Full wwPDB EM Validation Report ⓘ

Jun 23, 2025 – 06:54 pm BST

PDB ID	:	9R86 / pdb_00009r86
EMDB ID	:	EMD-53805
Title	:	Major Vault Protein from Human Brain
Authors	:	Lovestam, S.L.; Scheres, S.H.W.
Deposited on	:	2025-05-15
Resolution	:	3.10 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:

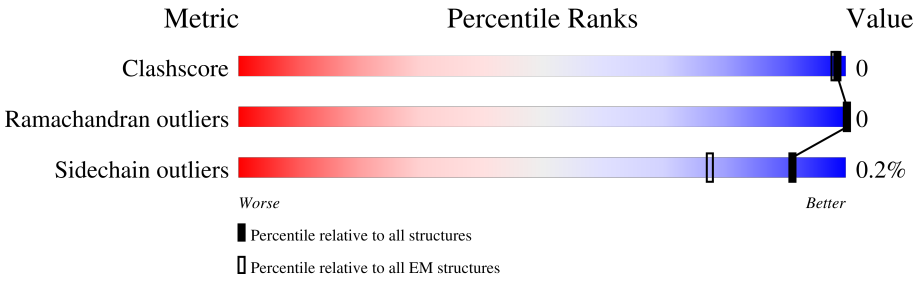
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A0	893	78% · 21%
1	A1	893	77% · 21%
1	A2	893	77% · 21%
1	A3	893	77% · 21%
1	A4	893	77% · 21%
1	A5	893	77% · 21%
1	A6	893	77% · 21%
1	A7	893	77% · 21%

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Mol	Chain	Length	Quality of chain
1	A8	893	76% 21%
1	A9	893	77% 21%
1	Ac	893	77% 21%
1	Ad	893	77% 21%
1	Ae	893	77% 21%
1	Af	893	77% 21%
1	Ag	893	77% 21%
1	Ah	893	77% 21%
1	Ai	893	77% 21%
1	Aj	893	77% 21%
1	Ak	893	77% 21%
1	Al	893	77% 21%
1	Am	893	77% 21%
1	An	893	77% 21%
1	Ap	893	77% 21%
1	Aq	893	77% 21%
1	Ar	893	77% 21%
1	As	893	77% 21%
1	At	893	77% 21%
1	Au	893	77% 21%
1	Av	893	77% 21%
1	Aw	893	77% 21%
1	Ax	893	77% 21%
1	Ay	893	77% 21%
1	Az	893	78% 21%

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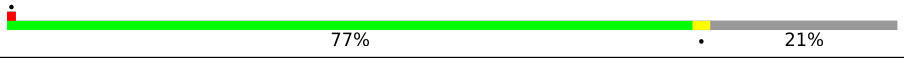
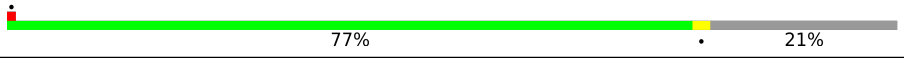
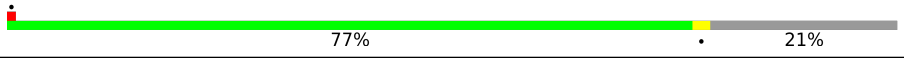
Mol	Chain	Length	Quality of chain
1	BA	893	
1	BB	893	
1	BC	893	
1	BD	893	
1	BE	893	
1	BF	893	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 440774 atoms, of which 220502 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 Major vault protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A0	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A1	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A2	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A3	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A4	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A5	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A6	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A7	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A8	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	A9	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ac	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ad	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ae	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Af	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ag	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ah	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ai	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Aj	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ak	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Al	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Am	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	An	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ap	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Aq	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ar	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	As	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	At	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Au	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Av	709	Total	C	H	N	O	S	0	0
			11298	3548	5650	1015	1076	9		
1	Aw	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ax	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Ay	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	Az	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	BA	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	BB	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	BC	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	BD	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		
1	BE	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		

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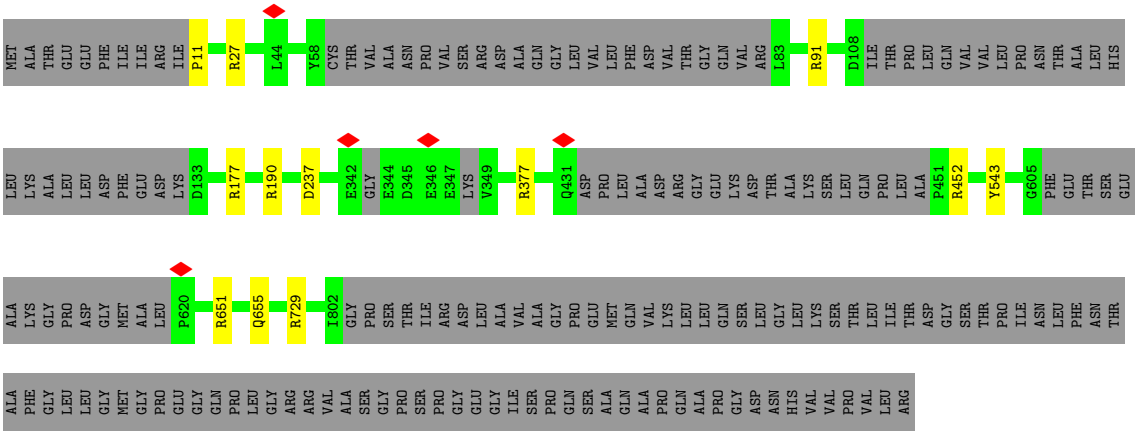
Mol	Chain	Residues	Atoms						AltConf	Trace
1	BF	709	Total	C	H	N	O	S	0	0
			11302	3548	5654	1015	1076	9		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

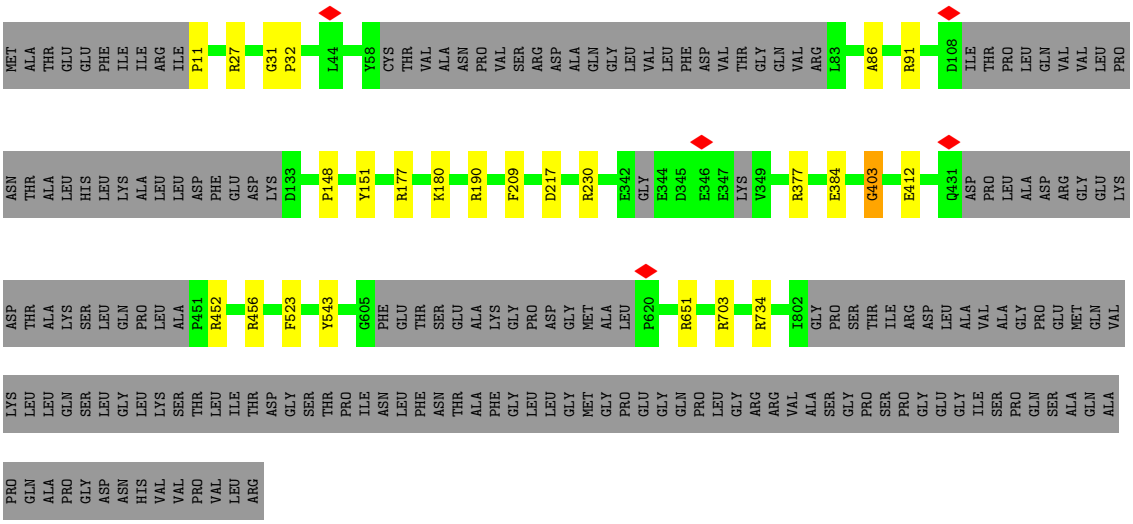
• Molecule 1: Major vault protein

Chain A0:



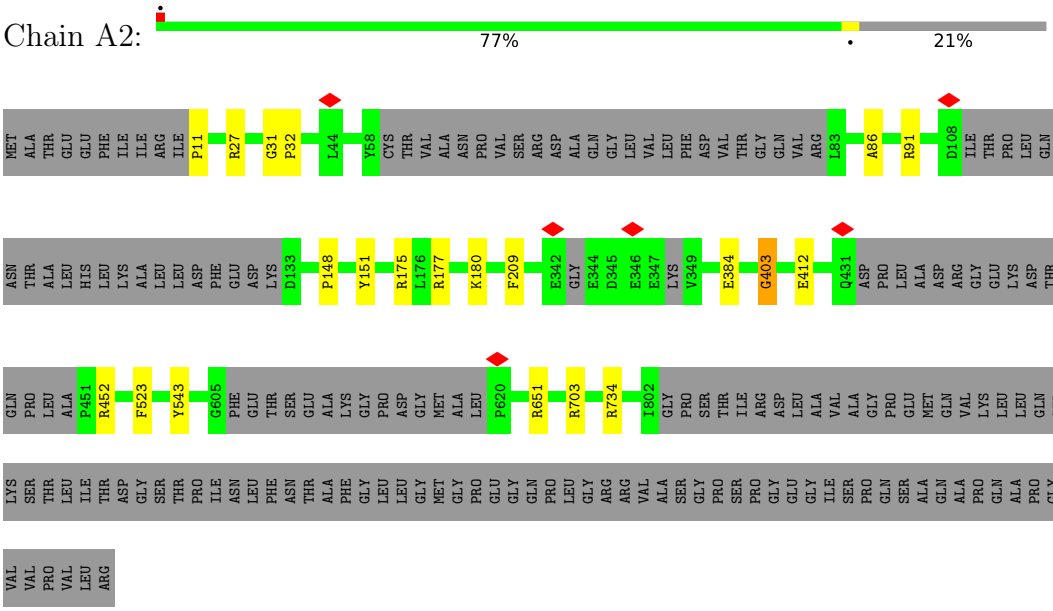
• Molecule 1: Major vault protein

Chain A1:



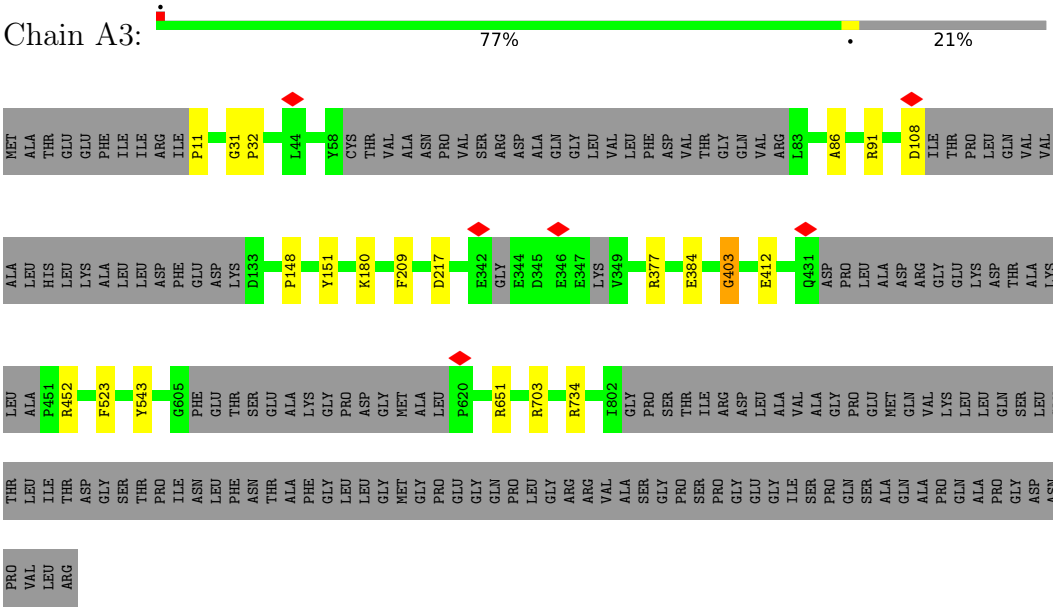
• Molecule 1: Major vault protein

Chain A2:



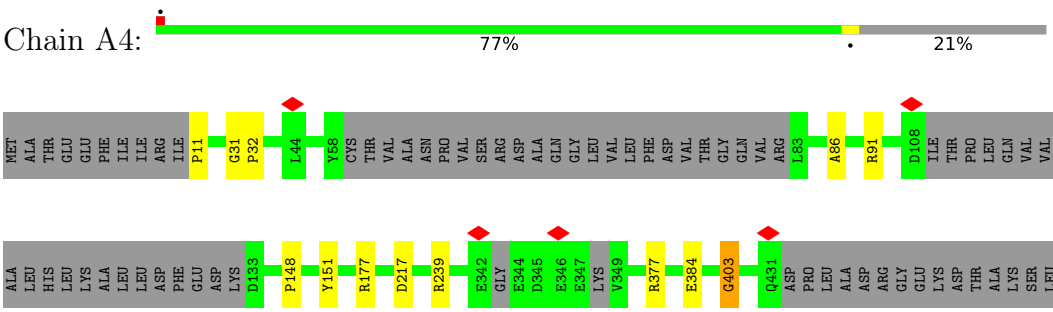
• Molecule 1: Major vault protein

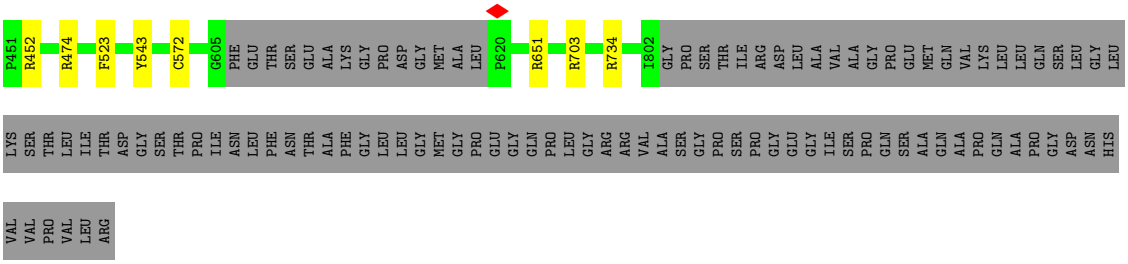
Chain A3:



• Molecule 1: Major vault protein

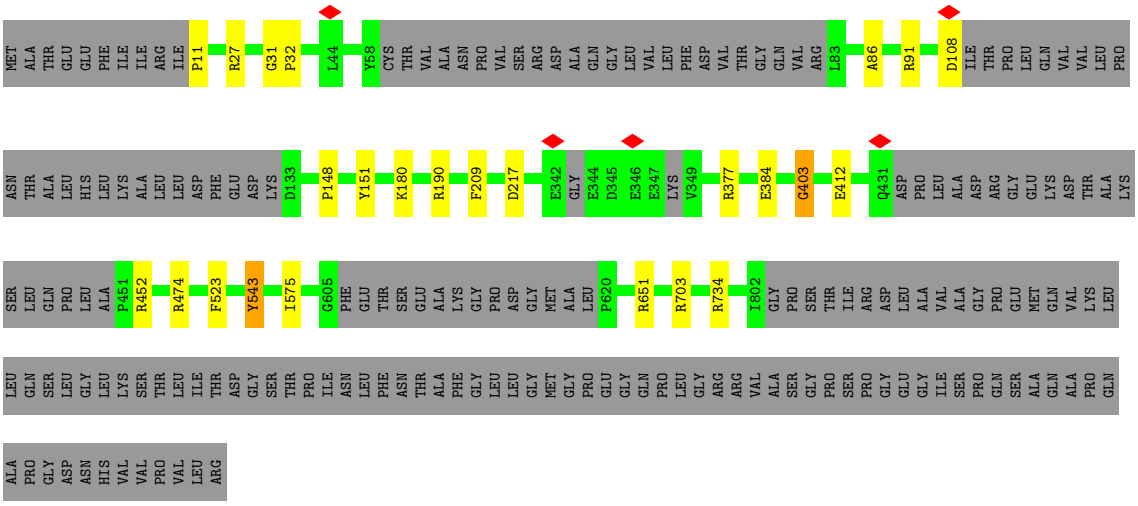
Chain A4:





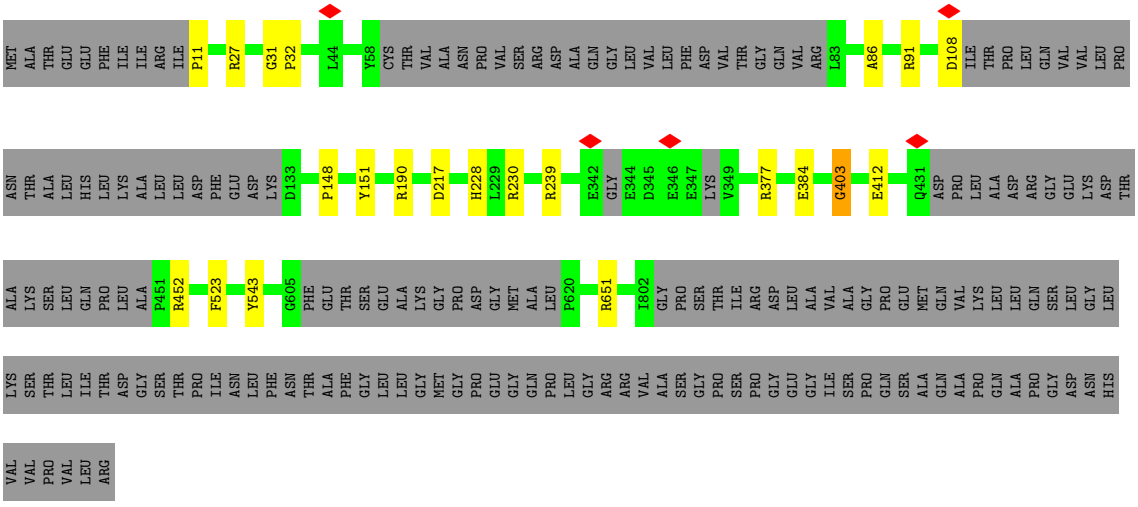
• Molecule 1: Major vault protein

Chain A5:



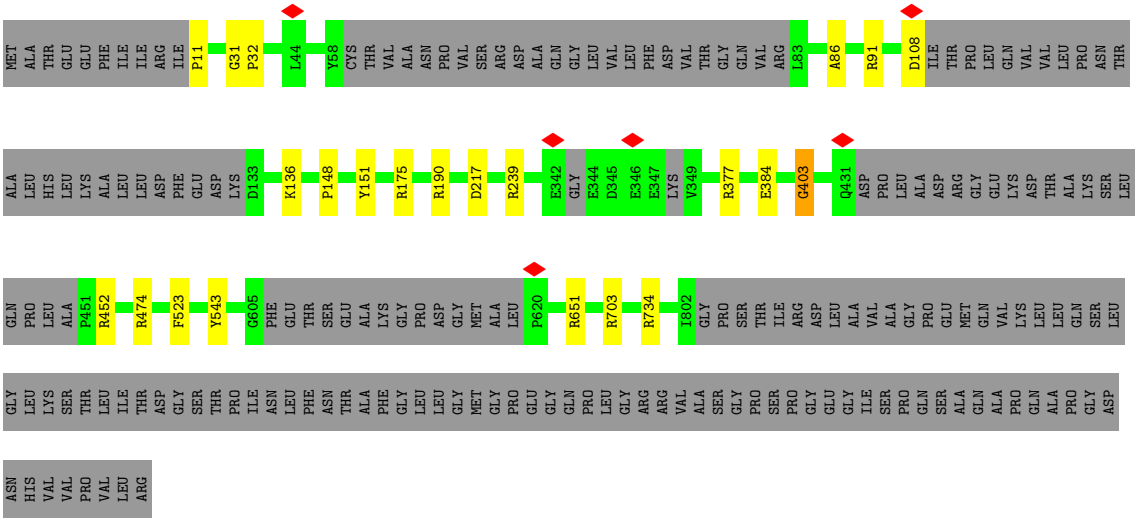
• Molecule 1: Major vault protein

Chain A6:



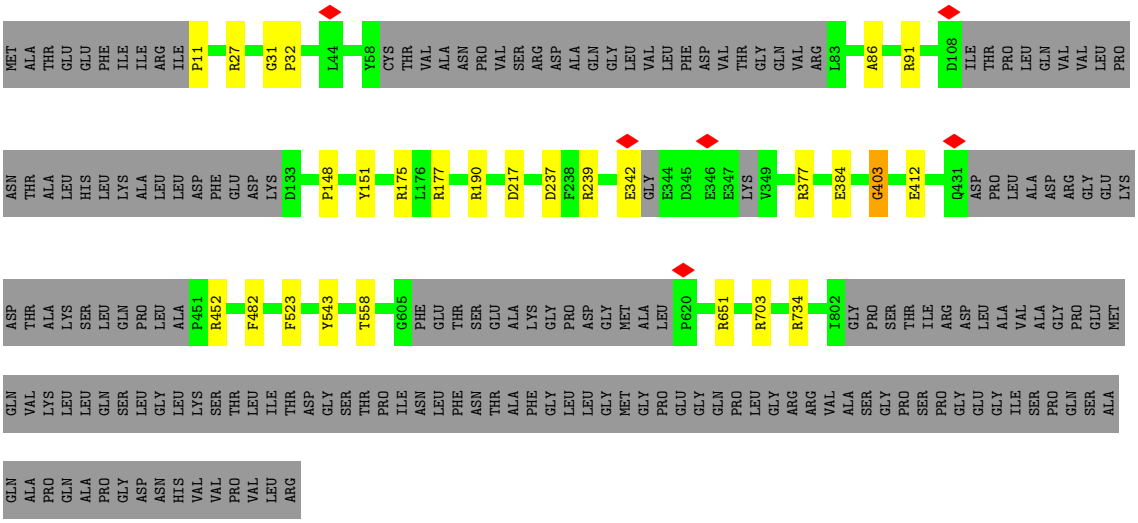
• Molecule 1: Major vault protein

Chain A7:



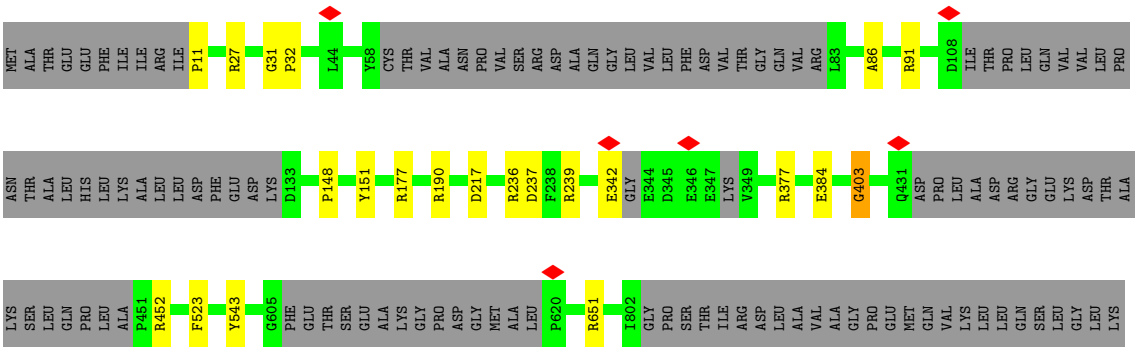
• Molecule 1: Major vault protein

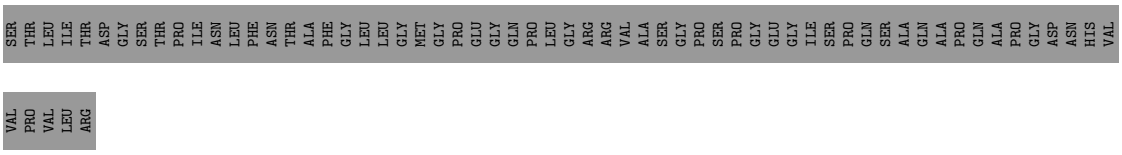
Chain A8:



• Molecule 1: Major vault protein

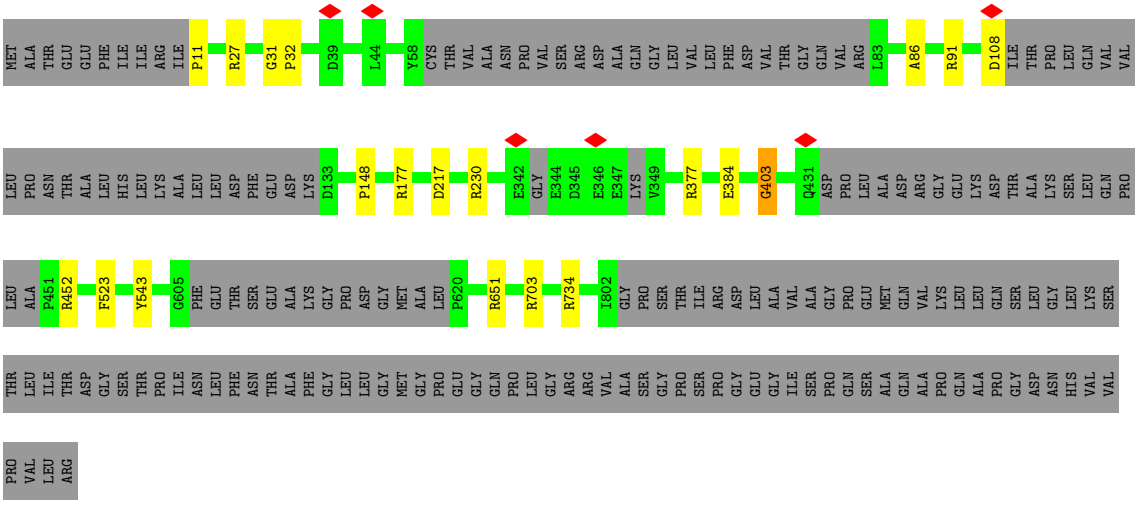
Chain A9:





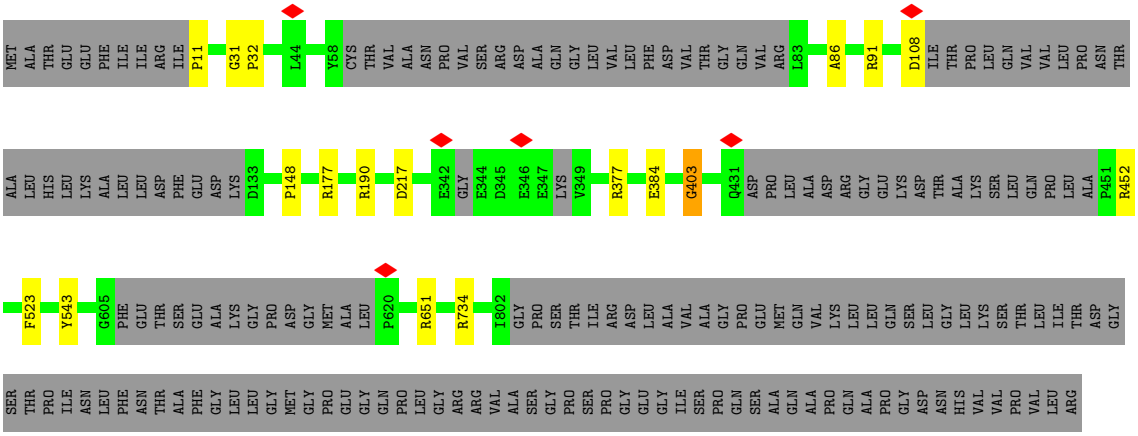
• Molecule 1: Major vault protein

Chain Ac:



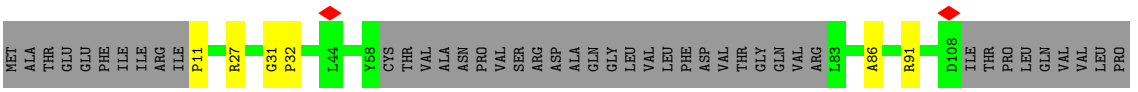
• Molecule 1: Major vault protein

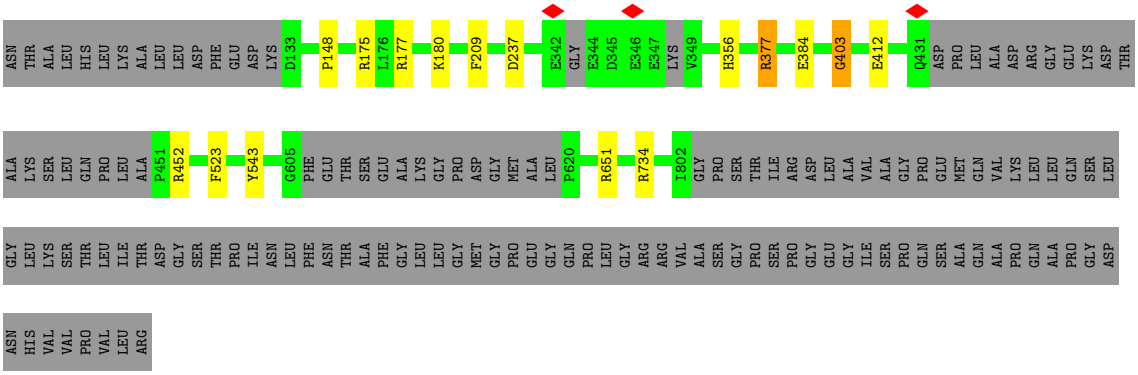
Chain Ad:



• Molecule 1: Major vault protein

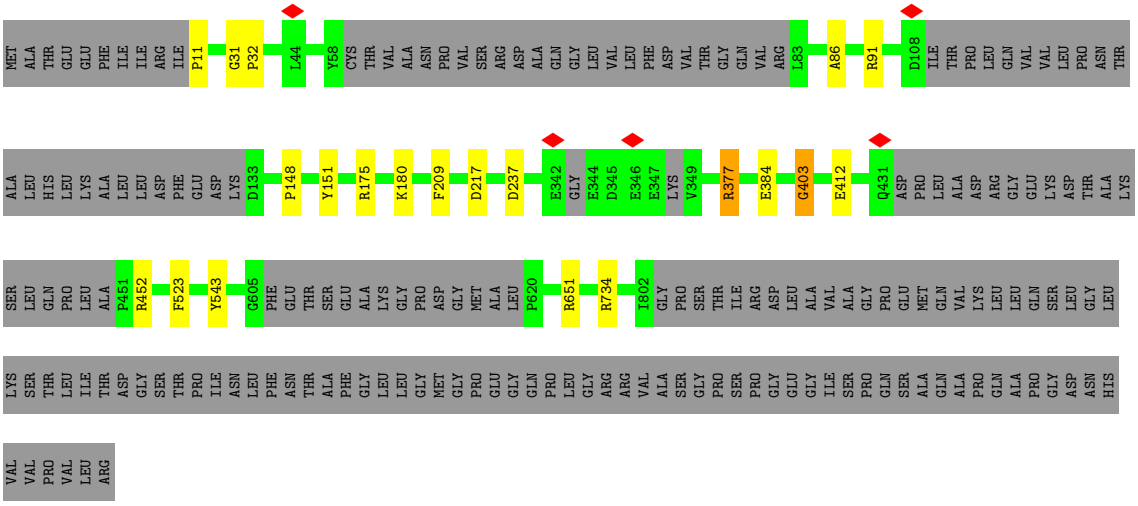
Chain Ae:





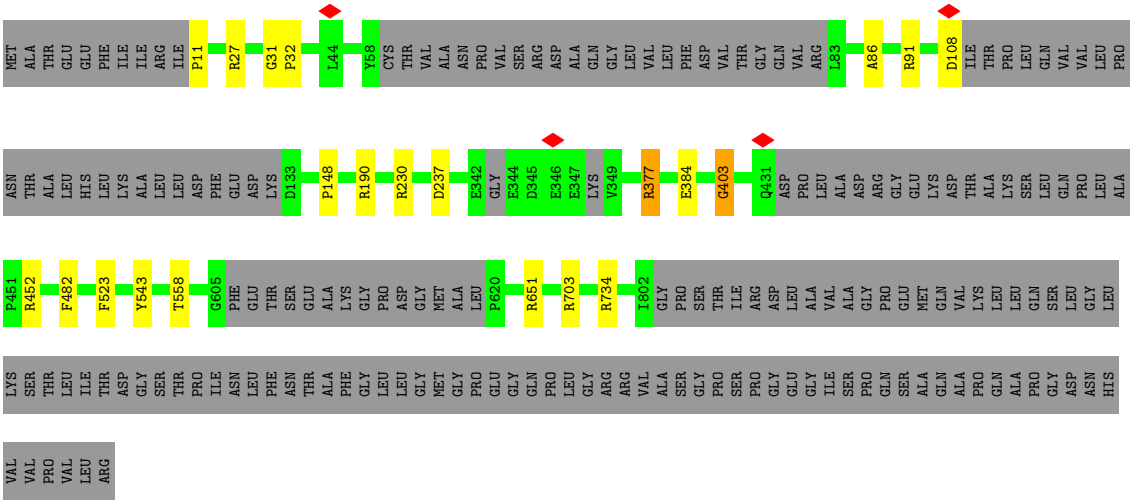
• Molecule 1: Major vault protein

Chain Af:



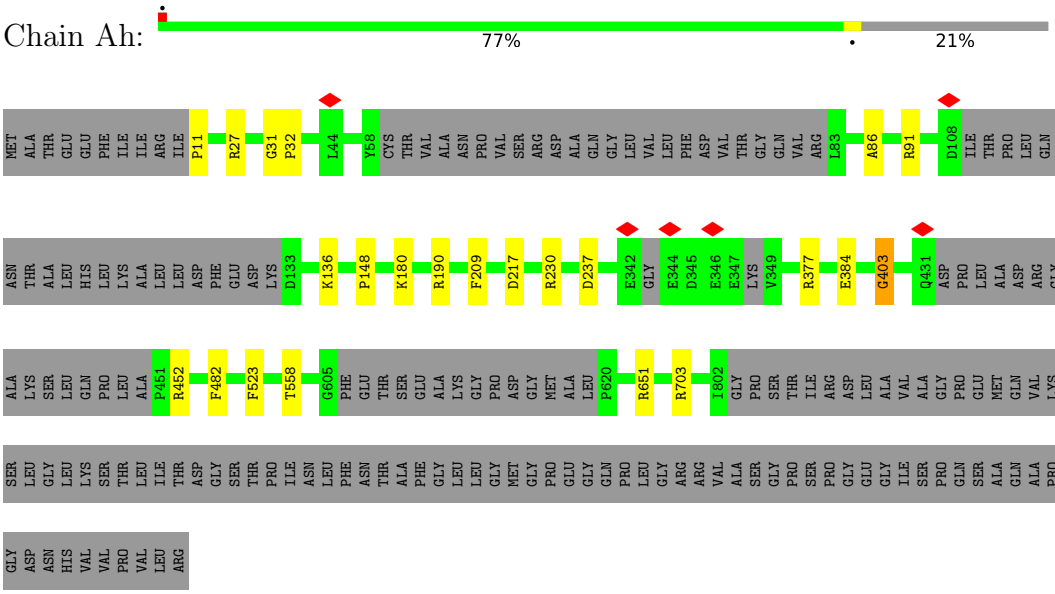
• Molecule 1: Major vault protein

Chain Ag:



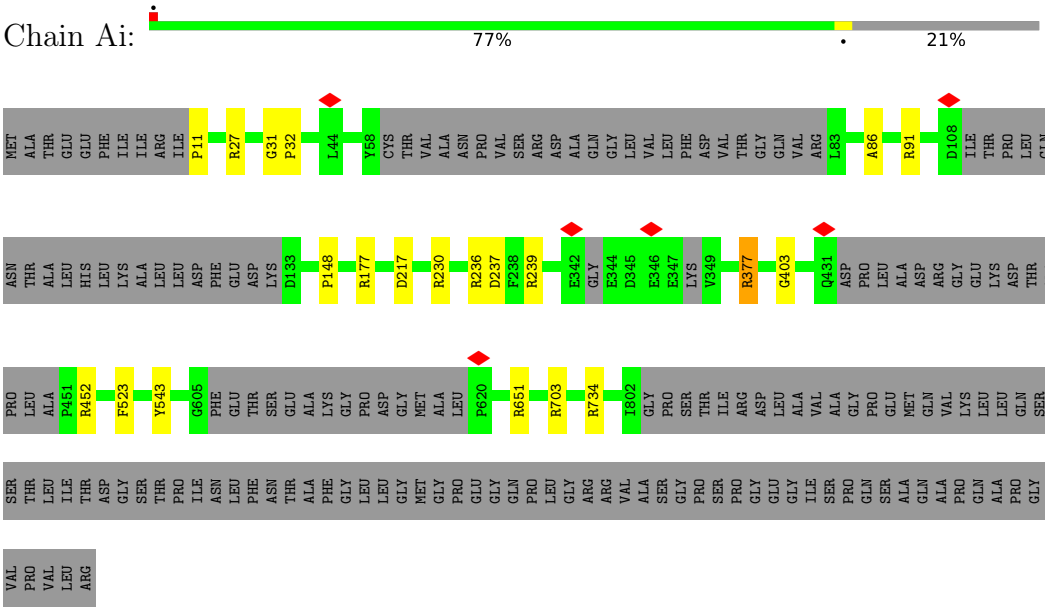
• Molecule 1: Major vault protein

Chain Ah:



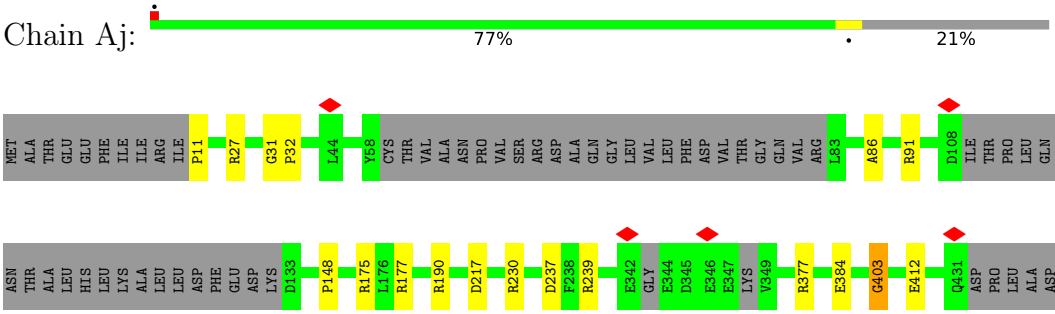
• Molecule 1: Major vault protein

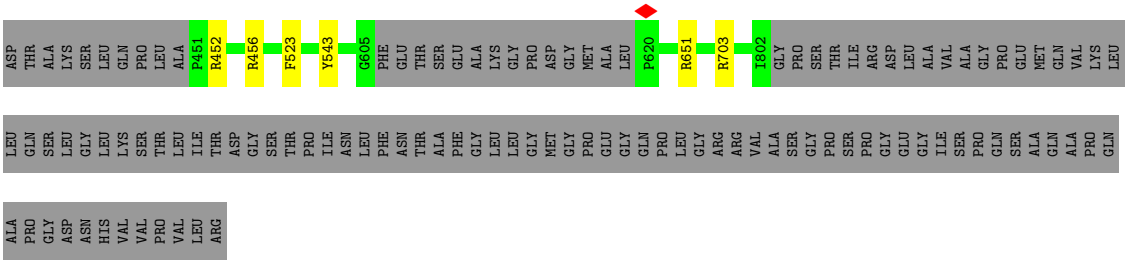
Chain Ai:



• Molecule 1: Major vault protein

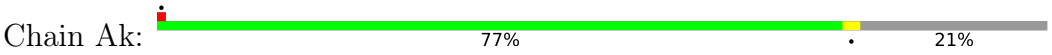
Chain Aj:

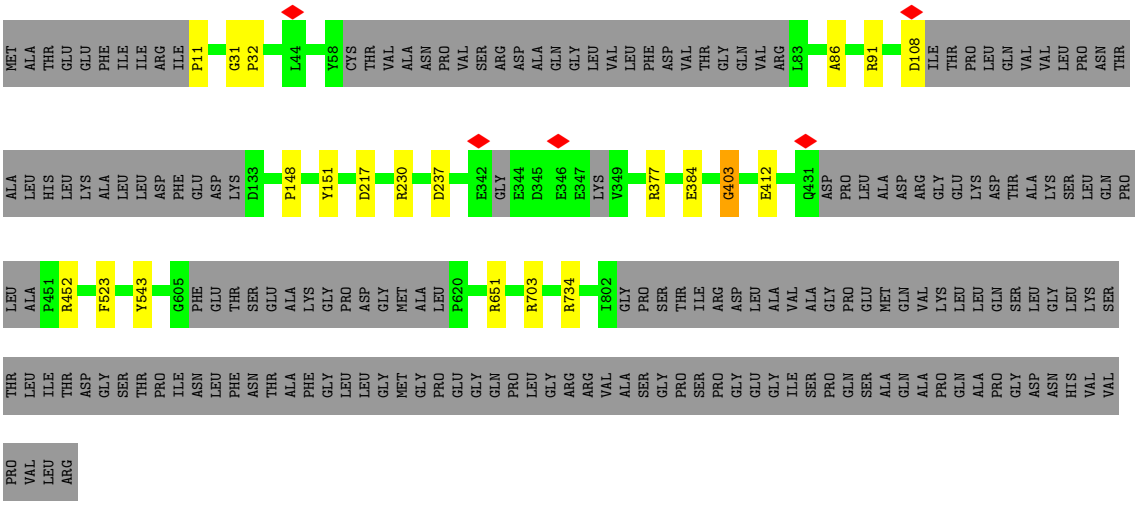




• Molecule 1: Major vault protein

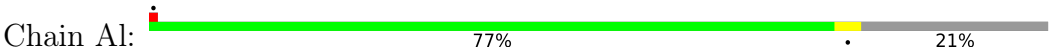
Chain Ak:

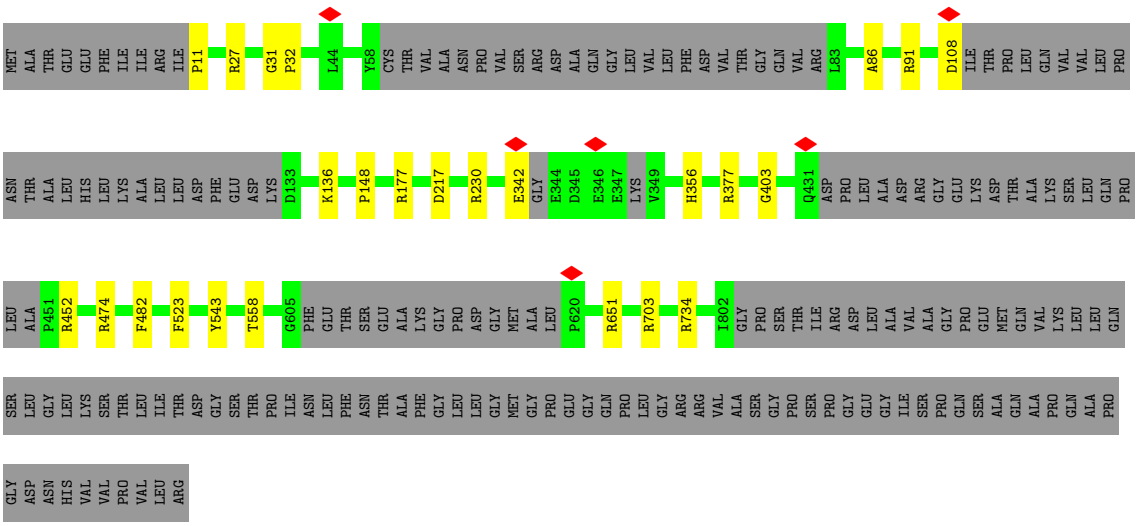




• Molecule 1: Major vault protein

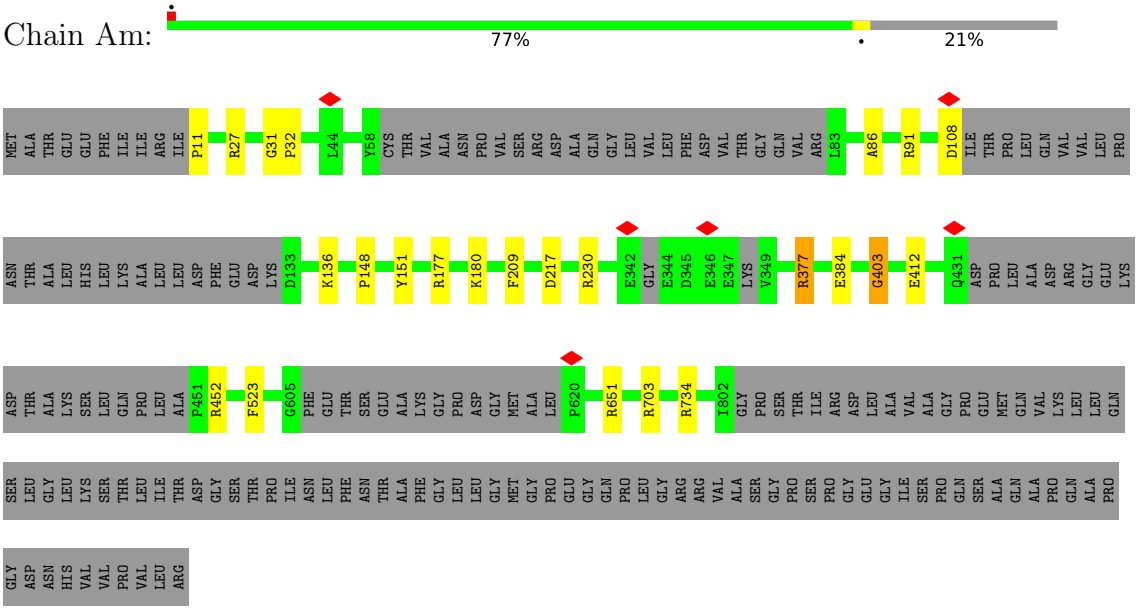
Chain Al:





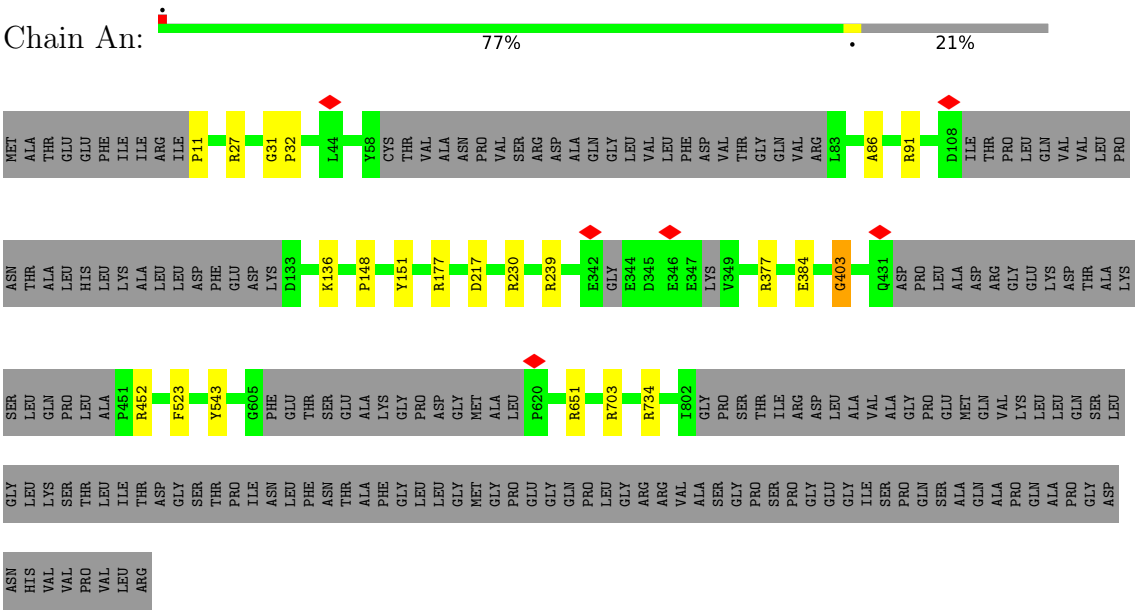
• Molecule 1: Major vault protein

Chain Am:



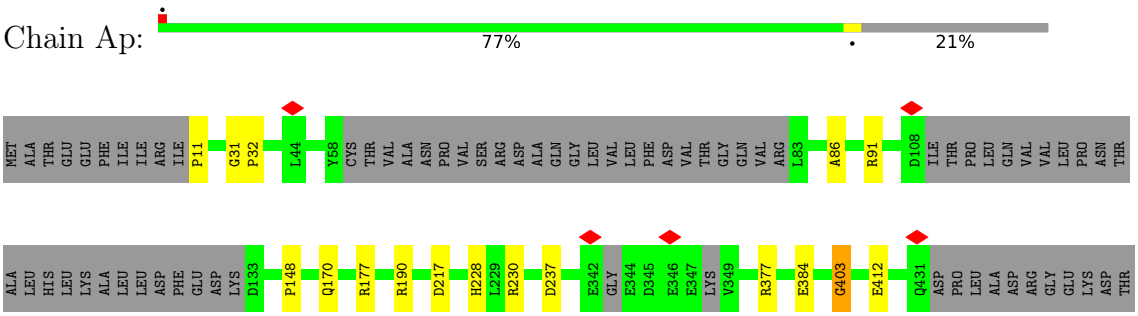
• Molecule 1: Major vault protein

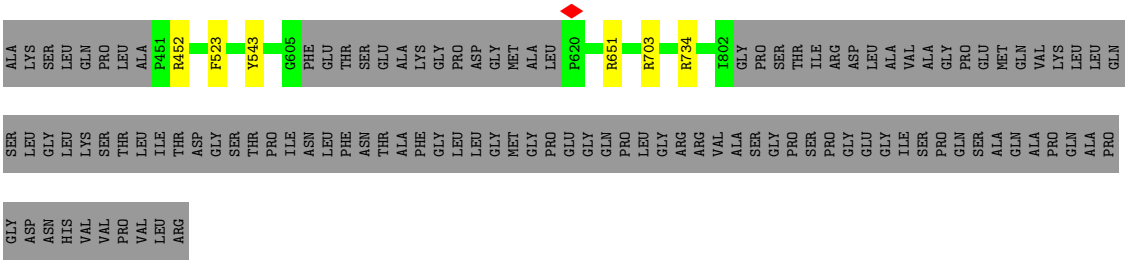
Chain An:



• Molecule 1: Major vault protein

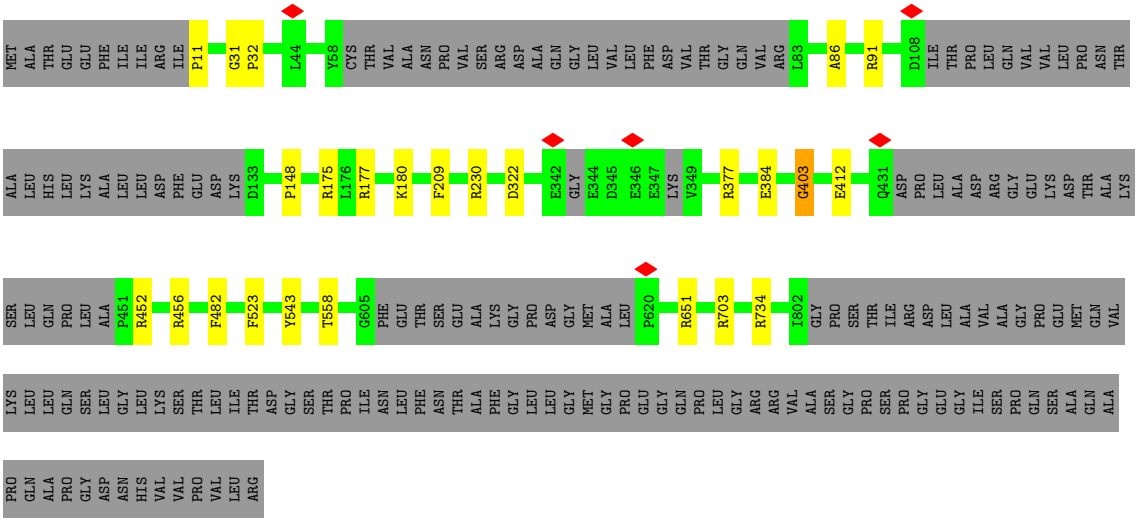
Chain Ap:





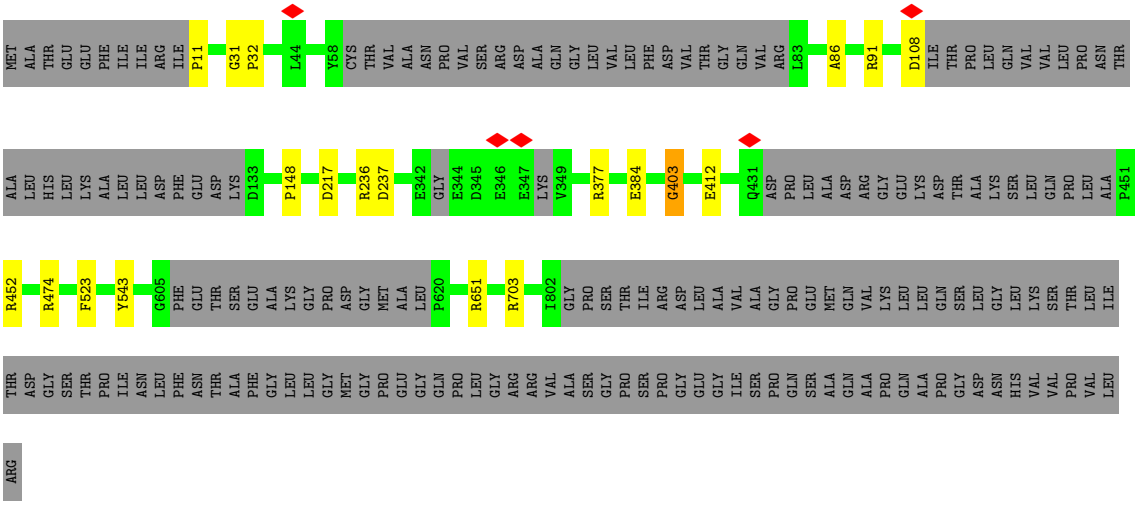
• Molecule 1: Major vault protein

Chain Aq:



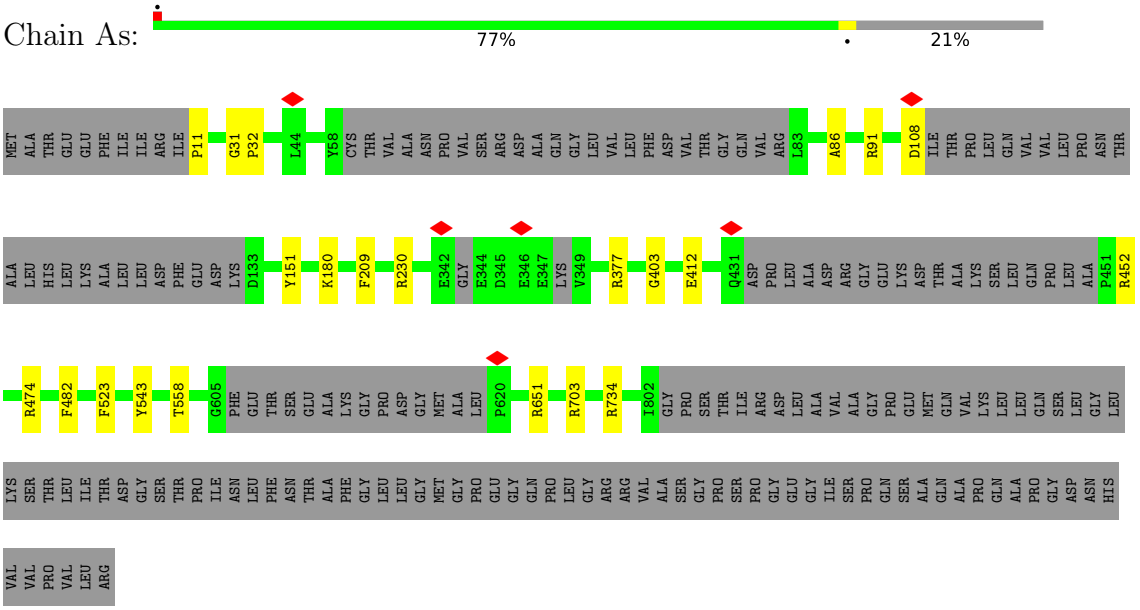
• Molecule 1: Major vault protein

Chain Ar:



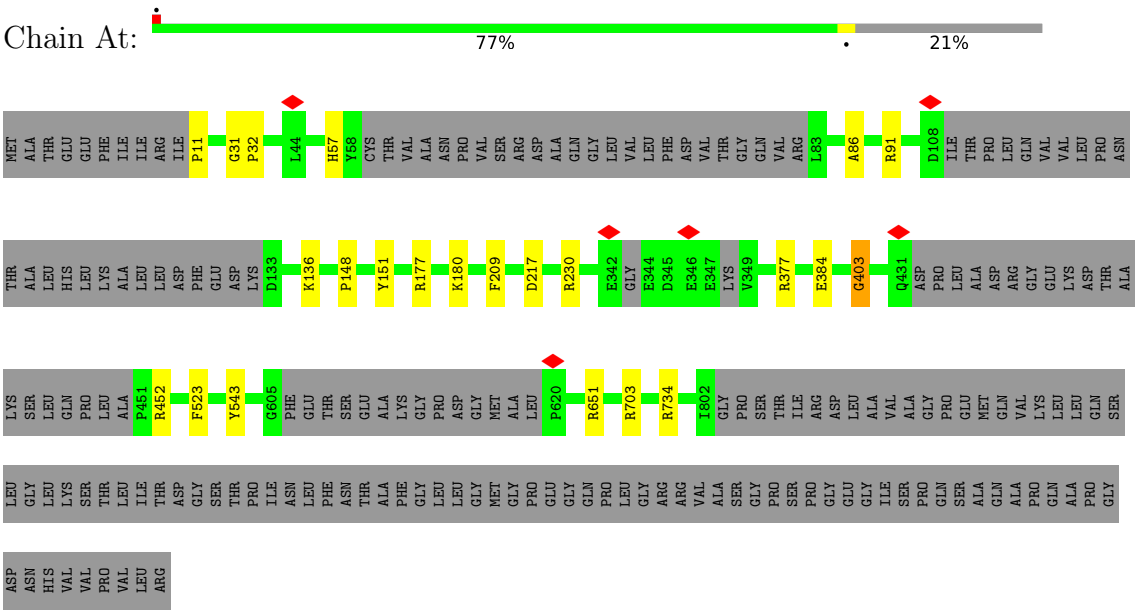
• Molecule 1: Major vault protein

Chain As:



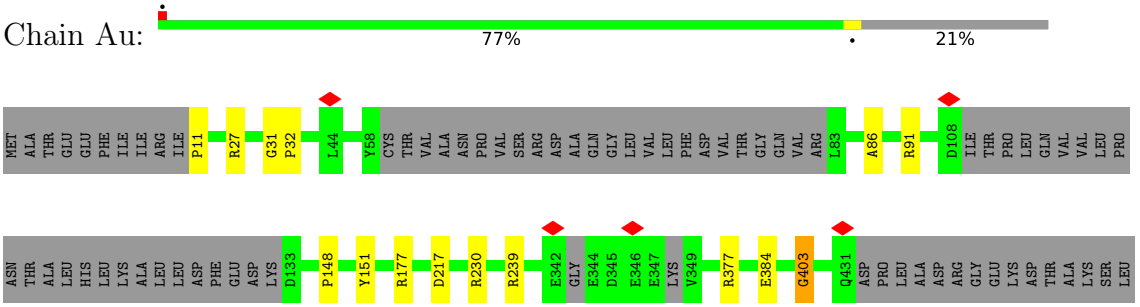
• Molecule 1: Major vault protein

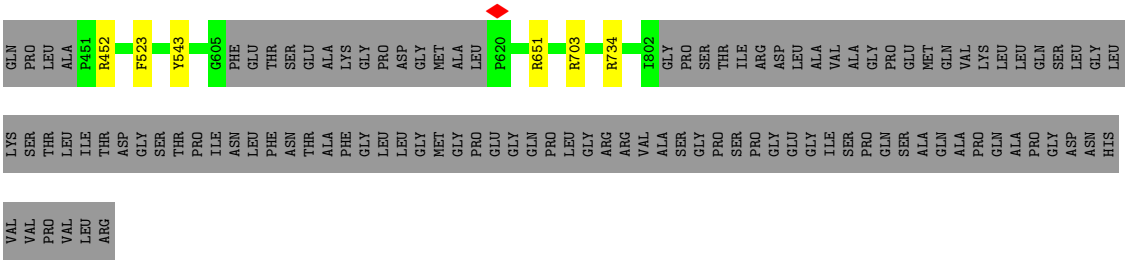
Chain At:



• Molecule 1: Major vault protein

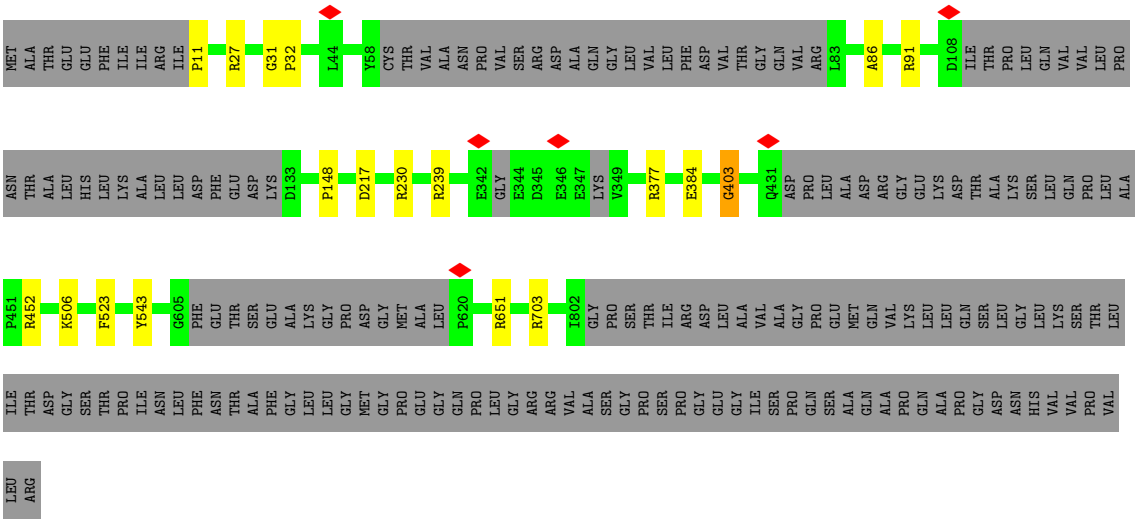
Chain Au:





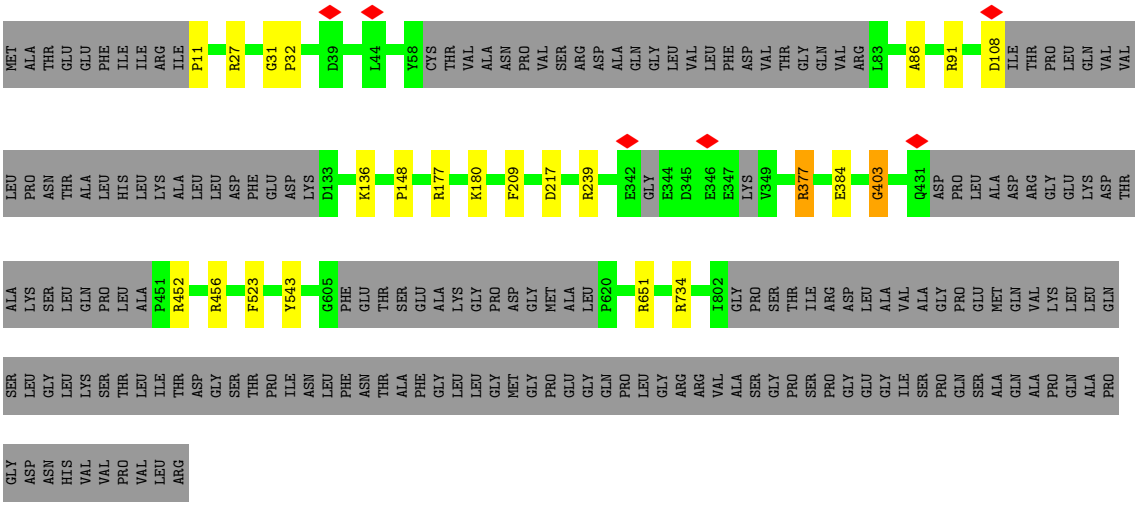
• Molecule 1: Major vault protein

Chain Av:



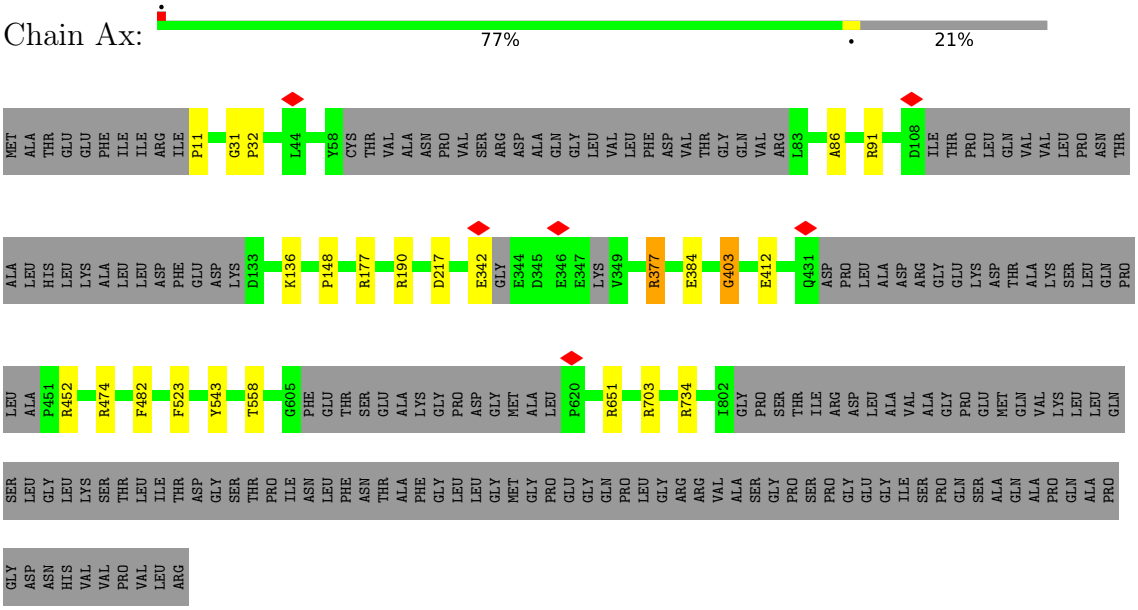
• Molecule 1: Major vault protein

Chain Aw:



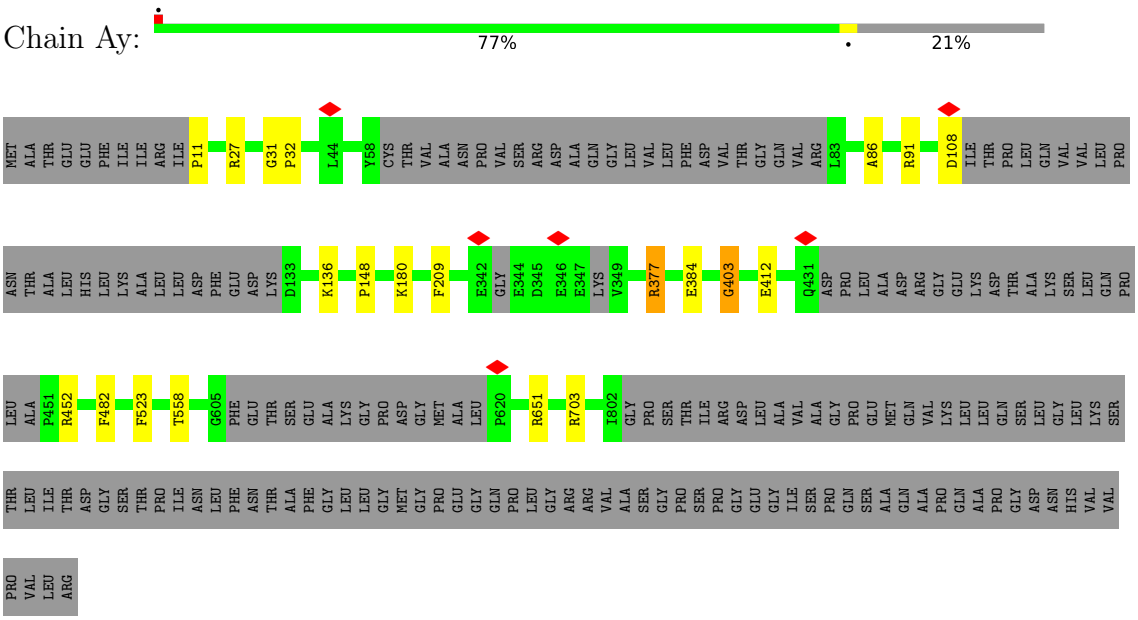
• Molecule 1: Major vault protein

Chain Ax:



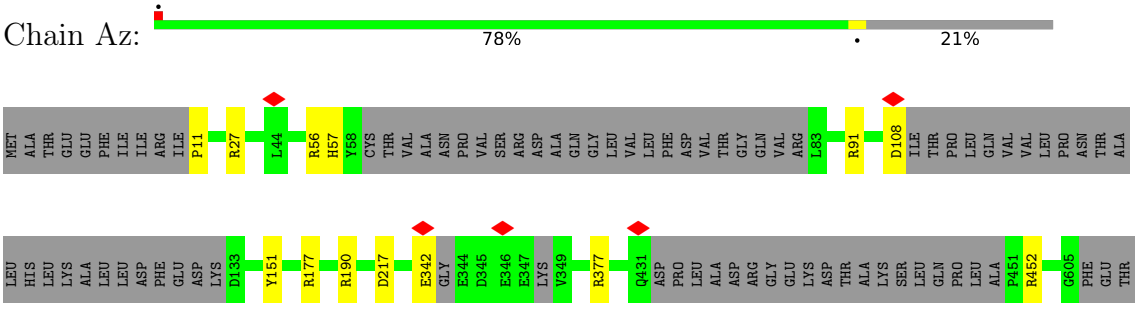
• Molecule 1: Major vault protein

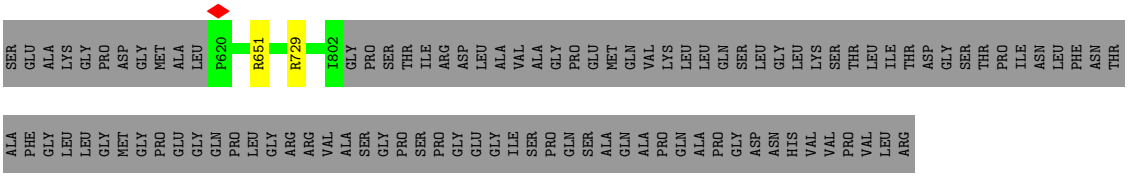
Chain Ay:



• Molecule 1: Major vault protein

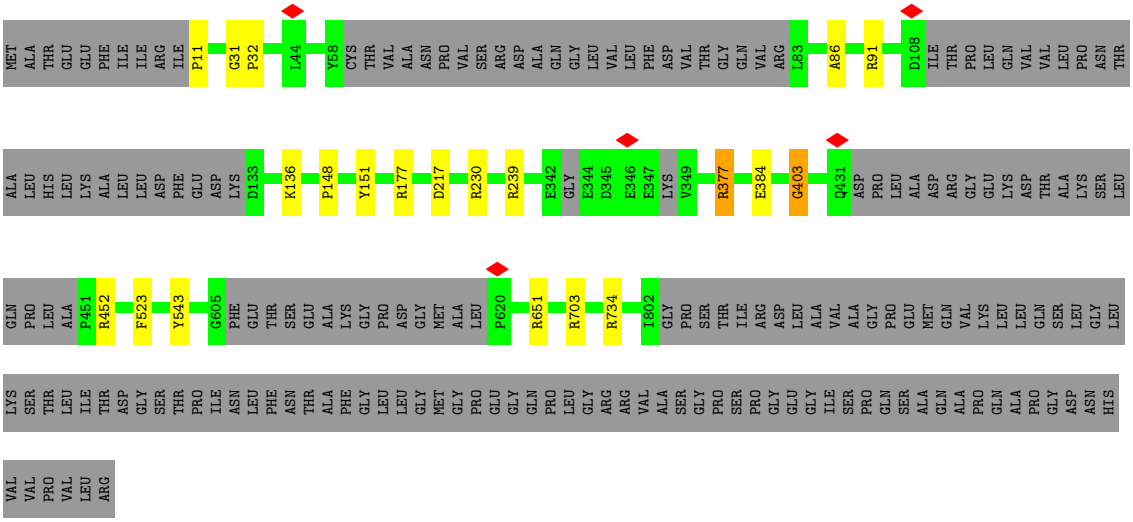
Chain Az:





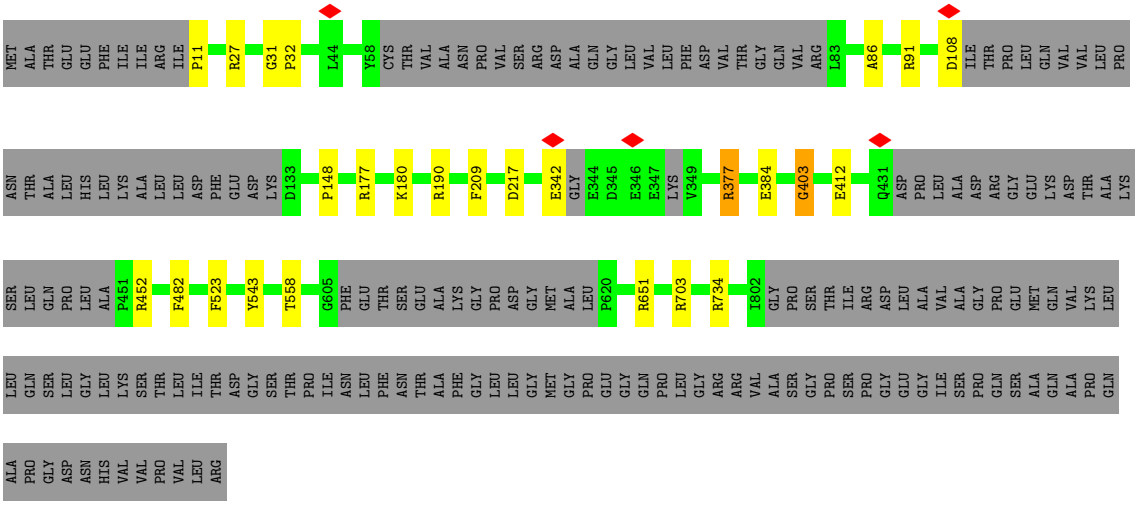
• Molecule 1: Major vault protein

Chain BA:



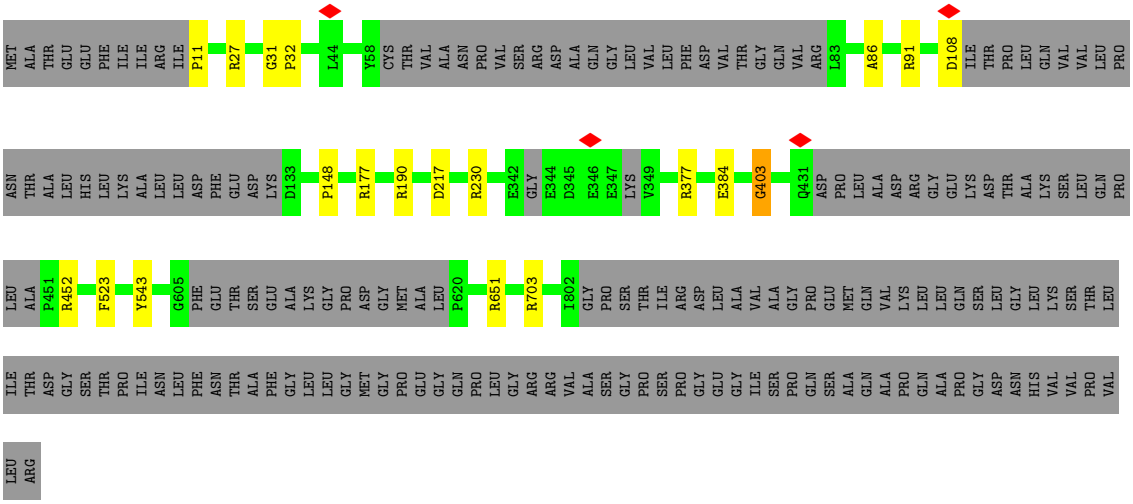
• Molecule 1: Major vault protein

Chain BB:



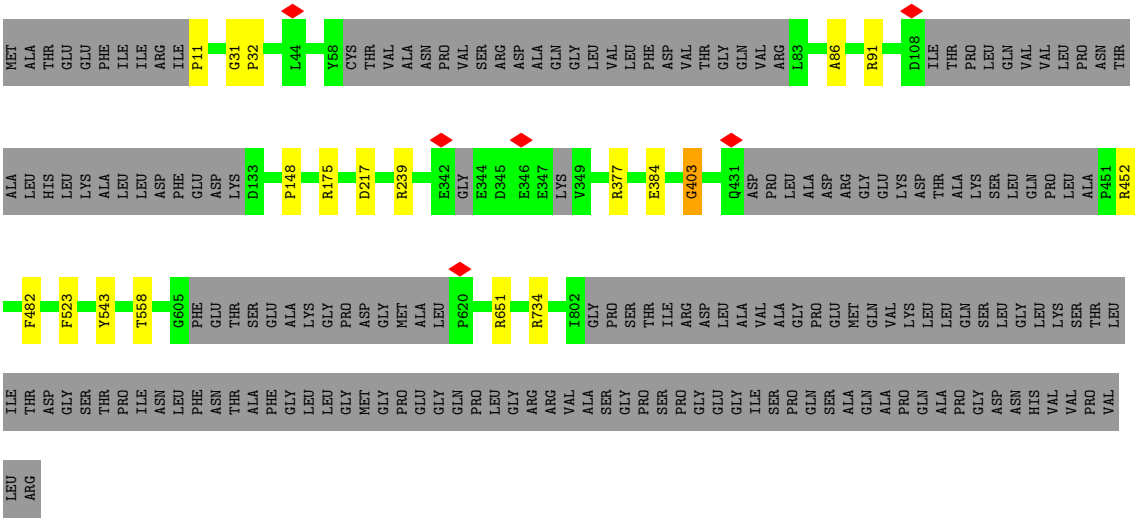
• Molecule 1: Major vault protein

Chain BC:



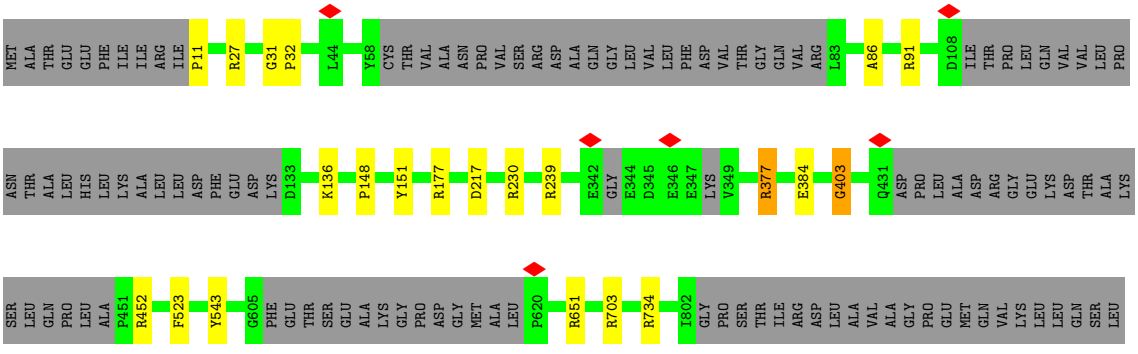
• Molecule 1: Major vault protein

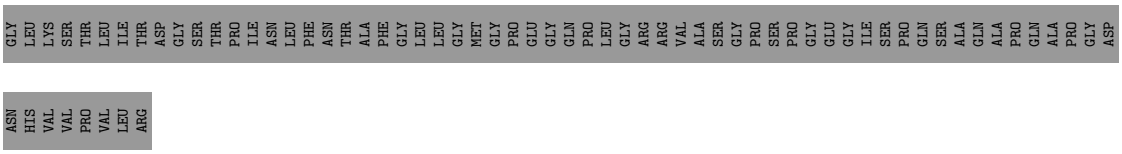
Chain BD:



• Molecule 1: Major vault protein

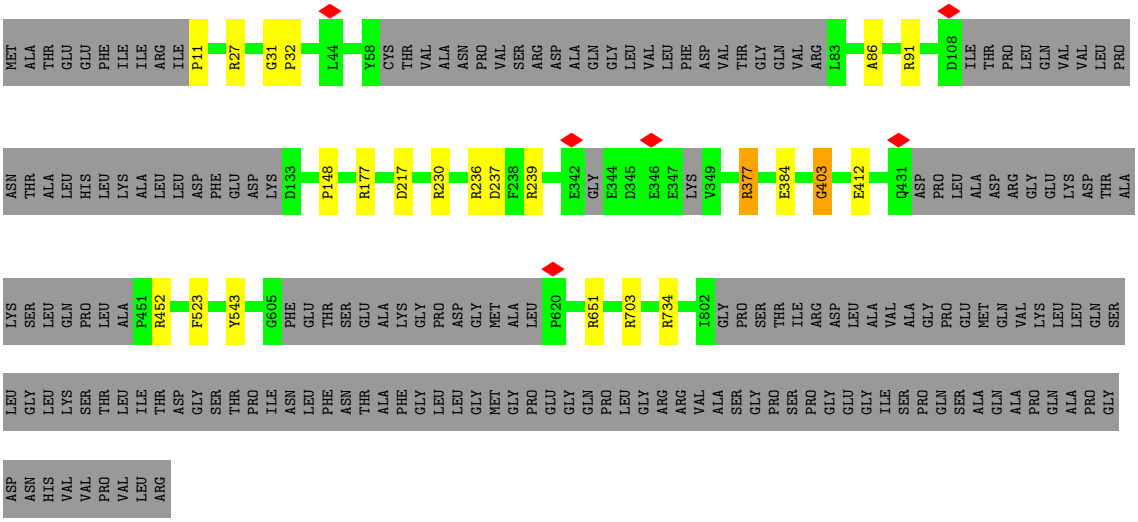
Chain BE:





• Molecule 1: Major vault protein

Chain BF:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00713	Depositor
Map size (Å)	736.0, 736.0, 736.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A0	0.72	0/5747	1.28	10/7784 (0.1%)
1	A1	0.72	0/5747	1.33	24/7784 (0.3%)
1	A2	0.72	0/5747	1.34	21/7784 (0.3%)
1	A3	0.72	0/5747	1.34	17/7784 (0.2%)
1	A4	0.72	0/5747	1.34	23/7784 (0.3%)
1	A5	0.72	0/5747	1.34	21/7784 (0.3%)
1	A6	0.72	0/5747	1.33	20/7784 (0.3%)
1	A7	0.72	0/5747	1.34	21/7784 (0.3%)
1	A8	0.72	0/5747	1.34	26/7784 (0.3%)
1	A9	0.72	0/5747	1.34	21/7784 (0.3%)
1	Ac	0.72	0/5747	1.34	19/7784 (0.2%)
1	Ad	0.72	0/5747	1.34	19/7784 (0.2%)
1	Ae	0.72	0/5747	1.34	22/7784 (0.3%)
1	Af	0.72	0/5747	1.34	22/7784 (0.3%)
1	Ag	0.72	0/5747	1.34	21/7784 (0.3%)
1	Ah	0.72	0/5747	1.34	22/7784 (0.3%)
1	Ai	0.72	0/5747	1.34	26/7784 (0.3%)
1	Aj	0.72	0/5747	1.34	25/7784 (0.3%)
1	Ak	0.72	0/5747	1.34	20/7784 (0.3%)
1	Al	0.72	0/5747	1.33	23/7784 (0.3%)
1	Am	0.72	0/5747	1.34	24/7784 (0.3%)
1	An	0.72	0/5747	1.34	23/7784 (0.3%)
1	Ap	0.72	0/5747	1.34	24/7784 (0.3%)
1	Aq	0.72	0/5747	1.34	23/7784 (0.3%)
1	Ar	0.72	0/5747	1.34	19/7784 (0.2%)
1	As	0.72	0/5747	1.34	15/7784 (0.2%)
1	At	0.72	0/5747	1.34	22/7784 (0.3%)
1	Au	0.72	0/5747	1.34	20/7784 (0.3%)
1	Av	0.72	0/5747	1.33	19/7784 (0.2%)
1	Aw	0.72	0/5747	1.33	21/7784 (0.3%)
1	Ax	0.72	0/5747	1.34	23/7784 (0.3%)
1	Ay	0.72	0/5747	1.34	18/7784 (0.2%)
1	Az	0.72	0/5747	1.28	12/7784 (0.2%)
1	BA	0.72	0/5747	1.34	23/7784 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	BB	0.72	0/5747	1.33	21/7784 (0.3%)
1	BC	0.72	0/5747	1.33	19/7784 (0.2%)
1	BD	0.72	0/5747	1.34	19/7784 (0.2%)
1	BE	0.72	0/5747	1.34	22/7784 (0.3%)
1	BF	0.72	0/5747	1.34	26/7784 (0.3%)
All	All	0.72	0/224133	1.33	816/303576 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A0	0	1
1	A1	0	2
1	A2	0	1
1	A3	0	2
1	A4	0	2
1	A5	0	3
1	A6	0	2
1	A7	0	3
1	A8	0	2
1	A9	0	2
1	Ac	0	1
1	Ad	0	1
1	Ae	0	1
1	Af	0	2
1	Ag	0	1
1	Ai	0	1
1	Aj	0	1
1	Ak	0	2
1	Al	0	2
1	Am	0	2
1	An	0	2
1	Ap	0	1
1	Aq	0	1
1	Ar	0	2
1	As	0	3
1	At	0	2
1	Au	0	2
1	Av	0	1
1	Aw	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ax	0	2
1	Ay	0	1
1	Az	0	2
1	BA	0	2
1	BB	0	1
1	BC	0	1
1	BD	0	1
1	BE	0	2
1	BF	0	1
All	All	0	62

There are no bond length outliers.

