



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:17 AM UTC

PDB ID : 8VSV / pdb_00008vsv
EMDB ID : EMD-43507
Title : Cryo-EM structure of SINV/EEEV in complex with a potentially neutralizing intact human antibody EEEV-373
Authors : Bandyopadhyay, A.; Klose, T.; Kuhn, R.J.
Deposited on : 2024-01-24
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

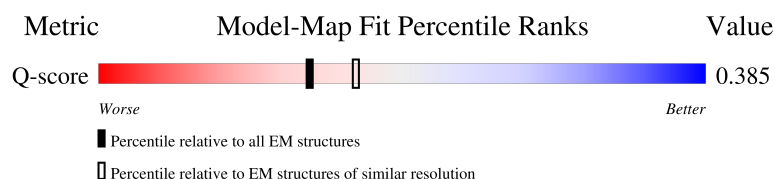
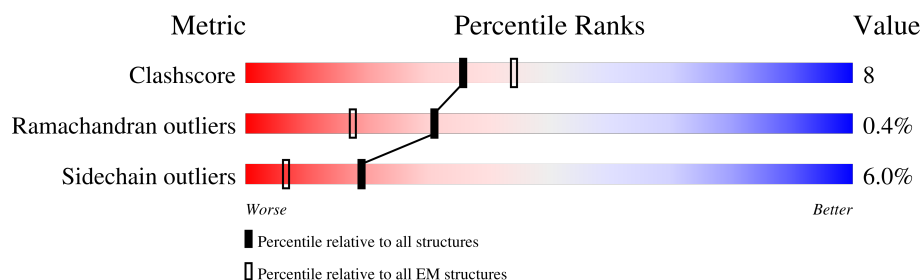
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

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

The reported resolution of this entry is 3.80 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.



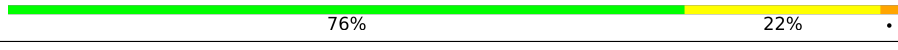
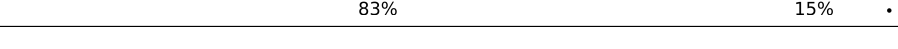
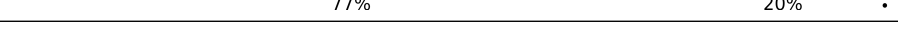
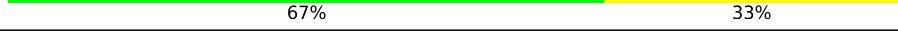
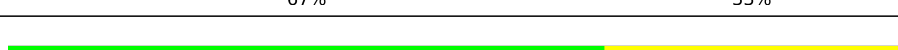
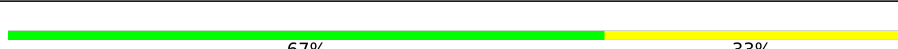
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	1	228	20% 100%
1	3	228	21% 100%
2	2	214	17% 100%
2	4	214	18% 100%

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Mol	Chain	Length	Quality of chain
3	A	400	
3	B	400	
3	C	400	
3	D	400	
3	E	400	
3	F	400	
4	a	338	
4	b	338	
4	c	338	
4	d	338	
4	e	338	
4	f	338	
5	G	3	
5	H	3	
5	I	3	
5	J	3	
5	K	3	
5	L	3	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38222 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 IgG EEEV-373 Heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	228	Total	C	N	O	0	0
			912	456	228	228		
1	3	228	Total	C	N	O	0	0
			912	456	228	228		

- Molecule 2 is a protein called IgG EEEV-373 Light chain..

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	214	Total	C	N	O	0	0
			856	428	214	214		
2	4	214	Total	C	N	O	0	0
			856	428	214	214		

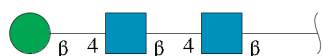
- Molecule 3 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	400	Total	C	N	O	S	0	0
			3064	1940	511	593	20		
3	B	400	Total	C	N	O	S	0	0
			3064	1940	511	593	20		
3	C	400	Total	C	N	O	S	0	0
			3064	1940	511	593	20		
3	D	400	Total	C	N	O	S	0	0
			3064	1940	511	593	20		
3	E	400	Total	C	N	O	S	0	0
			3064	1940	511	593	20		
3	F	400	Total	C	N	O	S	0	0
			3064	1940	511	593	20		

- Molecule 4 is a protein called E2 glycoprotein.

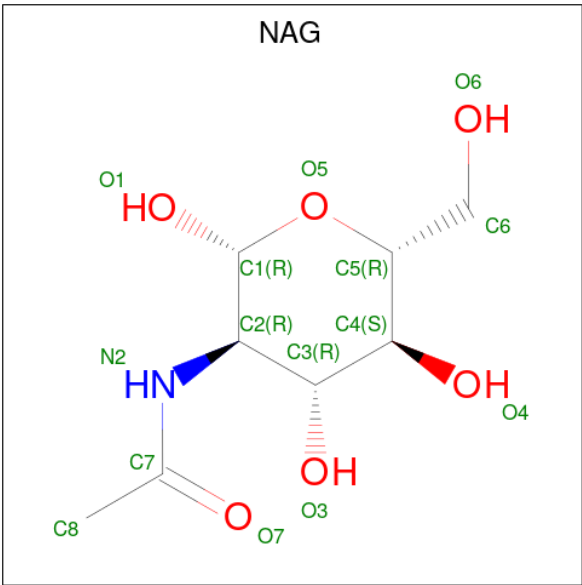
Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	338	Total	C	N	O	S	0	0
			2664	1673	491	484	16		
4	b	338	Total	C	N	O	S	0	0
			2664	1673	491	484	16		
4	c	338	Total	C	N	O	S	0	0
			2664	1673	491	484	16		
4	d	338	Total	C	N	O	S	0	0
			2664	1673	491	484	16		
4	e	338	Total	C	N	O	S	0	0
			2664	1673	491	484	16		
4	f	338	Total	C	N	O	S	0	0
			2664	1673	491	484	16		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	H	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	J	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		
5	L	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

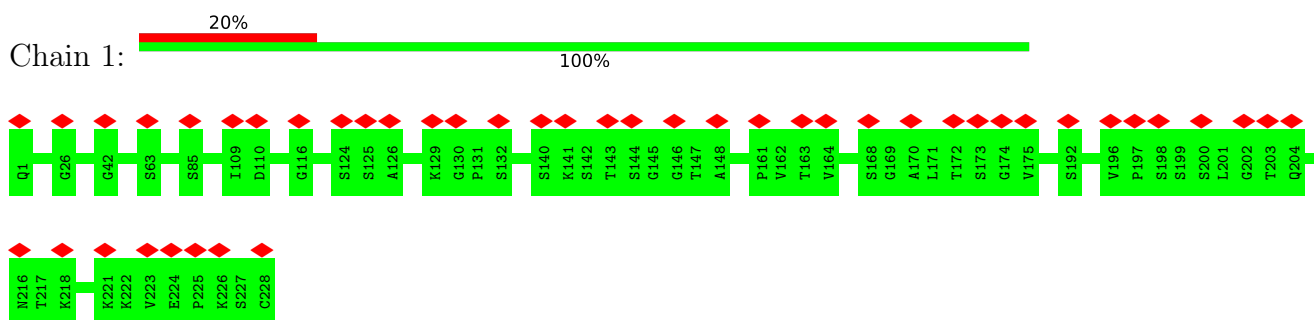


Mol	Chain	Residues	Atoms				AltConf
6	a	1	Total	C	N	O	0
			14	8	1	5	
6	b	1	Total	C	N	O	0
			14	8	1	5	
6	c	1	Total	C	N	O	0
			14	8	1	5	
6	d	1	Total	C	N	O	0
			14	8	1	5	
6	e	1	Total	C	N	O	0
			14	8	1	5	
6	f	1	Total	C	N	O	0
			14	8	1	5	

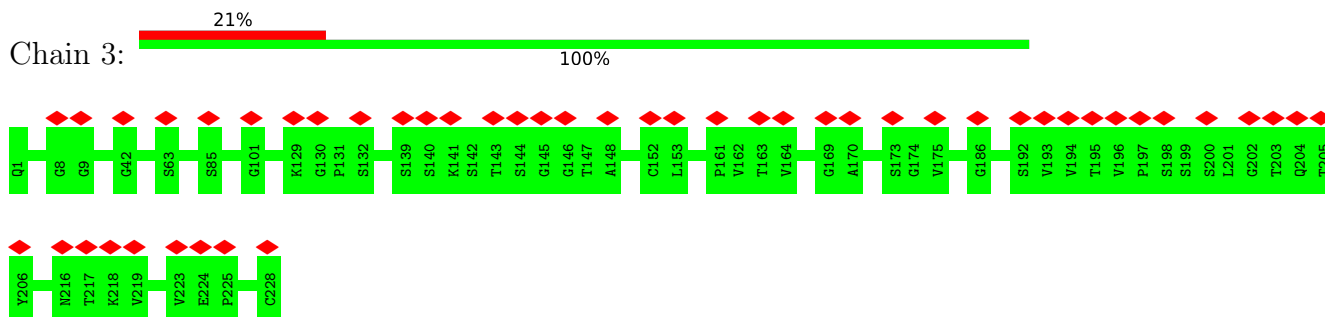
3 Residue-property plots [i](#)

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

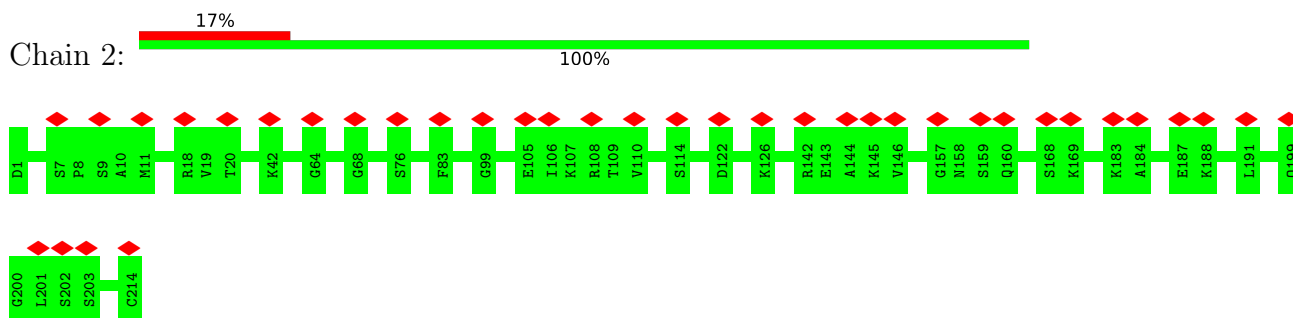
- Molecule 1: IgG EEEV-373 Heavy chain



- Molecule 1: IgG EEEV-373 Heavy chain

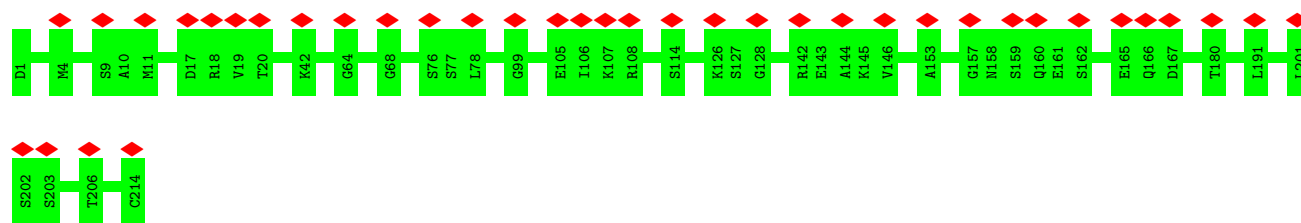


- Molecule 2: IgG EEEV-373 Light chain.



- Molecule 2: IgG EEEV-373 Light chain.





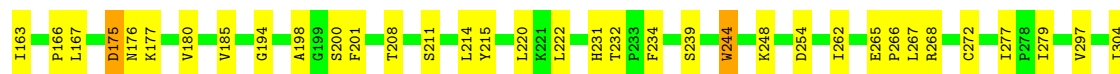
- Molecule 3: Spike glycoprotein E1

Chain A: 87% 12% .



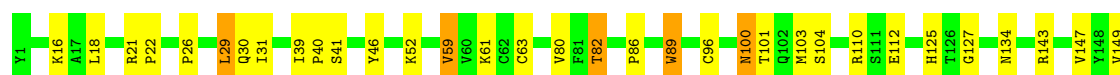
- Molecule 3: Spike glycoprotein E1

Chain B: 76% 22% .



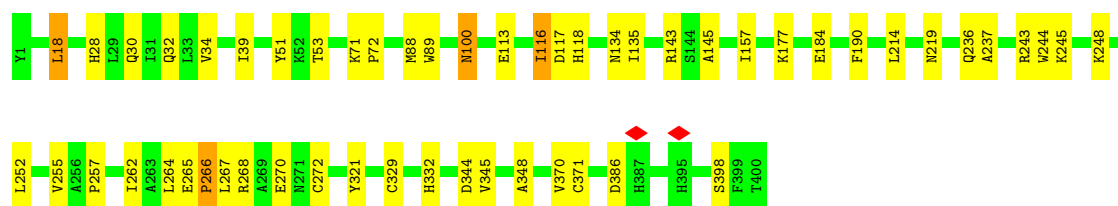
- Molecule 3: Spike glycoprotein E1

Chain C: 83% 15% .



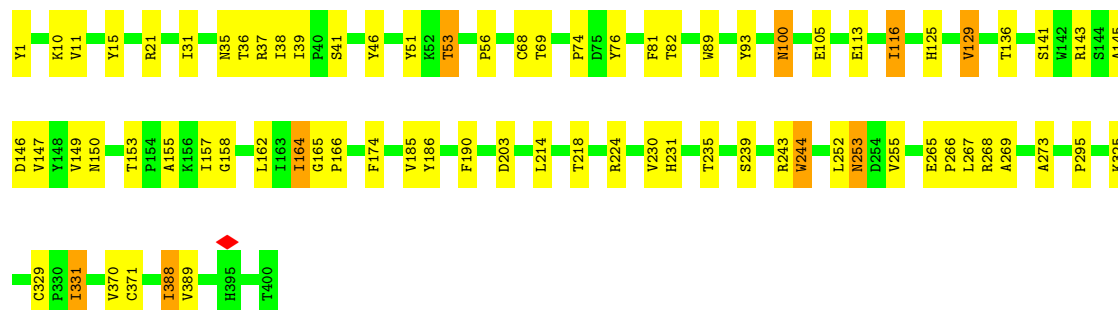
- Molecule 3: Spike glycoprotein E1

Chain D: 86% 12% .



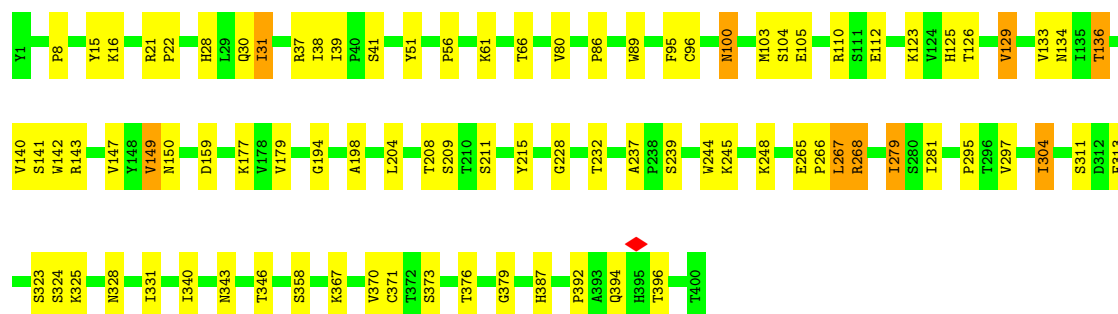
• Molecule 3: Spike glycoprotein E1

Chain E: 81% 17% .



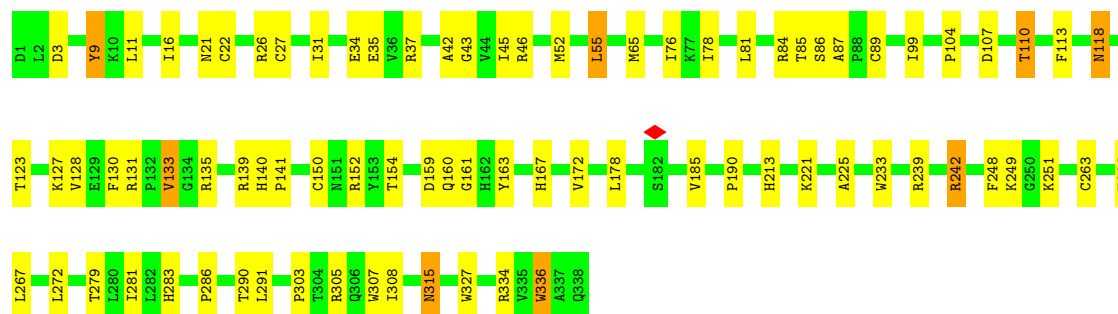
• Molecule 3: Spike glycoprotein E1

Chain F: 78% 20% .



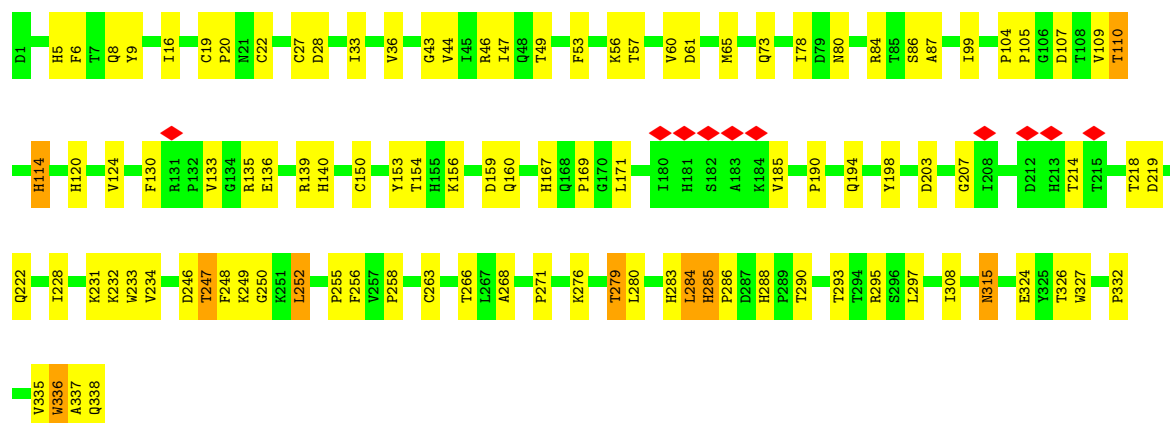
• Molecule 4: E2 glycoprotein

Chain a: 76% 22% .



