



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:36 AM UTC

PDB ID : 7E8S / pdb_00007e8s
EMDB ID : EMD-31021
Title : Intact TRAPP2 (state I).
Authors : Mi, C.C.; Sui, S.F.
Deposited on : 2021-03-02
Resolution : 4.36 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

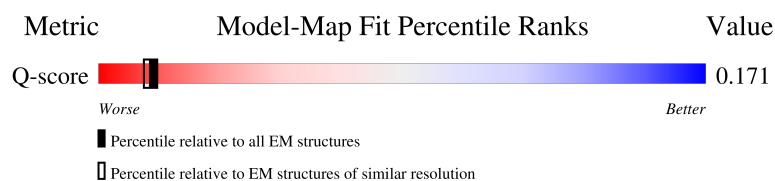
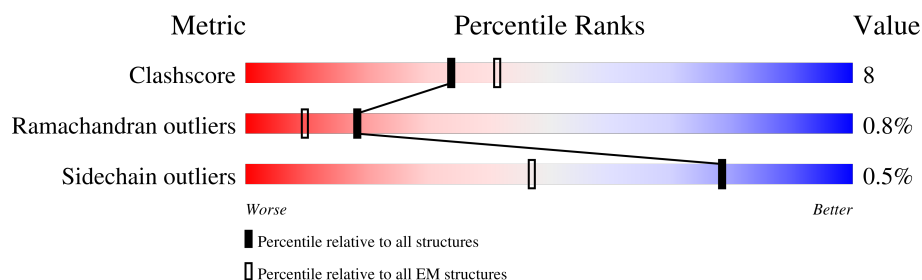
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.36 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3737 (3.87 - 4.86)

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	152	46% 82% 13% 5%
1	L	152	45% 82% 12% • 5%
2	B	268	25% 61% 13% • 25%
2	M	268	24% 60% 14% • 25%

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Mol	Chain	Length	Quality of chain
3	C	193	
3	F	193	
3	N	193	
3	Q	193	
4	D	159	
4	O	159	
5	E	219	
5	P	219	
6	G	283	
6	R	283	
7	H	175	
7	S	175	
8	I	1102	
8	T	1102	
9	J	1289	
9	U	1289	
10	K	560	
10	V	560	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 46554 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 TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	144	Total	C	N	O	S	0	0
			1160	753	182	221	4		
1	L	144	Total	C	N	O	S	0	0
			1160	753	182	221	4		

- Molecule 2 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	202	Total	C	N	O	S	0	0
			1630	1051	274	297	8		
2	M	202	Total	C	N	O	S	0	0
			1630	1051	274	297	8		

- Molecule 3 is a protein called Trafficking protein particle complex subunit BET3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	184	Total	C	N	O	S	0	0
			1482	947	244	280	11		
3	F	182	Total	C	N	O	S	0	0
			1470	939	242	278	11		
3	N	184	Total	C	N	O	S	0	0
			1482	947	244	280	11		
3	Q	182	Total	C	N	O	S	0	0
			1470	939	242	278	11		

- Molecule 4 is a protein called Trafficking protein particle complex subunit BET5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	151	Total	C	N	O	S	0	0
			1235	793	209	227	6		
4	O	151	Total	C	N	O	S	0	0
			1235	793	209	227	6		

- Molecule 5 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	161	Total	C	N	O	S	0	0
			1300	840	207	243	10		
5	P	161	Total	C	N	O	S	0	0
			1300	840	207	243	10		

- Molecule 6 is a protein called Trafficking protein particle complex subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	204	Total	C	N	O	S	0	0
			1646	1050	285	302	9		
6	R	204	Total	C	N	O	S	0	0
			1646	1050	285	302	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	108	SER	VAL	conflict	UNP Q03337
R	108	SER	VAL	conflict	UNP Q03337

- Molecule 7 is a protein called Trafficking protein particle complex subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	147	Total	C	N	O	S	0	0
			1180	763	195	217	5		
7	S	147	Total	C	N	O	S	0	0
			1180	763	195	217	5		

- Molecule 8 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	788	Total	C	N	O	S	0	0
			4199	2553	811	833	2		
8	T	788	Total	C	N	O	S	0	0
			4199	2553	811	833	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	464	LYS	TRP	conflict	UNP Q03660
T	464	LYS	TRP	conflict	UNP Q03660

- Molecule 9 is a protein called Trafficking protein particle complex II-specific subunit 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	872	Total	C	N	O	S	0	0
			6326	4028	1094	1185	19		
9	U	872	Total	C	N	O	S	0	0
			6326	4028	1094	1185	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1099	PHE	TYR	conflict	UNP Q04183
U	1099	PHE	TYR	conflict	UNP Q04183

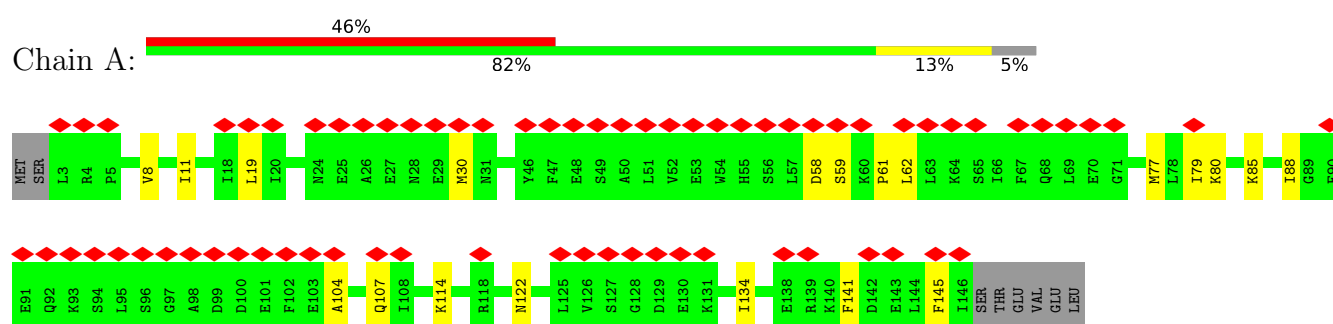
- Molecule 10 is a protein called Trafficking protein particle complex II-specific subunit 65.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	251	Total	C	N	O	S	0	0
			1649	1041	291	315	2		
10	V	251	Total	C	N	O	S	0	0
			1649	1041	291	315	2		

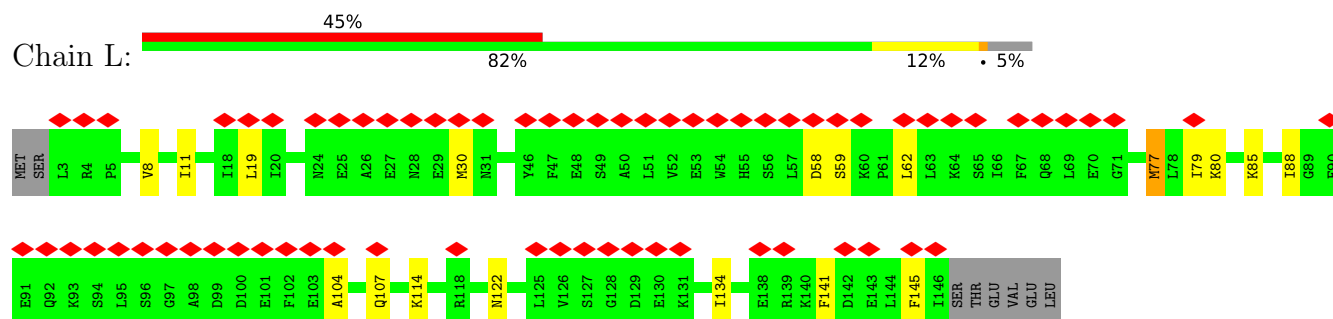
3 Residue-property plots

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: TRAPP-associated protein TCA17

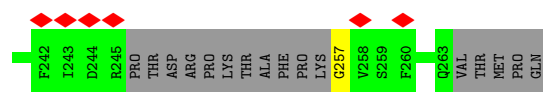


- Molecule 1: TRAPP-associated protein TCA17

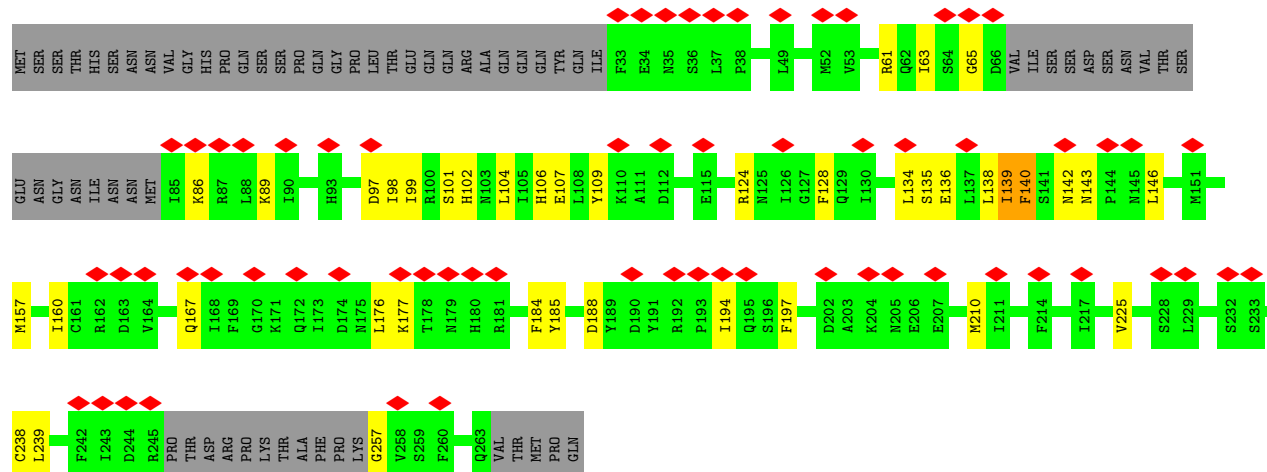


- Molecule 2: Trafficking protein particle complex subunit 33

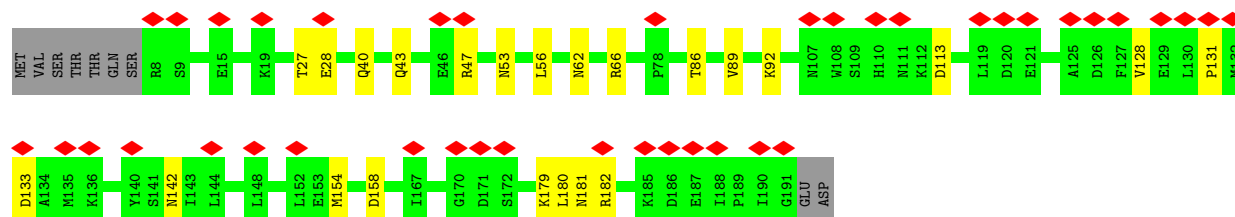
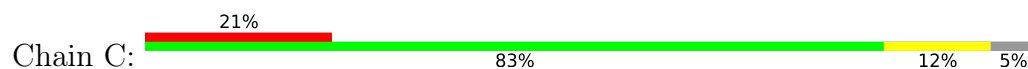




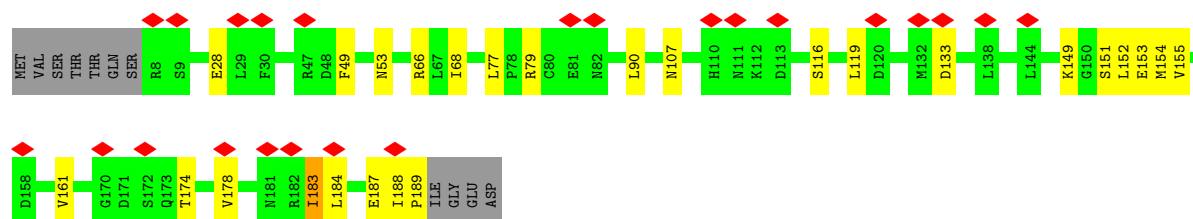
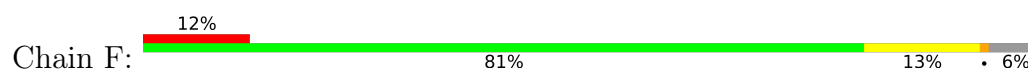
- Molecule 2: Trafficking protein particle complex subunit 33



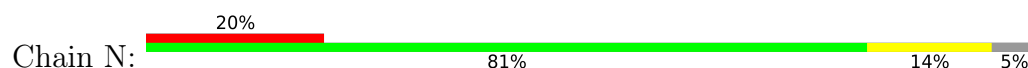
- Molecule 3: Trafficking protein particle complex subunit BET3

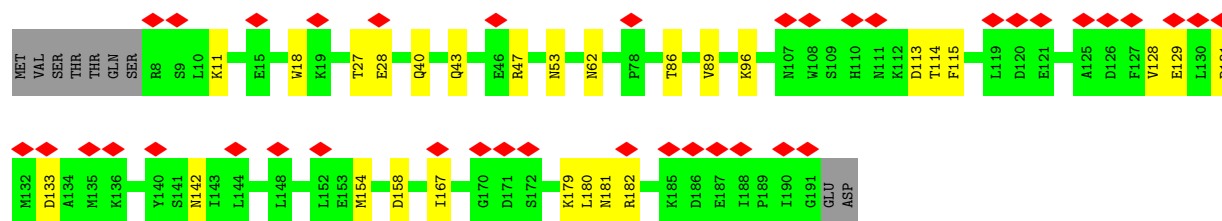


- Molecule 3: Trafficking protein particle complex subunit BET3

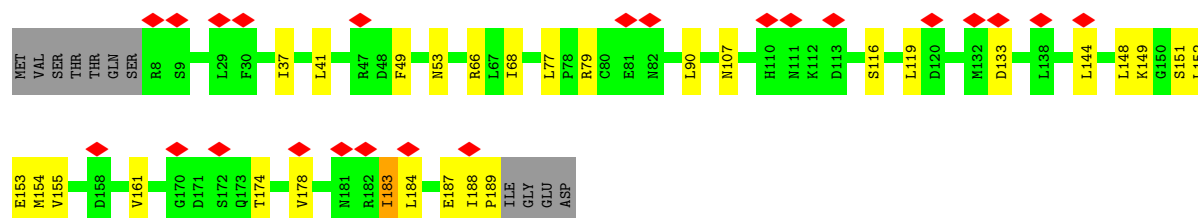
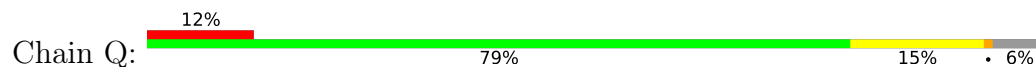


- Molecule 3: Trafficking protein particle complex subunit BET3

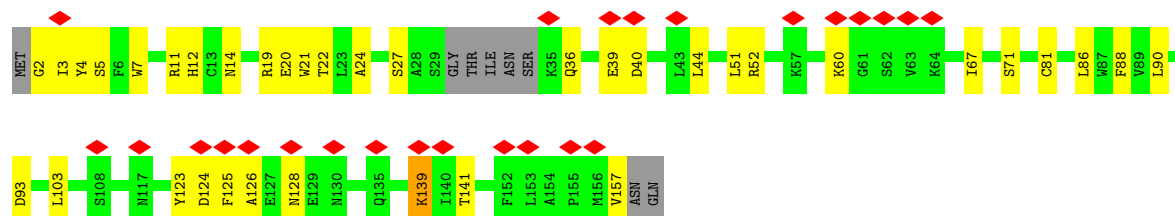




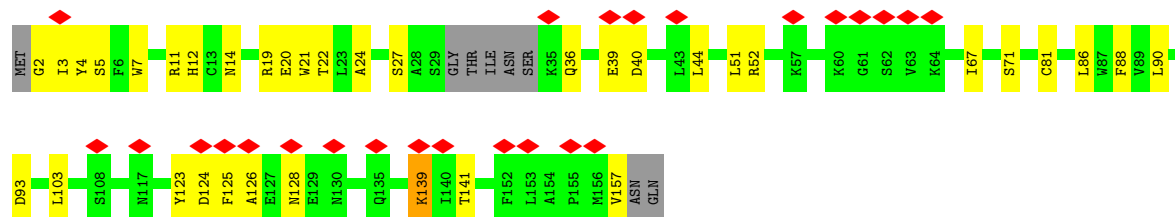
• Molecule 3: Trafficking protein particle complex subunit BET3



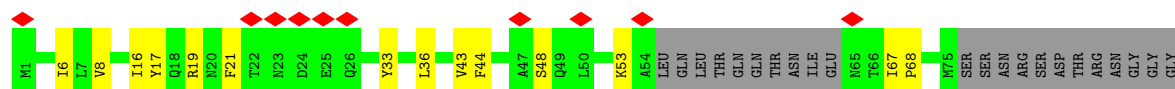
• Molecule 4: Trafficking protein particle complex subunit BET5

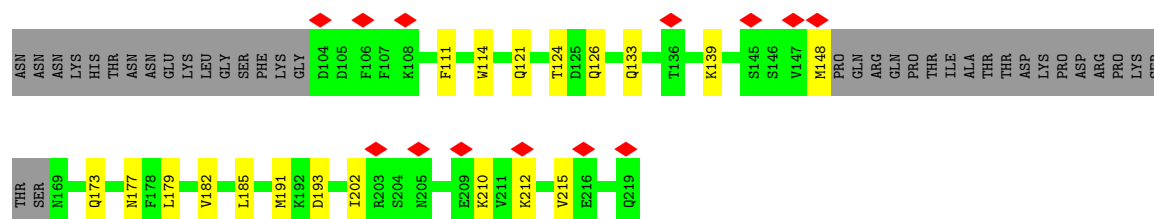


• Molecule 4: Trafficking protein particle complex subunit BET5

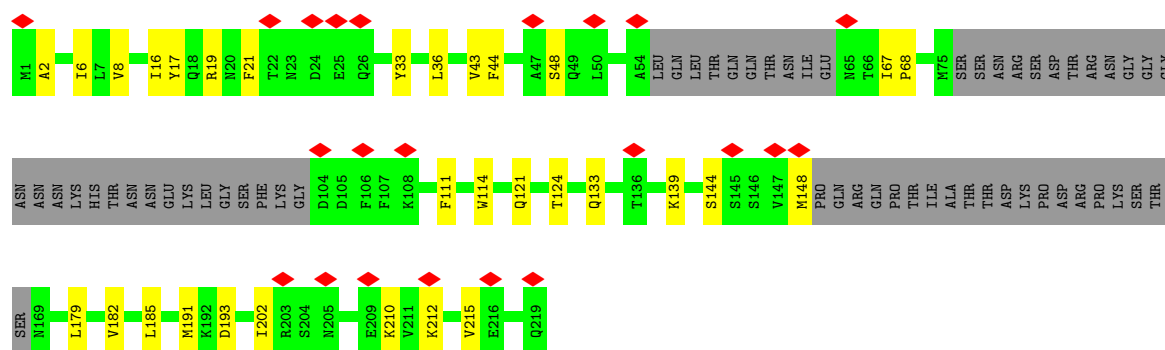


• Molecule 5: Trafficking protein particle complex subunit 23

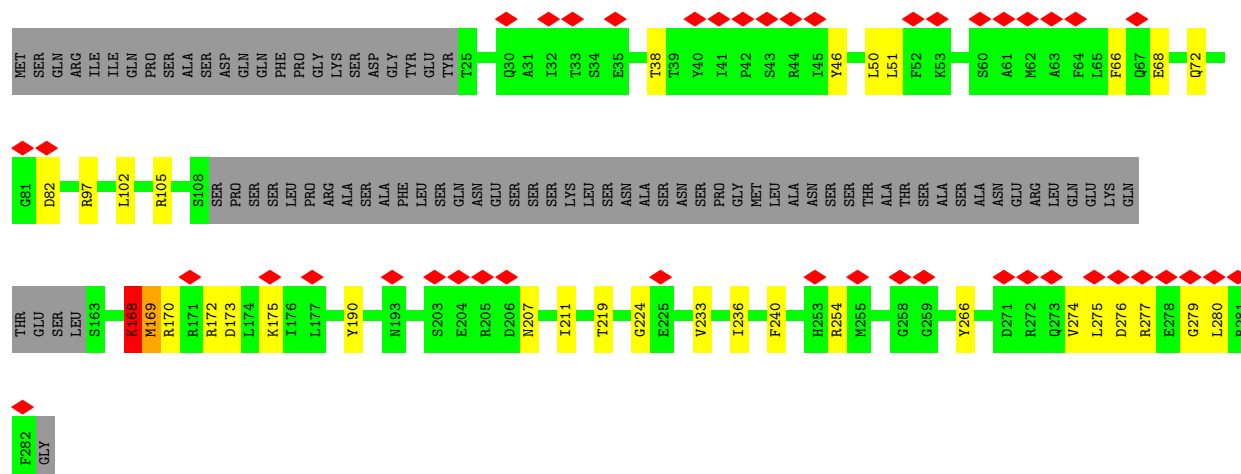




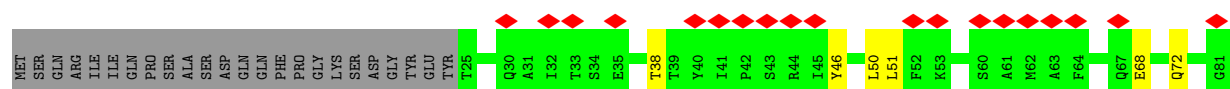
• Molecule 5: Trafficking protein particle complex subunit 23

