

Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 10:36 AM EST

PDB ID : 6X2I

EMDB ID : EMD-22008

Title : The Cutavirus (CuV) capsid structure Authors : Mietzsch, M.; Agbandje-McKenna, M.

Deposited on : 2020-05-20

Resolution : 2.87 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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $MapQ \quad : \quad 1.9.13$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

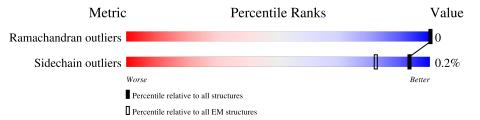
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.87 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
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	1	538	100%
1	2	538	100%
1	3	538	100%
1	4	538	100%
1	5	538	100%
1	6	538	100%
1	7	538	100%
1	8	538	100%
1	A	538	100%



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Mol	Chain	Length	Quality of chain
1	В	538	100%
1	С	538	100%
1	D	538	100%
1	Е	538	100%
1	F	538	100%
1	G	538	100%
1	Н	538	100%
1	I	538	100%
1	J	538	100%
1	K	538	100%
1	L	538	100%
1	M	538	100%
1	N	538	100%
1	О	538	100%
1	Р	538	100%
1	Q	538	100%
1	R	538	100%
1	S	538	100%
1	Т	538	100%
1	U	538	100%
1	V	538	100%
1	W	538	100%
1	X	538	100%
1	Y	538	100%
1	Z	538	100%



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Mol	Chain	Length	Quality of chain
1	a	538	100%
1	b	538	100%
1	c	538	100%
1	d	538	100%
1	е	538	100%
1	f	538	100%
1	g	538	100%
1	h	538	100%
1	i	538	100%
1	j	538	100%
1	k	538	100%
1	1	538	100%
1	m	538	100%
1	n	538	100%
1	О	538	100%
1	р	538	100%
1	q	538	100%
1	r	538	100%
1	s	538	100%
1	t	538	100%
1	u	538	100%
1	V	538	100%
1	W	538	100%
1	X	538	100%
1	у	538	100%
	J		1



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Mol	Chain	Length	Quality of chain
1	Z	538	100%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 259740 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 VP2.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	Λ	F 90	Total	С	N	О	S	0	0
1	A	538	4329	2737	760	816	16	0	0
1	D	F20	Total	С	N	О	S	0	0
1	В	538	4329	2737	760	816	16	0	0
1	С	538	Total	С	N	О	S	0	0
1	C	999	4329	2737	760	816	16	U	U
1	D	538	Total	С	N	О	S	0	0
1	D	990	4329	2737	760	816	16	U	U
1		538	Total	С	N	О	S	0	0
1	ъ	990	4329	2737	760	816	16	0	U
1	F	538	Total	С	N	О	S	0	0
1	Г	990	4329	2737	760	816	16	0	U
1	G	538	Total	С	N	О	S	0	0
1	G	936	4329	2737	760	816	16	0	U
1	Н	538	Total	С	N	О	S	0	0
1	11	990	4329	2737	760	816	16	U	
1	I	538	Total	С	N	О	S	0	0
1	1	990	4329	2737	760	816	16	U	U
1	J	538	Total	С	N	O	S	0	0
1	J	550	4329	2737	760	816	16	0	U
1	K	538	Total	\mathbf{C}	N	O	S	0	0
1	11	550	4329	2737	760	816	16	U	U
1	L	538	Total	\mathbf{C}	N	Ο	\mathbf{S}	0	0
1	п	550	4329	2737	760	816	16	O	U
1	M	538	Total	\mathbf{C}	N	Ο	\mathbf{S}	0	0
1	1V1	550	4329	2737	760	816	16	O	U
1	N	538	Total	С	N	Ο	S	0	0
1	11	550	4329	2737	760	816	16	O	U
1	O 538	538	Total	С	Ν	О	S	0	0
1		550	4329	2737	760	816	16	U	0
1	P 538	538	Total	С	N	О	\mathbf{S}	0	0
1		550	4329	2737	760	816	16	U	U
1	Q	538	Total	С	N	О	\mathbf{S}	0	0
1	\sim	990	4329	2737	760	816	16		0



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Mol	Chain	$oxed{ \mathbf{Residues} }$	<i>ye</i>	Δ+	oms			AltConf	Trace
IVIOI	Chain	recsiques	Total	$\frac{110}{C}$	N	0	S	711000111	Trace
1	R	538	4329	2737	760	816	16	0	0
1	S	538	Total	C	N	0	S	0	0
			4329 Total	$\frac{2737}{C}$	$\frac{760}{N}$	816 O	$\frac{16}{S}$		
1	T	538	4329	2737	760	816	16	0	0
1	U	538	Total	С	N	0	S	0	0
			4329 Total	$\frac{2737}{C}$	$\frac{760}{N}$	816 O	$\frac{16}{S}$		
1	V	538	4329	2737	760	816	16	0	0
1	W	538	Total	С	N	О	S	0	0
	**	000	4329	2737	760	816	16 S	0	
1	X	538	Total 4329	C 2737	N 760	O 816	5 16	0	0
1	Y	538	Total	С	N	О	S	0	0
	1	990	4329	2737	760	816	16	0	
1	Z	538	Total 4329	C 2737	N 760	O 816	S 16	0	0
1	_	F20	Total	C	N	0	S	0	0
1	a	538	4329	2737	760	816	16	0	0
1	b	538	Total 4329	C 2737	N 760	O 816	S 16	0	0
		* 20	Total	C	N	0	S 10		
1	С	538	4329	2737	760	816	16	0	0
1	d	538	Total	C	N 760	0	S	0	0
			4329 Total	$\frac{2737}{C}$	$\frac{760}{N}$	816 O	$\frac{16}{S}$		
1	е	538	4329	2737	760	816	16	0	0
1	f	538	Total	С	N	0	S	0	0
			4329 Total	$\frac{2737}{C}$	$\frac{760}{N}$	816 O	$\frac{16}{S}$		
1	g	538	4329	2737	760	816	16	0	0
1	h	538	Total	С	N	0	S	0	0
			4329 Total	$\frac{2737}{C}$	$\frac{760}{N}$	816 O	$\frac{16}{S}$		
1	i	538	4329	2737	760	816	3 16	0	0
1	j	538	Total	С	N	О	S	0	0
	J		4329 Total	2737 C	$\frac{760}{N}$	816 O	$\frac{16}{S}$		
1	k	538	4329	2737	760	816	5 16	0	0
1	1	538	Total	С	N	О	S	0	0
	1	000	4329	2737	760	816	$\frac{16}{C}$		



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Mol	Chain	$oxed{ egin{array}{c} \mathbf{Residues} \end{array} }$	<i>ye</i>	A t.	oms			AltConf	Trace
11101	Chain	residues	Total	$\frac{110}{\mathrm{C}}$	N	0	S	711000111	Trace
1	m	538	4329	2737	760	816	16	0	0
			Total	C	N	0	S		
1	n	538	4329	2737	760	816	16	0	0
		700	Total	C	N	О	S	0	
1	О	538	4329	2737	760	816	16	0	0
1		120	Total	С	N	О	S	0	0
1	p	538	4329	2737	760	816	16	0	0
1	a	538	Total	С	N	О	S	0	0
1	q	990	4329	2737	760	816	16	0	U
1	r	538	Total	\mathbf{C}	N	Ο	S	0	0
1	1	990	4329	2737	760	816	16		
1	s	538	Total	С	N	О	S	0	0
	~	000	4329	2737	760	816	16		Ů
1	t	538	Total	С	N	0	S	0	0
			4329	2737	760	816	16		
1	u	538	Total	C	N	0	S	0	0
			4329	2737	760	816	16		
1	V	538	Total	C	N 700	0	S	0	0
			4329	$\frac{2737}{C}$	$\frac{760}{N}$	816	$\frac{16}{S}$		
1	W	538	Total 4329	2737	760	O 816	5 16	0	0
			Total	C	N	0	S 10		
1	X	538	4329	2737	760	816	16	0	0
			Total	C	N	0	$\frac{10}{S}$		
1	У	538	4329	2737	760	816	16	0	0
			Total	C	N	0	S	_	_
1	Z	538	4329	2737	760	816	16	0	0
1	-	7 00	Total	С	N	О	S	0	0
1	1	538	4329	2737	760	816	16	0	0
1	2	£20	Total	С	N	О	S	0	0
1	2	538	4329	2737	760	816	16	0	0
1	3	538	Total	С	N	О	S	0	0
1	J	930	4329	2737	760	816	16	U	U
1	4	538	Total	\mathbf{C}	N	Ο	S	0	0
1	7	000	4329	2737	760	816	16	0	U
1	5	538	Total	С	N	О	S	0	0
			4329	2737	760	816	16		U
1	6	538	Total	С	N	0	S	0	0
	-		4329	2737	760	816	16	-	U
1	7	538	Total	C	N	0	S	0	0
			4329	2737	760	816	16		



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Mol	Chain	Residues	Atoms			AltConf	Trace		
1	8	538	Total 4329	C 2737	N 760	O 816	S 16	0	0



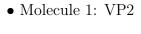
3 Residue-property plots (i)

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: VP2		
Chain A:	100%	
632 1,184 1,207 1,669		
• Molecule 1: VP2		
Chain B:	100%	
11.194 1.1207 1.1569		
• Molecule 1: VP2		
Chain C:	100%	
1.184 1.184		
• Molecule 1: VP2		
Chain D:	100%	
11.07 1.1.09 1.1.00 1.1		
• Molecule 1: VP2		
Chain E:	100%	
1.184 1.184		
• Molecule 1: VP2		
Chain F:	100%	



1184 1207 1569		
• Molecule 1: VP2		
Chain G:	100%	
1,184 1,184 1,267 1,269		
• Molecule 1: VP2		
Chain H:	100%	
1207 1207 1569		
• Molecule 1: VP2		
Chain I:	100%	
L184 L1207 L569		
• Molecule 1: VP2		
Chain J:	100%	
632 11184 11207 11569		
• Molecule 1: VP2		
Chain K:	100%	
L184 L1207 L569		
• Molecule 1: VP2		
Chain L:	100%	



Chain M: 100%



	4		0
2	00	0	9
63	17	12	15

• Molecule 1: VP2

Chain N:

100%



• Molecule 1: VP2

Chain O:



• Molecule 1: VP2

Chain P:



• Molecule 1: VP2

Chain Q: 100%



• Molecule 1: VP2

Chain R:



• Molecule 1: VP2

Chain S: 100%

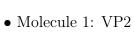


• Molecule 1: VP2

Chain T:



11 84 12 12 18 18 18 18 18 18 18 18 18 18 18 18 18	
• Molecule 1: VP2	
Chain U:	100%
120 134 150 150 150 150 150 150 150 150 150 150	
• Molecule 1: VP2	
Chain V:	100%
120 120 120 120 120 120 120 120 120 120	
• Molecule 1: VP2	
Chain W:	100%
1184 1207 1207 1569	
• Molecule 1: VP2	
Chain X:	100%
11 94 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
• Molecule 1: VP2	
Chain Y:	100%
1184 1207 1207 1569	
• Molecule 1: VP2	
Chain Z:	100%



Chain a: 100%



Chain h:

11 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 1 84 1 1 84 1 1 84 1 84 1 1 84 1	
• Molecule 1: VP2	
Chain b:	100%
L207	
• Molecule 1: VP2	
Chain c:	100%
12.07 12.07 12.07 15.68	
• Molecule 1: VP2	
Chain d:	100%
1184 1207 11689	
• Molecule 1: VP2	
Chain e:	100%
12	
• Molecule 1: VP2	
Chain f:	100%
1184 1207 1569	
• Molecule 1: VP2	
Chain g:	100%
L207	
• Molecule 1: VP2	



 \bullet Molecule 1: VP2

Chain o:

11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		
• Molecule 1: VP2		
Chain i:	100%	
L207 L184 L569		
• Molecule 1: VP2		
Chain j:	100%	
120 1207 1569		
• Molecule 1: VP2		
Chain k:	100%	
11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		
• Molecule 1: VP2		
Chain 1:	100%	
1207 1207 1568		
• Molecule 1: VP2		
Chain m:	100%	
11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		
• Molecule 1: VP2		
Chain n:	100%	
1184 1207 1269		



 \bullet Molecule 1: VP2

Chain v:

111 1184 1170 1170 1170 1170 1170 1170 1170 117	
• Molecule 1: VP2	
Chain p:	100%
11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
• Molecule 1: VP2	
Chain q:	100%
1184 1207 1569	
• Molecule 1: VP2	
Chain r:	100%
1207 1207 1207 1207 1207 1207 1207 1207	
• Molecule 1: VP2	
Chain s:	100%
1207 L207 L207 L569	
• Molecule 1: VP2	
Chain t:	100%
1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1.1	
• Molecule 1: VP2	
Chain u:	100%
1.1869 1.1869	



G32	L184	1 207	
•	Μ	ole	ecu
C	ha	in	W

ule 1: VP2

100%



• Molecule 1: VP2

Chain x:

100%



• Molecule 1: VP2

Chain y:

100%



• Molecule 1: VP2

Chain z:

100%



• Molecule 1: VP2

Chain 1:

100%



• Molecule 1: VP2

Chain 2:

100%



• Molecule 1: VP2

Chain 3:





• Molecule 1: VP2

Chain 4:

100%



• Molecule 1: VP2

Chain 5:

100%



• Molecule 1: VP2

Chain 6:

100%



• Molecule 1: VP2

Chain 7:

100%



• Molecule 1: VP2

Chain 8:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15296	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	16.659	Depositor
Minimum map value	-9.332	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	443.94, 443.94, 443.94	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	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).

Mal Chair		В	ond lengths	Bond angles		
Mol	Chain	RMSZ	# Z > 5	RMSZ	$\mid \# \mid Z \mid > 5 \mid$	
1	1	0.49	1/4478 (0.0%)	0.55	0/6135	
1	2	0.49	1/4478 (0.0%)	0.55	0/6135	
1	3	0.49	1/4478 (0.0%)	0.55	0/6135	
1	4	0.49	1/4478 (0.0%)	0.55	0/6135	
1	5	0.49	1/4478 (0.0%)	0.55	0/6135	
1	6	0.49	1/4478 (0.0%)	0.55	0/6135	
1	7	0.49	1/4478 (0.0%)	0.55	0/6135	
1	8	0.49	1/4478 (0.0%)	0.55	0/6135	
1	A	0.49	1/4478 (0.0%)	0.55	0/6135	
1	В	0.49	$1/4478 \; (0.0\%)$	0.55	0/6135	
1	С	0.49	1/4478~(0.0%)	0.55	0/6135	
1	D	0.49	1/4478~(0.0%)	0.55	0/6135	
1	Е	0.49	1/4478~(0.0%)	0.55	0/6135	
1	F	0.49	1/4478~(0.0%)	0.55	0/6135	
1	G	0.49	$1/4478 \; (0.0\%)$	0.55	0/6135	
1	Н	0.49	$1/4478 \; (0.0\%)$	0.55	0/6135	
1	I	0.49	$1/4478 \; (0.0\%)$	0.55	0/6135	
1	J	0.49	1/4478~(0.0%)	0.55	0/6135	
1	K	0.49	$1/4478 \; (0.0\%)$	0.55	0/6135	
1	L	0.49	1/4478~(0.0%)	0.55	0/6135	
1	M	0.49	1/4478~(0.0%)	0.55	0/6135	
1	N	0.49	1/4478~(0.0%)	0.55	0/6135	
1	О	0.49	1/4478~(0.0%)	0.55	0/6135	
1	Р	0.49	1/4478~(0.0%)	0.55	0/6135	
1	Q	0.49	1/4478~(0.0%)	0.55	0/6135	
1	R	0.49	1/4478~(0.0%)	0.55	0/6135	
1	S	0.49	1/4478~(0.0%)	0.55	0/6135	
1	Т	0.49	1/4478~(0.0%)	0.55	0/6135	
1	U	0.49	1/4478~(0.0%)	0.55	0/6135	
1	V	0.49	1/4478~(0.0%)	0.55	0/6135	
1	W	0.49	1/4478~(0.0%)	0.55	0/6135	
1	X	0.49	1/4478~(0.0%)	0.55	0/6135	
1	Y	0.49	1/4478~(0.0%)	0.55	0/6135	
1	Z	0.49	1/4478~(0.0%)	0.55	0/6135	



N/L-1	Chain Bond lengths			Bond	langles
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	a	0.49	1/4478~(0.0%)	0.55	0/6135
1	b	0.49	1/4478~(0.0%)	0.55	0/6135
1	С	0.49	1/4478~(0.0%)	0.55	0/6135
1	d	0.49	1/4478~(0.0%)	0.55	0/6135
1	е	0.49	1/4478~(0.0%)	0.55	0/6135
1	f	0.49	1/4478~(0.0%)	0.55	0/6135
1	g	0.49	1/4478~(0.0%)	0.55	0/6135
1	h	0.49	1/4478~(0.0%)	0.55	0/6135
1	i	0.49	1/4478~(0.0%)	0.55	0/6135
1	j	0.49	1/4478~(0.0%)	0.55	0/6135
1	k	0.49	1/4478~(0.0%)	0.55	0/6135
1	1	0.49	1/4478~(0.0%)	0.55	0/6135
1	m	0.49	1/4478~(0.0%)	0.55	0/6135
1	n	0.49	1/4478~(0.0%)	0.55	0/6135
1	О	0.49	1/4478~(0.0%)	0.55	0/6135
1	р	0.49	1/4478~(0.0%)	0.55	0/6135
1	q	0.49	1/4478~(0.0%)	0.55	0/6135
1	r	0.49	1/4478~(0.0%)	0.55	0/6135
1	s	0.49	1/4478~(0.0%)	0.55	0/6135
1	t	0.49	1/4478 (0.0%)	0.55	0/6135
1	u	0.49	1/4478~(0.0%)	0.55	0/6135
1	V	0.49	1/4478~(0.0%)	0.55	0/6135
1	W	0.49	1/4478~(0.0%)	0.55	0/6135
1	X	0.49	1/4478~(0.0%)	0.55	0/6135
1	У	0.49	1/4478~(0.0%)	0.55	0/6135
1	Z	0.49	1/4478~(0.0%)	0.55	0/6135
All	All	0.49	$60/268680 \ (0.0\%)$	0.55	0/368100

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
1	G	184	LEU	C-N	-5.12	1.22	1.34
1	р	184	LEU	C-N	-5.12	1.22	1.34
1	M	184	LEU	C-N	-5.12	1.22	1.34
1	Z	184	LEU	C-N	-5.12	1.22	1.34
1	h	184	LEU	C-N	-5.12	1.22	1.34
1	D	184	LEU	C-N	-5.11	1.22	1.34
1	k	184	LEU	C-N	-5.11	1.22	1.34
1	7	184	LEU	C-N	-5.10	1.22	1.34
1	С	184	LEU	C-N	-5.09	1.22	1.34
1	Q	184	LEU	C-N	-5.09	1.22	1.34
1	Т	184	LEU	C-N	-5.09	1.22	1.34



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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
1	V	184	LEU	C-N	-5.09	1.22	1.34
1	g	184	LEU	C-N	-5.09	1.22	1.34
1	m	184	LEU	C-N	-5.09	1.22	1.34
1	u	184	LEU	C-N	-5.09	1.22	1.34
1	X	184	LEU	C-N	-5.09	1.22	1.34
1	4	184	LEU	C-N	-5.09	1.22	1.34
1	K	184	LEU	C-N	-5.09	1.22	1.34
1	W	184	LEU	C-N	-5.09	1.22	1.34
1	A	184	LEU	C-N	-5.08	1.22	1.34
1	F	184	LEU	C-N	-5.08	1.22	1.34
1	a	184	LEU	C-N	-5.08	1.22	1.34
1	b	184	LEU	C-N	-5.08	1.22	1.34
1	С	184	LEU	C-N	-5.08	1.22	1.34
1	d	184	LEU	C-N	-5.08	1.22	1.34
1	е	184	LEU	C-N	-5.08	1.22	1.34
1	f	184	LEU	C-N	-5.08	1.22	1.34
1	n	184	LEU	C-N	-5.08	1.22	1.34
1	V	184	LEU	C-N	-5.08	1.22	1.34
1	У	184	LEU	C-N	-5.08	1.22	1.34
1	3	184	LEU	C-N	-5.08	1.22	1.34
1	6	184	LEU	C-N	-5.08	1.22	1.34
1	8	184	LEU	C-N	-5.08	1.22	1.34
1	J	184	LEU	C-N	-5.08	1.22	1.34
1	S	184	LEU	C-N	-5.08	1.22	1.34
1	X	184	LEU	C-N	-5.08	1.22	1.34
1	О	184	LEU	C-N	-5.08	1.22	1.34
1	r	184	LEU	C-N	-5.08	1.22	1.34
1	2	184	LEU	C-N	-5.08	1.22	1.34
1	H	184	LEU	C-N	-5.08	1.22	1.34
1	L	184	LEU	C-N	-5.08	1.22	1.34
1	U	184	LEU	C-N	-5.08	1.22	1.34
1	S	184	LEU	C-N	-5.08	1.22	1.34
1	Z	184	LEU	C-N	-5.08	1.22	1.34
1	5 N	184	LEU	C-N	-5.08	1.22	1.34
1	N	184	LEU	C-N	-5.07	1.22	1.34
1	P	184	LEU	C-N	-5.07	1.22	1.34
1	Y	184	LEU	C-N	-5.07	1.22	1.34
1	i	184	LEU	C-N	-5.07	1.22	1.34
1	j	184	LEU	C-N	-5.07	1.22	1.34
1	Е	184	LEU	C-N	-5.06	1.22	1.34
1	I	184	LEU	C-N	-5.06	1.22	1.34
1	О	184	LEU	C-N	-5.06	1.22	1.34



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	l	184	LEU	C-N	-5.06	1.22	1.34
1	t	184	LEU	C-N	-5.06	1.22	1.34
1	W	184	LEU	C-N	-5.06	1.22	1.34
1	В	184	LEU	C-N	-5.04	1.22	1.34
1	R	184	LEU	C-N	-5.04	1.22	1.34
1	q	184	LEU	C-N	-5.04	1.22	1.34
1	1	184	LEU	C-N	-5.04	1.22	1.34

There are no bond angle outliers.