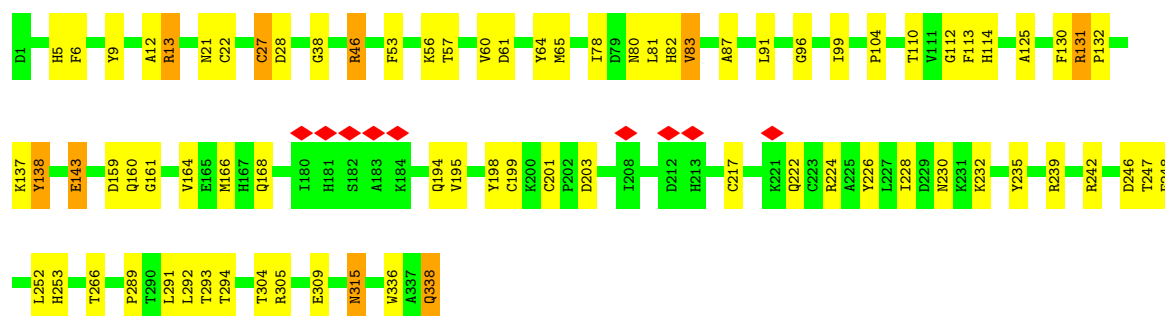
• Molecule 4: E2 glycoprotein

Chain b: 



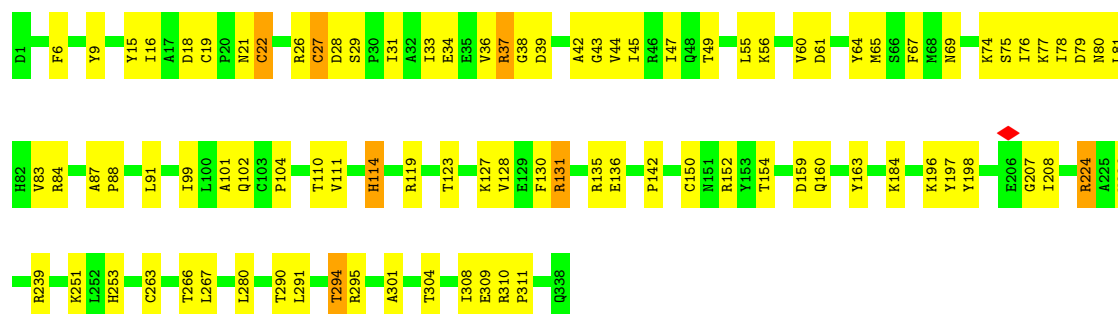
• Molecule 4: E2 glycoprotein

Chain c: 



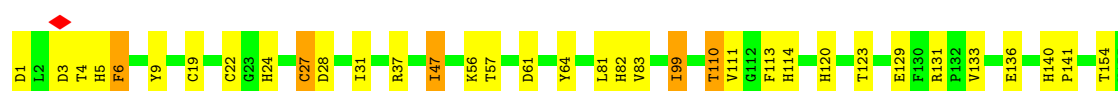
• Molecule 4: E2 glycoprotein

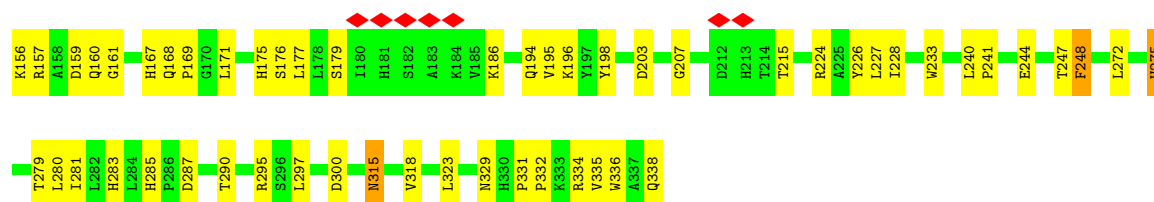
Chain d: 



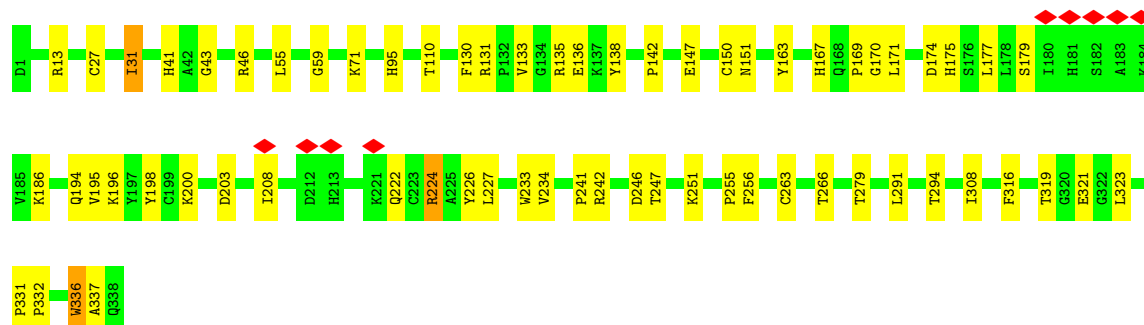
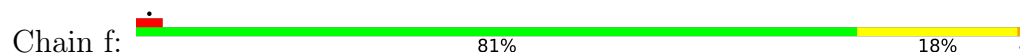
• Molecule 4: E2 glycoprotein

Chain e: 





• Molecule 4: E2 glycoprotein



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



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



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



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





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

Chain K:



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

Chain L:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	271460	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 ($e^-/\text{\AA}^2$)	35.49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	52.350	Depositor
Minimum map value	-27.772	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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: BMA, 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	1	0.71	0/911	1.07	0/1137
1	3	0.56	0/911	0.87	0/1137
2	2	0.74	0/855	1.09	0/1067
2	4	0.55	0/855	0.88	0/1067
3	A	0.59	1/3148 (0.0%)	1.01	0/4294
3	B	0.31	0/3148	0.57	0/4294
3	C	0.61	2/3148 (0.1%)	1.00	0/4294
3	D	0.49	0/3148	0.79	0/4294
3	E	0.45	0/3148	0.74	0/4294
3	F	0.21	0/3148	0.42	0/4294
4	a	0.53	0/2741	0.88	0/3729
4	b	0.47	0/2741	0.75	0/3729
4	c	0.65	0/2741	1.02	3/3729 (0.1%)
4	d	0.52	0/2741	0.85	3/3729 (0.1%)
4	e	0.49	0/2741	0.79	2/3729 (0.1%)
4	f	0.60	0/2741	0.92	0/3729
All	All	0.52	3/38866 (0.0%)	0.84	8/52546 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	1
3	C	0	2
4	a	0	3
4	d	0	4
4	f	0	2
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	TRP	C-O	-7.43	1.14	1.24
3	C	89	TRP	C-N	-5.77	1.25	1.33
3	A	391	TYR	N-CA	5.01	1.50	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	295	ARG	NE-CZ-NH2	6.72	125.25	119.20
4	c	46	ARG	NE-CZ-NH2	5.55	124.20	119.20
4	d	239	ARG	NE-CZ-NH2	5.54	124.18	119.20
4	e	295	ARG	NE-CZ-NH2	5.45	124.11	119.20
4	d	26	ARG	NE-CZ-NH2	5.36	124.03	119.20
4	c	239	ARG	NE-CZ-NH2	5.19	123.87	119.20
4	e	287	ASP	CA-CB-CG	5.10	117.70	112.60
4	c	222	GLN	OE1-CD-NE2	-5.04	117.56	122.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	93	TYR	Sidechain
3	C	391	TYR	Sidechain
3	C	46	TYR	Sidechain
4	a	242	ARG	Sidechain
4	a	334	ARG	Sidechain
4	a	9	TYR	Sidechain
4	d	15	TYR	Sidechain
4	d	197	TYR	Sidechain
4	d	198	TYR	Sidechain
4	d	224	ARG	Sidechain
4	f	13	ARG	Sidechain
4	f	224	ARG	Sidechain

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	1	912	0	262	0	0
1	3	912	0	262	0	0
2	2	856	0	230	0	0
2	4	856	0	230	0	0
3	A	3064	0	2949	27	0
3	B	3064	0	2949	54	0
3	C	3064	0	2949	34	0
3	D	3064	0	2949	30	0
3	E	3064	0	2949	44	0
3	F	3064	0	2949	70	0
4	a	2664	0	2602	58	0
4	b	2664	0	2602	62	0
4	c	2664	0	2602	69	0
4	d	2664	0	2603	62	0
4	e	2664	0	2602	47	0
4	f	2664	0	2602	54	0
5	G	39	0	34	1	0
5	H	39	0	34	0	0
5	I	39	0	34	1	0
5	J	39	0	34	0	0
5	K	39	0	34	0	0
5	L	39	0	34	1	0
6	a	14	0	13	0	0
6	b	14	0	13	0	0
6	c	14	0	13	0	0
6	d	14	0	13	0	0
6	e	14	0	13	0	0
6	f	14	0	13	0	0
All	All	38222	0	34573	565	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 8.

