Full wwPDB EM Validation Report ⓘ

Mar 12, 2024 – 12:18 pm GMT

PDB ID	:	7QCU
EMDB ID	:	EMD-13899
Title	:	Structure of the MUCIN-2 Cterminal domains partially deglycosylated.
Authors	:	Gallego, P.; Hansson, G.C.
Deposited on	:	2021-11-25
Resolution	:	3.25 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:

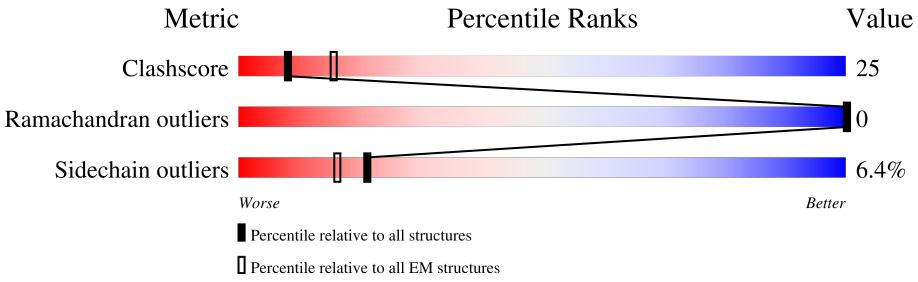
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	807	32% 21% • 45%
1	B	807	34% 20% • 45%
2	C	5	20% 40% 20% 40%
2	D	5	20% 60% 40%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7069 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 Mucin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total 3410	C 2127	N 564	O 666	S 53	0	0
1	B	445	Total 3423	C 2134	N 566	O 670	S 53	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4313	ALA	-	expression tag	UNP Q02817
A	4314	ALA	-	expression tag	UNP Q02817
A	4315	GLN	-	expression tag	UNP Q02817
A	4316	PRO	-	expression tag	UNP Q02817
A	4317	ALA	-	expression tag	UNP Q02817
A	4318	ARG	-	expression tag	UNP Q02817
A	4319	ARG	-	expression tag	UNP Q02817
A	4320	ALA	-	expression tag	UNP Q02817
A	4321	VAL	-	expression tag	UNP Q02817
A	4322	ARG	-	expression tag	UNP Q02817
A	4323	SER	-	expression tag	UNP Q02817
A	4324	SER	-	expression tag	UNP Q02817
A	4325	ARG	-	expression tag	UNP Q02817
A	4326	ARG	-	expression tag	UNP Q02817
A	4327	HIS	-	expression tag	UNP Q02817
A	4328	HIS	-	expression tag	UNP Q02817
A	4329	HIS	-	expression tag	UNP Q02817
A	4330	HIS	-	expression tag	UNP Q02817
A	4331	HIS	-	expression tag	UNP Q02817
A	4332	HIS	-	expression tag	UNP Q02817
A	4333	GLY	-	expression tag	UNP Q02817
A	4334	SER	-	expression tag	UNP Q02817
A	4335	GLY	-	expression tag	UNP Q02817
A	4336	LEU	-	expression tag	UNP Q02817
A	4337	GLU	-	expression tag	UNP Q02817
A	4338	VAL	-	expression tag	UNP Q02817

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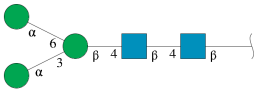
Chain	Residue	Modelled	Actual	Comment	Reference
A	4339	LEU	-	expression tag	UNP Q02817
A	4340	PHE	-	expression tag	UNP Q02817
A	4341	GLN	-	expression tag	UNP Q02817
A	4342	GLY	-	expression tag	UNP Q02817
A	4343	PRO	-	expression tag	UNP Q02817
A	4344	THR	-	expression tag	UNP Q02817
A	4345	PRO	-	expression tag	UNP Q02817
B	4313	ALA	-	expression tag	UNP Q02817
B	4314	ALA	-	expression tag	UNP Q02817
B	4315	GLN	-	expression tag	UNP Q02817
B	4316	PRO	-	expression tag	UNP Q02817
B	4317	ALA	-	expression tag	UNP Q02817
B	4318	ARG	-	expression tag	UNP Q02817
B	4319	ARG	-	expression tag	UNP Q02817
B	4320	ALA	-	expression tag	UNP Q02817
B	4321	VAL	-	expression tag	UNP Q02817
B	4322	ARG	-	expression tag	UNP Q02817
B	4323	SER	-	expression tag	UNP Q02817
B	4324	SER	-	expression tag	UNP Q02817
B	4325	ARG	-	expression tag	UNP Q02817
B	4326	ARG	-	expression tag	UNP Q02817
B	4327	HIS	-	expression tag	UNP Q02817
B	4328	HIS	-	expression tag	UNP Q02817
B	4329	HIS	-	expression tag	UNP Q02817
B	4330	HIS	-	expression tag	UNP Q02817
B	4331	HIS	-	expression tag	UNP Q02817
B	4332	HIS	-	expression tag	UNP Q02817
B	4333	GLY	-	expression tag	UNP Q02817
B	4334	SER	-	expression tag	UNP Q02817
B	4335	GLY	-	expression tag	UNP Q02817
B	4336	LEU	-	expression tag	UNP Q02817
B	4337	GLU	-	expression tag	UNP Q02817
B	4338	VAL	-	expression tag	UNP Q02817
B	4339	LEU	-	expression tag	UNP Q02817
B	4340	PHE	-	expression tag	UNP Q02817
B	4341	GLN	-	expression tag	UNP Q02817
B	4342	GLY	-	expression tag	UNP Q02817
B	4343	PRO	-	expression tag	UNP Q02817
B	4344	THR	-	expression tag	UNP Q02817
B	4345	PRO	-	expression tag	UNP Q02817

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

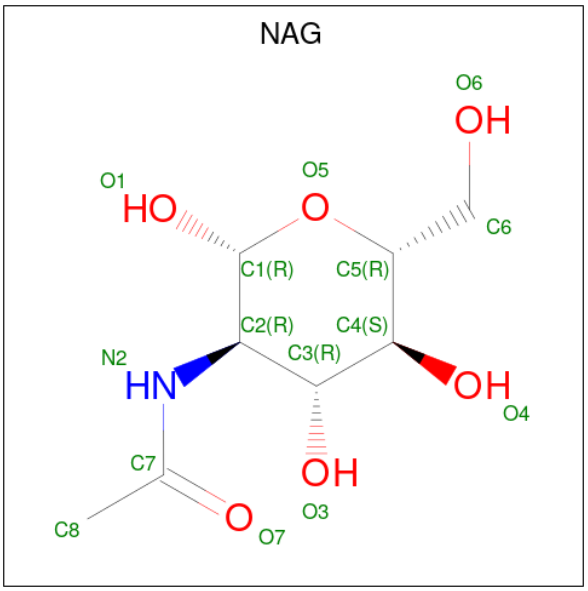


Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	5	Total	C	N	O	0	0
			61	34	2	25		
2	D	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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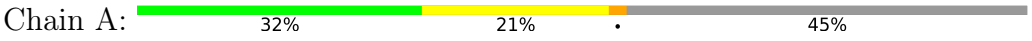
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

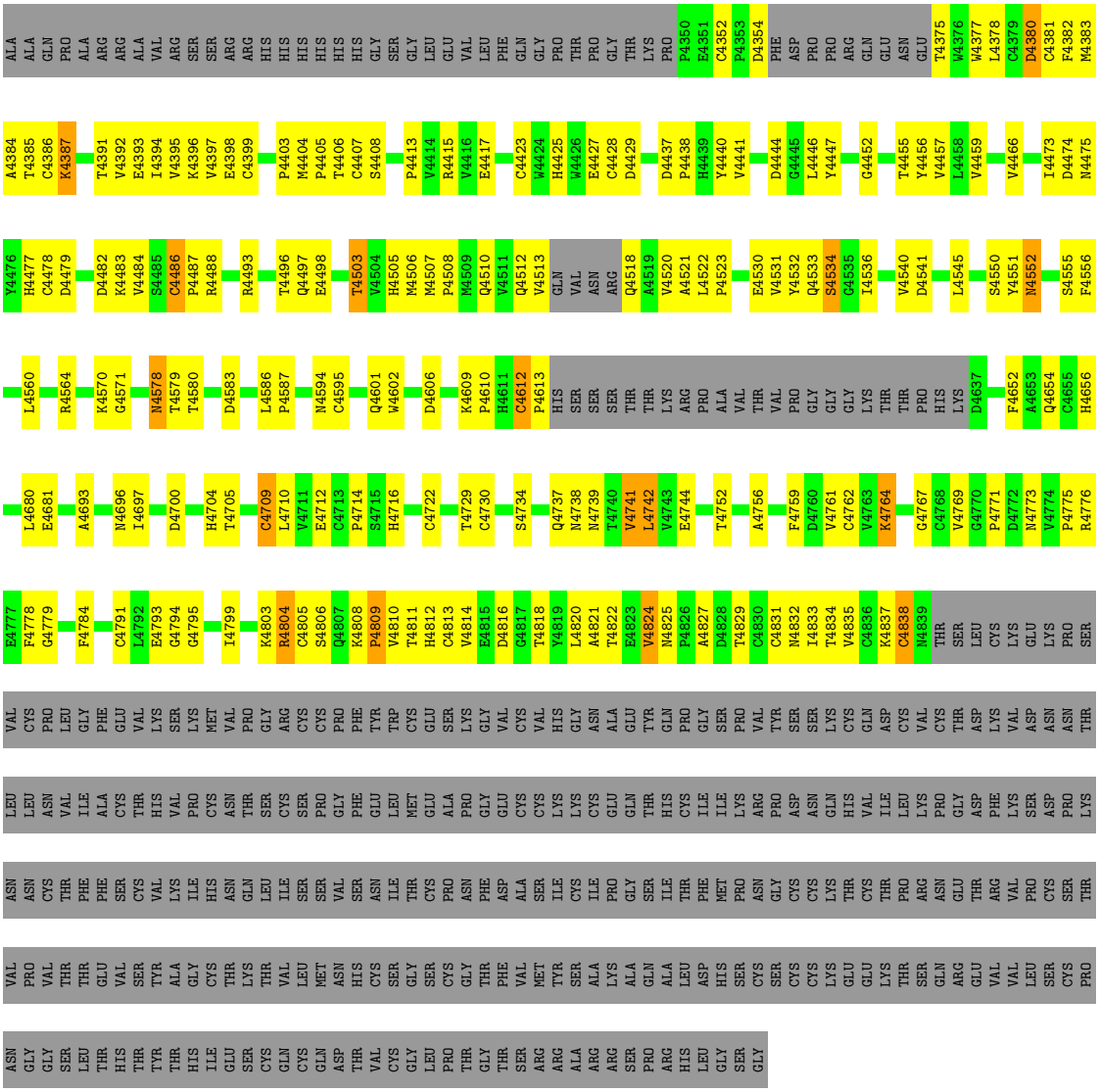
3 Residue-property plots (i)

