Full wwPDB EM Validation Report ⓘ

Aug 15, 2026 – 02:58 PM EDT

PDB ID	:	9YB3 / pdb_00009yb3
EMDB ID	:	EMD-72747
Title	:	Localized reconstruction of the asymmetric unit of SINV/EEEV.
Authors	:	Bandyopadhyay, A.; Klose, T.; Kuhn, R.J.
Deposited on	:	2025-09-16
Resolution	:	3.60 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:

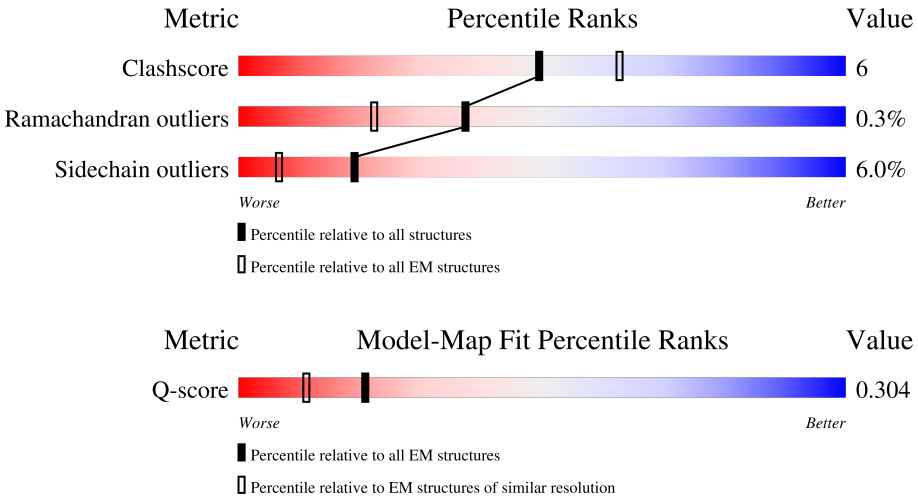
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.60 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	12797 (3.10 - 4.10)

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	441	84% 15%
1	B	441	82% 16%
1	C	441	87% 12%
1	D	441	84% 14%

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Mol	Chain	Length	Quality of chain
2	P	160	12% 82% 16%
2	Q	160	76% 21%
2	R	160	79% 18%
2	S	160	7% 77% 21%
3	a	418	82% 17%
3	d	418	82% 17%
4	b	419	79% 20%
4	c	419	84% 15%
5	E	3	33% 67% 33%
5	F	3	67% 33% 67%
5	G	3	67% 33% 67%
5	H	3	67% 33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	1	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31820 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called E1 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		
1	B	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		
1	C	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		
1	D	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		

- Molecule 2 is a protein called Capsid protein.

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

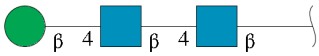
- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	418	Total	C	N	O	S	0	0
			3288	2080	596	588	24		
3	d	418	Total	C	N	O	S	0	0
			3288	2080	596	588	24		

- Molecule 4 is a protein called E2 glycoprotein.

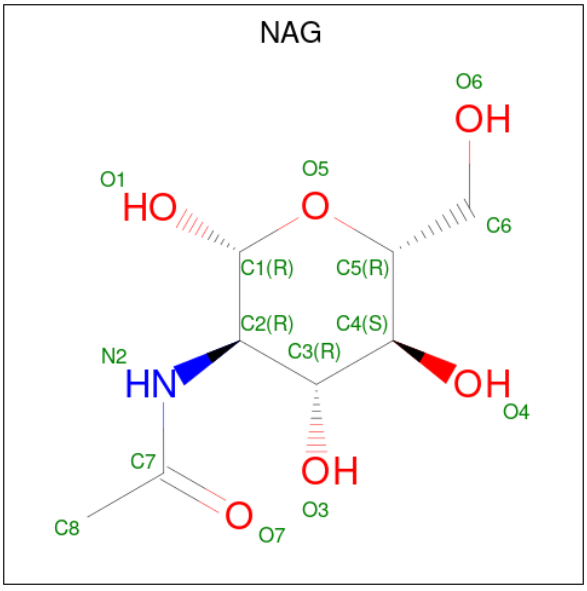
Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	419	Total	C	N	O	S	0	0
			3296	2084	597	591	24		
4	c	419	Total	C	N	O	S	0	0
			3296	2084	597	591	24		

- 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	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	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	G	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: $C_8H_{15}NO_6$).



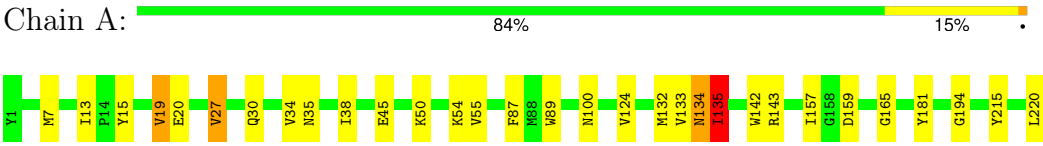
Mol	Chain	Residues	Atoms				AltConf
6	a	1	Total	C	N	O	0
			14	8	1	5	
6	b	1	Total	C	N	O	0
			14	8	1	5	
6	c	1	Total	C	N	O	0
			14	8	1	5	
6	d	1	Total	C	N	O	0
			14	8	1	5	

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.

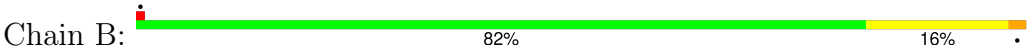
- Molecule 1: E1 glycoprotein

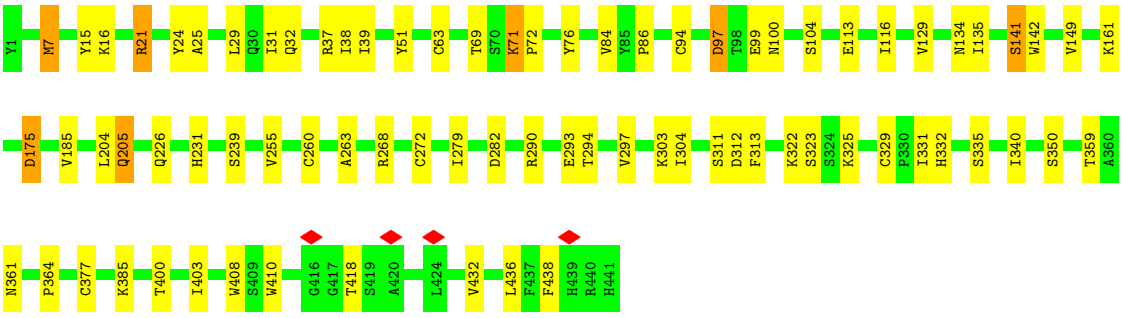
Chain A:



- Molecule 1: E1 glycoprotein

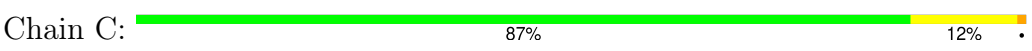
Chain B:

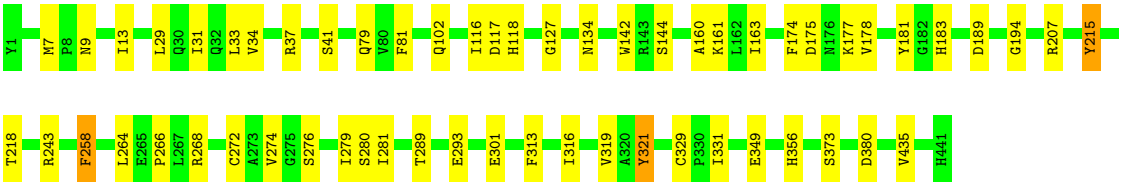




- Molecule 1: E1 glycoprotein

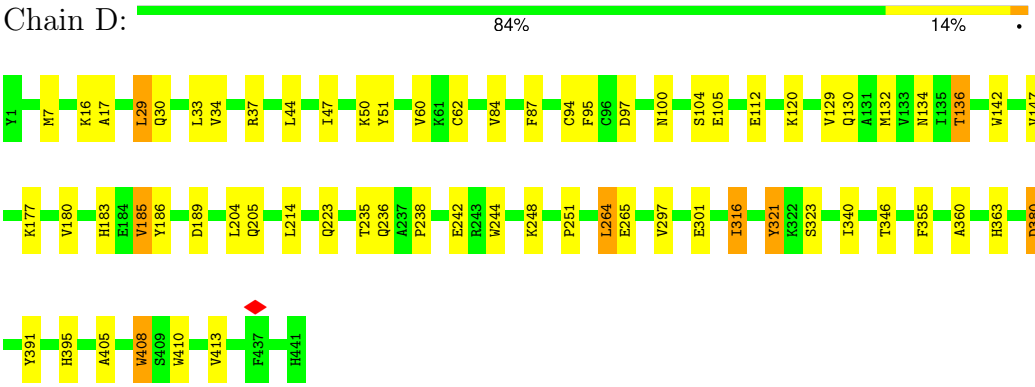
Chain C:





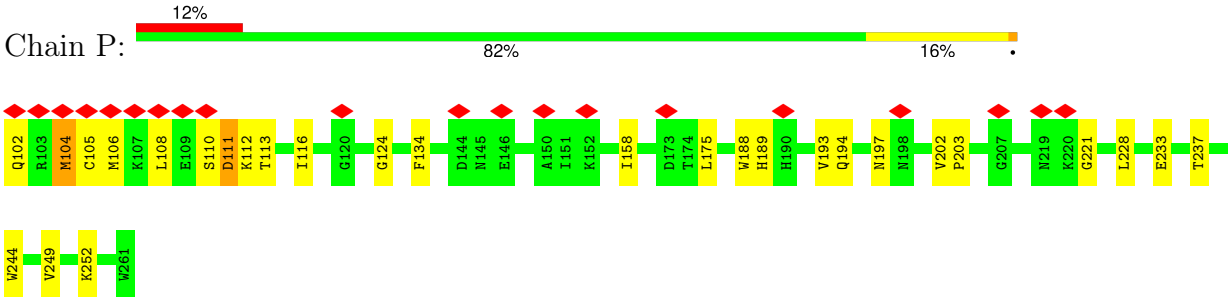
- Molecule 1: E1 glycoprotein

Chain D:



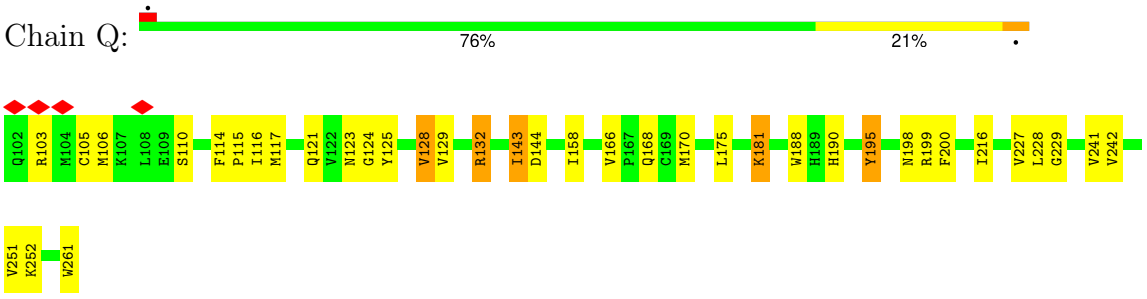
• Molecule 2: Capsid protein

Chain P:



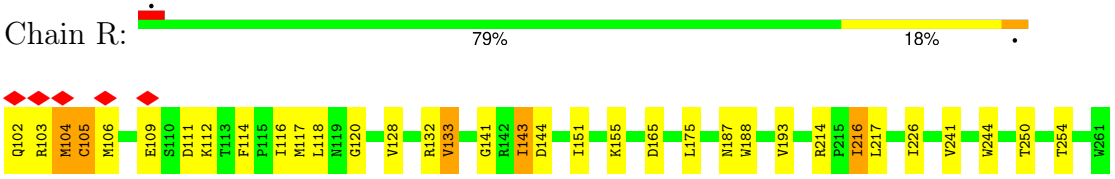
• Molecule 2: Capsid protein

Chain Q:



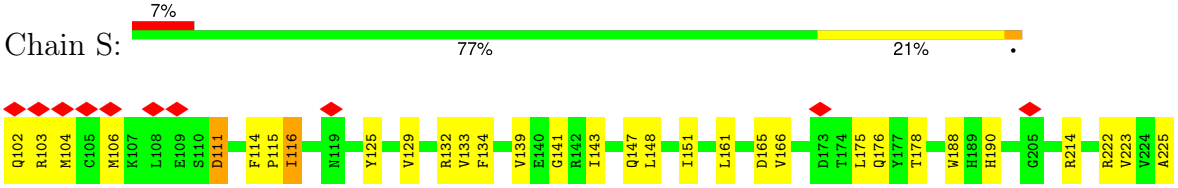
• Molecule 2: Capsid protein

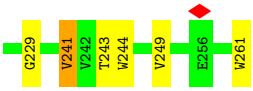
Chain R:



• Molecule 2: Capsid protein

Chain S:

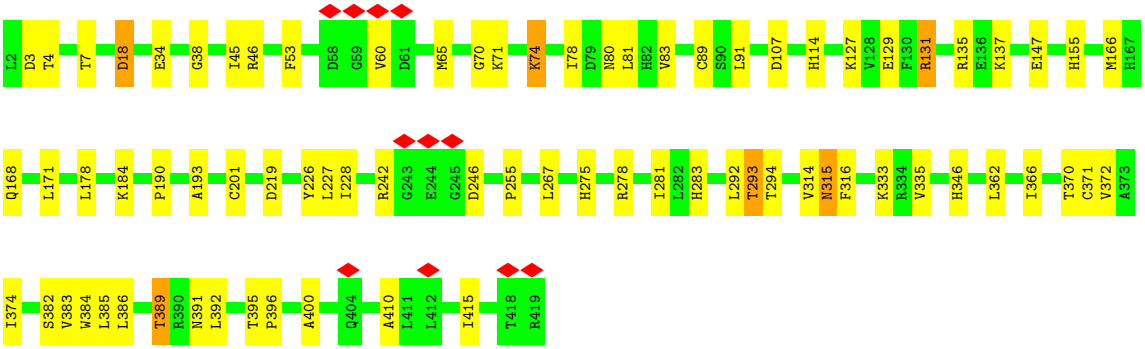




• Molecule 3: E2 glycoprotein

Chain a:

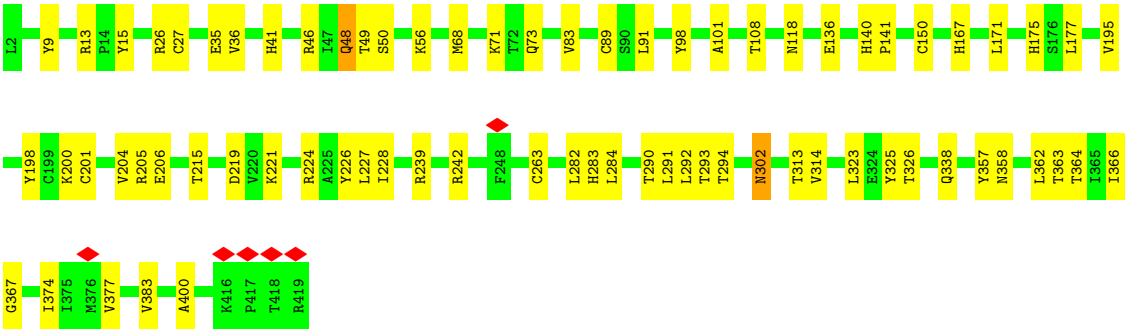




• Molecule 3: E2 glycoprotein

Chain d:

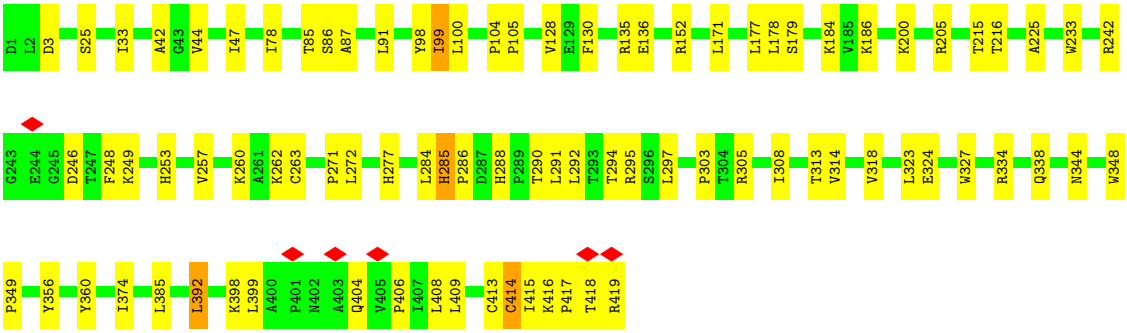




• Molecule 4: E2 glycoprotein

Chain b:





• Molecule 4: E2 glycoprotein

Chain c:





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

Chain F:





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

Chain E:





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

Chain H:





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

Chain G:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	820454	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 ($e^-/Å^2$)	31.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.723	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	291.84, 291.84, 291.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.79	1/3464 (0.0%)	1.28	3/4728 (0.1%)
1	B	0.82	3/3464 (0.1%)	1.28	6/4728 (0.1%)
1	C	0.74	1/3464 (0.0%)	1.24	3/4728 (0.1%)
1	D	0.82	1/3464 (0.0%)	1.18	7/4728 (0.1%)
2	P	0.88	0/1266	1.31	1/1711 (0.1%)
2	Q	0.79	0/1266	1.37	3/1711 (0.2%)
2	R	0.79	0/1266	1.33	5/1711 (0.3%)
2	S	0.80	0/1266	1.33	4/1711 (0.2%)
3	a	0.85	1/3383 (0.0%)	1.30	7/4613 (0.2%)
3	d	0.80	0/3383	1.29	5/4613 (0.1%)
4	b	0.86	2/3391 (0.1%)	1.29	7/4624 (0.2%)
4	c	0.84	1/3391 (0.0%)	1.28	10/4624 (0.2%)
All	All	0.81	10/32468 (0.0%)	1.28	61/44230 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	4
1	D	0	1
2	Q	0	2
2	R	0	1
2	S	0	1
3	a	0	5
3	d	0	4
4	b	0	4
4	c	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	30

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	ARG	CZ-NH2	-6.75	1.24	1.33
1	B	37	ARG	CZ-NH2	-5.82	1.25	1.33
1	B	400	THR	CB-OG1	-5.72	1.34	1.43
4	b	205	ARG	CZ-NH2	-5.68	1.26	1.33
3	a	333	LYS	CE-NZ	-5.55	1.32	1.49
4	c	37	ARG	CZ-NH2	-5.26	1.26	1.33
1	A	405	ALA	C-O	-5.24	1.17	1.24
1	D	346	THR	CB-OG1	-5.18	1.35	1.43
1	B	325	LYS	CE-NZ	-5.14	1.33	1.49
4	b	313	THR	CB-OG1	-5.04	1.35	1.43