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	Percen	tiles
1	1	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	2	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	3	$536/538 \; (100\%)$	521 (97%)	15 (3%)	0	100	100
1	4	$536/538 \; (100\%)$	522 (97%)	14 (3%)	0	100	100
1	5	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	6	$536/538 \; (100\%)$	521 (97%)	15 (3%)	0	100	100
1	7	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	8	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	A	536/538 (100%)	521 (97%)	15 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	В	$536/538\ (100\%)$	522 (97%)	14 (3%)	0	100	100
1	C	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	D	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	Е	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	F	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	G	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	Н	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	I	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	J	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	K	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	L	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	M	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	N	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	О	$536/538 \; (100\%)$	521 (97%)	15 (3%)	0	100	100
1	Р	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	Q	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	R	$536/538 \; (100\%)$	522 (97%)	14 (3%)	0	100	100
1	S	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	Т	$536/538 \; (100\%)$	522 (97%)	14 (3%)	0	100	100
1	U	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	V	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	W	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	X	$536/538 \; (100\%)$	522 (97%)	14 (3%)	0	100	100
1	Y	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	Z	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	a	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	b	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	c	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	d	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	e	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	f	536/538 (100%)	521 (97%)	15 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	g	$536/538 \; (100\%)$	521 (97%)	15 (3%)	0	100	100
1	h	$536/538 \; (100\%)$	522 (97%)	14 (3%)	0	100	100
1	i	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	j	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	k	536/538~(100%)	521 (97%)	15 (3%)	0	100	100
1	1	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	m	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	n	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	О	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	p	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	q	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	r	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	S	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	t	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	u	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	V	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	w	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
1	X	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	У	536/538 (100%)	521 (97%)	15 (3%)	0	100	100
1	Z	536/538 (100%)	522 (97%)	14 (3%)	0	100	100
All	All	32160/32280 (100%)	31282 (97%)	878 (3%)	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	1	469/469 (100%)	468 (100%)	1 (0%)	93 98



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	2	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	3	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93	98
1	4	$469/469\ (100\%)$	468 (100%)	1 (0%)	93	98
1	5	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93	98
1	6	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	7	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93	98
1	8	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	A	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93	98
1	В	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	С	469/469~(100%)	468 (100%)	1 (0%)	93	98
1	D	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	E	469/469~(100%)	468 (100%)	1 (0%)	93	98
1	F	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	G	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93	98
1	Н	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	I	469/469~(100%)	468 (100%)	1 (0%)	93	98
1	J	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	K	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93	98
1	L	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	M	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	N	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	О	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93	98
1	Р	$469/469\ (100\%)$	468 (100%)	1 (0%)	93	98
1	Q	$469/469\ (100\%)$	468 (100%)	1 (0%)	93	98
1	R	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	S	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	Т	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	U	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	V	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	W	469/469 (100%)	468 (100%)	1 (0%)	93	98
1	X	469/469 (100%)	468 (100%)	1 (0%)	93	98



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Mol	Chain	Analysed	Rotameric	Outliers	Percentile
1	Y	469/469~(100%)	468 (100%)	1 (0%)	93 98
1	Z	469/469~(100%)	468 (100%)	1 (0%)	93 98
1	a	469/469~(100%)	468 (100%)	1 (0%)	93 98
1	b	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93 98
1	c	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93 98
1	d	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93 98
1	e	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	f	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	g	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	h	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	i	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	j	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	k	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	1	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	m	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	n	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	О	$469/469 \; (100\%)$	468 (100%)	1 (0%)	93 98
1	p	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	q	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	r	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	S	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	t	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	u	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	V	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	W	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	X	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	У	469/469 (100%)	468 (100%)	1 (0%)	93 98
1	Z	469/469 (100%)	468 (100%)	1 (0%)	93 98
All	All	28140/28140 (100%)	28080 (100%)	60 (0%)	93 98

All (60) residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
1	A	207	LEU
1	В	207	LEU
1	С	207	LEU
1	C D	207	LEU
1	Е	207	LEU
1	F	207	LEU
1	G	207	LEU
1	Н	207	LEU
1	I	207	LEU
1	J	207	LEU
1	K	207	LEU
1	L	207	LEU
1	M	207	LEU
1	N	207	LEU
1	O P	207	LEU
1	Р	207	LEU
1	Q	207	LEU
1	R	207	LEU
1	S	207	LEU
1	Т	207	LEU
1	U	207	LEU
1	R S T U V W	207	LEU
1	W	207	LEU
1		207	LEU
1	Y	207	LEU
1	Z	207	LEU
1	a	207	LEU
1	b	207	LEU
1	С	207	LEU
1	d	207	LEU
1	е	207	LEU
1	f	207	LEU
1	g	207	LEU
1	h	207	LEU
1	i j	207	LEU
1		207	LEU
1	k	207	LEU
1	1	207	LEU
1	m	207	LEU
1	n	207	LEU
1	О	207	LEU
1	p	207	LEU
1	q	207	LEU



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Mol	Chain	Res	Type
1	r	207	LEU
1	s	207	LEU
1	t	207	LEU
1	u	207	LEU
1	V	207	LEU
1	W	207	LEU
1	X	207	LEU
1	у	207	LEU
1	Z	207	LEU
1	1	207	LEU
1	2	207	LEU
1	3	207	LEU
1	4	207	LEU
1	5	207	LEU
1	6	207	LEU
1	7	207	LEU
1	8	207	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1583) such side chains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	60	HIS
1	A	66	HIS
1	A	90	GLN
1	A	99	ASN
1	A	103	HIS
1	A	114	HIS
1	A	143	HIS
1	A	148	ASN
1	A	166	ASN
1	A	169	ASN
1	A	176	GLN
1	A	230	GLN
1	A	264	GLN
1	A	286	HIS
1	A	305	ASN
1	A	313	GLN
1	A	329	ASN
1	A	358	GLN
1	A	397	GLN
1	A	412	ASN

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Mol	Chain	Res	Type			
1	A	434	HIS			
1	A	446	HIS			
1	A	449	GLN			
1	A	471	HIS			
1	A	482	GLN			
1	В	44	ASN			
1	В	60	HIS			
1	В	66	HIS			
1	В	90	GLN			
1	В	99	ASN			
1	В	103	HIS			
1	В	114	HIS			
1	В	143	HIS			
1	В	148	ASN			
1	В	166	ASN			
1	В	169	ASN			
1	В	176	GLN			
1	В	230	GLN			
1	В	264	GLN			
1	В	286	HIS			
1	В	305	ASN			
1	В	313	GLN			
1	В	329	ASN			
1	В	358	GLN			
1	В	397	GLN			
1	В	399	ASN			
1	В	412	ASN			
1	В	434	HIS			
1	В	446	HIS			
1	В	449	GLN			
1	В	471	HIS			
1	В	482	GLN			
1		549	ASN			
1	С	44	ASN			
1	С	60	HIS			
1	С	66	HIS			
1	B C C C C C C C C C C C C C C C C C C C	90	GLN			
1	С	99	ASN			
1	С	103	HIS			
1	С	114	HIS			
1	С	143	HIS			
1	С	148	ASN			
	l .	l				



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Mol	Chain	Res	Type				
1	С	166	ASN				
1	С	169	ASN				
1	С	176	GLN				
1	С	230	GLN				
1	С	264	GLN				
1	С	286	HIS				
1	С	305	ASN				
1	С	313	GLN				
1	С	329	ASN				
1	С	358	GLN				
1	С	397	GLN				
1	С	399	ASN				
1	С	412	ASN				
1	C C C C C C C C C C C C C C C C C C C	434	HIS				
1	С	446	HIS				
1	С	449	GLN				
1	С	471	HIS				
1	С	482	GLN				
1	D	44	ASN				
1	D	60	HIS				
1	D	66	HIS				
1	D	90	GLN				
1	D	99	ASN				
1	D	103	HIS				
1	D	114	HIS				
1	D	143	HIS				
1	D	148	ASN				
1	D	166	ASN				
1	D	169	ASN				
1	D	176	GLN				
1	D	230	GLN				
1	D	264	GLN				
1	D	286	HIS				
1	D	305	ASN				
1	D	313	GLN				
1	D	329	ASN				
1	D	358	GLN				
1	D	397	GLN				
1	D	399	ASN				
1	D	412	ASN				
1	D	446	HIS				
1	D	449	GLN				



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Mol	Chain	Res	Type			
1	D	471	HIS			
1	D	482	GLN			
1	D	549	ASN			
1	Е	44	ASN			
1	Е	60	HIS			
1	Е	66	HIS			
1	Е	90	GLN			
1	Е	99	ASN			
1	Е	103	HIS			
1	Е	114	HIS			
1	Е	143	HIS			
1	Е	148	ASN			
1	Е	166	ASN			
1	Е	169	ASN			
1	Е	176	GLN			
1	Е	230	GLN			
1	Е	264	GLN			
1	Е	286	HIS			
1	Е	305	ASN			
1	Е	313	GLN			
1	Е	329	ASN			
1	Е	358	GLN			
1	Е	397	GLN			
1	Е	399	ASN			
1	Е	412	ASN			
1	Е	446	HIS			
1	Е	449	GLN			
1	Е	471	HIS			
1	Е	482	GLN			
1	F	44	ASN			
1	F	60	HIS			
1	F	66	HIS			
1	F	90	GLN			
1	F	99	ASN			
1	F	103	HIS			
1	F	114	HIS			
1	F	143	HIS			
1	F	148	ASN			
1	F	166	ASN			
1	F	169	ASN			
1	F	176	GLN			
1	F	230	GLN			



