Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 03:52 pm GMT

PDB ID	:	5N8N
EMDB ID	:	EMD-3600
Title	:	Contracted sheath of a Pseudomonas aeruginosa type six secretion system consisting of TssB1 and TssC1
Authors	:	Salih, O.; He, S.; Stach, L.; Macdonald, J.T.; Planamente, S.; Manoli, E.; Scheres, S.; Filloux, A.; Freemont, P.S.
Deposited on	:	2017-02-23
Resolution	:	3.28 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 (i) 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 (i)) were used in the production of this report:

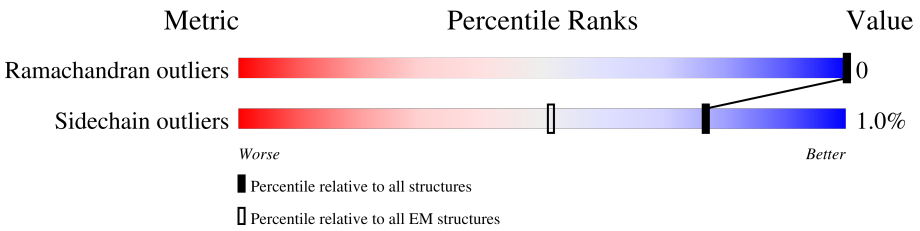
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.28 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)
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	132	93% 6% •
1	C	132	93% 6% •
1	E	132	93% 6% •
1	G	132	93% 6% •
1	I	132	93% 6% •
1	K	132	93% 6% •
1	M	132	93% 6% •
1	O	132	93% 6% •
1	Q	132	93% 6% •

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Mol	Chain	Length	Quality of chain
1	S	132	93% 6% •
1	U	132	93% 6% •
1	W	132	93% 6% •
1	Y	132	93% 6% •
1	a	132	93% 6% •
1	c	132	93% 6% •
2	B	461	5% 96% •
2	D	461	5% 96% •
2	F	461	• 96% •
2	H	461	5% 96% •
2	J	461	5% 96% •
2	L	461	• 96% •
2	N	461	• 96% •
2	P	461	5% 96% •
2	R	461	• 96% •
2	T	461	• 96% •
2	V	461	• 96% •
2	X	461	• 96% •
2	Z	461	• 96% •
2	b	461	• 96% •
2	d	461	• 96% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 70035 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 Type VI secretion protein, family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	132	1027	651	177	195	4	0	0
1	C	132	1027	651	177	195	4	0	0
1	E	132	1027	651	177	195	4	0	0
1	G	132	1027	651	177	195	4	0	0
1	I	132	1027	651	177	195	4	0	0
1	K	132	1027	651	177	195	4	0	0
1	M	132	1027	651	177	195	4	0	0
1	O	132	1027	651	177	195	4	0	0
1	Q	132	1027	651	177	195	4	0	0
1	S	132	1027	651	177	195	4	0	0
1	U	132	1027	651	177	195	4	0	0
1	W	132	1027	651	177	195	4	0	0
1	Y	132	1027	651	177	195	4	0	0
1	a	132	1027	651	177	195	4	0	0
1	c	132	1027	651	177	195	4	0	0

- Molecule 2 is a protein called EvpB family type VI secretion protein.

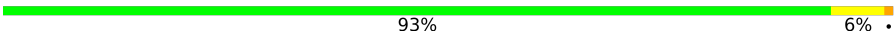
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	461	3642	2313	616	698	15	0	0
2	D	461	3642	2313	616	698	15	0	0
2	F	461	3642	2313	616	698	15	0	0
2	H	461	3642	2313	616	698	15	0	0
2	J	461	3642	2313	616	698	15	0	0
2	L	461	3642	2313	616	698	15	0	0
2	N	461	3642	2313	616	698	15	0	0
2	P	461	3642	2313	616	698	15	0	0
2	R	461	3642	2313	616	698	15	0	0
2	T	461	3642	2313	616	698	15	0	0
2	V	461	3642	2313	616	698	15	0	0
2	X	461	3642	2313	616	698	15	0	0
2	Z	461	3642	2313	616	698	15	0	0
2	b	461	3642	2313	616	698	15	0	0
2	d	461	3642	2313	616	698	15	0	0

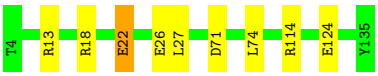
3 Residue-property plots (i)

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: Type VI secretion protein, family

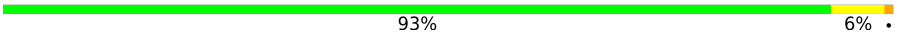
Chain A:

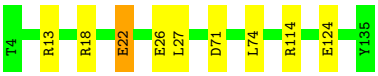




- Molecule 1: Type VI secretion protein, family

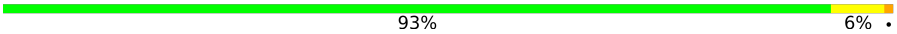
Chain C:

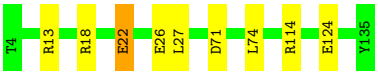




- Molecule 1: Type VI secretion protein, family

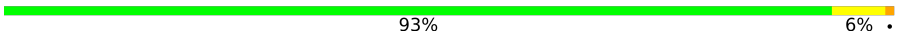
Chain E:

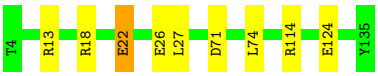




- Molecule 1: Type VI secretion protein, family

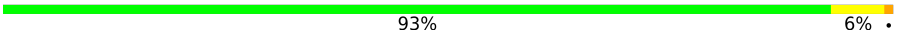
Chain G:

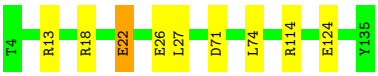




- Molecule 1: Type VI secretion protein, family

Chain I:





- Molecule 1: Type VI secretion protein, family

Chain K: 93% 6% •

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain M: 93% 6% •

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain O: 93% 6% •

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain Q: 93% 6% •

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain S: 93% 6% •

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain U: 93% 6% •

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain W: 93% 6% •

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain Y: 93% 6%

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain a: 93% 6%

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 1: Type VI secretion protein, family

Chain c: 93% 6%

T4 R13 R18 E22 E26 L27 D71 L74 R114 E124 Y135

• Molecule 2: EvpB family type VI secretion protein

Chain B: 5% 96%

R38 E39 R46 E50 H51 A52 L53 E54 Q55 T56 S57 L58 I59 S60 R99 E109 E150 Y160 Y168 E177 E181 Y239 A272 D273 K372 R390 R399 D410 E420 R423 D436 P437 A438 H439 S440 E458 E461 L473

L486 S494 A495 K496 E497 A498

• Molecule 2: EvpB family type VI secretion protein

Chain D: 5% 96%

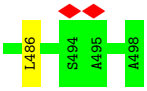
R38 E42 R46 A49 E50 E54 Q55 T56 S57 L58 I59 S60 R99 E109 E150 Y160 Y168 E177 E181 Y239 E261 A272 K372 R390 R399 D410 E420 R423 G435 D436 P437 A438 H439 S440 E458 E461

L473 L486 S494 A495 K496 E497 A498

• Molecule 2: EvpB family type VI secretion protein

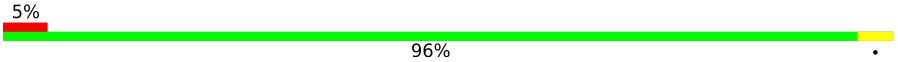
Chain F: 96%

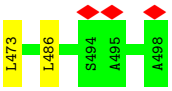
R38 E39 E42 R46 E50 H51 A52 L53 E54 Q55 T56 S57 L58 I59 S60 R99 E109 E150 Y160 Y168 E177 E181 Y239 A272 K372 R390 R399 D410 E420 R423 D436 P437 A438 H439 S440 E458 E461 L473



• Molecule 2: EvpB family type VI secretion protein

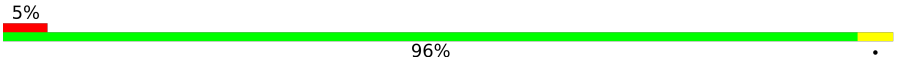
Chain H:

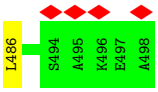




• Molecule 2: EvpB family type VI secretion protein

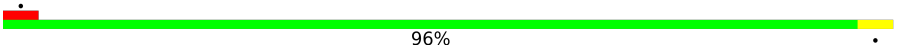
Chain J:

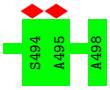




• Molecule 2: EvpB family type VI secretion protein

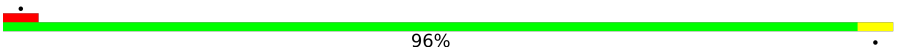
Chain L:

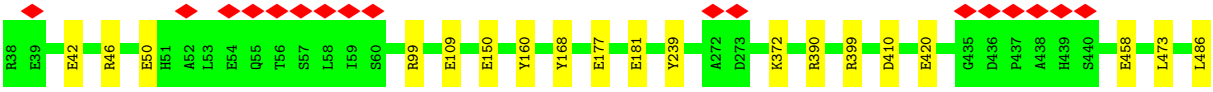




• Molecule 2: EvpB family type VI secretion protein

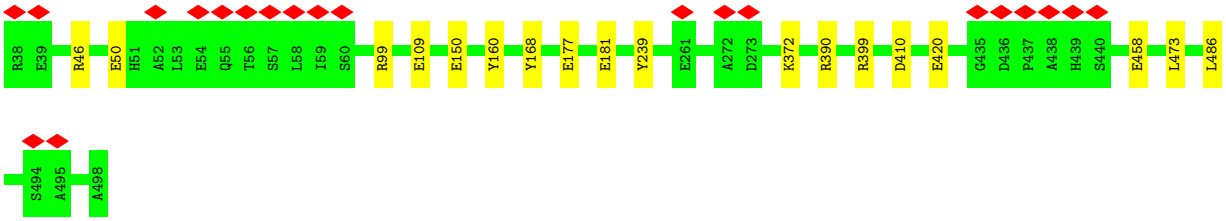
Chain N:





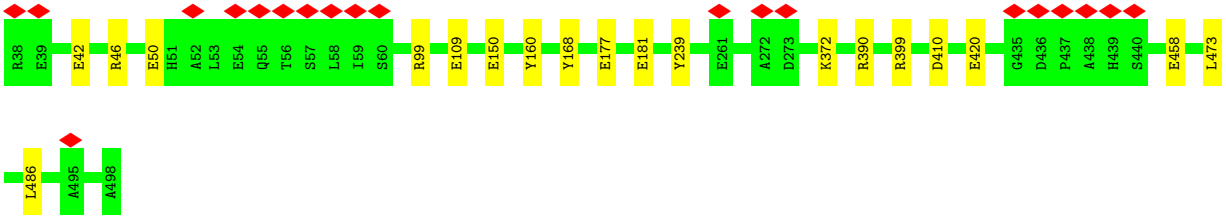
• Molecule 2: EvpB family type VI secretion protein

Chain P: 5% 96%



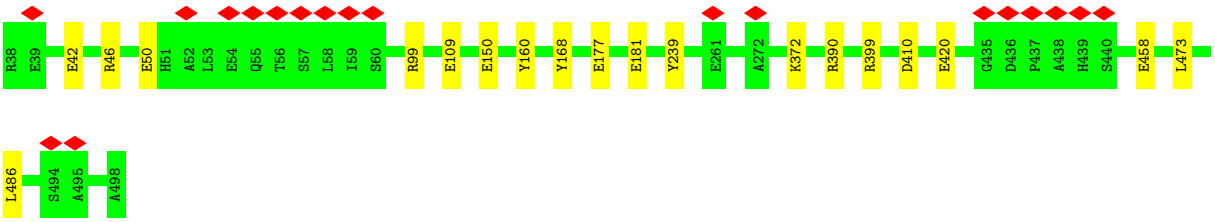
• Molecule 2: EvpB family type VI secretion protein

Chain R: 96%



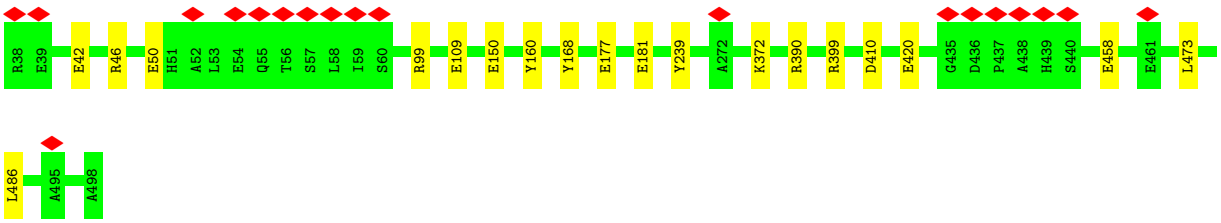
• Molecule 2: EvpB family type VI secretion protein

Chain T: 96%



• Molecule 2: EvpB family type VI secretion protein

Chain V: 96%

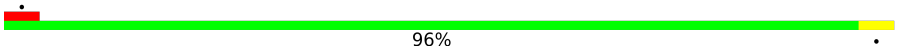


• Molecule 2: EvpB family type VI secretion protein

Chain X: 96%

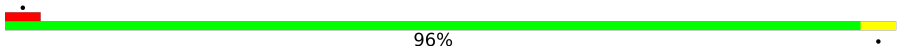
• Molecule 2: EvpB family type VI secretion protein

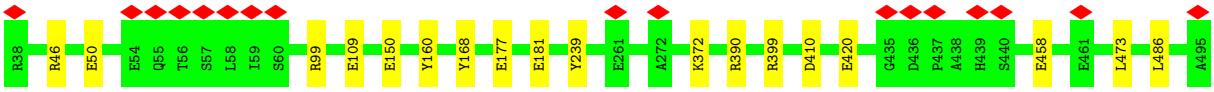
Chain Z:



• Molecule 2: EvpB family type VI secretion protein

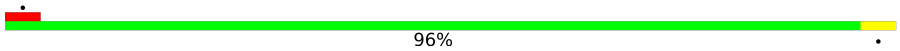
Chain b:

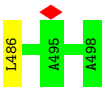




• Molecule 2: EvpB family type VI secretion protein

Chain d:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=27.7°, rise=20.2 Å, axial sym=C1	Depositor
Number of segments used	71264	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.512	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.0385	Depositor
Map size (Å)	335.0, 335.0, 335.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	C	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	E	1.00	5/1043 (0.5%)	0.92	6/1411 (0.4%)
1	G	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	I	1.00	5/1043 (0.5%)	0.92	6/1411 (0.4%)
1	K	1.00	5/1043 (0.5%)	0.92	6/1411 (0.4%)
1	M	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	O	1.00	5/1043 (0.5%)	0.92	6/1411 (0.4%)
1	Q	1.00	5/1043 (0.5%)	0.92	6/1411 (0.4%)
1	S	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	U	1.00	5/1043 (0.5%)	0.92	6/1411 (0.4%)
1	W	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	Y	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	a	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
1	c	1.00	5/1043 (0.5%)	0.93	6/1411 (0.4%)
2	B	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	D	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	F	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	H	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	J	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	L	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	N	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	P	1.00	9/3732 (0.2%)	0.77	8/5061 (0.2%)
2	R	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	T	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	V	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	X	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	Z	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
2	b	1.00	9/3732 (0.2%)	0.77	8/5061 (0.2%)
2	d	1.00	10/3732 (0.3%)	0.77	8/5061 (0.2%)
All	All	1.00	223/71625 (0.3%)	0.80	210/97080 (0.2%)

