



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 06:39 PM JST

PDB ID : 7ETM
EMDB ID : EMD-31299
Title : C6 portal vertex in the enveloped virion capsid
Authors : Li, Z.; Yu, X.
Deposited on : 2021-05-13
Resolution : 5.90 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

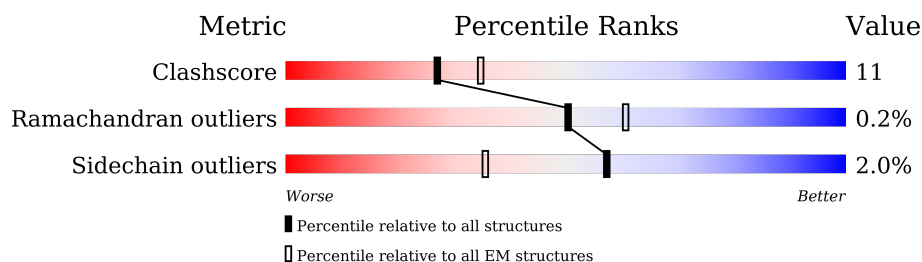
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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.





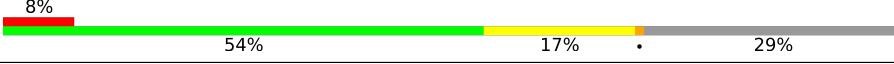

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	697	<div> <div>8%</div> <div>53%</div> <div>18%</div> <div>•</div> <div>29%</div> </div>
1	B	697	<div> <div>8%</div> <div>53%</div> <div>18%</div> <div>•</div> <div>29%</div> </div>
1	C	697	<div> <div>8%</div> <div>52%</div> <div>19%</div> <div>•</div> <div>29%</div> </div>
1	D	697	<div> <div>8%</div> <div>53%</div> <div>18%</div> <div>•</div> <div>29%</div> </div>
1	E	697	<div> <div>8%</div> <div>54%</div> <div>16%</div> <div>•</div> <div>29%</div> </div>
1	F	697	<div> <div>8%</div> <div>52%</div> <div>19%</div> <div>•</div> <div>29%</div> </div>
1	G	697	<div> <div>8%</div> <div>53%</div> <div>18%</div> <div>•</div> <div>29%</div> </div>
1	H	697	<div> <div>8%</div> <div>53%</div> <div>17%</div> <div>•</div> <div>29%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	697	
1	J	697	
1	K	697	
1	L	697	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45246 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

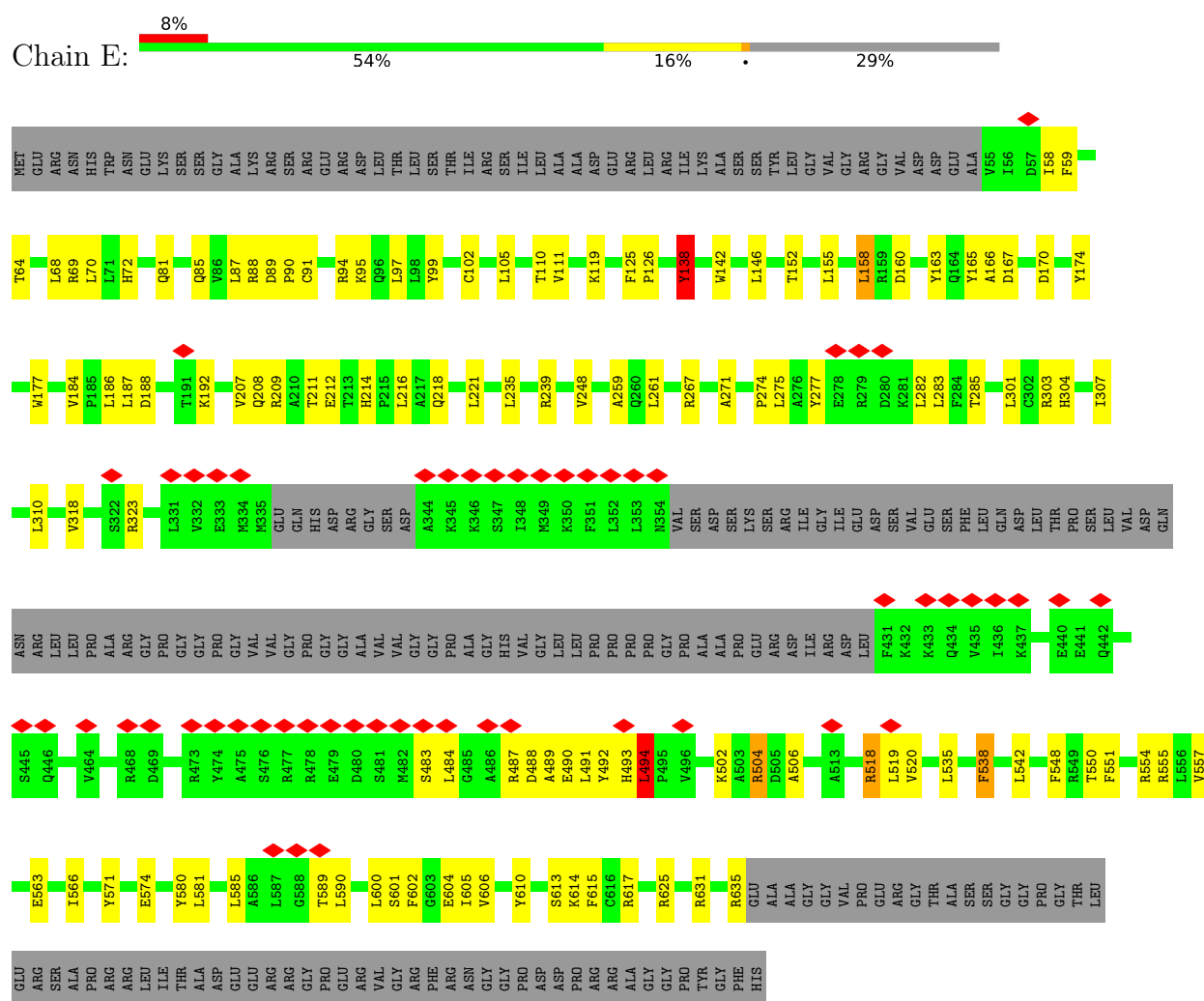
- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	497	Total	C	N	O	S	0	0
			3768	2395	683	678	12		
1	A	498	Total	C	N	O	S	0	0
			3773	2398	684	679	12		
1	H	497	Total	C	N	O	S	0	0
			3768	2395	683	678	12		
1	B	498	Total	C	N	O	S	0	0
			3773	2398	684	679	12		
1	I	497	Total	C	N	O	S	0	0
			3768	2395	683	678	12		
1	C	498	Total	C	N	O	S	0	0
			3773	2398	684	679	12		
1	J	497	Total	C	N	O	S	0	0
			3768	2395	683	678	12		
1	D	498	Total	C	N	O	S	0	0
			3773	2398	684	679	12		
1	K	497	Total	C	N	O	S	0	0
			3768	2395	683	678	12		
1	F	498	Total	C	N	O	S	0	0
			3773	2398	684	679	12		
1	L	497	Total	C	N	O	S	0	0
			3768	2395	683	678	12		
1	G	498	Total	C	N	O	S	0	0
			3773	2398	684	679	12		

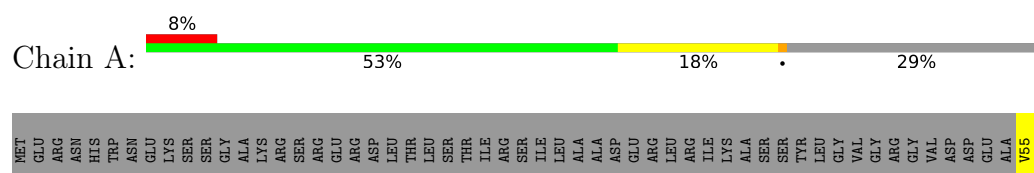
3 Residue-property plots

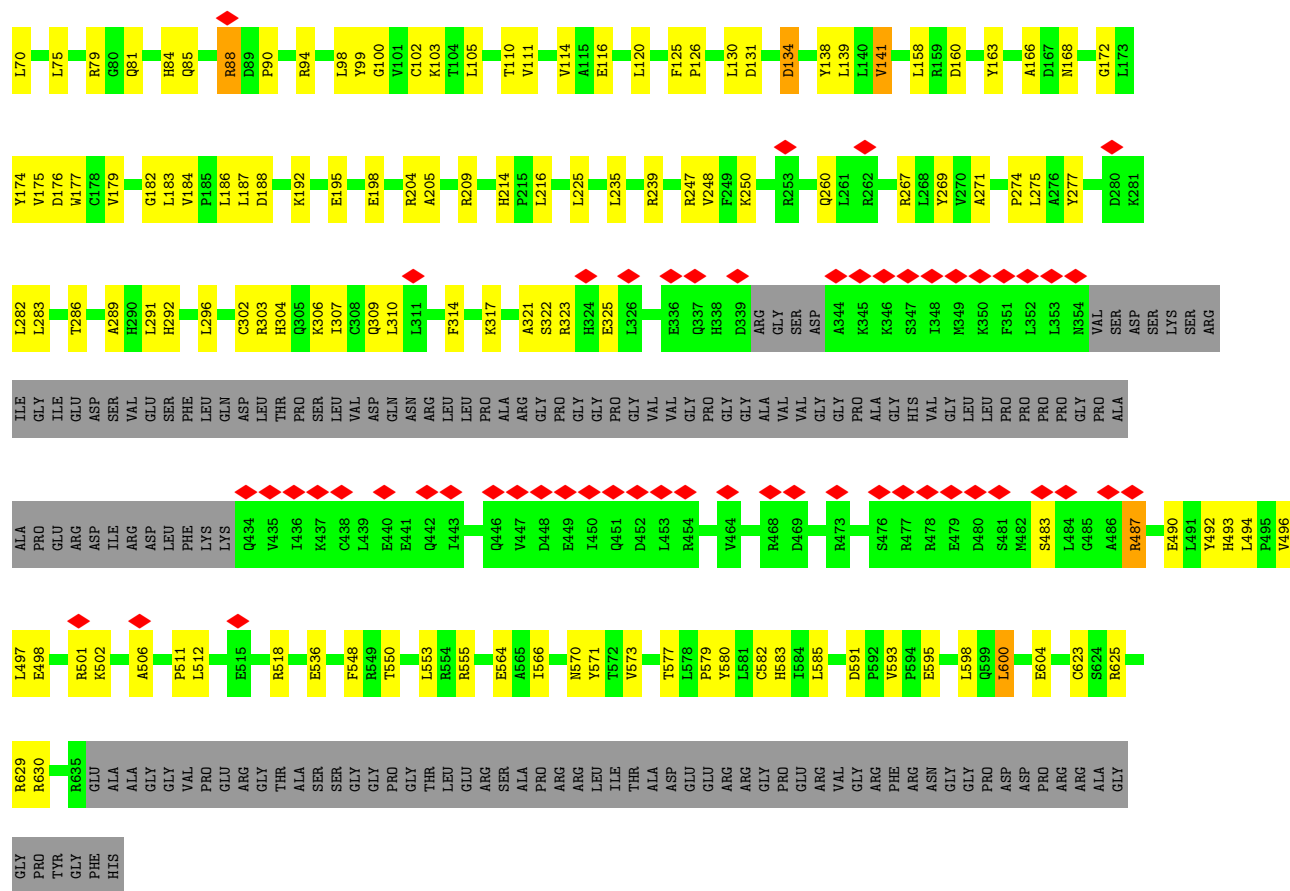
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Portal protein

