



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 10:43 AM JST

PDB ID : 7EA3
EMDB ID : EMD-31038
Title : Intact Ypt32-TRAPP2 (dimer).
Authors : Mi, C.C.; Sui, S.F.
Deposited on : 2021-03-06
Resolution : 4.31 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

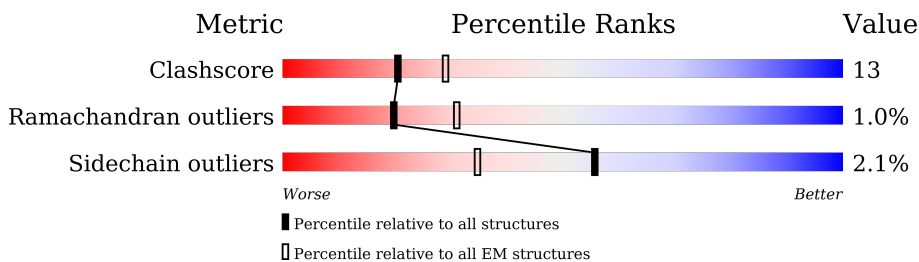
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.31 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	152	
1	N	152	
2	B	268	
2	O	268	
3	C	193	
3	F	193	
3	P	193	
3	S	193	

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Mol	Chain	Length	Quality of chain
4	D	154	<p>6% 77% 19% ..</p>
4	Q	154	<p>6% 78% 19% ..</p>
5	E	219	<p>5% 63% 10% 26%</p>
5	R	219	<p>5% 63% 10% 26%</p>
6	G	283	<p>9% 61% 9% . 29%</p>
6	T	283	<p>9% 61% 9% . 29%</p>
7	H	175	<p>17% 67% 17% 16%</p>
7	U	175	<p>17% 62% 18% 5% 16%</p>
8	I	1102	<p>8% 66% 5% . 28%</p>
8	V	1102	<p>8% 66% 5% . 28%</p>
9	J	1289	<p>7% 55% 12% . 31%</p>
9	W	1289	<p>7% 55% 12% . 31%</p>
10	K	560	<p>. 39% 5% . 55%</p>
10	X	560	<p>. 38% 6% . 55%</p>
11	L	222	<p>9% 58% 26% . 13%</p>
11	Y	222	<p>9% 58% 26% . 13%</p>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 49714 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
			Total	C	N	O	S		
1	A	144	Total	C	N	O	S	0	0
			1160	753	182	221	4		
1	N	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
			Total	C	N	O	S		
2	B	197	Total	C	N	O	S	0	0
			1590	1027	268	287	8		
2	O	197	Total	C	N	O	S	0	0
			1590	1027	268	287	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	185	Total	C	N	O	S	0	0
			1488	950	242	285	11		
3	F	183	Total	C	N	O	S	0	0
			1478	945	243	279	11		
3	P	185	Total	C	N	O	S	0	0
			1488	950	242	285	11		
3	S	183	Total	C	N	O	S	0	0
			1478	945	243	279	11		

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

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP Q03630
D	?	-	THR	deletion	UNP Q03630
D	?	-	ILE	deletion	UNP Q03630
D	?	-	ASN	deletion	UNP Q03630
D	?	-	SER	deletion	UNP Q03630
Q	?	-	GLY	deletion	UNP Q03630
Q	?	-	THR	deletion	UNP Q03630
Q	?	-	ILE	deletion	UNP Q03630
Q	?	-	ASN	deletion	UNP Q03630
Q	?	-	SER	deletion	UNP Q03630

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	162	1308	846	208	244	10	0	0
5	R	162	1308	846	208	244	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	202	1624	1035	280	300	9	0	0
6	T	202	1624	1035	280	300	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	788	Total	C	N	O	S	0	0
			4199	2553	811	833	2		
8	V	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
V	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
			Total	C	N	O	S		
9	J	883	Total	C	N	O	S	0	0
			6462	4120	1117	1206	19		
9	W	883	Total	C	N	O	S	0	0
			6462	4120	1117	1206	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1099	PHE	TYR	conflict	UNP Q04183
W	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
			Total	C	N	O	S		
10	K	251	Total	C	N	O	S	0	0
			1649	1041	291	315	2		
10	X	251	Total	C	N	O	S	0	0
			1649	1041	291	315	2		

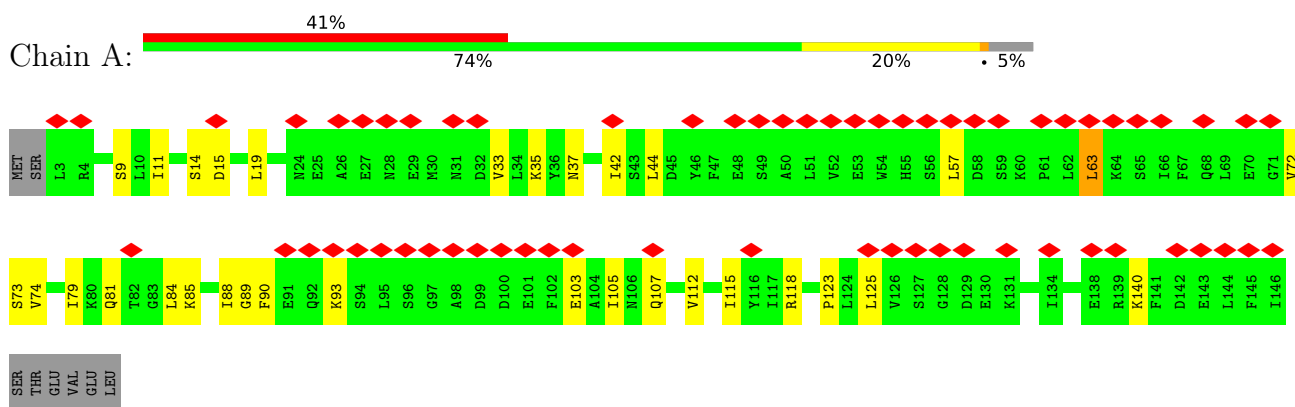
- Molecule 11 is a protein called GTP-binding protein YPT32/YPT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	194	Total	C	N	O	S	0	0
			1484	930	254	296	4		
11	Y	194	Total	C	N	O	S	0	0
			1484	930	254	296	4		

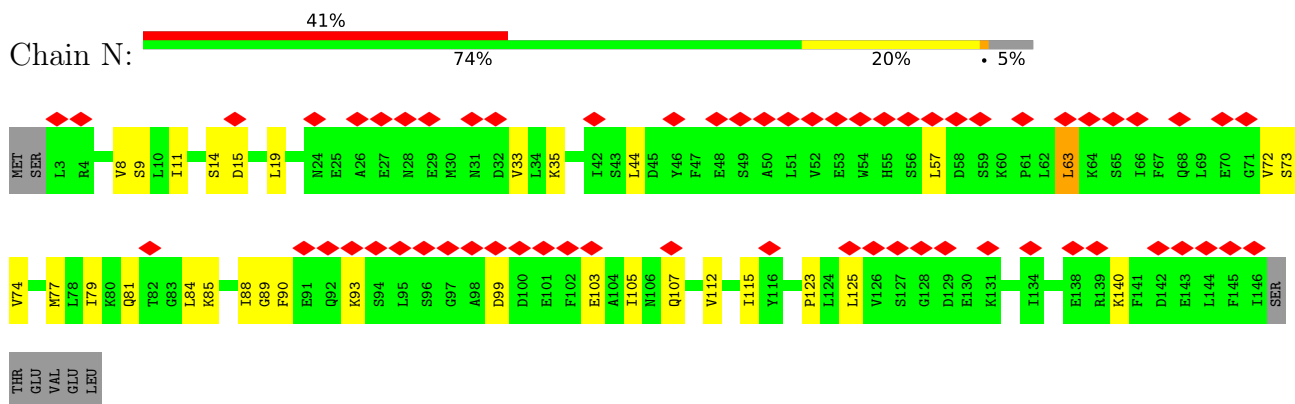
3 Residue-property plots i

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

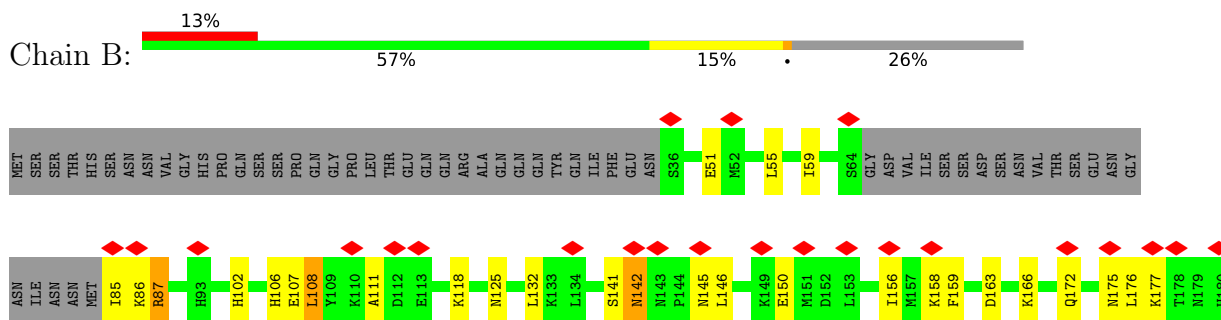
- Molecule 1: TRAPP-associated protein TCA17



- Molecule 1: TRAPP-associated protein TCA17

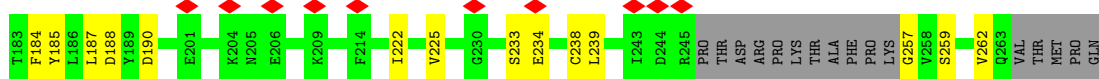
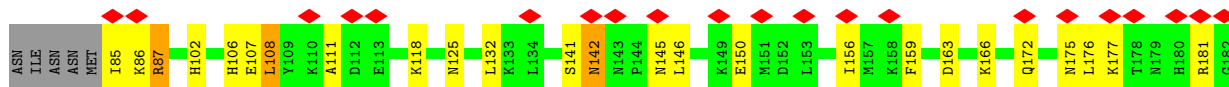
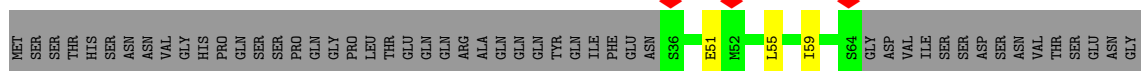


- Molecule 2: Trafficking protein particle complex subunit 33

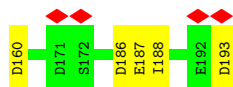
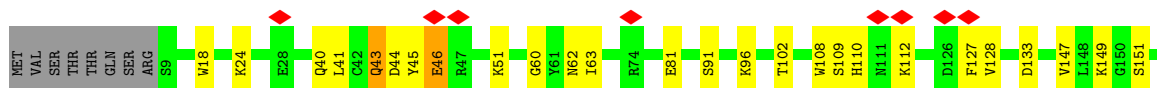
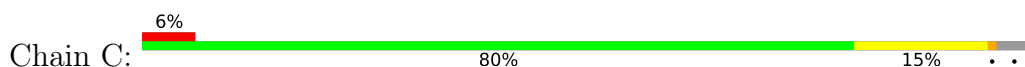




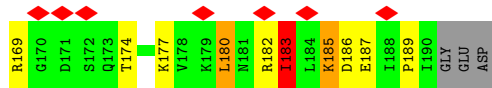
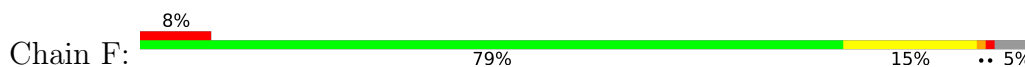
• Molecule 2: Trafficking protein particle complex subunit 33



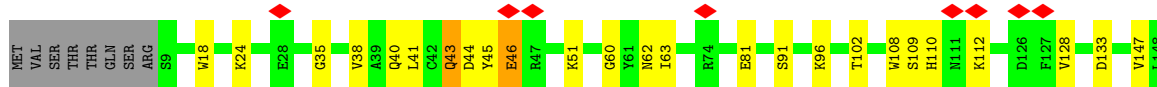
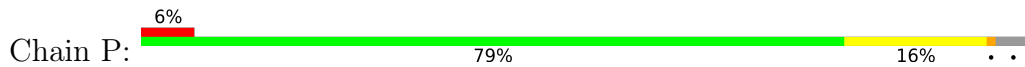
• Molecule 3: Trafficking protein particle complex subunit BET3

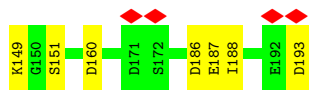


• Molecule 3: Trafficking protein particle complex subunit BET3

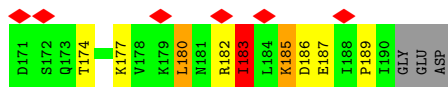
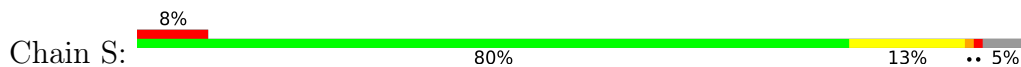


• Molecule 3: Trafficking protein particle complex subunit BET3

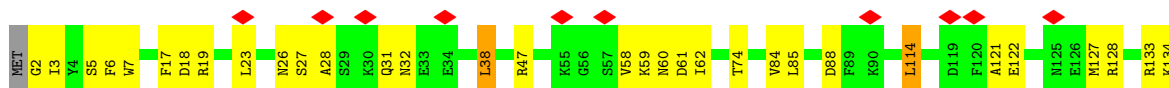
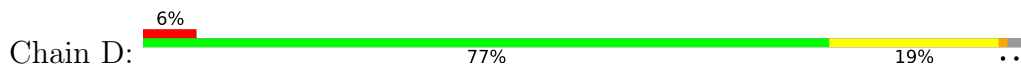




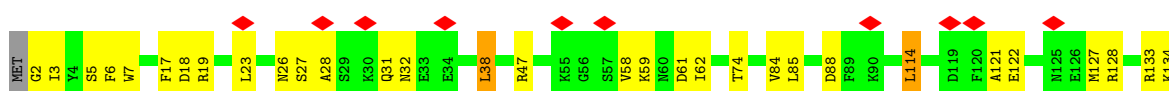
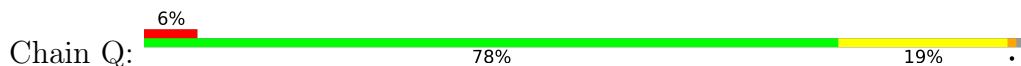
• Molecule 3: Trafficking protein particle complex subunit BET3



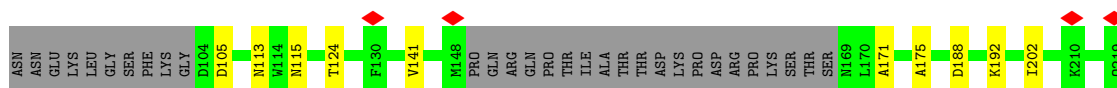
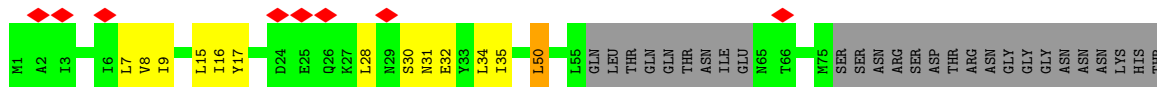
• Molecule 4: Trafficking protein particle complex subunit BET5



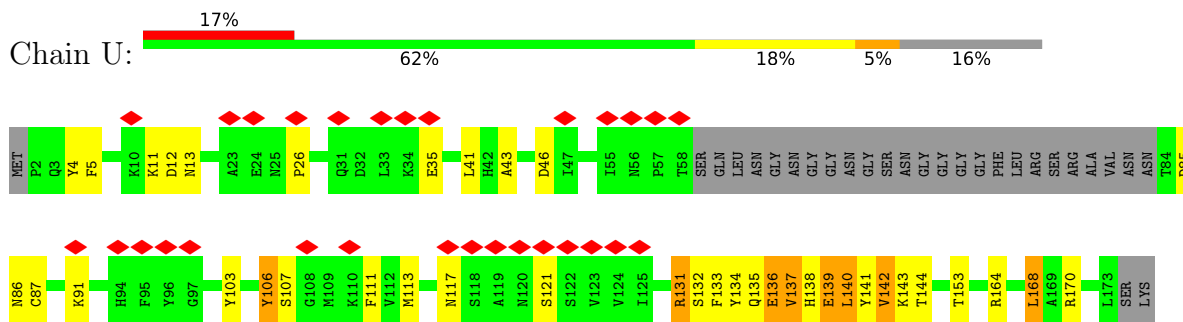
• Molecule 4: Trafficking protein particle complex subunit BET5



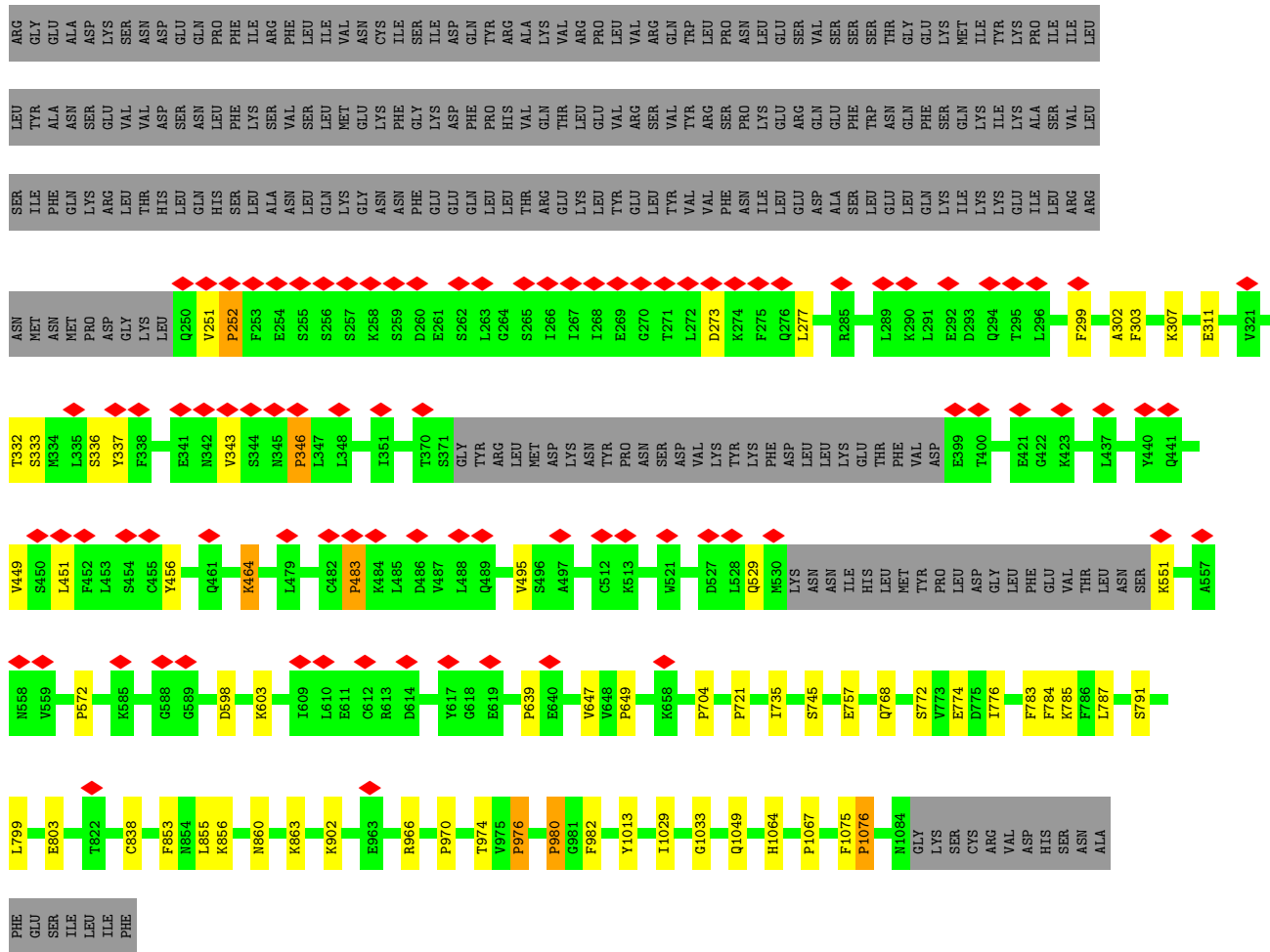
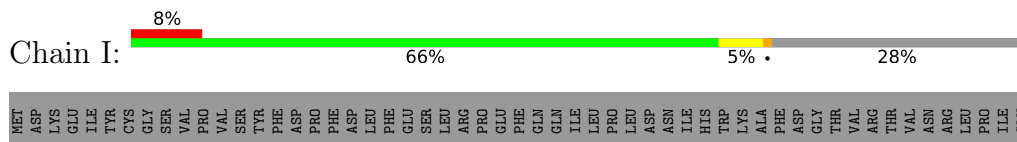
• Molecule 5: Trafficking protein particle complex subunit 23



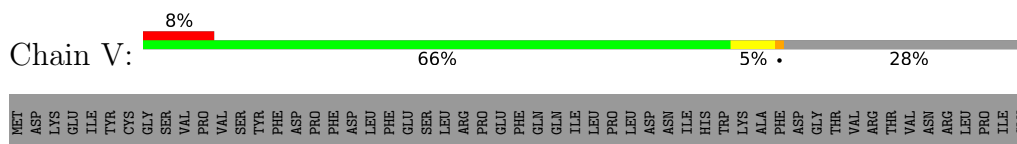
• Molecule 5: Trafficking protein particle complex subunit 23

