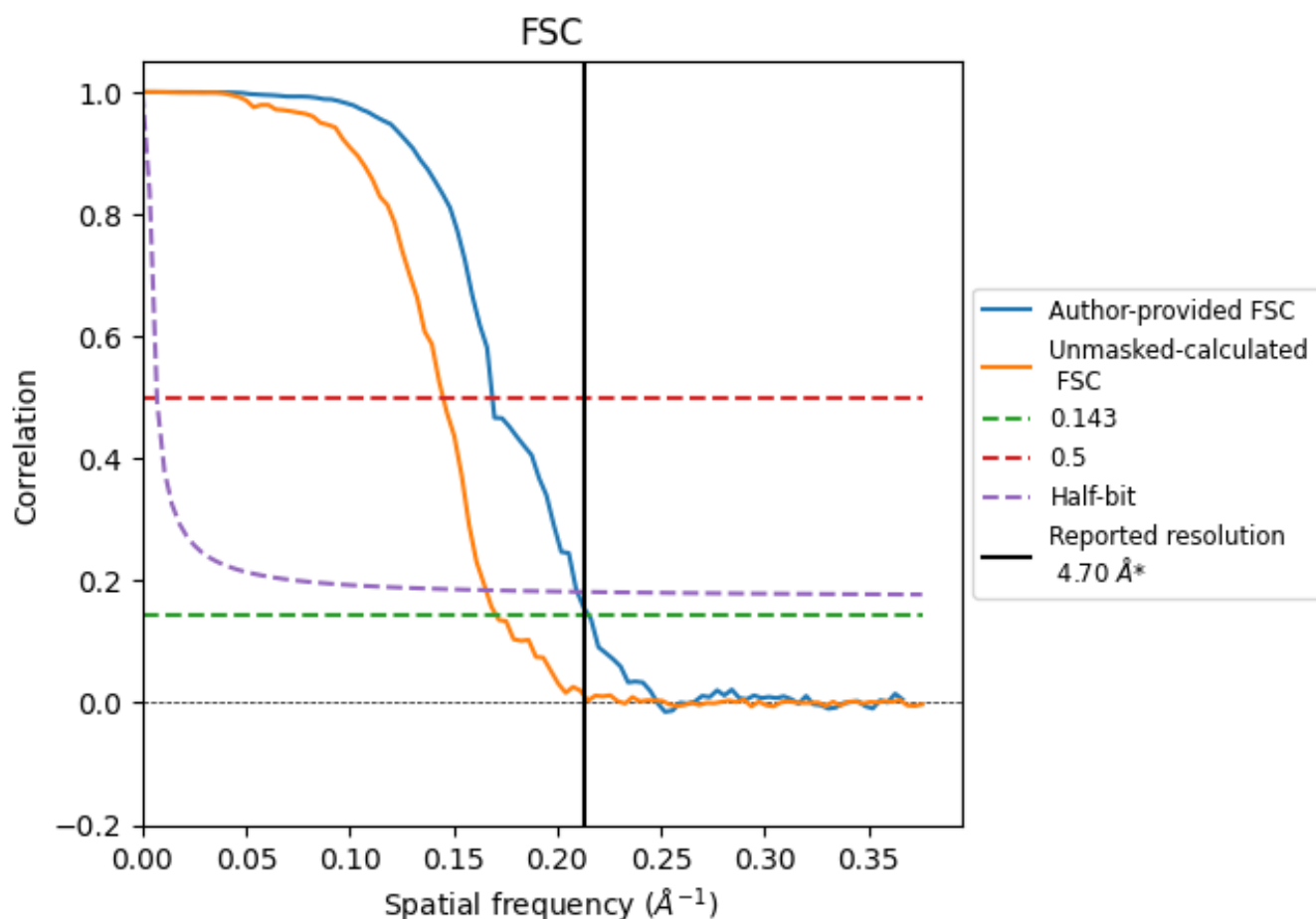


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 \AA^{-1}

8.2 Resolution estimates [i](#)

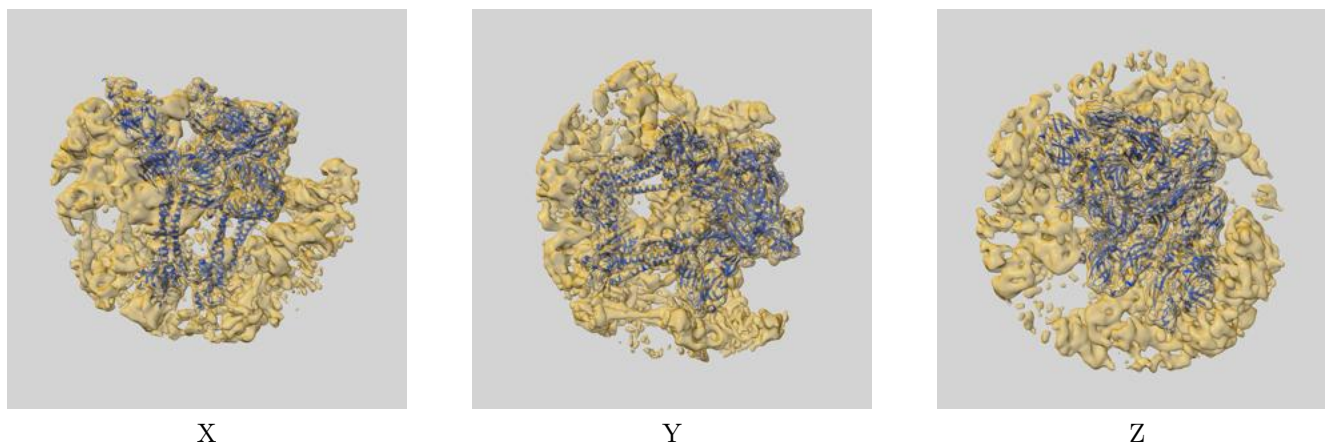
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.65	5.92	4.77
Unmasked-calculated*	5.86	6.90	6.04

*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 5.86 