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Conti	Continued from previous page						
Mol	Chain	Res	Type				
1	F	264	GLN				
1	F	286	HIS				
1	F	305	ASN				
1	F	313	GLN				
1	F	329	ASN				
1	F	358	GLN				
1	F	397	GLN				
1	F	412	ASN				
1	F	434	HIS				
1	F	446	HIS				
1	F	449	GLN				
1	F	471	HIS				
1	F	482	GLN				
1	G	44	ASN				
1	G	60	HIS				
1	G	66	HIS				
1	G	90	GLN				
1	G	99	ASN				
1	G	103	HIS				
1	G	114	HIS				
1	G	143	HIS				
1	G	148	ASN				
1	G	166	ASN				
1	G	169	ASN				
1	G	176	GLN				
1	G	230	GLN				
1	G	264	GLN				
1	G	286	HIS				
1	G	305	ASN				
1	G	313	GLN				
1	G G	329	ASN				
1	G	358	GLN				
1	G	397	GLN				
1	G	399	ASN				
1	G	412	ASN				
1	G	446	HIS				
1	G	449	GLN				
1	G	471	HIS				
1	G	482	GLN				
1	Н	44	ASN				
1	Н	60	HIS				
1	Н	66	HIS				



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			ous page
Mol	Chain	Res	Type
1	Н	90	GLN
1	Н	99	ASN
1	Н	103	HIS
1	Н	114	HIS
1	Н	143	HIS
1	Н	148	ASN
1	Н	166	ASN
1	Н	169	ASN
1	Н	176	GLN
1	Н	230	GLN
1	Н	264	GLN
1	Н	286	HIS
1	Н	305	ASN
1	Н	313	GLN
1	Н	329	ASN
1	Н	358	GLN
1	Н	397	GLN
1	Н	399	ASN
1	Н	412	ASN
1	Н	446	HIS
1	Н	449	GLN
1	Н	471	HIS
1	Н	482	GLN
1	I	44	ASN
1	I	60	HIS
1	I	66	HIS
1	I	90	GLN
1	I	99	ASN
1	I	103	HIS
1	I	114	HIS
1	I	143	HIS
1	I	148	ASN
1	I	166	ASN
1	I	169	ASN
1	I	176	GLN
1	I	230	GLN
1	I	264	GLN
1	I	286	HIS
1	I	305	ASN
1	I	313	GLN
1	I	329	ASN
1	I	358	GLN



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	Continued from previous page					
Mol	Chain	Res	Type			
1	I	397	GLN			
1	I	412	ASN			
1	I	446	HIS			
1	I	449	GLN			
1	I	471	HIS			
1	I	482	GLN			
1	J	44	ASN			
1	J	60	HIS			
1	J	66	HIS			
1	J	90	GLN			
1	J	99	ASN			
1	J	103	HIS			
1	J	114	HIS			
1	J	143	HIS			
1	J	148	ASN			
1	J	166	ASN			
1	J	169	ASN			
1	J	176	GLN			
1	J	230	GLN			
1	J	264	GLN			
1	J	286	HIS			
1	J	305	ASN			
1	J	313	GLN			
1	J	329	ASN			
1	J	358	GLN			
1	J	397	GLN			
1	J	412	ASN			
1	J	446	HIS			
1	J	449	GLN			
1	J	471	HIS			
1	J	482	GLN			
1	K	44	ASN			
1	K	60	HIS			
1	K	66	HIS			
1	K	90	GLN			
1	K	99	ASN			
1	K	103	HIS			
1	K	114	HIS			
1	K	143	HIS			
1	K	148	ASN			
1	K	166	ASN			
1	K	169	ASN			



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			ous page
Mol	Chain	Res	Type
1	K	176	GLN
1	K	230	GLN
1	K	264	GLN
1	K	286	HIS
1	K	305	ASN
1	K	313	GLN
1	K	329	ASN
1	K	358	GLN
1	K	397	GLN
1	K	399	ASN
1	K	412	ASN
1	K	446	HIS
1	K	449	GLN
1	K	471	HIS
1	K	482	GLN
1	L	44	ASN
1	L	60	HIS
1	L	66	HIS
1	L	90	GLN
1	L	99	ASN
1	L	103	HIS
1	L	114	HIS
1	L	143	HIS
1	L	148	ASN
1	L	166	ASN
1	L	169	ASN
1	L	176	GLN
1	L	230	GLN
1	L	264	GLN
1	L	286	HIS
1	L	305	ASN
1	L	313	GLN
1	L	329	ASN
1	L	358	GLN
1	L	397	GLN
1	L	399	ASN
1	L	412	ASN
1	L	446	HIS
1	L	449	GLN
1	L	471	HIS
1	L	482	GLN
1	M	44	ASN



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	Continued from previous page			
Mol	Chain	Res	Type	
1	M	60	HIS	
1	M	66	HIS	
1	M	90	GLN	
1	M	99	ASN	
1	M	103	HIS	
1	M	114	HIS	
1	M	143	HIS	
1	M	148	ASN	
1	M	166	ASN	
1	M	169	ASN	
1	M	176	GLN	
1	M	230	GLN	
1	M	264	GLN	
1	M	286	HIS	
1	M	305	ASN	
1	M	313	GLN	
1	M	329	ASN	
1	M	358	GLN	
1	M	397	GLN	
1	M	399	ASN	
1	M	412	ASN	
1	M	446	HIS	
1	M	449	GLN	
1	M	471	HIS	
1	M	482	GLN	
1	M	549	ASN	
1	N	44	ASN	
1	N	60	HIS	
1	N	66	HIS	
1	N	90	GLN	
1	N	99	ASN	
1	N	103	HIS	
1	N	114	HIS	
1	N	143	HIS	
1	N	148	ASN	
1	N	166	ASN	
1	N	169	ASN	
1	N	176	GLN	
1	N	230	GLN	
1	N	264	GLN	
1	N	286	HIS	
1	N	305	ASN	
		l		



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	Continued from previous page				
Mol	Chain	Res	Type		
1	N	313	GLN		
1	N	329	ASN		
1	N	358	GLN		
1	N	397	GLN		
1	N	412	ASN		
1	N	434	HIS		
1	N	446	HIS		
1	N	449	GLN		
1	N	471	HIS		
1	N	482	GLN		
1	О	44	ASN		
1	О	60	HIS		
1	О	66	HIS		
1	O O	90	GLN		
1	О	99	ASN		
1	О	103	HIS		
1	О	114	HIS		
1	O O	143	HIS		
1	О	148	ASN		
1	О	166	ASN		
1	0 0 0 0	169	ASN		
1	О	176	GLN		
1	О	230	GLN		
1	О	264	GLN		
1	О	286	HIS		
1	О	305	ASN		
1	O O	313	GLN		
1	О	329	ASN		
1	О	358	GLN		
1	О	397	GLN		
1	О	399	ASN		
1	О	412	ASN		
1	O O	446	HIS		
1		449	GLN		
1	О	471	HIS		
1	О	482	GLN		
1	Р	44	ASN		
1	P P	60	HIS		
1	Р	66	HIS		
1	Р	90	GLN		
1	Р	99	ASN		
1	Р	103	HIS		



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	Continued from previous page				
Mol	Chain	Res	Type		
1	Р	114	HIS		
1	Р	143	HIS		
1	Р	148	ASN		
1	P P	166	ASN		
1	Р	169	ASN		
1	P	176	GLN		
1	Р	230	GLN		
1	Р	264	GLN		
1	Р	286	HIS		
1	Р	305	ASN		
1	Р	313	GLN		
1	Р	329	ASN		
1	Р	358	GLN		
1	P P P P P P P	397	GLN		
1	Р	399	ASN		
1	Р	412	ASN		
1	P P	446	HIS		
1	Р	449	GLN		
1	Р	471	HIS		
1	Р	482	GLN		
1	Q	44	ASN		
1	Q	60	HIS		
1	Q Q Q Q Q Q	66	HIS		
1	Q	90	GLN		
1	Q	99	ASN		
1	Q	103	HIS		
1	Q	114	HIS		
1	Q	143	HIS		
1	Q	148	ASN		
1	Q	166	ASN		
1	Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q	169	ASN		
1	Q	176	GLN GLN		
1	Q	230	GLN		
1	Q	264	GLN HIS		
1	Q	286	HIS		
1	Q	305	ASN		
1	Q	313	ASN GLN		
1	Q	329	ASN		
1	Q	358	GLN		
1	Q	397	GLN		
1	Q	399	ASN		
1	Q	412	ASN		



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	Continued from previous page			
Mol	Chain	Res	Type	
1	Q	446	HIS	
1	Q	449	GLN	
1	Q Q Q	471	HIS	
1	Q	482	GLN	
1	R	44	ASN	
1	R	60	HIS	
1	R	66	HIS	
1	R	90	GLN	
1	R	99	ASN	
1	R	103	HIS	
1	R	114	HIS	
1	R	143	HIS	
1	R	148	ASN	
1	R	166	ASN	
1	R	169	ASN	
1	R	176	GLN	
1	R	230	GLN	
1	R	264	GLN	
1	R	286	HIS	
1	R	305	ASN	
1	R	313	GLN	
1	R	329	ASN	
1	R	358	GLN	
1	R	397	GLN	
1	R	412	ASN	
1	R	434	HIS	
1	R	446	HIS	
1	R	449	GLN	
1	R	471	HIS	
1	R	482	GLN	
1	R	549	ASN	
1	S	44	ASN	
1	S	60	HIS	
1	S S S	66	HIS	
1	S	90	GLN	
1		99	ASN	
1	S S	103	HIS	
1	S	114	HIS	
1	S	143	HIS	
1	S S	148	ASN	
1		166	ASN	
1	S	169	ASN	



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			ous page
Mol	Chain	Res	Type
1	S	176	GLN
1	S	230	GLN
1	S	264	GLN
1	S	286	HIS
1	S	305	ASN
1	S	313	GLN
1	S S S	329	ASN
1	S	358	GLN
1	S	397	GLN
1	S	399	ASN
1	S	412	ASN
1	S	446	HIS
1	S	449	GLN
1	S	471	HIS
1	S	482	GLN
1	Т	44	ASN
1	Т	60	HIS
1	Т	66	HIS
1	Т	90	GLN
1	Т	99	ASN
1	T T T T T T T T T T	103	HIS
1	Т	114	HIS
1	Т	143	HIS
1	Т	148	ASN
1	Т	166	ASN
1	Т	169	ASN
1	Т	176	GLN
1	Τ	230	GLN
1	Т	264	GLN
1	Т	286	HIS
1	Т	305	ASN
1	T T T T	313	GLN
1	Т	329	ASN
1	Т	358	GLN
1	Т	397	GLN
1	Т	412	ASN
1	T T	446	HIS
1	Т	449	GLN
1	Т	471	HIS
1	Т	482	GLN
1	U	44	ASN
1	U	60	HIS