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	42	GLU	CD-OE1	6.63	1.32	1.25
2	J	42	GLU	CD-OE1	6.62	1.32	1.25
2	T	42	GLU	CD-OE1	6.62	1.32	1.25
2	D	42	GLU	CD-OE1	6.61	1.32	1.25
2	V	42	GLU	CD-OE1	6.61	1.32	1.25
2	F	42	GLU	CD-OE1	6.61	1.32	1.25
2	L	42	GLU	CD-OE1	6.61	1.32	1.25
2	H	42	GLU	CD-OE1	6.59	1.32	1.25
1	Y	26	GLU	CD-OE1	6.59	1.32	1.25
2	R	42	GLU	CD-OE1	6.59	1.32	1.25
1	M	26	GLU	CD-OE1	6.59	1.32	1.25
1	W	26	GLU	CD-OE1	6.59	1.32	1.25
2	Z	42	GLU	CD-OE1	6.59	1.32	1.25
1	Q	26	GLU	CD-OE1	6.58	1.32	1.25
1	a	26	GLU	CD-OE1	6.58	1.32	1.25
2	N	42	GLU	CD-OE1	6.57	1.32	1.25
2	d	42	GLU	CD-OE1	6.57	1.32	1.25
1	G	26	GLU	CD-OE1	6.56	1.32	1.25
1	a	22	GLU	CD-OE1	6.55	1.32	1.25
1	K	22	GLU	CD-OE1	6.55	1.32	1.25
1	O	26	GLU	CD-OE1	6.54	1.32	1.25
1	U	26	GLU	CD-OE1	6.54	1.32	1.25
1	I	26	GLU	CD-OE1	6.54	1.32	1.25
1	S	26	GLU	CD-OE1	6.53	1.32	1.25
1	c	26	GLU	CD-OE1	6.53	1.32	1.25
1	I	22	GLU	CD-OE1	6.53	1.32	1.25
1	K	26	GLU	CD-OE1	6.53	1.32	1.25
1	M	22	GLU	CD-OE1	6.52	1.32	1.25
1	O	22	GLU	CD-OE1	6.51	1.32	1.25
1	C	26	GLU	CD-OE1	6.51	1.32	1.25
1	C	22	GLU	CD-OE1	6.51	1.32	1.25
1	G	22	GLU	CD-OE1	6.51	1.32	1.25
1	W	22	GLU	CD-OE1	6.50	1.32	1.25
1	c	22	GLU	CD-OE1	6.50	1.32	1.25
1	Y	22	GLU	CD-OE1	6.50	1.32	1.25
1	U	22	GLU	CD-OE1	6.50	1.32	1.25
1	A	26	GLU	CD-OE1	6.49	1.32	1.25
1	S	22	GLU	CD-OE1	6.49	1.32	1.25
1	E	26	GLU	CD-OE1	6.48	1.32	1.25
1	Q	22	GLU	CD-OE1	6.48	1.32	1.25
1	A	22	GLU	CD-OE1	6.47	1.32	1.25
1	E	22	GLU	CD-OE1	6.45	1.32	1.25
2	Z	150	GLU	CD-OE2	6.12	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	150	GLU	CD-OE1	6.11	1.32	1.25
2	D	150	GLU	CD-OE1	6.10	1.32	1.25
2	V	150	GLU	CD-OE1	6.10	1.32	1.25
2	X	150	GLU	CD-OE1	6.10	1.32	1.25
2	V	150	GLU	CD-OE2	6.10	1.32	1.25
2	R	150	GLU	CD-OE1	6.09	1.32	1.25
2	B	168	TYR	CE1-CZ	-6.08	1.30	1.38
2	H	150	GLU	CD-OE1	6.08	1.32	1.25
2	d	150	GLU	CD-OE1	6.08	1.32	1.25
2	J	150	GLU	CD-OE1	6.08	1.32	1.25
2	N	150	GLU	CD-OE1	6.08	1.32	1.25
2	F	150	GLU	CD-OE1	6.08	1.32	1.25
2	Z	150	GLU	CD-OE1	6.07	1.32	1.25
2	L	150	GLU	CD-OE1	6.07	1.32	1.25
2	B	150	GLU	CD-OE1	6.06	1.32	1.25
2	T	150	GLU	CD-OE1	6.06	1.32	1.25
2	V	168	TYR	CE1-CZ	-6.06	1.30	1.38
2	J	150	GLU	CD-OE2	6.06	1.32	1.25
2	X	150	GLU	CD-OE2	6.06	1.32	1.25
2	F	150	GLU	CD-OE2	6.06	1.32	1.25
2	b	150	GLU	CD-OE1	6.05	1.32	1.25
2	H	168	TYR	CE1-CZ	-6.05	1.30	1.38
2	d	150	GLU	CD-OE2	6.05	1.32	1.25
2	J	168	TYR	CE1-CZ	-6.05	1.30	1.38
2	T	168	TYR	CE1-CZ	-6.05	1.30	1.38
2	L	150	GLU	CD-OE2	6.04	1.32	1.25
2	P	150	GLU	CD-OE2	6.04	1.32	1.25
2	D	168	TYR	CE1-CZ	-6.04	1.30	1.38
2	H	150	GLU	CD-OE2	6.04	1.32	1.25
2	N	150	GLU	CD-OE2	6.04	1.32	1.25
2	R	150	GLU	CD-OE2	6.04	1.32	1.25
2	F	168	TYR	CE1-CZ	-6.03	1.30	1.38
2	R	168	TYR	CE1-CZ	-6.02	1.30	1.38
2	D	150	GLU	CD-OE2	6.02	1.32	1.25
2	P	168	TYR	CE1-CZ	-6.02	1.30	1.38
2	T	150	GLU	CD-OE2	6.02	1.32	1.25
2	b	150	GLU	CD-OE2	6.02	1.32	1.25
2	B	150	GLU	CD-OE2	6.02	1.32	1.25
2	d	168	TYR	CE1-CZ	-6.00	1.30	1.38
2	N	168	TYR	CE1-CZ	-5.99	1.30	1.38
2	L	168	TYR	CE1-CZ	-5.98	1.30	1.38
2	X	168	TYR	CE1-CZ	-5.97	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	168	TYR	CE1-CZ	-5.96	1.30	1.38
2	Z	168	TYR	CE1-CZ	-5.95	1.30	1.38
2	V	420	GLU	CD-OE1	5.93	1.32	1.25
2	P	420	GLU	CD-OE1	5.93	1.32	1.25
2	d	420	GLU	CD-OE1	5.92	1.32	1.25
2	X	420	GLU	CD-OE1	5.92	1.32	1.25
2	Z	420	GLU	CD-OE1	5.92	1.32	1.25
2	B	420	GLU	CD-OE1	5.91	1.32	1.25
2	L	420	GLU	CD-OE1	5.90	1.32	1.25
2	T	420	GLU	CD-OE1	5.88	1.32	1.25
2	J	420	GLU	CD-OE1	5.88	1.32	1.25
2	F	420	GLU	CD-OE1	5.88	1.32	1.25
2	H	420	GLU	CD-OE1	5.87	1.32	1.25
2	b	420	GLU	CD-OE1	5.84	1.32	1.25
2	N	420	GLU	CD-OE1	5.82	1.32	1.25
2	D	420	GLU	CD-OE1	5.82	1.32	1.25
2	R	420	GLU	CD-OE1	5.81	1.32	1.25
1	a	124	GLU	CD-OE1	5.73	1.31	1.25
1	c	124	GLU	CD-OE1	5.73	1.31	1.25
1	Q	124	GLU	CD-OE1	5.72	1.31	1.25
1	C	124	GLU	CD-OE1	5.72	1.31	1.25
1	K	124	GLU	CD-OE1	5.72	1.31	1.25
1	S	124	GLU	CD-OE1	5.72	1.31	1.25
1	W	124	GLU	CD-OE1	5.72	1.31	1.25
1	M	124	GLU	CD-OE1	5.71	1.31	1.25
1	U	124	GLU	CD-OE1	5.70	1.31	1.25
1	A	124	GLU	CD-OE1	5.70	1.31	1.25
1	E	124	GLU	CD-OE1	5.70	1.31	1.25
1	O	124	GLU	CD-OE1	5.70	1.31	1.25
2	B	177	GLU	CD-OE1	5.65	1.31	1.25
1	Y	124	GLU	CD-OE1	5.64	1.31	1.25
1	G	124	GLU	CD-OE1	5.63	1.31	1.25
2	N	177	GLU	CD-OE1	5.61	1.31	1.25
2	J	177	GLU	CD-OE1	5.61	1.31	1.25
2	L	177	GLU	CD-OE1	5.61	1.31	1.25
2	b	177	GLU	CD-OE1	5.61	1.31	1.25
1	I	124	GLU	CD-OE1	5.60	1.31	1.25
2	P	177	GLU	CD-OE1	5.59	1.31	1.25
2	d	177	GLU	CD-OE1	5.59	1.31	1.25
2	R	177	GLU	CD-OE1	5.59	1.31	1.25
2	V	177	GLU	CD-OE1	5.59	1.31	1.25
2	T	177	GLU	CD-OE1	5.58	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	177	GLU	CD-OE1	5.57	1.31	1.25
2	X	177	GLU	CD-OE1	5.57	1.31	1.25
2	H	177	GLU	CD-OE1	5.57	1.31	1.25
2	D	177	GLU	CD-OE1	5.54	1.31	1.25
2	Z	177	GLU	CD-OE1	5.53	1.31	1.25
2	J	181	GLU	CD-OE1	5.52	1.31	1.25
2	b	181	GLU	CD-OE1	5.48	1.31	1.25
2	H	181	GLU	CD-OE1	5.47	1.31	1.25
2	Z	181	GLU	CD-OE1	5.47	1.31	1.25
2	R	181	GLU	CD-OE1	5.46	1.31	1.25
2	L	181	GLU	CD-OE1	5.45	1.31	1.25
2	P	181	GLU	CD-OE1	5.45	1.31	1.25
2	B	181	GLU	CD-OE1	5.45	1.31	1.25
2	F	181	GLU	CD-OE1	5.45	1.31	1.25
2	D	181	GLU	CD-OE1	5.44	1.31	1.25
2	T	181	GLU	CD-OE1	5.43	1.31	1.25
2	V	181	GLU	CD-OE1	5.43	1.31	1.25
2	N	181	GLU	CD-OE1	5.42	1.31	1.25
2	X	181	GLU	CD-OE1	5.41	1.31	1.25
2	D	239	TYR	CE1-CZ	-5.41	1.31	1.38
2	Z	239	TYR	CE1-CZ	-5.41	1.31	1.38
2	d	181	GLU	CD-OE1	5.39	1.31	1.25
2	V	239	TYR	CE1-CZ	-5.38	1.31	1.38
1	K	13	ARG	CZ-NH1	5.37	1.40	1.33
2	X	239	TYR	CE1-CZ	-5.37	1.31	1.38
2	F	239	TYR	CE1-CZ	-5.36	1.31	1.38
2	J	239	TYR	CE1-CZ	-5.36	1.31	1.38
1	W	13	ARG	CZ-NH1	5.36	1.40	1.33
1	M	13	ARG	CZ-NH1	5.35	1.40	1.33
1	Q	13	ARG	CZ-NH1	5.35	1.40	1.33
2	T	239	TYR	CE1-CZ	-5.35	1.31	1.38
1	C	13	ARG	CZ-NH1	5.35	1.40	1.33
1	O	13	ARG	CZ-NH1	5.35	1.40	1.33
1	A	13	ARG	CZ-NH1	5.34	1.40	1.33
2	L	239	TYR	CE1-CZ	-5.34	1.31	1.38
1	S	13	ARG	CZ-NH1	5.34	1.40	1.33
1	I	13	ARG	CZ-NH1	5.34	1.40	1.33
2	N	239	TYR	CE1-CZ	-5.33	1.31	1.38
1	Y	13	ARG	CZ-NH1	5.33	1.40	1.33
2	H	239	TYR	CE1-CZ	-5.33	1.31	1.38
2	d	239	TYR	CE1-CZ	-5.33	1.31	1.38
2	B	239	TYR	CE1-CZ	-5.33	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	239	TYR	CE1-CZ	-5.33	1.31	1.38
1	E	13	ARG	CZ-NH1	5.33	1.40	1.33
2	R	239	TYR	CE1-CZ	-5.33	1.31	1.38
1	U	13	ARG	CZ-NH1	5.32	1.40	1.33
2	P	239	TYR	CE1-CZ	-5.32	1.31	1.38
1	c	13	ARG	CZ-NH1	5.31	1.40	1.33
1	a	13	ARG	CZ-NH1	5.30	1.40	1.33
1	G	13	ARG	CZ-NH1	5.28	1.40	1.33
2	N	50	GLU	CD-OE1	5.25	1.31	1.25
2	N	458	GLU	CD-OE1	5.25	1.31	1.25
2	P	50	GLU	CD-OE1	5.24	1.31	1.25
2	b	458	GLU	CD-OE1	5.23	1.31	1.25
2	F	458	GLU	CD-OE1	5.22	1.31	1.25
2	X	50	GLU	CD-OE1	5.22	1.31	1.25
2	X	458	GLU	CD-OE1	5.21	1.31	1.25
2	Z	458	GLU	CD-OE1	5.21	1.31	1.25
2	V	458	GLU	CD-OE1	5.21	1.31	1.25
2	H	50	GLU	CD-OE1	5.21	1.31	1.25
2	d	458	GLU	CD-OE1	5.20	1.31	1.25
2	D	50	GLU	CD-OE1	5.18	1.31	1.25
2	b	50	GLU	CD-OE1	5.18	1.31	1.25
2	P	458	GLU	CD-OE1	5.18	1.31	1.25
2	R	50	GLU	CD-OE1	5.18	1.31	1.25
2	T	50	GLU	CD-OE1	5.17	1.31	1.25
2	d	50	GLU	CD-OE1	5.17	1.31	1.25
2	R	458	GLU	CD-OE1	5.17	1.31	1.25
2	J	50	GLU	CD-OE1	5.16	1.31	1.25
2	J	458	GLU	CD-OE1	5.16	1.31	1.25
2	L	50	GLU	CD-OE1	5.16	1.31	1.25
2	L	458	GLU	CD-OE1	5.16	1.31	1.25
2	B	50	GLU	CD-OE1	5.15	1.31	1.25
2	B	458	GLU	CD-OE1	5.13	1.31	1.25
2	F	50	GLU	CD-OE1	5.13	1.31	1.25
2	H	458	GLU	CD-OE1	5.12	1.31	1.25
2	V	50	GLU	CD-OE1	5.11	1.31	1.25
2	Z	50	GLU	CD-OE1	5.11	1.31	1.25
2	D	458	GLU	CD-OE1	5.10	1.31	1.25
1	c	114	ARG	CZ-NH1	5.09	1.39	1.33
1	I	114	ARG	CZ-NH1	5.08	1.39	1.33
1	S	114	ARG	CZ-NH1	5.08	1.39	1.33
1	U	114	ARG	CZ-NH1	5.08	1.39	1.33
1	E	114	ARG	CZ-NH1	5.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	114	ARG	CZ-NH1	5.08	1.39	1.33
2	T	458	GLU	CD-OE1	5.08	1.31	1.25
1	K	114	ARG	CZ-NH1	5.07	1.39	1.33
1	Q	114	ARG	CZ-NH1	5.07	1.39	1.33
1	G	114	ARG	CZ-NH1	5.06	1.39	1.33
1	A	114	ARG	CZ-NH1	5.05	1.39	1.33
1	W	114	ARG	CZ-NH1	5.03	1.39	1.33
1	O	114	ARG	CZ-NH1	5.02	1.39	1.33
1	Y	114	ARG	CZ-NH1	5.02	1.39	1.33
2	B	497	GLU	CD-OE1	5.02	1.31	1.25
1	a	114	ARG	CZ-NH1	5.01	1.39	1.33
1	C	114	ARG	CZ-NH1	5.01	1.39	1.33