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: Mucin-2

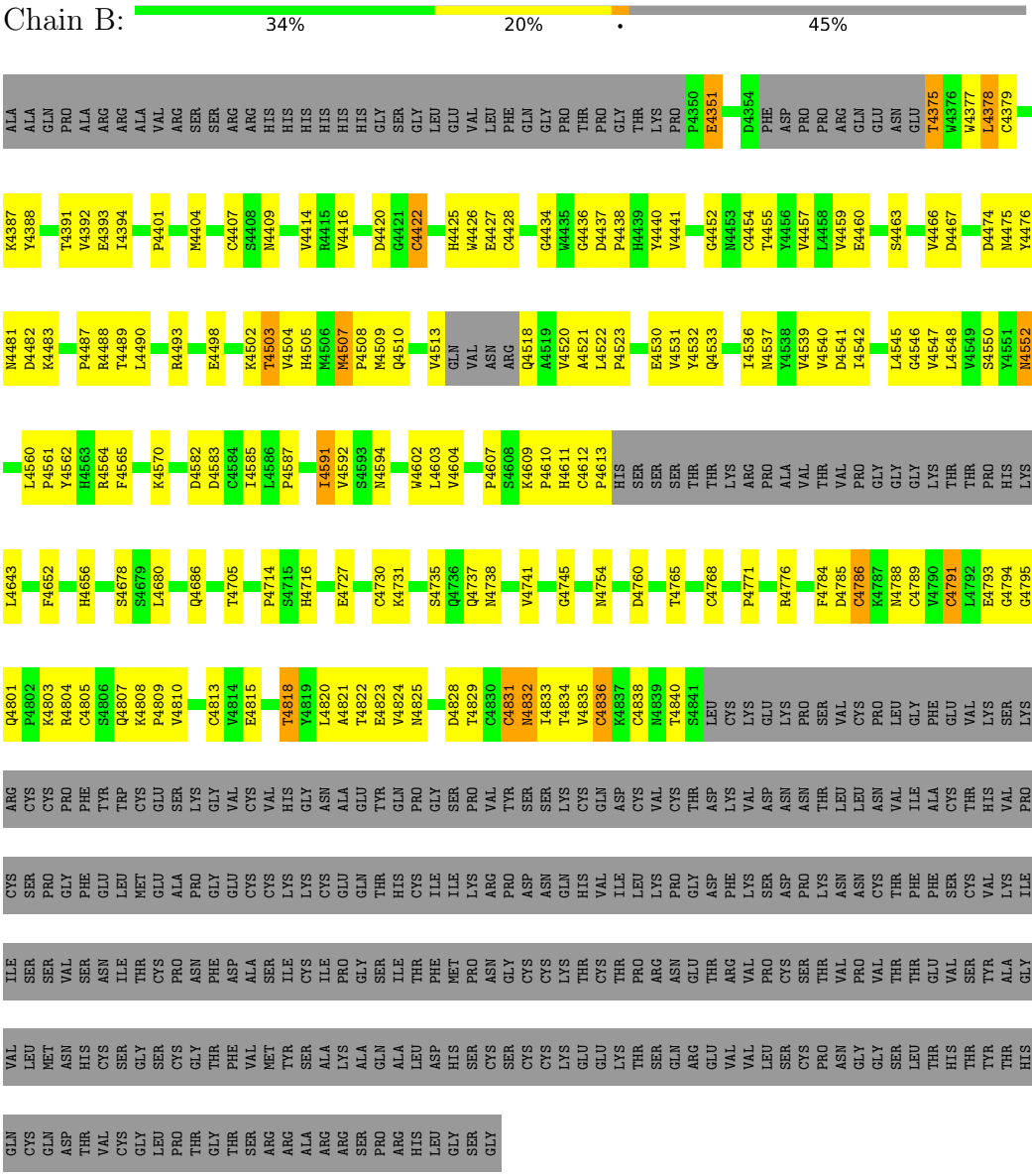
Chain A:





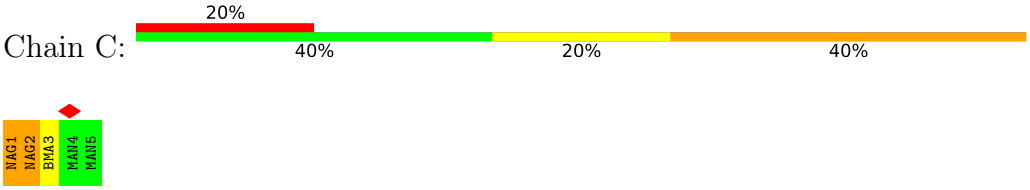
- Molecule 1: Mucin-2

Chain B:



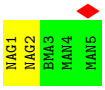
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:


NAG1
NAG2
BMA3
MAN4
MAN5

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	387288	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 ($e^-/Å^2$)	79	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.512	Depositor
Minimum map value	-0.249	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	354.24, 354.24, 354.24	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.69	5/3503 (0.1%)	1.13	27/4785 (0.6%)
1	B	0.59	0/3516	0.91	12/4803 (0.2%)
All	All	0.64	5/7019 (0.1%)	1.02	39/9588 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4809	PRO	N-CD	-11.42	1.31	1.47
1	A	4398	GLU	C-N	8.20	1.52	1.34
1	A	4610	PRO	N-CD	5.93	1.56	1.47
1	A	4555	SER	CA-CB	-5.67	1.44	1.52
1	A	4534	SER	CA-CB	-5.32	1.45	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4552	ASN	CB-CA-C	-12.77	84.85	110.40
1	A	4744	GLU	CB-CA-C	-11.13	88.15	110.40
1	A	4705	THR	CB-CA-C	-9.06	87.14	111.60
1	B	4637	ASP	N-CA-C	7.62	131.59	111.00
1	B	4440	TYR	CB-CA-C	-7.56	95.27	110.40
1	A	4809	PRO	CA-N-CD	7.47	122.16	111.70
1	A	4700	ASP	CB-CA-C	-7.37	95.66	110.40
1	A	4804	ARG	N-CA-CB	7.37	123.86	110.60
1	A	4812	HIS	N-CA-CB	7.11	123.40	110.60
1	A	4742	LEU	N-CA-CB	-7.10	96.19	110.40
1	B	4730	CYS	CA-CB-SG	-6.97	101.45	114.00
1	A	4503	THR	CB-CA-C	-6.83	93.16	111.60
1	A	4594	ASN	N-CA-CB	6.83	122.89	110.60
1	B	4507	MET	N-CA-CB	-6.83	98.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4375	THR	CA-CB-OG1	-6.75	94.84	109.00
1	A	4730	CYS	CA-CB-SG	-6.74	101.88	114.00
1	A	4403	PRO	CA-N-CD	-6.66	102.17	111.50
1	B	4351	GLU	CB-CA-C	6.42	123.24	110.40
1	A	4737	GLN	CB-CA-C	6.15	122.70	110.40
1	A	4496	THR	CB-CA-C	-6.11	95.10	111.60
1	B	4375	THR	N-CA-C	-6.04	94.68	111.00
1	A	4552	ASN	N-CA-C	-5.87	95.16	111.00
1	A	4809	PRO	N-CA-CB	-5.69	96.34	102.60
1	B	4503	THR	CB-CA-C	-5.69	96.24	111.60
1	A	4354	ASP	CB-CA-C	5.65	121.69	110.40
1	A	4712	GLU	C-N-CA	5.53	135.53	121.70
1	B	4441	VAL	CA-CB-CG2	5.27	118.80	110.90
1	B	4591	ILE	N-CA-CB	-5.25	98.72	110.80
1	A	4681	GLU	N-CA-CB	-5.21	101.21	110.60
1	B	4737	GLN	CB-CA-C	5.20	120.79	110.40
1	A	4816	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	4403	PRO	N-CA-CB	5.14	109.47	103.30
1	A	4606	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	4479	ASP	N-CA-C	-5.11	97.19	111.00
1	A	4764	LYS	CB-CA-C	-5.09	100.22	110.40
1	A	4551	TYR	CB-CA-C	-5.08	100.23	110.40
1	A	4741	VAL	N-CA-C	-5.04	97.40	111.00
1	B	4741	VAL	N-CA-C	-5.04	97.40	111.00
1	A	4762	CYS	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

There are no planarity outliers.

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	3410	0	3126	171	0
1	B	3423	0	3139	177	0
2	C	61	0	52	4	0
2	D	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	56	0	52	5	0
4	B	56	0	52	3	0
All	All	7069	0	6473	334	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 25.