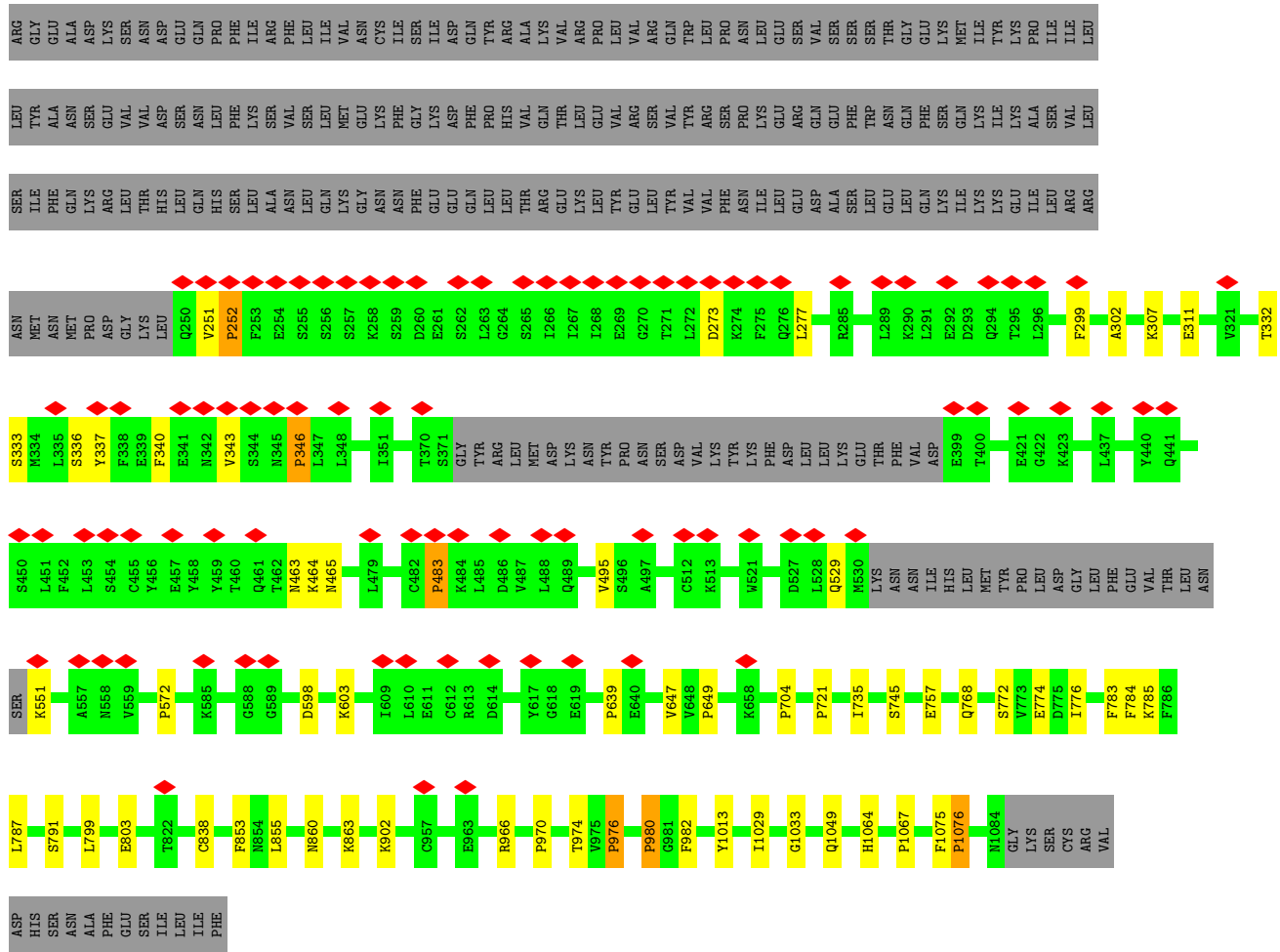


● Molecule 8: Trafficking protein particle complex II-specific subunit 130

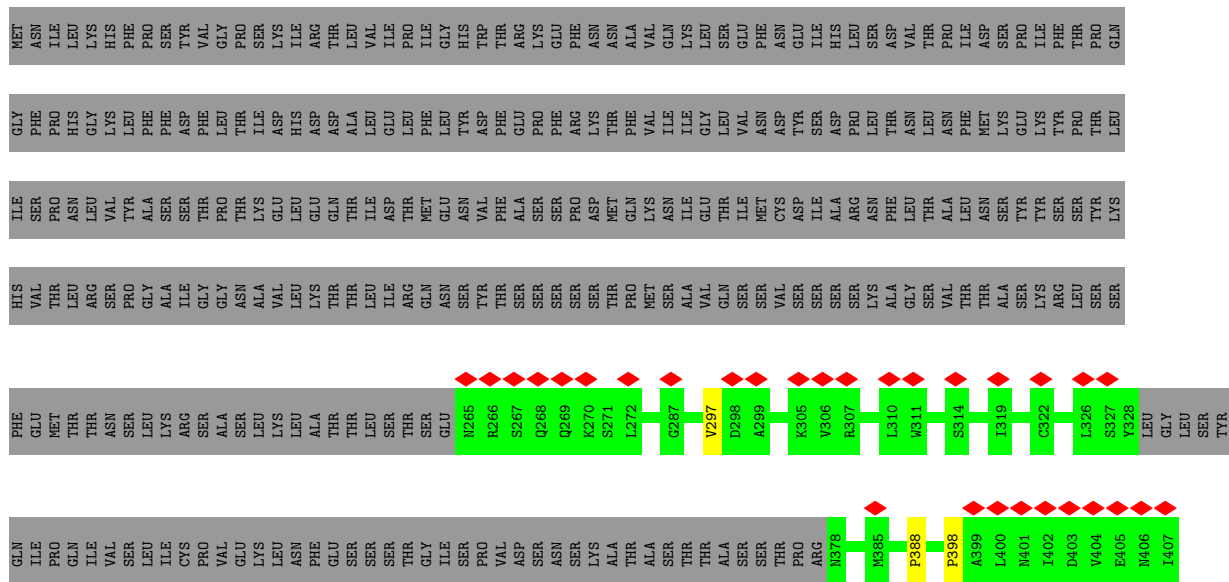


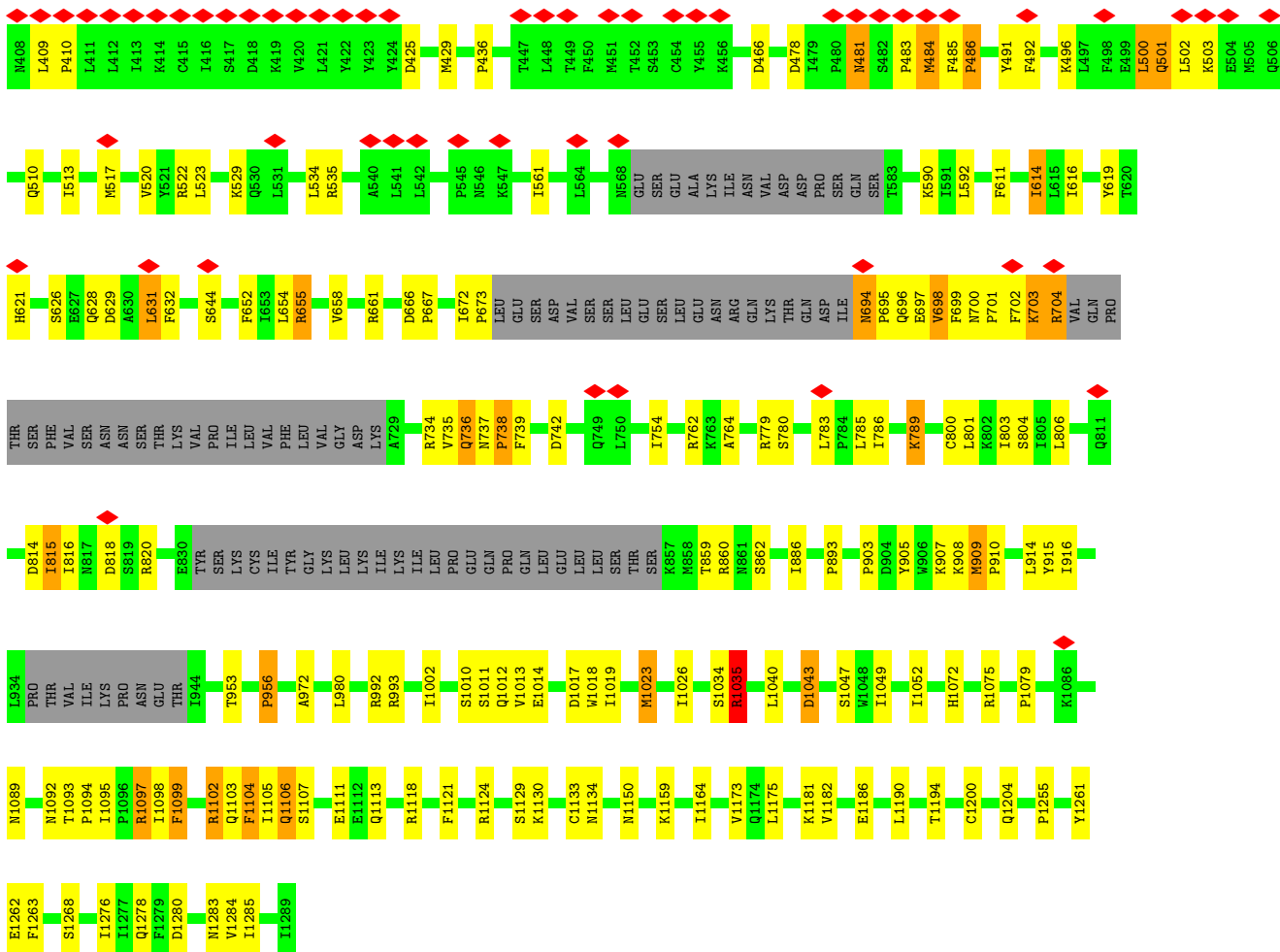
● Molecule 8: Trafficking protein particle complex II-specific subunit 130



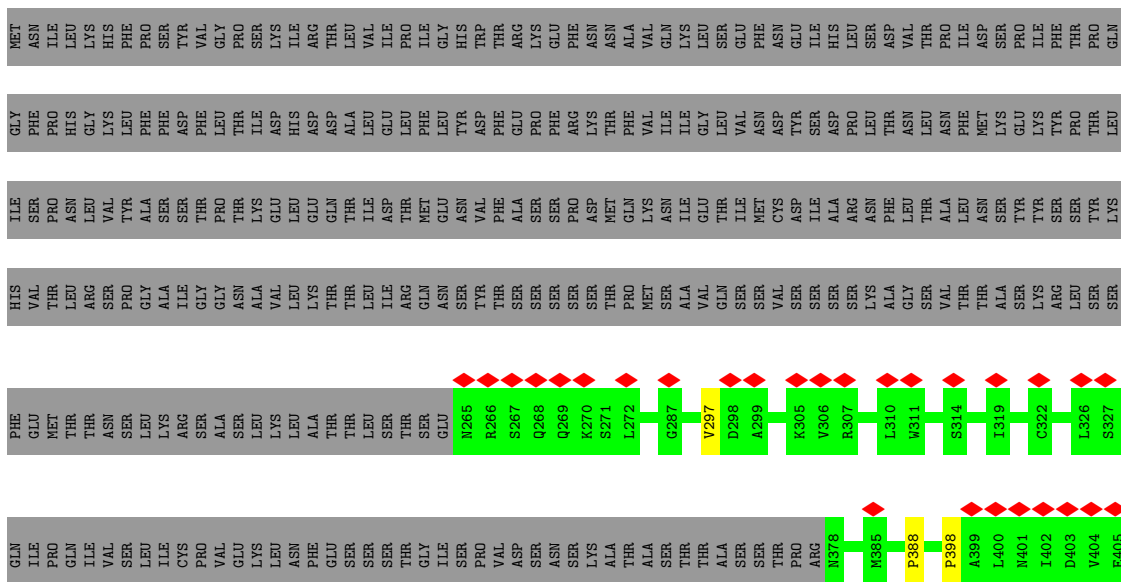


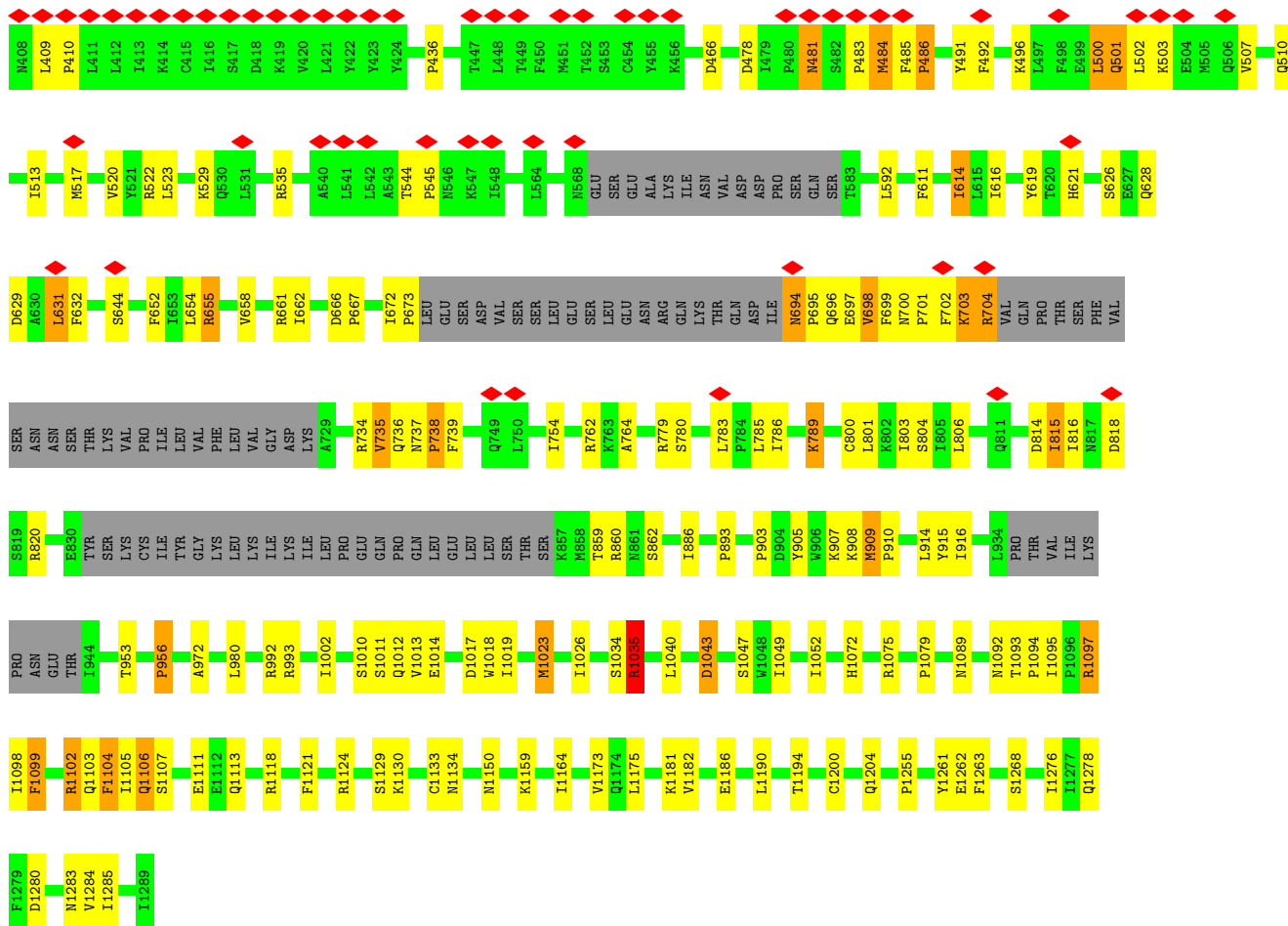
● Molecule 9: Trafficking protein particle complex II-specific subunit 120



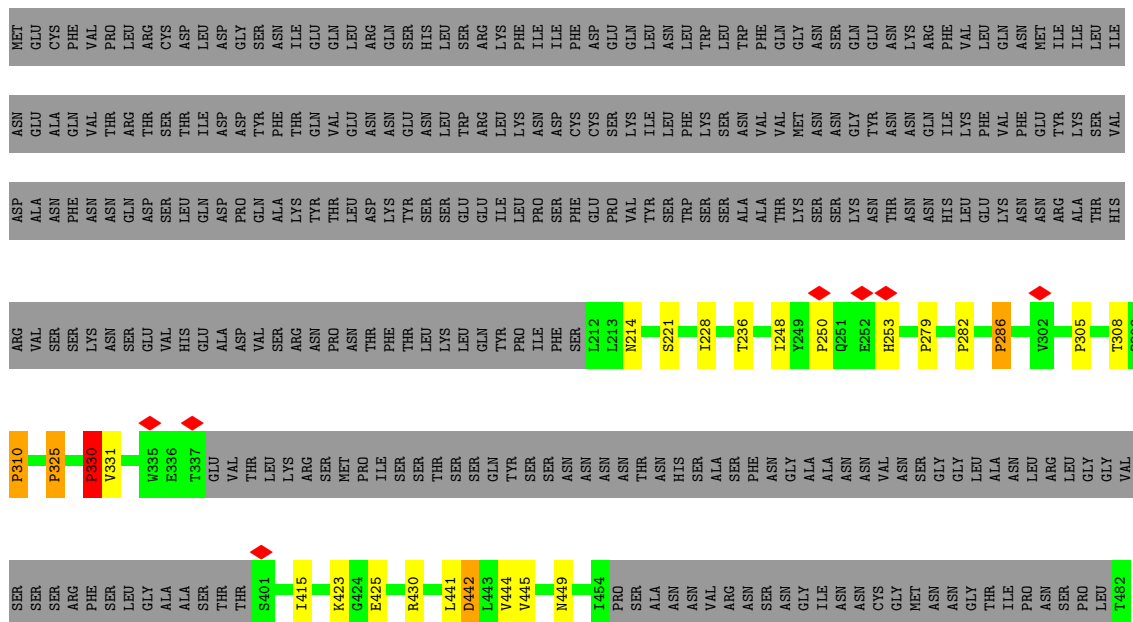
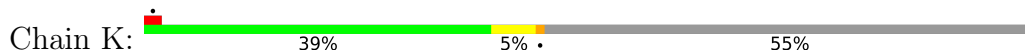


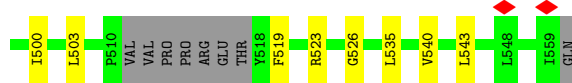
• Molecule 9: Trafficking protein particle complex II-specific subunit 120





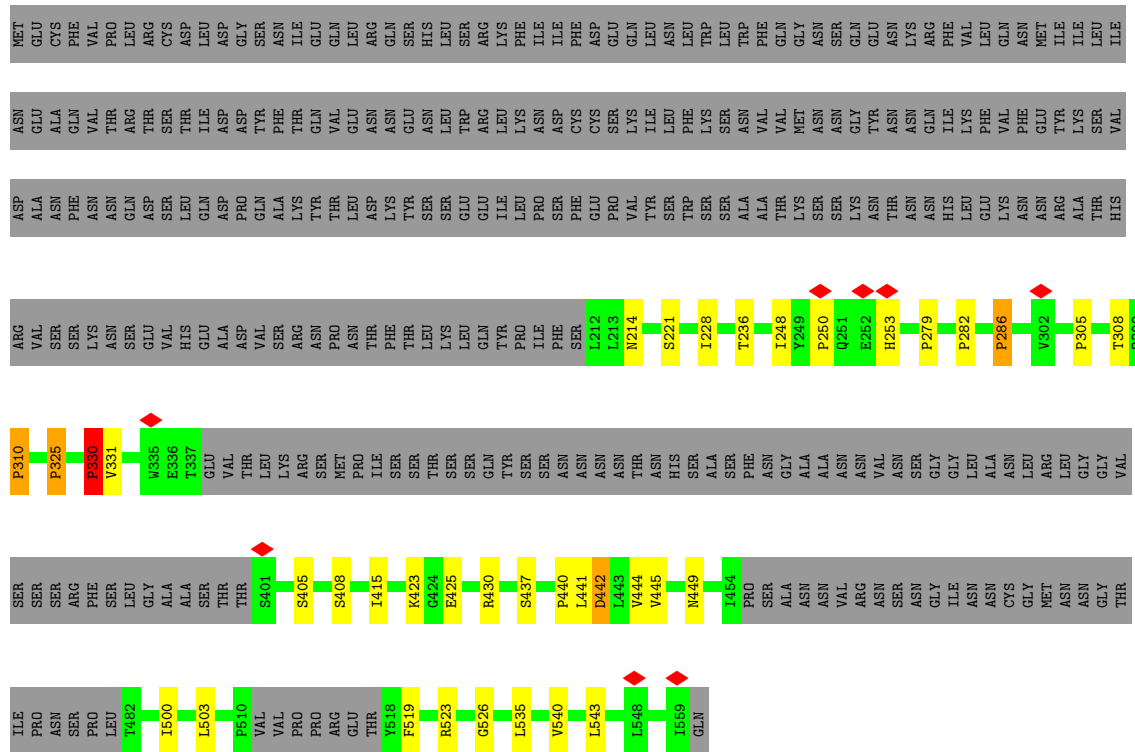
● Molecule 10: Trafficking protein particle complex II-specific subunit 65





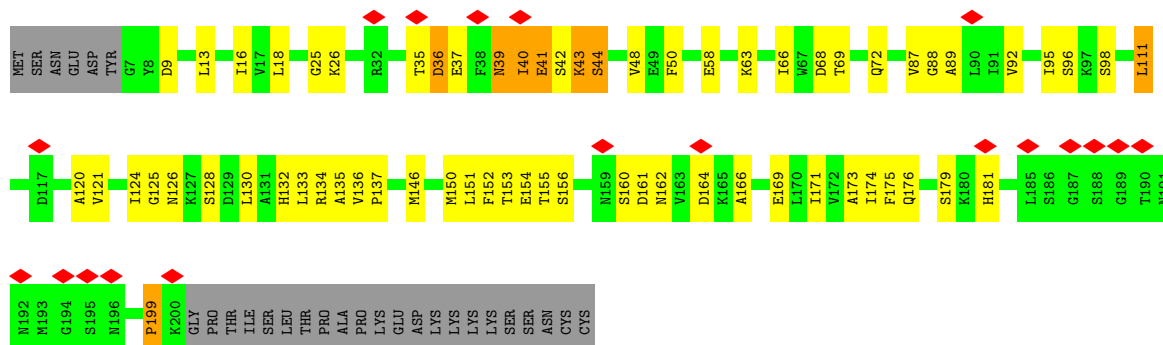
- Molecule 10: Trafficking protein particle complex II-specific subunit 65

Chain X: 38% 6% 55%



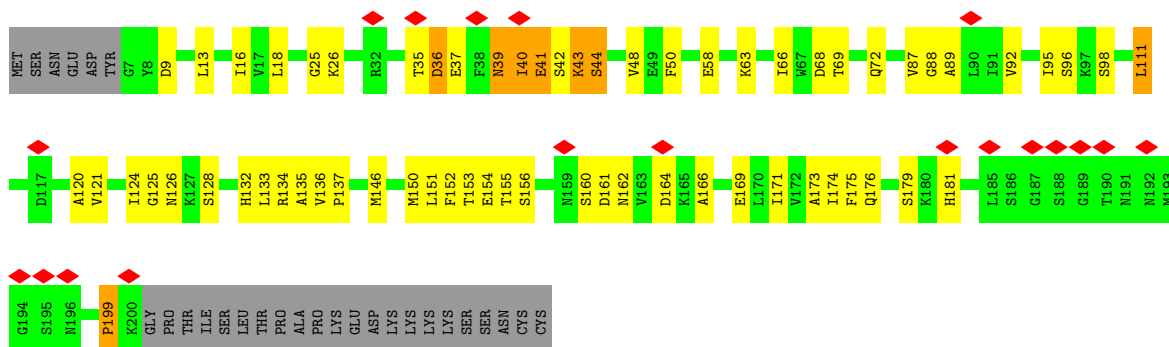
- Molecule 11: GTP-binding protein YPT32/YPT11

Chain L: 9% 58% 26% 13%



- Molecule 11: GTP-binding protein YPT32/YPT11

Chain Y: 9% 58% 26% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32394	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	0.036	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	521.82, 521.82, 521.82	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8697, 0.8697, 0.8697	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	0.39	0/1180	0.87	4/1592 (0.3%)
1	N	0.39	0/1180	0.87	4/1592 (0.3%)
2	B	0.43	0/1617	0.91	7/2174 (0.3%)
2	O	0.43	0/1617	0.91	7/2174 (0.3%)
3	C	0.47	0/1515	0.81	1/2049 (0.0%)
3	F	0.44	0/1505	0.80	4/2035 (0.2%)
3	P	0.47	0/1515	0.81	1/2049 (0.0%)
3	S	0.44	0/1505	0.80	4/2035 (0.2%)
4	D	0.45	0/1264	0.84	3/1707 (0.2%)
4	Q	0.45	0/1264	0.84	3/1707 (0.2%)
5	E	0.46	0/1332	0.84	2/1795 (0.1%)
5	R	0.46	0/1332	0.84	2/1795 (0.1%)
6	G	0.47	0/1658	0.80	2/2236 (0.1%)
6	T	0.46	0/1658	0.81	2/2236 (0.1%)
7	H	0.48	0/1211	0.95	5/1643 (0.3%)
7	U	0.49	0/1211	0.93	5/1643 (0.3%)
8	I	0.33	0/4219	0.65	14/5852 (0.2%)
8	V	0.32	0/4219	0.65	14/5852 (0.2%)
9	J	0.43	0/6572	0.85	26/8939 (0.3%)
9	W	0.43	0/6572	0.85	26/8939 (0.3%)
10	K	0.34	0/1663	0.83	11/2268 (0.5%)
10	X	0.34	0/1663	0.83	11/2268 (0.5%)
11	L	0.51	0/1507	0.83	3/2038 (0.1%)
11	Y	0.51	0/1507	0.83	3/2038 (0.1%)
All	All	0.42	0/50486	0.82	164/68656 (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
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	P	0	1
All	All	0	2

There are no bond length outliers.

