



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:35 AM UTC

PDB ID : 4UOM / pdb_00004uom
EMDB ID : EMD-2645
Title : Electron Cryo-microscopy of Venezuelan Equine Encephalitis Virus TC- 83 in complex with neutralizing antibody Fab F5
Authors : Porta, J.; Jose, J.; Roehrig, J.T.; Blair, C.D.; Kuhn, R.J.; Rossmann, M.G.
Deposited on : 2014-06-05
Resolution : 17.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

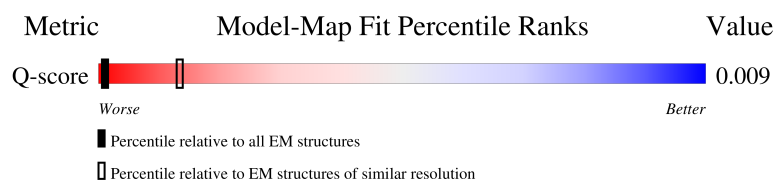
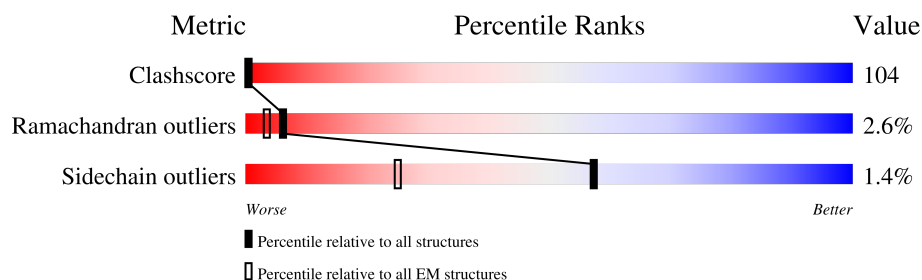
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	38 (16.50 - 17.50)

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

Mol	Chain	Length	Quality of chain
1	H	217	70% 53% 42% .
2	L	205	88% 58% 26% 11% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3206 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 FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	217	Total	C	N	O	S	0	0
			1645	1045	265	328	7		

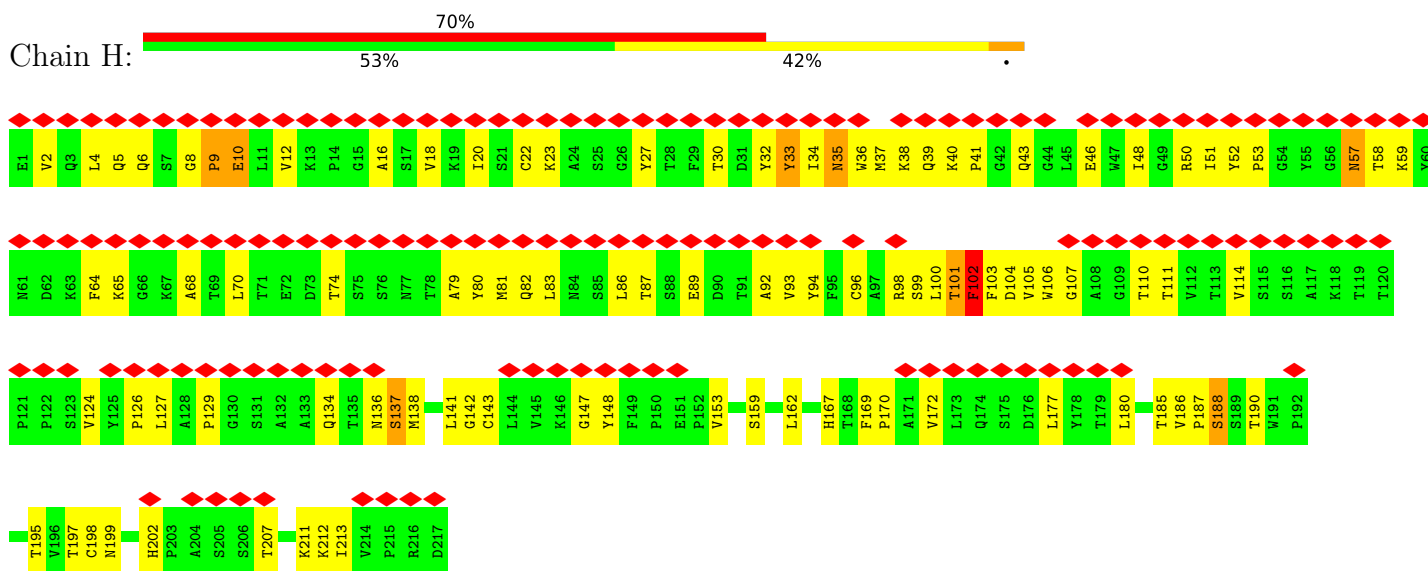
- Molecule 2 is a protein called FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	205	Total	C	N	O	S	0	0
			1561	969	262	325	5		

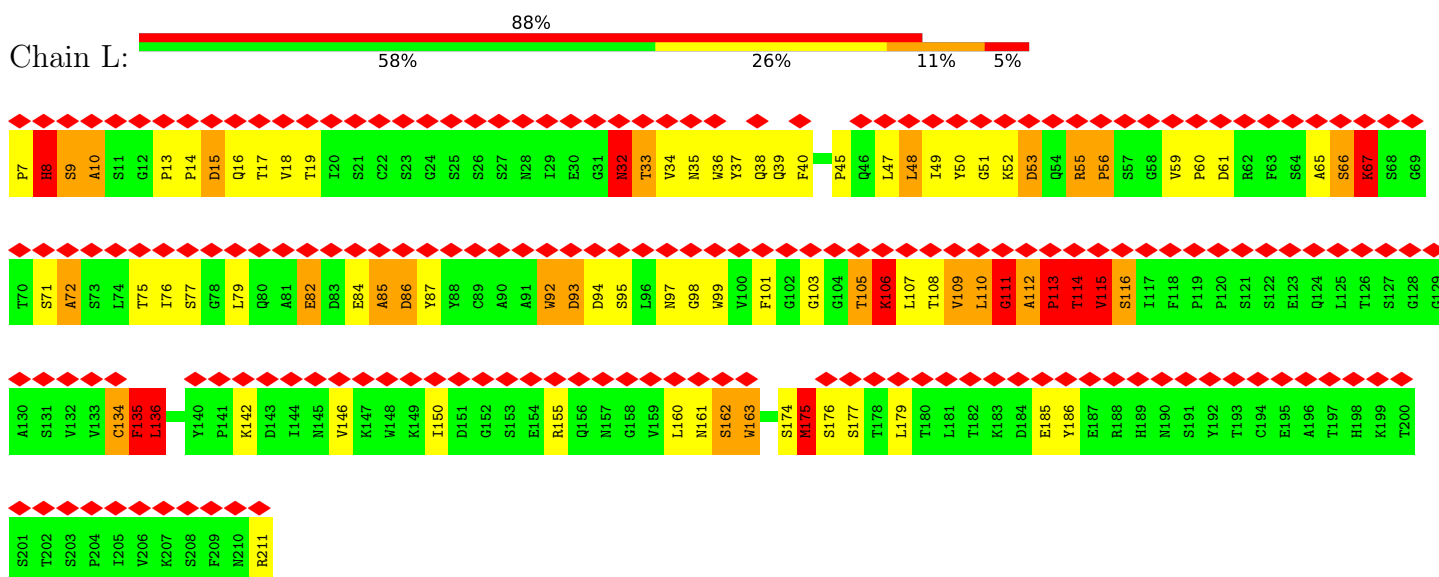
3 Residue-property plots

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: FAB FRAGMENT HEAVY CHAIN



• Molecule 2: FAB FRAGMENT LIGHT CHAIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1389	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	24	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60521	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.258	Depositor
Minimum map value	-8.635	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.740	Depositor
Recommended contour level	1.5	Depositor
Map size ($\text{\AA}$)	1095.68, 1095.68, 1095.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	4.28, 4.28, 4.28	Depositor

5 Model quality

5.1 Standard geometry

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	H	1.04	3/1689 (0.2%)	1.22	13/2309 (0.6%)
2	L	4.97	59/1600 (3.7%)	2.67	89/2177 (4.1%)
All	All	3.54	62/3289 (1.9%)	2.05	102/4486 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
2	L	3	8
All	All	3	10

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	111	GLY	CA-C	87.10	2.74	1.51
2	L	112	ALA	CA-CB	-56.76	0.91	1.53
2	L	163	TRP	CD2-CE2	51.24	2.28	1.41
2	L	134	CYS	C-N	46.62	1.99	1.33
2	L	111	GLY	N-CA	-40.40	0.86	1.45
2	L	114	THR	N-CA	-40.23	0.97	1.46
2	L	114	THR	CA-C	40.10	2.00	1.52
2	L	112	ALA	N-CA	-39.04	1.07	1.46
2	L	114	THR	CA-CB	35.94	2.08	1.53
2	L	135	PHE	N-CA	31.80	1.87	1.46
2	L	175	MET	CG-SD	30.48	2.56	1.80
2	L	113	PRO	CG-CD	-30.34	0.47	1.50
2	L	111	GLY	C-O	-30.30	0.83	1.23
2	L	113	PRO	N-CD	28.84	1.88	1.47
2	L	106	LYS	N-CA	-27.57	1.10	1.46
2	L	112	ALA	C-O	-27.22	0.94	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	163	TRP	NE1-CE2	26.07	1.66	1.37
2	L	112	ALA	CA-C	24.88	1.81	1.53
2	L	114	THR	C-O	-24.74	0.94	1.24
2	L	134	CYS	CA-CB	-22.48	1.20	1.52
2	L	114	THR	CB-CG2	-22.18	0.79	1.52
1	H	57	ASN	C-O	-22.08	0.96	1.24
2	L	175	MET	CB-CG	-21.48	0.88	1.52
2	L	135	PHE	CA-CB	-20.86	1.26	1.53
2	L	113	PRO	N-CA	-20.23	1.21	1.47
2	L	114	THR	CB-OG1	20.18	1.76	1.43
2	L	106	LYS	C-O	-20.15	0.98	1.24
2	L	134	CYS	C-O	17.39	1.45	1.23
2	L	163	TRP	CG-CD2	17.32	1.75	1.43
2	L	106	LYS	CA-C	15.04	1.73	1.52
2	L	106	LYS	CB-CG	-14.71	1.08	1.52
2	L	112	ALA	C-N	13.77	1.66	1.33
2	L	110	LEU	C-O	-13.62	1.10	1.24
2	L	134	CYS	CA-C	13.26	1.67	1.53
2	L	175	MET	SD-CE	13.23	2.12	1.79
2	L	106	LYS	CG-CD	-12.39	1.15	1.52
2	L	163	TRP	CD2-CE3	-12.38	1.20	1.40
2	L	163	TRP	CD1-NE1	12.05	1.63	1.37
2	L	9	SER	CA-C	-11.27	1.37	1.52
2	L	136	LEU	CG-CD1	-11.12	1.15	1.52
2	L	106	LYS	CE-NZ	-11.00	1.16	1.49
2	L	163	TRP	CG-CD1	10.88	1.64	1.36
2	L	135	PHE	CA-C	-10.27	1.39	1.52
2	L	135	PHE	C-N	-10.05	1.18	1.33
2	L	56	PRO	N-CD	-9.90	1.33	1.47
1	H	57	ASN	C-N	9.11	1.44	1.33
2	L	113	PRO	C-N	-9.06	1.21	1.33
2	L	175	MET	CA-CB	-8.55	1.32	1.54
2	L	67	LYS	CG-CD	-8.51	1.26	1.52
2	L	8	HIS	C-O	-7.94	1.13	1.24
2	L	86	ASP	N-CA	-7.32	1.37	1.46
1	H	57	ASN	CA-C	7.26	1.62	1.52
2	L	110	LEU	C-N	-7.21	1.23	1.33
2	L	115	VAL	N-CA	-6.86	1.37	1.46
2	L	33	THR	CB-CG2	-5.98	1.32	1.52
2	L	82	GLU	C-O	-5.98	1.16	1.24
2	L	162	SER	C-O	5.93	1.31	1.24
2	L	48	LEU	C-O	-5.67	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	163	TRP	CE2-CZ2	-5.60	1.28	1.39
2	L	113	PRO	C-O	-5.54	1.16	1.24
2	L	92	TRP	NE1-CE2	-5.30	1.31	1.37
2	L	32	ASN	CB-CG	-5.18	1.39	1.52