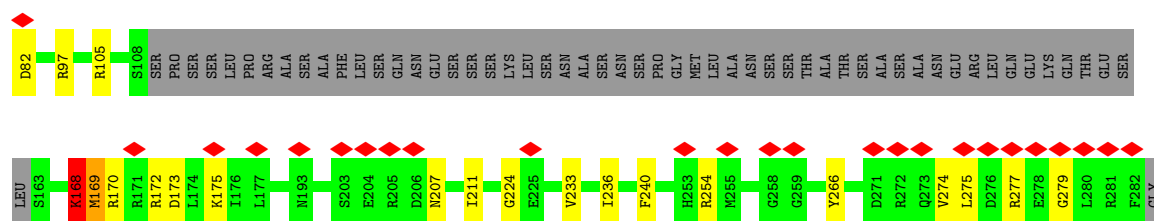


• Molecule 6: Trafficking protein particle complex subunit 31

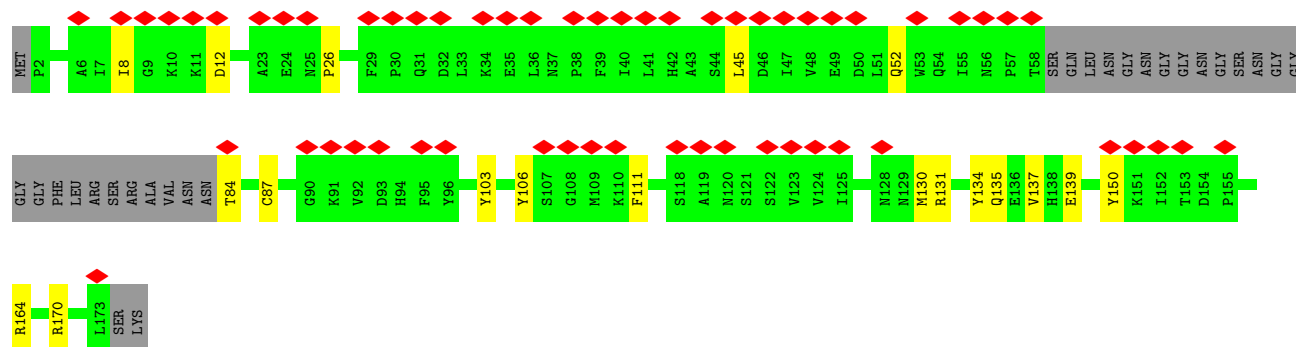
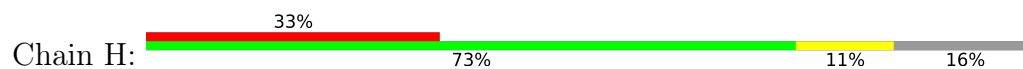


• Molecule 6: Trafficking protein particle complex subunit 31

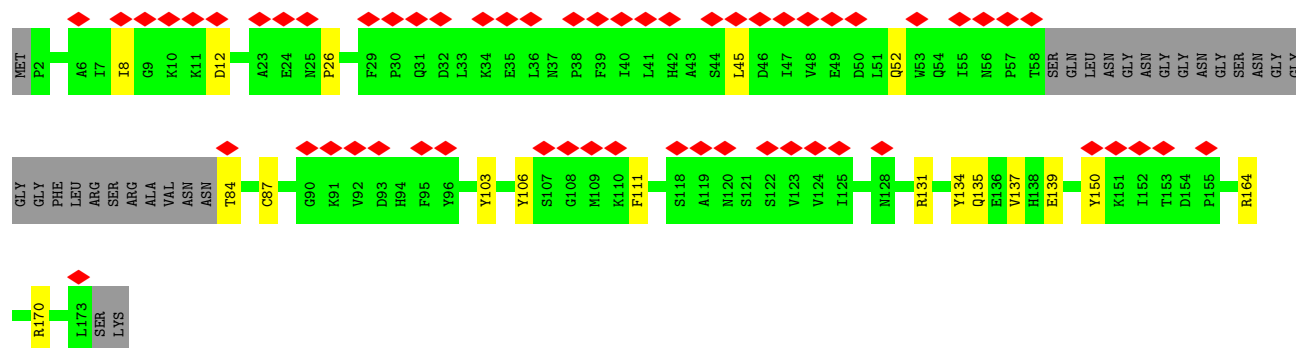
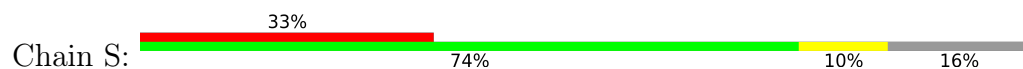




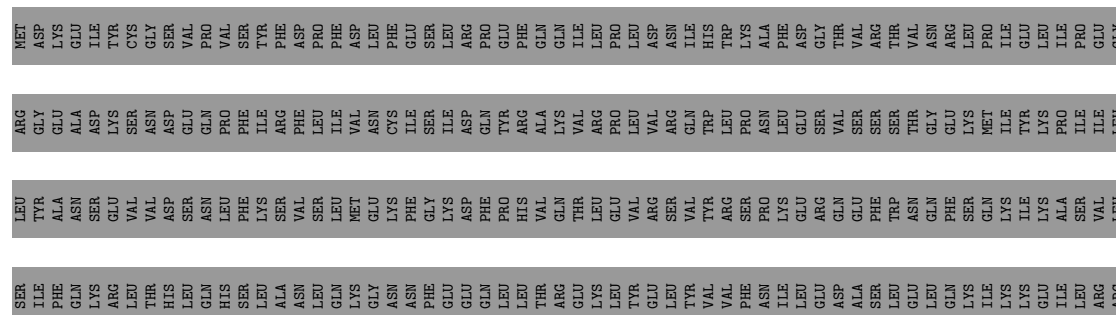
• Molecule 7: Trafficking protein particle complex subunit 20