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	46	ASP	CB-CG-OD1	10.23	127.51	118.30
7	U	46	ASP	CB-CG-OD1	10.23	127.51	118.30
3	P	186	ASP	CB-CG-OD1	9.62	126.96	118.30
3	C	186	ASP	CB-CG-OD1	9.60	126.94	118.30
9	W	783	LEU	CA-CB-CG	9.00	135.99	115.30
9	J	783	LEU	CA-CB-CG	8.97	135.94	115.30
9	J	815	ILE	CG1-CB-CG2	-8.87	91.88	111.40
9	W	815	ILE	CG1-CB-CG2	-8.84	91.95	111.40
4	Q	114	LEU	CA-CB-CG	7.98	133.64	115.30
9	J	592	LEU	CA-CB-CG	7.97	133.63	115.30
4	D	114	LEU	CA-CB-CG	7.95	133.59	115.30
9	W	592	LEU	CA-CB-CG	7.95	133.59	115.30
9	W	631	LEU	CA-CB-CG	7.93	133.54	115.30
9	J	631	LEU	CA-CB-CG	7.91	133.49	115.30
10	K	442	ASP	CB-CG-OD1	7.63	125.17	118.30
9	W	806	LEU	CA-CB-CG	7.61	132.79	115.30
9	J	806	LEU	CA-CB-CG	7.59	132.76	115.30
10	X	442	ASP	CB-CG-OD1	7.59	125.13	118.30
8	I	346	PRO	N-CA-CB	7.52	112.33	103.30
8	V	346	PRO	N-CA-CB	7.49	112.29	103.30
10	X	535	LEU	CA-CB-CG	7.23	131.93	115.30
10	K	535	LEU	CA-CB-CG	7.20	131.87	115.30
5	R	50	LEU	CA-CB-CG	7.16	131.76	115.30
5	E	50	LEU	CA-CB-CG	7.13	131.69	115.30
10	X	325	PRO	N-CA-CB	7.03	111.74	103.30
9	J	466	ASP	CB-CG-OD1	7.03	124.62	118.30
2	B	188	ASP	CB-CG-OD1	7.02	124.62	118.30
2	O	188	ASP	CB-CG-OD1	7.02	124.62	118.30
9	W	466	ASP	CB-CG-OD1	7.01	124.61	118.30
10	K	325	PRO	N-CA-CB	7.00	111.70	103.30
8	I	483	PRO	N-CA-CB	6.97	111.67	103.30
8	V	483	PRO	N-CA-CB	6.97	111.66	103.30
1	A	33	VAL	CA-CB-CG1	6.88	121.22	110.90
1	N	33	VAL	CA-CB-CG1	6.87	121.21	110.90
9	J	783	LEU	CB-CG-CD1	6.80	122.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	783	LEU	CB-CG-CD1	6.80	122.56	111.00
10	X	330	PRO	N-CA-CB	6.79	111.45	103.30
10	K	330	PRO	N-CA-CB	6.78	111.43	103.30
11	L	199	PRO	N-CA-CB	6.74	111.39	103.30
11	Y	199	PRO	N-CA-CB	6.70	111.34	103.30
2	B	132	LEU	CA-CB-CG	6.66	130.63	115.30
2	O	132	LEU	CA-CB-CG	6.63	130.54	115.30
9	J	481	ASN	C-N-CA	-6.58	105.25	121.70
9	W	481	ASN	C-N-CA	-6.58	105.26	121.70
10	X	310	PRO	N-CA-CB	6.43	111.02	103.30
9	W	1175	LEU	CA-CB-CG	6.37	129.94	115.30
10	K	310	PRO	N-CA-CB	6.36	110.93	103.30
9	J	1175	LEU	CA-CB-CG	6.35	129.90	115.30
4	D	38	LEU	CA-CB-CG	6.31	129.81	115.30
4	Q	38	LEU	CA-CB-CG	6.30	129.79	115.30
10	X	286	PRO	N-CA-CB	6.30	110.86	103.30
2	B	190	ASP	CB-CG-OD1	6.27	123.94	118.30
8	I	1067	PRO	N-CA-CB	6.26	110.82	103.30
10	K	286	PRO	N-CA-CB	6.26	110.81	103.30
8	V	976	PRO	N-CA-CB	6.26	110.81	103.30
2	O	190	ASP	CB-CG-OD1	6.25	123.93	118.30
8	V	649	PRO	N-CA-CB	6.25	110.80	103.30
7	U	46	ASP	CB-CG-OD2	-6.24	112.69	118.30
8	I	649	PRO	N-CA-CB	6.23	110.78	103.30
9	W	909	MET	CA-CB-CG	6.23	123.89	113.30
8	V	1076	PRO	N-CA-CB	6.22	110.77	103.30
8	I	976	PRO	N-CA-CB	6.22	110.77	103.30
8	V	1067	PRO	N-CA-CB	6.21	110.76	103.30
9	J	909	MET	CA-CB-CG	6.21	123.86	113.30
8	I	704	PRO	N-CA-CB	6.19	110.73	103.30
5	E	28	LEU	CA-CB-CG	6.19	129.54	115.30
8	V	704	PRO	N-CA-CB	6.19	110.73	103.30
7	H	46	ASP	CB-CG-OD2	-6.18	112.74	118.30
8	I	639	PRO	N-CA-CB	6.17	110.70	103.30
8	V	639	PRO	N-CA-CB	6.17	110.70	103.30
8	V	252	PRO	N-CA-CB	6.17	110.70	103.30
8	I	970	PRO	N-CA-CB	6.16	110.70	103.30
9	J	398	PRO	N-CA-CB	6.16	110.69	103.30
5	R	28	LEU	CA-CB-CG	6.16	129.46	115.30
8	I	1076	PRO	N-CA-CB	6.15	110.68	103.30
10	K	282	PRO	N-CA-CB	6.14	110.67	103.30
8	I	252	PRO	N-CA-CB	6.14	110.67	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	970	PRO	N-CA-CB	6.13	110.66	103.30
8	I	572	PRO	N-CA-CB	6.13	110.66	103.30
9	W	398	PRO	N-CA-CB	6.13	110.65	103.30
8	V	572	PRO	N-CA-CB	6.13	110.65	103.30
10	X	282	PRO	N-CA-CB	6.12	110.64	103.30
9	W	1043	ASP	CB-CG-OD1	6.08	123.77	118.30
9	J	1043	ASP	CB-CG-OD1	6.05	123.75	118.30
3	S	155	VAL	CA-CB-CG1	6.01	119.92	110.90
9	J	1255	PRO	N-CA-CB	6.00	110.50	103.30
9	W	1255	PRO	N-CA-CB	5.99	110.49	103.30
3	F	155	VAL	CA-CB-CG1	5.99	119.88	110.90
10	K	305	PRO	N-CA-CB	5.96	110.46	103.30
10	X	305	PRO	N-CA-CB	5.96	110.46	103.30
6	T	66	PHE	CB-CG-CD1	5.93	124.95	120.80
6	G	66	PHE	CB-CG-CD1	5.92	124.94	120.80
2	O	87	ARG	NE-CZ-NH1	5.89	123.25	120.30
10	K	279	PRO	N-CA-CB	5.89	110.36	103.30
10	X	441	LEU	CA-CB-CG	5.88	128.82	115.30
9	J	956	PRO	N-CA-CB	5.88	110.35	103.30
10	K	441	LEU	CA-CB-CG	5.87	128.81	115.30
10	X	279	PRO	N-CA-CB	5.85	110.32	103.30
9	J	1023	MET	CG-SD-CE	5.85	109.55	100.20
9	W	956	PRO	N-CA-CB	5.84	110.31	103.30
9	W	1023	MET	CG-SD-CE	5.84	109.54	100.20
10	K	250	PRO	N-CA-CB	5.83	110.30	103.30
10	X	250	PRO	N-CA-CB	5.83	110.30	103.30
3	S	180	LEU	CA-CB-CG	5.82	128.68	115.30
2	B	87	ARG	NE-CZ-NH1	5.82	123.21	120.30
3	F	180	LEU	CA-CB-CG	5.81	128.66	115.30
9	W	436	PRO	N-CA-CB	5.80	110.27	103.30
8	I	721	PRO	N-CA-CB	5.78	110.23	103.30
9	W	388	PRO	N-CA-CB	5.78	110.23	103.30
9	J	436	PRO	N-CA-CB	5.77	110.22	103.30
9	J	388	PRO	N-CA-CB	5.77	110.22	103.30
9	W	673	PRO	N-CA-CB	5.77	110.22	103.30
8	V	721	PRO	N-CA-CB	5.75	110.21	103.30
1	N	44	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	44	LEU	CA-CB-CG	5.72	128.46	115.30
9	J	673	PRO	N-CA-CB	5.72	110.16	103.30
9	J	410	PRO	N-CA-CB	5.65	110.08	103.30
8	I	799	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	A	63	LEU	CA-CB-CG	5.60	128.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	667	PRO	N-CA-CB	5.59	110.01	103.30
9	J	667	PRO	N-CA-CB	5.59	110.01	103.30
1	N	63	LEU	CA-CB-CG	5.59	128.15	115.30
8	V	799	LEU	CB-CG-CD1	-5.56	101.54	111.00
9	J	1035	ARG	CA-CB-CG	5.56	125.64	113.40
9	W	410	PRO	N-CA-CB	5.56	109.97	103.30
9	W	1035	ARG	CA-CB-CG	5.55	125.61	113.40
2	B	108	LEU	CA-CB-CG	5.53	128.02	115.30
7	H	26	PRO	N-CA-CB	5.53	109.93	103.30
7	U	26	PRO	N-CA-CB	5.51	109.91	103.30
2	O	108	LEU	CA-CB-CG	5.50	127.96	115.30
11	Y	9	ASP	CB-CG-OD1	5.47	123.23	118.30
6	T	267	LEU	CA-CB-CG	5.47	127.89	115.30
6	G	267	LEU	CA-CB-CG	5.47	127.88	115.30
8	I	980	PRO	N-CA-CB	5.46	109.86	103.30
11	L	9	ASP	CB-CG-OD1	5.46	123.22	118.30
2	O	150	GLU	CA-CB-CG	5.45	125.38	113.40
9	W	1052	ILE	CG1-CB-CG2	-5.44	99.43	111.40
7	U	131	ARG	NE-CZ-NH1	5.42	123.01	120.30
9	J	1052	ILE	CG1-CB-CG2	-5.42	99.48	111.40
2	B	150	GLU	CA-CB-CG	5.42	125.31	113.40
8	V	980	PRO	N-CA-CB	5.41	109.80	103.30
7	H	131	ARG	NE-CZ-NH1	5.39	122.99	120.30
4	D	58	VAL	CG1-CB-CG2	-5.37	102.31	110.90
4	Q	58	VAL	CG1-CB-CG2	-5.35	102.34	110.90
9	W	614	ILE	CG1-CB-CG2	-5.35	99.64	111.40
9	W	654	LEU	CA-CB-CG	5.35	127.60	115.30
9	J	614	ILE	CG1-CB-CG2	-5.34	99.64	111.40
9	J	1040	LEU	CA-CB-CG	5.34	127.57	115.30
9	J	654	LEU	CA-CB-CG	5.33	127.56	115.30
9	W	1040	LEU	CA-CB-CG	5.33	127.56	115.30
9	W	1190	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	125	LEU	CB-CG-CD1	5.22	119.87	111.00
9	J	1190	LEU	CA-CB-CG	5.21	127.29	115.30
1	N	125	LEU	CB-CG-CD1	5.19	119.83	111.00
11	Y	111	LEU	CB-CG-CD2	-5.19	102.18	111.00
11	L	111	LEU	CB-CG-CD2	-5.17	102.20	111.00
3	F	117	LEU	CA-CB-CG	5.17	127.20	115.30
3	S	117	LEU	CA-CB-CG	5.16	127.18	115.30
2	B	142	ASN	C-N-CA	5.09	134.43	121.70
2	O	142	ASN	C-N-CA	5.08	134.39	121.70
7	H	168	LEU	CB-CG-CD2	-5.04	102.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	168	LEU	CB-CG-CD2	-5.04	102.44	111.00
3	F	130	LEU	CA-CB-CG	5.01	126.83	115.30
3	S	130	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	43	GLN	Mainchain
3	P	43	GLN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1160	0	1184	17	0
1	N	1160	0	1184	17	0
2	B	1590	0	1612	28	0
2	O	1590	0	1612	27	0
3	C	1488	0	1487	32	0
3	F	1478	0	1487	22	0
3	P	1488	0	1487	32	0
3	S	1478	0	1487	20	0
4	D	1235	0	1203	19	0
4	Q	1235	0	1203	19	0
5	E	1308	0	1315	14	0
5	R	1308	0	1315	15	0
6	G	1624	0	1601	34	0
6	T	1624	0	1601	50	0
7	H	1180	0	1132	22	0
7	U	1180	0	1132	72	0
8	I	4199	0	2172	24	0
8	V	4199	0	2172	22	0
9	J	6462	0	5811	349	0
9	W	6462	0	5811	352	0
10	K	1649	0	1338	38	0
10	X	1649	0	1338	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	1484	0	1409	125	0
11	Y	1484	0	1409	123	0
All	All	49714	0	43502	1248	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 13.