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	135	PHE	CA-C-O	-36.84	76.78	120.62
2	L	113	PRO	N-CD-CG	27.36	144.24	103.20
2	L	112	ALA	CA-C-O	-27.00	87.38	120.87
2	L	113	PRO	N-CA-CB	-22.30	79.83	103.25
2	L	112	ALA	CA-C-N	20.59	145.57	119.84
2	L	112	ALA	C-N-CA	20.59	145.57	119.84
2	L	163	TRP	CD2-CE2-CZ2	-19.46	102.94	122.40
2	L	135	PHE	O-C-N	-19.14	96.92	122.77
2	L	163	TRP	NE1-CE2-CZ2	19.10	158.75	130.10
2	L	9	SER	N-CA-C	18.94	151.13	110.80
2	L	135	PHE	CA-CB-CG	18.32	132.12	113.80
2	L	113	PRO	CA-N-CD	-17.11	88.05	112.00
2	L	134	CYS	CB-CA-C	-16.73	87.47	111.23
2	L	106	LYS	O-C-N	-16.40	100.78	122.59
2	L	67	LYS	CG-CD-CE	16.05	148.21	111.30
2	L	135	PHE	CB-CA-C	15.20	133.78	110.67
2	L	175	MET	CB-CG-SD	14.81	157.13	112.70
2	L	134	CYS	CA-C-O	-13.99	101.58	120.47
2	L	134	CYS	N-CA-CB	12.87	133.22	110.95
2	L	111	GLY	N-CA-C	12.77	143.44	113.18
2	L	112	ALA	N-CA-CB	12.62	132.73	110.90
2	L	111	GLY	CA-C-O	12.25	141.89	120.57
2	L	32	ASN	CA-CB-CG	12.15	124.75	112.60
2	L	114	THR	CA-C-N	12.00	143.58	121.97
2	L	114	THR	C-N-CA	12.00	143.58	121.97
2	L	175	MET	CG-SD-CE	11.82	126.90	100.90
2	L	8	HIS	CA-C-O	-11.73	105.22	119.18
2	L	163	TRP	NE1-CE2-CD2	-11.64	92.27	107.40
2	L	10	ALA	N-CA-CB	11.22	129.45	110.49
2	L	110	LEU	N-CA-C	11.12	123.42	108.07
1	H	102	PHE	CA-CB-CG	11.00	124.80	113.80
2	L	8	HIS	CB-CA-C	-10.90	88.79	109.72
2	L	114	THR	O-C-N	-10.69	110.68	123.29
2	L	112	ALA	CB-CA-C	-9.79	97.94	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	9	SER	CA-C-O	-9.78	106.52	120.51
1	H	101	THR	CA-CB-CG2	9.78	127.12	110.50
2	L	8	HIS	CA-C-N	9.77	140.20	121.54
2	L	8	HIS	C-N-CA	9.77	140.20	121.54
2	L	111	GLY	O-C-N	-9.52	110.33	122.70
2	L	135	PHE	CA-C-N	9.48	138.11	123.23
2	L	135	PHE	C-N-CA	9.48	138.11	123.23
2	L	55	ARG	CA-C-N	9.18	129.12	119.85
2	L	55	ARG	C-N-CA	9.18	129.12	119.85
2	L	112	ALA	N-CA-C	9.13	126.27	110.02
2	L	115	VAL	N-CA-C	8.87	127.79	109.34
2	L	163	TRP	CA-CB-CG	8.63	130.01	113.60
2	L	93	ASP	CA-CB-CG	8.59	121.19	112.60
2	L	135	PHE	N-CA-CB	8.40	123.37	109.60
2	L	175	MET	N-CA-CB	-8.35	96.17	111.37
2	L	113	PRO	CB-CG-CD	-8.34	79.42	106.10
2	L	115	VAL	N-CA-CB	-8.34	97.47	111.23
2	L	175	MET	O-C-N	-8.34	112.98	123.24
2	L	8	HIS	O-C-N	8.30	134.20	122.41
2	L	113	PRO	CB-CA-C	8.01	124.77	111.56
2	L	106	LYS	CA-C-O	7.84	131.73	120.51
2	L	10	ALA	N-CA-C	7.78	127.37	110.80
2	L	9	SER	CA-CB-OG	-7.71	95.68	111.10
2	L	106	LYS	CA-CB-CG	7.67	129.44	114.10
2	L	33	THR	OG1-CB-CG2	7.54	124.37	109.30
2	L	162	SER	CB-CA-C	-7.37	100.02	110.34
2	L	175	MET	CB-CA-C	7.34	124.73	109.38
2	L	110	LEU	CA-C-O	7.34	131.23	121.47
2	L	106	LYS	N-CA-CB	7.28	122.79	110.49
2	L	134	CYS	CA-C-N	7.15	132.81	121.66
2	L	134	CYS	C-N-CA	7.15	132.81	121.66
2	L	113	PRO	N-CA-C	7.10	127.09	112.47
2	L	163	TRP	CZ3-CH2-CZ2	6.96	130.54	121.50
1	H	57	ASN	N-CA-C	6.93	125.57	110.80
1	H	110	THR	CA-CB-OG1	-6.84	99.34	109.60
1	H	57	ASN	CA-C-N	-6.77	108.17	121.91
1	H	57	ASN	C-N-CA	-6.77	108.17	121.91
2	L	56	PRO	N-CD-CG	6.75	113.32	103.20
1	H	35	ASN	OD1-CG-ND2	-6.70	115.90	122.60
2	L	163	TRP	CD1-NE1-CE2	6.66	120.89	108.90
2	L	32	ASN	CB-CG-ND2	6.56	126.24	116.40
1	H	58	THR	CA-CB-CG2	6.39	121.37	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	105	THR	O-C-N	6.34	131.02	122.59
2	L	32	ASN	CB-CG-OD1	-6.33	108.14	120.80
2	L	67	LYS	CB-CG-CD	6.27	125.73	111.30
1	H	101	THR	CA-C-N	6.23	132.92	121.70
1	H	101	THR	C-N-CA	6.23	132.92	121.70
2	L	32	ASN	CB-CA-C	6.10	122.56	110.42
2	L	53	ASP	O-C-N	-6.07	115.61	122.23
2	L	72	ALA	N-CA-CB	-6.03	100.08	111.00
2	L	116	SER	N-CA-C	-5.90	98.23	110.80
2	L	9	SER	CB-CA-C	-5.81	98.86	110.42
2	L	162	SER	N-CA-C	5.76	117.43	107.93
2	L	110	LEU	CA-C-N	-5.73	110.18	121.41
2	L	110	LEU	C-N-CA	-5.73	110.18	121.41
2	L	115	VAL	CA-C-N	5.66	132.35	121.54
2	L	115	VAL	C-N-CA	5.66	132.35	121.54
2	L	136	LEU	CB-CG-CD1	5.64	127.62	110.70
2	L	114	THR	CB-CA-C	5.56	119.34	109.72
1	H	110	THR	CA-CB-CG2	5.50	119.85	110.50
2	L	53	ASP	CA-C-O	5.45	125.19	119.03
2	L	66	SER	CA-C-O	-5.43	115.61	121.36
2	L	10	ALA	CB-CA-C	-5.29	99.88	110.42
2	L	86	ASP	N-CA-C	5.22	117.23	107.99
2	L	110	LEU	CB-CA-C	-5.21	102.41	114.41
1	H	58	THR	N-CA-C	5.21	116.44	108.42
2	L	135	PHE	N-CA-C	-5.16	101.72	109.15
1	H	188	SER	CB-CA-C	-5.15	99.45	110.32

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	L	9	SER	CA
2	L	112	ALA	CA
2	L	135	PHE	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	33	TYR	Sidechain
1	H	9	PRO	Mainchain
2	L	106	LYS	Mainchain
2	L	111	GLY	Peptide
2	L	113	PRO	Mainchain

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Mol	Chain	Res	Type	Group
2	L	114	THR	Peptide
2	L	115	VAL	Mainchain
2	L	135	PHE	Mainchain
2	L	175	MET	Mainchain
2	L	8	HIS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1645	0	1608	164	0
2	L	1561	0	1465	547	0
All	All	3206	0	3073	655	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 104.