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	13	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	a	13	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	G	13	ARG	NE-CZ-NH2	-11.93	114.33	120.30
1	S	13	ARG	NE-CZ-NH2	-11.91	114.34	120.30
1	O	13	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	A	13	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	U	13	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	W	13	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	c	13	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	I	13	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	C	13	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	E	13	ARG	NE-CZ-NH2	-11.81	114.40	120.30
1	K	13	ARG	NE-CZ-NH2	-11.79	114.40	120.30
1	Q	13	ARG	NE-CZ-NH2	-11.77	114.41	120.30
1	M	13	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	A	18	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	C	18	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	M	18	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	Y	18	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	K	18	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	G	18	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	W	18	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	I	18	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	c	18	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	O	18	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	a	18	ARG	NE-CZ-NH2	-9.08	115.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	18	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	U	18	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	S	18	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	Q	18	ARG	NE-CZ-NH2	-9.03	115.78	120.30
2	d	390	ARG	NE-CZ-NH2	-8.64	115.98	120.30
2	B	390	ARG	NE-CZ-NH2	-8.60	116.00	120.30
2	P	390	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	T	390	ARG	NE-CZ-NH2	-8.55	116.03	120.30
2	N	390	ARG	NE-CZ-NH2	-8.54	116.03	120.30
2	V	390	ARG	NE-CZ-NH2	-8.53	116.04	120.30
2	X	390	ARG	NE-CZ-NH2	-8.51	116.04	120.30
2	J	390	ARG	NE-CZ-NH2	-8.50	116.05	120.30
2	b	390	ARG	NE-CZ-NH2	-8.50	116.05	120.30
2	H	390	ARG	NE-CZ-NH2	-8.49	116.05	120.30
2	F	390	ARG	NE-CZ-NH2	-8.48	116.06	120.30
2	Z	390	ARG	NE-CZ-NH2	-8.48	116.06	120.30
2	D	390	ARG	NE-CZ-NH2	-8.47	116.06	120.30
2	R	390	ARG	NE-CZ-NH2	-8.47	116.06	120.30
2	L	390	ARG	NE-CZ-NH2	-8.46	116.07	120.30
2	R	150	GLU	OE1-CD-OE2	6.74	131.39	123.30
2	b	150	GLU	OE1-CD-OE2	6.74	131.39	123.30
2	X	150	GLU	OE1-CD-OE2	6.72	131.37	123.30
2	D	150	GLU	OE1-CD-OE2	6.72	131.36	123.30
2	F	150	GLU	OE1-CD-OE2	6.71	131.35	123.30
2	H	150	GLU	OE1-CD-OE2	6.71	131.35	123.30
2	T	150	GLU	OE1-CD-OE2	6.70	131.34	123.30
2	N	150	GLU	OE1-CD-OE2	6.70	131.34	123.30
2	J	150	GLU	OE1-CD-OE2	6.69	131.32	123.30
2	d	150	GLU	OE1-CD-OE2	6.68	131.32	123.30
2	L	150	GLU	OE1-CD-OE2	6.67	131.30	123.30
2	D	486	LEU	CB-CG-CD2	-6.67	99.67	111.00
2	B	150	GLU	OE1-CD-OE2	6.66	131.30	123.30
2	P	150	GLU	OE1-CD-OE2	6.66	131.30	123.30
2	V	150	GLU	OE1-CD-OE2	6.66	131.29	123.30
2	Z	150	GLU	OE1-CD-OE2	6.66	131.29	123.30
2	B	486	LEU	CB-CG-CD2	-6.65	99.69	111.00
2	N	486	LEU	CB-CG-CD2	-6.65	99.69	111.00
2	V	486	LEU	CB-CG-CD2	-6.65	99.69	111.00
2	L	486	LEU	CB-CG-CD2	-6.65	99.70	111.00
2	R	486	LEU	CB-CG-CD2	-6.65	99.70	111.00
2	X	486	LEU	CB-CG-CD2	-6.65	99.70	111.00
2	T	486	LEU	CB-CG-CD2	-6.64	99.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	486	LEU	CB-CG-CD2	-6.64	99.71	111.00
2	F	486	LEU	CB-CG-CD2	-6.64	99.71	111.00
2	b	486	LEU	CB-CG-CD2	-6.64	99.71	111.00
2	d	486	LEU	CB-CG-CD2	-6.64	99.72	111.00
2	H	486	LEU	CB-CG-CD2	-6.63	99.73	111.00
2	P	486	LEU	CB-CG-CD2	-6.63	99.73	111.00
2	Z	486	LEU	CB-CG-CD2	-6.63	99.73	111.00
2	N	109	GLU	OE1-CD-OE2	-6.03	116.07	123.30
2	d	109	GLU	OE1-CD-OE2	-6.02	116.07	123.30
2	V	109	GLU	OE1-CD-OE2	-6.02	116.08	123.30
2	D	109	GLU	OE1-CD-OE2	-6.00	116.10	123.30
2	R	109	GLU	OE1-CD-OE2	-6.00	116.10	123.30
2	P	109	GLU	OE1-CD-OE2	-6.00	116.10	123.30
2	J	109	GLU	OE1-CD-OE2	-6.00	116.11	123.30
2	F	109	GLU	OE1-CD-OE2	-5.99	116.11	123.30
2	L	109	GLU	OE1-CD-OE2	-5.98	116.12	123.30
2	Z	109	GLU	OE1-CD-OE2	-5.97	116.13	123.30
2	X	109	GLU	OE1-CD-OE2	-5.97	116.14	123.30
2	B	109	GLU	OE1-CD-OE2	-5.97	116.14	123.30
2	T	109	GLU	OE1-CD-OE2	-5.96	116.14	123.30
1	A	18	ARG	NH1-CZ-NH2	5.96	125.96	119.40
2	b	109	GLU	OE1-CD-OE2	-5.96	116.14	123.30
2	H	109	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	a	18	ARG	NH1-CZ-NH2	5.96	125.95	119.40
1	M	18	ARG	NH1-CZ-NH2	5.95	125.94	119.40
1	C	18	ARG	NH1-CZ-NH2	5.95	125.94	119.40
1	K	18	ARG	NH1-CZ-NH2	5.94	125.94	119.40
1	S	18	ARG	NH1-CZ-NH2	5.94	125.93	119.40
1	Y	18	ARG	NH1-CZ-NH2	5.94	125.93	119.40
1	W	18	ARG	NH1-CZ-NH2	5.93	125.92	119.40
1	G	18	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	Q	18	ARG	NH1-CZ-NH2	5.91	125.90	119.40
1	c	18	ARG	NH1-CZ-NH2	5.91	125.90	119.40
1	O	18	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	U	18	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	E	18	ARG	NH1-CZ-NH2	5.89	125.88	119.40
1	I	18	ARG	NH1-CZ-NH2	5.89	125.88	119.40
2	L	99	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	M	74	LEU	CB-CG-CD1	-5.61	101.47	111.00
1	G	74	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	I	74	LEU	CB-CG-CD1	-5.60	101.47	111.00
1	A	74	LEU	CB-CG-CD1	-5.60	101.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	74	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	Y	74	LEU	CB-CG-CD1	-5.59	101.50	111.00
2	J	99	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	C	74	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	Q	74	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	S	74	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	c	74	LEU	CB-CG-CD1	-5.58	101.51	111.00
2	H	99	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	U	74	LEU	CB-CG-CD1	-5.58	101.52	111.00
1	W	74	LEU	CB-CG-CD1	-5.57	101.52	111.00
1	E	74	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	K	74	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	Y	13	ARG	NH1-CZ-NH2	5.56	125.52	119.40
1	O	74	LEU	CB-CG-CD1	-5.56	101.55	111.00
2	X	99	ARG	NE-CZ-NH2	5.55	123.08	120.30
2	d	99	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	O	13	ARG	NH1-CZ-NH2	5.54	125.49	119.40
1	G	13	ARG	NH1-CZ-NH2	5.54	125.49	119.40
2	R	99	ARG	NE-CZ-NH2	5.53	123.07	120.30
2	Z	99	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	U	13	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	S	13	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	A	13	ARG	NH1-CZ-NH2	5.53	125.48	119.40
2	T	99	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	K	13	ARG	NH1-CZ-NH2	5.52	125.47	119.40
1	E	13	ARG	NH1-CZ-NH2	5.52	125.47	119.40
2	V	99	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	C	13	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	W	13	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	Q	13	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	a	13	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	c	13	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	I	13	ARG	NH1-CZ-NH2	5.49	125.43	119.40
2	F	99	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	B	99	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	M	13	ARG	NH1-CZ-NH2	5.48	125.42	119.40
2	N	99	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	b	99	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	P	99	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	D	99	ARG	NE-CZ-NH2	5.43	123.01	120.30
2	J	399	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	T	399	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	399	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	L	399	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	Z	399	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	R	399	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	D	399	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	d	399	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	N	399	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	P	372	LYS	CD-CE-NZ	-5.21	99.70	111.70
2	Z	372	LYS	CD-CE-NZ	-5.21	99.71	111.70
2	d	372	LYS	CD-CE-NZ	-5.21	99.72	111.70
2	b	372	LYS	CD-CE-NZ	-5.20	99.73	111.70
2	J	372	LYS	CD-CE-NZ	-5.20	99.74	111.70
2	N	372	LYS	CD-CE-NZ	-5.20	99.74	111.70
2	B	372	LYS	CD-CE-NZ	-5.20	99.75	111.70
2	H	372	LYS	CD-CE-NZ	-5.20	99.74	111.70
2	R	372	LYS	CD-CE-NZ	-5.20	99.75	111.70
2	V	372	LYS	CD-CE-NZ	-5.20	99.74	111.70
2	X	372	LYS	CD-CE-NZ	-5.20	99.74	111.70
2	L	372	LYS	CD-CE-NZ	-5.20	99.75	111.70
2	T	372	LYS	CD-CE-NZ	-5.19	99.76	111.70
2	V	399	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	F	399	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	X	399	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	D	372	LYS	CD-CE-NZ	-5.18	99.78	111.70
2	F	372	LYS	CD-CE-NZ	-5.18	99.79	111.70
2	b	399	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	B	399	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	71	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	a	71	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	71	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	M	71	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	Q	71	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	S	71	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	b	410	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	G	71	ASP	CB-CG-OD2	-5.13	113.68	118.30
2	P	399	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	V	410	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	W	71	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	Y	71	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	K	71	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	E	71	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	O	71	ASP	CB-CG-OD2	-5.11	113.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	410	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	d	410	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	I	71	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	L	410	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	c	71	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	H	410	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	U	71	ASP	CB-CG-OD2	-5.07	113.74	118.30
2	R	410	ASP	CB-CG-OD2	-5.06	113.74	118.30
2	J	410	ASP	CB-CG-OD2	-5.06	113.75	118.30
2	P	410	ASP	CB-CG-OD2	-5.05	113.75	118.30
2	Z	410	ASP	CB-CG-OD2	-5.04	113.76	118.30
2	T	410	ASP	CB-CG-OD2	-5.04	113.77	118.30
2	X	410	ASP	CB-CG-OD2	-5.04	113.77	118.30
2	D	410	ASP	CB-CG-OD2	-5.03	113.77	118.30
2	N	410	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	B	410	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	C	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	E	130/132 (98%)	121 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	I	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	K	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	M	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	O	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	Q	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	S	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	U	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	W	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	Y	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	a	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
1	c	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
2	B	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	D	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	F	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	H	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	J	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	L	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	N	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	P	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	R	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	T	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	V	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	X	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	Z	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	b	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
2	d	459/461 (100%)	442 (96%)	17 (4%)	0	100	100
All	All	8835/8895 (99%)	8445 (96%)	390 (4%)	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	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	C	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	E	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	G	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	I	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	K	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	M	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	O	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	Q	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	S	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	U	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	W	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	Y	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	a	110/110 (100%)	108 (98%)	2 (2%)	59	78
1	c	110/110 (100%)	108 (98%)	2 (2%)	59	78
2	B	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	D	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	F	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	H	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	J	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	L	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	N	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	P	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	R	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	T	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	V	384/384 (100%)	381 (99%)	3 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	Z	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	b	384/384 (100%)	381 (99%)	3 (1%)	81	89
2	d	384/384 (100%)	381 (99%)	3 (1%)	81	89
All	All	7410/7410 (100%)	7335 (99%)	75 (1%)	77	85