All (1248) 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)
9:J:903:PRO:HB3	9:J:1098:ILE:CG1	1.14	1.59
9:W:903:PRO:HB3	9:W:1098:ILE:CG1	1.14	1.58
9:W:903:PRO:CA	9:W:1098:ILE:HG21	1.37	1.53
9:J:661:ARG:HG2	9:J:736:GLN:CG	1.30	1.53
9:J:903:PRO:CA	9:J:1098:ILE:HG21	1.37	1.52
9:W:915:TYR:N	9:W:1102:ARG:HH22	1.07	1.50
9:J:915:TYR:H	9:J:1102:ARG:NH2	1.09	1.49
9:W:915:TYR:H	9:W:1102:ARG:NH2	1.09	1.48
9:W:903:PRO:CB	9:W:1098:ILE:HG12	1.44	1.47
9:J:903:PRO:CB	9:J:1098:ILE:HG12	1.44	1.46
7:U:103:TYR:OH	7:U:138:HIS:CE1	1.69	1.44
9:J:915:TYR:N	9:J:1102:ARG:HH22	1.07	1.41
9:J:661:ARG:CG	9:J:736:GLN:HG3	1.53	1.37
11:L:124:ILE:HG13	11:L:155:THR:OG1	1.18	1.35
9:J:916:ILE:N	9:J:1102:ARG:HH12	1.21	1.35
9:J:737:ASN:CG	9:J:785:LEU:HA	1.47	1.34
9:W:916:ILE:N	9:W:1102:ARG:HH12	1.21	1.34
6:T:169:MET:HG3	7:U:87:CYS:SG	1.67	1.34
9:J:698:VAL:HG21	11:L:166:ALA:CB	1.55	1.33
9:W:737:ASN:CG	9:W:785:LEU:HA	1.45	1.33
9:W:698:VAL:HG21	11:Y:166:ALA:CB	1.55	1.33
7:U:103:TYR:CE2	7:U:138:HIS:NE2	1.97	1.32
3:S:156:GLN:O	3:S:183:ILE:HG23	1.21	1.31
11:Y:132:HIS:C	11:Y:133:LEU:HD23	1.50	1.31
11:Y:124:ILE:HG13	11:Y:155:THR:OG1	1.18	1.31
11:L:132:HIS:C	11:L:133:LEU:HD23	1.50	1.31
7:U:139:GLU:OE2	7:U:143:LYS:HD3	1.25	1.29
11:L:128:SER:OG	11:L:156:SER:CA	1.81	1.29
9:W:903:PRO:HA	9:W:1098:ILE:CG2	1.62	1.29
9:J:903:PRO:HA	9:J:1098:ILE:CG2	1.62	1.28
9:W:907:LYS:NZ	9:W:1098:ILE:HG13	1.49	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:132:HIS:O	11:L:133:LEU:HD23	1.32	1.27
11:Y:128:SER:OG	11:Y:156:SER:CA	1.81	1.27
11:Y:132:HIS:O	11:Y:133:LEU:HD23	1.32	1.27
9:W:903:PRO:CB	9:W:1098:ILE:CG1	2.06	1.26
3:F:156:GLN:O	3:F:183:ILE:HG23	1.21	1.25
9:J:907:LYS:NZ	9:J:1098:ILE:HG13	1.49	1.24
11:Y:124:ILE:CG1	11:Y:155:THR:OG1	1.86	1.23
11:L:124:ILE:CG1	11:L:155:THR:OG1	1.86	1.22
9:J:701:PRO:HG3	11:L:150:MET:C	1.61	1.21
7:U:131:ARG:O	7:U:135:GLN:OE1	1.55	1.21
9:J:903:PRO:CB	9:J:1098:ILE:CG1	2.06	1.20
9:J:696:GLN:HA	11:L:162:ASN:OD1	1.03	1.19
9:J:702:PHE:C	9:J:703:LYS:HD2	1.61	1.19
9:J:903:PRO:CA	9:J:1098:ILE:CG2	2.19	1.19
9:W:701:PRO:HG3	11:Y:150:MET:C	1.61	1.19
9:W:696:GLN:HA	11:Y:162:ASN:OD1	1.03	1.18
9:W:702:PHE:C	9:W:703:LYS:HD2	1.61	1.18
9:W:737:ASN:OD1	9:W:785:LEU:CA	1.90	1.18
9:W:699:PHE:HB3	11:Y:152:PHE:H	1.06	1.18
11:L:128:SER:OG	11:L:156:SER:HA	1.03	1.18
11:Y:128:SER:OG	11:Y:156:SER:HA	1.03	1.18
6:T:168:LYS:HE3	7:U:85:ASP:OD2	1.40	1.17
9:W:1094:PRO:HG3	9:W:1118:ARG:CZ	1.74	1.16
9:W:737:ASN:ND2	9:W:785:LEU:HA	1.59	1.16
9:W:903:PRO:HG3	9:W:1098:ILE:HB	1.25	1.16
9:J:737:ASN:OD1	9:J:785:LEU:CA	1.92	1.16
7:U:139:GLU:OE2	7:U:143:LYS:CD	1.92	1.16
9:J:1094:PRO:HG3	9:J:1118:ARG:CZ	1.75	1.16
9:J:916:ILE:N	9:J:1102:ARG:NH1	1.93	1.15
9:W:916:ILE:N	9:W:1102:ARG:NH1	1.93	1.15
9:J:737:ASN:ND2	9:J:785:LEU:HA	1.59	1.15
9:W:903:PRO:CA	9:W:1098:ILE:CG2	2.19	1.15
9:J:702:PHE:CZ	11:L:120:ALA:HB1	1.84	1.13
9:J:903:PRO:HG3	9:J:1098:ILE:HB	1.25	1.13
9:J:696:GLN:CA	11:L:162:ASN:OD1	1.96	1.13
9:J:1049:ILE:O	9:W:1072:HIS:NE2	1.81	1.13
7:U:131:ARG:HG2	7:U:135:GLN:NE2	1.64	1.13
9:W:702:PHE:CZ	11:Y:120:ALA:HB1	1.84	1.12
9:J:702:PHE:HB3	11:L:173:ALA:HB1	1.13	1.12
9:W:696:GLN:CA	11:Y:162:ASN:OD1	1.96	1.12
9:W:910:PRO:HD3	9:W:1095:ILE:HG21	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:737:ASN:ND2	9:J:785:LEU:HD23	1.62	1.12
9:W:737:ASN:ND2	9:W:785:LEU:HD23	1.65	1.12
9:J:1072:HIS:NE2	9:W:1049:ILE:O	1.81	1.12
9:W:694:ASN:HB2	9:W:695:PRO:HD2	1.17	1.12
9:J:661:ARG:CG	9:J:736:GLN:CG	2.20	1.11
9:J:737:ASN:OD1	9:J:785:LEU:HA	1.48	1.11
9:W:1094:PRO:HB3	9:W:1118:ARG:CG	1.81	1.11
9:W:737:ASN:ND2	9:W:785:LEU:CA	2.12	1.11
9:W:1094:PRO:HG3	9:W:1118:ARG:NE	1.64	1.11
9:J:737:ASN:ND2	9:J:785:LEU:CA	2.14	1.11
9:J:910:PRO:HD3	9:J:1095:ILE:HG21	1.31	1.10
9:J:1094:PRO:HG3	9:J:1118:ARG:NE	1.64	1.10
9:W:702:PHE:HB3	11:Y:173:ALA:HB1	1.13	1.10
9:J:1094:PRO:HG3	9:J:1118:ARG:NH2	1.66	1.09
9:J:1094:PRO:HB3	9:J:1118:ARG:CG	1.81	1.09
7:U:103:TYR:HE2	7:U:138:HIS:NE2	1.35	1.09
10:K:519:PHE:HE2	9:W:860:ARG:CB	1.65	1.09
9:W:737:ASN:OD1	9:W:785:LEU:HA	1.45	1.09
9:J:903:PRO:HA	9:J:1098:ILE:HG21	1.19	1.08
9:J:860:ARG:CB	10:X:519:PHE:HE2	1.65	1.08
9:W:1094:PRO:HG3	9:W:1118:ARG:NH2	1.66	1.08
9:W:1098:ILE:HD11	9:W:1099:PHE:CD2	1.88	1.08
9:W:916:ILE:H	9:W:1102:ARG:NH1	1.47	1.08
9:J:698:VAL:CG2	11:L:166:ALA:HB2	1.83	1.07
9:J:694:ASN:HB2	9:J:695:PRO:HD2	1.17	1.07
9:J:903:PRO:HB3	9:J:1098:ILE:CD1	1.85	1.07
9:J:1098:ILE:HD11	9:J:1099:PHE:CD2	1.88	1.07
9:W:698:VAL:CG2	11:Y:166:ALA:HB2	1.84	1.07
9:J:699:PHE:HB3	11:L:152:PHE:H	1.06	1.07
9:J:1094:PRO:HB3	9:J:1118:ARG:HG2	1.28	1.07
9:W:903:PRO:HG3	9:W:1098:ILE:CB	1.84	1.07
9:J:737:ASN:HD21	9:J:785:LEU:CA	1.67	1.07
9:W:737:ASN:HD21	9:W:785:LEU:CA	1.66	1.06
9:W:1094:PRO:HB3	9:W:1118:ARG:HG2	1.28	1.06
9:J:992:ARG:NH2	10:X:519:PHE:H	1.54	1.06
9:J:916:ILE:H	9:J:1102:ARG:NH1	1.47	1.06
9:J:903:PRO:HG3	9:J:1098:ILE:CB	1.84	1.05
9:W:737:ASN:CG	9:W:785:LEU:CA	2.24	1.05
9:W:699:PHE:HE2	11:Y:146:MET:HE3	1.20	1.05
9:W:702:PHE:CB	11:Y:173:ALA:HB1	1.85	1.05
9:W:903:PRO:HB3	9:W:1098:ILE:CD1	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:907:LYS:NZ	9:W:1098:ILE:CG1	2.19	1.05
9:J:903:PRO:N	9:J:1098:ILE:HG21	1.71	1.05
9:J:702:PHE:CB	11:L:173:ALA:HB1	1.86	1.04
10:K:519:PHE:H	9:W:992:ARG:NH2	1.53	1.04
9:W:737:ASN:HD21	9:W:785:LEU:N	1.52	1.04
9:W:702:PHE:O	9:W:703:LYS:HD2	1.56	1.04
9:W:737:ASN:OD1	9:W:786:ILE:N	1.90	1.04
9:J:694:ASN:CB	9:J:695:PRO:HD2	1.86	1.04
9:J:907:LYS:NZ	9:J:1098:ILE:CG1	2.19	1.04
7:U:131:ARG:C	7:U:135:GLN:OE1	1.95	1.04
9:W:903:PRO:HA	9:W:1098:ILE:HG21	1.19	1.04
9:W:903:PRO:N	9:W:1098:ILE:HG21	1.71	1.04
9:J:702:PHE:O	9:J:703:LYS:HD2	1.56	1.04
9:W:694:ASN:CB	9:W:695:PRO:HD2	1.86	1.04
9:W:907:LYS:HZ1	9:W:1098:ILE:HG13	0.92	1.04
11:L:132:HIS:O	11:L:133:LEU:CD2	2.06	1.03
11:Y:132:HIS:O	11:Y:133:LEU:CD2	2.06	1.03
9:J:907:LYS:HZ1	9:J:1098:ILE:HG13	0.98	1.03
6:T:100:GLU:HA	7:U:106:TYR:CE2	1.94	1.02
9:J:903:PRO:CB	9:J:1098:ILE:HG21	1.90	1.02
7:U:103:TYR:CZ	7:U:138:HIS:CE1	2.47	1.02
9:J:737:ASN:HD21	9:J:785:LEU:N	1.57	1.01
9:J:992:ARG:HH22	10:X:519:PHE:N	1.58	1.01
10:K:519:PHE:N	9:W:992:ARG:HH22	1.58	1.01
9:J:737:ASN:CG	9:J:785:LEU:CA	2.26	1.01
9:J:702:PHE:CB	11:L:173:ALA:CB	2.38	1.01
6:G:170:ARG:HB3	6:G:170:ARG:HH11	1.21	1.01
9:J:737:ASN:OD1	9:J:786:ILE:N	1.93	1.01
9:W:702:PHE:CB	11:Y:173:ALA:CB	2.38	1.01
9:J:699:PHE:HE2	11:L:146:MET:HE3	1.23	1.00
9:J:734:ARG:HB2	9:J:736:GLN:OE1	1.60	1.00
9:J:800:CYS:SG	9:J:814:ASP:HA	2.01	1.00
9:W:903:PRO:CB	9:W:1098:ILE:HG21	1.90	1.00
9:W:702:PHE:HB3	11:Y:173:ALA:CB	1.91	1.00
9:W:800:CYS:SG	9:W:814:ASP:HA	2.01	1.00
9:J:661:ARG:HG2	9:J:736:GLN:CD	1.83	0.99
9:J:702:PHE:HB3	11:L:173:ALA:CB	1.91	0.99
9:W:699:PHE:CB	11:Y:152:PHE:H	1.76	0.99
9:W:737:ASN:ND2	9:W:785:LEU:N	2.11	0.98
9:W:907:LYS:HD2	9:W:1097:ARG:HG3	1.46	0.98
9:J:701:PRO:HG3	11:L:151:LEU:N	1.80	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:124:ILE:CD1	11:L:155:THR:OG1	2.12	0.97
9:J:1098:ILE:HD11	9:J:1099:PHE:CE2	2.00	0.97
9:W:696:GLN:HG2	11:Y:162:ASN:ND2	1.80	0.97
3:S:156:GLN:O	3:S:183:ILE:CG2	2.13	0.96
9:J:737:ASN:HD22	9:J:785:LEU:HD23	1.28	0.96
9:J:699:PHE:CB	11:L:152:PHE:H	1.76	0.96
9:W:907:LYS:HZ1	9:W:1098:ILE:CG1	1.76	0.96
9:W:907:LYS:HZ2	9:W:1098:ILE:H	1.02	0.96
9:W:1098:ILE:HD11	9:W:1099:PHE:CE2	2.00	0.96
11:Y:124:ILE:CD1	11:Y:155:THR:OG1	2.12	0.96
9:J:696:GLN:HG2	11:L:162:ASN:ND2	1.80	0.96
9:J:907:LYS:HD2	9:J:1097:ARG:HG3	1.46	0.96
9:J:1094:PRO:CG	9:J:1118:ARG:CZ	2.44	0.96
9:J:915:TYR:C	9:J:1102:ARG:HH12	1.69	0.95
9:W:903:PRO:HA	9:W:1098:ILE:HG23	1.47	0.95
9:J:694:ASN:HB2	9:J:695:PRO:CD	1.97	0.95
9:W:915:TYR:C	9:W:1102:ARG:HH12	1.69	0.95
9:W:1094:PRO:CG	9:W:1118:ARG:CZ	2.44	0.94
3:F:156:GLN:O	3:F:183:ILE:CG2	2.13	0.94
9:W:916:ILE:H	9:W:1102:ARG:HH12	0.95	0.94
3:C:188:ILE:CG2	11:L:42:SER:HB2	1.97	0.94
9:J:699:PHE:N	11:L:152:PHE:O	2.01	0.94
9:J:915:TYR:N	9:J:1102:ARG:NH2	1.82	0.94
9:W:701:PRO:HG3	11:Y:151:LEU:N	1.80	0.94
9:W:699:PHE:N	11:Y:152:PHE:O	2.01	0.94
11:Y:128:SER:OG	11:Y:156:SER:CB	2.16	0.94
11:L:128:SER:OG	11:L:156:SER:CB	2.16	0.94
9:J:704:ARG:HG3	9:J:704:ARG:HH11	1.33	0.93
11:L:124:ILE:HG13	11:L:155:THR:HG1	0.83	0.93
7:U:131:ARG:HG2	7:U:135:GLN:HE22	1.24	0.93
9:W:694:ASN:HB2	9:W:695:PRO:CD	1.97	0.93
9:W:737:ASN:ND2	9:W:785:LEU:H	1.65	0.93
11:Y:124:ILE:HG13	11:Y:155:THR:HG1	0.95	0.93
11:L:132:HIS:CD2	11:L:133:LEU:HD21	2.03	0.93
3:P:188:ILE:CG2	11:Y:42:SER:HB2	1.97	0.93
9:J:907:LYS:HZ2	9:J:1098:ILE:N	1.67	0.93
9:J:702:PHE:CE1	11:L:120:ALA:HB1	2.04	0.93
6:T:100:GLU:HA	7:U:106:TYR:CD2	2.03	0.93
9:W:1094:PRO:CG	9:W:1118:ARG:NE	2.31	0.93
9:W:702:PHE:CE1	11:Y:120:ALA:HB1	2.04	0.92
9:W:915:TYR:N	9:W:1102:ARG:NH2	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:132:HIS:CD2	11:Y:133:LEU:HD21	2.03	0.92
9:W:696:GLN:HG2	11:Y:162:ASN:HD21	1.31	0.92
9:J:903:PRO:HA	9:J:1098:ILE:HG23	1.47	0.92
9:W:704:ARG:HG3	9:W:704:ARG:HH11	1.33	0.92
9:J:1094:PRO:CG	9:J:1118:ARG:NE	2.31	0.92
9:W:914:LEU:C	9:W:1102:ARG:HH22	1.72	0.92
9:W:907:LYS:NZ	9:W:1098:ILE:H	1.68	0.92
9:W:698:VAL:HG21	11:Y:166:ALA:HB2	0.93	0.92
9:J:1094:PRO:CG	9:J:1118:ARG:NH2	2.33	0.92
9:J:914:LEU:C	9:J:1102:ARG:HH22	1.72	0.91
9:W:694:ASN:CB	9:W:695:PRO:CD	2.49	0.91
9:W:801:LEU:O	9:W:803:ILE:HD12	1.71	0.91
9:W:1094:PRO:HG3	9:W:1118:ARG:HE	1.33	0.91
9:J:801:LEU:O	9:J:803:ILE:HD12	1.71	0.91
7:U:103:TYR:OH	7:U:138:HIS:HE1	1.29	0.91
11:Y:124:ILE:HG13	11:Y:155:THR:CB	2.00	0.91
9:J:907:LYS:NZ	9:J:1098:ILE:H	1.68	0.91
9:W:661:ARG:HG2	9:W:736:GLN:HE21	1.33	0.91
9:J:698:VAL:HG21	11:L:166:ALA:HB2	0.93	0.91
11:L:124:ILE:HG13	11:L:155:THR:CB	2.00	0.91
9:W:500:LEU:HD12	9:W:502:LEU:HG	1.53	0.91
9:W:699:PHE:HB3	11:Y:152:PHE:N	1.86	0.91
9:J:737:ASN:ND2	9:J:785:LEU:N	2.15	0.91
9:J:500:LEU:HD12	9:J:502:LEU:HG	1.52	0.90
9:W:914:LEU:CB	9:W:1102:ARG:NH2	2.34	0.90
9:J:702:PHE:O	9:J:703:LYS:CD	2.19	0.90
9:J:914:LEU:CB	9:J:1102:ARG:NH2	2.34	0.90
6:T:168:LYS:CE	7:U:85:ASP:OD2	2.17	0.90
9:W:702:PHE:O	9:W:703:LYS:CD	2.19	0.90
9:W:737:ASN:HD22	9:W:785:LEU:HD23	1.32	0.90
10:K:519:PHE:CE2	9:W:860:ARG:CB	2.55	0.90
7:U:133:PHE:O	7:U:137:VAL:HG22	1.71	0.90
9:W:903:PRO:CG	9:W:1098:ILE:HG21	2.01	0.90
9:J:903:PRO:CG	9:J:1098:ILE:HG21	2.01	0.90
8:I:449:VAL:O	8:I:456:TYR:CB	2.19	0.90
9:W:907:LYS:HZ2	9:W:1098:ILE:N	1.70	0.90
3:P:188:ILE:HG23	11:Y:42:SER:HB2	1.52	0.90
9:W:1094:PRO:CG	9:W:1118:ARG:NH2	2.33	0.89
9:J:907:LYS:HZ3	9:J:1098:ILE:CG1	1.83	0.89
7:U:103:TYR:CE2	7:U:138:HIS:CE1	2.58	0.89
3:C:188:ILE:HG23	11:L:42:SER:HB2	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:694:ASN:CB	9:J:695:PRO:CD	2.49	0.89
9:J:699:PHE:HB3	11:L:152:PHE:N	1.86	0.89
9:J:860:ARG:CB	10:X:519:PHE:CE2	2.54	0.89
9:J:916:ILE:H	9:J:1102:ARG:HH12	0.95	0.89
9:W:801:LEU:H	9:W:801:LEU:HD23	1.38	0.89
3:P:188:ILE:HD12	11:Y:42:SER:HB3	1.55	0.88
6:T:169:MET:CG	7:U:87:CYS:SG	2.59	0.88
9:J:1094:PRO:HG3	9:J:1118:ARG:HE	1.33	0.88
9:J:737:ASN:ND2	9:J:785:LEU:H	1.70	0.88
9:J:696:GLN:HG2	11:L:162:ASN:HD21	1.31	0.88
9:J:907:LYS:HZ2	9:J:1098:ILE:H	0.92	0.88
9:W:903:PRO:CG	9:W:1098:ILE:CB	2.52	0.88
9:J:661:ARG:HG2	9:J:736:GLN:CB	2.02	0.88
9:W:661:ARG:CG	9:W:736:GLN:HE21	1.86	0.88
7:U:139:GLU:O	7:U:143:LYS:HB2	1.74	0.88
9:W:903:PRO:HB3	9:W:1098:ILE:CB	2.04	0.88
9:J:801:LEU:HD23	9:J:801:LEU:H	1.38	0.87
9:J:903:PRO:HB3	9:J:1098:ILE:CB	2.04	0.87
3:C:188:ILE:HD12	11:L:42:SER:HB3	1.55	0.87
6:T:169:MET:O	6:T:170:ARG:O	1.92	0.87
9:W:1094:PRO:CB	9:W:1118:ARG:HG2	2.05	0.87
9:J:661:ARG:HG2	9:J:736:GLN:HG3	0.89	0.87
7:U:134:TYR:O	7:U:137:VAL:HG23	1.75	0.87
6:G:170:ARG:HH11	6:G:170:ARG:CB	1.88	0.87
9:J:702:PHE:O	9:J:703:LYS:CE	2.23	0.87
9:W:661:ARG:HG2	9:W:736:GLN:CB	2.06	0.86
9:J:903:PRO:CB	9:J:1098:ILE:CB	2.53	0.86
9:J:903:PRO:CG	9:J:1098:ILE:CB	2.52	0.86
9:J:1094:PRO:CB	9:J:1118:ARG:HG2	2.05	0.86
9:W:903:PRO:CB	9:W:1098:ILE:CB	2.53	0.85
9:W:1098:ILE:CD1	9:W:1099:PHE:CD2	2.59	0.85
11:L:128:SER:HG	11:L:156:SER:CA	1.71	0.85
9:W:702:PHE:O	9:W:703:LYS:CE	2.23	0.85
9:W:661:ARG:CG	9:W:736:GLN:NE2	2.39	0.85
9:J:702:PHE:CZ	11:L:120:ALA:CB	2.60	0.85
9:J:1094:PRO:HG3	9:J:1118:ARG:HH21	1.38	0.85
9:W:1013:VAL:HG23	10:X:425:GLU:CD	1.97	0.85
9:W:903:PRO:CB	9:W:1098:ILE:CG2	2.53	0.85
11:Y:124:ILE:HG12	11:Y:155:THR:HG21	1.59	0.85
9:J:1098:ILE:CD1	9:J:1099:PHE:CD2	2.59	0.84
9:W:1094:PRO:HG3	9:W:1118:ARG:HH21	1.38	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:661:ARG:HG2	9:W:736:GLN:CG	2.07	0.84
11:Y:124:ILE:CG1	11:Y:155:THR:CB	2.55	0.84
9:J:1013:VAL:HG23	10:K:425:GLU:CD	1.97	0.84
7:U:131:ARG:CG	7:U:135:GLN:HE22	1.91	0.84
9:W:702:PHE:CZ	11:Y:120:ALA:CB	2.60	0.83
9:W:661:ARG:HG2	9:W:736:GLN:NE2	1.92	0.83
11:L:124:ILE:CG1	11:L:155:THR:HG1	1.76	0.83
3:C:45:TYR:O	3:C:46:GLU:OE1	1.96	0.83
11:L:124:ILE:CG1	11:L:155:THR:CB	2.55	0.83
11:L:124:ILE:HG12	11:L:155:THR:HG21	1.59	0.83
9:J:860:ARG:N	10:X:519:PHE:CZ	2.47	0.83
9:J:909:MET:HE2	9:J:1121:PHE:HB2	1.59	0.83
9:J:661:ARG:CG	9:J:736:GLN:CD	2.43	0.82
11:Y:40:ILE:HD12	11:Y:40:ILE:O	1.79	0.82
9:W:915:TYR:H	9:W:1102:ARG:CZ	1.91	0.82
10:K:519:PHE:HB2	9:W:992:ARG:NH2	1.95	0.82
9:W:701:PRO:CD	11:Y:151:LEU:HA	2.10	0.82
10:K:519:PHE:CZ	9:W:860:ARG:N	2.48	0.82
11:Y:128:SER:HG	11:Y:156:SER:CA	1.73	0.82
9:J:903:PRO:CB	9:J:1098:ILE:CG2	2.53	0.82
11:L:40:ILE:HD12	11:L:40:ILE:O	1.79	0.82
3:P:45:TYR:O	3:P:46:GLU:OE1	1.96	0.82
9:J:992:ARG:NH2	10:X:519:PHE:HB2	1.93	0.82
9:W:661:ARG:HD3	9:W:736:GLN:NE2	1.95	0.82
9:J:860:ARG:N	10:X:519:PHE:CE2	2.48	0.81
9:J:701:PRO:CD	11:L:151:LEU:HA	2.10	0.81
9:J:699:PHE:HE2	11:L:146:MET:CE	1.94	0.81
9:J:1094:PRO:HB3	9:J:1118:ARG:CD	2.11	0.81
10:K:519:PHE:CE2	9:W:860:ARG:N	2.49	0.81
9:J:1049:ILE:O	9:W:1072:HIS:CE1	2.34	0.81
9:J:1072:HIS:CE1	9:W:1049:ILE:O	2.34	0.81
9:W:699:PHE:HE2	11:Y:146:MET:CE	1.94	0.81
9:J:661:ARG:HG3	9:J:736:GLN:HG3	1.61	0.80
9:W:699:PHE:CE2	11:Y:146:MET:HE3	2.11	0.80
9:W:661:ARG:HG2	9:W:736:GLN:HB2	1.60	0.80
9:W:800:CYS:SG	9:W:814:ASP:OD1	2.39	0.80
9:J:800:CYS:SG	9:J:814:ASP:OD1	2.39	0.80
6:G:171:ARG:NH2	7:H:84:THR:HA	1.97	0.80
9:J:910:PRO:HD3	9:J:1095:ILE:CG2	2.11	0.80
9:W:1094:PRO:HB3	9:W:1118:ARG:CD	2.11	0.80
9:J:903:PRO:HG3	9:J:1098:ILE:CG2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:903:PRO:CB	9:W:1098:ILE:CD1	2.53	0.79
9:W:903:PRO:CG	9:W:1098:ILE:CG2	2.60	0.79
9:J:910:PRO:CD	9:J:1095:ILE:HG21	2.12	0.79
9:J:903:PRO:CG	9:J:1098:ILE:CG2	2.60	0.79
9:W:698:VAL:HG21	11:Y:166:ALA:HB1	1.63	0.79
9:W:702:PHE:CE1	11:Y:120:ALA:CB	2.66	0.79
9:W:910:PRO:HD3	9:W:1095:ILE:CG2	2.11	0.79
9:J:698:VAL:CG2	11:L:166:ALA:CB	2.51	0.79
9:J:915:TYR:H	9:J:1102:ARG:CZ	1.92	0.79
9:W:702:PHE:HB2	11:Y:173:ALA:CB	2.12	0.79
9:J:702:PHE:HB2	11:L:173:ALA:CB	2.13	0.78
9:J:1094:PRO:CD	9:J:1118:ARG:NH2	2.47	0.78
7:U:131:ARG:CG	7:U:135:GLN:NE2	2.46	0.78
9:W:737:ASN:OD1	9:W:785:LEU:C	2.22	0.78
9:J:702:PHE:CE1	11:L:120:ALA:CB	2.66	0.78
9:W:1094:PRO:CD	9:W:1118:ARG:NH2	2.47	0.78
8:I:853:PHE:HB2	8:I:974:THR:O	1.84	0.78
9:W:910:PRO:CD	9:W:1095:ILE:HG21	2.12	0.78
9:J:1094:PRO:HD3	9:J:1118:ARG:CZ	2.15	0.77
7:U:103:TYR:CZ	7:U:138:HIS:NE2	2.48	0.77
9:W:903:PRO:HG3	9:W:1098:ILE:CG2	2.12	0.77
9:J:1094:PRO:CB	9:J:1118:ARG:CG	2.61	0.77
7:U:141:TYR:O	7:U:144:THR:N	2.18	0.77
9:W:698:VAL:CG2	11:Y:166:ALA:CB	2.51	0.77
7:U:136:GLU:HA	7:U:136:GLU:OE1	1.83	0.77
6:T:100:GLU:HA	7:U:106:TYR:HE2	1.47	0.77
6:T:100:GLU:CA	7:U:106:TYR:HE2	1.97	0.77
9:J:698:VAL:HG21	11:L:166:ALA:HB1	1.63	0.77
6:T:169:MET:CE	6:T:170:ARG:N	2.48	0.77
9:W:703:LYS:HD2	9:W:703:LYS:N	1.99	0.77
6:T:169:MET:HE3	6:T:170:ARG:N	1.99	0.76
9:W:1094:PRO:HB3	9:W:1118:ARG:NE	2.00	0.76
9:J:903:PRO:CG	9:J:1098:ILE:HB	2.10	0.76
9:J:699:PHE:HD1	9:J:701:PRO:HD3	1.50	0.76
9:J:699:PHE:CE2	11:L:146:MET:HE3	2.15	0.76
9:J:1094:PRO:CB	9:J:1118:ARG:NE	2.48	0.76
9:W:699:PHE:HD1	9:W:701:PRO:HD3	1.50	0.76
9:W:1094:PRO:CB	9:W:1118:ARG:NE	2.48	0.76
9:W:1106:GLN:HE22	11:Y:133:LEU:HD22	1.49	0.76
9:J:859:THR:CB	10:X:519:PHE:CZ	2.68	0.76
9:J:1094:PRO:HB3	9:J:1118:ARG:NE	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:131:ARG:O	7:U:135:GLN:CD	2.24	0.76
8:V:853:PHE:HB2	8:V:974:THR:O	1.84	0.76
9:J:701:PRO:HD3	11:L:151:LEU:HA	1.67	0.76
9:W:1094:PRO:HD3	9:W:1118:ARG:CZ	2.15	0.76
6:T:100:GLU:CA	7:U:106:TYR:CE2	2.69	0.76
9:W:701:PRO:HD3	11:Y:151:LEU:HA	1.67	0.76
11:Y:124:ILE:HD11	11:Y:155:THR:CG2	2.16	0.75
9:J:907:LYS:HE3	9:J:1099:PHE:CE1	2.21	0.75
9:J:655:ARG:O	9:J:815:ILE:CG2	2.35	0.75
9:J:992:ARG:HH21	10:X:519:PHE:HB2	1.52	0.75
10:K:519:PHE:HE2	9:W:860:ARG:CA	2.00	0.75
9:W:907:LYS:HZ3	9:W:1098:ILE:CG1	1.96	0.75
9:J:1106:GLN:HE22	11:L:133:LEU:HD22	1.49	0.75
11:L:41:GLU:OE2	11:L:41:GLU:HA	1.87	0.75
9:W:907:LYS:HE3	9:W:1099:PHE:CE1	2.21	0.75
9:J:737:ASN:ND2	9:J:785:LEU:CD2	2.47	0.75
9:W:1263:PHE:O	9:W:1283:ASN:HA	1.87	0.75
10:K:519:PHE:CZ	9:W:859:THR:CB	2.69	0.74
11:L:124:ILE:HD11	11:L:155:THR:CG2	2.16	0.74
11:L:133:LEU:HD23	11:L:133:LEU:N	2.01	0.74
9:J:860:ARG:CA	10:X:519:PHE:HE2	2.00	0.74
9:W:655:ARG:O	9:W:815:ILE:CG2	2.35	0.74
9:J:859:THR:CB	10:X:519:PHE:HZ	2.00	0.74
11:Y:41:GLU:OE2	11:Y:41:GLU:HA	1.87	0.74
11:Y:133:LEU:HD23	11:Y:133:LEU:N	2.01	0.74
9:W:1094:PRO:CB	9:W:1118:ARG:CG	2.61	0.74
9:W:500:LEU:CD1	9:W:502:LEU:HG	2.18	0.73
9:W:704:ARG:HG3	9:W:704:ARG:NH1	2.02	0.73
9:J:801:LEU:O	9:J:803:ILE:CD1	2.35	0.73
6:T:168:LYS:HE2	6:T:169:MET:H	1.53	0.73
9:W:801:LEU:O	9:W:803:ILE:CD1	2.35	0.73
11:Y:96:SER:O	11:Y:135:ALA:HB2	1.88	0.73
9:W:661:ARG:CD	9:W:736:GLN:NE2	2.51	0.73
9:W:1013:VAL:CG2	10:X:425:GLU:CD	2.57	0.73
9:W:655:ARG:HG3	9:W:655:ARG:HH11	1.54	0.73
6:G:169:MET:CE	7:H:135:GLN:HE21	2.02	0.73
9:J:737:ASN:OD1	9:J:738:PRO:HD3	1.87	0.73
10:K:519:PHE:HZ	9:W:859:THR:CB	2.01	0.73
9:J:501:GLN:HB3	9:J:503:LYS:HE3	1.69	0.73
6:G:169:MET:HG2	7:H:87:CYS:CB	2.19	0.72
9:J:737:ASN:OD1	9:J:785:LEU:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:501:GLN:HB3	9:W:503:LYS:HE3	1.69	0.72
9:W:702:PHE:O	9:W:703:LYS:HE2	1.89	0.72
9:J:500:LEU:CD1	9:J:502:LEU:HG	2.18	0.72
9:J:702:PHE:HB2	11:L:173:ALA:HB2	1.70	0.72
11:L:96:SER:O	11:L:135:ALA:HB2	1.88	0.72
9:J:907:LYS:HD2	9:J:1097:ARG:CG	2.19	0.72
9:J:1013:VAL:CG2	10:K:425:GLU:CD	2.57	0.72
9:W:903:PRO:CG	9:W:1098:ILE:HD13	2.20	0.72
9:J:702:PHE:O	9:J:703:LYS:HE2	1.89	0.72
9:J:737:ASN:OD1	9:J:785:LEU:C	2.26	0.72
9:J:1094:PRO:HD3	9:J:1118:ARG:NH2	2.04	0.72
9:J:1263:PHE:O	9:J:1283:ASN:HA	1.87	0.72
9:W:903:PRO:CA	9:W:1098:ILE:HG12	2.20	0.72
9:J:655:ARG:HG3	9:J:655:ARG:HH11	1.54	0.72
9:J:1094:PRO:CD	9:J:1118:ARG:CZ	2.68	0.72
9:W:698:VAL:HG13	11:Y:151:LEU:HD11	1.71	0.72
3:C:188:ILE:HG21	11:L:42:SER:HB2	1.71	0.71
6:G:169:MET:HG2	7:H:87:CYS:SG	2.29	0.71
9:J:903:PRO:CB	9:J:1098:ILE:CD1	2.53	0.71