All (655) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:111:GLY:C	2:L:163:TRP:CE2	1.78	1.60
2:L:163:TRP:CG	2:L:163:TRP:CD2	1.74	1.59
2:L:111:GLY:C	2:L:163:TRP:CD2	1.80	1.55
2:L:111:GLY:CA	2:L:163:TRP:CE2	1.91	1.53
2:L:112:ALA:C	2:L:112:ALA:CA	1.81	1.51
1:H:37:MET:CE	2:L:101:PHE:HZ	1.25	1.50
2:L:111:GLY:CA	2:L:163:TRP:CD2	1.96	1.48
2:L:175:MET:CG	2:L:175:MET:CA	1.93	1.44
2:L:114:THR:C	2:L:136:LEU:HD12	1.42	1.42
2:L:112:ALA:CB	2:L:112:ALA:N	1.82	1.38
2:L:175:MET:SD	2:L:175:MET:CE	2.12	1.37
2:L:135:PHE:N	2:L:135:PHE:CA	1.87	1.37
2:L:114:THR:C	2:L:135:PHE:O	1.68	1.34
1:H:37:MET:CE	2:L:101:PHE:CZ	2.08	1.33
2:L:114:THR:C	2:L:114:THR:CA	2.00	1.32
2:L:114:THR:OG1	2:L:114:THR:CB	1.76	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:114:THR:CA	2:L:114:THR:CB	2.08	1.29
2:L:114:THR:HB	2:L:135:PHE:CG	1.66	1.28
2:L:111:GLY:C	2:L:163:TRP:CG	2.10	1.27
2:L:55:ARG:NH1	2:L:61:ASP:HA	1.50	1.26
2:L:32:ASN:HB2	2:L:33:THR:CB	1.66	1.24
2:L:163:TRP:CE2	2:L:163:TRP:CD2	2.28	1.21
2:L:111:GLY:C	2:L:163:TRP:CD1	2.19	1.21
2:L:112:ALA:C	2:L:112:ALA:CB	2.14	1.20
2:L:134:CYS:C	2:L:135:PHE:N	1.99	1.19
1:H:50:ARG:NH2	2:L:99:TRP:CE3	2.09	1.19
2:L:113:PRO:HD3	2:L:175:MET:SD	1.82	1.19
1:H:37:MET:HE1	2:L:101:PHE:CZ	1.74	1.18
2:L:111:GLY:HA2	2:L:163:TRP:CE2	1.68	1.18
2:L:7:PRO:O	2:L:106:LYS:HB3	1.41	1.16
2:L:111:GLY:C	2:L:163:TRP:NE1	2.03	1.16
2:L:92:TRP:HB3	2:L:95:SER:HB2	1.24	1.15
2:L:113:PRO:HB3	2:L:175:MET:CE	1.77	1.14
2:L:111:GLY:HA2	2:L:163:TRP:CZ2	1.83	1.14
2:L:115:VAL:HG23	2:L:136:LEU:CG	1.76	1.14
2:L:114:THR:C	2:L:135:PHE:N	2.06	1.13
2:L:111:GLY:O	2:L:175:MET:HG3	1.47	1.13
2:L:112:ALA:N	2:L:163:TRP:CE2	2.15	1.13
2:L:9:SER:N	2:L:106:LYS:HB2	1.63	1.12
2:L:113:PRO:CB	2:L:136:LEU:HD13	1.79	1.12
2:L:67:LYS:HB2	2:L:71:SER:O	1.49	1.12
2:L:112:ALA:C	2:L:175:MET:SD	2.32	1.12
1:H:37:MET:HE3	2:L:101:PHE:HZ	1.10	1.11
2:L:111:GLY:O	2:L:112:ALA:N	1.83	1.11
2:L:67:LYS:CB	2:L:72:ALA:HA	1.79	1.11
1:H:172:VAL:HG11	2:L:160:LEU:HD22	1.20	1.10
2:L:93:ASP:HB2	2:L:99:TRP:CE3	1.87	1.10
2:L:109:VAL:HG23	2:L:142:LYS:HE2	1.32	1.10
2:L:48:LEU:O	2:L:56:PRO:HD2	1.49	1.09
2:L:112:ALA:C	2:L:112:ALA:HB1	1.78	1.09
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.23	1.08
2:L:112:ALA:N	2:L:163:TRP:CD2	2.21	1.08
2:L:114:THR:CA	2:L:134:CYS:C	2.26	1.08
1:H:172:VAL:CG1	2:L:160:LEU:HD22	1.84	1.08
2:L:86:ASP:CA	2:L:105:THR:HG21	1.82	1.08
2:L:8:HIS:C	2:L:106:LYS:HB2	1.78	1.08
2:L:111:GLY:C	2:L:111:GLY:O	0.83	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:GLN:CD	2:L:48:LEU:HD21	1.78	1.07
2:L:92:TRP:HE1	2:L:94:ASP:HB2	1.10	1.07
2:L:115:VAL:CG2	2:L:136:LEU:HG	1.85	1.06
2:L:86:ASP:HA	2:L:105:THR:HG21	1.09	1.06
2:L:112:ALA:CB	2:L:112:ALA:HA	1.59	1.06
2:L:114:THR:C	2:L:135:PHE:C	2.22	1.06
2:L:34:VAL:HG11	2:L:67:LYS:HE3	1.35	1.05
2:L:112:ALA:C	2:L:175:MET:HG2	1.80	1.05
2:L:112:ALA:CA	2:L:112:ALA:O	2.00	1.05
2:L:135:PHE:N	2:L:135:PHE:O	1.88	1.05
2:L:112:ALA:CA	2:L:112:ALA:HB2	1.53	1.05
2:L:114:THR:CB	2:L:135:PHE:N	2.20	1.04
2:L:32:ASN:HB2	2:L:33:THR:HB	1.34	1.04
2:L:49:ILE:HD13	2:L:65:ALA:HB2	1.37	1.04
2:L:114:THR:HG1	2:L:135:PHE:N	1.55	1.04
2:L:175:MET:CA	2:L:175:MET:HG2	1.72	1.04
2:L:92:TRP:NE1	2:L:94:ASP:HB2	1.73	1.04
2:L:111:GLY:CA	2:L:163:TRP:NE1	2.22	1.03
2:L:113:PRO:CD	2:L:175:MET:SD	2.46	1.03
2:L:114:THR:HB	2:L:135:PHE:CB	1.87	1.03
1:H:37:MET:HE1	2:L:101:PHE:HZ	1.07	1.02
2:L:34:VAL:HG21	2:L:67:LYS:NZ	1.74	1.02
2:L:113:PRO:HB3	2:L:175:MET:HE2	1.05	1.02
2:L:106:LYS:C	2:L:107:LEU:HD12	1.84	1.01
2:L:112:ALA:CA	2:L:112:ALA:HB1	1.53	1.01
2:L:112:ALA:N	2:L:175:MET:SD	2.33	1.01
1:H:6:GLN:HE22	1:H:107:GLY:HA3	1.22	1.01
2:L:114:THR:CA	2:L:135:PHE:N	2.22	1.01
2:L:67:LYS:HB3	2:L:72:ALA:HA	1.39	1.00
2:L:112:ALA:CA	2:L:112:ALA:HB3	1.53	0.99
2:L:111:GLY:O	2:L:163:TRP:CD1	2.15	0.99
2:L:114:THR:CB	2:L:134:CYS:C	2.34	0.99
1:H:102:PHE:CE1	2:L:50:TYR:HB3	1.96	0.99
2:L:115:VAL:N	2:L:135:PHE:C	2.20	0.99
2:L:109:VAL:CG2	2:L:142:LYS:HE2	1.92	0.99
2:L:175:MET:CG	2:L:175:MET:HB3	1.48	0.99
2:L:111:GLY:N	2:L:163:TRP:CD2	2.31	0.99
2:L:86:ASP:HA	2:L:105:THR:CG2	1.94	0.98
2:L:175:MET:CG	2:L:175:MET:HB2	1.48	0.98
2:L:114:THR:HG23	2:L:134:CYS:O	1.64	0.98
2:L:114:THR:CG2	2:L:135:PHE:CD1	2.47	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:114:THR:OG1	2:L:134:CYS:C	2.05	0.97
2:L:32:ASN:HB2	2:L:33:THR:CA	1.93	0.97
2:L:33:THR:HG21	2:L:95:SER:HB2	1.44	0.97
2:L:7:PRO:HD2	2:L:106:LYS:HE2	1.46	0.97
2:L:114:THR:C	2:L:136:LEU:CD1	2.37	0.96
2:L:114:THR:O	2:L:134:CYS:SG	2.24	0.96
2:L:114:THR:CB	2:L:114:THR:HG22	1.44	0.96
2:L:110:LEU:O	2:L:163:TRP:CG	2.19	0.95
2:L:112:ALA:C	2:L:175:MET:CG	2.39	0.95
2:L:33:THR:OG1	2:L:92:TRP:HB2	1.67	0.95
2:L:113:PRO:HB2	2:L:136:LEU:HD13	1.44	0.94
1:H:170:PRO:HG2	2:L:162:SER:OG	1.67	0.94
1:H:102:PHE:CD1	2:L:50:TYR:HB3	2.03	0.94
2:L:175:MET:CG	2:L:175:MET:SD	2.57	0.94
2:L:114:THR:CB	2:L:114:THR:HG21	1.44	0.93
2:L:112:ALA:CA	2:L:175:MET:CG	2.46	0.93
2:L:114:THR:CB	2:L:114:THR:HG23	1.44	0.93
2:L:112:ALA:HB3	2:L:162:SER:C	1.94	0.93
2:L:114:THR:HG22	2:L:135:PHE:CD1	2.04	0.93
2:L:113:PRO:N	2:L:175:MET:CG	2.32	0.93
2:L:17:THR:HG22	2:L:77:SER:O	1.68	0.93
2:L:114:THR:HB	2:L:135:PHE:CA	1.98	0.93
2:L:10:ALA:HB2	2:L:106:LYS:NZ	1.84	0.92
2:L:112:ALA:CA	2:L:175:MET:SD	2.57	0.92
2:L:113:PRO:CD	2:L:175:MET:CG	2.47	0.92
2:L:113:PRO:N	2:L:175:MET:HG2	1.83	0.92
2:L:112:ALA:CB	2:L:162:SER:C	2.42	0.92
2:L:114:THR:CB	2:L:135:PHE:CA	2.48	0.91
2:L:87:TYR:O	2:L:105:THR:HB	1.70	0.91
2:L:34:VAL:HG21	2:L:67:LYS:HZ2	1.29	0.91
2:L:110:LEU:C	2:L:142:LYS:HE3	1.96	0.91
2:L:112:ALA:CA	2:L:112:ALA:CB	0.91	0.91
2:L:175:MET:HG2	2:L:175:MET:CB	1.38	0.90
2:L:114:THR:HB	2:L:135:PHE:CD1	2.05	0.90
2:L:114:THR:OG1	2:L:135:PHE:N	2.04	0.90
2:L:7:PRO:CD	2:L:106:LYS:HE2	2.02	0.89
1:H:50:ARG:HG2	1:H:59:LYS:HB2	1.52	0.89
2:L:113:PRO:HB2	2:L:136:LEU:CD1	2.01	0.89
2:L:10:ALA:HB2	2:L:106:LYS:HZ1	1.35	0.89
2:L:55:ARG:HH11	2:L:61:ASP:HA	1.18	0.89
2:L:175:MET:HG3	2:L:175:MET:CB	1.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:PRO:C	2:L:106:LYS:HB3	1.98	0.89
2:L:113:PRO:CA	2:L:136:LEU:HD13	2.01	0.89
1:H:35:ASN:HD22	1:H:103:PHE:HE1	1.21	0.88
1:H:37:MET:HE3	2:L:101:PHE:CZ	1.90	0.88
2:L:7:PRO:C	2:L:106:LYS:HD3	1.97	0.88
2:L:106:LYS:O	2:L:107:LEU:HD12	1.71	0.88
2:L:111:GLY:O	2:L:163:TRP:CG	2.26	0.88
2:L:33:THR:HG21	2:L:95:SER:CB	2.03	0.88
1:H:169:PHE:CE2	2:L:175:MET:C	2.52	0.88
2:L:115:VAL:HG23	2:L:136:LEU:HG	0.91	0.88
2:L:114:THR:CA	2:L:114:THR:CG2	2.52	0.88
2:L:175:MET:CG	2:L:175:MET:CB	0.88	0.87
2:L:113:PRO:C	2:L:136:LEU:HD13	1.99	0.87
2:L:87:TYR:H	2:L:105:THR:CB	1.87	0.87
2:L:112:ALA:HA	2:L:163:TRP:CE3	2.09	0.87
2:L:114:THR:OG1	2:L:114:THR:CG2	2.23	0.87
2:L:93:ASP:HB2	2:L:99:TRP:HE3	1.38	0.87
2:L:110:LEU:O	2:L:142:LYS:HE3	1.74	0.87
2:L:93:ASP:CA	2:L:99:TRP:HB3	2.05	0.86
2:L:115:VAL:H	2:L:135:PHE:C	1.81	0.86
2:L:114:THR:HB	2:L:114:THR:CG2	1.36	0.86
2:L:9:SER:CA	2:L:106:LYS:O	2.24	0.86
2:L:93:ASP:HA	2:L:99:TRP:HB3	1.58	0.85
2:L:49:ILE:CD1	2:L:65:ALA:HB2	2.06	0.85
2:L:85:ALA:O	2:L:107:LEU:HD22	1.77	0.85
2:L:8:HIS:O	2:L:106:LYS:C	2.20	0.85
2:L:18:VAL:HG12	2:L:76:ILE:HB	1.57	0.85
2:L:10:ALA:CB	2:L:106:LYS:HZ2	1.89	0.84