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	27	LEU
2	B	46	ARG
2	B	160	TYR
2	B	473	LEU
1	C	22	GLU
1	C	27	LEU
2	D	46	ARG
2	D	160	TYR
2	D	473	LEU
1	E	22	GLU
1	E	27	LEU
2	F	46	ARG
2	F	160	TYR
2	F	473	LEU
1	G	22	GLU
1	G	27	LEU
2	H	46	ARG
2	H	160	TYR
2	H	473	LEU
1	I	22	GLU
1	I	27	LEU
2	J	46	ARG
2	J	160	TYR
2	J	473	LEU
1	K	22	GLU
1	K	27	LEU
2	L	46	ARG
2	L	160	TYR
2	L	473	LEU
1	M	22	GLU
1	M	27	LEU

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Mol	Chain	Res	Type
2	N	46	ARG
2	N	160	TYR
2	N	473	LEU
1	O	22	GLU
1	O	27	LEU
2	P	46	ARG
2	P	160	TYR
2	P	473	LEU
1	Q	22	GLU
1	Q	27	LEU
2	R	46	ARG
2	R	160	TYR
2	R	473	LEU
1	S	22	GLU
1	S	27	LEU
2	T	46	ARG
2	T	160	TYR
2	T	473	LEU
1	U	22	GLU
1	U	27	LEU
2	V	46	ARG
2	V	160	TYR
2	V	473	LEU
1	W	22	GLU
1	W	27	LEU
2	X	46	ARG
2	X	160	TYR
2	X	473	LEU
1	Y	22	GLU
1	Y	27	LEU
2	Z	46	ARG
2	Z	160	TYR
2	Z	473	LEU
1	a	22	GLU
1	a	27	LEU
2	b	46	ARG
2	b	160	TYR
2	b	473	LEU
1	c	22	GLU
1	c	27	LEU
2	d	46	ARG
2	d	160	TYR

Continued on next page...