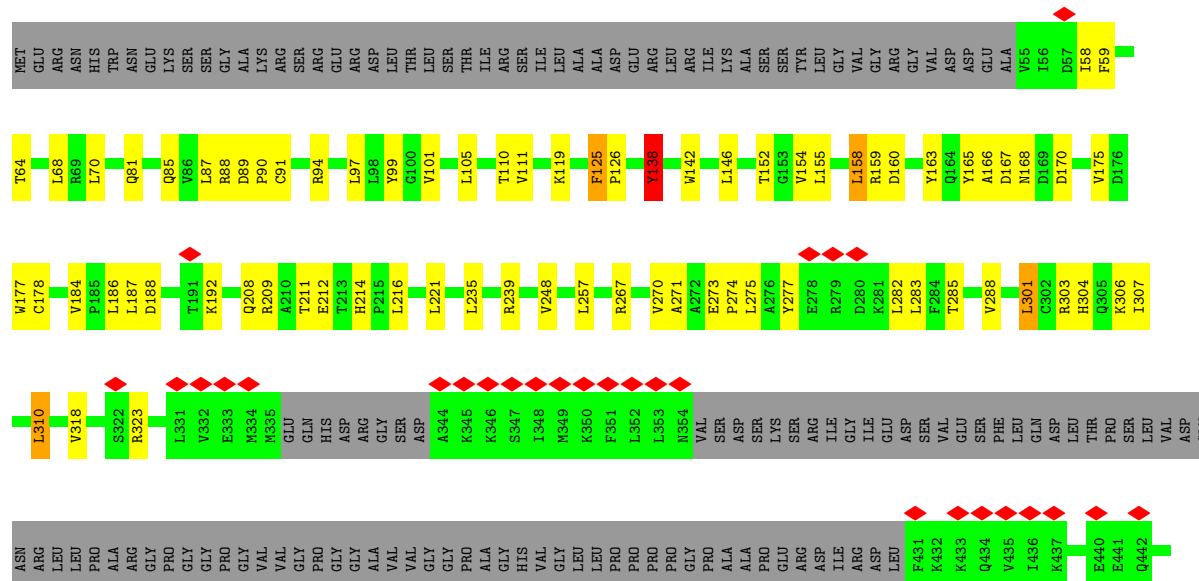


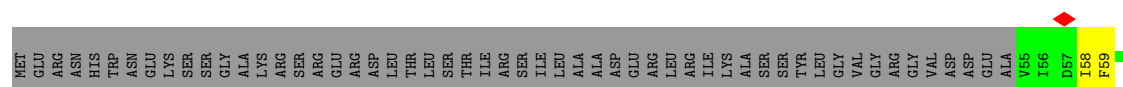
• Molecule 1: Portal protein

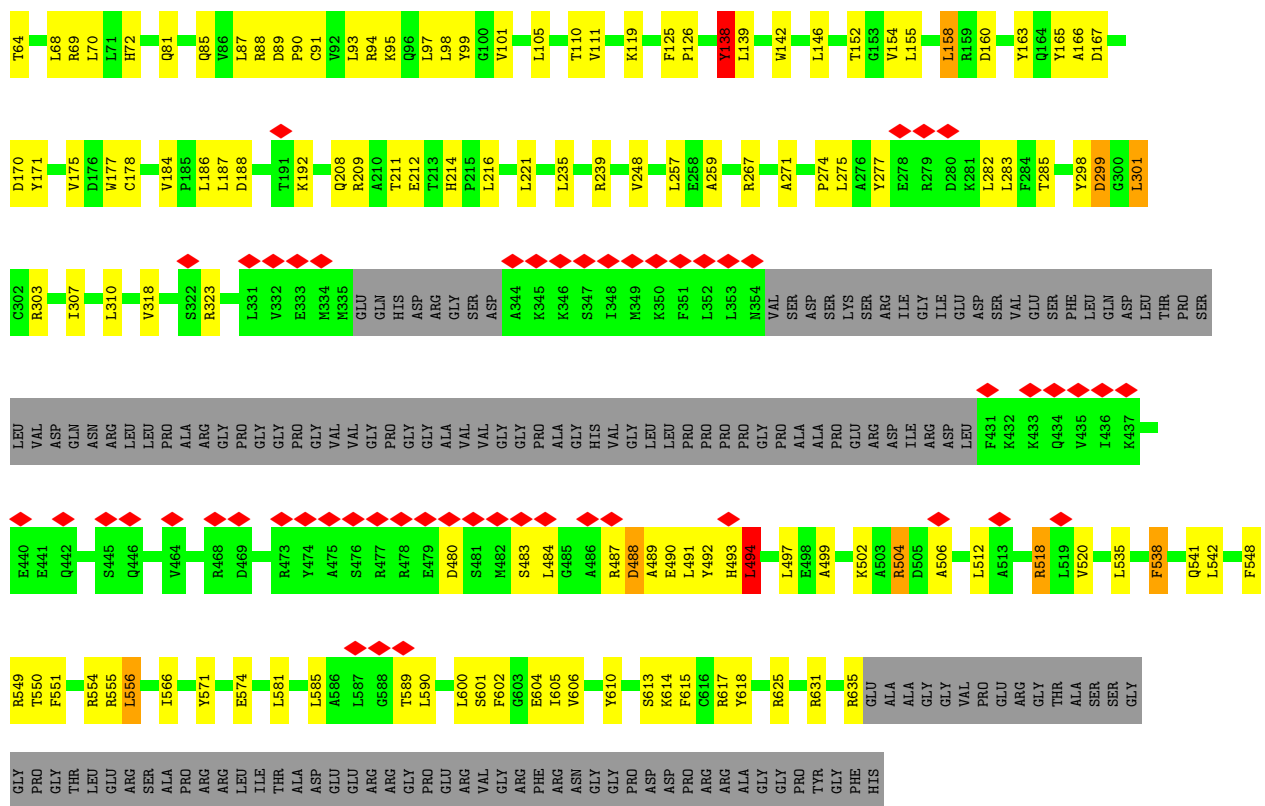




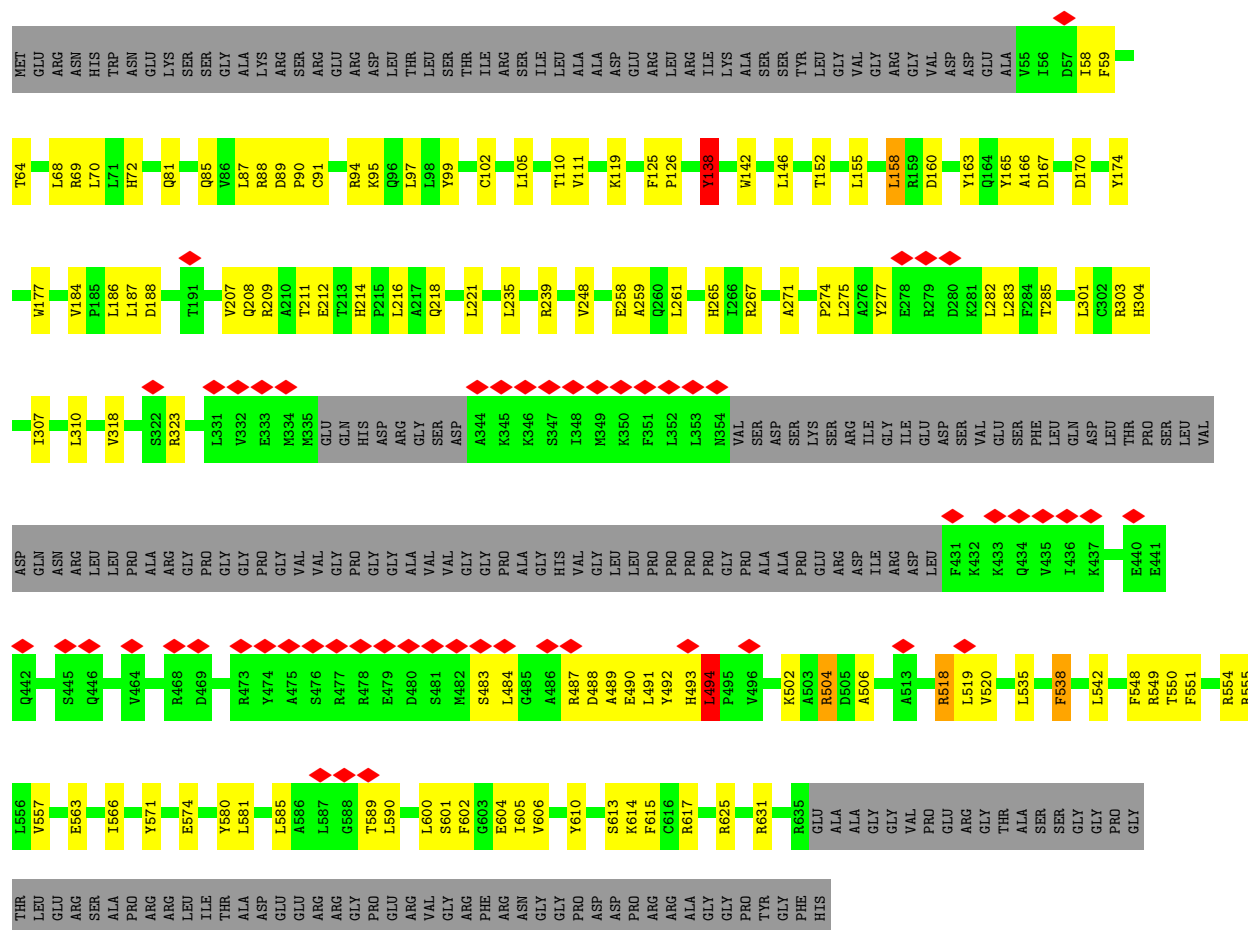
• Molecule 1: Portal protein



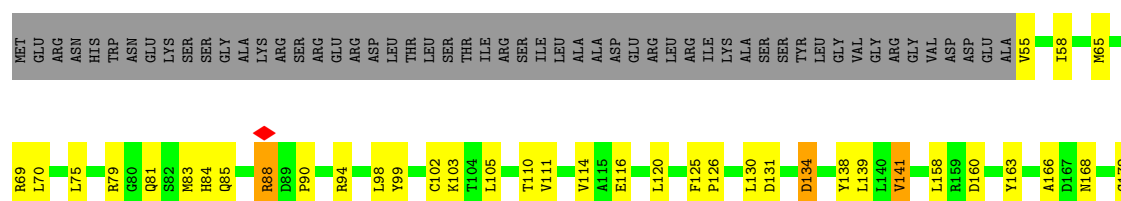




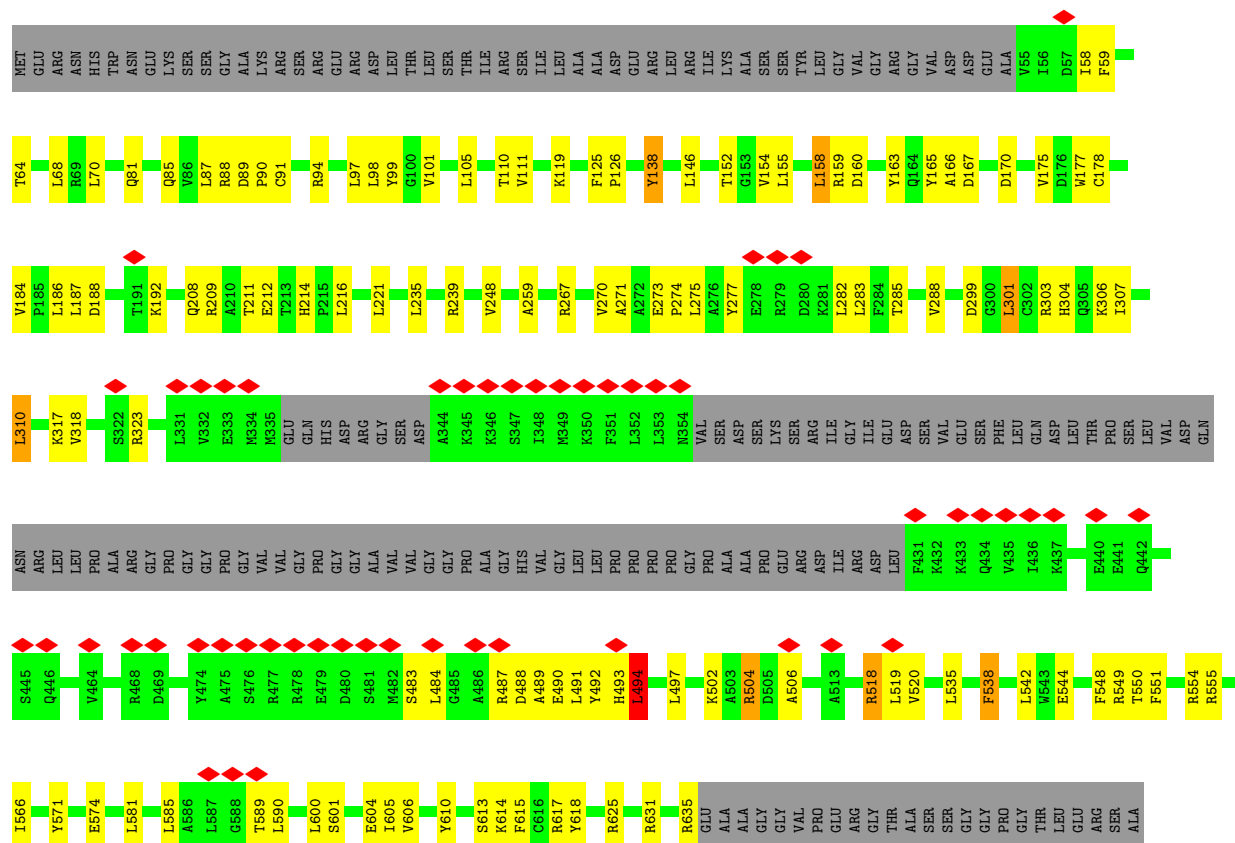
- Molecule 1: Portal protein



- Molecule 1: Portal protein



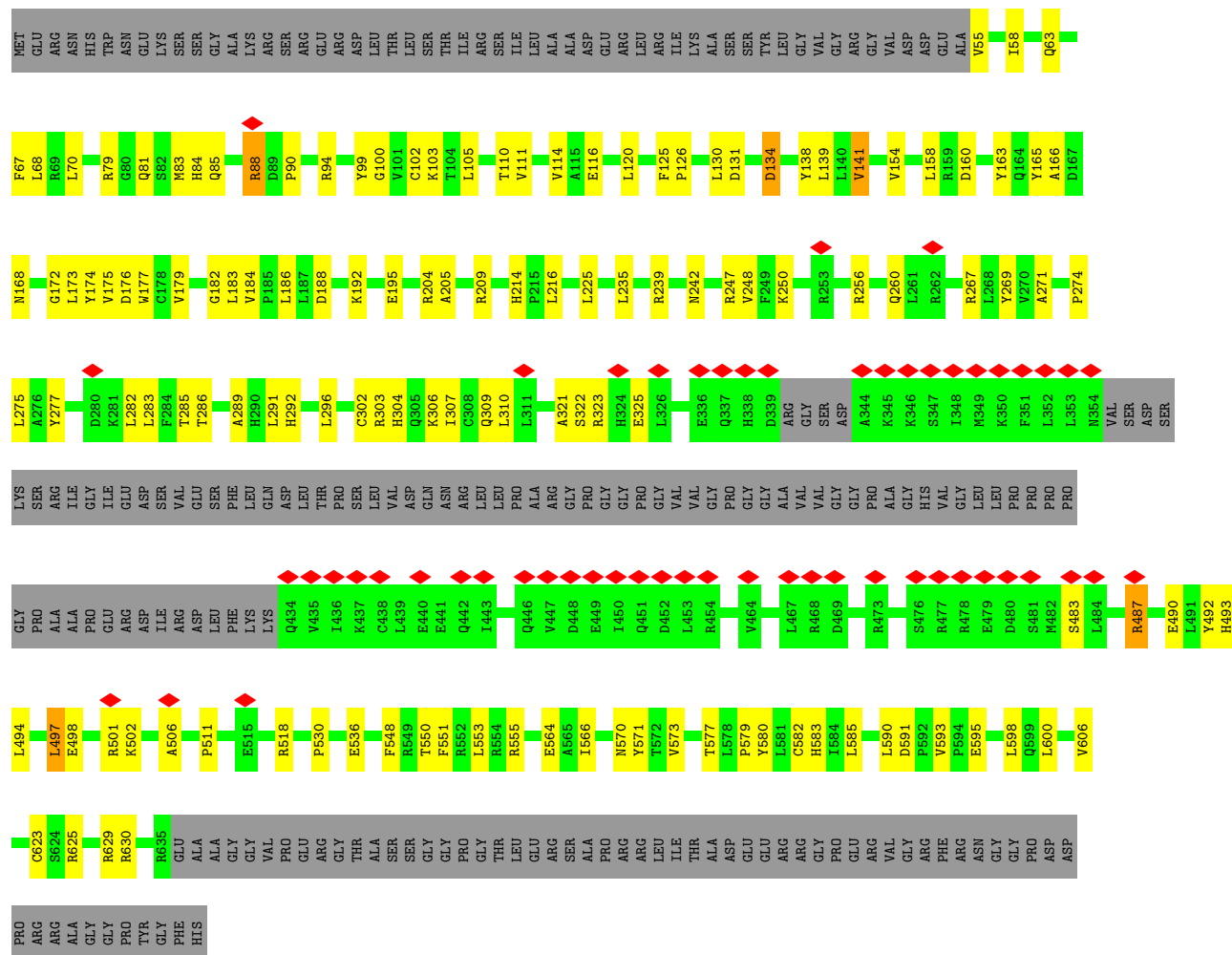
- Molecule 1: Portal protein



PRO ARG ARG ARG LEU LEU THR THR ALA ASP ASP GLU GLU ARG ARG GLY PRO PRO GLU GLU VAL VAL GLU GLU ARG ARG PHE ARG ASN GLY GLY PRO PRO ARG ARG ALA ALA GLY GLY PRO PRO TYR TYR GLY PHE HIS

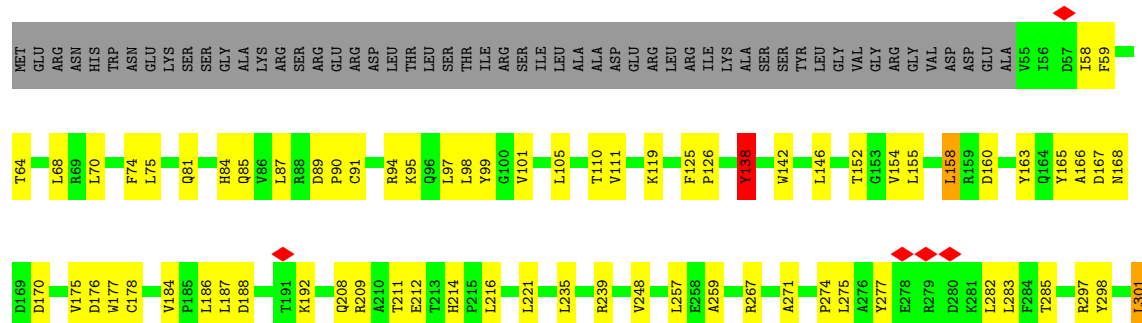
• Molecule 1: Portal protein

Chain F: 8% 52% 19% 29%

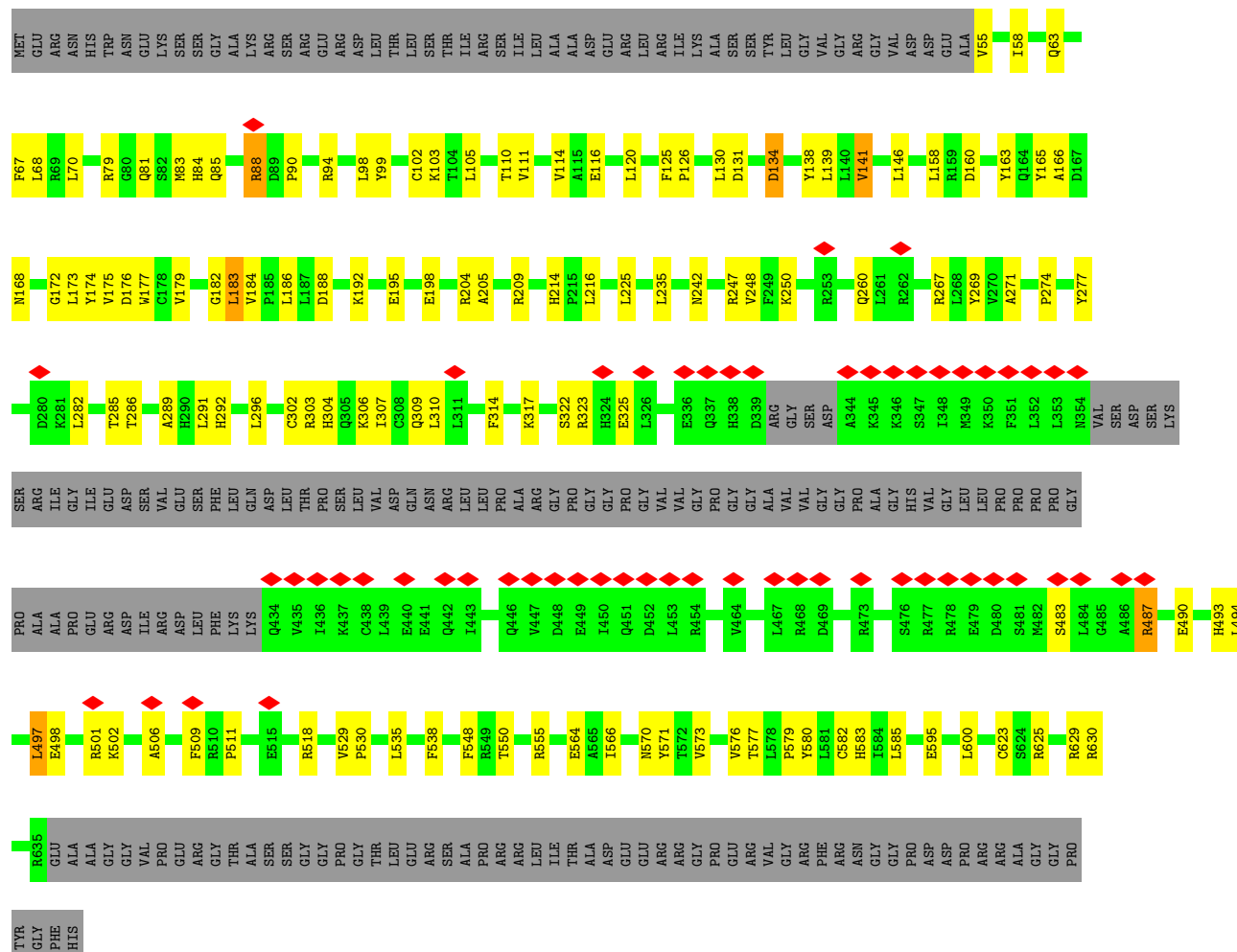


• Molecule 1: Portal protein

Chain L: 8% 53% 17% 29%



- Molecule 1: Portal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22087	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	390.0, 390.0, 390.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3842	0.77	7/5229 (0.1%)
1	B	0.43	0/3842	0.74	7/5229 (0.1%)
1	C	0.44	0/3842	0.75	6/5229 (0.1%)
1	D	0.43	0/3842	0.75	5/5229 (0.1%)
1	E	0.44	0/3837	0.79	11/5222 (0.2%)
1	F	0.43	0/3842	0.74	7/5229 (0.1%)
1	G	0.44	0/3842	0.75	6/5229 (0.1%)
1	H	0.44	0/3837	0.80	10/5222 (0.2%)
1	I	0.44	0/3837	0.81	12/5222 (0.2%)
1	J	0.44	0/3837	0.79	11/5222 (0.2%)
1	K	0.44	0/3837	0.80	10/5222 (0.2%)
1	L	0.44	0/3837	0.81	12/5222 (0.2%)
All	All	0.44	0/46074	0.78	104/62706 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	12