All (565) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:291:LEU:CD1	4:c:305:ARG:HD3	1.19	1.65
4:c:291:LEU:HD11	4:c:305:ARG:CD	1.15	1.59
3:F:95:PHE:CZ	4:f:200:LYS:HB2	1.40	1.54
3:F:95:PHE:CZ	4:f:200:LYS:CB	2.19	1.26
3:A:182:GLY:O	3:A:264:LEU:HD11	1.40	1.22
3:F:95:PHE:CE1	4:f:200:LYS:HB2	1.74	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:65:MET:HB2	4:a:78:ILE:CD1	1.74	1.18
4:a:65:MET:HB2	4:a:78:ILE:CG1	1.77	1.13
4:a:65:MET:HB2	4:a:78:ILE:HD11	1.25	1.11
4:c:83:VAL:HG12	4:c:91:LEU:CD2	1.82	1.09
4:d:83:VAL:HG21	4:d:91:LEU:HD21	1.11	1.09
3:F:95:PHE:HZ	4:f:200:LYS:HD2	1.10	1.08
4:c:83:VAL:CG1	4:c:91:LEU:CD2	2.32	1.08
4:d:91:LEU:HD23	4:d:101:ALA:HB2	1.30	1.07
4:d:83:VAL:CG2	4:d:91:LEU:HD21	1.85	1.06
3:F:95:PHE:CE2	4:f:200:LYS:HB2	1.90	1.06
4:c:56:LYS:HG2	4:c:57:THR:H	1.22	1.03
4:c:291:LEU:HD11	4:c:305:ARG:CG	1.87	1.03
4:c:293:THR:HG22	4:c:305:ARG:HG3	1.41	1.03
4:a:65:MET:CB	4:a:78:ILE:CG1	2.40	1.00
4:c:83:VAL:HG12	4:c:91:LEU:HD21	1.42	0.98
4:c:83:VAL:HG11	4:c:91:LEU:HD23	1.44	0.98
4:c:83:VAL:CG1	4:c:91:LEU:HD23	1.93	0.98
3:F:95:PHE:CZ	4:f:200:LYS:HD2	2.01	0.95
4:c:291:LEU:CD1	4:c:305:ARG:CD	2.01	0.93
3:F:95:PHE:CE1	4:f:222:GLN:HB2	2.03	0.93
3:F:95:PHE:CZ	4:f:200:LYS:CG	2.51	0.93
4:c:291:LEU:HD13	4:c:305:ARG:HD3	1.47	0.91
3:F:95:PHE:HZ	4:f:200:LYS:CD	1.84	0.91
4:d:91:LEU:HD22	4:d:99:ILE:HG22	1.51	0.91
4:c:83:VAL:CG1	4:c:91:LEU:HD21	1.97	0.90
4:a:21:ASN:HB3	4:a:123:THR:CG2	2.02	0.89
3:A:182:GLY:O	3:A:264:LEU:CD1	2.23	0.87
4:a:65:MET:CB	4:a:78:ILE:HG13	2.06	0.85
4:d:91:LEU:HD22	4:d:99:ILE:CG2	2.07	0.84
4:c:293:THR:HG22	4:c:305:ARG:CG	2.09	0.82
3:F:95:PHE:CZ	4:f:200:LYS:CD	2.62	0.79
4:b:185:VAL:HG13	4:b:218:THR:O	1.83	0.78
4:b:80:ASN:HB2	4:b:114:HIS:HB2	1.66	0.77
3:F:95:PHE:HE1	4:f:222:GLN:HB2	1.44	0.77
4:e:56:LYS:HB2	4:e:61:ASP:HB2	1.67	0.77
4:a:65:MET:CB	4:a:78:ILE:HD11	2.13	0.76
4:e:169:PRO:HD3	4:e:233:TRP:HA	1.65	0.76
4:d:83:VAL:HG21	4:d:91:LEU:CD2	2.05	0.76
4:c:83:VAL:HG11	4:c:91:LEU:CD2	2.04	0.76
4:d:91:LEU:CD2	4:d:101:ALA:HB2	2.16	0.74
3:F:95:PHE:CE1	4:f:200:LYS:CB	2.60	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:65:MET:HB3	4:a:78:ILE:HG13	1.67	0.74
3:E:41:SER:HB3	3:E:125:HIS:HB2	1.70	0.73
4:a:65:MET:HB2	4:a:78:ILE:HG12	1.71	0.73
3:F:15:TYR:HB2	3:F:31:ILE:HG23	1.70	0.72
3:F:95:PHE:CE2	4:f:200:LYS:CB	2.59	0.72
4:d:309:GLU:HG2	4:d:310:ARG:N	2.04	0.72
3:B:400:THR:HG23	3:B:400:THR:OXT	1.89	0.71
3:F:41:SER:HB3	3:F:125:HIS:HB2	1.73	0.71
4:c:56:LYS:CG	4:c:57:THR:H	2.01	0.71
3:D:143:ARG:NH2	3:D:157:ILE:O	2.23	0.70
4:a:65:MET:CB	4:a:78:ILE:HG12	2.21	0.70
4:d:80:ASN:HB2	4:d:114:HIS:HB2	1.72	0.70
4:c:168:GLN:H	4:c:248:PHE:HB2	1.55	0.70
4:d:45:ILE:CD1	4:d:128:VAL:HG11	2.21	0.69
4:a:21:ASN:HB3	4:a:123:THR:HG23	1.74	0.69
3:A:129:VAL:HG13	3:A:149:VAL:HB	1.73	0.69
4:a:21:ASN:HB3	4:a:123:THR:HG22	1.75	0.68
3:F:142:TRP:HB3	5:L:1:NAG:H5	1.75	0.68
4:c:56:LYS:HG2	4:c:57:THR:N	2.02	0.68
3:F:100:ASN:N	3:F:100:ASN:OD1	2.26	0.68
4:b:154:THR:HG22	4:b:156:LYS:H	1.58	0.68
3:F:8:PRO:O	3:F:15:TYR:OH	2.08	0.68
4:d:91:LEU:HD23	4:d:101:ALA:CB	2.17	0.67
4:d:74:LYS:HG2	4:d:76:ILE:HD11	1.78	0.66
3:F:295:PRO:HB3	3:F:325:LYS:HB2	1.77	0.66
4:a:281:ILE:HD13	4:a:315:ASN:HB3	1.77	0.66
4:d:309:GLU:HG2	4:d:310:ARG:H	1.58	0.66
4:e:19:CYS:HB3	4:e:22:CYS:HB2	1.77	0.66
4:e:61:ASP:HB3	4:e:64:TYR:HB2	1.78	0.65
4:b:135:ARG:NH2	4:b:326:THR:OG1	2.30	0.65
4:c:315:ASN:OD1	4:c:315:ASN:N	2.28	0.65
4:e:177:LEU:HD11	4:e:227:LEU:HD21	1.79	0.65
3:F:80:VAL:HG12	3:F:103:MET:HB3	1.79	0.65
4:f:198:TYR:HE1	4:f:203:ASP:H	1.45	0.65
3:F:95:PHE:CE2	4:f:200:LYS:CG	2.80	0.64
4:c:56:LYS:HB2	4:c:61:ASP:HB2	1.79	0.64
4:c:291:LEU:CD1	4:c:305:ARG:HD2	2.20	0.64
4:b:56:LYS:HB2	4:b:61:ASP:HB2	1.78	0.64
3:F:328:ASN:OD1	3:F:346:THR:OG1	2.16	0.63
3:B:59:VAL:HB	3:B:103:MET:HB3	1.79	0.63
4:b:293:THR:HG1	4:b:326:THR:HG1	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:308:ILE:HD11	4:b:327:TRP:HZ3	1.64	0.63
4:d:44:VAL:HG12	4:d:102:GLN:HG2	1.81	0.62
4:e:297:LEU:HD21	4:e:334:ARG:HE	1.65	0.62
3:F:95:PHE:CE2	4:f:200:LYS:HG3	2.34	0.62
4:d:196:LYS:HA	4:d:207:GLY:CA	2.30	0.62
4:b:198:TYR:HE1	4:b:203:ASP:H	1.47	0.61
4:f:170:GLY:HA3	4:f:241:PRO:O	2.00	0.61
3:F:245:LYS:O	3:F:248:LYS:NZ	2.33	0.61
3:B:254:ASP:OD2	4:b:135:ARG:NH1	2.34	0.61
3:C:61:LYS:NZ	3:C:63:CYS:O	2.34	0.61
3:E:253:ASN:OD1	3:E:253:ASN:N	2.33	0.61
4:d:42:ALA:HB3	4:d:152:ARG:HD3	1.82	0.61
4:a:135:ARG:HE	4:a:291:LEU:HD23	1.66	0.61
4:b:169:PRO:HB3	4:b:234:VAL:CG2	2.30	0.61
4:a:65:MET:HB3	4:a:78:ILE:CG1	2.22	0.61
3:B:76:TYR:OH	3:B:105:GLU:OE1	2.19	0.60
3:F:110:ARG:HG2	3:F:204:LEU:HD21	1.83	0.60
3:C:59:VAL:HB	3:C:103:MET:HE3	1.83	0.60
4:a:133:VAL:HG11	4:a:150:CYS:HB3	1.84	0.60
4:d:38:GLY:CA	4:d:45:ILE:HG13	2.32	0.60
3:C:59:VAL:HG23	3:C:103:MET:HG3	1.84	0.60
4:c:198:TYR:HE1	4:c:203:ASP:H	1.48	0.60
3:C:208:THR:HG22	3:C:211:SER:HB3	1.83	0.60
3:C:227:ALA:O	3:C:229:ILE:HG12	2.00	0.60
3:E:113:GLU:OE2	4:e:37:ARG:NH2	2.34	0.60
4:a:272:LEU:HB2	4:a:283:HIS:HB2	1.82	0.60
3:A:71:LYS:HB3	3:A:71:LYS:HZ2	1.65	0.60
4:e:194:GLN:HB3	4:e:228:ILE:HB	1.84	0.59
4:e:272:LEU:HB2	4:e:283:HIS:HB2	1.84	0.59
3:F:30:GLN:HB3	3:F:136:THR:HG23	1.83	0.59
3:F:56:PRO:HG2	3:F:105:GLU:HG3	1.84	0.59
4:c:138:TYR:CD1	4:c:266:THR:HG21	2.37	0.59
3:C:41:SER:HB2	3:C:125:HIS:HB3	1.83	0.59
3:F:313:PHE:HA	3:F:358:SER:HB3	1.84	0.59
3:E:100:ASN:OD1	3:E:100:ASN:N	2.34	0.59
4:b:276:LYS:HB2	4:b:279:THR:HG23	1.85	0.59
3:C:360:ALA:HB3	3:C:396:THR:HG23	1.85	0.58
3:E:129:VAL:HG22	3:E:149:VAL:HB	1.85	0.58
4:b:8:GLN:HB2	4:b:252:LEU:HD11	1.84	0.58
4:c:292:LEU:O	4:c:305:ARG:HG2	2.04	0.58
3:F:123:LYS:HE2	3:F:177:LYS:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:56:LYS:N	4:d:60:VAL:O	2.28	0.58
4:b:136:GLU:OE2	4:b:268:ALA:N	2.37	0.58
4:b:246:ASP:OD1	4:b:247:THR:N	2.37	0.58
4:b:295:ARG:NH2	4:b:324:GLU:OE2	2.36	0.58
3:B:359:THR:O	3:B:394:GLN:NE2	2.37	0.58
4:d:78:ILE:HD11	4:d:81:LEU:HD22	1.86	0.58
3:E:389:VAL:H	4:e:336:TRP:CD1	2.21	0.57
3:B:149:VAL:HG21	3:B:167:LEU:HG	1.86	0.57
4:d:43:GLY:HA2	4:d:130:PHE:CD1	2.38	0.57
4:b:169:PRO:HB3	4:b:234:VAL:HG22	1.86	0.57
4:a:22:CYS:HB3	4:a:27:CYS:H	1.70	0.57
4:f:196:LYS:HB3	4:f:226:TYR:HD2	1.68	0.57
4:d:76:ILE:HG22	4:d:77:LYS:H	1.70	0.57
4:b:288:HIS:O	4:b:290:THR:HG23	2.04	0.57
4:a:159:ASP:OD1	4:a:160:GLN:N	2.38	0.57
3:B:135:ILE:H	3:B:143:ARG:HB3	1.69	0.56
3:B:323:SER:OG	3:B:348:ALA:O	2.23	0.56
4:d:87:ALA:HB3	4:d:104:PRO:HG3	1.87	0.56
4:f:171:LEU:HD13	4:f:226:TYR:CG	2.40	0.56
4:a:85:THR:OG1	4:a:89:CYS:SG	2.63	0.56
4:e:154:THR:HG22	4:e:156:LYS:H	1.70	0.56
4:c:291:LEU:HD21	4:c:305:ARG:HH21	1.71	0.56
4:e:47:ILE:HG23	4:e:99:ILE:HG23	1.88	0.56
3:A:51:TYR:OH	3:A:237:ALA:O	2.24	0.56
3:D:100:ASN:OD1	3:D:100:ASN:N	2.24	0.56
4:d:91:LEU:CD2	4:d:99:ILE:CG2	2.83	0.56
3:C:40:PRO:HA	3:C:127:GLY:HA3	1.87	0.56
3:F:30:GLN:OE1	3:F:343:ASN:ND2	2.38	0.56
3:F:198:ALA:HB3	4:e:272:LEU:HD11	1.88	0.56
4:b:56:LYS:N	4:b:60:VAL:O	2.31	0.56
3:B:389:VAL:O	4:b:336:TRP:NE1	2.39	0.56
3:F:112:GLU:OE1	4:f:46:ARG:NH1	2.34	0.56
3:B:307:CYS:HA	3:B:315:GLY:HA2	1.88	0.55
3:F:268:ARG:H	3:F:268:ARG:HD3	1.72	0.55
4:f:150:CYS:SG	4:f:263:CYS:N	2.79	0.55
3:B:129:VAL:HG22	3:B:149:VAL:HB	1.86	0.55
4:d:163:TYR:HB2	4:d:251:LYS:HB2	1.88	0.55
3:D:71:LYS:HE2	3:D:72:PRO:HD2	1.88	0.55
4:c:159:ASP:O	4:c:253:HIS:ND1	2.34	0.55
4:f:46:ARG:NH1	4:f:256:PHE:O	2.39	0.55
4:c:56:LYS:N	4:c:60:VAL:O	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:42:ALA:HB3	4:a:152:ARG:HH11	1.71	0.55
3:C:96:CYS:O	3:C:100:ASN:ND2	2.40	0.54
4:e:198:TYR:HE1	4:e:203:ASP:H	1.53	0.54
3:C:334:PRO:HD3	3:C:369:GLN:HG2	1.89	0.54
3:A:207:ARG:HH22	3:A:213:ASP:HB3	1.72	0.54
3:B:305:THR:HB	3:B:316:ILE:HG13	1.88	0.54
4:d:19:CYS:HB3	4:d:22:CYS:HB2	1.90	0.54
3:D:30:GLN:O	3:D:135:ILE:HA	2.06	0.54
4:c:159:ASP:OD1	4:c:160:GLN:N	2.41	0.54
3:E:265:GLU:C	3:E:267:LEU:H	2.16	0.54
4:d:79:ASP:OD1	4:d:80:ASN:N	2.40	0.54
4:e:240:LEU:HD12	4:e:241:PRO:HD2	1.90	0.54
4:f:163:TYR:HB3	4:f:251:LYS:HB3	1.90	0.54
3:D:321:TYR:OH	3:D:348:ALA:N	2.40	0.53
4:f:294:THR:HB	4:f:323:LEU:HD11	1.90	0.53
3:A:38:ILE:HA	3:A:129:VAL:HG23	1.90	0.53
3:D:53:THR:OG1	3:D:236:GLN:OE1	2.25	0.53
4:c:81:LEU:HG	4:c:91:LEU:HD11	1.91	0.53
3:E:252:LEU:HA	3:E:255:VAL:HG22	1.90	0.53
4:a:11:LEU:HD22	4:a:233:TRP:HZ3	1.74	0.53
4:b:286:PRO:HB3	4:b:327:TRP:HH2	1.73	0.53
4:c:166:MET:SD	4:c:235:TYR:HA	2.48	0.53
4:e:318:VAL:HA	4:e:323:LEU:HD23	1.91	0.53
3:E:76:TYR:OH	3:E:105:GLU:OE1	2.26	0.53
4:b:271:PRO:HB3	4:b:284:LEU:HB3	1.91	0.53
3:A:136:THR:HG21	5:G:1:NAG:H5	1.90	0.53
3:D:257:PRO:HG3	4:d:301:ALA:HB2	1.91	0.53
3:D:268:ARG:NH2	3:D:270:GLU:OE2	2.42	0.53
4:d:45:ILE:HD12	4:d:128:VAL:HG11	1.90	0.53
4:c:164:VAL:HG23	4:c:166:MET:HE2	1.91	0.53
4:a:150:CYS:SG	4:a:263:CYS:N	2.82	0.52
4:b:185:VAL:CG1	4:b:218:THR:O	2.55	0.52
4:d:64:TYR:CZ	4:d:77:LYS:HG2	2.44	0.52
4:f:169:PRO:HB3	4:f:234:VAL:CG1	2.38	0.52
3:E:129:VAL:HG13	3:E:149:VAL:HG11	1.91	0.52
4:c:159:ASP:OD1	4:c:161:GLY:N	2.41	0.52
4:e:315:ASN:OD1	4:e:315:ASN:N	2.42	0.52
3:E:295:PRO:HB3	3:E:325:LYS:HB2	1.90	0.52
4:e:203:ASP:OD2	4:e:215:THR:N	2.42	0.52
4:f:142:PRO:HG2	4:f:266:THR:HB	1.90	0.52
3:F:194:GLY:HA2	3:F:215:TYR:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:112:GLU:OE1	4:b:46:ARG:NH1	2.41	0.52
3:C:100:ASN:OD1	3:C:100:ASN:N	2.43	0.52
3:B:400:THR:OXT	3:B:400:THR:CG2	2.58	0.52
4:a:9:TYR:CD1	4:a:55:LEU:HD21	2.45	0.52
4:a:163:TYR:HB3	4:a:251:LYS:HB3	1.91	0.52
4:d:56:LYS:NZ	4:d:75:SER:OG	2.41	0.52
4:f:246:ASP:OD1	4:f:247:THR:N	2.43	0.52
3:F:110:ARG:NH1	3:F:209:SER:O	2.42	0.52
4:c:12:ALA:O	4:c:13:ARG:NH2	2.42	0.52
4:c:53:PHE:O	4:c:96:GLY:N	2.43	0.52
4:c:83:VAL:HG12	4:c:91:LEU:CG	2.40	0.52
3:F:21:ARG:NH2	3:F:22:PRO:O	2.42	0.52
3:F:95:PHE:HE1	4:f:222:GLN:CB	2.18	0.52
4:b:153:TYR:HA	4:b:258:PRO:HA	1.91	0.52
3:D:18:LEU:HB2	3:D:332:HIS:CD2	2.45	0.51
3:E:53:THR:O	3:E:53:THR:OG1	2.27	0.51
3:F:133:VAL:HG22	3:F:134:ASN:N	2.25	0.51
3:F:265:GLU:C	3:F:267:LEU:H	2.17	0.51
4:a:286:PRO:HG3	4:a:327:TRP:HH2	1.74	0.51
4:e:129:GLU:OE2	4:e:131:ARG:NH1	2.36	0.51
3:D:39:ILE:H	3:D:268:ARG:HA	1.75	0.51
4:c:132:PRO:HG3	4:c:137:LYS:HA	1.91	0.51
4:e:27:CYS:SG	4:e:28:ASP:N	2.83	0.51
3:E:174:PHE:HE1	3:E:269:ALA:HB2	1.76	0.51
4:c:78:ILE:HD11	4:c:81:LEU:HD22	1.92	0.51
4:b:57:THR:HG22	4:b:73:GLN:HE22	1.75	0.51
4:c:87:ALA:HB3	4:c:104:PRO:HG2	1.91	0.51
4:e:159:ASP:OD1	4:e:160:GLN:N	2.44	0.51
4:b:159:ASP:OD1	4:b:160:GLN:N	2.44	0.51
4:d:6:PHE:HA	4:d:9:TYR:HB2	1.92	0.51
4:b:150:CYS:SG	4:b:263:CYS:N	2.84	0.51
4:d:135:ARG:HB3	4:d:291:LEU:HB3	1.92	0.51
4:b:185:VAL:HG23	4:b:214:THR:OG1	2.11	0.51
4:b:194:GLN:HB3	4:b:228:ILE:HB	1.93	0.51
3:A:94:CYS:HB2	3:A:100:ASN:HD21	1.76	0.51
3:B:265:GLU:C	3:B:267:LEU:H	2.18	0.51
3:F:95:PHE:CD1	4:f:200:LYS:HB2	2.39	0.51
4:a:52:MET:HE3	4:a:55:LEU:HD23	1.93	0.51
4:c:21:ASN:O	4:c:21:ASN:ND2	2.43	0.51
4:d:65:MET:HB2	4:d:78:ILE:HD13	1.93	0.51
4:f:95:HIS:CD2	4:f:255:PRO:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:198:ALA:HB3	4:a:272:LEU:HD11	1.93	0.51
4:c:246:ASP:OD1	4:c:247:THR:N	2.44	0.50
4:d:84:ARG:HB3	4:d:110:THR:HG23	1.93	0.50
3:C:21:ARG:HD2	3:C:22:PRO:HD2	1.93	0.50
3:E:136:THR:HG23	3:E:141:SER:HA	1.92	0.50
4:a:139:ARG:NH2	4:b:107:ASP:OD2	2.44	0.50
3:B:265:GLU:OE1	3:B:268:ARG:NE	2.45	0.50
4:a:34:GLU:OE2	4:a:239:ARG:NE	2.45	0.50
4:e:83:VAL:HG22	4:e:111:VAL:HG22	1.93	0.50
3:F:394:GLN:HB3	3:F:396:THR:HG22	1.93	0.50
4:d:81:LEU:HD23	4:d:91:LEU:CD1	2.41	0.50
3:D:145:ALA:HB1	3:D:157:ILE:HD12	1.93	0.50
3:F:143:ARG:NH2	3:F:159:ASP:H	2.09	0.50
3:C:29:LEU:HD23	3:C:30:GLN:H	1.76	0.50
3:E:74:PRO:HG3	3:E:214:LEU:HD21	1.94	0.50
4:c:80:ASN:HB3	4:c:114:HIS:HB3	1.92	0.50
3:B:14:PRO:HB2	3:B:16:LYS:HD3	1.92	0.50
3:D:219:ASN:ND2	3:D:219:ASN:O	2.41	0.50
3:E:155:ALA:HB3	3:E:162:LEU:HB3	1.93	0.50
3:B:116:ILE:HD11	4:b:258:PRO:HB2	1.94	0.50
3:F:95:PHE:CE1	4:f:222:GLN:CB	2.89	0.50
4:b:6:PHE:HA	4:b:9:TYR:HB2	1.94	0.50
4:a:315:ASN:OD1	4:a:315:ASN:N	2.45	0.50
4:c:61:ASP:HB3	4:c:64:TYR:HB2	1.94	0.50
4:b:43:GLY:HA2	4:b:130:PHE:CG	2.47	0.49
4:b:133:VAL:HG21	4:b:150:CYS:HA	1.95	0.49
4:b:315:ASN:N	4:b:315:ASN:OD1	2.45	0.49
4:d:152:ARG:NH2	4:d:263:CYS:SG	2.85	0.49
4:f:71:LYS:HB3	4:f:174:ASP:OD2	2.12	0.49
4:f:196:LYS:HB3	4:f:226:TYR:CD2	2.47	0.49
3:B:309:TYR:HD2	3:B:383:PRO:HB3	1.76	0.49
3:D:265:GLU:C	3:D:267:LEU:H	2.20	0.49
4:d:38:GLY:HA2	4:d:45:ILE:HG13	1.93	0.49
3:C:80:VAL:HG22	3:C:103:MET:HB3	1.95	0.49
4:b:249:LYS:HG3	4:b:250:GLY:H	1.77	0.49
4:b:33:ILE:HG22	4:b:49:THR:HG22	1.93	0.49
3:C:164:ILE:HB	3:C:279:ILE:HG22	1.94	0.49
4:d:114:HIS:HD2	4:d:119:ARG:HA	1.78	0.49
3:A:204:LEU:HD21	3:A:214:LEU:HD12	1.94	0.49
3:A:226:GLN:OE1	4:a:26:ARG:NH2	2.42	0.49