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c	239	ARG	NE-CZ-NH2	6.80	125.32	119.20
2	S	111	ASP	CA-CB-CG	6.46	119.06	112.60
4	c	84	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	D	380	ASP	CA-CB-CG	5.98	118.58	112.60
2	Q	199	ARG	N-CA-C	5.95	118.13	108.26
4	b	242	ARG	NE-CZ-NH2	5.95	124.55	119.20
4	c	135	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	B	312	ASP	CA-CB-CG	5.86	118.46	112.60
2	P	134	PHE	CA-CB-CG	5.85	119.65	113.80
2	Q	181	LYS	CB-CA-C	5.82	118.20	110.81
1	C	380	ASP	CA-CB-CG	5.80	118.41	112.60
2	S	161	LEU	CA-C-N	5.80	131.18	123.00
2	S	161	LEU	C-N-CA	5.80	131.18	123.00
3	d	26	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	D	363	HIS	CB-CG-CD2	-5.75	123.73	131.20
1	C	329	CYS	N-CA-C	5.69	113.34	108.22
2	R	165	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	97	ASP	CA-CB-CG	5.63	118.23	112.60
4	c	242	ARG	NE-CZ-NH2	5.62	124.26	119.20
3	d	73	GLN	OE1-CD-NE2	-5.53	117.07	122.60
2	R	111	ASP	CA-CB-CG	5.51	118.11	112.60
2	S	134	PHE	CA-CB-CG	5.50	119.30	113.80
1	B	226	GLN	OE1-CD-NE2	-5.49	117.11	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	PHE	CA-CB-CG	-5.48	108.32	113.80
3	a	3	ASP	CA-CB-CG	5.47	118.07	112.60
3	a	137	LYS	CB-CG-CD	5.47	123.87	111.30
3	a	131	ARG	NE-CZ-NH2	5.42	124.08	119.20
4	c	329	ASN	OD1-CG-ND2	-5.41	117.19	122.60
4	c	391	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	175	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	97	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	246	ARG	NE-CZ-NH2	5.34	124.00	119.20
4	b	334	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	a	242	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	B	231	HIS	CB-CG-CD2	-5.32	124.28	131.20
2	R	214	ARG	NE-CZ-NH2	5.31	123.98	119.20
4	b	414	CYS	N-CA-C	5.30	115.85	108.00
4	b	277	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	C	258	PHE	CA-CB-CG	5.24	119.04	113.80
1	B	205	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	D	205	GLN	OE1-CD-NE2	-5.22	117.38	122.60
3	d	167	HIS	CB-CG-CD2	-5.22	124.41	131.20
3	d	338	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	D	383	PRO	N-CA-CB	5.20	106.10	103.19
4	c	222	GLN	OE1-CD-NE2	-5.20	117.40	122.60
3	a	391	ASN	OD1-CG-ND2	-5.17	117.43	122.60
3	d	48	GLN	OE1-CD-NE2	-5.15	117.45	122.60
4	b	398	LYS	CA-C-N	5.14	131.36	121.54
4	b	398	LYS	C-N-CA	5.14	131.36	121.54
1	A	268	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	D	316	ILE	CA-C-O	-5.12	116.15	120.96
4	c	359	ARG	CD-NE-CZ	5.12	131.56	124.40
4	c	277	HIS	CB-CG-CD2	-5.08	124.60	131.20
4	b	295	ARG	NE-CZ-NH2	5.07	123.76	119.20
3	a	346	HIS	CB-CG-CD2	-5.05	124.63	131.20
3	a	283	HIS	CB-CG-CD2	-5.03	124.66	131.20
2	R	254	THR	CA-C-N	5.03	124.94	119.76
2	R	254	THR	C-N-CA	5.03	124.94	119.76
1	D	387	HIS	N-CA-C	5.02	119.03	113.01
4	c	359	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	Q	199	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	TYR	Sidechain
1	A	440	ARG	Sidechain
1	B	141	SER	Mainchain
1	B	21	ARG	Sidechain
1	C	181	TYR	Sidechain
1	C	207	ARG	Sidechain
1	C	215	TYR	Sidechain
1	C	321	TYR	Sidechain
1	D	391	TYR	Sidechain
2	Q	132	ARG	Sidechain
2	Q	195	TYR	Sidechain
2	R	132	ARG	Sidechain
2	S	222	ARG	Sidechain
3	a	131	ARG	Sidechain
3	a	135	ARG	Sidechain
3	a	278	ARG	Sidechain
3	a	46	ARG	Sidechain
3	a	53	PHE	Sidechain
4	b	135	ARG	Sidechain
4	b	360	TYR	Sidechain
4	b	419	ARG	Sidechain
4	b	98	TYR	Sidechain
4	c	131	ARG	Sidechain
4	c	135	ARG	Sidechain
4	c	139	ARG	Sidechain
4	c	153	TYR	Sidechain
3	d	13	ARG	Sidechain
3	d	239	ARG	Sidechain
3	d	242	ARG	Sidechain
3	d	46	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3371	0	3275	64	0
1	B	3371	0	3273	40	0
1	C	3371	0	3275	33	0
1	D	3371	0	3275	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1239	0	1225	14	0
2	Q	1239	0	1225	23	0
2	R	1239	0	1225	17	0
2	S	1239	0	1225	20	0
3	a	3288	0	3248	41	0
3	d	3288	0	3247	33	0
4	b	3296	0	3255	45	0
4	c	3296	0	3255	26	0
5	E	39	0	34	2	0
5	F	39	0	34	3	0
5	G	39	0	34	13	0
5	H	39	0	34	6	0
6	a	14	0	13	1	0
6	b	14	0	13	0	0
6	c	14	0	13	3	0
6	d	14	0	13	0	0
All	All	31820	0	31191	358	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 6.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:VAL:CG2	1:A:436:LEU:HD23	1.29	1.59
1:A:432:VAL:CG2	1:A:436:LEU:CD2	2.03	1.35
1:D:134:ASN:ND2	5:H:1:NAG:C1	1.92	1.32
1:A:432:VAL:HG23	1:A:436:LEU:CD2	1.69	1.20
1:A:432:VAL:HG22	1:A:436:LEU:CD2	1.64	1.15
1:D:134:ASN:HD21	5:H:1:NAG:C1	1.57	1.15
1:C:134:ASN:ND2	5:G:1:NAG:N2	2.00	1.09
1:A:432:VAL:HG23	1:A:436:LEU:HD23	1.33	1.02
1:C:134:ASN:ND2	5:G:1:NAG:C1	2.26	0.99
1:A:432:VAL:HG23	1:A:436:LEU:HD21	1.44	0.97
1:D:142:TRP:CZ2	5:H:2:NAG:H82	1.99	0.96
1:C:134:ASN:ND2	5:G:1:NAG:C7	2.32	0.92
1:C:134:ASN:HD21	5:G:1:NAG:C1	1.83	0.91
1:A:432:VAL:HG22	1:A:436:LEU:HD23	0.91	0.91
3:d:357:TYR:HA	3:d:364:THR:HG21	1.55	0.87
1:D:134:ASN:HD22	5:H:1:NAG:C1	1.86	0.86
1:A:436:LEU:HD13	1:A:440:ARG:NH2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:117:MET:HG2	2:R:144:ASP:HB2	1.63	0.78
2:S:114:PHE:HB2	2:S:143:ILE:HD11	1.64	0.78
1:A:429:THR:HG23	3:a:385:LEU:HD13	1.65	0.77
1:A:435:VAL:HA	1:A:439:HIS:HB2	1.64	0.77
1:D:405:ALA:HA	1:D:408:TRP:HB2	1.67	0.77
2:Q:216:ILE:HD11	2:Q:227:VAL:HG23	1.66	0.77
1:A:432:VAL:HG22	1:A:436:LEU:CG	2.14	0.77
1:C:134:ASN:ND2	5:G:1:NAG:C2	2.50	0.75
2:R:117:MET:CG	2:R:144:ASP:HB2	2.17	0.75
1:C:116:ILE:HD11	4:c:260:LYS:HB2	1.69	0.74
3:d:83:VAL:HG13	3:d:89:CYS:HB2	1.67	0.74
1:C:134:ASN:HD21	5:G:1:NAG:C2	2.01	0.73
2:R:118:LEU:HD13	2:R:141:GLY:HA2	1.70	0.72
1:A:425:GLY:HA2	3:a:385:LEU:HD11	1.72	0.71
1:A:432:VAL:CG1	1:A:433:ALA:N	2.54	0.71
1:B:141:SER:HB2	1:B:142:TRP:CD1	2.27	0.70
1:C:144:SER:CB	5:G:1:NAG:H82	2.21	0.70
1:C:144:SER:HB2	5:G:1:NAG:H82	1.75	0.69
3:d:302:ASN:HD22	3:d:302:ASN:C	2.01	0.68
1:A:432:VAL:HG13	1:A:433:ALA:N	2.08	0.68
4:c:196:LYS:HB3	4:c:228:ILE:HD11	1.75	0.68
1:A:432:VAL:CB	1:A:436:LEU:HD23	2.21	0.67
3:a:281:ILE:HD12	6:a:501:NAG:H81	1.76	0.66
1:D:37:ARG:HH22	1:D:132:MET:H	1.42	0.66
3:d:302:ASN:O	3:d:302:ASN:ND2	2.20	0.66
1:D:360:ALA:HB2	1:D:395:HIS:CD2	2.30	0.66
1:A:142:TRP:CD1	5:E:1:NAG:HO6	2.14	0.66
1:B:141:SER:HB2	1:B:142:TRP:HD1	1.59	0.65
1:D:223:GLN:HE22	1:D:235:THR:HG22	1.61	0.65
2:R:112:LYS:HD3	2:R:175:LEU:HD13	1.78	0.64
1:C:134:ASN:HD22	5:G:1:NAG:C7	2.12	0.63
4:b:286:PRO:HG3	4:b:308:ILE:HG22	1.80	0.63
1:A:440:ARG:HG2	2:P:249:VAL:HG11	1.78	0.62
3:a:83:VAL:HG13	3:a:89:CYS:HB2	1.81	0.62
3:d:68:MET:HE1	3:d:71:LYS:C	2.24	0.62
1:D:142:TRP:HZ2	5:H:2:NAG:H82	1.59	0.62
4:b:406:PRO:HB2	4:b:416:LYS:HD3	1.82	0.61
1:D:142:TRP:CE2	5:H:2:NAG:H82	2.36	0.60
4:b:87:ALA:HB3	4:b:104:PRO:HG3	1.83	0.60
3:d:294:THR:HG22	3:d:325:TYR:HB2	1.84	0.60
4:b:408:LEU:HB3	4:b:413:CYS:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TRP:CH2	3:a:70:GLY:HA2	2.37	0.59
2:Q:128:VAL:HG23	2:Q:166:VAL:HG21	1.83	0.59
1:D:183:HIS:HA	1:D:264:LEU:HD21	1.83	0.59
4:c:315:ASN:HB2	6:c:501:NAG:H82	1.84	0.59
1:A:432:VAL:HB	3:a:389:THR:HG22	1.84	0.59
1:A:436:LEU:HG	3:a:392:LEU:HB3	1.85	0.59
2:P:110:SER:O	2:P:111:ASP:C	2.46	0.58
4:c:315:ASN:H	6:c:501:NAG:H82	1.67	0.58
1:D:147:VAL:HG21	1:D:164:ILE:HG13	1.85	0.58
4:b:271:PRO:HB3	4:b:284:LEU:HD13	1.84	0.58
3:a:171:LEU:HD11	3:a:226:TYR:HB3	1.85	0.58
1:C:34:VAL:CG2	5:G:1:NAG:O7	2.52	0.58
1:A:436:LEU:HA	1:A:440:ARG:HH21	1.69	0.58
1:B:116:ILE:HD11	4:b:260:LYS:HB2	1.86	0.58
1:B:142:TRP:CD1	5:F:2:NAG:HO6	2.22	0.58
2:Q:115:PRO:HB2	2:Q:117:MET:HE1	1.86	0.58
2:R:117:MET:HG3	2:R:144:ASP:CG	2.28	0.57
3:a:168:GLN:H	3:a:168:GLN:CD	2.13	0.57
1:A:132:MET:HA	1:A:132:MET:HE2	1.86	0.57
1:A:437:PHE:O	1:A:441:HIS:N	2.37	0.57
2:S:151:ILE:HD12	2:S:151:ILE:H	1.69	0.57
2:Q:116:ILE:C	2:Q:117:MET:HE2	2.30	0.57
2:S:114:PHE:HB2	2:S:143:ILE:CD1	2.33	0.57
1:B:142:TRP:O	1:B:142:TRP:CE3	2.59	0.56
1:C:183:HIS:HA	1:C:264:LEU:HD11	1.86	0.56
2:S:115:PRO:HB3	2:S:125:TYR:CE2	2.41	0.56
4:b:91:LEU:HD11	4:b:99:ILE:HD11	1.88	0.56
4:c:373:ALA:O	4:c:377:VAL:HG13	2.06	0.56
1:A:437:PHE:CZ	2:P:158:ILE:HG12	2.41	0.55
1:A:134:ASN:O	1:A:135:ILE:HG23	2.07	0.55
1:B:113:GLU:CD	1:B:113:GLU:H	2.14	0.55
2:R:114:PHE:HB3	2:R:143:ILE:HD11	1.88	0.55
3:a:80:ASN:HD21	3:a:114:HIS:CE1	2.24	0.54
4:b:136:GLU:HB3	4:b:290:THR:HG22	1.88	0.54
4:c:366:ILE:O	4:c:370:THR:HG23	2.08	0.54
1:B:141:SER:CB	1:B:142:TRP:CD1	2.91	0.54
3:d:302:ASN:C	3:d:302:ASN:ND2	2.63	0.54
1:B:129:VAL:HG13	1:B:149:VAL:HB	1.90	0.54
1:B:410:TRP:CH2	4:b:349:PRO:HG3	2.42	0.54
4:b:404:GLN:HG2	4:b:416:LYS:C	2.32	0.54
4:c:98:TYR:CD2	4:c:255:PRO:HD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:PHE:O	1:A:438:PHE:C	2.50	0.54
1:A:388:ILE:HD13	3:a:335:VAL:HG13	1.90	0.54
1:D:37:ARG:NH1	1:D:130:GLN:HG3	2.23	0.54
1:A:89:TRP:CZ3	3:a:70:GLY:HA2	2.43	0.54
1:D:37:ARG:HH11	1:D:130:GLN:HG3	1.71	0.53
1:A:425:GLY:CA	3:a:385:LEU:HD11	2.38	0.53
1:D:244:TRP:CE3	1:D:248:LYS:HE2	2.43	0.53
4:c:142:PRO:HB3	4:c:266:THR:HG22	1.91	0.53
1:C:29:LEU:CD1	1:C:281:ILE:HG21	2.39	0.53
2:Q:117:MET:HE3	2:Q:144:ASP:HB2	1.91	0.52
2:R:120:GLY:HA3	2:S:147:GLN:HB3	1.92	0.52
1:A:362:ILE:HD12	1:A:362:ILE:H	1.75	0.52
1:A:414:LEU:HD21	3:a:371:CYS:HB2	1.92	0.52
4:b:262:LYS:HE3	4:b:262:LYS:HA	1.92	0.52
4:b:414:CYS:SG	4:b:415:ILE:N	2.83	0.52
4:c:39:ASP:HA	4:c:131:ARG:HH22	1.73	0.52
1:B:7:MET:HB3	1:B:279:ILE:HD11	1.91	0.52
1:D:95:PHE:HB2	3:d:224:ARG:HE	1.74	0.52
1:B:142:TRP:HB2	5:F:1:NAG:H61	1.91	0.52
1:A:435:VAL:O	1:A:436:LEU:C	2.53	0.52
1:A:432:VAL:CA	1:A:436:LEU:HD23	2.40	0.52
3:a:366:ILE:O	3:a:370:THR:HG22	2.08	0.52
6:c:501:NAG:H3	6:c:501:NAG:H83	1.92	0.52
3:d:283:HIS:ND1	3:d:313:THR:HG22	2.25	0.51
1:B:84:VAL:HG23	1:B:86:PRO:HD3	1.92	0.51
1:C:7:MET:HE3	1:C:279:ILE:HD11	1.93	0.51
1:B:418:THR:HG21	4:b:374:ILE:HD12	1.92	0.51
3:a:410:ALA:HA	3:a:415:ILE:HG23	1.92	0.51
4:b:284:LEU:HD12	4:b:327:TRP:CZ2	2.45	0.51
1:A:19:VAL:HB	1:A:27:VAL:HG12	1.92	0.51
1:D:297:VAL:HA	1:D:323:SER:HA	1.93	0.51
1:A:432:VAL:CG1	1:A:433:ALA:H	2.22	0.51
4:b:406:PRO:HB3	4:b:416:LYS:HB2	1.93	0.50
2:P:112:LYS:HD3	2:P:175:LEU:HG	1.93	0.50
2:S:190:HIS:CD2	2:S:214:ARG:HH12	2.30	0.50
3:d:219:ASP:OD1	3:d:221:LYS:HE2	2.11	0.50
1:C:142:TRP:CH2	5:G:2:NAG:H81	2.47	0.50
1:A:165:GLY:HA3	1:A:278:PRO:HG2	1.94	0.49
2:Q:228:LEU:HD11	2:Q:242:VAL:HG13	1.92	0.49
1:C:349:GLU:OE1	1:C:349:GLU:HA	2.11	0.49
2:P:249:VAL:HG13	3:a:396:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:404:GLN:HB3	4:b:417:PRO:O	2.12	0.49
1:A:436:LEU:O	1:A:440:ARG:HB2	2.13	0.49
2:S:129:VAL:HG12	2:S:175:LEU:HB2	1.94	0.49
4:b:291:LEU:HD21	4:b:305:ARG:HD2	1.94	0.49
1:A:388:ILE:HD11	3:a:275:HIS:CE1	2.48	0.49
2:Q:181:LYS:HE2	2:Q:200:PHE:CE1	2.47	0.48
3:a:382:SER:O	3:a:385:LEU:HG	2.13	0.48
4:b:288:HIS:O	4:b:290:THR:HG23	2.13	0.48
1:A:229:ILE:HD11	3:a:18:ASP:HB2	1.95	0.48
1:A:432:VAL:CB	3:a:389:THR:HG22	2.43	0.48
1:B:15:TYR:CD1	1:B:31:ILE:HG22	2.48	0.48
1:D:37:ARG:HH22	1:D:132:MET:N	2.08	0.48
3:a:315:ASN:HD22	3:a:315:ASN:H	1.62	0.48
1:B:311:SER:H	4:b:338:GLN:HE22	1.60	0.48
4:b:178:LEU:HD11	4:b:225:ALA:HB3	1.95	0.48
3:a:38:GLY:HA2	3:a:45:ILE:HG22	1.96	0.48
1:A:432:VAL:O	1:A:433:ALA:C	2.55	0.48
1:D:204:LEU:CD1	1:D:214:LEU:HD11	2.43	0.48
1:B:322:LYS:HA	1:B:350:SER:HA	1.96	0.48
1:D:410:TRP:HA	1:D:413:VAL:HG12	1.95	0.48
2:S:188:TRP:CZ2	2:S:190:HIS:HB2	2.48	0.48
1:A:405:ALA:HA	1:A:408:TRP:HB3	1.95	0.48
4:c:284:LEU:HD12	4:c:327:TRP:CZ2	2.50	0.47
3:d:201:CYS:SG	3:d:205:ARG:NH2	2.87	0.47
4:c:147:GLU:OE2	4:c:262:LYS:HE3	2.15	0.47
1:B:263:ALA:HB3	1:B:268:ARG:HG3	1.94	0.47
4:b:184:LYS:HD2	4:b:216:THR:HA	1.96	0.47
1:A:436:LEU:HD13	1:A:440:ARG:HH22	1.78	0.47
2:P:116:ILE:HG22	2:P:124:GLY:C	2.38	0.47
4:b:44:VAL:HG22	4:b:100:LEU:HD11	1.96	0.47
4:b:179:SER:O	4:b:186:LYS:N	2.41	0.47
4:c:125:ALA:HB2	3:d:140:HIS:HD2	1.78	0.47
4:c:194:GLN:HB3	4:c:228:ILE:HB	1.96	0.47
3:d:198:TYR:HA	3:d:206:GLU:OE1	2.15	0.47
1:A:388:ILE:C	1:A:388:ILE:HD12	2.39	0.47
2:R:216:ILE:HD12	2:R:217:LEU:H	1.79	0.47
3:d:366:ILE:HD12	3:d:367:GLY:N	2.30	0.47
1:C:316:ILE:HD12	1:C:356:HIS:ND1	2.30	0.47
4:c:381:THR:O	4:c:385:LEU:HD23	2.14	0.47
1:C:289:THR:OG1	1:C:293:GLU:OE1	2.21	0.47
1:A:437:PHE:CE1	2:P:158:ILE:HG12	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:102:GLN:O	2:P:106:MET:HG2	2.16	0.46
2:S:143:ILE:HG12	2:S:148:LEU:HB2	1.97	0.46
3:a:4:THR:HA	3:a:7:THR:HG23	1.97	0.46
3:a:395:THR:OG1	3:a:396:PRO:HD3	2.14	0.46
1:A:432:VAL:HG12	1:A:433:ALA:H	1.80	0.46
3:a:370:THR:O	3:a:374:ILE:HG22	2.16	0.46
4:b:85:THR:HG23	4:b:86:SER:H	1.81	0.46
3:a:292:LEU:HD21	3:a:316:PHE:HZ	1.81	0.46
4:c:199:CYS:HB3	4:c:205:ARG:HB2	1.98	0.46
4:b:297:LEU:HD21	4:b:324:GLU:HB2	1.98	0.46
4:c:87:ALA:HB3	4:c:104:PRO:HG3	1.97	0.46
3:d:91:LEU:HD12	3:d:91:LEU:H	1.80	0.46
1:A:367:LYS:HA	1:A:376:THR:HG22	1.96	0.46
1:B:255:VAL:HG23	4:b:303:PRO:HG3	1.98	0.46
1:D:186:TYR:CD1	1:D:251:PRO:HA	2.51	0.46
4:c:281:ILE:HD13	4:c:281:ILE:HA	1.78	0.46
1:B:263:ALA:HB3	1:B:268:ARG:CG	2.46	0.46
2:Q:106:MET:O	2:Q:110:SER:N	2.49	0.46
1:B:32:GLN:O	1:B:134:ASN:N	2.49	0.45
1:D:186:TYR:CZ	1:D:248:LYS:HD2	2.51	0.45
2:Q:114:PHE:HB3	2:Q:143:ILE:CD1	2.47	0.45
2:R:250:THR:HG21	4:c:399:LEU:HD11	1.98	0.45
1:C:142:TRP:CZ2	5:G:2:NAG:C8	2.99	0.45
3:a:107:ASP:HA	3:a:127:LYS:HA	1.99	0.45
1:B:25:ALA:HB2	1:B:294:THR:HG21	1.98	0.45
3:d:282:LEU:HB3	3:d:284:LEU:CD1	2.47	0.45
2:S:132:ARG:HE	2:S:165:ASP:HA	1.81	0.45
3:d:136:GLU:HB3	3:d:290:THR:HG22	1.99	0.45
1:A:437:PHE:O	1:A:440:ARG:N	2.50	0.45
3:a:65:MET:HE3	3:a:78:ILE:HG12	1.99	0.45
3:d:140:HIS:CG	3:d:141:PRO:HD2	2.51	0.45
1:D:321:TYR:HE1	1:D:323:SER:HB2	1.81	0.44
2:Q:158:ILE:HG12	4:b:392:LEU:HD22	1.99	0.44
4:b:233:TRP:CH2	4:b:248:PHE:CZ	3.05	0.44
1:B:359:THR:HG22	1:B:361:ASN:N	2.31	0.44
2:Q:195:TYR:CZ	2:Q:198:ASN:HA	2.52	0.44
1:A:34:VAL:HB	1:A:132:MET:HG3	2.00	0.44
1:A:432:VAL:O	1:A:436:LEU:N	2.50	0.44
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.88	0.44
1:B:71:LYS:HB3	1:B:76:TYR:CE2	2.53	0.44
3:a:71:LYS:H	3:a:71:LYS:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:371:CYS:SG	3:a:372:VAL:N	2.91	0.44
1:D:47:ILE:HG22	1:D:120:LYS:HA	1.99	0.44
2:Q:116:ILE:HG22	2:Q:124:GLY:C	2.43	0.44
1:A:35:ASN:H	1:A:132:MET:HB3	1.82	0.44
1:C:13:ILE:HD12	1:C:13:ILE:O	2.18	0.44
1:D:238:PRO:HD2	4:b:285:HIS:HB3	2.00	0.44
3:a:190:PRO:HG2	3:a:193:ALA:HB3	2.00	0.44
4:c:187:ILE:HG22	4:c:213:HIS:O	2.18	0.44
4:c:262:LYS:HE3	4:c:262:LYS:HA	1.99	0.44
2:S:176:GLN:O	2:S:223:VAL:HG12	2.18	0.44
4:b:406:PRO:CB	4:b:416:LYS:HB2	2.48	0.44
4:b:409:LEU:H	4:b:416:LYS:HE2	1.82	0.44
3:d:293:THR:OG1	3:d:326:THR:OG1	2.07	0.44
3:d:294:THR:HB	3:d:323:LEU:HD11	1.99	0.44
1:C:163:ILE:HB	1:C:280:SER:HB2	2.00	0.44
2:Q:114:PHE:HB3	2:Q:143:ILE:HD11	2.00	0.44
2:S:102:GLN:O	2:S:106:MET:HG2	2.18	0.43
2:S:116:ILE:HD12	2:S:141:GLY:HA3	2.00	0.43
4:b:344:ASN:OD1	4:b:344:ASN:C	2.60	0.43
1:B:304:ILE:HD11	1:B:377:CYS:HB3	1.99	0.43
4:c:147:GLU:HG3	4:c:262:LYS:HE2	1.99	0.43
1:A:134:ASN:C	1:A:135:ILE:HG23	2.43	0.43
1:B:359:THR:HG21	1:B:364:PRO:HB3	2.00	0.43
4:b:33:ILE:HD12	4:b:33:ILE:H	1.82	0.43
4:b:404:GLN:HG2	4:b:416:LYS:CA	2.48	0.43
1:D:17:ALA:HB3	1:D:29:LEU:HD21	2.00	0.43
2:S:244:TRP:CD1	3:d:400:ALA:HB2	2.53	0.43
4:b:284:LEU:HD12	4:b:327:TRP:CH2	2.54	0.43
4:b:294:THR:HB	4:b:323:LEU:HD11	2.00	0.43
2:Q:188:TRP:CH2	2:Q:190:HIS:HB2	2.53	0.43
1:C:194:GLY:HA2	1:C:215:TYR:CG	2.53	0.43
2:Q:117:MET:HE2	2:Q:117:MET:N	2.34	0.43
2:R:105:CYS:SG	2:R:106:MET:N	2.91	0.43
1:C:160:ALA:C	1:C:161:LYS:HE2	2.44	0.43
1:D:316:ILE:HD12	1:D:355:PHE:O	2.19	0.43
2:P:110:SER:O	2:P:113:THR:N	2.48	0.43
2:S:116:ILE:HD12	2:S:141:GLY:CA	2.49	0.43
4:b:404:GLN:HG2	4:b:416:LYS:HA	2.01	0.43
3:d:195:VAL:HG12	3:d:227:LEU:HA	2.01	0.43
3:d:362:LEU:HD12	3:d:363:THR:N	2.34	0.43
1:A:7:MET:HE3	1:A:15:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:O	1:A:135:ILE:HA	2.19	0.43
1:C:33:LEU:H	1:C:33:LEU:HD12	1.84	0.43
3:a:383:VAL:HA	3:a:386:LEU:HD12	1.99	0.43
4:b:233:TRP:CH2	4:b:248:PHE:CE2	3.07	0.43
4:c:114:HIS:CG	4:c:119:ARG:HH11	2.37	0.43
1:B:290:ARG:HB3	1:B:293:GLU:HG2	2.00	0.43
1:C:41:SER:H	1:C:127:GLY:CA	2.32	0.43
1:D:30:GLN:N	1:D:136:THR:O	2.52	0.42
2:P:108:LEU:HD22	2:P:221:GLY:HA3	2.01	0.42
1:C:174:PHE:HB3	1:C:178:VAL:HG11	2.01	0.42
2:Q:115:PRO:HA	2:Q:125:TYR:HA	2.00	0.42
4:b:42:ALA:HB3	4:b:152:ARG:HH12	1.84	0.42
1:C:79:GLN:HG2	1:C:81:PHE:CZ	2.55	0.42
1:D:180:VAL:HG13	1:D:185:VAL:HG12	2.02	0.42
1:D:223:GLN:NE2	1:D:235:THR:HG22	2.30	0.42
4:b:105:PRO:HG3	4:b:130:PHE:HB2	2.00	0.42
3:d:291:LEU:HD12	3:d:292:LEU:N	2.35	0.42
3:d:171:LEU:HA	3:d:228:ILE:HG22	2.01	0.42
1:A:436:LEU:CD1	1:A:440:ARG:NH2	2.77	0.42
2:S:116:ILE:HD11	2:S:139:VAL:HG22	2.01	0.42
3:a:281:ILE:HG22	3:a:315:ASN:HA	2.01	0.42
4:b:284:LEU:HD12	4:b:327:TRP:CE2	2.54	0.42
1:A:409:SER:HA	1:A:412:LYS:HE3	2.02	0.42
1:B:403:ILE:HG21	1:B:408:TRP:CD2	2.54	0.42
1:D:129:VAL:HG11	1:D:167:LEU:HD21	2.01	0.42
1:A:13:ILE:HD12	1:A:394:GLN:HA	2.01	0.42
1:B:304:ILE:HD12	1:B:304:ILE:N	2.34	0.42
2:Q:175:LEU:HD12	2:Q:175:LEU:H	1.83	0.42
3:a:83:VAL:HG12	3:a:91:LEU:CD2	2.49	0.42
4:b:292:LEU:HD21	4:b:314:VAL:HG21	2.01	0.42
1:A:133:VAL:HG22	1:A:135:ILE:HG23	2.00	0.42
1:A:254:ASP:HB3	3:a:293:THR:HG21	2.02	0.42
1:D:16:LYS:HE3	1:D:340:ILE:O	2.20	0.42
2:R:117:MET:HG3	2:R:144:ASP:CB	2.49	0.42
4:c:201:CYS:SG	4:c:205:ARG:NH2	2.92	0.42
3:d:200:LYS:HZ1	3:d:204:VAL:N	2.18	0.42
1:B:21:ARG:HD3	1:B:24:TYR:CE1	2.54	0.42
2:Q:116:ILE:HG23	2:Q:123:ASN:HB3	2.02	0.42
2:R:128:VAL:HG22	2:R:133:VAL:CG1	2.50	0.42
1:B:71:LYS:HG2	1:B:72:PRO:HD2	2.02	0.42
1:B:297:VAL:HA	1:B:323:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:HIS:HA	1:B:340:ILE:HD11	2.02	0.42
2:P:104:MET:SD	2:P:104:MET:N	2.92	0.42
2:S:188:TRP:CH2	2:S:190:HIS:HB2	2.55	0.42
2:P:202:VAL:HG22	2:P:203:PRO:HD2	2.02	0.41
2:Q:229:GLY:HA2	2:Q:261:TRP:CG	2.55	0.41
4:b:413:CYS:O	4:b:414:CYS:SG	2.75	0.41
2:P:244:TRP:CD1	3:a:400:ALA:HB2	2.56	0.41
2:Q:103:ARG:HD3	2:Q:103:ARG:N	2.35	0.41
2:R:102:GLN:O	2:R:106:MET:HG2	2.21	0.41
2:S:229:GLY:HA2	2:S:261:TRP:CG	2.55	0.41
1:A:429:THR:O	1:A:432:VAL:HG12	2.20	0.41
1:B:32:GLN:HG2	5:F:1:NAG:H82	2.01	0.41
1:B:161:LYS:HB3	1:B:282:ASP:HB3	2.02	0.41
2:R:105:CYS:O	2:R:109:GLU:HG3	2.21	0.41
2:S:225:ALA:HB1	2:S:241:VAL:HG12	2.02	0.41
4:b:47:ILE:HB	4:b:99:ILE:HG23	2.02	0.41
3:d:294:THR:HG22	3:d:325:TYR:CB	2.48	0.41
1:C:41:SER:H	1:C:127:GLY:HA3	1.86	0.41
2:P:188:TRP:CG	2:P:189:HIS:N	2.88	0.41
3:d:83:VAL:HG11	3:d:101:ALA:CB	2.51	0.41
1:B:38:ILE:N	1:B:38:ILE:HD12	2.36	0.41
1:C:9:ASN:H	1:C:276:SER:HA	1.86	0.41
1:C:142:TRP:CZ2	5:G:2:NAG:H82	2.55	0.41
1:C:266:PRO:HD2	1:C:268:ARG:NH2	2.36	0.41
2:S:148:LEU:HA	2:S:151:ILE:CD1	2.51	0.41
2:Q:105:CYS:SG	2:Q:106:MET:N	2.94	0.41
4:c:377:VAL:HA	4:c:380:VAL:HG22	2.02	0.41
3:d:91:LEU:HD12	3:d:91:LEU:N	2.35	0.41
3:d:374:ILE:HA	3:d:377:VAL:HG12	2.02	0.41
1:A:20:GLU:O	1:B:385:LYS:NZ	2.54	0.41
1:A:134:ASN:ND2	5:E:1:NAG:C1	2.84	0.41
1:D:51:TYR:CE1	1:D:236:GLN:NE2	2.89	0.41
2:R:104:MET:SD	2:R:104:MET:N	2.81	0.41
3:d:15:TYR:CE2	3:d:50:SER:HB3	2.55	0.41
1:B:260:CYS:HB3	1:B:272:CYS:HA	2.03	0.41
2:R:128:VAL:HG22	2:R:133:VAL:HG13	2.03	0.41
1:A:135:ILE:HG12	1:A:157:ILE:HG12	2.03	0.40
3:a:74:LYS:HE3	3:a:74:LYS:N	2.36	0.40
3:a:315:ASN:H	3:a:315:ASN:ND2	2.17	0.40
4:b:348:TRP:HB3	4:b:349:PRO:HD2	2.02	0.40
3:d:48:GLN:HB2	3:d:98:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLU:CD	1:C:293:GLU:C	2.89	0.40
4:c:174:ASP:OD1	4:c:176:SER:N	2.54	0.40
1:A:194:GLY:HA2	1:A:215:TYR:CD1	2.56	0.40
1:B:51:TYR:CE2	1:B:239:SER:HB2	2.55	0.40
2:Q:242:VAL:HG12	2:Q:252:LYS:HG3	2.03	0.40
3:a:168:GLN:CD	3:a:168:GLN:N	2.79	0.40
1:B:359:THR:HG22	1:B:361:ASN:H	1.86	0.40
2:Q:103:ARG:HD3	2:Q:103:ARG:H	1.85	0.40
2:R:244:TRP:CH2	4:c:400:ALA:HA	2.56	0.40
3:d:41:HIS:HB2	3:d:150:CYS:HB2	2.03	0.40
1:C:177:LYS:HE2	1:C:189:ASP:OD1	2.21	0.40
1:D:177:LYS:HE3	1:D:189:ASP:HA	2.02	0.40
3:a:382:SER:O	3:a:386:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/441 (100%)	398 (91%)	39 (9%)	2 (0%)	24	57
1	B	439/441 (100%)	406 (92%)	32 (7%)	1 (0%)	43	72
1	C	439/441 (100%)	406 (92%)	31 (7%)	2 (0%)	24	57
1	D	439/441 (100%)	403 (92%)	36 (8%)	0	100	100
2	P	158/160 (99%)	152 (96%)	5 (3%)	1 (1%)	21	54
2	Q	158/160 (99%)	148 (94%)	10 (6%)	0	100	100
2	R	158/160 (99%)	143 (90%)	15 (10%)	0	100	100
2	S	158/160 (99%)	147 (93%)	11 (7%)	0	100	100
3	a	416/418 (100%)	384 (92%)	28 (7%)	4 (1%)	12	45
3	d	416/418 (100%)	387 (93%)	29 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	b	417/419 (100%)	377 (90%)	37 (9%)	3 (1%)	18 51
4	c	417/419 (100%)	382 (92%)	35 (8%)	0	100 100
All	All	4054/4078 (99%)	3733 (92%)	308 (8%)	13 (0%)	37 65