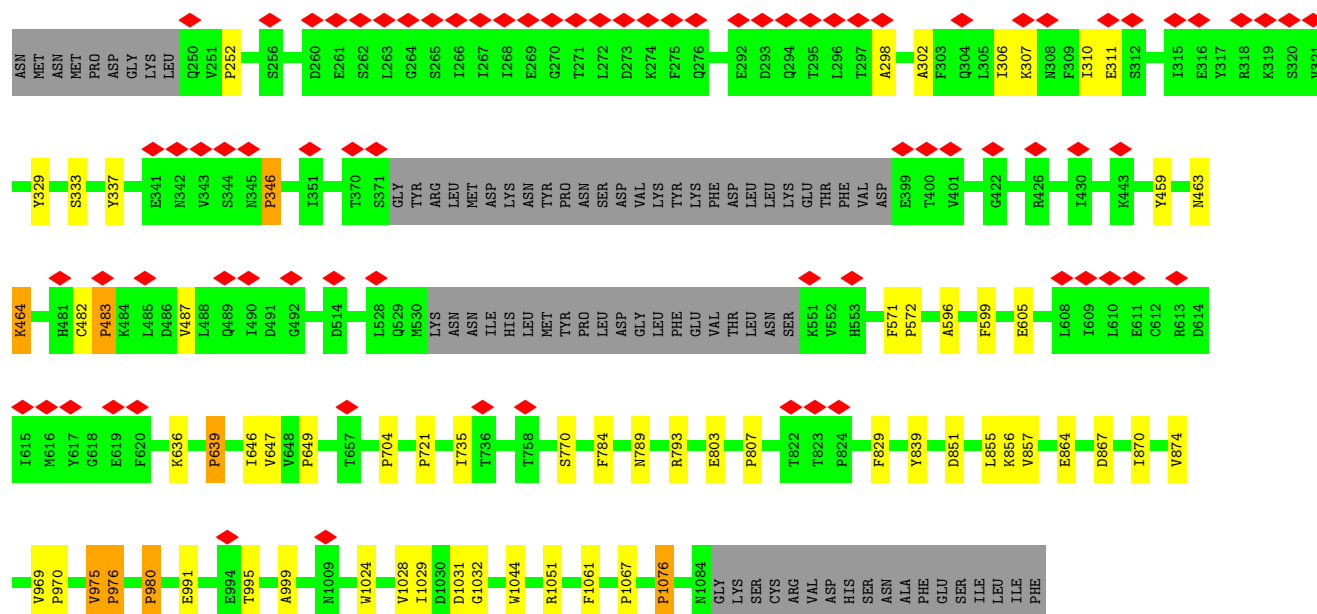


• Molecule 7: Trafficking protein particle complex subunit 20

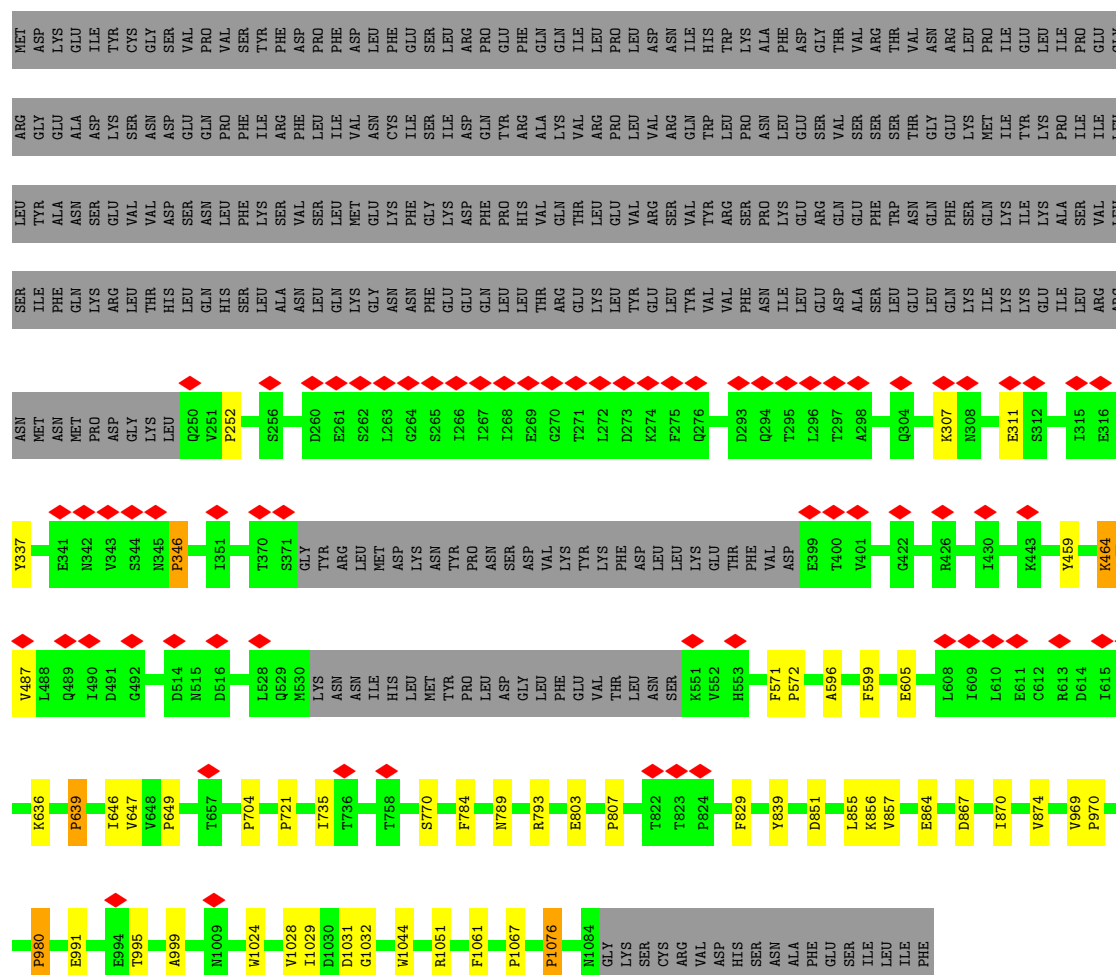


• Molecule 8: Trafficking protein particle complex II-specific subunit 130

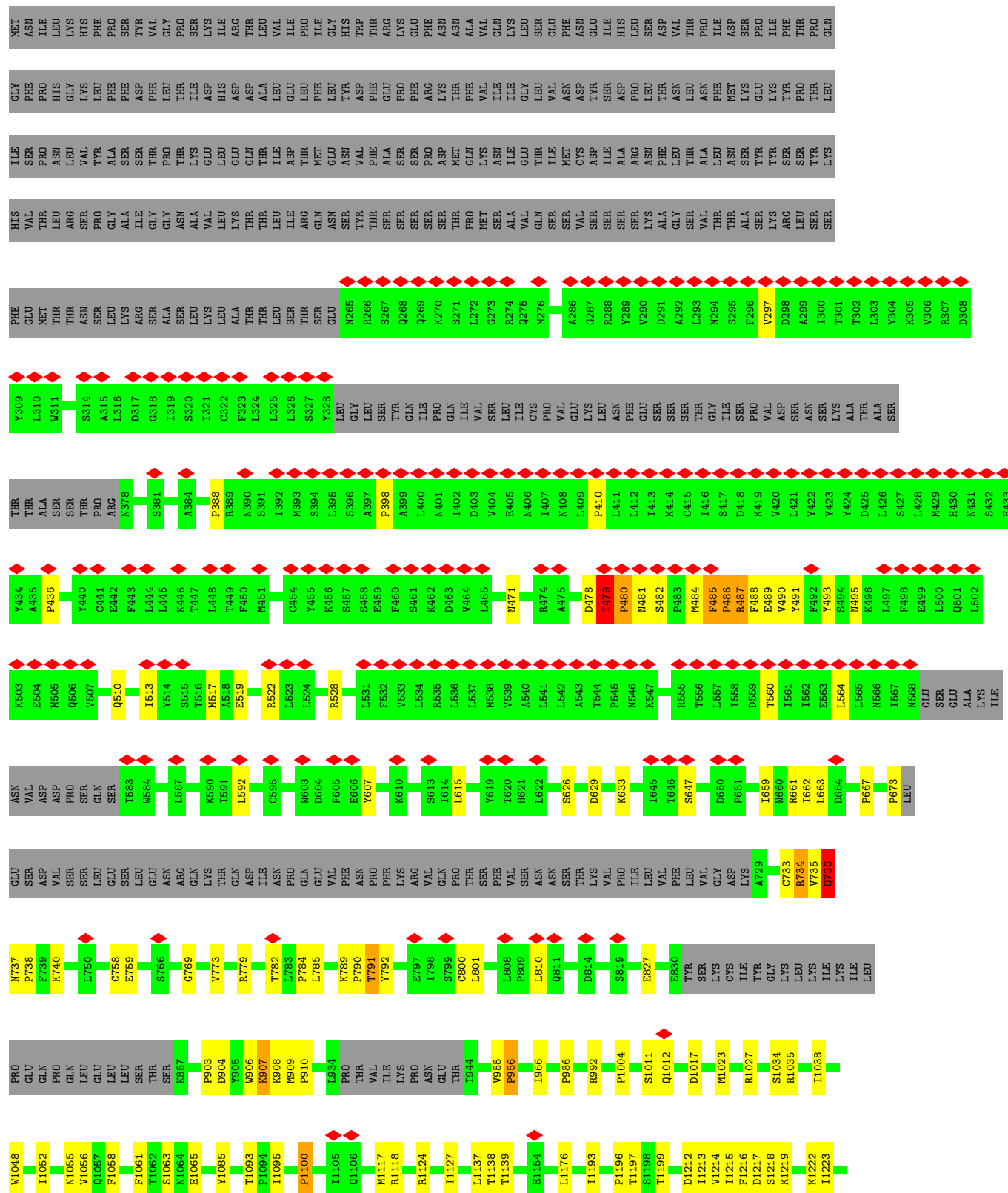


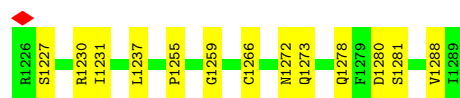


• Molecule 8: Trafficking protein particle complex II-specific subunit 130

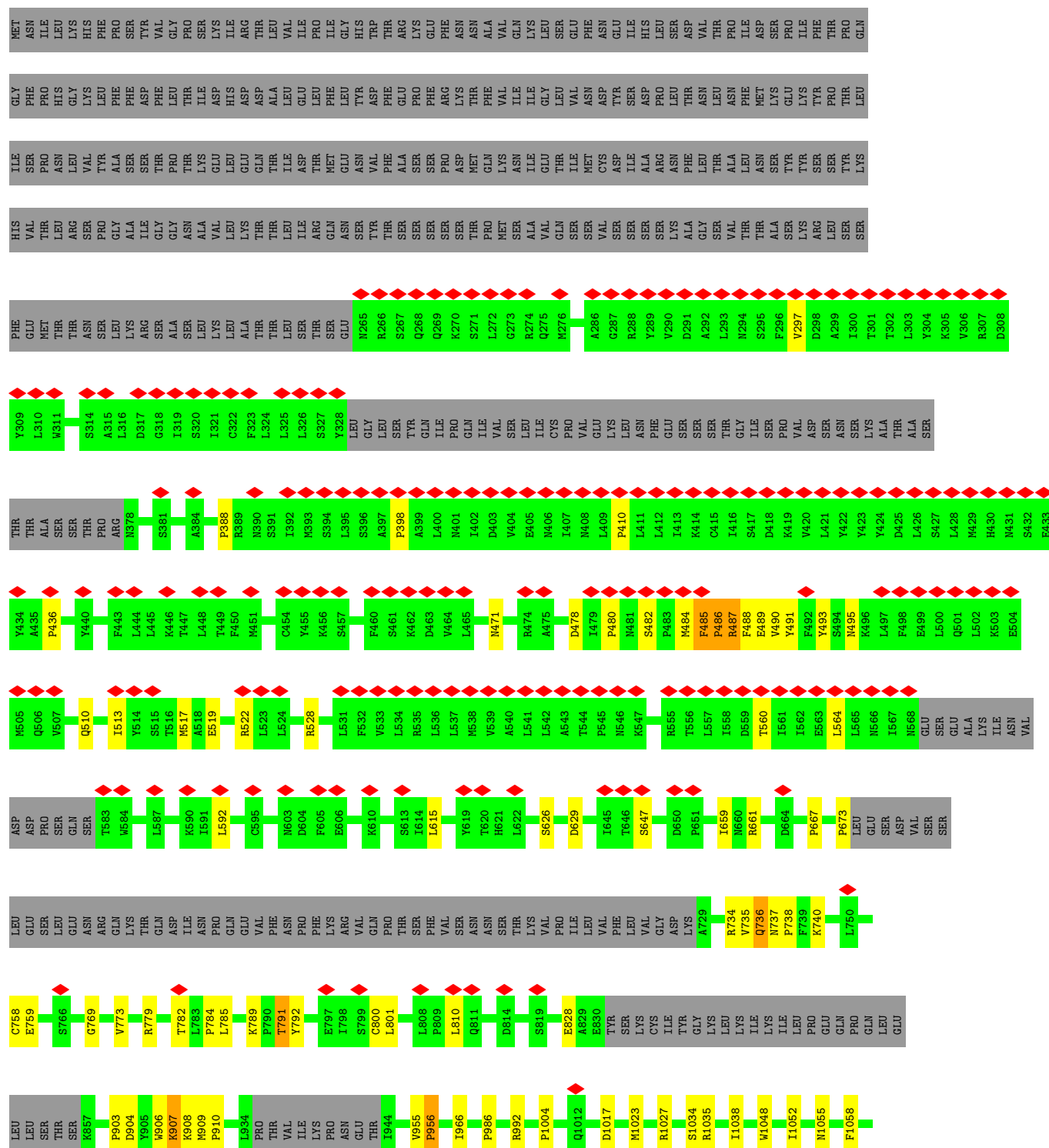


● Molecule 9: Trafficking protein particle complex II-specific subunit 120

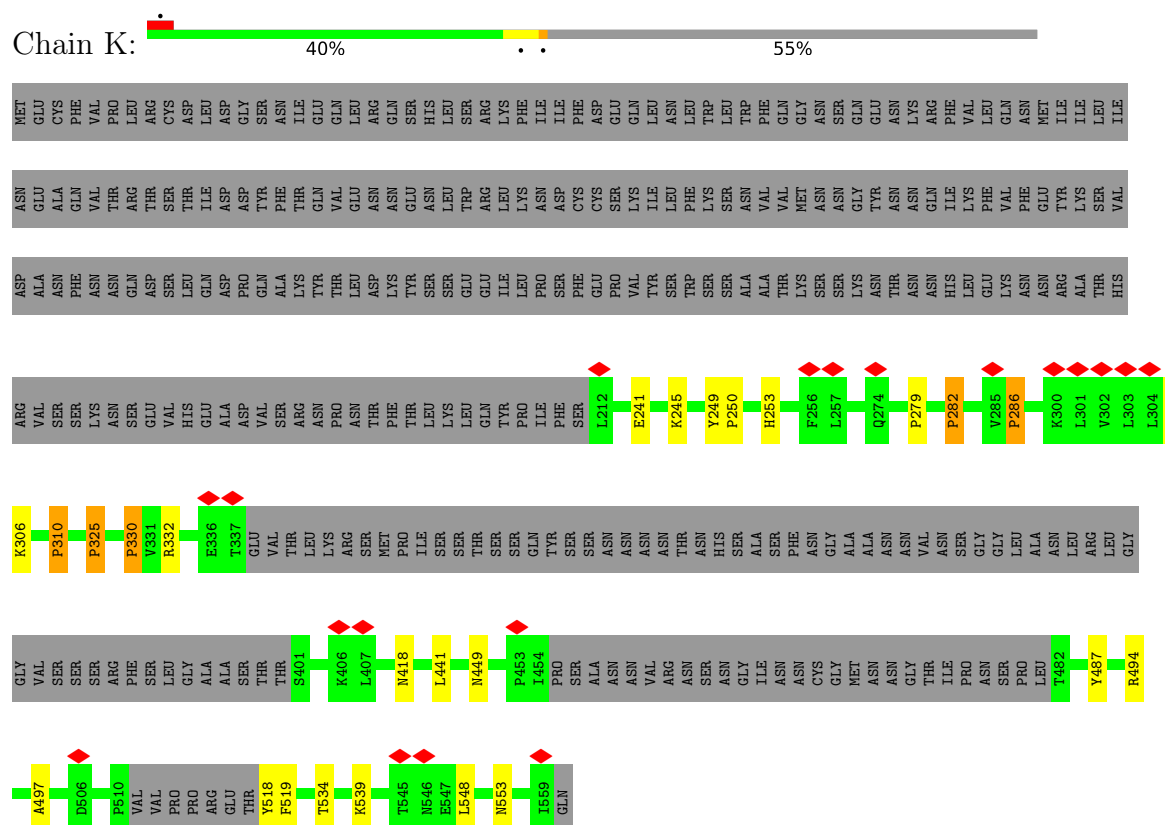




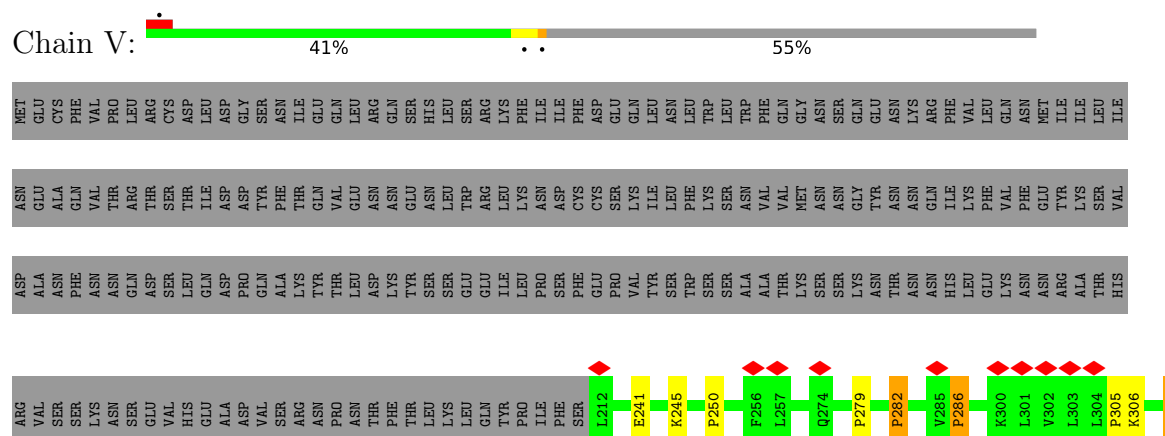
● Molecule 9: Trafficking protein particle complex II-specific subunit 120

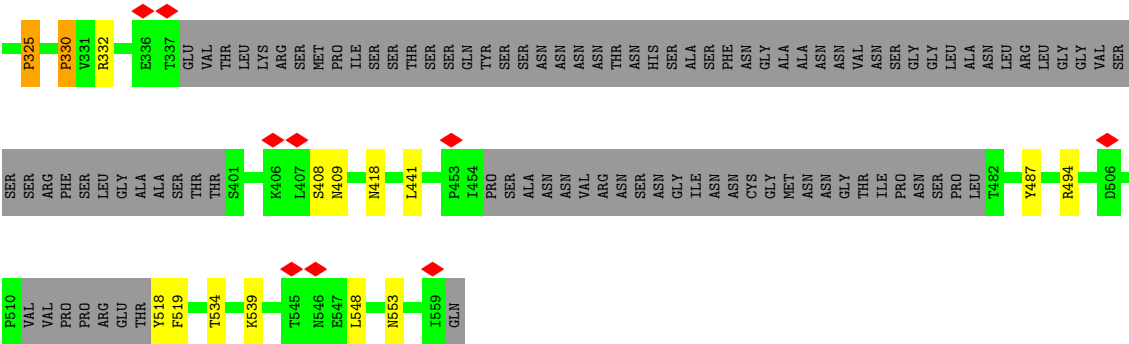


- Molecule 10: Trafficking protein particle complex II-specific subunit 65



- Molecule 10: Trafficking protein particle complex II-specific subunit 65





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36751	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.039	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	523.68, 523.68, 523.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	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	A	0.31	0/1180	0.73	0/1592
1	L	0.31	0/1180	0.73	0/1592
2	B	0.40	0/1658	0.84	0/2229
2	M	0.40	0/1658	0.84	0/2229
3	C	0.42	0/1509	0.90	2/2040 (0.1%)
3	F	0.37	0/1497	0.85	3/2024 (0.1%)
3	N	0.42	0/1509	0.90	4/2040 (0.2%)
3	Q	0.37	0/1497	0.85	3/2024 (0.1%)
4	D	0.42	0/1263	0.86	3/1704 (0.2%)
4	O	0.42	0/1263	0.86	3/1704 (0.2%)
5	E	0.38	0/1324	0.89	2/1784 (0.1%)
5	P	0.38	0/1324	0.89	2/1784 (0.1%)
6	G	0.35	0/1681	0.79	2/2266 (0.1%)
6	R	0.35	0/1681	0.79	2/2266 (0.1%)
7	H	0.34	0/1211	0.92	3/1643 (0.2%)
7	S	0.35	0/1211	0.92	3/1643 (0.2%)
8	I	0.32	0/4219	0.82	23/5852 (0.4%)
8	T	0.32	0/4219	0.82	23/5852 (0.4%)
9	J	0.41	2/6430 (0.0%)	0.94	18/8751 (0.2%)
9	U	0.39	1/6430 (0.0%)	0.91	14/8751 (0.2%)
10	K	0.31	0/1663	0.91	11/2268 (0.5%)
10	V	0.32	0/1663	0.91	11/2268 (0.5%)
All	All	0.37	3/47270 (0.0%)	0.87	132/64306 (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
9	J	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	481	ASN	N-CA	5.68	1.53	1.46
9	U	769	GLY	C-N	5.34	1.38	1.33
9	J	769	GLY	C-N	5.20	1.38	1.33

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	479	ILE	O-C-N	-16.02	102.84	121.10
3	F	155	VAL	N-CA-C	-9.49	103.16	112.17
3	Q	155	VAL	N-CA-C	-9.43	103.21	112.17
8	I	639	PRO	N-CA-CB	8.38	112.04	103.25
8	T	639	PRO	N-CA-CB	8.34	112.00	103.25
8	I	346	PRO	N-CA-CB	8.28	111.94	103.25
8	T	483	PRO	N-CA-CB	8.27	111.94	103.25
8	T	346	PRO	N-CA-CB	8.27	111.93	103.25
8	I	483	PRO	N-CA-CB	8.24	111.90	103.25
10	K	310	PRO	N-CA-CB	8.01	111.66	103.25
10	V	310	PRO	N-CA-CB	8.01	111.66	103.25
8	T	976	PRO	N-CA-CB	7.91	111.55	103.25
9	J	1052	ILE	CG1-CB-CG2	-7.90	87.00	110.70
9	U	1052	ILE	CG1-CB-CG2	-7.89	87.03	110.70
8	I	976	PRO	N-CA-CB	7.84	111.48	103.25
10	K	330	PRO	N-CA-CB	7.82	111.47	103.25
10	V	325	PRO	N-CA-CB	7.82	111.45	103.25
10	V	330	PRO	N-CA-CB	7.81	111.45	103.25
8	T	721	PRO	N-CA-CB	7.78	110.56	103.33
8	T	649	PRO	N-CA-CB	7.77	110.57	103.19
10	K	325	PRO	N-CA-CB	7.76	111.40	103.25
8	I	721	PRO	N-CA-CB	7.76	110.54	103.33
8	I	649	PRO	N-CA-CB	7.75	110.56	103.19
8	I	1076	PRO	N-CA-CB	7.69	111.33	103.25
10	K	286	PRO	N-CA-CB	7.67	111.31	103.25
8	T	1076	PRO	N-CA-CB	7.66	111.29	103.25
10	V	286	PRO	N-CA-CB	7.59	111.22	103.25
10	K	305	PRO	N-CA-CB	7.38	110.20	103.34
10	V	305	PRO	N-CA-CB	7.38	110.20	103.34
10	V	282	PRO	N-CA-CB	7.34	110.96	103.25
10	K	282	PRO	N-CA-CB	7.34	110.95	103.25
9	U	667	PRO	N-CA-CB	7.15	109.99	103.20
9	J	667	PRO	N-CA-CB	7.12	109.97	103.20
8	I	572	PRO	N-CA-CB	7.06	110.66	103.25
8	T	572	PRO	N-CA-CB	7.02	110.62	103.25
8	I	704	PRO	N-CA-CB	7.00	110.76	102.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	956	PRO	N-CA-CB	6.99	110.59	103.25
8	T	704	PRO	N-CA-CB	6.97	110.73	102.85
9	U	956	PRO	N-CA-CB	6.91	110.50	103.25
9	J	480	PRO	CA-C-O	-6.78	113.30	121.03
9	U	673	PRO	N-CA-CB	6.72	110.39	103.00
9	J	673	PRO	N-CA-CB	6.72	110.39	103.00
10	V	279	PRO	N-CA-CB	6.71	110.44	102.85
10	K	279	PRO	N-CA-CB	6.71	110.43	102.85
8	I	1067	PRO	N-CA-CB	6.51	110.09	103.25
8	T	1067	PRO	N-CA-CB	6.51	110.09	103.25
9	U	791	THR	OG1-CB-CG2	-6.43	96.43	109.30
9	J	791	THR	OG1-CB-CG2	-6.41	96.48	109.30
9	U	398	PRO	N-CA-CB	6.37	109.94	103.25
9	J	1100	PRO	N-CA-CB	6.36	109.92	103.25
9	J	398	PRO	N-CA-CB	6.32	109.89	103.25
8	I	646	ILE	CA-C-N	6.32	133.34	121.97
8	I	646	ILE	C-N-CA	6.32	133.34	121.97
8	T	980	PRO	N-CA-CB	6.30	109.87	103.25
8	T	646	ILE	CA-C-N	6.29	133.29	121.97
8	T	646	ILE	C-N-CA	6.29	133.29	121.97
9	U	1100	PRO	N-CA-CB	6.29	109.85	103.25
8	T	970	PRO	N-CA-CB	6.28	111.25	103.15
8	I	970	PRO	N-CA-CB	6.25	111.21	103.15
9	J	436	PRO	N-CA-CB	6.24	110.14	103.52
9	U	436	PRO	N-CA-CB	6.24	110.14	103.52
8	I	980	PRO	N-CA-CB	6.21	109.77	103.25
7	S	26	PRO	N-CA-CB	6.11	110.00	103.52
10	K	250	PRO	N-CA-CB	6.10	110.04	103.33
7	H	26	PRO	N-CA-CB	6.08	109.97	103.52
10	V	250	PRO	N-CA-CB	6.03	109.96	103.33
3	N	27	THR	CA-C-N	5.93	132.86	121.54
3	N	27	THR	C-N-CA	5.93	132.86	121.54
6	G	175	LYS	CB-CG-CD	5.93	124.93	111.30
9	J	410	PRO	N-CA-CB	5.92	110.07	103.44
6	R	175	LYS	CB-CG-CD	5.92	124.91	111.30
9	U	410	PRO	N-CA-CB	5.91	110.06	103.44
3	C	27	THR	CA-C-N	5.89	132.80	121.54
3	C	27	THR	C-N-CA	5.89	132.80	121.54
7	S	84	THR	CA-C-N	5.84	132.70	121.54
7	S	84	THR	C-N-CA	5.84	132.70	121.54
7	H	84	THR	CA-C-N	5.83	132.68	121.54
7	H	84	THR	C-N-CA	5.83	132.68	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	388	PRO	N-CA-CB	5.77	109.91	103.44
9	J	659	ILE	CG1-CB-CG2	-5.77	93.39	110.70
9	U	388	PRO	N-CA-CB	5.77	109.90	103.44
8	I	252	PRO	N-CA-CB	5.77	109.90	103.44
9	J	1255	PRO	N-CA-CB	5.76	110.59	103.15
8	T	252	PRO	N-CA-CB	5.75	109.88	103.44
9	U	659	ILE	CG1-CB-CG2	-5.75	93.46	110.70
9	U	1255	PRO	N-CA-CB	5.71	110.51	103.15
10	V	441	LEU	CA-C-N	5.68	130.71	122.36
10	V	441	LEU	C-N-CA	5.68	130.71	122.36
9	J	782	THR	CA-C-N	5.66	132.00	121.69
9	J	782	THR	C-N-CA	5.66	132.00	121.69
9	U	782	THR	CA-C-N	5.65	131.97	121.69
9	U	782	THR	C-N-CA	5.65	131.97	121.69
10	K	441	LEU	CA-C-N	5.63	130.63	122.36
10	K	441	LEU	C-N-CA	5.63	130.63	122.36
5	E	191	MET	CB-CG-SD	5.57	129.40	112.70
8	I	975	VAL	CA-C-N	5.57	126.80	119.84
8	I	975	VAL	C-N-CA	5.57	126.80	119.84
8	T	975	VAL	CA-C-N	5.56	126.79	119.84
8	T	975	VAL	C-N-CA	5.56	126.79	119.84
9	J	479	ILE	CA-C-N	-5.56	114.07	119.90
9	J	479	ILE	C-N-CA	-5.56	114.07	119.90
4	D	139	LYS	CA-CB-CG	5.55	125.21	114.10
5	P	191	MET	CB-CG-SD	5.55	129.35	112.70
4	O	139	LYS	CA-CB-CG	5.54	125.17	114.10
5	P	212	LYS	CB-CG-CD	5.52	124.00	111.30
5	E	212	LYS	CB-CG-CD	5.52	123.99	111.30
6	G	207	ASN	CA-CB-CG	5.51	118.11	112.60
6	R	207	ASN	CA-CB-CG	5.49	118.09	112.60
8	I	482	CYS	CA-C-N	5.44	126.64	119.84
8	I	482	CYS	C-N-CA	5.44	126.64	119.84
8	T	482	CYS	CA-C-N	5.42	126.62	119.84
8	T	482	CYS	C-N-CA	5.42	126.62	119.84
3	F	183	ILE	CA-C-N	5.26	131.58	121.54
3	F	183	ILE	C-N-CA	5.26	131.58	121.54
4	D	39	GLU	CA-C-N	5.22	131.51	121.54
4	D	39	GLU	C-N-CA	5.22	131.51	121.54
3	Q	183	ILE	CA-C-N	5.21	131.50	121.54
3	Q	183	ILE	C-N-CA	5.21	131.50	121.54
8	I	995	THR	CA-C-N	5.20	127.56	120.54
8	I	995	THR	C-N-CA	5.20	127.56	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	534	THR	CA-CB-CG2	5.19	119.32	110.50
4	O	39	GLU	CA-C-N	5.19	131.44	121.54
4	O	39	GLU	C-N-CA	5.19	131.44	121.54
10	V	534	THR	CA-CB-CG2	5.18	119.31	110.50
8	T	995	THR	CA-C-N	5.17	127.52	120.54
8	T	995	THR	C-N-CA	5.17	127.52	120.54
8	I	572	PRO	CA-C-N	5.14	131.37	121.54
8	I	572	PRO	C-N-CA	5.14	131.37	121.54
8	T	572	PRO	CA-C-N	5.14	131.36	121.54
8	T	572	PRO	C-N-CA	5.14	131.36	121.54
3	N	129	GLU	CA-C-N	5.02	128.28	120.60
3	N	129	GLU	C-N-CA	5.02	128.28	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	J	479	ILE	Mainchain

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	1160	0	1184	22	0
1	L	1160	0	1184	17	0
2	B	1630	0	1640	30	0
2	M	1630	0	1640	30	0
3	C	1482	0	1490	17	0
3	F	1470	0	1476	38	0
3	N	1482	0	1490	18	0
3	Q	1470	0	1476	40	0
4	D	1235	0	1202	36	0
4	O	1235	0	1202	34	0
5	E	1300	0	1304	38	0
5	P	1300	0	1304	36	0
6	G	1646	0	1623	36	0
6	R	1646	0	1623	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	1180	0	1132	23	0
7	S	1180	0	1132	22	0
8	I	4199	0	2172	31	0
8	T	4199	0	2172	23	0
9	J	6326	0	5648	151	0
9	U	6326	0	5648	124	0
10	K	1649	0	1338	20	0
10	V	1649	0	1338	19	0
All	All	46554	0	40418	712	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 8.