All (334) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4643:LEU:CD1	1:B:4705:THR:HG23	1.33	1.58
1:B:4643:LEU:HD11	1:B:4705:THR:CG2	1.44	1.45
1:A:4503:THR:HG23	1:A:4503:THR:O	1.43	1.13
1:A:4586:LEU:CD2	1:A:4587:PRO:HD2	1.83	1.08
1:B:4824:VAL:HA	1:B:4832:ASN:HB3	1.33	1.07
1:B:4404:MET:HG2	1:B:4426:TRP:HB2	1.30	1.07
1:A:4503:THR:O	1:A:4503:THR:CG2	2.00	1.06
1:A:4586:LEU:HD23	1:A:4587:PRO:HD2	1.42	1.02
1:A:4521:ALA:HB3	1:B:4794:GLY:HA3	1.42	1.01
1:A:4739:ASN:HD21	1:A:4741:VAL:CG2	1.77	0.97
1:A:4532:TYR:HE1	1:A:4534:SER:HB3	1.27	0.97
1:B:4476:TYR:CE1	1:B:4482:ASP:HA	2.01	0.96
1:B:4808:LYS:H	1:B:4833:ILE:HA	1.32	0.94
1:A:4503:THR:HA	1:A:4508:PRO:HA	1.48	0.93
1:A:4752:THR:HG22	1:A:4764:LYS:HG2	1.51	0.92
1:B:4420:ASP:OD2	1:B:4422:CYS:SG	2.27	0.92
1:A:4387:LYS:NZ	1:A:4391:THR:HG22	1.85	0.90
1:A:4586:LEU:HD23	1:A:4587:PRO:CD	2.03	0.89
1:B:4404:MET:HG2	1:B:4426:TRP:CB	2.05	0.87
1:A:4375:THR:HA	1:A:4385:THR:HA	1.57	0.87
1:A:4505:HIS:NE2	1:A:4506:MET:HG2	1.89	0.86
1:B:4475:ASN:HA	1:B:4488:ARG:HG2	1.56	0.85
1:A:4505:HIS:CG	1:A:4506:MET:H	1.92	0.84
1:A:4505:HIS:CD2	1:A:4506:MET:HG2	2.12	0.83
1:A:4383:MET:HB3	1:A:4395:VAL:HB	1.60	0.82
1:B:4503:THR:O	1:B:4503:THR:OG1	1.87	0.82
1:B:4541:ASP:HB3	1:B:4548:LEU:HD13	1.62	0.81
1:B:4705:THR:HG22	1:B:4705:THR:O	1.79	0.81
1:A:4446:LEU:HB2	1:A:4580:THR:HG23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4522:LEU:HD12	1:B:4533:GLN:HG3	1.64	0.80
1:B:4809:PRO:HB3	1:B:4834:THR:HG23	1.63	0.80
1:A:4709:CYS:C	1:A:4710:LEU:HD12	2.03	0.80
1:A:4457:VAL:HG11	1:A:4602:TRP:HE3	1.47	0.79
1:A:4654:GLN:HB2	1:A:4697:ILE:HG21	1.64	0.79
1:B:4643:LEU:CD1	1:B:4705:THR:CG2	2.27	0.79
1:A:4505:HIS:CG	1:A:4506:MET:N	2.47	0.78
1:A:4761:VAL:HG21	1:A:4769:VAL:HG21	1.63	0.78
1:A:4586:LEU:CG	1:A:4587:PRO:HD2	2.12	0.78
1:A:4742:LEU:N	1:A:4742:LEU:CD1	2.47	0.77
1:A:4697:ILE:O	1:A:4697:ILE:HG22	1.85	0.77
1:B:4810:VAL:HB	1:B:4836:CYS:HB2	1.66	0.77
1:A:4818:THR:HA	1:A:4838:CYS:HA	1.68	0.76
1:B:4825:ASN:HD21	1:B:4833:ILE:HG12	1.51	0.76
1:A:4387:LYS:HZ2	1:A:4391:THR:HG22	1.51	0.75
1:B:4810:VAL:HB	1:B:4836:CYS:H	1.52	0.75
1:B:4771:PRO:HG2	1:B:4784:PHE:CZ	2.22	0.75
1:A:4532:TYR:CE1	1:A:4534:SER:HB3	2.18	0.75
1:B:4822:THR:HG22	1:B:4834:THR:HB	1.67	0.75
1:A:4457:VAL:HG11	1:A:4602:TRP:CE3	2.21	0.75
1:A:4739:ASN:ND2	1:A:4741:VAL:CG2	2.49	0.74
1:B:4815:GLU:HB3	1:B:4818:THR:HG23	1.69	0.74
1:A:4824:VAL:HA	1:A:4832:ASN:HA	1.68	0.74
1:B:4507:MET:HG3	1:B:4507:MET:O	1.87	0.74
1:B:4455:THR:HG23	1:B:4604:VAL:HB	1.70	0.73
1:A:4522:LEU:HB3	1:A:4523:PRO:HD3	1.71	0.73
1:B:4428:CYS:O	1:B:4562:TYR:HB2	1.90	0.72
1:A:4804:ARG:O	1:A:4804:ARG:HG3	1.89	0.72
1:B:4481:ASN:HB2	1:B:4483:LYS:HE2	1.70	0.72
1:B:4788:ASN:HB2	1:B:4801:GLN:HE21	1.53	0.72
1:B:4825:ASN:OD1	1:B:4833:ILE:HG23	1.89	0.72
1:A:4739:ASN:HD21	1:A:4741:VAL:HG21	1.55	0.72
1:B:4545:LEU:HD23	1:B:4565:PHE:HZ	1.55	0.71
1:B:4466:VAL:HG21	1:B:4545:LEU:HD21	1.72	0.71
4:A:5205:NAG:H61	1:B:4829:THR:CG2	2.20	0.71
1:A:4693:ALA:O	1:A:4741:VAL:CG1	2.39	0.70
1:A:4654:GLN:CB	1:A:4697:ILE:HG21	2.22	0.70
1:A:4586:LEU:HG	1:A:4587:PRO:HD2	1.74	0.69
1:A:4384:ALA:HB1	1:A:4392:VAL:HG22	1.74	0.68
1:B:4475:ASN:CA	1:B:4488:ARG:HG2	2.23	0.68
1:B:4611:HIS:CD2	1:B:4613:PRO:HD3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4475:ASN:OD1	1:B:4475:ASN:O	2.11	0.67
1:B:4377:TRP:HA	1:B:4383:MET:HA	1.76	0.67
1:B:4807:GLN:HA	1:B:4832:ASN:O	1.95	0.66
1:A:4475:ASN:OD1	1:A:4488:ARG:HD2	1.95	0.66
1:B:4454:CYS:HA	1:B:4477:HIS:CD2	2.31	0.66
1:B:4727:GLU:OE2	1:B:4754:ASN:ND2	2.29	0.66
1:A:4586:LEU:CD1	1:A:4601:GLN:HG3	2.26	0.65
1:A:4393:GLU:HA	1:B:4391:THR:HA	1.78	0.65
1:A:4393:GLU:HG3	1:B:4391:THR:HG22	1.78	0.65
1:A:4387:LYS:HZ3	1:A:4391:THR:HG22	1.62	0.65
1:A:4520:VAL:HG12	1:B:4793:GLU:HG3	1.78	0.65
1:A:4771:PRO:HG2	1:A:4784:PHE:HZ	1.62	0.65
1:A:4818:THR:HG23	1:A:4818:THR:O	1.97	0.64
1:A:4487:PRO:O	1:A:4488:ARG:HG3	1.98	0.64
4:A:5205:NAG:H61	1:B:4829:THR:HG21	1.80	0.64
1:B:4531:VAL:HG22	1:B:4540:VAL:HG22	1.80	0.64
1:A:4383:MET:CB	1:A:4395:VAL:HB	2.27	0.63
1:A:4739:ASN:ND2	1:A:4741:VAL:HG23	2.14	0.63
1:A:4761:VAL:CG2	1:A:4769:VAL:HG21	2.29	0.63
1:B:4809:PRO:HB2	1:B:4820:LEU:HD22	1.80	0.63
1:B:4828:ASP:CB	1:B:4831:CYS:HB3	2.29	0.63
1:A:4532:TYR:HD1	1:A:4533:GLN:O	1.81	0.62
1:A:4794:GLY:HA3	1:B:4521:ALA:HB3	1.81	0.62
1:B:4425:HIS:HD2	1:B:4427:GLU:HG3	1.62	0.62
1:B:4716:HIS:NE2	1:B:4760:ASP:OD2	2.27	0.62
1:A:4523:PRO:HD2	1:B:4795:GLY:HA3	1.82	0.62
1:B:4507:MET:O	1:B:4507:MET:CG	2.45	0.62
1:A:4404:MET:HB2	1:A:4413:PRO:HG3	1.82	0.62
1:B:4809:PRO:HA	1:B:4835:VAL:HA	1.80	0.62
1:A:4457:VAL:HG12	1:A:4602:TRP:HB3	1.81	0.62
1:B:4404:MET:CG	1:B:4426:TRP:HB2	2.20	0.61
1:A:4385:THR:HG22	1:A:4393:GLU:HB2	1.83	0.61
1:A:4696:ASN:OD1	1:A:4741:VAL:HG22	1.99	0.61
1:B:4545:LEU:HD23	1:B:4565:PHE:CZ	2.35	0.61
1:A:4415:ARG:NH1	1:A:4417:GLU:OE2	2.34	0.60
1:A:4742:LEU:N	1:A:4742:LEU:HD12	2.16	0.60
1:A:4739:ASN:ND2	1:A:4741:VAL:HB	2.17	0.59
1:B:4831:CYS:O	1:B:4831:CYS:SG	2.60	0.59
1:B:4510:GLN:HE21	1:B:4522:LEU:HD13	1.68	0.59
1:B:4807:GLN:HG2	1:B:4834:THR:CG2	2.32	0.59
1:A:4586:LEU:HD23	1:A:4587:PRO:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4475:ASN:CB	1:B:4488:ARG:HG2	2.33	0.58
1:A:4810:VAL:O	1:A:4834:THR:HG22	2.03	0.58
1:A:4693:ALA:O	1:A:4741:VAL:HG11	2.04	0.58
1:A:4477:HIS:CE1	1:A:4609:LYS:HE2	2.39	0.58
1:A:4741:VAL:C	1:A:4742:LEU:HD12	2.24	0.58
1:A:4767:GLY:HA3	1:A:4776:ARG:O	2.03	0.57
1:B:4493:ARG:NH1	1:B:4498:GLU:OE1	2.36	0.57
1:A:4739:ASN:HD21	1:A:4741:VAL:CB	2.16	0.57
1:B:4476:TYR:HE1	1:B:4482:ASP:HA	1.65	0.57
1:A:4521:ALA:HB3	1:B:4794:GLY:CA	2.24	0.57
1:A:4455:THR:HA	1:A:4474:ASP:HA	1.85	0.57
1:A:4803:LYS:HG3	1:A:4804:ARG:N	2.20	0.57
4:A:5205:NAG:H61	1:B:4829:THR:HG22	1.86	0.57
1:B:4487:PRO:O	1:B:4488:ARG:HG3	2.04	0.57
1:A:4832:ASN:HD22	4:A:5205:NAG:H83	1.70	0.57
1:B:4570:LYS:CB	1:B:4585:ILE:HD11	2.34	0.57
1:A:4486:CYS:HA	1:A:4503:THR:CG2	2.35	0.56
1:A:4475:ASN:OD1	1:A:4488:ARG:CD	2.53	0.56
1:B:4807:GLN:HG2	1:B:4834:THR:HG22	1.87	0.56
1:B:4828:ASP:HB3	1:B:4831:CYS:HB3	1.86	0.56
1:B:4705:THR:CG2	1:B:4705:THR:O	2.49	0.56
1:B:4809:PRO:CB	1:B:4820:LEU:HD22	2.36	0.56
1:A:4821:ALA:O	1:A:4834:THR:HA	2.04	0.56
1:B:4585:ILE:HG22	1:B:4591:ILE:HG22	1.87	0.56
1:B:4609:LYS:HG3	1:B:4611:HIS:CE1	2.41	0.55
1:B:4821:ALA:O	1:B:4834:THR:HA	2.06	0.55
1:A:4709:CYS:O	1:A:4710:LEU:HD12	2.06	0.55
1:B:4454:CYS:HA	1:B:4477:HIS:HD2	1.70	0.55
1:A:4505:HIS:CD2	1:A:4506:MET:N	2.75	0.55
1:A:4795:GLY:H	1:B:4521:ALA:HB3	1.72	0.55
1:B:4587:PRO:HA	1:B:4602:TRP:CH2	2.42	0.55
1:B:4825:ASN:ND2	1:B:4833:ILE:HG12	2.20	0.55
1:B:4434:GLY:HA3	1:B:4556:PHE:CZ	2.41	0.55
1:A:4352:CYS:HB2	1:A:4375:THR:HG22	1.89	0.55
1:B:4825:ASN:H	1:B:4832:ASN:HA	1.73	0.54
1:A:4375:THR:CA	1:A:4385:THR:HA	2.35	0.54
1:A:4570:LYS:HD2	1:A:4602:TRP:HH2	1.73	0.54
1:B:4570:LYS:HB3	1:B:4585:ILE:HD11	1.90	0.54
1:B:4810:VAL:O	1:B:4813:CYS:SG	2.66	0.53
1:B:4561:PRO:HG2	1:B:4564:ARG:HB3	1.90	0.53
1:B:4807:GLN:HB3	4:B:5204:NAG:N2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4405:PRO:HB2	2:C:2:NAG:H62	1.90	0.53
1:A:4822:THR:HA	1:A:4834:THR:HA	1.90	0.53
1:A:4742:LEU:N	1:A:4742:LEU:HD13	2.24	0.53
1:B:4609:LYS:HE3	1:B:4612:CYS:HA	1.91	0.52
1:A:4531:VAL:HG22	1:A:4540:VAL:HG22	1.90	0.52
1:A:4793:GLU:HG3	1:B:4520:VAL:HG12	1.91	0.52
1:A:4825:ASN:HB3	1:A:4831:CYS:HB2	1.92	0.52
1:A:4391:THR:HA	1:B:4392:VAL:O	2.09	0.52
1:B:4387:LYS:HB2	1:B:4393:GLU:CD	2.29	0.52
1:B:4436:GLY:O	1:B:4488:ARG:CZ	2.58	0.52
1:B:4552:ASN:HD22	1:B:4553:GLY:H	1.57	0.52
1:A:4457:VAL:CG1	1:A:4602:TRP:CE3	2.92	0.52
1:A:4654:GLN:HB2	1:A:4697:ILE:CG2	2.39	0.52
1:B:4487:PRO:C	1:B:4488:ARG:HG3	2.30	0.52
1:B:4678:SER:HB2	1:B:4680:LEU:HD22	1.92	0.52
1:A:4771:PRO:HG2	1:A:4784:PHE:CZ	2.45	0.52
1:B:4387:LYS:HB2	1:B:4393:GLU:OE2	2.10	0.52
1:A:4378:LEU:HB3	1:A:4382:PHE:HB2	1.92	0.51