2:L:55:ARG:NH1	2:L:61:ASP:CA	2.39	0.84
2:L:10:ALA:CA	2:L:106:LYS:HZ2	1.91	0.84
2:L:112:ALA:CA	2:L:175:MET:HG3	2.08	0.83
2:L:7:PRO:HG2	2:L:106:LYS:CE	2.08	0.83
2:L:113:PRO:HG2	2:L:136:LEU:CG	2.08	0.83
2:L:10:ALA:CB	2:L:106:LYS:NZ	2.41	0.83
2:L:55:ARG:HH12	2:L:61:ASP:HA	1.44	0.83
2:L:105:THR:HG23	2:L:105:THR:O	1.76	0.83
2:L:67:LYS:HZ3	2:L:72:ALA:HB1	1.43	0.82
2:L:113:PRO:HD3	2:L:175:MET:CG	2.09	0.82
2:L:111:GLY:HA3	2:L:163:TRP:NE1	1.92	0.82
2:L:52:LYS:HD2	2:L:67:LYS:O	1.79	0.82
2:L:114:THR:CB	2:L:135:PHE:CG	2.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:93:ASP:CB	2:L:99:TRP:CE3	2.62	0.81
1:H:33:TYR:CD1	1:H:53:PRO:HD2	2.16	0.81
1:H:172:VAL:HG11	2:L:160:LEU:CD2	2.08	0.81
2:L:113:PRO:CB	2:L:146:VAL:HG21	2.10	0.81
2:L:114:THR:OG1	2:L:134:CYS:CA	2.29	0.81
2:L:114:THR:CB	2:L:134:CYS:O	2.28	0.81
2:L:49:ILE:HD13	2:L:65:ALA:CB	2.10	0.80
2:L:8:HIS:O	2:L:106:LYS:CA	2.29	0.80
2:L:113:PRO:C	2:L:175:MET:C	2.49	0.80
2:L:39:GLN:O	2:L:85:ALA:HB1	1.81	0.80
2:L:111:GLY:CA	2:L:163:TRP:CZ2	2.47	0.80
2:L:110:LEU:O	2:L:142:LYS:CE	2.30	0.80
2:L:7:PRO:HG2	2:L:106:LYS:HE2	1.62	0.80
2:L:112:ALA:O	2:L:175:MET:HE3	1.83	0.79
1:H:170:PRO:CG	2:L:162:SER:OG	2.30	0.79
2:L:111:GLY:C	2:L:112:ALA:CB	2.54	0.79
1:H:6:GLN:NE2	1:H:107:GLY:HA3	1.97	0.79
2:L:32:ASN:CB	2:L:33:THR:HB	2.12	0.79
2:L:111:GLY:C	2:L:175:MET:HG3	2.05	0.79
2:L:8:HIS:C	2:L:106:LYS:CB	2.55	0.79
2:L:112:ALA:N	2:L:163:TRP:CE3	2.50	0.79
1:H:101:THR:H	1:H:102:PHE:HB3	1.48	0.79
2:L:114:THR:CB	2:L:114:THR:CG2	0.79	0.79
2:L:7:PRO:HD2	2:L:106:LYS:CE	2.12	0.79
2:L:112:ALA:HB2	2:L:175:MET:HG3	1.65	0.79
1:H:33:TYR:CE2	1:H:52:TYR:HB2	2.18	0.78
2:L:67:LYS:HD2	2:L:72:ALA:CB	2.13	0.78
2:L:111:GLY:CA	2:L:163:TRP:CG	2.66	0.78
2:L:110:LEU:O	2:L:142:LYS:NZ	2.14	0.78
2:L:113:PRO:HD2	2:L:175:MET:HB3	1.65	0.78
2:L:113:PRO:N	2:L:175:MET:SD	2.56	0.78
2:L:110:LEU:N	2:L:142:LYS:HE3	1.99	0.78
2:L:113:PRO:HG2	2:L:136:LEU:HD22	1.64	0.78
2:L:8:HIS:O	2:L:106:LYS:HA	1.84	0.78
1:H:169:PHE:CD1	2:L:176:SER:HB2	2.19	0.77
2:L:92:TRP:CD1	2:L:94:ASP:H	2.02	0.77
1:H:37:MET:HE1	2:L:101:PHE:CE1	2.20	0.77
2:L:112:ALA:N	2:L:163:TRP:CZ2	2.51	0.77
2:L:33:THR:HG23	2:L:33:THR:O	1.85	0.77
2:L:111:GLY:O	2:L:112:ALA:CA	2.32	0.76
1:H:37:MET:SD	2:L:101:PHE:CZ	2.79	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:PRO:CA	2:L:106:LYS:HD3	2.14	0.76
2:L:7:PRO:CG	2:L:106:LYS:HE2	2.15	0.76
2:L:38:GLN:NE2	2:L:48:LEU:HD21	2.00	0.76
2:L:113:PRO:HB3	2:L:146:VAL:HG21	1.68	0.76
2:L:8:HIS:C	2:L:106:LYS:CA	2.59	0.76
2:L:33:THR:HG21	2:L:92:TRP:HB3	1.68	0.75
2:L:34:VAL:CG2	2:L:67:LYS:NZ	2.48	0.75
2:L:113:PRO:CB	2:L:136:LEU:CD1	2.61	0.75
2:L:114:THR:CA	2:L:136:LEU:HD12	2.16	0.75
2:L:114:THR:CG2	2:L:134:CYS:O	2.35	0.75
2:L:8:HIS:CA	2:L:106:LYS:HB2	2.16	0.75
2:L:87:TYR:N	2:L:105:THR:CB	2.50	0.75
2:L:112:ALA:O	2:L:175:MET:SD	2.44	0.75
1:H:159:SER:H	1:H:199:ASN:HD21	1.35	0.75
2:L:18:VAL:HG11	2:L:76:ILE:HD12	1.69	0.74
1:H:30:THR:HG22	1:H:74:THR:HB	1.68	0.74
2:L:163:TRP:CD2	2:L:163:TRP:CD1	2.75	0.74
2:L:113:PRO:CG	2:L:136:LEU:HD22	2.18	0.74
2:L:110:LEU:CA	2:L:142:LYS:HE3	2.17	0.74
1:H:18:VAL:HG12	1:H:86:LEU:HD11	1.69	0.74
2:L:114:THR:HG21	2:L:135:PHE:CD1	2.22	0.74
2:L:113:PRO:CG	2:L:175:MET:SD	2.67	0.74
2:L:112:ALA:CB	2:L:162:SER:O	2.35	0.73
2:L:10:ALA:N	2:L:106:LYS:HZ2	1.86	0.73
2:L:38:GLN:OE1	2:L:48:LEU:HD11	1.88	0.73
2:L:111:GLY:CA	2:L:163:TRP:CD1	2.71	0.73
2:L:114:THR:CB	2:L:135:PHE:O	2.34	0.73
2:L:40:PHE:HA	2:L:85:ALA:HB2	1.69	0.73
1:H:70:LEU:HD12	1:H:80:TYR:O	1.89	0.72
2:L:112:ALA:O	2:L:175:MET:CE	2.37	0.72
2:L:114:THR:O	2:L:136:LEU:HD12	1.82	0.72
1:H:6:GLN:HE21	1:H:96:CYS:H	1.37	0.72
2:L:105:THR:O	2:L:107:LEU:N	2.23	0.72
2:L:113:PRO:CB	2:L:175:MET:HE2	2.02	0.72
2:L:113:PRO:O	2:L:175:MET:C	2.32	0.72
2:L:18:VAL:CG1	2:L:76:ILE:HB	2.19	0.72
2:L:87:TYR:N	2:L:105:THR:HB	2.05	0.72
1:H:36:TRP:CD1	1:H:81:MET:HE2	2.25	0.72
2:L:112:ALA:CB	2:L:175:MET:CG	2.68	0.72
2:L:114:THR:N	2:L:136:LEU:CD1	2.53	0.72
1:H:27:TYR:CE1	1:H:98:ARG:HD3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:9:SER:O	2:L:106:LYS:O	2.07	0.71
2:L:113:PRO:HG2	2:L:136:LEU:CD2	2.19	0.71
2:L:114:THR:O	2:L:135:PHE:N	2.22	0.71
1:H:2:VAL:HG23	1:H:27:TYR:CD2	2.26	0.71
2:L:114:THR:O	2:L:134:CYS:C	2.33	0.71
2:L:115:VAL:H	2:L:136:LEU:CA	2.03	0.71
1:H:101:THR:HG23	1:H:102:PHE:HB2	1.71	0.71
2:L:115:VAL:HB	2:L:136:LEU:HA	1.73	0.71
2:L:32:ASN:CB	2:L:33:THR:CA	2.69	0.71
1:H:170:PRO:CD	2:L:162:SER:OG	2.38	0.70
2:L:110:LEU:O	2:L:163:TRP:CD1	2.44	0.70
2:L:146:VAL:HG21	2:L:175:MET:HE2	1.71	0.70
1:H:38:LYS:HZ3	1:H:64:PHE:HZ	1.39	0.70
2:L:53:ASP:OD1	2:L:53:ASP:O	2.09	0.70
2:L:115:VAL:H	2:L:136:LEU:N	1.88	0.70
2:L:34:VAL:CG2	2:L:67:LYS:HZ1	2.05	0.70
2:L:48:LEU:C	2:L:56:PRO:HG2	2.17	0.70
1:H:169:PHE:CG	2:L:176:SER:HB2	2.26	0.70
2:L:48:LEU:O	2:L:56:PRO:CD	2.36	0.70
2:L:7:PRO:C	2:L:106:LYS:CB	2.64	0.69
2:L:105:THR:CG2	2:L:105:THR:O	2.39	0.69
1:H:170:PRO:HG2	2:L:162:SER:HG	1.58	0.69
2:L:114:THR:CG2	2:L:135:PHE:CG	2.75	0.69
2:L:114:THR:C	2:L:134:CYS:C	2.61	0.69
2:L:67:LYS:HD2	2:L:72:ALA:HB2	1.75	0.69
1:H:138:MET:HE3	1:H:185:THR:HG22	1.74	0.69
1:H:136:ASN:O	1:H:188:SER:HB3	1.92	0.68
2:L:115:VAL:H	2:L:136:LEU:HA	1.57	0.68
1:H:9:PRO:HB2	1:H:111:THR:O	1.93	0.68
2:L:53:ASP:HA	2:L:65:ALA:HB3	1.75	0.68
2:L:112:ALA:HB3	2:L:163:TRP:N	2.07	0.68
2:L:32:ASN:HB2	2:L:33:THR:HA	1.76	0.68
2:L:40:PHE:CE1	2:L:82:GLU:O	2.46	0.68
2:L:10:ALA:CA	2:L:106:LYS:NZ	2.56	0.68
2:L:112:ALA:CB	2:L:175:MET:HG3	2.23	0.68
2:L:114:THR:N	2:L:134:CYS:C	2.51	0.68
2:L:175:MET:HG2	2:L:175:MET:C	2.18	0.68
2:L:113:PRO:C	2:L:175:MET:O	2.37	0.67
2:L:113:PRO:O	2:L:175:MET:O	2.11	0.67
1:H:159:SER:H	1:H:199:ASN:ND2	1.91	0.67
2:L:66:SER:O	2:L:67:LYS:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:9:SER:HA	2:L:106:LYS:HD2	1.75	0.67
2:L:114:THR:H	2:L:134:CYS:C	2.03	0.67
1:H:50:ARG:NH1	2:L:94:ASP:OD1	2.27	0.67
2:L:111:GLY:HA2	2:L:163:TRP:CH2	2.30	0.67
2:L:67:LYS:NZ	2:L:72:ALA:HB1	2.10	0.66
2:L:92:TRP:HD1	2:L:94:ASP:C	2.02	0.66
1:H:50:ARG:NE	2:L:99:TRP:CZ3	2.63	0.66
1:H:169:PHE:CE2	2:L:175:MET:O	2.49	0.66
1:H:93:VAL:HG22	1:H:111:THR:HG22	1.77	0.66
2:L:66:SER:C	2:L:67:LYS:HG2	2.20	0.66
2:L:92:TRP:CD1	2:L:94:ASP:HB2	2.29	0.66
2:L:52:LYS:O	2:L:65:ALA:HB1	1.96	0.66
2:L:110:LEU:H	2:L:142:LYS:HE3	1.61	0.66
2:L:47:LEU:HD23	2:L:56:PRO:HG2	1.77	0.66
2:L:111:GLY:CA	2:L:163:TRP:CH2	2.78	0.66
2:L:112:ALA:HA	2:L:163:TRP:CZ3	2.30	0.66
2:L:113:PRO:CG	2:L:136:LEU:HD13	2.26	0.66
2:L:113:PRO:O	2:L:136:LEU:N	2.29	0.66
2:L:67:LYS:HB2	2:L:72:ALA:HA	1.75	0.65
2:L:114:THR:N	2:L:134:CYS:O	2.29	0.65
2:L:67:LYS:CD	2:L:72:ALA:CB	2.73	0.65
2:L:112:ALA:HB2	2:L:175:MET:CG	2.26	0.65
2:L:113:PRO:HG2	2:L:136:LEU:CB	2.27	0.65
2:L:111:GLY:O	2:L:163:TRP:NE1	2.30	0.65
1:H:169:PHE:HE2	2:L:175:MET:CA	2.09	0.65
2:L:18:VAL:CG1	2:L:76:ILE:HD12	2.27	0.65
2:L:86:ASP:C	2:L:105:THR:HG21	2.22	0.65
2:L:114:THR:C	2:L:136:LEU:N	2.53	0.65
2:L:10:ALA:N	2:L:106:LYS:NZ	2.45	0.64
1:H:38:LYS:HD3	1:H:94:TYR:CZ	2.31	0.64
2:L:66:SER:O	2:L:67:LYS:CG	2.45	0.64
2:L:87:TYR:N	2:L:105:THR:HG21	2.12	0.64
2:L:113:PRO:CD	2:L:175:MET:HB3	2.27	0.64
2:L:115:VAL:HG23	2:L:136:LEU:CD1	2.24	0.64
