



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:41 AM UTC

PDB ID : 7E93 / pdb_00007e93
EMDB ID : EMD-31027
Title : Intact TRAPP2 (state III).
Authors : Mi, C.C.; Sui, S.F.
Deposited on : 2021-03-03
Resolution : 6.54 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

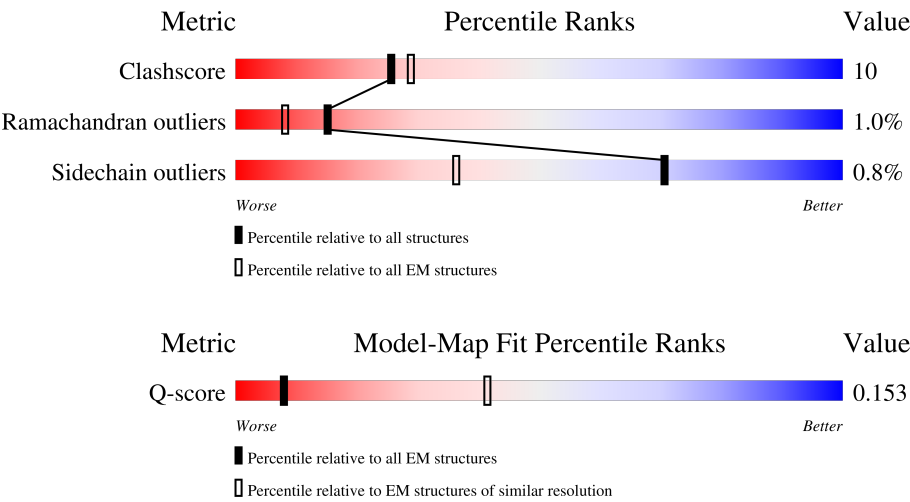
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.54 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	501 (6.04 - 7.04)

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	71% 72% 24% ..
1	L	152	71% 72% 24% ..
2	B	268	26% 53% 18% • 27%
2	M	268	26% 52% 20% • 27%

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 45998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	150	Total	C	N	O	S	0	0
			1206	781	188	233	4		
1	L	150	Total	C	N	O	S	0	0
			1206	781	188	233	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	195	Total	C	N	O	S	0	0
			1459	940	247	264	8		
2	M	195	Total	C	N	O	S	0	0
			1459	940	247	264	8		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	161	Total	C	N	O	S	0	0
			1295	839	205	242	9		
5	P	161	Total	C	N	O	S	0	0
			1297	840	206	242	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	203	Total	C	N	O	S	0	0
			1610	1027	282	292	9		
6	R	203	Total	C	N	O	S	0	0
			1610	1027	282	292	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	41	TYR	ILE	conflict	UNP Q03337
G	42	ILE	PRO	conflict	UNP Q03337
G	108	SER	VAL	conflict	UNP Q03337
R	41	TYR	ILE	conflict	UNP Q03337
R	42	ILE	PRO	conflict	UNP Q03337
R	108	SER	VAL	conflict	UNP Q03337

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	146	Total	C	N	O	S	0	0
			1173	759	194	215	5		
7	S	146	Total	C	N	O	S	0	0
			1173	759	194	215	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	799	Total	C	N	O	S	0	0
			4244	2578	822	842	2		
8	T	799	Total	C	N	O	S	0	0
			4244	2578	822	842	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	873	Total	C	N	O	S	0	0
			6256	3979	1085	1173	19		
9	U	873	Total	C	N	O	S	0	0
			6256	3979	1085	1173	19		

There are 2 discrepancies between the modelled and reference sequences:

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

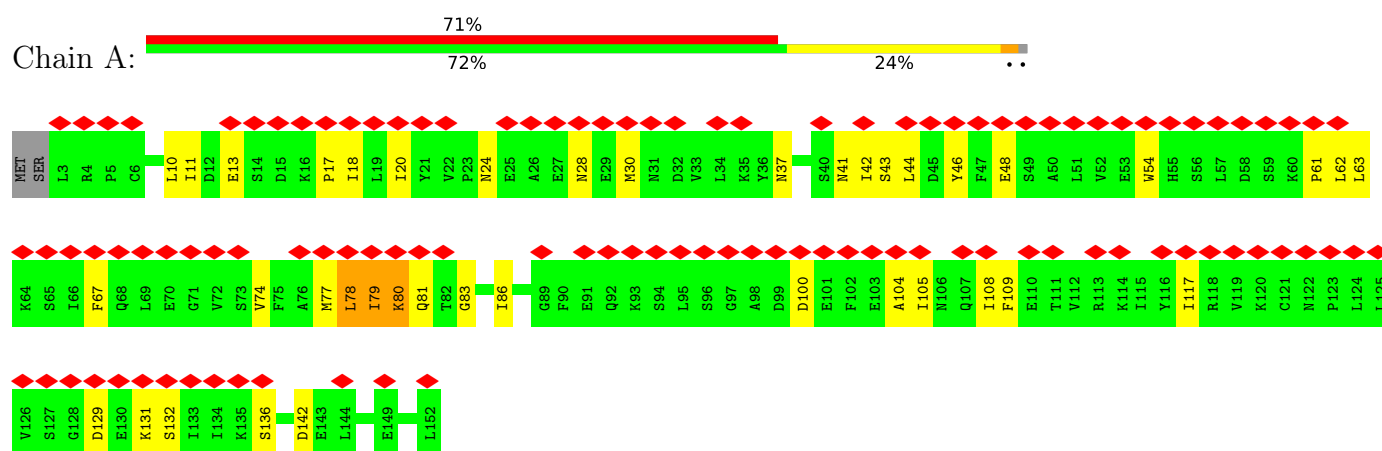
- Molecule 10 is a protein called Trafficking protein particle complex II-specific subunit 65.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	251	Total	C	N	O	S	0	0
			1568	988	278	300	2		
10	V	251	Total	C	N	O	S	0	0
			1568	988	278	300	2		

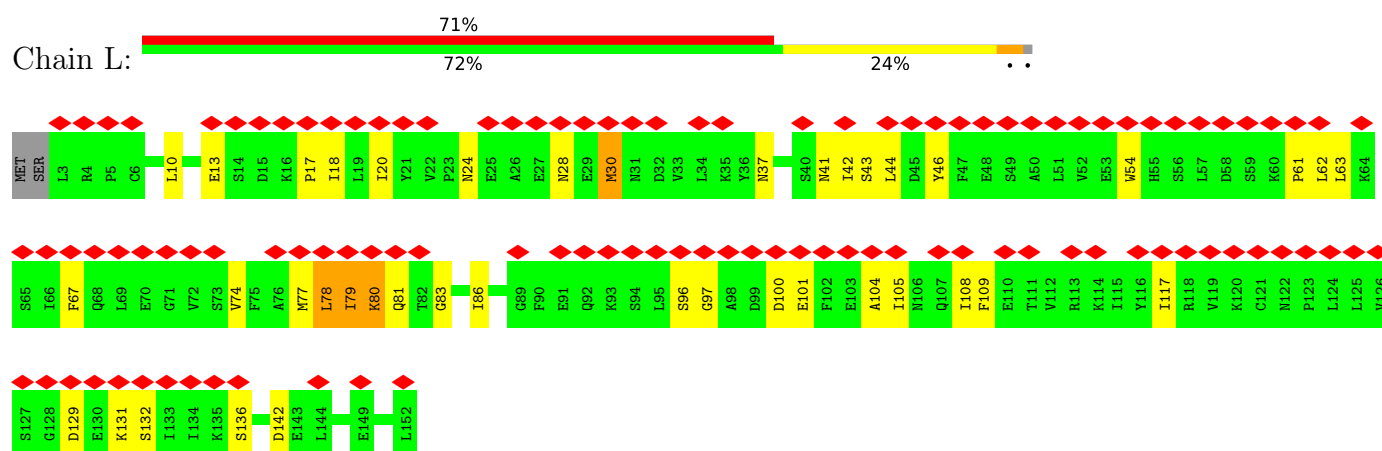
3 Residue-property plots [i](#)

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.

