



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 09:01 pm BST

PDB ID : 9TIF / pdb_00009tif
EMDB ID : EMD-55954
Title : Phage 812 baseplate in the pre-contraction state - lower arm
Authors : Binovsky, J.; Plevka, P.
Deposited on : 2025-12-05
Resolution : 5.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

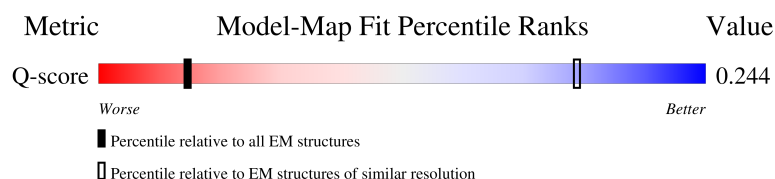
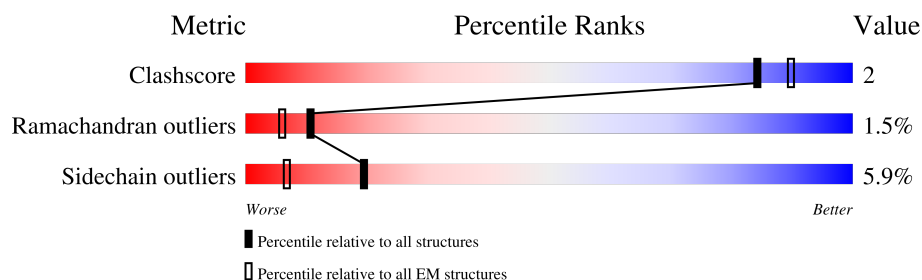
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 5.60 Å.

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



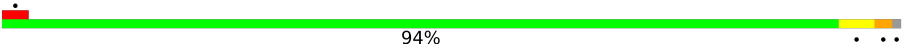
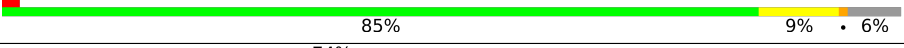
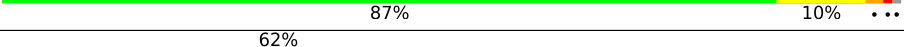
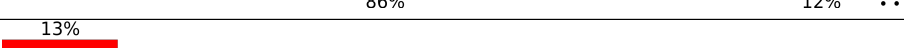




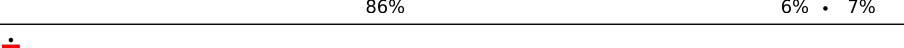



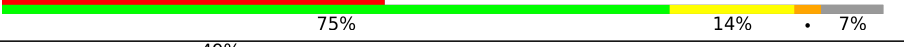
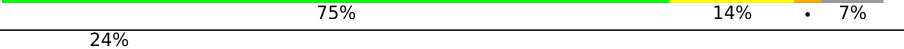




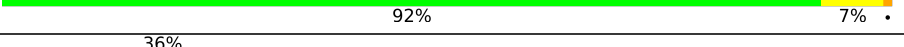
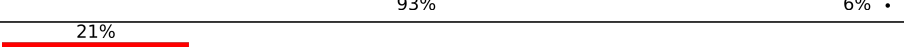
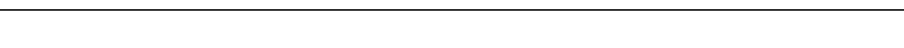



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	513 (5.10 - 6.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	640	<div> <div>26%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	640	<div> <div>28%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	J	640	<div> <div>18%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	D	173	<div> <div>61%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	173	
2	I	173	
2	K	173	
2	L	173	
2	N	173	
2	O	173	
2	P	173	
2	Q	173	
2	R	173	
2	V	173	
2	c	173	
3	F	295	
4	G	124	
5	H	1152	
5	d	1152	
5	e	1152	
5	f	1152	
5	g	1152	
5	h	1152	
6	M	808	
7	S	458	
7	T	458	
7	U	458	
8	b	1019	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 100209 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 CBM-cenC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
1	B	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
1	J	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		

- Molecule 2 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	E	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	I	163	Total	C	N	O	S	0	0
			1277	817	208	251	1		
2	K	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	L	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	N	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	O	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	P	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	Q	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	R	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	V	161	Total	C	N	O	S	0	0
			1266	809	207	249	1		
2	c	162	Total	C	N	O	S	0	0
			1272	812	208	251	1		

- Molecule 3 is a protein called ORF57.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	139	Total	C	N	O	S	0	0
			1157	739	177	239	2		

- Molecule 4 is a protein called ORF67.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	71	Total	C	N	O		0	0
			597	390	94	113			

- Molecule 5 is a protein called ORF65.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	d	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	e	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	f	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	g	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		
5	h	1066	Total	C	N	O	S	0	0
			8390	5275	1402	1688	25		

- Molecule 6 is a protein called ORF56.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	136	Total	C	N	O	S	0	0
			1064	682	193	186	3		

- Molecule 7 is a protein called ORF68.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
7	T	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
7	U	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		

- Molecule 8 is a protein called ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	b	628	5070	3240	807	1013	10	0	0

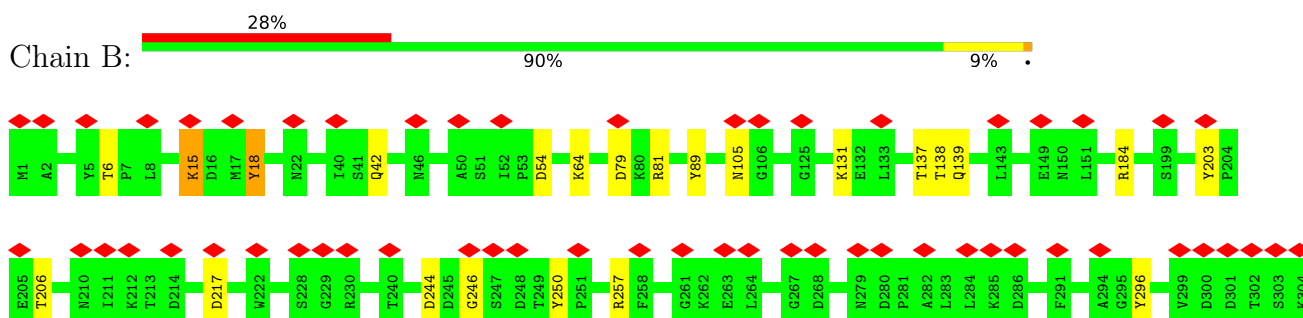
3 Residue-property plots

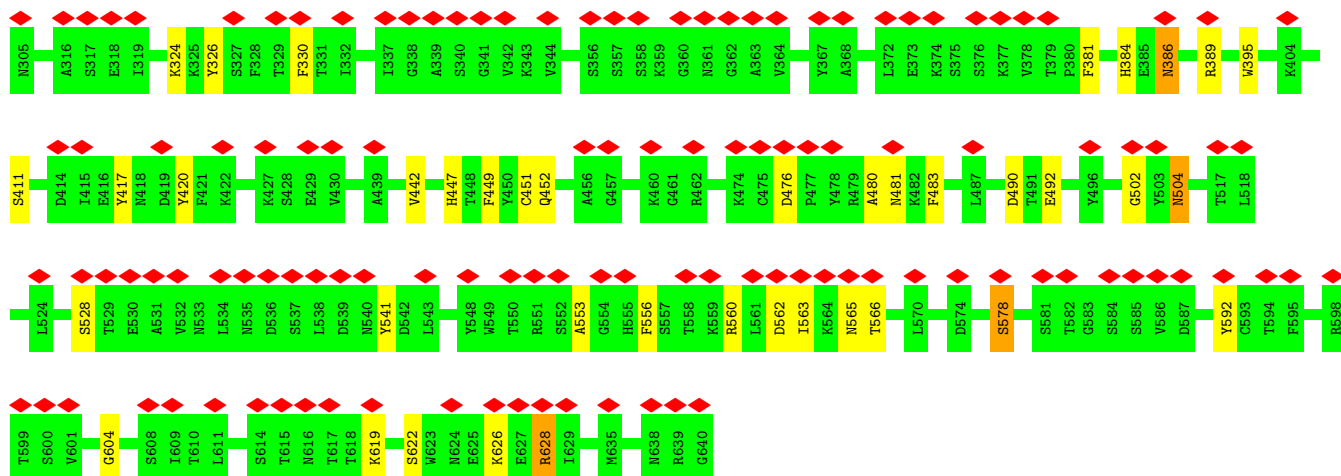
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CBM-cenC domain-containing protein

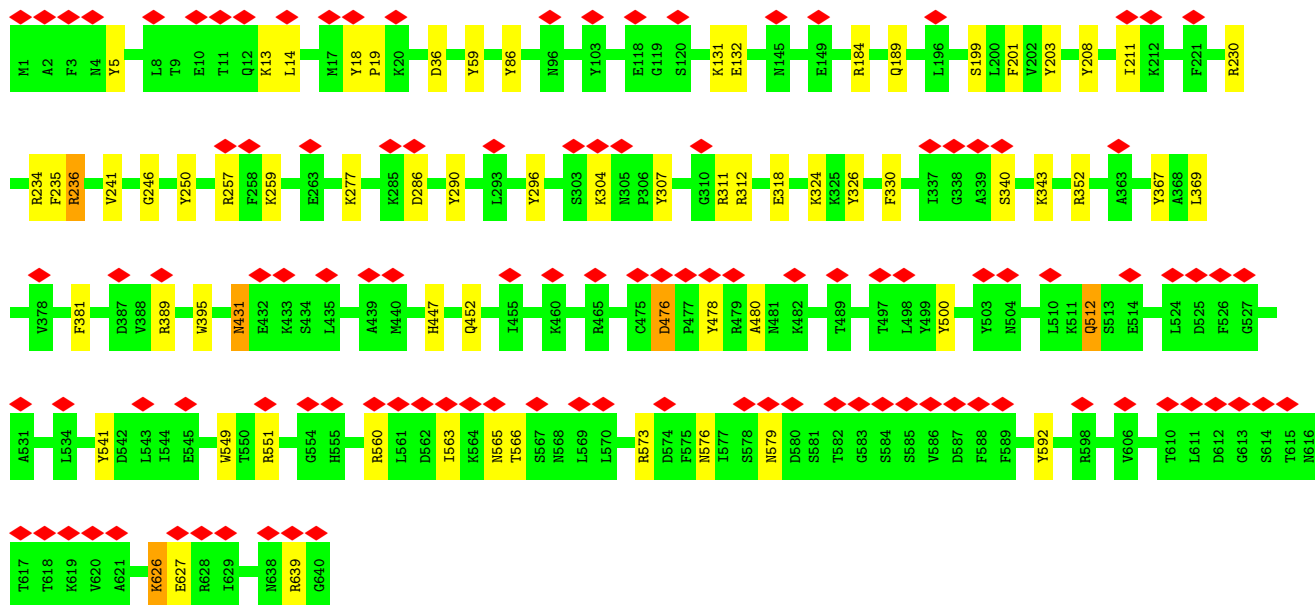
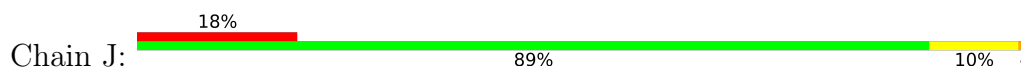


• Molecule 1: CBM-cenC domain-containing protein

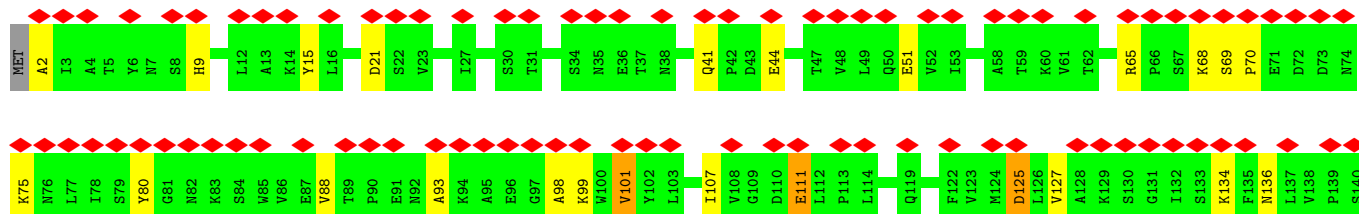
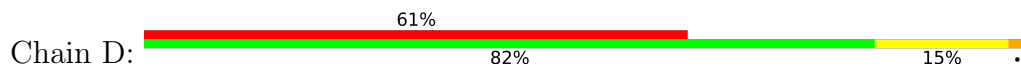


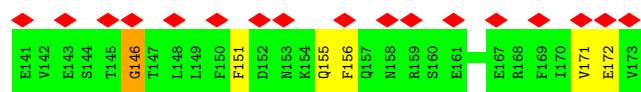


• Molecule 1: CBM-cenC domain-containing protein

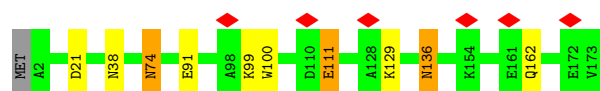
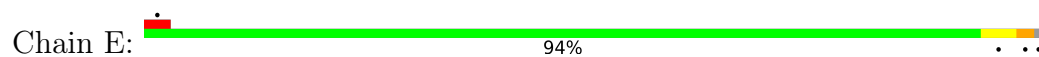


• Molecule 2: ORF64

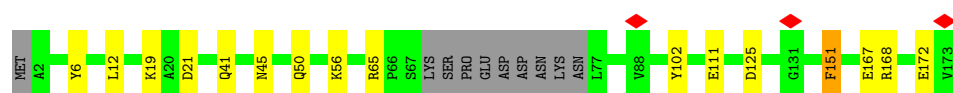
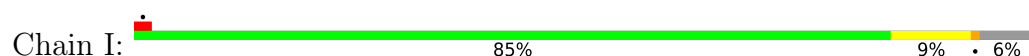




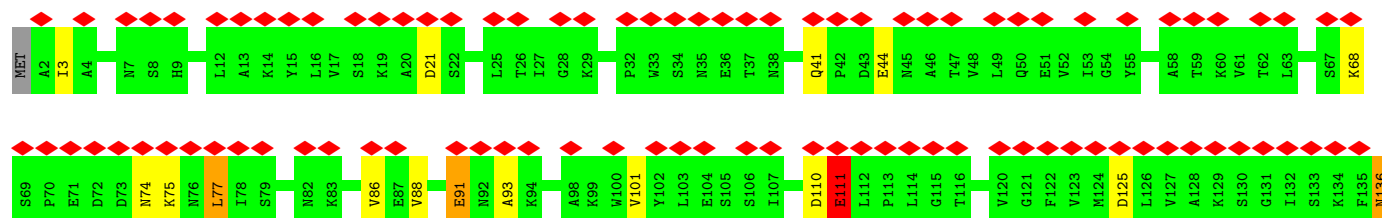
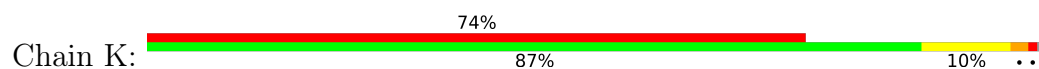
• Molecule 2: ORF64



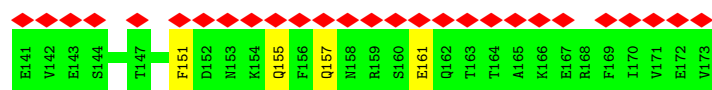
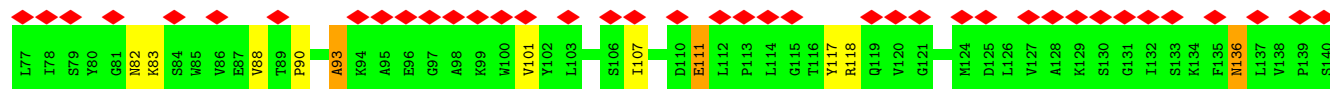
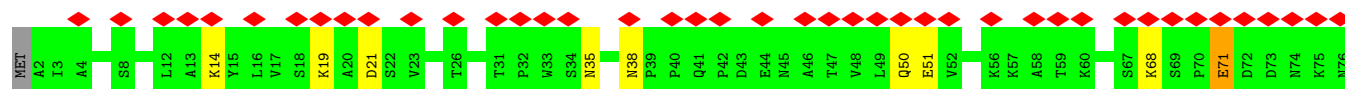
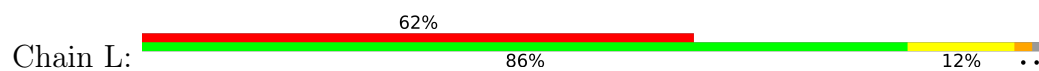
• Molecule 2: ORF64




• Molecule 2: ORF64

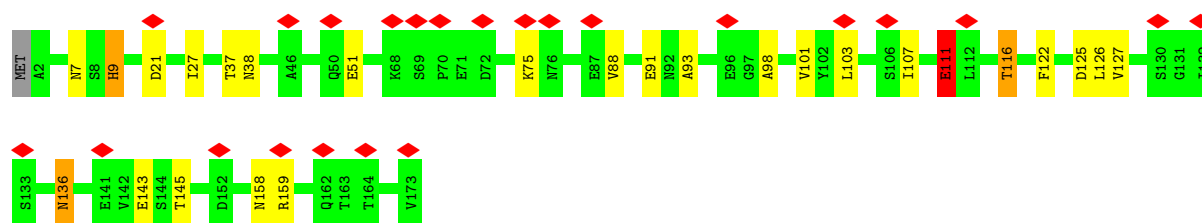


• Molecule 2: ORF64




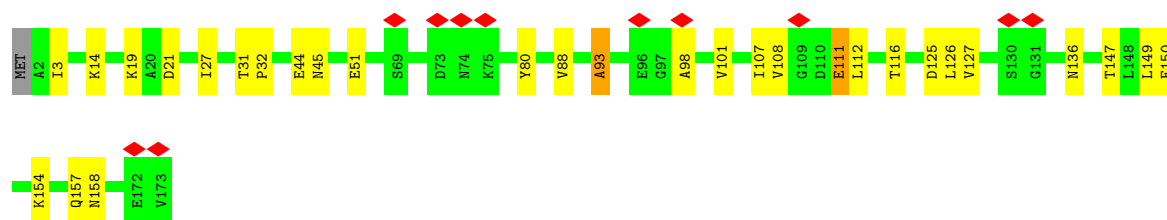
• Molecule 2: ORF64

Chain N: 




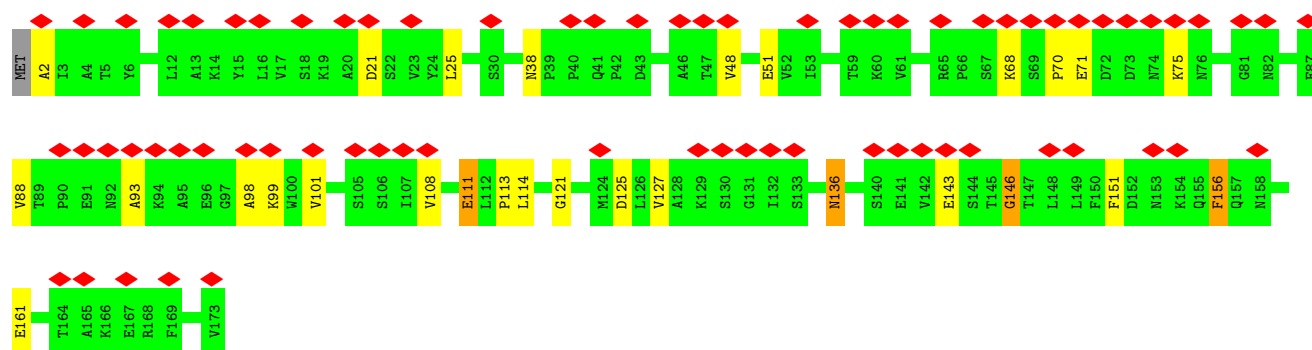
• Molecule 2: ORF64

Chain O: 




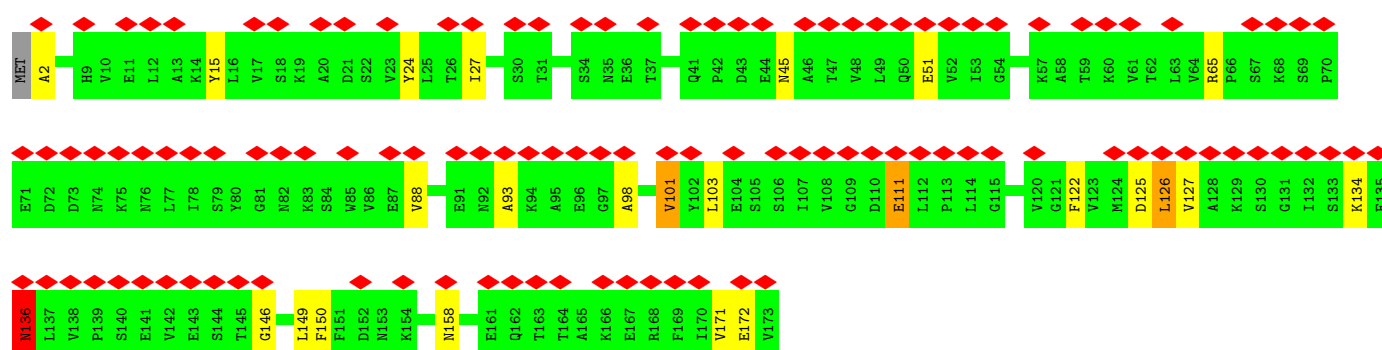
• Molecule 2: ORF64

Chain P: 

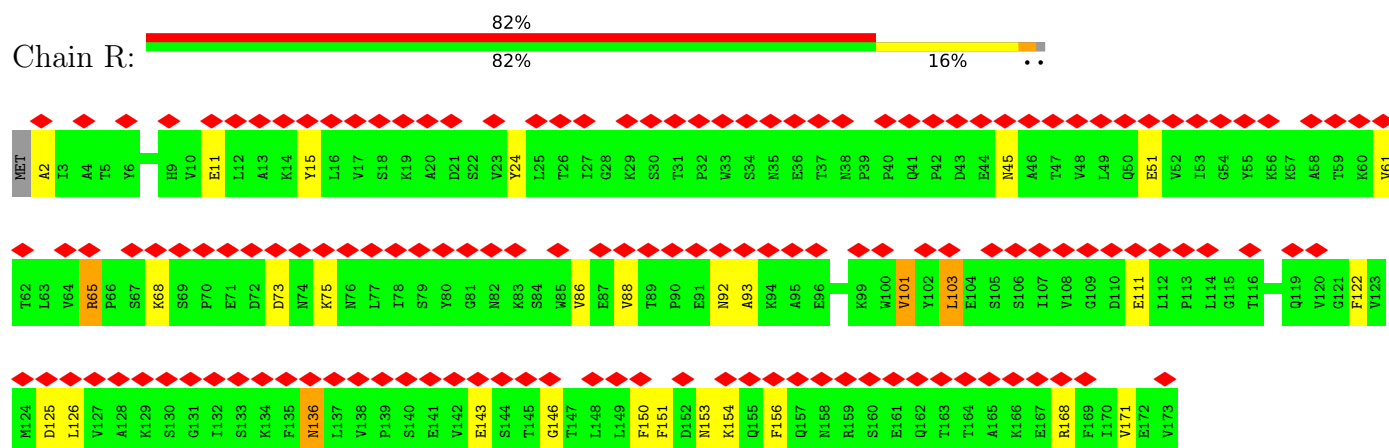


• Molecule 2: ORF64

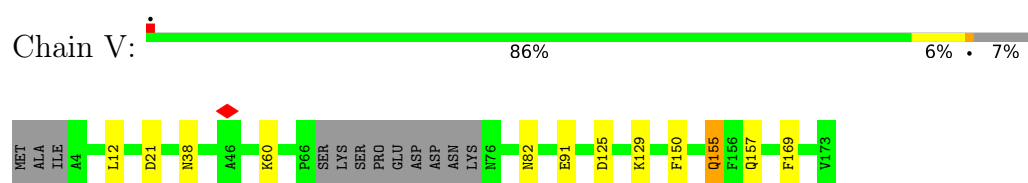
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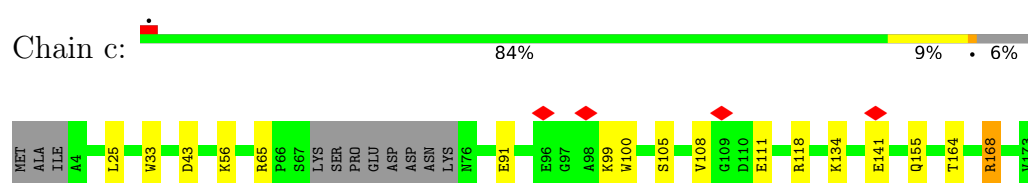
- Molecule 2: ORF64



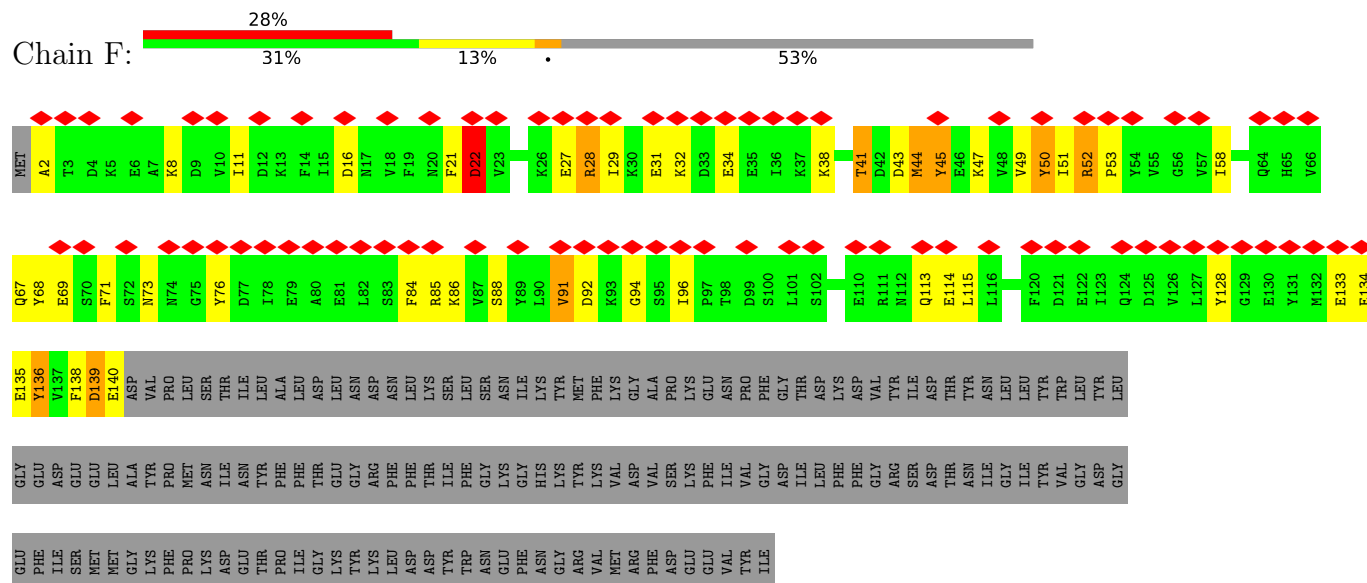
- Molecule 2: ORF64



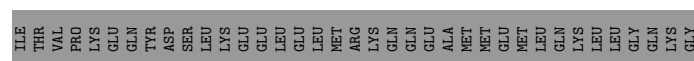
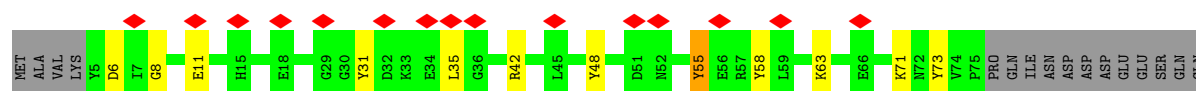
- Molecule 2: ORF64