All (712) 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:A:77:MET:HE1	1:A:79:ILE:CG2	1.28	1.60
5:E:44:PHE:CE1	3:F:189:PRO:HG3	1.49	1.45
5:P:44:PHE:CE1	3:Q:189:PRO:HG3	1.49	1.43
9:U:737:ASN:OD1	9:U:785:LEU:HA	1.24	1.37
9:J:734:ARG:NH2	9:J:827:GLU:HG2	1.40	1.32
8:T:459:TYR:O	8:T:464:LYS:HB3	1.19	1.31
9:J:737:ASN:OD1	9:J:785:LEU:HA	1.30	1.29
8:T:459:TYR:O	8:T:464:LYS:CB	1.79	1.27
1:A:77:MET:CE	1:A:79:ILE:HG23	1.62	1.27
9:J:1216:PHE:CD1	9:J:1222:LYS:HB3	1.71	1.24
9:U:1216:PHE:CD1	9:U:1222:LYS:HB3	1.71	1.24
9:J:734:ARG:NH2	9:J:827:GLU:CG	2.08	1.16
9:J:737:ASN:CG	9:J:785:LEU:HA	1.70	1.15
5:E:44:PHE:HE1	3:F:189:PRO:CG	1.61	1.14
8:I:459:TYR:O	8:I:464:LYS:HB2	1.44	1.13
3:N:181:ASN:O	3:N:182:ARG:HG2	1.48	1.13
5:P:44:PHE:HE1	3:Q:189:PRO:CG	1.61	1.12
9:J:662:ILE:H	9:J:736:GLN:CG	1.43	1.12
3:C:181:ASN:O	3:C:182:ARG:HG2	1.48	1.10
3:Q:188:ILE:HG23	3:Q:189:PRO:HD3	1.30	1.09
9:J:662:ILE:H	9:J:736:GLN:HG2	1.07	1.09
1:A:77:MET:CE	1:A:79:ILE:CG2	2.22	1.08
3:F:188:ILE:HG23	3:F:189:PRO:HD3	1.30	1.08
9:J:1216:PHE:CE1	9:J:1222:LYS:HB3	1.87	1.08
9:U:1216:PHE:CE1	9:U:1222:LYS:HB3	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:907:LYS:HE3	9:U:908:LYS:HA	1.36	1.07
1:A:62:LEU:O	1:A:77:MET:HG2	1.54	1.06
9:U:907:LYS:HE3	9:U:908:LYS:CA	1.87	1.04
9:J:907:LYS:HE3	9:J:908:LYS:CA	1.87	1.04
5:P:44:PHE:CE1	3:Q:189:PRO:CG	2.39	1.04
6:G:168:LYS:HA	7:H:135:GLN:HE22	1.22	1.03
6:G:169:MET:HG3	7:H:87:CYS:SG	1.98	1.03
6:R:169:MET:HG3	7:S:87:CYS:SG	1.99	1.03
1:A:77:MET:HE1	1:A:79:ILE:HG22	1.36	1.03
5:P:133:GLN:NE2	3:Q:189:PRO:HG2	1.74	1.03
5:E:133:GLN:NE2	3:F:189:PRO:HG2	1.74	1.02
9:J:907:LYS:HE3	9:J:908:LYS:HA	1.36	1.02
5:E:44:PHE:CE1	3:F:189:PRO:CG	2.39	1.01
6:R:168:LYS:HA	7:S:135:GLN:HE22	1.23	1.00
9:U:737:ASN:CG	9:U:785:LEU:HA	1.87	1.00
9:J:734:ARG:HH12	9:J:827:GLU:HA	1.24	0.99
3:Q:188:ILE:CG2	3:Q:189:PRO:HD3	1.94	0.98
3:F:188:ILE:CG2	3:F:189:PRO:HD3	1.94	0.97
8:T:459:TYR:O	8:T:464:LYS:CG	2.12	0.97
2:B:134:LEU:O	2:B:138:LEU:HD23	1.66	0.95
9:J:662:ILE:N	9:J:736:GLN:CG	2.25	0.94
2:M:134:LEU:O	2:M:138:LEU:HD23	1.66	0.94
9:J:907:LYS:HE3	9:J:908:LYS:N	1.84	0.93
4:D:19:ARG:NH1	4:D:24:ALA:O	2.02	0.93
9:J:737:ASN:ND2	9:J:785:LEU:HA	1.84	0.92
4:O:19:ARG:NH1	4:O:24:ALA:O	2.02	0.92
9:U:661:ARG:HB2	9:U:736:GLN:HB3	1.49	0.92
5:P:133:GLN:HE22	3:Q:189:PRO:HG2	1.34	0.92
9:U:907:LYS:HE3	9:U:908:LYS:N	1.84	0.91
5:E:68:PRO:HD2	5:E:111:PHE:O	1.71	0.91
9:J:734:ARG:NH1	9:J:827:GLU:HA	1.85	0.91
5:P:133:GLN:HE22	3:Q:189:PRO:CG	1.84	0.91
9:J:734:ARG:CZ	9:J:827:GLU:HG2	2.01	0.91
5:E:133:GLN:HE22	3:F:189:PRO:CG	1.84	0.90
9:J:992:ARG:HH22	10:V:518:TYR:HA	1.36	0.90
4:O:11:ARG:HH22	4:O:125:PHE:HD1	1.18	0.90
5:P:68:PRO:HD2	5:P:111:PHE:O	1.71	0.89
9:J:478:ASP:HB2	9:J:486:PRO:HG2	1.54	0.89
9:J:662:ILE:N	9:J:736:GLN:HG2	1.85	0.89
9:U:737:ASN:OD1	9:U:785:LEU:CA	2.19	0.88
5:E:133:GLN:HE22	3:F:189:PRO:HG2	1.34	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:734:ARG:HH22	9:J:827:GLU:CA	1.86	0.88
10:K:518:TYR:HA	9:U:992:ARG:HH22	1.37	0.88
9:U:661:ARG:HB2	9:U:736:GLN:CB	2.03	0.88
4:D:11:ARG:HH22	4:D:125:PHE:HD1	1.18	0.87
9:U:1216:PHE:CD1	9:U:1222:LYS:CB	2.58	0.86
9:J:1216:PHE:CD1	9:J:1222:LYS:CB	2.58	0.86
9:J:487:ARG:O	9:J:491:TYR:CE1	2.29	0.86
9:J:737:ASN:OD1	9:J:785:LEU:CA	2.22	0.85
9:U:478:ASP:HB2	9:U:486:PRO:HG2	1.54	0.85
8:I:463:ASN:CB	8:I:464:LYS:HE2	2.06	0.85
9:J:908:LYS:O	9:J:908:LYS:HD3	1.76	0.85
9:U:487:ARG:O	9:U:491:TYR:CE1	2.29	0.85
6:R:168:LYS:HD3	7:S:131:ARG:NH1	1.92	0.85
3:C:113:ASP:OD2	3:C:179:LYS:HE3	1.77	0.84
8:I:459:TYR:O	8:I:464:LYS:CB	2.24	0.84
9:U:908:LYS:O	9:U:908:LYS:HD3	1.76	0.84
5:P:133:GLN:NE2	3:Q:189:PRO:CG	2.41	0.84
3:N:113:ASP:OD2	3:N:179:LYS:HE3	1.77	0.83
2:M:134:LEU:O	2:M:138:LEU:CD2	2.27	0.83
6:G:168:LYS:HD3	7:H:131:ARG:NH1	1.93	0.83
9:J:1216:PHE:CE2	10:K:487:TYR:HE2	1.97	0.83
5:E:133:GLN:NE2	3:F:189:PRO:CG	2.41	0.83
2:B:134:LEU:O	2:B:138:LEU:CD2	2.27	0.82
9:J:907:LYS:CE	9:J:908:LYS:HA	2.09	0.82
9:U:907:LYS:CE	9:U:908:LYS:HA	2.09	0.82
10:K:241:GLU:O	10:K:245:LYS:HB2	1.80	0.81
9:U:1216:PHE:CE2	10:V:487:TYR:HE2	1.97	0.81
9:J:1214:VAL:O	9:J:1215:ILE:HD13	1.82	0.80
10:V:241:GLU:O	10:V:245:LYS:HB2	1.80	0.80
6:R:168:LYS:HD3	7:S:131:ARG:HH11	1.47	0.79
8:I:464:LYS:HE2	8:I:464:LYS:H	1.45	0.79
9:U:1214:VAL:O	9:U:1215:ILE:HD13	1.82	0.79
8:I:463:ASN:CB	8:I:464:LYS:NZ	2.46	0.78
5:P:44:PHE:HE1	3:Q:189:PRO:HG3	0.73	0.78
6:G:168:LYS:HD3	7:H:131:ARG:HH11	1.45	0.78
9:J:737:ASN:ND2	9:J:785:LEU:CA	2.43	0.78
6:G:168:LYS:HA	7:H:135:GLN:NE2	1.98	0.78
5:P:133:GLN:NE2	3:Q:189:PRO:HB2	2.00	0.77
5:P:133:GLN:NE2	3:Q:189:PRO:CB	2.47	0.77
5:E:133:GLN:NE2	3:F:189:PRO:CB	2.47	0.77
6:R:168:LYS:HA	7:S:135:GLN:NE2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:ARG:NH2	4:D:125:PHE:CD1	2.53	0.77
9:J:661:ARG:HB2	9:J:736:GLN:HB3	1.67	0.77
5:E:133:GLN:NE2	3:F:189:PRO:HB2	2.00	0.76
3:Q:187:GLU:OE2	3:Q:187:GLU:N	2.18	0.76
5:E:44:PHE:HE1	3:F:189:PRO:HG3	0.73	0.76
4:O:11:ARG:NH2	4:O:125:PHE:CD1	2.53	0.76
4:D:4:TYR:OH	4:D:93:ASP:OD2	2.03	0.75
1:A:77:MET:HE1	1:A:79:ILE:HG23	0.77	0.75
3:F:187:GLU:OE2	3:F:187:GLU:N	2.18	0.74
9:J:734:ARG:HH22	9:J:827:GLU:C	1.93	0.74
5:P:133:GLN:CD	3:Q:189:PRO:HG2	2.11	0.74
5:E:133:GLN:CD	3:F:189:PRO:HG2	2.11	0.74
3:F:188:ILE:HG23	3:F:189:PRO:CD	2.15	0.74
8:I:463:ASN:CB	8:I:464:LYS:CE	2.66	0.74
9:J:908:LYS:HD3	9:J:908:LYS:C	2.11	0.74
9:U:908:LYS:HD3	9:U:908:LYS:C	2.11	0.74
9:U:1216:PHE:HE2	10:V:487:TYR:HE2	1.36	0.74
9:J:661:ARG:HB2	9:J:736:GLN:CB	2.17	0.73
1:L:62:LEU:O	1:L:77:MET:HG3	1.88	0.73
6:R:168:LYS:CA	7:S:135:GLN:HE22	2.02	0.73
9:J:734:ARG:NH2	9:J:827:GLU:CD	2.47	0.73
6:R:169:MET:HG3	7:S:87:CYS:CB	2.19	0.73
9:J:734:ARG:HH22	9:J:827:GLU:CG	2.02	0.72
9:J:906:TRP:HZ3	9:J:1095:ILE:N	1.80	0.72
9:U:906:TRP:HZ3	9:U:1095:ILE:N	1.80	0.72
5:E:133:GLN:HE22	3:F:189:PRO:CB	2.02	0.72
4:O:4:TYR:OH	4:O:93:ASP:OD2	2.03	0.72
9:U:907:LYS:CE	9:U:908:LYS:CA	2.67	0.72
6:G:168:LYS:CA	7:H:135:GLN:HE22	2.01	0.72
9:J:1216:PHE:HE2	10:K:487:TYR:HE2	1.36	0.72
9:J:907:LYS:HE3	9:J:907:LYS:C	2.15	0.72
5:P:133:GLN:HE22	3:Q:189:PRO:CB	2.02	0.72
9:U:906:TRP:CZ3	9:U:1095:ILE:N	2.58	0.71
8:I:464:LYS:HE2	8:I:464:LYS:N	2.03	0.71
6:G:169:MET:HG3	7:H:87:CYS:CB	2.20	0.71
4:O:20:GLU:OE2	4:O:36:GLN:HB2	1.91	0.71
9:U:909:MET:HE3	9:U:910:PRO:HD3	1.73	0.71
9:U:907:LYS:HE3	9:U:907:LYS:C	2.15	0.71
9:J:906:TRP:CZ3	9:J:1095:ILE:N	2.58	0.70
4:D:20:GLU:OE2	4:D:36:GLN:HB2	1.91	0.70
1:L:62:LEU:O	1:L:77:MET:CG	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:188:ILE:HG23	3:Q:189:PRO:CD	2.15	0.70
2:B:135:SER:O	2:B:139:ILE:HD13	1.92	0.69
9:J:909:MET:HE3	9:J:910:PRO:HD3	1.73	0.69
9:J:907:LYS:CE	9:J:908:LYS:CA	2.67	0.69
2:M:135:SER:O	2:M:139:ILE:HD13	1.92	0.68
4:D:11:ARG:NH2	4:D:125:PHE:HD1	1.91	0.67
9:J:907:LYS:CE	9:J:908:LYS:N	2.58	0.67
9:J:1216:PHE:CE2	10:K:487:TYR:CE2	2.83	0.67
6:R:172:ARG:HH22	7:S:52:GLN:HB2	1.60	0.66
9:J:734:ARG:NH2	9:J:827:GLU:CA	2.59	0.66
9:J:560:THR:O	9:J:564:LEU:HB2	1.96	0.65
9:U:1216:PHE:HZ	10:V:487:TYR:CD2	2.14	0.65
4:D:86:LEU:HD12	4:D:124:ASP:OD2	1.97	0.65
9:J:487:ARG:O	9:J:491:TYR:CD1	2.50	0.65
9:J:1216:PHE:HZ	10:K:487:TYR:CD2	2.14	0.65
6:G:172:ARG:HH22	7:H:52:GLN:HB2	1.60	0.65
9:J:487:ARG:HD3	9:J:490:VAL:HG12	1.78	0.65
9:U:487:ARG:HD3	9:U:490:VAL:HG12	1.78	0.65
9:U:1216:PHE:CE2	10:V:487:TYR:CE2	2.83	0.65
5:E:133:GLN:HE22	3:F:189:PRO:HB2	1.61	0.65
5:P:133:GLN:HE22	3:Q:189:PRO:HB2	1.61	0.65
9:U:907:LYS:CE	9:U:908:LYS:N	2.58	0.65
9:U:560:THR:O	9:U:564:LEU:HB2	1.96	0.65
9:J:734:ARG:CZ	9:J:827:GLU:HA	2.27	0.64
4:O:86:LEU:HD12	4:O:124:ASP:OD2	1.97	0.64
9:J:907:LYS:O	9:J:910:PRO:HD2	1.98	0.64
2:B:143:ASN:HD21	2:B:146:LEU:CD2	2.11	0.63
1:L:11:ILE:HB	1:L:85:LYS:HB2	1.81	0.63
9:U:907:LYS:O	9:U:910:PRO:HD2	1.98	0.63
9:U:903:PRO:O	9:U:907:LYS:HB3	1.99	0.63
9:U:487:ARG:O	9:U:491:TYR:CD1	2.50	0.63
2:M:143:ASN:HD21	2:M:146:LEU:CD2	2.11	0.63
8:I:463:ASN:CB	8:I:464:LYS:HZ3	2.11	0.63
9:J:903:PRO:O	9:J:907:LYS:HB3	1.99	0.63
8:T:459:TYR:O	8:T:464:LYS:HG3	1.99	0.63
9:J:734:ARG:NH2	9:J:827:GLU:HA	2.14	0.62
9:U:904:ASP:O	9:U:907:LYS:HG3	1.98	0.62
9:J:734:ARG:HH22	9:J:827:GLU:HA	1.64	0.62
1:A:11:ILE:HB	1:A:85:LYS:HB2	1.81	0.62
4:D:5:SER:HG	4:D:7:TRP:NE1	1.97	0.62
9:J:734:ARG:HH21	9:J:827:GLU:HG2	1.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:904:ASP:O	9:J:907:LYS:HG3	1.99	0.62
4:O:3:ILE:HD11	4:O:21:TRP:CZ2	2.35	0.62
9:J:758:CYS:SG	9:J:759:GLU:N	2.73	0.62
7:H:103:TYR:HB3	7:H:111:PHE:HB2	1.82	0.61
9:J:478:ASP:HB2	9:J:486:PRO:CG	2.29	0.61
9:U:737:ASN:ND2	9:U:785:LEU:HA	2.15	0.61
4:D:3:ILE:HD11	4:D:21:TRP:CZ2	2.35	0.61
4:O:11:ARG:NH2	4:O:125:PHE:HD1	1.91	0.61
9:J:734:ARG:HH21	9:J:827:GLU:CD	2.07	0.61
4:O:22:THR:HG22	4:O:22:THR:O	2.01	0.61
9:U:487:ARG:HG2	9:U:487:ARG:HH11	1.66	0.61
6:G:168:LYS:O	7:H:135:GLN:NE2	2.33	0.61
9:J:487:ARG:HH11	9:J:487:ARG:CG	2.14	0.60
6:R:168:LYS:O	7:S:135:GLN:NE2	2.33	0.60
9:U:909:MET:SD	9:U:1117:MET:CE	2.90	0.60
4:O:11:ARG:NH2	4:O:125:PHE:CE1	2.70	0.60
7:S:103:TYR:HB3	7:S:111:PHE:HB2	1.81	0.60
4:D:11:ARG:NH2	4:D:125:PHE:CE1	2.70	0.60
9:J:487:ARG:HD3	9:J:490:VAL:CG1	2.32	0.60
10:K:518:TYR:CA	9:U:992:ARG:HH22	2.13	0.60
9:J:909:MET:SD	9:J:1117:MET:CE	2.89	0.60
9:J:1215:ILE:O	9:J:1222:LYS:HB2	2.02	0.60
9:U:487:ARG:HD3	9:U:490:VAL:CG1	2.32	0.60
9:U:487:ARG:HH11	9:U:487:ARG:CG	2.14	0.60
4:D:4:TYR:O	4:D:21:TRP:HB2	2.02	0.59
9:U:758:CYS:SG	9:U:759:GLU:N	2.73	0.59
9:J:487:ARG:HH11	9:J:487:ARG:HG2	1.66	0.59
6:R:169:MET:HG3	7:S:87:CYS:HB3	1.84	0.59
9:U:1215:ILE:O	9:U:1222:LYS:HB2	2.02	0.59
4:O:4:TYR:O	4:O:21:TRP:HB2	2.02	0.59
4:D:5:SER:OG	4:D:7:TRP:NE1	2.36	0.59
4:D:20:GLU:OE2	4:D:36:GLN:CB	2.51	0.59
4:D:22:THR:O	4:D:22:THR:HG22	2.01	0.59
5:E:68:PRO:CD	5:E:111:PHE:O	2.49	0.59
4:O:20:GLU:OE2	4:O:36:GLN:CB	2.51	0.59
1:A:77:MET:HE3	1:A:77:MET:O	2.02	0.59
4:O:5:SER:OG	4:O:7:TRP:NE1	2.36	0.59
9:U:738:PRO:HG2	9:U:784:PRO:HG2	1.86	0.58
2:B:101:SER:OG	3:C:62:ASN:OD1	2.22	0.58
3:N:181:ASN:O	3:N:182:ARG:CG	2.39	0.58
9:U:661:ARG:HB2	9:U:736:GLN:HB2	1.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:1216:PHE:CZ	10:V:487:TYR:CE2	2.91	0.58
8:I:459:TYR:C	8:I:464:LYS:HB2	2.27	0.58
5:P:68:PRO:CD	5:P:111:PHE:O	2.49	0.58
9:J:992:ARG:HH22	10:V:518:TYR:CA	2.13	0.58
5:E:44:PHE:CD1	3:F:189:PRO:HG3	2.28	0.57
1:A:77:MET:CE	1:A:79:ILE:HG22	2.11	0.57
10:V:539:LYS:HB3	10:V:548:LEU:HD11	1.86	0.57
9:J:1216:PHE:CZ	10:K:487:TYR:CE2	2.92	0.57
2:M:101:SER:OG	3:N:62:ASN:OD1	2.22	0.57
3:C:181:ASN:O	3:C:182:ARG:CG	2.39	0.57
9:J:738:PRO:HG2	9:J:784:PRO:HG2	1.86	0.57
6:G:168:LYS:CA	7:H:135:GLN:NE2	2.65	0.57
3:N:158:ASP:O	3:N:180:LEU:O	2.24	0.56
2:B:135:SER:HB3	2:B:225:VAL:HG12	1.88	0.56