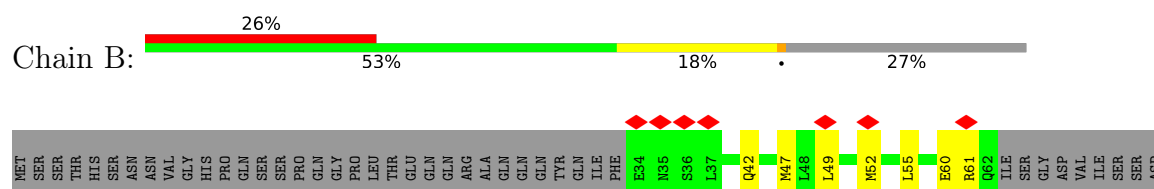
• Molecule 1: TRAPP-associated protein TCA17

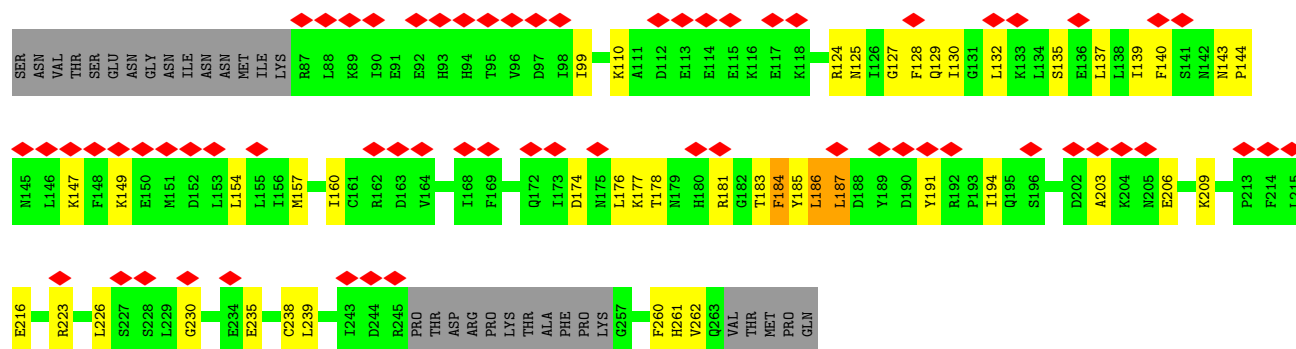


• Molecule 1: TRAPP-associated protein TCA17

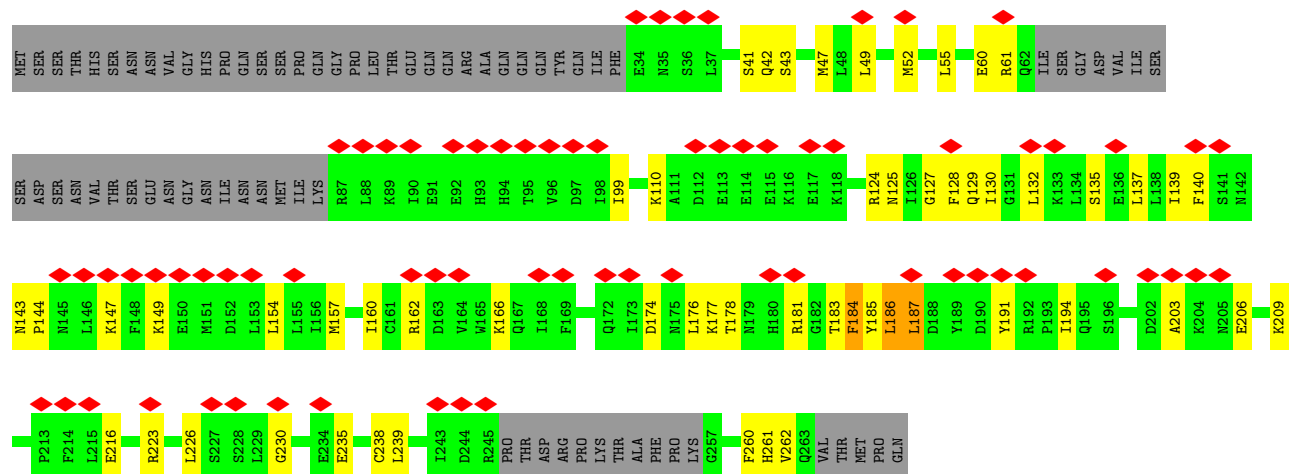


• Molecule 2: Trafficking protein particle complex subunit 33

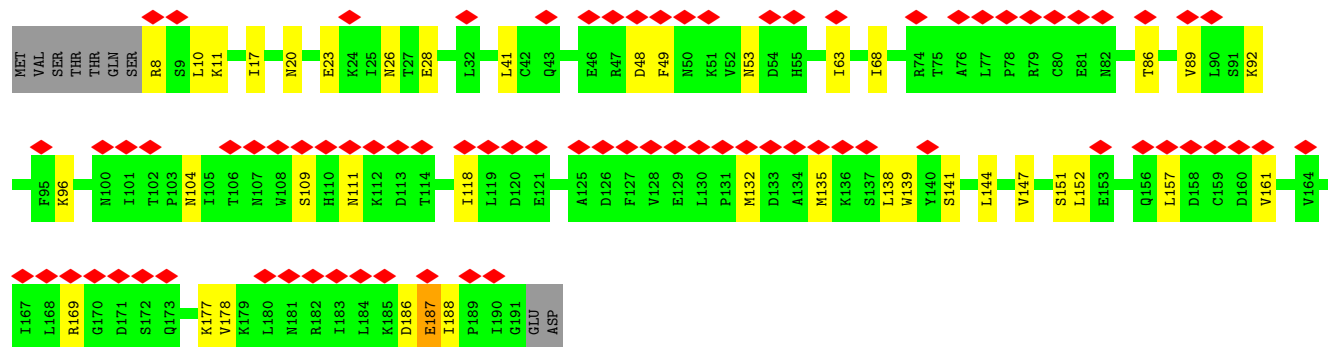
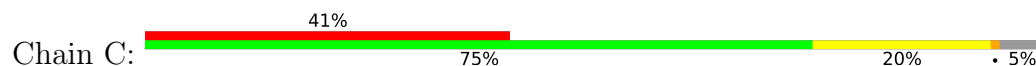




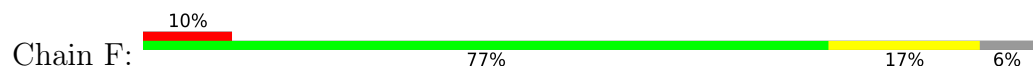
• Molecule 2: Trafficking protein particle complex subunit 33

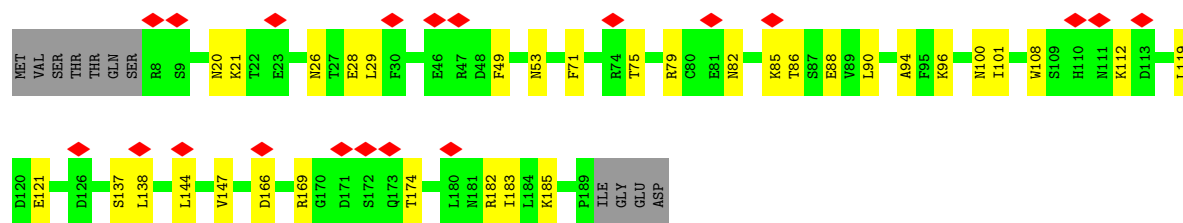


• Molecule 3: Trafficking protein particle complex subunit BET3

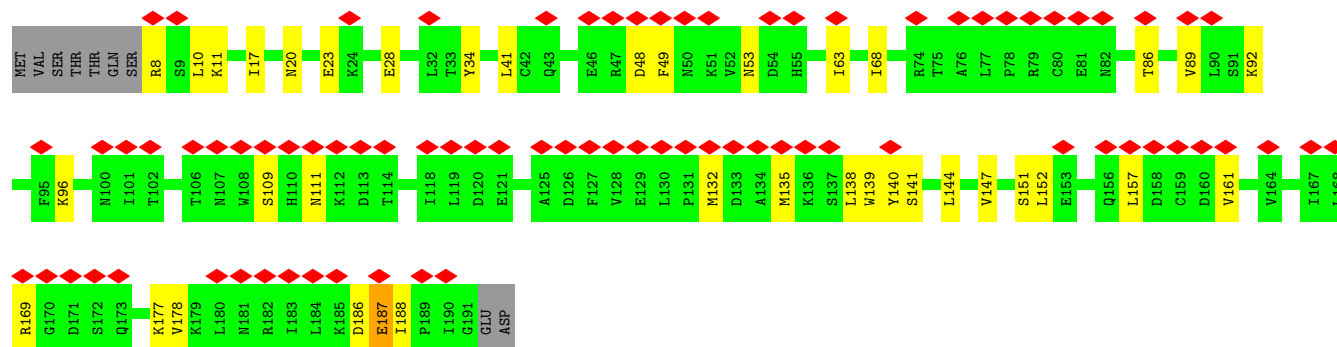
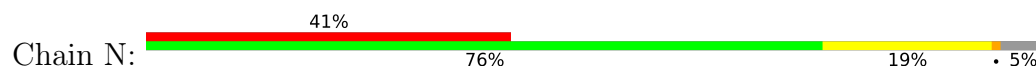


• Molecule 3: Trafficking protein particle complex subunit BET3

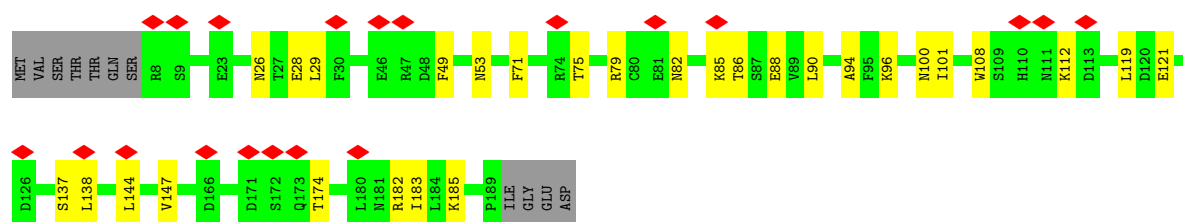
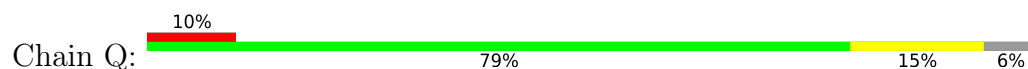