1:B:4385:THR:HB	1:B:4393:GLU:HB2	1.92	0.51
1:A:4497:GLN:HG2	1:A:4512:GLN:HE22	1.76	0.51
1:A:4477:HIS:ND1	1:A:4609:LYS:HE2	2.26	0.51
1:B:4466:VAL:HG12	1:B:4467:ASP:N	2.25	0.51
1:A:4399:CYS:N	1:A:4423:CYS:SG	2.84	0.50
1:B:4503:THR:HA	1:B:4508:PRO:HA	1.93	0.50
1:B:4825:ASN:HD21	1:B:4833:ILE:CG1	2.22	0.50
1:A:4444:ASP:HB2	1:A:4583:ASP:OD2	2.12	0.50
1:B:4532:TYR:CZ	1:B:4539:VAL:HG11	2.45	0.50
1:A:4804:ARG:HH12	1:A:4806:SER:HB2	1.77	0.50
1:B:4643:LEU:HD13	1:B:4705:THR:HG23	1.67	0.49
1:A:4652:PHE:O	1:A:4656:HIS:ND1	2.42	0.49
1:B:4771:PRO:HG2	1:B:4784:PHE:HZ	1.73	0.49
1:B:4607:PRO:O	1:B:4610:PRO:HD3	2.11	0.49
1:A:4380:ASP:HB2	1:B:4379:CYS:SG	2.52	0.49
1:B:4825:ASN:HD21	1:B:4833:ILE:HG23	1.78	0.49
1:A:4483:LYS:HG3	1:A:4484:VAL:N	2.28	0.49
1:A:4761:VAL:HG21	1:A:4769:VAL:CG2	2.40	0.49
1:A:4739:ASN:ND2	1:A:4741:VAL:CB	2.75	0.49
1:B:4550:SER:HB2	1:B:4557:SER:OG	2.11	0.49
1:A:4466:VAL:HG21	1:A:4545:LEU:HD11	1.95	0.49
1:B:4612:CYS:O	1:B:4613:PRO:C	2.51	0.49
1:B:4434:GLY:HA3	1:B:4556:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4739:ASN:HD21	1:A:4741:VAL:HB	1.78	0.49
1:A:4784:PHE:CZ	1:B:4784:PHE:HE2	2.31	0.48
1:A:4395:VAL:HG12	1:A:4396:LYS:N	2.28	0.48
1:A:4475:ASN:HA	1:A:4488:ARG:HG2	1.96	0.48
1:A:4493:ARG:NH2	1:A:4498:GLU:OE1	2.45	0.48
1:A:4570:LYS:HB2	1:A:4602:TRP:CH2	2.48	0.48
1:B:4552:ASN:ND2	1:B:4553:GLY:H	2.11	0.48
1:A:4457:VAL:CG1	1:A:4602:TRP:HB3	2.43	0.48
1:B:4822:THR:HA	1:B:4833:ILE:O	2.13	0.48
1:B:4513:VAL:O	1:B:4518:GLN:N	2.47	0.48
1:A:4779:GLY:N	1:A:4791:CYS:O	2.45	0.48
1:B:4807:GLN:CD	1:B:4807:GLN:H	2.16	0.48
1:A:4408:SER:HB2	1:A:4444:ASP:O	2.14	0.48
1:A:4394:ILE:HG12	1:B:4392:VAL:HG13	1.96	0.48
1:B:4387:LYS:HG2	1:B:4388:TYR:CD2	2.48	0.48
1:B:4522:LEU:HB2	1:B:4523:PRO:HD3	1.95	0.48
1:A:4486:CYS:HA	1:A:4503:THR:HG21	1.96	0.47
1:A:4803:LYS:HG3	1:A:4805:CYS:H	1.80	0.47
1:B:4437:ASP:HB3	1:B:4438:PRO:HD3	1.96	0.47
1:A:4714:PRO:HB2	1:A:4716:HIS:CE1	2.50	0.47
1:B:4414:VAL:HG13	1:B:4416:VAL:HG23	1.97	0.47
1:B:4805:CYS:HB3	1:B:4831:CYS:HB2	1.61	0.47
1:B:4820:LEU:HB3	1:B:4834:THR:OG1	2.15	0.47
1:A:4586:LEU:HG	1:A:4587:PRO:CD	2.41	0.47
1:B:4436:GLY:O	1:B:4488:ARG:NH2	2.48	0.47
1:B:4823:GLU:OE2	1:B:4833:ILE:HG13	2.14	0.47
1:A:4507:MET:O	1:A:4507:MET:HG3	2.15	0.47
1:B:4375:THR:HG23	1:B:4375:THR:O	2.14	0.47
1:B:4611:HIS:CG	1:B:4613:PRO:HD3	2.50	0.47
1:A:4739:ASN:CG	1:A:4741:VAL:HG23	2.36	0.46
1:B:4825:ASN:ND2	1:B:4833:ILE:HG23	2.30	0.46
1:A:4486:CYS:O	1:A:4486:CYS:SG	2.73	0.46
1:B:4479:ASP:HB2	1:B:4481:ASN:OD1	2.15	0.46
1:A:4586:LEU:CG	1:A:4587:PRO:CD	2.90	0.46
1:B:4476:TYR:CZ	1:B:4487:PRO:HA	2.50	0.46
1:B:4807:GLN:H	4:B:5204:NAG:HN2	1.64	0.46
1:A:4385:THR:CG2	1:A:4393:GLU:HB2	2.45	0.46
1:A:4437:ASP:HB3	1:A:4438:PRO:HD3	1.98	0.46
1:A:4452:GLY:HA3	1:A:4456:TYR:HE2	1.81	0.46
1:B:4547:VAL:HG22	1:B:4560:LEU:HD22	1.98	0.46
1:A:4441:VAL:HG12	1:A:4447:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4769:VAL:HG22	1:A:4775:PRO:HA	1.99	0.45
1:B:4652:PHE:O	1:B:4656:HIS:ND1	2.47	0.45
1:A:4808:LYS:HA	1:A:4809:PRO:HD3	1.56	0.45
1:A:4521:ALA:CB	1:B:4794:GLY:HA3	2.28	0.45
1:B:4457:VAL:HG12	1:B:4602:TRP:HB3	1.98	0.45
1:A:4532:TYR:HD1	1:A:4533:GLN:C	2.20	0.45
1:B:4825:ASN:HB2	1:B:4831:CYS:O	2.16	0.45
1:A:4497:GLN:HG2	1:A:4512:GLN:NE2	2.32	0.45
1:A:4761:VAL:CG1	1:A:4773:ASN:HB3	2.47	0.45
1:B:4401:PRO:HG2	1:B:4425:HIS:HA	1.99	0.45
1:B:4714:PRO:HB2	1:B:4716:HIS:CE1	2.52	0.45
1:B:4828:ASP:HB2	1:B:4831:CYS:HB3	1.99	0.45
1:A:4429:ASP:N	1:A:4429:ASP:OD1	2.46	0.45
1:A:4778:PHE:CE2	1:A:4793:GLU:HB3	2.52	0.45
1:B:4825:ASN:CG	1:B:4833:ILE:HG23	2.37	0.45
1:A:4813:CYS:C	1:A:4818:THR:HG21	2.38	0.45
1:B:4457:VAL:HG21	1:B:4460:GLU:HG3	1.99	0.44
1:A:4803:LYS:HG3	1:A:4804:ARG:H	1.80	0.44
1:B:4530:GLU:HB3	1:B:4541:ASP:OD1	2.17	0.44
1:B:4822:THR:HG22	1:B:4834:THR:CB	2.42	0.44
1:A:4808:LYS:HD2	1:A:4809:PRO:HD2	1.99	0.44
1:B:4510:GLN:NE2	1:B:4522:LEU:HD13	2.32	0.44
1:A:4571:GLY:HA2	1:A:4602:TRP:CD2	2.53	0.44
1:B:4545:LEU:HB3	1:B:4547:VAL:HG23	2.00	0.44
1:B:4552:ASN:OD1	1:B:4686:GLN:NE2	2.50	0.44
1:B:4680:LEU:HD23	1:B:4680:LEU:H	1.83	0.44
1:B:4776:ARG:HB2	1:B:4791:CYS:SG	2.58	0.44
1:B:4475:ASN:O	1:B:4475:ASN:CG	2.55	0.44
1:B:4536:ILE:HG23	1:B:4745:GLY:HA2	2.00	0.44
1:A:4818:THR:O	1:A:4818:THR:CG2	2.62	0.44
1:B:4477:HIS:CD2	1:B:4609:LYS:HD3	2.53	0.44
1:A:4530:GLU:HB3	1:A:4541:ASP:OD1	2.18	0.44
1:B:4786:CYS:O	1:B:4803:LYS:HB2	2.18	0.44
1:B:4542:ILE:O	1:B:4546:GLY:N	2.51	0.43
1:B:4807:GLN:HG2	1:B:4834:THR:HG21	2.00	0.43
1:A:4505:HIS:CE1	1:A:4506:MET:HG2	2.50	0.43
1:A:4578:ASN:O	2:C:1:NAG:N2	2.51	0.43
1:A:4739:ASN:OD1	1:A:4741:VAL:HG23	2.18	0.43
1:B:4375:THR:N	1:B:4384:ALA:O	2.51	0.43
1:B:4785:ASP:CG	1:B:4786:CYS:H	2.21	0.43
1:A:4381:CYS:SG	1:A:4397:VAL:HB	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4487:PRO:C	1:A:4488:ARG:HG3	2.38	0.43
1:B:4643:LEU:HD11	1:B:4705:THR:HG23	0.50	0.43
1:B:4788:ASN:HB2	1:B:4801:GLN:NE2	2.25	0.43
1:A:4680:LEU:HD23	1:A:4680:LEU:HA	1.75	0.42
1:A:4825:ASN:HD21	1:A:4827:ALA:HB3	1.84	0.42
1:A:4811:THR:HB	1:A:4820:LEU:HD21	2.01	0.42
1:A:4756:ALA:HB3	1:A:4759:PHE:HD2	1.84	0.42
1:B:4808:LYS:N	1:B:4833:ILE:HA	2.15	0.42
1:A:4811:THR:HA	1:A:4820:LEU:HG	2.01	0.42
1:B:4455:THR:HA	1:B:4474:ASP:HA	2.00	0.42
1:B:4466:VAL:CG1	1:B:4467:ASP:N	2.82	0.42
1:B:4735:SER:O	4:B:5203:NAG:N2	2.52	0.42
1:A:4459:VAL:HG21	1:A:4560:LEU:HD11	2.02	0.42
1:A:4473:ILE:HD12	1:A:4473:ILE:HA	1.97	0.42
1:A:4510:GLN:NE2	1:A:4522:LEU:HA	2.35	0.42
1:A:4654:GLN:HB3	1:A:4697:ILE:HG21	2.01	0.42
1:B:4504:VAL:HG22	1:B:4509:MET:HG2	2.01	0.42
1:A:4784:PHE:HE2	1:B:4771:PRO:HG3	1.84	0.42
1:B:4592:VAL:HG12	1:B:4594:ASN:H	1.84	0.42
1:A:4466:VAL:HG11	1:A:4545:LEU:HD11	2.02	0.42
1:A:4586:LEU:HD11	1:A:4601:GLN:HG3	1.99	0.42
1:A:4824:VAL:HG23	1:A:4829:THR:O	2.20	0.41
1:A:4825:ASN:HB2	1:A:4833:ILE:HG22	2.03	0.41
1:B:4789:CYS:HB3	1:B:4798:ILE:CG2	2.49	0.41
1:B:4808:LYS:O	1:B:4835:VAL:HG13	2.19	0.41
1:B:4457:VAL:HB	1:B:4604:VAL:CG2	2.50	0.41
1:A:4837:LYS:HA	1:A:4837:LYS:HD2	1.91	0.41
1:A:4704:HIS:CE1	4:A:5202:NAG:H83	2.56	0.41
1:B:4384:ALA:HA	1:B:4394:ILE:HA	2.02	0.41
1:B:4798:ILE:N	1:B:4798:ILE:HD12	2.35	0.41
1:B:4378:LEU:HA	1:B:4378:LEU:HD23	1.73	0.41
1:B:4474:ASP:CG	1:B:4477:HIS:HB3	2.41	0.41
1:A:4440:TYR:CE1	1:A:4556:PHE:HZ	2.38	0.41
1:A:4488:ARG:NH2	1:A:4556:PHE:CE1	2.88	0.41
1:B:4452:GLY:O	1:B:4475:ASN:ND2	2.54	0.41
1:B:4552:ASN:HD22	1:B:4553:GLY:N	2.19	0.41
1:A:4586:LEU:HD12	1:A:4601:GLN:HG3	2.00	0.41
1:A:4804:ARG:NH1	1:A:4806:SER:HB2	2.35	0.41
1:B:4351:GLU:HB3	1:B:4375:THR:HG21	2.03	0.41
1:B:4807:GLN:CD	1:B:4807:GLN:N	2.74	0.41
1:A:4425:HIS:HD2	1:A:4427:GLU:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4489:THR:HG22	1:B:4502:LYS:HB2	2.03	0.41
1:B:4537:ASN:OD1	1:B:4552:ASN:HB2	2.21	0.41
1:B:4809:PRO:HA	1:B:4834:THR:C	2.42	0.41
2:C:2:NAG:H83	2:C:3:BMA:H62	2.03	0.41
1:A:4612:CYS:HA	1:A:4613:PRO:HD2	1.93	0.41
1:B:4490:LEU:HD12	1:B:4490:LEU:HA	1.92	0.41
2:C:2:NAG:H5	2:C:2:NAG:N2	2.36	0.41
1:A:4513:VAL:O	1:A:4518:GLN:N	2.53	0.40
1:B:4541:ASP:HA	1:B:4547:VAL:O	2.22	0.40
1:A:4784:PHE:CZ	1:B:4784:PHE:CE2	3.09	0.40
1:B:4459:VAL:HA	1:B:4570:LYS:O	2.22	0.40
1:A:4820:LEU:HD12	1:A:4820:LEU:N	2.36	0.40
1:B:4542:ILE:HG22	1:B:4545:LEU:H	1.87	0.40
1:B:4731:LYS:HA	1:B:4731:LYS:HD3	1.85	0.40
1:A:4377:TRP:HA	1:A:4383:MET:HA	2.03	0.40
1:A:4493:ARG:HB2	1:A:4493:ARG:NH1	2.37	0.40
1:A:4824:VAL:HA	1:A:4832:ASN:CG	2.42	0.40
1:B:4804:ARG:HA	1:B:4804:ARG:HD2	1.81	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	435/807 (54%)	406 (93%)	29 (7%)	0	100	100
1	B	437/807 (54%)	406 (93%)	31 (7%)	0	100	100
All	All	872/1614 (54%)	812 (93%)	60 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	395/719 (55%)	368 (93%)	27 (7%)	16 44
1	B	397/719 (55%)	373 (94%)	24 (6%)	19 49
All	All	792/1438 (55%)	741 (94%)	51 (6%)	21 47