All (816) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	An	403	GLY	N-CA-C	7.02	124.33	115.21
1	Az	11	PRO	CA-N-CD	-6.87	102.39	112.00
1	Ar	403	GLY	N-CA-C	6.73	123.96	115.21
1	Ac	403	GLY	N-CA-C	6.65	123.86	115.21
1	Ak	11	PRO	CA-N-CD	-6.65	102.69	112.00
1	At	403	GLY	N-CA-C	6.64	123.85	115.21
1	A7	31	GLY	N-CA-C	6.59	125.78	112.34
1	A8	11	PRO	CA-N-CD	-6.59	102.78	112.00
1	A0	11	PRO	CA-N-CD	-6.58	102.79	112.00
1	A4	11	PRO	CA-N-CD	-6.57	102.81	112.00
1	Ar	11	PRO	CA-N-CD	-6.57	102.81	112.00
1	Aq	91	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	Ah	11	PRO	CA-N-CD	-6.54	102.84	112.00
1	Ai	11	PRO	CA-N-CD	-6.53	102.86	112.00
1	Af	403	GLY	N-CA-C	6.53	124.33	115.32
1	A7	11	PRO	CA-N-CD	-6.53	102.86	112.00
1	Ap	11	PRO	CA-N-CD	-6.52	102.87	112.00
1	Al	11	PRO	CA-N-CD	-6.51	102.88	112.00
1	Ay	11	PRO	CA-N-CD	-6.51	102.88	112.00
1	Ac	91	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	Ac	11	PRO	CA-N-CD	-6.51	102.89	112.00
1	A6	11	PRO	CA-N-CD	-6.51	102.89	112.00
1	A5	11	PRO	CA-N-CD	-6.50	102.90	112.00
1	Aj	11	PRO	CA-N-CD	-6.50	102.90	112.00
1	An	11	PRO	CA-N-CD	-6.50	102.90	112.00
1	A1	91	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	Au	11	PRO	CA-N-CD	-6.49	102.92	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BE	11	PRO	CA-N-CD	-6.49	102.92	112.00
1	Am	91	ARG	NE-CZ-NH2	6.47	125.02	119.20
1	BC	11	PRO	CA-N-CD	-6.47	102.95	112.00
1	A9	403	GLY	N-CA-C	6.46	124.24	115.32
1	Ae	11	PRO	CA-N-CD	-6.46	102.95	112.00
1	BA	11	PRO	CA-N-CD	-6.46	102.95	112.00
1	Ag	11	PRO	CA-N-CD	-6.46	102.96	112.00
1	A2	11	PRO	CA-N-CD	-6.46	102.96	112.00
1	At	11	PRO	CA-N-CD	-6.45	102.97	112.00
1	Aq	11	PRO	CA-N-CD	-6.45	102.97	112.00
1	Aw	11	PRO	CA-N-CD	-6.43	102.99	112.00
1	A9	11	PRO	CA-N-CD	-6.43	103.00	112.00
1	Aw	91	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	As	11	PRO	CA-N-CD	-6.42	103.02	112.00
1	BB	11	PRO	CA-N-CD	-6.40	103.04	112.00
1	Ap	523	PHE	CA-CB-CG	6.39	120.19	113.80
1	Ax	91	ARG	NE-CZ-NH2	6.39	124.96	119.20
1	Av	11	PRO	CA-N-CD	-6.39	103.06	112.00
1	A2	31	GLY	N-CA-C	6.39	125.37	112.34
1	Ag	91	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A3	11	PRO	CA-N-CD	-6.38	103.07	112.00
1	Az	91	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	BA	31	GLY	N-CA-C	6.38	125.34	112.34
1	A2	91	ARG	NE-CZ-NH2	6.37	124.94	119.20
1	BA	403	GLY	N-CA-C	6.37	124.11	115.32
1	Ag	31	GLY	N-CA-C	6.37	125.33	112.34
1	Aw	403	GLY	N-CA-C	6.37	124.11	115.32
1	Av	403	GLY	N-CA-C	6.36	124.10	115.32
1	Aq	31	GLY	N-CA-C	6.36	125.31	112.34
1	BB	523	PHE	CA-CB-CG	6.36	120.16	113.80
1	Af	11	PRO	CA-N-CD	-6.34	103.12	112.00
1	Al	31	GLY	N-CA-C	6.34	125.28	112.34
1	BE	31	GLY	N-CA-C	6.34	125.28	112.34
1	As	31	GLY	N-CA-C	6.34	125.27	112.34
1	Af	31	GLY	N-CA-C	6.34	125.27	112.34
1	Au	403	GLY	N-CA-C	6.34	124.06	115.32
1	BD	11	PRO	CA-N-CD	-6.33	103.13	112.00
1	Am	31	GLY	N-CA-C	6.33	125.25	112.34
1	BD	91	ARG	NE-CZ-NH2	6.33	124.90	119.20
1	Ak	31	GLY	N-CA-C	6.33	125.25	112.34
1	Am	11	PRO	CA-N-CD	-6.33	103.14	112.00
1	BF	91	ARG	NE-CZ-NH2	6.33	124.90	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	31	GLY	N-CA-C	6.32	125.23	112.34
1	Ad	11	PRO	CA-N-CD	-6.32	103.16	112.00
1	Aw	31	GLY	N-CA-C	6.32	125.23	112.34
1	BC	403	GLY	N-CA-C	6.31	124.02	115.32
1	BC	31	GLY	N-CA-C	6.30	125.19	112.34
1	BB	91	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	Ad	31	GLY	N-CA-C	6.30	125.18	112.34
1	BA	91	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	BB	403	GLY	N-CA-C	6.30	124.01	115.32
1	Ax	11	PRO	CA-N-CD	-6.29	103.19	112.00
1	A6	31	GLY	N-CA-C	6.29	125.18	112.34
1	Ap	403	GLY	N-CA-C	6.28	123.99	115.32
1	Ai	403	GLY	N-CA-C	6.28	123.99	115.32
1	A1	11	PRO	CA-N-CD	-6.28	103.21	112.00
1	A4	31	GLY	N-CA-C	6.27	125.14	112.34
1	A8	91	ARG	NE-CZ-NH2	6.27	124.85	119.20
1	Au	91	ARG	NE-CZ-NH2	6.27	124.85	119.20
1	Ar	31	GLY	N-CA-C	6.26	125.12	112.34
1	Ap	31	GLY	N-CA-C	6.26	125.10	112.34
1	BD	403	GLY	N-CA-C	6.25	123.94	115.32
1	A2	403	GLY	N-CA-C	6.25	123.94	115.32
1	Ah	31	GLY	N-CA-C	6.24	125.08	112.34
1	A7	403	GLY	N-CA-C	6.24	123.94	115.32
1	BF	31	GLY	N-CA-C	6.24	125.06	112.34
1	Ar	91	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	BE	91	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	A3	31	GLY	N-CA-C	6.23	125.05	112.34
1	Al	403	GLY	N-CA-C	6.21	123.89	115.32
1	A8	403	GLY	N-CA-C	6.21	123.89	115.32
1	Ay	31	GLY	N-CA-C	6.20	125.00	112.34
1	BC	91	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A5	31	GLY	N-CA-C	6.20	124.99	112.34
1	Ac	31	GLY	N-CA-C	6.20	124.98	112.34
1	A4	91	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	At	31	GLY	N-CA-C	6.19	124.97	112.34
1	Af	91	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	BB	31	GLY	N-CA-C	6.19	124.96	112.34
1	At	91	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	BF	11	PRO	CA-N-CD	-6.17	103.36	112.00
1	Al	452	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	Av	31	GLY	N-CA-C	6.17	124.92	112.34
1	Ak	452	ARG	NE-CZ-NH2	6.17	124.75	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ak	91	ARG	NE-CZ-NH2	6.16	124.75	119.20
1	Aj	403	GLY	N-CA-C	6.16	123.82	115.32
1	An	31	GLY	N-CA-C	6.16	124.90	112.34
1	Ap	91	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	Ai	91	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	BE	403	GLY	N-CA-C	6.16	123.81	115.32
1	Ai	31	GLY	N-CA-C	6.15	124.88	112.34
1	Ah	91	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	Ae	31	GLY	N-CA-C	6.14	124.86	112.34
1	As	91	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	Aj	91	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	A8	31	GLY	N-CA-C	6.13	124.85	112.34
1	Au	31	GLY	N-CA-C	6.13	124.85	112.34
1	Ax	31	GLY	N-CA-C	6.13	124.85	112.34
1	BD	31	GLY	N-CA-C	6.12	124.83	112.34
1	Aw	452	ARG	NE-CZ-NH2	6.12	124.70	119.20
1	A9	31	GLY	N-CA-C	6.11	124.81	112.34
1	Ae	91	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	Ay	91	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	Ag	403	GLY	N-CA-C	6.11	123.75	115.32
1	Aj	31	GLY	N-CA-C	6.10	124.79	112.34
1	Av	91	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	Am	403	GLY	N-CA-C	6.10	123.74	115.32
1	Ad	403	GLY	N-CA-C	6.10	123.73	115.32
1	Ah	403	GLY	N-CA-C	6.10	123.73	115.32
1	Ai	523	PHE	CA-CB-CG	6.10	119.90	113.80
1	BF	452	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	Ax	523	PHE	CA-CB-CG	6.08	119.88	113.80
1	Am	452	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A9	91	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	Ad	91	ARG	NE-CZ-NH2	6.07	124.67	119.20
1	Aw	148	PRO	CA-C-N	6.06	127.91	120.51
1	Aw	148	PRO	C-N-CA	6.06	127.91	120.51
1	A2	452	ARG	NE-CZ-NH2	6.06	124.66	119.20
1	A3	403	GLY	N-CA-C	6.05	123.67	115.32
1	Ax	452	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	Ad	523	PHE	CA-CB-CG	6.05	119.85	113.80
1	A0	91	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	Ay	452	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	As	523	PHE	CA-CB-CG	6.04	119.84	113.80
1	BF	403	GLY	N-CA-C	6.04	123.65	115.32
1	BE	148	PRO	CA-C-N	6.04	127.87	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BE	148	PRO	C-N-CA	6.04	127.87	120.51
1	Aj	452	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	Ap	452	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	BC	452	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	Ay	523	PHE	CA-CB-CG	6.01	119.81	113.80
1	Aq	403	GLY	N-CA-C	6.00	123.60	115.32
1	A5	91	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	A8	523	PHE	CA-CB-CG	5.99	119.79	113.80
1	A9	148	PRO	CA-C-N	5.99	127.82	120.51
1	A9	148	PRO	C-N-CA	5.99	127.82	120.51
1	A4	523	PHE	CA-CB-CG	5.97	119.77	113.80
1	Al	91	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A1	403	GLY	N-CA-C	5.97	123.56	115.32
1	Au	148	PRO	CA-C-N	5.97	127.79	120.51
1	Au	148	PRO	C-N-CA	5.97	127.79	120.51
1	Aw	523	PHE	CA-CB-CG	5.97	119.77	113.80
1	Ar	452	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A3	148	PRO	CA-C-N	5.95	127.77	120.51
1	A3	148	PRO	C-N-CA	5.95	127.77	120.51
1	Ak	86	ALA	CA-C-N	5.95	132.91	121.54
1	Ak	86	ALA	C-N-CA	5.95	132.91	121.54
1	BA	452	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	Ag	452	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	A3	91	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	A7	452	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	Ag	523	PHE	CA-CB-CG	5.93	119.73	113.80
1	Ay	403	GLY	N-CA-C	5.93	123.51	115.32
1	A7	91	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	A6	452	ARG	NE-CZ-NH2	5.93	124.53	119.20
1	Ay	86	ALA	CA-C-N	5.92	132.85	121.54
1	Ay	86	ALA	C-N-CA	5.92	132.85	121.54
1	Aw	86	ALA	CA-C-N	5.92	132.84	121.54
1	Aw	86	ALA	C-N-CA	5.92	132.84	121.54
1	An	523	PHE	CA-CB-CG	5.91	119.71	113.80
1	Ay	86	ALA	N-CA-C	-5.91	104.19	111.40
1	As	452	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	Av	86	ALA	CA-C-N	5.90	132.80	121.54
1	Av	86	ALA	C-N-CA	5.90	132.80	121.54
1	Au	452	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A5	452	ARG	NE-CZ-NH2	5.88	124.50	119.20
1	BC	523	PHE	CA-CB-CG	5.88	119.68	113.80
1	A4	452	ARG	NE-CZ-NH2	5.88	124.49	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A7	86	ALA	CA-C-N	5.86	132.74	121.54
1	A7	86	ALA	C-N-CA	5.86	132.74	121.54
1	Aj	148	PRO	CA-C-N	5.86	127.66	120.51
1	Aj	148	PRO	C-N-CA	5.86	127.66	120.51
1	BE	452	ARG	NE-CZ-NH2	5.86	124.48	119.20
1	At	523	PHE	CA-CB-CG	5.86	119.66	113.80
1	A9	523	PHE	CA-CB-CG	5.85	119.65	113.80
1	Aq	452	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	Af	452	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	BD	452	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	Ai	86	ALA	CA-C-N	5.84	132.69	121.54
1	Ai	86	ALA	C-N-CA	5.84	132.69	121.54
1	Ak	523	PHE	CA-CB-CG	5.84	119.64	113.80
1	Av	148	PRO	CA-C-N	5.84	127.63	120.51
1	Av	148	PRO	C-N-CA	5.84	127.63	120.51
1	Ae	452	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	Ax	403	GLY	N-CA-C	5.81	123.34	115.32
1	BD	148	PRO	CA-C-N	5.81	127.60	120.51
1	BD	148	PRO	C-N-CA	5.81	127.60	120.51
1	Ah	452	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	A4	403	GLY	N-CA-C	5.81	123.33	115.32
1	Ad	452	ARG	NE-CZ-NH2	5.79	124.42	119.20
1	Aq	148	PRO	CA-C-N	5.79	127.58	120.51
1	Aq	148	PRO	C-N-CA	5.79	127.58	120.51
1	Af	148	PRO	CA-C-N	5.79	127.58	120.51
1	Af	148	PRO	C-N-CA	5.79	127.58	120.51
1	BA	523	PHE	CA-CB-CG	5.79	119.59	113.80
1	A4	86	ALA	N-CA-C	-5.79	104.34	111.40
1	A6	91	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	An	91	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	As	86	ALA	CA-C-N	5.78	132.57	121.54
1	As	86	ALA	C-N-CA	5.78	132.57	121.54
1	A5	403	GLY	N-CA-C	5.77	123.29	115.32
1	A6	403	GLY	N-CA-C	5.77	123.29	115.32
1	A8	452	ARG	NE-CZ-NH2	5.77	124.40	119.20
1	Al	86	ALA	CA-C-N	5.77	132.56	121.54
1	Al	86	ALA	C-N-CA	5.77	132.56	121.54
1	Ac	452	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A2	523	PHE	CA-CB-CG	5.76	119.56	113.80
1	BC	86	ALA	N-CA-C	-5.76	104.37	111.40
1	A6	651	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	Ae	86	ALA	N-CA-C	-5.76	104.38	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	An	452	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	Av	452	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	A5	523	PHE	CA-CB-CG	5.75	119.55	113.80
1	Ah	86	ALA	CA-C-N	5.75	132.52	121.54
1	Ah	86	ALA	C-N-CA	5.75	132.52	121.54
1	A0	452	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	Ac	148	PRO	CA-C-N	5.75	127.52	120.51
1	Ac	148	PRO	C-N-CA	5.75	127.52	120.51
1	As	403	GLY	N-CA-C	5.75	123.25	115.32
1	A1	452	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	Ae	86	ALA	CA-C-N	5.74	132.50	121.54
1	Ae	86	ALA	C-N-CA	5.74	132.50	121.54
1	Ae	403	GLY	N-CA-C	5.73	123.23	115.32
1	Am	523	PHE	CA-CB-CG	5.73	119.53	113.80
1	Az	217	ASP	CA-CB-CG	5.73	118.33	112.60
1	Af	523	PHE	CA-CB-CG	5.73	119.53	113.80
1	Aj	523	PHE	CA-CB-CG	5.72	119.52	113.80
1	A4	148	PRO	CA-C-N	5.72	127.49	120.51
1	A4	148	PRO	C-N-CA	5.72	127.49	120.51
1	A5	86	ALA	CA-C-N	5.72	132.46	121.54
1	A5	86	ALA	C-N-CA	5.72	132.46	121.54
1	A9	452	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	Aj	651	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A8	86	ALA	CA-C-N	5.70	132.43	121.54
1	A8	86	ALA	C-N-CA	5.70	132.43	121.54
1	At	86	ALA	CA-C-N	5.70	132.43	121.54
1	At	86	ALA	C-N-CA	5.70	132.43	121.54
1	Av	523	PHE	CA-CB-CG	5.69	119.49	113.80
1	A7	86	ALA	N-CA-C	-5.69	104.46	111.40
1	A6	523	PHE	CA-CB-CG	5.68	119.48	113.80
1	BA	86	ALA	CA-C-N	5.68	132.39	121.54
1	BA	86	ALA	C-N-CA	5.68	132.39	121.54
1	A3	86	ALA	N-CA-C	-5.68	104.47	111.40
1	Au	523	PHE	CA-CB-CG	5.68	119.48	113.80
1	Ay	377	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	A3	32	PRO	N-CA-C	-5.66	106.15	113.57
1	Ak	403	GLY	N-CA-C	5.66	123.13	115.32
1	BD	86	ALA	CA-C-N	5.66	132.35	121.54
1	BD	86	ALA	C-N-CA	5.66	132.35	121.54
1	Ai	32	PRO	N-CA-C	-5.66	106.16	113.57
1	Ag	86	ALA	N-CA-C	-5.66	104.50	111.40
1	A5	148	PRO	CA-C-N	5.65	127.41	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A5	148	PRO	C-N-CA	5.65	127.41	120.51
1	BB	452	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	BB	651	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	Ae	523	PHE	CA-CB-CG	5.64	119.44	113.80
1	Aj	86	ALA	CA-C-N	5.64	132.31	121.54
1	Aj	86	ALA	C-N-CA	5.64	132.31	121.54
1	Ai	452	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	A3	452	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	Al	523	PHE	CA-CB-CG	5.63	119.43	113.80
1	Ah	32	PRO	N-CA-C	-5.63	106.20	113.57
1	Al	86	ALA	N-CA-C	-5.63	104.53	111.40
1	A1	523	PHE	CA-CB-CG	5.62	119.42	113.80
1	Ac	86	ALA	CA-C-N	5.62	132.28	121.54
1	Ac	86	ALA	C-N-CA	5.62	132.28	121.54
1	Aw	86	ALA	N-CA-C	-5.62	104.55	111.40
1	BF	148	PRO	CA-C-N	5.62	127.36	120.51
1	BF	148	PRO	C-N-CA	5.62	127.36	120.51
1	BE	86	ALA	CA-C-N	5.61	132.26	121.54
1	BE	86	ALA	C-N-CA	5.61	132.26	121.54
1	A3	86	ALA	CA-C-N	5.61	132.25	121.54
1	A3	86	ALA	C-N-CA	5.61	132.25	121.54
1	Ay	148	PRO	CA-C-N	5.61	127.35	120.51
1	Ay	148	PRO	C-N-CA	5.61	127.35	120.51
1	At	32	PRO	N-CA-C	-5.61	106.23	113.57
1	BF	32	PRO	N-CA-C	-5.61	106.23	113.57
1	A2	86	ALA	CA-C-N	5.59	132.22	121.54
1	A2	86	ALA	C-N-CA	5.59	132.22	121.54
1	Al	651	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	At	651	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	At	452	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	A8	32	PRO	N-CA-C	-5.58	106.26	113.57
1	As	651	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A4	32	PRO	N-CA-C	-5.58	106.26	113.57
1	Ae	32	PRO	N-CA-C	-5.58	106.26	113.57
1	Aq	32	PRO	N-CA-C	-5.58	106.26	113.57
1	Ag	148	PRO	CA-C-N	5.58	127.31	120.51
1	Ag	148	PRO	C-N-CA	5.58	127.31	120.51
1	A7	148	PRO	CA-C-N	5.57	127.31	120.51
1	A7	148	PRO	C-N-CA	5.57	127.31	120.51
1	A2	148	PRO	CA-C-N	5.57	127.31	120.51
1	A2	148	PRO	C-N-CA	5.57	127.31	120.51
1	A9	86	ALA	CA-C-N	5.57	132.18	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A9	86	ALA	C-N-CA	5.57	132.18	121.54
1	Ae	651	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	BD	523	PHE	CA-CB-CG	5.57	119.37	113.80
1	A8	651	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	A7	523	PHE	CA-CB-CG	5.56	119.36	113.80
1	Aq	86	ALA	CA-C-N	5.56	132.17	121.54
1	Aq	86	ALA	C-N-CA	5.56	132.17	121.54
1	Ad	86	ALA	CA-C-N	5.56	132.16	121.54
1	Ad	86	ALA	C-N-CA	5.56	132.16	121.54
1	Ai	148	PRO	CA-C-N	5.56	127.29	120.51
1	Ai	148	PRO	C-N-CA	5.56	127.29	120.51
1	A5	32	PRO	N-CA-C	-5.56	106.29	113.57
1	A9	86	ALA	N-CA-C	-5.56	104.62	111.40
1	Af	86	ALA	N-CA-C	-5.56	104.62	111.40
1	A5	86	ALA	N-CA-C	-5.55	104.62	111.40
1	A5	651	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	Al	32	PRO	N-CA-C	-5.55	106.30	113.57
1	Ac	86	ALA	N-CA-C	-5.54	104.64	111.40
1	A3	651	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	Av	703	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	Ax	86	ALA	N-CA-C	-5.53	104.66	111.40
1	BF	86	ALA	CA-C-N	5.53	132.10	121.54
1	BF	86	ALA	C-N-CA	5.53	132.10	121.54
1	Am	32	PRO	N-CA-C	-5.52	106.34	113.57
1	Ac	32	PRO	N-CA-C	-5.52	106.34	113.57
1	A9	27	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	Ay	32	PRO	N-CA-C	-5.52	106.34	113.57
1	A1	32	PRO	N-CA-C	-5.51	106.35	113.57
1	Ag	32	PRO	N-CA-C	-5.51	106.35	113.57
1	Ar	523	PHE	CA-CB-CG	5.51	119.31	113.80
1	Ap	86	ALA	N-CA-C	-5.50	104.68	111.40
1	An	86	ALA	N-CA-C	-5.50	104.69	111.40
1	BD	86	ALA	N-CA-C	-5.50	104.69	111.40
1	A1	86	ALA	N-CA-C	-5.50	104.69	111.40
1	Aj	32	PRO	N-CA-C	-5.50	106.37	113.57
1	A6	86	ALA	CA-C-N	5.50	132.03	121.54
1	A6	86	ALA	C-N-CA	5.50	132.03	121.54
1	Ac	523	PHE	CA-CB-CG	5.50	119.30	113.80
1	Ae	27	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	Am	86	ALA	CA-C-N	5.49	132.03	121.54
1	Am	86	ALA	C-N-CA	5.49	132.03	121.54
1	BC	651	ARG	NE-CZ-NH2	5.49	124.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Af	651	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	Ai	651	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	An	86	ALA	CA-C-N	5.49	132.02	121.54
1	An	86	ALA	C-N-CA	5.49	132.02	121.54
1	Az	651	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	Aj	86	ALA	N-CA-C	-5.48	104.71	111.40
1	A9	651	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A4	86	ALA	CA-C-N	5.47	132.00	121.54
1	A4	86	ALA	C-N-CA	5.47	132.00	121.54
1	As	32	PRO	N-CA-C	-5.47	106.40	113.57
1	Am	734	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	Ay	703	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	Ad	148	PRO	CA-C-N	5.47	127.18	120.51
1	Ad	148	PRO	C-N-CA	5.47	127.18	120.51
1	As	412	GLU	N-CA-C	5.47	118.97	110.17
1	Au	86	ALA	CA-C-N	5.47	131.98	121.54
1	Au	86	ALA	C-N-CA	5.47	131.98	121.54
1	Af	86	ALA	CA-C-N	5.46	131.98	121.54
1	Af	86	ALA	C-N-CA	5.46	131.98	121.54
1	BC	32	PRO	N-CA-C	-5.46	106.41	113.57
1	Af	734	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	Ar	32	PRO	N-CA-C	-5.46	106.42	113.57
1	A6	32	PRO	N-CA-C	-5.46	106.42	113.57
1	Ap	32	PRO	N-CA-C	-5.46	106.42	113.57
1	BF	651	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	Ae	734	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	Av	651	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	Ap	651	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	Ax	734	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	Ac	651	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	Am	148	PRO	CA-C-N	5.45	127.16	120.51
1	Am	148	PRO	C-N-CA	5.45	127.16	120.51
1	At	86	ALA	N-CA-C	-5.45	104.76	111.40
1	BD	651	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	Ah	523	PHE	CA-CB-CG	5.44	119.24	113.80
1	Ap	86	ALA	CA-C-N	5.44	131.93	121.54
1	Ap	86	ALA	C-N-CA	5.44	131.93	121.54
1	Aw	734	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	A2	651	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	Ak	217	ASP	CA-CB-CG	5.43	118.03	112.60
1	Ap	703	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	Ak	651	ARG	NE-CZ-NH2	5.43	124.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Av	217	ASP	CA-CB-CG	5.43	118.03	112.60
1	BE	523	PHE	CA-CB-CG	5.43	119.23	113.80
1	A0	651	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	BA	148	PRO	CA-C-N	5.42	127.13	120.51
1	BA	148	PRO	C-N-CA	5.42	127.13	120.51
1	Ag	86	ALA	CA-C-N	5.42	131.89	121.54
1	Ag	86	ALA	C-N-CA	5.42	131.89	121.54
1	Aw	217	ASP	CA-CB-CG	5.42	118.02	112.60
1	Ai	86	ALA	N-CA-C	-5.41	104.80	111.40
1	BC	86	ALA	CA-C-N	5.41	131.87	121.54
1	BC	86	ALA	C-N-CA	5.41	131.87	121.54
1	Ap	148	PRO	CA-C-N	5.41	127.11	120.51
1	Ap	148	PRO	C-N-CA	5.41	127.11	120.51
1	An	32	PRO	N-CA-C	-5.40	106.49	113.57
1	Av	86	ALA	N-CA-C	-5.40	104.81	111.40
1	Aw	32	PRO	N-CA-C	-5.40	106.49	113.57
1	BF	523	PHE	CA-CB-CG	5.40	119.20	113.80
1	BD	734	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	Au	32	PRO	N-CA-C	-5.39	106.50	113.57
1	A8	703	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	BE	734	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A1	86	ALA	CA-C-N	5.39	131.83	121.54
1	A1	86	ALA	C-N-CA	5.39	131.83	121.54
1	A3	734	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A8	86	ALA	N-CA-C	-5.39	104.83	111.40
1	BA	651	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A1	651	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	Aq	523	PHE	CA-CB-CG	5.38	119.18	113.80
1	A1	148	PRO	CA-C-N	5.38	127.07	120.51
1	A1	148	PRO	C-N-CA	5.38	127.07	120.51
1	Af	32	PRO	N-CA-C	-5.38	106.53	113.57
1	A3	523	PHE	CA-CB-CG	5.37	119.17	113.80
1	A6	86	ALA	N-CA-C	-5.37	104.85	111.40
1	Au	86	ALA	N-CA-C	-5.37	104.85	111.40
1	BF	217	ASP	CA-CB-CG	5.37	117.97	112.60
1	A1	703	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	An	651	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A7	651	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	Ad	86	ALA	N-CA-C	-5.37	104.85	111.40
1	BF	86	ALA	N-CA-C	-5.37	104.85	111.40
1	Am	651	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	Ap	412	GLU	N-CA-C	5.36	118.80	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ar	86	ALA	N-CA-C	-5.36	104.86	111.40
1	Az	452	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	BA	32	PRO	N-CA-C	-5.36	106.54	113.57
1	A4	651	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	Ar	651	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	Az	57	HIS	N-CA-C	5.36	117.81	111.33
1	A0	729	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A9	239	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	Ah	651	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	BA	734	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	Ak	32	PRO	N-CA-C	-5.35	106.56	113.57
1	BA	86	ALA	N-CA-C	-5.35	104.87	111.40
1	Au	703	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	Ak	86	ALA	N-CA-C	-5.35	104.87	111.40
1	BD	32	PRO	N-CA-C	-5.35	106.56	113.57
1	Ah	148	PRO	CA-C-N	5.35	127.03	120.51
1	Ah	148	PRO	C-N-CA	5.35	127.03	120.51
1	Aw	651	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	BC	230	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	BE	86	ALA	N-CA-C	-5.34	104.88	111.40
1	Aq	86	ALA	N-CA-C	-5.34	104.88	111.40
1	BB	86	ALA	CA-C-N	5.34	131.74	121.54
1	BB	86	ALA	C-N-CA	5.34	131.74	121.54
1	Ag	651	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	Ah	86	ALA	N-CA-C	-5.34	104.89	111.40
1	Am	86	ALA	N-CA-C	-5.34	104.89	111.40
1	A2	86	ALA	N-CA-C	-5.33	104.90	111.40
1	A6	230	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	Av	32	PRO	N-CA-C	-5.33	106.59	113.57
1	BF	734	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	BC	148	PRO	CA-C-N	5.32	127.01	120.51
1	BC	148	PRO	C-N-CA	5.32	127.01	120.51
1	As	703	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	Ap	237	ASP	CA-C-N	5.32	128.14	120.38
1	Ap	237	ASP	C-N-CA	5.32	128.14	120.38
1	Ar	86	ALA	CA-C-N	5.31	131.69	121.54
1	Ar	86	ALA	C-N-CA	5.31	131.69	121.54
1	BB	217	ASP	CA-CB-CG	5.31	117.91	112.60
1	BF	230	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	Aj	412	GLU	N-CA-C	5.30	118.71	110.17
1	Ax	651	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	BE	136	LYS	N-CA-C	5.30	118.22	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ah	377	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	BB	32	PRO	N-CA-C	-5.29	106.64	113.57
1	An	703	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	Ag	734	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	Ar	148	PRO	CA-C-N	5.29	126.96	120.51
1	Ar	148	PRO	C-N-CA	5.29	126.96	120.51
1	Ax	86	ALA	CA-C-N	5.28	131.63	121.54
1	Ax	86	ALA	C-N-CA	5.28	131.63	121.54
1	BE	651	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	BF	377	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	An	148	PRO	CA-C-N	5.28	126.95	120.51
1	An	148	PRO	C-N-CA	5.28	126.95	120.51
1	BB	86	ALA	N-CA-C	-5.28	104.96	111.40
1	Ah	703	ARG	NE-CZ-NH2	5.27	123.95	119.20
1	Aj	217	ASP	CA-CB-CG	5.27	117.87	112.60
1	A2	32	PRO	N-CA-C	-5.27	106.67	113.57
1	A1	27	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A3	703	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	Ah	217	ASP	CA-CB-CG	5.26	117.86	112.60
1	A8	177	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	As	86	ALA	N-CA-C	-5.26	104.98	111.40
1	Ac	217	ASP	CA-CB-CG	5.26	117.86	112.60
1	Ak	148	PRO	CA-C-N	5.25	126.92	120.51
1	Ak	148	PRO	C-N-CA	5.25	126.92	120.51
1	A6	148	PRO	CA-C-N	5.25	126.92	120.51
1	A6	148	PRO	C-N-CA	5.25	126.92	120.51
1	BD	217	ASP	CA-CB-CG	5.25	117.85	112.60
1	A5	412	GLU	N-CA-C	5.25	118.62	110.17
1	Aq	703	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	BA	230	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A6	217	ASP	CA-CB-CG	5.25	117.84	112.60
1	Ap	190	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	Ap	734	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	At	734	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A7	217	ASP	CA-CB-CG	5.24	117.84	112.60
1	Ar	703	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A6	412	GLU	N-CA-C	5.24	118.60	110.17
1	Av	239	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	Ag	230	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	Ah	190	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	Ad	734	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	At	148	PRO	CA-C-N	5.23	126.89	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	At	148	PRO	C-N-CA	5.23	126.89	120.51
1	BE	230	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A1	230	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A8	239	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A8	734	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	Al	148	PRO	CA-C-N	5.23	126.89	120.51
1	Al	148	PRO	C-N-CA	5.23	126.89	120.51
1	Aq	230	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A8	148	PRO	CA-C-N	5.22	126.88	120.51
1	A8	148	PRO	C-N-CA	5.22	126.88	120.51
1	Ad	217	ASP	CA-CB-CG	5.22	117.83	112.60
1	Ac	27	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A9	236	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	Ae	148	PRO	CA-C-N	5.22	126.88	120.51
1	Ae	148	PRO	C-N-CA	5.22	126.88	120.51
1	Ad	651	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	Aj	175	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	An	217	ASP	CA-CB-CG	5.22	117.82	112.60
1	Ah	237	ASP	CA-C-N	5.21	127.99	120.38
1	Ah	237	ASP	C-N-CA	5.21	127.99	120.38
1	Ar	217	ASP	CA-CB-CG	5.21	117.81	112.60
1	BB	27	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	BB	148	PRO	CA-C-N	5.21	126.86	120.51
1	BB	148	PRO	C-N-CA	5.21	126.86	120.51
1	A0	190	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A7	703	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A9	217	ASP	CA-CB-CG	5.21	117.81	112.60
1	Ae	237	ASP	CA-C-N	5.21	127.98	120.38
1	Ae	237	ASP	C-N-CA	5.21	127.98	120.38
1	Am	412	GLU	N-CA-C	5.20	118.55	110.17
1	Au	651	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A2	177	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A9	32	PRO	N-CA-C	-5.20	106.76	113.57
1	BD	175	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	Ai	734	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	At	217	ASP	CA-CB-CG	5.19	117.79	112.60
1	BA	703	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Al	27	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Av	230	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	BF	236	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	Ad	32	PRO	CA-C-N	5.18	130.41	120.97
1	Ad	32	PRO	C-N-CA	5.18	130.41	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	703	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	Am	177	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	BF	27	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	Ad	177	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A8	217	ASP	CA-CB-CG	5.18	117.78	112.60
1	Ai	230	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	Az	27	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A9	190	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	Al	217	ASP	CA-CB-CG	5.17	117.78	112.60
1	BD	239	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	A4	217	ASP	CA-CB-CG	5.17	117.77	112.60
1	Ac	177	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	Am	230	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	BE	32	PRO	N-CA-C	-5.17	106.80	113.57
1	A8	32	PRO	CA-C-N	5.16	130.37	120.97
1	A8	32	PRO	C-N-CA	5.16	130.37	120.97
1	Aj	190	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	Al	136	LYS	N-CA-C	5.16	117.98	108.58
1	An	230	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	Au	27	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	Ay	651	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	At	177	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Al	703	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Ak	734	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Aq	456	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Ai	177	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	At	57	HIS	N-CA-C	5.15	117.56	111.33
1	Ax	32	PRO	N-CA-C	-5.15	106.82	113.57
1	Az	56	ARG	CA-C-N	5.15	127.44	120.38
1	Az	56	ARG	C-N-CA	5.15	127.44	120.38
1	Ae	356	HIS	CA-CB-CG	5.15	118.95	113.80
1	BC	217	ASP	CA-CB-CG	5.15	117.75	112.60
1	BA	136	LYS	N-CA-C	5.15	117.95	108.58
1	Ai	27	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	Aq	651	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	Ag	703	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	Ah	136	LYS	N-CA-C	5.14	117.94	108.58
1	Al	177	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	A4	474	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	Ag	27	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	Aj	27	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	Aj	177	ARG	NE-CZ-NH2	5.14	123.82	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Am	27	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	Ah	27	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	Aq	177	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	Au	177	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	Au	239	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A8	27	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A9	177	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	An	136	LYS	N-CA-C	5.13	117.92	108.58
1	A7	190	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	Ai	237	ASP	CA-C-N	5.13	127.87	120.38
1	Ai	237	ASP	C-N-CA	5.13	127.87	120.38
1	BD	32	PRO	CA-C-N	5.13	130.31	120.97
1	BD	32	PRO	C-N-CA	5.13	130.31	120.97
1	A9	237	ASP	CA-C-N	5.13	127.87	120.38
1	A9	237	ASP	C-N-CA	5.13	127.87	120.38
1	Ai	32	PRO	CA-C-N	5.13	130.30	120.97
1	Ai	32	PRO	C-N-CA	5.13	130.30	120.97
1	Aw	136	LYS	N-CA-C	5.13	117.91	108.58
1	Ay	136	LYS	N-CA-C	5.13	117.91	108.58
1	BE	239	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A4	734	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A7	734	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A2	27	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A2	734	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	Ax	148	PRO	CA-C-N	5.12	126.76	120.51
1	Ax	148	PRO	C-N-CA	5.12	126.76	120.51
1	A4	32	PRO	CA-C-N	5.12	130.29	120.97
1	A4	32	PRO	C-N-CA	5.12	130.29	120.97
1	BB	190	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A5	27	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A7	136	LYS	N-CA-C	5.12	117.89	108.58
1	Ag	190	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	Ar	237	ASP	CA-C-N	5.12	127.85	120.38
1	Ar	237	ASP	C-N-CA	5.12	127.85	120.38
1	Ax	190	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	Af	175	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	Ah	230	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A1	217	ASP	CA-CB-CG	5.11	117.71	112.60
1	A0	177	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A2	175	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	Ad	190	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A1	32	PRO	CA-C-N	5.11	130.27	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	32	PRO	C-N-CA	5.11	130.27	120.97
1	An	177	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	BC	703	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	Aj	237	ASP	CA-C-N	5.11	127.83	120.38
1	Aj	237	ASP	C-N-CA	5.11	127.83	120.38
1	A1	734	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	Af	412	GLU	N-CA-C	5.10	118.39	110.17
1	A4	177	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	Ar	412	GLU	N-CA-C	5.10	118.38	110.17
1	At	230	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A5	217	ASP	CA-CB-CG	5.10	117.70	112.60
1	A6	239	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	Ae	177	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	An	734	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	BB	703	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	Ad	32	PRO	N-CA-C	-5.10	106.89	113.57
1	Ag	237	ASP	CA-C-N	5.10	127.82	120.38
1	Ag	237	ASP	C-N-CA	5.10	127.82	120.38
1	Al	32	PRO	CA-C-N	5.10	130.25	120.97
1	Al	32	PRO	C-N-CA	5.10	130.25	120.97
1	A7	239	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	Aq	734	ARG	NE-CZ-NH2	5.09	123.79	119.20
1	BA	239	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A5	703	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	Au	734	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	BE	377	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	Aw	177	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	Aw	239	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	Az	177	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	Ax	217	ASP	CA-CB-CG	5.09	117.69	112.60
1	Af	32	PRO	CA-C-N	5.09	130.23	120.97
1	Af	32	PRO	C-N-CA	5.09	130.23	120.97
1	Aq	322	ASP	CA-CB-CG	5.09	117.69	112.60
1	Ax	377	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	Ak	412	GLU	N-CA-C	5.08	118.36	110.17
1	Ap	217	ASP	CA-CB-CG	5.08	117.69	112.60
1	Ax	32	PRO	CA-C-N	5.08	130.22	120.97
1	Ax	32	PRO	C-N-CA	5.08	130.22	120.97
1	A4	703	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	Ai	236	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	BE	217	ASP	CA-CB-CG	5.08	117.68	112.60
1	Az	190	ARG	NE-CZ-NH2	5.08	123.77	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Am	217	ASP	CA-CB-CG	5.08	117.68	112.60
1	Aq	32	PRO	CA-C-N	5.08	130.22	120.97
1	Aq	32	PRO	C-N-CA	5.08	130.22	120.97
1	Af	237	ASP	CA-C-N	5.08	127.80	120.38
1	Af	237	ASP	C-N-CA	5.08	127.80	120.38
1	Av	506	LYS	N-CA-C	5.08	117.37	111.02
1	Ap	177	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	Am	32	PRO	CA-C-N	5.08	130.21	120.97
1	Am	32	PRO	C-N-CA	5.08	130.21	120.97
1	BF	703	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	BB	734	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	BE	177	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	Ac	703	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	Ai	217	ASP	CA-CB-CG	5.07	117.67	112.60
1	BA	32	PRO	CA-C-N	5.07	130.20	120.97
1	BA	32	PRO	C-N-CA	5.07	130.20	120.97
1	BA	217	ASP	CA-CB-CG	5.07	117.67	112.60
1	A6	190	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	Ak	237	ASP	CA-C-N	5.07	127.78	120.38
1	Ak	237	ASP	C-N-CA	5.07	127.78	120.38
1	BB	377	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A8	190	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	At	703	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	Az	729	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	Aj	230	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	A5	734	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	Aw	27	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	BA	377	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	BF	230	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	Ag	377	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	BF	412	GLU	N-CA-C	5.06	118.31	110.17
1	Al	230	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	Ae	377	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	Aj	456	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	A7	175	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	Ap	170	GLN	N-CA-C	5.05	116.78	111.28
1	Aq	175	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	As	734	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	BC	27	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	A1	456	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	Af	377	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	Am	377	ARG	NE-CZ-NH2	5.05	123.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ax	412	GLU	N-CA-C	5.05	118.29	110.17
1	Ak	703	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A6	27	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	Ax	136	LYS	N-CA-C	5.04	117.76	108.58
1	BB	412	GLU	N-CA-C	5.04	118.29	110.17
1	A5	32	PRO	CA-C-N	5.04	130.14	120.97
1	A5	32	PRO	C-N-CA	5.04	130.14	120.97
1	A7	32	PRO	CA-C-N	5.04	129.75	121.39
1	A7	32	PRO	C-N-CA	5.04	129.75	121.39
1	Ai	377	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	BC	177	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	Am	703	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	Ai	703	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	As	230	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	Ac	230	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	Af	217	ASP	CA-CB-CG	5.03	117.63	112.60
1	Aj	703	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	Aw	456	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A2	32	PRO	CA-C-N	5.03	130.13	120.97
1	A2	32	PRO	C-N-CA	5.03	130.13	120.97
1	A1	412	GLU	N-CA-C	5.03	118.27	110.17
1	Al	734	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	Au	217	ASP	CA-CB-CG	5.03	117.63	112.60
1	BE	703	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A8	412	GLU	N-CA-C	5.03	118.27	110.17
1	Ac	734	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	Ax	177	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	BA	177	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	A1	190	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	A6	228	HIS	CA-CB-CG	5.03	118.83	113.80
1	Ae	175	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	BE	27	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	Ap	230	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	Ar	236	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	An	239	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	At	32	PRO	CA-C-N	5.02	130.11	120.97
1	At	32	PRO	C-N-CA	5.02	130.11	120.97
1	A8	237	ASP	CA-C-N	5.02	127.71	120.38
1	A8	237	ASP	C-N-CA	5.02	127.71	120.38
1	BB	177	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A5	190	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	Al	356	HIS	CA-CB-CG	5.02	118.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Am	136	LYS	N-CA-C	5.02	117.71	108.58
1	Av	27	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	Aw	377	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	Ay	412	GLU	N-CA-C	5.02	118.25	110.17
1	BF	239	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	An	32	PRO	CA-C-N	5.02	130.10	120.97
1	An	32	PRO	C-N-CA	5.02	130.10	120.97
1	Ap	228	HIS	CA-CB-CG	5.02	118.82	113.80
1	A0	237	ASP	CA-C-N	5.02	127.70	120.38
1	A0	237	ASP	C-N-CA	5.02	127.70	120.38
1	A4	572	CYS	CA-C-N	5.02	127.00	120.28
1	A4	572	CYS	C-N-CA	5.02	127.00	120.28
1	A0	27	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	Ai	239	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	An	27	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	Au	230	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	Ak	230	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	BF	237	ASP	CA-C-N	5.01	127.70	120.38
1	BF	237	ASP	C-N-CA	5.01	127.70	120.38
1	A1	177	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	Ae	412	GLU	N-CA-C	5.01	118.24	110.17
1	Ay	27	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	Aq	412	GLU	N-CA-C	5.01	118.23	110.17
1	Ax	703	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A3	217	ASP	CA-CB-CG	5.01	117.61	112.60
1	A4	239	ARG	NE-CZ-NH2	5.01	123.70	119.20
1	A8	175	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	Aj	239	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	BC	190	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	BF	177	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	A2	412	GLU	N-CA-C	5.00	118.23	110.17
1	A3	412	GLU	N-CA-C	5.00	118.22	110.17
1	At	136	LYS	N-CA-C	5.00	117.68	108.58