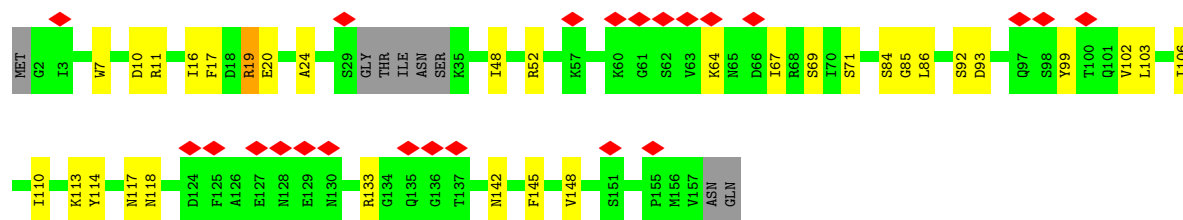
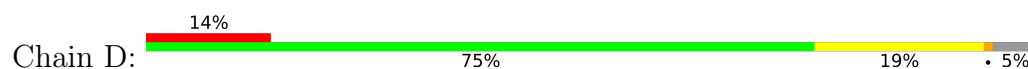
• Molecule 3: Trafficking protein particle complex subunit BET3



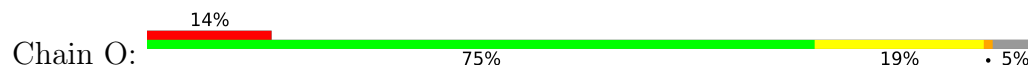
• Molecule 3: Trafficking protein particle complex subunit BET3

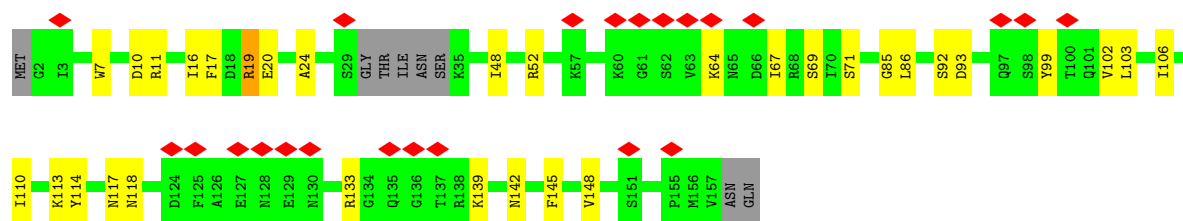


• Molecule 4: Trafficking protein particle complex subunit BET5

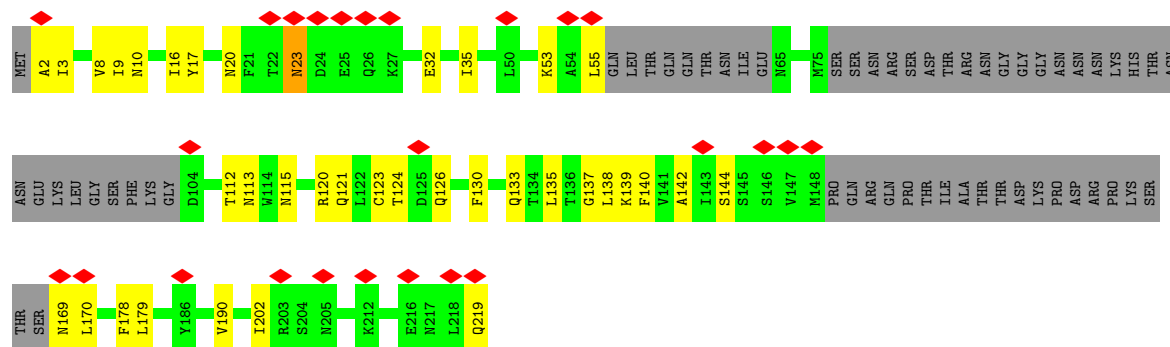


• Molecule 4: Trafficking protein particle complex subunit BET5

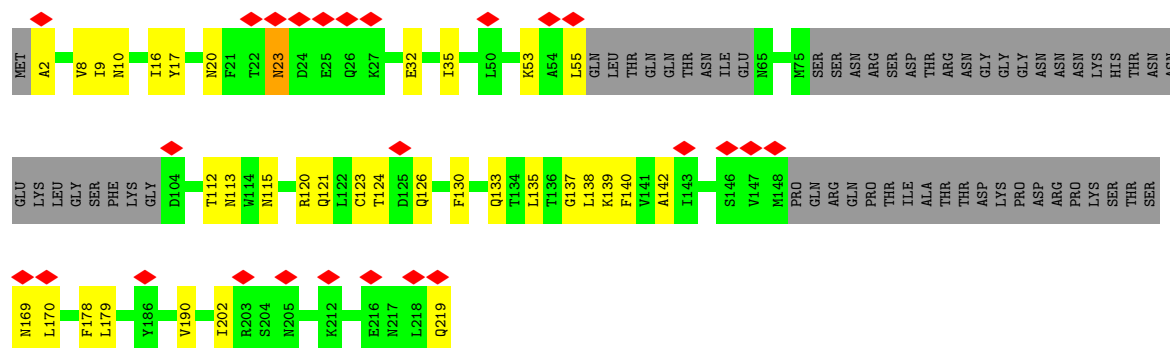




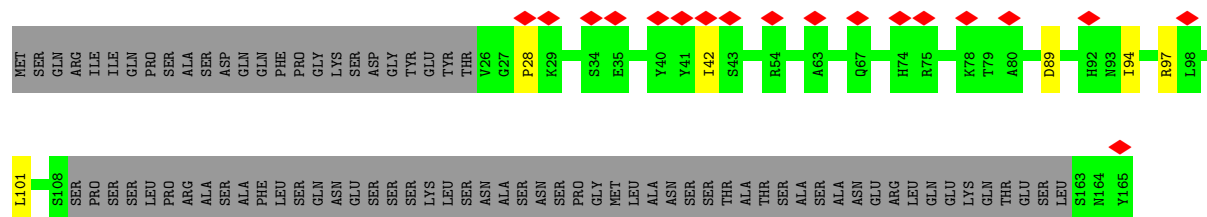
• Molecule 5: Trafficking protein particle complex subunit 23



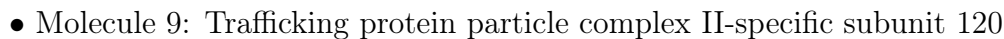
• Molecule 5: Trafficking protein particle complex subunit 23



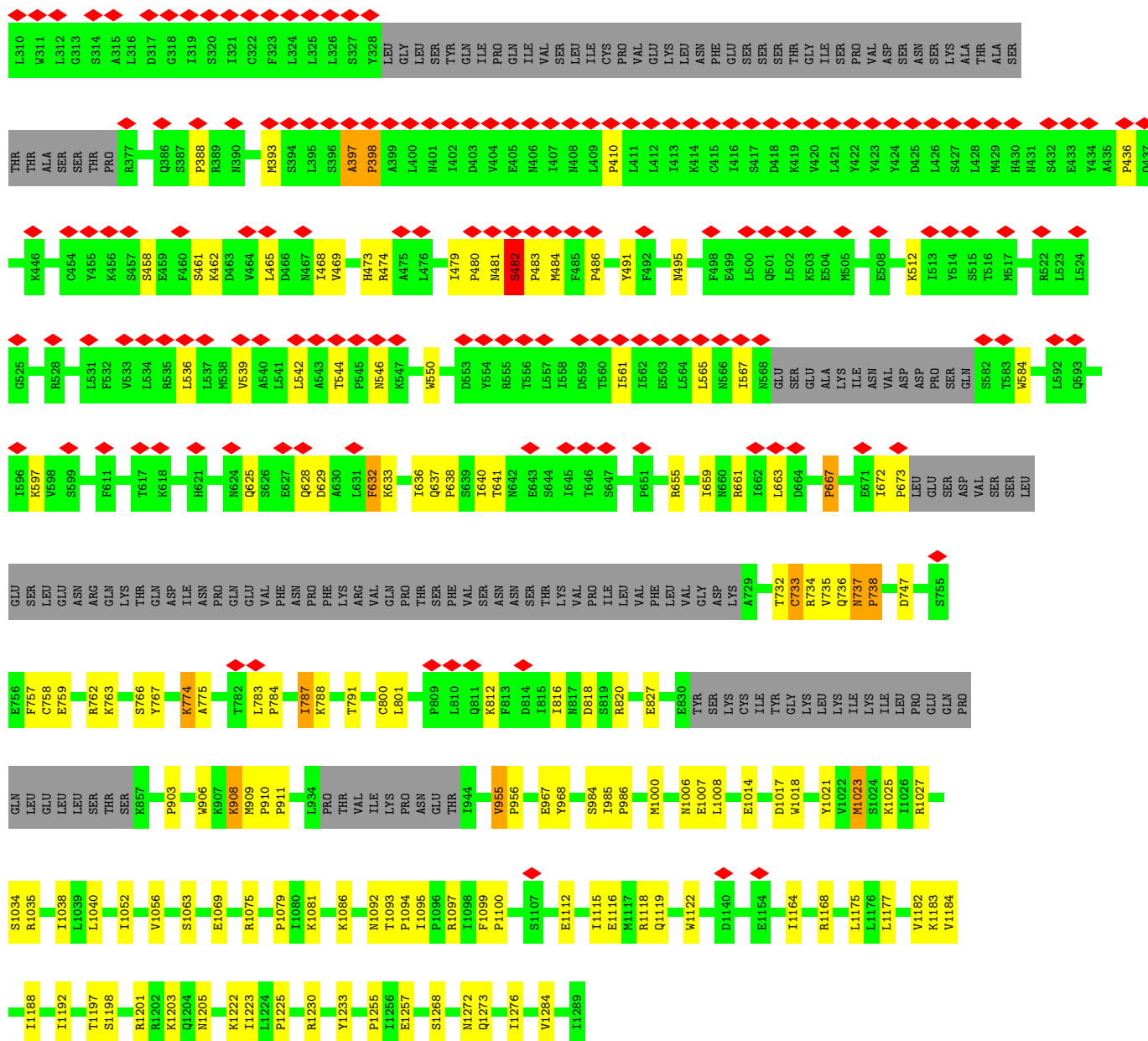
• Molecule 6: Trafficking protein particle complex subunit 31