3:P:188:ILE:HG21	11:Y:42:SER:HB2	1.71	0.71
9:W:702:PHE:HB2	11:Y:173:ALA:HB2	1.70	0.71
9:W:1094:PRO:CD	9:W:1118:ARG:CZ	2.68	0.71
9:J:914:LEU:CA	9:J:1102:ARG:HH22	2.04	0.71
9:J:698:VAL:HG13	11:L:151:LEU:HD11	1.71	0.71
9:W:1106:GLN:OE1	9:W:1106:GLN:HA	1.91	0.71
9:J:903:PRO:CA	9:J:1098:ILE:HG12	2.20	0.71
9:W:914:LEU:CA	9:W:1102:ARG:HH22	2.04	0.71
3:S:183:ILE:HD12	3:S:183:ILE:N	2.06	0.71
7:U:136:GLU:HB3	7:U:168:LEU:HD21	1.72	0.71
9:W:737:ASN:OD1	9:W:785:LEU:N	2.23	0.71
9:J:903:PRO:CG	9:J:1098:ILE:HD13	2.20	0.70
9:W:903:PRO:CG	9:W:1098:ILE:HB	2.10	0.70
9:J:702:PHE:CZ	11:L:120:ALA:CA	2.74	0.70
9:W:702:PHE:CZ	11:Y:120:ALA:CA	2.74	0.70
9:W:737:ASN:OD1	9:W:738:PRO:HD3	1.91	0.70
3:F:183:ILE:HD12	3:F:183:ILE:N	2.06	0.70
6:T:169:MET:HE3	6:T:169:MET:C	2.12	0.70
3:C:45:TYR:CE2	3:C:51:LYS:HB3	2.27	0.70
3:P:45:TYR:CE2	3:P:51:LYS:HB3	2.27	0.70
9:W:662:ILE:N	9:W:736:GLN:HG2	2.06	0.70
9:J:699:PHE:CE2	11:L:146:MET:CE	2.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:155:THR:HG22	11:Y:155:THR:O	1.91	0.70
11:L:155:THR:O	11:L:155:THR:HG22	1.90	0.69
9:J:661:ARG:CD	9:J:736:GLN:CD	2.61	0.69
9:J:661:ARG:HD3	9:J:736:GLN:CD	2.13	0.69
9:J:1106:GLN:OE1	9:J:1106:GLN:HA	1.91	0.69
10:K:519:PHE:HB2	9:W:992:ARG:HH21	1.53	0.69
9:W:907:LYS:HD2	9:W:1097:ARG:CG	2.20	0.69
9:W:1094:PRO:HD3	9:W:1118:ARG:NH2	2.04	0.69
11:Y:36:ASP:OD1	11:Y:37:GLU:N	2.25	0.69
7:U:131:ARG:HG2	7:U:135:GLN:CD	2.12	0.69
10:X:444:VAL:O	10:X:540:VAL:HA	1.93	0.69
9:W:903:PRO:CB	9:W:1098:ILE:HD13	2.23	0.69
9:J:703:LYS:HD2	9:J:703:LYS:N	1.99	0.69
9:J:915:TYR:CA	9:J:1102:ARG:HH12	2.06	0.69
11:Y:132:HIS:C	11:Y:133:LEU:CD2	2.45	0.68
9:J:903:PRO:CB	9:J:1098:ILE:HD13	2.23	0.68
9:J:903:PRO:CG	9:J:1098:ILE:CG1	2.71	0.68
9:W:915:TYR:CA	9:W:1102:ARG:HH12	2.06	0.68
10:K:444:VAL:O	10:K:540:VAL:HA	1.93	0.68
11:L:124:ILE:CG1	11:L:155:THR:HG21	2.23	0.68
11:Y:128:SER:OG	11:Y:156:SER:HB2	1.92	0.68
3:P:40:GLN:O	3:P:44:ASP:HB2	1.93	0.68
6:T:168:LYS:CE	7:U:85:ASP:CG	2.61	0.68
9:W:699:PHE:CE2	11:Y:146:MET:CE	2.73	0.68
9:J:903:PRO:CD	9:J:1098:ILE:HG21	2.24	0.68
9:J:907:LYS:HZ3	9:J:1098:ILE:HG12	1.58	0.68
7:U:139:GLU:OE2	7:U:143:LYS:HD2	1.92	0.68
9:W:737:ASN:ND2	9:W:785:LEU:CD2	2.49	0.68
7:U:131:ARG:CD	7:U:135:GLN:HE22	2.08	0.67
9:W:737:ASN:CG	9:W:785:LEU:N	2.44	0.67
11:Y:124:ILE:CG1	11:Y:155:THR:HG21	2.23	0.67
3:C:40:GLN:O	3:C:44:ASP:HB2	1.93	0.67
8:V:299:PHE:O	8:V:302:ALA:HB3	1.95	0.67
9:J:1261:TYR:O	9:J:1285:ILE:HA	1.95	0.67
11:L:36:ASP:OD1	11:L:37:GLU:N	2.25	0.67
9:J:907:LYS:HE3	9:J:1099:PHE:HE1	1.60	0.67
8:I:299:PHE:O	8:I:302:ALA:HB3	1.95	0.67
4:Q:122:GLU:H	4:Q:127:MET:HG3	1.60	0.67
10:K:519:PHE:CE2	9:W:860:ARG:CA	2.78	0.66
9:W:903:PRO:CD	9:W:1098:ILE:HG21	2.24	0.66
9:J:737:ASN:CG	9:J:785:LEU:N	2.46	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:128:SER:OG	11:L:156:SER:HB2	1.92	0.66
4:D:122:GLU:H	4:D:127:MET:HG3	1.60	0.66
9:J:915:TYR:N	9:J:1102:ARG:CZ	2.54	0.66
9:W:909:MET:CE	9:W:1121:PHE:HB2	2.26	0.66
9:J:914:LEU:CA	9:J:1102:ARG:NH2	2.59	0.66
10:K:519:PHE:H	9:W:992:ARG:HH22	0.75	0.66
9:W:1261:TYR:O	9:W:1285:ILE:HA	1.95	0.66
10:K:519:PHE:N	9:W:992:ARG:NH2	2.29	0.66
9:W:661:ARG:HA	9:W:736:GLN:HB3	1.77	0.66
11:L:43:LYS:O	11:L:44:SER:HB2	1.95	0.66
11:Y:43:LYS:O	11:Y:44:SER:HB2	1.95	0.66
9:J:860:ARG:CA	10:X:519:PHE:CE2	2.78	0.65
9:W:903:PRO:CG	9:W:1098:ILE:CG1	2.71	0.65
11:Y:124:ILE:HD11	11:Y:155:THR:OG1	1.96	0.65
9:J:737:ASN:CG	9:J:785:LEU:H	2.00	0.65
6:G:171:ARG:HH22	7:H:84:THR:HA	1.60	0.65
9:J:801:LEU:HD23	9:J:801:LEU:N	2.09	0.65
10:K:519:PHE:HZ	9:W:860:ARG:N	1.95	0.65
9:W:737:ASN:CG	9:W:785:LEU:H	1.99	0.65
9:W:914:LEU:CA	9:W:1102:ARG:NH2	2.59	0.65
9:W:907:LYS:HE3	9:W:1099:PHE:HE1	1.60	0.65
11:L:124:ILE:CG1	11:L:155:THR:CG2	2.75	0.64
11:L:128:SER:HG	11:L:156:SER:HA	0.77	0.64
9:W:915:TYR:N	9:W:1102:ARG:CZ	2.54	0.64
11:Y:124:ILE:CG1	11:Y:155:THR:CG2	2.75	0.64
9:J:909:MET:CE	9:J:1121:PHE:HB2	2.26	0.64
9:W:501:GLN:HG3	9:W:503:LYS:HE3	1.79	0.64
9:J:704:ARG:HG3	9:J:704:ARG:NH1	2.02	0.64
2:O:184:PHE:H	2:O:262:VAL:HG22	1.63	0.64
9:W:801:LEU:HD23	9:W:801:LEU:N	2.09	0.64
9:W:701:PRO:HG3	11:Y:150:MET:O	1.97	0.63
2:B:176:LEU:HA	2:B:185:TYR:O	1.99	0.63
9:J:501:GLN:HG3	9:J:503:LYS:HE3	1.79	0.63
9:J:655:ARG:NH1	9:J:816:ILE:CD1	2.62	0.63
11:L:132:HIS:C	11:L:133:LEU:CD2	2.45	0.63
3:C:45:TYR:C	3:C:46:GLU:OE1	2.37	0.63
9:W:655:ARG:HG3	9:W:655:ARG:NH1	2.14	0.63
9:J:992:ARG:NH2	10:X:519:PHE:N	2.29	0.62
9:W:655:ARG:NH1	9:W:816:ILE:CD1	2.62	0.62
11:L:43:LYS:O	11:L:44:SER:CB	2.47	0.62
3:P:45:TYR:C	3:P:46:GLU:OE1	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:124:ILE:HD11	11:L:155:THR:OG1	1.96	0.62
2:O:176:LEU:HA	2:O:185:TYR:O	1.99	0.62
6:T:169:MET:HG3	7:U:87:CYS:CB	2.29	0.62
8:V:463:ASN:O	8:V:465:ASN:N	2.32	0.62
6:T:168:LYS:HE3	7:U:85:ASP:CG	2.18	0.62
3:P:188:ILE:HD12	11:Y:42:SER:CB	2.29	0.62
7:U:13:ASN:HD21	7:U:153:THR:HG22	1.65	0.62
2:B:184:PHE:H	2:B:262:VAL:HG22	1.63	0.62
9:J:661:ARG:HA	9:J:736:GLN:HB2	1.80	0.62
2:B:159:PHE:O	2:B:163:ASP:HB2	2.00	0.61
9:J:628:GLN:HA	9:J:631:LEU:HB3	1.83	0.61
9:J:860:ARG:N	10:X:519:PHE:HZ	1.93	0.61
11:Y:43:LYS:O	11:Y:44:SER:CB	2.47	0.61
11:Y:132:HIS:CD2	11:Y:133:LEU:CD2	2.82	0.61
9:J:655:ARG:NH1	9:J:816:ILE:HD13	2.15	0.61
2:O:159:PHE:O	2:O:163:ASP:HB2	2.00	0.61
9:W:701:PRO:CG	11:Y:151:LEU:N	2.60	0.61
6:G:170:ARG:HH11	6:G:170:ARG:CG	2.14	0.61
11:L:132:HIS:CD2	11:L:133:LEU:CD2	2.82	0.61
10:K:519:PHE:CB	9:W:992:ARG:NH2	2.63	0.61
6:T:100:GLU:OE2	7:U:107:SER:OG	2.19	0.61
9:W:909:MET:HE2	9:W:1121:PHE:HB2	1.83	0.61
11:Y:128:SER:HG	11:Y:156:SER:HA	0.77	0.61
9:W:628:GLN:HA	9:W:631:LEU:HB3	1.82	0.61
11:Y:124:ILE:HD11	11:Y:155:THR:HG23	1.83	0.61
2:B:239:LEU:O	2:B:257:GLY:C	2.39	0.61
2:O:239:LEU:O	2:O:257:GLY:C	2.39	0.61
9:W:655:ARG:NH1	9:W:816:ILE:HD13	2.15	0.61
9:W:1095:ILE:O	9:W:1095:ILE:HG22	2.01	0.60
11:L:44:SER:OG	11:L:72:GLN:NE2	2.34	0.60
9:J:701:PRO:HG3	11:L:150:MET:O	1.97	0.60
3:C:188:ILE:HD12	11:L:42:SER:CB	2.29	0.60
9:J:992:ARG:NH2	10:X:519:PHE:CB	2.62	0.60
9:W:661:ARG:CD	9:W:736:GLN:CD	2.69	0.60
11:Y:44:SER:OG	11:Y:72:GLN:NE2	2.35	0.60
10:K:445:VAL:HG12	10:K:540:VAL:HG12	1.83	0.60
9:W:702:PHE:HZ	11:Y:120:ALA:C	2.05	0.60
9:J:501:GLN:HB3	9:J:503:LYS:HG3	1.83	0.60
9:W:903:PRO:HG2	9:W:1098:ILE:HD13	1.84	0.60
10:X:445:VAL:HG12	10:X:540:VAL:HG12	1.83	0.60
9:J:1095:ILE:HG22	9:J:1095:ILE:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:13:ASN:HD21	7:H:153:THR:HG22	1.65	0.59
9:J:701:PRO:CG	11:L:151:LEU:N	2.60	0.59
9:W:1094:PRO:CG	9:W:1118:ARG:HH21	2.07	0.59
9:J:702:PHE:HZ	11:L:120:ALA:C	2.05	0.59
9:W:501:GLN:HB3	9:W:503:LYS:HG3	1.83	0.59
9:W:1013:VAL:HG22	10:X:425:GLU:OE1	2.02	0.59
9:W:655:ARG:CZ	9:W:816:ILE:HD13	2.33	0.59
9:W:903:PRO:HB3	9:W:1098:ILE:HG12	0.60	0.59
9:J:655:ARG:HG3	9:J:655:ARG:NH1	2.14	0.59
9:J:655:ARG:CZ	9:J:816:ILE:HD13	2.33	0.59
9:J:903:PRO:HB3	9:J:1098:ILE:HG12	0.60	0.59
9:J:903:PRO:HG2	9:J:1098:ILE:HD13	1.83	0.59
9:W:628:GLN:O	9:W:632:PHE:HB2	2.03	0.59
9:J:737:ASN:OD1	9:J:738:PRO:CD	2.51	0.59
6:T:30:GLN:OE1	9:W:621:HIS:ND1	2.35	0.59
9:J:1013:VAL:HG22	10:K:425:GLU:OE1	2.03	0.59
9:W:626:SER:HA	9:W:629:ASP:HB2	1.85	0.59
9:W:699:PHE:CD1	9:W:701:PRO:HD3	2.36	0.59
3:P:18:TRP:NE1	3:P:96:LYS:O	2.35	0.58
7:U:132:SER:HA	7:U:135:GLN:OE1	2.03	0.58
11:Y:124:ILE:CD1	11:Y:155:THR:CG2	2.81	0.58
2:B:59:ILE:CG1	3:C:44:ASP:OD2	2.51	0.58
6:G:170:ARG:HB3	6:G:170:ARG:NH1	2.04	0.58
8:I:784:PHE:O	8:I:838:CYS:HA	2.03	0.58
9:J:626:SER:HA	9:J:629:ASP:HB2	1.85	0.58
9:J:992:ARG:HH22	10:X:519:PHE:H	0.75	0.58
9:J:1094:PRO:CG	9:J:1118:ARG:HH21	2.08	0.58
2:O:59:ILE:CG1	3:P:44:ASP:OD2	2.51	0.58
9:J:734:ARG:O	9:J:736:GLN:HG2	2.04	0.58
3:P:188:ILE:HG23	11:Y:42:SER:CB	2.31	0.58
11:L:124:ILE:HD11	11:L:155:THR:HG23	1.83	0.58
6:T:100:GLU:CD	7:U:107:SER:OG	2.42	0.58
7:U:140:LEU:HD11	7:U:164:ARG:HB3	1.85	0.58
9:J:628:GLN:O	9:J:632:PHE:HB2	2.03	0.58
2:B:175:ASN:HB3	2:B:187:LEU:HB2	1.85	0.57
7:U:139:GLU:O	7:U:143:LYS:CB	2.51	0.57
8:V:784:PHE:O	8:V:838:CYS:HA	2.03	0.57
6:G:30:GLN:OE1	9:J:621:HIS:ND1	2.35	0.57
9:J:1013:VAL:HG13	9:J:1019:ILE:HG21	1.86	0.57
11:L:98:SER:HB2	11:L:135:ALA:HB1	1.86	0.57
9:W:737:ASN:HD21	9:W:785:LEU:CB	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1094:PRO:CG	9:W:1118:ARG:HE	2.04	0.57
10:K:519:PHE:HD2	9:W:992:ARG:CZ	2.17	0.57
11:L:124:ILE:CD1	11:L:155:THR:CG2	2.81	0.57
4:D:47:ARG:NH1	4:D:61:ASP:OD2	2.38	0.57
4:Q:47:ARG:NH1	4:Q:61:ASP:OD2	2.37	0.57
9:J:699:PHE:CD1	9:J:701:PRO:HD3	2.36	0.57
9:J:907:LYS:HZ1	9:J:1098:ILE:CG1	1.88	0.57
9:J:1103:GLN:CD	9:J:1103:GLN:H	2.08	0.57
9:W:661:ARG:CG	9:W:736:GLN:CG	2.80	0.57
11:Y:124:ILE:HG12	11:Y:155:THR:CG2	2.32	0.57
2:O:175:ASN:HB3	2:O:187:LEU:HB2	1.85	0.57
9:W:611:PHE:HA	9:W:614:ILE:HG22	1.87	0.57
9:W:1013:VAL:HG13	9:W:1019:ILE:HG21	1.86	0.57
9:J:1094:PRO:CG	9:J:1118:ARG:HE	2.04	0.57
9:W:661:ARG:HD2	9:W:736:GLN:HG2	1.87	0.57
9:W:1103:GLN:H	9:W:1103:GLN:CD	2.08	0.57
9:W:915:TYR:CA	9:W:1102:ARG:NH1	2.68	0.56
9:J:992:ARG:CZ	10:X:519:PHE:HD2	2.17	0.56
3:C:18:TRP:NE1	3:C:96:LYS:O	2.35	0.56
9:J:915:TYR:CA	9:J:1102:ARG:NH1	2.68	0.56
10:K:519:PHE:HE2	9:W:860:ARG:N	1.97	0.56
9:W:661:ARG:HD3	9:W:736:GLN:CD	2.25	0.56
9:J:909:MET:CB	9:J:1095:ILE:HD12	2.36	0.56
11:Y:98:SER:HB2	11:Y:135:ALA:HB1	1.86	0.56
3:C:188:ILE:HG23	11:L:42:SER:CB	2.31	0.56
3:F:138:LEU:O	3:F:169:ARG:NH1	2.39	0.56
7:H:117:ASN:HB2	7:H:121:SER:HB3	1.88	0.56
9:W:734:ARG:HB2	9:W:736:GLN:HE22	1.71	0.56
9:J:1103:GLN:H	9:J:1103:GLN:NE2	2.04	0.56
9:W:501:GLN:CB	9:W:503:LYS:HE3	2.36	0.56
11:Y:58:GLU:OE1	11:Y:176:GLN:NE2	2.38	0.56
9:J:501:GLN:CB	9:J:503:LYS:HE3	2.36	0.56
7:U:132:SER:N	7:U:135:GLN:OE1	2.38	0.56
6:G:169:MET:CE	7:H:135:GLN:NE2	2.68	0.56
5:R:8:VAL:HB	5:R:17:TYR:HB3	1.88	0.56
9:W:1103:GLN:H	9:W:1103:GLN:NE2	2.04	0.56
11:Y:175:PHE:O	11:Y:179:SER:N	2.35	0.56
2:B:55:LEU:HD11	3:C:41:LEU:HD21	1.88	0.56
3:S:138:LEU:O	3:S:169:ARG:NH1	2.39	0.56
5:E:8:VAL:HB	5:E:17:TYR:HB3	1.88	0.56
11:L:58:GLU:OE1	11:L:176:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:117:ASN:HB2	7:U:121:SER:HB3	1.88	0.56
6:T:169:MET:HB3	7:U:87:CYS:HB2	1.87	0.55
9:W:701:PRO:CD	11:Y:151:LEU:CA	2.83	0.55
9:W:909:MET:CB	9:W:1095:ILE:HD12	2.36	0.55
3:C:45:TYR:O	3:C:46:GLU:HB2	2.06	0.55
9:W:701:PRO:HD2	11:Y:151:LEU:HB2	1.89	0.55
9:J:501:GLN:CG	9:J:503:LYS:HE3	2.36	0.55
9:J:702:PHE:CE1	11:L:120:ALA:HA	2.41	0.55
9:J:737:ASN:HD21	9:J:785:LEU:CB	2.17	0.55
3:P:45:TYR:O	3:P:46:GLU:HB2	2.06	0.55
9:J:611:PHE:HA	9:J:614:ILE:HG22	1.87	0.55
3:C:108:TRP:HE1	3:C:112:LYS:HE2	1.72	0.55
9:J:699:PHE:HB2	11:L:152:PHE:HB3	1.89	0.55
9:J:1262:GLU:HA	9:J:1284:VAL:O	2.07	0.55
9:W:694:ASN:HB3	9:W:695:PRO:CD	2.36	0.55
9:W:1262:GLU:HA	9:W:1284:VAL:O	2.07	0.55
3:P:108:TRP:HE1	3:P:112:LYS:HE2	1.72	0.55
9:W:501:GLN:CG	9:W:503:LYS:HE3	2.36	0.55
9:W:662:ILE:N	9:W:736:GLN:CG	2.69	0.55
11:Y:161:ASP:O	11:Y:164:ASP:N	2.40	0.55
1:A:37:ASN:OD1	8:I:464:LYS:HD2	2.07	0.55
2:O:55:LEU:HD11	3:P:41:LEU:HD21	1.88	0.55
11:Y:18:LEU:HD12	11:Y:68:ASP:HB3	1.89	0.55
2:O:166:LYS:NZ	2:O:172:GLN:OE1	2.37	0.54
2:B:51:GLU:HB3	4:D:114:LEU:HD11	1.89	0.54
2:B:59:ILE:HG13	3:C:44:ASP:OD2	2.07	0.54
6:T:100:GLU:HA	7:U:106:TYR:HD2	1.66	0.54
9:J:702:PHE:CZ	11:L:120:ALA:C	2.81	0.54
9:W:702:PHE:CE1	11:Y:120:ALA:HA	2.41	0.54
6:T:169:MET:HE1	6:T:170:ARG:N	2.21	0.54
5:E:113:ASN:ND2	5:E:115:ASN:OD1	2.41	0.54
9:W:907:LYS:NZ	9:W:1098:ILE:N	2.42	0.54
10:K:500:ILE:HA	10:K:526:GLY:HA2	1.89	0.54
11:L:161:ASP:O	11:L:164:ASP:N	2.40	0.54
9:W:737:ASN:OD1	9:W:738:PRO:CD	2.56	0.54
9:J:737:ASN:HD21	9:J:785:LEU:CG	2.21	0.54
9:J:1043:ASP:HB3	9:J:1075:ARG:HG2	1.90	0.54
5:R:31:ASN:HA	5:R:34:LEU:HD13	1.90	0.54
9:J:694:ASN:HB3	9:J:695:PRO:CD	2.37	0.54
9:J:907:LYS:CD	9:J:1097:ARG:HG3	2.29	0.54
11:L:125:GLY:O	11:L:154:GLU:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:59:ILE:HG13	3:P:44:ASP:OD2	2.07	0.54
10:X:500:ILE:HA	10:X:526:GLY:HA2	1.89	0.54
9:J:701:PRO:HD2	11:L:151:LEU:HB2	1.89	0.54
9:W:702:PHE:CZ	11:Y:120:ALA:C	2.81	0.54
11:L:18:LEU:HD12	11:L:68:ASP:HB3	1.89	0.53
9:W:699:PHE:HB2	11:Y:152:PHE:HB3	1.89	0.53
2:B:233:SER:OG	2:B:234:GLU:N	2.42	0.53
2:O:177:LYS:HB3	2:O:185:TYR:HB2	1.91	0.53
5:R:35:ILE:CD1	11:Y:39:ASN:OD1	2.56	0.53
9:W:702:PHE:CE2	11:Y:120:ALA:HB1	2.41	0.53
5:R:113:ASN:ND2	5:R:115:ASN:OD1	2.41	0.53
2:O:233:SER:OG	2:O:234:GLU:N	2.42	0.53
9:W:492:PHE:O	9:W:496:LYS:NZ	2.41	0.53
9:W:661:ARG:CG	9:W:736:GLN:HG2	2.39	0.53
9:W:907:LYS:HZ3	9:W:1098:ILE:HG12	1.74	0.53
5:R:32:GLU:HA	5:R:35:ILE:HG12	1.90	0.53
9:W:1043:ASP:HB3	9:W:1075:ARG:HG2	1.90	0.53
1:A:63:LEU:HD11	1:A:105:ILE:HG22	1.91	0.53
9:J:492:PHE:O	9:J:496:LYS:NZ	2.41	0.53
11:L:175:PHE:O	11:L:179:SER:N	2.35	0.53
9:W:699:PHE:CB	11:Y:152:PHE:N	2.59	0.53
4:Q:26:ASN:O	4:Q:134:LYS:NZ	2.38	0.53
11:Y:95:ILE:O	11:Y:135:ALA:N	2.26	0.53
11:Y:125:GLY:O	11:Y:154:GLU:O	2.26	0.53
5:E:31:ASN:HA	5:E:34:LEU:HD13	1.90	0.53
5:E:32:GLU:HA	5:E:35:ILE:HG12	1.91	0.53
5:E:35:ILE:CD1	11:L:39:ASN:OD1	2.56	0.53
9:J:1017:ASP:N	9:J:1017:ASP:OD1	2.42	0.53
9:W:522:ARG:HE	9:W:523:LEU:HD22	1.74	0.53
2:B:177:LYS:HB3	2:B:185:TYR:HB2	1.91	0.53
2:O:51:GLU:HB3	4:Q:114:LEU:HD11	1.90	0.53
3:C:109:SER:OG	3:C:110:HIS:N	2.42	0.52
9:J:694:ASN:OD1	9:J:694:ASN:N	2.42	0.52
3:P:109:SER:OG	3:P:110:HIS:N	2.42	0.52
3:S:159:CYS:HA	3:S:180:LEU:HA	1.91	0.52
6:G:166:ILE:O	6:G:166:ILE:HG22	2.10	0.52
9:J:907:LYS:NZ	9:J:1098:ILE:N	2.42	0.52
1:N:63:LEU:HD11	1:N:105:ILE:HG22	1.91	0.52
1:N:115:ILE:HD11	1:N:140:LYS:HB3	1.92	0.52
9:J:522:ARG:HE	9:J:523:LEU:HD22	1.73	0.52
4:D:6:PHE:O	4:D:18:ASP:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:1034:SER:OG	9:J:1035:ARG:N	2.41	0.52
9:W:909:MET:HB3	9:W:1095:ILE:HD12	1.92	0.52
9:W:1017:ASP:OD1	9:W:1017:ASP:N	2.42	0.52
1:A:81:GLN:NE2	2:B:146:LEU:O	2.42	0.52
9:J:701:PRO:CD	11:L:151:LEU:CA	2.83	0.52
9:J:860:ARG:N	10:X:519:PHE:HE2	1.97	0.52
9:J:909:MET:HB3	9:J:1095:ILE:HD12	1.92	0.52
6:T:169:MET:C	6:T:170:ARG:O	2.48	0.52
6:G:47:SER:HB2	7:H:164:ARG:HH22	1.75	0.52
11:L:95:ILE:O	11:L:135:ALA:N	2.26	0.52
6:T:168:LYS:HZ1	7:U:85:ASP:CG	2.13	0.52
4:D:28:ALA:HB1	4:D:32:ASN:HB3	1.92	0.52
8:I:529:GLN:O	8:I:551:LYS:N	2.43	0.52
9:J:478:ASP:OD2	9:J:491:TYR:OH	2.28	0.52
4:Q:74:THR:HG22	4:Q:84:VAL:HG12	1.90	0.52
3:S:156:GLN:HG2	3:S:185:LYS:O	2.10	0.52
9:W:694:ASN:OD1	9:W:694:ASN:N	2.42	0.52
3:C:81:GLU:OE2	4:D:59:LYS:NZ	2.42	0.52
3:F:70:ASP:OD1	3:F:74:ARG:NH2	2.43	0.52
3:F:159:CYS:HA	3:F:180:LEU:HA	1.91	0.52
9:W:661:ARG:HG2	9:W:736:GLN:CD	2.29	0.52
3:S:70:ASP:OD1	3:S:74:ARG:NH2	2.43	0.51
9:W:801:LEU:N	9:W:801:LEU:CD2	2.73	0.51
5:E:105:ASP:OD1	5:E:105:ASP:N	2.43	0.51
4:Q:6:PHE:O	4:Q:18:ASP:HA	2.10	0.51
6:T:276:ASP:OD1	6:T:276:ASP:N	2.43	0.51
9:W:737:ASN:HD21	9:W:785:LEU:CG	2.22	0.51
9:W:1129:SER:OG	9:W:1130:LYS:NZ	2.43	0.51
4:D:74:THR:HG22	4:D:84:VAL:HG12	1.90	0.51
5:E:7:LEU:HB3	5:E:141:VAL:HB	1.92	0.51
1:A:79:ILE:HG12	1:A:84:LEU:HB3	1.93	0.51
1:A:115:ILE:HD11	1:A:140:LYS:HB3	1.92	0.51
9:J:702:PHE:CE1	11:L:120:ALA:CA	2.94	0.51
9:W:704:ARG:NH1	9:W:704:ARG:CG	2.73	0.51
8:I:1013:TYR:HA	8:I:1064:HIS:HA	1.93	0.51
6:T:104:PHE:HB2	7:U:106:TYR:OH	2.11	0.51
1:A:57:LEU:HA	2:B:145:ASN:HB3	1.93	0.51
9:J:702:PHE:CE2	11:L:120:ALA:HB1	2.41	0.51
9:J:1200:CYS:O	9:J:1204:GLN:NE2	2.42	0.51
1:N:81:GLN:NE2	2:O:146:LEU:O	2.42	0.51
4:Q:28:ALA:HB1	4:Q:32:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:47:SER:HB2	7:U:164:ARG:HH22	1.75	0.51
9:W:1200:CYS:O	9:W:1204:GLN:NE2	2.42	0.51
8:I:776:ILE:HB	8:I:783:PHE:HB2	1.93	0.51
9:J:801:LEU:N	9:J:801:LEU:CD2	2.73	0.51
2:B:166:LYS:NZ	2:B:172:GLN:OE1	2.37	0.51
9:J:698:VAL:HA	11:L:152:PHE:O	2.11	0.51
2:O:141:SER:OG	2:O:142:ASN:N	2.44	0.51
9:W:481:ASN:O	9:W:484:MET:SD	2.69	0.51
9:W:915:TYR:C	9:W:1102:ARG:NH1	2.49	0.51
3:C:45:TYR:CD2	3:C:51:LYS:HB3	2.46	0.51
3:F:156:GLN:HG2	3:F:185:LYS:O	2.10	0.51
6:G:170:ARG:CG	6:G:170:ARG:NH1	2.73	0.51
5:R:7:LEU:HB3	5:R:141:VAL:HB	1.92	0.51
8:V:529:GLN:O	8:V:551:LYS:N	2.43	0.51
9:W:907:LYS:CD	9:W:1097:ARG:HG3	2.29	0.51
2:B:85:ILE:O	2:B:87:ARG:NH1	2.44	0.50
11:L:124:ILE:HG12	11:L:155:THR:CG2	2.32	0.50
1:N:57:LEU:HA	2:O:145:ASN:HB3	1.93	0.50
9:J:915:TYR:C	9:J:1102:ARG:NH1	2.49	0.50
8:V:803:GLU:O	8:V:855:LEU:HA	2.12	0.50
9:W:700:ASN:HB3	9:W:703:LYS:HD3	1.93	0.50
9:W:1034:SER:OG	9:W:1035:ARG:N	2.41	0.50
9:J:485:PHE:HB2	9:J:486:PRO:HD3	1.93	0.50
6:T:100:GLU:O	7:U:106:TYR:HE2	1.95	0.50
8:V:1013:TYR:HA	8:V:1064:HIS:HA	1.93	0.50
9:W:483:PRO:C	9:W:484:MET:SD	2.89	0.50
9:W:909:MET:HE1	9:W:1121:PHE:HB2	1.92	0.50
9:J:700:ASN:HB3	9:J:703:LYS:HD3	1.93	0.50
6:T:100:GLU:OE2	7:U:106:TYR:CD2	2.64	0.50
8:V:776:ILE:HB	8:V:783:PHE:HB2	1.93	0.50
9:W:698:VAL:HA	11:Y:152:PHE:O	2.11	0.50
10:K:442:ASP:HB2	10:K:543:LEU:HD12	1.93	0.50
9:W:818:ASP:HB3	9:W:820:ARG:HG2	1.93	0.50
10:X:442:ASP:HB2	10:X:543:LEU:HD12	1.93	0.50
9:J:483:PRO:C	9:J:484:MET:SD	2.90	0.50
6:T:169:MET:CG	7:U:87:CYS:CB	2.89	0.50
6:T:163:SER:OG	6:T:164:ASN:N	2.44	0.50
1:A:14:SER:OG	1:A:15:ASP:N	2.45	0.50
2:B:141:SER:OG	2:B:142:ASN:N	2.44	0.50
8:I:803:GLU:O	8:I:855:LEU:HA	2.12	0.50
9:W:485:PHE:HB2	9:W:486:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:702:PHE:CE1	11:Y:120:ALA:CA	2.94	0.50
2:O:59:ILE:HG12	3:P:44:ASP:OD2	2.12	0.50
9:W:661:ARG:CD	9:W:736:GLN:HG2	2.42	0.50
9:W:1013:VAL:HG23	10:X:425:GLU:OE2	2.12	0.50
6:G:276:ASP:OD1	6:G:276:ASP:N	2.43	0.49
9:J:481:ASN:O	9:J:484:MET:SD	2.69	0.49
9:J:779:ARG:NH2	9:J:780:SER:O	2.45	0.49
1:N:79:ILE:HG12	1:N:84:LEU:HB3	1.93	0.49
3:P:45:TYR:CD2	3:P:51:LYS:HB3	2.46	0.49
9:W:779:ARG:NH2	9:W:780:SER:O	2.45	0.49
2:B:59:ILE:HG12	3:C:44:ASP:OD2	2.12	0.49
11:L:26:LYS:HB3	11:L:92:VAL:HG11	1.94	0.49
1:N:14:SER:OG	1:N:15:ASP:N	2.45	0.49
5:R:105:ASP:OD1	5:R:105:ASP:N	2.43	0.49
6:G:169:MET:N	6:G:169:MET:HE2	2.27	0.49
9:J:1129:SER:OG	9:J:1130:LYS:NZ	2.43	0.49
9:J:1159:LYS:NZ	10:K:449:ASN:O	2.41	0.49
2:O:85:ILE:O	2:O:87:ARG:NH1	2.44	0.49
9:W:1098:ILE:CD1	9:W:1099:PHE:CG	2.95	0.49
5:E:188:ASP:OD1	5:E:192:LYS:NZ	2.45	0.49
9:W:1013:VAL:HA	10:X:425:GLU:OE2	2.13	0.49
11:Y:40:ILE:HD12	11:Y:40:ILE:C	2.33	0.49
4:Q:2:GLY:N	4:Q:88:ASP:OD2	2.46	0.49
11:Y:26:LYS:HB3	11:Y:92:VAL:HG11	1.94	0.49
6:G:207:ASN:ND2	6:G:270:PHE:O	2.45	0.49
9:J:1098:ILE:CD1	9:J:1099:PHE:CG	2.95	0.49
11:L:136:VAL:HG13	11:L:137:PRO:HD2	1.94	0.49
3:P:133:ASP:N	3:P:133:ASP:OD1	2.41	0.49
7:U:106:TYR:CD1	7:U:106:TYR:N	2.73	0.49
5:E:9:ILE:HA	5:E:15:LEU:HA	1.95	0.49
9:J:818:ASP:HB3	9:J:820:ARG:HG2	1.93	0.49
11:Y:136:VAL:HG13	11:Y:137:PRO:HD2	1.94	0.49
2:B:239:LEU:O	2:B:257:GLY:O	2.31	0.49
3:F:187:GLU:HG2	3:F:189:PRO:HD2	1.95	0.49
6:G:227:VAL:HG22	6:G:230:GLU:HB2	1.94	0.49
7:H:11:LYS:O	7:H:11:LYS:HD3	2.11	0.49
3:S:187:GLU:HG2	3:S:189:PRO:HD2	1.95	0.49
7:U:11:LYS:O	7:U:11:LYS:HD3	2.11	0.49