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	494	LEU	CA-CB-CG	9.04	136.09	115.30
1	J	494	LEU	CA-CB-CG	9.04	136.09	115.30
1	H	494	LEU	CA-CB-CG	8.80	135.54	115.30
1	K	494	LEU	CA-CB-CG	8.69	135.29	115.30
1	I	494	LEU	CA-CB-CG	8.33	134.47	115.30
1	L	494	LEU	CA-CB-CG	8.31	134.42	115.30
1	K	519	LEU	CA-CB-CG	7.42	132.37	115.30
1	H	519	LEU	CA-CB-CG	7.40	132.32	115.30
1	E	519	LEU	CA-CB-CG	7.38	132.28	115.30
1	J	519	LEU	CA-CB-CG	7.31	132.11	115.30
1	B	68	LEU	CA-CB-CG	7.09	131.60	115.30
1	F	68	LEU	CA-CB-CG	7.09	131.60	115.30
1	A	68	LEU	CA-CB-CG	6.98	131.36	115.30
1	I	68	LEU	CA-CB-CG	6.93	131.24	115.30
1	G	68	LEU	CA-CB-CG	6.85	131.06	115.30
1	C	68	LEU	CA-CB-CG	6.85	131.05	115.30
1	L	68	LEU	CA-CB-CG	6.83	131.00	115.30
1	E	68	LEU	CA-CB-CG	6.76	130.84	115.30
1	J	68	LEU	CA-CB-CG	6.76	130.84	115.30
1	B	158	LEU	CB-CG-CD1	6.75	122.48	111.00
1	F	158	LEU	CB-CG-CD1	6.75	122.48	111.00
1	H	600	LEU	CA-CB-CG	6.67	130.64	115.30
1	K	600	LEU	CA-CB-CG	6.66	130.61	115.30
1	E	600	LEU	CA-CB-CG	6.57	130.42	115.30
1	I	600	LEU	CA-CB-CG	6.57	130.41	115.30
1	J	600	LEU	CA-CB-CG	6.54	130.34	115.30
1	L	600	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	275	LEU	CA-CB-CG	6.43	130.10	115.30
1	G	134	ASP	CB-CG-OD1	6.27	123.95	118.30
1	A	134	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	134	ASP	CB-CG-OD1	6.23	123.91	118.30
1	G	291	LEU	CA-CB-CG	6.23	129.62	115.30
1	C	134	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	291	LEU	CA-CB-CG	6.21	129.59	115.30
1	B	134	ASP	CB-CG-OD1	6.21	123.89	118.30
1	F	134	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	75	LEU	CA-CB-CG	6.21	129.57	115.30
1	E	221	LEU	CA-CB-CG	6.20	129.55	115.30
1	J	221	LEU	CA-CB-CG	6.20	129.55	115.30
1	D	75	LEU	CA-CB-CG	6.17	129.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	221	LEU	CA-CB-CG	6.03	129.16	115.30
1	K	221	LEU	CA-CB-CG	6.03	129.16	115.30
1	D	291	LEU	CA-CB-CG	5.65	128.29	115.30
1	I	556	LEU	CB-CG-CD2	5.63	120.57	111.00
1	L	221	LEU	CA-CB-CG	5.62	128.24	115.30
1	I	221	LEU	CA-CB-CG	5.62	128.22	115.30
1	J	261	LEU	CA-CB-CG	5.58	128.13	115.30
1	E	261	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	291	LEU	CA-CB-CG	5.47	127.87	115.30
1	F	291	LEU	CA-CB-CG	5.47	127.87	115.30
1	E	158	LEU	CB-CG-CD1	5.46	120.28	111.00
1	J	158	LEU	CB-CG-CD1	5.45	120.27	111.00
1	I	158	LEU	CB-CG-CD1	5.44	120.24	111.00
1	D	275	LEU	CA-CB-CG	5.43	127.79	115.30
1	L	158	LEU	CB-CG-CD1	5.42	120.22	111.00
1	L	556	LEU	CB-CG-CD2	5.42	120.22	111.00
1	I	556	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	I	518	ARG	CA-CB-CG	-5.39	101.55	113.40
1	L	518	ARG	CA-CB-CG	-5.37	101.58	113.40
1	C	146	LEU	CA-CB-CG	5.37	127.65	115.30
1	G	146	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	275	LEU	CA-CB-CG	5.35	127.61	115.30
1	F	275	LEU	CA-CB-CG	5.35	127.61	115.30
1	E	318	VAL	CA-CB-CG2	5.35	118.93	110.90
1	A	291	LEU	CA-CB-CG	5.35	127.60	115.30
1	J	318	VAL	CA-CB-CG2	5.33	118.90	110.90
1	L	556	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	K	68	LEU	CA-CB-CG	5.18	127.21	115.30
1	I	138	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	H	318	VAL	CA-CB-CG2	5.14	118.62	110.90
1	I	318	VAL	CA-CB-CG2	5.14	118.62	110.90
1	L	488	ASP	CB-CG-OD1	5.14	122.93	118.30
1	G	183	LEU	CA-CB-CG	5.14	127.12	115.30
1	E	138	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	J	138	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	600	LEU	CA-CB-CG	5.13	127.09	115.30
1	D	600	LEU	CA-CB-CG	5.13	127.09	115.30
1	H	158	LEU	CB-CG-CD1	5.12	119.71	111.00
1	G	600	LEU	CA-CB-CG	5.12	127.08	115.30
1	K	318	VAL	CA-CB-CG2	5.12	118.58	110.90
1	C	183	LEU	CA-CB-CG	5.12	127.07	115.30
1	K	158	LEU	CB-CG-CD1	5.12	119.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	600	LEU	CA-CB-CG	5.11	127.06	115.30
1	I	488	ASP	CB-CG-OD1	5.11	122.90	118.30
1	L	318	VAL	CA-CB-CG2	5.10	118.55	110.90
1	F	600	LEU	CA-CB-CG	5.09	127.01	115.30
1	E	518	ARG	CA-CB-CG	-5.09	102.20	113.40
1	B	600	LEU	CA-CB-CG	5.09	127.00	115.30
1	B	183	LEU	CA-CB-CG	5.08	127.00	115.30
1	F	183	LEU	CA-CB-CG	5.08	127.00	115.30
1	H	138	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	J	518	ARG	CA-CB-CG	-5.08	102.22	113.40
1	K	138	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	K	518	ARG	CA-CB-CG	-5.08	102.23	113.40
1	L	138	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	H	518	ARG	CA-CB-CG	-5.07	102.24	113.40
1	I	146	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	183	LEU	CA-CB-CG	5.05	126.92	115.30
1	L	146	LEU	CA-CB-CG	5.05	126.92	115.30
1	H	146	LEU	CA-CB-CG	5.03	126.86	115.30
1	K	146	LEU	CA-CB-CG	5.02	126.85	115.30
1	E	146	LEU	CA-CB-CG	5.02	126.84	115.30
1	H	68	LEU	CA-CB-CG	5.02	126.84	115.30
1	J	146	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	TYR	Peptide
1	B	277	TYR	Peptide
1	C	277	TYR	Peptide
1	D	277	TYR	Peptide
1	E	277	TYR	Peptide
1	F	277	TYR	Peptide
1	G	277	TYR	Peptide
1	H	277	TYR	Peptide
1	I	277	TYR	Peptide
1	J	277	TYR	Peptide
1	K	277	TYR	Peptide
1	L	277	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3773	0	3581	92	0
1	B	3773	0	3581	96	0
1	C	3773	0	3581	102	0
1	D	3773	0	3581	93	0
1	E	3768	0	3579	90	0
1	F	3773	0	3581	97	0
1	G	3773	0	3581	95	0
1	H	3768	0	3579	96	0
1	I	3768	0	3579	98	0
1	J	3768	0	3579	90	0
1	K	3768	0	3579	95	0
1	L	3768	0	3579	97	0
All	All	45246	0	42960	961	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 11.