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4380	ASP
1	A	4386	CYS
1	A	4387	LYS
1	A	4406	THR
1	A	4407	CYS
1	A	4428	CYS
1	A	4478	CYS
1	A	4482	ASP
1	A	4486	CYS
1	A	4536	ILE
1	A	4550	SER
1	A	4552	ASN
1	A	4564	ARG
1	A	4578	ASN
1	A	4579	THR
1	A	4595	CYS
1	A	4612	CYS
1	A	4709	CYS
1	A	4722	CYS
1	A	4729	THR
1	A	4734	SER
1	A	4738	ASN
1	A	4799	ILE
1	A	4814	VAL
1	A	4824	VAL
1	A	4835	VAL
1	A	4838	CYS

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Mol	Chain	Res	Type
1	B	4378	LEU
1	B	4407	CYS
1	B	4409	ASN
1	B	4422	CYS
1	B	4463	SER
1	B	4478	CYS
1	B	4505	HIS
1	B	4552	ASN
1	B	4582	ASP
1	B	4583	ASP
1	B	4603	LEU
1	B	4639	THR
1	B	4738	ASN
1	B	4765	THR
1	B	4768	CYS
1	B	4786	CYS
1	B	4791	CYS
1	B	4800	CYS
1	B	4818	THR
1	B	4831	CYS
1	B	4832	ASN
1	B	4836	CYS
1	B	4838	CYS
1	B	4840	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4512	GLN
1	A	4739	ASN
1	B	4425	HIS
1	B	4477	HIS
1	B	4510	GLN
1	B	4801	GLN
1	B	4825	ASN

5.3.3 RNA

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)

10 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	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.50	0	17,19,21	1.78	4 (23%)
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.96	1 (5%)
2	BMA	C	3	2	11,11,12	0.18	0	15,15,17	0.60	0
2	MAN	C	4	2	11,11,12	0.22	0	15,15,17	0.66	0
2	MAN	C	5	2	11,11,12	0.21	0	15,15,17	0.63	0
2	NAG	D	1	2,1	14,14,15	0.43	0	17,19,21	2.22	6 (35%)
2	NAG	D	2	2	14,14,15	0.82	1 (7%)	17,19,21	0.98	1 (5%)
2	BMA	D	3	2	11,11,12	0.21	0	15,15,17	0.59	0
2	MAN	D	4	2	11,11,12	0.20	0	15,15,17	0.61	0
2	MAN	D	5	2	11,11,12	0.22	0	15,15,17	0.57	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
2	NAG	C	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	5/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C1	2.72	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C3-C4-C5	4.33	117.97	110.24
2	D	1	NAG	C4-C3-C2	4.29	117.31	111.02
2	D	1	NAG	O5-C5-C6	3.93	113.37	107.20
2	D	2	NAG	C1-O5-C5	3.73	117.25	112.19
2	D	1	NAG	O5-C1-C2	3.52	116.85	111.29
2	D	1	NAG	C2-N2-C7	3.50	127.89	122.90
2	C	1	NAG	C1-O5-C5	-3.29	107.73	112.19
2	D	1	NAG	C1-O5-C5	3.04	116.31	112.19
2	C	1	NAG	C4-C3-C2	2.92	115.30	111.02
2	D	1	NAG	C3-C4-C5	2.36	114.46	110.24
2	C	2	NAG	O5-C5-C6	2.23	110.69	107.20
2	C	1	NAG	O5-C1-C2	-2.12	107.94	111.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	D	5	MAN	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

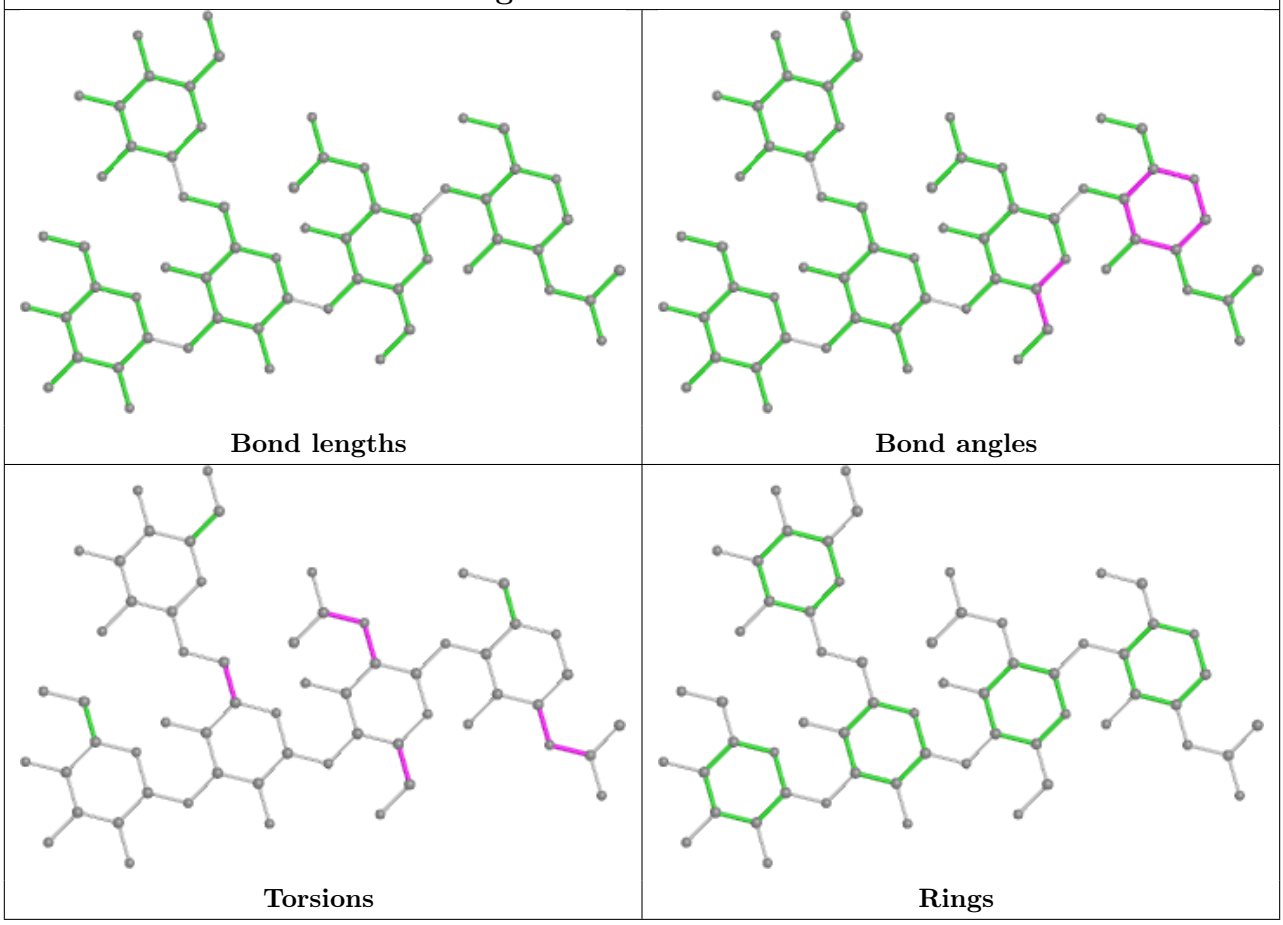
There are no ring outliers.