9:J:1034:SER:OG	9:J:1035:ARG:N	2.38	0.56
6:G:169:MET:HG3	7:H:87:CYS:HB3	1.86	0.56
2:M:135:SER:HB3	2:M:225:VAL:HG12	1.88	0.56
8:T:864:GLU:HA	8:T:867:ASP:HB2	1.87	0.56
3:C:158:ASP:O	3:C:180:LEU:O	2.24	0.56
4:O:5:SER:HG	4:O:7:TRP:NE1	2.02	0.56
9:U:800:CYS:SG	9:U:801:LEU:N	2.79	0.56
9:U:478:ASP:HB2	9:U:486:PRO:CG	2.30	0.56
10:K:539:LYS:HB3	10:K:548:LEU:HD11	1.86	0.56
9:J:488:PHE:HA	9:J:491:TYR:CZ	2.41	0.56
9:J:661:ARG:HB2	9:J:736:GLN:HB2	1.88	0.56
9:U:735:VAL:HG23	9:U:735:VAL:O	2.05	0.56
1:A:122:ASN:ND2	3:C:128:VAL:O	2.39	0.55
4:D:5:SER:HG	4:D:7:TRP:CD1	2.24	0.55
9:U:1034:SER:OG	9:U:1035:ARG:N	2.38	0.55
6:G:168:LYS:C	6:G:168:LYS:HD2	2.32	0.55
4:O:67:ILE:HA	5:P:124:THR:HG22	1.88	0.55
9:U:487:ARG:HD3	9:U:490:VAL:HB	1.88	0.55
8:I:864:GLU:HA	8:I:867:ASP:HB2	1.87	0.55
9:J:1216:PHE:CZ	10:K:487:TYR:CD2	2.95	0.55
9:U:1035:ARG:O	9:U:1035:ARG:NH2	2.40	0.55
4:D:67:ILE:HA	5:E:124:THR:HG22	1.89	0.55
2:B:167:GLN:NE2	3:C:28:GLU:OE2	2.40	0.55
9:J:487:ARG:HD3	9:J:490:VAL:HB	1.88	0.55
9:J:489:GLU:OE2	9:J:493:TYR:HE2	1.90	0.55
6:R:275:LEU:O	6:R:279:GLY:N	2.40	0.55
9:U:489:GLU:OE2	9:U:493:TYR:HE2	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:1216:PHE:CZ	10:V:487:TYR:CD2	2.95	0.55
5:E:8:VAL:HB	5:E:17:TYR:HB3	1.89	0.55
6:G:275:LEU:O	6:G:279:GLY:N	2.40	0.55
5:P:33:TYR:HA	5:P:36:LEU:HG	1.89	0.55
1:L:122:ASN:ND2	3:N:128:VAL:O	2.39	0.54
2:M:167:GLN:NE2	3:N:28:GLU:OE2	2.40	0.54
5:P:8:VAL:HB	5:P:17:TYR:HB3	1.89	0.54
9:U:488:PHE:HA	9:U:491:TYR:CZ	2.42	0.54
9:J:487:ARG:CZ	9:J:487:ARG:CB	2.86	0.54
9:U:1216:PHE:HE2	10:V:487:TYR:CE2	2.22	0.54
4:D:3:ILE:O	4:D:3:ILE:HG13	2.08	0.54
9:J:800:CYS:SG	9:J:801:LEU:N	2.79	0.54
9:J:1124:ARG:HA	9:J:1127:ILE:HG12	1.88	0.54
9:J:1035:ARG:O	9:J:1035:ARG:NH2	2.40	0.54
5:E:33:TYR:HA	5:E:36:LEU:HG	1.89	0.54
4:O:126:ALA:O	4:O:128:ASN:N	2.38	0.54
9:U:1124:ARG:HA	9:U:1127:ILE:HG12	1.88	0.54
4:O:5:SER:HG	4:O:7:TRP:CD1	2.25	0.53
4:O:3:ILE:HG13	4:O:3:ILE:O	2.08	0.53
8:T:329:TYR:O	8:T:333:SER:N	2.40	0.53
2:B:188:ASP:O	2:B:257:GLY:N	2.41	0.53
4:D:52:ARG:NH1	4:D:81:CYS:SG	2.81	0.53
4:O:52:ARG:NH1	4:O:81:CYS:SG	2.81	0.53
5:P:44:PHE:CD1	3:Q:189:PRO:HG3	2.28	0.53
1:A:114:LYS:HG2	2:B:140:PHE:CE2	2.44	0.53
8:I:329:TYR:O	8:I:333:SER:N	2.40	0.53
9:J:735:VAL:HG12	9:J:735:VAL:O	2.08	0.53
9:U:487:ARG:CZ	9:U:487:ARG:CB	2.86	0.53
2:B:99:ILE:HG21	2:B:104:LEU:HD13	1.91	0.53
5:E:48:SER:OG	3:F:188:ILE:HG13	2.09	0.53
7:H:8:ILE:HG21	7:H:45:LEU:HD11	1.90	0.53
7:H:12:ASP:OD2	9:J:528:ARG:NH1	2.42	0.53
1:L:114:LYS:HG2	2:M:140:PHE:CE2	2.44	0.53
6:R:168:LYS:CA	7:S:135:GLN:NE2	2.66	0.53
7:S:8:ILE:HG21	7:S:45:LEU:HD11	1.90	0.53
3:F:188:ILE:CG2	3:F:189:PRO:CD	2.80	0.53
2:M:143:ASN:HD21	2:M:146:LEU:HD22	1.74	0.53
7:S:12:ASP:OD2	9:U:528:ARG:NH1	2.42	0.53
2:M:99:ILE:HG21	2:M:104:LEU:HD13	1.91	0.53
5:P:48:SER:OG	3:Q:188:ILE:HG13	2.09	0.53
2:B:143:ASN:HD21	2:B:146:LEU:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:82:ASP:OD1	6:R:82:ASP:N	2.41	0.52
3:Q:133:ASP:OD1	3:Q:133:ASP:N	2.41	0.52
9:J:1223:ILE:HG21	9:J:1230:ARG:HG3	1.90	0.52
5:P:48:SER:OG	3:Q:188:ILE:CG1	2.58	0.52
6:R:168:LYS:HD2	6:R:168:LYS:C	2.34	0.52
9:U:1223:ILE:HG21	9:U:1230:ARG:HG3	1.90	0.52
5:E:193:ASP:O	3:F:66:ARG:NH2	2.42	0.52
2:M:188:ASP:O	2:M:257:GLY:N	2.41	0.52
9:U:487:ARG:CG	9:U:487:ARG:NH1	2.73	0.52
3:C:133:ASP:OD1	3:C:133:ASP:N	2.43	0.52
1:L:62:LEU:O	1:L:77:MET:HG2	2.08	0.52
2:M:61:ARG:NH2	2:M:107:GLU:OE1	2.43	0.52
4:D:126:ALA:O	4:D:128:ASN:N	2.38	0.52
9:J:1216:PHE:HE2	10:K:487:TYR:CE2	2.22	0.52
9:J:1278:GLN:NE2	9:J:1280:ASP:OD2	2.43	0.52
10:K:418:ASN:ND2	10:K:553:ASN:OD1	2.43	0.52
9:J:1216:PHE:HZ	10:K:487:TYR:HD2	1.57	0.52
6:R:274:VAL:O	6:R:277:ARG:HB3	2.10	0.52
3:F:133:ASP:OD1	3:F:133:ASP:N	2.41	0.52
9:U:1093:THR:OG1	9:U:1118:ARG:NH2	2.43	0.52
6:G:82:ASP:OD1	6:G:82:ASP:N	2.41	0.51
9:U:487:ARG:CB	9:U:487:ARG:NH1	2.73	0.51
5:E:68:PRO:HG3	5:E:111:PHE:CE2	2.45	0.51
2:B:61:ARG:NH2	2:B:107:GLU:OE1	2.43	0.51
9:J:487:ARG:CB	9:J:487:ARG:NH1	2.73	0.51
10:V:418:ASN:ND2	10:V:553:ASN:OD1	2.43	0.51
4:D:27:SER:O	4:D:36:GLN:NE2	2.42	0.51
4:D:139:LYS:HG2	4:D:141:THR:HG22	1.92	0.51
9:J:1093:THR:OG1	9:J:1118:ARG:NH2	2.43	0.51
5:P:193:ASP:O	3:Q:66:ARG:NH2	2.42	0.51
1:A:77:MET:SD	1:A:77:MET:C	2.94	0.51
5:E:48:SER:OG	3:F:188:ILE:CG1	2.58	0.51
9:J:734:ARG:NH2	9:J:827:GLU:CB	2.73	0.51
5:P:68:PRO:HG3	5:P:111:PHE:CE2	2.45	0.51
9:U:909:MET:SD	9:U:909:MET:C	2.94	0.51
1:L:58:ASP:OD1	1:L:58:ASP:N	2.44	0.51
9:U:1278:GLN:NE2	9:U:1280:ASP:OD2	2.43	0.51
8:I:464:LYS:N	8:I:464:LYS:CD	2.73	0.51
2:B:102:HIS:O	2:B:106:HIS:ND1	2.42	0.51
6:G:274:VAL:O	6:G:277:ARG:HB3	2.10	0.51
9:J:909:MET:SD	9:J:909:MET:C	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:27:SER:O	4:O:36:GLN:NE2	2.42	0.51
3:Q:90:LEU:HD11	3:Q:152:LEU:HD11	1.92	0.51
9:U:737:ASN:ND2	9:U:785:LEU:CA	2.73	0.51
1:A:58:ASP:OD1	1:A:58:ASP:N	2.44	0.51
9:U:1216:PHE:HZ	10:V:487:TYR:HD2	1.57	0.50
5:P:114:TRP:NE1	3:Q:77:LEU:O	2.42	0.50
9:U:661:ARG:CB	9:U:736:GLN:HB3	2.33	0.50
3:F:90:LEU:HD11	3:F:152:LEU:HD11	1.92	0.50
8:I:999:ALA:O	8:I:1024:TRP:NE1	2.45	0.50
9:J:733:CYS:O	9:J:734:ARG:CZ	2.59	0.50
9:J:906:TRP:CH2	9:J:1095:ILE:HG22	2.47	0.50
9:J:1217:ASP:O	9:J:1219:LYS:N	2.44	0.50
2:M:177:LYS:HB3	2:M:185:TYR:HB2	1.94	0.50
8:T:991:GLU:HA	8:T:1032:GLY:HA2	1.93	0.50
9:U:1212:ASP:HB3	9:U:1266:CYS:HB3	1.94	0.50
9:J:489:GLU:OE2	9:J:493:TYR:CE2	2.65	0.50
9:J:734:ARG:HH22	9:J:827:GLU:CB	2.22	0.50
9:J:1055:ASN:HD21	9:J:1065:GLU:HG2	1.77	0.50
8:T:307:LYS:O	8:T:311:GLU:N	2.45	0.50
8:T:999:ALA:O	8:T:1024:TRP:NE1	2.45	0.50
9:U:1217:ASP:O	9:U:1219:LYS:N	2.44	0.50
6:G:46:TYR:O	7:H:164:ARG:NH2	2.44	0.50
9:U:489:GLU:OE2	9:U:493:TYR:CE2	2.65	0.50
9:U:906:TRP:CH2	9:U:1095:ILE:HG22	2.47	0.50
9:J:1216:PHE:HA	9:J:1222:LYS:HA	1.94	0.49
6:R:46:TYR:O	7:S:164:ARG:NH2	2.44	0.49
6:R:169:MET:CG	7:S:87:CYS:SG	2.88	0.49
9:U:1055:ASN:HD21	9:U:1065:GLU:HG2	1.77	0.49
4:D:88:PHE:HB3	4:D:103:LEU:HD22	1.95	0.49
8:I:991:GLU:HA	8:I:1032:GLY:HA2	1.93	0.49
4:O:139:LYS:HG2	4:O:141:THR:HG22	1.93	0.49
1:L:19:LEU:HD13	1:L:134:ILE:HG23	1.94	0.49
9:J:626:SER:HA	9:J:629:ASP:HB2	1.95	0.49
9:U:1058:PHE:HB3	9:U:1061:PHE:HB3	1.94	0.49
2:B:177:LYS:HB3	2:B:185:TYR:HB2	1.94	0.49
1:A:19:LEU:HD13	1:A:134:ILE:HG23	1.93	0.49
1:A:61:PRO:HB2	1:A:77:MET:SD	2.53	0.49
3:F:79:ARG:NH1	3:F:187:GLU:OE2	2.45	0.49
9:U:487:ARG:NH1	9:U:487:ARG:HB3	2.28	0.49
6:G:68:GLU:OE2	6:G:72:GLN:NE2	2.46	0.49
9:J:966:ILE:HA	9:J:986:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:1212:ASP:HB3	9:J:1266:CYS:HB3	1.94	0.49
9:U:626:SER:HA	9:U:629:ASP:HB2	1.95	0.49
8:I:464:LYS:CE	8:I:464:LYS:N	2.73	0.49
9:J:907:LYS:C	9:J:907:LYS:CD	2.85	0.48
9:U:1017:ASP:OD1	9:U:1017:ASP:N	2.45	0.48
8:I:793:ARG:NH2	8:I:829:PHE:O	2.47	0.48
9:J:1004:PRO:HB3	9:J:1038:ILE:HG22	1.95	0.48
9:J:1017:ASP:N	9:J:1017:ASP:OD1	2.45	0.48
9:J:1058:PHE:HB3	9:J:1061:PHE:HB3	1.94	0.48
3:Q:79:ARG:NH1	3:Q:187:GLU:OE2	2.45	0.48
9:U:485:PHE:N	9:U:486:PRO:CD	2.76	0.48
9:U:907:LYS:C	9:U:907:LYS:CD	2.85	0.48
9:U:1216:PHE:HA	9:U:1222:LYS:HA	1.94	0.48
9:J:487:ARG:CG	9:J:487:ARG:NH1	2.73	0.48
2:M:102:HIS:O	2:M:106:HIS:ND1	2.42	0.48
9:U:491:TYR:O	9:U:495:ASN:ND2	2.43	0.48
10:V:306:LYS:HA	10:V:332:ARG:HA	1.95	0.48
9:J:487:ARG:HD3	9:J:490:VAL:CB	2.43	0.48
4:O:88:PHE:HB3	4:O:103:LEU:HD22	1.95	0.48
4:D:40:ASP:O	4:D:44:LEU:CB	2.62	0.48
3:F:161:VAL:HG13	3:F:178:VAL:HG22	1.95	0.48
6:G:97:ARG:NH1	7:H:150:TYR:O	2.46	0.48
6:R:97:ARG:NH1	7:S:150:TYR:O	2.46	0.48
1:A:59:SER:HB3	2:B:142:ASN:O	2.14	0.48
9:J:510:GLN:HA	9:J:513:ILE:HG22	1.96	0.48
2:M:63:ILE:HG13	2:M:65:GLY:H	1.78	0.48
4:O:40:ASP:O	4:O:44:LEU:CB	2.62	0.48
2:B:109:TYR:HD1	2:B:210:MET:HE3	1.79	0.48
9:J:487:ARG:NH1	9:J:487:ARG:HB3	2.28	0.48
9:J:1023:MET:O	9:J:1027:ARG:HB2	2.14	0.48
9:U:907:LYS:CE	9:U:907:LYS:C	2.85	0.48
9:J:491:TYR:O	9:J:495:ASN:ND2	2.42	0.48
1:A:104:ALA:HA	1:A:107:GLN:HG2	1.96	0.47
4:D:4:TYR:O	4:D:21:TRP:N	2.41	0.47
6:G:168:LYS:HZ2	6:G:169:MET:HB2	1.79	0.47
9:U:487:ARG:HD3	9:U:490:VAL:CB	2.43	0.47
8:I:807:PRO:HG3	8:I:851:ASP:HB3	1.96	0.47
1:L:59:SER:HB3	2:M:142:ASN:O	2.14	0.47
2:B:63:ILE:HG13	2:B:65:GLY:H	1.78	0.47
3:C:53:ASN:O	3:C:142:ASN:ND2	2.47	0.47
9:J:485:PHE:N	9:J:486:PRO:CD	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:793:ARG:NH2	8:T:829:PHE:O	2.47	0.47
8:T:807:PRO:HG3	8:T:851:ASP:HB3	1.96	0.47
1:A:114:LYS:HG2	2:B:140:PHE:HE2	1.79	0.47
6:G:50:LEU:O	6:G:105:ARG:NH1	2.47	0.47
9:U:966:ILE:HA	9:U:986:PRO:HA	1.95	0.47
10:K:306:LYS:HA	10:K:332:ARG:HA	1.94	0.47
3:N:53:ASN:O	3:N:142:ASN:ND2	2.47	0.47
9:J:740:LYS:HD3	9:J:784:PRO:HG3	1.96	0.47
2:M:89:LYS:HZ1	2:M:98:ILE:HG12	1.79	0.47
3:N:133:ASP:N	3:N:133:ASP:OD1	2.43	0.47
4:O:2:GLY:HA2	4:O:157:VAL:O	2.15	0.47
4:O:5:SER:O	4:O:90:LEU:HD12	2.15	0.47
6:R:173:ASP:OD1	6:R:173:ASP:N	2.45	0.47
6:R:224:GLY:O	6:R:254:ARG:NH1	2.48	0.47
9:U:1004:PRO:HB3	9:U:1038:ILE:HG22	1.95	0.47
9:U:1023:MET:O	9:U:1027:ARG:HB2	2.14	0.47
9:U:510:GLN:HA	9:U:513:ILE:HG22	1.96	0.47
4:D:5:SER:O	4:D:90:LEU:HD12	2.15	0.47
2:M:124:ARG:O	2:M:128:PHE:HB2	2.15	0.47
2:M:194:ILE:HA	2:M:197:PHE:HD2	1.80	0.47
2:B:194:ILE:HA	2:B:197:PHE:HD2	1.80	0.47
3:Q:161:VAL:HG13	3:Q:178:VAL:HG22	1.96	0.47
6:R:50:LEU:O	6:R:105:ARG:NH1	2.47	0.47
6:G:224:GLY:O	6:G:254:ARG:NH1	2.48	0.46
3:N:86:THR:HA	3:N:89:VAL:HG12	1.97	0.46
2:M:134:LEU:O	2:M:138:LEU:HD22	2.14	0.46
9:U:1048:TRP:HE1	9:U:1137:LEU:HD21	1.81	0.46
6:G:168:LYS:NZ	6:G:169:MET:HB2	2.31	0.46
6:G:233:VAL:O	6:G:236:ILE:HB	2.15	0.46
8:I:307:LYS:O	8:I:311:GLU:N	2.45	0.46
9:J:662:ILE:H	9:J:736:GLN:CB	2.18	0.46
5:P:133:GLN:HA	5:P:139:LYS:HA	1.97	0.46
6:R:233:VAL:O	6:R:236:ILE:HB	2.15	0.46
4:D:2:GLY:HA2	4:D:157:VAL:O	2.15	0.46
6:G:51:LEU:HA	6:G:105:ARG:HD3	1.97	0.46
9:U:740:LYS:HD3	9:U:784:PRO:HG3	1.96	0.46
9:U:1216:PHE:CE1	9:U:1222:LYS:CB	2.80	0.46
2:B:124:ARG:O	2:B:128:PHE:HB2	2.15	0.46
4:D:123:TYR:H	4:D:123:TYR:HD1	1.62	0.46
9:J:647:SER:HA	9:J:810:LEU:HD13	1.96	0.46
9:U:1214:VAL:C	9:U:1215:ILE:HD13	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:1214:VAL:C	9:J:1215:ILE:HD13	2.40	0.46
1:L:104:ALA:HA	1:L:107:GLN:HG2	1.96	0.46
6:R:68:GLU:OE2	6:R:72:GLN:NE2	2.46	0.46
9:J:1048:TRP:HE1	9:J:1137:LEU:HD21	1.81	0.46
9:U:647:SER:HA	9:U:810:LEU:HD13	1.96	0.46
2:B:89:LYS:HZ1	2:B:98:ILE:HG12	1.79	0.46
9:J:1197:THR:HG23	9:J:1199:THR:H	1.81	0.46
8:I:599:PHE:HA	8:I:636:LYS:HA	1.98	0.46
2:M:109:TYR:HD1	2:M:210:MET:HE3	1.79	0.46
9:U:487:ARG:CZ	9:U:487:ARG:HB2	2.46	0.46
8:I:770:SER:N	8:I:789:ASN:O	2.49	0.46
9:J:907:LYS:CE	9:J:907:LYS:C	2.86	0.46
9:J:992:ARG:HH21	10:V:519:PHE:H	1.65	0.46
9:U:908:LYS:C	9:U:908:LYS:CD	2.88	0.46
9:U:1085:TYR:OH	9:U:1196:PRO:O	2.34	0.46