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Continued from previous page			
Mol	Chain	Res	Type
1	U	66	HIS
1	U	90	GLN
1	U	99	ASN
1	U	103	HIS
1	U	114	HIS
1	U	143	HIS
1	U	148	ASN
1	U	166	ASN
1	U	169	ASN
1	U	176	GLN
1	U	230	GLN
1	U	264	GLN
1	U	286	HIS
1	U	305	ASN
1	U	313	GLN
1	U	329	ASN
1	U	358	GLN
1	U	397	GLN
1	U	399	ASN
1	U	412	ASN
1	U	446	HIS
1	U	449	GLN
1	U	471	HIS
1	U	482	GLN
1	V	44	ASN
1	V	60	HIS
1	V	66	HIS
1	V	90	GLN
1	V	99	ASN
1	V	103	HIS
1	V	114	HIS
1	V	143	HIS
1	V	148	ASN
1	V	166	ASN
1	V	169	ASN
1	V	176	GLN
1	V	230	GLN
1	V	264	GLN
1	V	286	HIS
1	V	305	ASN
1	V	313	GLN
1	V	329	ASN
	i		



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Conti	Continued from previous page			
Mol	Chain	Res	Type	
1	V	358	GLN	
1	V	397	GLN	
1	V	399	ASN	
1	V	412	ASN	
1	V	434	HIS	
1	V	446	HIS	
1	V V	449	GLN	
1	V	471	HIS	
1	V	482	GLN	
1	V	549	ASN	
1	W	44	ASN	
1	W	60	HIS	
1	W	66	HIS	
1	W	90	GLN	
1	W	99	ASN	
1	W	103	HIS	
1	W	114	HIS	
1	W	143	HIS	
1	W	148	ASN	
1	W	166	ASN	
1	W	169	ASN	
1	W	176	GLN	
1	W	230	GLN	
1	W	264	GLN	
1	W	286	HIS	
1	W	305	ASN	
1	W	313	GLN	
1	W	329	ASN	
1	W	358	GLN	
1	W	397	GLN	
1	W	399	ASN	
1	W	412	ASN	
1	W	446	HIS	
1	W	449	GLN	
1	W	471	HIS	
1	W	482	GLN	
1	X	44	ASN	
1	X	60	HIS	
1	X	66	HIS	
1	X	90	GLN	
1	X	99	ASN	
1	X	103	HIS	



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Conti	Continued from previous page			
Mol	Chain	Res	Type	
1	X	114	HIS	
1	X	143	HIS	
1	X X	148	ASN	
1	X	166	ASN	
1	X	169	ASN	
1	X	176	GLN	
1	X	230	GLN	
1	X	264	GLN	
1	X	286	HIS	
1	X	305	ASN	
1	X	313	GLN	
1	X	329	ASN	
1	X	358	GLN	
1	X	397	GLN	
1	X	399	ASN	
1	X	412	ASN	
1	X X	446	HIS	
1	X	449	GLN	
1	X	471	HIS	
1	X	482	GLN	
1	X Y Y Y Y Y	549	ASN	
1	Y	44	ASN	
1	Y	60	HIS	
1	Y	66	HIS	
1	Y	90	GLN	
1	Y	99	ASN	
1	Y	103	HIS	
1	Y	114	HIS	
1	Y	143	HIS	
1	Y	148	ASN	
1	Y	166	ASN	
1	Y	169	ASN	
1	Y	176	GLN	
1	Y Y	230	GLN	
1	Y	264	GLN	
1	Y	286	HIS	
1	Y	305	ASN	
1	Y	313	GLN	
1	Y	329	ASN	
1	Y	358	GLN	
1	Y Y	397	GLN	
1	Y	412	ASN	

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Conti	Continued from previous page			
Mol	Chain	Res	Type	
1	Y	434	HIS	
1	Y	446	HIS	
1	Y	449	GLN	
1	Y	471	HIS	
1	Y	482	GLN	
1	Y Y Y Y Z Z	44	ASN	
1	Z	60	HIS	
1	Z	66	HIS	
1	Z	90	GLN	
1	Z	99	ASN	
1	Z Z	103	HIS	
1	Z	114	HIS	
1	Z	143	HIS	
1	Z	148	ASN	
1	Z Z Z	166	ASN	
1	Z	169	ASN	
1	Z	176	GLN	
1	Z	230	GLN	
1	Z Z Z	264	GLN	
1	Z	286	HIS	
1	Z	305	ASN	
1	Z	313	GLN	
1	Z Z Z	329	ASN	
1	Z	358	GLN	
1	Z	397	GLN	
1	Z	399	ASN	
1	Z	412	ASN	
1	Z	446	HIS	
1	Z	449	GLN	
1	Z	471	HIS	
1	Z	482	GLN	
1	a	44	ASN	
1	a	60	HIS	
1	a	66	HIS	
1	a	90	GLN	
1	a	99	ASN	
1	a	103	HIS	
1	a	114	HIS	
1	a	143	HIS	
1	a	148	ASN	
1	a	166	ASN	
1	a	169	ASN	



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	Continued from previous page			
Mol	Chain	Res	Type	
1	a	176	GLN	
1	a	230	GLN	
1	a	264	GLN	
1	a	286	HIS	
1	a	305	ASN	
1	a	313	GLN	
1	a	329	ASN	
1	a	358	GLN	
1	a	397	GLN	
1	a	399	ASN	
1	a	412	ASN	
1	a	434	HIS	
1	a	446	HIS	
1	a	449	GLN	
1	a	471	HIS	
1	a	482	GLN	
1	b	44	ASN	
1	b	60	HIS	
1	b	66	HIS	
1	b	90	GLN	
1	b	99	ASN	
1	b	103	HIS	
1	b	114	HIS	
1	b	143	HIS	
1	b	148	ASN	
1	b	166	ASN	
1	b	169	ASN	
1	b	176	GLN	
1	b	230	GLN	
1	b	264	GLN	
1	b	286	HIS	
1	b	305	ASN	
1	b	313	GLN	
1	b	329	ASN	
1	b	358	GLN	
1	b	397	GLN	
1	b	399	ASN	
1	b	412	ASN	
1	b	446	HIS	
1	b	449	GLN	
1	b	471	HIS	
1	b	482	GLN	



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Conti	Continued from previous page			
Mol	Chain	Res	Type	
1	c	44	ASN	
1	С	60	HIS	
1	c	66	HIS	
1	С	90	GLN	
1	c	99	ASN	
1	С	103	HIS	
1	С	114	HIS	
1	c	143	HIS	
1	С	148	ASN	
1	С	166	ASN	
1	С	169	ASN	
1	С	176	GLN	
1	С	230	GLN	
1	С	264	GLN	
1	С	286	HIS	
1	С	305	ASN	
1	С	313	GLN	
1	С	329	ASN	
1	С	358	GLN	
1	c	397	GLN	
1	С	399	ASN	
1	С	412	ASN	
1	С	446	HIS	
1	С	449	GLN	
1	С	471	HIS	
1	С	482	GLN	
1	c	549	ASN	
1	d	44	ASN	
1	d	60	HIS	
1	d	66	HIS	
1	d	90	GLN	
1	d	99	ASN	
1	d	103	HIS	
1	d	114	HIS	
1	d	143	HIS	
1	d	148	ASN	
1	d	166	ASN	
1	d	169	ASN	
1	d	176	GLN	
1	d	230	GLN	
1	d	264	GLN	
1	d	286	HIS	



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Conti	Continued from previous page			
Mol	Chain	Res	Type	
1	d	305	ASN	
1	d	313	GLN	
1	d	329	ASN	
1	d	358	GLN	
1	d	397	GLN	
1	d	399	ASN	
1	d	412	ASN	
1	d	434	HIS	
1	d	446	HIS	
1	d	449	GLN	
1	d	471	HIS	
1	d	482	GLN	
1	е	44	ASN	
1	е	60	HIS	
1	е	66	HIS	
1	е	90	GLN	
1	е	99	ASN	
1	е	103	HIS	
1	е	114	HIS	
1	е	143	HIS	
1	е	148	ASN	
1	е	166	ASN	
1	е	169	ASN	
1	е	176	GLN	
1	е	230	GLN	
1	е	264	GLN	
1	е	286	HIS	
1	е	305	ASN	
1	е	313	GLN	
1	е	329	ASN	
1	е	358	GLN	
1	е	397	GLN	
1	е	399	ASN	
1	е	412	ASN	
1	е	446	HIS	
1	е	449	GLN	
1	е	471	HIS	
1	е	482	GLN	
1	е	549	ASN	
1	f	44	ASN	
1	f	60	HIS	
1	f	66	HIS	



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			ous page
Mol	Chain	Res	Type
1	f	90	GLN
1	f	99	ASN
1	f	103	HIS
1	f	114	HIS
1	f	143	HIS
1	f	148	ASN
1	f	166	ASN
1	f	169	ASN
1	f	176	GLN
1	f	230	GLN
1	f	264	GLN
1	f	286	HIS
1	f	305	ASN
1	f	313	GLN
1	f	329	ASN
1	f	358	GLN
1	f	397	GLN
1	f	399	ASN
1	f	412	ASN
1	f	446	HIS
1	f	449	GLN
1	f	471	HIS
1	f	482	GLN
1	g	44	ASN
1	g	60	HIS
1	g	66	HIS
1	g	90	GLN
1	g	99	ASN
1	g	103	HIS
1	g	114	HIS
1	g	143	HIS
1	g	148	ASN
1	g	166	ASN
1	g	169	ASN
1	g	176	GLN
1	g	230	GLN
1	g	264	GLN
1	g	286	HIS
1	g	305	ASN
1	g	313	GLN
1	g	329	ASN
1	g	358	GLN



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		n previo	ous page
Mol	Chain	Res	Type
1	g	397	GLN
1	g	399	ASN
1	g	412	ASN
1	g	434	HIS
1	g	446	HIS
1	g	449	GLN
1	g	471	HIS
1	g	482	GLN
1	g	549	ASN
1	h	44	ASN
1	h	60	HIS
1	h	66	HIS
1	h	90	GLN
1	h	99	ASN
1	h	103	HIS
1	h	114	HIS
1	h	143	HIS
1	h	148	ASN
1	h	166	ASN
1	h	169	ASN
1	h	176	GLN
1	h	230	GLN
1	h	264	GLN
1	h	286	HIS
1	h	305	ASN
1	h	313	GLN
1	h	329	ASN
1	h	358	GLN
1	h	397	GLN
1	h	399	ASN
1	h	412	ASN
1	h	446	HIS
1	h	449	GLN
1	h	471	HIS
1	h	482	GLN
1	h	549	ASN
1	i	44	ASN
1	i	60	HIS
1	i	66	HIS
1	i	90	GLN
1	i	99	ASN
1	i	103	HIS