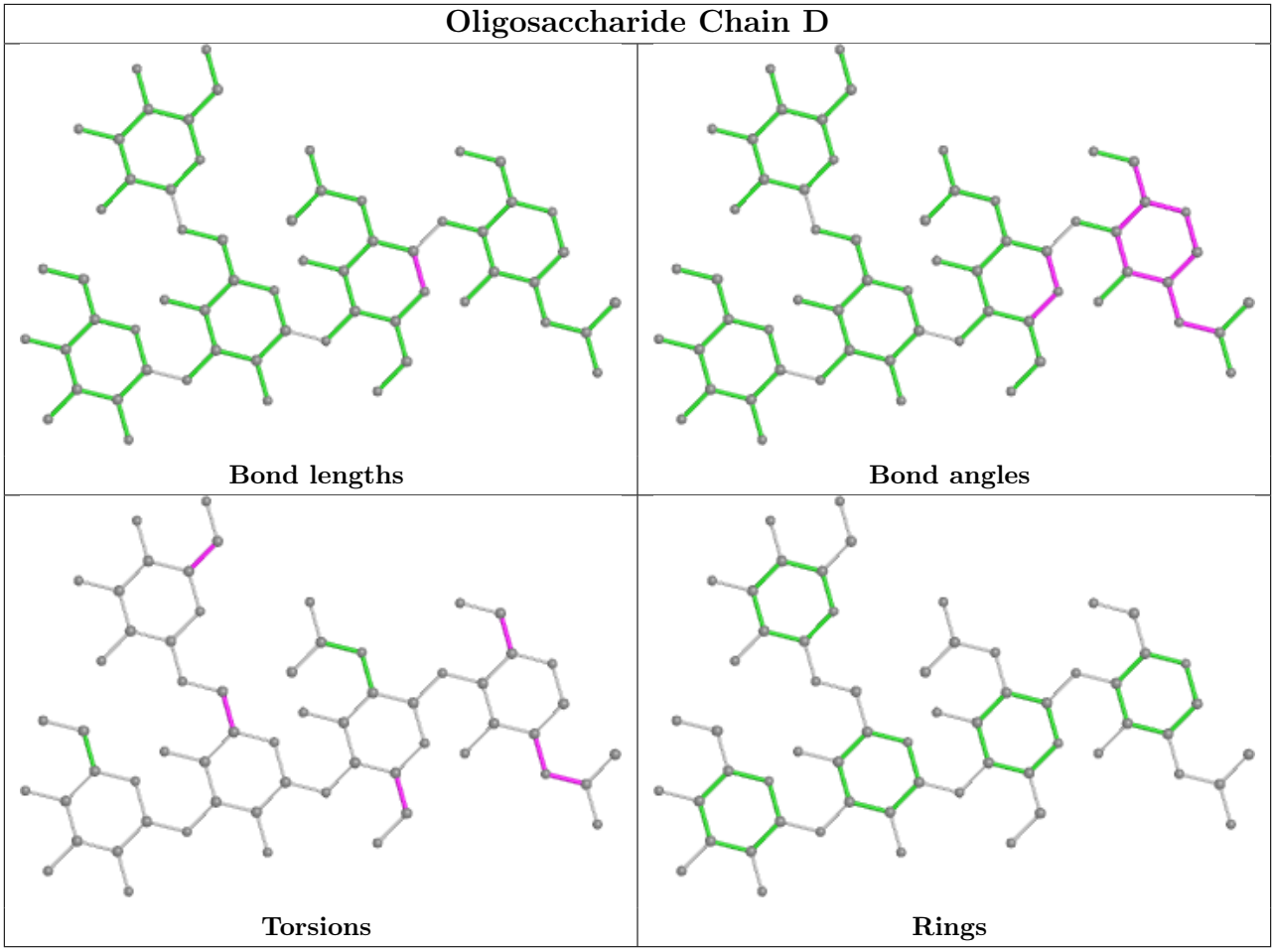
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	1	0
2	C	1	NAG	1	0
2	C	2	NAG	3	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.

Oligosaccharide Chain C





5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	5205	1	14,14,15	0.30	0	17,19,21	0.65	0
4	NAG	B	5202	1	14,14,15	0.30	0	17,19,21	0.72	0
4	NAG	B	5204	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	A	5204	1	14,14,15	0.32	0	17,19,21	0.79	1 (5%)
4	NAG	B	5203	1	14,14,15	0.30	0	17,19,21	0.59	0
4	NAG	A	5202	1	14,14,15	0.71	0	17,19,21	2.65	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	5205	1	14,14,15	0.30	0	17,19,21	0.74	0
4	NAG	A	5203	1	14,14,15	0.51	0	17,19,21	1.58	3 (17%)

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	A	5205	1	-	3/6/23/26	0/1/1/1
4	NAG	B	5202	1	-	2/6/23/26	0/1/1/1
4	NAG	B	5204	1	-	3/6/23/26	0/1/1/1
4	NAG	A	5204	1	-	2/6/23/26	0/1/1/1
4	NAG	B	5203	1	-	2/6/23/26	0/1/1/1
4	NAG	A	5202	1	-	4/6/23/26	0/1/1/1
4	NAG	B	5205	1	-	2/6/23/26	0/1/1/1
4	NAG	A	5203	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5202	NAG	C1-O5-C5	8.73	124.02	112.19
4	A	5202	NAG	O5-C5-C6	-5.03	99.32	107.20
4	A	5203	NAG	C1-C2-N2	3.88	117.12	110.49
4	A	5202	NAG	O5-C1-C2	-2.66	107.08	111.29
4	A	5203	NAG	O5-C5-C6	2.60	111.28	107.20
4	A	5203	NAG	C1-O5-C5	-2.43	108.90	112.19
4	A	5204	NAG	C4-C3-C2	-2.21	107.78	111.02

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5202	NAG	C8-C7-N2-C2
4	A	5202	NAG	O7-C7-N2-C2
4	A	5203	NAG	C8-C7-N2-C2
4	A	5203	NAG	O7-C7-N2-C2
4	A	5205	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	5205	NAG	O7-C7-N2-C2
4	B	5202	NAG	C8-C7-N2-C2
4	B	5202	NAG	O7-C7-N2-C2
4	B	5203	NAG	O7-C7-N2-C2
4	B	5204	NAG	C8-C7-N2-C2
4	B	5204	NAG	O7-C7-N2-C2
4	A	5203	NAG	C4-C5-C6-O6
4	B	5203	NAG	C8-C7-N2-C2
4	B	5205	NAG	C8-C7-N2-C2
4	B	5205	NAG	O7-C7-N2-C2
4	A	5203	NAG	O5-C5-C6-O6
4	A	5205	NAG	C1-C2-N2-C7
4	B	5204	NAG	C1-C2-N2-C7
4	A	5204	NAG	C8-C7-N2-C2
4	A	5202	NAG	O5-C5-C6-O6
4	A	5204	NAG	O7-C7-N2-C2
4	A	5202	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5205	NAG	4	0
4	B	5204	NAG	2	0
4	B	5203	NAG	1	0
4	A	5202	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.

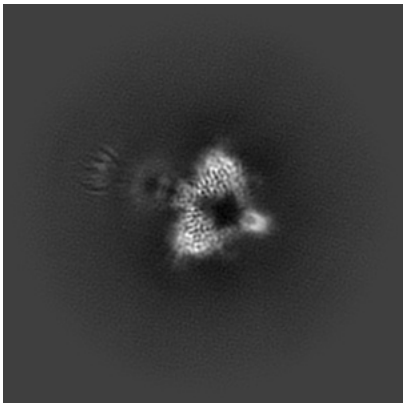
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13899. These allow visual inspection of the internal detail of the map and identification of artifacts.

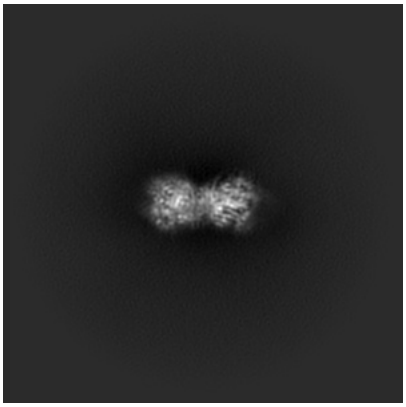
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

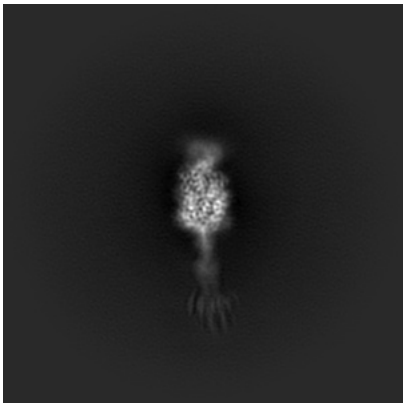
6.1.1 Primary map



X



Y

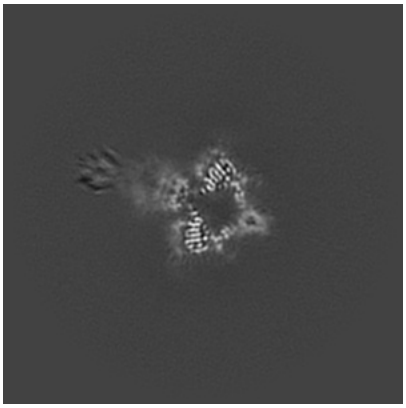


Z

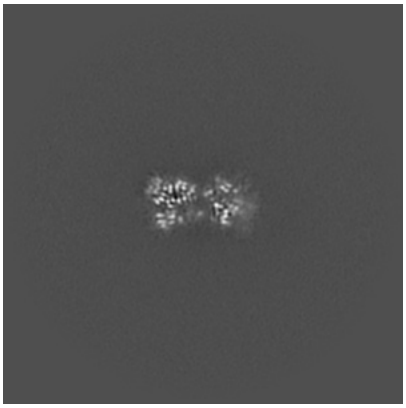
The images above show the map projected in three orthogonal directions.

6.2 Central slices

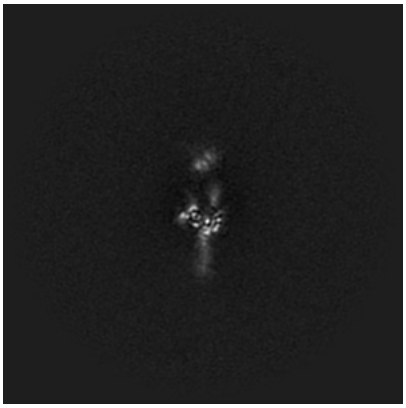
6.2.1 Primary map



X Index: 216



Y Index: 216

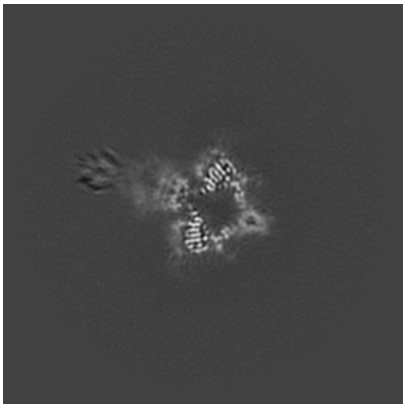


Z Index: 216

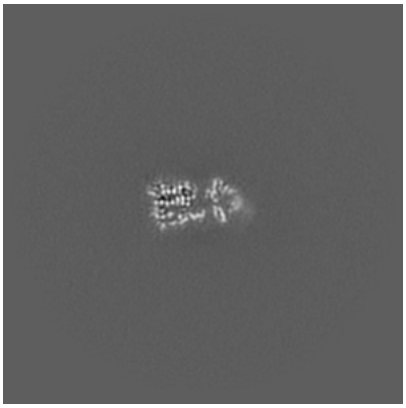
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

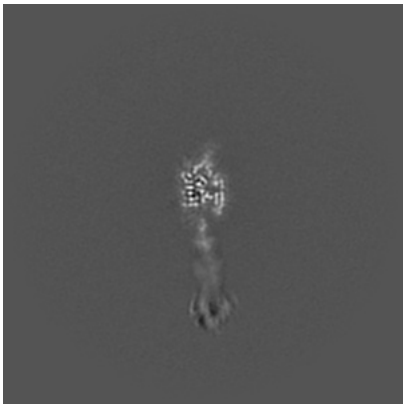
6.3.1 Primary map



X Index: 216



Y Index: 211

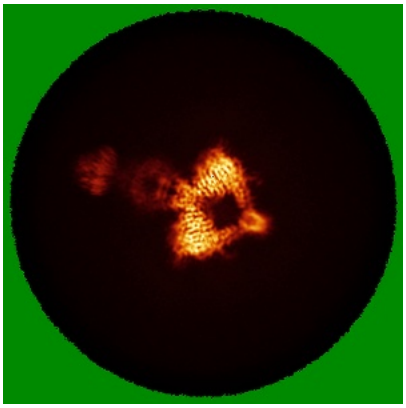


Z Index: 242

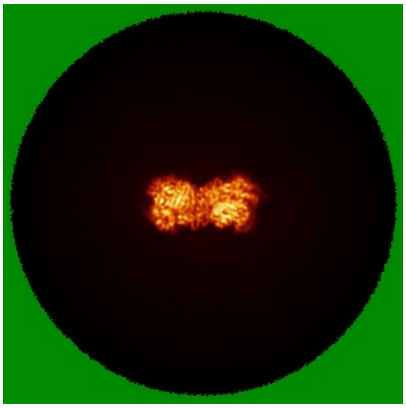
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