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ILE
1	B	97	ASP
2	P	111	ASP
1	C	218	THR
1	A	134	ASN
3	a	255	PRO
1	C	313	PHE
3	a	60	VAL
3	a	201	CYS
3	a	362	LEU
4	b	25	SER
4	b	399	LEU
4	b	78	ILE

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	370/370 (100%)	343 (93%)	27 (7%)	13 40
1	B	370/370 (100%)	347 (94%)	23 (6%)	16 44
1	C	370/370 (100%)	355 (96%)	15 (4%)	27 53
1	D	370/370 (100%)	346 (94%)	24 (6%)	15 43
2	P	134/134 (100%)	125 (93%)	9 (7%)	15 42
2	Q	134/134 (100%)	125 (93%)	9 (7%)	15 42
2	R	134/134 (100%)	120 (90%)	14 (10%)	7 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S	134/134 (100%)	124 (92%)	10 (8%)	12 39
3	a	366/366 (100%)	345 (94%)	21 (6%)	18 46
3	d	366/366 (100%)	349 (95%)	17 (5%)	24 51
4	b	367/367 (100%)	348 (95%)	19 (5%)	21 48
4	c	367/367 (100%)	347 (95%)	20 (5%)	20 47
All	All	3482/3482 (100%)	3274 (94%)	208 (6%)	19 45

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	27	VAL
1	A	38	ILE
1	A	45	GLU
1	A	50	LYS
1	A	54	LYS
1	A	55	VAL
1	A	87	PHE
1	A	100	ASN
1	A	124	VAL
1	A	135	ILE
1	A	143	ARG
1	A	159	ASP
1	A	220	LEU
1	A	226	GLN
1	A	232	THR
1	A	272	CYS
1	A	283	ILE
1	A	332	HIS
1	A	349	GLU
1	A	359	THR
1	A	373	SER
1	A	391	TYR
1	A	403	ILE
1	A	410	TRP
1	A	421	PHE
1	A	434	LEU
1	B	7	MET
1	B	16	LYS
1	B	29	LEU

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Mol	Chain	Res	Type
1	B	63	CYS
1	B	69	THR
1	B	71	LYS
1	B	94	CYS
1	B	99	GLU
1	B	100	ASN
1	B	104	SER
1	B	135	ILE
1	B	175	ASP
1	B	185	VAL
1	B	204	LEU
1	B	205	GLN
1	B	303	LYS
1	B	313	PHE
1	B	329	CYS
1	B	331	ILE
1	B	335	SER
1	B	432	VAL
1	B	436	LEU
1	B	438	PHE
1	C	31	ILE
1	C	102	GLN
1	C	117	ASP
1	C	118	HIS
1	C	175	ASP
1	C	243	ARG
1	C	258	PHE
1	C	272	CYS
1	C	274	VAL
1	C	301	GLU
1	C	319	VAL
1	C	321	TYR
1	C	331	ILE
1	C	373	SER
1	C	435	VAL
1	D	7	MET
1	D	29	LEU
1	D	33	LEU
1	D	34	VAL
1	D	44	LEU
1	D	50	LYS
1	D	60	VAL

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Mol	Chain	Res	Type
1	D	62	CYS
1	D	84	VAL
1	D	87	PHE
1	D	94	CYS
1	D	100	ASN
1	D	104	SER
1	D	105	GLU
1	D	112	GLU
1	D	136	THR
1	D	185	VAL
1	D	242	GLU
1	D	264	LEU
1	D	265	GLU
1	D	301	GLU
1	D	321	TYR
1	D	380	ASP
1	D	408	TRP
2	P	104	MET
2	P	105	CYS
2	P	193	VAL
2	P	194	GLN
2	P	197	ASN
2	P	228	LEU
2	P	233	GLU
2	P	237	THR
2	P	252	LYS
2	Q	121	GLN
2	Q	128	VAL
2	Q	129	VAL
2	Q	132	ARG
2	Q	143	ILE
2	Q	168	GLN
2	Q	170	MET
2	Q	241	VAL
2	Q	251	VAL
2	R	103	ARG
2	R	104	MET
2	R	105	CYS
2	R	116	ILE
2	R	133	VAL
2	R	143	ILE
2	R	151	ILE