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			ous page
Mol	Chain	Res	Type
1	i	114	HIS
1	i	143	HIS
1	i	148	ASN
1	i	166	ASN
1	i	169	ASN
1	i	176	GLN
1	i	230	GLN
1	i	264	GLN
1	i	286	HIS
1	i	305	ASN
1	i	313	GLN
1	i	329	ASN
1	i	358	GLN
1	i	397	GLN
1	i	412	ASN
1	i	434	HIS
1	i	446	HIS
1	i	449	GLN
1	i	471	HIS
1	i	482	GLN
1	j	44	ASN
1	j	60	HIS
1	j	66	HIS
1	j	90	GLN
1	j	99	ASN
1	j	103	HIS
1	j j	114	HIS
1	j	143	HIS
1	j	148	ASN
1	j	166	ASN
1	j	169	ASN
1	j	176	GLN
1	j j j j j j	230	GLN GLN
1	j	264	GLN
1	j	286	HIS
1	j	305	ASN
1	j	313	GLN
1	j	329	ASN
1	j	358	GLN
1	j	397	GLN
1	j	399	ASN
1	j	412	ASN



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Conti			ous page
Mol	Chain	Res	Type
1	j	446	HIS
1	j j	449	GLN
1	j	471	HIS
1	j	482	GLN
1	k	44	ASN
1	k	60	HIS
1	k	66	HIS
1	k	90	GLN
1	k	99	ASN
1	k	103	HIS
1	k	114	HIS
1	k	143	HIS
1	k	148	ASN
1	k	166	ASN
1	k	169	ASN
1	k	176	GLN
1	k	230	GLN
1	k	264	GLN
1	k	286	HIS
1	k	305	ASN
1	k	313	GLN
1	k	329	ASN
1	k	358	GLN
1	k	397	GLN
1	k	399	ASN
1	k	412	ASN
1	k	446	HIS
1	k	449	GLN
1	k	471	HIS
1	k	482	GLN
1	k	549	ASN
1	1	44	ASN
1	1	60	HIS
1	1	66	HIS
1	1	90	GLN
1	1	99	ASN
1	1	103	HIS
1	1	114	HIS
1	1	143	HIS
1	1	148	ASN
1	1	166	ASN
1	1	169	ASN



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			ous page
Mol	Chain	Res	Type
1	1	176	GLN
1	1	230	GLN
1	1	264	GLN
1	1	286	HIS
1	1	305	ASN
1	1	313	GLN
1	1	329	ASN
1	1	358	GLN
1	1	397	GLN
1	1	399	ASN
1	1	412	ASN
1	1	446	HIS
1	1	449	GLN
1	1	471	HIS
1	1	482	GLN
1	m	44	ASN
1	m	60	HIS
1	m	66	HIS
1	m	90	GLN
1	m	99	ASN
1	m	103	HIS
1	m	114	HIS
1	m	143	HIS
1	m	148	ASN
1	m	166	ASN
1	m	169	ASN
1	m	176	GLN
1	m	230	GLN
1	m	264	GLN
1	m	286	HIS
1	m	305	ASN
1	m	313	GLN
1	m	329	ASN
1	m	358	GLN
1	m	397	GLN
1	m	399	ASN
1	m	412	ASN
1	m	446	HIS
1	m	449	GLN
1	m	471	HIS
1	m	482	GLN
1	n	44	ASN



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Conti		n previo	ous page
Mol	Chain	Res	Type
1	n	60	HIS
1	n	66	HIS
1	n	90	GLN
1	n	99	ASN
1	n	103	HIS
1	n	114	HIS
1	n	143	HIS
1	n	148	ASN
1	n	166	ASN
1	n	169	ASN
1	n	176	GLN
1	n	230	GLN
1	n	264	GLN
1	n	286	HIS
1	n	305	ASN
1	n	313	GLN
1	n	329	ASN
1	n	358	GLN
1	n	397	GLN
1	n	399	ASN
1	n	412	ASN
1	n	434	HIS
1	n	446	HIS
1	n	449	GLN
1	n	471	HIS
1	n	482	GLN
1	О	44	ASN
1	О	60	HIS
1	О	66	HIS
1	О	90	GLN
1	О	99	ASN
1	О	103	HIS
1	О	114	HIS
1	О	143	HIS
1	О	148	ASN
1	О	166	ASN
1	О	169	ASN
1	О	176	GLN
1	О	230	GLN
1	О	264	GLN
1	О	286	HIS
1	О	305	ASN



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			ous page
Mol	Chain	Res	Type
1	О	313	GLN
1	О	329	ASN
1	О	358	GLN
1	О	397	GLN
1	О	399	ASN
1	О	412	ASN
1	О	446	HIS
1	О	449	GLN
1	О	471	HIS
1	О	482	GLN
1	О	549	ASN
1	p	44	ASN
1	p	60	HIS
1	p	66	HIS
1	p	90	GLN
1	p	99	ASN
1	p	103	HIS
1	р	114	HIS
1	р	143	HIS
1	р	148	ASN
1	р	166	ASN
1	р	169	ASN
1	р	176	GLN
1	р	230	GLN
1	р	264	GLN
1	р	286	HIS
1	р	305	ASN
1	р	313	GLN
1	р	329	ASN
1	p	358	GLN
1	p	397	GLN
1	p	399	ASN
1	p	412	ASN
1	p	434	HIS
1	p	446	HIS
1	p	449	GLN
1	p	471	HIS
1	p	482	GLN
1	p	549	ASN
1	q	44	ASN
1	q	60	HIS
1	q	66	HIS



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			ous page
Mol	Chain	Res	Type
1	q	90	GLN
1	q	99	ASN
1	q	103	HIS
1	q	114	HIS
1	q	143	HIS
1	q	148	ASN
1	q	166	ASN
1	q	169	ASN
1	q	176	GLN
1	q	230	GLN
1	q	264	GLN
1	q	286	HIS
1	q	305	ASN
1	q	313	GLN
1	q	329	ASN
1	q	358	GLN
1	q	397	GLN
1	q	412	ASN
1	q	434	HIS
1	q	446	HIS
1	q	449	GLN
1	q	471	HIS
1	q	482	GLN
1	q	549	ASN
1	r	44	ASN
1	r	60	HIS
1	r	66	HIS
1	r	90	GLN
1	r	99	ASN
1	r	103	HIS
1	r	114	HIS
1	r	143	HIS
1	r	148	ASN
1	r	166	ASN
1	r	169	ASN
1	r	176	GLN
1	r	230	GLN
1	r	264	GLN
1	r	286	HIS
1	r	305	ASN
1	r	313	GLN
1	r	329	ASN
	1		



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Conti	Continued from previous page			
Mol	Chain	Res	Type	
1	r	358	GLN	
1	r	397	GLN	
1	r	399	ASN	
1	r	412	ASN	
1	r	446	HIS	
1	r	449	GLN	
1	r	471	HIS	
1	r	482	GLN	
1	S	44	ASN	
1	S	60	HIS	
1	S	66	HIS	
1	S	90	GLN	
1	S	99	ASN	
1	S	103	HIS	
1	S	114	HIS	
1	S	143	HIS	
1	S	148	ASN	
1	S	166	ASN	
1	S	169	ASN	
1	S	176	GLN	
1	s	230	GLN	
1	S	264	GLN	
1	s	286	HIS	
1	S	305	ASN	
1	S	313	GLN	
1	s	329	ASN	
1	S	358	GLN	
1	s	397	GLN	
1	S	399	ASN	
1	S	412	ASN	
1	s	446	HIS	
1	s	449	GLN	
1	s	471	HIS	
1	s	482	GLN	
1	t	44	ASN	
1	t	60	HIS	
1	t	66	HIS	
1	t	90	GLN	
1	t	99	ASN	
1	t	103	HIS	
1	t	114	HIS	
1	t	143	HIS	



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			ous page
Mol	Chain	Res	Type
1	t	148	ASN
1	t	166	ASN
1	t	169	ASN
1	t	176	GLN
1	t	230	GLN
1	t	264	GLN
1	t	286	HIS
1	t	305	ASN
1	t	313	GLN
1	t	329	ASN
1	t	358	GLN
1	t	397	GLN
1	t	399	ASN
1	t	412	ASN
1	t	446	HIS
1	t	449	GLN
1	t	471	HIS
1	t	482	GLN
1	u	44	ASN
1	u	60	HIS
1	u	66	HIS
1	u	90	GLN
1	u	99	ASN
1	u	103	HIS
1	u	114	HIS
1	u	143	HIS
1	u	148	ASN
1	u	166	ASN
1	u	169	ASN
1	u	176	GLN
1	u	230	GLN
1	u	264	GLN
1	u	286	HIS
1	u	305	ASN
1	u	313	GLN
1	u	329	ASN
1	u	358	GLN
1	u	397	GLN
1	u	399	ASN
1	u	412	ASN
1	u	446	HIS
1	u	449	GLN



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	Continued from previous page				
Mol	Chain	Res	Type		
1	u	471	HIS		
1	u	482	GLN		
1	V	44	ASN		
1	V	60	HIS		
1	V	66	HIS		
1	V	90	GLN		
1	V	99	ASN		
1	V	103	HIS		
1	V	114	HIS		
1	V	143	HIS		
1	V	148	ASN		
1	V	166	ASN		
1	v	169	ASN		
1	V	176	GLN		
1	V	230	GLN		
1	V	264	GLN		
1	V	286	HIS		
1	V	305	ASN		
1	V	313	GLN		
1	V	329	ASN		
1	V	358	GLN		
1	V	397	GLN		
1	V	412	ASN		
1	V	434	HIS		
1	V	446	HIS		
1	V	449	GLN		
1	V	471	HIS		
1	V	482	GLN		
1	W	44	ASN		
1	W	60	HIS		
1	W	66	HIS		
1	W	90	GLN		
1	W	99	ASN		
1	W	103	HIS		
1	W	114	HIS		
1	W	143	HIS		
1	W	148	ASN		
1	W	166	ASN		
1	W	169	ASN		
1	W	176	GLN		
1	W	230	GLN		
1	W	264	GLN		