2:L:52:LYS:O	2:L:65:ALA:CB	2.46	0.64
1:H:99:SER:HB3	1:H:103:PHE:CD1	2.31	0.64
2:L:113:PRO:HG3	2:L:175:MET:SD	2.36	0.64
2:L:113:PRO:HD2	2:L:136:LEU:HB2	1.80	0.64
2:L:114:THR:N	2:L:136:LEU:HD12	2.12	0.64
2:L:86:ASP:CA	2:L:105:THR:CG2	2.62	0.64
2:L:113:PRO:HG2	2:L:136:LEU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:40:PHE:HE1	2:L:82:GLU:O	1.80	0.64
1:H:6:GLN:NE2	1:H:96:CYS:H	1.96	0.63
2:L:113:PRO:C	2:L:136:LEU:CD1	2.70	0.63
2:L:34:VAL:CG1	2:L:67:LYS:HE3	2.20	0.63
2:L:111:GLY:HA3	2:L:163:TRP:CD1	2.33	0.63
2:L:9:SER:CB	2:L:106:LYS:O	2.47	0.63
2:L:87:TYR:H	2:L:105:THR:CG2	2.12	0.63
2:L:40:PHE:HA	2:L:85:ALA:CB	2.28	0.63
2:L:108:THR:C	2:L:109:VAL:HG13	2.24	0.63
2:L:32:ASN:CB	2:L:33:THR:HA	2.29	0.62
2:L:84:GLU:O	2:L:85:ALA:HB2	1.99	0.62
2:L:7:PRO:CB	2:L:106:LYS:HD3	2.29	0.62
2:L:34:VAL:HG11	2:L:67:LYS:CE	2.21	0.62
2:L:114:THR:CB	2:L:135:PHE:CD1	2.73	0.62
1:H:101:THR:N	1:H:102:PHE:HB3	2.14	0.62
2:L:114:THR:N	2:L:136:LEU:HD13	2.15	0.62
2:L:66:SER:O	2:L:67:LYS:CB	2.47	0.62
1:H:38:LYS:HD2	1:H:92:ALA:HB3	1.82	0.62
1:H:20:ILE:CG1	1:H:81:MET:HB3	2.29	0.62
2:L:114:THR:CA	2:L:134:CYS:O	2.46	0.62
2:L:7:PRO:CG	2:L:106:LYS:CE	2.75	0.62
1:H:27:TYR:CZ	1:H:98:ARG:HD3	2.34	0.62
1:H:36:TRP:CD1	1:H:70:LEU:HD13	2.35	0.61
2:L:114:THR:OG1	2:L:134:CYS:N	2.32	0.61
2:L:7:PRO:CG	2:L:106:LYS:CD	2.78	0.61
1:H:136:ASN:HA	1:H:188:SER:OG	2.01	0.61
2:L:8:HIS:CA	2:L:106:LYS:CB	2.78	0.61
2:L:142:LYS:HZ2	2:L:163:TRP:CG	2.19	0.61
2:L:163:TRP:CD2	2:L:163:TRP:CB	2.73	0.61
2:L:55:ARG:HH12	2:L:61:ASP:CA	2.09	0.60
2:L:87:TYR:H	2:L:105:THR:HG21	1.66	0.60
2:L:67:LYS:CG	2:L:72:ALA:HA	2.31	0.60
2:L:110:LEU:N	2:L:142:LYS:CE	2.64	0.60
2:L:111:GLY:C	2:L:111:GLY:CA	2.74	0.60
2:L:8:HIS:C	2:L:106:LYS:C	2.69	0.60
2:L:92:TRP:CD1	2:L:94:ASP:N	2.68	0.60
2:L:114:THR:C	2:L:135:PHE:CA	2.75	0.60
2:L:33:THR:CG2	2:L:95:SER:CB	2.80	0.60
2:L:67:LYS:HD2	2:L:72:ALA:CA	2.32	0.60
2:L:112:ALA:HB1	2:L:162:SER:O	2.02	0.60
2:L:67:LYS:CD	2:L:72:ALA:HA	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:106:LYS:C	2:L:107:LEU:CD1	2.67	0.60
2:L:113:PRO:CD	2:L:175:MET:CB	2.79	0.59
2:L:36:TRP:C	2:L:37:TYR:HD1	2.09	0.59
2:L:110:LEU:H	2:L:142:LYS:CE	2.14	0.59
1:H:167:HIS:NE2	2:L:174:SER:OG	2.35	0.59
1:H:169:PHE:CZ	2:L:175:MET:O	2.55	0.59
2:L:112:ALA:CA	2:L:175:MET:HG2	2.30	0.59
2:L:135:PHE:N	2:L:135:PHE:C	2.54	0.59
2:L:112:ALA:N	2:L:175:MET:HG3	2.15	0.59
2:L:142:LYS:HZ2	2:L:163:TRP:CD1	2.20	0.59
1:H:32:TYR:CE2	1:H:98:ARG:NH1	2.71	0.58
1:H:2:VAL:HG21	1:H:98:ARG:HH21	1.68	0.58
1:H:169:PHE:CE2	2:L:175:MET:CA	2.84	0.58
2:L:14:PRO:O	2:L:15:ASP:HB3	2.03	0.58
1:H:172:VAL:HG12	2:L:160:LEU:HD22	1.82	0.58
2:L:9:SER:N	2:L:106:LYS:CB	2.52	0.58
2:L:67:LYS:CD	2:L:72:ALA:CA	2.81	0.58
2:L:92:TRP:HD1	2:L:95:SER:N	2.02	0.58
2:L:111:GLY:O	2:L:112:ALA:CB	2.52	0.57
2:L:112:ALA:CB	2:L:175:MET:HG2	2.34	0.57
2:L:111:GLY:O	2:L:112:ALA:HB2	2.04	0.57
2:L:7:PRO:CB	2:L:106:LYS:CD	2.82	0.57
2:L:79:LEU:HD23	2:L:79:LEU:C	2.30	0.57
2:L:112:ALA:C	2:L:175:MET:CE	2.77	0.57
2:L:33:THR:HG21	2:L:92:TRP:CB	2.32	0.57
1:H:170:PRO:O	2:L:162:SER:OG	2.19	0.57
1:H:50:ARG:NH2	2:L:99:TRP:CZ3	2.68	0.57
2:L:87:TYR:N	2:L:105:THR:CG2	2.68	0.57
1:H:6:GLN:HE21	1:H:96:CYS:HB3	1.70	0.57
1:H:38:LYS:HB2	1:H:48:ILE:CD1	2.16	0.57
1:H:20:ILE:HD12	1:H:36:TRP:CZ3	2.40	0.57
2:L:8:HIS:C	2:L:106:LYS:HA	2.27	0.57
2:L:115:VAL:CB	2:L:136:LEU:HA	2.35	0.56
1:H:106:TRP:CZ2	2:L:45:PRO:HB2	2.40	0.56
2:L:55:ARG:HH12	2:L:61:ASP:CB	2.18	0.56
2:L:7:PRO:CD	2:L:106:LYS:HD3	2.36	0.56
2:L:15:ASP:OD1	2:L:15:ASP:O	2.24	0.56
2:L:66:SER:O	2:L:67:LYS:HB3	2.04	0.56
1:H:50:ARG:CG	1:H:59:LYS:HB2	2.30	0.56
2:L:108:THR:O	2:L:109:VAL:HG13	2.06	0.56
1:H:87:THR:OG1	1:H:89:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:PRO:HG2	1:H:190:THR:OG1	2.05	0.56
1:H:167:HIS:CE1	2:L:174:SER:OG	2.59	0.56
2:L:14:PRO:O	2:L:15:ASP:CB	2.53	0.56
2:L:87:TYR:C	2:L:105:THR:HB	2.31	0.56
2:L:33:THR:CG2	2:L:95:SER:OG	2.54	0.55
2:L:113:PRO:CG	2:L:136:LEU:CD2	2.83	0.55
1:H:169:PHE:CG	2:L:176:SER:CB	2.90	0.55
2:L:47:LEU:CD2	2:L:56:PRO:HG3	2.36	0.55
2:L:105:THR:O	2:L:106:LYS:C	2.49	0.55
2:L:67:LYS:HB2	2:L:71:SER:C	2.29	0.55
2:L:111:GLY:O	2:L:175:MET:CG	2.39	0.55
2:L:7:PRO:CD	2:L:106:LYS:CE	2.77	0.55
1:H:40:LYS:HD2	1:H:43:GLN:OE1	2.06	0.55
2:L:108:THR:O	2:L:109:VAL:CG1	2.55	0.55
2:L:47:LEU:HD23	2:L:56:PRO:CG	2.38	0.54
2:L:113:PRO:CG	2:L:136:LEU:CG	2.84	0.54
2:L:33:THR:HG1	2:L:92:TRP:HB2	1.73	0.54
2:L:7:PRO:CG	2:L:106:LYS:HD3	2.38	0.54
1:H:102:PHE:CD1	2:L:50:TYR:CB	2.86	0.54
2:L:9:SER:C	2:L:106:LYS:HG3	2.33	0.54
2:L:7:PRO:C	2:L:106:LYS:CD	2.76	0.54
2:L:163:TRP:CZ2	2:L:175:MET:SD	3.01	0.54
1:H:197:THR:HG22	1:H:212:LYS:HA	1.90	0.54
2:L:33:THR:CB	2:L:92:TRP:HB2	2.37	0.53
2:L:112:ALA:CB	2:L:112:ALA:O	2.44	0.53
2:L:52:LYS:CD	2:L:67:LYS:O	2.56	0.53
1:H:39:GLN:C	1:H:92:ALA:HB1	2.34	0.53
2:L:7:PRO:HB2	2:L:106:LYS:HD2	1.90	0.53
1:H:34:ILE:HD12	1:H:79:ALA:HB2	1.91	0.53
2:L:112:ALA:HB3	2:L:163:TRP:CE3	2.43	0.53
1:H:22:CYS:SG	1:H:96:CYS:SG	3.07	0.53
1:H:102:PHE:HZ	2:L:56:PRO:HG3	1.74	0.53
1:H:37:MET:SD	1:H:46:GLU:C	2.92	0.53
2:L:67:LYS:NZ	2:L:72:ALA:CB	2.71	0.53
2:L:114:THR:HG21	2:L:135:PHE:CE1	2.44	0.53
1:H:20:ILE:HD11	1:H:81:MET:HB3	1.90	0.52
1:H:12:VAL:HG22	1:H:16:ALA:HB3	1.90	0.52
2:L:93:ASP:OD1	2:L:94:ASP:N	2.42	0.52
2:L:7:PRO:O	2:L:106:LYS:HD3	2.09	0.52
2:L:34:VAL:HG22	2:L:67:LYS:HZ1	1.74	0.52
2:L:87:TYR:HB2	2:L:105:THR:OG1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:GLN:CG	1:H:23:LYS:HB3	2.39	0.52
1:H:8:GLY:N	1:H:9:PRO:CD	2.73	0.52
1:H:51:ILE:HG13	1:H:57:ASN:O	2.09	0.52
2:L:114:THR:CG2	2:L:134:CYS:C	2.83	0.52
2:L:92:TRP:CD1	2:L:94:ASP:CA	2.93	0.52
1:H:20:ILE:HG12	1:H:81:MET:HB3	1.90	0.52
2:L:8:HIS:O	2:L:107:LEU:N	2.43	0.52
2:L:112:ALA:HB1	2:L:162:SER:H	1.75	0.52
1:H:8:GLY:N	1:H:9:PRO:HD2	2.25	0.52
2:L:84:GLU:O	2:L:85:ALA:CB	2.58	0.51
1:H:6:GLN:HE22	1:H:107:GLY:CA	2.08	0.51
2:L:112:ALA:N	2:L:163:TRP:CZ3	2.77	0.51
1:H:169:PHE:HD2	2:L:162:SER:O	1.93	0.51
1:H:2:VAL:HG23	1:H:27:TYR:CE2	2.45	0.51
2:L:92:TRP:HB3	2:L:95:SER:CB	2.17	0.51
2:L:107:LEU:C	2:L:108:THR:HG23	2.35	0.51
2:L:113:PRO:CD	2:L:136:LEU:HD13	2.34	0.51
2:L:113:PRO:HB2	2:L:136:LEU:HD11	1.90	0.51
2:L:86:ASP:HB3	2:L:105:THR:HG22	1.92	0.51
1:H:5:GLN:HG3	1:H:23:LYS:HB3	1.93	0.51
2:L:47:LEU:CD2	2:L:56:PRO:CG	2.89	0.51
1:H:12:VAL:HG11	1:H:86:LEU:HD13	1.92	0.51
1:H:50:ARG:NH1	2:L:94:ASP:CG	2.69	0.51
1:H:124:VAL:O	1:H:211:LYS:HE3	2.10	0.51
2:L:34:VAL:HG13	2:L:52:LYS:HA	1.93	0.50
1:H:129:PRO:HB3	1:H:134:GLN:NE2	2.26	0.50
1:H:170:PRO:HG3	2:L:163:TRP:O	2.11	0.50
2:L:93:ASP:CB	2:L:99:TRP:HE3	2.14	0.50
2:L:115:VAL:CG2	2:L:136:LEU:CG	2.65	0.50
1:H:136:ASN:CG	1:H:137:SER:H	2.20	0.50
2:L:112:ALA:N	2:L:175:MET:CG	2.68	0.50
1:H:83:LEU:HB3	1:H:86:LEU:HD21	1.94	0.50
1:H:33:TYR:CZ	1:H:52:TYR:HB2	2.47	0.50
1:H:38:LYS:CG	1:H:92:ALA:HB3	2.42	0.50
2:L:32:ASN:HB2	2:L:33:THR:OG1	2.08	0.50
1:H:134:GLN:O	1:H:134:GLN:HG3	2.12	0.50
2:L:107:LEU:O	2:L:108:THR:HG23	2.12	0.50
2:L:155:ARG:NH2	2:L:185:GLU:OE2	2.45	0.50
1:H:27:TYR:CE1	1:H:98:ARG:CD	2.94	0.49
1:H:102:PHE:CZ	2:L:56:PRO:HG3	2.48	0.49
1:H:170:PRO:HD2	2:L:162:SER:OG	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:112:ALA:HB3	2:L:162:SER:CA	2.41	0.49