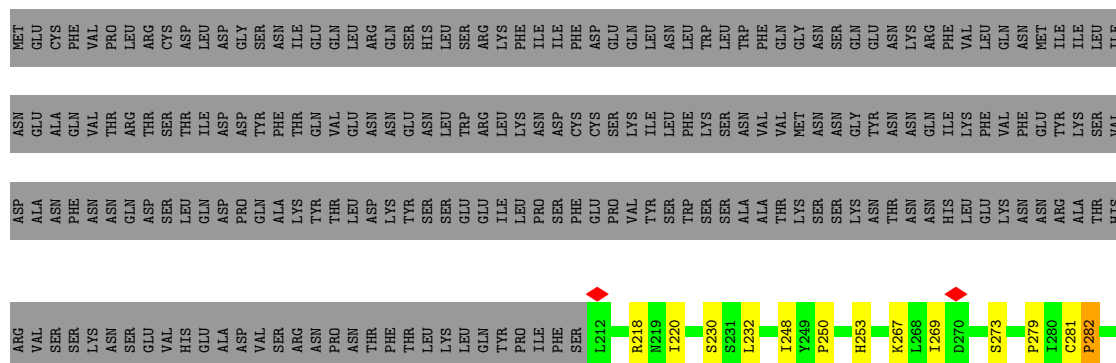


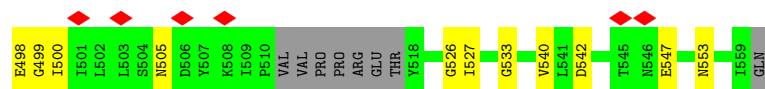
PHE	HIS	ILE	GLY	MET
GLU	VAL	SER	PHE	ASN
MET	THR	PRO	PRO	PRO
THR	LEU	ASN	HIS	LEU
ASN	ARG	VAL	GLY	LYS
SER	PRO	TYR	LEU	HIS
LEU	GLY	ALA	PHE	PHE
LYS	ALA	SER	PHE	PRO
ARG	ILE	SER	ASP	SER
SER	GLY	THR	PHE	TYR
ALA	GLY	PRO	LEU	VAL
SER	ASN	THR	THR	GLY
LEU	ALA	LYS	ILE	PRO
LEU	VAL	GLU	ASP	SER
LEU	LEU	LEU	HIS	LYS
ALA	LYS	GLU	ASP	ILE
THR	THR	GLN	ASP	THR
THR	THR	THR	ALA	LEU
LEU	LEU	ILE	VAL	VAL
SER	ILE	ASP	GLU	ILE
THR	ARG	THR	LEU	PRO
SER	GLN	MET	PHE	ILE
GLU	ASN	GLU	LEU	GLY
ASN	SER	ASN	TYR	HIS
R266	TYR	VAL	ASP	TRP
R267	THR	PHE	PHE	THR
Q268	SER	ALA	GLU	ARG
Q269	SER	SER	PRO	LYS
R270	SER	PRO	PHE	GLU
R271	SER	ASP	LYS	PHE
S272	THR	MET	THR	ASN
L272	PRO	GLN	PHE	ALA
	MET	LYS	VAL	VAL
F282	SER	ASN	ILE	GLN
	ALA	ILE	ILE	GLN
L285	VAL	GLU	GLY	LEU
A286	GLN	THR	LEU	SER
Q287	SER	ILE	VAL	GLU
R288	SER	MET	ASN	PHE
Y289	VAL	CYS	ASP	ASN
Y290	SER	ASP	TYR	GLU
D291	SER	ILE	SER	ILE
A292	SER	ALA	ASP	HIS
L293	LYS	ASN	PRO	LEU
M294	ALA	PHE	LEU	SER
S295	GLY	LEU	THR	ASP
F296	VAL	THR	ASN	VAL
Y297	THR	LEU	LEU	THR
D298	ALA	SER	PHE	ILE
A299	SER	TYR	LYS	THR
I300	ARG	SER	TYR	PRO
T301	LEU	SER	THR	THR
	SER	TYR	LEU	GLN



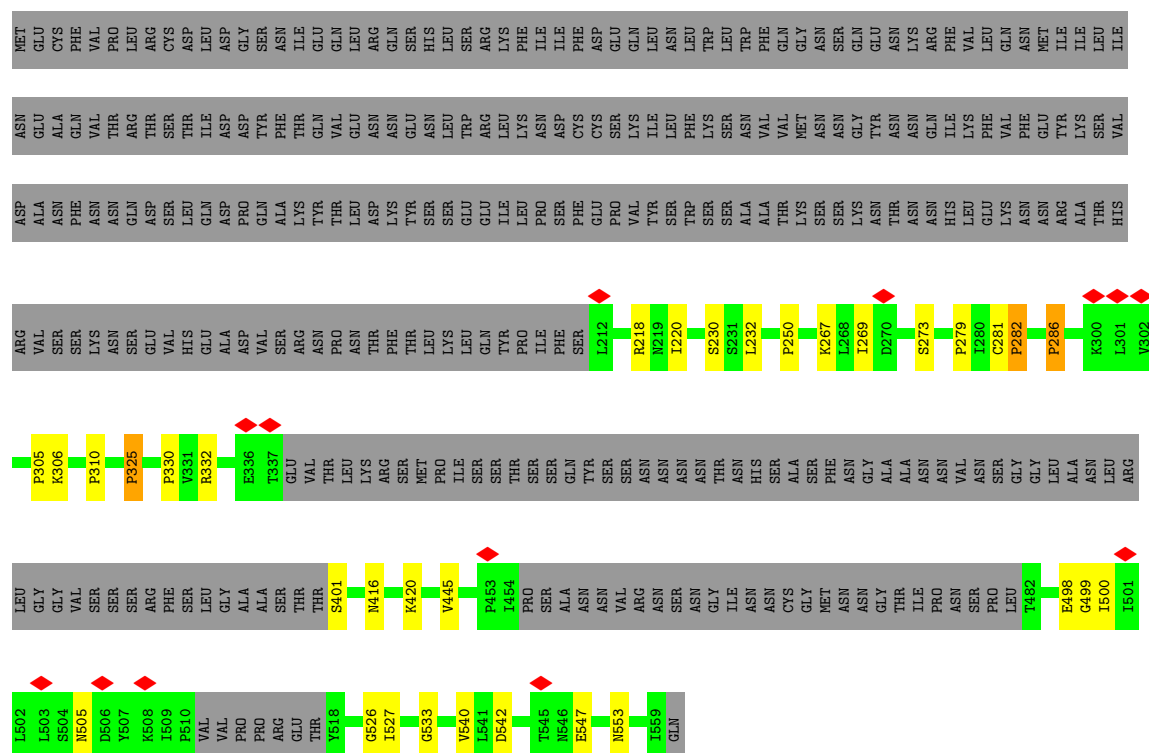
• Molecule 10: Trafficking protein particle complex II-specific subunit 65