10:X:221:SER:O	10:X:228:ILE:HA	2.13	0.49
3:C:193:ASP:OD1	3:C:193:ASP:N	2.46	0.48
11:L:40:ILE:HD12	11:L:40:ILE:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:207:ASN:ND2	6:T:270:PHE:O	2.45	0.48
11:Y:171:ILE:HA	11:Y:174:ILE:HG22	1.95	0.48
4:Q:19:ARG:HH22	4:Q:23:LEU:HA	1.79	0.48
7:U:103:TYR:HE2	7:U:138:HIS:HE2	0.63	0.48
9:W:699:PHE:HD1	9:W:701:PRO:CD	2.23	0.48
9:W:907:LYS:CE	9:W:1099:PHE:CE1	2.95	0.48
1:A:9:SER:HA	1:A:19:LEU:O	2.14	0.48
9:J:699:PHE:CB	11:L:152:PHE:N	2.59	0.48
6:T:227:VAL:HG22	6:T:230:GLU:HB2	1.94	0.48
9:W:655:ARG:NH1	9:W:816:ILE:HD11	2.27	0.48
9:W:700:ASN:CB	11:Y:169:GLU:OE1	2.58	0.48
9:W:915:TYR:N	9:W:1102:ARG:NH1	2.62	0.48
2:B:125:ASN:OD1	3:C:40:GLN:NE2	2.39	0.48
6:G:254:ARG:HG2	6:G:264:THR:HG22	1.96	0.48
9:J:1013:VAL:HG23	10:K:425:GLU:OE2	2.12	0.48
9:W:696:GLN:CG	11:Y:162:ASN:HD21	2.16	0.48
3:C:40:GLN:OE1	3:C:43:GLN:NE2	2.40	0.48
9:W:698:VAL:HG13	11:Y:151:LEU:CD1	2.41	0.48
3:C:133:ASP:OD1	3:C:133:ASP:N	2.41	0.48
3:F:182:ARG:C	3:F:183:ILE:HG13	2.34	0.48
9:J:655:ARG:NH1	9:J:816:ILE:HD11	2.27	0.48
9:J:909:MET:HB2	9:J:1095:ILE:HG23	1.96	0.48
10:K:415:ILE:HD13	10:K:430:ARG:HG2	1.95	0.48
1:N:9:SER:HA	1:N:19:LEU:O	2.14	0.48
5:R:188:ASP:OD1	5:R:192:LYS:NZ	2.45	0.48
9:W:478:ASP:OD2	9:W:491:TYR:OH	2.28	0.48
4:D:19:ARG:HH22	4:D:23:LEU:HA	1.78	0.48
6:G:169:MET:HB2	6:G:169:MET:HE3	1.52	0.48
10:K:221:SER:O	10:K:228:ILE:HA	2.13	0.48
5:R:9:ILE:HA	5:R:15:LEU:HA	1.95	0.48
4:D:26:ASN:O	4:D:134:LYS:NZ	2.38	0.48
4:D:27:SER:O	4:D:31:GLN:NE2	2.45	0.48
9:J:1013:VAL:HA	10:K:425:GLU:OE2	2.13	0.48
2:O:239:LEU:O	2:O:257:GLY:O	2.31	0.48
6:T:173:ASP:OD1	6:T:173:ASP:N	2.47	0.48
9:J:628:GLN:O	9:J:632:PHE:CB	2.62	0.48
4:D:2:GLY:N	4:D:88:ASP:OD2	2.46	0.47
11:L:171:ILE:HA	11:L:174:ILE:HG22	1.96	0.47
9:W:909:MET:HB2	9:W:1095:ILE:HG23	1.96	0.47
3:F:29:LEU:HD12	6:G:191:LEU:HD22	1.96	0.47
9:J:698:VAL:HG13	11:L:151:LEU:CD1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:254:ARG:HG2	6:T:264:THR:HG22	1.96	0.47
11:Y:16:ILE:HA	11:Y:88:GLY:O	2.13	0.47
11:Y:124:ILE:CD1	11:Y:155:THR:HG21	2.44	0.47
9:J:1013:VAL:CG2	10:K:425:GLU:OE1	2.62	0.47
10:X:415:ILE:HD13	10:X:430:ARG:HG2	1.95	0.47
8:I:772:SER:HB3	8:I:787:LEU:HB3	1.96	0.47
3:S:29:LEU:HD12	6:T:191:LEU:HD22	1.96	0.47
9:J:738:PRO:HD3	9:J:786:ILE:H	1.80	0.47
3:P:149:LYS:NZ	3:P:160:ASP:OD1	2.44	0.47
3:P:193:ASP:OD1	3:P:193:ASP:N	2.46	0.47
4:Q:5:SER:OG	4:Q:7:TRP:NE1	2.46	0.47
9:W:700:ASN:O	9:W:703:LYS:HG2	2.14	0.47
9:W:701:PRO:HG3	11:Y:151:LEU:CA	2.45	0.47
9:W:738:PRO:HD3	9:W:786:ILE:H	1.80	0.47
9:J:484:MET:SD	9:J:484:MET:N	2.88	0.47
9:J:698:VAL:HG11	11:L:166:ALA:HA	1.96	0.47
11:L:89:ALA:HB1	11:L:111:LEU:HD21	1.96	0.47
7:U:103:TYR:HB3	7:U:111:PHE:HB2	1.96	0.47
9:W:698:VAL:HG11	11:Y:166:ALA:HA	1.96	0.47
9:W:1018:TRP:HB2	9:W:1079:PRO:HG3	1.97	0.47
3:F:109:SER:HB3	3:F:114:THR:H	1.80	0.47
8:I:333:SER:O	8:I:337:TYR:N	2.48	0.47
9:J:903:PRO:CG	9:J:1098:ILE:CD1	2.85	0.47
9:J:915:TYR:N	9:J:1102:ARG:NH1	2.62	0.47
11:L:16:ILE:HA	11:L:88:GLY:O	2.13	0.47
3:S:182:ARG:C	3:S:183:ILE:HG13	2.34	0.47
8:V:772:SER:HB3	8:V:787:LEU:HB3	1.96	0.47
9:W:628:GLN:O	9:W:632:PHE:CB	2.62	0.47
9:W:655:ARG:O	9:W:815:ILE:HG23	2.15	0.47
9:J:658:VAL:HG23	9:J:739:PHE:HB3	1.96	0.47
9:J:1018:TRP:HB2	9:J:1079:PRO:HG3	1.97	0.47
4:Q:27:SER:O	4:Q:31:GLN:NE2	2.45	0.47
9:W:484:MET:SD	9:W:484:MET:N	2.88	0.47
9:W:658:VAL:HG23	9:W:739:PHE:HB3	1.96	0.47
9:W:903:PRO:CG	9:W:1098:ILE:CD1	2.85	0.47
9:W:993:ARG:O	9:W:1047:SER:OG	2.33	0.47
4:D:7:TRP:HA	4:D:17:PHE:O	2.15	0.47
6:G:180:LEU:HB3	6:G:199:LEU:HD21	1.96	0.47
9:J:700:ASN:O	9:J:703:LYS:HG2	2.14	0.47
9:J:737:ASN:HD21	9:J:785:LEU:HD23	1.66	0.47
9:J:1092:ASN:N	9:J:1092:ASN:HD22	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:100:GLU:O	7:U:106:TYR:CE2	2.68	0.47
3:C:149:LYS:NZ	3:C:160:ASP:OD1	2.44	0.47
9:W:1092:ASN:N	9:W:1092:ASN:HD22	2.12	0.46
7:H:43:ALA:HB1	9:J:529:LYS:HD2	1.96	0.46
9:J:1124:ARG:NH2	9:J:1150:ASN:O	2.48	0.46
4:Q:3:ILE:HD12	4:Q:85:LEU:HD11	1.96	0.46
3:S:109:SER:HB3	3:S:114:THR:H	1.80	0.46
9:W:1013:VAL:CG2	10:X:425:GLU:OE1	2.62	0.46
6:T:180:LEU:HA	6:T:183:ILE:HG22	1.97	0.46
6:T:180:LEU:HB3	6:T:199:LEU:HD21	1.96	0.46
9:W:907:LYS:NZ	9:W:1098:ILE:HG12	2.21	0.46
9:W:1104:PHE:HD1	9:W:1104:PHE:O	1.99	0.46
9:W:1159:LYS:NZ	10:X:449:ASN:O	2.41	0.46
11:Y:25:GLY:O	11:Y:126:ASN:ND2	2.49	0.46
4:D:5:SER:OG	4:D:7:TRP:NE1	2.46	0.46
7:H:103:TYR:HB3	7:H:111:PHE:HB2	1.96	0.46
1:N:112:VAL:HA	1:N:115:ILE:HG22	1.97	0.46
4:Q:7:TRP:HA	4:Q:17:PHE:O	2.15	0.46
7:U:43:ALA:HB1	9:W:529:LYS:HD2	1.96	0.46
11:Y:50:PHE:HA	11:Y:66:ILE:O	2.15	0.46
7:U:134:TYR:HA	7:U:137:VAL:CG2	2.45	0.46
8:V:307:LYS:O	8:V:311:GLU:N	2.47	0.46
2:B:177:LYS:HD2	2:B:177:LYS:HA	1.80	0.46
11:L:41:GLU:HB3	11:L:42:SER:H	1.61	0.46
8:V:333:SER:O	8:V:337:TYR:N	2.48	0.46
11:Y:89:ALA:HB1	11:Y:111:LEU:HD21	1.96	0.46
8:I:307:LYS:O	8:I:311:GLU:N	2.47	0.46
11:Y:16:ILE:HG12	11:Y:88:GLY:HA3	1.97	0.46
9:J:1104:PHE:HD1	9:J:1104:PHE:O	1.99	0.46
9:W:754:ILE:O	9:W:804:SER:OG	2.32	0.46
9:W:1268:SER:HA	9:W:1276:ILE:HA	1.97	0.46
10:X:503:LEU:HB2	10:X:523:ARG:HG3	1.98	0.46
4:D:3:ILE:HD12	4:D:85:LEU:HD11	1.97	0.46
5:E:16:ILE:HD12	5:E:202:ILE:HD11	1.97	0.46
11:L:124:ILE:CD1	11:L:155:THR:HG21	2.44	0.46
7:U:132:SER:CA	7:U:135:GLN:OE1	2.63	0.46
6:G:38:THR:HA	7:H:170:ARG:HD3	1.98	0.46
6:G:173:ASP:OD1	6:G:173:ASP:N	2.47	0.46
9:J:702:PHE:CZ	11:L:120:ALA:HA	2.51	0.46
9:W:915:TYR:CB	9:W:1102:ARG:NH1	2.79	0.46
6:G:180:LEU:HA	6:G:183:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:478:ASP:HB2	9:J:486:PRO:HG2	1.98	0.45
9:J:703:LYS:HE2	9:J:703:LYS:HA	1.98	0.45
9:J:754:ILE:O	9:J:804:SER:OG	2.32	0.45
11:L:25:GLY:O	11:L:126:ASN:ND2	2.49	0.45
11:L:48:VAL:HG22	11:L:69:THR:HA	1.98	0.45
3:F:133:ASP:OD1	3:F:133:ASP:N	2.46	0.45
9:J:701:PRO:HG3	11:L:151:LEU:CA	2.45	0.45
9:J:915:TYR:CB	9:J:1102:ARG:NH1	2.79	0.45
9:W:1013:VAL:HG22	10:X:425:GLU:CD	2.37	0.45
1:A:112:VAL:HA	1:A:115:ILE:HG22	1.97	0.45
9:J:699:PHE:HD1	9:J:701:PRO:CD	2.23	0.45
9:J:914:LEU:CB	9:J:1102:ARG:HH22	2.16	0.45
9:J:1268:SER:HA	9:J:1276:ILE:HA	1.97	0.45
10:K:503:LEU:HB2	10:K:523:ARG:HG3	1.98	0.45
6:T:169:MET:HE1	6:T:170:ARG:H	1.81	0.45
9:W:1173:VAL:HG12	9:W:1194:THR:HG23	1.99	0.45
9:W:1181:LYS:HD3	9:W:1181:LYS:HA	1.80	0.45
11:L:16:ILE:HG12	11:L:88:GLY:HA3	1.97	0.45
9:J:655:ARG:O	9:J:815:ILE:HG23	2.15	0.45
9:J:1089:ASN:ND2	9:J:1092:ASN:ND2	2.64	0.45
9:J:1133:CYS:SG	9:J:1134:ASN:N	2.89	0.45
9:J:1173:VAL:HG12	9:J:1194:THR:HG23	1.99	0.45
9:W:661:ARG:C	9:W:736:GLN:HG2	2.36	0.45
9:J:661:ARG:HD3	9:J:736:GLN:OE1	2.15	0.45
2:B:118:LYS:HE3	2:B:118:LYS:HB2	1.85	0.45
9:J:700:ASN:CB	11:L:169:GLU:OE1	2.58	0.45
11:L:153:THR:CG2	11:L:162:ASN:HB3	2.46	0.45
2:O:86:LYS:NZ	2:O:107:GLU:OE2	2.44	0.45
4:Q:121:ALA:O	4:Q:133:ARG:NH2	2.50	0.45
5:R:16:ILE:HD12	5:R:202:ILE:HD11	1.98	0.45
9:W:703:LYS:HE2	9:W:703:LYS:HA	1.98	0.45
11:Y:48:VAL:HG22	11:Y:69:THR:HA	1.98	0.45
6:G:170:ARG:HB3	6:G:171:ARG:H	1.55	0.45
11:L:50:PHE:HA	11:L:66:ILE:O	2.16	0.45
4:Q:62:ILE:HA	5:R:124:THR:HG22	1.99	0.45
11:Y:153:THR:CG2	11:Y:162:ASN:HB3	2.47	0.45
8:I:860:ASN:ND2	8:I:966:ARG:O	2.48	0.45
9:J:734:ARG:CB	9:J:736:GLN:OE1	2.49	0.45
7:U:35:GLU:HB2	9:W:535:ARG:HH22	1.82	0.45
8:V:774:GLU:HB3	8:V:785:LYS:HB3	1.99	0.45
5:E:30:SER:OG	5:E:32:GLU:OE1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:167:ILE:HG23	3:F:174:THR:HG23	1.99	0.45
9:J:1104:PHE:O	9:J:1104:PHE:CD1	2.70	0.45
9:W:1089:ASN:ND2	9:W:1092:ASN:ND2	2.64	0.45
9:W:1133:CYS:SG	9:W:1134:ASN:N	2.90	0.45
6:T:53:LYS:HE2	6:T:53:LYS:HB2	1.83	0.44
9:W:478:ASP:HB2	9:W:486:PRO:HG2	1.98	0.44
9:W:1278:GLN:HG2	9:W:1280:ASP:HB2	1.98	0.44
9:J:699:PHE:CE2	11:L:146:MET:HE2	2.50	0.44
9:J:1278:GLN:HG2	9:J:1280:ASP:HB2	1.98	0.44
2:O:238:CYS:HB2	2:O:259:SER:HB2	1.99	0.44
3:S:182:ARG:O	3:S:183:ILE:HG13	2.18	0.44
9:J:907:LYS:CE	9:J:1099:PHE:CE1	2.95	0.44
3:P:91:SER:O	3:P:102:THR:OG1	2.34	0.44
6:T:38:THR:HA	7:U:170:ARG:HD3	1.98	0.44
9:W:893:PRO:HG2	9:W:953:THR:HA	2.00	0.44
7:H:35:GLU:HB2	9:J:535:ARG:HH22	1.82	0.44
9:J:702:PHE:CB	11:L:173:ALA:HB2	2.28	0.44
9:J:993:ARG:O	9:J:1047:SER:OG	2.33	0.44
3:S:167:ILE:HG23	3:S:174:THR:HG23	1.99	0.44
8:V:745:SER:HA	8:V:757:GLU:HA	1.99	0.44
9:W:1124:ARG:NH2	9:W:1150:ASN:O	2.49	0.44
11:Y:153:THR:HG22	11:Y:162:ASN:HB3	1.99	0.44
9:J:652:PHE:HD2	9:J:816:ILE:HG22	1.83	0.44
1:N:73:SER:O	1:N:89:GLY:HA2	2.18	0.44
3:P:147:VAL:O	3:P:151:SER:CB	2.66	0.44
9:W:1104:PHE:O	9:W:1104:PHE:CD1	2.70	0.44
9:J:661:ARG:CD	9:J:736:GLN:NE2	2.81	0.44
9:J:893:PRO:HG2	9:J:953:THR:HA	2.00	0.44
9:J:907:LYS:HD2	9:J:1097:ARG:CB	2.47	0.44
7:U:141:TYR:O	7:U:142:VAL:C	2.55	0.44
2:B:102:HIS:O	2:B:106:HIS:ND1	2.49	0.44
2:B:146:LEU:HD22	2:B:156:ILE:HG22	2.00	0.44
9:W:915:TYR:N	9:W:1102:ARG:HH12	2.16	0.44
4:D:62:ILE:HA	5:E:124:THR:HG22	1.99	0.44
2:O:108:LEU:HA	2:O:111:ALA:HB2	2.00	0.44
9:W:652:PHE:HD2	9:W:816:ILE:HG22	1.83	0.44
2:B:158:LYS:HD2	2:B:158:LYS:HA	1.86	0.44
9:W:517:MET:HA	9:W:520:VAL:HG12	2.00	0.44
9:W:544:THR:HA	9:W:545:PRO:HD3	1.90	0.44
9:W:764:ALA:HB1	9:W:786:ILE:HD11	1.99	0.44
1:A:73:SER:O	1:A:89:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:163:SER:HB3	7:H:139:GLU:HG3	1.99	0.43
2:O:177:LYS:HD2	2:O:177:LYS:HA	1.79	0.43
3:P:81:GLU:OE2	4:Q:59:LYS:NZ	2.42	0.43
5:R:171:ALA:O	5:R:175:ALA:HB2	2.18	0.43
4:D:121:ALA:O	4:D:133:ARG:NH2	2.50	0.43
6:T:169:MET:O	6:T:170:ARG:C	2.54	0.43
7:U:141:TYR:O	7:U:143:LYS:N	2.51	0.43
9:W:907:LYS:HD2	9:W:1097:ARG:CB	2.47	0.43
8:I:774:GLU:HB3	8:I:785:LYS:HB3	1.99	0.43
1:N:99:ASP:OD1	1:N:99:ASP:N	2.47	0.43
11:Y:87:VAL:HG22	11:Y:174:ILE:HD11	2.01	0.43
5:E:171:ALA:O	5:E:175:ALA:HB2	2.18	0.43
11:L:153:THR:HG22	11:L:162:ASN:HB3	1.99	0.43
3:F:182:ARG:O	3:F:183:ILE:HG13	2.18	0.43
3:P:40:GLN:OE1	3:P:43:GLN:NE2	2.40	0.43
11:Y:41:GLU:HB3	11:Y:42:SER:H	1.61	0.43
2:B:238:CYS:HB2	2:B:259:SER:HB2	1.99	0.43
9:J:701:PRO:CG	11:L:151:LEU:CA	2.97	0.43
1:N:103:GLU:O	1:N:107:GLN:OE1	2.37	0.43
8:V:598:ASP:HA	8:V:603:LYS:HA	2.01	0.43
9:W:510:GLN:HA	9:W:513:ILE:HG22	2.01	0.43
10:X:248:ILE:O	10:X:253:HIS:N	2.51	0.43
3:F:186:ASP:N	3:F:186:ASP:OD1	2.52	0.43
7:H:88:TYR:OH	7:H:130:MET:SD	2.65	0.43
9:J:734:ARG:O	9:J:736:GLN:N	2.52	0.43
8:V:1033:GLY:HA2	8:V:1049:GLN:HA	2.01	0.43
6:G:171:ARG:HG3	6:G:171:ARG:O	2.18	0.43
9:W:500:LEU:H	9:W:500:LEU:HG	1.57	0.43
9:W:661:ARG:CD	9:W:736:GLN:CG	2.97	0.43
9:W:701:PRO:CG	11:Y:151:LEU:CA	2.96	0.43
9:W:702:PHE:CZ	11:Y:120:ALA:HA	2.51	0.43
3:C:147:VAL:O	3:C:151:SER:CB	2.66	0.43
8:I:745:SER:HA	8:I:757:GLU:HA	1.99	0.43
9:J:764:ALA:HB1	9:J:786:ILE:HD11	1.99	0.43
9:J:1089:ASN:HB3	9:J:1092:ASN:HD21	1.84	0.43
11:L:89:ALA:HB3	11:L:121:VAL:HG22	2.01	0.43
9:W:1182:VAL:HG13	9:W:1186:GLU:HB2	2.01	0.43
10:X:308:THR:HA	10:X:330:PRO:HA	2.01	0.43
1:A:123:PRO:HD2	3:C:128:VAL:HG13	2.01	0.43
2:B:108:LEU:HA	2:B:111:ALA:HB2	2.00	0.43
11:L:87:VAL:HG22	11:L:174:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:19:LYS:HA	3:S:19:LYS:HD2	1.78	0.43
6:T:74:HIS:HB3	11:Y:181:HIS:HD2	1.84	0.43
6:T:169:MET:O	7:U:85:ASP:OD1	2.37	0.43
3:C:187:GLU:HG3	4:D:128:ARG:HG3	2.01	0.42
4:D:60:ASN:OD1	4:D:60:ASN:N	2.51	0.42
6:G:164:ASN:OD1	6:G:164:ASN:N	2.45	0.42
8:I:768:GLN:O	8:I:791:SER:N	2.52	0.42
9:J:517:MET:HA	9:J:520:VAL:HG12	2.00	0.42
9:J:644:SER:O	9:J:644:SER:OG	2.34	0.42
9:J:972:ALA:HA	9:J:980:LEU:HG	2.01	0.42
9:J:1010:SER:OG	10:K:423:LYS:CE	2.67	0.42
2:O:102:HIS:O	2:O:106:HIS:ND1	2.49	0.42
2:O:146:LEU:HD22	2:O:156:ILE:HG22	2.00	0.42
8:V:768:GLN:O	8:V:791:SER:N	2.52	0.42
8:I:303:PHE:O	8:I:307:LYS:N	2.47	0.42
9:J:501:GLN:N	9:J:501:GLN:CD	2.73	0.42
3:P:60:GLY:HA2	3:P:63:ILE:HG22	2.01	0.42
7:U:4:TYR:HE2	7:U:41:LEU:HD22	1.84	0.42
9:W:501:GLN:N	9:W:501:GLN:OE1	2.51	0.42
9:W:1092:ASN:N	9:W:1092:ASN:ND2	2.67	0.42
9:W:1098:ILE:HD12	9:W:1099:PHE:CD2	2.51	0.42
1:A:103:GLU:O	1:A:107:GLN:OE1	2.37	0.42
9:W:501:GLN:N	9:W:501:GLN:CD	2.73	0.42
9:W:644:SER:O	9:W:644:SER:OG	2.34	0.42
9:W:862:SER:HA	9:W:992:ARG:HB2	2.01	0.42
6:G:169:MET:HE1	7:H:135:GLN:NE2	2.35	0.42
9:J:501:GLN:N	9:J:501:GLN:OE1	2.51	0.42
9:J:510:GLN:HA	9:J:513:ILE:HG22	2.01	0.42
9:J:915:TYR:N	9:J:1102:ARG:HH12	2.16	0.42
9:J:1181:LYS:HA	9:J:1181:LYS:HD3	1.79	0.42
9:J:1268:SER:O	9:J:1268:SER:OG	2.38	0.42
10:K:214:ASN:HA	10:K:236:THR:HA	2.01	0.42
2:O:118:LYS:HE3	2:O:118:LYS:HB2	1.85	0.42
9:W:737:ASN:HD21	9:W:785:LEU:CD2	2.30	0.42
9:W:905:TYR:HA	9:W:908:LYS:HB2	2.02	0.42
3:C:60:GLY:HA2	3:C:63:ILE:HG22	2.01	0.42
10:K:308:THR:HA	10:K:330:PRO:HA	2.01	0.42
1:N:123:PRO:HD2	3:P:128:VAL:HG13	2.01	0.42
2:O:125:ASN:OD1	3:P:40:GLN:NE2	2.39	0.42
11:Y:89:ALA:HB3	11:Y:121:VAL:HG22	2.01	0.42
8:I:598:ASP:HA	8:I:603:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:49:PHE:HA	3:S:52:VAL:HG22	2.01	0.42
9:W:616:ILE:HG22	9:W:619:TYR:HE2	1.85	0.42
9:W:762:ARG:HB3	9:W:789:LYS:HE3	2.02	0.42
2:B:86:LYS:NZ	2:B:107:GLU:OE2	2.44	0.42
8:I:863:LYS:NZ	8:I:902:LYS:O	2.53	0.42
9:J:1099:PHE:HD1	9:J:1099:PHE:O	2.03	0.42
11:L:13:LEU:HA	11:L:63:LYS:O	2.20	0.42
3:P:147:VAL:O	3:P:151:SER:HB3	2.20	0.42
3:C:91:SER:O	3:C:102:THR:OG1	2.34	0.42
8:I:856:LYS:HE3	8:I:856:LYS:HB3	1.86	0.42
9:W:1023:MET:HA	9:W:1026:ILE:HG22	2.01	0.42
7:H:4:TYR:HE2	7:H:41:LEU:HD22	1.84	0.42
11:L:124:ILE:HD11	11:L:155:THR:CB	2.50	0.42
3:S:74:ARG:HH21	3:S:98:PHE:HE1	1.68	0.42
3:S:162:TRP:HE1	3:S:177:LYS:HD2	1.84	0.42
9:W:1010:SER:OG	10:X:423:LYS:CE	2.67	0.42
10:X:405:SER:OG	10:X:408:SER:O	2.30	0.42
9:J:661:ARG:HD3	9:J:736:GLN:NE2	2.35	0.42
9:J:1023:MET:HA	9:J:1026:ILE:HG22	2.01	0.42
10:K:503:LEU:N	10:K:523:ARG:O	2.46	0.42
8:V:860:ASN:ND2	8:V:966:ARG:O	2.49	0.42
11:Y:13:LEU:HA	11:Y:63:LYS:O	2.20	0.42
1:A:11:ILE:HB	1:A:85:LYS:HB2	2.02	0.41
3:C:147:VAL:O	3:C:151:SER:HB3	2.20	0.41
3:F:74:ARG:HH21	3:F:98:PHE:HE1	1.68	0.41
6:G:74:HIS:HB3	11:L:181:HIS:HD2	1.84	0.41
8:I:1033:GLY:HA2	8:I:1049:GLN:HA	2.01	0.41
9:J:862:SER:HA	9:J:992:ARG:HB2	2.01	0.41
9:J:1092:ASN:N	9:J:1092:ASN:ND2	2.67	0.41
1:N:11:ILE:HB	1:N:85:LYS:HB2	2.02	0.41
9:W:1099:PHE:HD1	9:W:1099:PHE:O	2.03	0.41
9:J:500:LEU:H	9:J:500:LEU:HG	1.57	0.41
9:J:698:VAL:HA	11:L:153:THR:HA	2.02	0.41
9:J:742:ASP:O	9:J:779:ARG:N	2.52	0.41
9:J:1010:SER:OG	10:K:423:LYS:NZ	2.53	0.41
9:J:1099:PHE:CD1	9:J:1099:PHE:N	2.88	0.41
3:P:187:GLU:HG3	4:Q:128:ARG:HG3	2.01	0.41
6:T:169:MET:HB3	7:U:87:CYS:CB	2.50	0.41
9:W:1089:ASN:HB3	9:W:1092:ASN:HD21	1.84	0.41
11:Y:124:ILE:HD11	11:Y:155:THR:CB	2.50	0.41
3:F:162:TRP:HE1	3:F:177:LYS:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:34:LYS:O	9:J:590:LYS:NZ	2.42	0.41
9:J:485:PHE:N	9:J:486:PRO:CD	2.84	0.41
9:J:616:ILE:HG22	9:J:619:TYR:HE2	1.85	0.41
9:J:1182:VAL:HG13	9:J:1186:GLU:HB2	2.01	0.41
8:V:863:LYS:NZ	8:V:902:LYS:O	2.53	0.41
3:F:49:PHE:HA	3:F:52:VAL:HG22	2.01	0.41
3:S:186:ASP:OD1	3:S:186:ASP:N	2.52	0.41
9:W:698:VAL:HA	11:Y:153:THR:HA	2.02	0.41
7:H:5:PHE:HD1	7:H:113:MET:HB2	1.85	0.41
9:W:1010:SER:OG	10:X:423:LYS:NZ	2.53	0.41
9:J:483:PRO:O	9:J:484:MET:SD	2.79	0.41
9:J:905:TYR:HA	9:J:908:LYS:HB2	2.02	0.41
4:Q:5:SER:HG	4:Q:7:TRP:HE1	1.66	0.41
5:R:30:SER:OG	5:R:32:GLU:OE1	2.27	0.41
9:J:737:ASN:ND2	9:J:785:LEU:CB	2.80	0.41
6:T:168:LYS:NZ	7:U:85:ASP:CG	2.74	0.41
8:V:332:THR:O	8:V:336:SER:N	2.54	0.41
3:F:63:ILE:HG12	6:G:68:GLU:HG3	2.03	0.41
1:N:8:VAL:HG12	1:N:88:ILE:HG13	2.03	0.41
1:N:74:VAL:HA	1:N:88:ILE:O	2.21	0.41
3:S:87:SER:HB2	3:S:105:ILE:HG12	2.02	0.41
6:T:172:ARG:HH21	7:U:86:ASN:HB3	1.85	0.41
9:W:483:PRO:O	9:W:484:MET:SD	2.79	0.41
9:W:972:ALA:HA	9:W:980:LEU:HG	2.02	0.41
10:X:437:SER:HA	10:X:440:PRO:HB3	2.03	0.41
1:A:74:VAL:HA	1:A:88:ILE:O	2.21	0.41
3:F:87:SER:HB2	3:F:105:ILE:HG12	2.02	0.41
6:G:100:GLU:OE2	7:H:107:SER:N	2.50	0.41
9:J:425:ASP:O	9:J:429:MET:N	2.54	0.41
9:J:736:GLN:HE21	9:J:736:GLN:HB3	1.61	0.41
9:J:762:ARG:HB3	9:J:789:LYS:HE3	2.02	0.41
9:J:1002:ILE:HG12	9:J:1164:ILE:HD11	2.03	0.41
9:J:1049:ILE:C	9:W:1072:HIS:HE2	2.14	0.41
8:V:982:PHE:HB2	8:V:1075:PHE:HA	2.03	0.41
9:W:696:GLN:HG2	11:Y:162:ASN:CG	2.39	0.41
10:X:214:ASN:HA	10:X:236:THR:HA	2.01	0.41
1:A:42:ILE:HD12	1:A:42:ILE:HA	1.95	0.41
1:A:118:ARG:HD3	3:C:127:PHE:HB3	2.03	0.41
3:F:19:LYS:HD2	3:F:19:LYS:HA	1.78	0.41
8:I:273:ASP:O	8:I:277:LEU:N	2.53	0.41
6:T:100:GLU:C	7:U:106:TYR:HE2	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1002:ILE:HG12	9:W:1164:ILE:HD11	2.03	0.41
1:A:72:VAL:HA	1:A:90:PHE:O	2.21	0.40
6:G:172:ARG:HH21	7:H:86:ASN:HB3	1.85	0.40
8:I:332:THR:O	8:I:336:SER:N	2.54	0.40
4:Q:38:LEU:HD12	5:R:50:LEU:HD23	2.03	0.40
7:U:5:PHE:HD1	7:U:113:MET:HB2	1.85	0.40
8:V:336:SER:O	8:V:340:PHE:N	2.54	0.40
9:W:507:VAL:O	9:W:510:GLN:N	2.54	0.40
9:J:534:LEU:HB3	9:J:561:ILE:HD12	2.03	0.40
9:J:1103:GLN:O	9:J:1104:PHE:HB3	2.21	0.40
11:L:130:LEU:N	11:L:130:LEU:CD2	2.84	0.40
1:N:72:VAL:HA	1:N:90:PHE:O	2.22	0.40
1:N:77:MET:SD	1:N:79:ILE:HG22	2.62	0.40
8:V:273:ASP:O	8:V:277:LEU:N	2.53	0.40
9:W:485:PHE:N	9:W:486:PRO:CD	2.84	0.40
3:F:182:ARG:C	3:F:183:ILE:CG1	2.89	0.40
8:I:982:PHE:HB2	8:I:1075:PHE:HA	2.03	0.40
9:J:1098:ILE:HD12	9:J:1099:PHE:CD2	2.51	0.40
10:K:248:ILE:O	10:K:253:HIS:N	2.51	0.40
2:O:222:ILE:HA	2:O:225:VAL:HG22	2.04	0.40
3:P:35:GLY:HA2	3:P:38:VAL:HG12	2.04	0.40
3:S:182:ARG:C	3:S:183:ILE:CG1	2.89	0.40
2:B:222:ILE:HA	2:B:225:VAL:HG22	2.04	0.40
5:R:31:ASN:OD1	5:R:31:ASN:N	2.54	0.40
9:W:734:ARG:O	9:W:736:GLN:N	2.54	0.40
9:W:909:MET:HE1	9:W:1121:PHE:HA	2.03	0.40
4:D:38:LEU:HD12	5:E:50:LEU:HD23	2.03	0.40
9:W:662:ILE:H	9:W:736:GLN:CG	2.33	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%)	131 (92%)	11 (8%)	0	100	100
1	N	142/152 (93%)	131 (92%)	11 (8%)	0	100	100
2	B	191/268 (71%)	172 (90%)	19 (10%)	0	100	100
2	O	191/268 (71%)	172 (90%)	19 (10%)	0	100	100
3	C	183/193 (95%)	165 (90%)	17 (9%)	1 (0%)	29	68
3	F	181/193 (94%)	161 (89%)	19 (10%)	1 (1%)	25	65
3	P	183/193 (95%)	165 (90%)	17 (9%)	1 (0%)	29	68
3	S	181/193 (94%)	161 (89%)	19 (10%)	1 (1%)	25	65
4	D	149/154 (97%)	130 (87%)	19 (13%)	0	100	100
4	Q	149/154 (97%)	130 (87%)	19 (13%)	0	100	100
5	E	154/219 (70%)	137 (89%)	17 (11%)	0	100	100
5	R	154/219 (70%)	137 (89%)	17 (11%)	0	100	100
6	G	198/283 (70%)	178 (90%)	20 (10%)	0	100	100
6	T	198/283 (70%)	180 (91%)	17 (9%)	1 (0%)	29	68
7	H	143/175 (82%)	134 (94%)	9 (6%)	0	100	100
7	U	143/175 (82%)	132 (92%)	10 (7%)	1 (1%)	22	62
8	I	782/1102 (71%)	646 (83%)	123 (16%)	13 (2%)	9	43
8	V	782/1102 (71%)	651 (83%)	118 (15%)	13 (2%)	9	43
9	J	869/1289 (67%)	730 (84%)	128 (15%)	11 (1%)	12	48
9	W	869/1289 (67%)	728 (84%)	130 (15%)	11 (1%)	12	48
10	K	243/560 (43%)	205 (84%)	33 (14%)	5 (2%)	7	39
10	X	243/560 (43%)	205 (84%)	33 (14%)	5 (2%)	7	39
11	L	192/222 (86%)	169 (88%)	20 (10%)	3 (2%)	9	45
11	Y	192/222 (86%)	169 (88%)	20 (10%)	3 (2%)	9	45
All	All	6854/9620 (71%)	5919 (86%)	865 (13%)	70 (1%)	20	54