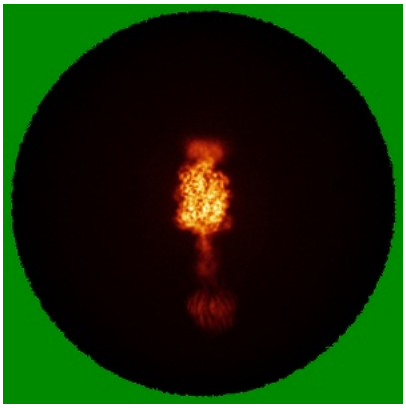
6.4.1 Primary map



X



Y

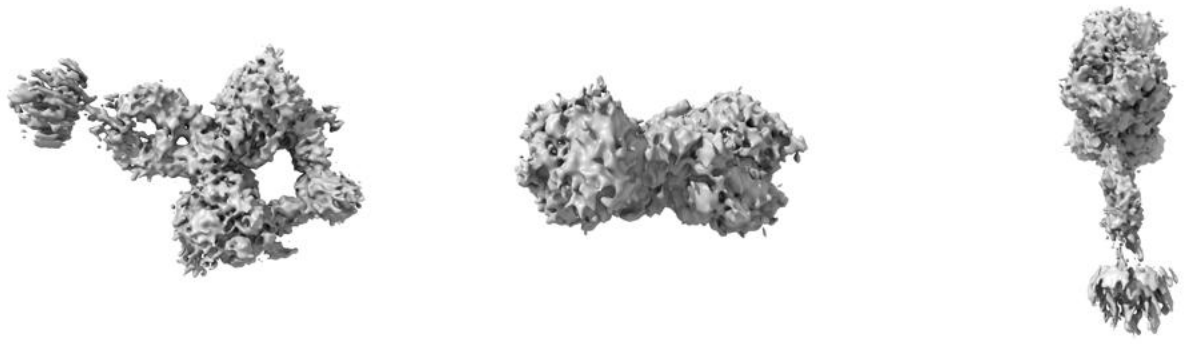


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

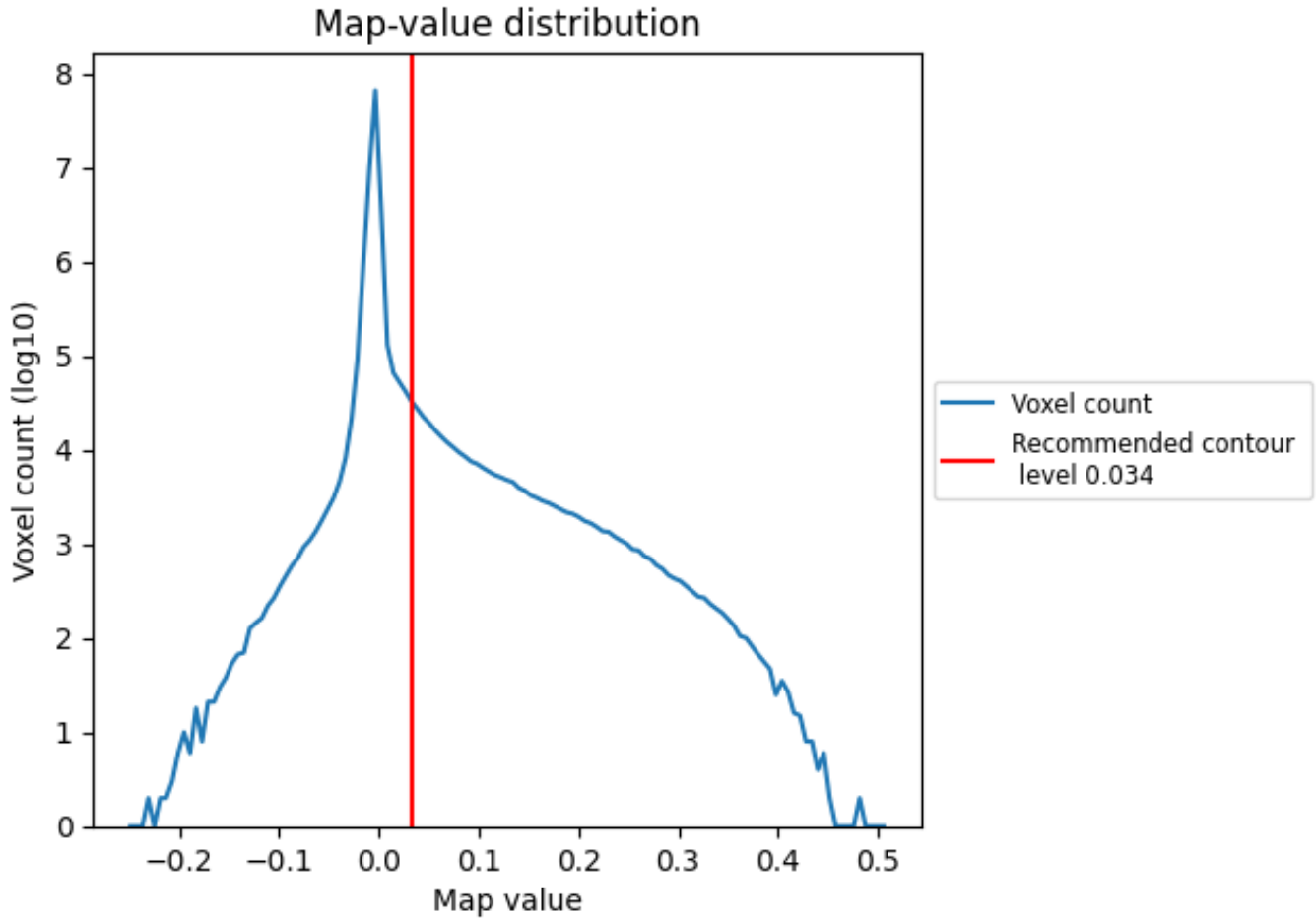
6.6 Mask visualisation (i)

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

7 Map analysis

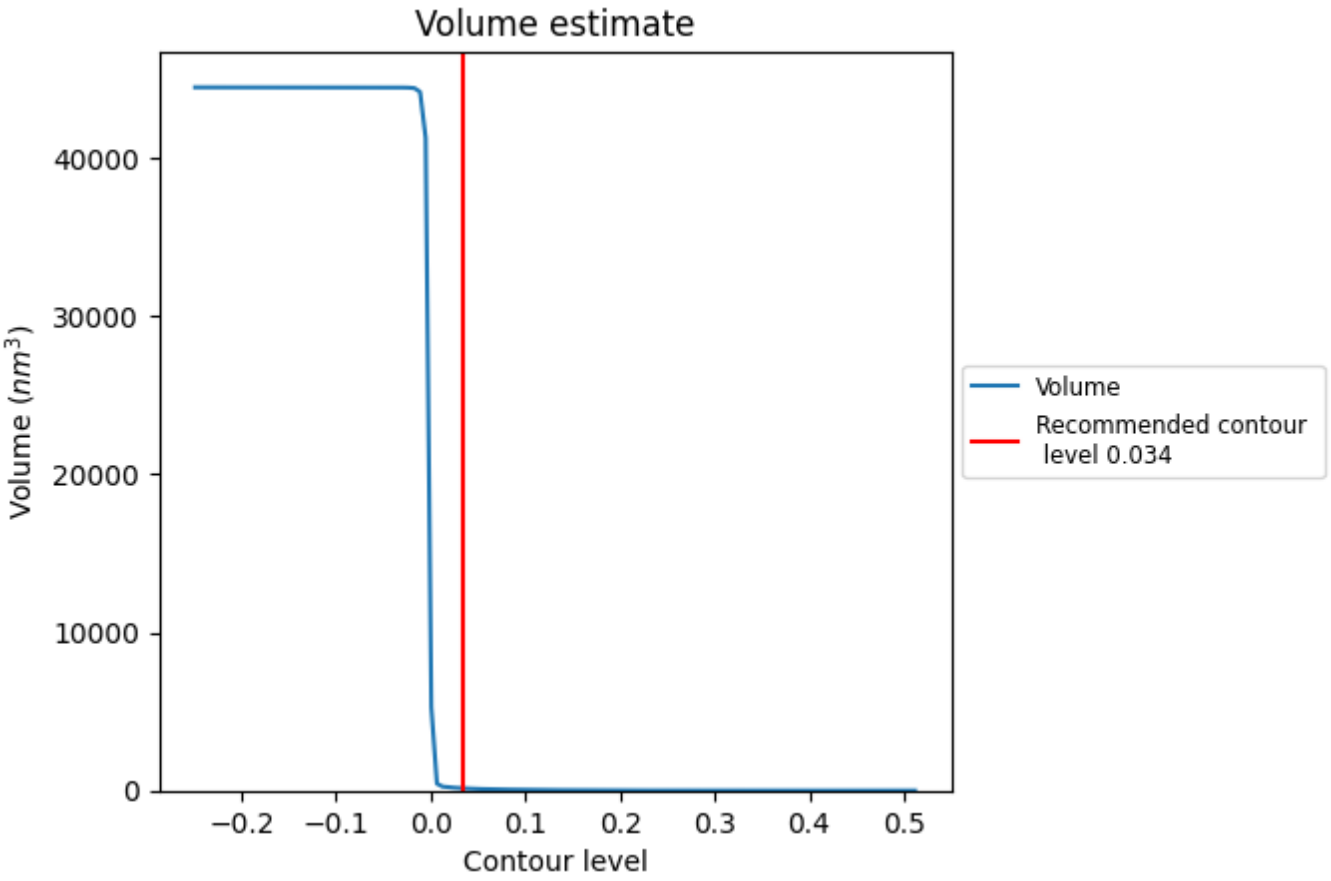
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