Chain K: 39% 6% 55%





Chain V: 39% 5% 55%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15858	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	0.029	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	523.68, 523.68, 523.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/1226	0.91	4/1655 (0.2%)
1	L	0.38	0/1226	0.91	4/1655 (0.2%)
2	B	0.42	0/1481	0.87	0/2000
2	M	0.42	0/1481	0.87	0/2000
3	C	0.36	0/1509	0.81	2/2040 (0.1%)
3	F	0.40	0/1497	0.85	1/2024 (0.0%)
3	N	0.36	0/1509	0.81	2/2040 (0.1%)
3	Q	0.40	0/1497	0.85	1/2024 (0.0%)
4	D	0.42	0/1263	0.86	1/1704 (0.1%)
4	O	0.42	0/1263	0.86	1/1704 (0.1%)
5	E	0.42	0/1318	0.77	2/1775 (0.1%)
5	P	0.42	0/1321	0.77	2/1781 (0.1%)
6	G	0.43	0/1643	0.84	3/2214 (0.1%)
6	R	0.43	0/1643	0.84	3/2214 (0.1%)
7	H	0.48	0/1204	0.92	3/1633 (0.2%)
7	S	0.48	0/1204	0.92	3/1633 (0.2%)
8	I	0.38	0/4263	0.88	16/5914 (0.3%)
8	T	0.38	0/4263	0.88	16/5914 (0.3%)
9	J	0.45	1/6358 (0.0%)	0.98	26/8657 (0.3%)
9	U	0.45	1/6358 (0.0%)	0.98	27/8657 (0.3%)
10	K	0.47	0/1582	1.03	10/2169 (0.5%)
10	V	0.47	0/1582	1.03	10/2169 (0.5%)
All	All	0.42	2/46691 (0.0%)	0.91	137/63576 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	738	PRO	N-CD	10.11	1.61	1.47
9	J	738	PRO	N-CD	10.04	1.61	1.47

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	346	PRO	N-CA-CB	10.52	110.17	102.28
8	I	346	PRO	N-CA-CB	10.46	110.12	102.28
9	J	737	ASN	N-CA-C	10.31	125.90	109.40
9	U	737	ASN	N-CA-C	10.29	125.87	109.40
8	I	976	PRO	N-CA-CB	9.15	112.86	103.25
8	T	976	PRO	N-CA-CB	9.13	112.83	103.25
8	I	1076	PRO	N-CA-CB	8.43	112.10	103.25
8	T	1076	PRO	N-CA-CB	8.39	112.06	103.25
7	S	26	PRO	N-CA-CB	8.20	111.86	103.25
7	H	26	PRO	N-CA-CB	8.20	111.86	103.25
10	V	325	PRO	N-CA-CB	8.14	111.80	103.25
10	K	325	PRO	N-CA-CB	8.14	111.80	103.25
8	T	704	PRO	N-CA-CB	7.89	111.54	103.25
8	I	704	PRO	N-CA-CB	7.89	111.54	103.25
9	U	673	PRO	N-CA-CB	7.84	111.63	103.00
9	J	673	PRO	N-CA-CB	7.81	111.59	103.00
8	I	970	PRO	N-CA-CB	7.78	110.56	103.33
8	T	970	PRO	N-CA-CB	7.78	110.56	103.33
8	T	649	PRO	N-CA-CB	7.75	110.54	103.33
9	J	667	PRO	N-CA-CB	7.72	111.36	103.25
9	U	667	PRO	N-CA-CB	7.72	111.36	103.25
8	I	649	PRO	N-CA-CB	7.66	110.45	103.33
8	T	721	PRO	N-CA-CB	7.58	110.06	103.31
8	T	252	PRO	N-CA-CB	7.57	111.19	103.25
8	I	721	PRO	N-CA-CB	7.56	110.03	103.31
8	I	252	PRO	N-CA-CB	7.55	111.17	103.25
10	V	330	PRO	N-CA-CB	7.51	111.13	103.25
10	K	330	PRO	N-CA-CB	7.48	111.11	103.25
10	V	282	PRO	N-CA-CB	7.40	111.02	103.25
10	K	282	PRO	N-CA-CB	7.36	110.98	103.25
9	U	1255	PRO	N-CA-CB	7.33	110.26	103.15
8	T	483	PRO	N-CA-CB	7.32	110.93	103.25
9	J	1255	PRO	N-CA-CB	7.30	110.23	103.15
8	I	483	PRO	N-CA-CB	7.28	110.90	103.25
10	K	310	PRO	N-CA-CB	7.15	110.93	102.85
10	V	310	PRO	N-CA-CB	7.15	110.93	102.85
8	I	1067	PRO	N-CA-CB	7.04	110.64	103.25
8	T	1067	PRO	N-CA-CB	7.01	110.61	103.25
6	R	42	ILE	CG1-CB-CG2	-6.97	89.79	110.70
6	G	42	ILE	CG1-CB-CG2	-6.96	89.83	110.70
9	J	1100	PRO	N-CA-CB	6.93	109.78	103.20
9	U	1100	PRO	N-CA-CB	6.92	109.77	103.20
7	S	25	ASN	CA-C-N	6.83	128.38	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	25	ASN	C-N-CA	6.83	128.38	119.84
10	K	305	PRO	N-CA-CB	6.81	110.53	103.38
10	V	305	PRO	N-CA-CB	6.80	110.53	103.38
10	V	279	PRO	N-CA-CB	6.79	110.38	103.25
7	H	25	ASN	CA-C-N	6.79	128.33	119.84
7	H	25	ASN	C-N-CA	6.79	128.33	119.84
10	K	279	PRO	N-CA-CB	6.77	110.36	103.25
9	J	956	PRO	N-CA-CB	6.72	109.90	103.52
9	U	956	PRO	N-CA-CB	6.65	109.84	103.52
8	T	381	PRO	N-CA-CB	6.61	110.19	103.25
8	T	980	PRO	N-CA-CB	6.57	110.15	103.25
8	I	381	PRO	N-CA-CB	6.56	110.14	103.25
9	U	783	LEU	CA-CB-CG	6.56	139.25	116.30
9	J	783	LEU	CA-CB-CG	6.55	139.23	116.30
8	I	980	PRO	N-CA-CB	6.51	110.08	103.25
4	D	16	ILE	CG1-CB-CG2	-6.46	91.31	110.70
4	O	16	ILE	CG1-CB-CG2	-6.46	91.32	110.70
9	U	632	PHE	CA-C-N	6.46	133.88	121.54
9	U	632	PHE	C-N-CA	6.46	133.88	121.54
9	J	632	PHE	CA-C-N	6.44	133.84	121.54
9	J	632	PHE	C-N-CA	6.44	133.84	121.54
9	U	398	PRO	N-CA-CB	6.44	110.01	103.25
8	T	646	ILE	CA-C-N	6.42	133.53	121.97
8	T	646	ILE	C-N-CA	6.42	133.53	121.97
3	F	185	LYS	CA-CB-CG	6.42	126.94	114.10
9	J	398	PRO	N-CA-CB	6.42	109.99	103.25
3	Q	185	LYS	CA-CB-CG	6.41	126.92	114.10
8	I	646	ILE	CA-C-N	6.40	133.48	121.97
8	I	646	ILE	C-N-CA	6.40	133.48	121.97
8	T	639	PRO	N-CA-CB	6.37	109.94	103.25
8	I	639	PRO	N-CA-CB	6.36	109.93	103.25
8	I	572	PRO	N-CA-CB	6.36	109.92	103.25
8	T	572	PRO	N-CA-CB	6.32	109.89	103.25
9	J	410	PRO	N-CA-CB	6.30	110.20	103.52
9	U	410	PRO	N-CA-CB	6.28	110.17	103.52
9	U	986	PRO	N-CA-CB	6.23	109.79	103.25
9	J	986	PRO	N-CA-CB	6.22	109.78	103.25
6	R	28	PRO	N-CA-CB	6.22	110.40	103.44
9	J	733	CYS	CA-C-N	6.19	131.91	122.93
9	J	733	CYS	C-N-CA	6.19	131.91	122.93
9	U	733	CYS	CA-C-N	6.19	131.91	122.93
9	U	733	CYS	C-N-CA	6.19	131.91	122.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	388	PRO	N-CA-CB	6.16	110.05	103.52
9	U	388	PRO	N-CA-CB	6.16	110.05	103.52
10	K	250	PRO	N-CA-CB	6.13	110.08	103.33
6	G	28	PRO	N-CA-CB	6.12	110.30	103.44
10	V	250	PRO	N-CA-CB	6.09	110.03	103.33
10	V	533	GLY	CA-C-N	6.08	133.16	121.54
10	V	533	GLY	C-N-CA	6.08	133.16	121.54
10	K	533	GLY	CA-C-N	6.05	133.10	121.54
10	K	533	GLY	C-N-CA	6.05	133.10	121.54
9	U	436	PRO	N-CA-CB	5.98	110.14	103.44
10	V	286	PRO	N-CA-CB	5.96	109.50	103.25
9	J	436	PRO	N-CA-CB	5.94	110.09	103.44
10	K	286	PRO	N-CA-CB	5.94	109.48	103.25
9	J	787	ILE	CG1-CB-CG2	-5.68	93.65	110.70
9	U	787	ILE	CG1-CB-CG2	-5.68	93.66	110.70
9	U	908	LYS	CA-C-N	5.59	135.45	121.80
9	U	908	LYS	C-N-CA	5.59	135.45	121.80
9	J	908	LYS	CA-C-N	5.59	135.44	121.80
9	J	908	LYS	C-N-CA	5.59	135.44	121.80
9	J	763	LYS	CA-CB-CG	5.52	125.15	114.10
9	U	763	LYS	CA-CB-CG	5.50	125.10	114.10
9	J	550	TRP	CA-C-N	5.45	140.87	121.59
9	J	550	TRP	C-N-CA	5.45	140.87	121.59
9	U	550	TRP	CA-C-N	5.45	140.87	121.59
9	U	550	TRP	C-N-CA	5.45	140.87	121.59
9	U	738	PRO	CA-N-CD	-5.39	104.45	112.00
1	A	131	LYS	CA-C-N	5.38	131.81	121.54
1	A	131	LYS	C-N-CA	5.38	131.81	121.54
1	L	131	LYS	CA-C-N	5.38	131.81	121.54
1	L	131	LYS	C-N-CA	5.38	131.81	121.54
9	J	738	PRO	CA-N-CD	-5.35	104.52	112.00
3	C	187	GLU	CA-C-N	5.32	131.97	122.13
3	C	187	GLU	C-N-CA	5.32	131.97	122.13
3	N	187	GLU	CA-C-N	5.29	131.92	122.13
3	N	187	GLU	C-N-CA	5.29	131.92	122.13
1	A	30	MET	CA-C-N	5.24	131.54	121.54
1	A	30	MET	C-N-CA	5.24	131.54	121.54
1	L	30	MET	CA-C-N	5.22	131.51	121.54
1	L	30	MET	C-N-CA	5.22	131.51	121.54
5	P	23	ASN	CA-C-N	5.19	131.45	121.54
5	P	23	ASN	C-N-CA	5.19	131.45	121.54
9	J	909	MET	N-CA-C	-5.16	98.40	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	909	MET	N-CA-C	-5.16	98.40	109.81
5	E	23	ASN	CA-C-N	5.14	131.35	121.54
5	E	23	ASN	C-N-CA	5.14	131.35	121.54
6	G	101	LEU	CA-CB-CG	5.14	134.28	116.30
6	R	101	LEU	CA-CB-CG	5.13	134.24	116.30
9	J	1023	MET	CB-CG-SD	5.12	128.07	112.70
9	U	1023	MET	CB-CG-SD	5.11	128.04	112.70
9	J	1052	ILE	CG1-CB-CG2	-5.02	95.65	110.70
9	U	1052	ILE	CG1-CB-CG2	-5.01	95.67	110.70
9	U	774	LYS	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