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

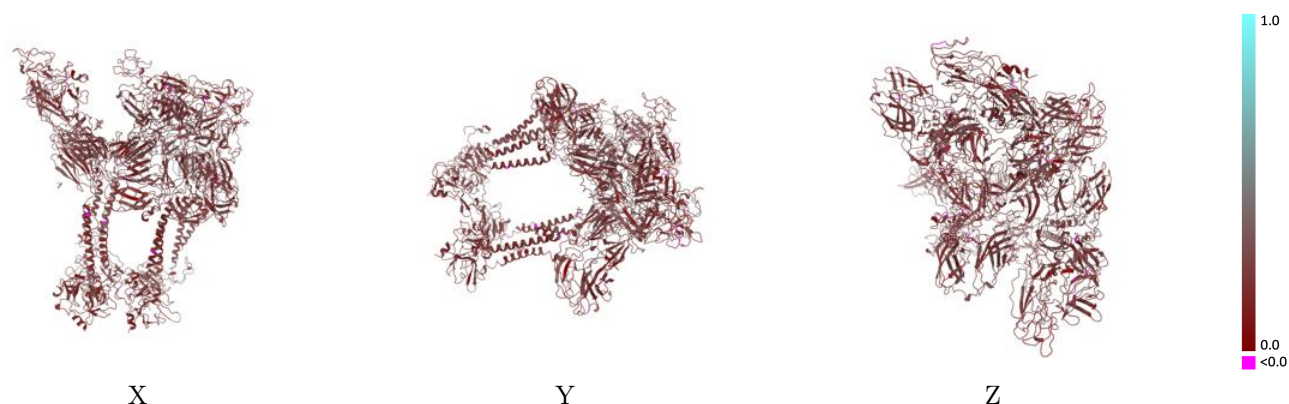
This section contains information regarding the fit between EMDB map EMD-72745 and PDB model 9YB1. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



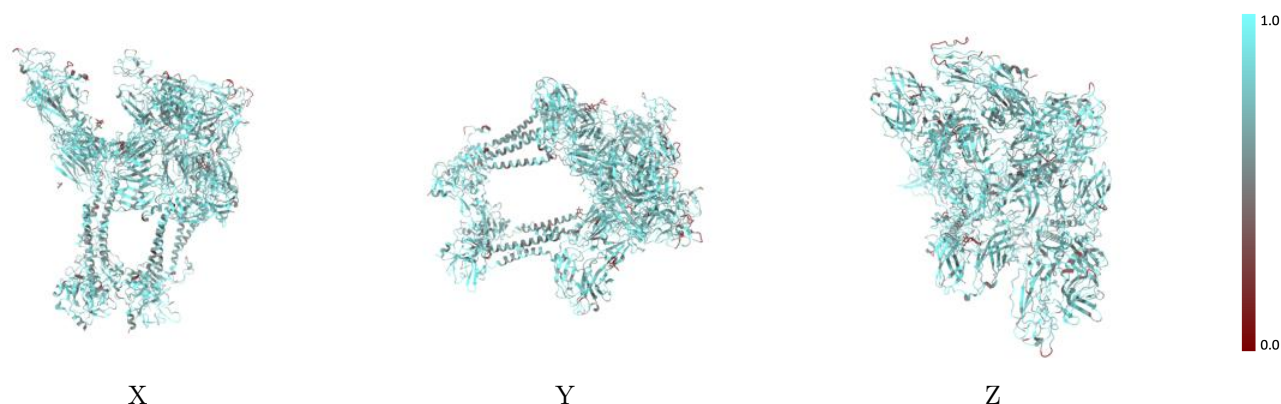
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