3:B:39:ILE:H	3:B:268:ARG:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:GLU:CD	4:c:46:ARG:HH12	2.21	0.49
3:F:95:PHE:CD1	4:f:222:GLN:HB2	2.48	0.49
4:c:168:GLN:OE1	4:c:230:ASN:ND2	2.46	0.48
4:f:135:ARG:HB3	4:f:291:LEU:HB3	1.95	0.48
3:E:388:ILE:HG12	4:e:275:HIS:CG	2.48	0.48
3:A:394:GLN:O	3:A:395:HIS:C	2.55	0.48
3:E:143:ARG:HD2	3:E:157:ILE:HG22	1.95	0.48
4:a:178:LEU:HG	4:a:225:ALA:HB2	1.96	0.48
3:A:250:ALA:HA	4:a:305:ARG:HH21	1.79	0.48
3:F:104:SER:HB2	3:F:232:THR:HG23	1.95	0.48
4:f:294:THR:HG21	4:f:316:PHE:CE1	2.48	0.48
3:B:39:ILE:HG12	3:B:268:ARG:HB3	1.94	0.48
4:c:194:GLN:HB3	4:c:228:ILE:HB	1.94	0.48
4:e:5:HIS:HB2	4:e:9:TYR:CZ	2.48	0.48
4:c:289:PRO:HB3	4:c:309:GLU:HG2	1.96	0.48
4:d:196:LYS:HA	4:d:207:GLY:HA3	1.93	0.48
4:f:169:PRO:HB3	4:f:234:VAL:HG13	1.95	0.48
3:B:194:GLY:HA2	3:B:215:TYR:CG	2.49	0.48
3:C:82:THR:HG23	3:C:101:THR:HG22	1.95	0.48
4:b:326:THR:HG22	4:b:332:PRO:HB3	1.95	0.48
3:D:243:ARG:O	3:D:244:TRP:HB3	2.12	0.48
3:E:203:ASP:OD1	3:E:203:ASP:N	2.47	0.48
4:c:81:LEU:HA	4:c:113:PHE:HA	1.96	0.48
4:f:169:PRO:HD3	4:f:233:TRP:HA	1.95	0.48
4:f:319:THR:HG23	4:f:321:GLU:H	1.79	0.48
4:f:31:ILE:HD13	4:f:31:ILE:H	1.79	0.48
3:B:313:PHE:HA	3:B:358:SER:HB3	1.96	0.47
3:E:39:ILE:H	3:E:268:ARG:HA	1.79	0.47
4:b:231:LYS:HG3	4:b:232:LYS:HG3	1.96	0.47
4:d:142:PRO:HG3	4:d:266:THR:HB	1.96	0.47
3:B:38:ILE:HA	3:B:129:VAL:HB	1.96	0.47
3:C:104:SER:HB2	3:C:232:THR:HG23	1.97	0.47
3:F:311:SER:HB3	3:F:392:PRO:HA	1.96	0.47
4:a:291:LEU:HD11	4:a:305:ARG:HE	1.78	0.47
4:b:87:ALA:HB3	4:b:104:PRO:HG2	1.97	0.47
3:F:105:GLU:OE2	4:f:242:ARG:NH1	2.42	0.47
4:d:294:THR:HG22	4:d:304:THR:HB	1.95	0.47
3:B:341:LYS:HD3	3:B:356:HIS:HB2	1.95	0.47
3:E:35:ASN:OD1	3:E:36:THR:N	2.47	0.47
3:B:7:MET:HB3	3:B:277:ILE:HG13	1.95	0.47
3:C:39:ILE:HG12	3:C:268:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:TYR:OH	3:D:237:ALA:O	2.31	0.47
4:d:196:LYS:HA	4:d:207:GLY:HA2	1.95	0.47
4:e:281:ILE:HG13	4:e:315:ASN:HB3	1.96	0.47
4:a:336:TRP:CD1	4:a:336:TRP:C	2.93	0.47
3:B:149:VAL:HG22	3:B:166:PRO:HA	1.96	0.47
3:F:51:TYR:CE2	3:F:239:SER:HA	2.50	0.47
4:c:82:HIS:ND1	4:c:112:GLY:O	2.47	0.47
4:a:110:THR:HG22	4:a:123:THR:OG1	2.15	0.47
4:b:46:ARG:HD3	4:b:256:PHE:HB2	1.98	0.47
4:b:56:LYS:HG2	4:b:57:THR:H	1.80	0.47
4:e:159:ASP:OD1	4:e:161:GLY:N	2.47	0.47
3:D:244:TRP:O	3:D:248:LYS:HB3	2.15	0.46
3:E:56:PRO:HG2	3:E:105:GLU:HG3	1.97	0.46
3:F:38:ILE:HA	3:F:129:VAL:HB	1.95	0.46
4:c:13:ARG:HB2	4:c:232:LYS:HB3	1.97	0.46
4:e:168:GLN:HB3	4:e:248:PHE:CD2	2.50	0.46
3:B:58:PRO:HG3	3:B:232:THR:HG23	1.98	0.46
3:C:265:GLU:OE1	3:C:268:ARG:NE	2.49	0.46
3:F:304:ILE:HG12	3:F:379:GLY:HA3	1.96	0.46
3:B:175:ASP:OD1	3:B:175:ASP:N	2.45	0.46
3:B:359:THR:HG21	3:B:364:PRO:HB3	1.96	0.46
3:E:38:ILE:HA	3:E:129:VAL:HB	1.98	0.46
3:E:46:TYR:OH	3:E:190:PHE:HB2	2.15	0.46
4:d:56:LYS:HG3	4:d:61:ASP:HB2	1.98	0.46
4:d:159:ASP:OD1	4:d:160:GLN:N	2.47	0.46
3:C:265:GLU:C	3:C:267:LEU:H	2.23	0.46
3:F:208:THR:HG22	3:F:211:SER:HB2	1.96	0.46
3:B:68:CYS:SG	3:B:103:MET:HE3	2.56	0.46
3:F:370:VAL:O	3:F:373:SER:HB3	2.15	0.46
4:c:336:TRP:CZ3	4:c:338:GLN:HA	2.50	0.46
4:f:175:HIS:C	4:f:177:LEU:N	2.74	0.46
4:a:65:MET:SD	4:a:78:ILE:HG12	2.55	0.46
4:b:36:VAL:HG12	4:b:47:ILE:HG12	1.98	0.46
4:c:27:CYS:SG	4:c:28:ASP:N	2.89	0.46
4:b:43:GLY:HA2	4:b:130:PHE:CD2	2.50	0.46
4:d:67:PHE:HE2	4:d:69:ASN:HB3	1.81	0.46
3:C:247:ASP:N	3:C:247:ASP:OD1	2.49	0.46
4:d:27:CYS:SG	4:d:28:ASP:N	2.88	0.46
4:d:83:VAL:HG22	4:d:111:VAL:HG12	1.98	0.46
4:d:251:LYS:O	4:d:251:LYS:HG3	2.16	0.46
4:f:133:VAL:HG11	4:f:150:CYS:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:87:ALA:HB3	4:a:104:PRO:HG3	1.97	0.46
4:b:86:SER:OG	4:b:105:PRO:O	2.31	0.46
4:d:81:LEU:CD2	4:d:91:LEU:CD1	2.94	0.45
3:A:244:TRP:O	3:A:248:LYS:HB3	2.15	0.45
4:a:159:ASP:OD1	4:a:161:GLY:N	2.48	0.45
3:D:243:ARG:C	3:D:245:LYS:H	2.24	0.45
3:E:10:LYS:HD2	3:E:273:ALA:HB1	1.98	0.45
4:d:39:ASP:OD1	4:d:131:ARG:NH1	2.49	0.45
4:e:3:ASP:HA	4:e:6:PHE:HD1	1.81	0.45
3:B:208:THR:O	3:B:211:SER:OG	2.31	0.45
4:d:84:ARG:HG3	4:d:88:PRO:HA	1.97	0.45
4:f:43:GLY:HA2	4:f:130:PHE:CG	2.51	0.45
3:B:321:TYR:HE2	3:B:353:PHE:N	2.14	0.45
3:D:184:GLU:N	3:D:184:GLU:OE1	2.49	0.45
3:E:146:ASP:OD1	3:E:146:ASP:N	2.46	0.45
4:a:85:THR:HG22	4:a:86:SER:H	1.80	0.45
4:b:20:PRO:HG3	4:b:124:VAL:HG23	1.99	0.45
3:A:3:HIS:HB3	3:A:281:ILE:HD13	1.99	0.45
3:B:222:LEU:H	3:B:222:LEU:HD12	1.81	0.45
4:a:45:ILE:HD11	4:a:130:PHE:HE1	1.82	0.45
4:f:43:GLY:HA2	4:f:130:PHE:CD1	2.51	0.45
4:a:35:GLU:OE1	4:a:37:ARG:NH1	2.49	0.45
3:F:304:ILE:H	3:F:304:ILE:HG13	1.51	0.45
3:C:265:GLU:C	3:C:267:LEU:N	2.75	0.44
3:F:129:VAL:HG13	3:F:149:VAL:HG11	1.99	0.44
4:b:219:ASP:HB3	4:b:222:GLN:HE21	1.82	0.44
4:c:291:LEU:HD11	4:c:305:ARG:HD3	0.50	0.44
4:d:21:ASN:HB3	4:d:123:THR:HG23	1.99	0.44
3:A:74:PRO:HG3	3:A:214:LEU:HD21	1.98	0.44
3:F:37:ARG:HB3	3:F:268:ARG:HB3	1.98	0.44
3:F:136:THR:HB	3:F:141:SER:O	2.17	0.44
4:b:337:ALA:O	4:b:338:GLN:OXT	2.35	0.44
3:B:265:GLU:C	3:B:267:LEU:N	2.76	0.44
3:F:265:GLU:C	3:F:267:LEU:N	2.75	0.44
4:b:140:HIS:ND1	4:c:125:ALA:HB2	2.32	0.44
4:e:196:LYS:HB3	4:e:226:TYR:HD2	1.83	0.44
3:B:180:VAL:HG22	3:B:185:VAL:HG22	1.99	0.44
3:B:310:ALA:HB2	3:B:384:PRO:HG3	2.00	0.44
4:e:31:ILE:HD12	4:e:111:VAL:HG12	2.00	0.44
4:f:177:LEU:HD11	4:f:227:LEU:HD21	1.99	0.44
3:B:176:ASN:ND2	3:B:177:LYS:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:150:ASN:OD1	3:E:153:THR:N	2.50	0.44
4:a:26:ARG:NH1	4:c:143:GLU:O	2.37	0.44
4:e:196:LYS:HB3	4:e:226:TYR:CD2	2.52	0.44
3:E:15:TYR:HB2	3:E:31:ILE:HB	2.00	0.44
3:F:39:ILE:HG12	3:F:268:ARG:HG3	1.99	0.44
3:F:297:VAL:CG2	3:F:371:CYS:HB2	2.48	0.44
4:e:1:ASP:O	4:e:4:THR:OG1	2.30	0.44
3:F:140:VAL:O	3:F:141:SER:HB2	2.18	0.44
3:E:116:ILE:H	3:E:116:ILE:HD13	1.82	0.44
4:b:135:ARG:HH22	4:b:326:THR:HG1	1.64	0.44
4:c:91:LEU:HD22	4:c:99:ILE:CG2	2.47	0.44
3:D:88:MET:O	3:D:89:TRP:CD1	2.70	0.44
3:D:265:GLU:OE1	3:D:266:PRO:HD2	2.18	0.44
3:E:243:ARG:HE	4:d:311:PRO:HB2	1.82	0.44
3:F:16:LYS:HB3	3:F:28:HIS:NE2	2.33	0.44
3:D:265:GLU:C	3:D:267:LEU:N	2.76	0.43
4:a:140:HIS:CG	4:a:141:PRO:HD2	2.53	0.43
4:c:143:GLU:H	4:c:143:GLU:HG3	1.58	0.43
4:d:45:ILE:HD12	4:d:128:VAL:CG1	2.48	0.43
3:B:40:PRO:HA	3:B:127:GLY:HA3	1.99	0.43
4:f:136:GLU:N	4:f:136:GLU:OE1	2.51	0.43
3:B:50:LYS:HE2	3:B:50:LYS:HB3	1.84	0.43
3:B:321:TYR:HE2	3:B:353:PHE:H	1.64	0.43
4:d:91:LEU:CD2	4:d:99:ILE:HG21	2.48	0.43
3:B:18:LEU:HD12	3:B:332:HIS:HB3	2.01	0.43
3:B:244:TRP:O	3:B:248:LYS:HB3	2.19	0.43
3:D:18:LEU:HD12	3:D:332:HIS:HB3	2.00	0.43
3:E:143:ARG:NH2	3:E:158:GLY:HA3	2.34	0.43
4:e:175:HIS:C	4:e:177:LEU:N	2.74	0.43
3:A:3:HIS:HB3	3:A:281:ILE:CD1	2.47	0.43
4:a:43:GLY:HA2	4:a:130:PHE:CD1	2.53	0.43
4:b:167:HIS:O	4:b:233:TRP:HB3	2.19	0.43
4:e:82:HIS:O	4:e:82:HIS:ND1	2.51	0.43
4:c:168:GLN:NE2	4:c:246:ASP:O	2.48	0.43
4:b:27:CYS:SG	4:b:28:ASP:N	2.92	0.43
4:d:45:ILE:CD1	4:d:128:VAL:CG1	2.95	0.43
4:e:175:HIS:O	4:e:176:SER:C	2.61	0.43
3:B:16:LYS:HA	3:B:29:LEU:O	2.18	0.43
3:D:32:GLN:HB2	3:D:134:ASN:HB3	2.01	0.43
4:c:224:ARG:HB3	4:c:226:TYR:CZ	2.54	0.43
4:e:136:GLU:CD	4:e:136:GLU:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:175:HIS:C	4:f:177:LEU:H	2.27	0.43
4:b:169:PRO:HB3	4:b:234:VAL:HG21	1.98	0.43
4:c:168:GLN:N	4:c:248:PHE:HB2	2.29	0.43
4:e:56:LYS:HG2	4:e:57:THR:H	1.84	0.43
3:B:28:HIS:HD2	3:B:330:PRO:HB3	1.84	0.42
3:B:200:SER:OG	3:B:201:PHE:N	2.51	0.42
3:B:220:LEU:HD11	3:B:234:PHE:HB2	2.01	0.42
3:C:59:VAL:HG13	4:c:242:ARG:HB3	2.00	0.42
4:b:19:CYS:HB3	4:b:22:CYS:HB2	2.00	0.42
4:d:110:THR:HB	4:d:123:THR:HB	2.01	0.42
3:F:297:VAL:HG21	3:F:371:CYS:HB2	2.01	0.42
3:B:118:HIS:O	3:B:118:HIS:ND1	2.51	0.42
3:D:116:ILE:HD13	3:D:116:ILE:H	1.85	0.42
3:D:177:LYS:HD2	3:D:190:PHE:CZ	2.55	0.42
4:c:291:LEU:CD1	4:c:305:ARG:CG	2.77	0.42
4:f:41:HIS:HD2	4:f:151:ASN:HB2	1.84	0.42
3:B:37:ARG:HG2	3:B:268:ARG:HD2	2.00	0.42
3:B:277:ILE:HD12	3:B:279:ILE:HD11	2.01	0.42
3:C:110:ARG:NH1	3:C:209:SER:O	2.53	0.42
3:C:134:ASN:ND2	5:I:1:NAG:O7	2.52	0.42
4:a:249:LYS:HD2	4:a:249:LYS:HA	1.87	0.42
4:c:294:THR:HG22	4:c:304:THR:HB	2.01	0.42
3:E:1:TYR:HB2	3:E:21:ARG:HD3	2.02	0.42
3:F:51:TYR:OH	3:F:237:ALA:O	2.36	0.42
4:a:167:HIS:HA	4:a:248:PHE:HB3	2.01	0.42
4:d:136:GLU:N	4:d:136:GLU:OE1	2.52	0.42
4:e:179:SER:N	4:e:186:LYS:O	2.53	0.42
3:E:39:ILE:HG12	3:E:268:ARG:HB3	2.01	0.42
3:A:112:GLU:OE1	4:a:46:ARG:NH2	2.38	0.42
4:f:179:SER:N	4:f:186:LYS:O	2.53	0.42
3:A:46:TYR:OH	3:A:190:PHE:HB2	2.20	0.42
3:B:10:LYS:HG2	3:B:13:ILE:HD12	2.02	0.42
3:C:86:PRO:HA	3:C:228:GLY:O	2.19	0.42
4:a:9:TYR:CE1	4:a:55:LEU:HD21	2.55	0.42
4:e:248:PHE:HD1	4:e:248:PHE:HA	1.79	0.42
4:a:84:ARG:HB2	4:a:110:THR:OG1	2.20	0.42
3:D:89:TRP:CE2	4:d:16:ILE:HD11	2.54	0.42
4:c:38:GLY:O	4:c:131:ARG:NH1	2.52	0.42
3:A:300:LEU:HD23	3:A:300:LEU:H	1.85	0.41
3:C:179:VAL:N	3:C:186:TYR:O	2.41	0.41
3:E:145:ALA:HB2	3:E:157:ILE:HG21	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:86:PRO:HA	3:F:228:GLY:O	2.20	0.41
4:e:171:LEU:HD13	4:e:226:TYR:CG	2.55	0.41
3:E:37:ARG:HB3	3:E:268:ARG:HD3	2.02	0.41
3:E:331:ILE:HG22	3:E:370:VAL:HG13	2.02	0.41
4:c:199:CYS:HB3	4:c:217:CYS:SG	2.60	0.41
3:C:391:TYR:CG	3:C:392:PRO:HD2	2.55	0.41
3:F:367:LYS:HA	3:F:376:THR:HA	2.03	0.41
4:b:65:MET:HE3	4:b:78:ILE:HG13	2.02	0.41
4:b:136:GLU:HA	4:b:290:THR:HG22	2.03	0.41
4:c:6:PHE:HA	4:c:9:TYR:HB2	2.02	0.41
4:f:336:TRP:CG	4:f:337:ALA:N	2.88	0.41
3:D:113:GLU:OE2	4:d:37:ARG:NH2	2.54	0.41
3:E:149:VAL:O	3:E:165:GLY:HA3	2.21	0.41
3:E:68:CYS:SG	3:E:69:THR:N	2.92	0.41
4:a:118:ASN:OD1	4:a:118:ASN:N	2.52	0.41
3:F:96:CYS:O	3:F:100:ASN:ND2	2.39	0.41
4:c:53:PHE:N	4:c:96:GLY:O	2.48	0.41
4:d:22:CYS:SG	4:d:29:SER:OG	2.79	0.41
3:F:95:PHE:CD2	4:f:200:LYS:HB2	2.51	0.41
3:F:396:THR:O	3:F:396:THR:OG1	2.38	0.41
4:b:5:HIS:HB2	4:b:9:TYR:CE2	2.56	0.41
3:A:51:TYR:CE2	3:A:239:SER:HA	2.55	0.41
3:C:18:LEU:HD11	3:C:26:PRO:HB2	2.02	0.41
4:a:291:LEU:HD13	4:a:307:TRP:CE2	2.56	0.41
4:e:31:ILE:HD13	4:e:113:PHE:HD1	1.85	0.41
3:A:134:ASN:OD1	3:A:136:THR:HG23	2.20	0.41
3:A:192:GLU:OE1	3:A:193:TYR:N	2.41	0.41
3:A:255:VAL:HG12	4:a:303:PRO:HB3	2.03	0.41
3:B:51:TYR:CE2	3:B:239:SER:HA	2.56	0.41
3:B:341:LYS:HE2	3:B:341:LYS:HB2	1.96	0.41
3:E:51:TYR:CE2	3:E:239:SER:HA	2.56	0.41
3:E:81:PHE:CG	3:E:224:ARG:HG2	2.56	0.41
3:E:186:TYR:HD2	3:E:244:TRP:CH2	2.39	0.41
4:b:44:VAL:HG23	4:b:153:TYR:HD2	1.86	0.41
4:b:84:ARG:HB2	4:b:110:THR:OG1	2.20	0.41
4:b:255:PRO:HB2	4:b:256:PHE:CD1	2.56	0.41
4:c:13:ARG:HA	4:c:13:ARG:HD3	1.88	0.41
4:c:166:MET:HE3	4:c:252:LEU:HD21	2.02	0.41
4:f:194:GLN:NE2	4:f:208:ILE:HG12	2.36	0.41
4:f:331:PRO:HA	4:f:332:PRO:HD3	1.99	0.41
3:D:344:ASP:OD1	3:D:345:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:149:VAL:O	3:E:166:PRO:HA	2.21	0.41
4:a:45:ILE:HD11	4:a:130:PHE:CE1	2.56	0.41
4:d:150:CYS:SG	4:d:263:CYS:N	2.93	0.41
4:e:198:TYR:HB3	4:e:224:ARG:HD2	2.03	0.41
3:A:389:VAL:HB	4:a:336:TRP:CD1	2.56	0.40
3:C:199:GLY:HA3	4:b:285:HIS:CD2	2.56	0.40
3:C:308:THR:OG1	3:C:314:GLY:HA3	2.21	0.40
3:D:116:ILE:HG12	3:D:117:ASP:N	2.36	0.40
3:E:147:VAL:HG21	3:E:164:ILE:HG21	2.04	0.40
4:a:11:LEU:HB3	4:a:233:TRP:HE3	1.86	0.40
3:A:73:HIS:HB2	3:A:76:TYR:HB2	2.03	0.40
3:E:265:GLU:C	3:E:267:LEU:N	2.79	0.40
4:e:110:THR:HB	4:e:123:THR:HB	2.02	0.40
4:e:331:PRO:HA	4:e:332:PRO:HD3	1.92	0.40
3:C:214:LEU:C	3:C:214:LEU:HD12	2.46	0.40
3:C:307:CYS:HA	3:C:315:GLY:HA2	2.04	0.40
3:F:323:SER:OG	3:F:324:SER:N	2.55	0.40
4:b:280:LEU:HD12	4:b:335:VAL:HG11	2.03	0.40
4:c:65:MET:HB3	4:c:78:ILE:HD13	2.01	0.40
4:e:140:HIS:CG	4:e:141:PRO:HD2	2.57	0.40
4:e:329:ASN:OD1	4:e:329:ASN:N	2.48	0.40
3:A:219:ASN:O	3:A:219:ASN:ND2	2.55	0.40
3:D:252:LEU:HA	3:D:255:VAL:HG22	2.03	0.40
3:F:279:ILE:HD11	3:F:281:ILE:HG23	2.03	0.40
4:e:31:ILE:HD13	4:e:113:PHE:CD1	2.56	0.40
4:a:107:ASP:HA	4:a:127:LYS:HA	2.02	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	1	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
1	3	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
2	2	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
2	4	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
3	A	398/400 (100%)	360 (90%)	36 (9%)	2 (0%)	24	57
3	B	398/400 (100%)	372 (94%)	25 (6%)	1 (0%)	36	67
3	C	398/400 (100%)	370 (93%)	25 (6%)	3 (1%)	16	48
3	D	398/400 (100%)	354 (89%)	41 (10%)	3 (1%)	16	48
3	E	398/400 (100%)	365 (92%)	32 (8%)	1 (0%)	36	67
3	F	398/400 (100%)	357 (90%)	39 (10%)	2 (0%)	24	57
4	a	336/338 (99%)	294 (88%)	41 (12%)	1 (0%)	36	67
4	b	336/338 (99%)	284 (84%)	50 (15%)	2 (1%)	21	54
4	c	336/338 (99%)	290 (86%)	46 (14%)	0	100	100
4	d	336/338 (99%)	295 (88%)	39 (12%)	2 (1%)	21	54
4	e	336/338 (99%)	285 (85%)	50 (15%)	1 (0%)	36	67
4	f	336/338 (99%)	288 (86%)	47 (14%)	1 (0%)	36	67
All	All	5280/5312 (99%)	4766 (90%)	495 (9%)	19 (0%)	31	62