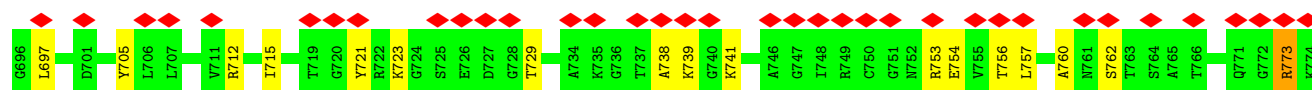
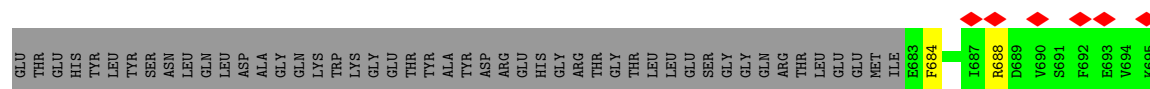
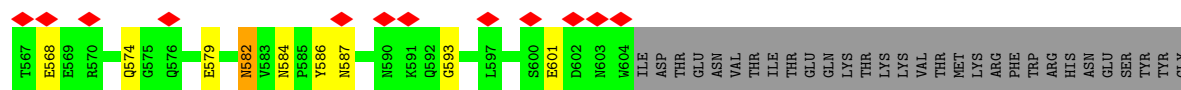
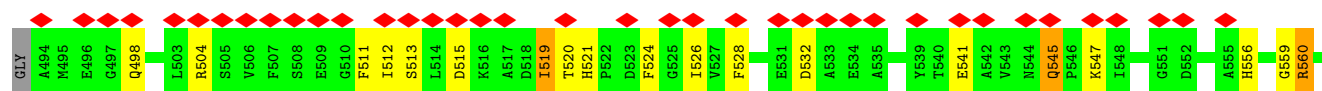
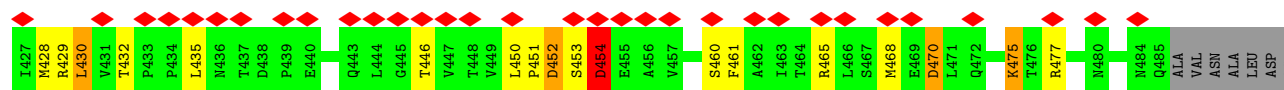
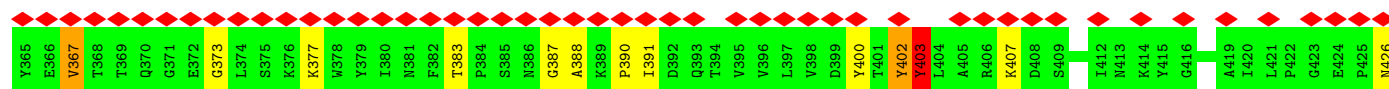
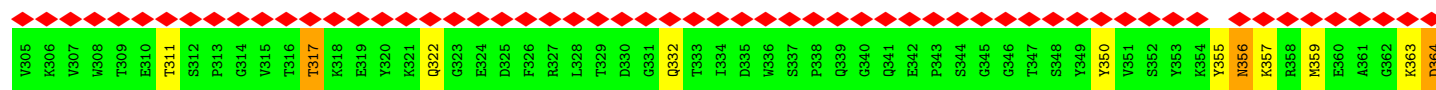
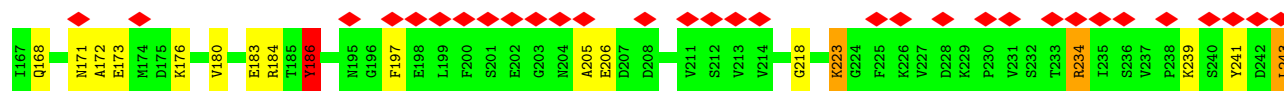
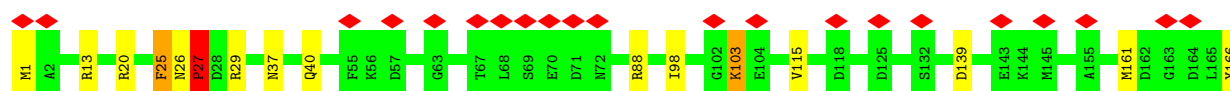
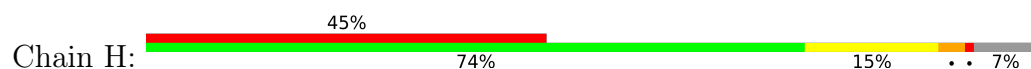
- Molecule 3: ORF57

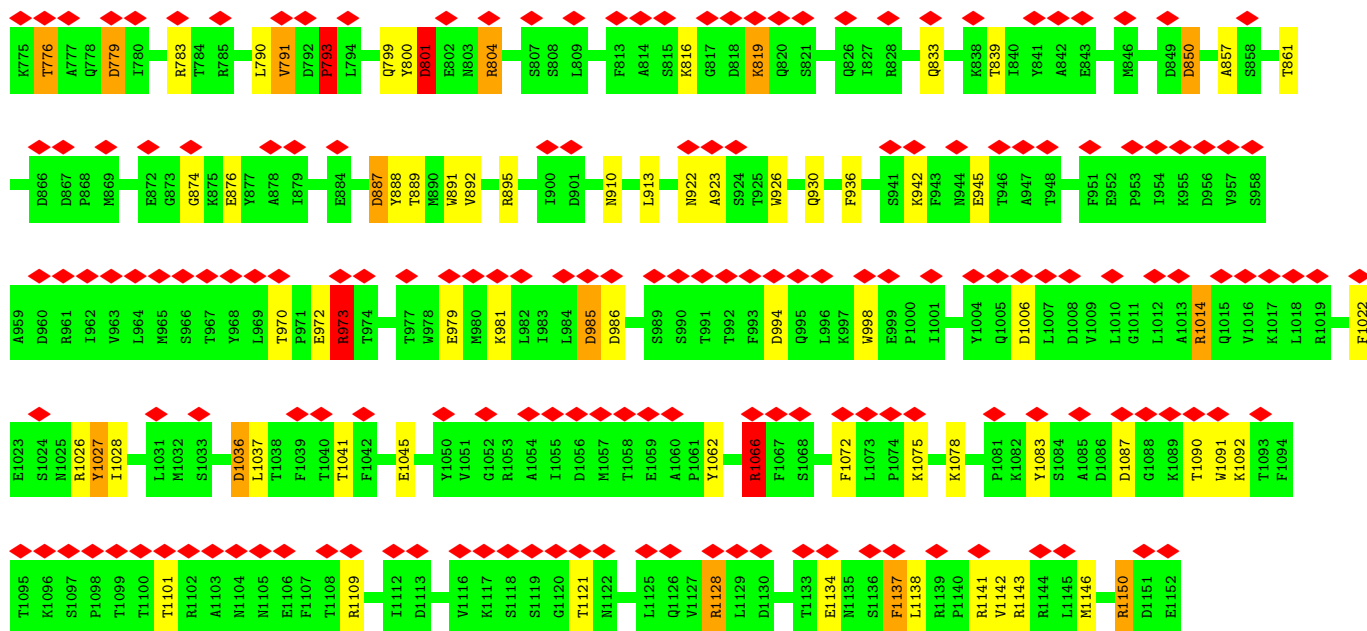


- Molecule 4: ORF67

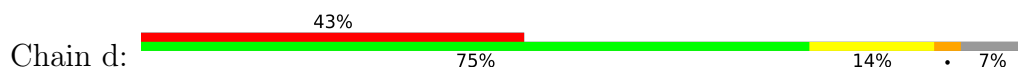


• Molecule 5: ORF65

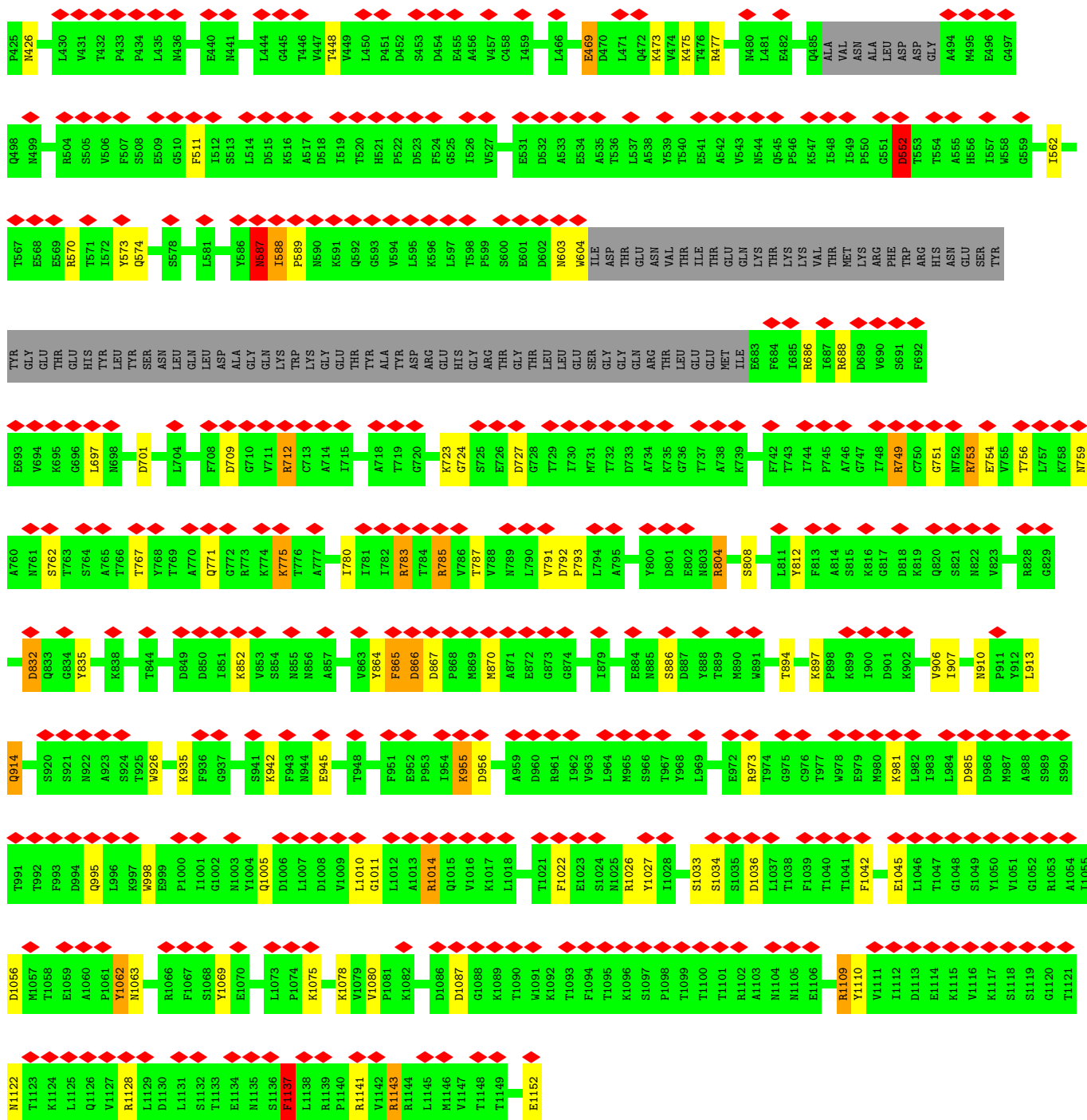




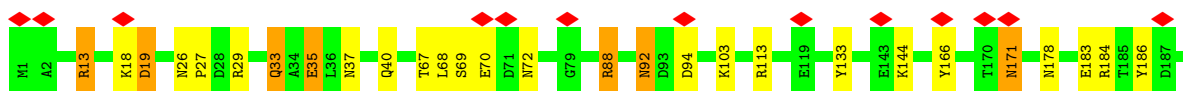
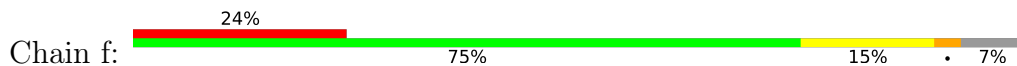
• Molecule 5: ORF65

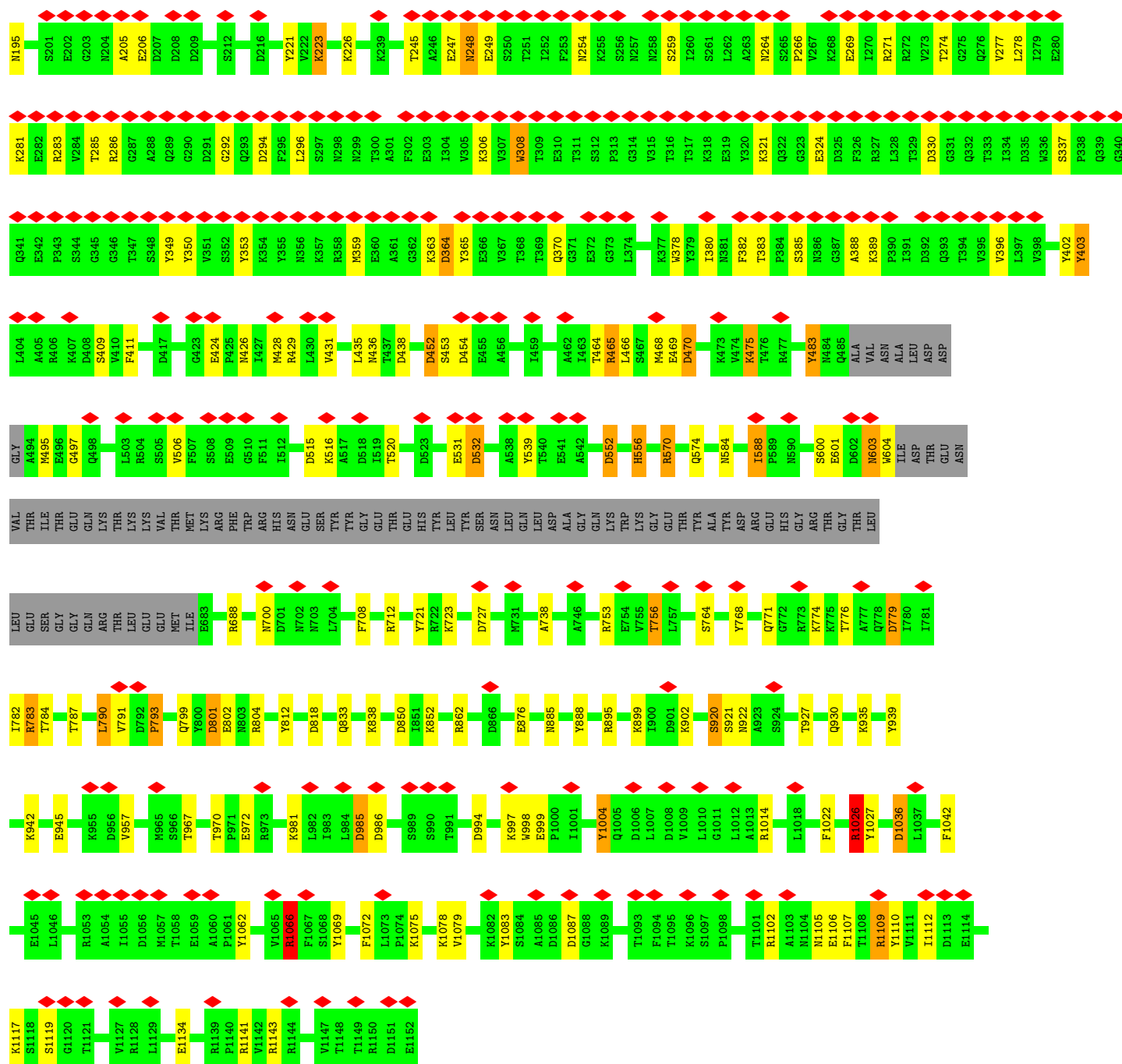




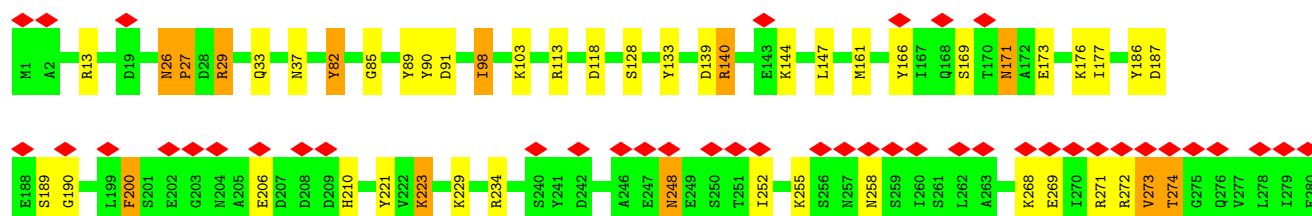
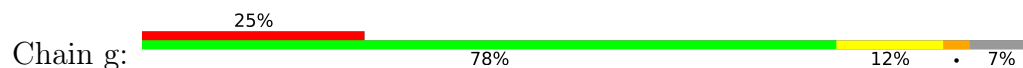


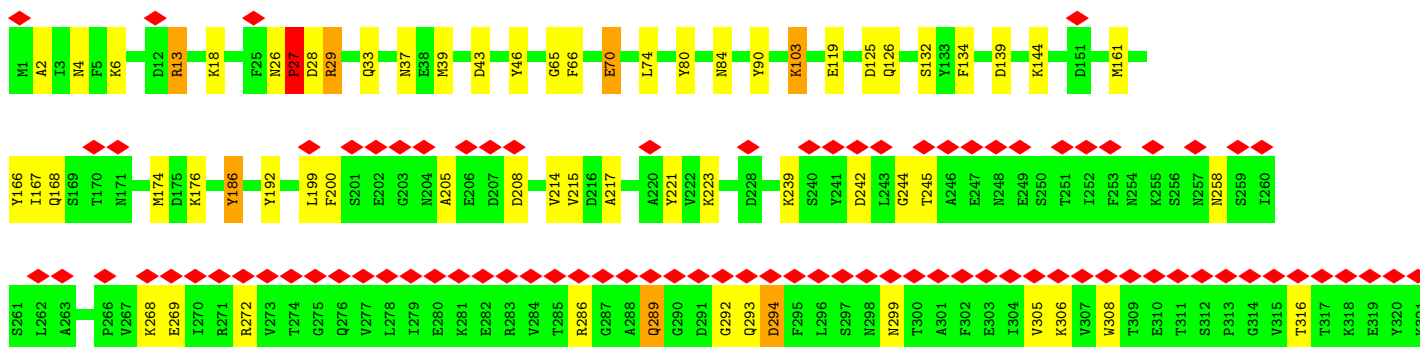
• Molecule 5: ORF65

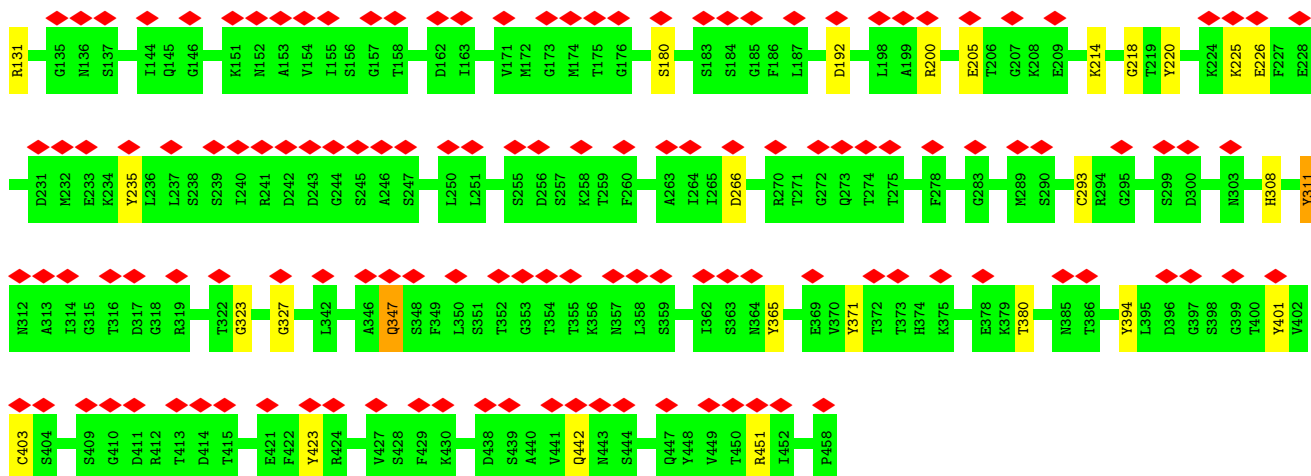




• Molecule 5: ORF65

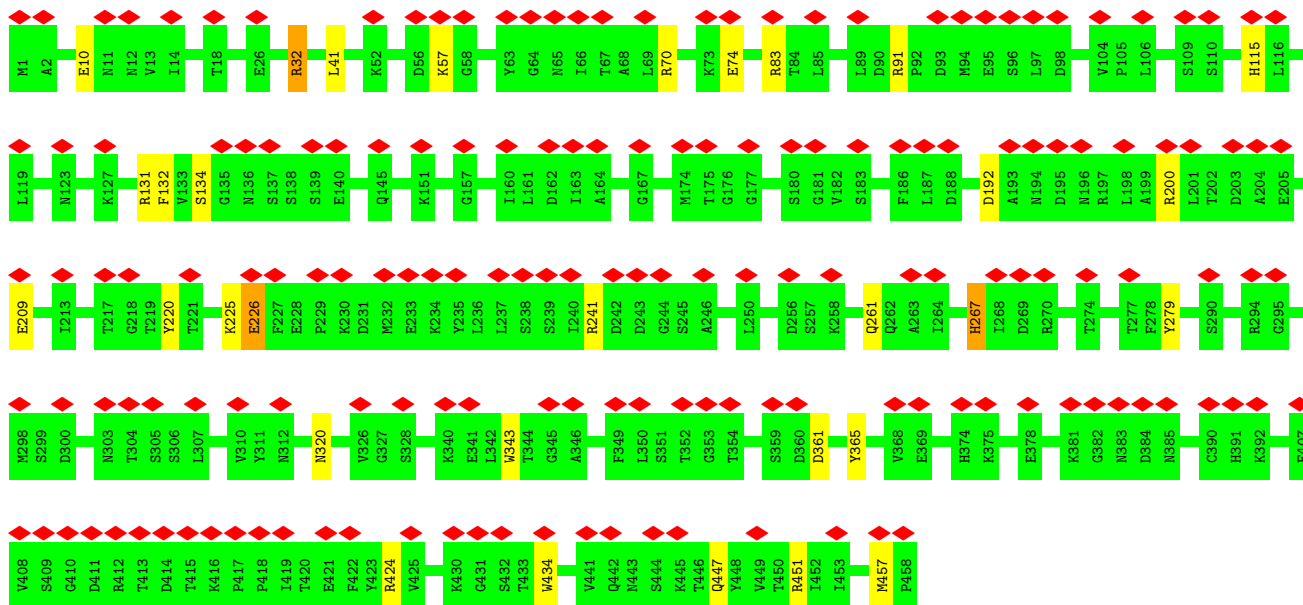






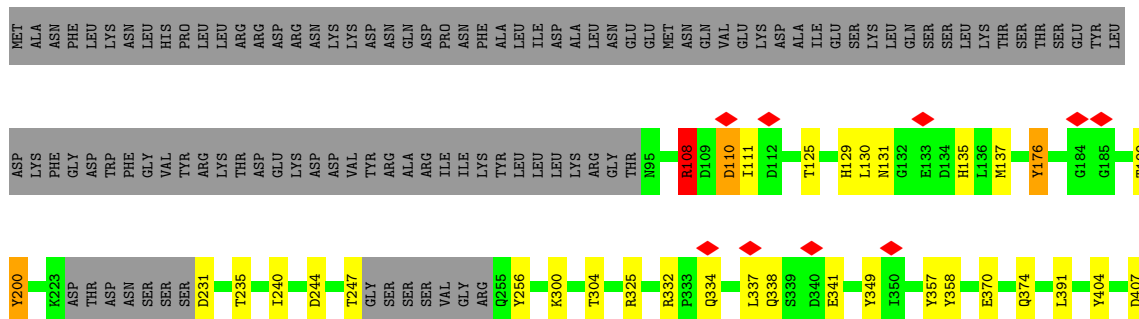
• Molecule 7: ORF68

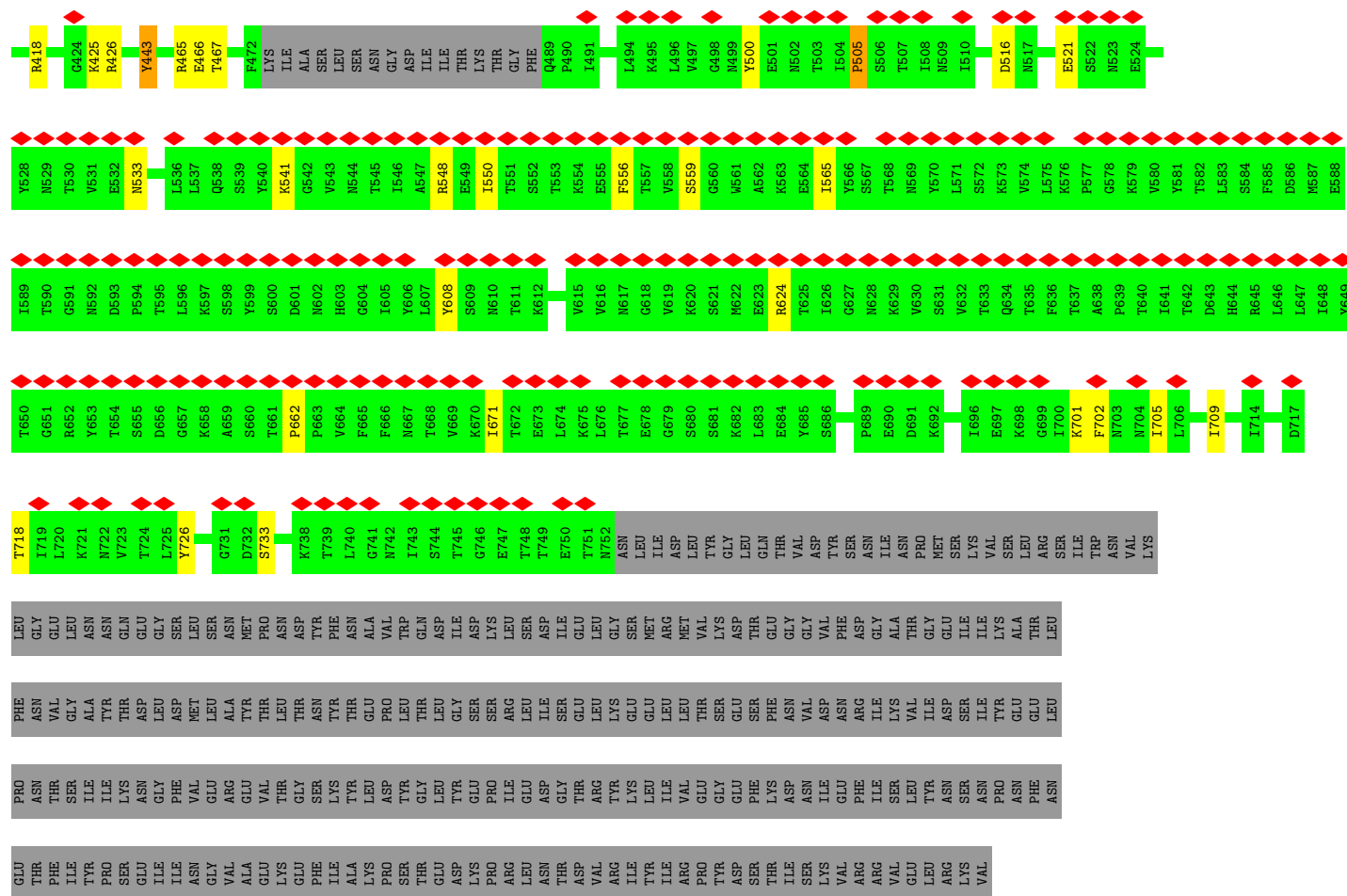
Chain U: 36% 93% 6% •



• Molecule 8: ORF63

Chain b: 21% 55% 6% 38%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	600.192, 600.192, 600.192	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.6672001, 1.6672001, 1.6672001	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	A	0.74	0/5253	1.30	17/7135 (0.2%)
1	B	0.75	0/5253	1.31	22/7135 (0.3%)
1	J	0.74	0/5253	1.31	19/7135 (0.3%)
2	D	0.75	0/1377	1.48	9/1872 (0.5%)
2	E	0.71	0/1377	1.29	5/1872 (0.3%)
2	I	0.71	0/1303	1.27	3/1771 (0.2%)
2	K	0.80	0/1377	1.51	9/1872 (0.5%)
2	L	0.78	0/1377	1.46	11/1872 (0.6%)
2	N	0.70	0/1377	1.42	8/1872 (0.4%)
2	O	0.73	0/1377	1.39	7/1872 (0.4%)
2	P	0.74	0/1377	1.43	8/1872 (0.4%)
2	Q	0.76	0/1377	1.46	7/1872 (0.4%)
2	R	0.80	0/1377	1.47	8/1872 (0.4%)
2	V	0.71	0/1292	1.29	1/1756 (0.1%)
2	c	0.73	0/1298	1.21	3/1764 (0.2%)
3	F	0.78	0/1178	1.59	11/1593 (0.7%)
4	G	0.77	0/613	1.32	0/830
5	H	0.81	0/8552	1.50	71/11599 (0.6%)
5	d	0.79	0/8552	1.46	63/11599 (0.5%)
5	e	0.77	0/8552	1.41	48/11599 (0.4%)
5	f	0.77	0/8552	1.41	61/11599 (0.5%)
5	g	0.77	0/8552	1.44	55/11599 (0.5%)
5	h	0.77	0/8552	1.46	71/11599 (0.6%)
6	M	0.80	0/1097	1.43	7/1482 (0.5%)
7	S	0.72	0/3619	1.26	14/4913 (0.3%)
7	T	0.75	0/3619	1.29	12/4913 (0.2%)
7	U	0.72	0/3619	1.27	11/4913 (0.2%)
8	b	0.76	0/5179	1.30	15/7040 (0.2%)
All	All	0.76	0/102281	1.39	576/138822 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	11
1	J	0	16
2	D	0	2
2	I	0	2
2	L	0	2
2	N	0	1
2	O	0	1
2	Q	0	1
2	R	0	3
2	V	0	1
2	c	0	1
3	F	0	5
4	G	0	6
5	H	0	17
5	d	0	25
5	e	0	23
5	f	0	21
5	g	0	19
5	h	0	30
6	M	0	8
7	S	0	10
7	T	0	9
7	U	0	7
8	b	0	14
All	All	0	247

There are no bond length outliers.