There are no planarity outliers.

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	1206	0	1228	72	0
1	L	1206	0	1228	72	0
2	B	1459	0	1381	57	0
2	M	1459	0	1381	56	0
3	C	1482	0	1490	29	0
3	F	1470	0	1476	24	0
3	N	1482	0	1490	27	0
3	Q	1470	0	1476	20	0
4	D	1235	0	1202	26	0
4	O	1235	0	1202	25	0
5	E	1295	0	1296	26	0
5	P	1297	0	1299	24	0
6	G	1610	0	1547	33	0
6	R	1610	0	1547	30	0
7	H	1173	0	1125	51	0
7	S	1173	0	1125	52	0
8	I	4244	0	2176	26	0
8	T	4244	0	2176	25	0
9	J	6256	0	5486	119	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	U	6256	0	5486	111	0
10	K	1568	0	1147	13	0
10	V	1568	0	1147	12	0
All	All	45998	0	39111	872	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 10.

All (872) 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:U:481:ASN:HD22	9:U:484:MET:CE	1.33	1.41
1:L:79:ILE:CG2	1:L:81:GLN:OE1	1.67	1.41
1:A:79:ILE:CG2	1:A:81:GLN:OE1	1.68	1.40
9:J:482:SER:HB3	9:J:483:PRO:CD	1.53	1.33
1:A:63:LEU:HD12	1:A:77:MET:CE	1.58	1.33
1:L:63:LEU:HD12	1:L:77:MET:CE	1.58	1.31
9:U:481:ASN:ND2	9:U:484:MET:HE2	1.42	1.31
9:U:482:SER:HB3	9:U:483:PRO:CD	1.62	1.25
9:J:481:ASN:CB	9:J:484:MET:HE2	1.71	1.19
1:A:63:LEU:HD12	1:A:77:MET:HE1	1.19	1.18
7:S:37:ASN:HB3	7:S:38:PRO:CD	1.73	1.18
7:H:37:ASN:HB3	7:H:38:PRO:CD	1.73	1.16
7:S:32:ASP:OD1	7:S:36:LEU:HD23	1.46	1.15
2:M:177:LYS:CB	2:M:185:TYR:HE1	1.60	1.15
6:R:168:LYS:HD3	6:R:170:ARG:HH22	1.01	1.15
2:B:177:LYS:CB	2:B:185:TYR:HE1	1.60	1.14
7:H:32:ASP:OD1	7:H:36:LEU:HD23	1.46	1.13
6:G:168:LYS:HD3	6:G:170:ARG:HH22	1.01	1.13
9:J:479:ILE:HG22	9:J:480:PRO:HD2	1.24	1.11
2:B:177:LYS:HB2	2:B:185:TYR:CE1	1.85	1.11
9:J:481:ASN:HB2	9:J:484:MET:HE2	1.27	1.10
1:L:63:LEU:HD12	1:L:77:MET:HE1	1.19	1.10
2:M:177:LYS:HB2	2:M:185:TYR:CE1	1.85	1.09
9:U:482:SER:HB3	9:U:483:PRO:HD3	1.18	1.09
7:H:37:ASN:CB	7:H:38:PRO:HD2	1.83	1.09
2:M:177:LYS:HB2	2:M:185:TYR:HE1	0.96	1.08
1:A:63:LEU:HA	1:A:77:MET:HE1	1.07	1.07
9:J:482:SER:CB	9:J:483:PRO:HD2	1.83	1.07
1:L:63:LEU:HA	1:L:77:MET:CE	1.84	1.07
7:S:37:ASN:CB	7:S:38:PRO:HD2	1.83	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:LEU:HA	1:L:77:MET:HE1	1.07	1.07
1:A:79:ILE:HG23	1:A:81:GLN:CD	1.79	1.06
2:B:177:LYS:HB2	2:B:185:TYR:HE1	0.96	1.06
1:L:79:ILE:HG23	1:L:81:GLN:CD	1.79	1.06
7:S:37:ASN:CB	7:S:38:PRO:CD	2.35	1.05
1:A:63:LEU:HA	1:A:77:MET:CE	1.84	1.05
9:J:1069:GLU:OE1	9:U:1069:GLU:OE1	1.73	1.04
1:A:79:ILE:HG23	1:A:81:GLN:OE1	0.86	1.03
1:L:79:ILE:HG23	1:L:81:GLN:OE1	0.85	1.02
1:A:63:LEU:CD1	1:A:77:MET:HE1	1.89	1.02
7:H:37:ASN:CB	7:H:38:PRO:CD	2.35	1.01
1:L:61:PRO:HB2	1:L:79:ILE:HD13	1.41	1.01
1:A:63:LEU:CD1	1:A:77:MET:CE	2.39	1.01
1:L:63:LEU:CD1	1:L:77:MET:HE1	1.89	1.01
1:A:63:LEU:CA	1:A:77:MET:HE1	1.91	0.99
1:L:63:LEU:CD1	1:L:77:MET:CE	2.39	0.99
1:A:79:ILE:HG22	1:A:81:GLN:H	1.22	0.99
1:L:63:LEU:CA	1:L:77:MET:HE1	1.91	0.99
9:U:481:ASN:CG	9:U:484:MET:HE2	1.88	0.99
9:U:481:ASN:ND2	9:U:484:MET:CE	2.10	0.98
9:U:482:SER:CB	9:U:483:PRO:CD	2.42	0.98
1:A:61:PRO:HB2	1:A:79:ILE:HD13	1.41	0.97
1:L:79:ILE:HG22	1:L:81:GLN:H	1.22	0.97
9:U:481:ASN:HD22	9:U:484:MET:HE2	0.94	0.96
7:S:37:ASN:O	7:S:41:LEU:HG	1.66	0.96
7:S:37:ASN:HB3	7:S:38:PRO:HD2	0.96	0.95
7:H:37:ASN:O	7:H:41:LEU:HG	1.66	0.95
6:R:168:LYS:HD2	6:R:170:ARG:HH12	1.32	0.94
6:R:168:LYS:HD3	6:R:170:ARG:NH2	1.83	0.94
7:H:37:ASN:HB3	7:H:38:PRO:HD2	0.96	0.94
6:G:168:LYS:HD3	6:G:170:ARG:NH2	1.82	0.93
9:J:482:SER:HB3	9:J:483:PRO:HD2	0.93	0.92
6:G:168:LYS:HD2	6:G:170:ARG:HH12	1.32	0.91
9:U:481:ASN:CB	9:U:484:MET:HE2	1.99	0.91
2:M:177:LYS:CB	2:M:185:TYR:CE1	2.49	0.91
2:M:176:LEU:HB2	2:M:186:LEU:CD1	2.01	0.91
2:B:176:LEU:HB2	2:B:186:LEU:CD1	2.01	0.91
1:A:54:TRP:NE1	1:A:78:LEU:HD12	1.86	0.90
1:L:54:TRP:NE1	1:L:78:LEU:HD12	1.86	0.89
2:M:174:ASP:O	2:M:187:LEU:HD23	1.73	0.89
2:B:174:ASP:O	2:B:187:LEU:HD23	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:37:ASN:CG	7:S:38:PRO:HD3	1.98	0.88
1:A:62:LEU:O	1:A:77:MET:SD	2.31	0.88
1:L:62:LEU:O	1:L:77:MET:SD	2.31	0.87
1:A:61:PRO:HG2	1:A:79:ILE:HA	1.55	0.87
7:H:37:ASN:CG	7:H:38:PRO:HD3	1.99	0.87
9:J:482:SER:CB	9:J:483:PRO:CD	2.45	0.87
1:L:61:PRO:HG2	1:L:79:ILE:HA	1.55	0.86
2:B:177:LYS:CB	2:B:185:TYR:CE1	2.49	0.85
2:B:187:LEU:HD23	2:B:187:LEU:O	1.77	0.84
2:B:176:LEU:HB2	2:B:186:LEU:HD11	1.59	0.84
2:M:176:LEU:HB2	2:M:186:LEU:HD11	1.59	0.84