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Mol	Chain	Res	Type
2	R	155	LYS
2	R	187	ASN
2	R	188	TRP
2	R	193	VAL
2	R	216	ILE
2	R	226	ILE
2	R	241	VAL
2	S	103	ARG
2	S	104	MET
2	S	111	ASP
2	S	116	ILE
2	S	133	VAL
2	S	166	VAL
2	S	178	THR
2	S	241	VAL
2	S	243	THR
2	S	249	VAL
3	a	18	ASP
3	a	34	GLU
3	a	74	LYS
3	a	81	LEU
3	a	129	GLU
3	a	147	GLU
3	a	155	HIS
3	a	166	MET
3	a	178	LEU
3	a	184	LYS
3	a	219	ASP
3	a	227	LEU
3	a	228	ILE
3	a	246	ASP
3	a	267	LEU
3	a	293	THR
3	a	294	THR
3	a	314	VAL
3	a	315	ASN
3	a	384	TRP
3	a	389	THR
4	b	3	ASP
4	b	99	ILE
4	b	128	VAL
4	b	171	LEU

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Mol	Chain	Res	Type
4	b	177	LEU
4	b	200	LYS
4	b	215	THR
4	b	246	ASP
4	b	249	LYS
4	b	253	HIS
4	b	257	VAL
4	b	263	CYS
4	b	272	LEU
4	b	285	HIS
4	b	318	VAL
4	b	356	TYR
4	b	385	LEU
4	b	392	LEU
4	b	418	THR
4	c	18	ASP
4	c	34	GLU
4	c	48	GLN
4	c	76	ILE
4	c	108	THR
4	c	118	ASN
4	c	124	VAL
4	c	200	LYS
4	c	249	LYS
4	c	254	VAL
4	c	281	ILE
4	c	294	THR
4	c	314	VAL
4	c	324	GLU
4	c	359	ARG
4	c	362	LEU
4	c	371	CYS
4	c	398	LYS
4	c	399	LEU
4	c	415	ILE
3	d	9	TYR
3	d	27	CYS
3	d	35	GLU
3	d	36	VAL
3	d	49	THR
3	d	56	LYS
3	d	108	THR

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Mol	Chain	Res	Type
3	d	118	ASN
3	d	175	HIS
3	d	177	LEU
3	d	215	THR
3	d	226	TYR
3	d	263	CYS
3	d	302	ASN
3	d	314	VAL
3	d	358	ASN
3	d	383	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	134	ASN
1	A	223	GLN
1	B	3	HIS
1	B	79	GLN
1	B	223	GLN
1	C	9	ASN
1	C	30	GLN
1	C	125	HIS
1	C	134	ASN
1	C	223	GLN
1	C	231	HIS
1	C	394	GLN
1	D	134	ASN
1	D	236	GLN
1	D	332	HIS
1	D	369	GLN
1	D	395	HIS
2	P	189	HIS
2	P	194	GLN
2	P	246	GLN
2	R	187	ASN
2	S	121	GLN
2	S	190	HIS
2	S	232	ASN
3	a	114	HIS
3	a	140	HIS
3	a	285	HIS

Continued on next page...

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Mol	Chain	Res	Type
3	a	350	HIS
3	a	391	ASN
4	b	24	HIS
4	b	73	GLN
4	b	275	HIS
4	c	48	GLN
4	c	230	ASN
4	c	236	ASN
4	c	402	ASN
3	d	69	ASN
3	d	140	HIS
3	d	168	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	1	5	14,14,15	0.39	0	17,19,21	0.55	0
5	NAG	E	2	5	14,14,15	0.40	0	17,19,21	0.39	0
5	BMA	E	3	5	11,11,12	0.17	0	15,15,17	0.48	0
5	NAG	F	1	1,5	14,14,15	0.39	0	17,19,21	0.55	0
5	NAG	F	2	5	14,14,15	0.40	0	17,19,21	0.39	0
5	BMA	F	3	5	11,11,12	0.17	0	15,15,17	0.49	0
5	NAG	G	1	5	14,14,15	0.40	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	G	2	5	14,14,15	0.41	0	17,19,21	0.39	0
5	BMA	G	3	5	11,11,12	0.17	0	15,15,17	0.48	0
5	NAG	H	1	5	14,14,15	0.40	0	17,19,21	0.55	0
5	NAG	H	2	5	14,14,15	0.38	0	17,19,21	0.38	0
5	BMA	H	3	5	11,11,12	0.16	0	15,15,17	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1
5	NAG	G	1	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	NAG	H	1	5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

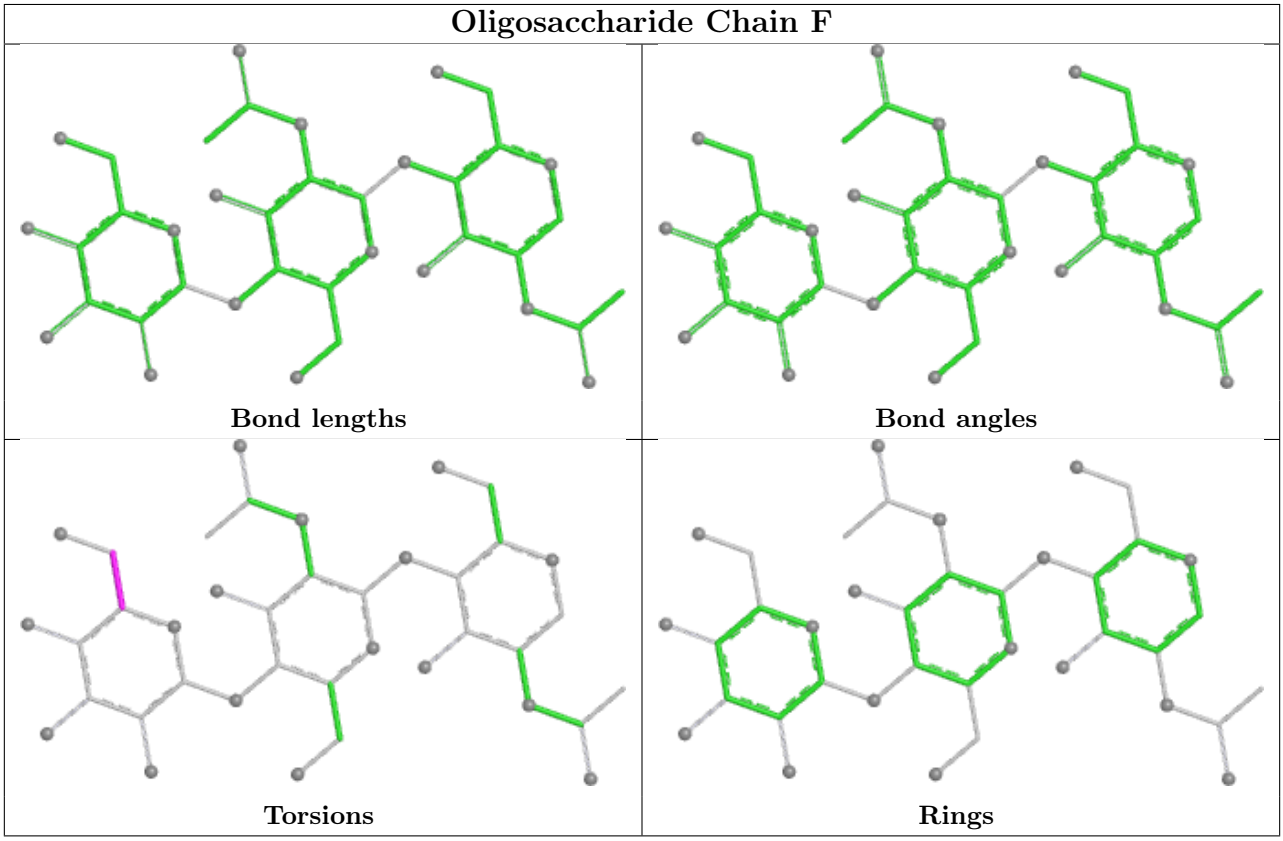
Mol	Chain	Res	Type	Atoms
5	F	3	BMA	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6

There are no ring outliers.

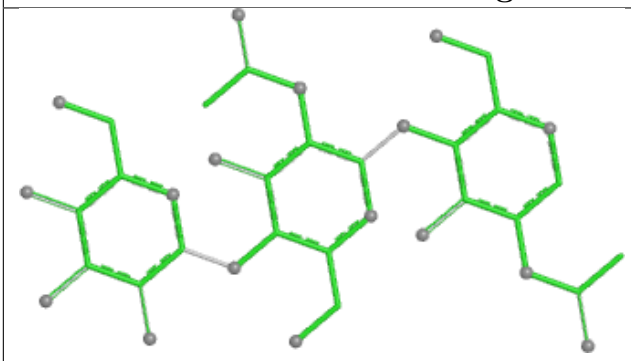
7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	2	0
5	E	1	NAG	2	0
5	H	2	NAG	3	0
5	F	2	NAG	1	0
5	G	2	NAG	3	0
5	G	1	NAG	10	0
5	H	1	NAG	3	0

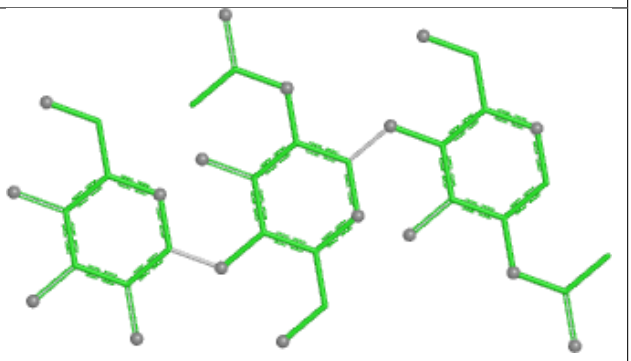
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