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A0	377	ARG	Sidechain
1	A1	151	TYR	Sidechain
1	A1	377	ARG	Sidechain
1	A2	151	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A3	151	TYR	Sidechain
1	A3	377	ARG	Sidechain
1	A4	151	TYR	Sidechain
1	A4	377	ARG	Sidechain
1	A5	151	TYR	Sidechain
1	A5	377	ARG	Sidechain
1	A5	474	ARG	Sidechain
1	A6	151	TYR	Sidechain
1	A6	377	ARG	Sidechain
1	A7	151	TYR	Sidechain
1	A7	377	ARG	Sidechain
1	A7	474	ARG	Sidechain
1	A8	151	TYR	Sidechain
1	A8	377	ARG	Sidechain
1	A9	151	TYR	Sidechain
1	A9	377	ARG	Sidechain
1	Ac	377	ARG	Sidechain
1	Ad	377	ARG	Sidechain
1	Ae	377	ARG	Sidechain
1	Af	151	TYR	Sidechain
1	Af	377	ARG	Sidechain
1	Ag	377	ARG	Sidechain
1	Ai	377	ARG	Sidechain
1	Aj	377	ARG	Sidechain
1	Ak	151	TYR	Sidechain
1	Ak	377	ARG	Sidechain
1	Al	377	ARG	Sidechain
1	Al	474	ARG	Sidechain
1	Am	151	TYR	Sidechain
1	Am	377	ARG	Sidechain
1	An	151	TYR	Sidechain
1	An	377	ARG	Sidechain
1	Ap	377	ARG	Sidechain
1	Aq	377	ARG	Sidechain
1	Ar	377	ARG	Sidechain
1	Ar	474	ARG	Sidechain
1	As	151	TYR	Sidechain
1	As	377	ARG	Sidechain
1	As	474	ARG	Sidechain
1	At	151	TYR	Sidechain
1	At	377	ARG	Sidechain
1	Au	151	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	Au	377	ARG	Sidechain
1	Av	377	ARG	Sidechain
1	Aw	377	ARG	Sidechain
1	Ax	377	ARG	Sidechain
1	Ax	474	ARG	Sidechain
1	Ay	377	ARG	Sidechain
1	Az	151	TYR	Sidechain
1	Az	377	ARG	Sidechain
1	BA	151	TYR	Sidechain
1	BA	377	ARG	Sidechain
1	BB	377	ARG	Sidechain
1	BC	377	ARG	Sidechain
1	BD	377	ARG	Sidechain
1	BE	151	TYR	Sidechain
1	BE	377	ARG	Sidechain
1	BF	377	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	5648	5654	5652	0	0
1	A1	5648	5654	5652	2	0
1	A2	5648	5654	5652	2	0
1	A3	5648	5654	5652	2	0
1	A4	5648	5654	5652	1	0
1	A5	5648	5654	5652	3	0
1	A6	5648	5654	5652	1	0
1	A7	5648	5654	5652	1	0
1	A8	5648	5654	5652	2	0
1	A9	5648	5654	5652	1	0
1	Ac	5648	5654	5652	1	0
1	Ad	5648	5654	5652	1	0
1	Ae	5648	5654	5652	2	0
1	Af	5648	5654	5652	2	0
1	Ag	5648	5654	5652	2	0
1	Ah	5648	5654	5652	3	0
1	Ai	5648	5654	5652	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aj	5648	5654	5652	1	0
1	Ak	5648	5654	5652	1	0
1	Al	5648	5654	5652	1	0
1	Am	5648	5654	5652	2	0
1	An	5648	5654	5652	1	0
1	Ap	5648	5654	5652	1	0
1	Aq	5648	5654	5652	3	0
1	Ar	5648	5654	5652	1	0
1	As	5648	5654	5652	2	0
1	At	5648	5654	5652	2	0
1	Au	5648	5654	5652	1	0
1	Av	5648	5650	5652	1	0
1	Aw	5648	5654	5652	2	0
1	Ax	5648	5654	5652	2	0
1	Ay	5648	5654	5652	3	0
1	Az	5648	5654	5652	0	0
1	BA	5648	5654	5652	1	0
1	BB	5648	5654	5652	3	0
1	BC	5648	5654	5652	1	0
1	BD	5648	5654	5652	2	0
1	BE	5648	5654	5652	1	0
1	BF	5648	5654	5652	1	0
All	All	220272	220502	220428	59	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 0.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A6:384:GLU:HA	1:A6:403:GLY:HA2	1.98	0.46
1:An:384:GLU:HA	1:An:403:GLY:HA2	1.98	0.46
1:Am:384:GLU:HA	1:Am:403:GLY:HA2	1.99	0.45
1:Ac:384:GLU:HA	1:Ac:403:GLY:HA2	1.99	0.45
1:BD:384:GLU:HA	1:BD:403:GLY:HA2	1.99	0.44
1:Ax:384:GLU:HA	1:Ax:403:GLY:HA2	2.00	0.44
1:Au:384:GLU:HA	1:Au:403:GLY:HA2	2.00	0.44
1:BF:384:GLU:HA	1:BF:403:GLY:HA2	2.00	0.44
1:A2:384:GLU:HA	1:A2:403:GLY:HA2	2.00	0.44
1:Ah:180:LYS:HE2	1:Ah:209:PHE:CE1	2.53	0.44
1:Ak:384:GLU:HA	1:Ak:403:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:384:GLU:HA	1:Ay:403:GLY:HA2	2.00	0.44
1:A7:384:GLU:HA	1:A7:403:GLY:HA2	1.99	0.44
1:BC:384:GLU:HA	1:BC:403:GLY:HA2	2.00	0.44
1:Av:384:GLU:HA	1:Av:403:GLY:HA2	2.00	0.43
1:A9:384:GLU:HA	1:A9:403:GLY:HA2	2.00	0.43
1:Ad:384:GLU:HA	1:Ad:403:GLY:HA2	1.99	0.43
1:Aw:384:GLU:HA	1:Aw:403:GLY:HA2	2.00	0.43
1:Af:384:GLU:HA	1:Af:403:GLY:HA2	1.99	0.43
1:BE:384:GLU:HA	1:BE:403:GLY:HA2	2.01	0.43
1:Ap:384:GLU:HA	1:Ap:403:GLY:HA2	2.01	0.43
1:Ar:384:GLU:HA	1:Ar:403:GLY:HA2	2.01	0.43
1:A3:180:LYS:HE2	1:A3:209:PHE:CE1	2.54	0.43
1:A4:384:GLU:HA	1:A4:403:GLY:HA2	2.01	0.43
1:Ah:384:GLU:HA	1:Ah:403:GLY:HA2	2.00	0.43
1:A2:180:LYS:HE2	1:A2:209:PHE:CE1	2.54	0.42
1:Aj:384:GLU:HA	1:Aj:403:GLY:HA2	2.01	0.42
1:A3:384:GLU:HA	1:A3:403:GLY:HA2	2.01	0.42
1:Ay:482:PHE:CZ	1:Ay:558:THR:HG23	2.54	0.42
1:A1:384:GLU:HA	1:A1:403:GLY:HA2	2.02	0.42
1:Ae:180:LYS:HE2	1:Ae:209:PHE:CE1	2.55	0.42
1:Ae:384:GLU:HA	1:Ae:403:GLY:HA2	2.01	0.42
1:Af:180:LYS:HE2	1:Af:209:PHE:CE1	2.54	0.42
1:BB:180:LYS:HE2	1:BB:209:PHE:CE1	2.55	0.42
1:A8:384:GLU:HA	1:A8:403:GLY:HA2	2.02	0.42
1:Ag:384:GLU:HA	1:Ag:403:GLY:HA2	2.00	0.42
1:BA:384:GLU:HA	1:BA:403:GLY:HA2	2.02	0.42
1:At:384:GLU:HA	1:At:403:GLY:HA2	2.02	0.42
1:Aq:482:PHE:CZ	1:Aq:558:THR:HG23	2.55	0.42
1:Aq:384:GLU:HA	1:Aq:403:GLY:HA2	2.01	0.41
1:BD:482:PHE:CZ	1:BD:558:THR:HG23	2.55	0.41
1:A5:543:TYR:CE1	1:A5:575:ILE:HG21	2.55	0.41
1:BB:384:GLU:HA	1:BB:403:GLY:HA2	2.02	0.41
1:A5:384:GLU:HA	1:A5:403:GLY:HA2	2.03	0.41
1:As:180:LYS:HE2	1:As:209:PHE:CE1	2.56	0.41
1:Ay:180:LYS:HE2	1:Ay:209:PHE:CE1	2.56	0.41
1:Ah:482:PHE:CZ	1:Ah:558:THR:HG23	2.56	0.41
1:As:482:PHE:CZ	1:As:558:THR:HG23	2.55	0.41
1:Aw:180:LYS:HE2	1:Aw:209:PHE:CE1	2.56	0.41
1:A5:180:LYS:HE2	1:A5:209:PHE:CE1	2.56	0.41
1:A1:180:LYS:HE2	1:A1:209:PHE:CE1	2.55	0.41
1:A8:482:PHE:CZ	1:A8:558:THR:HG23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:180:LYS:HE2	1:Am:209:PHE:CE1	2.55	0.41
1:At:180:LYS:HE2	1:At:209:PHE:CE1	2.56	0.41
1:BB:482:PHE:CZ	1:BB:558:THR:HG23	2.56	0.40
1:Aq:180:LYS:HE2	1:Aq:209:PHE:CE1	2.55	0.40
1:Ag:482:PHE:CZ	1:Ag:558:THR:HG23	2.56	0.40
1:Ax:482:PHE:CZ	1:Ax:558:THR:HG23	2.57	0.40
1:Al:482:PHE:CZ	1:Al:558:THR:HG23	2.57	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	A0	699/893 (78%)	675 (97%)	24 (3%)	0	100	100
1	A1	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	A2	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	A3	699/893 (78%)	676 (97%)	23 (3%)	0	100	100
1	A4	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	A5	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	A6	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	A7	699/893 (78%)	676 (97%)	23 (3%)	0	100	100
1	A8	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	A9	699/893 (78%)	676 (97%)	23 (3%)	0	100	100
1	Ac	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	Ad	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Ae	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Af	699/893 (78%)	679 (97%)	20 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ag	699/893 (78%)	679 (97%)	20 (3%)	0	100	100
1	Ah	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Ai	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Aj	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Ak	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	Al	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Am	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	An	699/893 (78%)	679 (97%)	20 (3%)	0	100	100
1	Ap	699/893 (78%)	679 (97%)	20 (3%)	0	100	100
1	Aq	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	Ar	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	As	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	At	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	Au	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	Av	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Aw	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	Ax	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Ay	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	Az	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	BA	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	BB	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	BC	699/893 (78%)	678 (97%)	21 (3%)	0	100	100
1	BD	699/893 (78%)	677 (97%)	22 (3%)	0	100	100
1	BE	699/893 (78%)	676 (97%)	23 (3%)	0	100	100
1	BF	699/893 (78%)	676 (97%)	23 (3%)	0	100	100
All	All	27261/34827 (78%)	26413 (97%)	848 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	A1	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	A2	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	A3	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	A4	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	A5	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	A6	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	A7	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	A8	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	A9	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	Ac	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	Ad	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	Ae	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Af	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Ag	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	Ah	607/755 (80%)	607 (100%)	0	100	100
1	Ai	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Aj	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Ak	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	Al	607/755 (80%)	604 (100%)	3 (0%)	86	92
1	Am	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	An	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Ap	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Aq	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Ar	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	As	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	At	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Au	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Av	607/755 (80%)	606 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aw	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	Ax	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	Ay	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	Az	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	BA	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	BB	607/755 (80%)	604 (100%)	3 (0%)	86	92
1	BC	607/755 (80%)	605 (100%)	2 (0%)	91	95
1	BD	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	BE	607/755 (80%)	606 (100%)	1 (0%)	92	96
1	BF	607/755 (80%)	606 (100%)	1 (0%)	92	96
All	All	23673/29445 (80%)	23614 (100%)	59 (0%)	91	96

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	543	TYR
1	A0	655	GLN
1	A1	543	TYR
1	A2	543	TYR
1	A3	108	ASP
1	A3	543	TYR
1	A4	543	TYR
1	A5	108	ASP
1	A5	543	TYR
1	A6	108	ASP
1	A6	543	TYR
1	A7	108	ASP
1	A7	543	TYR
1	A8	342	GLU
1	A8	543	TYR
1	A9	342	GLU
1	A9	543	TYR
1	Ac	108	ASP
1	Ac	543	TYR
1	Ad	108	ASP
1	Ad	543	TYR
1	Ae	543	TYR
1	Af	543	TYR