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	89	TRP
3	A	267	LEU
3	A	395	HIS
3	D	386	ASP
3	F	89	TRP
4	d	226	TYR
3	C	191	PRO
3	F	266	PRO
4	f	59	GLY
3	D	398	SER
4	d	208	ILE
3	E	266	PRO
4	b	190	PRO
3	B	266	PRO
3	C	266	PRO
3	D	266	PRO

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Mol	Chain	Res	Type
4	e	207	GLY
4	a	190	PRO
4	b	207	GLY

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	
3	A	339/339 (100%)	322 (95%)	17 (5%)	22	47
3	B	339/339 (100%)	318 (94%)	21 (6%)	16	42
3	C	339/339 (100%)	323 (95%)	16 (5%)	23	48
3	D	339/339 (100%)	326 (96%)	13 (4%)	29	53
3	E	339/339 (100%)	319 (94%)	20 (6%)	18	43
3	F	339/339 (100%)	320 (94%)	19 (6%)	19	45
4	a	294/294 (100%)	268 (91%)	26 (9%)	9	33
4	b	294/294 (100%)	274 (93%)	20 (7%)	14	40
4	c	294/294 (100%)	280 (95%)	14 (5%)	23	47
4	d	294/294 (100%)	271 (92%)	23 (8%)	11	36
4	e	294/294 (100%)	269 (92%)	25 (8%)	10	33
4	f	294/294 (100%)	281 (96%)	13 (4%)	25	49
All	All	3798/3798 (100%)	3571 (94%)	227 (6%)	19	43

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	VAL
3	A	28	HIS
3	A	31	ILE
3	A	55	VAL
3	A	71	LYS
3	A	79	GLN
3	A	89	TRP

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Mol	Chain	Res	Type
3	A	116	ILE
3	A	147	VAL
3	A	167	LEU
3	A	171	TRP
3	A	185	VAL
3	A	226	GLN
3	A	244	TRP
3	A	281	ILE
3	A	387	HIS
3	A	400	THR
3	B	11	VAL
3	B	16	LYS
3	B	18	LEU
3	B	66	THR
3	B	100	ASN
3	B	118	HIS
3	B	129	VAL
3	B	156	LYS
3	B	163	ILE
3	B	175	ASP
3	B	214	LEU
3	B	231	HIS
3	B	244	TRP
3	B	262	ILE
3	B	272	CYS
3	B	297	VAL
3	B	304	ILE
3	B	345	VAL
3	B	359	THR
3	B	386	ASP
3	B	391	TYR
3	C	16	LYS
3	C	29	LEU
3	C	31	ILE
3	C	52	LYS
3	C	59	VAL
3	C	82	THR
3	C	100	ASN
3	C	143	ARG
3	C	147	VAL
3	C	149	VAL
3	C	164	ILE

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Mol	Chain	Res	Type
3	C	219	ASN
3	C	244	TRP
3	C	262	ILE
3	C	272	CYS
3	C	389	VAL
3	D	18	LEU
3	D	28	HIS
3	D	34	VAL
3	D	100	ASN
3	D	116	ILE
3	D	118	HIS
3	D	214	LEU
3	D	262	ILE
3	D	264	LEU
3	D	272	CYS
3	D	329	CYS
3	D	370	VAL
3	D	371	CYS
3	E	11	VAL
3	E	53	THR
3	E	82	THR
3	E	89	TRP
3	E	93	TYR
3	E	100	ASN
3	E	116	ILE
3	E	129	VAL
3	E	164	ILE
3	E	185	VAL
3	E	218	THR
3	E	230	VAL
3	E	231	HIS
3	E	235	THR
3	E	244	TRP
3	E	253	ASN
3	E	329	CYS
3	E	331	ILE
3	E	371	CYS
3	E	388	ILE
3	F	31	ILE
3	F	61	LYS
3	F	66	THR
3	F	100	ASN

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Mol	Chain	Res	Type
3	F	126	THR
3	F	129	VAL
3	F	136	THR
3	F	147	VAL
3	F	149	VAL
3	F	150	ASN
3	F	179	VAL
3	F	244	TRP
3	F	267	LEU
3	F	268	ARG
3	F	279	ILE
3	F	304	ILE
3	F	331	ILE
3	F	340	ILE
3	F	387	HIS
4	a	3	ASP
4	a	16	ILE
4	a	31	ILE
4	a	55	LEU
4	a	76	ILE
4	a	81	LEU
4	a	99	ILE
4	a	110	THR
4	a	113	PHE
4	a	118	ASN
4	a	128	VAL
4	a	131	ARG
4	a	133	VAL
4	a	154	THR
4	a	172	VAL
4	a	185	VAL
4	a	213	HIS
4	a	221	LYS
4	a	242	ARG
4	a	266	THR
4	a	267	LEU
4	a	279	THR
4	a	290	THR
4	a	308	ILE
4	a	315	ASN
4	a	336	TRP
4	b	16	ILE

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Mol	Chain	Res	Type
4	b	53	PHE
4	b	99	ILE
4	b	109	VAL
4	b	110	THR
4	b	114	HIS
4	b	120	HIS
4	b	139	ARG
4	b	171	LEU
4	b	247	THR
4	b	248	PHE
4	b	252	LEU
4	b	266	THR
4	b	279	THR
4	b	283	HIS
4	b	284	LEU
4	b	285	HIS
4	b	297	LEU
4	b	315	ASN
4	b	336	TRP
4	c	5	HIS
4	c	13	ARG
4	c	22	CYS
4	c	27	CYS
4	c	83	VAL
4	c	110	THR
4	c	130	PHE
4	c	131	ARG
4	c	138	TYR
4	c	143	GLU
4	c	195	VAL
4	c	201	CYS
4	c	315	ASN
4	c	338	GLN
4	d	18	ASP
4	d	22	CYS
4	d	27	CYS
4	d	31	ILE
4	d	33	ILE
4	d	34	GLU
4	d	36	VAL
4	d	37	ARG
4	d	47	ILE

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Mol	Chain	Res	Type
4	d	49	THR
4	d	55	LEU
4	d	114	HIS
4	d	127	LYS
4	d	131	ARG
4	d	154	THR
4	d	184	LYS
4	d	224	ARG
4	d	253	HIS
4	d	267	LEU
4	d	280	LEU
4	d	290	THR
4	d	294	THR
4	d	308	ILE
4	e	6	PHE
4	e	24	HIS
4	e	27	CYS
4	e	47	ILE
4	e	81	LEU
4	e	99	ILE
4	e	110	THR
4	e	114	HIS
4	e	120	HIS
4	e	133	VAL
4	e	157	ARG
4	e	167	HIS
4	e	195	VAL
4	e	244	GLU
4	e	247	THR
4	e	248	PHE
4	e	275	HIS
4	e	279	THR
4	e	280	LEU
4	e	285	HIS
4	e	290	THR
4	e	300	ASP
4	e	315	ASN
4	e	335	VAL
4	e	338	GLN
4	f	27	CYS
4	f	31	ILE
4	f	55	LEU

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Mol	Chain	Res	Type
4	f	110	THR
4	f	131	ARG
4	f	138	TYR
4	f	147	GLU
4	f	167	HIS
4	f	195	VAL
4	f	224	ARG
4	f	279	THR
4	f	308	ILE
4	f	336	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	32	GLN
3	A	100	ASN
3	A	356	HIS
3	A	361	ASN
3	A	363	HIS
3	B	3	HIS
3	B	217	ASN
3	B	394	GLN
3	C	30	GLN
3	C	35	ASN
3	C	125	HIS
3	C	183	HIS
3	D	3	HIS
3	D	231	HIS
3	D	356	HIS
3	E	43	ASN
3	E	77	GLN
3	E	187	ASN
3	E	363	HIS
3	F	231	HIS
3	F	253	ASN
3	F	395	HIS
4	a	95	HIS
4	a	120	HIS
4	a	167	HIS
4	a	213	HIS
4	a	275	HIS
4	a	329	ASN

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Mol	Chain	Res	Type
4	b	69	ASN
4	b	73	GLN
4	b	95	HIS
4	b	194	GLN
4	b	222	GLN
4	b	302	ASN
4	c	41	HIS
4	c	48	GLN
4	c	120	HIS
4	c	277	HIS
4	d	69	ASN
4	d	126	HIS
4	d	167	HIS
4	d	181	HIS
4	e	73	GLN
4	e	80	ASN
4	e	114	HIS
4	e	140	HIS
4	e	194	GLN
4	f	21	ASN
4	f	24	HIS
4	f	73	GLN
4	f	151	ASN
4	f	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

18 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	G	1	3,5	14,14,15	0.40	0	17,19,21	0.45	0
5	NAG	G	2	5	14,14,15	0.39	0	17,19,21	0.55	0
5	BMA	G	3	5	11,11,12	0.21	0	15,15,17	0.44	0
5	NAG	H	1	3,5	14,14,15	0.41	0	17,19,21	0.48	0
5	NAG	H	2	5	14,14,15	0.39	0	17,19,21	0.87	1 (5%)
5	BMA	H	3	5	11,11,12	0.17	0	15,15,17	0.47	0
5	NAG	I	1	3,5	14,14,15	0.40	0	17,19,21	1.57	3 (17%)
5	NAG	I	2	5	14,14,15	0.41	0	17,19,21	0.49	0
5	BMA	I	3	5	11,11,12	0.17	0	15,15,17	0.46	0
5	NAG	J	1	3,5	14,14,15	0.39	0	17,19,21	0.48	0
5	NAG	J	2	5	14,14,15	0.39	0	17,19,21	0.85	1 (5%)
5	BMA	J	3	5	11,11,12	0.18	0	15,15,17	0.51	0
5	NAG	K	1	3,5	14,14,15	0.38	0	17,19,21	0.69	1 (5%)
5	NAG	K	2	5	14,14,15	0.40	0	17,19,21	0.60	0
5	BMA	K	3	5	11,11,12	0.17	0	15,15,17	0.51	0
5	NAG	L	1	3,5	14,14,15	0.42	0	17,19,21	1.93	3 (17%)
5	NAG	L	2	5	14,14,15	0.39	0	17,19,21	0.41	0
5	BMA	L	3	5	11,11,12	0.21	0	15,15,17	0.44	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	G	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	NAG	H	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	NAG	I	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	1/2/19/22	0/1/1/1
5	NAG	J	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	K	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	NAG	L	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1	NAG	C2-N2-C7	5.30	130.01	122.90
5	L	1	NAG	C1-C2-N2	4.32	117.24	110.43
5	I	1	NAG	O5-C1-C2	-4.04	105.04	111.29
5	I	1	NAG	C1-C2-N2	3.81	116.43	110.43
5	I	1	NAG	C2-N2-C7	2.68	126.50	122.90
5	J	2	NAG	C2-N2-C7	2.43	126.16	122.90
5	H	2	NAG	C2-N2-C7	2.35	126.05	122.90
5	L	1	NAG	O5-C1-C2	2.31	114.86	111.29
5	K	1	NAG	C2-N2-C7	2.27	125.94	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

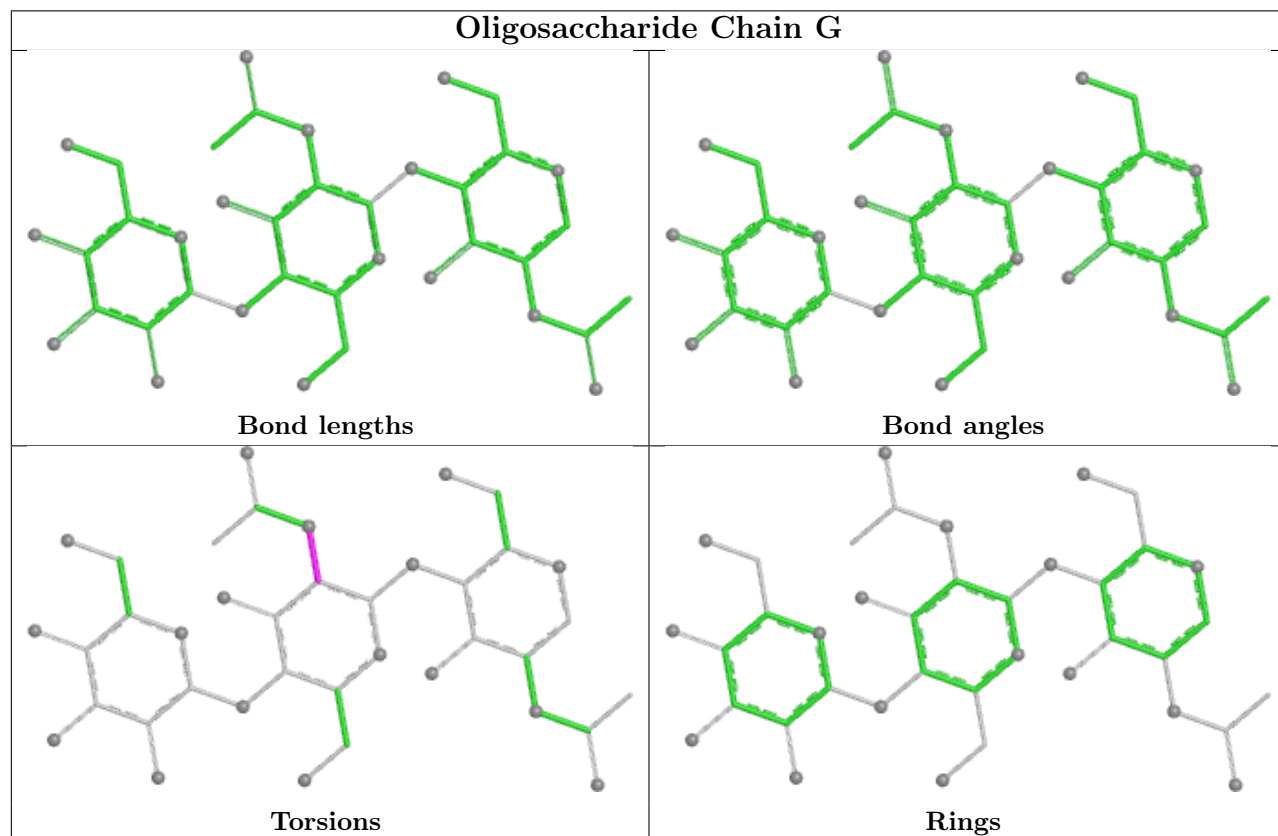
Mol	Chain	Res	Type	Atoms
5	L	1	NAG	C1-C2-N2-C7
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
5	L	1	NAG	C8-C7-N2-C2
5	I	3	BMA	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7
5	L	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C1-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7
5	J	2	NAG	C3-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
5	G	2	NAG	C3-C2-N2-C7

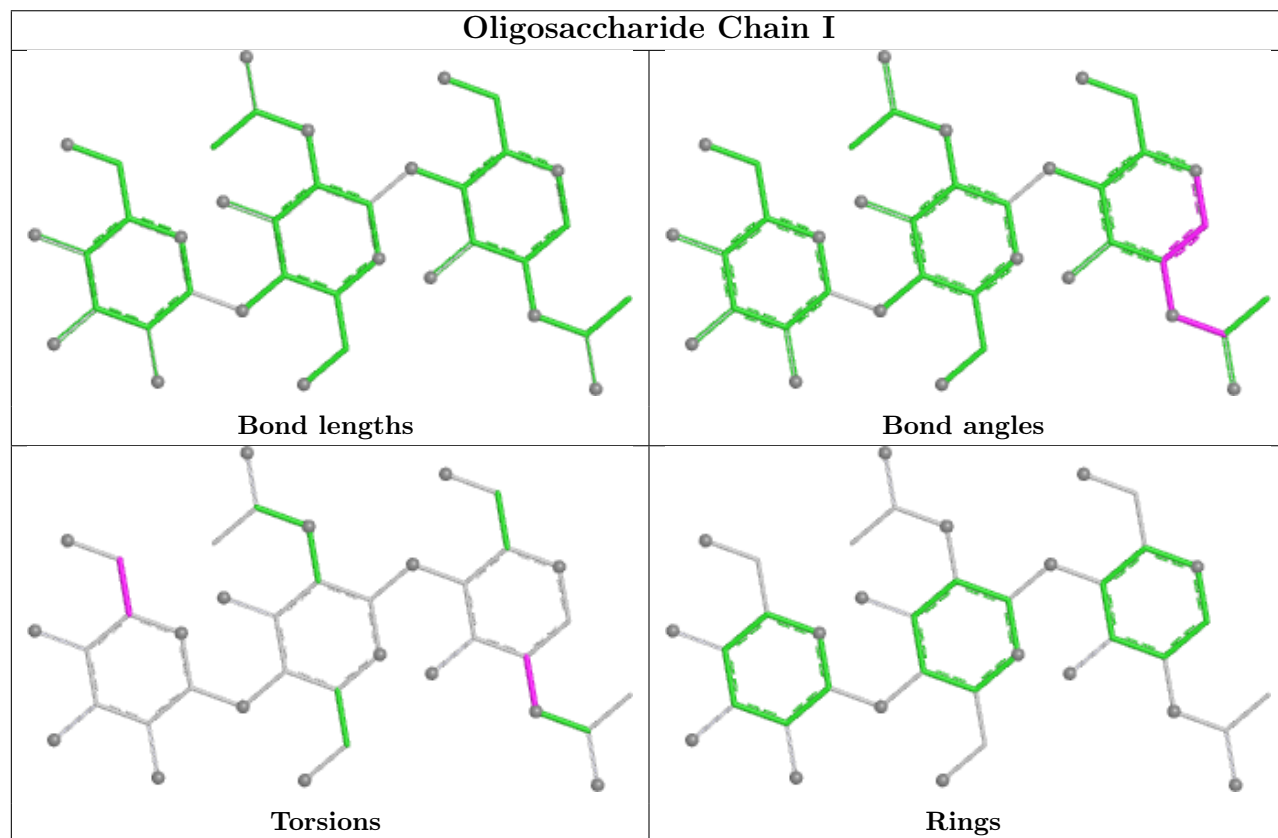
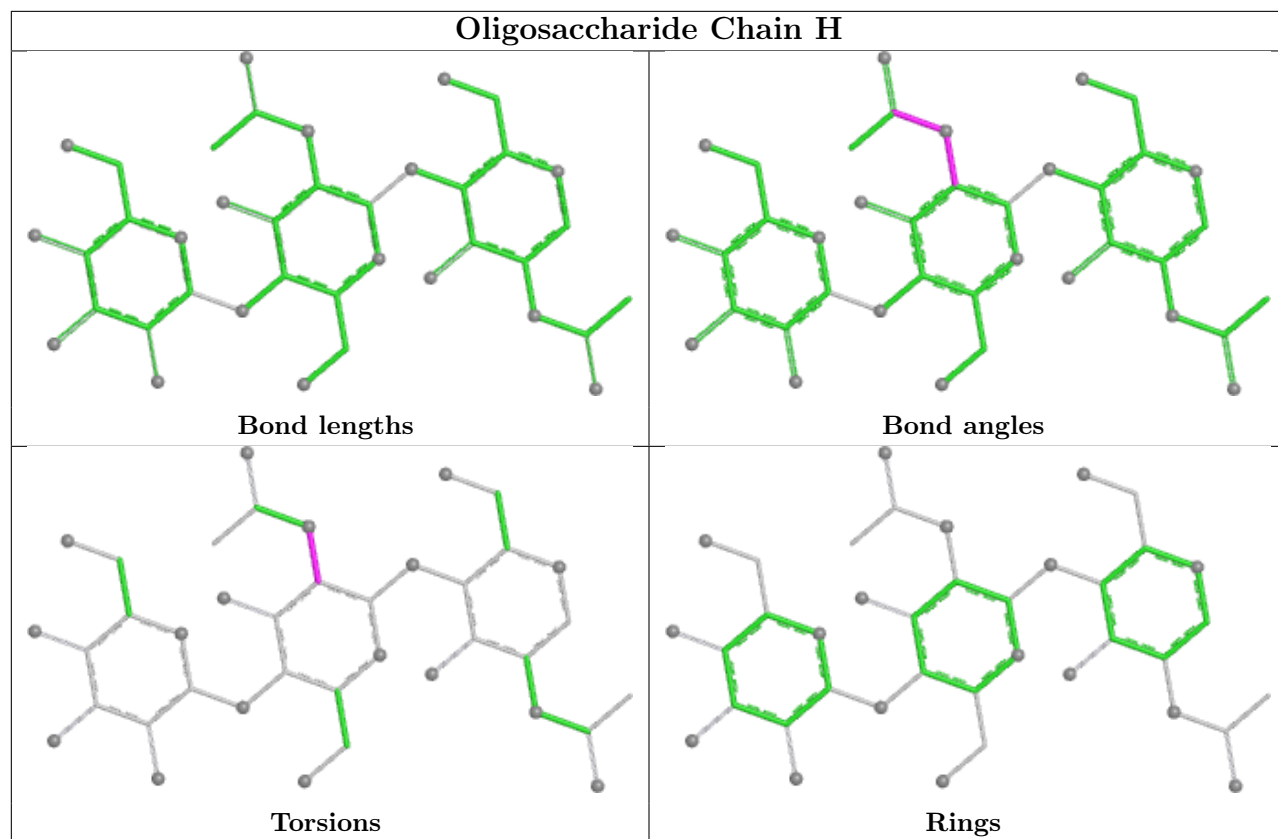
There are no ring outliers.