1:L:114:LYS:HG2	2:M:140:PHE:HE2	1.79	0.45
3:C:86:THR:HA	3:C:89:VAL:HG12	1.97	0.45
1:L:77:MET:HE3	1:L:79:ILE:HG23	1.99	0.45
5:E:16:ILE:HD12	5:E:202:ILE:HD11	1.98	0.45
8:T:599:PHE:HA	8:T:636:LYS:HA	1.98	0.45
5:E:133:GLN:HA	5:E:139:LYS:HA	1.97	0.45
4:O:12:HIS:O	4:O:14:ASN:ND2	2.49	0.45
10:V:539:LYS:HD3	10:V:548:LEU:HD21	1.98	0.45
6:R:51:LEU:HA	6:R:105:ARG:HD3	1.97	0.45
9:U:1197:THR:HG23	9:U:1199:THR:H	1.81	0.45
9:J:487:ARG:CZ	9:J:487:ARG:HB2	2.46	0.45
9:J:908:LYS:C	9:J:908:LYS:CD	2.87	0.45
4:O:51:LEU:HD21	5:P:43:VAL:HG21	1.99	0.45
9:U:1216:PHE:CZ	9:U:1222:LYS:HD3	2.51	0.45
2:B:86:LYS:HE2	2:B:97:ASP:HB3	1.98	0.45
4:D:71:SER:HB3	5:E:121:GLN:HG2	1.99	0.45
5:E:179:LEU:HA	5:E:182:VAL:HG12	1.99	0.45
8:I:298:ALA:O	8:I:302:ALA:N	2.48	0.45
4:O:4:TYR:O	4:O:21:TRP:N	2.41	0.45
10:K:519:PHE:H	9:U:992:ARG:HH21	1.65	0.45
9:U:734:ARG:NH2	9:U:828:GLU:O	2.43	0.45
3:F:68:ILE:HD13	3:F:151:SER:HB2	1.99	0.45
9:J:1011:SER:OG	9:J:1012:GLN:N	2.45	0.45
10:K:539:LYS:HD3	10:K:548:LEU:HD21	1.98	0.45
2:M:86:LYS:HE2	2:M:97:ASP:HB3	1.98	0.45
2:M:238:CYS:SG	2:M:239:LEU:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:16:ILE:HD12	5:P:202:ILE:HD11	1.98	0.45
5:E:21:PHE:HZ	5:E:215:VAL:HG21	1.82	0.45
3:F:49:PHE:O	3:F:53:ASN:ND2	2.50	0.45
8:I:803:GLU:HB3	8:I:856:LYS:HB3	1.99	0.45
4:O:71:SER:HB3	5:P:121:GLN:HG2	1.99	0.45
3:Q:49:PHE:O	3:Q:53:ASN:ND2	2.50	0.45
4:D:51:LEU:HD21	5:E:43:VAL:HG21	1.98	0.44
9:J:909:MET:SD	9:J:1117:MET:HE3	2.57	0.44
9:J:1216:PHE:CZ	9:J:1222:LYS:HD3	2.51	0.44
3:Q:188:ILE:CG2	3:Q:189:PRO:CD	2.80	0.44
6:R:169:MET:SD	7:S:106:TYR:OH	2.61	0.44
7:S:134:TYR:HA	7:S:137:VAL:HG12	2.00	0.44
8:T:459:TYR:C	8:T:464:LYS:CB	2.77	0.44
6:G:169:MET:SD	7:H:106:TYR:OH	2.60	0.44
5:P:6:ILE:HG22	5:P:19:ARG:HB2	1.98	0.44
3:Q:188:ILE:N	3:Q:189:PRO:CD	2.81	0.44
6:R:236:ILE:O	6:R:240:PHE:N	2.50	0.44
3:C:154:MET:HE2	3:C:154:MET:HB3	1.79	0.44
9:J:1085:TYR:OH	9:J:1196:PRO:O	2.34	0.44
9:U:789:LYS:NZ	9:U:791:THR:OG1	2.40	0.44
9:U:909:MET:SD	9:U:1117:MET:HE3	2.57	0.44
10:V:408:SER:OG	10:V:409:ASN:N	2.50	0.44
2:B:134:LEU:O	2:B:138:LEU:HD22	2.14	0.44
3:C:40:GLN:HE22	3:C:43:GLN:HE21	1.64	0.44
4:D:12:HIS:O	4:D:14:ASN:ND2	2.49	0.44
3:F:188:ILE:N	3:F:189:PRO:CD	2.81	0.44
3:N:40:GLN:HE22	3:N:43:GLN:HE21	1.64	0.44
4:O:4:TYR:C	4:O:21:TRP:HB2	2.41	0.44
5:P:133:GLN:OE1	3:Q:189:PRO:HG2	2.17	0.44
9:J:789:LYS:NZ	9:J:791:THR:OG1	2.40	0.44
3:Q:188:ILE:HG22	3:Q:189:PRO:HD3	1.93	0.44
8:T:803:GLU:HB3	8:T:856:LYS:HB3	2.00	0.44
8:T:1031:ASP:HA	8:T:1051:ARG:HA	1.99	0.44
5:E:114:TRP:NE1	3:F:77:LEU:O	2.42	0.44
6:G:168:LYS:C	7:H:135:GLN:NE2	2.76	0.44
3:Q:68:ILE:HD13	3:Q:151:SER:HB2	1.99	0.44
5:E:6:ILE:HG22	5:E:19:ARG:HB2	1.99	0.44
5:E:185:LEU:HD13	5:E:210:LYS:HB3	1.99	0.44
6:G:236:ILE:O	6:G:240:PHE:N	2.50	0.44
7:H:134:TYR:HA	7:H:137:VAL:HG12	2.00	0.44
2:B:238:CYS:SG	2:B:239:LEU:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:992:ARG:NH2	10:V:519:PHE:H	2.16	0.44
10:K:449:ASN:ND2	10:K:497:ALA:O	2.49	0.44
4:D:4:TYR:C	4:D:21:TRP:HB2	2.41	0.43
8:I:1031:ASP:HA	8:I:1051:ARG:HA	2.00	0.43
9:J:909:MET:SD	9:J:1117:MET:HE1	2.58	0.43
9:J:1216:PHE:CE1	9:J:1222:LYS:CB	2.80	0.43
2:M:176:LEU:HD11	2:M:184:PHE:HB3	2.00	0.43
3:Q:37:ILE:HD13	3:Q:37:ILE:HA	1.89	0.43
9:U:1213:ILE:HB	9:U:1237:LEU:HB3	2.00	0.43
5:E:173:GLN:O	5:E:177:ASN:ND2	2.49	0.43
8:I:464:LYS:N	8:I:464:LYS:HD3	2.31	0.43
5:P:179:LEU:HA	5:P:182:VAL:HG12	1.99	0.43
6:R:168:LYS:C	7:S:135:GLN:NE2	2.76	0.43
3:N:11:LYS:HB2	3:N:11:LYS:HE3	1.77	0.43
5:P:21:PHE:HZ	5:P:215:VAL:HG21	1.82	0.43
9:U:592:LEU:HD11	9:U:615:LEU:HD13	2.00	0.43
9:U:791:THR:HG22	9:U:792:TYR:H	1.83	0.43
1:A:30:MET:HG3	1:A:30:MET:O	2.19	0.43
1:A:80:LYS:NZ	2:B:146:LEU:O	2.43	0.43
3:F:119:LEU:O	3:F:174:THR:OG1	2.37	0.43
9:J:517:MET:HE2	9:J:517:MET:HB3	1.87	0.43
9:J:791:THR:HG22	9:J:792:TYR:H	1.83	0.43
10:K:519:PHE:H	9:U:992:ARG:NH2	2.16	0.43
5:P:185:LEU:HD13	5:P:210:LYS:HB3	2.00	0.43
2:B:143:ASN:HD21	2:B:146:LEU:HD23	1.82	0.43
2:B:176:LEU:HD11	2:B:184:PHE:HB3	2.00	0.43
9:U:1217:ASP:O	9:U:1218:SER:C	2.62	0.43
9:J:734:ARG:HA	9:J:734:ARG:HD3	1.62	0.43
9:U:487:ARG:C	9:U:491:TYR:CE1	2.97	0.43
9:U:909:MET:SD	9:U:1117:MET:HE1	2.58	0.43
9:U:1227:SER:OG	9:U:1227:SER:O	2.36	0.43
9:J:1213:ILE:HB	9:J:1237:LEU:HB3	2.00	0.43
4:O:123:TYR:HD1	4:O:123:TYR:H	1.62	0.43
3:F:149:LYS:O	3:F:153:GLU:N	2.50	0.43
9:J:592:LEU:HD11	9:J:615:LEU:HD13	2.00	0.43
2:M:177:LYS:HD2	2:M:177:LYS:HA	1.81	0.43
4:O:3:ILE:O	4:O:21:TRP:CG	2.72	0.43
1:A:141:PHE:O	1:A:145:PHE:N	2.51	0.42
3:C:47:ARG:HH22	3:C:131:PRO:HG2	1.84	0.42
4:D:4:TYR:OH	4:D:93:ASP:HB3	2.19	0.42
1:L:141:PHE:O	1:L:145:PHE:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:211:ILE:HG23	6:R:266:TYR:HB2	2.01	0.42
9:U:789:LYS:HZ2	9:U:789:LYS:HG2	1.64	0.42
5:E:133:GLN:OE1	3:F:189:PRO:HG2	2.17	0.42
3:F:107:ASN:HB2	3:F:116:SER:HB3	2.01	0.42
3:Q:119:LEU:O	3:Q:174:THR:OG1	2.37	0.42
3:Q:144:LEU:O	3:Q:148:LEU:N	2.48	0.42
6:G:169:MET:CG	7:H:87:CYS:SG	2.88	0.42
2:M:143:ASN:HD21	2:M:146:LEU:HD23	1.82	0.42
3:N:47:ARG:HH22	3:N:131:PRO:HG2	1.84	0.42
3:N:18:TRP:NE1	3:N:96:LYS:O	2.47	0.42
6:R:168:LYS:NZ	6:R:169:MET:HB2	2.34	0.42
6:G:173:ASP:OD1	6:G:173:ASP:N	2.45	0.42
8:I:306:ILE:O	8:I:310:ILE:N	2.46	0.42
8:I:333:SER:O	8:I:337:TYR:N	2.49	0.42
9:J:1227:SER:OG	9:J:1231:ILE:O	2.29	0.42
3:Q:107:ASN:HB2	3:Q:116:SER:HB3	2.01	0.42
3:Q:149:LYS:O	3:Q:153:GLU:N	2.50	0.42
8:T:770:SER:N	8:T:789:ASN:O	2.49	0.42
9:U:471:ASN:ND2	9:U:495:ASN:OD1	2.52	0.42
9:U:773:VAL:HG23	9:U:779:ARG:HB3	2.01	0.42
9:U:1227:SER:OG	9:U:1231:ILE:O	2.29	0.42
6:G:50:LEU:HD22	7:H:139:GLU:HG3	2.02	0.42
9:J:663:LEU:HA	9:J:736:GLN:NE2	2.35	0.42
5:P:148:MET:HE2	5:P:148:MET:HB3	1.89	0.42
8:T:784:PHE:HB2	8:T:839:TYR:HB2	2.01	0.42
4:D:3:ILE:O	4:D:21:TRP:CG	2.72	0.42
5:E:68:PRO:HG3	5:E:111:PHE:CD2	2.54	0.42
4:O:40:ASP:O	4:O:44:LEU:HB3	2.19	0.42
5:P:68:PRO:HG3	5:P:111:PHE:CD2	2.54	0.42
6:G:211:ILE:HG23	6:G:266:TYR:HB2	2.02	0.42
6:G:276:ASP:O	6:G:280:LEU:N	2.53	0.42
7:H:130:MET:HE2	7:H:130:MET:HB3	1.88	0.42
9:J:633:LYS:HA	9:J:633:LYS:HD2	1.80	0.42
9:J:1056:VAL:H	9:J:1063:SER:HG	1.68	0.42
9:J:1217:ASP:O	9:J:1218:SER:C	2.62	0.42
1:L:30:MET:O	1:L:30:MET:HG3	2.19	0.42
3:Q:68:ILE:HG21	3:Q:154:MET:HB3	2.02	0.42
9:U:1004:PRO:HA	9:U:1038:ILE:HA	2.01	0.42
9:U:1176:LEU:HD11	9:U:1193:ILE:HD11	2.02	0.42
3:C:56:LEU:HD23	3:C:56:LEU:HA	1.94	0.42
3:C:92:LYS:HB3	3:C:92:LYS:HE2	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:ASP:O	4:D:44:LEU:HB3	2.19	0.42
9:J:773:VAL:HG23	9:J:779:ARG:HB3	2.01	0.42
5:E:148:MET:HE2	5:E:148:MET:HB3	1.88	0.41
9:J:479:ILE:O	9:J:480:PRO:C	2.57	0.41
4:O:4:TYR:OH	4:O:93:ASP:HB3	2.19	0.41
8:I:784:PHE:HB2	8:I:839:TYR:HB2	2.02	0.41
9:J:1272:ASN:ND2	9:J:1273:GLN:O	2.54	0.41
9:U:1272:ASN:ND2	9:U:1273:GLN:O	2.54	0.41
5:E:53:LYS:HA	5:E:53:LYS:HD3	1.90	0.41
9:J:1176:LEU:HD11	9:J:1193:ILE:HD11	2.02	0.41
3:Q:41:LEU:HD23	3:Q:41:LEU:HA	1.96	0.41
9:U:903:PRO:HA	9:U:906:TRP:HB2	2.02	0.41
9:J:471:ASN:ND2	9:J:495:ASN:OD1	2.53	0.41
9:J:487:ARG:C	9:J:491:TYR:CE1	2.97	0.41
8:T:770:SER:O	8:T:789:ASN:N	2.53	0.41
2:B:177:LYS:HA	2:B:177:LYS:HD2	1.81	0.41
9:J:1004:PRO:HA	9:J:1038:ILE:HA	2.01	0.41
9:J:1259:GLY:HA2	9:J:1288:VAL:H	1.86	0.41
9:U:484:MET:O	9:U:484:MET:SD	2.79	0.41
1:A:8:VAL:HG12	1:A:88:ILE:HG23	2.03	0.41
2:B:59:ILE:HD12	2:B:59:ILE:HA	1.88	0.41
3:C:66:ARG:HA	3:C:66:ARG:HD3	1.87	0.41
3:F:183:ILE:HG13	3:F:184:LEU:H	1.86	0.41
4:D:5:SER:HG	4:D:7:TRP:HE1	1.66	0.41
3:F:68:ILE:HG21	3:F:154:MET:HB3	2.02	0.41
1:L:77:MET:HE2	1:L:77:MET:HB3	1.71	0.41
5:P:2:ALA:O	5:P:144:SER:OG	2.33	0.41
8:T:596:ALA:HA	8:T:605:GLU:HA	2.03	0.41
9:U:482:SER:O	9:U:484:MET:CE	2.68	0.41
4:D:60:LYS:O	5:E:126:GLN:NE2	2.46	0.41
8:I:855:LEU:HD13	8:I:857:VAL:HG23	2.03	0.41
8:I:1044:TRP:O	8:I:1061:PHE:N	2.54	0.41
9:J:482:SER:O	9:J:484:MET:CE	2.68	0.41
9:J:484:MET:O	9:J:484:MET:SD	2.79	0.41
9:J:607:TYR:HD1	9:J:607:TYR:HA	1.80	0.41
9:J:758:CYS:HA	9:J:801:LEU:HB2	2.03	0.41
3:Q:183:ILE:HG13	3:Q:184:LEU:H	1.86	0.41
9:U:758:CYS:HA	9:U:801:LEU:HB2	2.03	0.41
9:J:1138:THR:HG23	9:J:1139:THR:HG23	2.03	0.41
1:L:80:LYS:NZ	2:M:146:LEU:O	2.43	0.41
2:M:136:GLU:O	2:M:139:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:870:ILE:O	8:T:874:VAL:CB	2.69	0.41
3:F:28:GLU:OE1	6:G:190:TYR:OH	2.37	0.40
9:J:1281:SER:HB2	10:K:494:ARG:HH12	1.86	0.40
1:L:8:VAL:HG12	1:L:88:ILE:HG23	2.03	0.40
3:F:188:ILE:HG22	3:F:189:PRO:HD3	1.92	0.40
6:G:38:THR:HA	7:H:170:ARG:HD3	2.03	0.40
6:G:66:PHE:HE2	6:G:219:THR:HB	1.87	0.40
9:J:789:LYS:NZ	9:J:790:PRO:O	2.54	0.40
2:M:157:MET:HA	2:M:160:ILE:HG22	2.03	0.40
8:T:333:SER:O	8:T:337:TYR:N	2.49	0.40
6:G:102:LEU:HD23	6:G:102:LEU:HA	1.93	0.40
8:I:870:ILE:O	8:I:874:VAL:CB	2.69	0.40
9:J:519:GLU:HG3	9:J:522:ARG:HH22	1.86	0.40
3:N:114:THR:OG1	3:N:115:PHE:N	2.55	0.40
3:N:154:MET:HB3	3:N:154:MET:HE2	1.79	0.40
6:R:38:THR:HA	7:S:170:ARG:HD3	2.03	0.40
8:T:855:LEU:HD13	8:T:857:VAL:HG23	2.03	0.40
9:U:519:GLU:HG3	9:U:522:ARG:HH22	1.86	0.40
9:U:1259:GLY:HA2	9:U:1288:VAL:H	1.86	0.40
9:J:903:PRO:HA	9:J:906:TRP:HB2	2.02	0.40
3:N:167:ILE:HD13	3:N:167:ILE:HA	1.95	0.40
8:T:1044:TRP:O	8:T:1061:PHE:N	2.54	0.40
9:U:1216:PHE:CE1	9:U:1222:LYS:HD3	2.57	0.40
9:U:1281:SER:HB2	10:V:494:ARG:HH12	1.86	0.40
2:B:104:LEU:HD12	2:B:104:LEU:HA	1.93	0.40
3:C:62:ASN:C	3:C:62:ASN:HD22	2.28	0.40
8:I:596:ALA:HA	8:I:605:GLU:HA	2.03	0.40
10:K:249:TYR:HA	10:K:253:HIS:H	1.87	0.40
3:N:62:ASN:C	3:N:62:ASN:HD22	2.28	0.40
6:R:50:LEU:HD22	7:S:139:GLU:HG3	2.02	0.40
9:U:517:MET:HE2	9:U:517:MET:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
1	L	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
2	B	196/268 (73%)	186 (95%)	10 (5%)	0	100	100
2	M	196/268 (73%)	186 (95%)	10 (5%)	0	100	100
3	C	182/193 (94%)	167 (92%)	15 (8%)	0	100	100
3	F	180/193 (93%)	172 (96%)	8 (4%)	0	100	100
3	N	182/193 (94%)	167 (92%)	15 (8%)	0	100	100
3	Q	180/193 (93%)	172 (96%)	8 (4%)	0	100	100
4	D	147/159 (92%)	137 (93%)	10 (7%)	0	100	100
4	O	147/159 (92%)	137 (93%)	10 (7%)	0	100	100
5	E	153/219 (70%)	145 (95%)	8 (5%)	0	100	100
5	P	153/219 (70%)	145 (95%)	8 (5%)	0	100	100
6	G	200/283 (71%)	187 (94%)	11 (6%)	2 (1%)	12	47
6	R	200/283 (71%)	187 (94%)	11 (6%)	2 (1%)	12	47
7	H	143/175 (82%)	134 (94%)	9 (6%)	0	100	100
7	S	143/175 (82%)	134 (94%)	9 (6%)	0	100	100
8	I	782/1102 (71%)	679 (87%)	89 (11%)	14 (2%)	6	33
8	T	782/1102 (71%)	679 (87%)	89 (11%)	14 (2%)	6	33
9	J	860/1289 (67%)	730 (85%)	124 (14%)	6 (1%)	18	55
9	U	860/1289 (67%)	731 (85%)	123 (14%)	6 (1%)	18	55
10	K	243/560 (43%)	212 (87%)	26 (11%)	5 (2%)	5	30
10	V	243/560 (43%)	212 (87%)	26 (11%)	5 (2%)	5	30
All	All	6456/9186 (70%)	5773 (89%)	629 (10%)	54 (1%)	18	52