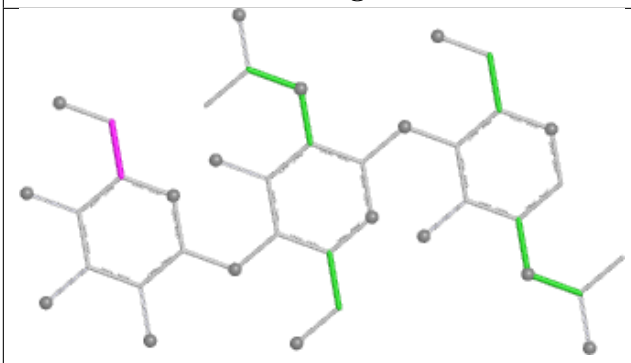
Oligosaccharide Chain E



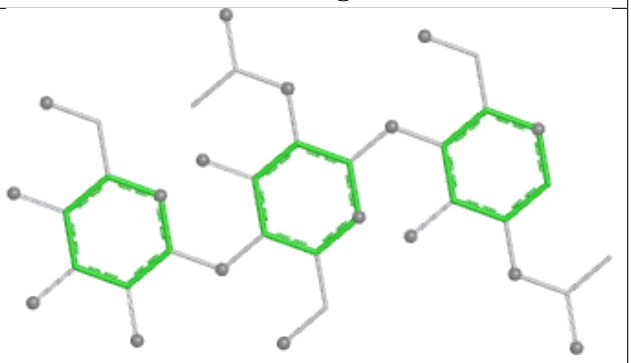
Bond lengths



Bond angles

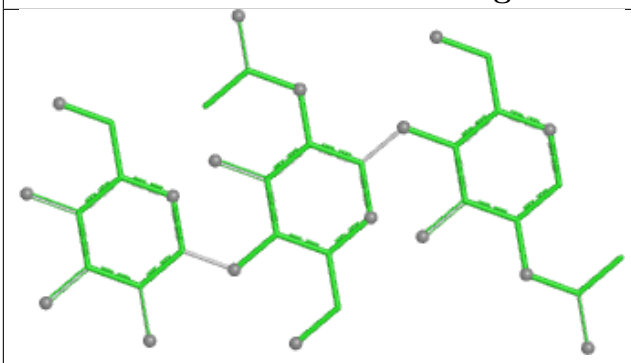


Torsions

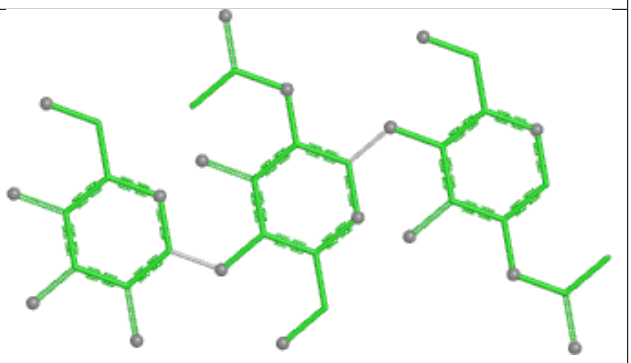


Rings

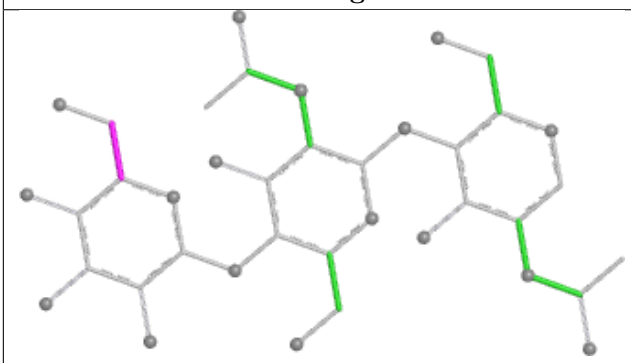
Oligosaccharide Chain H



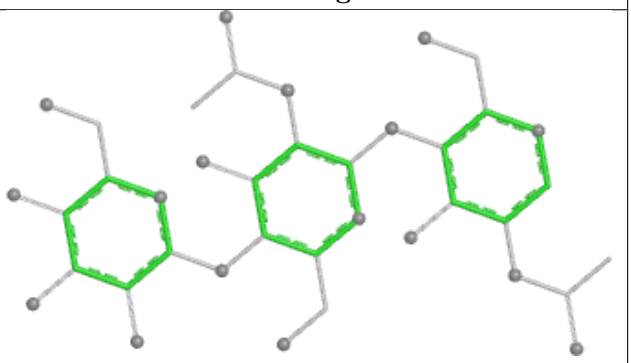
Bond lengths



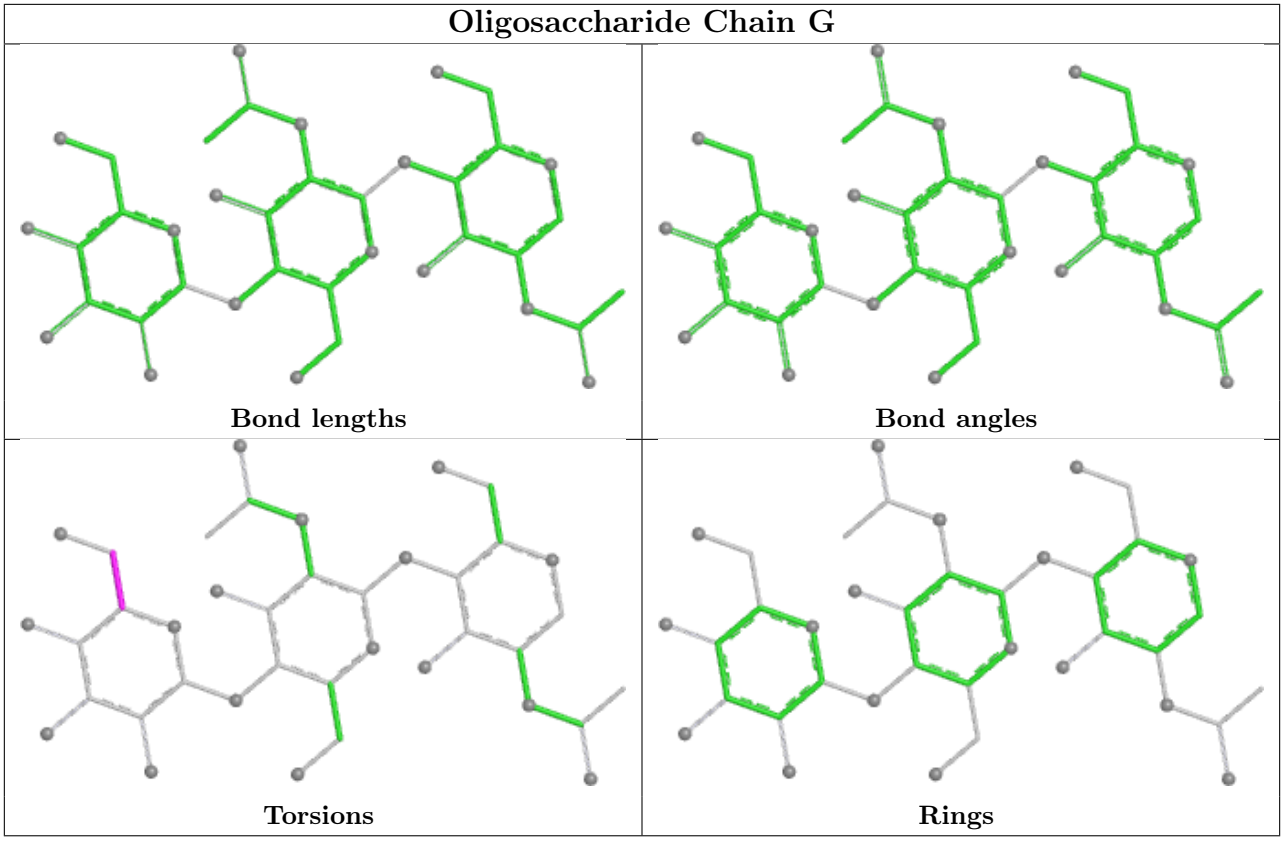
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	a	501	3	14,14,15	0.39	0	17,19,21	1.17	3 (17%)
6	NAG	d	501	3	14,14,15	0.39	0	17,19,21	0.98	2 (11%)
6	NAG	b	501	4	14,14,15	0.37	0	17,19,21	1.49	2 (11%)
6	NAG	c	501	4	14,14,15	0.38	0	17,19,21	2.07	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
6	NAG	a	501	3	-	3/6/23/26	0/1/1/1
6	NAG	d	501	3	-	3/6/23/26	0/1/1/1
6	NAG	b	501	4	-	3/6/23/26	0/1/1/1
6	NAG	c	501	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	c	501	NAG	C2-N2-C7	7.55	133.01	122.90
6	b	501	NAG	C2-N2-C7	4.37	128.76	122.90
6	b	501	NAG	C1-C2-N2	3.74	116.33	110.43
6	a	501	NAG	C2-N2-C7	3.18	127.17	122.90
6	d	501	NAG	C2-N2-C7	3.11	127.06	122.90
6	a	501	NAG	C1-C2-N2	2.75	114.76	110.43
6	c	501	NAG	C1-C2-N2	2.59	114.51	110.43
6	a	501	NAG	C1-O5-C5	2.13	115.03	112.19
6	c	501	NAG	C1-O5-C5	2.06	114.94	112.19
6	d	501	NAG	C1-C2-N2	2.05	113.67	110.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	a	501	NAG	1	0
6	c	501	NAG	3	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.

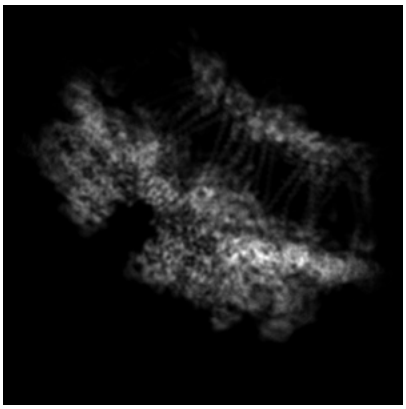
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72747. These allow visual inspection of the internal detail of the map and identification of artifacts.

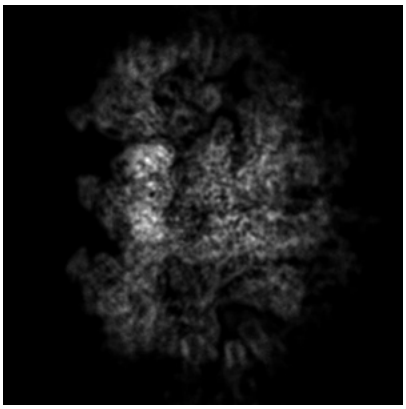
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

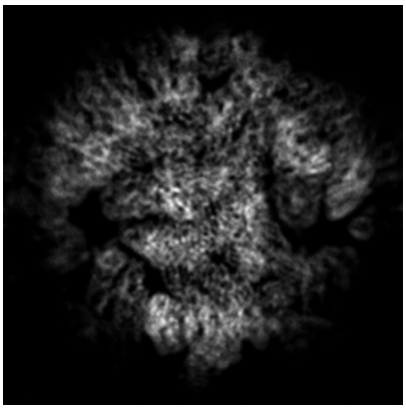
6.1.1 Primary map



X

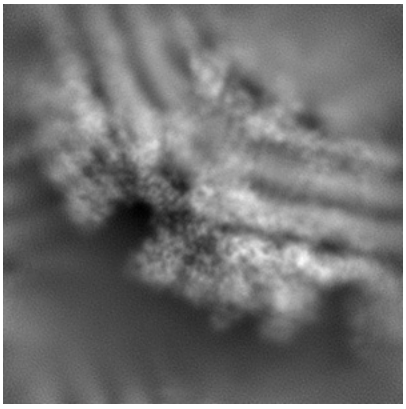


Y

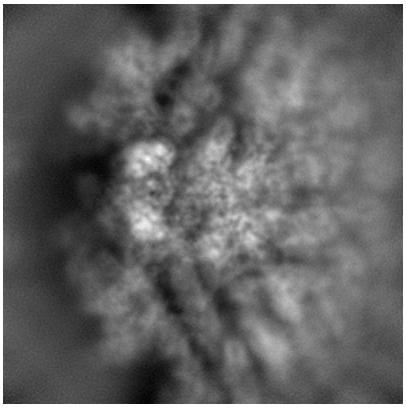


Z

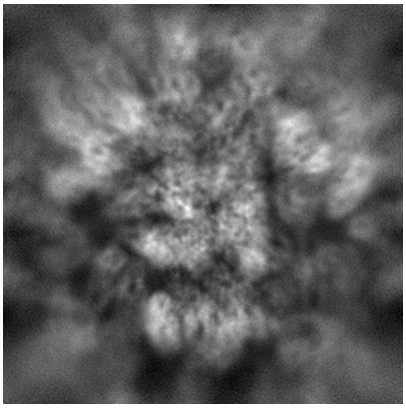
6.1.2 Raw map



X



Y

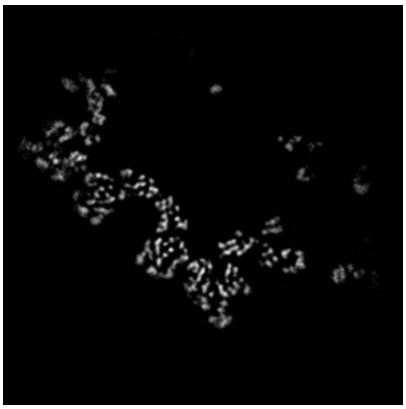


Z

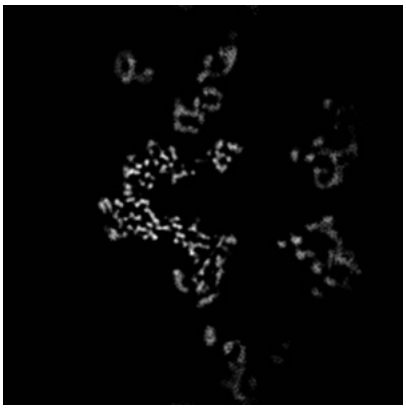
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

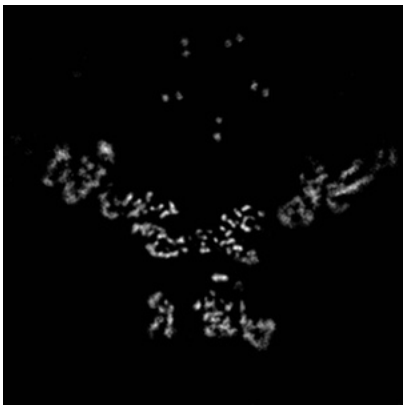
6.2.1 Primary map



X Index: 128

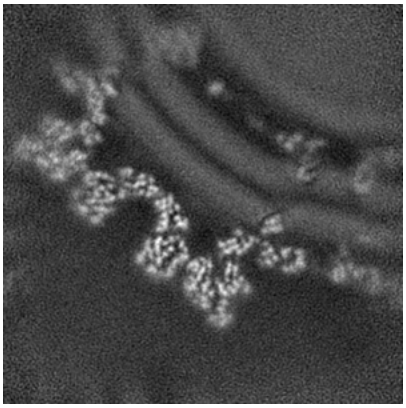


Y Index: 128

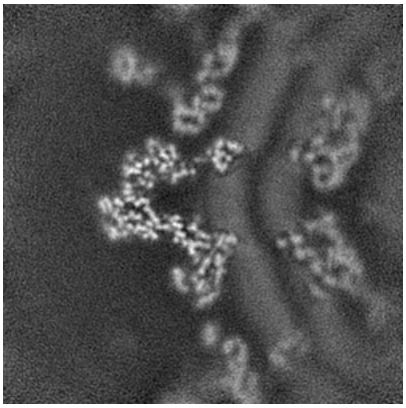


Z Index: 128

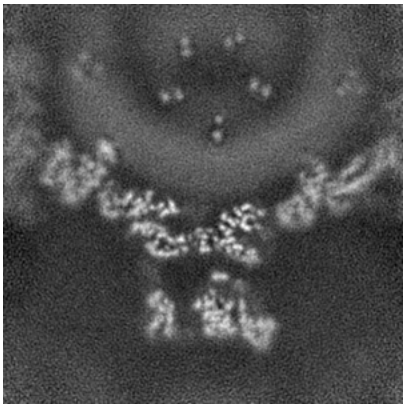
6.2.2 Raw map



X Index: 128



Y Index: 128

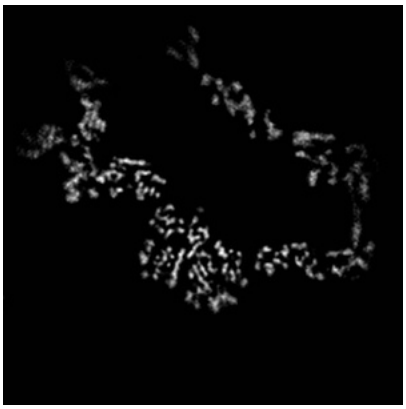


Z Index: 128

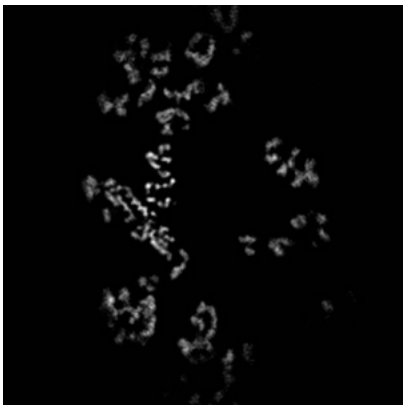
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 119

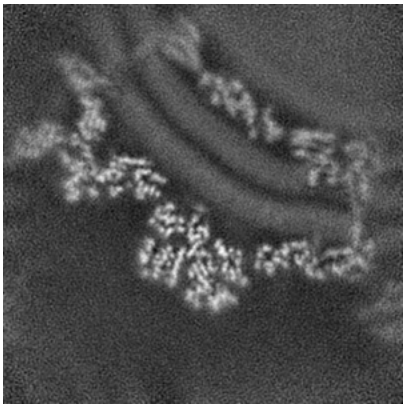


Y Index: 148

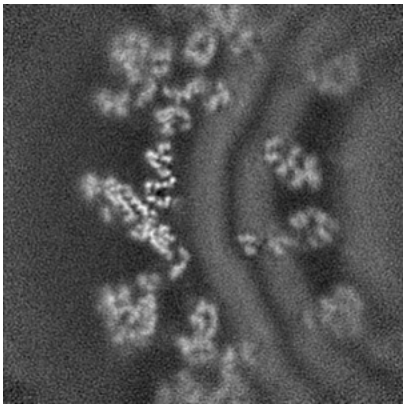


Z Index: 92

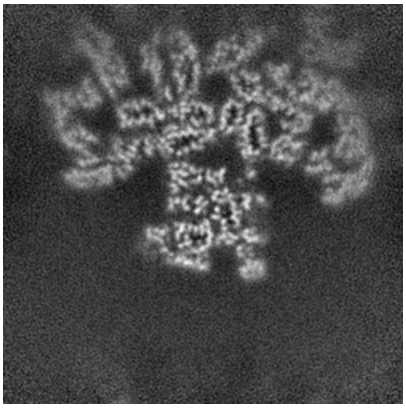
6.3.2 Raw map



X Index: 119



Y Index: 148

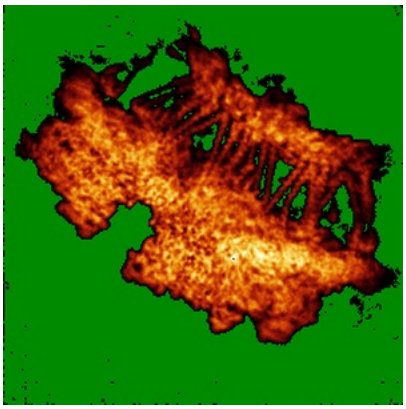


Z Index: 92

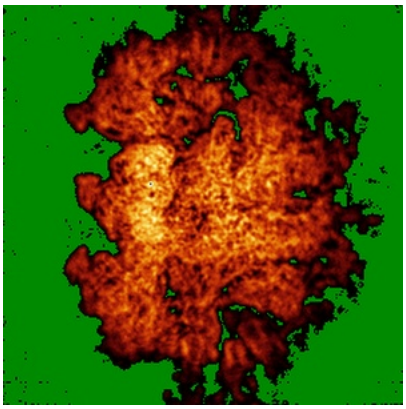
The images above show the largest variance slices of the map in three orthogonal directions.