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1 w 286 HIS 1 w 305 ASN 1 w 313 GLN 1 w 329 ASN 1 w 358 GLN 1 w 397 GLN 1 w 399 ASN 1 w 446 HIS 1 w 446 HIS 1 w 447 HIS 1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 44 ASN 1 x 66 HIS 1 x 99 ASN 1 x 103 HIS 1 x 144 HIS 1 x 143 HIS 1 x 143 HIS 1 x 148		inued from		
1 w 305 ASN 1 w 313 GLN 1 w 329 ASN 1 w 358 GLN 1 w 397 GLN 1 w 399 ASN 1 w 442 ASN 1 w 446 HIS 1 w 449 GLN 1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 99 ASN 1 x 103 HIS 1 x 144 HIS 1 x 143 HIS 1 x 148 ASN		Chain	Res	Type
1 w 313 GLN 1 w 329 ASN 1 w 358 GLN 1 w 397 GLN 1 w 399 ASN 1 w 412 ASN 1 w 446 HIS 1 w 449 GLN 1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 66 HIS 1 x 66 HIS 1 x 99 ASN 1 x 103 HIS 1 x 144 HIS 1 x 143 HIS 1 x 148 ASN		W	286	
1 w 329 ASN 1 w 358 GLN 1 w 397 GLN 1 w 399 ASN 1 w 412 ASN 1 w 446 HIS 1 w 449 GLN 1 w 449 GLN 1 w 442 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 144 HIS 1 x 143 HIS 1 x 148 ASN	1	W		
1 w 358 GLN 1 w 397 GLN 1 w 399 ASN 1 w 412 ASN 1 w 446 HIS 1 w 446 HIS 1 w 447 HIS 1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	313	
1 w 397 GLN 1 w 399 ASN 1 w 412 ASN 1 w 446 HIS 1 w 449 GLN 1 w 471 HIS 1 w 482 GLN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 144 HIS 1 x 143 HIS 1 x 148 ASN	1	W	329	
1 w 399 ASN 1 w 412 ASN 1 w 446 HIS 1 w 449 GLN 1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	358	GLN
1 w 412 ASN 1 w 446 HIS 1 w 449 GLN 1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	397	GLN
1 w 446 HIS 1 w 449 GLN 1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	399	ASN
1 w 449 GLN 1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	412	ASN
1 w 471 HIS 1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	446	
1 w 482 GLN 1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	449	GLN
1 x 44 ASN 1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	471	HIS
1 x 60 HIS 1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	W	482	GLN
1 x 66 HIS 1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	X	44	ASN
1 x 90 GLN 1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	X	60	
1 x 99 ASN 1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	X	66	HIS
1 x 103 HIS 1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	X	90	GLN
1 x 114 HIS 1 x 143 HIS 1 x 148 ASN	1	X	99	ASN
1 x 143 HIS 1 x 148 ASN	1	X	103	HIS
1 x 148 ASN	1	X	114	HIS
	1	X	143	HIS
1 100 AOM	1	X	148	ASN
1 X 100 ASN	1	X	166	ASN
1 x 169 ASN	1	X	169	ASN
1 x 176 GLN	1	X	176	GLN
1 x 230 GLN	1	X	230	GLN
1 x 264 GLN	1	X	264	GLN
1 x 286 HIS	1	X	286	HIS
1 x 305 ASN	1	X	305	ASN
1 x 313 GLN	1	X	313	GLN
1 x 329 ASN	1	X	329	ASN
1 x 358 GLN	1	X	358	GLN
1 x 397 GLN	1	X	397	GLN
1 x 399 ASN	1	X	399	
1 x 412 ASN	1	X	412	
1 x 446 HIS	1	X	446	
1 x 449 GLN	1	X	449	
1 x 471 HIS	1	X	471	HIS
1 x 482 GLN	1	X		GLN
1 y 44 ASN	1	у	44	ASN
1 y 60 HIS	1		60	HIS
1 y 66 HIS	1		66	HIS
1 y 90 GLN	1		90	



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Continued from previous page			
Mol	Chain	Res	Type
1	у	99	ASN
1	У	103	HIS
1	у	114	HIS
1	у	143	HIS
1	у	148	ASN
1	у	166	ASN
1	у	169	ASN
1	у	176	GLN
1	у	230	GLN
1	У	264	GLN
1	У	286	HIS
1	У	305	ASN
1	у	313	GLN
1	у	329	ASN
1	у	358	GLN
1	у	397	GLN
1	у	399	ASN
1	у	412	ASN
1	у	434	HIS
1	у	446	HIS
1	у	449	GLN
1	у	471	HIS
1	у	482	GLN
1	Z	44	ASN
1	Z	60	HIS
1	Z	66	HIS
1	Z	90	GLN
1	Z	99	ASN
1	Z	103	HIS
1	Z	114	HIS
1	Z	143	HIS
1	Z	148	ASN
1	Z	166	ASN
1	Z	169	ASN
1	Z	176	GLN
1	Z	230	GLN
1	Z	264	GLN
1	Z	286	HIS
1	Z	305	ASN
1	Z	313	GLN
1	Z	329	ASN
1	Z	358	GLN

Z | 358 | GLN | Continued on next page...



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Continued from previous page			
Mol	Chain	Res	Type
1	Z	397	GLN
1	Z	399	ASN
1	Z	412	ASN
1	Z	446	HIS
1	Z	449	GLN
1	Z	471	HIS
1	Z	482	GLN
1	1	44	ASN
1	1	60	HIS
1	1	66	HIS
1	1	90	GLN
1	1	99	ASN
1	1	103	HIS
1	1	114	HIS
1	1	143	HIS
1	1	148	ASN
1	1	166	ASN
1	1	169	ASN
1	1	176	GLN
1	1	230	GLN
1	1	264	GLN
1	1	286	HIS
1	1	305	ASN
1	1	313	GLN
1	1	329	ASN
1	1	358	GLN
1	1	397	GLN
1	1	399	ASN
1	1	412	ASN
1	1	446	HIS
1	1	449	GLN
1	1	471	HIS
1	1	482	GLN
1	1	549	ASN
1	2	44	ASN
1	2	60	HIS
1	2	66	HIS
1	2	90	GLN
1	2	99	ASN
1	2	103	HIS
1	2	114	HIS
1	2	143	HIS



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Continued from previous page			
Mol	Chain	Res	Type
1	2	148	ASN
1	2	166	ASN
1	2	169	ASN
1	2	176	GLN
1	2	230	GLN
1	2	264	GLN
1	2	286	HIS
1	2	305	ASN
1	2	313	GLN
1	2	329	ASN
1	2	358	GLN
1	2	397	GLN
1	2	412	ASN
1	2	434	HIS
1	2	446	HIS
1	2	449	GLN
1	2	471	HIS
1	2	482	GLN
1	3	44	ASN
1	3	60	HIS
1	3	66	HIS
1	3	90	GLN
1	3	99	ASN
1	3	103	HIS
1	3	114	HIS
1	3	143	HIS
1	3	148	ASN
1	3	166	ASN
1	3	169	ASN
1	3	176	GLN
1	3	230	GLN
1	3	264	GLN
1	3	286	HIS
1	3	305	ASN
1	3	313	GLN
1	3	329	ASN
1	3	358	GLN
1	3	397	GLN
1	3	399	ASN
1	3	412	ASN
1	3	434	HIS
1	3	446	HIS



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Continued from previous page			
Mol	Chain	Res	Type
1	3	449	GLN
1	3	471	HIS
1	3	482	GLN
1	4	44	ASN
1	4	60	HIS
1	4	66	HIS
1	4	90	GLN
1	4	99	ASN
1	4	103	HIS
1	4	114	HIS
1	4	143	HIS
1	4	148	ASN
1	4	166	ASN
1	4	169	ASN
1	4	176	GLN
1	4	230	GLN
1	4	264	GLN
1	4	286	HIS
1	4	305	ASN
1	4	313	GLN
1	4	329	ASN
1	4	358	GLN
1	4	397	GLN
1	4	399	ASN
1	4	412	ASN
1	4	446	HIS
1	4	449	GLN
1	4	471	HIS
1	4	482	GLN
1	5	44	ASN
1	5	60	HIS
1	5	66	HIS
1	5	90	GLN
1	5	99	ASN
1	5	103	HIS
1	5	114	HIS
1	5	143	HIS
1	5	148	ASN
1	5	166	ASN
1	5	169	ASN
1	5	176	GLN
1	5	230	GLN



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Mol	Chain	Res	Type
1	5	264	GLN
1	5	286	HIS
1	5	305	ASN
1	5	313	GLN
1	5	329	ASN
1	5	358	GLN
1	5	397	GLN
1	5	399	ASN
1	5	412	ASN
1	5	446	HIS
1	5	449	GLN
1	5	471	HIS
1	5	482	GLN
1	6	44	ASN
1	6	60	HIS
1	6	66	HIS
1	6	90	GLN
1	6	99	ASN
1	6	103	HIS
1	6	114	HIS
1	6	143	HIS
1	6	148	ASN
1	6	166	ASN
1	6	169	ASN
1	6	176	GLN
1	6	230	GLN
1	6	264	GLN
1	6	286	HIS
1	6	305	ASN
1	6	313	GLN
1	6	329	ASN
1	6	358	GLN
1	6	397	GLN
1	6	399	ASN
1	6	412	ASN
1	6	446	HIS
1	6	449	GLN
1	6	471	HIS
1	6	482	GLN
1	7	44	ASN
1	7	60	HIS
1	7	66	HIS



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Mol	Chain	Res	Type
1	7	90	GLN
1	7 7	99	ASN
1		103	HIS
1	7	114	HIS
1	7	143	HIS
1	7	148	ASN
1	7	166	ASN
1	7	169	ASN
1	7	176	GLN
1	7	230	GLN
1	7	264	GLN
1	7	286	HIS
1	7	305	ASN
1	7 7	313	GLN
1		329	ASN
1	7	358	GLN
1	7	397	GLN
1	7	412	ASN
1	7 7	434	HIS
1	7	446	HIS
1	7	449	GLN
1	7	471	HIS
1	7	482	GLN
1	8	44	ASN
1	8	60	HIS
1	8	66	HIS
1	8	90	GLN
1	8	99	ASN
1	8	103	HIS
1	8	114	HIS
1	8	143	HIS
1	8	148	ASN
1	8	166	ASN
1	8	169	ASN
1	8	176	GLN
1	8	230	GLN
1	8	264	GLN
1	8	286	HIS
1	8	305	ASN
1	8	313	GLN
1	8	329	ASN
1	8	358	GLN



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Mol	Chain	Res	Type
1	8	397	GLN
1	8	399	ASN
1	8	412	ASN
1	8	446	HIS
1	8	449	GLN
1	8	471	HIS
1	8	482	GLN
1	8	549	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.