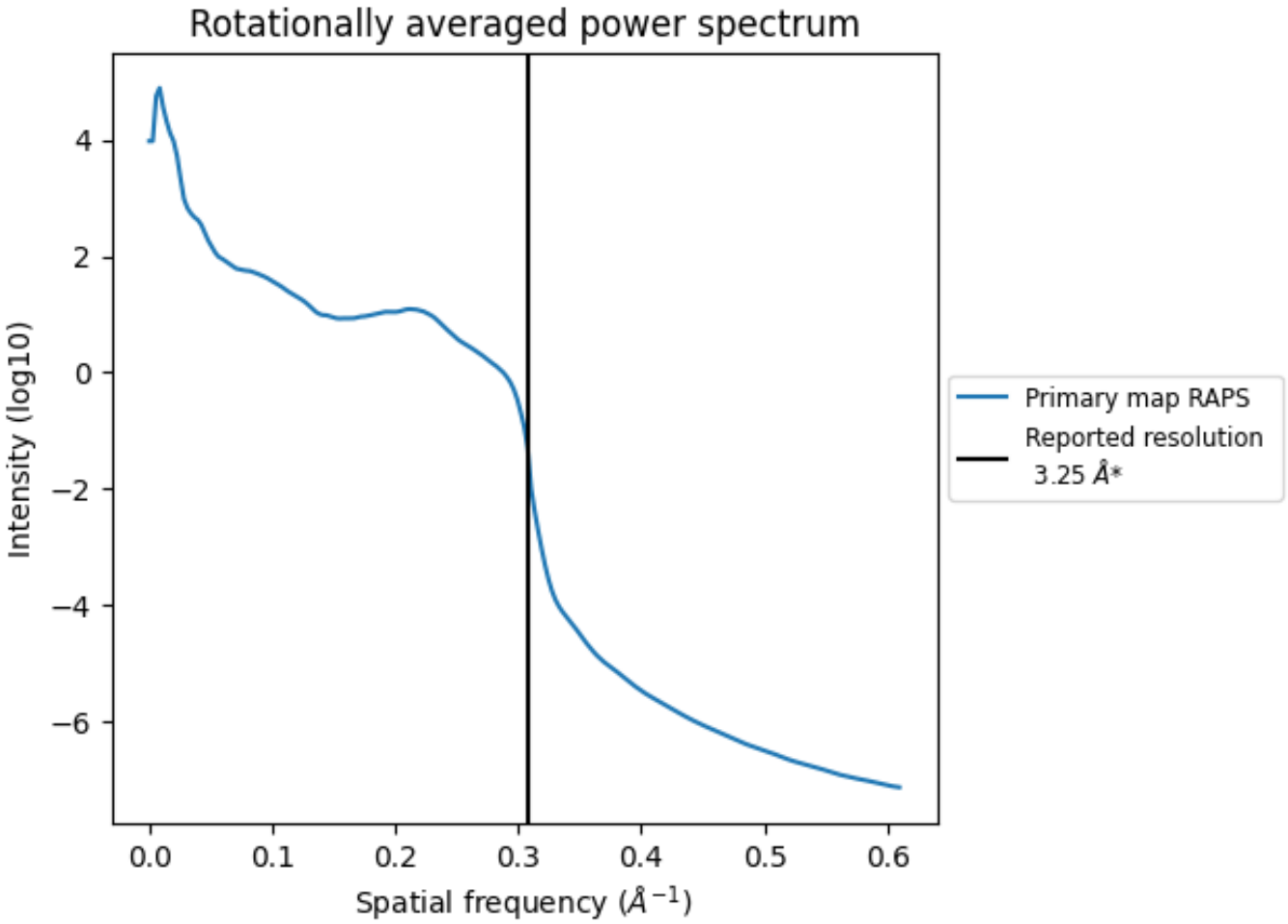
7.2 Volume estimate



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.308 Å^{-1}

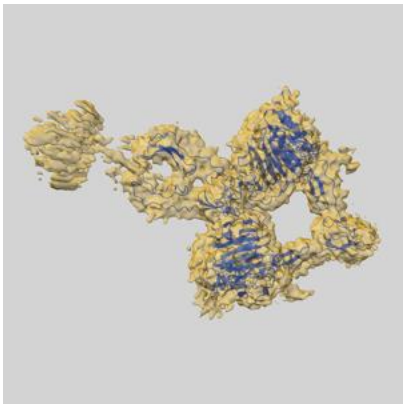
8 Fourier-Shell correlation (i)

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

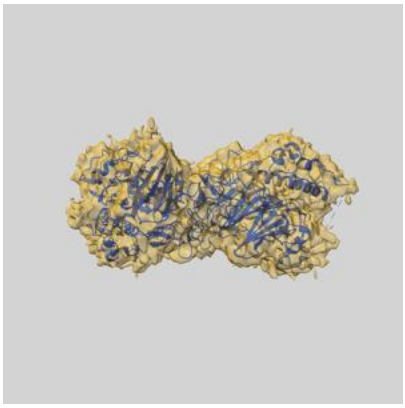
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13899 and PDB model 7QCU. Per-residue inclusion information can be found in section 3 on page 7.

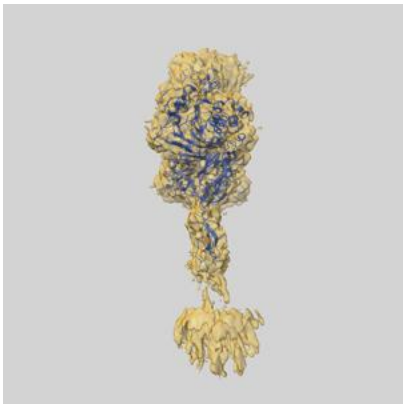
9.1 Map-model overlay



X



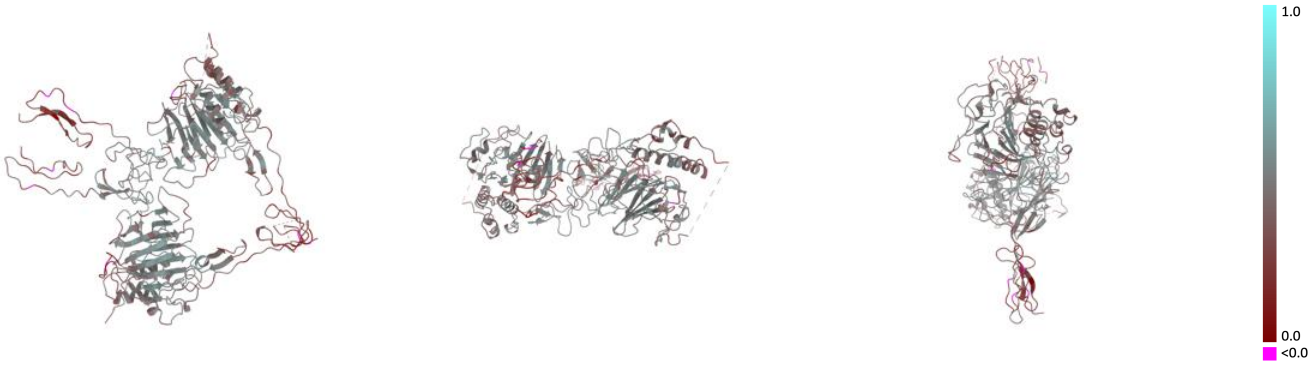
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.034 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.

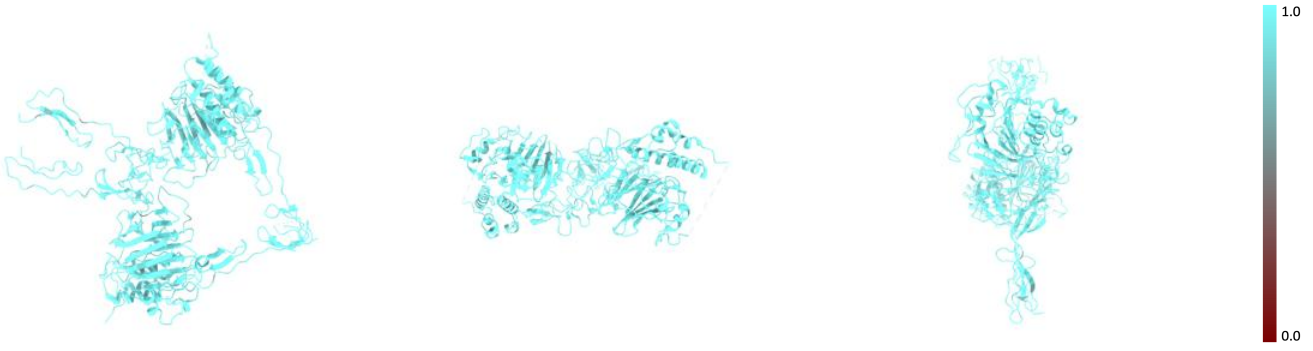
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

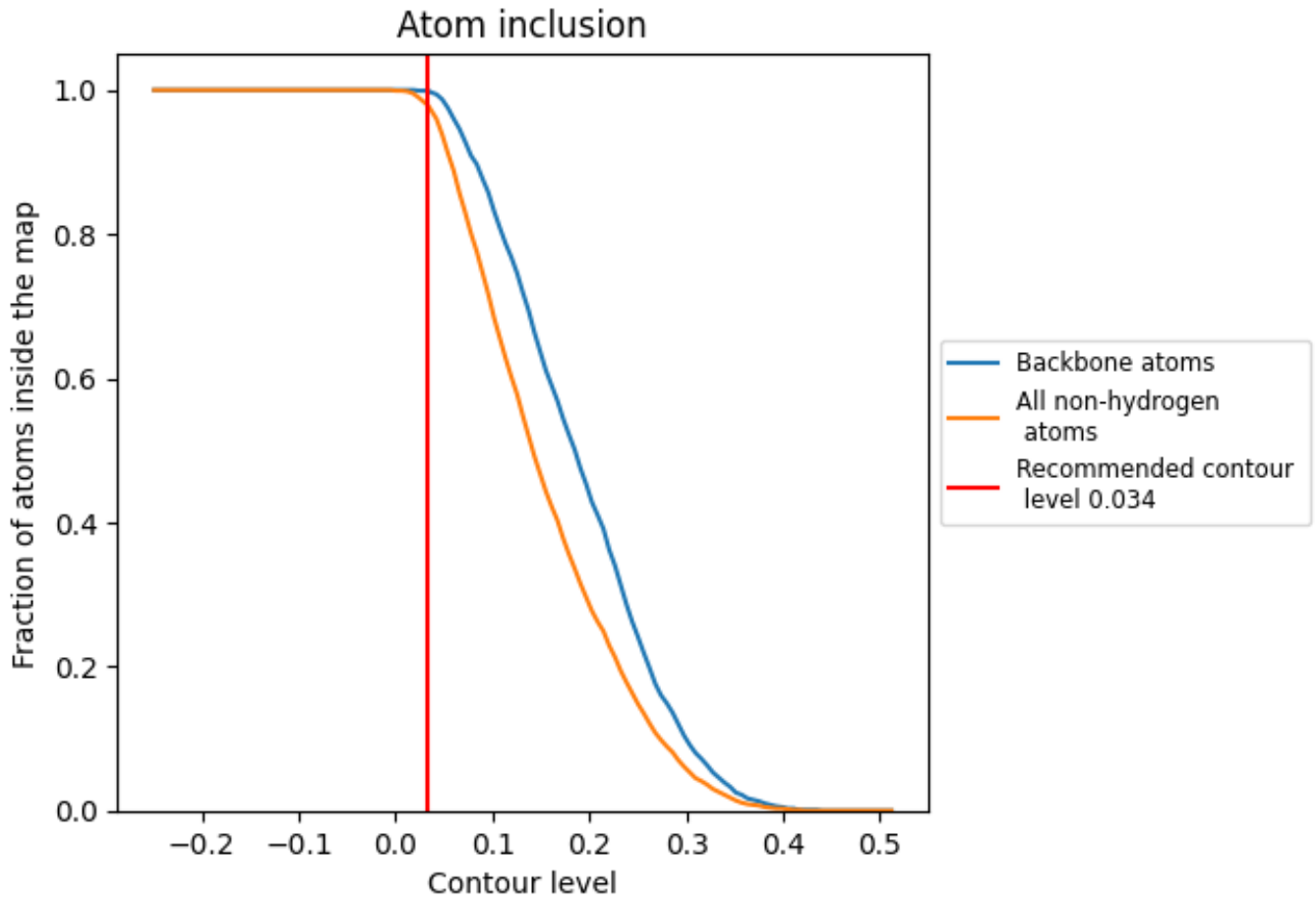
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.034).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9780	0.4040
A	0.9820	0.4060
B	0.9830	0.4060
C	0.7870	0.3060
D	0.6890	0.2180