All (576) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	171	ASN	CA-CB-CG	11.87	124.47	112.60
5	e	552	ASP	CA-CB-CG	11.68	124.28	112.60
5	H	243	LEU	CA-C-N	10.48	129.68	121.61
5	H	243	LEU	C-N-CA	10.48	129.68	121.61
5	h	43	ASP	CA-CB-CG	-9.52	103.08	112.60
5	h	530	PHE	CA-CB-CG	9.45	123.25	113.80
5	e	866	ASP	CA-CB-CG	9.29	121.89	112.60
3	F	134	GLU	N-CA-C	9.08	121.86	108.60
5	h	866	ASP	CA-CB-CG	9.03	121.63	112.60
5	d	1137	PHE	CA-CB-CG	8.76	122.56	113.80
5	h	785	ARG	NE-CZ-NH2	8.76	127.08	119.20
5	f	171	ASN	CA-CB-CG	8.70	121.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	801	ASP	CA-CB-CG	8.63	121.23	112.60
5	d	530	PHE	CA-CB-CG	8.60	122.39	113.80
2	V	169	PHE	CA-CB-CG	8.56	122.36	113.80
5	d	866	ASP	CA-CB-CG	8.54	121.14	112.60
5	f	779	ASP	CA-CB-CG	8.47	121.07	112.60
5	f	1066	ARG	NE-CZ-NH2	8.36	126.72	119.20
5	H	470	ASP	CA-CB-CG	8.35	120.95	112.60
1	J	389	ARG	NE-CZ-NH2	8.35	126.71	119.20
5	H	850	ASP	CA-CB-CG	8.28	120.88	112.60
5	g	272	ARG	CA-C-N	8.28	131.38	122.11
5	g	272	ARG	C-N-CA	8.28	131.38	122.11
5	h	26	ASN	CA-C-N	8.26	130.16	119.84
5	h	26	ASN	C-N-CA	8.26	130.16	119.84
5	H	684	PHE	CA-CB-CG	8.18	121.98	113.80
2	K	21	ASP	CA-CB-CG	-8.09	104.51	112.60
5	H	1137	PHE	CA-CB-CG	8.01	121.81	113.80
5	h	727	ASP	CA-CB-CG	-7.94	104.66	112.60
2	P	136	ASN	CA-CB-CG	7.93	120.53	112.60
5	H	26	ASN	CA-C-N	7.93	129.75	119.84
5	H	26	ASN	C-N-CA	7.93	129.75	119.84
5	g	428	MET	N-CA-C	7.91	122.62	112.34
5	d	603	ASN	OD1-CG-ND2	-7.90	114.70	122.60
5	H	779	ASP	CA-CB-CG	7.87	120.47	112.60
5	h	29	ARG	N-CA-C	7.67	119.52	110.31
5	g	1109	ARG	NE-CZ-NH2	7.53	125.98	119.20
2	N	21	ASP	CA-CB-CG	-7.47	105.13	112.60
5	f	688	ARG	NE-CZ-NH2	7.46	125.92	119.20
5	H	887	ASP	CA-CB-CG	7.45	120.05	112.60
5	H	1143	ARG	NE-CZ-NH2	7.42	125.88	119.20
5	d	779	ASP	CA-CB-CG	7.40	120.00	112.60
7	U	451	ARG	NE-CZ-NH2	7.37	125.83	119.20
5	f	26	ASN	N-CA-C	7.35	114.84	108.22
5	H	37	ASN	CA-C-N	7.35	130.86	120.28
5	H	37	ASN	C-N-CA	7.35	130.86	120.28
2	D	21	ASP	CA-CB-CG	-7.34	105.26	112.60
5	H	1066	ARG	CD-NE-CZ	7.32	134.64	124.40
5	g	783	ARG	NE-CZ-NH2	7.31	125.78	119.20
5	g	470	ASP	CA-CB-CG	-7.30	105.30	112.60
3	F	134	GLU	CA-C-N	7.24	135.37	121.54
3	F	134	GLU	C-N-CA	7.24	135.37	121.54
2	L	136	ASN	CA-CB-CG	7.22	119.82	112.60
5	e	294	ASP	CA-CB-CG	7.21	119.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	h	560	ARG	NE-CZ-NH2	7.21	125.69	119.20
5	d	985	ASP	CA-CB-CG	7.21	119.81	112.60
5	e	1014	ARG	NE-CZ-NH2	7.20	125.68	119.20
5	f	532	ASP	CA-CB-CG	7.20	119.80	112.60
5	f	92	ASN	CA-CB-CG	7.12	119.72	112.60
5	g	1014	ARG	NE-CZ-NH2	7.12	125.61	119.20
5	e	200	PHE	CA-CB-CG	7.11	120.91	113.80
5	f	895	ARG	NE-CZ-NH2	7.09	125.58	119.20
5	g	712	ARG	NE-CZ-NH2	7.08	125.58	119.20
8	b	426	ARG	NE-CZ-NH2	7.06	125.55	119.20
2	D	172	GLU	N-CA-CB	-7.04	99.45	110.44
5	e	832	ASP	CA-C-N	7.03	134.96	121.54
5	e	832	ASP	C-N-CA	7.03	134.96	121.54
2	L	21	ASP	CA-CB-CG	-7.01	105.59	112.60
5	h	603	ASN	CA-CB-CG	7.01	119.61	112.60
5	e	286	ARG	NE-CZ-NH2	6.98	125.48	119.20
5	e	1005	GLN	OE1-CD-NE2	-6.97	115.63	122.60
1	A	539	ASP	CA-CB-CG	-6.95	105.65	112.60
5	H	20	ARG	NE-CZ-NH2	6.95	125.45	119.20
5	g	779	ASP	CA-CB-CG	6.94	119.54	112.60
5	d	603	ASN	CA-CB-CG	6.93	119.53	112.60
5	f	804	ARG	NE-CZ-NH2	6.91	125.42	119.20
5	e	727	ASP	CA-CB-CG	-6.91	105.69	112.60
5	h	1141	ARG	NE-CZ-NH2	6.88	125.39	119.20
5	H	461	PHE	CA-CB-CG	6.87	120.67	113.80
5	H	1036	ASP	CA-CB-CG	-6.86	105.74	112.60
7	U	74	GLU	CB-CG-CD	-6.83	100.99	112.60
5	h	294	ASP	CA-CB-CG	6.83	119.43	112.60
7	T	200	ARG	NE-CZ-NH2	6.82	125.34	119.20
1	B	217	ASP	CA-CB-CG	-6.82	105.78	112.60
5	h	556	HIS	CA-CB-CG	-6.81	106.99	113.80
3	F	85	ARG	NE-CZ-NH2	6.81	125.33	119.20
5	H	1066	ARG	NE-CZ-NH2	6.77	125.29	119.20
1	A	389	ARG	NE-CZ-NH2	6.76	125.28	119.20
5	H	783	ARG	NE-CZ-NH2	6.76	125.28	119.20
5	d	33	GLN	OE1-CD-NE2	-6.76	115.84	122.60
1	A	560	ARG	NE-CZ-NH2	6.73	125.26	119.20
2	P	156	PHE	CA-CB-CG	6.73	120.53	113.80
7	S	412	ARG	NE-CZ-NH2	6.71	125.24	119.20
2	I	151	PHE	CA-CB-CG	6.70	120.50	113.80
5	g	13	ARG	NE-CZ-NH2	6.70	125.23	119.20
5	h	1004	TYR	CA-C-N	6.70	133.89	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	h	1004	TYR	C-N-CA	6.70	133.89	122.37
5	h	13	ARG	NE-CZ-NH2	6.66	125.19	119.20
5	h	477	ARG	NE-CZ-NH2	6.59	125.13	119.20
5	d	943	PHE	CA-CB-CG	-6.59	107.21	113.80
5	f	19	ASP	CA-CB-CG	6.57	119.17	112.60
5	H	1128	ARG	NE-CZ-NH2	6.56	125.10	119.20
1	B	560	ARG	NE-CZ-NH2	6.55	125.10	119.20
5	g	531	GLU	CA-C-N	6.55	131.82	120.68
5	g	531	GLU	C-N-CA	6.55	131.82	120.68
5	f	1109	ARG	NE-CZ-NH2	6.54	125.08	119.20
2	c	155	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	A	81	ARG	NE-CZ-NH2	6.53	125.07	119.20
5	h	1022	PHE	CA-CB-CG	6.53	120.33	113.80
5	e	1143	ARG	NE-CZ-NH1	-6.51	114.98	121.50
5	f	556	HIS	CB-CG-CD2	-6.50	122.75	131.20
5	g	255	LYS	CA-C-N	6.50	129.87	120.38
5	g	255	LYS	C-N-CA	6.50	129.87	120.38
7	U	447	GLN	OE1-CD-NE2	-6.50	116.10	122.60
5	d	477	ARG	NE-CZ-NH2	6.48	125.03	119.20
3	F	22	ASP	CA-CB-CG	6.47	119.07	112.60
5	f	712	ARG	NE-CZ-NH2	6.47	125.02	119.20
5	f	1143	ARG	NE-CZ-NH2	6.46	125.02	119.20
5	H	248	ASN	CA-CB-CG	6.45	119.05	112.60
7	T	451	ARG	NE-CZ-NH2	6.44	125.00	119.20
5	e	1022	PHE	CA-CB-CG	6.43	120.23	113.80
2	N	136	ASN	CA-CB-CG	6.42	119.03	112.60
5	f	13	ARG	NE-CZ-NH1	-6.42	115.08	121.50
5	H	373	GLY	N-CA-C	6.41	122.94	111.02
5	f	603	ASN	CA-CB-CG	6.40	119.00	112.60
2	R	136	ASN	OD1-CG-ND2	-6.40	116.20	122.60
2	K	136	ASN	CA-CB-CG	6.39	118.99	112.60
2	R	65	ARG	NE-CZ-NH2	6.38	124.94	119.20
5	e	477	ARG	NE-CZ-NH2	6.38	124.94	119.20
2	R	136	ASN	CA-CB-CG	6.35	118.95	112.60
5	H	773	ARG	NE-CZ-NH2	6.34	124.91	119.20
7	S	32	ARG	NE-CZ-NH2	6.31	124.88	119.20
5	H	1141	ARG	NE-CZ-NH2	6.31	124.88	119.20
5	h	973	ARG	CD-NE-CZ	6.31	133.23	124.40
1	B	452	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	J	512	GLN	OE1-CD-NE2	-6.29	116.31	122.60
5	g	994	ASP	CA-CB-CG	-6.28	106.32	112.60
7	T	7	THR	CA-C-N	6.27	129.14	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	7	THR	C-N-CA	6.27	129.14	120.49
2	R	111	GLU	CA-C-N	6.25	137.05	121.80
2	R	111	GLU	C-N-CA	6.25	137.05	121.80
5	d	94	ASP	CA-CB-CG	6.24	118.84	112.60
5	e	753	ARG	NE-CZ-NH2	6.24	124.82	119.20
5	H	27	PRO	N-CA-C	6.24	125.32	112.47
1	B	562	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	389	ARG	NE-CZ-NH2	6.23	124.81	119.20
5	g	1042	PHE	CA-CB-CG	6.23	120.03	113.80
5	f	364	ASP	CA-CB-CG	6.23	118.83	112.60
5	g	1143	ARG	NE-CZ-NH2	6.23	124.81	119.20
5	h	472	GLN	OE1-CD-NE2	-6.22	116.38	122.60
8	b	108	ARG	NE-CZ-NH2	6.20	124.78	119.20
8	b	135	HIS	CB-CG-CD2	-6.19	123.15	131.20
5	e	749	ARG	NE-CZ-NH2	6.19	124.77	119.20
5	h	688	ARG	NE-CZ-NH2	6.18	124.77	119.20
5	H	688	ARG	NE-CZ-NH2	6.18	124.76	119.20
5	d	920	SER	N-CA-C	6.17	116.23	108.45
5	d	727	ASP	CA-CB-CG	-6.16	106.44	112.60
2	L	111	GLU	CA-C-N	6.16	136.82	121.80
2	L	111	GLU	C-N-CA	6.16	136.82	121.80
2	P	146	GLY	N-CA-C	6.14	120.42	112.68
2	I	50	GLN	OE1-CD-NE2	-6.14	116.46	122.60
5	g	302	PHE	CA-CB-CG	6.12	119.92	113.80
5	g	26	ASN	CA-C-N	6.10	127.47	119.84
5	g	26	ASN	C-N-CA	6.10	127.47	119.84
5	H	528	PHE	CA-CB-CG	6.10	119.90	113.80
5	H	286	ARG	NE-CZ-NH2	6.09	124.68	119.20
5	d	113	ARG	NE-CZ-NH2	6.08	124.67	119.20
5	d	175	ASP	CA-C-N	6.07	130.41	120.63
5	d	175	ASP	C-N-CA	6.07	130.41	120.63
2	Q	65	ARG	NE-CZ-NH2	6.06	124.65	119.20
5	H	712	ARG	NE-CZ-NH2	6.04	124.64	119.20
5	e	759	ASN	CA-CB-CG	6.04	118.64	112.60
5	d	688	ARG	NE-CZ-NH2	6.04	124.63	119.20
5	e	234	ARG	NE-CZ-NH2	6.04	124.63	119.20
5	e	1109	ARG	NE-CZ-NH2	6.03	124.63	119.20
5	h	504	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	J	257	ARG	NE-CZ-NH2	6.03	124.62	119.20
5	H	243	LEU	N-CA-C	6.02	118.48	110.53
5	h	125	ASP	CA-CB-CG	-6.02	106.58	112.60
5	e	1056	ASP	CA-CB-CG	-6.02	106.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	521	HIS	CA-CB-CG	-6.02	107.78	113.80
5	e	139	ASP	CA-CB-CG	6.02	118.62	112.60
5	g	504	ARG	NE-CZ-NH2	6.02	124.62	119.20
5	d	1014	ARG	NE-CZ-NH2	6.02	124.61	119.20
5	f	688	ARG	NE-CZ-NH1	-6.01	115.49	121.50
5	f	1026	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	J	36	ASP	CA-CB-CG	-5.99	106.61	112.60
5	d	804	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	184	ARG	NE-CZ-NH2	5.98	124.58	119.20
7	U	361	ASP	CA-CB-CG	-5.98	106.62	112.60
2	D	155	GLN	OE1-CD-NE2	-5.98	116.62	122.60
5	H	88	ARG	NE-CZ-NH2	5.98	124.58	119.20
7	U	200	ARG	NE-CZ-NH2	5.98	124.58	119.20
5	h	850	ASP	CA-CB-CG	5.97	118.58	112.60
7	T	266	ASP	CA-CB-CG	5.96	118.56	112.60
7	S	424	ARG	NE-CZ-NH1	-5.95	115.55	121.50
5	h	272	ARG	NE-CZ-NH2	5.95	124.55	119.20
5	d	773	ARG	NE-CZ-NH2	5.92	124.53	119.20
5	g	753	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	77	ARG	NE-CZ-NH2	5.91	124.52	119.20
5	d	294	ASP	CA-CB-CG	5.91	118.50	112.60
5	f	790	LEU	CB-CA-C	5.90	121.04	109.35
5	e	365	TYR	N-CA-C	5.90	117.22	108.60
5	H	25	PHE	CA-C-N	5.90	128.75	122.26
5	H	25	PHE	C-N-CA	5.90	128.75	122.26
6	M	759	HIS	CA-CB-CG	5.90	119.70	113.80
5	f	1022	PHE	CA-CB-CG	5.90	119.70	113.80
1	A	573	ARG	NE-CZ-NH2	5.90	124.51	119.20
5	f	1102	ARG	NE-CZ-NH2	5.89	124.50	119.20
5	g	521	HIS	CA-CB-CG	-5.89	107.91	113.80
5	h	920	SER	N-CA-C	5.88	115.86	108.45
5	g	406	ARG	NE-CZ-NH2	5.88	124.49	119.20
5	d	429	ARG	NE-CZ-NH2	5.88	124.49	119.20
5	H	753	ARG	NE-CZ-NH2	5.87	124.48	119.20
5	f	469	GLU	CA-C-N	5.87	128.07	120.44
5	f	469	GLU	C-N-CA	5.87	128.07	120.44
7	T	442	GLN	OE1-CD-NE2	-5.86	116.74	122.60
7	S	227	PHE	CA-CB-CG	-5.86	107.94	113.80
5	d	1141	ARG	NE-CZ-NH2	5.86	124.47	119.20
7	U	241	ARG	NE-CZ-NH2	5.85	124.47	119.20
5	f	470	ASP	CA-CB-CG	5.85	118.45	112.60
5	g	1087	ASP	CA-CB-CG	5.85	118.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	356	ASN	CB-CA-C	5.84	121.41	112.00
5	f	783	ARG	NE-CZ-NH2	5.84	124.46	119.20
5	g	560	ARG	NE-CZ-NH2	5.84	124.46	119.20
5	d	26	ASN	CA-C-N	5.84	127.14	119.84
5	d	26	ASN	C-N-CA	5.84	127.14	119.84
7	S	131	ARG	NE-CZ-NH2	5.84	124.45	119.20
2	N	111	GLU	CA-C-N	5.83	135.56	121.68
2	N	111	GLU	C-N-CA	5.83	135.56	121.68
2	D	21	ASP	N-CA-C	5.82	117.71	111.36
5	H	428	MET	N-CA-C	5.82	123.20	110.80
5	d	1143	ARG	NE-CZ-NH2	5.82	124.44	119.20
5	d	528	PHE	CA-CB-CG	5.82	119.62	113.80
5	h	918	PHE	CA-CB-CG	5.82	119.62	113.80
5	g	426	ASN	N-CA-C	5.82	116.26	108.23
2	N	159	ARG	NE-CZ-NH2	5.81	124.43	119.20
5	f	94	ASP	CA-CB-CG	5.81	118.41	112.60
5	g	778	GLN	CA-C-N	5.80	128.33	120.38
5	g	778	GLN	C-N-CA	5.80	128.33	120.38
5	H	1150	ARG	NE-CZ-NH2	5.80	124.42	119.20
5	f	248	ASN	CA-CB-CG	5.80	118.40	112.60
5	h	453	SER	N-CA-C	5.80	123.15	110.80
5	d	521	HIS	CB-CG-CD2	-5.80	123.66	131.20
2	Q	111	GLU	N-CA-C	5.79	118.59	109.39
7	S	424	ARG	NE-CZ-NH2	5.79	124.41	119.20
5	H	560	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	A	256	ASN	OD1-CG-ND2	-5.77	116.83	122.60
2	D	9	HIS	CA-CB-CG	5.77	119.57	113.80
5	g	271	ARG	NE-CZ-NH2	5.77	124.39	119.20
5	d	452	ASP	CA-C-N	5.76	132.54	121.54
5	d	452	ASP	C-N-CA	5.76	132.54	121.54
7	S	83	ARG	NE-CZ-NH2	5.75	124.38	119.20
5	d	778	GLN	CA-C-N	5.75	127.99	120.28
5	d	778	GLN	C-N-CA	5.75	127.99	120.28
5	g	140	ARG	NE-CZ-NH2	5.75	124.38	119.20
3	F	84	PHE	CA-CB-CG	5.74	119.54	113.80
5	h	126	GLN	OE1-CD-NE2	-5.74	116.86	122.60
5	f	283	ARG	NE-CZ-NH2	5.74	124.36	119.20
5	H	1014	ARG	NE-CZ-NH2	5.73	124.36	119.20
5	f	985	ASP	CA-C-N	5.73	132.48	121.54
5	f	985	ASP	C-N-CA	5.73	132.48	121.54
7	U	267	HIS	CB-CG-CD2	-5.72	123.77	131.20
5	h	1019	ARG	NE-CZ-NH2	5.71	124.34	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	773	ARG	NE-CZ-NH2	5.71	124.34	119.20
7	U	131	ARG	NE-CZ-NH2	5.71	124.34	119.20
5	h	1014	ARG	NE-CZ-NH2	5.71	124.33	119.20
5	h	37	ASN	CA-C-N	5.70	127.86	120.44
5	h	37	ASN	C-N-CA	5.70	127.86	120.44
5	H	454	ASP	CA-CB-CG	5.70	118.30	112.60
5	H	364	ASP	CA-CB-CG	5.70	118.30	112.60
7	S	374	HIS	CB-CG-CD2	-5.69	123.80	131.20
5	f	885	ASN	CA-CB-CG	5.69	118.29	112.60
5	g	804	ARG	NE-CZ-NH2	5.68	124.31	119.20
2	O	21	ASP	CA-CB-CG	-5.68	106.92	112.60
5	e	184	ARG	NE-CZ-NH2	5.67	124.30	119.20
8	b	418	ARG	NE-CZ-NH2	5.66	124.30	119.20
5	h	498	GLN	OE1-CD-NE2	-5.66	116.94	122.60
2	L	82	ASN	CA-CB-CG	5.66	118.26	112.60
8	b	129	HIS	CA-CB-CG	-5.66	108.14	113.80
5	d	272	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	J	560	ARG	NE-CZ-NH2	5.66	124.29	119.20
5	d	833	GLN	OE1-CD-NE2	-5.66	116.94	122.60
2	R	146	GLY	N-CA-C	5.66	119.17	112.33
2	N	9	HIS	CB-CG-CD2	-5.66	123.85	131.20
5	d	523	ASP	CA-CB-CG	5.66	118.26	112.60
2	Q	111	GLU	CA-C-N	5.65	132.42	122.08
2	Q	111	GLU	C-N-CA	5.65	132.42	122.08
5	f	799	GLN	OE1-CD-NE2	-5.65	116.95	122.60
5	g	98	ILE	CA-CB-CG1	5.64	119.99	110.40
5	H	1072	PHE	CA-CB-CG	5.63	119.43	113.80
2	Q	136	ASN	CA-CB-CG	5.63	118.23	112.60
5	g	785	ARG	NE-CZ-NH2	5.63	124.27	119.20
5	f	603	ASN	OD1-CG-ND2	-5.62	116.97	122.60
5	h	408	ASP	CA-CB-CG	5.62	118.22	112.60
7	S	266	ASP	CA-CB-CG	5.62	118.22	112.60
2	K	136	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	5	TYR	N-CA-C	5.62	117.99	110.35
2	D	111	GLU	N-CA-C	5.62	118.32	109.39
2	O	111	GLU	CA-C-N	5.62	135.50	121.80
2	O	111	GLU	C-N-CA	5.62	135.50	121.80
5	d	299	ASN	CA-C-N	5.62	128.82	120.17
5	d	299	ASN	C-N-CA	5.62	128.82	120.17
5	g	1108	THR	CA-C-N	5.62	131.02	122.65
5	g	1108	THR	C-N-CA	5.62	131.02	122.65
5	d	809	LEU	CA-C-N	5.61	126.42	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	809	LEU	C-N-CA	5.61	126.42	122.33
1	A	257	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	L	136	ASN	OD1-CG-ND2	-5.61	116.99	122.60
5	d	178	ASN	CA-CB-CG	-5.61	106.99	112.60
5	H	271	ARG	NE-CZ-NH1	-5.61	115.89	121.50
5	f	69	SER	CA-C-N	5.61	128.35	120.28
5	f	69	SER	C-N-CA	5.61	128.35	120.28
5	g	173	GLU	N-CA-C	5.60	118.92	111.30
1	J	230	ARG	NE-CZ-NH2	5.59	124.23	119.20
7	U	424	ARG	NE-CZ-NH2	5.59	124.23	119.20
5	g	210	HIS	CA-CB-CG	5.59	119.39	113.80
2	E	111	GLU	CA-C-N	5.58	131.19	122.26
2	E	111	GLU	C-N-CA	5.58	131.19	122.26
5	h	84	ASN	CA-CB-CG	-5.58	107.02	112.60
5	e	1042	PHE	CA-CB-CG	5.57	119.37	113.80
2	K	111	GLU	CA-C-N	5.56	135.38	121.80
2	K	111	GLU	C-N-CA	5.56	135.38	121.80
8	b	341	GLU	CB-CG-CD	-5.56	103.14	112.60
5	d	13	ARG	NE-CZ-NH2	5.56	124.21	119.20
5	e	995	GLN	OE1-CD-NE2	-5.56	117.04	122.60
7	U	32	ARG	NE-CZ-NH2	5.56	124.20	119.20
5	f	13	ARG	NE-CZ-NH2	5.56	124.20	119.20
5	g	477	ARG	NE-CZ-NH2	5.55	124.20	119.20
5	e	1128	ARG	CD-NE-CZ	5.55	132.17	124.40
5	H	1022	PHE	CA-CB-CG	5.54	119.34	113.80
5	H	556	HIS	CB-CG-CD2	-5.54	124.00	131.20
5	e	262	LEU	CA-C-N	5.54	128.15	120.29
5	e	262	LEU	C-N-CA	5.54	128.15	120.29
5	h	29	ARG	NE-CZ-NH2	5.53	124.18	119.20
5	e	172	ALA	CA-C-N	5.52	132.08	121.54
5	e	172	ALA	C-N-CA	5.52	132.08	121.54
5	h	920	SER	CA-C-N	5.52	129.44	120.23
5	h	920	SER	C-N-CA	5.52	129.44	120.23
5	H	322	GLN	OE1-CD-NE2	-5.51	117.08	122.60
1	B	565	ASN	OD1-CG-ND2	-5.51	117.09	122.60
5	d	295	PHE	CA-CB-CG	5.51	119.31	113.80
5	e	4	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	J	476	ASP	CB-CA-C	5.50	115.39	110.44
5	H	521	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	B	628	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	J	184	ARG	NE-CZ-NH2	5.47	124.13	119.20
2	P	111	GLU	CB-CG-CD	5.47	121.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	247	GLU	CA-C-N	5.47	132.00	121.54
5	f	247	GLU	C-N-CA	5.47	132.00	121.54
2	E	136	ASN	CA-CB-CG	5.47	118.07	112.60
2	O	136	ASN	OD1-CG-ND2	-5.47	117.13	122.60
5	f	429	ARG	NE-CZ-NH2	5.47	124.12	119.20
5	e	1143	ARG	NE-CZ-NH2	5.46	124.12	119.20
6	M	784	ASN	CA-CB-CG	-5.46	107.14	112.60
2	K	151	PHE	N-CA-C	5.46	116.56	108.60
5	e	1141	ARG	NE-CZ-NH2	5.45	124.11	119.20
3	F	52	ARG	NE-CZ-NH2	5.45	124.11	119.20
2	R	103	LEU	N-CA-CB	-5.45	101.36	110.57
1	A	6	THR	CA-C-N	5.45	126.65	119.84
1	A	6	THR	C-N-CA	5.45	126.65	119.84
5	d	461	PHE	CA-CB-CG	5.45	119.25	113.80
5	H	532	ASP	CA-CB-CG	5.44	118.04	112.60
2	K	169	PHE	CA-CB-CG	5.44	119.24	113.80
8	b	662	PRO	N-CA-CB	5.44	106.05	103.22
5	f	727	ASP	CA-CB-CG	-5.44	107.16	112.60
5	h	602	ASP	N-CA-C	5.43	117.34	108.76
1	B	490	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	79	ASP	CA-CB-CG	5.42	118.03	112.60
1	J	389	ARG	NE-CZ-NH1	-5.42	116.08	121.50
5	e	32	GLN	OE1-CD-NE2	-5.41	117.19	122.60
5	h	867	ASP	CA-CB-CG	5.41	118.01	112.60
2	N	116	THR	CA-CB-OG1	5.40	117.71	109.60
2	P	136	ASN	OD1-CG-ND2	-5.40	117.20	122.60
5	g	850	ASP	CA-CB-CG	5.40	118.00	112.60
5	h	1139	ARG	NE-CZ-NH2	5.40	124.06	119.20
7	S	447	GLN	OE1-CD-NE2	-5.40	117.20	122.60
2	K	168	ARG	NE-CZ-NH2	5.39	124.05	119.20
5	h	406	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	I	21	ASP	CA-CB-CG	-5.39	107.21	112.60
3	F	58	ILE	CA-C-N	5.38	129.26	122.16
3	F	58	ILE	C-N-CA	5.38	129.26	122.16
5	d	372	GLU	N-CA-C	5.38	117.56	109.23
5	h	1102	ARG	NE-CZ-NH2	5.37	124.04	119.20
2	R	101	VAL	CB-CA-C	5.37	118.14	110.84
5	e	804	ARG	NE-CZ-NH2	5.37	124.03	119.20
5	f	178	ASN	CA-CB-CG	-5.37	107.23	112.60
1	B	257	ARG	NE-CZ-NH2	5.36	124.03	119.20
5	h	833	GLN	OE1-CD-NE2	-5.36	117.24	122.60
5	d	603	ASN	CB-CG-ND2	5.36	124.44	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	J	312	ARG	NE-CZ-NH2	5.36	124.02	119.20
5	h	993	PHE	CA-C-N	5.36	127.77	120.54
5	h	993	PHE	C-N-CA	5.36	127.77	120.54
7	T	36	ASP	CA-CB-CG	5.36	117.95	112.60
8	b	624	ARG	CA-C-N	5.35	128.31	120.71
8	b	624	ARG	C-N-CA	5.35	128.31	120.71
5	f	37	ASN	CA-C-N	5.35	127.72	120.44
5	f	37	ASN	C-N-CA	5.35	127.72	120.44
5	h	327	ARG	NE-CZ-NH2	5.35	124.02	119.20
5	H	587	ASN	OD1-CG-ND2	-5.35	117.25	122.60
7	S	442	GLN	OE1-CD-NE2	-5.34	117.26	122.60
3	F	50	TYR	CB-CA-C	5.34	120.26	110.11
2	L	50	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	B	244	ASP	CA-CB-CG	5.33	117.93	112.60
1	J	452	GLN	OE1-CD-NE2	-5.33	117.27	122.60
5	H	403	TYR	N-CA-C	5.33	117.17	109.07
5	h	603	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	J	14	LEU	CA-C-N	5.32	127.67	120.38
1	J	14	LEU	C-N-CA	5.32	127.67	120.38
1	J	352	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	579	ASN	OD1-CG-ND2	-5.31	117.29	122.60
2	Q	101	VAL	CB-CA-C	5.31	118.31	110.77
5	e	342	GLU	N-CA-C	5.31	114.41	108.25
7	T	35	PHE	CA-CB-CG	5.31	119.11	113.80
2	P	21	ASP	CA-CB-CG	-5.30	107.30	112.60
5	h	560	ARG	CD-NE-CZ	5.30	131.82	124.40
1	B	184	ARG	NE-CZ-NH2	5.30	123.97	119.20
5	f	801	ASP	CA-CB-CG	5.30	117.90	112.60
5	H	300	THR	CA-C-N	5.29	128.22	120.71
5	H	300	THR	C-N-CA	5.29	128.22	120.71
5	H	985	ASP	CA-C-N	5.29	130.83	120.99
5	H	985	ASP	C-N-CA	5.29	130.83	120.99
8	b	129	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	J	277	LYS	CG-CD-CE	5.28	123.44	111.30
7	T	131	ARG	NE-CZ-NH2	5.28	123.95	119.20
5	g	785	ARG	NE-CZ-NH1	-5.28	116.22	121.50
2	O	32	PRO	N-CA-C	5.28	119.50	111.11
5	f	783	ARG	CA-C-N	5.28	128.84	121.24
5	f	783	ARG	C-N-CA	5.28	128.84	121.24
5	g	360	GLU	CA-C-N	5.27	129.12	120.63
5	g	360	GLU	C-N-CA	5.27	129.12	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	401	THR	CA-C-N	5.27	129.41	120.81
5	d	401	THR	C-N-CA	5.27	129.41	120.81
5	f	552	ASP	CA-CB-CG	5.27	117.87	112.60
1	J	447	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	L	155	GLN	OE1-CD-NE2	-5.26	117.34	122.60
5	h	29	ARG	NE-CZ-NH1	-5.26	116.24	121.50
7	U	320	ASN	OD1-CG-ND2	-5.26	117.34	122.60
8	b	334	GLN	OE1-CD-NE2	-5.25	117.34	122.60
5	H	1090	THR	CA-CB-OG1	5.25	117.48	109.60
5	f	40	GLN	CB-CG-CD	-5.25	103.68	112.60
5	g	570	ARG	CA-C-N	5.24	127.31	120.28
5	g	570	ARG	C-N-CA	5.24	127.31	120.28
5	f	793	PRO	CA-N-CD	-5.24	104.67	112.00
5	h	29	ARG	N-CA-CB	-5.24	103.75	109.72
5	H	367	VAL	CA-CB-CG2	5.24	119.30	110.40
1	B	42	GLN	OE1-CD-NE2	-5.23	117.37	122.60
5	H	521	HIS	CA-CB-CG	-5.23	108.57	113.80
5	f	531	GLU	CA-C-N	5.23	129.44	120.71
5	f	531	GLU	C-N-CA	5.23	129.44	120.71
5	e	1137	PHE	CA-CB-CG	5.23	119.03	113.80
5	h	168	GLN	OE1-CD-NE2	-5.23	117.37	122.60
5	h	293	GLN	OE1-CD-NE2	-5.23	117.37	122.60
5	H	936	PHE	CA-C-N	5.22	126.14	122.33
5	H	936	PHE	C-N-CA	5.22	126.14	122.33
1	J	5	TYR	N-CA-C	5.22	117.86	110.50
5	h	862	ARG	NE-CZ-NH2	5.22	123.90	119.20
5	H	930	GLN	OE1-CD-NE2	-5.22	117.38	122.60
5	g	29	ARG	CB-CG-CD	5.22	123.31	111.30
5	e	1036	ASP	CA-CB-CG	-5.22	107.38	112.60
2	L	71	GLU	CB-CG-CD	-5.22	103.73	112.60
2	D	41	GLN	OE1-CD-NE2	-5.21	117.39	122.60
5	h	772	GLY	CA-C-N	5.21	131.50	121.54
5	h	772	GLY	C-N-CA	5.21	131.50	121.54
5	h	465	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	B	79	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	386	ASN	OD1-CG-ND2	-5.20	117.40	122.60
5	d	587	ASN	CA-CB-CG	5.20	117.80	112.60
5	g	248	ASN	CA-CB-CG	5.20	117.80	112.60
5	H	26	ASN	N-CA-CB	-5.19	102.90	111.78
5	h	453	SER	CA-C-N	5.19	130.54	122.49
5	h	453	SER	C-N-CA	5.19	130.54	122.49
5	h	712	ARG	NE-CZ-NH2	5.19	123.87	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	477	ARG	NE-CZ-NH2	5.18	123.86	119.20
5	f	920	SER	N-CA-C	5.18	116.86	109.14
1	B	447	HIS	CB-CG-CD2	-5.18	124.47	131.20
5	h	539	TYR	CA-CB-CG	5.18	123.22	113.90
5	g	29	ARG	N-CA-C	5.17	118.15	110.39
5	d	84	ASN	CA-CB-CG	-5.17	107.43	112.60
7	S	200	ARG	NE-CZ-NH2	5.17	123.85	119.20
5	d	422	PRO	CA-C-N	5.17	126.67	121.35
5	d	422	PRO	C-N-CA	5.17	126.67	121.35
5	h	1143	ARG	NE-CZ-NH1	-5.17	116.33	121.50
7	T	347	GLN	OE1-CD-NE2	-5.16	117.44	122.60
5	g	358	ARG	NE-CZ-NH2	5.16	123.84	119.20
5	H	450	LEU	CB-CA-C	5.16	120.33	110.17
5	e	688	ARG	NE-CZ-NH2	5.16	123.84	119.20
5	e	712	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	O	31	THR	CA-C-N	5.16	125.15	119.89
2	O	31	THR	C-N-CA	5.16	125.15	119.89
5	f	1141	ARG	NE-CZ-NH2	5.16	123.84	119.20
5	e	785	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	A	490	ASP	CA-CB-CG	5.15	117.75	112.60
2	P	71	GLU	CB-CG-CD	-5.15	103.85	112.60
5	d	956	ASP	CB-CA-C	5.15	118.63	111.63
5	d	917	LEU	N-CA-CB	-5.15	102.47	110.29
8	b	505	PRO	N-CA-CB	5.14	107.82	103.35
2	c	168	ARG	NE-CZ-NH2	5.14	123.83	119.20
5	h	588	ILE	CA-C-N	5.14	126.27	119.84
5	h	588	ILE	C-N-CA	5.14	126.27	119.84
5	g	1143	ARG	NE-CZ-NH1	-5.13	116.36	121.50
5	h	372	GLU	N-CA-C	5.13	116.99	109.24
5	h	429	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	6	THR	CA-C-N	5.13	125.13	119.89
1	B	6	THR	C-N-CA	5.13	125.13	119.89
2	N	111	GLU	CB-CG-CD	5.13	121.32	112.60
7	S	11	ASN	OD1-CG-ND2	-5.13	117.47	122.60
7	S	15	ARG	NE-CZ-NH2	5.12	123.81	119.20
5	d	516	LYS	CA-C-N	5.12	127.98	120.71
5	d	516	LYS	C-N-CA	5.12	127.98	120.71
2	E	162	GLN	OE1-CD-NE2	-5.12	117.48	122.60
5	H	234	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	L	93	ALA	CA-C-N	5.12	127.45	120.54
2	L	93	ALA	C-N-CA	5.12	127.45	120.54
8	b	374	GLN	OE1-CD-NE2	-5.12	117.48	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	ASN	CA-CB-CG	5.11	117.71	112.60
6	M	683	HIS	CA-CB-CG	5.11	118.91	113.80
5	d	477	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
5	d	850	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	277	LYS	CB-CG-CD	-5.10	99.57	111.30
5	f	1042	PHE	CA-CB-CG	5.10	118.90	113.80
5	g	768	TYR	N-CA-C	-5.10	102.94	110.48
5	e	570	ARG	NE-CZ-NH2	5.09	123.78	119.20
5	H	504	ARG	NE-CZ-NH2	5.09	123.78	119.20
5	H	283	ARG	NE-CZ-NH2	5.08	123.78	119.20
5	f	113	ARG	NE-CZ-NH2	5.08	123.77	119.20
5	h	521	HIS	CB-CG-CD2	-5.08	124.60	131.20
2	D	65	ARG	NE-CZ-NH2	5.07	123.77	119.20
5	e	395	VAL	N-CA-C	5.07	115.88	108.58
5	f	26	ASN	CA-C-N	5.06	124.67	119.05
5	f	26	ASN	C-N-CA	5.06	124.67	119.05
5	e	33	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	54	ASP	CA-CB-CG	5.06	117.66	112.60
2	D	146	GLY	N-CA-C	5.06	120.70	112.61
2	P	151	PHE	N-CA-C	5.06	115.21	108.38
5	f	259	SER	N-CA-C	5.06	115.98	108.60
5	e	382	PHE	CB-CA-C	5.05	119.00	111.88
5	h	28	ASP	CA-CB-CG	5.05	117.65	112.60
5	e	914	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	K	155	GLN	OE1-CD-NE2	-5.05	117.55	122.60
5	e	587	ASN	OD1-CG-ND2	-5.05	117.55	122.60
5	f	88	ARG	NE-CZ-NH2	5.04	123.74	119.20
5	d	916	VAL	CA-C-N	5.04	129.76	121.39
5	d	916	VAL	C-N-CA	5.04	129.76	121.39
5	f	171	ASN	OD1-CG-ND2	-5.04	117.56	122.60
2	Q	146	GLY	N-CA-C	5.04	119.03	112.68
8	b	304	THR	N-CA-C	5.04	117.61	110.10
7	T	22	ASN	OD1-CG-ND2	-5.04	117.56	122.60
5	g	749	ARG	NE-CZ-NH2	5.04	123.73	119.20
5	h	956	ASP	CB-CA-C	5.04	119.56	111.66
6	M	725	GLY	CA-C-N	5.03	125.57	119.98
6	M	725	GLY	C-N-CA	5.03	125.57	119.98
5	d	761	ASN	CA-CB-CG	5.03	117.63	112.60
5	H	172	ALA	CA-C-N	5.03	129.26	122.07
5	H	172	ALA	C-N-CA	5.03	129.26	122.07
3	F	113	GLN	OE1-CD-NE2	-5.02	117.58	122.60
5	h	895	ARG	NE-CZ-NH2	5.02	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	21	ASP	CA-CB-CG	-5.02	107.58	112.60
1	J	234	ARG	NE-CZ-NH2	5.02	123.72	119.20
8	b	332	ARG	NE-CZ-NH2	5.01	123.71	119.20
5	d	1019	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	J	369	LEU	O-C-N	-5.01	119.22	121.53
7	T	32	ARG	NE-CZ-NH2	5.01	123.71	119.20
5	g	37	ASN	OD1-CG-ND2	-5.01	117.59	122.60
6	M	747	GLN	OE1-CD-NE2	-5.01	117.59	122.60
2	c	65	ARG	NE-CZ-NH2	5.01	123.70	119.20
5	d	20	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	411	SER	N-CA-C	5.00	116.19	109.83
5	H	289	GLN	OE1-CD-NE2	-5.00	117.59	122.60
1	B	442	VAL	CA-C-N	5.00	125.47	120.52
1	B	442	VAL	C-N-CA	5.00	125.47	120.52
5	g	570	ARG	NE-CZ-NH2	5.00	123.70	119.20
6	M	789	ARG	NE-CZ-NH2	5.00	123.70	119.20
5	e	151	ASP	CA-C-N	5.00	125.93	120.83
5	e	151	ASP	C-N-CA	5.00	125.93	120.83