All (961) 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:E:323:ARG:H	1:B:518:ARG:HB3	1.50	0.77
1:J:323:ARG:H	1:F:518:ARG:HB3	1.50	0.76
1:K:323:ARG:H	1:G:518:ARG:HB3	1.53	0.74
1:H:323:ARG:H	1:C:518:ARG:HB3	1.53	0.73
1:A:518:ARG:HB3	1:L:323:ARG:H	1.56	0.71
1:L:518:ARG:HG3	1:G:323:ARG:H	1.56	0.70
1:I:518:ARG:HG3	1:C:323:ARG:H	1.56	0.69
1:I:323:ARG:H	1:D:518:ARG:HB3	1.56	0.69
1:J:625:ARG:HH21	1:D:126:PRO:HA	1.59	0.67
1:K:518:ARG:HG3	1:F:323:ARG:H	1.60	0.67
1:J:518:ARG:HG3	1:D:323:ARG:H	1.60	0.67
1:K:589:THR:HG23	1:K:590:LEU:HD12	1.76	0.67
1:K:625:ARG:HH21	1:F:126:PRO:HA	1.59	0.67
1:E:518:ARG:HG3	1:A:323:ARG:H	1.60	0.67
1:H:589:THR:HG23	1:H:590:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:625:ARG:HH21	1:C:126:PRO:HA	1.59	0.67
1:L:625:ARG:HH21	1:G:126:PRO:HA	1.59	0.67
1:H:625:ARG:HH21	1:B:126:PRO:HA	1.59	0.66
1:J:589:THR:HG23	1:J:590:LEU:HD12	1.76	0.66
1:E:625:ARG:HH21	1:A:126:PRO:HA	1.59	0.66
1:E:492:TYR:O	1:H:303:ARG:NH2	2.29	0.66
1:H:518:ARG:HG3	1:B:323:ARG:H	1.60	0.66
1:L:589:THR:HG23	1:L:590:LEU:HD12	1.76	0.66
1:E:589:THR:HG23	1:E:590:LEU:HD12	1.76	0.65
1:I:589:THR:HG23	1:I:590:LEU:HD12	1.76	0.65
1:J:492:TYR:O	1:K:303:ARG:NH2	2.29	0.65
1:K:492:TYR:O	1:L:303:ARG:NH2	2.30	0.65
1:K:518:ARG:NH2	1:F:325:GLU:O	2.30	0.65
1:A:70:LEU:O	1:A:81:GLN:NE2	2.30	0.65
1:H:492:TYR:O	1:I:303:ARG:NH2	2.31	0.64
1:D:70:LEU:O	1:D:81:GLN:NE2	2.30	0.64
1:L:70:LEU:O	1:L:81:GLN:NE2	2.31	0.64
1:E:483:SER:HA	1:E:487:ARG:HG2	1.80	0.63
1:H:518:ARG:NH2	1:B:325:GLU:O	2.30	0.63
1:I:70:LEU:O	1:I:81:GLN:NE2	2.32	0.63
1:E:518:ARG:NH2	1:A:325:GLU:O	2.30	0.63
1:E:59:PHE:O	1:E:64:THR:OG1	2.16	0.63
1:I:492:TYR:O	1:J:303:ARG:NH2	2.32	0.63
1:H:483:SER:HA	1:H:487:ARG:HG2	1.81	0.63
1:E:303:ARG:NH2	1:L:492:TYR:O	2.32	0.62
1:G:173:LEU:HD11	1:G:242:ASN:HB3	1.81	0.62
1:C:70:LEU:O	1:C:81:GLN:NE2	2.32	0.62
1:L:548:PHE:HZ	1:L:566:ILE:HD13	1.64	0.62
1:E:542:LEU:HD13	1:A:79:ARG:HA	1.82	0.62
1:G:70:LEU:O	1:G:81:GLN:NE2	2.32	0.62
1:K:90:PRO:O	1:G:571:TYR:OH	2.15	0.62
1:I:548:PHE:HZ	1:I:566:ILE:HD13	1.64	0.62
1:K:542:LEU:HD13	1:F:79:ARG:HA	1.82	0.62
1:B:70:LEU:O	1:B:81:GLN:NE2	2.33	0.62
1:C:173:LEU:HD11	1:C:242:ASN:HB3	1.81	0.62
1:J:483:SER:HA	1:J:487:ARG:HG2	1.80	0.62
1:K:177:TRP:HB3	1:K:184:VAL:HG12	1.81	0.62
1:E:99:TYR:HB2	1:E:605:ILE:HD11	1.82	0.61
1:J:542:LEU:HD13	1:D:79:ARG:HA	1.82	0.61
1:J:99:TYR:HB2	1:J:605:ILE:HD11	1.82	0.61
1:H:542:LEU:HD13	1:B:79:ARG:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:TYR:HB2	1:I:605:ILE:HD11	1.83	0.61
1:J:518:ARG:NH2	1:D:325:GLU:O	2.31	0.61
1:F:70:LEU:O	1:F:81:GLN:NE2	2.33	0.61
1:J:90:PRO:O	1:F:571:TYR:OH	2.16	0.61
1:I:299:ASP:OD2	1:I:299:ASP:N	2.30	0.61
1:L:99:TYR:HB2	1:L:605:ILE:HD11	1.82	0.61
1:H:177:TRP:HB3	1:H:184:VAL:HG12	1.81	0.61
1:J:102:CYS:HA	1:J:105:LEU:HB2	1.83	0.61
1:A:235:LEU:HA	1:A:585:LEU:HD12	1.82	0.61
1:F:173:LEU:HD11	1:F:242:ASN:HB3	1.82	0.61
1:B:173:LEU:HD11	1:B:242:ASN:HB3	1.82	0.60
1:K:487:ARG:HH11	1:K:491:LEU:HD21	1.66	0.60
1:I:275:LEU:HB2	1:I:283:LEU:HB3	1.83	0.60
1:J:323:ARG:O	1:F:518:ARG:NH1	2.35	0.60
1:L:59:PHE:O	1:L:64:THR:OG1	2.16	0.60
1:E:70:LEU:O	1:E:81:GLN:NE2	2.35	0.60
1:E:275:LEU:HB2	1:E:283:LEU:HB3	1.83	0.60
1:K:483:SER:HA	1:K:487:ARG:HG2	1.82	0.60
1:F:502:LYS:O	1:F:506:ALA:HB2	2.02	0.60
1:A:94:ARG:NH2	1:A:166:ALA:O	2.35	0.60
1:E:102:CYS:HA	1:E:105:LEU:HB2	1.83	0.59
1:B:502:LYS:O	1:B:506:ALA:HB2	2.02	0.59
1:H:487:ARG:HH11	1:H:491:LEU:HD21	1.67	0.59
1:J:70:LEU:O	1:J:81:GLN:NE2	2.35	0.59
1:E:323:ARG:O	1:B:518:ARG:NH1	2.35	0.59
1:J:301:LEU:HD21	1:J:535:LEU:HD11	1.84	0.59
1:H:70:LEU:O	1:H:81:GLN:NE2	2.36	0.59
1:H:59:PHE:O	1:H:64:THR:OG1	2.16	0.59
1:B:94:ARG:NH2	1:B:166:ALA:O	2.36	0.59
1:C:502:LYS:O	1:C:506:ALA:HB2	2.03	0.59
1:J:275:LEU:HB2	1:J:283:LEU:HB3	1.84	0.59
1:L:275:LEU:HB2	1:L:283:LEU:HB3	1.83	0.59
1:H:323:ARG:O	1:C:518:ARG:NH1	2.36	0.59
1:D:188:ASP:OD1	1:D:267:ARG:NH2	2.36	0.59
1:K:70:LEU:O	1:K:81:GLN:NE2	2.36	0.59
1:I:155:LEU:HA	1:I:158:LEU:HG	1.85	0.59
1:K:155:LEU:HA	1:K:158:LEU:HG	1.85	0.59
1:K:275:LEU:HB2	1:K:283:LEU:HB3	1.84	0.59
1:E:301:LEU:HD21	1:E:535:LEU:HD11	1.84	0.59
1:A:502:LYS:O	1:A:506:ALA:HB2	2.03	0.58
1:K:323:ARG:O	1:G:518:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:PHE:O	1:J:64:THR:OG1	2.16	0.58
1:J:554:ARG:NH1	1:D:564:GLU:OE1	2.37	0.58
1:D:502:LYS:O	1:D:506:ALA:HB2	2.04	0.58
1:G:502:LYS:O	1:G:506:ALA:HB2	2.03	0.58
1:H:275:LEU:HB2	1:H:283:LEU:HB3	1.84	0.58
1:I:90:PRO:O	1:D:571:TYR:OH	2.17	0.58
1:J:187:LEU:HB2	1:J:239:ARG:HB2	1.85	0.58
1:F:94:ARG:NH2	1:F:166:ALA:O	2.36	0.58
1:D:94:ARG:NH2	1:D:166:ALA:O	2.36	0.58
1:K:91:CYS:SG	1:K:94:ARG:NH1	2.76	0.58
1:E:187:LEU:HB2	1:E:239:ARG:HB2	1.85	0.58
1:H:91:CYS:SG	1:H:94:ARG:NH1	2.76	0.58
1:H:99:TYR:HB2	1:H:605:ILE:HD11	1.86	0.58
1:I:554:ARG:NH1	1:C:564:GLU:OE1	2.36	0.58
1:A:571:TYR:OH	1:L:90:PRO:O	2.17	0.58
1:H:155:LEU:HA	1:H:158:LEU:HG	1.85	0.58
1:K:89:ASP:OD1	1:K:89:ASP:N	2.37	0.58
1:I:483:SER:HA	1:I:487:ARG:HG2	1.85	0.58
1:D:548:PHE:HZ	1:D:566:ILE:HD13	1.69	0.58
1:K:101:VAL:O	1:K:105:LEU:HB2	2.03	0.58
1:L:483:SER:HA	1:L:487:ARG:HG2	1.85	0.58
1:H:101:VAL:O	1:H:105:LEU:HB2	2.03	0.58
1:K:99:TYR:HB2	1:K:605:ILE:HD11	1.86	0.57
1:F:548:PHE:HZ	1:F:566:ILE:HD13	1.69	0.57
1:E:155:LEU:HA	1:E:158:LEU:HG	1.85	0.57
1:A:548:PHE:HZ	1:A:566:ILE:HD13	1.69	0.57
1:B:548:PHE:HZ	1:B:566:ILE:HD13	1.69	0.57
1:H:504:ARG:NH2	1:C:511:PRO:O	2.37	0.57
1:J:323:ARG:N	1:F:518:ARG:HB3	2.20	0.57
1:L:155:LEU:HA	1:L:158:LEU:HG	1.85	0.57
1:J:617:ARG:HG2	1:D:141:VAL:HG23	1.87	0.57
1:G:58:ILE:HB	1:G:248:VAL:HG13	1.86	0.57
1:A:511:PRO:O	1:L:504:ARG:NH2	2.37	0.57
1:J:155:LEU:HA	1:J:158:LEU:HG	1.85	0.57
1:J:89:ASP:OD1	1:J:89:ASP:N	2.37	0.57
1:E:554:ARG:NH1	1:A:564:GLU:OE1	2.37	0.57
1:H:90:PRO:O	1:C:571:TYR:OH	2.15	0.57
1:H:187:LEU:HB2	1:H:239:ARG:HB2	1.87	0.57
1:I:91:CYS:SG	1:I:94:ARG:NH1	2.78	0.57
1:I:487:ARG:HH11	1:I:491:LEU:HD21	1.69	0.57
1:C:58:ILE:HB	1:C:248:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:554:ARG:NH1	1:G:564:GLU:OE1	2.36	0.57
1:I:617:ARG:HG2	1:C:141:VAL:HG23	1.87	0.56
1:A:58:ILE:HB	1:A:248:VAL:HG13	1.86	0.56
1:H:554:ARG:NH1	1:B:564:GLU:OE1	2.38	0.56
1:C:94:ARG:NH2	1:C:166:ALA:O	2.38	0.56
1:K:187:LEU:HB2	1:K:239:ARG:HB2	1.87	0.56
1:K:554:ARG:NH1	1:F:564:GLU:OE1	2.38	0.56
1:E:90:PRO:O	1:B:571:TYR:OH	2.16	0.56
1:E:91:CYS:SG	1:E:94:ARG:NH1	2.79	0.56
1:H:617:ARG:HG2	1:B:141:VAL:HG23	1.87	0.56
1:D:58:ILE:HB	1:D:248:VAL:HG13	1.86	0.56
1:L:487:ARG:HH11	1:L:491:LEU:HD21	1.69	0.56
1:L:518:ARG:NH2	1:G:325:GLU:O	2.29	0.56
1:G:94:ARG:NH2	1:G:166:ALA:O	2.38	0.56
1:G:573:VAL:O	1:G:577:THR:OG1	2.21	0.56
1:B:58:ILE:HB	1:B:248:VAL:HG13	1.86	0.56
1:D:235:LEU:HD22	1:D:585:LEU:HD13	1.88	0.56
1:H:323:ARG:N	1:C:518:ARG:HB3	2.21	0.56
1:I:89:ASP:N	1:I:89:ASP:OD1	2.37	0.56
1:I:494:LEU:O	1:J:303:ARG:NH2	2.39	0.56
1:K:504:ARG:NH2	1:G:511:PRO:O	2.37	0.56
1:I:504:ARG:NH2	1:D:511:PRO:O	2.37	0.56
1:J:163:TYR:O	1:F:583:HIS:NE2	2.39	0.56
1:K:617:ARG:HG2	1:F:141:VAL:HG23	1.87	0.56
1:L:542:LEU:HD13	1:G:79:ARG:HA	1.88	0.56
1:I:187:LEU:HB2	1:I:239:ARG:HB2	1.88	0.56
1:G:188:ASP:OD1	1:G:267:ARG:NH2	2.38	0.56
1:I:541:GLN:HG3	1:C:79:ARG:HD2	1.88	0.56
1:E:504:ARG:NH2	1:B:511:PRO:O	2.38	0.56
1:K:59:PHE:O	1:K:64:THR:OG1	2.16	0.56
1:A:188:ASP:OD1	1:A:267:ARG:NH2	2.38	0.55
1:H:163:TYR:O	1:C:583:HIS:NE2	2.39	0.55
1:F:58:ILE:HB	1:F:248:VAL:HG13	1.86	0.55
1:G:548:PHE:HZ	1:G:566:ILE:HD13	1.72	0.55
1:I:59:PHE:O	1:I:64:THR:OG1	2.16	0.55
1:F:629:ARG:O	1:F:629:ARG:NH1	2.40	0.55
1:B:629:ARG:O	1:B:629:ARG:NH1	2.40	0.55
1:J:504:ARG:NH2	1:F:511:PRO:O	2.38	0.55
1:L:541:GLN:HG3	1:G:79:ARG:HD2	1.88	0.55
1:E:617:ARG:HG2	1:A:141:VAL:HG23	1.87	0.55
1:I:323:ARG:O	1:D:518:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:629:ARG:O	1:G:629:ARG:NH1	2.40	0.55
1:A:494:LEU:O	1:B:303:ARG:NH2	2.40	0.55
1:H:89:ASP:OD1	1:H:89:ASP:N	2.37	0.55
1:C:629:ARG:O	1:C:629:ARG:NH1	2.40	0.55
1:L:91:CYS:SG	1:L:94:ARG:NH1	2.78	0.55
1:E:89:ASP:N	1:E:89:ASP:OD1	2.36	0.55
1:E:186:LEU:HD21	1:E:267:ARG:HG2	1.89	0.55
1:K:58:ILE:HB	1:K:248:VAL:HG13	1.89	0.55
1:E:303:ARG:NH2	1:L:494:LEU:O	2.39	0.55
1:A:518:ARG:HB3	1:L:323:ARG:N	2.22	0.55
1:A:629:ARG:NH1	1:A:629:ARG:O	2.40	0.55
1:E:160:ASP:OD2	1:E:160:ASP:N	2.40	0.55
1:I:542:LEU:HD13	1:C:79:ARG:HA	1.88	0.55
1:D:494:LEU:O	1:F:303:ARG:NH2	2.40	0.55
1:L:617:ARG:HG2	1:G:141:VAL:HG23	1.87	0.55
1:A:573:VAL:O	1:A:577:THR:OG1	2.24	0.54
1:I:110:THR:OG1	1:I:111:VAL:N	2.41	0.54
1:D:629:ARG:O	1:D:629:ARG:NH1	2.40	0.54
1:H:94:ARG:NH2	1:H:166:ALA:O	2.40	0.54
1:C:205:ALA:O	1:C:209:ARG:NH1	2.41	0.54
1:K:94:ARG:NH2	1:K:166:ALA:O	2.40	0.54
1:L:110:THR:OG1	1:L:111:VAL:N	2.41	0.54
1:A:518:ARG:NH1	1:L:323:ARG:O	2.39	0.54
1:C:548:PHE:HZ	1:C:566:ILE:HD13	1.72	0.54
1:D:205:ALA:O	1:D:209:ARG:NH1	2.41	0.54
1:K:163:TYR:O	1:G:583:HIS:NE2	2.39	0.54
1:A:205:ALA:O	1:A:209:ARG:NH1	2.40	0.54
1:H:58:ILE:HB	1:H:248:VAL:HG13	1.89	0.54
1:I:186:LEU:HD21	1:I:267:ARG:HG2	1.90	0.54
1:L:187:LEU:HB2	1:L:239:ARG:HB2	1.90	0.54
1:E:163:TYR:O	1:B:583:HIS:NE2	2.39	0.54
1:C:494:LEU:O	1:D:303:ARG:NH2	2.41	0.54
1:D:55:VAL:N	1:D:250:LYS:O	2.40	0.54
1:F:188:ASP:OD1	1:F:267:ARG:NH2	2.38	0.54
1:E:110:THR:OG1	1:E:111:VAL:N	2.41	0.54
1:L:89:ASP:N	1:L:89:ASP:OD1	2.37	0.54
1:H:186:LEU:HD21	1:H:267:ARG:HG2	1.90	0.54
1:J:186:LEU:HD21	1:J:267:ARG:HG2	1.89	0.54
1:D:498:GLU:OE2	1:D:501:ARG:NH2	2.41	0.54
1:L:101:VAL:O	1:L:105:LEU:HB2	2.08	0.54
1:H:110:THR:OG1	1:H:111:VAL:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:VAL:O	1:I:105:LEU:HB2	2.08	0.54
1:J:110:THR:OG1	1:J:111:VAL:N	2.41	0.54
1:F:494:LEU:O	1:G:303:ARG:NH2	2.41	0.54
1:B:494:LEU:O	1:C:303:ARG:NH2	2.40	0.54
1:F:85:GLN:HE22	1:F:88:ARG:HD2	1.73	0.54
1:E:323:ARG:N	1:B:518:ARG:HB3	2.20	0.53
1:A:303:ARG:NH2	1:G:494:LEU:O	2.41	0.53
1:D:182:GLY:O	1:D:271:ALA:N	2.39	0.53
1:G:55:VAL:N	1:G:250:LYS:O	2.41	0.53
1:G:85:GLN:HE22	1:G:88:ARG:HD2	1.73	0.53
1:E:94:ARG:NH2	1:E:166:ALA:O	2.41	0.53
1:B:205:ALA:O	1:B:209:ARG:NH1	2.41	0.53
1:H:160:ASP:N	1:H:160:ASP:OD2	2.40	0.53
1:B:85:GLN:HE22	1:B:88:ARG:HD2	1.73	0.53
1:L:94:ARG:NH2	1:L:166:ALA:O	2.41	0.53
1:A:85:GLN:HE22	1:A:88:ARG:HD2	1.73	0.53
1:A:214:HIS:CE1	1:A:216:LEU:HB3	2.43	0.53
1:J:487:ARG:HH11	1:J:491:LEU:HD21	1.73	0.53
1:C:55:VAL:N	1:C:250:LYS:O	2.41	0.53
1:J:94:ARG:NH2	1:J:166:ALA:O	2.41	0.53
1:K:613:SER:OG	1:K:614:LYS:N	2.41	0.53
1:E:487:ARG:HH11	1:E:491:LEU:HD21	1.73	0.53
1:A:498:GLU:OE2	1:A:501:ARG:NH2	2.41	0.53
1:B:188:ASP:OD1	1:B:267:ARG:NH2	2.38	0.53
1:I:323:ARG:N	1:D:518:ARG:HB3	2.22	0.53
1:I:613:SER:OG	1:I:614:LYS:N	2.42	0.53
1:J:91:CYS:SG	1:J:94:ARG:NH1	2.79	0.53
1:J:613:SER:OG	1:J:614:LYS:N	2.41	0.53
1:G:205:ALA:O	1:G:209:ARG:NH1	2.41	0.53
1:E:613:SER:OG	1:E:614:LYS:N	2.41	0.53
1:A:55:VAL:N	1:A:250:LYS:O	2.41	0.53
1:B:55:VAL:N	1:B:250:LYS:O	2.42	0.53
1:B:214:HIS:CE1	1:B:216:LEU:HB3	2.44	0.53
1:I:58:ILE:HB	1:I:248:VAL:HG13	1.90	0.53
1:L:160:ASP:OD2	1:L:160:ASP:N	2.40	0.53
1:L:574:GLU:OE1	1:G:163:TYR:OH	2.27	0.53
1:G:498:GLU:OE2	1:G:501:ARG:NH2	2.42	0.53
1:D:139:LEU:HD13	1:D:623:CYS:HA	1.91	0.53
1:F:55:VAL:N	1:F:250:LYS:O	2.42	0.53
1:F:235:LEU:HG	1:F:585:LEU:HD13	1.91	0.53
1:E:58:ILE:HB	1:E:248:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD13	1:A:623:CYS:HA	1.91	0.53
1:I:94:ARG:NH2	1:I:166:ALA:O	2.41	0.53
1:C:498:GLU:OE2	1:C:501:ARG:NH2	2.42	0.53
1:L:186:LEU:HD21	1:L:267:ARG:HG2	1.91	0.53
1:I:574:GLU:OE1	1:C:163:TYR:OH	2.27	0.53
1:C:177:TRP:HB3	1:C:184:VAL:HG22	1.91	0.53
1:B:235:LEU:HG	1:B:585:LEU:HD13	1.91	0.52
1:C:179:VAL:O	1:C:286:THR:OG1	2.27	0.52
1:C:214:HIS:CE1	1:C:216:LEU:HB3	2.44	0.52
1:K:110:THR:OG1	1:K:111:VAL:N	2.41	0.52
1:K:186:LEU:HD21	1:K:267:ARG:HG2	1.90	0.52
1:F:179:VAL:O	1:F:286:THR:OG1	2.27	0.52
1:G:214:HIS:CE1	1:G:216:LEU:HB3	2.44	0.52
1:H:544:GLU:OE1	1:H:555:ARG:NH2	2.42	0.52
1:L:58:ILE:HB	1:L:248:VAL:HG13	1.90	0.52
1:H:613:SER:OG	1:H:614:LYS:N	2.41	0.52
1:I:160:ASP:OD2	1:I:160:ASP:N	2.40	0.52
1:F:498:GLU:OE2	1:F:501:ARG:NH2	2.42	0.52
1:E:574:GLU:OE1	1:A:163:TYR:OH	2.28	0.52
1:H:59:PHE:HB2	1:H:248:VAL:HG12	1.92	0.52
1:H:574:GLU:OE1	1:B:163:TYR:OH	2.28	0.52
1:B:498:GLU:OE2	1:B:501:ARG:NH2	2.42	0.52
1:J:58:ILE:HB	1:J:248:VAL:HG13	1.90	0.52
1:D:214:HIS:CE1	1:D:216:LEU:HB3	2.44	0.52
1:F:214:HIS:CE1	1:F:216:LEU:HB3	2.44	0.52
1:G:555:ARG:HE	1:G:566:ILE:HD11	1.74	0.52
1:E:69:ARG:HD2	1:B:283:LEU:HD22	1.91	0.52
1:D:85:GLN:HE22	1:D:88:ARG:HD2	1.73	0.52
1:F:205:ALA:O	1:F:209:ARG:NH1	2.41	0.52
1:J:160:ASP:OD2	1:J:160:ASP:N	2.40	0.52
1:I:490:GLU:HG3	1:I:494:LEU:HG	1.92	0.52
1:C:85:GLN:HE22	1:C:88:ARG:HD2	1.74	0.52
1:C:555:ARG:HE	1:C:566:ILE:HD11	1.74	0.52
1:L:177:TRP:HB3	1:L:184:VAL:HG22	1.92	0.52
1:L:613:SER:OG	1:L:614:LYS:N	2.42	0.52
1:G:235:LEU:HG	1:G:585:LEU:HD13	1.92	0.52
1:B:139:LEU:HD13	1:B:623:CYS:HA	1.92	0.52
1:I:163:TYR:O	1:D:583:HIS:NE2	2.43	0.52
1:D:555:ARG:HE	1:D:566:ILE:HD11	1.75	0.52
1:C:235:LEU:HG	1:C:585:LEU:HD13	1.92	0.52
1:F:139:LEU:HD13	1:F:623:CYS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:631:ARG:HE	1:A:130:LEU:HD22	1.75	0.52
1:K:574:GLU:OE1	1:F:163:TYR:OH	2.28	0.52
1:A:177:TRP:HB3	1:A:184:VAL:HG22	1.91	0.51
1:B:179:VAL:O	1:B:286:THR:OG1	2.27	0.51
1:J:69:ARG:HD2	1:F:283:LEU:HD22	1.91	0.51
1:D:177:TRP:HB3	1:D:184:VAL:HG22	1.91	0.51
1:D:573:VAL:O	1:D:577:THR:OG1	2.23	0.51
1:D:179:VAL:O	1:D:286:THR:OG1	2.28	0.51
1:K:544:GLU:OE1	1:K:555:ARG:NH2	2.42	0.51
1:L:490:GLU:HG3	1:L:494:LEU:HG	1.92	0.51
1:C:490:GLU:HG3	1:C:494:LEU:HD23	1.91	0.51
1:J:631:ARG:HE	1:D:130:LEU:HD22	1.75	0.51
1:K:323:ARG:N	1:G:518:ARG:HB3	2.21	0.51
1:I:152:THR:HA	1:I:155:LEU:HG	1.92	0.51
1:I:177:TRP:HB3	1:I:184:VAL:HG22	1.92	0.51
1:G:179:VAL:O	1:G:286:THR:OG1	2.27	0.51
1:G:177:TRP:HB3	1:G:184:VAL:HG22	1.91	0.51
1:C:304:HIS:HD2	1:C:530:PRO:HG3	1.76	0.51
1:K:631:ARG:HE	1:F:130:LEU:HD22	1.76	0.51
1:L:209:ARG:NH1	1:L:212:GLU:OE1	2.43	0.51
1:C:134:ASP:O	1:C:138:TYR:HB2	2.11	0.51
1:C:573:VAL:O	1:C:577:THR:OG1	2.21	0.51
1:D:490:GLU:HG3	1:D:494:LEU:HD23	1.92	0.51
1:G:490:GLU:HG3	1:G:494:LEU:HD23	1.91	0.51
1:A:179:VAL:O	1:A:286:THR:OG1	2.28	0.51