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

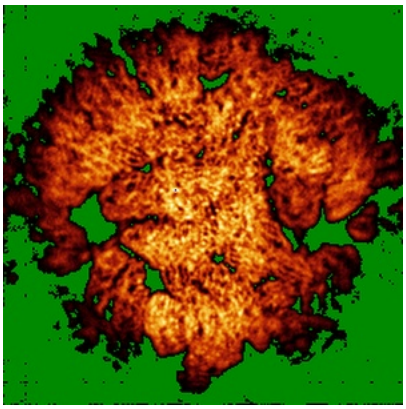
6.4.1 Primary map



X

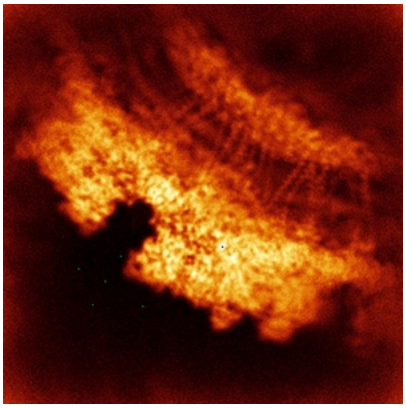


Y

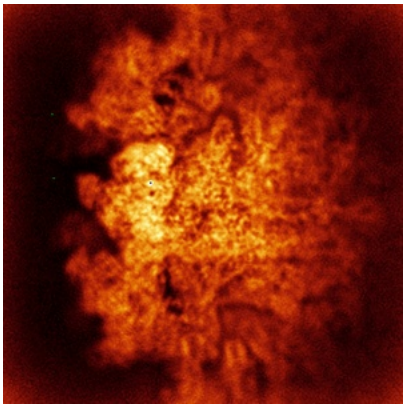


Z

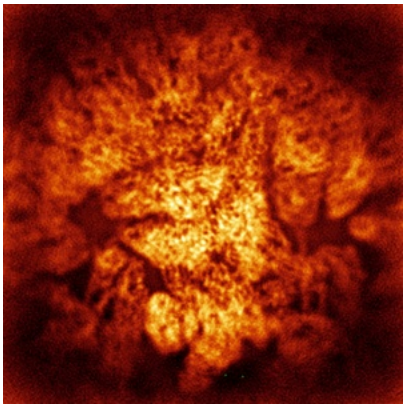
6.4.2 Raw map



X



Y

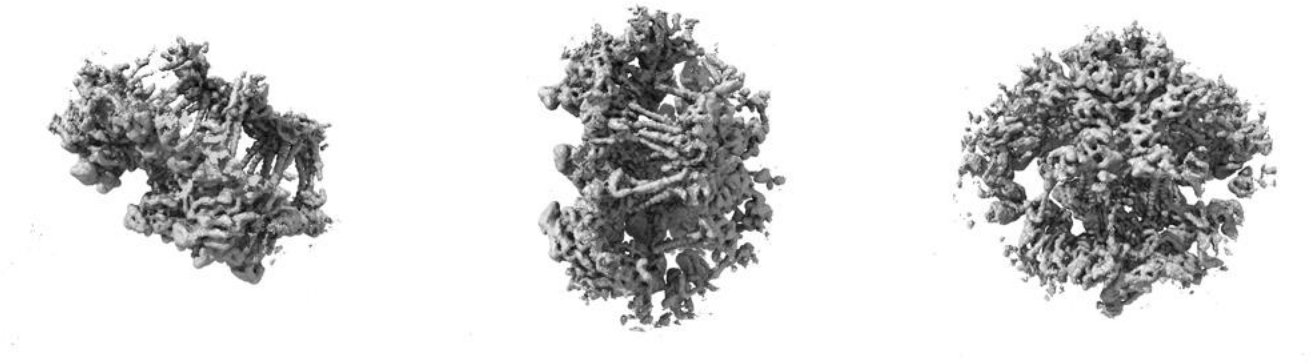


Z

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



X Y Z

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

6.5.2 Raw map



X Y Z

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

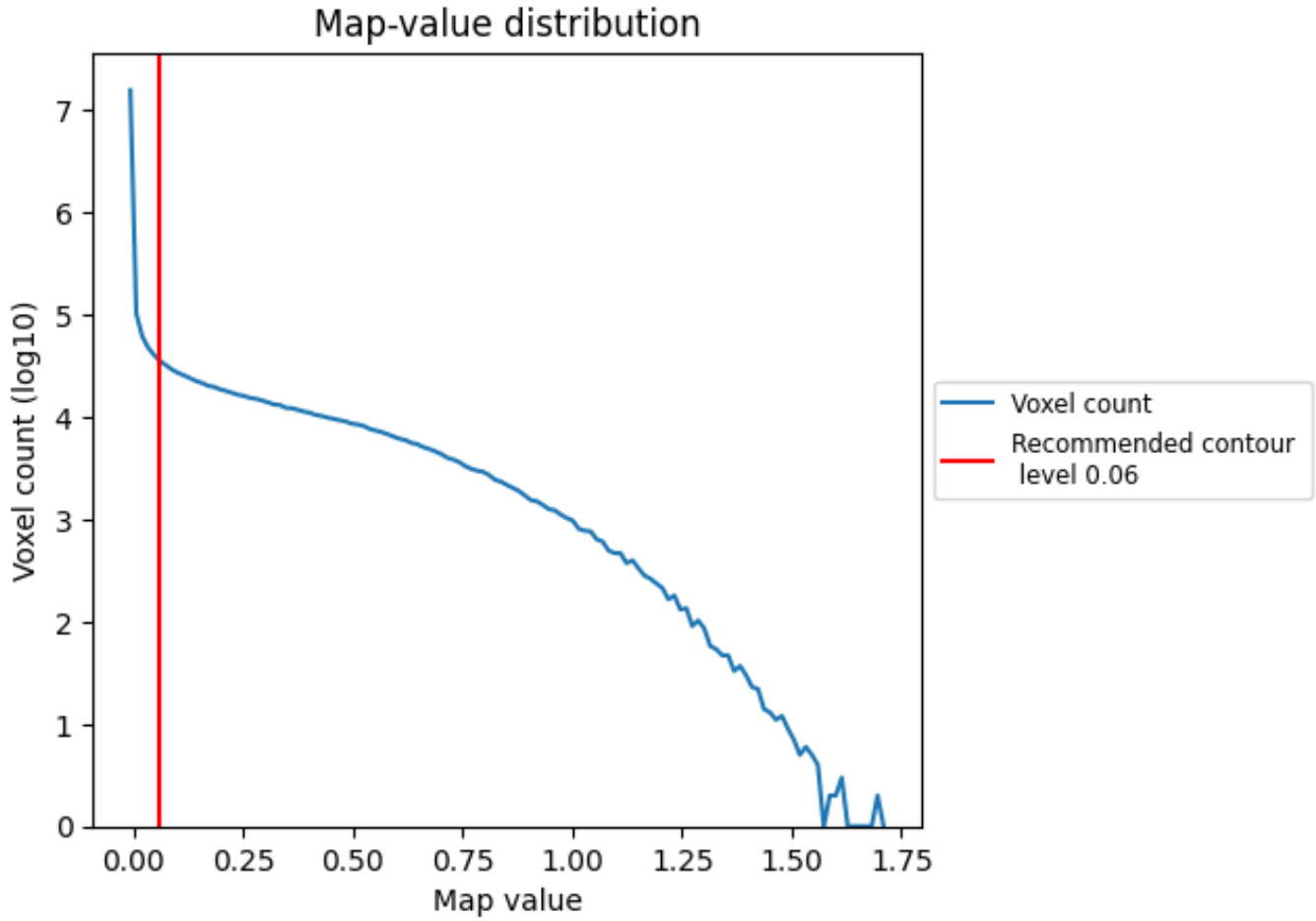
6.6 Mask visualisation (i)

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

7 Map analysis

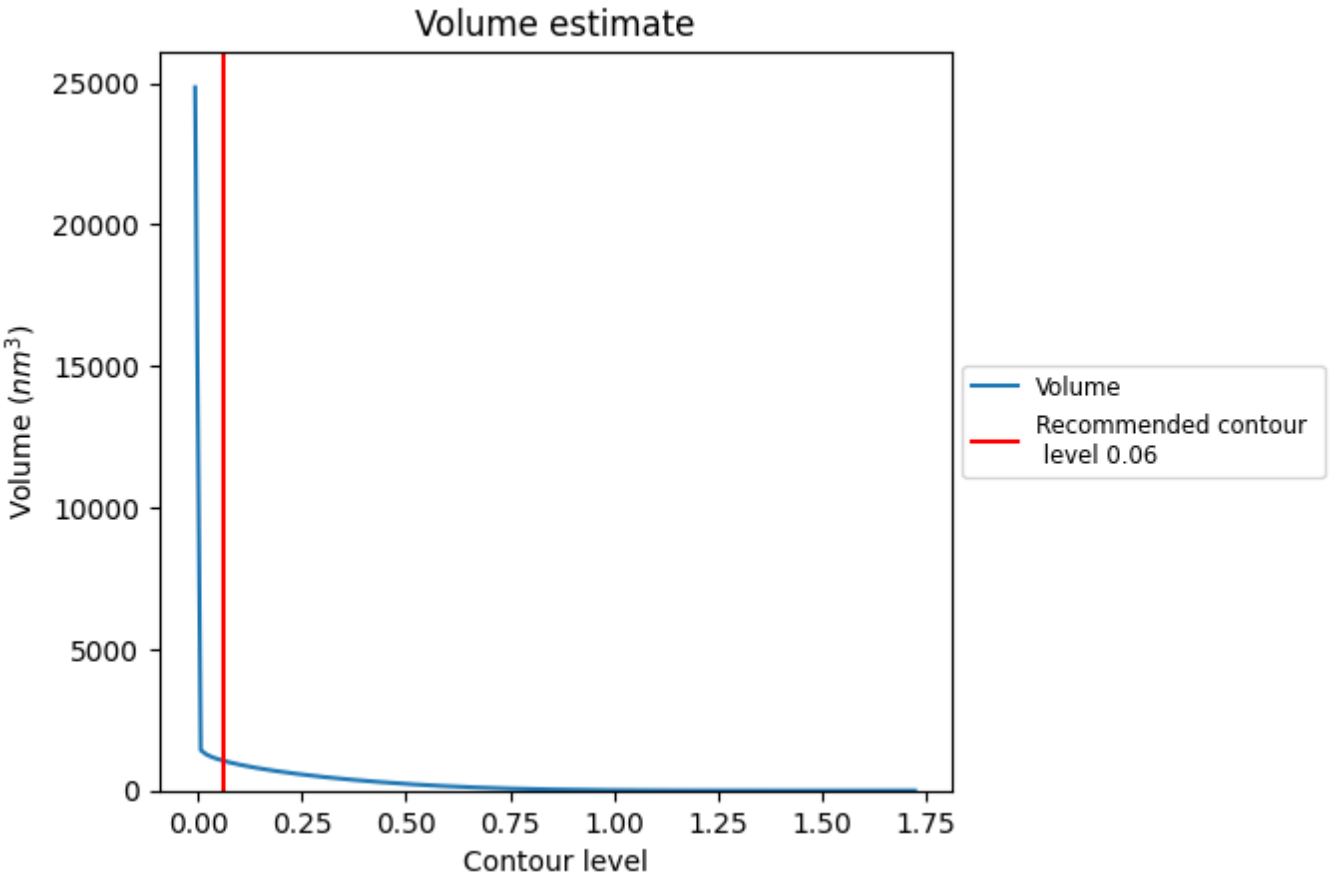
This section contains the results of statistical analysis of the map.

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.

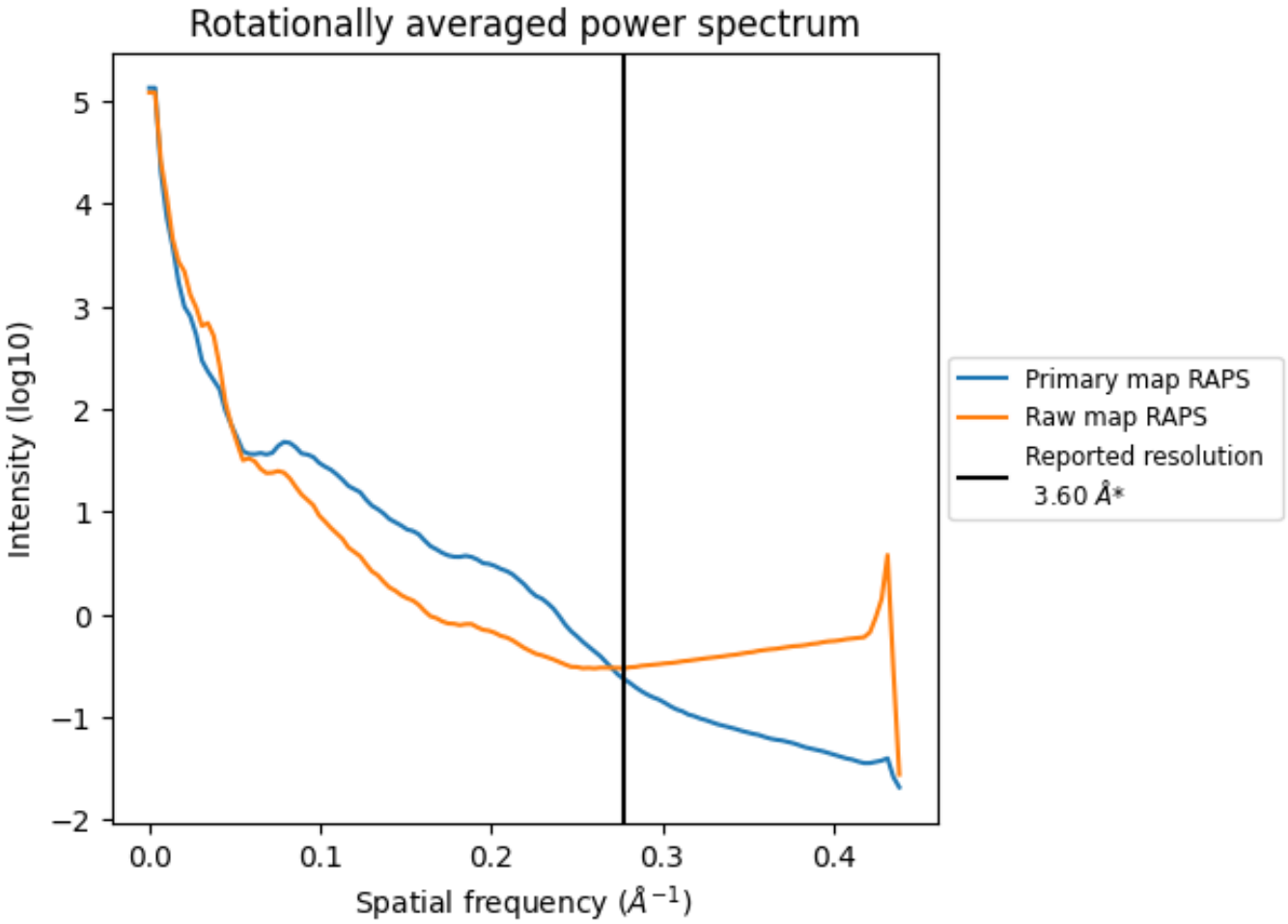
7.2 Volume estimate



The volume at the recommended contour level is 1060 nm^3; this corresponds to an approximate mass of 957 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)