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Mol	Chain	Res	Type
2	d	473	LEU

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

Mol	Chain	Res	Type
1	A	54	GLN
2	B	113	GLN
2	B	291	ASN
1	C	54	GLN
1	C	131	ASN
2	D	113	GLN
2	D	291	ASN
1	E	54	GLN
2	F	113	GLN
2	F	291	ASN
1	G	54	GLN
2	H	113	GLN
2	H	291	ASN
1	I	54	GLN
2	J	113	GLN
2	J	291	ASN
1	K	54	GLN
2	L	113	GLN
2	L	291	ASN
1	M	54	GLN
2	N	113	GLN
2	N	291	ASN
1	O	54	GLN
2	P	113	GLN
2	P	291	ASN
1	Q	54	GLN
2	R	113	GLN
2	R	291	ASN
1	S	54	GLN
2	T	113	GLN
2	T	291	ASN
1	U	54	GLN
2	V	113	GLN
2	V	291	ASN
1	W	54	GLN
2	X	113	GLN
2	X	291	ASN

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Mol	Chain	Res	Type
1	Y	54	GLN
2	Z	113	GLN
2	Z	291	ASN
1	a	54	GLN
1	a	87	ASN
2	b	113	GLN
2	b	291	ASN
1	c	54	GLN
1	c	87	ASN
1	c	131	ASN
2	d	113	GLN
2	d	291	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

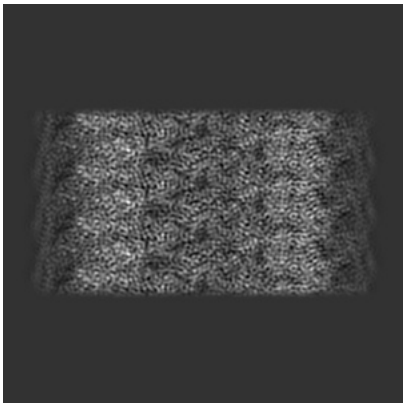
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3600. These allow visual inspection of the internal detail of the map and identification of artifacts.

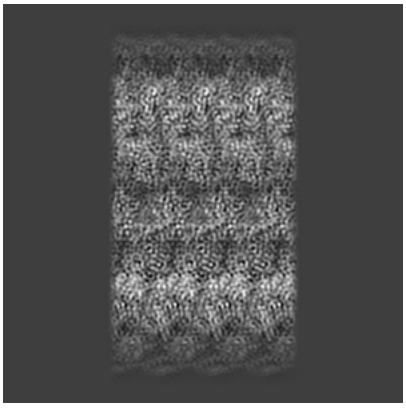
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

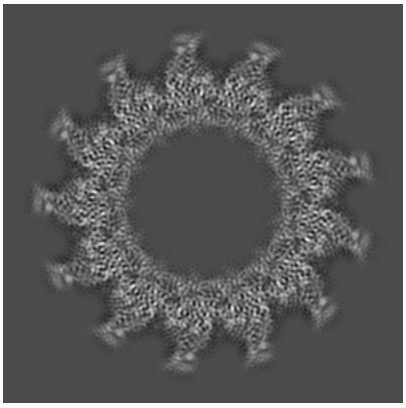
6.1.1 Primary map



X



Y

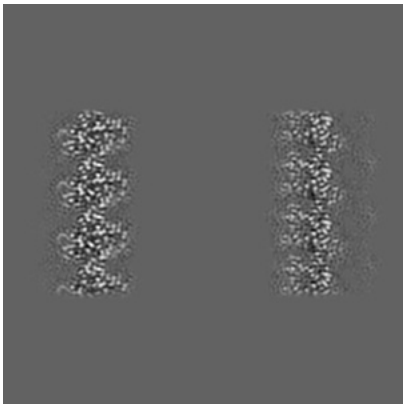


Z

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

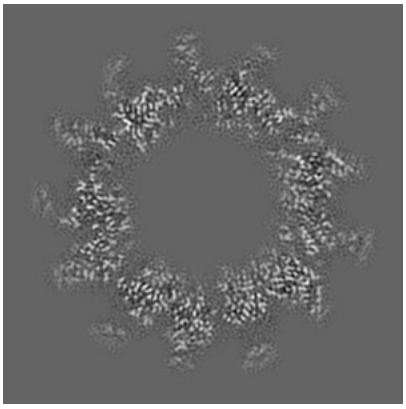
6.2 Central slices (i)

6.2.1 Primary map



X Index: 125

Y Index: 125

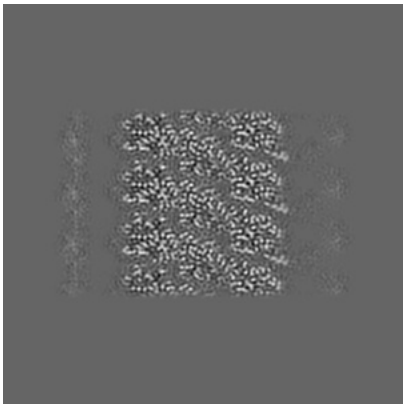


Z Index: 125

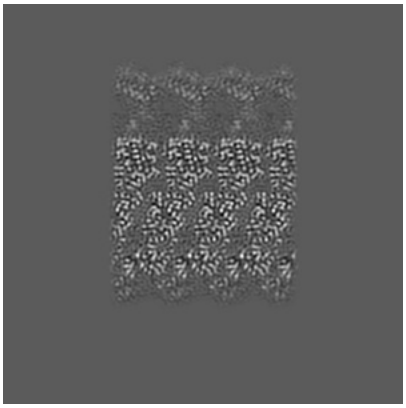
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

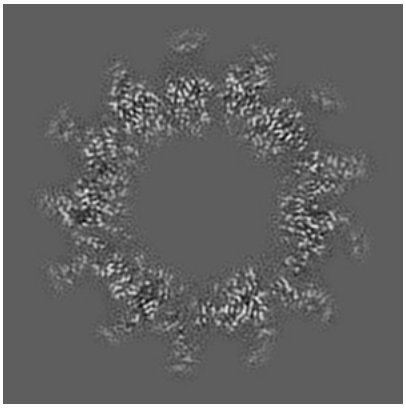
6.3.1 Primary map



X Index: 60



Y Index: 59

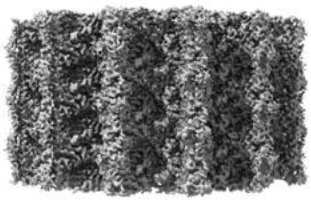


Z Index: 117

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

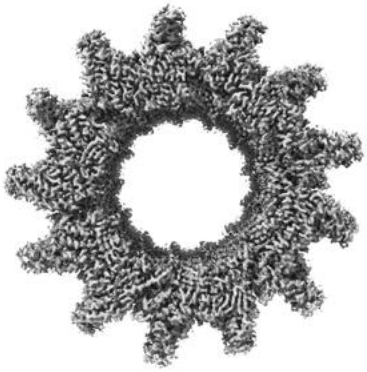
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0385. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

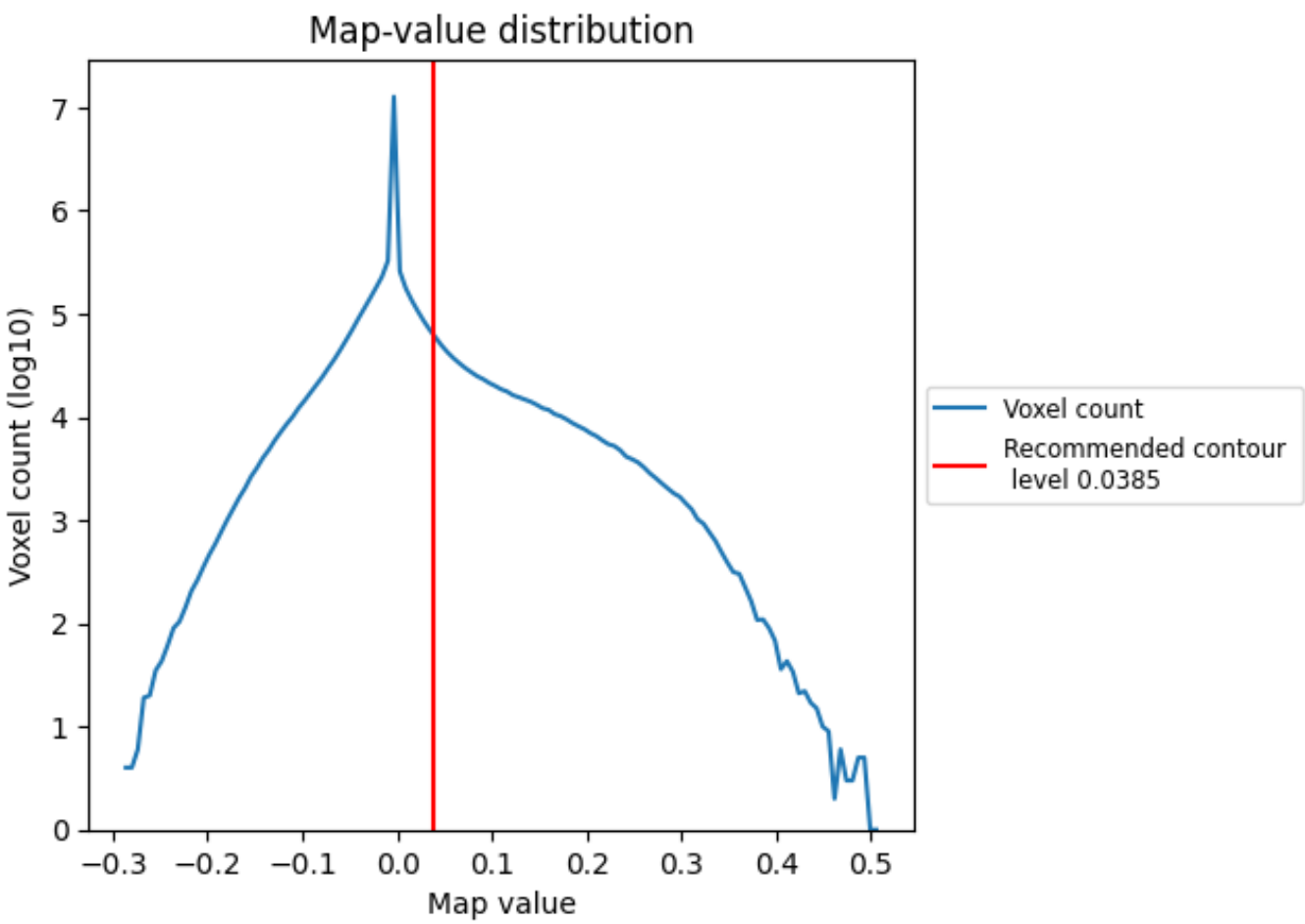
6.5 Mask visualisation (i)