There are no chirality outliers.

All (247) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	TYR	Sidechain
1	A	18	TYR	Sidechain
1	A	208	TYR	Sidechain
1	A	250	TYR	Sidechain
1	A	389	ARG	Sidechain
1	A	391	TYR	Sidechain
1	A	472	TYR	Sidechain
1	A	5	TYR	Sidechain
1	A	500	TYR	Sidechain
1	A	541	TYR	Sidechain
1	A	548	TYR	Sidechain
1	A	93	TYR	Sidechain
1	B	18	TYR	Sidechain
1	B	203	TYR	Sidechain
1	B	250	TYR	Sidechain
1	B	296	TYR	Sidechain
1	B	417	TYR	Sidechain
1	B	420	TYR	Sidechain
1	B	483	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	B	541	TYR	Sidechain
1	B	592	TYR	Sidechain
1	B	81	ARG	Sidechain
1	B	89	TYR	Sidechain
2	D	15	TYR	Sidechain
2	D	80	TYR	Sidechain
3	F	128	TYR	Sidechain
3	F	136	TYR	Sidechain
3	F	22	ASP	Sidechain
3	F	50	TYR	Sidechain
3	F	76	TYR	Sidechain
4	G	31	TYR	Sidechain
4	G	42	ARG	Sidechain
4	G	48	TYR	Sidechain
4	G	55	TYR	Sidechain
4	G	58	TYR	Sidechain
4	G	73	TYR	Sidechain
5	H	1062	TYR	Sidechain
5	H	1109	ARG	Sidechain
5	H	1150	ARG	Sidechain
5	H	13	ARG	Sidechain
5	H	166	TYR	Sidechain
5	H	184	ARG	Sidechain
5	H	186	TYR	Sidechain
5	H	29	ARG	Sidechain
5	H	400	TYR	Sidechain
5	H	402	TYR	Sidechain
5	H	403	TYR	Sidechain
5	H	429	ARG	Sidechain
5	H	705	TYR	Sidechain
5	H	800	TYR	Sidechain
5	H	804	ARG	Sidechain
5	H	895	ARG	Sidechain
5	H	973	ARG	Sidechain
2	I	6	TYR	Sidechain
2	I	65	ARG	Sidechain
1	J	203	TYR	Sidechain
1	J	208	TYR	Sidechain
1	J	236	ARG	Sidechain
1	J	250	TYR	Sidechain
1	J	290	TYR	Sidechain
1	J	296	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	J	307	TYR	Sidechain
1	J	311	ARG	Sidechain
1	J	367	TYR	Sidechain
1	J	478	TYR	Sidechain
1	J	500	TYR	Sidechain
1	J	541	TYR	Sidechain
1	J	573	ARG	Sidechain
1	J	59	TYR	Sidechain
1	J	592	TYR	Sidechain
1	J	86	TYR	Sidechain
2	L	117	TYR	Sidechain
2	L	118	ARG	Sidechain
6	M	695	TYR	Sidechain
6	M	702	TYR	Sidechain
6	M	704	TYR	Sidechain
6	M	707	ARG	Sidechain
6	M	736	ARG	Sidechain
6	M	757	TYR	Sidechain
6	M	768	ASP	Sidechain
6	M	789	ARG	Sidechain
2	N	9	HIS	Sidechain
2	O	80	TYR	Sidechain
2	Q	15	TYR	Sidechain
2	R	15	TYR	Sidechain
2	R	156	PHE	Sidechain
2	R	65	ARG	Sidechain
7	S	227	PHE	Sidechain
7	S	270	ARG	Sidechain
7	S	294	ARG	Sidechain
7	S	365	TYR	Sidechain
7	S	371	TYR	Sidechain
7	S	394	TYR	Sidechain
7	S	412	ARG	Sidechain
7	S	424	ARG	Sidechain
7	S	79	TYR	Sidechain
7	S	91	ARG	Sidechain
7	T	220	TYR	Sidechain
7	T	235	TYR	Sidechain
7	T	311	TYR	Sidechain
7	T	365	TYR	Sidechain
7	T	371	TYR	Sidechain
7	T	394	TYR	Sidechain

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Mol	Chain	Res	Type	Group
7	T	401	TYR	Sidechain
7	T	423	TYR	Sidechain
7	T	70	ARG	Sidechain
7	U	115	HIS	Sidechain
7	U	220	TYR	Sidechain
7	U	267	HIS	Sidechain
7	U	279	TYR	Sidechain
7	U	365	TYR	Sidechain
7	U	70	ARG	Sidechain
7	U	91	ARG	Sidechain
2	V	125	ASP	Sidechain
8	b	108	ARG	Sidechain
8	b	176	TYR	Sidechain
8	b	200	TYR	Sidechain
8	b	256	TYR	Sidechain
8	b	325	ARG	Sidechain
8	b	349	TYR	Sidechain
8	b	357	TYR	Sidechain
8	b	358	TYR	Sidechain
8	b	404	TYR	Sidechain
8	b	407	ASP	Sidechain
8	b	443	TYR	Sidechain
8	b	500	TYR	Sidechain
8	b	608	TYR	Sidechain
8	b	726	TYR	Sidechain
2	c	168	ARG	Sidechain
5	d	1062	TYR	Sidechain
5	d	1066	ARG	Sidechain
5	d	113	ARG	Sidechain
5	d	1150	ARG	Sidechain
5	d	13	ARG	Sidechain
5	d	133	TYR	Sidechain
5	d	166	TYR	Sidechain
5	d	186	TYR	Sidechain
5	d	221	TYR	Sidechain
5	d	29	ARG	Sidechain
5	d	320	TYR	Sidechain
5	d	358	ARG	Sidechain
5	d	400	TYR	Sidechain
5	d	403	TYR	Sidechain
5	d	530	PHE	Sidechain
5	d	586	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	d	712	ARG	Sidechain
5	d	721	TYR	Sidechain
5	d	768	TYR	Sidechain
5	d	773	ARG	Sidechain
5	d	785	ARG	Sidechain
5	d	862	ARG	Sidechain
5	d	895	ARG	Sidechain
5	d	968	TYR	Sidechain
5	d	973	ARG	Sidechain
5	e	1027	TYR	Sidechain
5	e	1062	TYR	Sidechain
5	e	1109	ARG	Sidechain
5	e	14	PHE	Sidechain
5	e	158	TYR	Sidechain
5	e	166	TYR	Sidechain
5	e	192	TYR	Sidechain
5	e	272	ARG	Sidechain
5	e	286	ARG	Sidechain
5	e	29	ARG	Sidechain
5	e	320	TYR	Sidechain
5	e	353	TYR	Sidechain
5	e	355	TYR	Sidechain
5	e	365	TYR	Sidechain
5	e	400	TYR	Sidechain
5	e	403	TYR	Sidechain
5	e	573	TYR	Sidechain
5	e	712	ARG	Sidechain
5	e	80	TYR	Sidechain
5	e	804	ARG	Sidechain
5	e	835	TYR	Sidechain
5	e	865	PHE	Sidechain
5	e	90	TYR	Sidechain
5	f	1004	TYR	Sidechain
5	f	1062	TYR	Sidechain
5	f	1066	ARG	Sidechain
5	f	1083	TYR	Sidechain
5	f	1109	ARG	Sidechain
5	f	13	ARG	Sidechain
5	f	133	TYR	Sidechain
5	f	166	TYR	Sidechain
5	f	184	ARG	Sidechain
5	f	221	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	f	29	ARG	Sidechain
5	f	349	TYR	Sidechain
5	f	403	TYR	Sidechain
5	f	483	TYR	Sidechain
5	f	539	TYR	Sidechain
5	f	556	HIS	Sidechain
5	f	570	ARG	Sidechain
5	f	753	ARG	Sidechain
5	f	862	ARG	Sidechain
5	f	88	ARG	Sidechain
5	f	888	TYR	Sidechain
5	g	1027	TYR	Sidechain
5	g	1062	TYR	Sidechain
5	g	113	ARG	Sidechain
5	g	1139	ARG	Sidechain
5	g	1143	ARG	Sidechain
5	g	166	TYR	Sidechain
5	g	221	TYR	Sidechain
5	g	286	ARG	Sidechain
5	g	29	ARG	Sidechain
5	g	353	TYR	Sidechain
5	g	365	TYR	Sidechain
5	g	403	TYR	Sidechain
5	g	712	ARG	Sidechain
5	g	749	ARG	Sidechain
5	g	804	ARG	Sidechain
5	g	82	TYR	Sidechain
5	g	835	TYR	Sidechain
5	g	841	TYR	Sidechain
5	g	90	TYR	Sidechain
5	h	1050	TYR	Sidechain
5	h	1062	TYR	Sidechain
5	h	1069	TYR	Sidechain
5	h	1083	TYR	Sidechain
5	h	1109	ARG	Sidechain
5	h	1150	ARG	Sidechain
5	h	13	ARG	Sidechain
5	h	166	TYR	Sidechain
5	h	186	TYR	Sidechain
5	h	192	TYR	Sidechain
5	h	221	TYR	Sidechain
5	h	289	GLN	Peptide

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Mol	Chain	Res	Type	Group
5	h	29	ARG	Sidechain
5	h	358	ARG	Sidechain
5	h	403	TYR	Sidechain
5	h	415	TYR	Sidechain
5	h	429	ARG	Sidechain
5	h	46	TYR	Sidechain
5	h	465	ARG	Sidechain
5	h	539	TYR	Sidechain
5	h	556	HIS	Sidechain
5	h	560	ARG	Sidechain
5	h	712	ARG	Sidechain
5	h	749	ARG	Sidechain
5	h	80	TYR	Sidechain
5	h	862	ARG	Sidechain
5	h	864	TYR	Sidechain
5	h	895	ARG	Sidechain
5	h	90	TYR	Sidechain
5	h	968	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5127	0	4969	16	0
1	B	5127	0	4969	16	0
1	J	5127	0	4969	17	0
2	D	1349	0	1339	8	0
2	E	1349	0	1339	5	0
2	I	1277	0	1274	6	0
2	K	1349	0	1339	7	0
2	L	1349	0	1339	6	0
2	N	1349	0	1339	6	0
2	O	1349	0	1339	8	0
2	P	1349	0	1339	5	0
2	Q	1349	0	1339	7	0
2	R	1349	0	1339	8	0
2	V	1266	0	1259	3	0
2	c	1272	0	1264	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1157	0	1111	14	0
4	G	597	0	570	3	0
5	H	8390	0	8229	61	0
5	d	8390	0	8229	49	0
5	e	8390	0	8229	55	0
5	f	8390	0	8229	52	0
5	g	8390	0	8229	39	0
5	h	8390	0	8229	43	0
6	M	1064	0	1039	14	0
7	S	3548	0	3468	12	0
7	T	3548	0	3468	10	0
7	U	3548	0	3468	7	0
8	b	5070	0	4932	12	0
All	All	100209	0	98185	452	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 2.