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Mol	Chain	Res	Type
1	Ag	108	ASP
1	Ag	543	TYR
1	Ai	543	TYR
1	Aj	543	TYR
1	Ak	108	ASP
1	Ak	543	TYR
1	Al	108	ASP
1	Al	342	GLU
1	Al	543	TYR
1	Am	108	ASP
1	An	543	TYR
1	Ap	543	TYR
1	Aq	543	TYR
1	Ar	108	ASP
1	Ar	543	TYR
1	As	108	ASP
1	As	543	TYR
1	At	543	TYR
1	Au	543	TYR
1	Av	543	TYR
1	Aw	108	ASP
1	Aw	543	TYR
1	Ax	342	GLU
1	Ax	543	TYR
1	Ay	108	ASP
1	Az	108	ASP
1	Az	342	GLU
1	BA	543	TYR
1	BB	108	ASP
1	BB	342	GLU
1	BB	543	TYR
1	BC	108	ASP
1	BC	543	TYR
1	BD	543	TYR
1	BE	543	TYR
1	BF	543	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (388) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	280	ASN
1	A0	294	ASN

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Mol	Chain	Res	Type
1	A0	318	GLN
1	A0	321	GLN
1	A0	410	GLN
1	A0	469	GLN
1	A0	630	GLN
1	A0	749	GLN
1	A0	776	GLN
1	A1	280	ASN
1	A1	295	GLN
1	A1	329	GLN
1	A1	338	GLN
1	A1	469	GLN
1	A1	494	GLN
1	A1	630	GLN
1	A1	669	GLN
1	A1	749	GLN
1	A1	776	GLN
1	A2	295	GLN
1	A2	329	GLN
1	A2	338	GLN
1	A2	469	GLN
1	A2	669	GLN
1	A2	682	GLN
1	A2	691	GLN
1	A2	749	GLN
1	A2	776	GLN
1	A2	786	GLN
1	A2	797	GLN
1	A3	295	GLN
1	A3	329	GLN
1	A3	338	GLN
1	A3	469	GLN
1	A3	494	GLN
1	A3	630	GLN
1	A3	682	GLN
1	A3	696	GLN
1	A3	749	GLN
1	A3	776	GLN
1	A4	38	GLN
1	A4	295	GLN
1	A4	329	GLN
1	A4	338	GLN

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Mol	Chain	Res	Type
1	A4	469	GLN
1	A4	630	GLN
1	A4	749	GLN
1	A4	776	GLN
1	A5	38	GLN
1	A5	295	GLN
1	A5	329	GLN
1	A5	338	GLN
1	A5	469	GLN
1	A5	682	GLN
1	A5	749	GLN
1	A5	776	GLN
1	A6	38	GLN
1	A6	280	ASN
1	A6	295	GLN
1	A6	329	GLN
1	A6	338	GLN
1	A6	469	GLN
1	A6	494	GLN
1	A6	682	GLN
1	A6	749	GLN
1	A6	776	GLN
1	A7	38	GLN
1	A7	295	GLN
1	A7	329	GLN
1	A7	338	GLN
1	A7	469	GLN
1	A7	494	GLN
1	A7	630	GLN
1	A7	669	GLN
1	A7	682	GLN
1	A7	749	GLN
1	A7	776	GLN
1	A7	786	GLN
1	A8	38	GLN
1	A8	280	ASN
1	A8	295	GLN
1	A8	338	GLN
1	A8	469	GLN
1	A8	494	GLN
1	A8	682	GLN
1	A8	691	GLN

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Mol	Chain	Res	Type
1	A8	749	GLN
1	A8	776	GLN
1	A8	797	GLN
1	A9	38	GLN
1	A9	295	GLN
1	A9	329	GLN
1	A9	469	GLN
1	A9	630	GLN
1	A9	682	GLN
1	A9	691	GLN
1	A9	749	GLN
1	A9	776	GLN
1	Ac	295	GLN
1	Ac	329	GLN
1	Ac	338	GLN
1	Ac	469	GLN
1	Ac	494	GLN
1	Ac	630	GLN
1	Ac	682	GLN
1	Ac	749	GLN
1	Ac	776	GLN
1	Ad	38	GLN
1	Ad	295	GLN
1	Ad	329	GLN
1	Ad	338	GLN
1	Ad	469	GLN
1	Ad	630	GLN
1	Ad	682	GLN
1	Ad	691	GLN
1	Ad	749	GLN
1	Ad	776	GLN
1	Ad	786	GLN
1	Ad	797	GLN
1	Ae	38	GLN
1	Ae	295	GLN
1	Ae	329	GLN
1	Ae	338	GLN
1	Ae	469	GLN
1	Ae	494	GLN
1	Ae	630	GLN
1	Ae	749	GLN
1	Ae	776	GLN

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Mol	Chain	Res	Type
1	Ae	797	GLN
1	Af	38	GLN
1	Af	295	GLN
1	Af	329	GLN
1	Af	338	GLN
1	Af	469	GLN
1	Af	494	GLN
1	Af	630	GLN
1	Af	682	GLN
1	Af	776	GLN
1	Ag	38	GLN
1	Ag	280	ASN
1	Ag	295	GLN
1	Ag	318	GLN
1	Ag	338	GLN
1	Ag	469	GLN
1	Ag	630	GLN
1	Ag	682	GLN
1	Ag	776	GLN
1	Ag	786	GLN
1	Ah	38	GLN
1	Ah	329	GLN
1	Ah	338	GLN
1	Ah	469	GLN
1	Ah	669	GLN
1	Ah	682	GLN
1	Ah	749	GLN
1	Ah	776	GLN
1	Ai	280	ASN
1	Ai	295	GLN
1	Ai	356	HIS
1	Ai	469	GLN
1	Ai	494	GLN
1	Ai	630	GLN
1	Ai	669	GLN
1	Ai	749	GLN
1	Ai	776	GLN
1	Aj	295	GLN
1	Aj	318	GLN
1	Aj	329	GLN
1	Aj	469	GLN
1	Aj	494	GLN

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Mol	Chain	Res	Type
1	Aj	630	GLN
1	Aj	669	GLN
1	Aj	682	GLN
1	Aj	696	GLN
1	Aj	749	GLN
1	Aj	776	GLN
1	Aj	786	GLN
1	Ak	280	ASN
1	Ak	295	GLN
1	Ak	329	GLN
1	Ak	338	GLN
1	Ak	469	GLN
1	Ak	630	GLN
1	Ak	682	GLN
1	Ak	749	GLN
1	Ak	776	GLN
1	Ak	786	GLN
1	Ak	797	GLN
1	Al	38	GLN
1	Al	295	GLN
1	Al	329	GLN
1	Al	338	GLN
1	Al	469	GLN
1	Al	494	GLN
1	Al	630	GLN
1	Al	682	GLN
1	Al	749	GLN
1	Al	776	GLN
1	Al	786	GLN
1	Am	295	GLN
1	Am	318	GLN
1	Am	329	GLN
1	Am	338	GLN
1	Am	469	GLN
1	Am	630	GLN
1	Am	682	GLN
1	Am	749	GLN
1	Am	776	GLN
1	Am	786	GLN
1	An	38	GLN
1	An	295	GLN
1	An	329	GLN

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Mol	Chain	Res	Type
1	An	338	GLN
1	An	469	GLN
1	An	494	GLN
1	An	630	GLN
1	An	682	GLN
1	An	749	GLN
1	An	776	GLN
1	An	797	GLN
1	Ap	38	GLN
1	Ap	329	GLN
1	Ap	338	GLN
1	Ap	469	GLN
1	Ap	630	GLN
1	Ap	682	GLN
1	Ap	691	GLN
1	Ap	749	GLN
1	Ap	776	GLN
1	Aq	38	GLN
1	Aq	280	ASN
1	Aq	295	GLN
1	Aq	329	GLN
1	Aq	338	GLN
1	Aq	469	GLN
1	Aq	682	GLN
1	Aq	749	GLN
1	Aq	776	GLN
1	Ar	38	GLN
1	Ar	329	GLN
1	Ar	338	GLN
1	Ar	469	GLN
1	Ar	494	GLN
1	Ar	630	GLN
1	Ar	682	GLN
1	Ar	749	GLN
1	Ar	776	GLN
1	As	295	GLN
1	As	329	GLN
1	As	338	GLN
1	As	469	GLN
1	As	749	GLN
1	As	776	GLN
1	At	38	GLN

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Mol	Chain	Res	Type
1	At	295	GLN
1	At	338	GLN
1	At	351	HIS
1	At	469	GLN
1	At	494	GLN
1	At	630	GLN
1	At	749	GLN
1	At	776	GLN
1	Au	280	ASN
1	Au	295	GLN
1	Au	329	GLN
1	Au	338	GLN
1	Au	469	GLN
1	Au	494	GLN
1	Au	669	GLN
1	Au	749	GLN
1	Au	776	GLN
1	Au	786	GLN
1	Av	280	ASN
1	Av	295	GLN
1	Av	318	GLN
1	Av	329	GLN
1	Av	338	GLN
1	Av	469	GLN
1	Av	682	GLN
1	Av	749	GLN
1	Av	776	GLN
1	Aw	295	GLN
1	Aw	329	GLN
1	Aw	338	GLN
1	Aw	351	HIS
1	Aw	469	GLN
1	Aw	494	GLN
1	Aw	630	GLN
1	Aw	682	GLN
1	Aw	691	GLN
1	Aw	749	GLN
1	Aw	776	GLN
1	Ax	295	GLN
1	Ax	329	GLN
1	Ax	338	GLN
1	Ax	469	GLN

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Mol	Chain	Res	Type
1	Ax	630	GLN
1	Ax	682	GLN
1	Ax	749	GLN
1	Ax	776	GLN
1	Ax	786	GLN
1	Ay	38	GLN
1	Ay	295	GLN
1	Ay	338	GLN
1	Ay	469	GLN
1	Ay	494	GLN
1	Ay	630	GLN
1	Ay	669	GLN
1	Ay	691	GLN
1	Ay	696	GLN
1	Ay	749	GLN
1	Ay	776	GLN
1	Az	294	ASN
1	Az	295	GLN
1	Az	318	GLN
1	Az	338	GLN
1	Az	410	GLN
1	Az	469	GLN
1	Az	655	GLN
1	Az	682	GLN
1	Az	691	GLN
1	Az	749	GLN
1	Az	776	GLN
1	Az	797	GLN
1	BA	38	GLN
1	BA	280	ASN
1	BA	295	GLN
1	BA	318	GLN
1	BA	329	GLN
1	BA	469	GLN
1	BA	494	GLN
1	BA	682	GLN
1	BA	749	GLN
1	BA	776	GLN
1	BA	797	GLN
1	BB	38	GLN
1	BB	295	GLN
1	BB	329	GLN

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Mol	Chain	Res	Type
1	BB	338	GLN
1	BB	469	GLN
1	BB	630	GLN
1	BB	669	GLN
1	BB	682	GLN
1	BB	691	GLN
1	BB	749	GLN
1	BB	776	GLN
1	BC	280	ASN
1	BC	295	GLN
1	BC	329	GLN
1	BC	338	GLN
1	BC	351	HIS
1	BC	469	GLN
1	BC	494	GLN
1	BC	669	GLN
1	BC	691	GLN
1	BC	749	GLN
1	BC	776	GLN
1	BD	38	GLN
1	BD	295	GLN
1	BD	329	GLN
1	BD	338	GLN
1	BD	469	GLN
1	BD	494	GLN
1	BD	630	GLN
1	BD	669	GLN
1	BD	749	GLN
1	BD	776	GLN
1	BD	786	GLN
1	BE	38	GLN
1	BE	295	GLN
1	BE	329	GLN
1	BE	338	GLN
1	BE	469	GLN
1	BE	669	GLN
1	BE	682	GLN
1	BE	749	GLN
1	BE	776	GLN
1	BE	797	GLN
1	BF	38	GLN
1	BF	295	GLN

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Mol	Chain	Res	Type
1	BF	329	GLN
1	BF	338	GLN
1	BF	469	GLN
1	BF	630	GLN
1	BF	682	GLN
1	BF	696	GLN
1	BF	749	GLN
1	BF	776	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

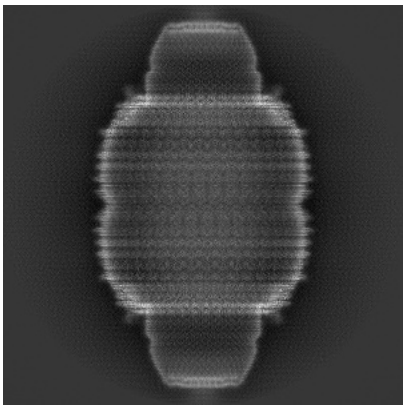
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53805. These allow visual inspection of the internal detail of the map and identification of artifacts.

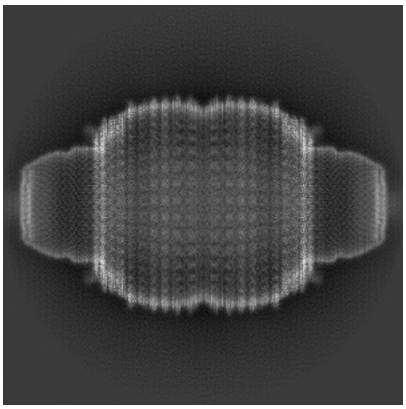
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

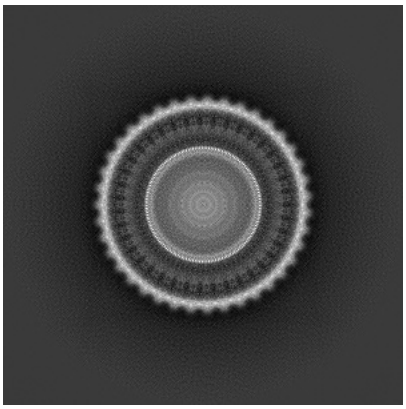
6.1.1 Primary map



X

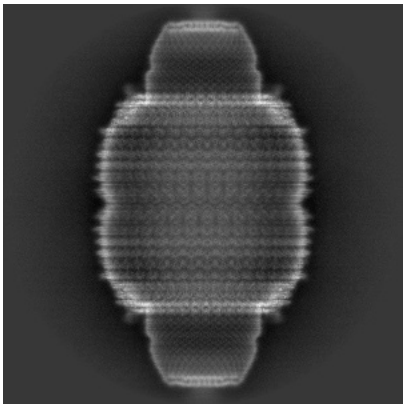


Y

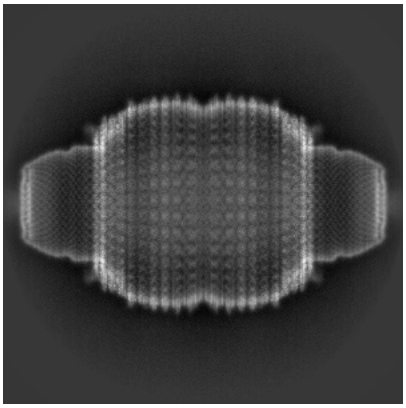


Z

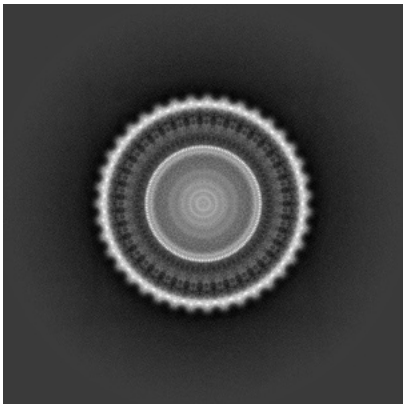
6.1.2 Raw map



X



Y

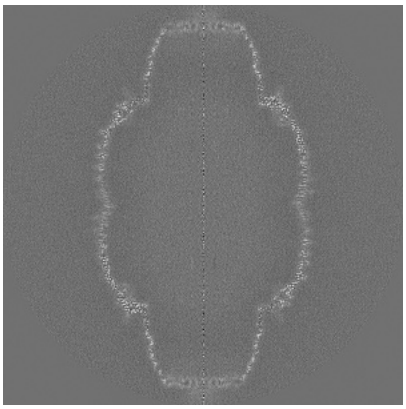


Z

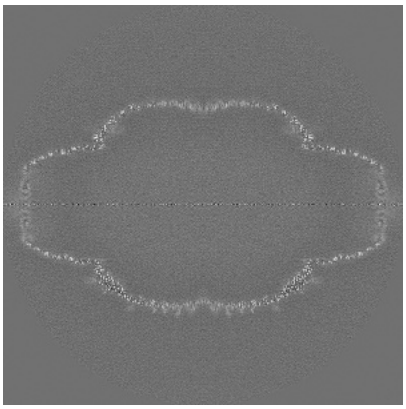
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

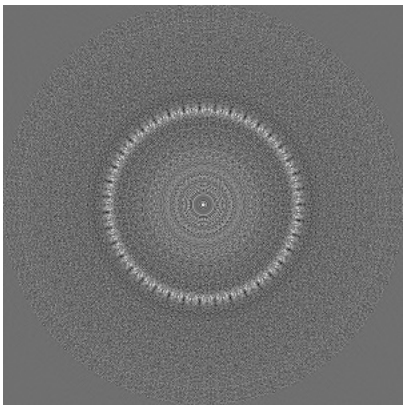
6.2.1 Primary map



X Index: 320

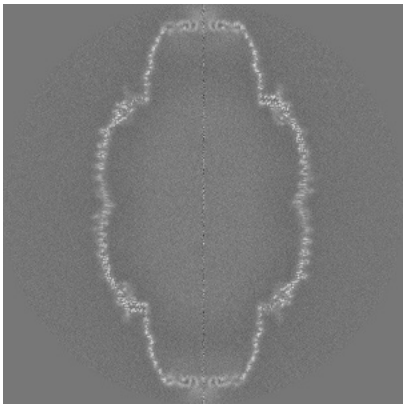


Y Index: 320

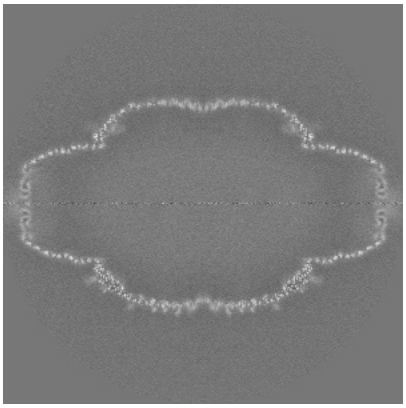


Z Index: 320

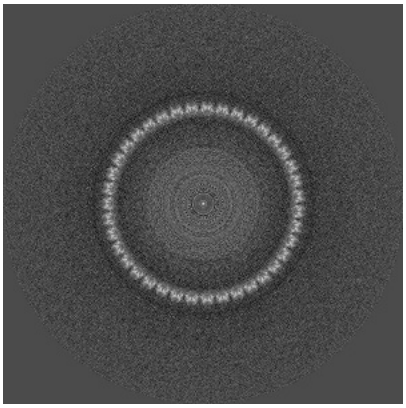
6.2.2 Raw map



X Index: 320



Y Index: 320

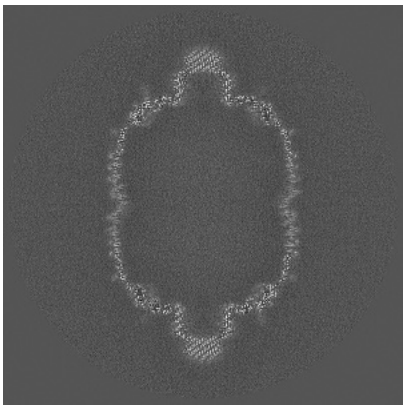


Z Index: 320

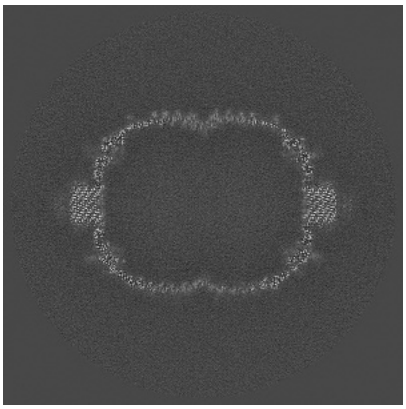
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

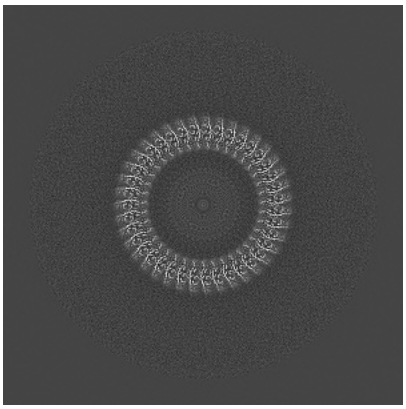
6.3.1 Primary map



X Index: 402

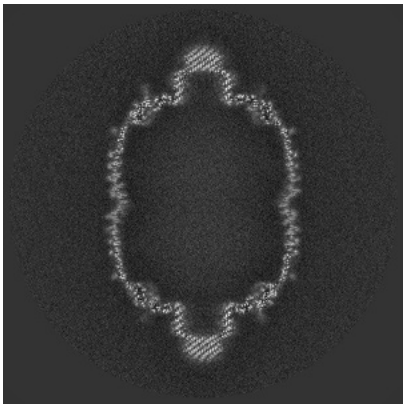


Y Index: 231

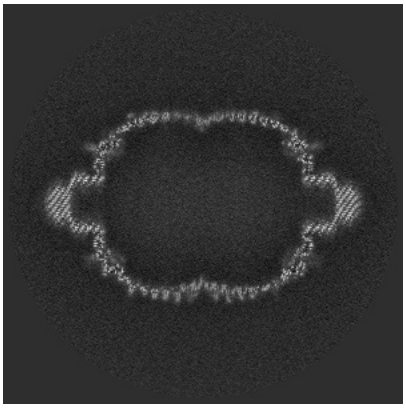


Z Index: 160

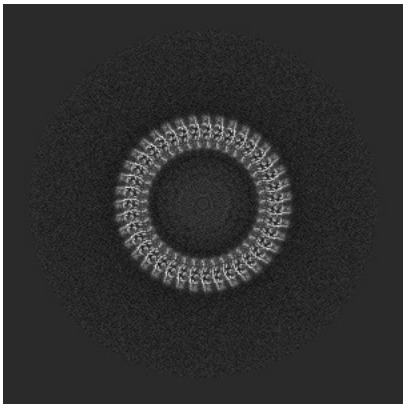
6.3.2 Raw map



X Index: 402



Y Index: 238

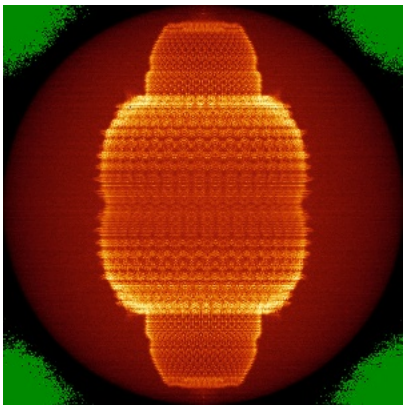


Z Index: 160

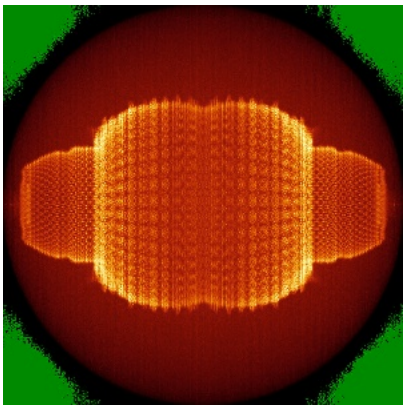
The images above show the largest variance slices of the map in three orthogonal directions.