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

7 Map analysis (i)

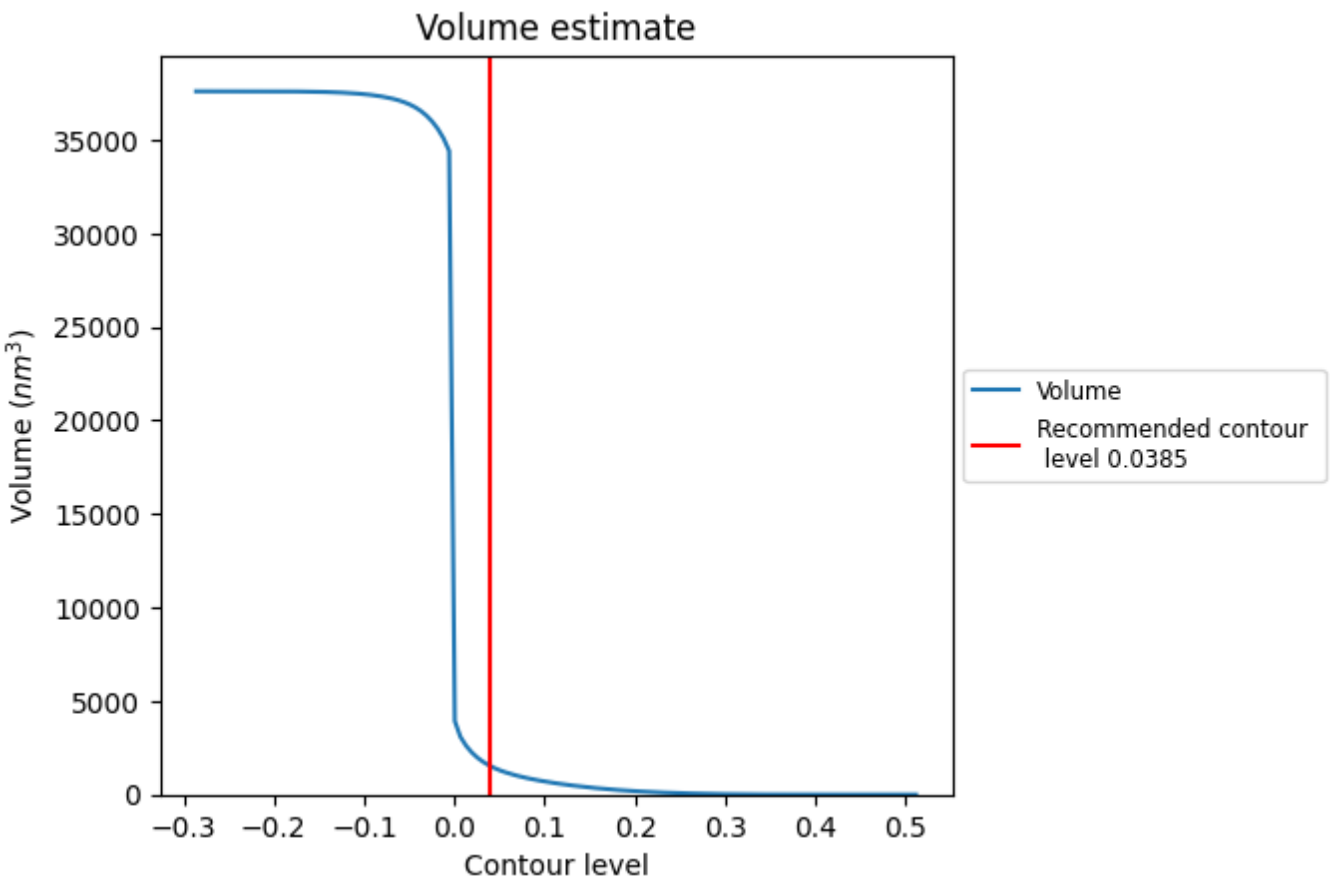
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

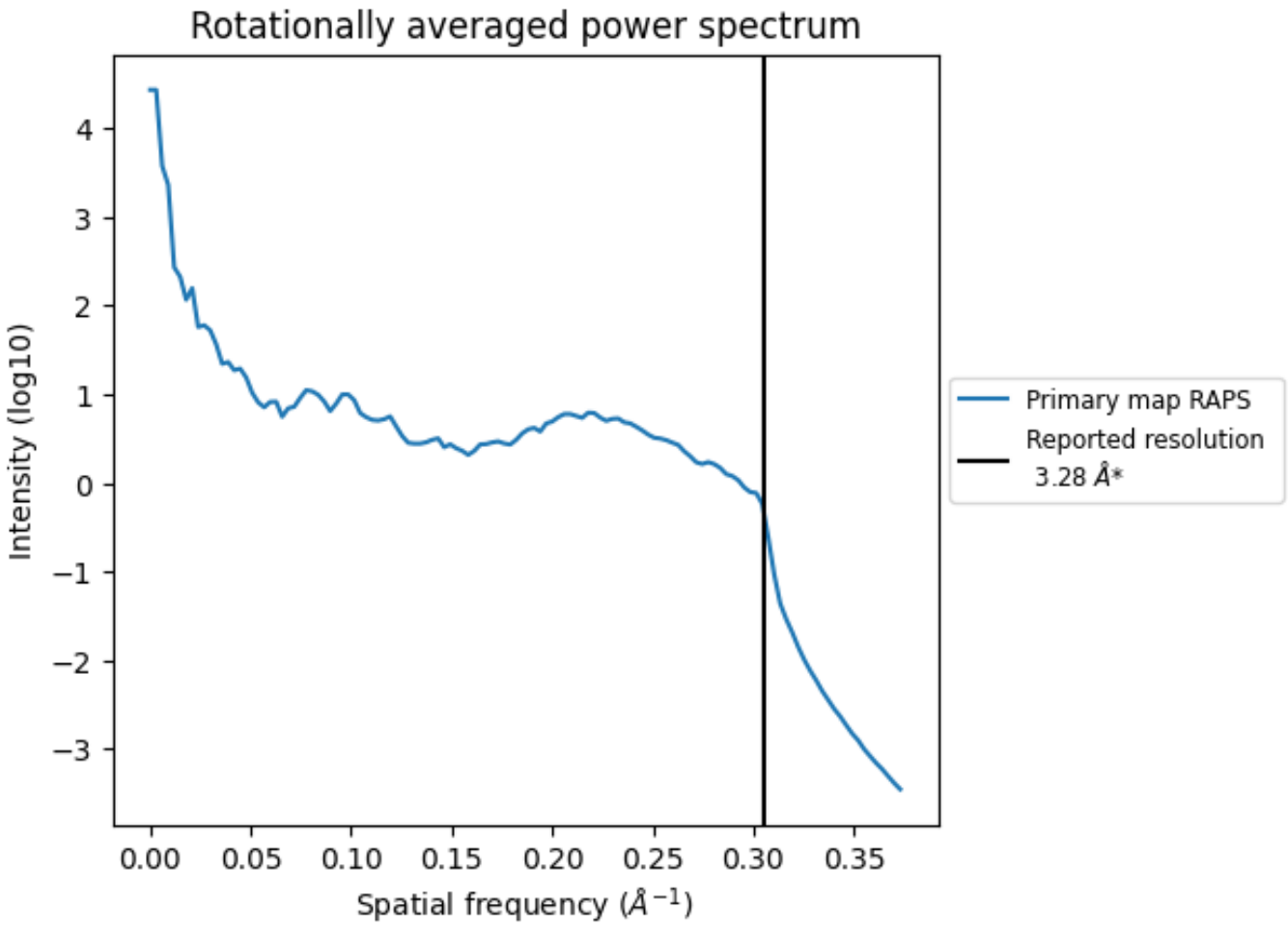
7.2 Volume estimate (i)



The volume at the recommended contour level is 1563 nm^3; this corresponds to an approximate mass of 1412 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 0.305 Å^{-1}

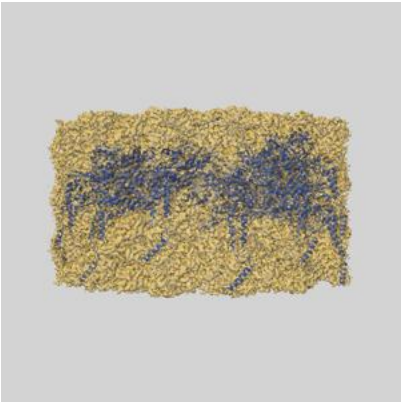
8 Fourier-Shell correlation (i)

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

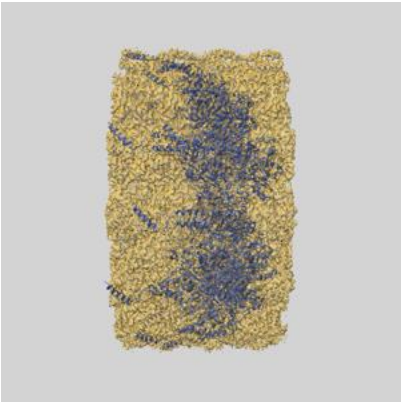
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3600 and PDB model 5N8N. Per-residue inclusion information can be found in section 3 on page 6.