2:L:9:SER:CA	2:L:106:LYS:HG3	2.42	0.49
2:L:10:ALA:HA	2:L:106:LYS:NZ	2.26	0.49
2:L:8:HIS:N	2:L:106:LYS:HB2	2.28	0.49
2:L:49:ILE:HG21	2:L:65:ALA:CB	2.42	0.49
1:H:186:VAL:HB	1:H:187:PRO:HD2	1.94	0.49
2:L:7:PRO:HG2	2:L:106:LYS:CD	2.40	0.49
2:L:113:PRO:CB	2:L:175:MET:SD	2.99	0.49
1:H:169:PHE:HE2	2:L:175:MET:N	2.10	0.49
2:L:113:PRO:CG	2:L:136:LEU:CD1	2.91	0.49
2:L:114:THR:CG2	2:L:176:SER:HA	2.43	0.49
1:H:169:PHE:CE1	2:L:176:SER:HB2	2.48	0.48
1:H:180:LEU:C	1:H:180:LEU:HD12	2.38	0.48
1:H:35:ASN:OD1	1:H:50:ARG:CB	2.61	0.48
1:H:40:LYS:CG	1:H:41:PRO:HD2	2.44	0.48
2:L:8:HIS:CA	2:L:106:LYS:HA	2.42	0.48
2:L:37:TYR:HD1	2:L:37:TYR:N	2.11	0.48
2:L:110:LEU:C	2:L:163:TRP:CD2	2.91	0.48
2:L:93:ASP:HA	2:L:99:TRP:CB	2.38	0.48
2:L:112:ALA:CA	2:L:163:TRP:CE3	2.91	0.48
2:L:7:PRO:HB2	2:L:106:LYS:CD	2.42	0.48
2:L:146:VAL:HG21	2:L:175:MET:CE	2.43	0.48
1:H:33:TYR:CE2	1:H:52:TYR:CB	2.96	0.48
1:H:34:ILE:HD12	1:H:79:ALA:CB	2.44	0.48
2:L:113:PRO:HD2	2:L:175:MET:CG	2.42	0.48
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.95	0.48
1:H:127:LEU:HB2	1:H:142:GLY:CA	2.44	0.48
1:H:9:PRO:C	1:H:10:GLU:HG2	2.39	0.48
2:L:86:ASP:CB	2:L:105:THR:HG22	2.44	0.47
2:L:175:MET:HG3	2:L:175:MET:HB2	1.37	0.47
1:H:202:HIS:HB3	1:H:207:THR:HB	1.96	0.47
2:L:113:PRO:HA	2:L:177:SER:N	2.29	0.47
2:L:47:LEU:HD23	2:L:47:LEU:C	2.39	0.47
1:H:38:LYS:HG2	1:H:92:ALA:HB3	1.97	0.47
1:H:143:CYS:SG	1:H:198:CYS:SG	3.13	0.47
2:L:9:SER:C	2:L:106:LYS:O	2.57	0.47
1:H:50:ARG:CZ	2:L:99:TRP:CZ3	2.98	0.47
1:H:169:PHE:CE2	2:L:176:SER:N	2.83	0.47
2:L:92:TRP:CD1	2:L:94:ASP:C	2.89	0.47
2:L:13:PRO:HG2	2:L:16:GLN:HG3	1.97	0.47
2:L:33:THR:HG22	2:L:95:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:108:THR:C	2:L:109:VAL:CG1	2.88	0.47
2:L:34:VAL:HG13	2:L:34:VAL:O	2.14	0.47
2:L:37:TYR:N	2:L:37:TYR:CD1	2.82	0.47
1:H:20:ILE:CD1	1:H:81:MET:HB3	2.45	0.46
1:H:38:LYS:CD	1:H:92:ALA:HB3	2.44	0.46
1:H:100:LEU:O	1:H:100:LEU:HD23	2.16	0.46
2:L:186:TYR:CZ	2:L:211:ARG:HD3	2.50	0.46
2:L:175:MET:CG	2:L:175:MET:HA	2.24	0.46
1:H:40:LYS:HA	1:H:92:ALA:HB2	1.97	0.46
1:H:101:THR:HG23	1:H:102:PHE:CB	2.44	0.46
2:L:7:PRO:HG2	2:L:106:LYS:NZ	2.29	0.46
1:H:8:GLY:H	1:H:9:PRO:HD2	1.81	0.46
1:H:40:LYS:HB3	1:H:43:GLN:OE1	2.15	0.46
1:H:170:PRO:CD	2:L:163:TRP:O	2.64	0.46
2:L:113:PRO:HB3	2:L:175:MET:SD	2.55	0.46
2:L:38:GLN:NE2	2:L:40:PHE:HE2	2.13	0.46
2:L:38:GLN:HB3	2:L:48:LEU:HD11	1.96	0.46
1:H:106:TRP:CE3	2:L:45:PRO:HD2	2.51	0.46
1:H:38:LYS:HG2	1:H:92:ALA:CB	2.46	0.46
2:L:109:VAL:HB	2:L:142:LYS:HD3	1.97	0.46
1:H:38:LYS:CD	1:H:94:TYR:CZ	2.99	0.45
2:L:52:LYS:HG3	2:L:67:LYS:HG2	1.97	0.45
2:L:86:ASP:CB	2:L:105:THR:CG2	2.94	0.45
2:L:112:ALA:N	2:L:163:TRP:CH2	2.81	0.45
2:L:61:ASP:OD1	2:L:61:ASP:O	2.34	0.45
1:H:4:LEU:HD21	1:H:27:TYR:OH	2.17	0.45
1:H:136:ASN:C	1:H:188:SER:HB3	2.41	0.45
2:L:48:LEU:C	2:L:56:PRO:HD2	2.32	0.45
2:L:114:THR:HG22	2:L:176:SER:HA	1.98	0.45
2:L:51:GLY:O	2:L:52:LYS:HB3	2.16	0.45
2:L:107:LEU:O	2:L:108:THR:CG2	2.65	0.45
2:L:114:THR:HG1	2:L:134:CYS:C	2.20	0.45
2:L:92:TRP:CD1	2:L:94:ASP:CB	2.99	0.44
2:L:93:ASP:CB	2:L:99:TRP:HB3	2.48	0.44
1:H:102:PHE:HD1	2:L:35:ASN:OD1	2.00	0.44
1:H:147:GLY:HA2	1:H:177:LEU:HB3	1.99	0.44
2:L:53:ASP:CG	2:L:65:ALA:O	2.60	0.44
2:L:111:GLY:CA	2:L:163:TRP:CZ3	3.00	0.44
2:L:115:VAL:N	2:L:136:LEU:HG	2.32	0.44
1:H:40:LYS:HG3	1:H:41:PRO:HD2	2.00	0.44
2:L:67:LYS:HD3	2:L:72:ALA:CA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:TYR:CZ	1:H:98:ARG:NH1	2.86	0.44
1:H:126:PRO:HD3	1:H:211:LYS:HG2	1.99	0.44
2:L:52:LYS:O	2:L:65:ALA:HB3	2.16	0.44
2:L:67:LYS:HZ3	2:L:72:ALA:CB	2.21	0.44
1:H:50:ARG:CZ	2:L:99:TRP:CE3	2.96	0.44
1:H:195:THR:HG22	1:H:197:THR:HG23	1.99	0.44
2:L:113:PRO:N	2:L:175:MET:CB	2.79	0.44
1:H:50:ARG:HH11	2:L:94:ASP:CG	2.26	0.44
1:H:6:GLN:NE2	1:H:96:CYS:HB3	2.33	0.44
1:H:6:GLN:HE21	1:H:96:CYS:CB	2.31	0.44
2:L:38:GLN:CD	2:L:48:LEU:CD2	2.71	0.44
1:H:101:THR:CG2	1:H:102:PHE:HB2	2.43	0.43
1:H:169:PHE:CD2	2:L:162:SER:O	2.70	0.43
2:L:85:ALA:O	2:L:107:LEU:CD2	2.60	0.43
2:L:114:THR:CB	2:L:114:THR:HG1	2.18	0.43
1:H:98:ARG:O	1:H:104:ASP:OD1	2.36	0.43
1:H:22:CYS:HB3	1:H:79:ALA:HB3	1.99	0.43
1:H:33:TYR:CD2	1:H:52:TYR:HB2	2.53	0.43
1:H:172:VAL:HG21	2:L:160:LEU:HB3	2.01	0.43
2:L:92:TRP:NE1	2:L:94:ASP:CB	2.62	0.43
1:H:167:HIS:CD2	2:L:174:SER:OG	2.72	0.43
1:H:170:PRO:CG	2:L:162:SER:HG	2.23	0.43
2:L:113:PRO:CB	2:L:175:MET:CE	2.71	0.43
2:L:163:TRP:CE2	2:L:175:MET:SD	3.12	0.43
1:H:68:ALA:HA	1:H:82:GLN:O	2.19	0.42
1:H:136:ASN:HA	1:H:188:SER:CB	2.49	0.42
2:L:7:PRO:N	2:L:106:LYS:HD3	2.34	0.42
2:L:17:THR:CG2	2:L:77:SER:O	2.53	0.42
2:L:114:THR:C	2:L:114:THR:N	2.52	0.42
1:H:141:LEU:HD22	1:H:213:ILE:HG21	2.01	0.42
2:L:59:VAL:HA	2:L:60:PRO:HD3	1.85	0.42
2:L:93:ASP:N	2:L:99:TRP:HB3	2.33	0.42
2:L:113:PRO:HD2	2:L:113:PRO:O	2.18	0.42
2:L:115:VAL:HG12	2:L:115:VAL:O	2.18	0.42
1:H:12:VAL:O	1:H:114:VAL:HA	2.18	0.42
1:H:32:TYR:CG	1:H:98:ARG:HD2	2.54	0.42
1:H:33:TYR:CE1	1:H:53:PRO:HD2	2.54	0.42
2:L:101:PHE:N	2:L:101:PHE:CD1	2.87	0.42
2:L:112:ALA:CB	2:L:163:TRP:N	2.74	0.42
2:L:48:LEU:C	2:L:56:PRO:CG	2.91	0.42
2:L:67:LYS:CD	2:L:72:ALA:HB1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:114:THR:C	2:L:136:LEU:HG	2.44	0.42
2:L:7:PRO:CD	2:L:106:LYS:CD	2.97	0.42
2:L:67:LYS:HD3	2:L:72:ALA:HA	2.02	0.41
1:H:33:TYR:CD2	1:H:52:TYR:CB	3.03	0.41
2:L:19:THR:HG22	2:L:75:THR:HG22	2.01	0.41
2:L:112:ALA:CA	2:L:163:TRP:CD2	2.89	0.41
2:L:13:PRO:HG2	2:L:16:GLN:CG	2.51	0.41
1:H:148:TYR:CE2	1:H:153:VAL:HG13	2.54	0.41
1:H:170:PRO:CG	2:L:163:TRP:O	2.68	0.41
1:H:2:VAL:HG21	1:H:105:VAL:HG21	2.03	0.41
2:L:35:ASN:CB	2:L:37:TYR:HE1	2.34	0.41
2:L:113:PRO:N	2:L:175:MET:CE	2.83	0.41
2:L:175:MET:HG2	2:L:175:MET:HA	1.85	0.41
2:L:17:THR:HG22	2:L:77:SER:C	2.43	0.40
2:L:7:PRO:HG2	2:L:106:LYS:HZ3	1.86	0.40
2:L:112:ALA:HB2	2:L:163:TRP:HA	2.02	0.40
1:H:2:VAL:HG23	1:H:27:TYR:HD2	1.83	0.40
1:H:106:TRP:CD1	2:L:45:PRO:O	2.75	0.40
2:L:32:ASN:CB	2:L:33:THR:CB	2.62	0.40
2:L:113:PRO:O	2:L:136:LEU:HB2	2.22	0.40
2:L:97:ASN:HA	2:L:98:GLY:HA2	1.80	0.40
2:L:111:GLY:CA	2:L:163:TRP:CE3	2.76	0.40
2:L:161:ASN:OD1	2:L:175:MET:HE3	2.21	0.40
2:L:163:TRP:CD2	2:L:163:TRP:NE1	2.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	215/217 (99%)	203 (94%)	9 (4%)	3 (1%)	9 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	203/205 (99%)	181 (89%)	14 (7%)	8 (4%)	2	19
All	All	418/422 (99%)	384 (92%)	23 (6%)	11 (3%)	6	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	10	GLU
1	H	102	PHE
1	H	137	SER
2	L	67	LYS
2	L	85	ALA
2	L	106	LYS
2	L	109	VAL
2	L	116	SER
2	L	32	ASN
2	L	103	GLY
2	L	15	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	187/187 (100%)	185 (99%)	2 (1%)	65	76
2	L	177/177 (100%)	174 (98%)	3 (2%)	53	69
All	All	364/364 (100%)	359 (99%)	5 (1%)	57	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	65	LYS
1	H	162	LEU
2	L	113	PRO
2	L	114	THR
2	L	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	6	GLN
1	H	82	GLN
1	H	134	GLN
1	H	199	ASN
2	L	32	ASN
2	L	124	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	134:CYS	C	135:PHE	N	1.99
1	L	112:ALA	C	113:PRO	N	1.66
1	L	135:PHE	C	136:LEU	N	1.18