1:A:555:ARG:HE	1:A:566:ILE:HD11	1.75	0.51
1:I:209:ARG:NH1	1:I:212:GLU:OE1	2.43	0.51
1:K:59:PHE:HB2	1:K:248:VAL:HG12	1.92	0.51
1:K:160:ASP:OD2	1:K:160:ASP:N	2.40	0.51
1:A:490:GLU:HG3	1:A:494:LEU:HD23	1.92	0.51
1:H:494:LEU:O	1:I:303:ARG:NH2	2.43	0.51
1:C:139:LEU:HD13	1:C:623:CYS:HA	1.93	0.51
1:H:490:GLU:HG3	1:H:494:LEU:HG	1.93	0.50
1:J:574:GLU:OE1	1:D:163:TYR:OH	2.28	0.50
1:G:134:ASP:O	1:G:138:TYR:HB2	2.11	0.50
1:L:187:LEU:N	1:L:239:ARG:O	2.43	0.50
1:L:631:ARG:HE	1:G:130:LEU:HD22	1.76	0.50
1:I:549:ARG:HE	1:C:83:MET:HE1	1.76	0.50
1:K:548:PHE:HZ	1:K:566:ILE:HD13	1.76	0.50
1:B:177:TRP:HB3	1:B:184:VAL:HG22	1.93	0.50
1:K:299:ASP:OD2	1:K:299:ASP:N	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ASP:HB2	1:F:630:ARG:HB3	1.94	0.50
1:L:59:PHE:HB2	1:L:248:VAL:HG12	1.93	0.50
1:B:182:GLY:O	1:B:271:ALA:N	2.38	0.50
1:I:489:ALA:O	1:I:493:HIS:ND1	2.45	0.50
1:I:535:LEU:HA	1:I:538:PHE:HB3	1.94	0.50
1:I:631:ARG:HE	1:C:130:LEU:HD22	1.76	0.50
1:F:555:ARG:HE	1:F:566:ILE:HD11	1.76	0.50
1:G:502:LYS:O	1:G:506:ALA:CB	2.60	0.50
1:E:571:TYR:OH	1:A:90:PRO:O	2.29	0.50
1:H:631:ARG:HE	1:B:130:LEU:HD22	1.76	0.50
1:L:571:TYR:OH	1:G:90:PRO:O	2.29	0.50
1:G:304:HIS:HD2	1:G:530:PRO:HG3	1.76	0.50
1:D:131:ASP:HB2	1:D:630:ARG:HB3	1.94	0.50
1:G:139:LEU:HD13	1:G:623:CYS:HA	1.93	0.50
1:A:160:ASP:N	1:A:160:ASP:OD2	2.45	0.50
1:L:152:THR:HA	1:L:155:LEU:HG	1.92	0.50
1:C:188:ASP:OD1	1:C:267:ARG:NH2	2.38	0.49
1:L:167:ASP:OD1	1:L:170:ASP:N	2.45	0.49
1:G:131:ASP:HB2	1:G:630:ARG:HB3	1.94	0.49
1:G:235:LEU:HA	1:G:585:LEU:HD22	1.94	0.49
1:F:177:TRP:HB3	1:F:184:VAL:HG22	1.93	0.49
1:J:555:ARG:HE	1:J:566:ILE:HD11	1.78	0.49
1:F:160:ASP:N	1:F:160:ASP:OD2	2.44	0.49
1:A:131:ASP:HB2	1:A:630:ARG:HB3	1.94	0.49
1:H:548:PHE:HZ	1:H:566:ILE:HD13	1.76	0.49
1:I:59:PHE:HB2	1:I:248:VAL:HG12	1.94	0.49
1:C:289:ALA:HA	1:C:292:HIS:HB2	1.94	0.49
1:C:502:LYS:O	1:C:506:ALA:CB	2.60	0.49
1:J:307:ILE:HA	1:J:310:LEU:HD12	1.95	0.49
1:D:134:ASP:O	1:D:138:TYR:HB2	2.13	0.49
1:L:549:ARG:HE	1:G:83:MET:HE1	1.76	0.49
1:G:302:CYS:SG	1:G:303:ARG:N	2.85	0.49
1:H:571:TYR:OH	1:B:90:PRO:O	2.29	0.49
1:B:160:ASP:OD2	1:B:160:ASP:N	2.44	0.49
1:B:490:GLU:HG3	1:B:494:LEU:HD23	1.94	0.49
1:B:502:LYS:O	1:B:506:ALA:CB	2.60	0.49
1:B:555:ARG:HE	1:B:566:ILE:HD11	1.76	0.49
1:J:490:GLU:HG3	1:J:494:LEU:HG	1.94	0.49
1:K:494:LEU:O	1:L:303:ARG:NH2	2.45	0.49
1:F:502:LYS:O	1:F:506:ALA:CB	2.60	0.49
1:F:570:ASN:N	1:F:595:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:518:ARG:HB2	1:G:322:SER:HA	1.95	0.49
1:G:182:GLY:O	1:G:271:ALA:N	2.39	0.49
1:B:302:CYS:SG	1:B:303:ARG:N	2.85	0.49
1:D:570:ASN:N	1:D:595:GLU:OE1	2.45	0.49
1:E:85:GLN:HG2	1:B:550:THR:HG22	1.93	0.49
1:C:302:CYS:SG	1:C:303:ARG:N	2.85	0.49
1:D:160:ASP:OD2	1:D:160:ASP:N	2.45	0.49
1:B:134:ASP:O	1:B:138:TYR:HB2	2.13	0.49
1:F:99:TYR:OH	1:F:103:LYS:NZ	2.40	0.49
1:F:235:LEU:HA	1:F:585:LEU:HD22	1.95	0.49
1:B:235:LEU:HA	1:B:585:LEU:HD22	1.95	0.49
1:F:134:ASP:O	1:F:138:TYR:HB2	2.13	0.49
1:E:490:GLU:HG3	1:E:494:LEU:HG	1.94	0.48
1:A:182:GLY:O	1:A:271:ALA:N	2.39	0.48
1:A:302:CYS:SG	1:A:303:ARG:N	2.86	0.48
1:J:85:GLN:HG2	1:F:550:THR:HG22	1.93	0.48
1:E:307:ILE:HA	1:E:310:LEU:HD12	1.95	0.48
1:I:69:ARG:HD2	1:D:283:LEU:HD22	1.95	0.48
1:I:85:GLN:HG2	1:D:550:THR:HG22	1.95	0.48
1:I:571:TYR:OH	1:C:90:PRO:O	2.29	0.48
1:C:235:LEU:HA	1:C:585:LEU:HD22	1.94	0.48
1:D:302:CYS:SG	1:D:303:ARG:N	2.86	0.48
1:A:134:ASP:O	1:A:138:TYR:HB2	2.13	0.48
1:H:301:LEU:HD21	1:H:535:LEU:HD11	1.96	0.48
1:C:160:ASP:N	1:C:160:ASP:OD2	2.45	0.48
1:J:59:PHE:HB2	1:J:248:VAL:HG12	1.94	0.48
1:F:573:VAL:O	1:F:577:THR:OG1	2.24	0.48
1:L:535:LEU:HA	1:L:538:PHE:HB3	1.94	0.48
1:B:131:ASP:HB2	1:B:630:ARG:HB3	1.94	0.48
1:K:490:GLU:HG3	1:K:494:LEU:HG	1.94	0.48
1:E:555:ARG:HE	1:E:566:ILE:HD11	1.78	0.48
1:C:102:CYS:HA	1:C:105:LEU:HB2	1.95	0.48
1:C:131:ASP:HB2	1:C:630:ARG:HB3	1.94	0.48
1:K:502:LYS:O	1:K:506:ALA:HB2	2.13	0.48
1:G:198:GLU:OE1	1:G:198:GLU:N	2.46	0.48
1:I:167:ASP:OD1	1:I:170:ASP:N	2.46	0.48
1:J:489:ALA:O	1:J:493:HIS:ND1	2.44	0.48
1:K:549:ARG:HE	1:F:83:MET:HE1	1.78	0.48
1:F:302:CYS:SG	1:F:303:ARG:N	2.85	0.48
1:L:488:ASP:HA	1:L:491:LEU:HG	1.95	0.48
1:E:59:PHE:HB2	1:E:248:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:489:ALA:O	1:H:493:HIS:ND1	2.45	0.48
1:I:307:ILE:HA	1:I:310:LEU:HD12	1.96	0.48
1:D:289:ALA:HA	1:D:292:HIS:HB2	1.95	0.48
1:K:187:LEU:N	1:K:239:ARG:O	2.47	0.48
1:G:102:CYS:HA	1:G:105:LEU:HB2	1.95	0.48
1:I:518:ARG:HB2	1:C:322:SER:HA	1.95	0.48
1:F:490:GLU:HG3	1:F:494:LEU:HD23	1.94	0.48
1:E:488:ASP:HA	1:E:491:LEU:HG	1.96	0.48
1:C:84:HIS:NE2	1:C:176:ASP:OD1	2.42	0.48
1:C:182:GLY:O	1:C:271:ALA:N	2.38	0.48
1:J:488:ASP:HA	1:J:491:LEU:HG	1.96	0.48
1:J:548:PHE:HZ	1:J:566:ILE:HD13	1.79	0.48
1:L:307:ILE:HA	1:L:310:LEU:HD12	1.96	0.47
1:G:289:ALA:HA	1:G:292:HIS:HB2	1.94	0.47
1:G:535:LEU:HA	1:G:538:PHE:HB3	1.96	0.47
1:E:548:PHE:HZ	1:E:566:ILE:HD13	1.79	0.47
1:B:289:ALA:HA	1:B:292:HIS:HB2	1.95	0.47
1:D:493:HIS:HE2	1:F:296:LEU:HD13	1.80	0.47
1:K:301:LEU:HD21	1:K:535:LEU:HD11	1.96	0.47
1:F:274:PRO:HB2	1:F:282:LEU:HD12	1.96	0.47
1:E:489:ALA:O	1:E:493:HIS:ND1	2.44	0.47
1:B:102:CYS:HA	1:B:105:LEU:HB2	1.97	0.47
1:H:167:ASP:OD1	1:H:170:ASP:N	2.47	0.47
1:K:167:ASP:OD1	1:K:170:ASP:N	2.47	0.47
1:F:79:ARG:N	1:F:536:GLU:OE1	2.47	0.47
1:F:289:ALA:HA	1:F:292:HIS:HB2	1.95	0.47
1:G:84:HIS:NE2	1:G:176:ASP:OD1	2.42	0.47
1:A:550:THR:HG22	1:L:85:GLN:HG2	1.96	0.47
1:H:549:ARG:HE	1:B:83:MET:HE1	1.78	0.47
1:I:188:ASP:OD1	1:I:267:ARG:NH2	2.44	0.47
1:J:152:THR:HA	1:J:155:LEU:HG	1.96	0.47
1:K:489:ALA:O	1:K:493:HIS:ND1	2.46	0.47
1:L:502:LYS:O	1:L:506:ALA:HB2	2.15	0.47
1:E:152:THR:HA	1:E:155:LEU:HG	1.96	0.47
1:B:274:PRO:HB2	1:B:282:LEU:HD12	1.96	0.47
1:I:488:ASP:HA	1:I:491:LEU:HG	1.95	0.47
1:I:502:LYS:O	1:I:506:ALA:HB2	2.15	0.47
1:C:535:LEU:HA	1:C:538:PHE:HB3	1.96	0.47
1:J:188:ASP:OD1	1:J:267:ARG:NH2	2.45	0.47
1:D:204:ARG:HH12	1:D:225:LEU:HD21	1.80	0.47
1:D:274:PRO:HB2	1:D:282:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:HD21	1:A:604:GLU:HG3	1.97	0.47
1:L:489:ALA:O	1:L:493:HIS:ND1	2.45	0.47
1:G:98:LEU:HD11	1:G:158:LEU:HD22	1.97	0.47
1:E:138:TYR:O	1:E:142:TRP:HB2	2.15	0.47
1:A:102:CYS:HA	1:A:105:LEU:HB2	1.97	0.47
1:A:493:HIS:HE2	1:B:296:LEU:HD13	1.80	0.47
1:H:152:THR:HA	1:H:155:LEU:HG	1.97	0.47
1:H:488:ASP:HA	1:H:491:LEU:HG	1.97	0.47
1:H:502:LYS:O	1:H:506:ALA:HB2	2.14	0.47
1:J:571:TYR:OH	1:D:90:PRO:O	2.29	0.47
1:E:167:ASP:OD1	1:E:170:ASP:N	2.47	0.47
1:B:204:ARG:HH12	1:B:225:LEU:HD21	1.79	0.47
1:B:570:ASN:N	1:B:595:GLU:OE1	2.45	0.47
1:C:110:THR:OG1	1:C:111:VAL:N	2.48	0.47
1:H:606:VAL:O	1:H:610:TYR:HB2	2.16	0.46
1:F:204:ARG:HH12	1:F:225:LEU:HD21	1.79	0.46
1:A:502:LYS:O	1:A:506:ALA:CB	2.63	0.46
1:J:167:ASP:OD1	1:J:170:ASP:N	2.47	0.46
1:J:535:LEU:HA	1:J:538:PHE:HB3	1.98	0.46
1:D:600:LEU:HD21	1:D:604:GLU:HG3	1.97	0.46
1:K:488:ASP:HA	1:K:491:LEU:HG	1.97	0.46
1:L:94:ARG:HE	1:L:166:ALA:HB3	1.80	0.46
1:E:192:LYS:HA	1:E:192:LYS:HD3	1.73	0.46
1:D:186:LEU:HD21	1:D:267:ARG:HG2	1.97	0.46
1:D:502:LYS:O	1:D:506:ALA:CB	2.63	0.46
1:G:160:ASP:OD2	1:G:160:ASP:N	2.45	0.46
1:B:186:LEU:HD21	1:B:267:ARG:HG2	1.98	0.46
1:E:490:GLU:O	1:E:494:LEU:N	2.36	0.46
1:A:289:ALA:HA	1:A:292:HIS:HB2	1.98	0.46
1:K:535:LEU:HA	1:K:538:PHE:HB3	1.98	0.46
1:G:99:TYR:OH	1:G:103:LYS:NZ	2.41	0.46
1:E:209:ARG:NH1	1:E:212:GLU:OE2	2.46	0.46
1:E:520:VAL:HB	1:A:321:ALA:H	1.80	0.46
1:E:535:LEU:HA	1:E:538:PHE:HB3	1.98	0.46
1:A:98:LEU:HD11	1:A:158:LEU:HD22	1.97	0.46
1:B:110:THR:OG1	1:B:111:VAL:N	2.49	0.46
1:I:555:ARG:HE	1:I:566:ILE:HD11	1.81	0.46
1:D:172:GLY:HA2	1:D:175:VAL:HG22	1.98	0.46
1:K:97:LEU:HA	1:K:590:LEU:HD23	1.98	0.46
1:K:606:VAL:O	1:K:610:TYR:HB2	2.16	0.46
1:H:187:LEU:N	1:H:239:ARG:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:VAL:O	1:B:577:THR:OG1	2.24	0.46
1:C:186:LEU:HD21	1:C:267:ARG:HG2	1.98	0.46
1:J:239:ARG:HA	1:J:239:ARG:HD3	1.77	0.46
1:A:186:LEU:HD21	1:A:267:ARG:HG2	1.98	0.46
1:I:94:ARG:HE	1:I:166:ALA:HB3	1.80	0.46
1:C:204:ARG:HH12	1:C:225:LEU:HD21	1.81	0.46
1:J:97:LEU:HA	1:J:590:LEU:HD23	1.98	0.46
1:K:91:CYS:HA	1:K:94:ARG:HG3	1.97	0.46
1:E:271:ALA:HA	1:A:168:ASN:HD21	1.81	0.46
1:E:502:LYS:O	1:E:506:ALA:HB2	2.15	0.46
1:E:581:LEU:HA	1:E:585:LEU:HB2	1.98	0.46
1:A:304:HIS:HA	1:A:307:ILE:HG12	1.98	0.46
1:H:209:ARG:NH1	1:H:212:GLU:OE2	2.46	0.46
1:I:91:CYS:HA	1:I:94:ARG:HG3	1.98	0.46
1:I:512:LEU:HD12	1:C:509:PHE:HB2	1.97	0.46
1:J:502:LYS:O	1:J:506:ALA:HB2	2.16	0.46
1:K:152:THR:HA	1:K:155:LEU:HG	1.97	0.46
1:F:102:CYS:HA	1:F:105:LEU:HB2	1.97	0.46
1:F:182:GLY:O	1:F:271:ALA:N	2.38	0.46
1:L:97:LEU:HA	1:L:590:LEU:HD23	1.97	0.46
1:G:110:THR:OG1	1:G:111:VAL:N	2.48	0.46
1:E:177:TRP:HB3	1:E:184:VAL:HG22	1.98	0.45
1:E:239:ARG:HD3	1:E:239:ARG:HA	1.77	0.45
1:A:204:ARG:HH12	1:A:225:LEU:HD21	1.82	0.45
1:H:535:LEU:HA	1:H:538:PHE:HB3	1.98	0.45
1:J:94:ARG:HE	1:J:166:ALA:HB3	1.81	0.45
1:D:98:LEU:HD11	1:D:158:LEU:HD22	1.97	0.45
1:K:520:VAL:HB	1:F:321:ALA:H	1.82	0.45
1:L:192:LYS:HD3	1:L:192:LYS:HA	1.73	0.45
1:H:91:CYS:HA	1:H:94:ARG:HG3	1.97	0.45
1:I:89:ASP:HB2	1:D:571:TYR:OH	2.16	0.45
1:I:97:LEU:HA	1:I:590:LEU:HD23	1.97	0.45
1:C:99:TYR:OH	1:C:103:LYS:NZ	2.41	0.45
1:J:520:VAL:HB	1:D:321:ALA:H	1.80	0.45
1:D:102:CYS:HA	1:D:105:LEU:HB2	1.97	0.45
1:K:94:ARG:HE	1:K:166:ALA:HB3	1.81	0.45
1:L:91:CYS:HA	1:L:94:ARG:HG3	1.98	0.45
1:E:89:ASP:HB2	1:B:571:TYR:OH	2.17	0.45
1:E:97:LEU:HA	1:E:590:LEU:HD23	1.98	0.45
1:I:187:LEU:N	1:I:239:ARG:O	2.48	0.45
1:C:98:LEU:HD11	1:C:158:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:GLN:O	1:H:211:THR:OG1	2.33	0.45
1:J:138:TYR:O	1:J:142:TRP:HB2	2.15	0.45
1:J:271:ALA:HA	1:D:168:ASN:HD21	1.81	0.45
1:F:186:LEU:HD21	1:F:267:ARG:HG2	1.98	0.45
1:L:480:ASP:O	1:L:483:SER:OG	2.34	0.45
1:L:581:LEU:HA	1:L:585:LEU:HB2	1.99	0.45
1:A:570:ASN:N	1:A:595:GLU:OE1	2.45	0.45
1:H:89:ASP:HB2	1:C:571:TYR:OH	2.17	0.45
1:J:187:LEU:N	1:J:239:ARG:O	2.50	0.45
1:D:235:LEU:HA	1:D:585:LEU:HD22	1.99	0.45
1:L:484:LEU:O	1:L:487:ARG:HG3	2.16	0.45
1:L:512:LEU:HD12	1:G:509:PHE:HB2	1.97	0.45
1:G:98:LEU:HD12	1:G:98:LEU:HA	1.81	0.45
1:H:94:ARG:HE	1:H:166:ALA:HB3	1.81	0.45
1:B:79:ARG:N	1:B:536:GLU:OE1	2.47	0.45
1:I:480:ASP:O	1:I:483:SER:OG	2.35	0.45
1:I:484:LEU:O	1:I:487:ARG:HG3	2.16	0.45
1:F:110:THR:OG1	1:F:111:VAL:N	2.49	0.45
1:E:187:LEU:N	1:E:239:ARG:O	2.50	0.45
1:A:110:THR:OG1	1:A:111:VAL:N	2.48	0.45
1:A:198:GLU:OE1	1:A:198:GLU:N	2.48	0.45
1:H:484:LEU:O	1:H:487:ARG:HG3	2.17	0.45
1:H:520:VAL:HB	1:B:321:ALA:H	1.82	0.45
1:J:89:ASP:HB2	1:F:571:TYR:OH	2.17	0.45
1:D:110:THR:OG1	1:D:111:VAL:N	2.48	0.45
1:D:505:ASP:OD1	1:D:505:ASP:N	2.44	0.45
1:G:186:LEU:HD21	1:G:267:ARG:HG2	1.98	0.45
1:H:97:LEU:HA	1:H:590:LEU:HD23	1.98	0.45
1:B:593:VAL:HG11	1:B:598:LEU:HD13	1.99	0.45
1:I:518:ARG:NH2	1:C:325:GLU:O	2.29	0.45
1:C:502:LYS:HB2	1:C:502:LYS:HE2	1.85	0.45
1:J:177:TRP:HB3	1:J:184:VAL:HG22	1.98	0.45
1:D:192:LYS:HB2	1:D:195:GLU:HG3	1.97	0.45
1:K:89:ASP:HB2	1:G:571:TYR:OH	2.17	0.45
1:G:192:LYS:HA	1:G:192:LYS:HD3	1.75	0.45
1:B:492:TYR:O	1:C:303:ARG:NH2	2.50	0.45
1:D:492:TYR:O	1:F:303:ARG:NH2	2.50	0.45
1:K:85:GLN:HG2	1:G:550:THR:HG22	1.98	0.45
1:F:492:TYR:O	1:G:303:ARG:NH2	2.50	0.45
1:L:298:TYR:HA	1:L:301:LEU:HD23	1.98	0.45
1:A:239:ARG:HD3	1:A:239:ARG:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:TYR:OH	1:L:89:ASP:HB2	2.17	0.44
1:K:88:ARG:HA	1:K:175:VAL:HG21	1.99	0.44
1:F:593:VAL:HG11	1:F:598:LEU:HD13	1.99	0.44
1:L:239:ARG:HA	1:L:239:ARG:HD3	1.78	0.44
1:L:555:ARG:HE	1:L:566:ILE:HD11	1.81	0.44
1:E:484:LEU:O	1:E:487:ARG:HG3	2.17	0.44
1:A:192:LYS:HB2	1:A:195:GLU:HG3	1.99	0.44
1:A:492:TYR:O	1:B:303:ARG:NH2	2.50	0.44
1:K:208:GLN:O	1:K:211:THR:OG1	2.33	0.44
1:L:188:ASP:OD1	1:L:267:ARG:NH2	2.43	0.44
1:H:154:VAL:HG22	1:H:158:LEU:HD23	1.98	0.44
1:H:581:LEU:HD13	1:H:585:LEU:HB2	1.99	0.44
1:C:198:GLU:OE1	1:C:198:GLU:N	2.46	0.44
1:J:91:CYS:HA	1:J:94:ARG:HG3	1.99	0.44
1:J:581:LEU:HA	1:J:585:LEU:HB2	1.98	0.44
1:K:154:VAL:HG22	1:K:158:LEU:HD23	1.98	0.44
1:F:63:GLN:HE22	1:F:67:PHE:HD1	1.65	0.44
1:L:271:ALA:HA	1:G:168:ASN:HD21	1.83	0.44
1:L:610:TYR:CZ	1:L:615:PHE:HB3	2.53	0.44
1:E:91:CYS:HA	1:E:94:ARG:HG3	1.99	0.44
1:I:285:THR:OG1	1:C:88:ARG:NE	2.51	0.44
1:C:172:GLY:HA2	1:C:175:VAL:HG22	1.99	0.44
1:D:593:VAL:HG11	1:D:598:LEU:HD13	2.00	0.44
1:L:74:PHE:HB3	1:L:75:LEU:HD22	2.00	0.44
1:E:94:ARG:HE	1:E:166:ALA:HB3	1.81	0.44
1:H:581:LEU:HA	1:H:585:LEU:HB2	1.99	0.44
1:A:114:VAL:HG12	1:A:216:LEU:HD11	2.00	0.44
1:H:239:ARG:HD3	1:H:239:ARG:HA	1.78	0.44
1:H:271:ALA:HA	1:B:168:ASN:HD21	1.83	0.44
1:C:570:ASN:N	1:C:595:GLU:OE1	2.50	0.44
1:D:99:TYR:OH	1:D:103:LYS:NZ	2.40	0.44
1:K:484:LEU:O	1:K:487:ARG:HG3	2.17	0.44
1:G:165:TYR:HE2	1:G:235:LEU:HB2	1.83	0.44
1:A:187:LEU:HB2	1:A:239:ARG:HB2	2.00	0.44
1:J:88:ARG:NE	1:F:285:THR:HG21	2.33	0.44
1:J:484:LEU:O	1:J:487:ARG:HG3	2.17	0.44
1:F:629:ARG:HA	1:F:629:ARG:HD2	1.79	0.44
1:B:63:GLN:HE22	1:B:67:PHE:HD1	1.65	0.44
1:J:610:TYR:CZ	1:J:615:PHE:HB3	2.53	0.44
1:F:590:LEU:H	1:F:590:LEU:HG	1.58	0.44
1:E:248:VAL:HA	1:E:259:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:PRO:HB2	1:E:282:LEU:HD12	1.99	0.44
1:E:285:THR:OG1	1:A:88:ARG:NE	2.51	0.44
1:H:126:PRO:HA	1:C:625:ARG:HE	1.82	0.44
1:H:188:ASP:OD1	1:H:267:ARG:NH2	2.44	0.44
1:I:610:TYR:CZ	1:I:615:PHE:HB3	2.53	0.44
1:K:581:LEU:HD13	1:K:585:LEU:HB2	1.99	0.44
1:F:165:TYR:HE2	1:F:235:LEU:HB2	1.83	0.44
1:G:304:HIS:HA	1:G:307:ILE:HG12	2.00	0.44
1:A:79:ARG:N	1:A:536:GLU:OE1	2.51	0.43
1:A:593:VAL:HG11	1:A:598:LEU:HD13	1.99	0.43
1:H:85:GLN:HG2	1:C:550:THR:HG22	1.98	0.43
1:I:139:LEU:HD23	1:I:139:LEU:HA	1.89	0.43
1:J:208:GLN:O	1:J:211:THR:OG1	2.34	0.43
1:D:79:ARG:N	1:D:536:GLU:OE1	2.50	0.43
1:L:285:THR:OG1	1:G:88:ARG:NE	2.50	0.43
1:G:274:PRO:HB2	1:G:282:LEU:HD12	1.99	0.43
1:B:165:TYR:HE2	1:B:235:LEU:HB2	1.83	0.43
1:I:581:LEU:HA	1:I:585:LEU:HB2	1.99	0.43
1:K:188:ASP:OD1	1:K:267:ARG:NH2	2.44	0.43
1:K:271:ALA:HA	1:F:168:ASN:HD21	1.83	0.43
1:K:310:LEU:HD12	1:G:304:HIS:CE1	2.53	0.43
1:K:483:SER:HB3	1:K:487:ARG:HE	1.83	0.43
1:K:555:ARG:HE	1:K:566:ILE:HD11	1.83	0.43
1:G:204:ARG:HH12	1:G:225:LEU:HD21	1.81	0.43