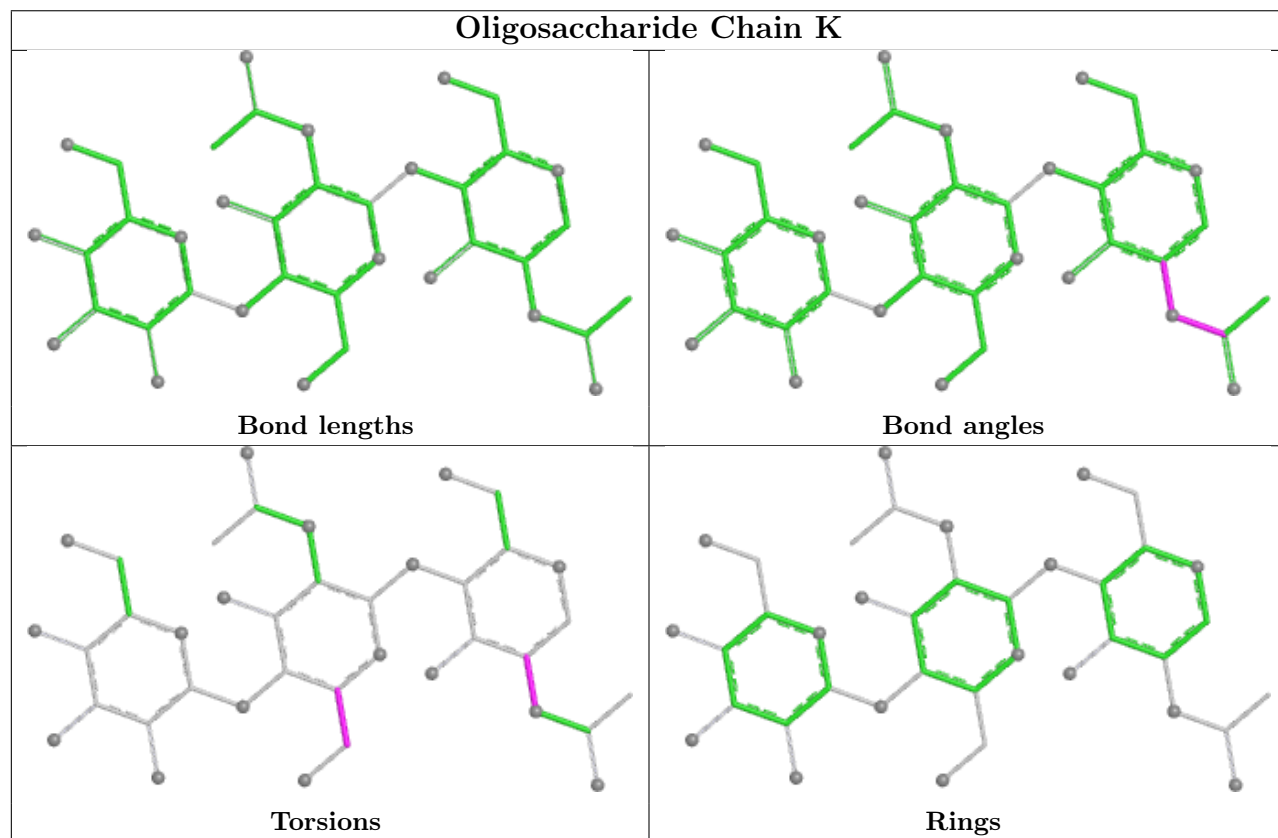
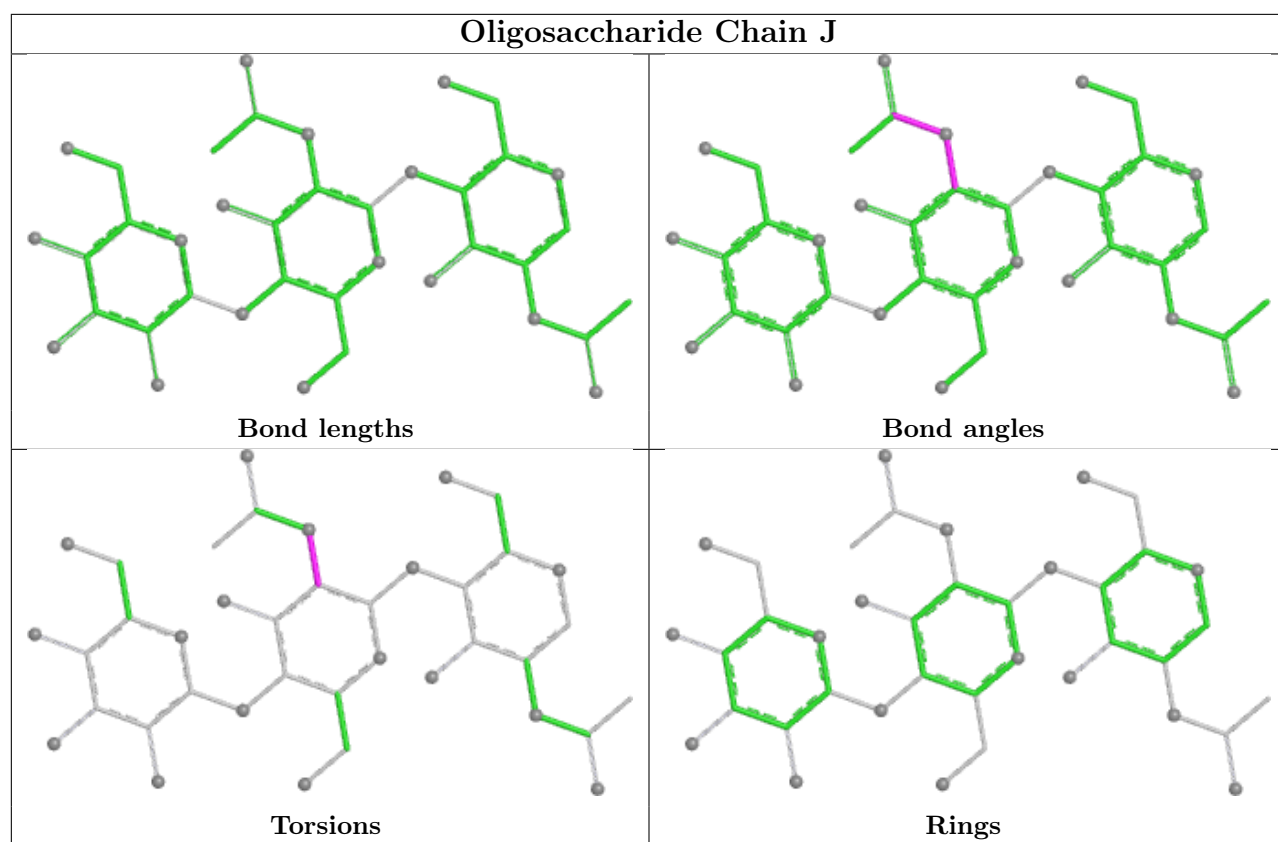
3 monomers are involved in 3 short contacts:

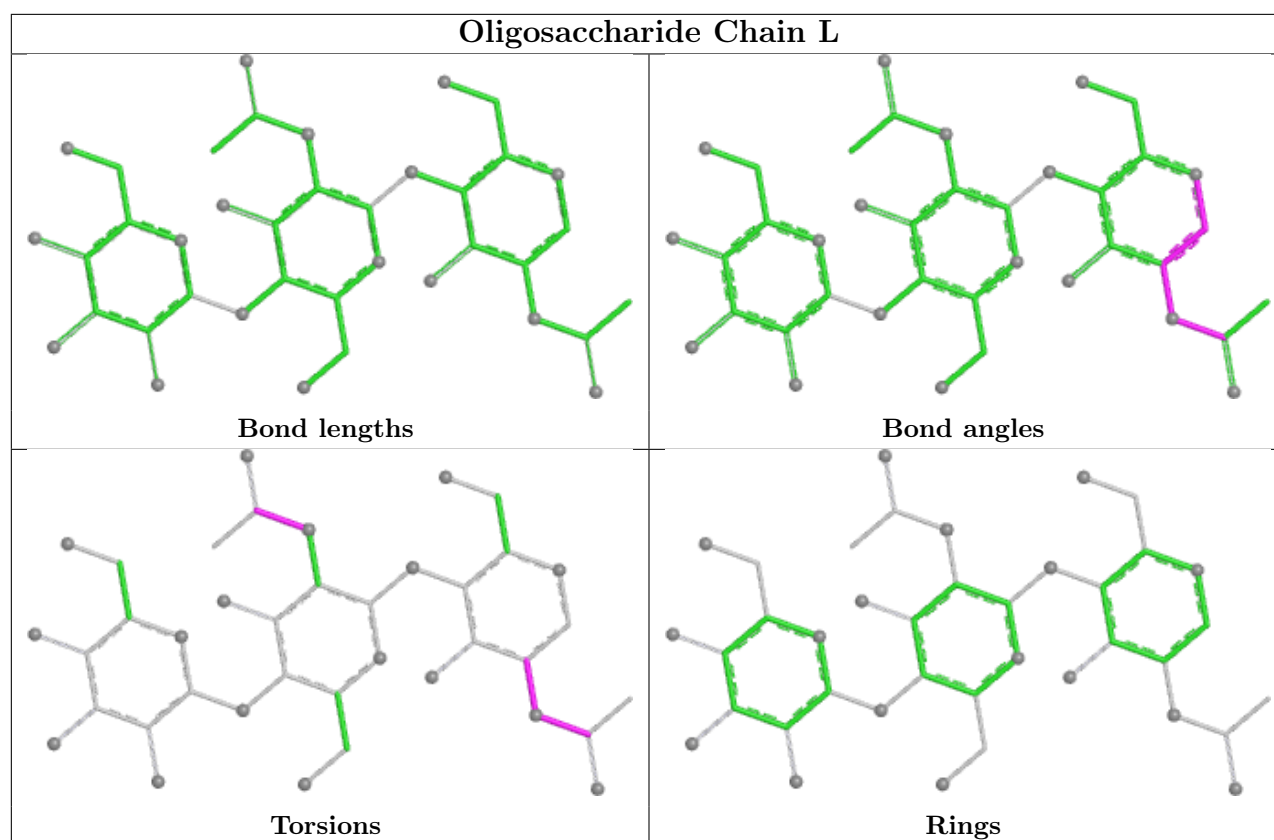
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	1	0
5	G	1	NAG	1	0
5	L	1	NAG	1	0

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](#)

6 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	c	401	4	14,14,15	0.39	0	17,19,21	0.95	1 (5%)
6	NAG	a	401	4	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
6	NAG	d	401	-	14,14,15	1.01	1 (7%)	17,19,21	1.56	4 (23%)
6	NAG	f	401	4	14,14,15	0.40	0	17,19,21	0.33	0
6	NAG	e	401	4	14,14,15	0.41	0	17,19,21	1.32	2 (11%)
6	NAG	b	401	4	14,14,15	0.41	0	17,19,21	0.35	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
6	NAG	c	401	4	-	3/6/23/26	0/1/1/1
6	NAG	a	401	4	-	1/6/23/26	0/1/1/1
6	NAG	d	401	-	-	1/6/23/26	0/1/1/1
6	NAG	f	401	4	-	0/6/23/26	0/1/1/1
6	NAG	e	401	4	-	3/6/23/26	0/1/1/1
6	NAG	b	401	4	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	401	NAG	O5-C1	2.37	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	e	401	NAG	C2-N2-C7	3.80	128.00	122.90
6	e	401	NAG	C1-C2-N2	3.26	115.57	110.43
6	c	401	NAG	O5-C1-C2	2.95	115.86	111.29
6	d	401	NAG	C3-C4-C5	2.95	115.57	110.23
6	d	401	NAG	O5-C1-C2	-2.68	107.14	111.29
6	d	401	NAG	C4-C3-C2	-2.61	107.19	111.02
6	a	401	NAG	C2-N2-C7	2.57	126.35	122.90
6	d	401	NAG	C1-C2-N2	2.31	114.07	110.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	c	401	NAG	C1-C2-N2-C7
6	c	401	NAG	C8-C7-N2-C2
6	c	401	NAG	O7-C7-N2-C2
6	d	401	NAG	C1-C2-N2-C7
6	e	401	NAG	C1-C2-N2-C7
6	e	401	NAG	C8-C7-N2-C2
6	e	401	NAG	O7-C7-N2-C2
6	b	401	NAG	O5-C5-C6-O6
6	a	401	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

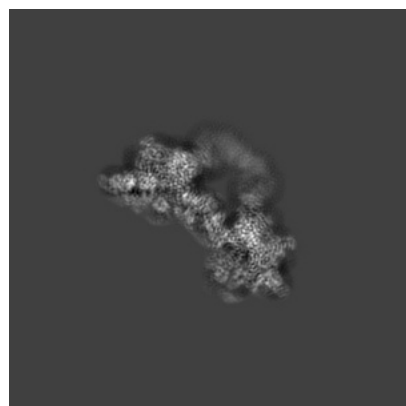
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43507. These allow visual inspection of the internal detail of the map and identification of artifacts.

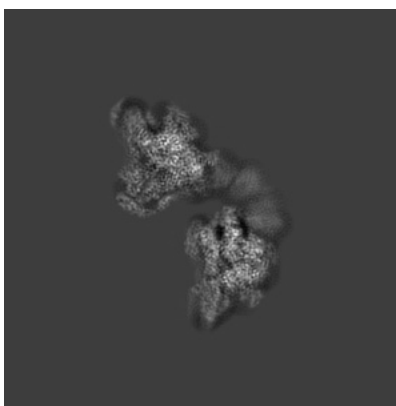
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

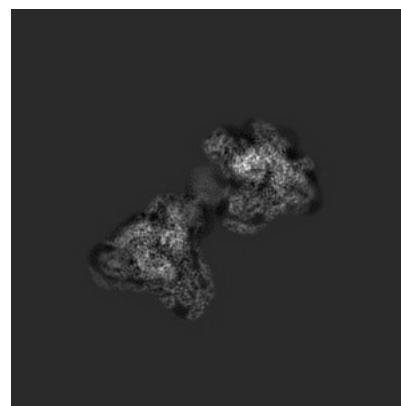
6.1.1 Primary map



X

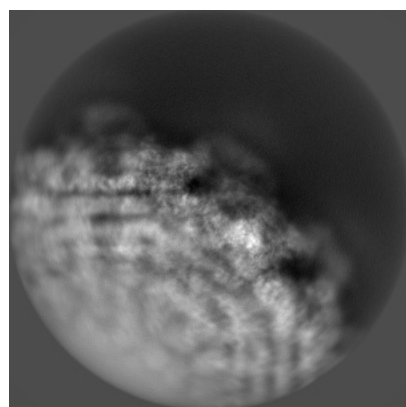


Y

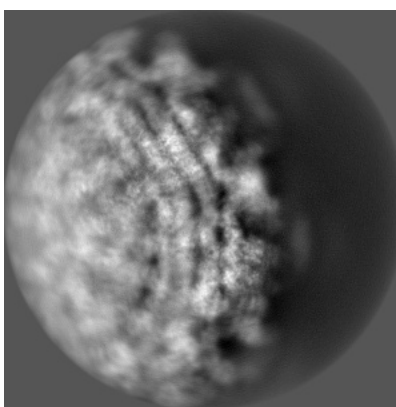


Z

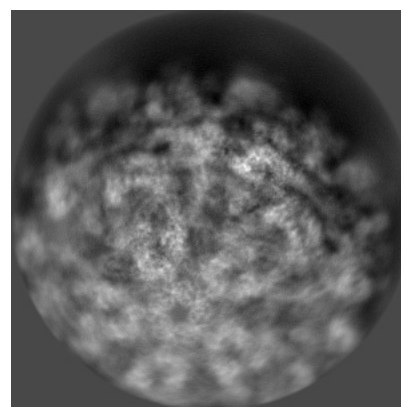
6.1.2 Raw map



X



Y

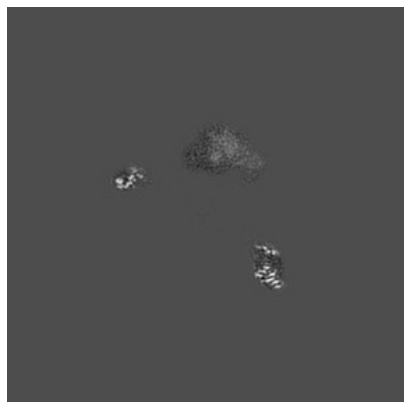


Z

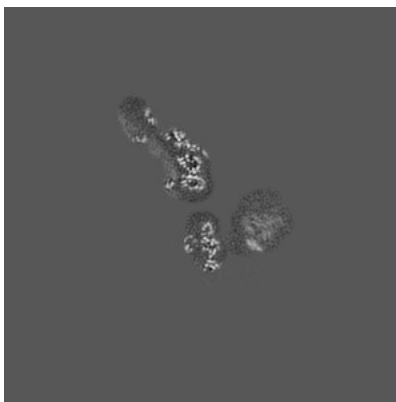
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