2:M:187:LEU:HD23	2:M:187:LEU:O	1.77	0.84
9:U:481:ASN:HB3	9:U:484:MET:HG2	1.57	0.84
9:J:479:ILE:HG22	9:J:480:PRO:CD	2.09	0.83
1:A:61:PRO:HG2	1:A:79:ILE:HD12	1.60	0.82
5:E:169:ASN:CB	5:E:169:ASN:C	2.52	0.82
1:A:79:ILE:CG2	1:A:81:GLN:HB2	2.10	0.82
1:L:61:PRO:HG2	1:L:79:ILE:HD12	1.60	0.81
9:J:479:ILE:CG2	9:J:480:PRO:HD2	2.09	0.81
2:M:181:ARG:HA	2:M:184:PHE:CE1	2.16	0.80
1:L:61:PRO:CG	1:L:79:ILE:HD12	2.11	0.80
2:B:181:ARG:HA	2:B:184:PHE:CE1	2.16	0.80
1:L:79:ILE:CG2	1:L:81:GLN:HB2	2.10	0.80
1:A:61:PRO:CG	1:A:79:ILE:HD12	2.11	0.80
1:A:61:PRO:HD2	1:A:79:ILE:HD12	1.64	0.79
7:S:32:ASP:O	7:S:36:LEU:HG	1.83	0.79
7:H:38:PRO:O	7:H:42:HIS:N	2.16	0.79
7:S:38:PRO:HB3	9:U:584:TRP:CZ2	2.18	0.78
7:H:38:PRO:HB3	9:J:584:TRP:CZ2	2.18	0.78
7:S:38:PRO:O	7:S:42:HIS:N	2.16	0.78
1:A:54:TRP:CE2	1:A:78:LEU:HD12	2.19	0.77
2:M:174:ASP:O	2:M:187:LEU:CD2	2.32	0.77
2:M:177:LYS:O	2:M:185:TYR:CE1	2.37	0.77
1:L:54:TRP:CE2	1:L:78:LEU:HD12	2.19	0.77
1:L:61:PRO:HD2	1:L:79:ILE:HD12	1.64	0.77
7:S:37:ASN:CG	7:S:38:PRO:CD	2.57	0.77
7:H:32:ASP:O	7:H:36:LEU:HG	1.84	0.77
7:H:37:ASN:CG	7:H:38:PRO:CD	2.57	0.77
2:B:177:LYS:O	2:B:185:TYR:CE1	2.37	0.76
9:J:481:ASN:HB2	9:J:484:MET:CE	2.14	0.76
1:L:61:PRO:CD	1:L:79:ILE:HD12	2.15	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:LEU:HD12	1:L:77:MET:HE2	1.67	0.76
2:B:174:ASP:O	2:B:187:LEU:CD2	2.32	0.76
9:U:479:ILE:C	9:U:481:ASN:H	1.92	0.76
1:A:61:PRO:CD	1:A:79:ILE:HD12	2.15	0.75
6:R:168:LYS:CD	6:R:170:ARG:HH22	1.93	0.75
9:U:482:SER:CB	9:U:483:PRO:HD2	2.17	0.74
1:A:61:PRO:CB	1:A:79:ILE:HD13	2.16	0.74
9:J:735:VAL:HG23	9:J:735:VAL:O	1.88	0.74
9:J:491:TYR:O	9:J:495:ASN:HB2	1.88	0.73
1:L:61:PRO:CB	1:L:79:ILE:HD13	2.16	0.73
1:A:63:LEU:HD12	1:A:77:MET:HE2	1.67	0.73
1:L:61:PRO:HG2	1:L:79:ILE:CD1	2.19	0.73
9:U:491:TYR:O	9:U:495:ASN:HB2	1.88	0.73
1:A:61:PRO:HG2	1:A:79:ILE:CD1	2.19	0.72
9:U:735:VAL:HG23	9:U:735:VAL:O	1.88	0.72
1:A:61:PRO:CG	1:A:79:ILE:CD1	2.67	0.72
6:G:168:LYS:CD	6:G:170:ARG:HH22	1.93	0.72
1:L:61:PRO:CG	1:L:79:ILE:CD1	2.67	0.72
2:M:176:LEU:HD13	2:M:186:LEU:HD13	1.73	0.71
9:J:481:ASN:HD22	9:J:484:MET:CE	2.03	0.71
1:A:61:PRO:CG	1:A:79:ILE:HA	2.21	0.71
1:A:79:ILE:HG22	1:A:81:GLN:N	2.03	0.70
2:B:176:LEU:HD13	2:B:186:LEU:HD13	1.73	0.70
1:L:79:ILE:HG22	1:L:81:GLN:N	2.03	0.70
1:L:54:TRP:HE1	1:L:78:LEU:HD12	1.57	0.69
1:L:61:PRO:CG	1:L:79:ILE:HA	2.21	0.68
1:A:77:MET:HB3	1:A:109:PHE:CE1	2.28	0.68
9:J:481:ASN:HB3	9:J:484:MET:HG2	1.74	0.68
1:A:79:ILE:HG21	1:A:81:GLN:HB2	1.76	0.68
7:H:38:PRO:O	7:H:42:HIS:HB2	1.94	0.68
7:H:36:LEU:HD12	7:H:36:LEU:C	2.19	0.68
7:S:36:LEU:C	7:S:36:LEU:HD12	2.19	0.68
9:J:800:CYS:SG	9:J:801:LEU:N	2.67	0.67
1:L:77:MET:HB3	1:L:109:PHE:CE1	2.28	0.67
1:L:79:ILE:HG21	1:L:81:GLN:HB2	1.76	0.67
7:S:38:PRO:O	7:S:42:HIS:HB2	1.94	0.67
9:U:481:ASN:HB2	9:U:484:MET:HE2	1.76	0.67
1:L:61:PRO:HD2	1:L:79:ILE:CD1	2.25	0.67
2:B:47:MET:HB2	3:C:63:ILE:HD11	1.78	0.66
1:A:54:TRP:HE1	1:A:78:LEU:HD12	1.57	0.66
1:A:61:PRO:HD2	1:A:79:ILE:CD1	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:2:PRO:HB2	7:H:29:PHE:CE1	2.31	0.65
7:S:2:PRO:HB2	7:S:29:PHE:CE1	2.31	0.65
1:A:54:TRP:CZ2	1:A:78:LEU:CD1	2.80	0.64
1:L:54:TRP:CZ2	1:L:78:LEU:CD1	2.80	0.64
2:M:47:MET:HB2	3:N:63:ILE:HD11	1.78	0.64
9:U:479:ILE:O	9:U:481:ASN:N	2.29	0.64
7:S:52:GLN:HG3	7:S:104:ILE:HG21	1.78	0.64
9:J:628:GLN:O	9:J:632:PHE:HB2	1.98	0.64
9:U:628:GLN:O	9:U:632:PHE:HB2	1.98	0.64
7:H:52:GLN:HG3	7:H:104:ILE:HG21	1.78	0.64
2:B:183:THR:C	2:B:184:PHE:HD1	2.06	0.63
2:M:183:THR:C	2:M:184:PHE:HD1	2.06	0.63
4:O:20:GLU:HB2	4:O:24:ALA:CB	2.28	0.63
7:H:36:LEU:HA	7:H:40:ILE:HG21	1.80	0.63
2:M:177:LYS:O	2:M:185:TYR:CD1	2.51	0.63
1:A:61:PRO:HG2	1:A:79:ILE:CA	2.27	0.63
2:B:177:LYS:O	2:B:185:TYR:CD1	2.51	0.63
4:D:20:GLU:HB2	4:D:24:ALA:CB	2.28	0.62
3:N:49:PHE:HB3	3:N:138:LEU:HB2	1.81	0.62
3:N:187:GLU:H	4:O:133:ARG:HH11	1.48	0.62
5:E:140:PHE:HB3	5:E:179:LEU:HD12	1.81	0.62
9:J:1182:VAL:HG11	9:J:1188:ILE:HD11	1.82	0.62
7:S:36:LEU:HA	7:S:40:ILE:HG21	1.80	0.62
1:L:61:PRO:HG2	1:L:79:ILE:CA	2.27	0.62
9:U:800:CYS:SG	9:U:801:LEU:N	2.67	0.62
9:U:1182:VAL:HG11	9:U:1188:ILE:HD11	1.82	0.62
9:J:393:MET:O	9:J:397:ALA:HB3	2.00	0.62
9:J:481:ASN:CG	9:J:484:MET:HE2	2.25	0.62
5:P:140:PHE:HB3	5:P:179:LEU:HD12	1.81	0.62
3:C:187:GLU:H	4:D:133:ARG:HH11	1.48	0.61
9:U:393:MET:O	9:U:397:ALA:HB3	2.00	0.61