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	170	ARG
8	I	346	PRO
8	I	483	PRO
8	I	639	PRO
8	I	969	VAL
8	I	976	PRO

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Mol	Chain	Res	Type
8	I	980	PRO
8	I	1076	PRO
10	K	286	PRO
10	K	310	PRO
10	K	325	PRO
10	K	330	PRO
6	R	170	ARG
8	T	346	PRO
8	T	483	PRO
8	T	639	PRO
8	T	969	VAL
8	T	976	PRO
8	T	980	PRO
8	T	1076	PRO
10	V	286	PRO
10	V	310	PRO
10	V	325	PRO
10	V	330	PRO
8	I	647	VAL
8	I	735	ILE
9	J	1100	PRO
6	R	168	LYS
8	T	647	VAL
9	U	1100	PRO
6	G	168	LYS
9	J	956	PRO
8	T	735	ILE
9	U	956	PRO
9	J	486	PRO
9	J	736	GLN
9	U	486	PRO
10	K	282	PRO
10	V	282	PRO
8	I	1028	VAL
9	J	955	VAL
8	T	1028	VAL
9	U	955	VAL
8	I	487	VAL
8	I	975	VAL
8	I	1029	ILE
8	T	487	VAL
8	T	975	VAL

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Mol	Chain	Res	Type
8	T	1029	ILE
9	J	297	VAL
9	U	297	VAL
8	I	571	PHE
8	T	571	PHE
9	U	480	PRO

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	134/142 (94%)	134 (100%)	0	100	100
1	L	134/142 (94%)	133 (99%)	1 (1%)	76	79
2	B	180/248 (73%)	178 (99%)	2 (1%)	65	74
2	M	180/248 (73%)	178 (99%)	2 (1%)	65	74
3	C	169/178 (95%)	169 (100%)	0	100	100
3	F	168/178 (94%)	168 (100%)	0	100	100
3	N	169/178 (95%)	169 (100%)	0	100	100
3	Q	168/178 (94%)	168 (100%)	0	100	100
4	D	135/145 (93%)	135 (100%)	0	100	100
4	O	135/145 (93%)	135 (100%)	0	100	100
5	E	147/199 (74%)	146 (99%)	1 (1%)	76	79
5	P	147/199 (74%)	146 (99%)	1 (1%)	76	79
6	G	181/249 (73%)	179 (99%)	2 (1%)	65	74
6	R	181/249 (73%)	179 (99%)	2 (1%)	65	74
7	H	127/152 (84%)	127 (100%)	0	100	100
7	S	127/152 (84%)	127 (100%)	0	100	100
8	I	78/1023 (8%)	77 (99%)	1 (1%)	61	72
8	T	78/1023 (8%)	77 (99%)	1 (1%)	61	72
9	J	574/1213 (47%)	569 (99%)	5 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	U	574/1213 (47%)	570 (99%)	4 (1%)	76	79
10	K	121/518 (23%)	121 (100%)	0	100	100
10	V	121/518 (23%)	121 (100%)	0	100	100
All	All	4028/8490 (47%)	4006 (100%)	22 (0%)	78	81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	ILE
2	B	140	PHE
5	E	67	ILE
6	G	168	LYS
6	G	169	MET
8	I	464	LYS
9	J	485	PHE
9	J	487	ARG
9	J	734	ARG
9	J	736	GLN
9	J	907	LYS
1	L	77	MET
2	M	139	ILE
2	M	140	PHE
5	P	67	ILE
6	R	168	LYS
6	R	169	MET
8	T	464	LYS
9	U	485	PHE
9	U	487	ARG
9	U	736	GLN
9	U	907	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	107	GLN
2	B	50	ASN
2	B	142	ASN
2	B	143	ASN
3	C	40	GLN

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Mol	Chain	Res	Type
4	D	96	GLN
4	D	130	ASN
4	D	142	ASN
5	E	23	ASN
5	E	133	GLN
3	F	40	GLN
3	F	104	ASN
3	F	142	ASN
6	G	30	GLN
6	G	55	GLN
7	H	129	ASN
7	H	135	GLN
8	I	854	ASN
9	J	603	ASN
9	J	637	GLN
9	J	823	ASN
9	J	1012	GLN
9	J	1089	ASN
9	J	1092	ASN
9	J	1134	ASN
9	J	1234	ASN
10	K	448	ASN
10	K	490	HIS
10	K	544	ASN
1	L	92	GLN
1	L	107	GLN
2	M	50	ASN
2	M	142	ASN
2	M	143	ASN
3	N	40	GLN
4	O	96	GLN
4	O	130	ASN
4	O	142	ASN
5	P	23	ASN
5	P	133	GLN
3	Q	40	GLN
3	Q	104	ASN
3	Q	142	ASN
6	R	30	GLN
6	R	55	GLN
7	S	129	ASN
7	S	135	GLN

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Mol	Chain	Res	Type
8	T	854	ASN
9	U	603	ASN
9	U	637	GLN
9	U	823	ASN
9	U	1089	ASN
9	U	1134	ASN
9	U	1234	ASN
10	V	448	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

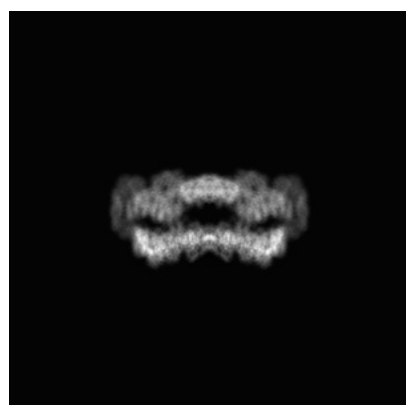
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31021. These allow visual inspection of the internal detail of the map and identification of artifacts.

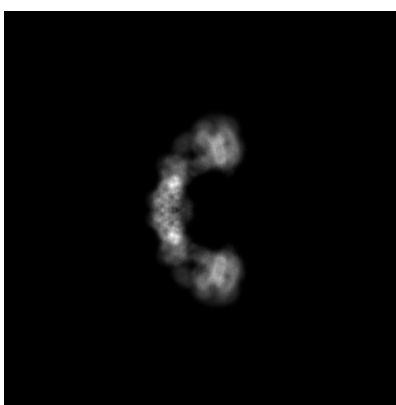
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

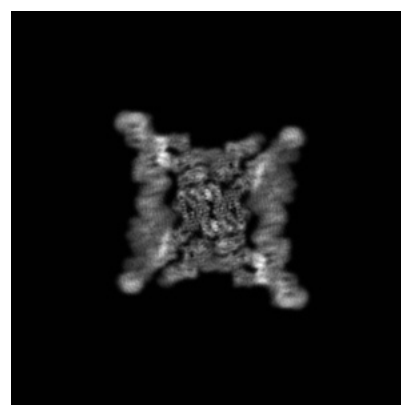
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

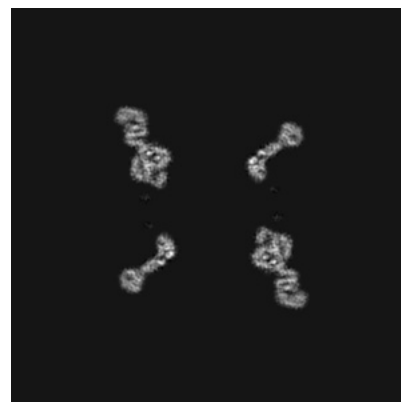
6.2.1 Primary map



X Index: 240



Y Index: 240

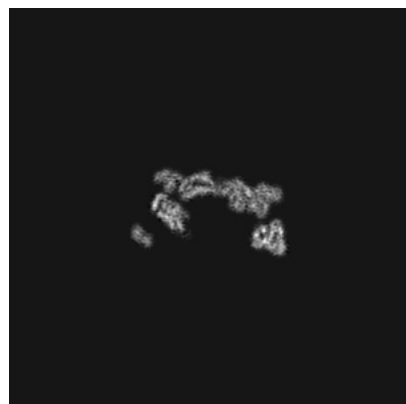


Z Index: 240

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

6.3 Largest variance slices [i](#)

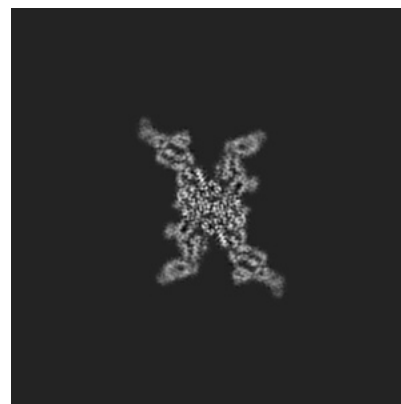
6.3.1 Primary map



X Index: 182



Y Index: 181

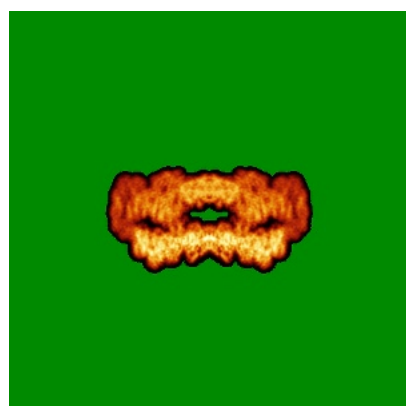


Z Index: 205

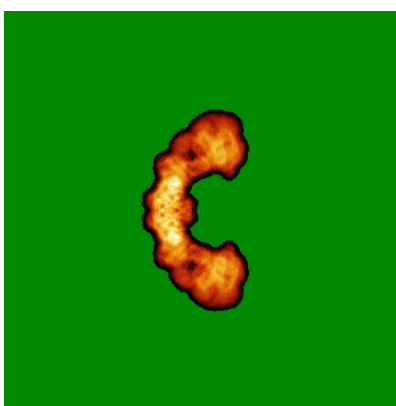
The images above show the largest variance slices of the map in three orthogonal directions.

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

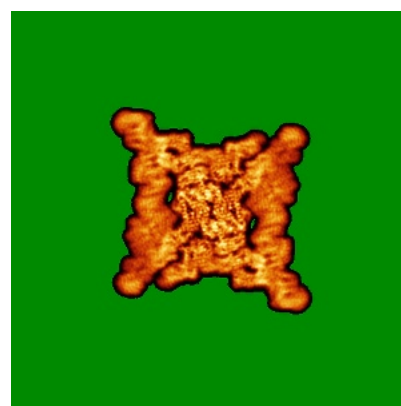
6.4.1 Primary map



X



Y

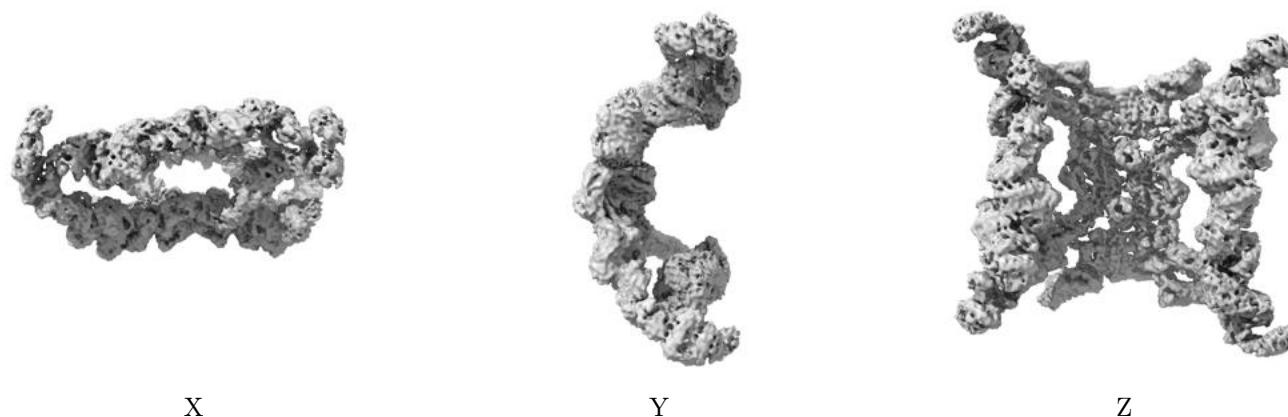


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

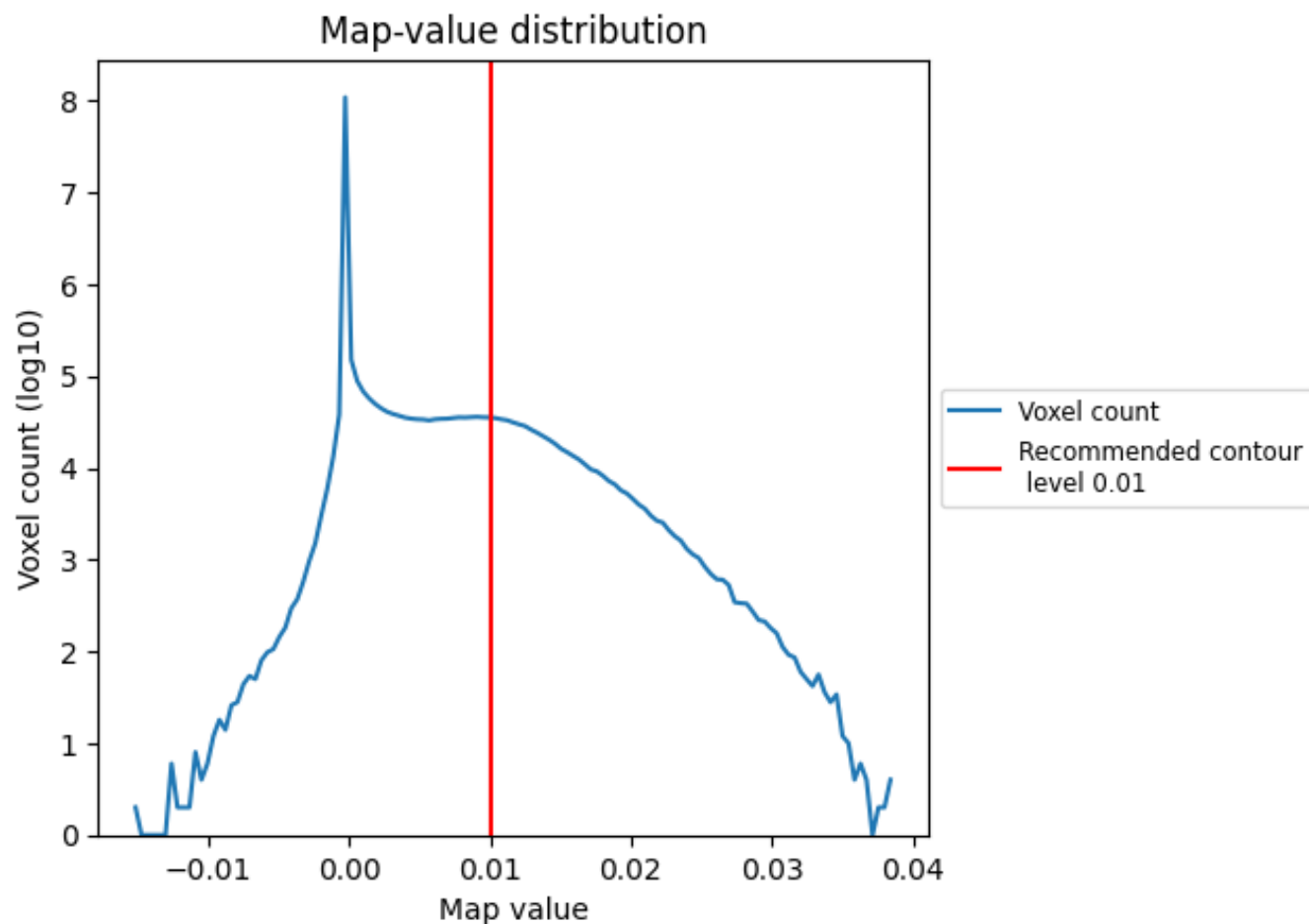
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