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	46	GLU
8	I	346	PRO
8	I	451	LEU
8	I	483	PRO
8	I	976	PRO
9	J	956	PRO

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Mol	Chain	Res	Type
10	K	325	PRO
10	K	330	PRO
11	L	199	PRO
3	P	46	GLU
6	T	170	ARG
8	V	346	PRO
8	V	483	PRO
8	V	976	PRO
9	W	956	PRO
10	X	325	PRO
10	X	330	PRO
11	Y	199	PRO
3	F	183	ILE
8	I	252	PRO
8	I	495	VAL
8	I	980	PRO
8	I	1076	PRO
9	J	486	PRO
11	L	44	SER
3	S	183	ILE
8	V	252	PRO
8	V	464	LYS
8	V	495	VAL
8	V	980	PRO
8	V	1076	PRO
9	W	486	PRO
11	Y	44	SER
8	I	343	VAL
8	V	343	VAL
8	I	251	VAL
8	I	735	ILE
9	J	409	LEU
9	J	735	VAL
10	K	310	PRO
11	L	36	ASP
8	V	251	VAL
8	V	735	ILE
9	W	409	LEU
9	W	735	VAL
10	X	310	PRO
11	Y	36	ASP
9	J	666	ASP

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Mol	Chain	Res	Type
9	J	1014	GLU
9	W	666	ASP
9	W	1014	GLU
9	J	738	PRO
9	J	1102	ARG
10	K	286	PRO
7	U	142	VAL
9	W	738	PRO
9	W	1102	ARG
10	X	286	PRO
9	J	672	ILE
10	K	331	VAL
9	W	672	ILE
10	X	331	VAL
8	I	1029	ILE
9	J	886	ILE
8	V	1029	ILE
9	W	886	ILE
8	I	647	VAL
9	J	297	VAL
8	V	647	VAL
9	W	297	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	134/142 (94%)	132 (98%)	2 (2%)	65 80
1	N	134/142 (94%)	132 (98%)	2 (2%)	65 80
2	B	176/248 (71%)	175 (99%)	1 (1%)	86 92
2	O	176/248 (71%)	175 (99%)	1 (1%)	86 92
3	C	170/178 (96%)	168 (99%)	2 (1%)	71 84
3	F	169/178 (95%)	167 (99%)	2 (1%)	71 84
3	P	170/178 (96%)	168 (99%)	2 (1%)	71 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	169/178 (95%)	167 (99%)	2 (1%)	71	84
4	D	135/141 (96%)	135 (100%)	0	100	100
4	Q	135/141 (96%)	135 (100%)	0	100	100
5	E	148/199 (74%)	148 (100%)	0	100	100
5	R	148/199 (74%)	148 (100%)	0	100	100
6	G	179/249 (72%)	175 (98%)	4 (2%)	52	71
6	T	179/249 (72%)	176 (98%)	3 (2%)	60	78
7	H	127/152 (84%)	125 (98%)	2 (2%)	62	79
7	U	127/152 (84%)	120 (94%)	7 (6%)	21	49
8	I	78/1023 (8%)	77 (99%)	1 (1%)	69	82
8	V	78/1023 (8%)	78 (100%)	0	100	100
9	J	595/1213 (49%)	572 (96%)	23 (4%)	32	57
9	W	595/1213 (49%)	572 (96%)	23 (4%)	32	57
10	K	121/518 (23%)	121 (100%)	0	100	100
10	X	121/518 (23%)	121 (100%)	0	100	100
11	L	152/189 (80%)	145 (95%)	7 (5%)	27	53
11	Y	152/189 (80%)	145 (95%)	7 (5%)	27	53
All	All	4368/8860 (49%)	4277 (98%)	91 (2%)	56	72

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	93	LYS
2	B	181	ARG
3	C	24	LYS
3	C	62	ASN
3	F	183	ILE
3	F	185	LYS
6	G	164	ASN
6	G	167	THR
6	G	169	MET
6	G	170	ARG
7	H	12	ASP
7	H	91	LYS
8	I	464	LYS

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Mol	Chain	Res	Type
9	J	484	MET
9	J	500	LEU
9	J	501	GLN
9	J	655	ARG
9	J	694	ASN
9	J	697	GLU
9	J	698	VAL
9	J	703	LYS
9	J	704	ARG
9	J	736	GLN
9	J	789	LYS
9	J	1011	SER
9	J	1012	GLN
9	J	1035	ARG
9	J	1093	THR
9	J	1097	ARG
9	J	1099	PHE
9	J	1104	PHE
9	J	1105	ILE
9	J	1106	GLN
9	J	1107	SER
9	J	1111	GLU
9	J	1113	GLN
11	L	35	THR
11	L	39	ASN
11	L	40	ILE
11	L	41	GLU
11	L	43	LYS
11	L	134	ARG
11	L	160	SER
1	N	35	LYS
1	N	93	LYS
2	O	181	ARG
3	P	24	LYS
3	P	62	ASN
3	S	183	ILE
3	S	185	LYS
6	T	167	THR
6	T	168	LYS
6	T	169	MET
7	U	12	ASP
7	U	91	LYS

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Mol	Chain	Res	Type
7	U	106	TYR
7	U	136	GLU
7	U	137	VAL
7	U	139	GLU
7	U	140	LEU
9	W	484	MET
9	W	500	LEU
9	W	501	GLN
9	W	655	ARG
9	W	694	ASN
9	W	697	GLU
9	W	698	VAL
9	W	703	LYS
9	W	704	ARG
9	W	735	VAL
9	W	789	LYS
9	W	1011	SER
9	W	1012	GLN
9	W	1035	ARG
9	W	1093	THR
9	W	1097	ARG
9	W	1099	PHE
9	W	1104	PHE
9	W	1105	ILE
9	W	1106	GLN
9	W	1107	SER
9	W	1111	GLU
9	W	1113	GLN
11	Y	35	THR
11	Y	39	ASN
11	Y	40	ILE
11	Y	41	GLU
11	Y	43	LYS
11	Y	134	ARG
11	Y	160	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	113	ASN
7	H	135	GLN
9	J	694	ASN

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Mol	Chain	Res	Type
9	J	1092	ASN
9	J	1103	GLN
11	L	72	GLN
11	L	132	HIS
5	R	113	ASN
3	S	53	ASN
7	U	138	HIS
9	W	694	ASN
9	W	736	GLN
9	W	1092	ASN
9	W	1103	GLN
11	Y	72	GLN
11	Y	132	HIS

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.