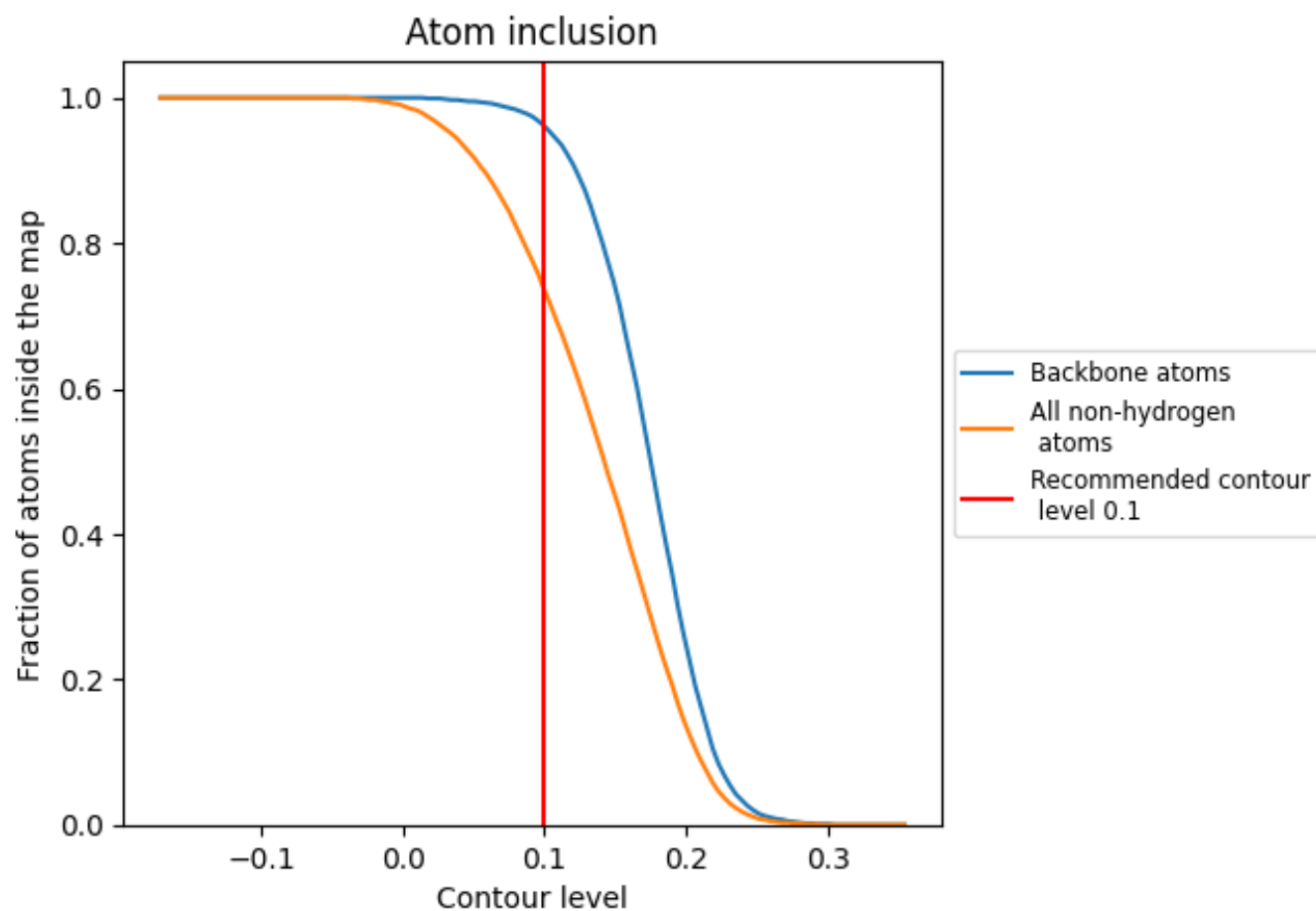
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 74% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7350	<div></div> 0.2440
A	<div></div> 0.7540	<div></div> 0.2590
B	<div></div> 0.7440	<div></div> 0.2540
C	<div></div> 0.7510	<div></div> 0.2520
D	<div></div> 0.7570	<div></div> 0.2580
E	<div></div> 0.4100	<div></div> 0.1550
F	<div></div> 0.3080	<div></div> 0.2150
G	<div></div> 0.2310	<div></div> 0.1250
H	<div></div> 0.2560	<div></div> 0.1740
P	<div></div> 0.7480	<div></div> 0.2270
Q	<div></div> 0.7700	<div></div> 0.2380
R	<div></div> 0.7880	<div></div> 0.2410
S	<div></div> 0.7400	<div></div> 0.2280
a	<div></div> 0.7120	<div></div> 0.2430
b	<div></div> 0.6980	<div></div> 0.2310
c	<div></div> 0.7200	<div></div> 0.2430
d	<div></div> 0.7270	<div></div> 0.2340

1.0

0.0

<0.0