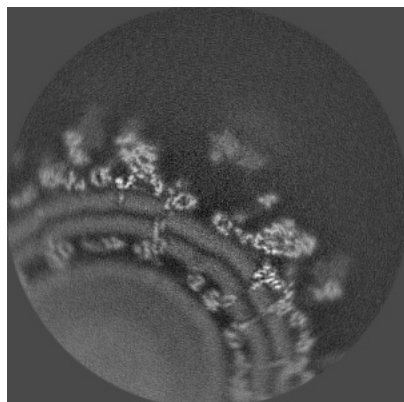


Y Index: 200

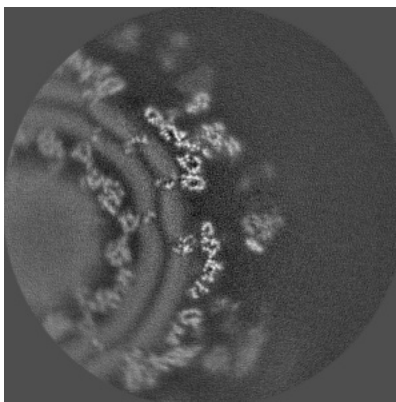


Z Index: 200

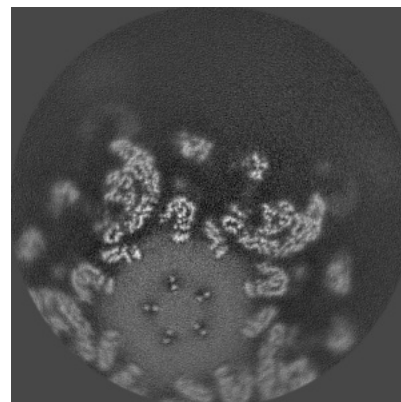
6.2.2 Raw map



X Index: 200



Y Index: 200

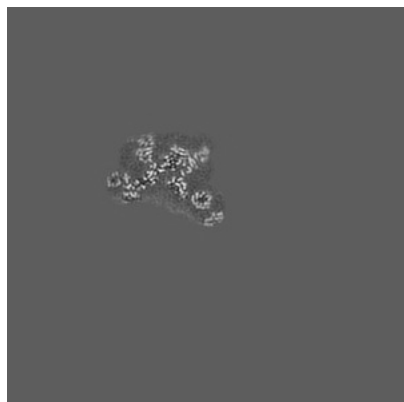


Z Index: 200

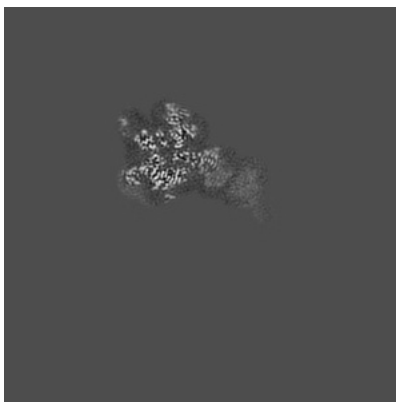
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

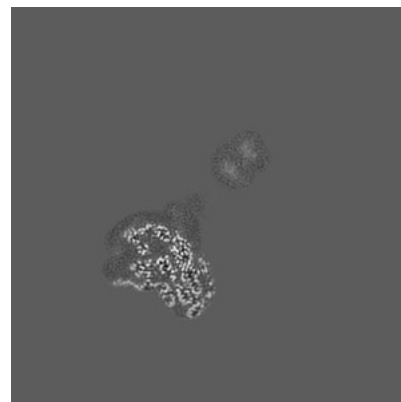
6.3.1 Primary map



X Index: 157

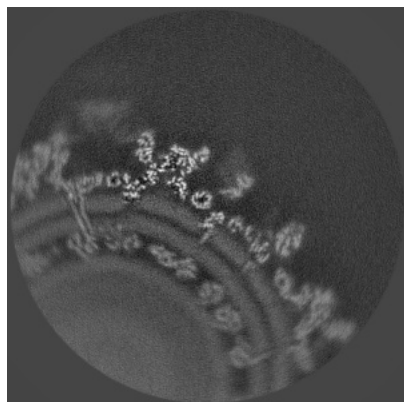


Y Index: 243

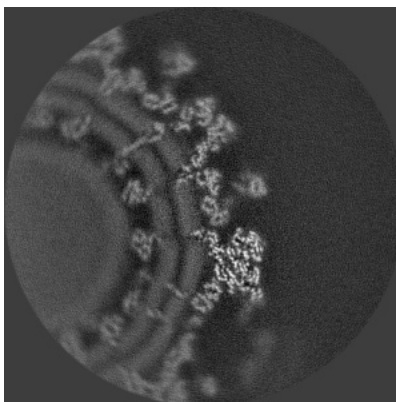


Z Index: 228

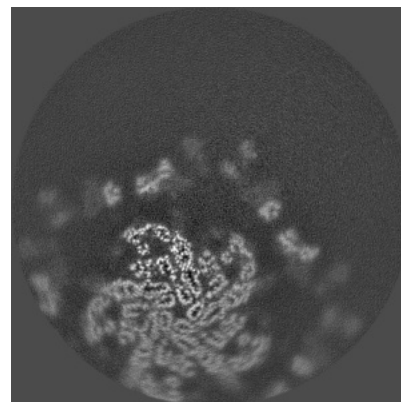
6.3.2 Raw map



X Index: 157



Y Index: 174

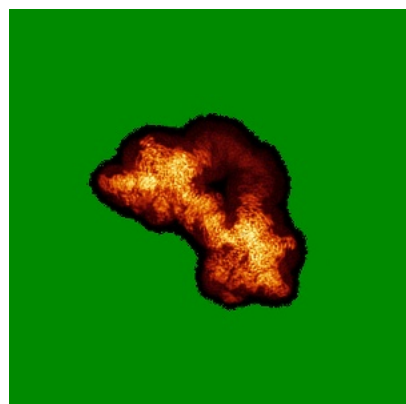


Z Index: 228

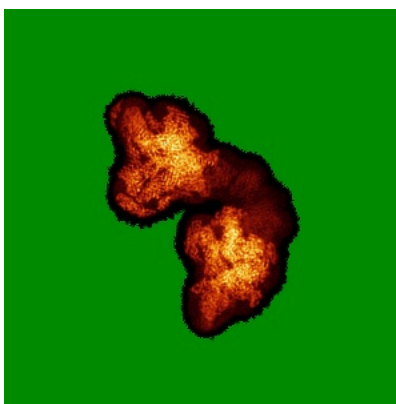
The images above show the largest variance slices of the map in three orthogonal directions.

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

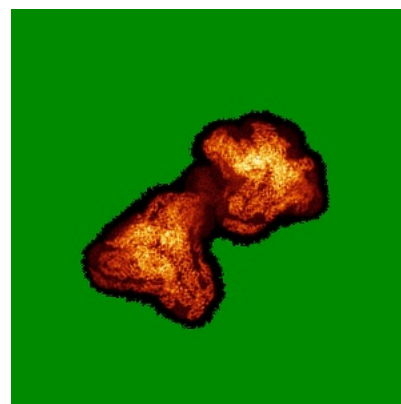
6.4.1 Primary map



X

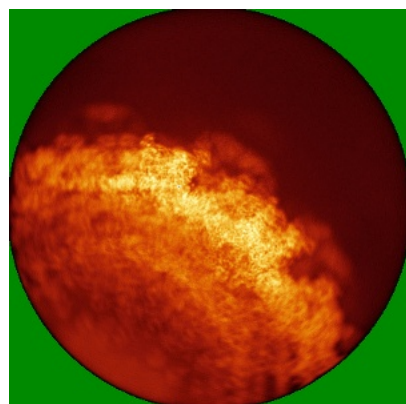


Y

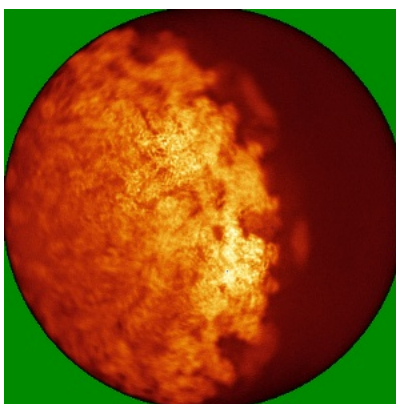


Z

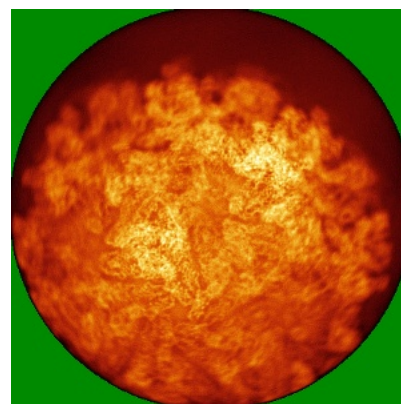
6.4.2 Raw map



X



Y

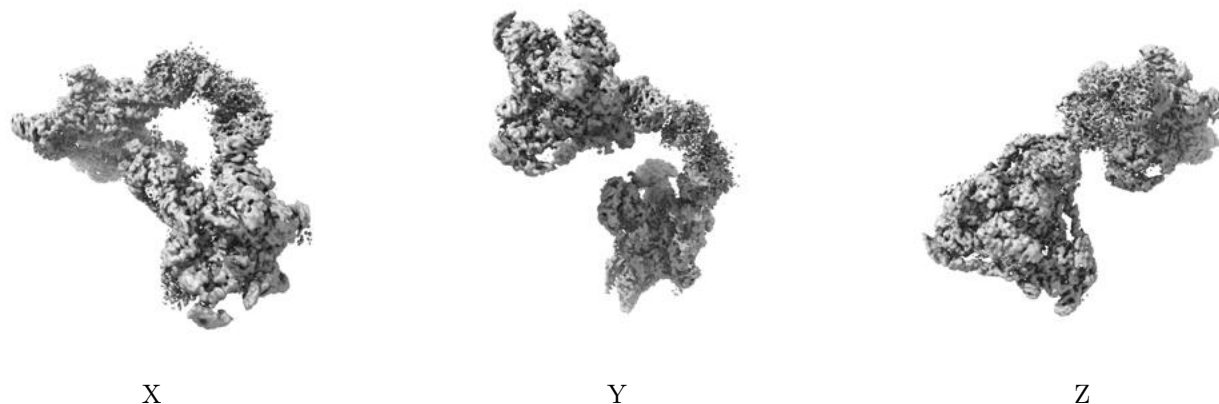


Z

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

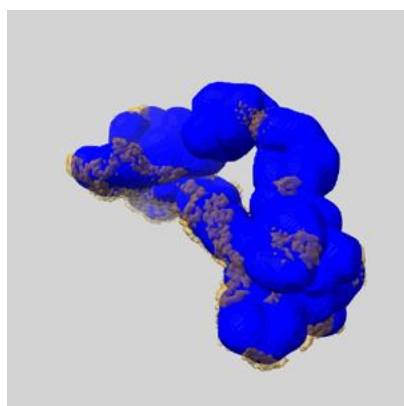
6.6 Mask visualisation [i](#)

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

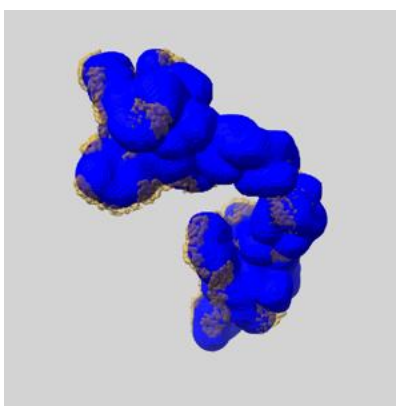
A mask typically either:

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

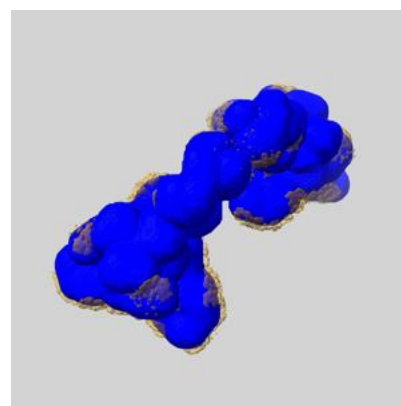
6.6.1 emd_43507_msk_1.map [i](#)



X



Y

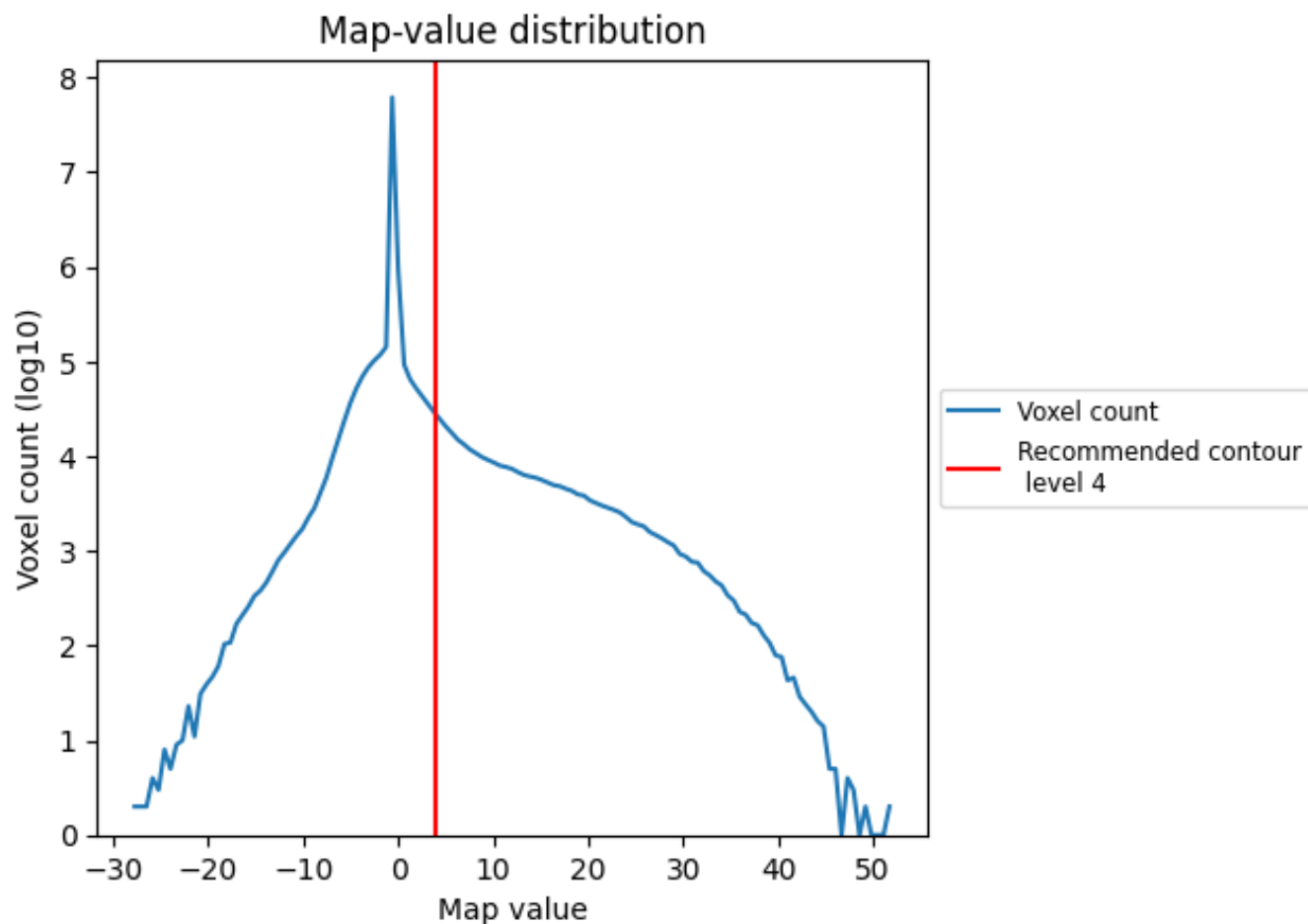


Z

7 Map analysis [i](#)

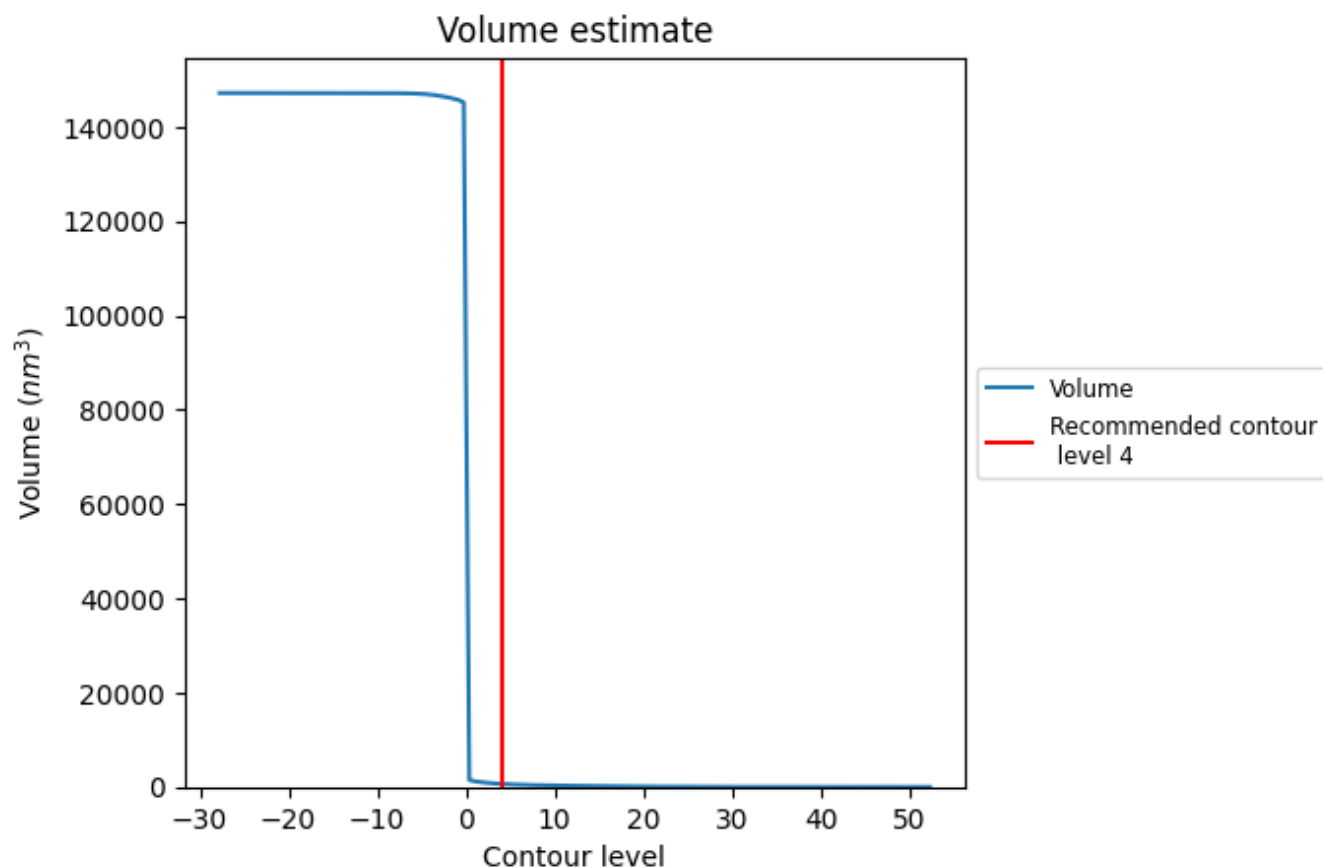
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