All (452) 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)
7:S:424:ARG:NH1	7:T:380:THR:HG21	2.01	0.75
3:F:53:PRO:HB3	6:M:782:THR:HG23	1.70	0.71
5:d:33:GLN:HE21	5:e:27:PRO:HA	1.57	0.70
2:I:12:LEU:HD21	2:V:12:LEU:HD22	1.76	0.68
2:N:116:THR:HG22	2:N:158:ASN:HA	1.76	0.68
6:M:696:LYS:HE3	5:d:903:PRO:HD2	1.77	0.67
5:f:186:TYR:CD1	5:f:223:LYS:HE2	2.31	0.66
5:g:469:GLU:CD	5:g:469:GLU:H	2.02	0.66
7:S:424:ARG:HH12	7:T:380:THR:HG21	1.60	0.66
4:G:55:TYR:HB2	1:J:626:LYS:HE3	1.78	0.66
2:c:108:VAL:HA	2:c:164:THR:HG22	1.80	0.64
6:M:763:VAL:HA	6:M:775:ILE:HG22	1.80	0.62
5:d:981:LYS:HA	5:d:981:LYS:CE	2.30	0.61
5:H:582:ASN:HA	5:H:889:THR:HG22	1.83	0.61
5:h:103:LYS:HE3	5:h:161:MET:SD	2.42	0.60
1:B:131:LYS:HZ3	1:B:395:TRP:CD1	2.20	0.60
5:d:981:LYS:HA	5:d:981:LYS:HE2	1.84	0.60
2:E:91:GLU:H	2:E:91:GLU:CD	2.10	0.59
3:F:51:ILE:HB	6:M:781:ALA:O	2.03	0.59
6:M:683:HIS:CD2	6:M:706:ARG:HH22	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:PHE:CE1	2:Q:158:ASN:ND2	2.70	0.58
5:d:277:VAL:HG12	5:d:278:LEU:H	1.68	0.58
5:H:355:TYR:CE2	5:H:357:LYS:HA	2.38	0.58
5:h:1070:GLU:CD	5:h:1103:ALA:HB1	2.29	0.58
5:H:981:LYS:HE3	5:H:998:TRP:CE2	2.38	0.58
2:P:113:PRO:HB3	8:b:705:ILE:O	2.03	0.58
5:d:1078:LYS:HE2	5:d:1080:VAL:HG22	1.86	0.58
5:f:68:LEU:HD11	5:f:72:ASN:HA	1.86	0.58
5:e:147:LEU:HD23	5:e:148:THR:N	2.18	0.58
7:T:32:ARG:HH11	7:T:36:ASP:HB3	1.70	0.57
2:R:75:LYS:HE2	2:R:86:VAL:HG22	1.87	0.56
5:H:475:LYS:C	5:H:475:LYS:HE3	2.30	0.56
5:h:998:TRP:CG	5:h:1019:ARG:HH12	2.24	0.56
2:K:77:LEU:HD13	2:L:38:ASN:ND2	2.21	0.55
5:f:981:LYS:HE3	5:f:998:TRP:CE2	2.40	0.55
5:g:511:PHE:CD2	5:g:1143:ARG:HA	2.42	0.55
5:H:186:TYR:CD1	5:H:223:LYS:HE2	2.41	0.55
5:d:812:TYR:CE1	5:d:935:LYS:HE2	2.41	0.55
5:H:299:ASN:HA	5:H:332:GLN:HB3	1.89	0.55
5:h:1072:PHE:HB2	5:h:1107:PHE:CD1	2.42	0.55
7:U:83:ARG:CD	7:U:83:ARG:H	2.19	0.54
5:h:981:LYS:HE2	5:h:981:LYS:HA	1.87	0.54
1:A:206:THR:HA	1:J:431:ASN:CG	2.32	0.54
5:H:593:GLY:CA	5:H:697:LEU:HD21	2.38	0.54
6:M:706:ARG:HH11	6:M:778:HIS:CG	2.25	0.54
5:f:281:LYS:HE2	5:f:350:TYR:CD1	2.43	0.54
5:H:593:GLY:HA3	5:H:697:LEU:HD21	1.90	0.53
5:f:365:TYR:CD1	5:f:380:ILE:HG23	2.43	0.53
5:f:33:GLN:NE2	5:h:27:PRO:HA	2.24	0.53
5:f:1078:LYS:HE2	5:f:1078:LYS:HA	1.90	0.53
5:H:268:LYS:HB2	5:H:403:TYR:CZ	2.44	0.53
5:h:857:ALA:HB2	5:h:891:TRP:CD2	2.44	0.53
5:h:981:LYS:HA	5:h:981:LYS:CE	2.38	0.53
5:H:833:GLN:CD	5:H:833:GLN:H	2.17	0.53
5:g:912:TYR:CZ	5:g:914:GLN:HB2	2.44	0.53
2:D:134:LYS:HE2	2:D:136:ASN:O	2.09	0.52
1:B:622:SER:HB3	1:B:628:ARG:CZ	2.39	0.52
5:d:365:TYR:CG	5:d:380:ILE:HG23	2.45	0.52
5:d:468:MET:HE1	5:e:192:TYR:CE2	2.44	0.52
2:K:74:ASN:HA	2:L:35:ASN:HD22	1.74	0.52
5:e:751:GLY:HA3	5:e:753:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:55:TYR:CB	1:J:626:LYS:HE3	2.39	0.52
5:f:274:THR:O	5:f:396:VAL:HG13	2.10	0.52
5:d:336:TRP:C	5:d:338:PRO:HD2	2.35	0.52
5:e:1078:LYS:HE2	5:e:1080:VAL:HG22	1.92	0.51
5:H:275:GLY:C	5:H:356:ASN:HA	2.36	0.51
2:I:102:TYR:CD1	2:I:168:ARG:HD3	2.45	0.51
5:e:106:ILE:HG23	5:e:147:LEU:HD21	1.92	0.51
5:g:992:THR:H	5:g:995:GLN:NE2	2.09	0.51
2:V:155:GLN:HE21	2:V:155:GLN:HA	1.75	0.51
2:K:74:ASN:HA	2:L:35:ASN:ND2	2.26	0.51
5:H:268:LYS:HA	5:H:268:LYS:HE3	1.92	0.51
5:h:470:ASP:HA	5:h:473:LYS:HE2	1.93	0.51
5:H:186:TYR:CD1	5:H:223:LYS:CE	2.94	0.50
5:H:697:LEU:HD22	5:H:762:SER:HB3	1.92	0.50
2:c:56:LYS:HZ2	2:c:111:GLU:CD	2.19	0.50
5:h:409:SER:HB3	5:h:411:PHE:CE2	2.46	0.50
5:e:382:PHE:HB3	5:e:389:LYS:HE2	1.93	0.50
2:K:77:LEU:HB2	2:L:38:ASN:OD1	2.11	0.50
2:K:91:GLU:CD	2:K:91:GLU:H	2.19	0.50
2:R:153:ASN:O	2:R:154:LYS:HE3	2.12	0.50
1:B:476:ASP:O	1:B:480:ALA:HB3	2.12	0.50
5:H:1078:LYS:HA	5:H:1078:LYS:HE2	1.93	0.50
1:J:476:ASP:O	1:J:480:ALA:HB3	2.12	0.50
5:h:872:GLU:CD	5:h:875:LYS:HZ2	2.20	0.50
8:b:200:TYR:CE1	2:c:164:THR:HG23	2.46	0.50
5:f:436:ASN:HD21	5:f:438:ASP:HB3	1.77	0.50
5:f:603:ASN:CG	5:f:771:GLN:H	2.20	0.50
2:K:75:LYS:HE2	2:K:86:VAL:HG21	1.94	0.50
5:g:588:ILE:HG13	5:g:792:ASP:H	1.76	0.50
5:h:470:ASP:HA	5:h:473:LYS:CE	2.42	0.50
2:D:2:ALA:HA	2:R:151:PHE:O	2.12	0.49
7:U:225:LYS:HE3	7:U:226:GLU:O	2.12	0.49
5:d:981:LYS:HE3	5:d:997:LYS:O	2.12	0.49
2:N:91:GLU:CD	2:N:91:GLU:H	2.19	0.49
5:f:927:THR:HG21	5:h:65:GLY:CA	2.42	0.49
5:h:580:THR:HG21	5:h:814:ALA:CB	2.42	0.49
7:S:215:LYS:HZ3	7:T:205:GLU:CD	2.21	0.49
5:f:1112:ILE:HD12	5:f:1112:ILE:H	1.77	0.49
5:d:103:LYS:HE3	5:d:161:MET:SD	2.52	0.49
5:e:1:MET:HA	5:e:112:GLU:OE2	2.12	0.49
5:f:782:ILE:HG22	5:f:784:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:981:LYS:HE3	5:e:998:TRP:CD1	2.48	0.49
5:e:96:VAL:HG11	5:e:147:LEU:HD22	1.94	0.49
3:F:2:ALA:N	3:F:73:ASN:HD22	2.11	0.49
5:e:303:GLU:CD	5:e:354:LYS:HZ3	2.21	0.49
1:A:431:ASN:CG	1:B:206:THR:HA	2.38	0.48
6:M:707:ARG:NE	6:M:714:VAL:H	2.10	0.48
5:e:588:ILE:HD13	5:e:589:PRO:HD2	1.94	0.48
5:g:470:ASP:HA	5:g:473:LYS:HE3	1.95	0.48
5:g:751:GLY:HA3	5:g:753:ARG:HH11	1.78	0.48
5:H:311:THR:HG23	5:H:317:THR:HG21	1.93	0.48
5:H:403:TYR:CG	5:H:452:ASP:HB2	2.48	0.48
5:d:334:ILE:HD12	5:d:334:ILE:H	1.77	0.48
5:d:857:ALA:HB2	5:d:891:TRP:CD2	2.48	0.48
5:e:865:PHE:C	5:e:867:ASP:H	2.21	0.48
5:g:835:TYR:CE2	5:g:926:TRP:HB2	2.48	0.48
5:h:176:LYS:H	5:h:176:LYS:HD2	1.79	0.48
2:c:99:LYS:HE3	2:c:100:TRP:CZ2	2.48	0.48
5:d:1082:LYS:HE2	5:d:1091:TRP:CG	2.48	0.48
5:f:424:GLU:O	5:f:431:VAL:HG23	2.13	0.48
2:D:151:PHE:O	2:R:2:ALA:HA	2.14	0.48
7:U:343:TRP:CG	7:U:434:TRP:HE1	2.32	0.48
5:d:244:GLY:H	5:d:403:TYR:HA	1.78	0.48
5:g:572:ILE:HD12	5:g:800:TYR:CE1	2.49	0.48
5:h:981:LYS:HE3	5:h:997:LYS:C	2.39	0.48
5:H:266:PRO:HG3	5:H:451:PRO:O	2.13	0.48
1:J:431:ASN:CG	1:J:431:ASN:O	2.56	0.48
2:O:107:ILE:HD12	2:O:107:ILE:H	1.78	0.48
2:Q:24:TYR:HB2	2:Q:126:LEU:HD21	1.94	0.48
5:f:756:THR:HG22	5:f:764:SER:O	2.13	0.48
5:f:306:LYS:HE3	5:f:308:TRP:CD2	2.48	0.48
5:h:723:LYS:HE2	5:h:724:GLY:O	2.14	0.48
5:H:773:ARG:HH22	5:H:776:THR:HG23	1.78	0.48
5:e:812:TYR:CE2	5:e:935:LYS:HE2	2.49	0.48
5:g:793:PRO:HG2	5:g:926:TRP:CH2	2.47	0.48
1:A:605:MET:HE2	1:J:579:ASN:OD1	2.14	0.47
7:S:224:LYS:HZ2	7:T:226:GLU:CD	2.21	0.47
5:f:266:PRO:HA	5:f:378:TRP:CZ3	2.49	0.47
5:f:774:LYS:HE3	5:f:1004:TYR:CG	2.49	0.47
5:g:103:LYS:HE3	5:g:161:MET:SD	2.54	0.47
5:H:545:GLN:HE22	5:H:1036:ASP:HA	1.78	0.47
1:J:235:PHE:CE2	1:J:236:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:469:GLU:C	5:e:473:LYS:HE3	2.40	0.47
5:h:846:MET:HA	5:h:846:MET:HE2	1.96	0.47
2:R:75:LYS:HE2	2:R:86:VAL:CG2	2.45	0.47
6:M:706:ARG:HH11	6:M:778:HIS:CD2	2.32	0.47
1:A:476:ASP:O	1:A:480:ALA:HB3	2.15	0.47
2:E:74:ASN:C	2:E:74:ASN:HD22	2.22	0.47
5:H:377:LYS:HE2	5:H:377:LYS:HA	1.97	0.47
6:M:799:LYS:HE3	6:M:799:LYS:HA	1.97	0.47
5:d:603:ASN:HB2	5:d:775:LYS:HE2	1.97	0.47
5:f:1066:ARG:HG2	5:f:1066:ARG:HH21	1.79	0.47
5:g:27:PRO:HA	5:h:33:GLN:NE2	2.30	0.47
5:d:1078:LYS:HE2	5:d:1080:VAL:CG2	2.44	0.47
5:e:587:ASN:ND2	5:e:886:SER:H	2.13	0.47
5:f:600:SER:HA	5:f:768:TYR:CE2	2.50	0.47
2:L:151:PHE:O	2:P:2:ALA:HA	2.15	0.46
8:b:443:TYR:CD2	8:b:443:TYR:C	2.93	0.46
5:g:274:THR:HB	5:g:397:LEU:H	1.80	0.46
5:H:243:LEU:HD23	5:H:403:TYR:CD2	2.50	0.46
5:d:176:LYS:H	5:d:176:LYS:HD2	1.80	0.46
5:e:955:LYS:HZ3	5:e:956:ASP:CG	2.23	0.46
5:h:306:LYS:HE3	5:h:308:TRP:CE3	2.50	0.46
5:H:206:GLU:H	5:H:206:GLU:CD	2.23	0.46
5:e:241:TYR:HA	5:e:403:TYR:CE2	2.51	0.46
5:e:274:THR:O	5:e:357:LYS:HE2	2.16	0.46
1:A:86:TYR:CE2	1:A:103:TYR:CD1	3.03	0.46
5:f:997:LYS:HZ1	5:f:999:GLU:CD	2.24	0.46
2:E:99:LYS:HE3	2:E:100:TRP:CZ2	2.51	0.46
2:E:111:GLU:CG	2:E:136:ASN:HD21	2.28	0.46
5:H:223:LYS:HE2	5:H:223:LYS:HA	1.98	0.46
4:G:8:GLY:H	4:G:11:GLU:CD	2.24	0.46
5:H:301:ALA:HA	5:H:355:TYR:HA	1.98	0.46
5:H:791:VAL:H	5:H:923:ALA:HB3	1.81	0.46
5:e:793:PRO:HG2	5:e:926:TRP:CZ3	2.51	0.46
5:h:286:ARG:HH22	5:h:292:GLY:C	2.23	0.46
1:J:549:TRP:CZ2	1:J:551:ARG:HA	2.50	0.46
5:f:833:GLN:CD	5:f:833:GLN:H	2.24	0.46
1:A:543:LEU:HD23	1:A:562:ASP:HA	1.97	0.46
1:J:324:LYS:HE3	1:J:326:TYR:CE2	2.51	0.46
5:d:380:ILE:HG22	5:d:382:PHE:CZ	2.51	0.46
5:f:600:SER:HA	5:f:768:TYR:CD2	2.51	0.46
5:f:812:TYR:CD2	5:f:935:LYS:HE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:981:LYS:HG3	5:f:998:TRP:CZ3	2.51	0.46
8:b:176:TYR:CD2	8:b:176:TYR:C	2.94	0.46
5:e:219:LYS:HE2	5:e:228:ASP:CG	2.40	0.46
5:h:705:TYR:HB3	5:h:729:THR:HG22	1.96	0.46
2:D:101:VAL:HB	2:D:171:VAL:CG2	2.47	0.45
5:e:281:LYS:HE3	5:e:281:LYS:HA	1.98	0.45
5:e:812:TYR:CD2	5:e:935:LYS:HE2	2.51	0.45
5:e:1062:TYR:CZ	5:e:1122:ASN:HB2	2.51	0.45
5:h:377:LYS:HE2	5:h:377:LYS:HA	1.97	0.45
5:h:812:TYR:CZ	5:h:935:LYS:HE2	2.51	0.45
1:A:559:LYS:HE2	1:A:571:TYR:O	2.17	0.45
5:e:166:TYR:C	5:e:166:TYR:CD2	2.95	0.45
5:H:801:ASP:HB2	5:e:166:TYR:CE2	2.52	0.45
5:f:403:TYR:CE2	5:f:452:ASP:CG	2.94	0.45
1:A:99:TYR:CE2	1:A:113:SER:HB3	2.51	0.45
5:H:721:TYR:CE1	5:H:738:ALA:HA	2.51	0.45
6:M:694:HIS:CG	6:M:716:LEU:HB3	2.52	0.45
7:S:187:LEU:HD12	7:S:200:ARG:O	2.16	0.45
7:S:10:GLU:H	7:S:10:GLU:CD	2.24	0.45
7:U:261:GLN:CD	7:U:261:GLN:H	2.25	0.45
5:e:562:ILE:HD11	5:e:1034:SER:HB3	1.98	0.45
5:h:336:TRP:C	5:h:338:PRO:HD2	2.42	0.45
1:A:324:LYS:HE2	1:A:326:TYR:CE2	2.52	0.45
5:H:1066:ARG:HH12	5:H:1146:MET:HB2	1.82	0.45
7:T:225:LYS:HE3	7:T:226:GLU:O	2.17	0.45
5:f:70:GLU:CD	5:f:70:GLU:H	2.25	0.45
5:g:186:TYR:CE2	5:g:223:LYS:HE3	2.51	0.45
3:F:51:ILE:HG22	6:M:781:ALA:HA	1.97	0.45
1:J:324:LYS:HE3	1:J:326:TYR:CZ	2.51	0.45
2:Q:134:LYS:HE2	2:Q:136:ASN:O	2.17	0.44
5:d:286:ARG:HH22	5:d:292:GLY:C	2.25	0.44
5:h:244:GLY:H	5:h:403:TYR:HA	1.82	0.44
2:R:103:LEU:HD11	2:R:122:PHE:CD2	2.52	0.44
5:g:945:GLU:N	5:g:945:GLU:CD	2.75	0.44
2:O:19:LYS:HE2	2:O:19:LYS:HA	1.99	0.44
5:e:64:LEU:HD11	5:e:81:VAL:HB	2.00	0.44
8:b:556:PHE:CE1	8:b:671:ILE:HG21	2.52	0.44
5:d:208:ASP:O	5:d:239:LYS:HE3	2.17	0.44
5:e:171:ASN:C	5:e:173:GLU:N	2.75	0.44
5:f:721:TYR:CE1	5:f:738:ALA:HA	2.53	0.44
5:g:469:GLU:O	5:g:473:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:199:LEU:HD23	5:h:215:VAL:HG22	1.99	0.44
2:E:91:GLU:CD	2:E:91:GLU:N	2.75	0.44
1:J:381:PHE:CD1	1:J:381:PHE:C	2.96	0.44
5:g:702:ASN:CG	5:g:731:MET:HE3	2.42	0.44
5:H:234:ARG:HH22	5:e:709:ASP:CG	2.26	0.44
2:c:25:LEU:HD22	2:c:105:SER:HB3	1.99	0.44
1:B:137:THR:HG21	1:B:139:GLN:HE21	1.82	0.44
5:H:715:ILE:HD11	5:H:757:LEU:HD13	1.98	0.44
8:b:550:ILE:HD11	8:b:565:ILE:HB	2.00	0.44
2:N:7:ASN:HB3	2:O:147:THR:HG23	1.99	0.44
5:d:981:LYS:HE3	5:d:997:LYS:C	2.43	0.44
5:f:812:TYR:CE2	5:f:935:LYS:HE2	2.53	0.44
5:H:511:PHE:CE2	5:H:1142:VAL:HG23	2.53	0.43
1:J:18:TYR:CD1	1:J:19:PRO:HD3	2.53	0.43
2:N:91:GLU:CD	2:N:91:GLU:N	2.76	0.43
5:g:791:VAL:C	5:g:793:PRO:HD3	2.43	0.43
2:D:101:VAL:HB	2:D:171:VAL:HG22	1.99	0.43
5:H:816:LYS:HA	5:H:888:TYR:CD1	2.54	0.43
1:J:131:LYS:HE2	1:J:395:TRP:CG	2.54	0.43
5:d:697:LEU:HD22	5:d:762:SER:HB3	2.00	0.43
5:e:985:ASP:HA	5:e:1014:ARG:CZ	2.47	0.43
5:H:519:ILE:HG22	5:H:524:PHE:CZ	2.53	0.43
5:d:787:THR:HG23	5:d:839:THR:HA	1.99	0.43
5:e:260:ILE:HG21	5:e:396:VAL:HG21	2.00	0.43
5:f:409:SER:HB3	5:f:411:PHE:CE2	2.53	0.43
5:g:311:THR:HG23	5:g:317:THR:HG21	1.99	0.43
1:B:324:LYS:HE2	1:B:326:TYR:CZ	2.54	0.43
1:J:201:PHE:CD2	1:J:241:VAL:HG13	2.53	0.43
5:d:239:LYS:HE2	5:d:453:SER:O	2.19	0.43
5:g:1091:TRP:CD1	5:g:1128:ARG:HH21	2.36	0.43
1:A:18:TYR:CD1	1:A:18:TYR:C	2.96	0.43
5:e:171:ASN:C	5:e:173:GLU:H	2.25	0.43
5:e:1011:GLY:HA2	5:e:1137:PHE:CE2	2.54	0.43
5:H:512:ILE:HD12	5:H:513:SER:N	2.33	0.43
6:M:702:TYR:CD1	6:M:702:TYR:N	2.86	0.43
7:S:267:HIS:CE1	7:S:270:ARG:NH1	2.86	0.43
5:d:562:ILE:HD11	5:d:1034:SER:HB3	2.00	0.43
5:f:296:LEU:HD22	5:f:353:TYR:CE1	2.54	0.43
5:H:281:LYS:HE3	5:H:350:TYR:CG	2.54	0.43
5:H:582:ASN:ND2	5:H:584:ASN:H	2.17	0.43
5:H:833:GLN:HA	5:d:171:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:808:SER:HB3	5:e:864:TYR:CE2	2.53	0.43
3:F:21:PHE:CE1	3:F:32:LYS:HD2	2.54	0.43
2:O:116:THR:HG22	2:O:158:ASN:HA	2.00	0.43
7:U:83:ARG:H	7:U:83:ARG:HD3	1.84	0.43
5:e:723:LYS:HE2	5:e:724:GLY:O	2.19	0.43
5:f:1117:LYS:HE2	5:f:1119:SER:O	2.19	0.43
5:g:1026:ARG:C	5:g:1026:ARG:HD3	2.43	0.43
1:B:449:PHE:CD1	1:B:449:PHE:C	2.97	0.42
2:D:125:ASP:O	2:D:146:GLY:HA3	2.19	0.42
3:F:43:ASP:CG	3:F:47:LYS:HZ2	2.26	0.42
7:S:267:HIS:CE1	7:S:270:ARG:HH12	2.37	0.42
5:g:206:GLU:CD	5:g:206:GLU:H	2.27	0.42
5:h:336:TRP:CZ3	5:h:343:PRO:HD3	2.53	0.42
1:A:556:PHE:CD1	1:B:566:THR:HA	2.53	0.42
3:F:16:ASP:OD2	3:F:32:LYS:HE2	2.19	0.42
5:d:277:VAL:HG12	5:d:278:LEU:N	2.32	0.42
5:d:981:LYS:HE3	5:d:996:LEU:O	2.20	0.42
5:f:783:ARG:HH12	5:f:1036:ASP:CG	2.27	0.42
5:g:273:VAL:HG22	5:g:365:TYR:CE2	2.54	0.42
1:B:481:ASN:HB3	1:B:502:GLY:HA3	2.01	0.42
5:H:407:LYS:CG	5:H:446:THR:HB	2.49	0.42
5:H:545:GLN:HE22	5:H:1036:ASP:CA	2.32	0.42
2:I:19:LYS:HZ1	2:I:125:ASP:CG	2.28	0.42
5:d:970:THR:HG22	5:d:1030:PRO:HB3	2.01	0.42
5:f:787:THR:HG22	5:f:838:LYS:C	2.44	0.42
5:g:89:TYR:CE2	5:g:91:ASP:HB2	2.54	0.42
5:h:973:ARG:HE	5:h:973:ARG:CA	2.32	0.42
5:H:253:PHE:CD1	5:H:390:PRO:HG2	2.55	0.42
2:O:107:ILE:HD12	2:O:107:ILE:N	2.34	0.42
2:P:25:LEU:HD12	2:P:121:GLY:O	2.20	0.42
2:Q:150:PHE:CE2	2:Q:171:VAL:HG11	2.54	0.42
7:U:10:GLU:H	7:U:10:GLU:CD	2.27	0.42
5:f:475:LYS:C	5:f:475:LYS:HE3	2.44	0.42
1:B:131:LYS:HE2	1:B:395:TRP:CG	2.55	0.42
2:N:37:THR:HG23	8:b:733:SER:HB2	2.02	0.42
5:f:385:SER:HA	5:f:389:LYS:HE3	2.02	0.42
5:f:1026:ARG:NH1	5:f:1027:TYR:CE1	2.87	0.42
3:F:8:LYS:HA	3:F:11:ILE:HB	2.01	0.42
3:F:28:ARG:HH21	3:F:28:ARG:HG3	1.85	0.42
5:H:874:GLY:O	5:e:179:LYS:HE2	2.18	0.42
5:e:363:LYS:HE3	5:e:363:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:1069:TYR:CE1	5:f:1110:TYR:HB2	2.54	0.42
5:h:199:LEU:CD2	5:h:215:VAL:HG22	2.50	0.42
3:F:49:VAL:HA	3:F:52:ARG:CG	2.50	0.42
5:d:88:ARG:N	5:d:88:ARG:CD	2.83	0.42
5:d:411:PHE:CZ	5:d:436:ASN:CB	3.03	0.42
5:d:1085:ALA:HB1	5:d:1122:ASN:HD21	1.83	0.42
5:e:229:LYS:HE2	5:e:231:VAL:CG2	2.50	0.42
5:e:894:THR:HG21	5:e:897:LYS:HE3	2.01	0.42
5:H:40:GLN:HB2	5:d:22:LYS:HE3	2.02	0.42
7:S:10:GLU:CD	7:S:10:GLU:N	2.78	0.42
5:d:403:TYR:CE1	5:d:452:ASP:HB2	2.55	0.42
5:f:465:ARG:C	5:f:466:LEU:HD22	2.45	0.42
5:h:580:THR:HG21	5:h:814:ALA:HB2	2.02	0.42
1:B:528:SER:HA	1:B:626:LYS:HE2	2.02	0.42
5:H:25:PHE:CE2	5:e:36:LEU:HD12	2.55	0.42
5:H:857:ALA:HB2	5:H:891:TRP:CD2	2.55	0.42
1:J:324:LYS:CE	1:J:326:TYR:CZ	3.03	0.42
1:J:551:ARG:HH21	1:J:627:GLU:HB3	1.85	0.42
2:R:150:PHE:CE1	2:R:171:VAL:HG11	2.55	0.42
7:T:214:LYS:HE2	7:T:218:GLY:O	2.19	0.42
7:U:132:PHE:CE2	7:U:134:SER:HB2	2.55	0.42
2:V:91:GLU:N	2:V:91:GLU:CD	2.78	0.42
5:e:109:LYS:HZ1	5:e:151:ASP:CG	2.27	0.42
3:F:45:TYR:CD1	3:F:45:TYR:C	2.97	0.42
2:I:12:LEU:HD23	2:I:12:LEU:C	2.45	0.42
2:I:167:GLU:N	2:I:167:GLU:CD	2.78	0.42
7:S:402:VAL:HG13	7:S:424:ARG:HD2	2.02	0.42
5:d:267:VAL:HB	5:d:378:TRP:CD2	2.55	0.42
5:e:19:ASP:O	5:e:21:THR:HG23	2.20	0.42
5:h:208:ASP:O	5:h:239:LYS:HE3	2.20	0.42
5:H:253:PHE:CD2	5:H:390:PRO:HB2	2.54	0.41
5:H:403:TYR:CD2	5:H:452:ASP:HB2	2.55	0.41
2:K:151:PHE:O	2:Q:2:ALA:HA	2.19	0.41
2:O:149:LEU:HD23	2:O:150:PHE:CE2	2.54	0.41
5:d:70:GLU:N	5:d:70:GLU:CD	2.78	0.41
5:H:239:LYS:HZ3	5:H:454:ASP:CG	2.29	0.41
5:H:793:PRO:HG2	5:H:926:TRP:CH2	2.54	0.41
7:T:32:ARG:HH11	7:T:36:ASP:CB	2.33	0.41
5:e:604:TRP:CE3	5:e:686:ARG:CZ	3.03	0.41
5:f:206:GLU:CD	5:f:206:GLU:N	2.79	0.41
5:f:708:PHE:CD1	5:f:708:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:1075:LYS:HZ1	5:g:1134:GLU:CD	2.27	0.41
5:h:981:LYS:HE3	5:h:997:LYS:O	2.19	0.41
1:A:15:LYS:HE3	1:A:16:ASP:OD1	2.20	0.41
1:A:263:GLU:CD	1:A:263:GLU:H	2.28	0.41
5:H:791:VAL:H	5:H:923:ALA:CB	2.33	0.41
2:P:125:ASP:O	2:P:146:GLY:HA3	2.20	0.41
5:d:336:TRP:CZ3	5:d:343:PRO:HD3	2.55	0.41
1:B:15:LYS:HE3	1:B:15:LYS:O	2.20	0.41
1:B:381:PHE:CD1	1:B:381:PHE:C	2.99	0.41
3:F:44:MET:SD	3:F:47:LYS:HD2	2.61	0.41
5:H:1083:TYR:CE2	5:H:1092:LYS:HD2	2.55	0.41
2:P:113:PRO:CB	8:b:705:ILE:O	2.69	0.41
8:b:505:PRO:HG2	8:b:541:LYS:HB3	2.02	0.41
5:e:603:ASN:O	5:e:775:LYS:HE2	2.20	0.41
5:f:27:PRO:HA	5:g:33:GLN:HE22	1.84	0.41
5:f:277:VAL:HG12	5:f:278:LEU:H	1.85	0.41
1:A:86:TYR:CZ	1:A:103:TYR:CD1	3.08	0.41
3:F:27:GLU:CD	3:F:27:GLU:H	2.28	0.41
7:T:308:HIS:CE1	7:T:327:GLY:H	2.39	0.41
8:b:337:LEU:H	8:b:338:GLN:NE2	2.19	0.41
8:b:548:ARG:HD3	8:b:548:ARG:H	1.85	0.41
5:e:1026:ARG:C	5:e:1026:ARG:HD3	2.46	0.41
5:f:264:ASN:HB3	5:f:402:TYR:CE2	2.55	0.41
5:f:286:ARG:HH12	5:f:292:GLY:N	2.19	0.41
5:g:229:LYS:HE3	5:g:416:GLY:HA3	2.03	0.41
5:g:326:PHE:HB3	5:g:336:TRP:CZ3	2.55	0.41
5:h:570:ARG:HD3	5:h:939:TYR:CZ	2.56	0.41
3:F:51:ILE:C	3:F:51:ILE:HD12	2.46	0.41
5:H:103:LYS:HE3	5:H:161:MET:SD	2.61	0.41
5:H:526:ILE:C	5:H:526:ILE:HD12	2.46	0.41
2:O:112:LEU:HD23	2:O:112:LEU:HA	1.92	0.41
5:g:177:ILE:H	5:g:177:ILE:HD12	1.85	0.41
5:g:382:PHE:O	5:g:389:LYS:HE2	2.20	0.41
5:h:66:PHE:CD1	5:h:74:LEU:HD11	2.56	0.41
5:h:70:GLU:CD	5:h:70:GLU:N	2.78	0.41
5:d:1062:TYR:CD1	5:d:1062:TYR:C	2.99	0.41
5:g:381:ASN:HB2	5:g:383:THR:HG23	2.02	0.41
5:g:403:TYR:CD1	5:g:452:ASP:HB2	2.55	0.41
5:g:702:ASN:OD1	5:g:731:MET:HE3	2.21	0.41
1:A:197:LYS:HE2	1:A:384:HIS:CE1	2.56	0.41
5:H:364:ASP:HA	5:H:387:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:56:LYS:HZ2	2:I:111:GLU:CD	2.28	0.41
2:L:14:LYS:HE2	2:L:90:PRO:O	2.20	0.41
5:d:470:ASP:HA	5:d:473:LYS:HE2	2.03	0.41
5:f:584:ASN:HD21	5:f:588:ILE:N	2.19	0.41
5:g:82:TYR:OH	5:g:85:GLY:HA2	2.21	0.41
2:D:69:SER:HB2	2:D:70:PRO:HD3	2.03	0.41
5:H:243:LEU:CD2	5:H:403:TYR:CD2	3.04	0.41
5:H:253:PHE:HA	5:H:260:ILE:HG22	2.01	0.41
5:H:1066:ARG:HH12	5:H:1146:MET:CB	2.34	0.41
6:M:675:LYS:HE3	6:M:676:TYR:CZ	2.56	0.41
7:S:261:GLN:H	7:S:261:GLN:CD	2.29	0.41
7:T:311:TYR:CE2	7:T:323:GLY:HA3	2.56	0.41
5:d:33:GLN:HE21	5:e:27:PRO:CA	2.31	0.41
5:e:511:PHE:CD1	5:e:1143:ARG:HA	2.55	0.41
5:e:697:LEU:HD22	5:e:762:SER:HB3	2.02	0.41
5:e:780:ILE:HG21	5:e:1033:SER:HB2	2.02	0.41
5:f:245:THR:HG23	5:f:271:ARG:HH22	1.86	0.41
5:g:363:LYS:HA	5:g:363:LYS:CE	2.51	0.41
1:B:556:PHE:CD1	1:J:566:THR:HA	2.56	0.41
5:H:1027:TYR:O	5:H:1028:ILE:HD13	2.21	0.41
2:N:103:LEU:HD11	2:N:122:PHE:CD2	2.56	0.41
2:O:14:LYS:HE2	2:O:93:ALA:CB	2.51	0.41
2:c:134:LYS:HZ1	2:c:141:GLU:CD	2.28	0.41
5:g:200:PHE:CD1	5:g:200:PHE:N	2.89	0.41
1:A:488:PHE:CE2	1:A:496:TYR:HB2	2.55	0.40
8:b:702:PHE:CE2	8:b:709:ILE:HD11	2.56	0.40
5:d:603:ASN:N	5:d:775:LYS:HE2	2.35	0.40
5:e:1063:ASN:HD21	5:e:1152:GLU:N	2.19	0.40
5:f:468:MET:SD	5:h:465:ARG:HA	2.61	0.40
5:h:200:PHE:CE1	5:h:214:VAL:HB	2.56	0.40
5:H:402:TYR:C	5:H:403:TYR:CD1	2.99	0.40
2:Q:103:LEU:HD11	2:Q:122:PHE:CD2	2.56	0.40
5:d:358:ARG:HH22	5:d:359:MET:C	2.29	0.40
5:d:511:PHE:CD1	5:d:1143:ARG:HA	2.57	0.40
5:e:945:GLU:CD	5:e:945:GLU:H	2.29	0.40
5:f:570:ARG:HD3	5:f:939:TYR:CZ	2.56	0.40
5:g:363:LYS:HA	5:g:363:LYS:HE3	2.03	0.40
5:h:593:GLY:HA3	5:h:697:LEU:HD21	2.02	0.40
1:B:384:HIS:CE1	1:B:386:ASN:HB2	2.57	0.40
5:d:308:TRP:CD1	5:d:316:THR:HG1	2.39	0.40
5:e:1069:TYR:CZ	5:e:1110:TYR:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:128:SER:HA	5:g:133:TYR:CD1	2.57	0.40
5:h:957:VAL:HG12	5:h:958:SER:N	2.36	0.40
6:M:689:GLN:HA	6:M:690:PRO:HD3	1.91	0.40
2:Q:150:PHE:CZ	2:Q:171:VAL:HG11	2.57	0.40
2:R:24:TYR:CE1	2:R:126:LEU:HD11	2.56	0.40
2:c:33:TRP:CD1	2:c:118:ARG:HD3	2.57	0.40
5:e:791:VAL:O	5:e:793:PRO:HD3	2.20	0.40
5:f:35:GLU:CD	5:g:140:ARG:HH12	2.30	0.40
5:f:1072:PHE:HB2	5:f:1107:PHE:CD1	2.56	0.40
5:h:787:THR:HG21	5:h:840:ILE:HD12	2.03	0.40
5:h:980:MET:O	5:h:981:LYS:HE2	2.22	0.40
1:B:384:HIS:CE1	1:B:386:ASN:HD22	2.39	0.40
5:H:197:PHE:CE1	5:H:218:GLY:C	3.00	0.40
5:H:1091:TRP:CE3	5:H:1128:ARG:HD3	2.56	0.40
7:S:225:LYS:HE3	7:S:226:GLU:O	2.21	0.40
2:c:91:GLU:CD	2:c:91:GLU:N	2.79	0.40
5:d:1:MET:H2	5:d:112:GLU:CD	2.29	0.40
5:d:90:TYR:HA	5:d:145:MET:SD	2.62	0.40
5:d:318:LYS:HE2	5:d:320:TYR:CE2	2.57	0.40
5:e:336:TRP:CH2	5:e:343:PRO:CD	3.04	0.40
5:f:186:TYR:CE1	5:f:223:LYS:HE2	2.56	0.40
5:h:812:TYR:CE2	5:h:935:LYS:HE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	638/640 (100%)	607 (95%)	29 (4%)	2 (0%)	36	72
1	B	638/640 (100%)	604 (95%)	30 (5%)	4 (1%)	21	59
1	J	638/640 (100%)	607 (95%)	25 (4%)	6 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	170/173 (98%)	149 (88%)	19 (11%)	2 (1%)	10	43
2	E	170/173 (98%)	155 (91%)	15 (9%)	0	100	100
2	I	159/173 (92%)	150 (94%)	9 (6%)	0	100	100
2	K	170/173 (98%)	150 (88%)	16 (9%)	4 (2%)	4	26
2	L	170/173 (98%)	154 (91%)	14 (8%)	2 (1%)	10	43
2	N	170/173 (98%)	153 (90%)	14 (8%)	3 (2%)	6	33
2	O	170/173 (98%)	155 (91%)	13 (8%)	2 (1%)	10	43
2	P	170/173 (98%)	148 (87%)	17 (10%)	5 (3%)	3	23
2	Q	170/173 (98%)	152 (89%)	16 (9%)	2 (1%)	10	43
2	R	170/173 (98%)	149 (88%)	18 (11%)	3 (2%)	6	33
2	V	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
2	c	158/173 (91%)	151 (96%)	7 (4%)	0	100	100
3	F	137/295 (46%)	104 (76%)	25 (18%)	8 (6%)	1	13
4	G	69/124 (56%)	59 (86%)	8 (12%)	2 (3%)	3	23
5	H	1060/1152 (92%)	916 (86%)	120 (11%)	24 (2%)	5	27
5	d	1060/1152 (92%)	896 (84%)	134 (13%)	30 (3%)	4	24
5	e	1060/1152 (92%)	920 (87%)	117 (11%)	23 (2%)	5	28
5	f	1060/1152 (92%)	930 (88%)	113 (11%)	17 (2%)	7	36
5	g	1060/1152 (92%)	928 (88%)	118 (11%)	14 (1%)	9	41
5	h	1060/1152 (92%)	933 (88%)	98 (9%)	29 (3%)	4	24
6	M	134/808 (17%)	115 (86%)	18 (13%)	1 (1%)	18	55
7	S	456/458 (100%)	440 (96%)	15 (3%)	1 (0%)	43	77
7	T	456/458 (100%)	434 (95%)	21 (5%)	1 (0%)	43	77
7	U	456/458 (100%)	436 (96%)	19 (4%)	1 (0%)	43	77
8	b	620/1019 (61%)	568 (92%)	45 (7%)	7 (1%)	11	45
All	All	12606/14528 (87%)	11316 (90%)	1097 (9%)	193 (2%)	11	38