1:A:99:TYR:OH	1:A:103:LYS:NZ	2.40	0.43
1:I:126:PRO:HA	1:D:625:ARG:HE	1.83	0.43
1:J:285:THR:OG1	1:D:88:ARG:NE	2.51	0.43
1:D:205:ALA:HB1	1:D:209:ARG:HH12	1.83	0.43
1:K:581:LEU:HA	1:K:585:LEU:HB2	2.00	0.43
1:H:88:ARG:HA	1:H:175:VAL:HG21	1.99	0.43
1:H:555:ARG:HE	1:H:566:ILE:HD11	1.83	0.43
1:C:165:TYR:HE2	1:C:235:LEU:HB2	1.83	0.43
1:D:114:VAL:HG12	1:D:216:LEU:HD11	2.00	0.43
1:K:571:TYR:OH	1:F:90:PRO:O	2.29	0.43
1:F:99:TYR:HA	1:F:102:CYS:SG	2.58	0.43
1:F:239:ARG:HD3	1:F:239:ARG:HA	1.86	0.43
1:L:98:LEU:HA	1:L:98:LEU:HD12	1.80	0.43
1:G:314:PHE:HB3	1:G:317:LYS:HE3	2.00	0.43
1:E:610:TYR:CZ	1:E:615:PHE:HB3	2.53	0.43
1:H:310:LEU:HD12	1:C:304:HIS:CE1	2.53	0.43
1:H:483:SER:HB3	1:H:487:ARG:HE	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:274:PRO:HB2	1:I:282:LEU:HD12	2.01	0.43
1:J:248:VAL:HA	1:J:259:ALA:HA	2.00	0.43
1:G:99:TYR:HA	1:G:102:CYS:SG	2.59	0.43
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.80	0.43
1:A:99:TYR:HA	1:A:102:CYS:SG	2.58	0.43
1:A:100:GLY:HA2	1:A:591:ASP:H	1.83	0.43
1:A:174:TYR:CZ	1:A:580:TYR:HB2	2.54	0.43
1:A:306:LYS:HA	1:A:309:GLN:HE21	1.83	0.43
1:H:629:ARG:HA	1:H:629:ARG:HD2	1.85	0.43
1:I:581:LEU:HD13	1:I:585:LEU:HB2	2.01	0.43
1:K:98:LEU:HD12	1:K:98:LEU:HA	1.82	0.43
1:K:126:PRO:HA	1:G:625:ARG:HE	1.82	0.43
1:K:610:TYR:CZ	1:K:615:PHE:HB3	2.54	0.43
1:F:172:GLY:HA2	1:F:175:VAL:HG22	2.00	0.43
1:F:205:ALA:HB1	1:F:209:ARG:HH12	1.84	0.43
1:G:139:LEU:HD23	1:G:139:LEU:HA	1.91	0.43
1:E:88:ARG:NE	1:B:285:THR:HG21	2.33	0.43
1:H:257:LEU:HD13	1:H:257:LEU:HA	1.90	0.43
1:B:114:VAL:HG12	1:B:216:LEU:HD11	2.01	0.43
1:B:192:LYS:HD3	1:B:192:LYS:HA	1.75	0.43
1:D:99:TYR:HA	1:D:102:CYS:SG	2.58	0.43
1:F:192:LYS:HA	1:F:192:LYS:HD3	1.75	0.43
1:L:257:LEU:HD13	1:L:257:LEU:HA	1.90	0.43
1:E:188:ASP:OD1	1:E:267:ARG:NH2	2.45	0.43
1:A:205:ALA:HB1	1:A:209:ARG:HH12	1.83	0.43
1:H:274:PRO:HB2	1:H:282:LEU:HD12	2.01	0.43
1:I:257:LEU:HD13	1:I:257:LEU:HA	1.90	0.43
1:C:63:GLN:HE22	1:C:67:PHE:HD1	1.67	0.43
1:K:306:LYS:O	1:K:310:LEU:HB2	2.19	0.43
1:F:483:SER:N	1:F:487:ARG:HH12	2.17	0.43
1:G:172:GLY:HA2	1:G:175:VAL:HG22	1.99	0.43
1:G:306:LYS:HA	1:G:309:GLN:HE21	1.84	0.43
1:C:205:ALA:HB1	1:C:209:ARG:HH12	1.83	0.43
1:F:502:LYS:HB2	1:F:502:LYS:HE2	1.86	0.43
1:A:625:ARG:HE	1:L:126:PRO:HA	1.83	0.43
1:H:306:LYS:O	1:H:310:LEU:HB2	2.19	0.43
1:C:274:PRO:HB2	1:C:282:LEU:HD12	2.00	0.43
1:F:114:VAL:HG12	1:F:216:LEU:HD11	2.01	0.43
1:L:208:GLN:O	1:L:211:THR:OG1	2.35	0.43
1:G:205:ALA:HB1	1:G:209:ARG:HH12	1.83	0.43
1:C:497:LEU:HD23	1:C:497:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:SER:HB3	1:E:604:GLU:HG3	2.01	0.42
1:A:172:GLY:HA2	1:A:175:VAL:HG22	2.00	0.42
1:H:285:THR:OG1	1:B:88:ARG:NE	2.52	0.42
1:H:610:TYR:CZ	1:H:615:PHE:HB3	2.54	0.42
1:B:304:HIS:HA	1:B:307:ILE:HG12	2.01	0.42
1:B:629:ARG:HA	1:B:629:ARG:HD2	1.79	0.42
1:I:271:ALA:HA	1:C:168:ASN:HD21	1.83	0.42
1:L:581:LEU:HD13	1:L:585:LEU:HB2	2.01	0.42
1:G:292:HIS:O	1:G:296:LEU:HG	2.19	0.42
1:E:214:HIS:CE1	1:E:216:LEU:HB3	2.55	0.42
1:H:125:PHE:O	1:C:625:ARG:NH2	2.49	0.42
1:B:99:TYR:HA	1:B:102:CYS:SG	2.58	0.42
1:B:172:GLY:HA2	1:B:175:VAL:HG22	2.00	0.42
1:I:93:LEU:HD13	1:I:171:TYR:HB2	2.00	0.42
1:I:165:TYR:CE2	1:I:235:LEU:HB3	2.55	0.42
1:C:114:VAL:HG12	1:C:216:LEU:HD11	2.01	0.42
1:E:606:VAL:O	1:E:610:TYR:HB2	2.20	0.42
1:A:84:HIS:NE2	1:A:176:ASP:OD1	2.44	0.42
1:I:165:TYR:HE2	1:I:235:LEU:HB3	1.84	0.42
1:I:186:LEU:HD11	1:I:267:ARG:HE	1.85	0.42
1:C:304:HIS:HA	1:C:307:ILE:HG12	2.00	0.42
1:J:186:LEU:HD11	1:J:267:ARG:HE	1.85	0.42
1:J:209:ARG:NH1	1:J:212:GLU:OE2	2.46	0.42
1:J:601:SER:HB3	1:J:604:GLU:HG3	2.01	0.42
1:D:306:LYS:HA	1:D:309:GLN:HE21	1.84	0.42
1:A:490:GLU:HA	1:A:493:HIS:ND1	2.35	0.42
1:A:583:HIS:NE2	1:L:163:TYR:O	2.52	0.42
1:B:174:TYR:CZ	1:B:580:TYR:HB2	2.55	0.42
1:I:239:ARG:HD3	1:I:239:ARG:HA	1.78	0.42
1:C:99:TYR:HA	1:C:102:CYS:SG	2.59	0.42
1:J:557:VAL:HG22	1:J:563:GLU:HA	2.02	0.42
1:K:209:ARG:NH1	1:K:212:GLU:OE2	2.46	0.42
1:L:248:VAL:HA	1:L:259:ALA:HA	2.01	0.42
1:L:274:PRO:HB2	1:L:282:LEU:HD12	2.01	0.42
1:G:114:VAL:HG12	1:G:216:LEU:HD11	2.01	0.42
1:H:304:HIS:HA	1:H:307:ILE:HG12	2.02	0.42
1:I:298:TYR:HA	1:I:301:LEU:HD23	2.01	0.42
1:J:274:PRO:HB2	1:J:282:LEU:HD12	2.00	0.42
1:J:304:HIS:HA	1:J:307:ILE:HG12	2.02	0.42
1:J:606:VAL:O	1:J:610:TYR:HB2	2.20	0.42
1:D:174:TYR:CZ	1:D:580:TYR:HB2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:GLU:HA	1:D:493:HIS:ND1	2.34	0.42
1:K:285:THR:OG1	1:F:88:ARG:NE	2.52	0.42
1:G:629:ARG:HD2	1:G:629:ARG:HA	1.79	0.42
1:E:557:VAL:HG22	1:E:563:GLU:HA	2.02	0.42
1:E:581:LEU:HD13	1:E:585:LEU:HB2	2.01	0.42
1:A:579:PRO:HA	1:A:582:CYS:SG	2.59	0.42
1:H:601:SER:HB3	1:H:604:GLU:HG3	2.01	0.42
1:B:483:SER:N	1:B:487:ARG:HH12	2.17	0.42
1:D:70:LEU:HD11	1:D:288:VAL:HG13	2.01	0.42
1:D:98:LEU:HA	1:D:98:LEU:HD12	1.81	0.42
1:D:629:ARG:HA	1:D:629:ARG:HD2	1.78	0.42
1:K:274:PRO:HB2	1:K:282:LEU:HD12	2.01	0.42
1:L:631:ARG:HG2	1:L:635:ARG:HH12	1.84	0.42
1:G:63:GLN:HE22	1:G:67:PHE:HD1	1.67	0.42
1:C:140:LEU:O	1:C:143:SER:OG	2.38	0.42
1:J:207:VAL:HG23	1:J:218:GLN:HG3	2.02	0.42
1:L:165:TYR:CE2	1:L:235:LEU:HB3	2.55	0.42
1:L:550:THR:OG1	1:L:551:PHE:N	2.53	0.42
1:G:116:GLU:O	1:G:120:LEU:HG	2.20	0.42
1:A:483:SER:N	1:A:487:ARG:HH12	2.18	0.42
1:H:165:TYR:CE2	1:H:235:LEU:HB3	2.55	0.42
1:H:186:LEU:HD11	1:H:267:ARG:HE	1.85	0.42
1:H:214:HIS:CE1	1:H:216:LEU:HB3	2.55	0.42
1:H:270:VAL:HB	1:H:273:GLU:HB3	2.01	0.42
1:B:99:TYR:OH	1:B:103:LYS:NZ	2.40	0.42
1:B:205:ALA:HB1	1:B:209:ARG:HH12	1.84	0.42
1:I:192:LYS:HA	1:I:192:LYS:HD3	1.73	0.42
1:I:214:HIS:CE1	1:I:216:LEU:HB3	2.54	0.42
1:D:306:LYS:O	1:D:310:LEU:HB2	2.20	0.42
1:K:270:VAL:HB	1:K:273:GLU:HB3	2.01	0.42
1:G:483:SER:N	1:G:487:ARG:HH12	2.18	0.42
1:E:126:PRO:HA	1:B:625:ARG:HE	1.85	0.42
1:E:304:HIS:HA	1:E:307:ILE:HG12	2.02	0.42
1:C:292:HIS:O	1:C:296:LEU:HG	2.19	0.42
1:C:490:GLU:HA	1:C:493:HIS:ND1	2.35	0.42
1:K:492:TYR:CD1	1:L:297:ARG:HA	2.55	0.42
1:F:497:LEU:HD23	1:F:497:LEU:H	1.85	0.42
1:L:95:LYS:HG2	1:L:602:PHE:HD2	1.85	0.42
1:L:154:VAL:HG22	1:L:158:LEU:HD23	2.01	0.42
1:L:629:ARG:HD2	1:L:629:ARG:HA	1.85	0.42
1:E:186:LEU:HD11	1:E:267:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:HB2	1:A:282:LEU:HD12	2.02	0.41
1:B:100:GLY:HA2	1:B:591:ASP:H	1.84	0.41
1:B:497:LEU:H	1:B:497:LEU:HD23	1.85	0.41
1:D:314:PHE:HB3	1:D:317:LYS:HD3	2.02	0.41
1:D:317:LYS:HE3	1:D:512:LEU:HD22	2.01	0.41
1:D:483:SER:N	1:D:487:ARG:HH12	2.18	0.41
1:K:186:LEU:HD11	1:K:267:ARG:HE	1.85	0.41
1:K:317:LYS:HE2	1:K:317:LYS:HB2	1.86	0.41
1:K:601:SER:HB3	1:K:604:GLU:HG3	2.01	0.41
1:F:304:HIS:HA	1:F:307:ILE:HG12	2.01	0.41
1:F:550:THR:OG1	1:F:551:PHE:N	2.53	0.41
1:L:186:LEU:HD11	1:L:267:ARG:HE	1.85	0.41
1:L:214:HIS:CE1	1:L:216:LEU:HB3	2.54	0.41
1:G:579:PRO:HA	1:G:582:CYS:SG	2.60	0.41
1:A:116:GLU:O	1:A:120:LEU:HG	2.20	0.41
1:A:317:LYS:HE3	1:A:512:LEU:HD22	2.01	0.41
1:C:239:ARG:HA	1:C:239:ARG:HD3	1.87	0.41
1:C:314:PHE:HB3	1:C:317:LYS:HE3	2.01	0.41
1:J:549:ARG:HE	1:D:83:MET:HE1	1.85	0.41
1:K:165:TYR:CE2	1:K:235:LEU:HB3	2.55	0.41
1:L:175:VAL:HA	1:L:178:CYS:SG	2.60	0.41
1:G:192:LYS:HB2	1:G:195:GLU:HG3	2.01	0.41
1:B:84:HIS:NE2	1:B:176:ASP:OD1	2.41	0.41
1:I:550:THR:OG1	1:I:551:PHE:N	2.53	0.41
1:J:214:HIS:CE1	1:J:216:LEU:HB3	2.55	0.41
1:J:483:SER:HB3	1:J:487:ARG:HE	1.85	0.41
1:K:248:VAL:HA	1:K:259:ALA:HA	2.03	0.41
1:I:154:VAL:HG22	1:I:158:LEU:HD23	2.01	0.41
1:C:483:SER:N	1:C:487:ARG:HH12	2.18	0.41
1:J:165:TYR:CE2	1:J:235:LEU:HB3	2.56	0.41
1:D:116:GLU:O	1:D:120:LEU:HG	2.20	0.41
1:K:304:HIS:HA	1:K:307:ILE:HG12	2.02	0.41
1:E:174:TYR:CZ	1:E:580:TYR:HB2	2.56	0.41
1:E:483:SER:HB3	1:E:487:ARG:HE	1.85	0.41
1:I:208:GLN:O	1:I:211:THR:OG1	2.35	0.41
1:C:629:ARG:HD2	1:C:629:ARG:HA	1.79	0.41
1:J:126:PRO:HA	1:F:625:ARG:HE	1.85	0.41
1:F:116:GLU:O	1:F:120:LEU:HG	2.20	0.41
1:L:84:HIS:NE2	1:L:176:ASP:OD2	2.46	0.41
1:G:497:LEU:H	1:G:497:LEU:HD23	1.85	0.41
1:H:138:TYR:O	1:H:142:TRP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:ASN:N	1:H:168:ASN:OD1	2.53	0.41
1:B:490:GLU:HA	1:B:493:HIS:ND1	2.35	0.41
1:I:248:VAL:HA	1:I:259:ALA:HA	2.01	0.41
1:I:606:VAL:O	1:I:610:TYR:HB2	2.21	0.41
1:J:258:GLU:OE1	1:J:265:HIS:ND1	2.48	0.41
1:E:208:GLN:O	1:E:211:THR:OG1	2.34	0.41
1:E:550:THR:OG1	1:E:551:PHE:N	2.54	0.41
1:H:555:ARG:HA	1:H:566:ILE:HG12	2.02	0.41
1:B:154:VAL:HG21	1:B:606:VAL:HG21	2.03	0.41
1:I:601:SER:HB3	1:I:604:GLU:HG3	2.01	0.41
1:C:116:GLU:O	1:C:120:LEU:HG	2.20	0.41
1:C:306:LYS:HA	1:C:309:GLN:HE21	1.84	0.41
1:C:579:PRO:HA	1:C:582:CYS:SG	2.60	0.41
1:D:304:HIS:HA	1:D:307:ILE:HG12	2.01	0.41
1:K:159:ARG:HH22	1:G:582:CYS:HB3	1.86	0.41
1:K:214:HIS:CE1	1:K:216:LEU:HB3	2.55	0.41
1:F:247:ARG:HG3	1:F:260:GLN:HB2	2.02	0.41
1:G:490:GLU:HA	1:G:493:HIS:ND1	2.35	0.41
1:E:165:TYR:CE2	1:E:235:LEU:HB3	2.56	0.41
1:E:518:ARG:HB2	1:A:322:SER:HA	2.03	0.41
1:E:631:ARG:HG2	1:E:635:ARG:HH12	1.86	0.41
1:H:304:HIS:CE1	1:B:310:LEU:HD12	2.56	0.41
1:I:175:VAL:HA	1:I:178:CYS:SG	2.60	0.41
1:I:631:ARG:HG2	1:I:635:ARG:HH12	1.84	0.41
1:C:204:ARG:HA	1:C:204:ARG:HD3	1.93	0.41
1:F:174:TYR:CZ	1:F:580:TYR:HB2	2.55	0.41
1:F:306:LYS:HA	1:F:309:GLN:HE21	1.85	0.41
1:F:548:PHE:CE1	1:F:553:LEU:HB2	2.56	0.41
1:A:317:LYS:HA	1:A:317:LYS:HD2	1.85	0.41
1:H:496:VAL:H	1:H:496:VAL:HG22	1.65	0.41
1:B:116:GLU:O	1:B:120:LEU:HG	2.20	0.41
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.88	0.41
1:B:548:PHE:CE1	1:B:553:LEU:HB2	2.56	0.41
1:I:138:TYR:O	1:I:142:TRP:HB2	2.21	0.41
1:C:174:TYR:CZ	1:C:580:TYR:HB2	2.56	0.41
1:C:256:ARG:HD3	1:C:256:ARG:HA	1.95	0.41
1:C:257:LEU:HD13	1:C:257:LEU:HA	1.97	0.41
1:C:517:ASN:OD1	1:C:517:ASN:N	2.48	0.41
1:J:95:LYS:HG2	1:J:602:PHE:HD2	1.86	0.41
1:J:550:THR:OG1	1:J:551:PHE:N	2.54	0.41
1:J:581:LEU:HD13	1:J:585:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:HIS:NE2	1:D:176:ASP:OD1	2.44	0.41
1:D:548:PHE:CE1	1:D:553:LEU:HB2	2.55	0.41
1:D:579:PRO:HA	1:D:582:CYS:SG	2.60	0.41
1:K:518:ARG:HB2	1:F:322:SER:HA	2.02	0.41
1:K:614:LYS:O	1:K:618:TYR:N	2.53	0.41
1:F:100:GLY:HA2	1:F:591:ASP:H	1.84	0.41
1:F:579:PRO:HA	1:F:582:CYS:SG	2.61	0.41
1:L:168:ASN:OD1	1:L:168:ASN:N	2.52	0.41
1:L:601:SER:HB3	1:L:604:GLU:HG3	2.01	0.41
1:L:606:VAL:O	1:L:610:TYR:HB2	2.21	0.41
1:G:570:ASN:N	1:G:595:GLU:OE1	2.50	0.41
1:A:306:LYS:O	1:A:310:LEU:HB2	2.20	0.41
1:H:545:ASN:O	1:B:82:SER:OG	2.27	0.41
1:H:573:VAL:O	1:H:577:THR:OG1	2.31	0.41
1:H:614:LYS:O	1:H:618:TYR:N	2.53	0.41
1:I:72:HIS:CD2	1:D:285:THR:HA	2.56	0.41
1:C:192:LYS:HB2	1:C:195:GLU:HG3	2.01	0.41
1:J:72:HIS:CD2	1:F:285:THR:HA	2.56	0.41
1:L:165:TYR:HE2	1:L:235:LEU:HB3	1.85	0.41
1:A:314:PHE:HB3	1:A:317:LYS:HD3	2.02	0.40
1:A:548:PHE:CE1	1:A:553:LEU:HB2	2.55	0.40
1:B:306:LYS:HA	1:B:309:GLN:HE21	1.85	0.40
1:I:491:LEU:HD22	1:I:499:ALA:HB1	2.03	0.40
1:C:98:LEU:HD12	1:C:98:LEU:HA	1.81	0.40
1:C:487:ARG:HA	1:C:490:GLU:HB3	2.03	0.40
1:J:518:ARG:HB2	1:D:322:SER:HA	2.03	0.40
1:K:555:ARG:HA	1:K:566:ILE:HG12	2.02	0.40
1:F:84:HIS:NE2	1:F:176:ASP:OD1	2.41	0.40
1:F:154:VAL:HG21	1:F:606:VAL:HG21	2.03	0.40
1:F:256:ARG:HD3	1:F:256:ARG:HA	1.95	0.40
1:A:292:HIS:O	1:A:296:LEU:HG	2.22	0.40
1:B:247:ARG:HG3	1:B:260:GLN:HB2	2.02	0.40
1:B:550:THR:OG1	1:B:551:PHE:N	2.53	0.40
1:B:579:PRO:HA	1:B:582:CYS:SG	2.61	0.40
1:I:88:ARG:NE	1:D:285:THR:HG21	2.36	0.40
1:I:95:LYS:HG2	1:I:602:PHE:HD2	1.86	0.40
1:I:520:VAL:HB	1:C:321:ALA:H	1.86	0.40
1:C:79:ARG:N	1:C:536:GLU:OE1	2.52	0.40
1:D:65:MET:O	1:D:69:ARG:HG2	2.21	0.40
1:D:247:ARG:HG3	1:D:260:GLN:HB2	2.03	0.40
1:K:175:VAL:HA	1:K:178:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:LYS:HA	1:K:192:LYS:HD3	1.74	0.40
1:F:306:LYS:O	1:F:310:LEU:HB2	2.21	0.40
1:L:491:LEU:HD22	1:L:499:ALA:HB1	2.03	0.40
1:E:72:HIS:CD2	1:B:285:THR:HA	2.57	0.40
1:E:207:VAL:HG23	1:E:218:GLN:HG3	2.02	0.40
1:E:548:PHE:CZ	1:E:566:ILE:HD13	2.55	0.40
1:A:492:TYR:HD1	1:B:297:ARG:HA	1.86	0.40
1:A:496:VAL:H	1:A:496:VAL:HG22	1.67	0.40
1:B:502:LYS:HB2	1:B:502:LYS:HE2	1.85	0.40
1:I:614:LYS:O	1:I:618:TYR:N	2.54	0.40
1:C:65:MET:O	1:C:69:ARG:HG2	2.21	0.40
1:D:487:ARG:HA	1:D:490:GLU:HB3	2.04	0.40
1:K:88:ARG:NE	1:G:285:THR:HG21	2.36	0.40
1:K:550:THR:OG1	1:K:551:PHE:N	2.55	0.40
1:F:192:LYS:HB2	1:F:195:GLU:HG3	2.03	0.40
1:F:490:GLU:HA	1:F:493:HIS:ND1	2.35	0.40
1:G:306:LYS:O	1:G:310:LEU:HB2	2.21	0.40
1:G:487:ARG:HA	1:G:490:GLU:HB3	2.03	0.40
1:E:95:LYS:HG2	1:E:602:PHE:HD2	1.86	0.40
1:A:247:ARG:HG3	1:A:260:GLN:HB2	2.02	0.40
1:A:502:LYS:HE2	1:A:502:LYS:HB2	1.85	0.40
1:H:192:LYS:HA	1:H:192:LYS:HD3	1.74	0.40
1:C:247:ARG:HG3	1:C:260:GLN:HB2	2.03	0.40
1:D:239:ARG:HA	1:D:239:ARG:HD3	1.90	0.40
1:G:174:TYR:OH	1:G:576:VAL:O	2.24	0.40
1:G:174:TYR:CZ	1:G:580:TYR:HB2	2.56	0.40
1:A:487:ARG:HA	1:A:490:GLU:HB3	2.04	0.40
1:H:159:ARG:HH22	1:C:582:CYS:HB3	1.86	0.40
1:H:175:VAL:HA	1:H:178:CYS:SG	2.61	0.40
1:H:631:ARG:HG2	1:H:635:ARG:HH12	1.85	0.40
1:B:192:LYS:HB2	1:B:195:GLU:HG3	2.03	0.40
1:B:487:ARG:HA	1:B:490:GLU:HB3	2.04	0.40
1:I:98:LEU:HD12	1:I:98:LEU:HA	1.80	0.40
1:C:574:GLU:H	1:C:574:GLU:HG3	1.77	0.40
1:J:165:TYR:HE2	1:J:235:LEU:HB3	1.86	0.40
1:J:174:TYR:CZ	1:J:580:TYR:HB2	2.56	0.40
1:J:548:PHE:CZ	1:J:566:ILE:HD13	2.56	0.40
1:K:239:ARG:HD3	1:K:239:ARG:HA	1.78	0.40
1:K:631:ARG:HG2	1:K:635:ARG:HH12	1.85	0.40
1:F:304:HIS:HD2	1:F:530:PRO:HG3	1.87	0.40
1:L:138:TYR:O	1:L:142:TRP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:301:LEU:HD21	1:L:535:LEU:HD11	2.04	0.40
1:L:614:LYS:O	1:L:618:TYR:N	2.54	0.40
1:G:247:ARG:HG3	1:G:260:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/697 (71%)	466 (95%)	25 (5%)	1 (0%)	47	81
1	B	492/697 (71%)	466 (95%)	25 (5%)	1 (0%)	47	81
1	C	492/697 (71%)	465 (94%)	26 (5%)	1 (0%)	47	81
1	D	492/697 (71%)	466 (95%)	25 (5%)	1 (0%)	47	81
1	E	491/697 (70%)	472 (96%)	18 (4%)	1 (0%)	47	81
1	F	492/697 (71%)	466 (95%)	25 (5%)	1 (0%)	47	81
1	G	492/697 (71%)	466 (95%)	25 (5%)	1 (0%)	47	81
1	H	491/697 (70%)	471 (96%)	19 (4%)	1 (0%)	47	81
1	I	491/697 (70%)	472 (96%)	18 (4%)	1 (0%)	47	81
1	J	491/697 (70%)	472 (96%)	18 (4%)	1 (0%)	47	81
1	K	491/697 (70%)	471 (96%)	19 (4%)	1 (0%)	47	81
1	L	491/697 (70%)	471 (96%)	19 (4%)	1 (0%)	47	81
All	All	5898/8364 (70%)	5624 (95%)	262 (4%)	12 (0%)	50	81