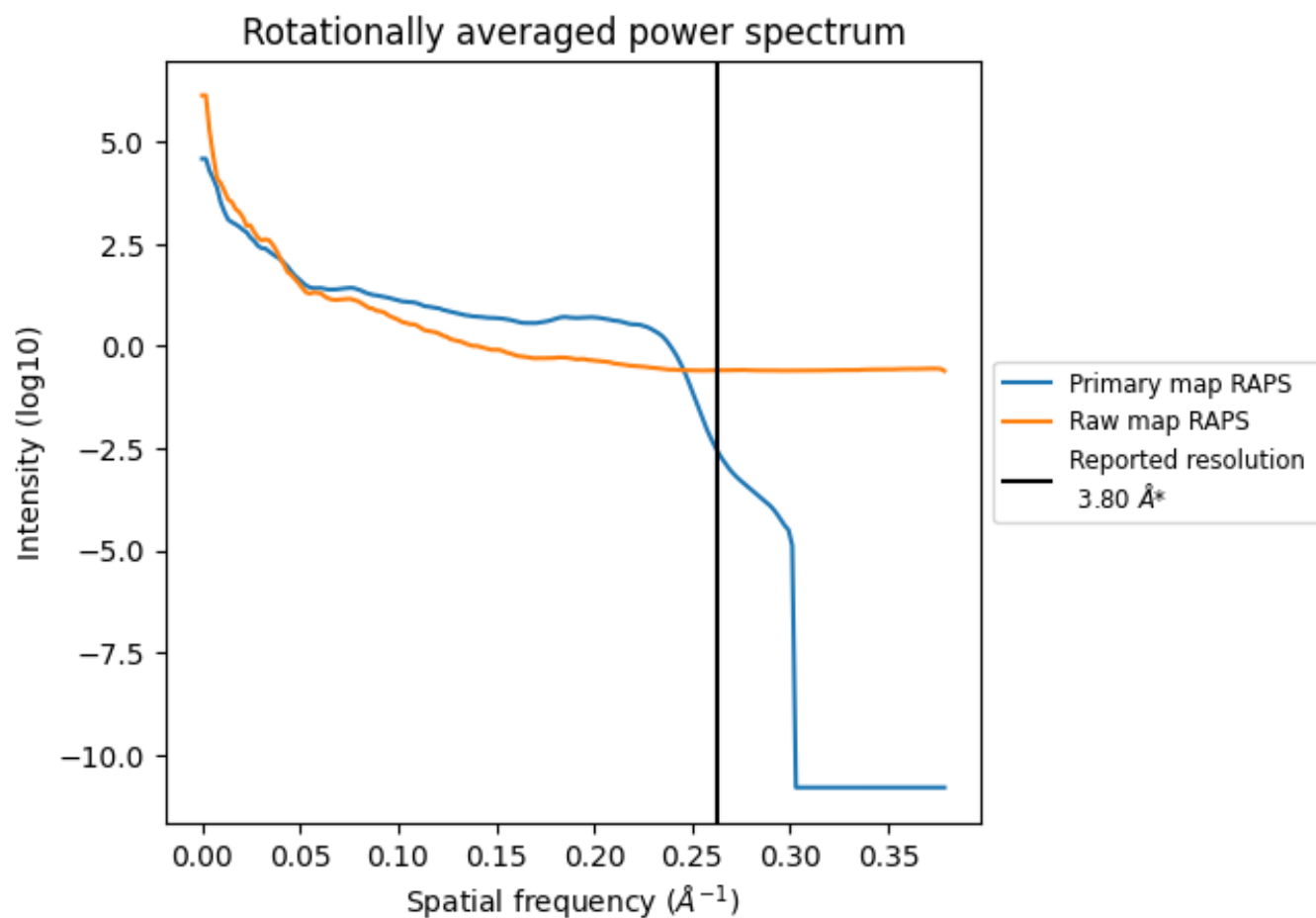
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 655 nm^3 ; this corresponds to an approximate mass of 592 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 ⓘ

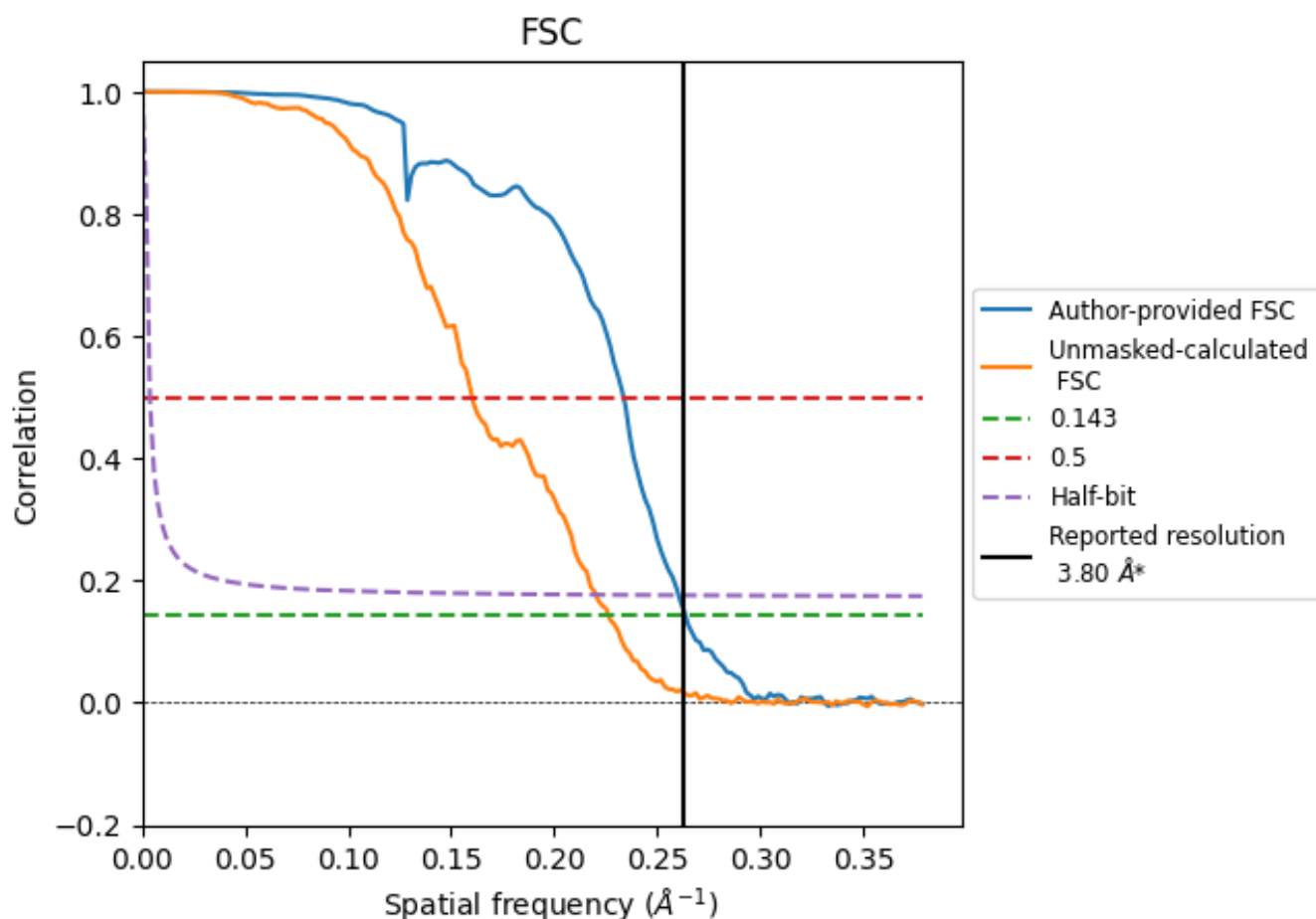


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

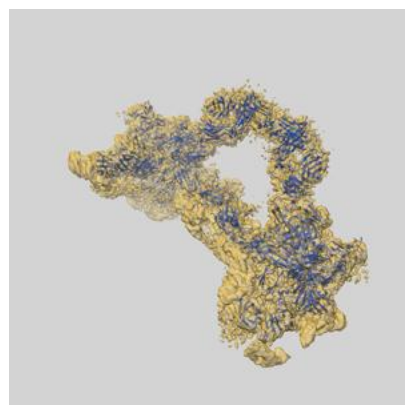
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.28	3.84
Unmasked-calculated*	4.42	6.24	4.54

*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 4.42 differs from the reported value 3.8 by more than 10 %

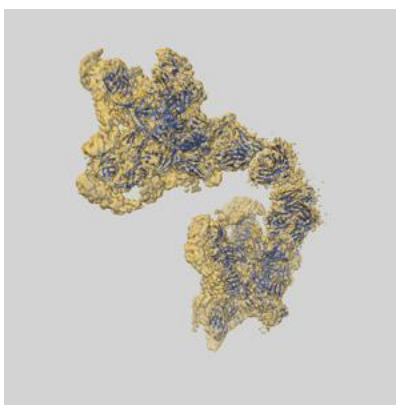
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43507 and PDB model 8VSV. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

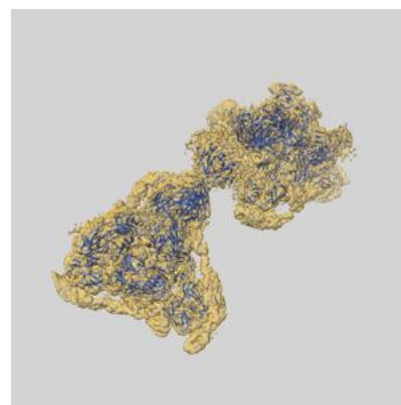
9.1 Map-model overlay [i](#)



X



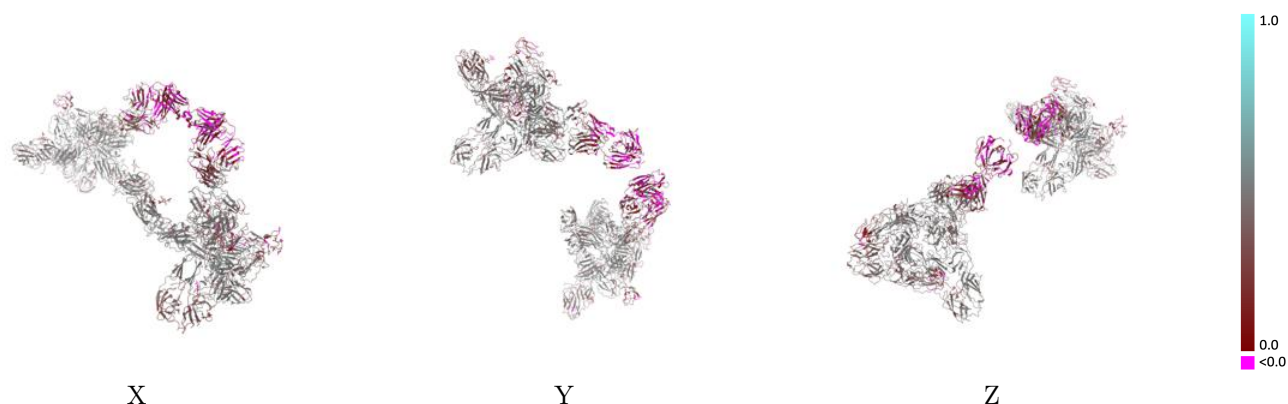
Y



Z

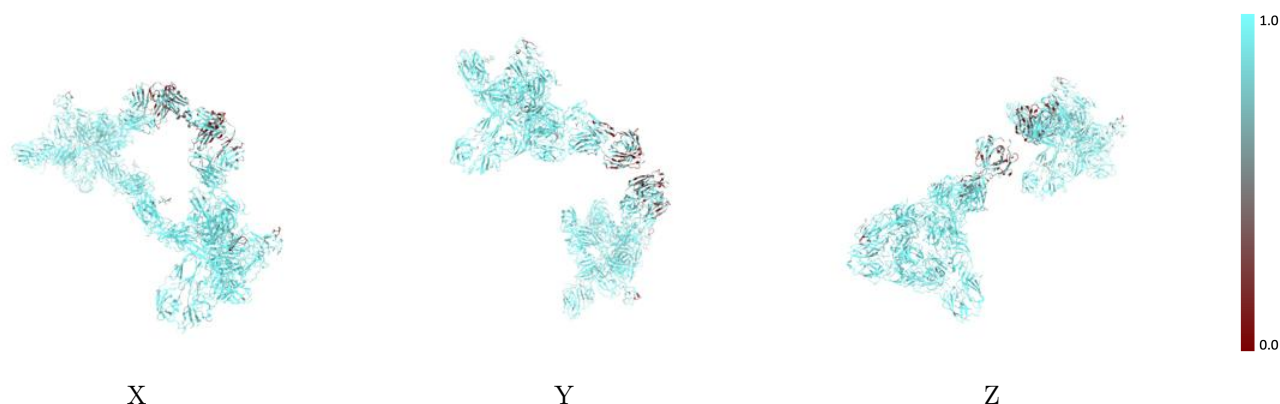
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



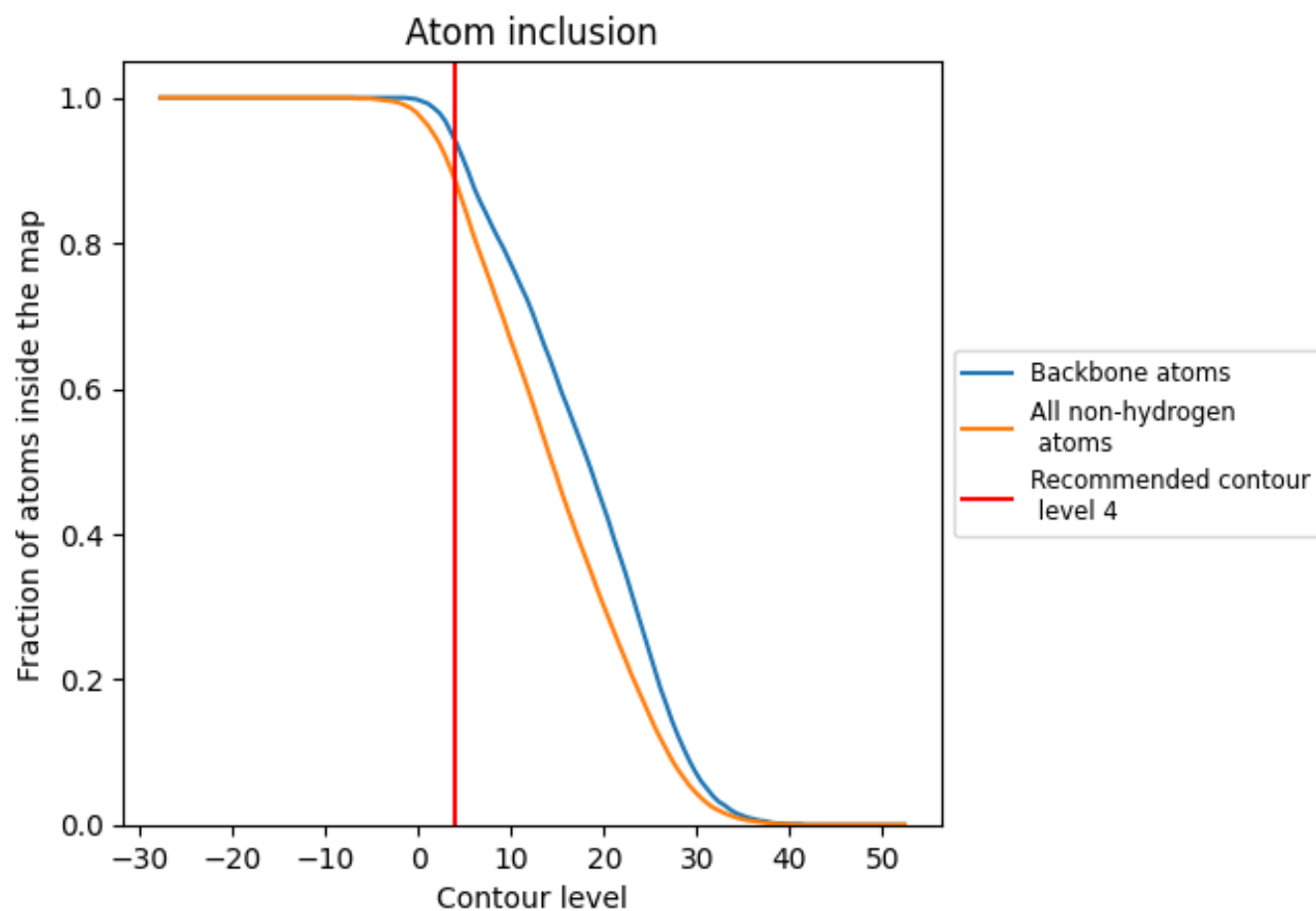
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.3850
1	 0.6960	 0.1890
2	 0.6950	 0.1360
3	 0.6910	 0.1850
4	 0.7110	 0.1370
A	 0.9150	 0.4310
B	 0.9030	 0.3970
C	 0.9150	 0.4320
D	 0.9170	 0.4310
E	 0.9000	 0.3950
F	 0.9220	 0.4310
G	 0.8210	 0.2370
H	 0.6920	 0.1750
I	 0.7950	 0.2930
J	 0.9230	 0.3470
K	 0.7180	 0.1410
L	 0.5900	 0.1130
a	 0.9240	 0.4210
b	 0.8810	 0.3850
c	 0.8910	 0.3960
d	 0.9150	 0.4120
e	 0.8940	 0.3880
f	 0.8790	 0.3840