All (193) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
5	H	452	ASP
5	H	791	VAL

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Mol	Chain	Res	Type
2	L	93	ALA
2	N	93	ALA
2	O	93	ALA
2	P	93	ALA
2	P	114	LEU
2	R	93	ALA
8	b	108	ARG
5	d	337	SER
5	d	453	SER
5	d	784	THR
5	d	997	LYS
5	e	189	SER
5	e	832	ASP
5	e	973	ARG
5	f	793	PRO
5	f	922	ASN
5	f	972	GLU
5	g	171	ASN
5	g	189	SER
5	g	773	ARG
5	g	922	ASN
5	g	973	ARG
5	h	337	SER
5	h	773	ARG
5	h	791	VAL
5	h	793	PRO
5	h	913	LEU
5	h	922	ASN
5	h	997	LYS
1	B	553	ALA
1	B	578	SER
2	D	93	ALA
3	F	135	GLU
5	H	241	TYR
5	H	276	GLN
5	H	426	ASN
5	H	922	ASN
5	H	972	GLU
5	H	1037	LEU
1	J	246	GLY
2	K	111	GLU
2	N	98	ALA

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Mol	Chain	Res	Type
2	N	111	GLU
2	Q	93	ALA
7	S	93	ASP
5	d	330	ASP
5	d	791	VAL
5	d	922	ASN
5	e	171	ASN
5	e	190	GLY
5	e	300	THR
5	f	428	MET
5	f	452	ASP
5	f	453	SER
5	f	497	GLY
5	f	791	VAL
5	f	930	GLN
5	g	190	GLY
5	g	388	ALA
5	g	930	GLN
5	h	2	ALA
5	h	299	ASN
5	h	330	ASP
5	h	426	ASN
5	h	428	MET
5	h	589	PRO
5	h	930	GLN
5	h	973	ARG
3	F	38	LYS
3	F	91	VAL
3	F	139	ASP
4	G	71	LYS
5	H	388	ALA
5	H	430	LEU
5	H	453	SER
5	H	973	ARG
2	O	98	ALA
2	R	92	ASN
8	b	125	THR
8	b	425	LYS
5	d	243	LEU
5	d	256	SER
5	d	332	GLN
5	d	414	LYS

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Mol	Chain	Res	Type
5	d	769	THR
5	d	793	PRO
5	d	1075	LYS
5	d	1089	LYS
5	d	1104	ASN
5	e	173	GLU
5	e	552	ASP
5	e	771	GLN
5	e	783	ARG
5	e	913	LEU
5	f	337	SER
5	f	426	ASN
5	f	435	LEU
5	f	921	SER
5	g	1075	LYS
5	h	4	ASN
5	h	132	SER
5	h	217	ALA
5	h	242	ASP
5	h	453	SER
5	h	1076	GLY
3	F	41	THR
3	F	133	GLU
5	H	205	ALA
5	H	460	SER
1	J	189	GLN
1	J	304	LYS
1	J	340	SER
2	K	93	ALA
2	K	110	ASP
2	P	98	ALA
2	Q	98	ALA
2	R	73	ASP
7	T	180	SER
7	U	226	GLU
8	b	110	ASP
8	b	300	LYS
8	b	533	ASN
5	d	172	ALA
5	d	382	PHE
5	d	426	ASN
5	d	599	PRO

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Mol	Chain	Res	Type
5	d	760	ALA
5	d	953	PRO
5	d	973	ARG
5	e	288	ALA
5	e	388	ALA
5	e	389	LYS
5	f	382	PHE
5	f	388	ALA
5	h	697	LEU
5	h	733	ASP
1	B	246	GLY
2	D	98	ALA
3	F	22	ASP
4	G	35	LEU
5	H	186	TYR
5	H	291	ASP
5	H	468	MET
5	H	819	LYS
1	J	211	ILE
2	L	71	GLU
6	M	715	PRO
5	d	84	ASN
5	d	239	LYS
5	d	242	ASP
5	d	301	ALA
5	d	924	SER
5	e	176	LYS
5	e	256	SER
5	e	275	GLY
5	e	361	ALA
5	e	866	ASP
5	f	33	GLN
5	g	357	LYS
5	g	390	PRO
5	h	316	THR
5	h	384	PRO
5	h	760	ALA
3	F	94	GLY
5	H	27	PRO
5	H	435	LEU
5	H	760	ALA
5	H	913	LEU

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Mol	Chain	Res	Type
1	J	199	SER
2	K	143	GLU
8	b	131	ASN
5	d	169	SER
5	d	874	GLY
5	e	28	ASP
5	e	337	SER
5	f	205	ALA
5	h	205	ALA
5	H	559	GLY
5	h	27	PRO
5	h	559	GLY
5	H	793	PRO
5	e	907	ILE
1	A	7	PRO
1	B	604	GLY
2	P	108	VAL
5	e	384	PRO
5	g	791	VAL
2	P	70	PRO
5	g	559	GLY
5	g	907	ILE

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	A	577/577 (100%)	566 (98%)	11 (2%)	50	66
1	B	577/577 (100%)	565 (98%)	12 (2%)	47	65
1	J	577/577 (100%)	563 (98%)	14 (2%)	43	63
2	D	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	E	152/153 (99%)	149 (98%)	3 (2%)	48	66
2	I	143/153 (94%)	139 (97%)	4 (3%)	38	59
2	K	152/153 (99%)	141 (93%)	11 (7%)	13	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	N	152/153 (99%)	138 (91%)	14 (9%)	8	26
2	O	152/153 (99%)	138 (91%)	14 (9%)	8	26
2	P	152/153 (99%)	138 (91%)	14 (9%)	8	26
2	Q	152/153 (99%)	140 (92%)	12 (8%)	11	31
2	R	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	V	142/153 (93%)	134 (94%)	8 (6%)	19	40
2	c	143/153 (94%)	142 (99%)	1 (1%)	76	80
3	F	132/271 (49%)	109 (83%)	23 (17%)	2	10
4	G	63/112 (56%)	61 (97%)	2 (3%)	34	55
5	H	936/1010 (93%)	848 (91%)	88 (9%)	8	25
5	d	936/1010 (93%)	865 (92%)	71 (8%)	12	32
5	e	936/1010 (93%)	871 (93%)	65 (7%)	14	36
5	f	936/1010 (93%)	859 (92%)	77 (8%)	10	30
5	g	936/1010 (93%)	863 (92%)	73 (8%)	11	32
5	h	936/1010 (93%)	875 (94%)	61 (6%)	15	37
6	M	105/695 (15%)	95 (90%)	10 (10%)	8	25
7	S	405/405 (100%)	399 (98%)	6 (2%)	57	71
7	T	405/405 (100%)	398 (98%)	7 (2%)	53	68
7	U	405/405 (100%)	399 (98%)	6 (2%)	57	71
8	b	573/928 (62%)	553 (96%)	20 (4%)	32	53
All	All	11231/12848 (87%)	10571 (94%)	660 (6%)	19	39

All (660) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	138	THR
1	A	322	GLU
1	A	330	PHE
1	A	379	THR
1	A	418	ASN
1	A	431	ASN
1	A	432	GLU
1	A	563	ILE

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Mol	Chain	Res	Type
1	A	565	ASN
1	A	576	ASN
1	B	15	LYS
1	B	18	TYR
1	B	64	LYS
1	B	105	ASN
1	B	138	THR
1	B	330	PHE
1	B	451	CYS
1	B	492	GLU
1	B	504	ASN
1	B	563	ILE
1	B	578	SER
1	B	619	LYS
2	D	44	GLU
2	D	51	GLU
2	D	68	LYS
2	D	75	LYS
2	D	88	VAL
2	D	99	LYS
2	D	101	VAL
2	D	107	ILE
2	D	111	GLU
2	D	125	ASP
2	D	127	VAL
2	E	38	ASN
2	E	74	ASN
2	E	129	LYS
3	F	22	ASP
3	F	28	ARG
3	F	29	ILE
3	F	31	GLU
3	F	34	GLU
3	F	41	THR
3	F	44	MET
3	F	45	TYR
3	F	67	GLN
3	F	68	TYR
3	F	69	GLU
3	F	71	PHE
3	F	86	LYS
3	F	88	SER

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Mol	Chain	Res	Type
3	F	91	VAL
3	F	92	ASP
3	F	96	ILE
3	F	114	GLU
3	F	115	LEU
3	F	136	TYR
3	F	138	PHE
3	F	139	ASP
3	F	140	GLU
4	G	6	ASP
4	G	63	LYS
5	H	1	MET
5	H	27	PRO
5	H	98	ILE
5	H	103	LYS
5	H	115	VAL
5	H	139	ASP
5	H	168	GLN
5	H	173	GLU
5	H	176	LYS
5	H	180	VAL
5	H	183	GLU
5	H	223	LYS
5	H	248	ASN
5	H	249	GLU
5	H	254	ASN
5	H	264	ASN
5	H	268	LYS
5	H	269	GLU
5	H	294	ASP
5	H	317	THR
5	H	359	MET
5	H	363	LYS
5	H	367	VAL
5	H	383	THR
5	H	391	ILE
5	H	430	LEU
5	H	432	THR
5	H	454	ASP
5	H	465	ARG
5	H	470	ASP
5	H	475	LYS

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Mol	Chain	Res	Type
5	H	498	GLN
5	H	515	ASP
5	H	519	ILE
5	H	520	THR
5	H	541	GLU
5	H	545	GLN
5	H	547	LYS
5	H	560	ARG
5	H	568	GLU
5	H	574	GLN
5	H	579	GLU
5	H	582	ASN
5	H	586	TYR
5	H	601	GLU
5	H	723	LYS
5	H	729	THR
5	H	739	LYS
5	H	741	LYS
5	H	754	GLU
5	H	756	THR
5	H	776	THR
5	H	779	ASP
5	H	790	LEU
5	H	793	PRO
5	H	799	GLN
5	H	801	ASP
5	H	804	ARG
5	H	819	LYS
5	H	839	THR
5	H	850	ASP
5	H	861	THR
5	H	876	GLU
5	H	887	ASP
5	H	892	VAL
5	H	910	ASN
5	H	942	LYS
5	H	945	GLU
5	H	970	THR
5	H	973	ARG
5	H	979	GLU
5	H	985	ASP
5	H	986	ASP

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Mol	Chain	Res	Type
5	H	994	ASP
5	H	1006	ASP
5	H	1014	ARG
5	H	1026	ARG
5	H	1027	TYR
5	H	1041	THR
5	H	1045	GLU
5	H	1066	ARG
5	H	1075	LYS
5	H	1087	ASP
5	H	1101	THR
5	H	1121	THR
5	H	1134	GLU
5	H	1137	PHE
5	H	1138	LEU
2	I	41	GLN
2	I	45	ASN
2	I	151	PHE
2	I	172	GLU
1	J	13	LYS
1	J	132	GLU
1	J	259	LYS
1	J	286	ASP
1	J	318	GLU
1	J	330	PHE
1	J	343	LYS
1	J	431	ASN
1	J	512	GLN
1	J	563	ILE
1	J	565	ASN
1	J	576	ASN
1	J	626	LYS
1	J	639	ARG
2	K	3	ILE
2	K	41	GLN
2	K	44	GLU
2	K	68	LYS
2	K	77	LEU
2	K	88	VAL
2	K	91	GLU
2	K	101	VAL
2	K	111	GLU

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Mol	Chain	Res	Type
2	K	125	ASP
2	K	136	ASN
2	L	19	LYS
2	L	51	GLU
2	L	68	LYS
2	L	83	LYS
2	L	88	VAL
2	L	101	VAL
2	L	107	ILE
2	L	111	GLU
2	L	136	ASN
2	L	157	GLN
2	L	161	GLU
6	M	689	GLN
6	M	695	TYR
6	M	700	THR
6	M	702	TYR
6	M	714	VAL
6	M	747	GLN
6	M	759	HIS
6	M	780	TYR
6	M	790	THR
6	M	799	LYS
2	N	27	ILE
2	N	38	ASN
2	N	51	GLU
2	N	75	LYS
2	N	88	VAL
2	N	101	VAL
2	N	107	ILE
2	N	111	GLU
2	N	125	ASP
2	N	126	LEU
2	N	127	VAL
2	N	136	ASN
2	N	143	GLU
2	N	145	THR
2	O	3	ILE
2	O	27	ILE
2	O	44	GLU
2	O	45	ASN
2	O	51	GLU

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Mol	Chain	Res	Type
2	O	88	VAL
2	O	101	VAL
2	O	108	VAL
2	O	111	GLU
2	O	125	ASP
2	O	126	LEU
2	O	127	VAL
2	O	154	LYS
2	O	157	GLN
2	P	38	ASN
2	P	48	VAL
2	P	51	GLU
2	P	68	LYS
2	P	75	LYS
2	P	88	VAL
2	P	99	LYS
2	P	101	VAL
2	P	111	GLU
2	P	127	VAL
2	P	136	ASN
2	P	143	GLU
2	P	156	PHE
2	P	161	GLU
2	Q	27	ILE
2	Q	45	ASN
2	Q	51	GLU
2	Q	88	VAL
2	Q	101	VAL
2	Q	111	GLU
2	Q	125	ASP
2	Q	126	LEU
2	Q	127	VAL
2	Q	136	ASN
2	Q	149	LEU
2	Q	172	GLU
2	R	11	GLU
2	R	45	ASN
2	R	51	GLU
2	R	61	VAL
2	R	68	LYS
2	R	88	VAL
2	R	101	VAL

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Mol	Chain	Res	Type
2	R	125	ASP
2	R	136	ASN
2	R	143	GLU
2	R	168	ARG
7	S	70	ARG
7	S	83	ARG
7	S	111	LYS
7	S	192	ASP
7	S	235	TYR
7	S	436	LEU
7	T	14	ILE
7	T	91	ARG
7	T	94	MET
7	T	192	ASP
7	T	293	CYS
7	T	347	GLN
7	T	403	CYS
7	U	32	ARG
7	U	41	LEU
7	U	57	LYS
7	U	192	ASP
7	U	209	GLU
7	U	457	MET
2	V	21	ASP
2	V	38	ASN
2	V	60	LYS
2	V	82	ASN
2	V	129	LYS
2	V	150	PHE
2	V	155	GLN
2	V	157	GLN
8	b	110	ASP
8	b	111	ILE
8	b	130	LEU
8	b	137	MET
8	b	199	THR
8	b	231	ASP
8	b	235	THR
8	b	240	ILE
8	b	244	ASP
8	b	247	THR
8	b	370	GLU