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PHE

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Mol	Chain	Res	Type
1	B	125	PHE
1	C	125	PHE
1	D	125	PHE
1	F	125	PHE
1	G	125	PHE
1	E	125	PHE
1	H	125	PHE
1	I	125	PHE
1	J	125	PHE
1	K	125	PHE
1	L	125	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	358/589 (61%)	352 (98%)	6 (2%)	60	78
1	B	358/589 (61%)	353 (99%)	5 (1%)	67	80
1	C	358/589 (61%)	351 (98%)	7 (2%)	55	74
1	D	358/589 (61%)	353 (99%)	5 (1%)	67	80
1	E	358/589 (61%)	352 (98%)	6 (2%)	60	78
1	F	358/589 (61%)	353 (99%)	5 (1%)	67	80
1	G	358/589 (61%)	351 (98%)	7 (2%)	55	74
1	H	358/589 (61%)	348 (97%)	10 (3%)	43	65
1	I	358/589 (61%)	348 (97%)	10 (3%)	43	65
1	J	358/589 (61%)	352 (98%)	6 (2%)	60	78
1	K	358/589 (61%)	348 (97%)	10 (3%)	43	65
1	L	358/589 (61%)	349 (98%)	9 (2%)	47	68
All	All	4296/7068 (61%)	4210 (98%)	86 (2%)	57	74

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	87	LEU
1	E	119	LYS
1	E	138	TYR
1	E	494	LEU
1	E	504	ARG
1	E	538	PHE
1	A	88	ARG
1	A	141	VAL
1	A	269	TYR
1	A	283	LEU
1	A	487	ARG
1	A	497	LEU
1	H	87	LEU
1	H	119	LYS
1	H	138	TYR
1	H	288	VAL
1	H	301	LEU
1	H	310	LEU
1	H	494	LEU
1	H	497	LEU
1	H	504	ARG
1	H	538	PHE
1	B	88	ARG
1	B	141	VAL
1	B	269	TYR
1	B	487	ARG
1	B	497	LEU
1	I	87	LEU
1	I	119	LYS
1	I	138	TYR
1	I	299	ASP
1	I	301	LEU
1	I	494	LEU
1	I	497	LEU
1	I	504	ARG
1	I	538	PHE
1	I	556	LEU
1	C	88	ARG
1	C	141	VAL
1	C	183	LEU
1	C	269	TYR
1	C	487	ARG
1	C	497	LEU

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Mol	Chain	Res	Type
1	C	529	VAL
1	J	87	LEU
1	J	119	LYS
1	J	138	TYR
1	J	494	LEU
1	J	504	ARG
1	J	538	PHE
1	D	88	ARG
1	D	141	VAL
1	D	269	TYR
1	D	487	ARG
1	D	497	LEU
1	K	87	LEU
1	K	119	LYS
1	K	138	TYR
1	K	288	VAL
1	K	301	LEU
1	K	310	LEU
1	K	494	LEU
1	K	497	LEU
1	K	504	ARG
1	K	538	PHE
1	F	88	ARG
1	F	141	VAL
1	F	269	TYR
1	F	487	ARG
1	F	497	LEU
1	L	87	LEU
1	L	119	LYS
1	L	138	TYR
1	L	301	LEU
1	L	494	LEU
1	L	497	LEU
1	L	504	ARG
1	L	538	PHE
1	L	556	LEU
1	G	88	ARG
1	G	141	VAL
1	G	183	LEU
1	G	269	TYR
1	G	487	ARG
1	G	497	LEU

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Mol	Chain	Res	Type
1	G	529	VAL

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

Mol	Chain	Res	Type
1	E	304	HIS
1	A	72	HIS
1	A	85	GLN
1	A	304	HIS
1	A	309	GLN
1	A	527	GLN
1	H	260	GLN
1	H	304	HIS
1	B	63	GLN
1	B	72	HIS
1	B	85	GLN
1	B	292	HIS
1	B	304	HIS
1	B	309	GLN
1	I	260	GLN
1	I	304	HIS
1	I	632	GLN
1	C	63	GLN
1	C	72	HIS
1	C	85	GLN
1	C	292	HIS
1	C	304	HIS
1	C	309	GLN
1	J	304	HIS
1	J	632	GLN
1	D	72	HIS
1	D	85	GLN
1	D	304	HIS
1	D	309	GLN
1	D	527	GLN
1	K	121	HIS
1	K	260	GLN
1	K	304	HIS
1	K	632	GLN
1	F	63	GLN
1	F	72	HIS
1	F	85	GLN

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Mol	Chain	Res	Type
1	F	292	HIS
1	F	304	HIS
1	F	309	GLN
1	L	260	GLN
1	L	304	HIS
1	L	632	GLN
1	G	63	GLN
1	G	72	HIS
1	G	85	GLN
1	G	292	HIS
1	G	304	HIS
1	G	309	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

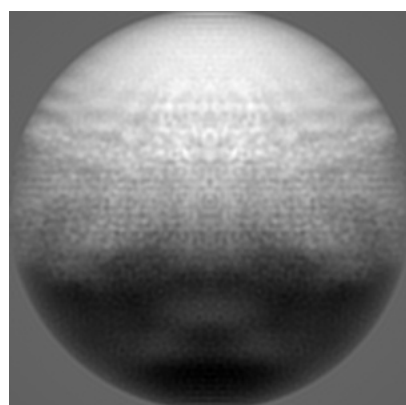
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31299. These allow visual inspection of the internal detail of the map and identification of artifacts.

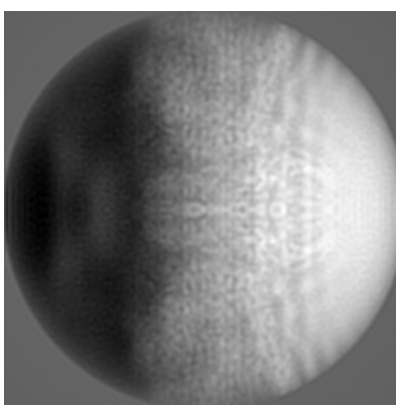
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

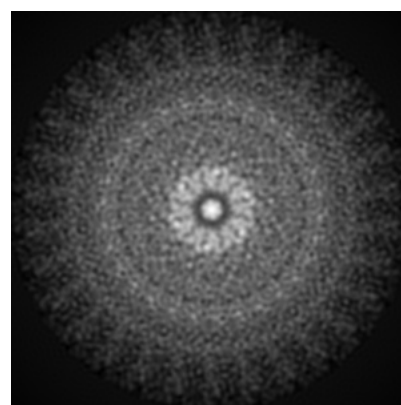
6.1.1 Primary map



X



Y

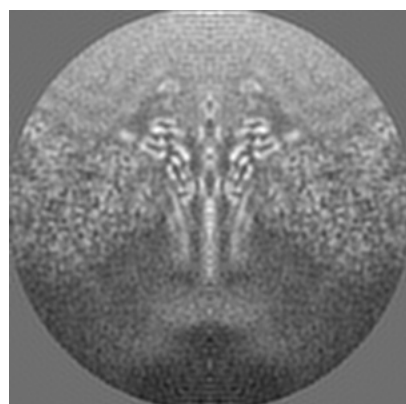


Z

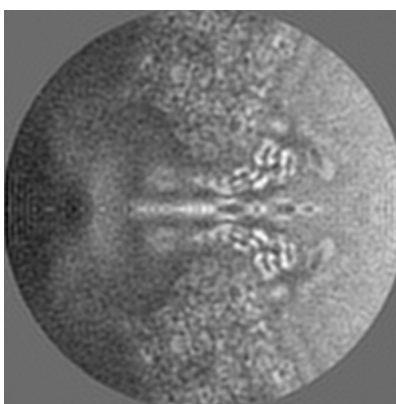
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

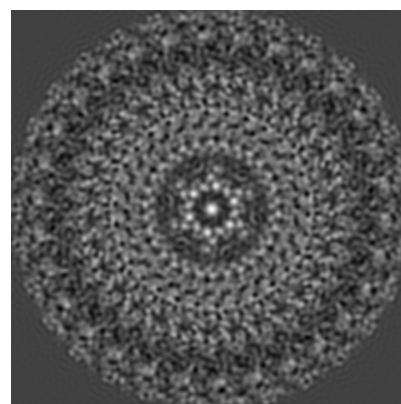
6.2.1 Primary map



X Index: 120



Y Index: 120

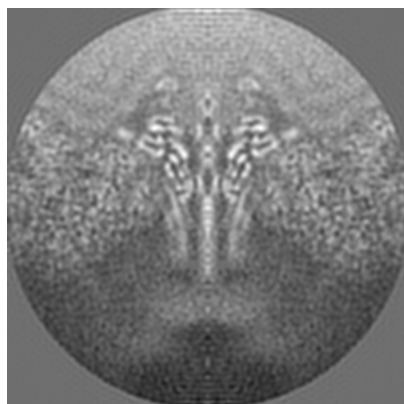


Z Index: 120

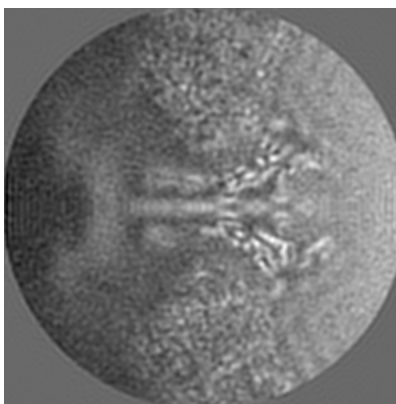
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

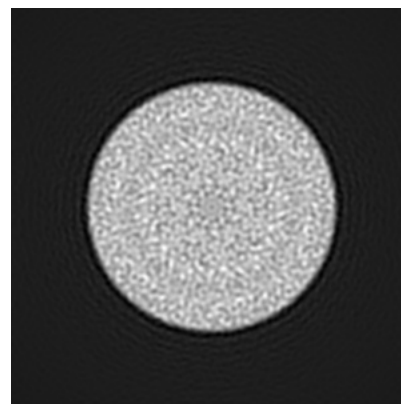
6.3.1 Primary map



X Index: 120



Y Index: 122



Z Index: 216

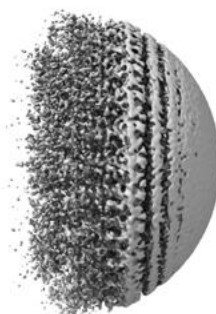
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

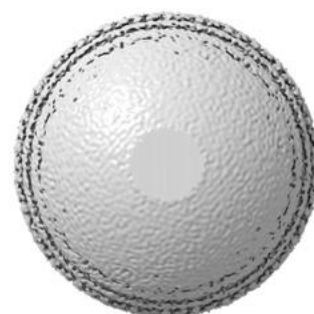
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