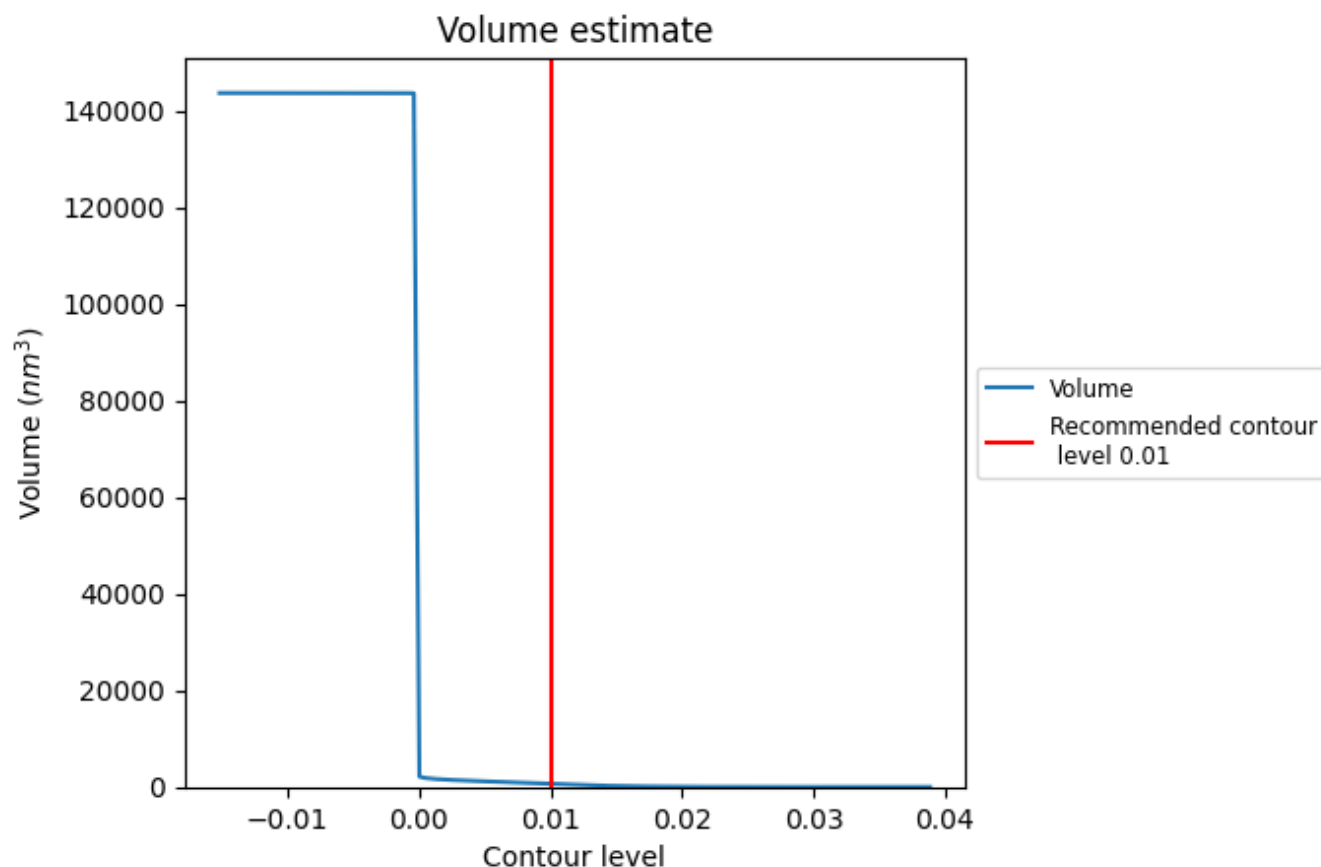
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

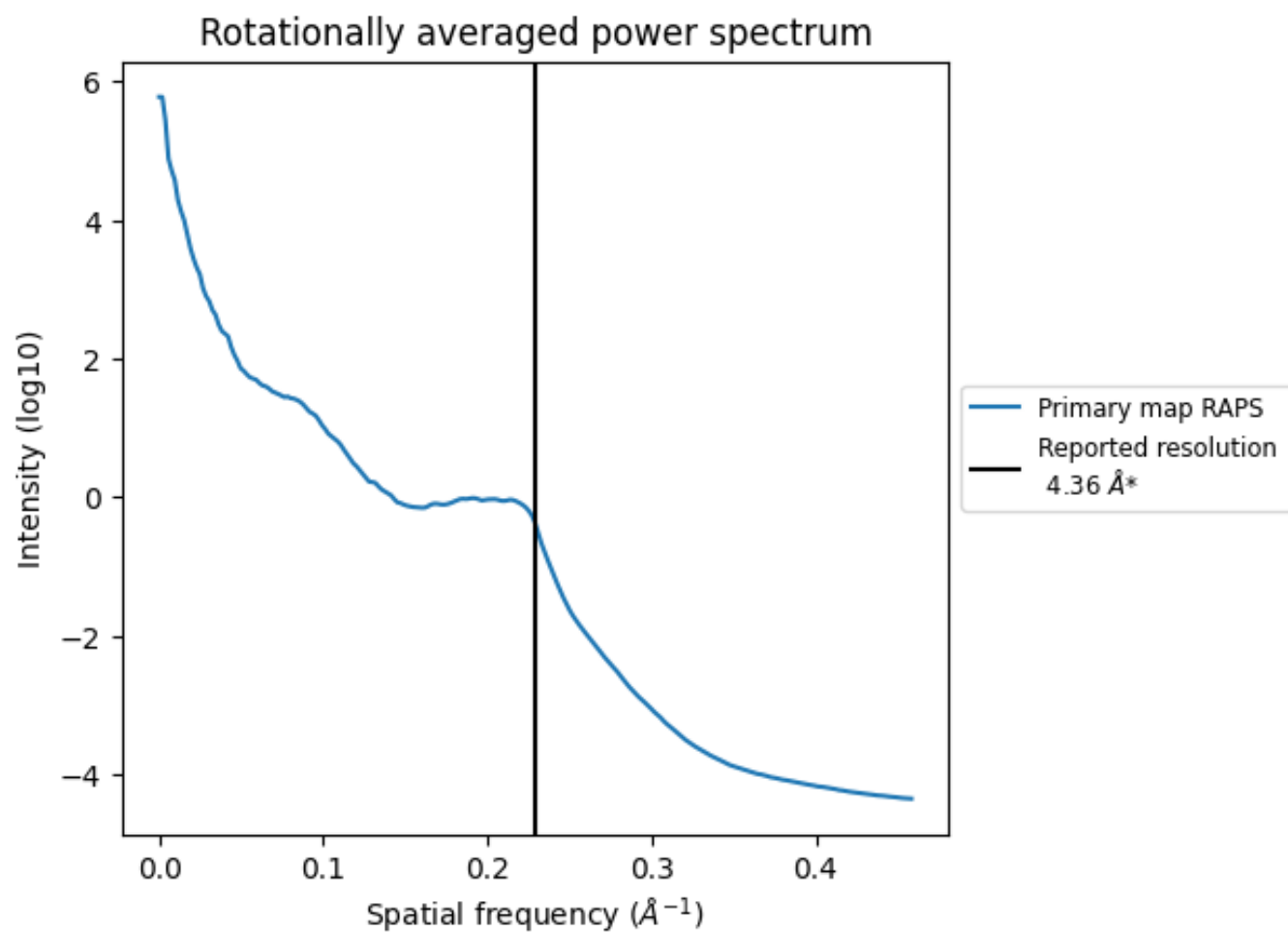
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 633 nm^3 ; this corresponds to an approximate mass of 571 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 0.229 $\text{\AA}^{-1}$

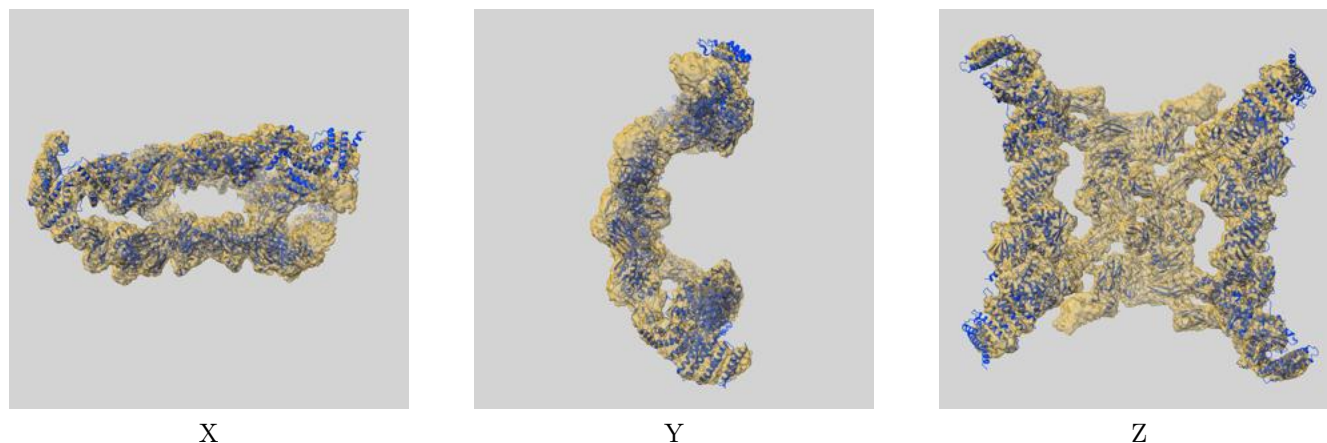
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

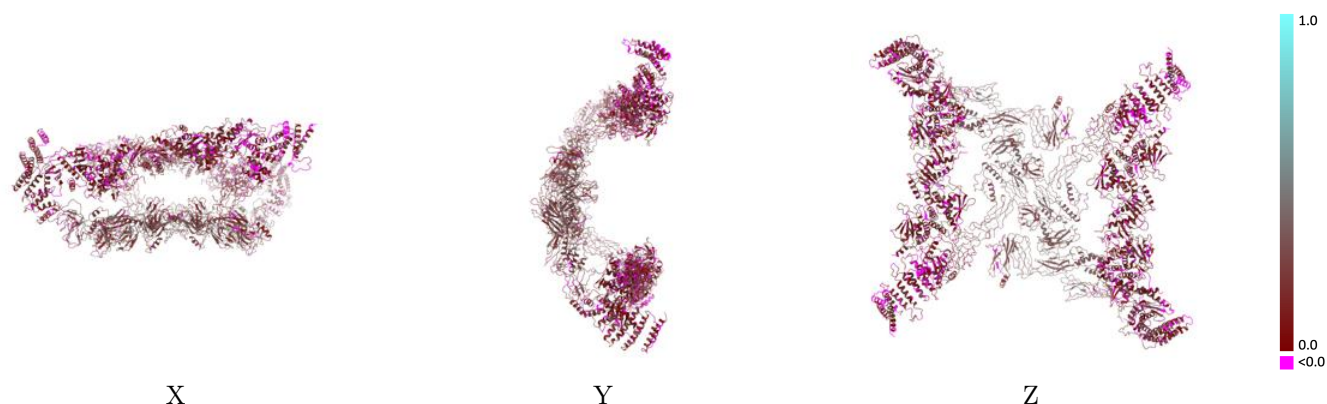
This section contains information regarding the fit between EMDB map EMD-31021 and PDB model 7E8S. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



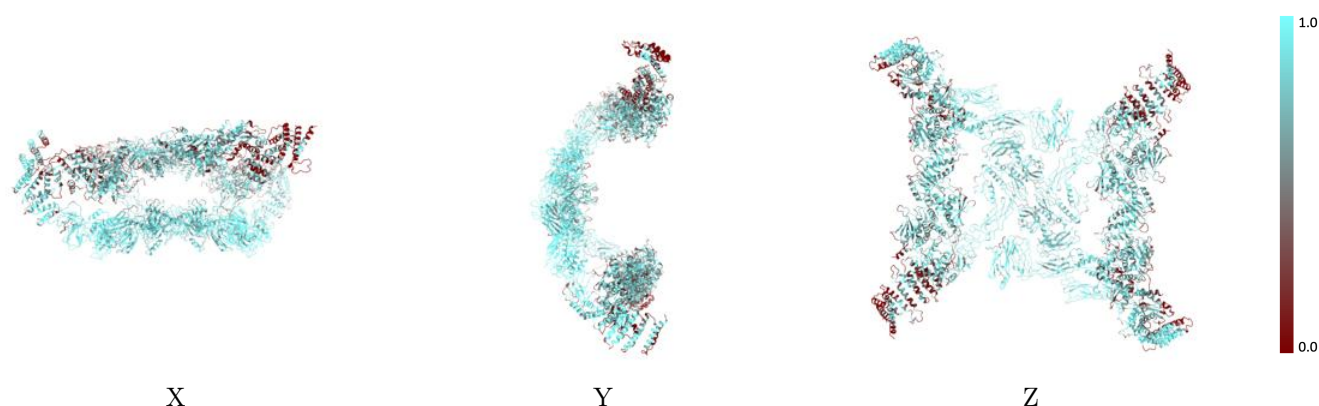
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



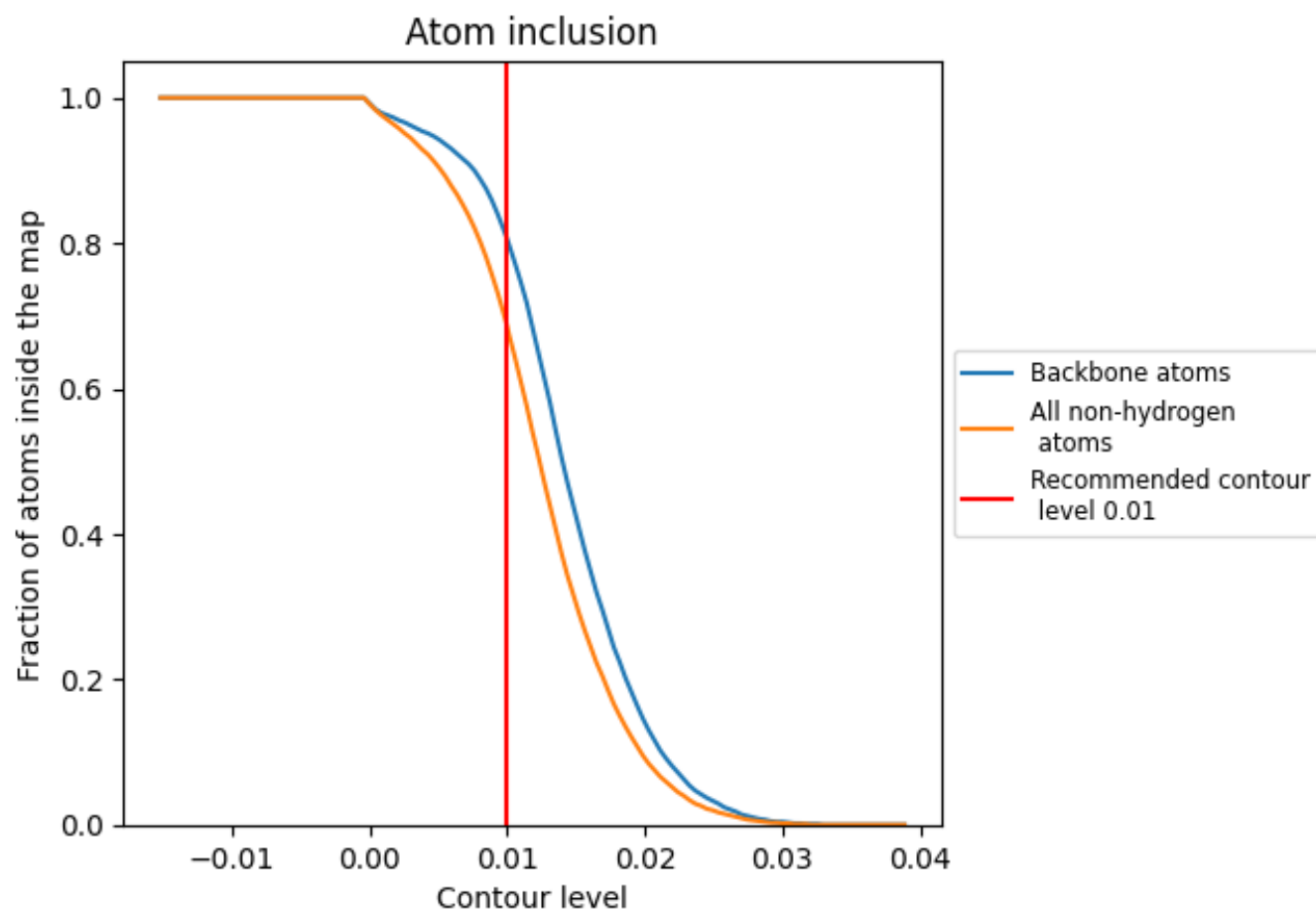
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 69% 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	 0.6860	 0.1710
A	 0.4140	 0.0930
B	 0.5580	 0.1000
C	 0.6310	 0.1440
D	 0.6900	 0.1180
E	 0.6860	 0.1510
F	 0.7010	 0.1530
G	 0.6100	 0.1470
H	 0.5360	 0.0650
I	 0.8550	 0.2280
J	 0.6780	 0.2030
K	 0.8100	 0.2300
L	 0.4150	 0.0880
M	 0.5570	 0.1000
N	 0.6330	 0.1400
O	 0.6900	 0.1190
P	 0.6880	 0.1490
Q	 0.7000	 0.1530
R	 0.6080	 0.1440
S	 0.5360	 0.0630
T	 0.8540	 0.2310
U	 0.6780	 0.2000
V	 0.8090	 0.2310