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

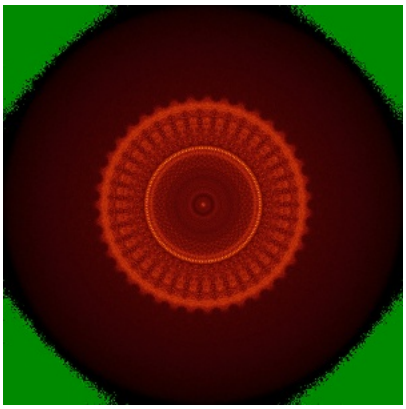
6.4.1 Primary map



X

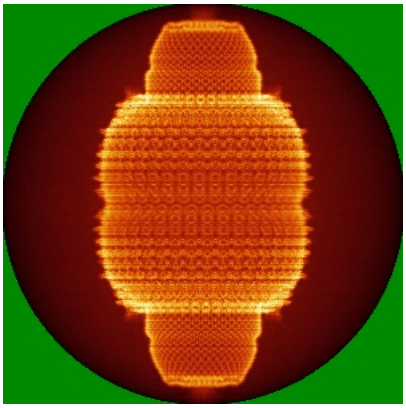


Y

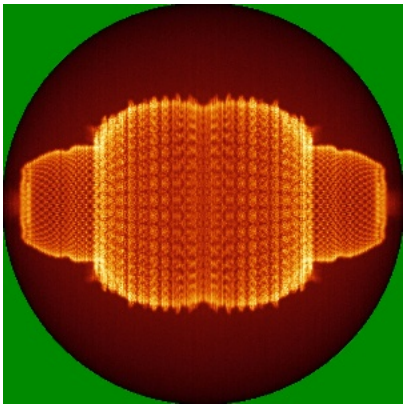


Z

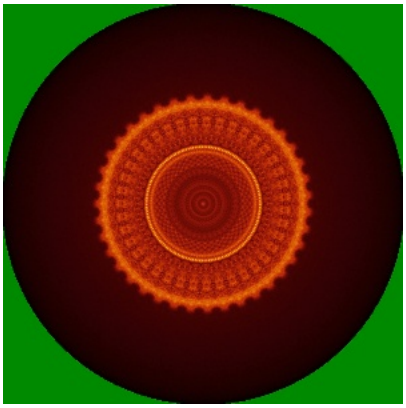
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00713. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

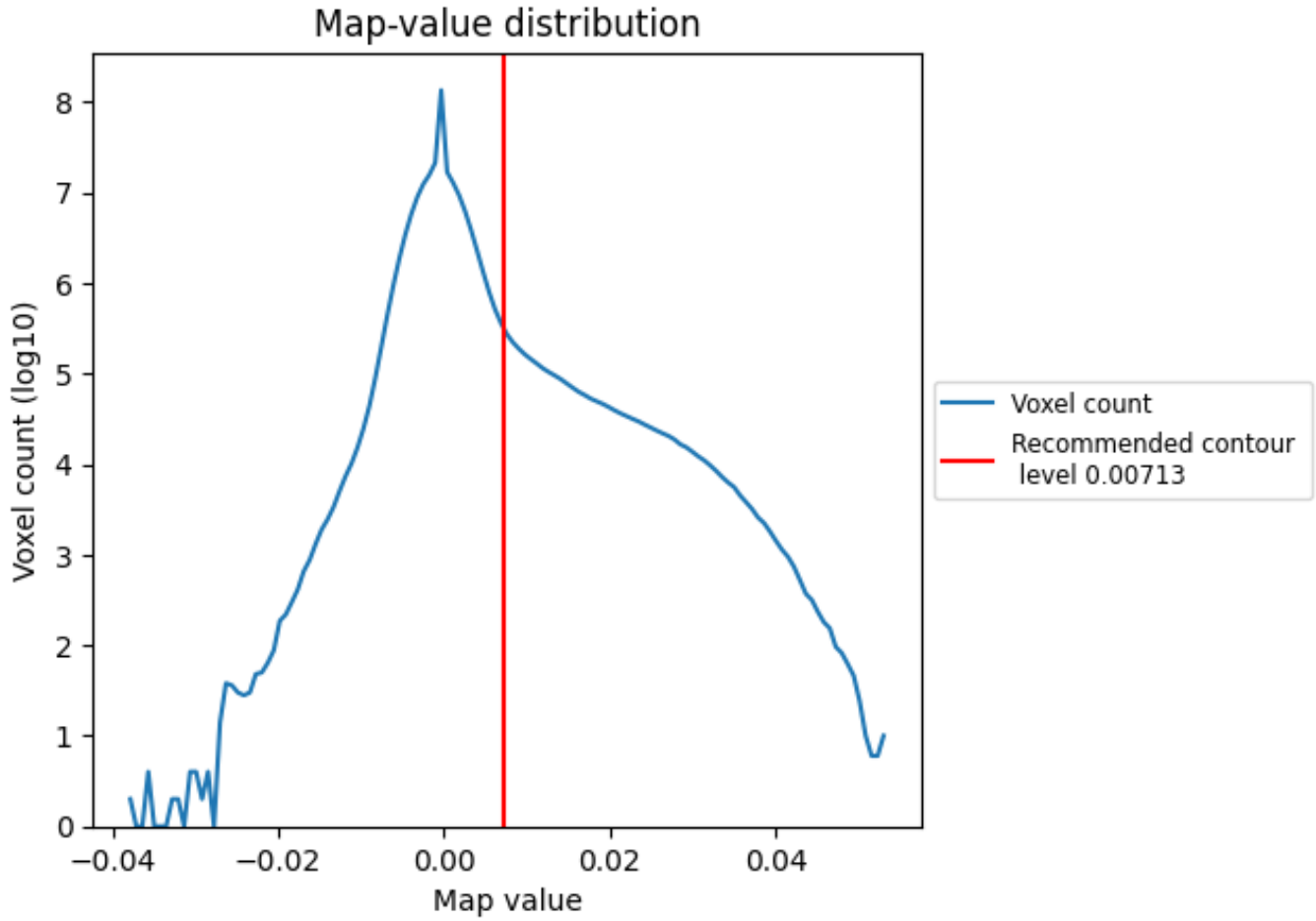
6.6 Mask visualisation (i)

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

7 Map analysis

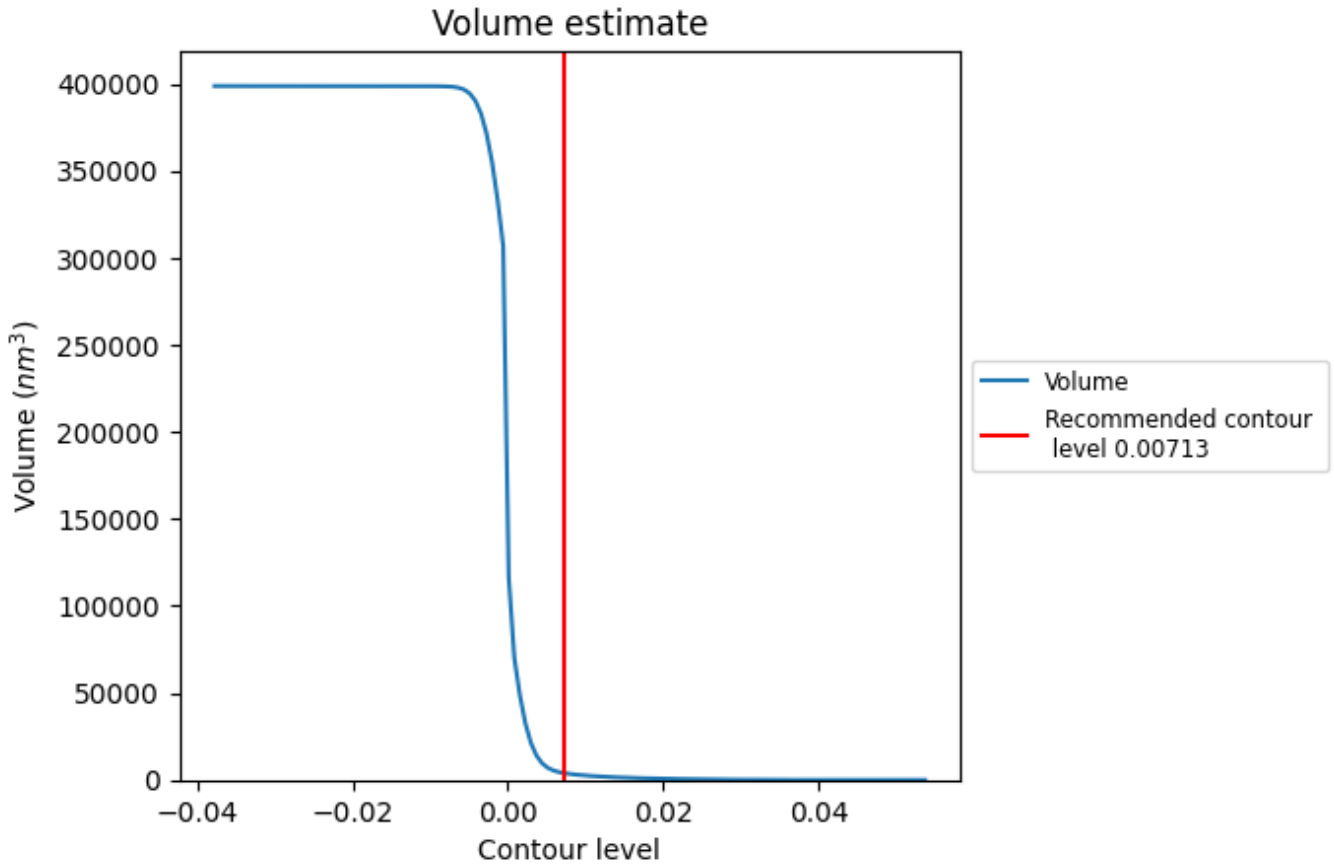
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

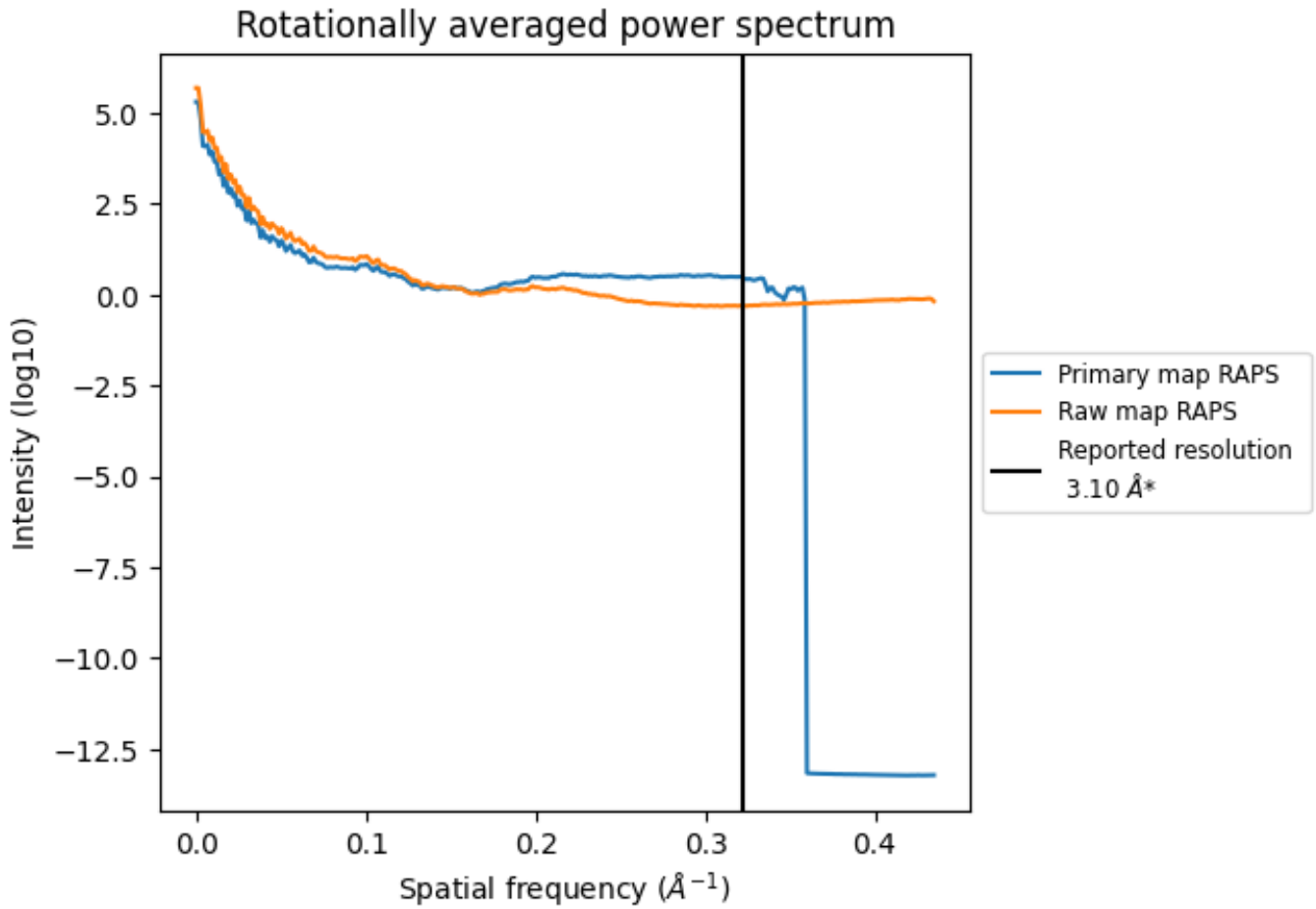
7.2 Volume estimate



The volume at the recommended contour level is 4041 nm^3; this corresponds to an approximate mass of 3650 kDa.

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

7.3 Rotationally averaged power spectrum (i)

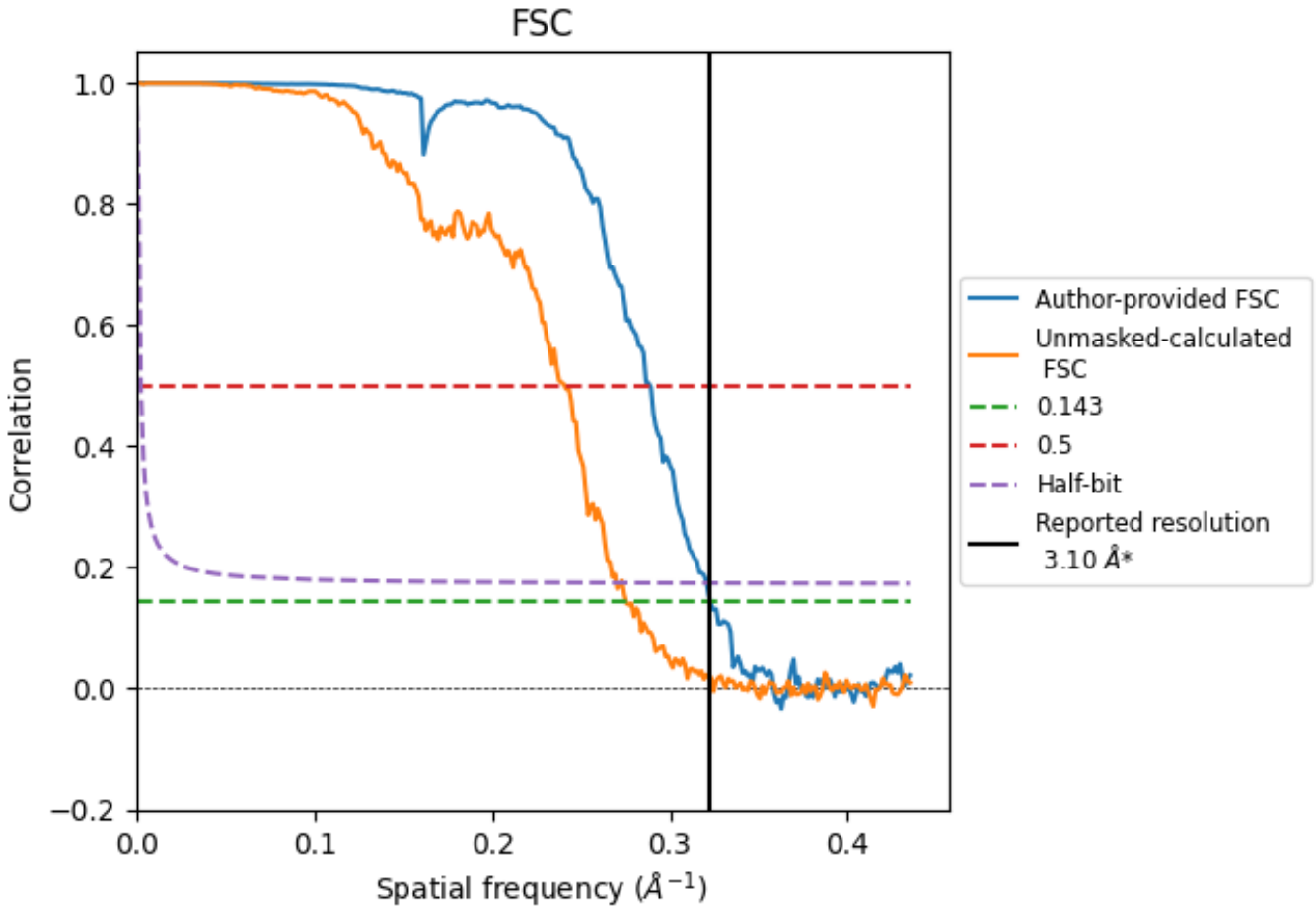


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

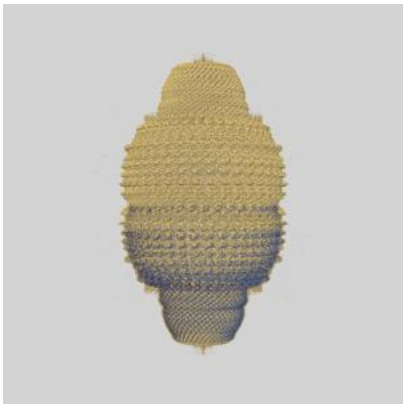
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.46	3.12
Unmasked-calculated*	3.63	4.15	3.71

*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 3.63 differs from the reported value 3.1 by more than 10 %

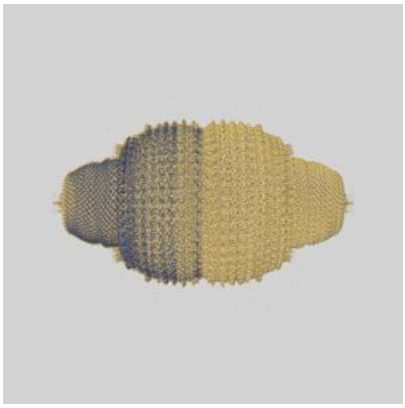
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53805 and PDB model 9R86. Per-residue inclusion information can be found in section 3 on page 8.

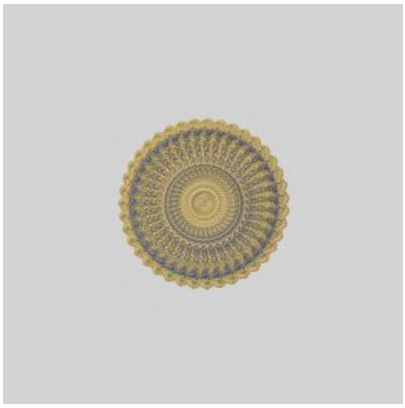
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00713 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

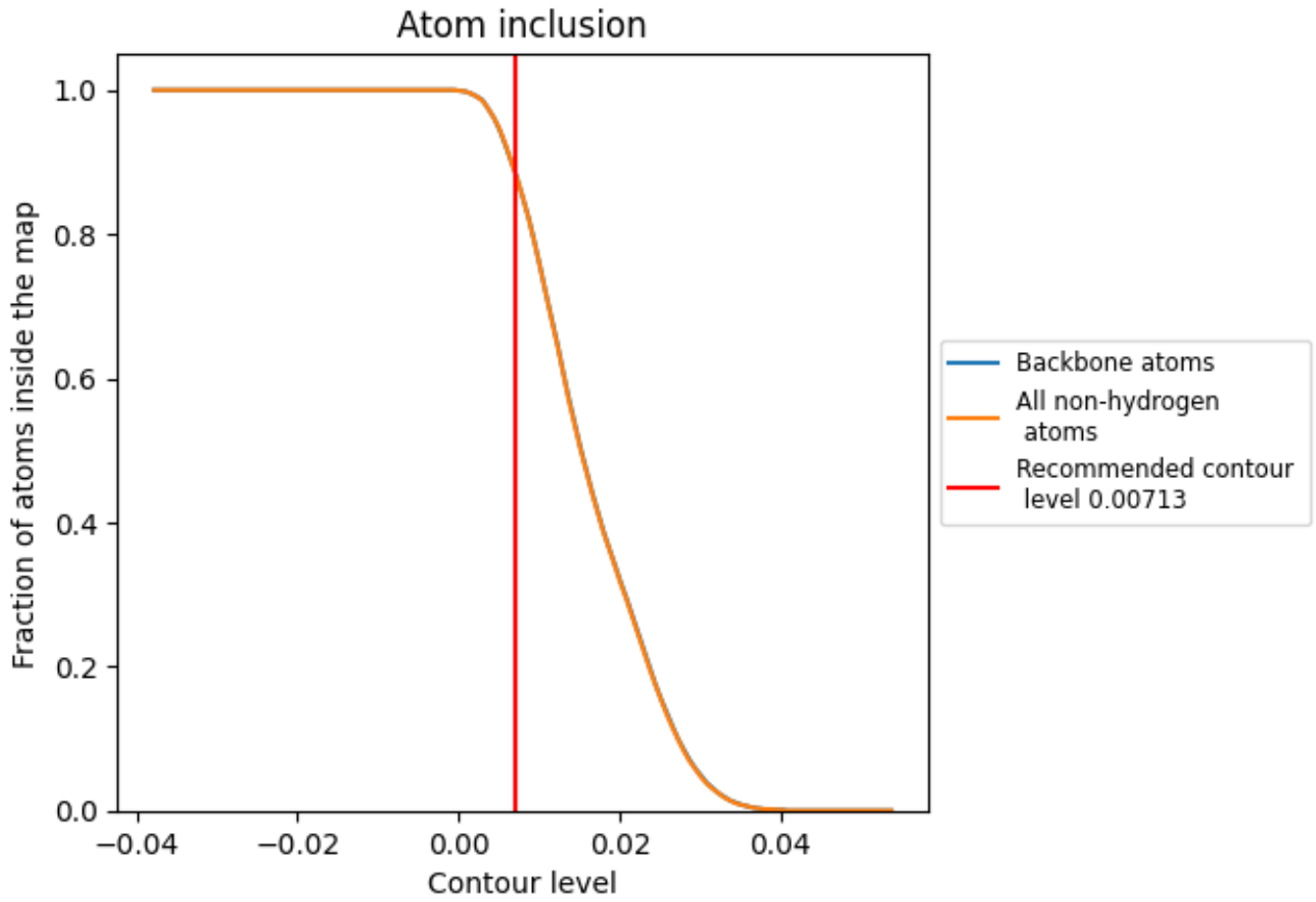
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00713).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.00713) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.5450
A0	0.8940	0.5480
A1	0.8900	0.5440
A2	0.8910	0.5440
A3	0.8930	0.5440
A4	0.8880	0.5440
A5	0.8920	0.5460
A6	0.8920	0.5440
A7	0.8890	0.5450
A8	0.8890	0.5450
A9	0.8910	0.5440
Ac	0.8930	0.5450
Ad	0.8900	0.5440
Ae	0.8890	0.5440
Af	0.8890	0.5440
Ag	0.8900	0.5440
Ah	0.8910	0.5450
Ai	0.8890	0.5450
Aj	0.8880	0.5450
Ak	0.8910	0.5450
Al	0.8890	0.5440
Am	0.8910	0.5450
An	0.8900	0.5450
Ap	0.8910	0.5450
Aq	0.8920	0.5440
Ar	0.8910	0.5450
As	0.8910	0.5450
At	0.8890	0.5440
Au	0.8890	0.5440
Av	0.8910	0.5450
Aw	0.8900	0.5440
Ax	0.8920	0.5440
Ay	0.8940	0.5450
Az	0.8920	0.5460
BA	0.8910	0.5440

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Chain	Atom inclusion	Q-score
BB	0.8910	0.5450
BC	0.8880	0.5450
BD	0.8900	0.5450
BE	0.8930	0.5450
BF	0.8920	0.5440