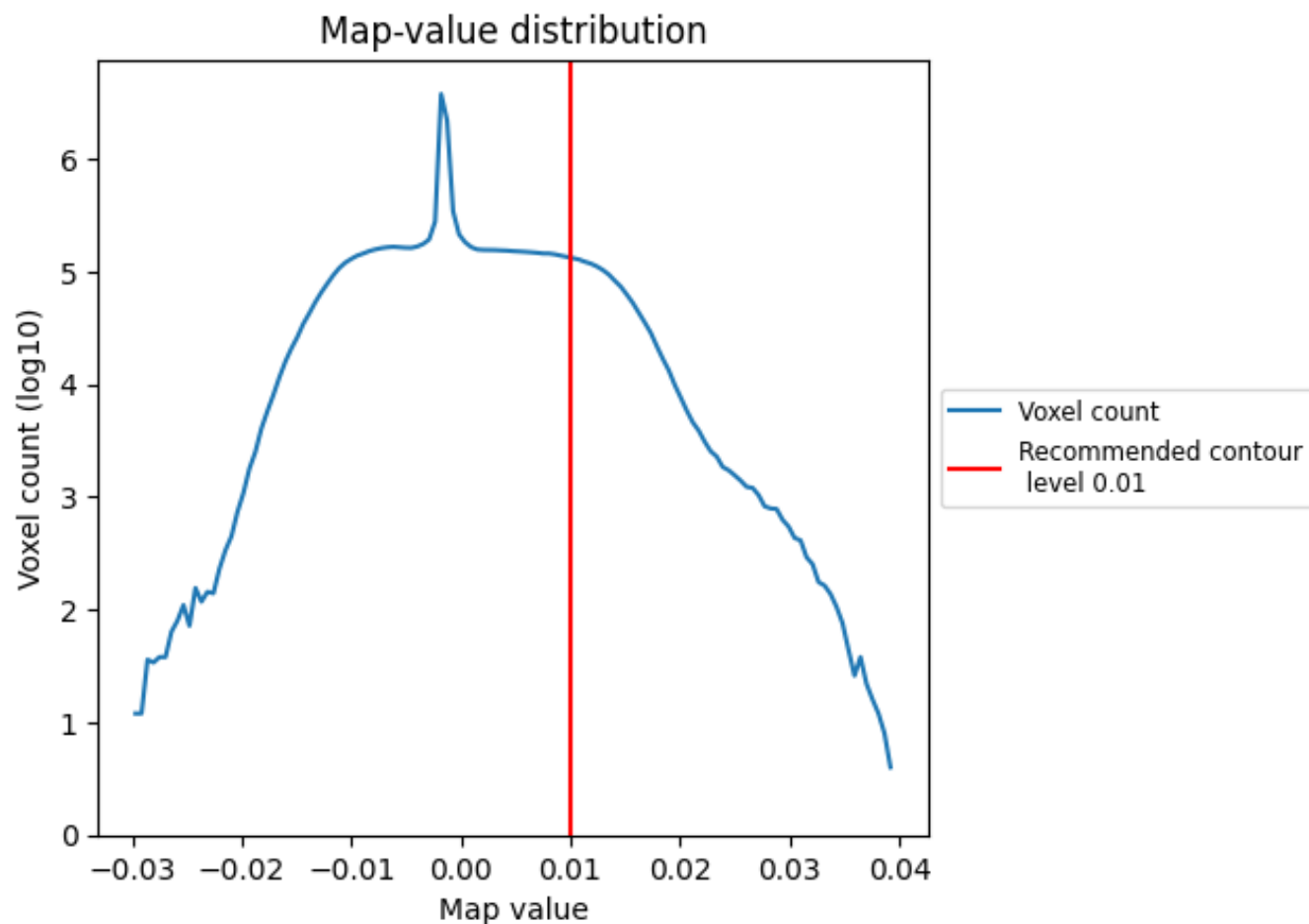
6.5 Mask visualisation

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

7 Map analysis [i](#)

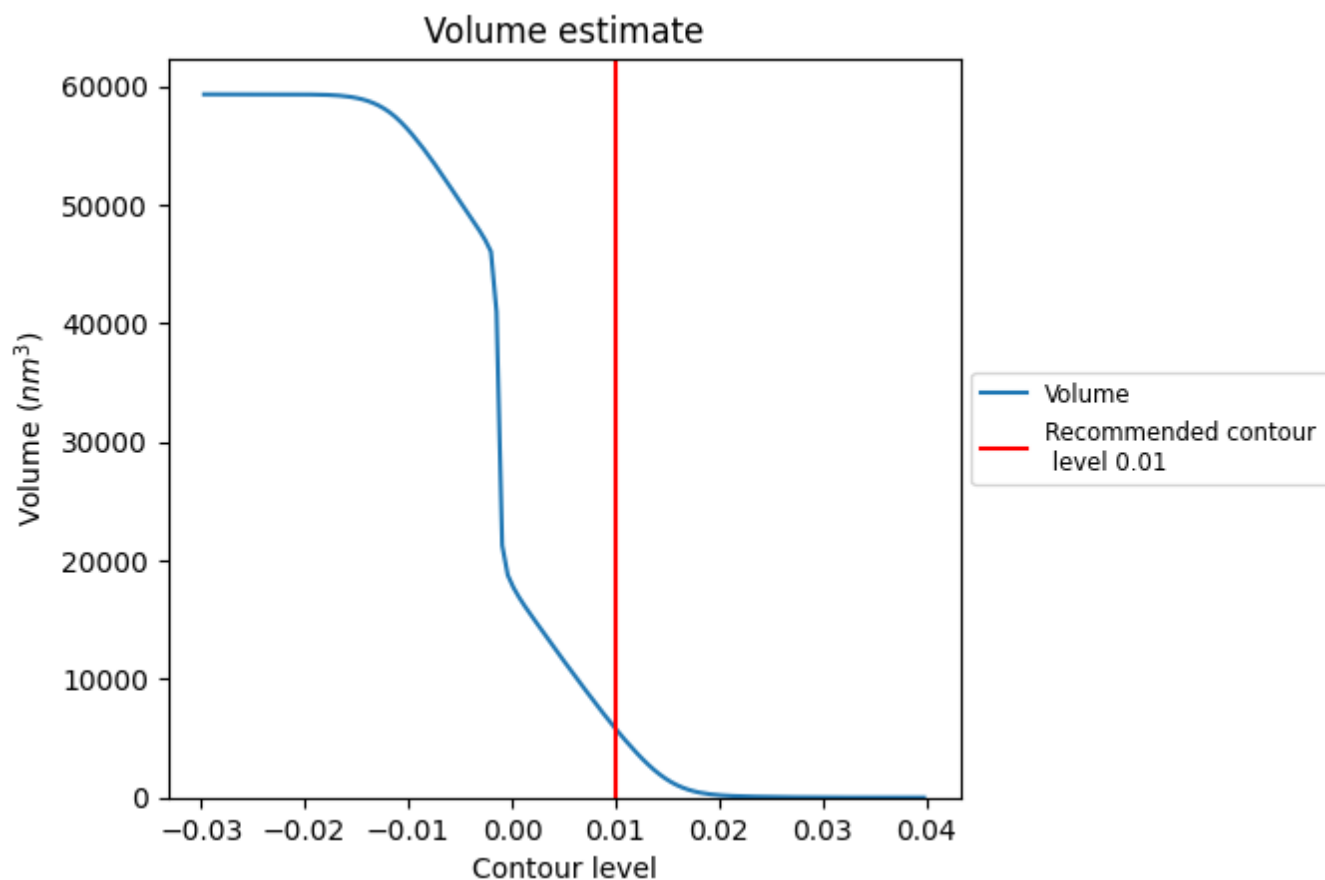
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

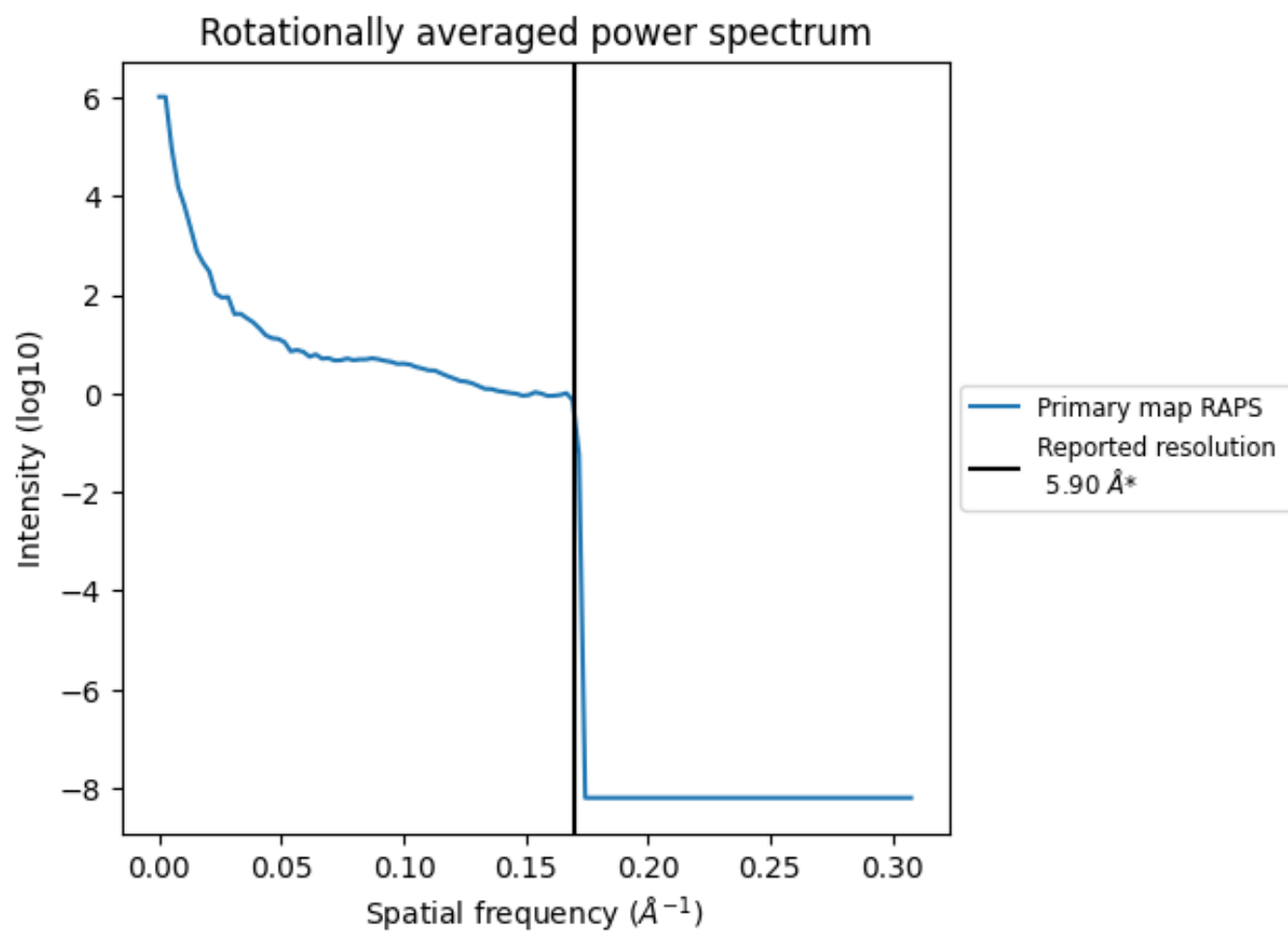
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5826 nm³; this corresponds to an approximate mass of 5263 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

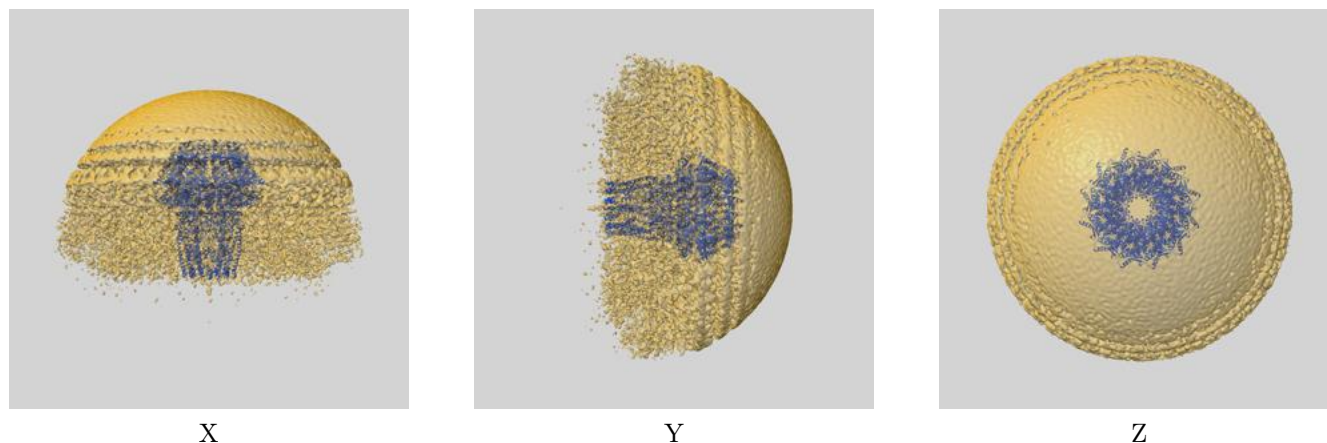
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

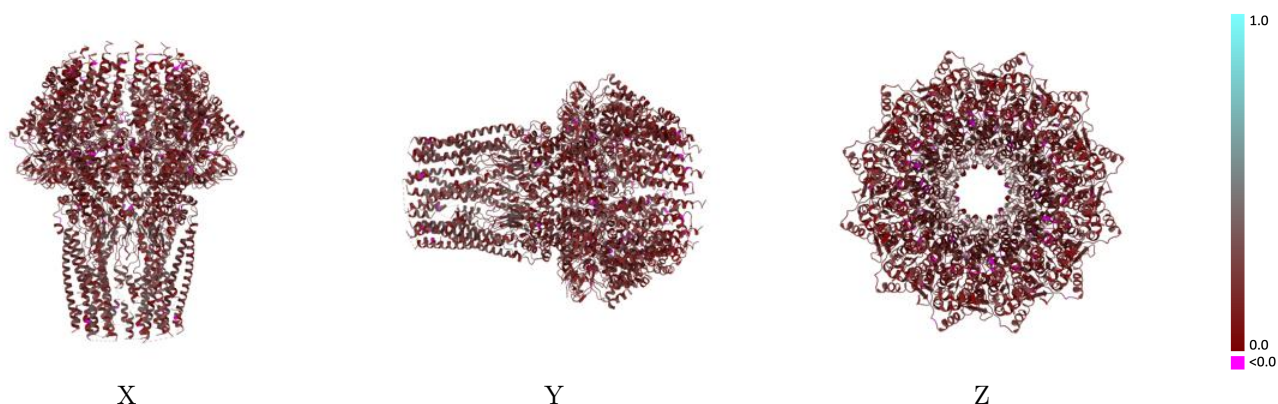
This section contains information regarding the fit between EMDB map EMD-31299 and PDB model 7ETM. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



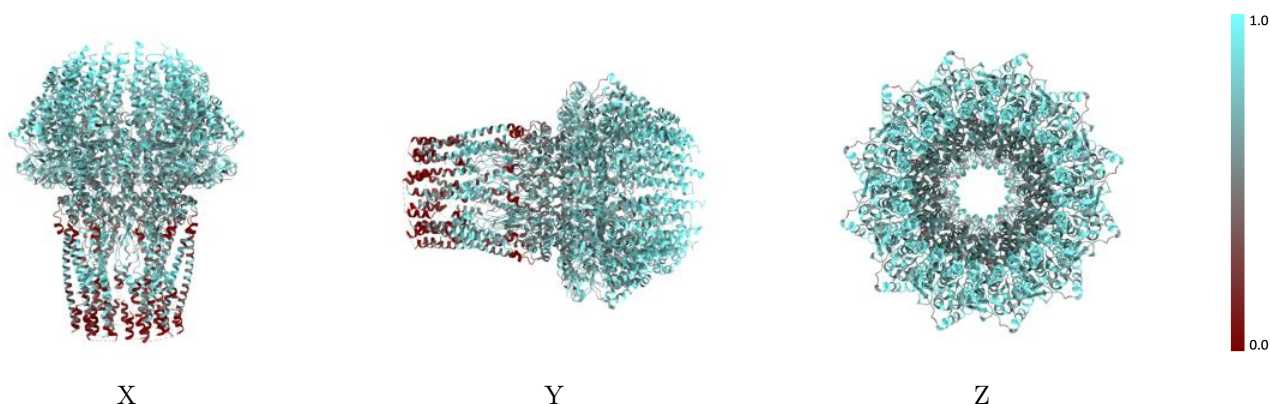
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



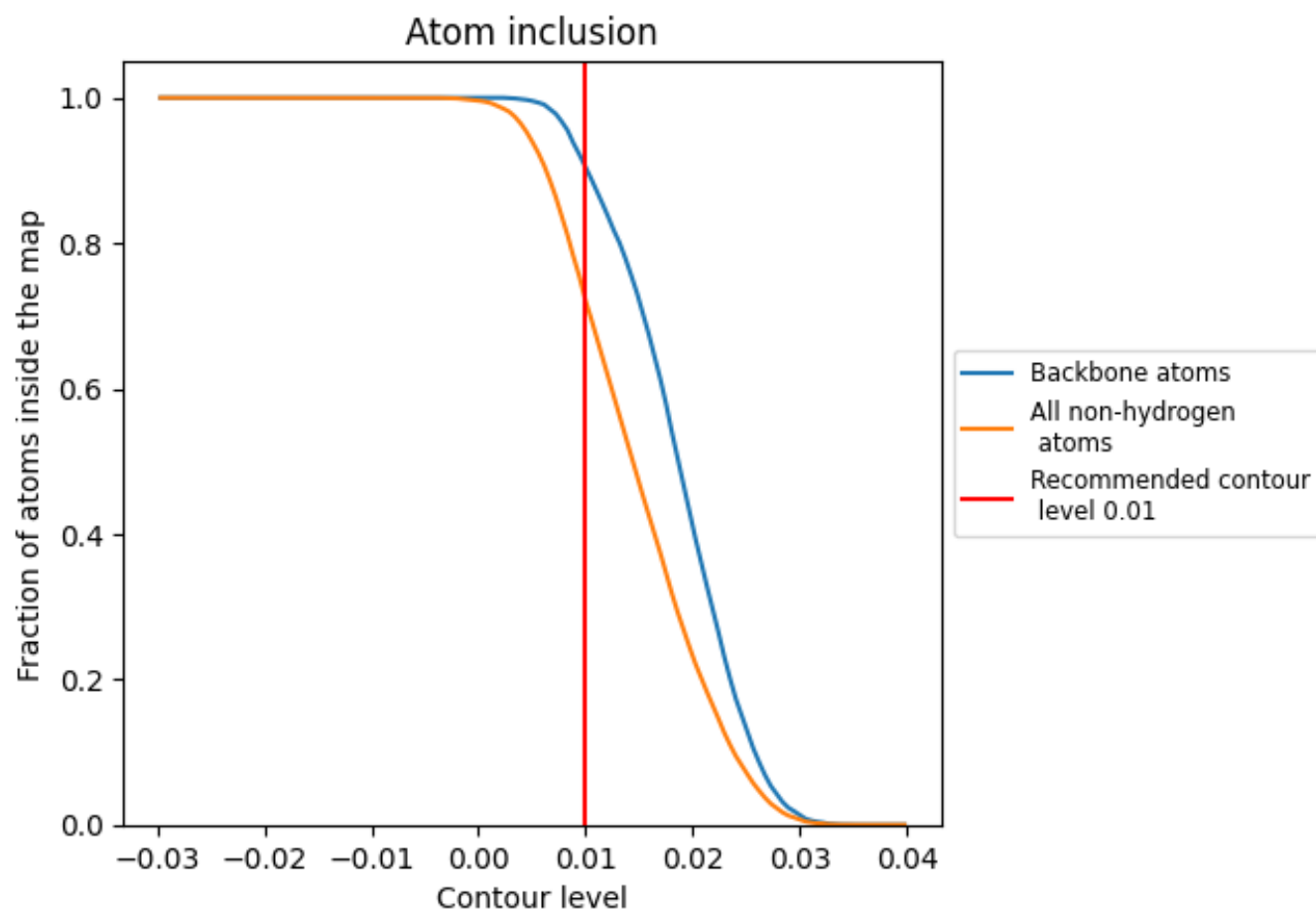
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 72% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7204	<div></div> 0.1860
A	<div></div> 0.7158	<div></div> 0.1860
B	<div></div> 0.7198	<div></div> 0.1870
C	<div></div> 0.7158	<div></div> 0.1880
D	<div></div> 0.7163	<div></div> 0.1860
E	<div></div> 0.7244	<div></div> 0.1870
F	<div></div> 0.7198	<div></div> 0.1850
G	<div></div> 0.7158	<div></div> 0.1860
H	<div></div> 0.7244	<div></div> 0.1870
I	<div></div> 0.7225	<div></div> 0.1870
J	<div></div> 0.7241	<div></div> 0.1860
K	<div></div> 0.7244	<div></div> 0.1850
L	<div></div> 0.7222	<div></div> 0.1870

1.0

0.0

<0.0