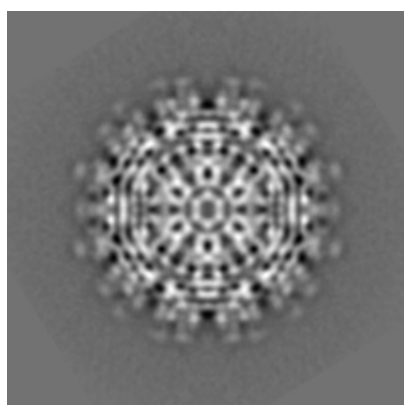
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2645. These allow visual inspection of the internal detail of the map and identification of artifacts.

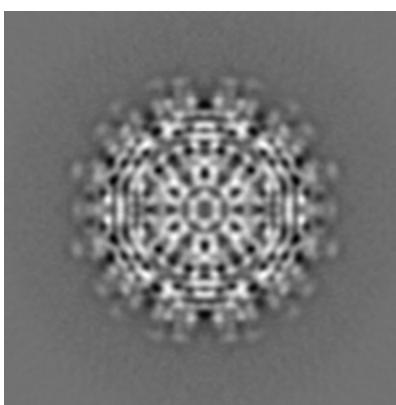
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

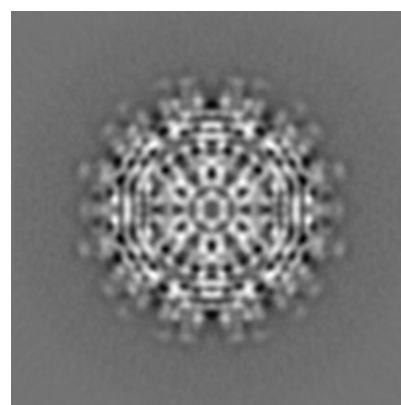
6.1.1 Primary map



X



Y

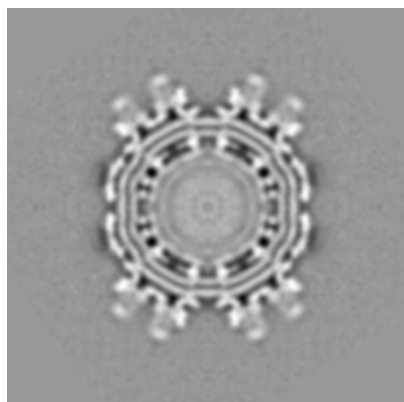


Z

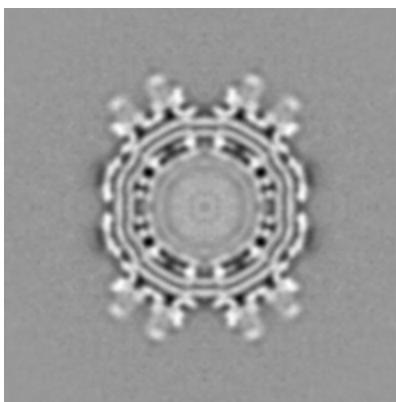
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

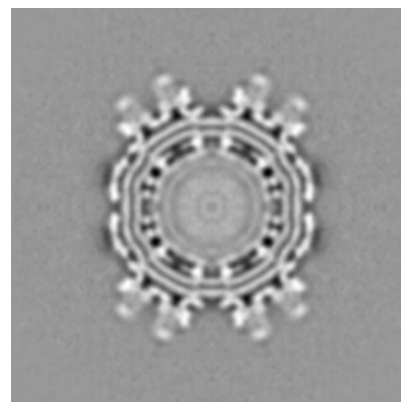
6.2.1 Primary map



X Index: 128



Y Index: 128

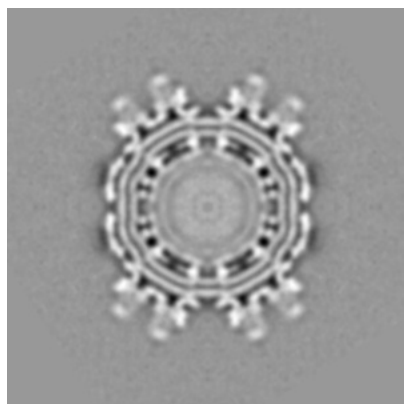


Z Index: 128

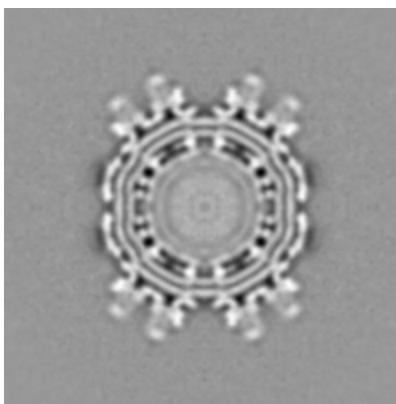
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

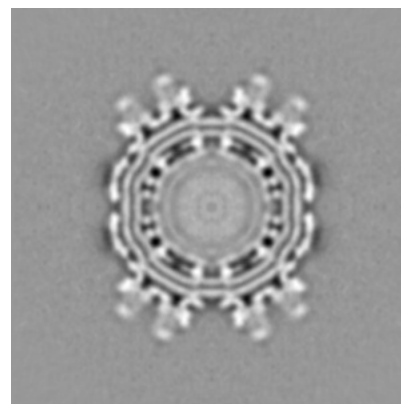
6.3.1 Primary map



X Index: 128



Y Index: 128

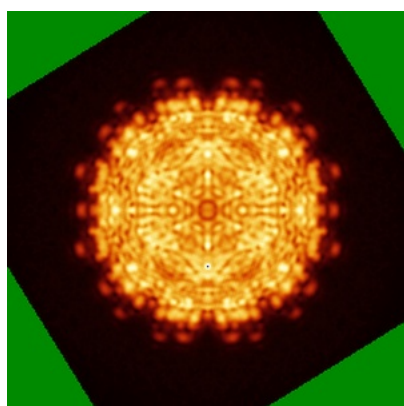


Z Index: 128

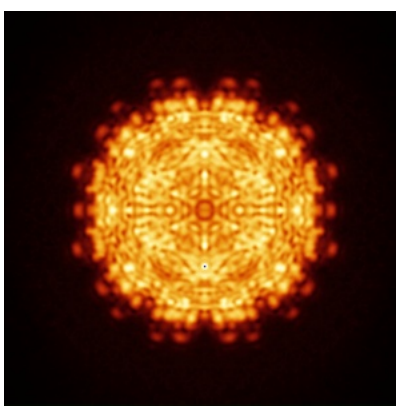
The images above show the largest variance slices of the map in three orthogonal directions.

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

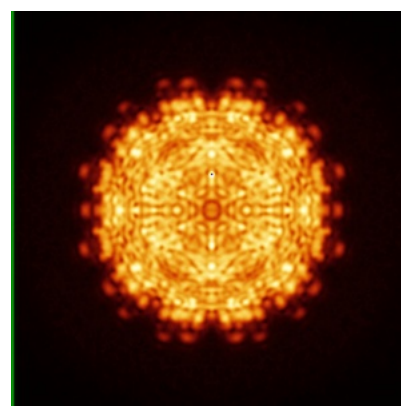
6.4.1 Primary map



X



Y

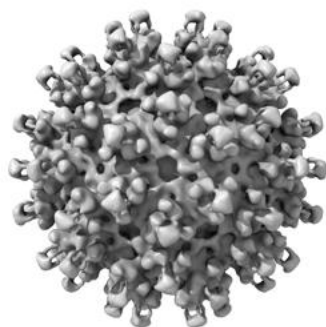


Z

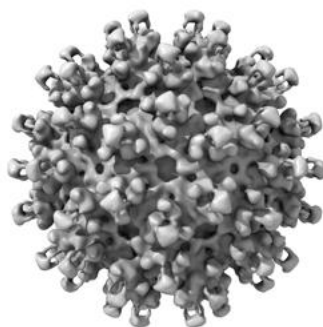
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

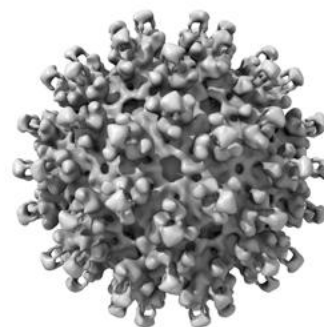
6.5.1 Primary map



X



Y



Z

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

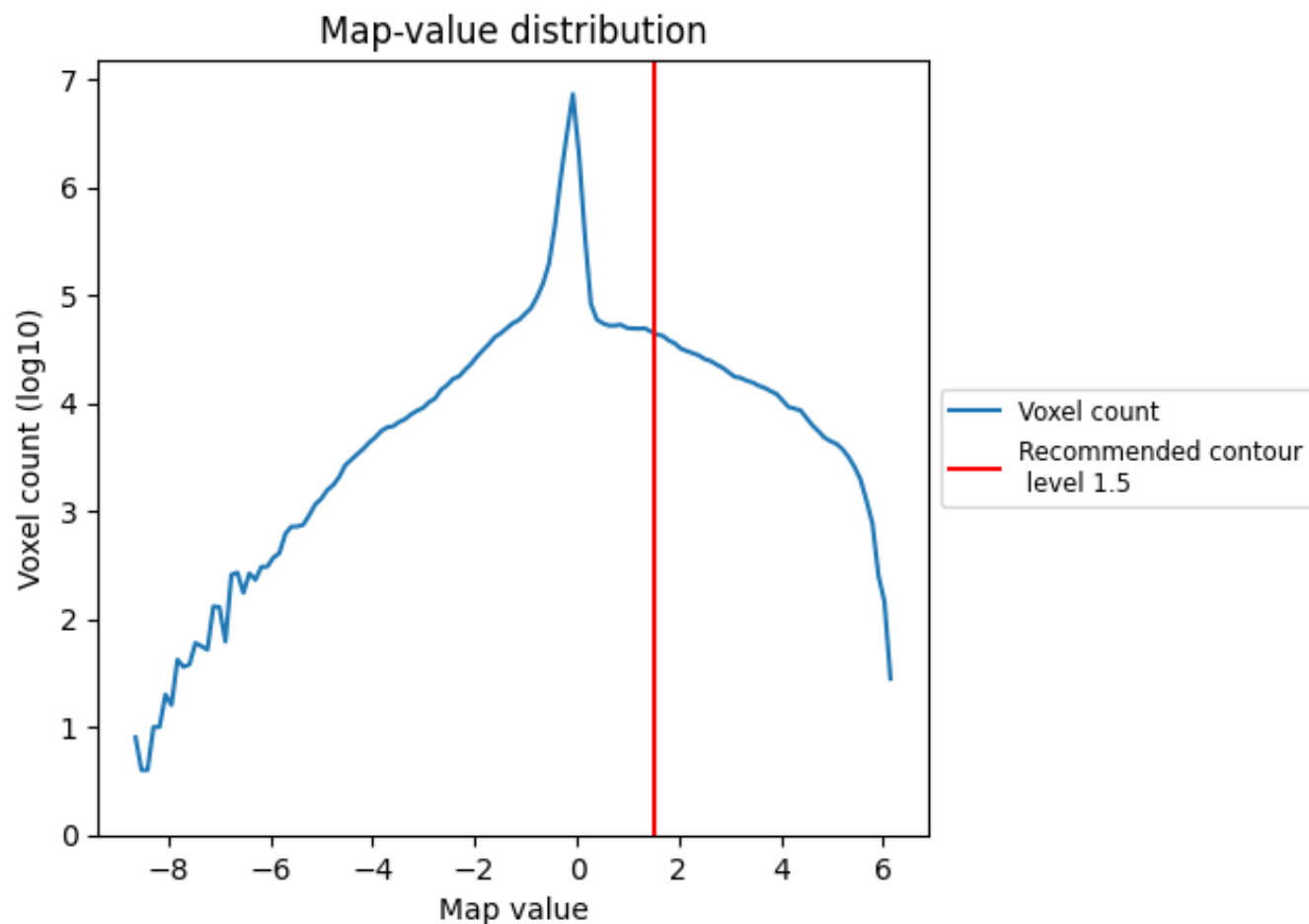
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