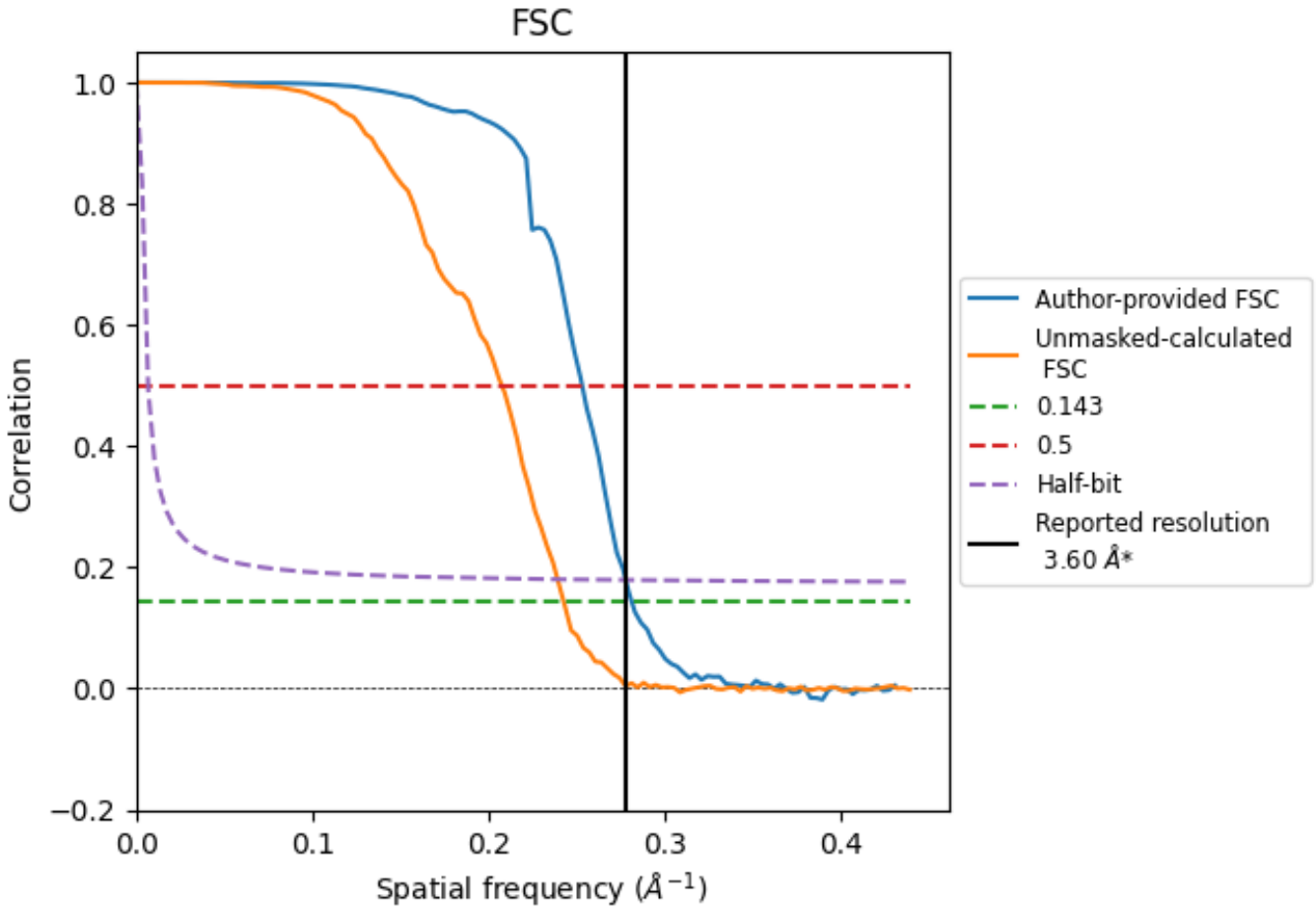


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

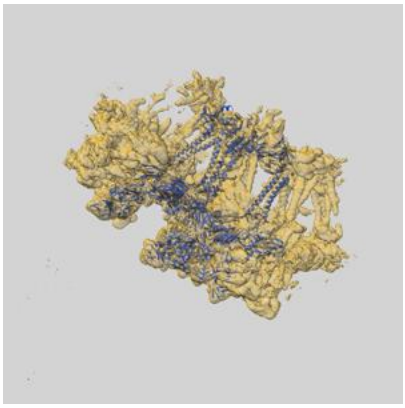
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.56	3.95	3.60
Unmasked-calculated*	4.12	4.82	4.18

*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 4.12 differs from the reported value 3.6 by more than 10 %

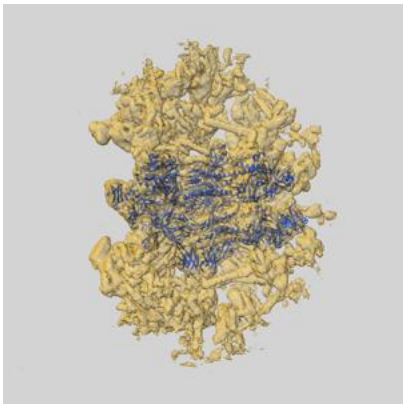
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72747 and PDB model 9YB3. Per-residue inclusion information can be found in section 3 on page 7.

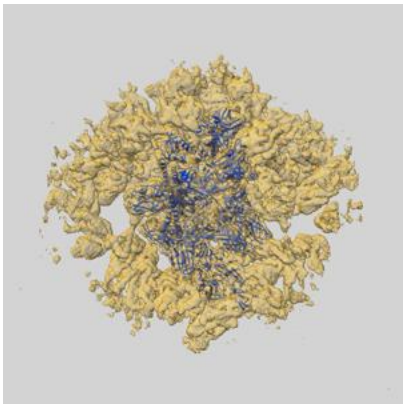
9.1 Map-model overlay



X



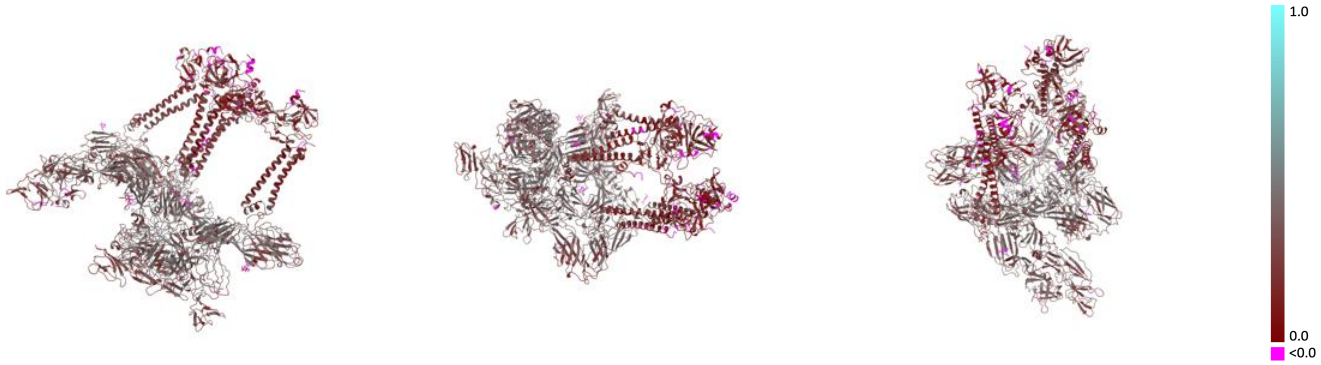
Y



Z

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

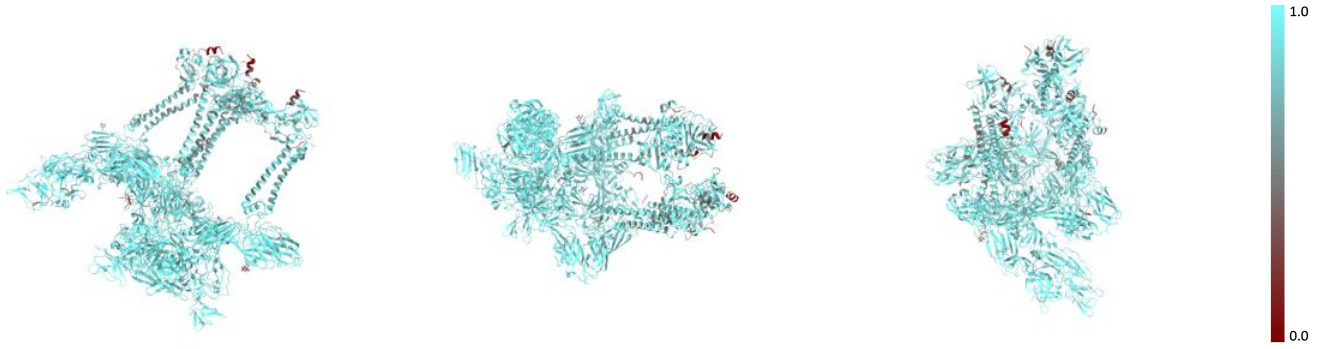
9.2 Q-score mapped to coordinate model (i)



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.

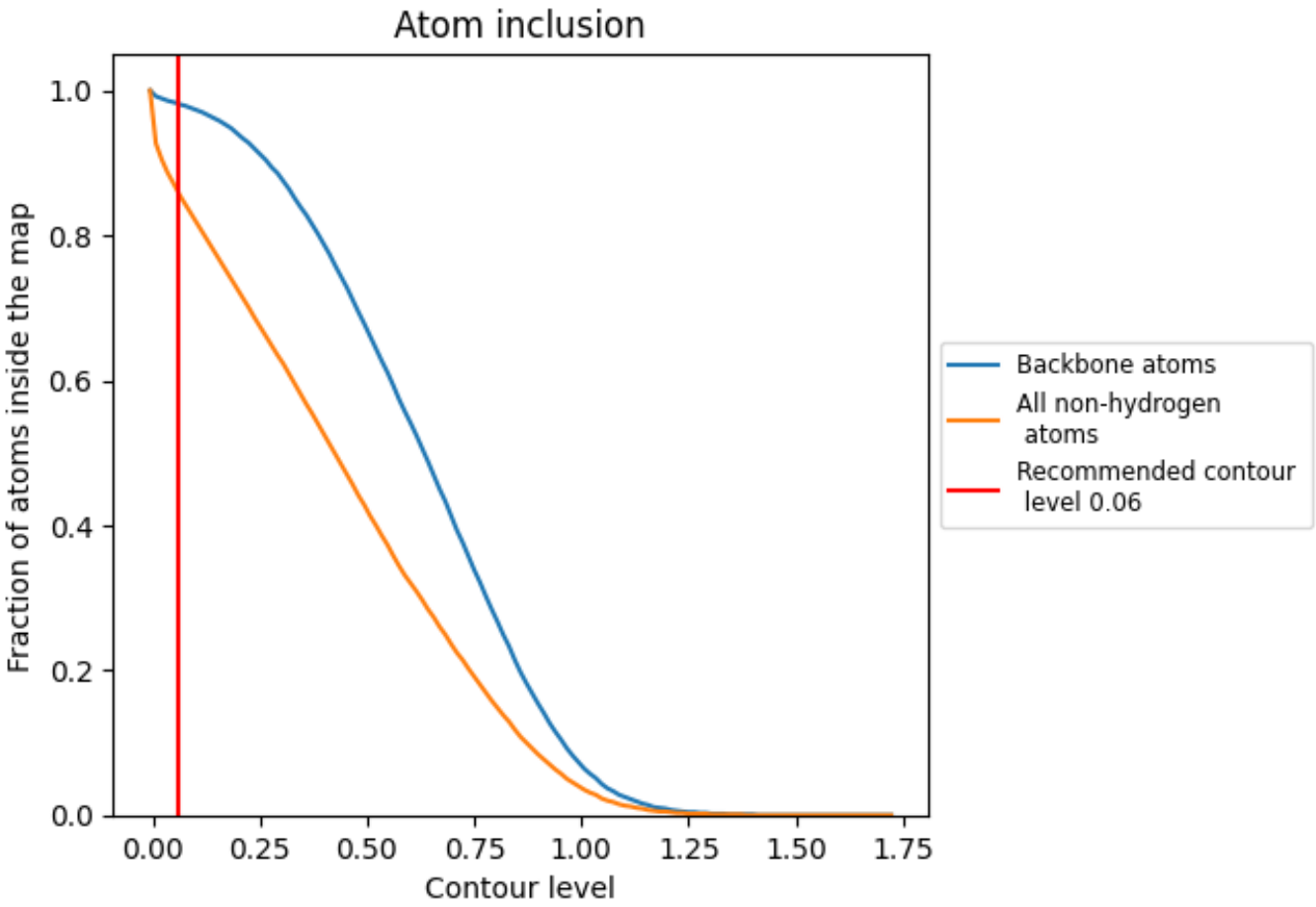
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.3040
A	0.8770	0.3330
B	0.8800	0.3150
C	0.8930	0.3500
D	0.8850	0.3470
E	0.3850	0.0770
F	0.4360	0.0950
G	0.4620	0.0950
H	0.4620	0.0870
P	0.6940	0.1340
Q	0.7690	0.1770
R	0.7800	0.2140
S	0.7400	0.1750
a	0.8700	0.2970
b	0.8840	0.3230
c	0.8880	0.3350
d	0.8790	0.3340