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Mol	Chain	Res	Type
8	b	391	LEU
8	b	465	ARG
8	b	466	GLU
8	b	467	THR
8	b	516	ASP
8	b	521	GLU
8	b	559	SER
8	b	701	LYS
8	b	718	THR
2	c	43	ASP
5	d	26	ASN
5	d	70	GLU
5	d	75	THR
5	d	88	ARG
5	d	91	ASP
5	d	92	ASN
5	d	93	ASP
5	d	94	ASP
5	d	103	LYS
5	d	116	THR
5	d	119	GLU
5	d	134	PHE
5	d	139	ASP
5	d	174	MET
5	d	175	ASP
5	d	186	TYR
5	d	223	LYS
5	d	248	ASN
5	d	258	ASN
5	d	260	ILE
5	d	268	LYS
5	d	269	GLU
5	d	289	GLN
5	d	294	ASP
5	d	305	VAL
5	d	334	ILE
5	d	358	ARG
5	d	363	LYS
5	d	370	GLN
5	d	377	LYS
5	d	448	THR
5	d	449	VAL

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Mol	Chain	Res	Type
5	d	453	SER
5	d	523	ASP
5	d	531	GLU
5	d	540	THR
5	d	552	ASP
5	d	562	ILE
5	d	574	GLN
5	d	579	GLU
5	d	588	ILE
5	d	603	ASN
5	d	701	ASP
5	d	756	THR
5	d	761	ASN
5	d	773	ARG
5	d	776	THR
5	d	779	ASP
5	d	787	THR
5	d	793	PRO
5	d	818	ASP
5	d	833	GLN
5	d	850	ASP
5	d	852	LYS
5	d	870	MET
5	d	876	GLU
5	d	884	GLU
5	d	887	ASP
5	d	905	GLU
5	d	981	LYS
5	d	985	ASP
5	d	997	LYS
5	d	999	GLU
5	d	1014	ARG
5	d	1022	PHE
5	d	1075	LYS
5	d	1078	LYS
5	d	1087	ASP
5	d	1121	THR
5	d	1127	VAL
5	d	1137	PHE
5	e	19	ASP
5	e	20	ARG
5	e	67	THR

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Mol	Chain	Res	Type
5	e	75	THR
5	e	118	ASP
5	e	119	GLU
5	e	139	ASP
5	e	144	LYS
5	e	169	SER
5	e	171	ASN
5	e	188	GLU
5	e	200	PHE
5	e	223	LYS
5	e	234	ARG
5	e	245	THR
5	e	248	ASN
5	e	268	LYS
5	e	269	GLU
5	e	273	VAL
5	e	274	THR
5	e	277	VAL
5	e	281	LYS
5	e	283	ARG
5	e	291	ASP
5	e	294	ASP
5	e	299	ASN
5	e	303	GLU
5	e	329	THR
5	e	332	GLN
5	e	341	GLN
5	e	357	LYS
5	e	363	LYS
5	e	364	ASP
5	e	377	LYS
5	e	383	THR
5	e	426	ASN
5	e	448	THR
5	e	469	GLU
5	e	475	LYS
5	e	552	ASP
5	e	574	GLN
5	e	587	ASN
5	e	588	ILE
5	e	701	ASP
5	e	749	ARG

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Mol	Chain	Res	Type
5	e	754	GLU
5	e	756	THR
5	e	767	THR
5	e	775	LYS
5	e	783	ARG
5	e	785	ARG
5	e	787	THR
5	e	792	ASP
5	e	852	LYS
5	e	870	MET
5	e	906	VAL
5	e	910	ASN
5	e	914	GLN
5	e	942	LYS
5	e	955	LYS
5	e	1010	LEU
5	e	1045	GLU
5	e	1075	LYS
5	e	1087	ASP
5	e	1137	PHE
5	f	18	LYS
5	f	19	ASP
5	f	35	GLU
5	f	67	THR
5	f	92	ASN
5	f	103	LYS
5	f	144	LYS
5	f	171	ASN
5	f	183	GLU
5	f	195	ASN
5	f	223	LYS
5	f	226	LYS
5	f	248	ASN
5	f	249	GLU
5	f	254	ASN
5	f	269	GLU
5	f	285	THR
5	f	294	ASP
5	f	308	TRP
5	f	321	LYS
5	f	324	GLU
5	f	330	ASP

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Mol	Chain	Res	Type
5	f	359	MET
5	f	363	LYS
5	f	364	ASP
5	f	370	GLN
5	f	383	THR
5	f	454	ASP
5	f	464	THR
5	f	465	ARG
5	f	470	ASP
5	f	475	LYS
5	f	483	TYR
5	f	495	MET
5	f	506	VAL
5	f	515	ASP
5	f	516	LYS
5	f	520	THR
5	f	532	ASP
5	f	552	ASP
5	f	574	GLN
5	f	588	ILE
5	f	601	GLU
5	f	604	TRP
5	f	700	ASN
5	f	723	LYS
5	f	756	THR
5	f	776	THR
5	f	779	ASP
5	f	790	LEU
5	f	801	ASP
5	f	802	GLU
5	f	818	ASP
5	f	850	ASP
5	f	852	LYS
5	f	876	GLU
5	f	899	LYS
5	f	902	LYS
5	f	920	SER
5	f	942	LYS
5	f	945	GLU
5	f	957	VAL
5	f	967	THR
5	f	970	THR

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Mol	Chain	Res	Type
5	f	985	ASP
5	f	986	ASP
5	f	994	ASP
5	f	1014	ARG
5	f	1026	ARG
5	f	1036	ASP
5	f	1066	ARG
5	f	1075	LYS
5	f	1079	VAL
5	f	1087	ASP
5	f	1105	ASN
5	f	1106	GLU
5	f	1134	GLU
5	g	26	ASN
5	g	27	PRO
5	g	98	ILE
5	g	118	ASP
5	g	139	ASP
5	g	144	LYS
5	g	147	LEU
5	g	169	SER
5	g	171	ASN
5	g	176	LYS
5	g	187	ASP
5	g	200	PHE
5	g	223	LYS
5	g	234	ARG
5	g	248	ASN
5	g	252	ILE
5	g	258	ASN
5	g	268	LYS
5	g	269	GLU
5	g	273	VAL
5	g	274	THR
5	g	283	ARG
5	g	294	ASP
5	g	302	PHE
5	g	303	GLU
5	g	308	TRP
5	g	329	THR
5	g	357	LYS
5	g	363	LYS

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Mol	Chain	Res	Type
5	g	377	LYS
5	g	427	ILE
5	g	443	GLN
5	g	453	SER
5	g	455	GLU
5	g	469	GLU
5	g	475	LYS
5	g	498	GLN
5	g	506	VAL
5	g	520	THR
5	g	571	THR
5	g	574	GLN
5	g	579	GLU
5	g	587	ASN
5	g	588	ILE
5	g	601	GLU
5	g	604	TRP
5	g	700	ASN
5	g	729	THR
5	g	753	ARG
5	g	756	THR
5	g	776	THR
5	g	779	ASP
5	g	783	ARG
5	g	787	THR
5	g	818	ASP
5	g	824	VAL
5	g	846	MET
5	g	850	ASP
5	g	852	LYS
5	g	867	ASP
5	g	887	ASP
5	g	910	ASN
5	g	942	LYS
5	g	945	GLU
5	g	955	LYS
5	g	970	THR
5	g	973	ARG
5	g	1010	LEU
5	g	1042	PHE
5	g	1075	LYS
5	g	1087	ASP

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Mol	Chain	Res	Type
5	g	1106	GLU
5	g	1137	PHE
5	h	6	LYS
5	h	18	LYS
5	h	27	PRO
5	h	39	MET
5	h	70	GLU
5	h	103	LYS
5	h	119	GLU
5	h	134	PHE
5	h	139	ASP
5	h	144	LYS
5	h	167	ILE
5	h	174	MET
5	h	186	TYR
5	h	223	LYS
5	h	245	THR
5	h	258	ASN
5	h	268	LYS
5	h	269	GLU
5	h	289	GLN
5	h	294	ASP
5	h	305	VAL
5	h	332	GLN
5	h	363	LYS
5	h	370	GLN
5	h	377	LYS
5	h	383	THR
5	h	417	ASP
5	h	448	THR
5	h	455	GLU
5	h	515	ASP
5	h	532	ASP
5	h	603	ASN
5	h	700	ASN
5	h	713	CYS
5	h	729	THR
5	h	741	LYS
5	h	756	THR
5	h	778	GLN
5	h	780	ILE
5	h	787	THR

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Mol	Chain	Res	Type
5	h	793	PRO
5	h	818	ASP
5	h	822	ASN
5	h	833	GLN
5	h	846	MET
5	h	850	ASP
5	h	852	LYS
5	h	853	VAL
5	h	866	ASP
5	h	876	GLU
5	h	884	GLU
5	h	887	ASP
5	h	942	LYS
5	h	973	ARG
5	h	981	LYS
5	h	987	MET
5	h	997	LYS
5	h	1014	ARG
5	h	1066	ARG
5	h	1075	LYS
5	h	1087	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	139	GLN
1	A	469	GLN
1	A	633	ASN
1	B	126	ASN
1	B	139	GLN
1	B	384	HIS
1	B	444	GLN
1	B	602	GLN
2	E	7	ASN
2	E	38	ASN
2	E	74	ASN
5	H	33	GLN
5	H	195	ASN
5	H	264	ASN
5	H	443	GLN
5	H	484	ASN

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Mol	Chain	Res	Type
5	H	582	ASN
5	H	587	ASN
5	H	799	GLN
5	H	914	GLN
2	I	119	GLN
2	I	157	GLN
2	I	158	ASN
1	J	105	ASN
1	J	126	ASN
1	J	139	GLN
1	J	210	ASN
1	J	469	GLN
1	J	540	ASN
1	J	602	GLN
2	K	38	ASN
2	K	157	GLN
2	L	119	GLN
2	L	153	ASN
2	N	7	ASN
2	N	119	GLN
2	N	153	ASN
2	N	158	ASN
2	O	7	ASN
2	O	38	ASN
2	O	162	GLN
2	P	38	ASN
2	P	45	ASN
2	P	50	GLN
2	P	119	GLN
2	P	153	ASN
2	Q	50	GLN
2	Q	162	GLN
2	R	119	GLN
7	S	44	ASN
7	S	115	HIS
7	T	124	ASN
7	T	142	GLN
7	T	267	HIS
7	U	102	HIS
7	U	150	ASN
7	U	262	GLN
7	U	273	GLN

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Mol	Chain	Res	Type
7	U	303	ASN
2	V	38	ASN
2	V	155	GLN
2	V	157	GLN
8	b	163	ASN
8	b	268	ASN
8	b	320	ASN
8	b	338	GLN
8	b	389	ASN
8	b	523	ASN
8	b	533	ASN
8	b	569	ASN
8	b	710	GLN
5	d	72	ASN
5	d	126	GLN
5	d	195	ASN
5	d	257	ASN
5	d	393	GLN
5	d	441	ASN
5	d	480	ASN
5	d	484	ASN
5	d	556	HIS
5	d	576	GLN
5	d	587	ASN
5	d	752	ASN
5	d	778	GLN
5	d	820	GLN
5	e	61	GLN
5	e	171	ASN
5	e	254	ASN
5	e	257	ASN
5	e	339	GLN
5	e	393	GLN
5	e	443	GLN
5	e	587	ASN
5	e	820	GLN
5	e	914	GLN
5	e	1126	GLN
5	f	171	ASN
5	f	299	ASN
5	f	370	GLN
5	f	480	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	f	576	GLN
5	f	584	ASN
5	f	778	GLN
5	f	820	GLN
5	f	910	ASN
5	f	1005	GLN
5	f	1015	GLN
5	g	386	ASN
5	g	443	GLN
5	g	484	ASN
5	g	761	ASN
5	g	799	GLN
5	g	820	GLN
5	g	995	GLN
5	h	248	ASN
5	h	289	GLN
5	h	339	GLN
5	h	356	ASN
5	h	441	ASN
5	h	472	GLN
5	h	698	ASN
5	h	778	GLN
5	h	930	GLN
5	h	944	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 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](#)

There are no chain breaks in this entry.

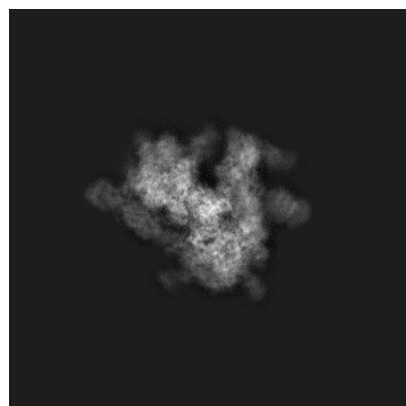
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55954. These allow visual inspection of the internal detail of the map and identification of artifacts.

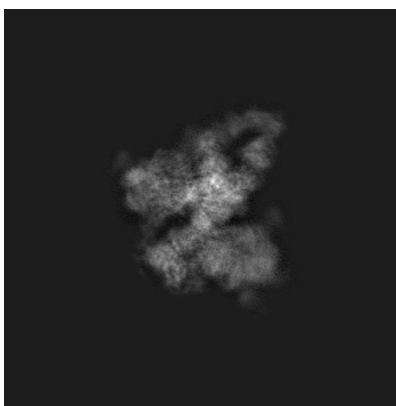
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

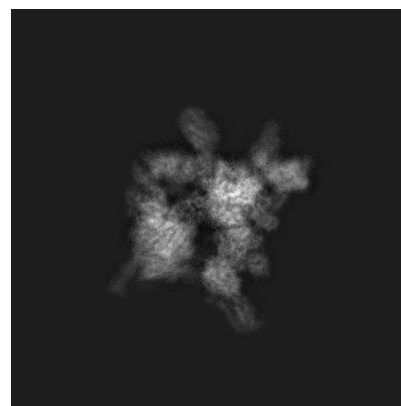
6.1.1 Primary map



X

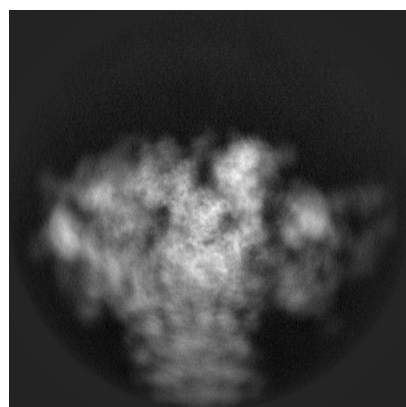


Y

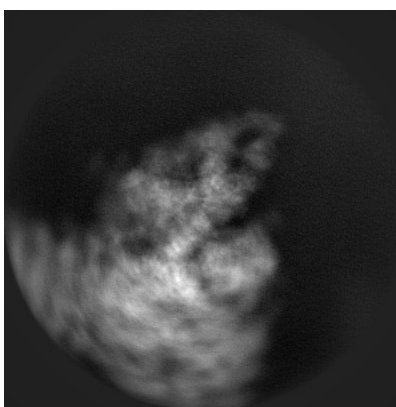


Z

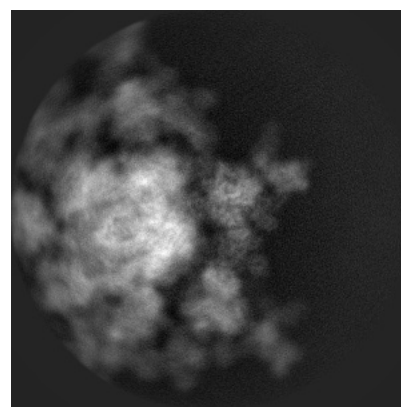
6.1.2 Raw map



X



Y

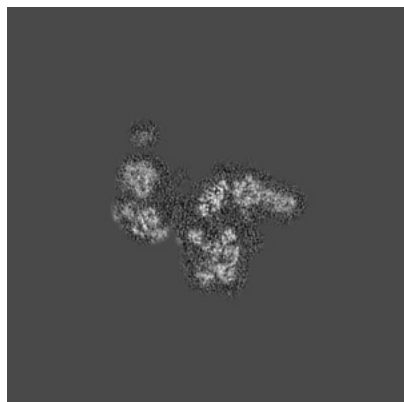


Z

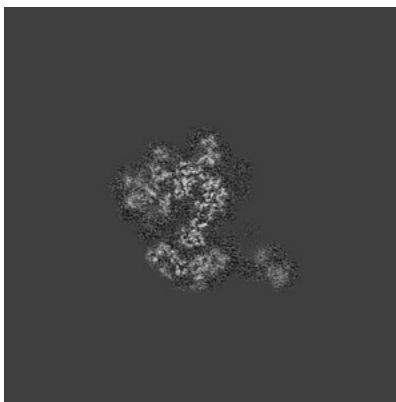
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

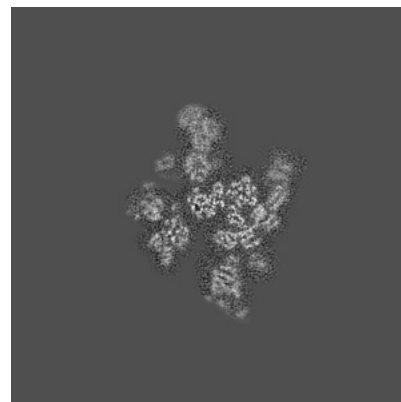
6.2.1 Primary map



X Index: 180

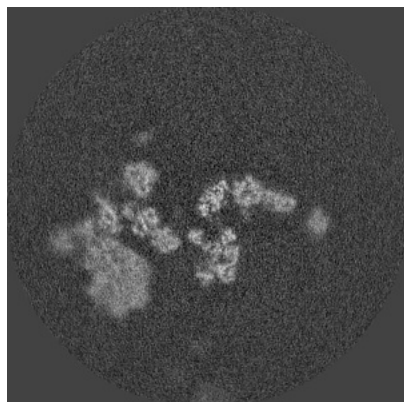


Y Index: 180

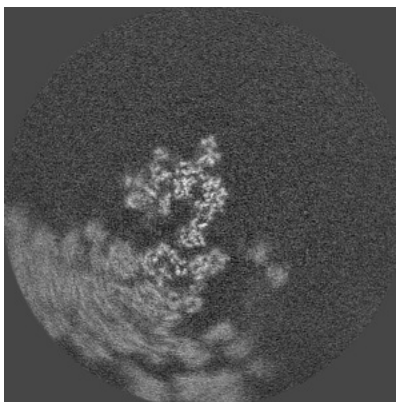


Z Index: 180

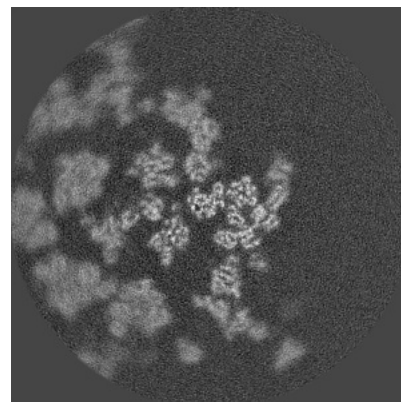
6.2.2 Raw map



X Index: 180



Y Index: 180

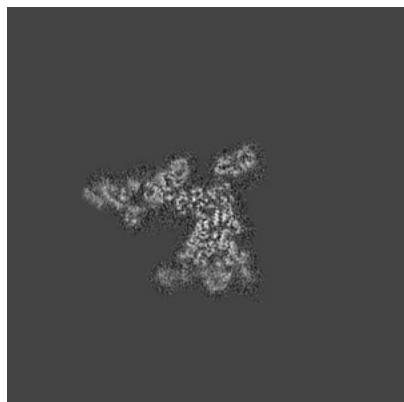


Z Index: 180

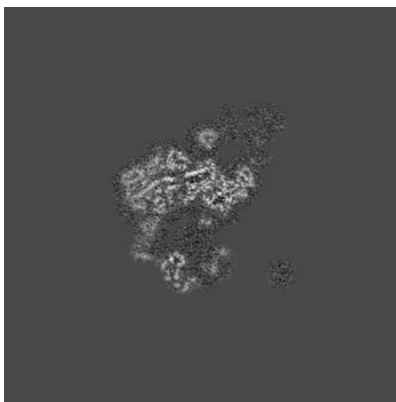
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

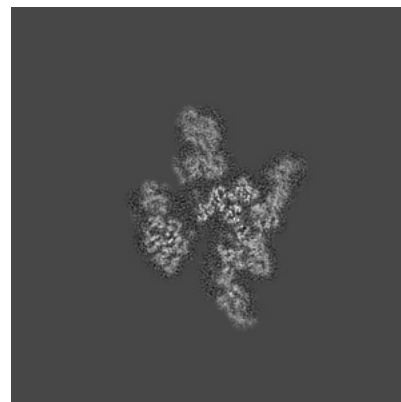
6.3.1 Primary map



X Index: 204

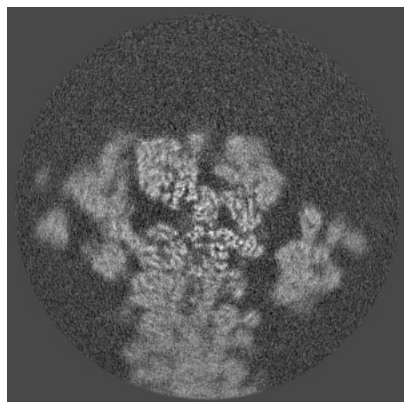


Y Index: 192

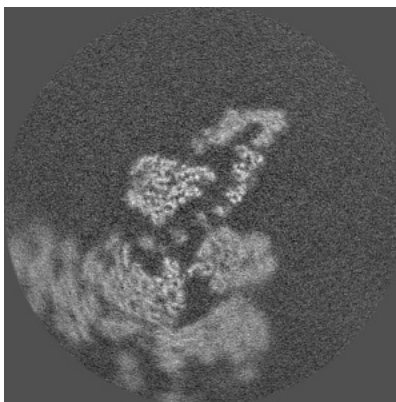


Z Index: 186

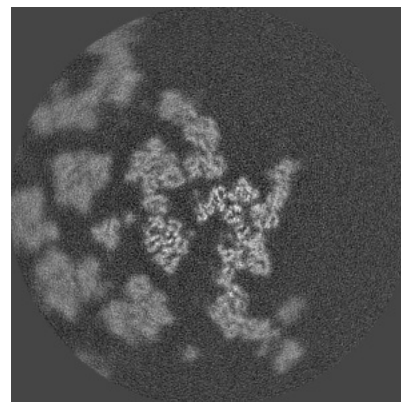
6.3.2 Raw map



X Index: 127



Y Index: 203

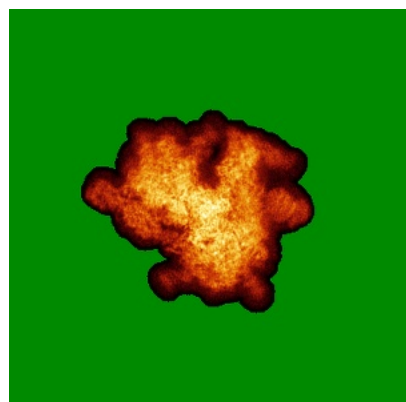


Z Index: 186

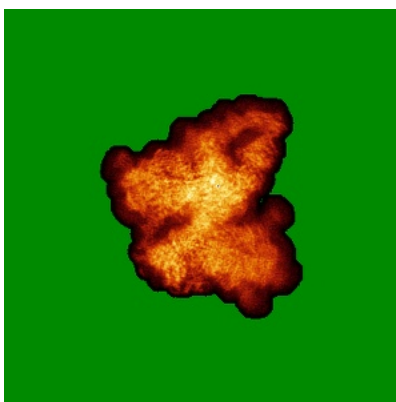
The images above show the largest variance slices of the map in three orthogonal directions.