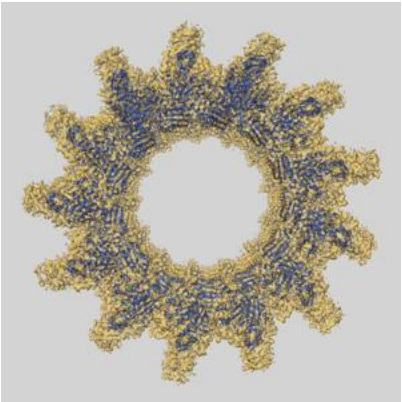
9.1 Map-model overlay (i)



X



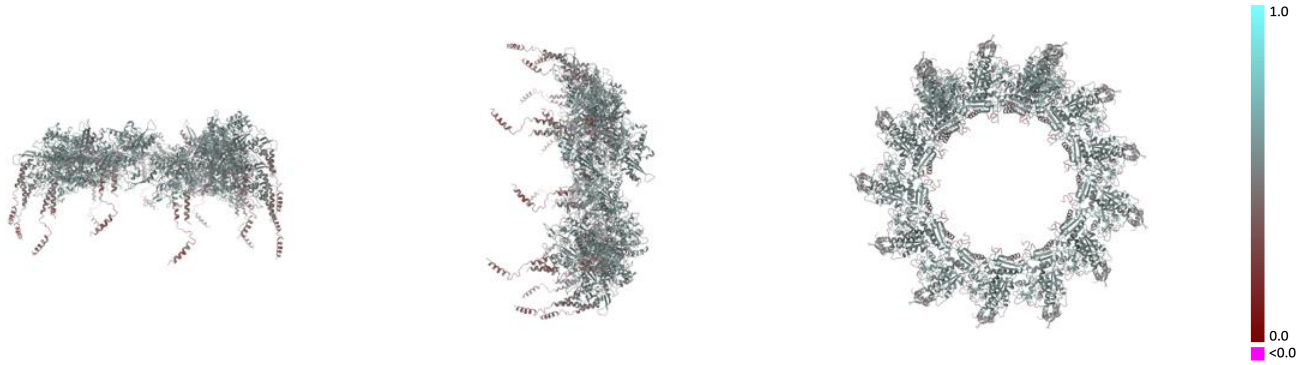
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0385 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.

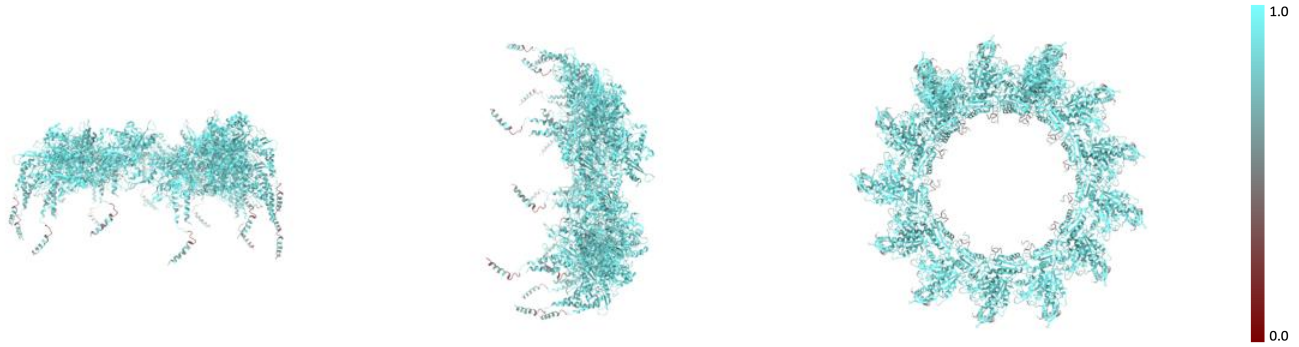
9.2 Q-score mapped to coordinate model (i)



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.

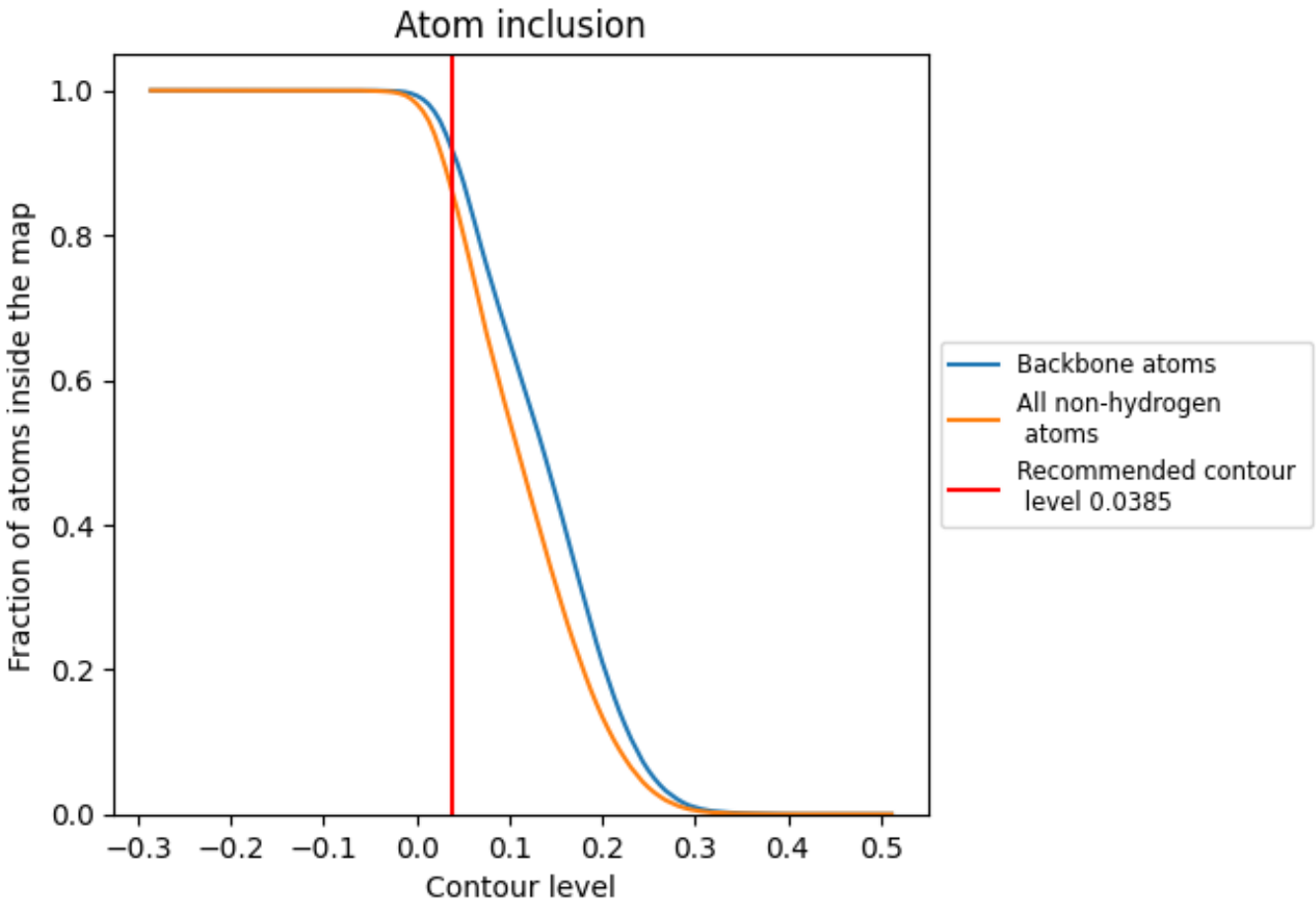
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0385).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0385) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8599	0.5090
A	0.8532	0.5010
B	0.8525	0.5080
C	0.8552	0.5040
D	0.8545	0.5080
E	0.8581	0.4990
F	0.8612	0.5110
G	0.8601	0.5000
H	0.8589	0.5110
I	0.8532	0.5030
J	0.8606	0.5120
K	0.8591	0.5050
L	0.8564	0.5120
M	0.8581	0.5050
N	0.8640	0.5130
O	0.8681	0.5060
P	0.8612	0.5130
Q	0.8631	0.5050
R	0.8592	0.5100
S	0.8581	0.5020
T	0.8595	0.5130
U	0.8542	0.5030
V	0.8668	0.5120
W	0.8641	0.5050
X	0.8626	0.5100
Y	0.8512	0.5030
Z	0.8654	0.5100
a	0.8591	0.5050
b	0.8592	0.5100
c	0.8641	0.5060
d	0.8626	0.5090