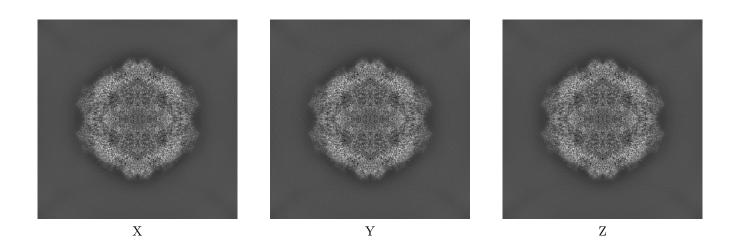
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22008. 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)

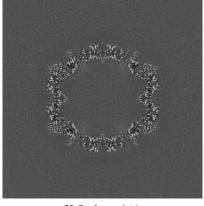
6.1.1 Primary map



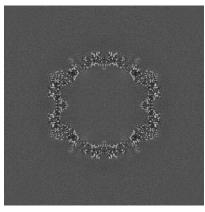
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

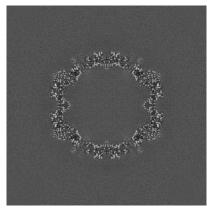
6.2.1 Primary map







Y Index: 210



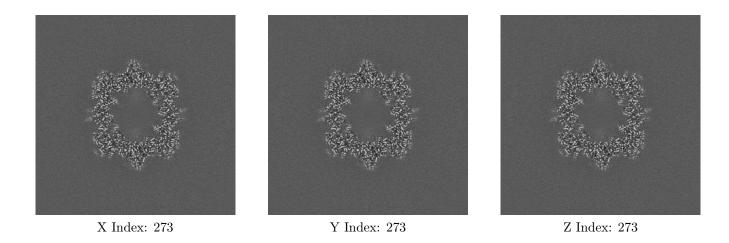
Z Index: 210



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

6.3 Largest variance slices (i)

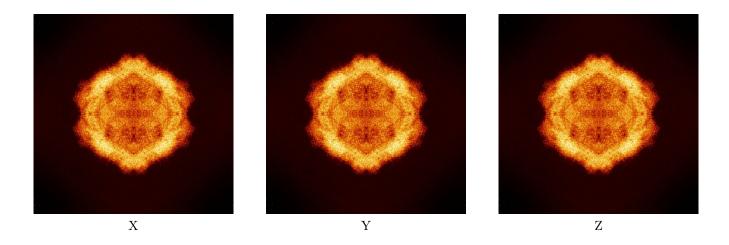
6.3.1 Primary map



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

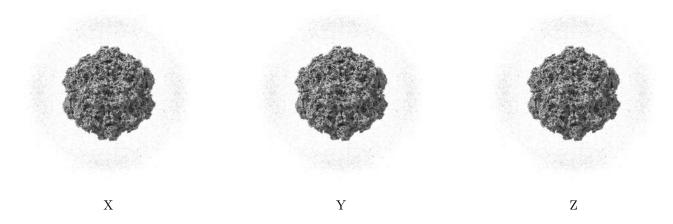


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

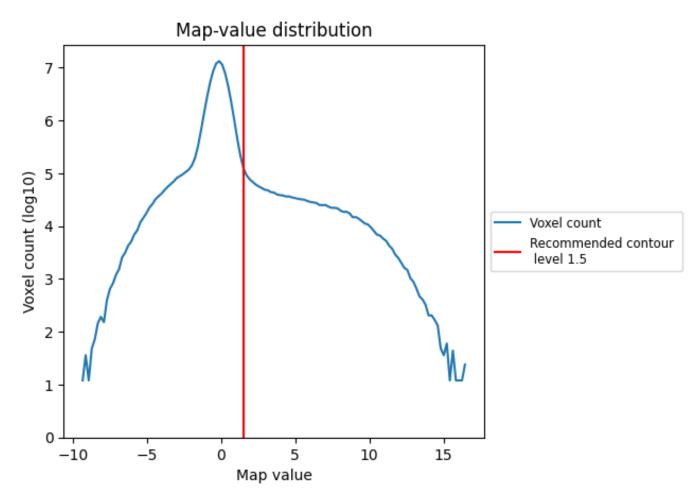
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

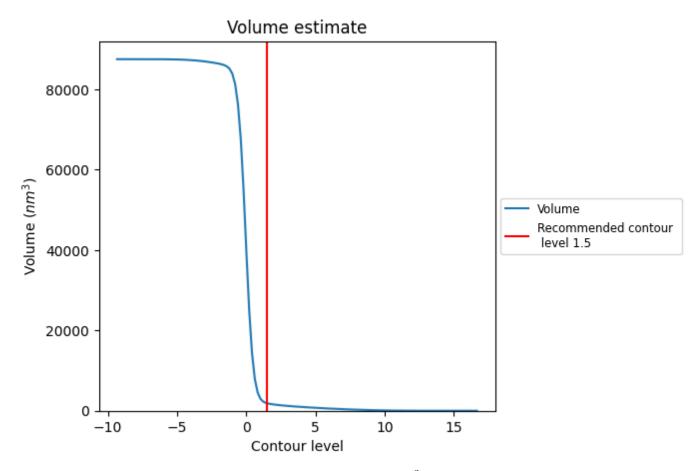
7.1 Map-value distribution (i)



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)

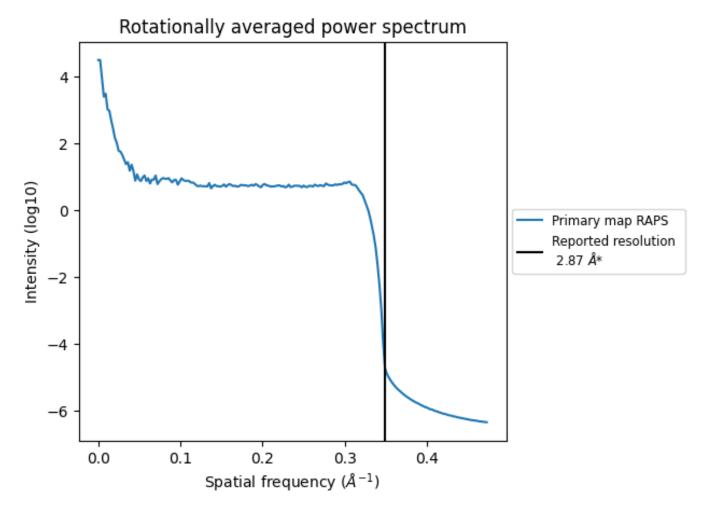


The volume at the recommended contour level is 1874 nm^3 ; this corresponds to an approximate mass of 1693 kDa.

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 0.348 $\rm \mathring{A}^{-1}$



8 Fourier-Shell correlation (i)

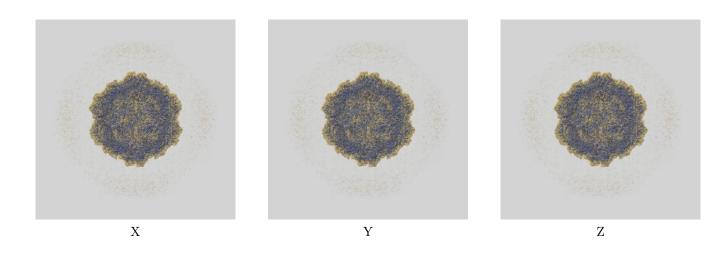
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22008 and PDB model 6X2I. Per-residue inclusion information can be found in section 3 on page 10.

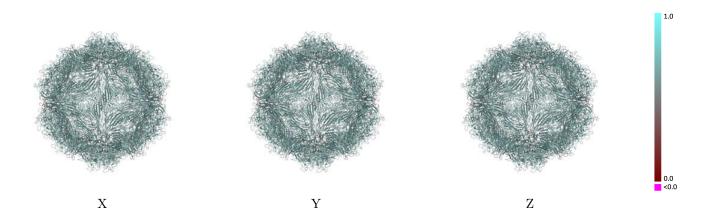
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

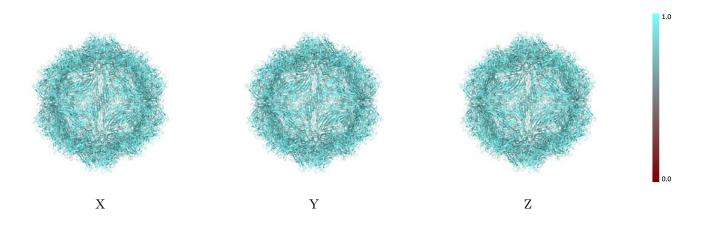


9.2 Q-score mapped to coordinate model (i)



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

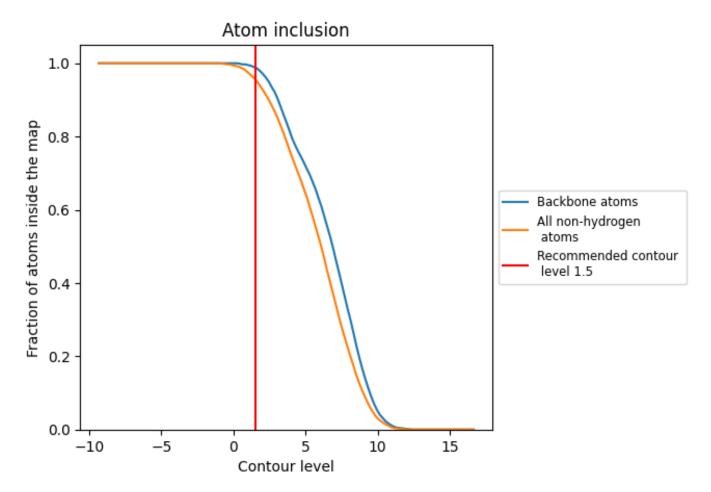
9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).



9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.6120
1	0.9560	0.6130
2	0.9560	0.6130
3	0.9560	0.6120
4	0.9570	0.6120
5	0.9550	0.6120
6	0.9530	0.6130
7	0.9530	0.6110
8	0.9550	0.6120
A	0.9560	0.6130
В	0.9560	0.6130
С	0.9570	0.6120
D	0.9530	0.6120
Е	0.9550	0.6110
F	0.9560	0.6110
G	0.9550	0.6110
Н	0.9550	0.6120
I	0.9570	0.6120
J	0.9560	0.6130
K	0.9570	0.6130
L	0.9560	0.6140
M	0.9550	0.6120
N	0.9550	0.6120
О	0.9550	0.6120
P	0.9550	0.6130
Q	0.9570	0.6130
R	0.9560	0.6140
S	0.9560	0.6130
T	0.9570	0.6140
U	0.9560	0.6140
V	0.9570	0.6130
W	0.9540	0.6130
X	0.9550	0.6120
Y	0.9550	0.6130
Z	0.9550	0.6120





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Chain	Atom inclusion	Q-score
a	0.9560	0.6120
b	0.9560	0.6130
С	0.9560	0.6130
d	0.9560	0.6130
e	0.9560	0.6120
f	0.9560	0.6130
g	0.9570	0.6120
h	0.9550	0.6120
i	0.9550	0.6120
j	0.9550	0.6120
k	0.9530	0.6120
1	0.9550	0.6120
m	0.9570	0.6140
n	0.9560	0.6130
0	0.9550	0.6120
p	0.9570	0.6120
q	0.9560	0.6130
r	0.9560	0.6130
S	0.9560	0.6130
t	0.9550	0.6120
u	0.9570	0.6120
V	0.9560	0.6120
W	0.9550	0.6110
X	0.9570	0.6120
У	0.9560	0.6120
Z	0.9560	0.6140