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

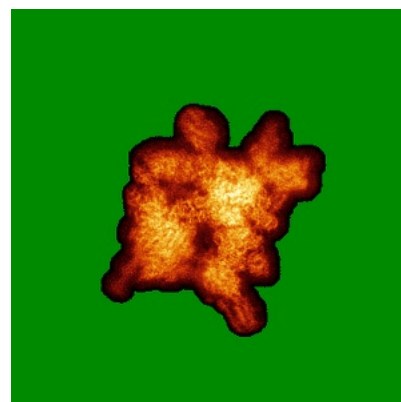
6.4.1 Primary map



X

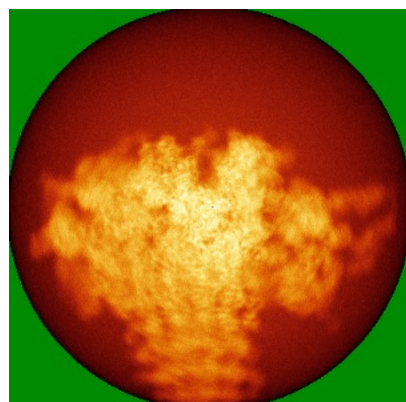


Y

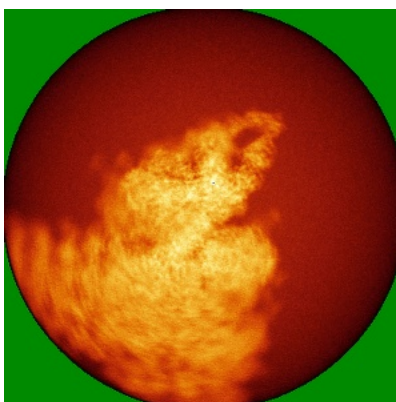


Z

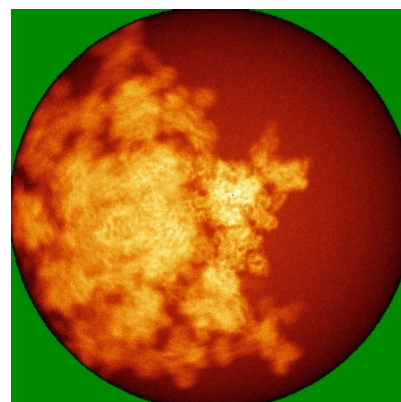
6.4.2 Raw map



X



Y

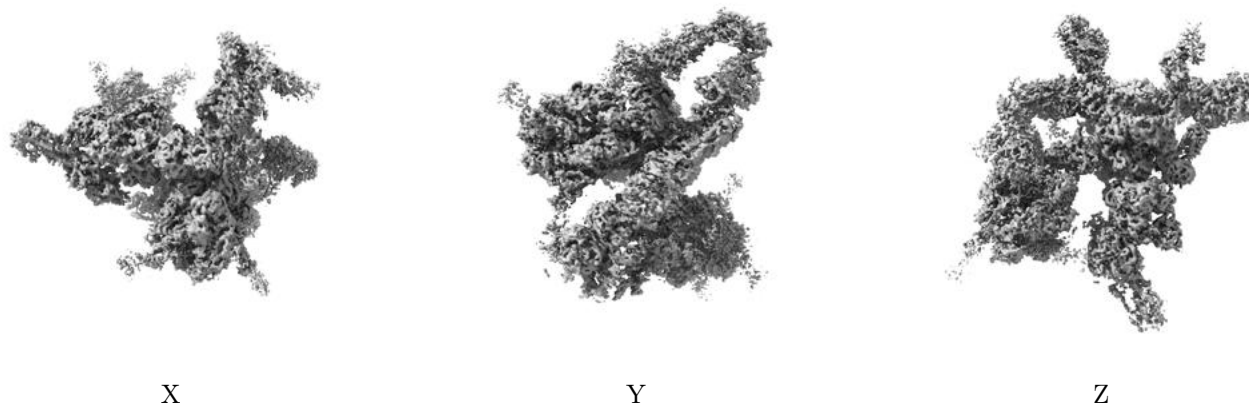


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

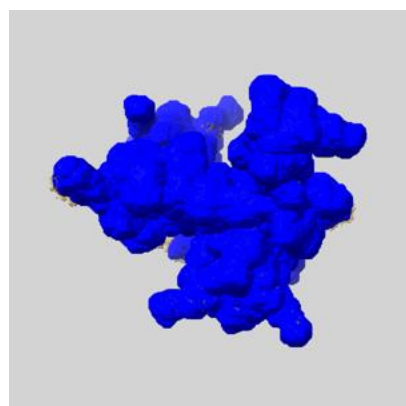
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

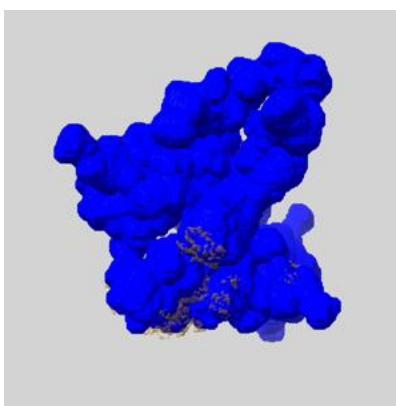
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

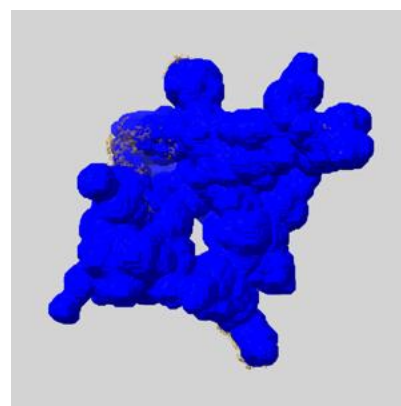
6.6.1 emd_55954_msk_1.map [i](#)



X



Y

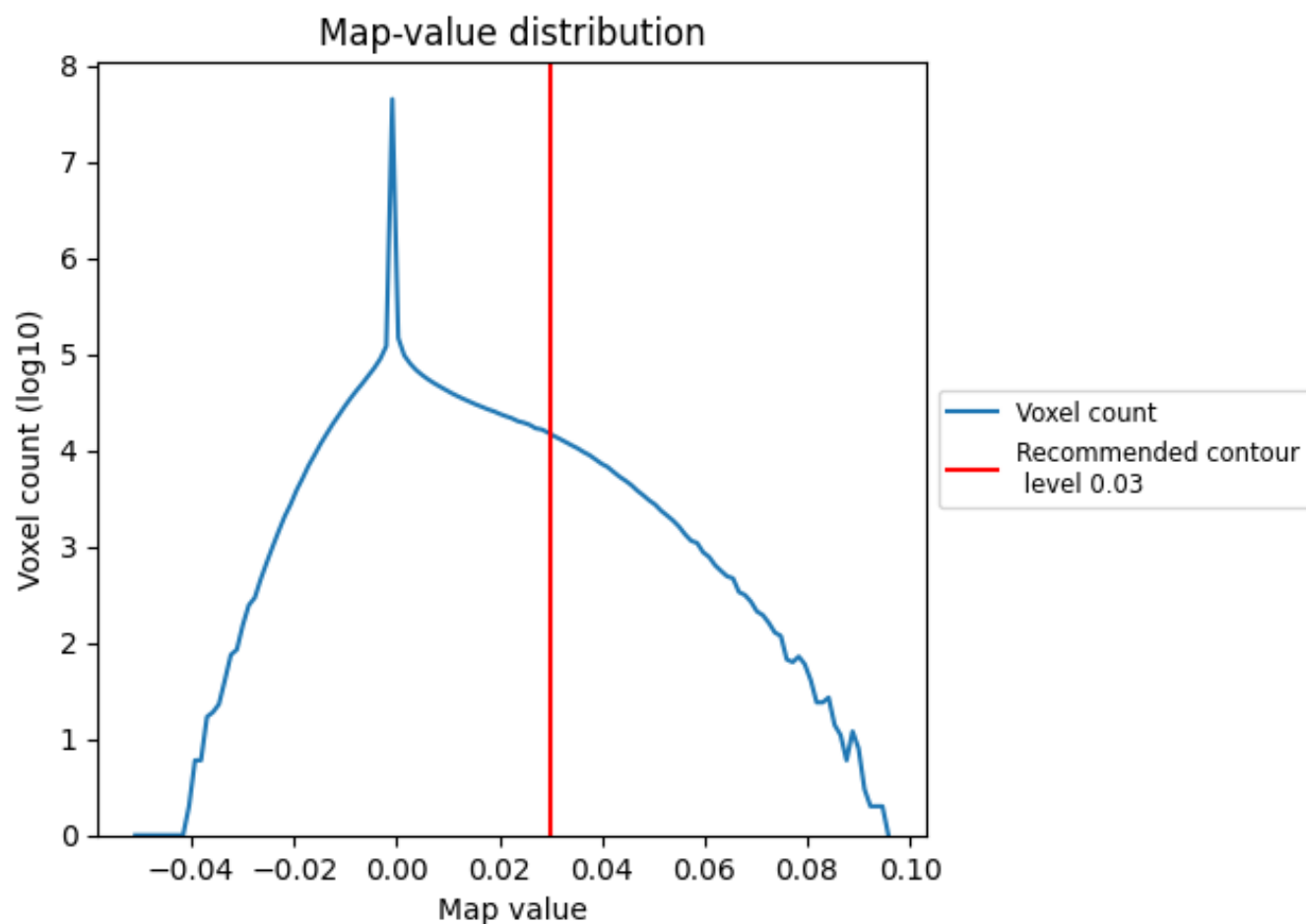


Z

7 Map analysis [i](#)

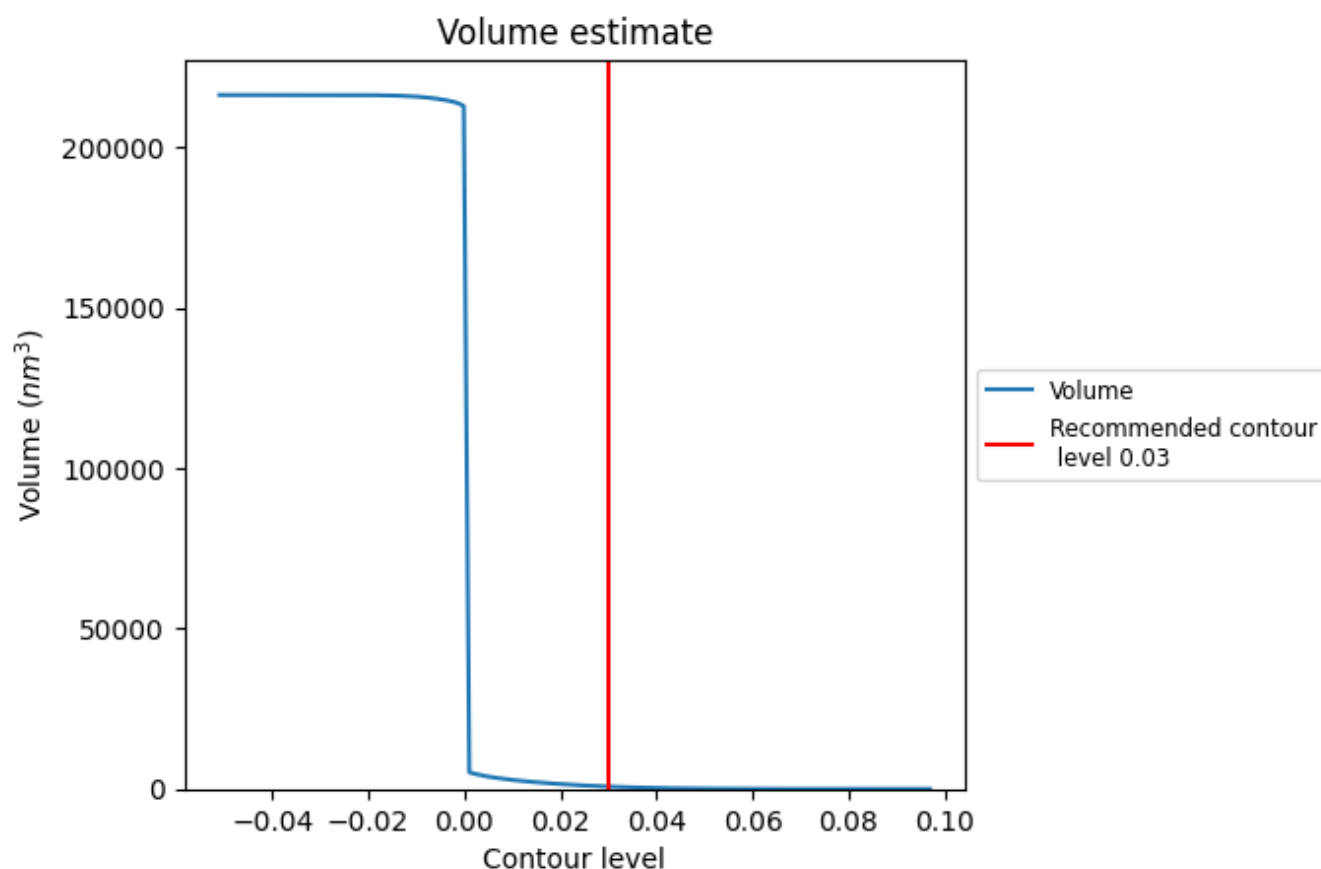
This section contains the results of statistical analysis of the map.

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.

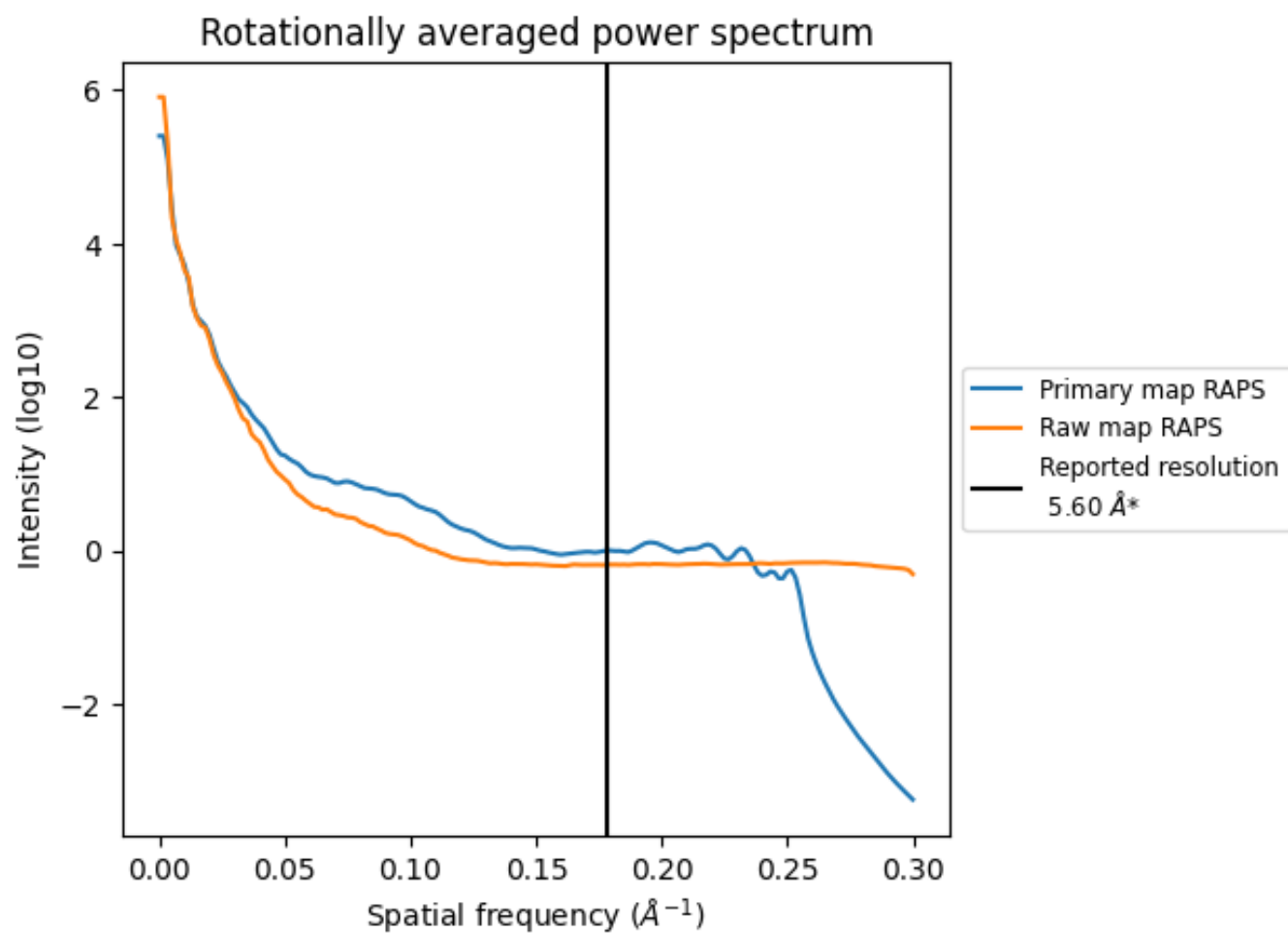
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 745 nm^3 ; this corresponds to an approximate mass of 673 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 ⓘ

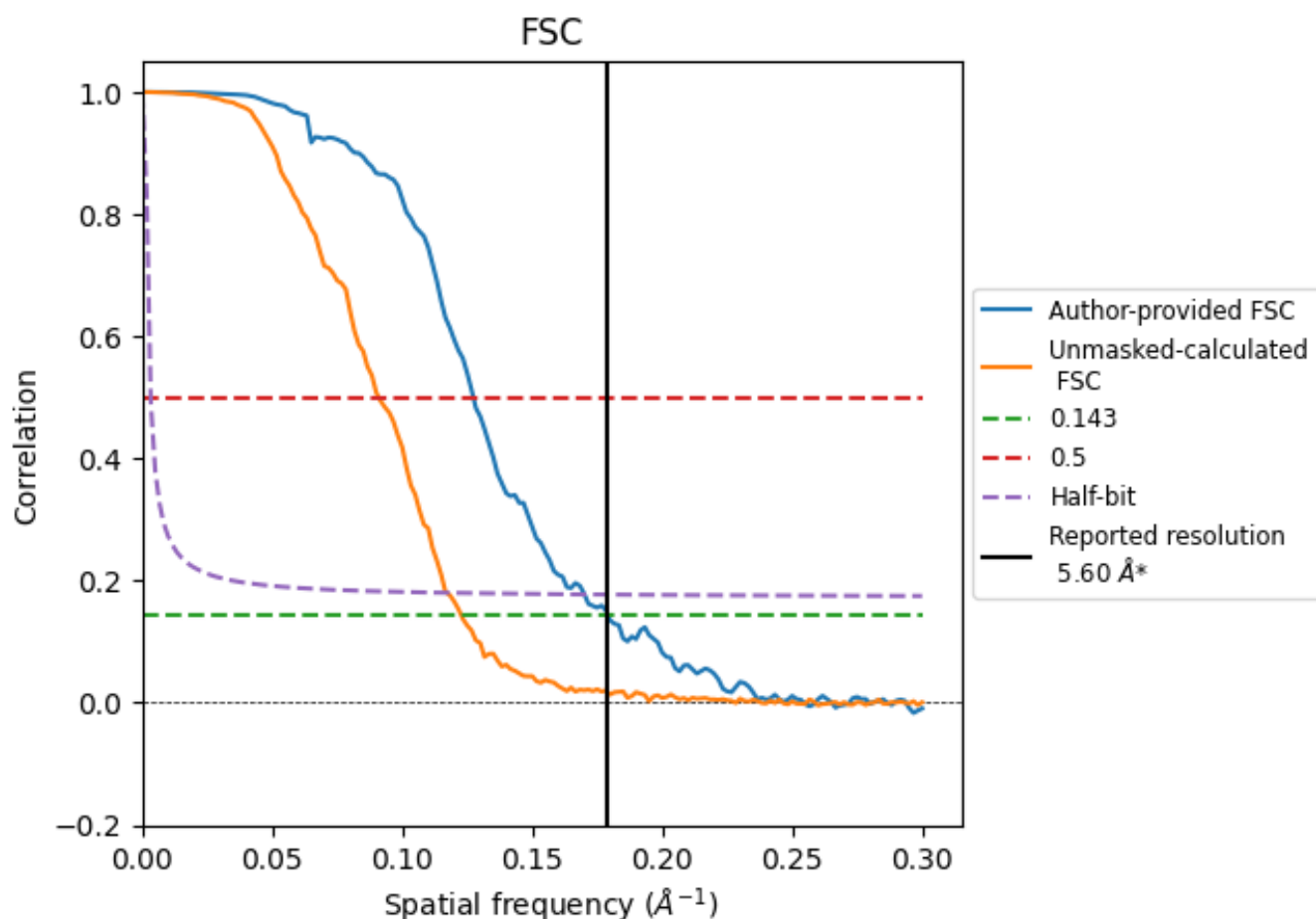


*Reported resolution corresponds to spatial frequency of 0.179 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.179 \AA^{-1}

8.2 Resolution estimates [i](#)

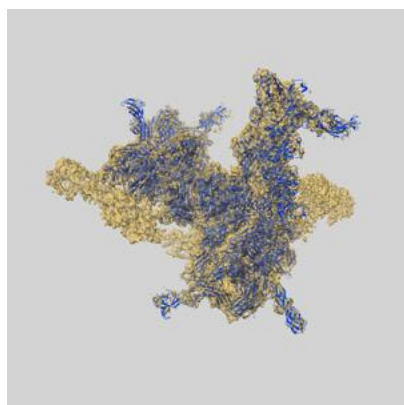
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	5.58	7.86	5.88
Unmasked-calculated*	8.15	10.99	8.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.15 differs from the reported value 5.6 by more than 10 %

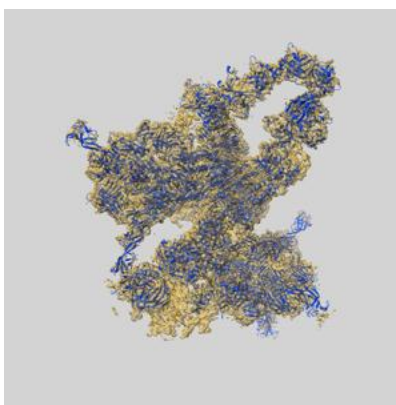
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55954 and PDB model 9TIF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

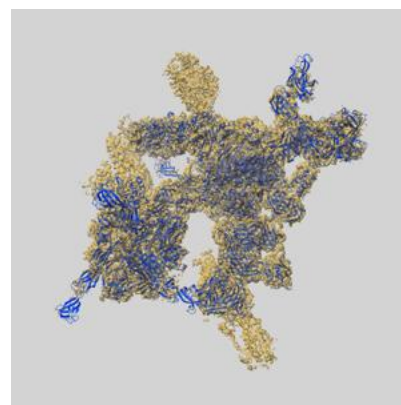
9.1 Map-model overlay [i](#)



X



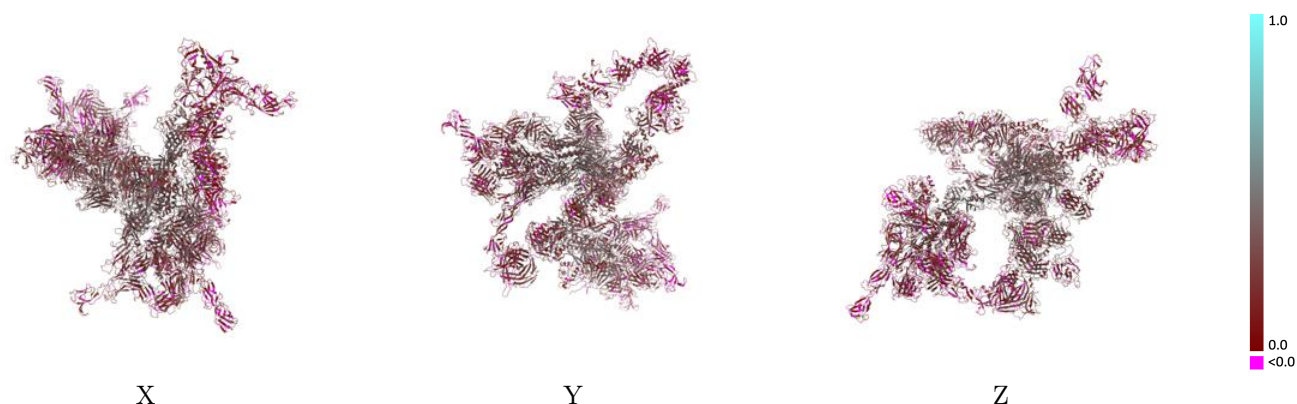
Y



Z

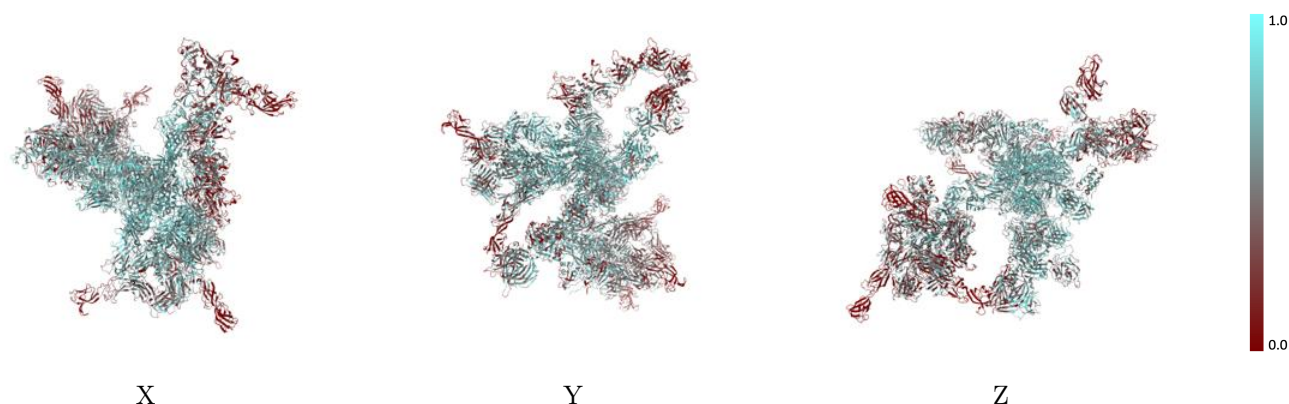
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



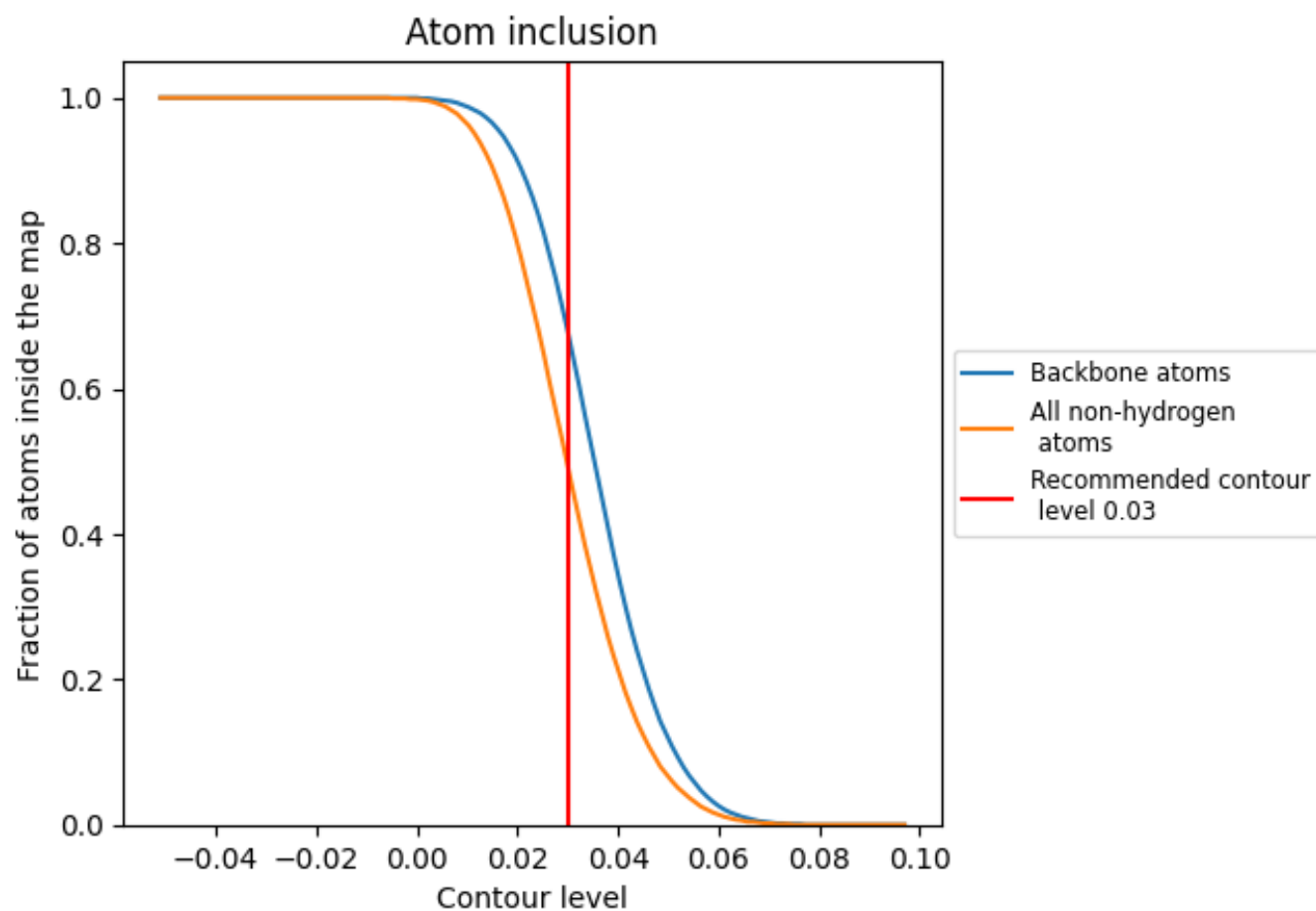
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4940	 0.2440
A	 0.5570	 0.2400
B	 0.5450	 0.2410
D	 0.3340	 0.1580
E	 0.6980	 0.3590
F	 0.3580	 0.2340
G	 0.5740	 0.2920
H	 0.4060	 0.2010
I	 0.7060	 0.3670
J	 0.6040	 0.2880
K	 0.2670	 0.1480
L	 0.3060	 0.1710
M	 0.4790	 0.1960
N	 0.5770	 0.2800
O	 0.6600	 0.3150
P	 0.4480	 0.2330
Q	 0.2940	 0.1620
R	 0.1980	 0.1520
S	 0.4730	 0.2210
T	 0.4910	 0.2260
U	 0.4940	 0.2360
V	 0.7080	 0.3820
b	 0.5210	 0.2880
c	 0.7310	 0.3880
d	 0.4200	 0.2280
e	 0.3790	 0.1950
f	 0.5520	 0.2650
g	 0.5460	 0.2640
h	 0.5420	 0.2550