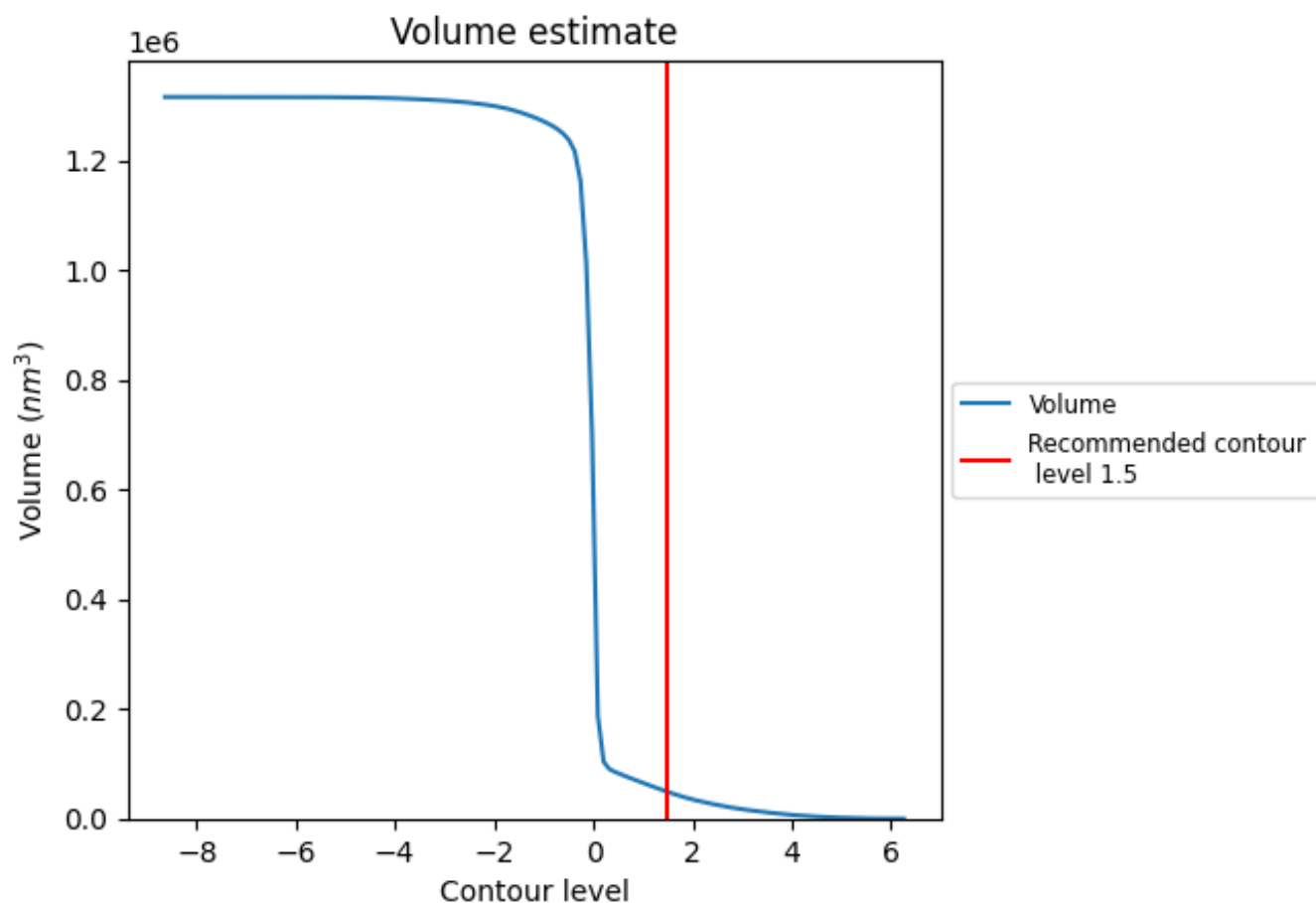
This section contains the results of statistical analysis of the map.

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.

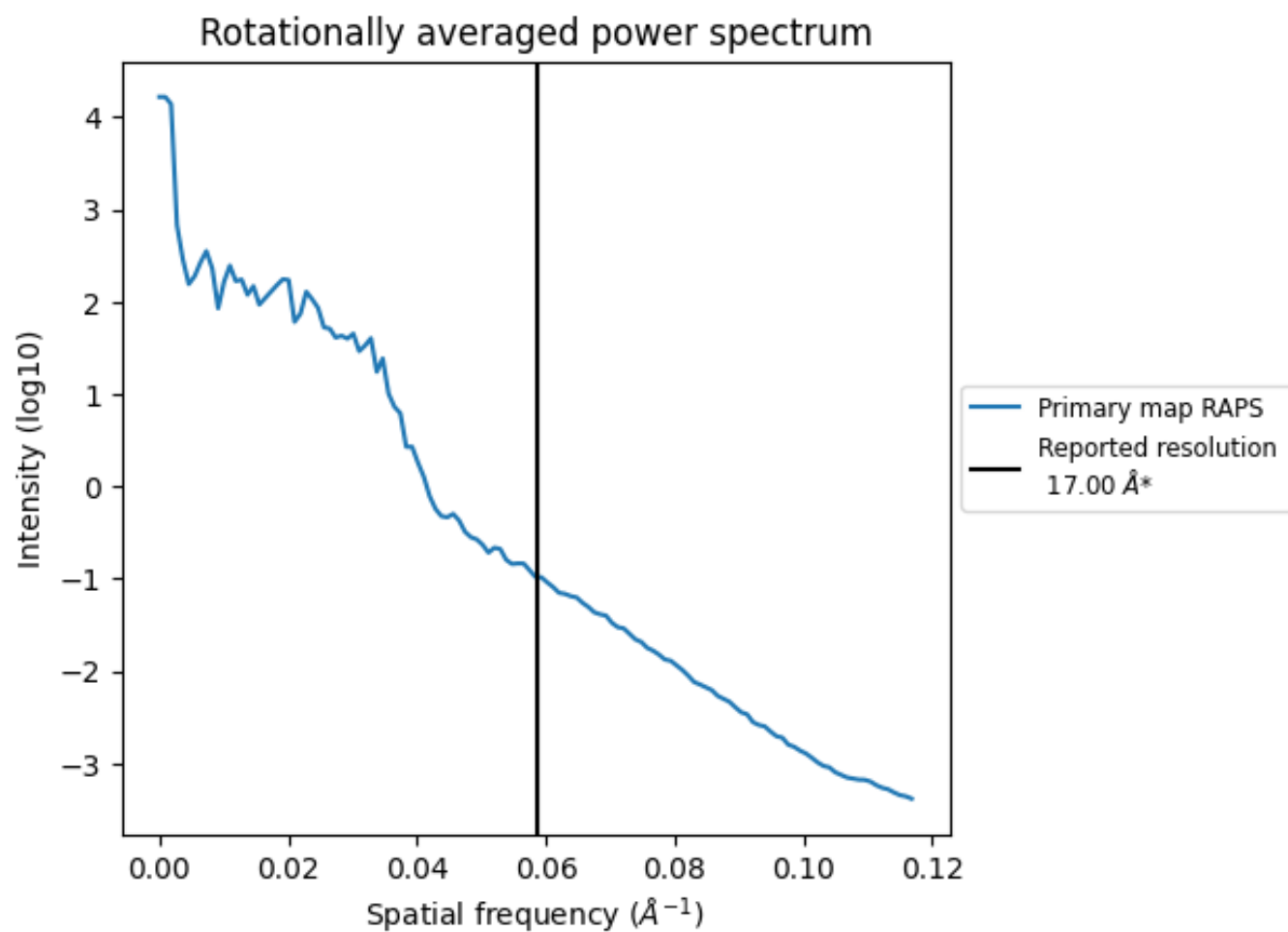
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48587 nm³; this corresponds to an approximate mass of 43890 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

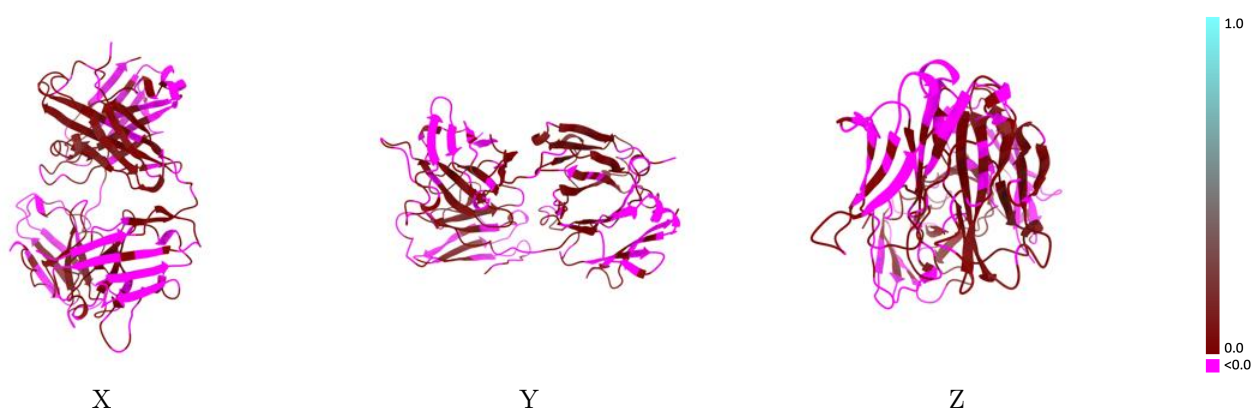
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2645 and PDB model 4UOM. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

This section was not generated.

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

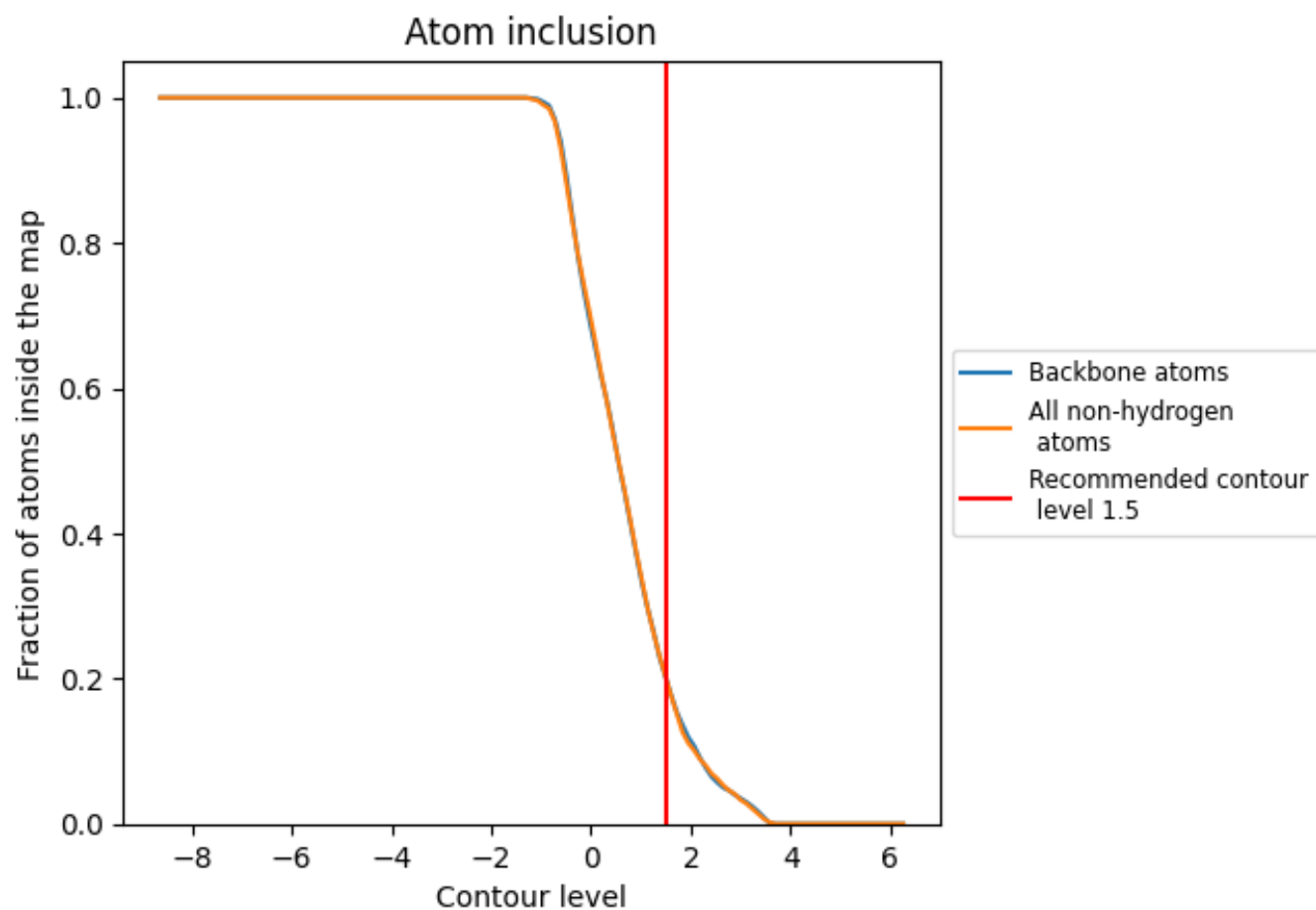


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 20% of all backbone atoms, 20% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2010	0.0090
H	0.2850	0.0300
L	0.1130	-0.0130