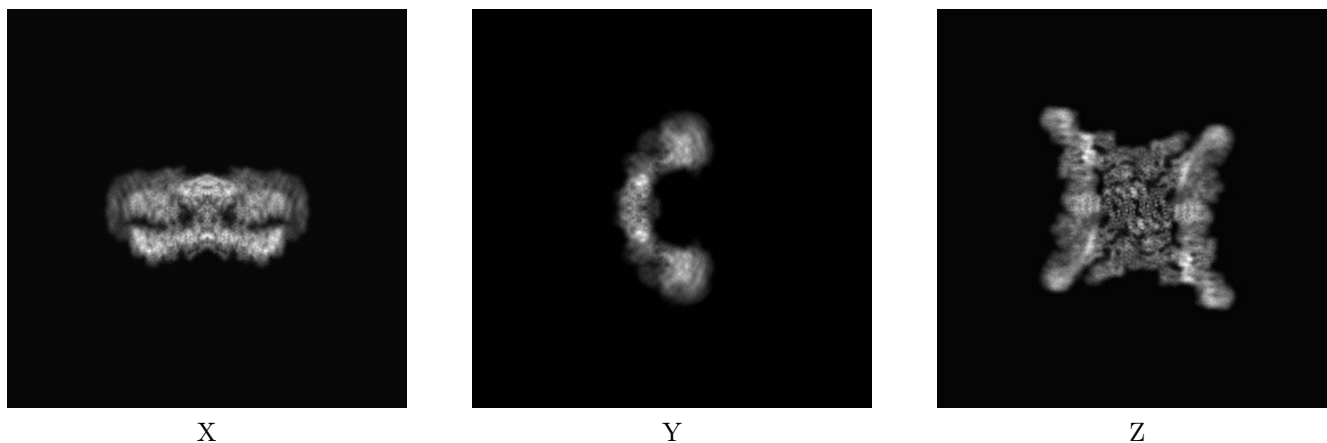
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31038. 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](#)

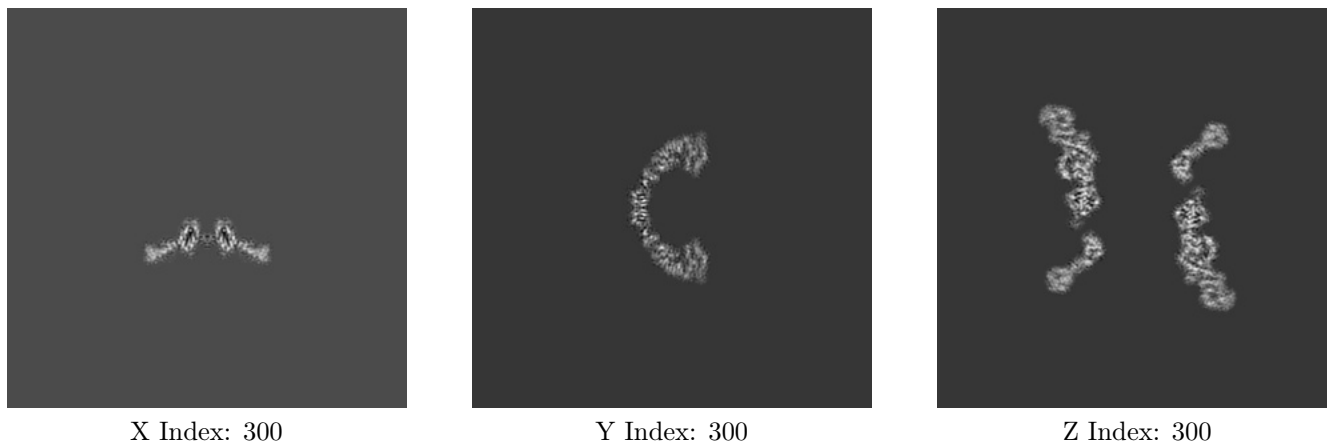
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

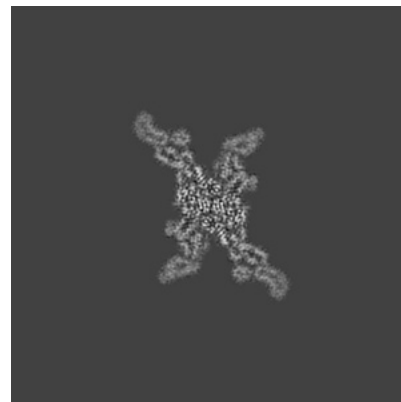
6.3.1 Primary map



X Index: 228



Y Index: 297

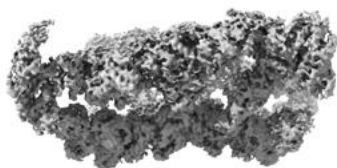


Z Index: 256

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

6.4 Orthogonal surface views [i](#)

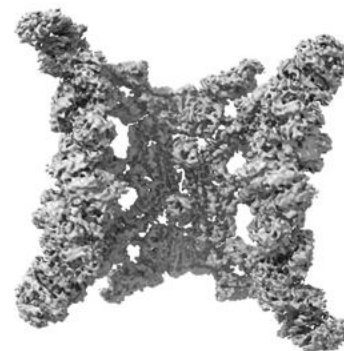
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

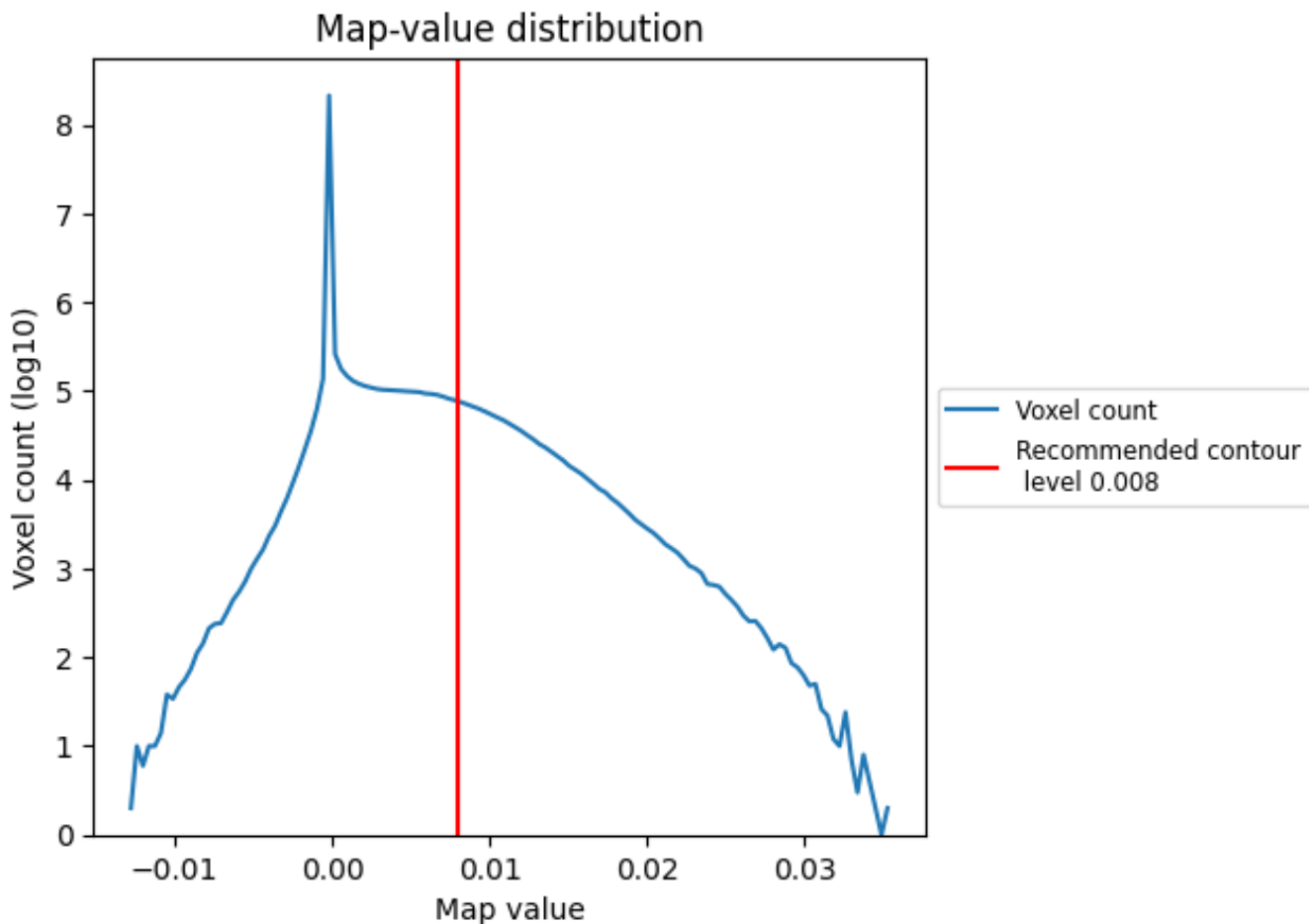
6.5 Mask visualisation

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

7 Map analysis [i](#)

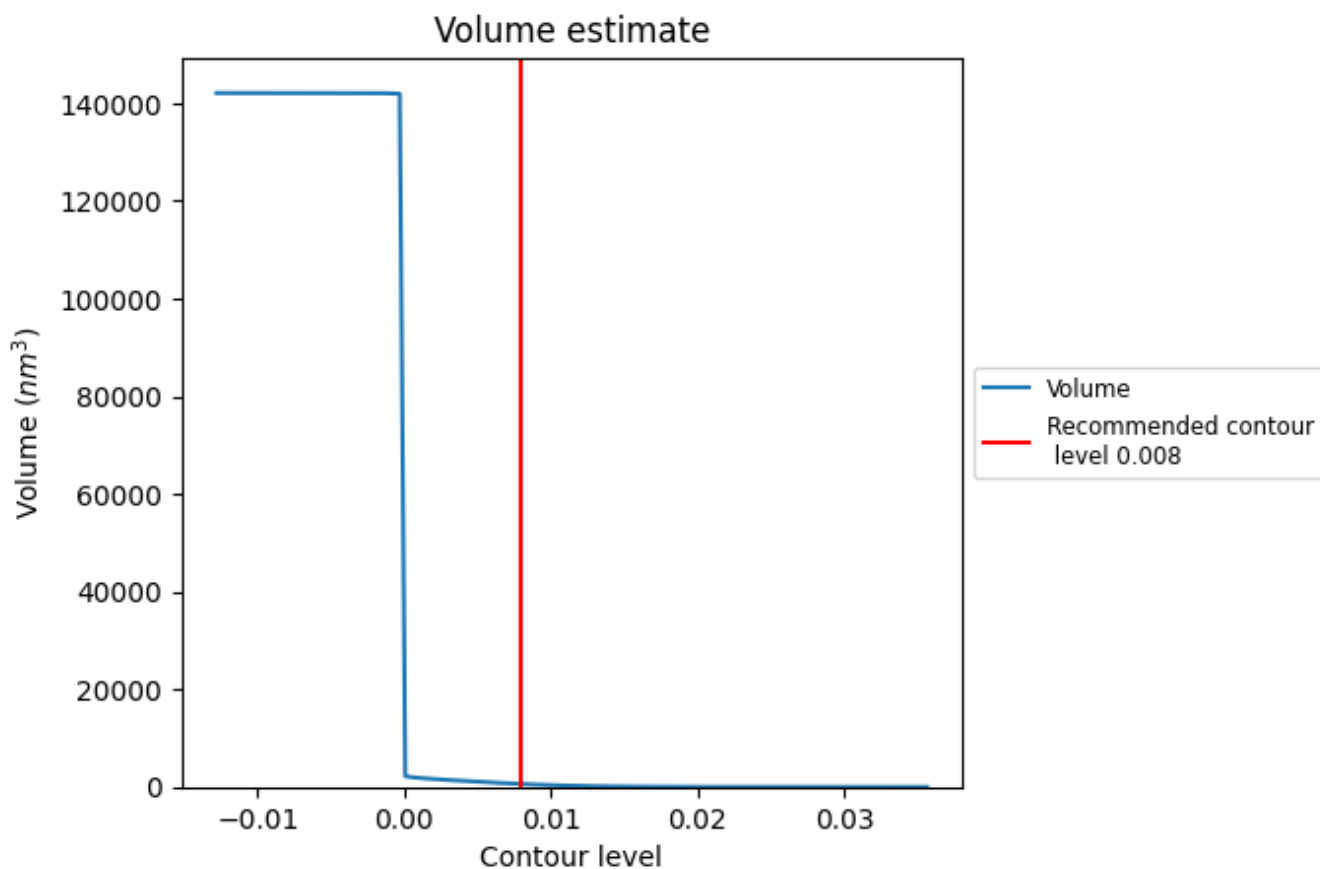
This section contains the results of statistical analysis of the map.

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.

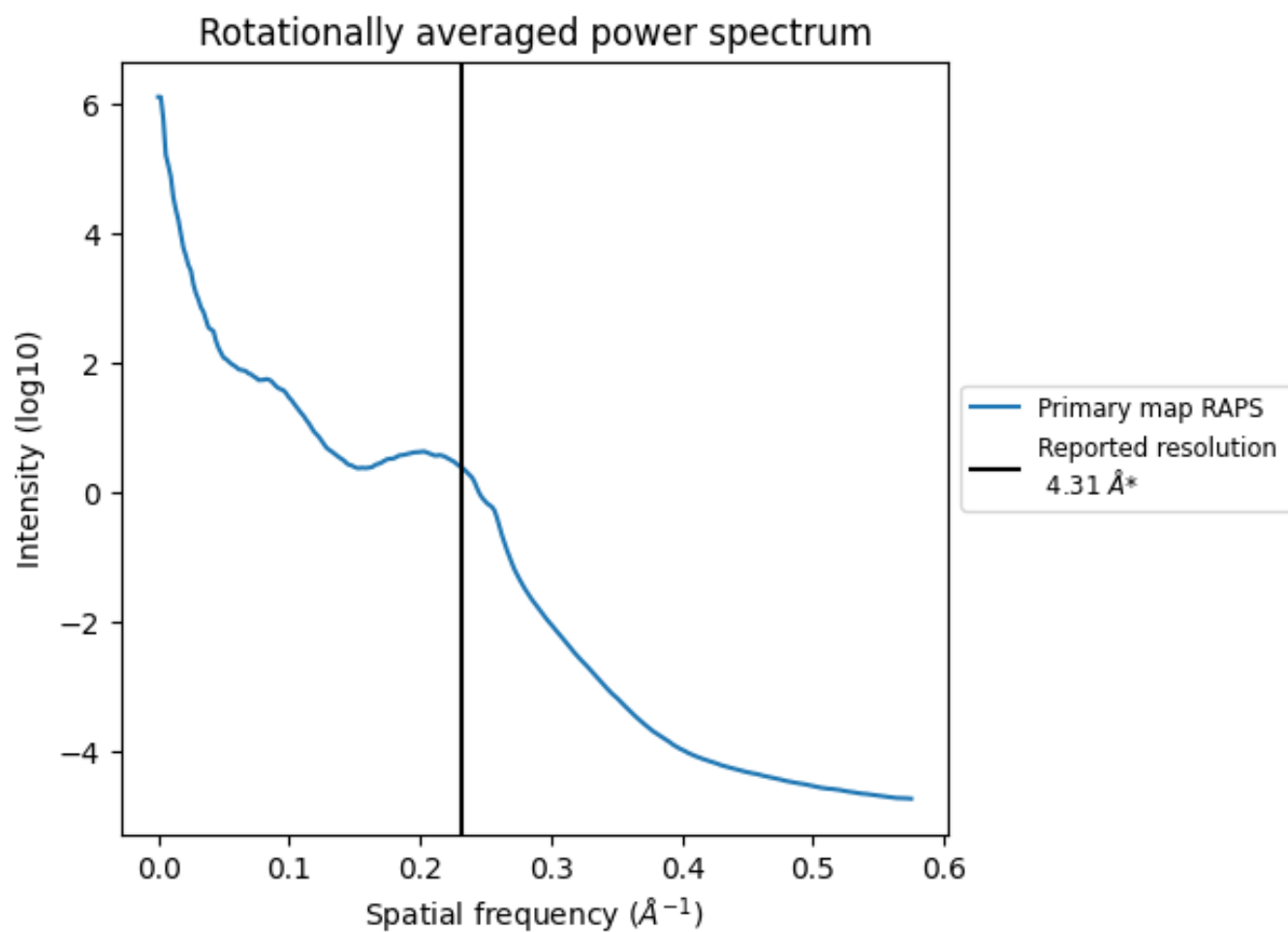
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 609 nm³; this corresponds to an approximate mass of 551 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.232\AA^{-1}

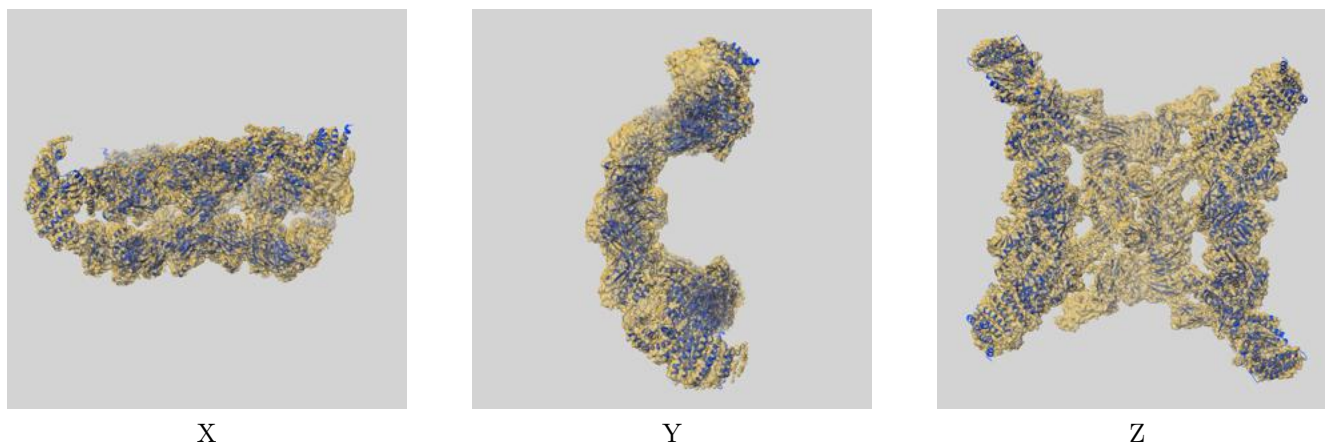
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

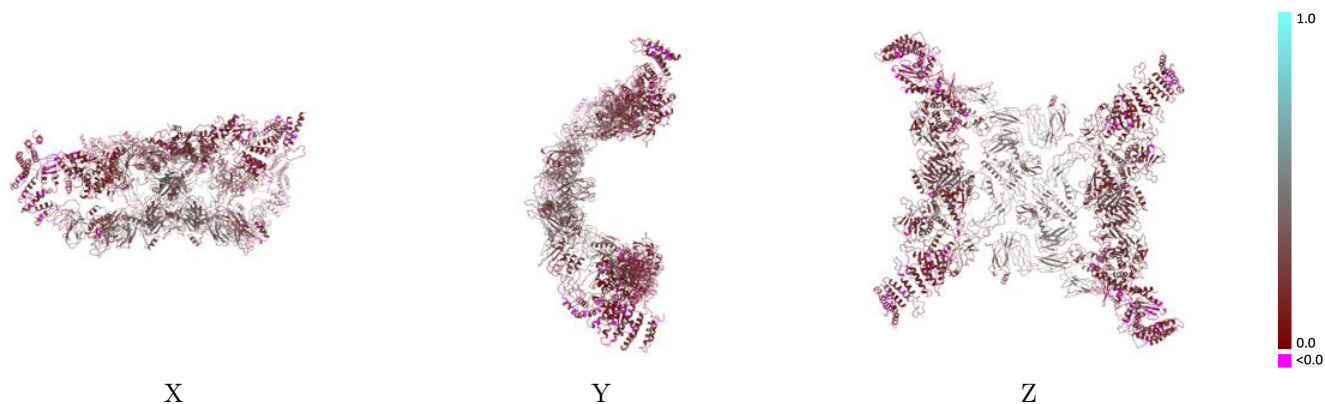
This section contains information regarding the fit between EMDB map EMD-31038 and PDB model 7EA3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



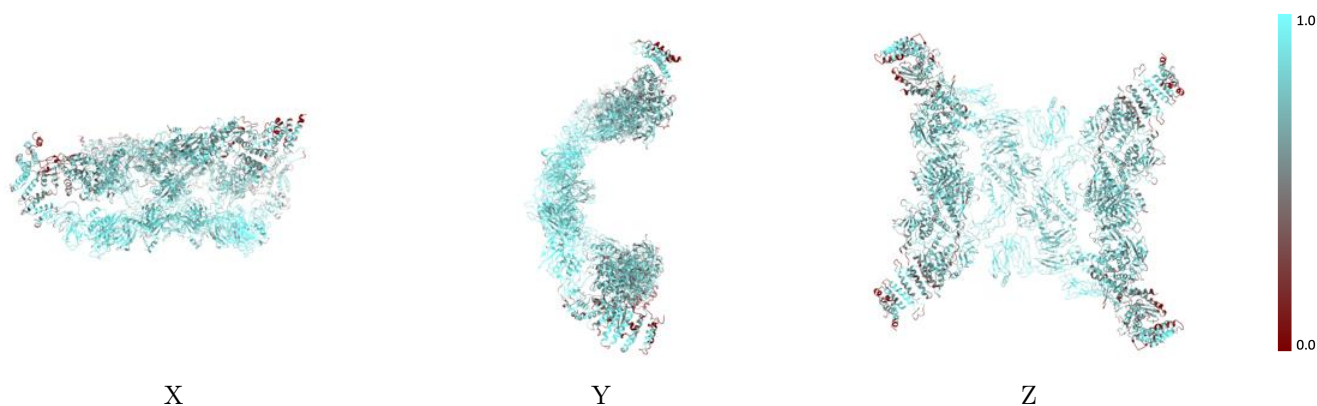
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



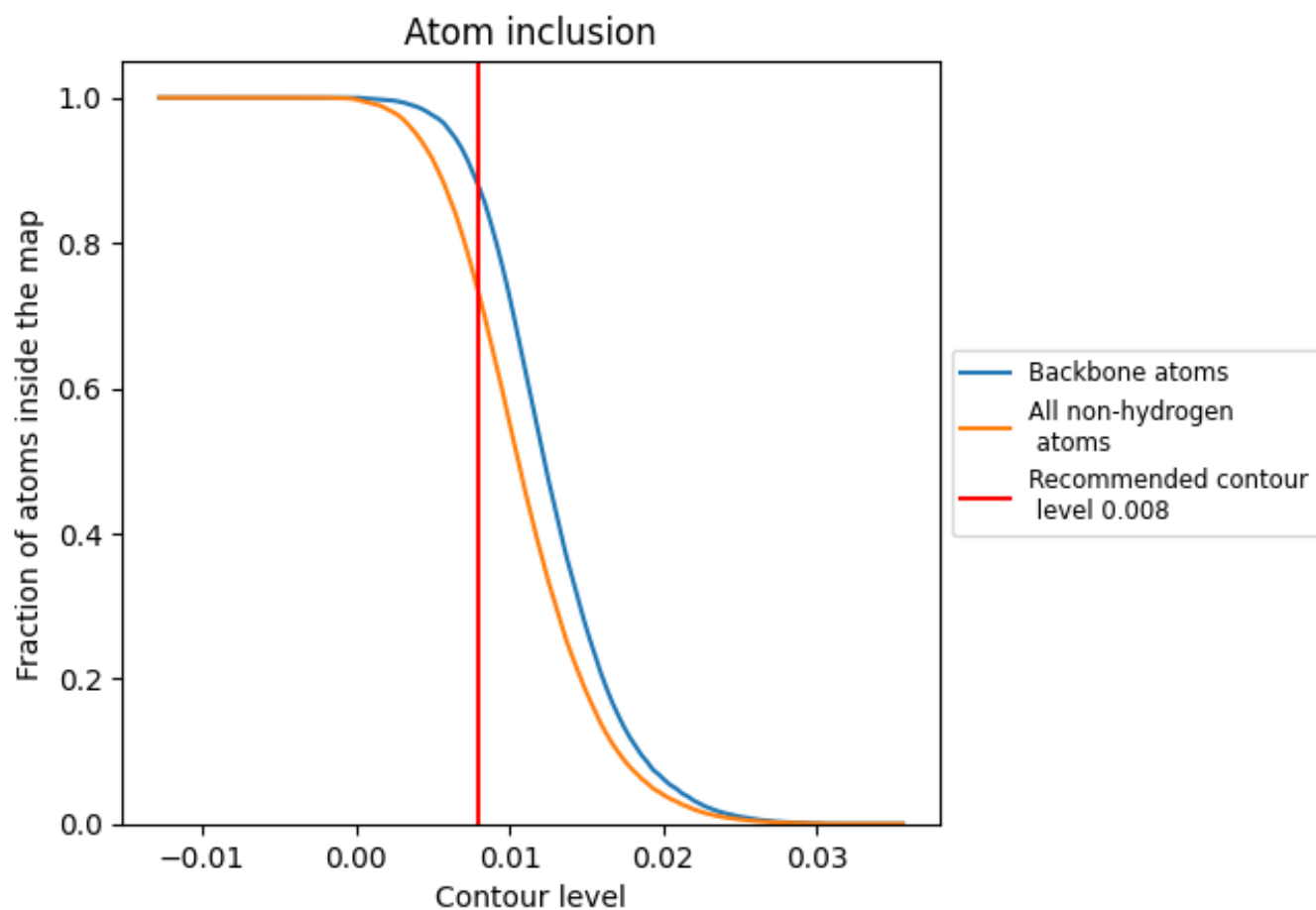
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 73% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7321	 0.2410
A	 0.4281	 0.0990
B	 0.6275	 0.1750
C	 0.7212	 0.2360
D	 0.7488	 0.2360
E	 0.7310	 0.2520
F	 0.6990	 0.2320
G	 0.6866	 0.2290
H	 0.6250	 0.1710
I	 0.8268	 0.2450
J	 0.7601	 0.2670
K	 0.8416	 0.3010
L	 0.7353	 0.3180
N	 0.4298	 0.0980
O	 0.6275	 0.1740
P	 0.7205	 0.2370
Q	 0.7454	 0.2360
R	 0.7302	 0.2470
S	 0.6990	 0.2300
T	 0.6872	 0.2210
U	 0.6284	 0.1710
V	 0.8249	 0.2450
W	 0.7598	 0.2680
X	 0.8404	 0.3010
Y	 0.7366	 0.3180