9:J:481:ASN:CB	9:J:484:MET:CE	2.65	0.61
3:C:49:PHE:HB3	3:C:138:LEU:HB2	1.81	0.61
7:H:35:GLU:O	7:H:40:ILE:CG2	2.49	0.61
7:H:87:CYS:SG	7:H:88:TYR:N	2.74	0.61
1:A:79:ILE:HG21	1:A:81:GLN:OE1	1.90	0.61
9:J:481:ASN:HB3	9:J:484:MET:HE2	1.74	0.61
7:S:35:GLU:O	7:S:40:ILE:CG2	2.49	0.61
7:S:87:CYS:SG	7:S:88:TYR:N	2.74	0.60
9:J:1112:GLU:O	9:J:1116:GLU:HB2	2.02	0.60
9:U:1075:ARG:HD2	10:V:505:ASN:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:4:TYR:HB3	7:H:114:ILE:HB	1.84	0.60
3:C:68:ILE:HD13	3:C:151:SER:HB2	1.84	0.60
1:A:54:TRP:CE2	1:A:78:LEU:CD1	2.85	0.60
6:R:168:LYS:CD	6:R:170:ARG:HH12	2.11	0.60
7:S:4:TYR:HB3	7:S:114:ILE:HB	1.84	0.60
1:L:54:TRP:CE2	1:L:78:LEU:CD1	2.85	0.60
10:V:445:VAL:HG12	10:V:540:VAL:HG12	1.83	0.60
10:K:445:VAL:HG12	10:K:540:VAL:HG12	1.83	0.59
3:N:68:ILE:HD13	3:N:151:SER:HB2	1.84	0.59
2:M:181:ARG:C	2:M:184:PHE:HE1	2.11	0.59
9:U:1112:GLU:O	9:U:1116:GLU:HB2	2.02	0.59
2:M:181:ARG:HA	2:M:184:PHE:HE1	1.67	0.59
1:A:63:LEU:CD1	1:A:77:MET:HE3	2.32	0.59
3:F:101:ILE:HD11	3:F:121:GLU:HG3	1.85	0.59
1:L:63:LEU:CD1	1:L:77:MET:HE3	2.32	0.59
1:L:105:ILE:HA	1:L:108:ILE:HG12	1.85	0.59
9:J:1075:ARG:HD2	10:K:505:ASN:HB2	1.83	0.58
9:J:481:ASN:ND2	9:J:484:MET:HE2	2.17	0.58
7:S:47:ILE:O	7:S:51:LEU:HB2	2.04	0.58
3:N:92:LYS:O	3:N:96:LYS:HB2	2.04	0.58
1:A:61:PRO:CB	1:A:79:ILE:HA	2.34	0.58
3:Q:101:ILE:HD11	3:Q:121:GLU:HG3	1.85	0.58
2:B:181:ARG:C	2:B:184:PHE:HE1	2.11	0.58
9:J:479:ILE:CG1	9:J:485:PHE:HB2	2.33	0.58
9:U:659:ILE:HG23	9:U:738:PRO:HB3	1.86	0.58
7:H:47:ILE:O	7:H:51:LEU:HB2	2.04	0.58
9:U:1175:LEU:HG	9:U:1192:ILE:HG22	1.85	0.58
10:V:416:ASN:O	10:V:420:LYS:NZ	2.37	0.58
1:A:105:ILE:HA	1:A:108:ILE:HG12	1.85	0.58
4:O:20:GLU:HB2	4:O:24:ALA:HB1	1.86	0.58
9:J:659:ILE:HG23	9:J:738:PRO:HB3	1.86	0.57
3:Q:108:TRP:HB3	3:Q:112:LYS:HA	1.85	0.57
8:T:1003:THR:O	9:U:1230:ARG:NH2	2.37	0.57
9:U:661:ARG:NH2	9:U:733:CYS:HA	2.19	0.57
3:C:92:LYS:O	3:C:96:LYS:HB2	2.04	0.57
5:E:169:ASN:CB	5:E:170:LEU:N	2.68	0.57
9:J:1175:LEU:HG	9:J:1192:ILE:HG22	1.85	0.57
7:S:29:PHE:CD1	7:S:29:PHE:N	2.73	0.57
1:L:61:PRO:CB	1:L:79:ILE:HA	2.34	0.57
2:M:157:MET:HA	2:M:160:ILE:HG22	1.87	0.57
7:H:29:PHE:N	7:H:29:PHE:CD1	2.73	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:416:ASN:O	10:K:420:LYS:NZ	2.37	0.57
1:L:79:ILE:HG21	1:L:81:GLN:OE1	1.90	0.57
8:I:1003:THR:O	9:J:1230:ARG:NH2	2.37	0.57
1:L:62:LEU:C	1:L:77:MET:SD	2.88	0.57
3:F:108:TRP:HB3	3:F:112:LYS:HA	1.85	0.56
7:H:37:ASN:O	7:H:41:LEU:CG	2.49	0.56
2:B:42:GLN:H	3:C:23:GLU:HB3	1.69	0.56
4:D:20:GLU:HB2	4:D:24:ALA:HB1	1.86	0.56
2:M:42:GLN:H	3:N:23:GLU:HB3	1.69	0.56
7:S:88:TYR:OH	7:S:130:MET:SD	2.62	0.56
9:J:661:ARG:NH2	9:J:733:CYS:HA	2.20	0.56
6:G:277:ARG:HH11	7:H:53:TRP:HB3	1.71	0.56
1:A:62:LEU:C	1:A:77:MET:SD	2.88	0.56
4:D:19:ARG:HH22	4:D:20:GLU:HG2	1.69	0.56
4:O:19:ARG:HH22	4:O:20:GLU:HG2	1.69	0.56
9:U:458:SER:O	9:U:462:LYS:NZ	2.39	0.56
6:G:168:LYS:CD	6:G:170:ARG:HH12	2.11	0.56
7:H:88:TYR:OH	7:H:130:MET:SD	2.62	0.56
5:P:10:ASN:HA	5:P:138:LEU:HD23	1.88	0.56
2:B:157:MET:HA	2:B:160:ILE:HG22	1.87	0.56
2:B:181:ARG:HA	2:B:184:PHE:HE1	1.66	0.56
3:Q:29:LEU:HD12	6:R:191:LEU:HD22	1.88	0.56
6:R:277:ARG:HH11	7:S:53:TRP:HB3	1.71	0.55
2:B:238:CYS:SG	2:B:239:LEU:N	2.78	0.55
9:U:1115:ILE:HD11	9:U:1201:ARG:HH21	1.72	0.55
8:I:599:PHE:HA	8:I:636:LYS:HA	1.88	0.55
9:U:542:LEU:HD11	9:U:597:LYS:HB3	1.88	0.55
9:J:1115:ILE:HD11	9:J:1201:ARG:HH21	1.72	0.55
3:F:29:LEU:HD12	6:G:191:LEU:HD22	1.88	0.55
9:J:458:SER:O	9:J:462:LYS:NZ	2.39	0.55
2:B:187:LEU:HD23	2:B:187:LEU:C	2.31	0.54
7:H:32:ASP:HA	7:H:35:GLU:CD	2.32	0.54
9:J:542:LEU:HD11	9:J:597:LYS:HB3	1.88	0.54
9:U:481:ASN:ND2	9:U:484:MET:SD	2.76	0.54
9:U:1008:LEU:O	9:U:1023:MET:SD	2.66	0.54
1:A:63:LEU:CB	1:A:77:MET:HE1	2.37	0.54
1:L:80:LYS:O	1:L:80:LYS:HG2	2.08	0.54
7:S:32:ASP:HA	7:S:35:GLU:CD	2.32	0.54
9:U:1017:ASP:OD1	9:U:1017:ASP:N	2.40	0.54
2:B:184:PHE:HD1	2:B:184:PHE:N	2.05	0.54
1:L:63:LEU:CB	1:L:77:MET:HE1	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:SER:HG	2:M:43:SER:HG	1.54	0.54
8:T:599:PHE:HA	8:T:636:LYS:HA	1.89	0.54
5:E:10:ASN:HA	5:E:138:LEU:HD23	1.88	0.54
5:E:190:VAL:HG21	5:E:202:ILE:HG23	1.90	0.54
9:J:737:ASN:OD1	9:J:737:ASN:C	2.51	0.54
2:M:184:PHE:CD1	2:M:184:PHE:N	2.76	0.54
6:R:168:LYS:HD2	6:R:170:ARG:NH1	2.14	0.54
2:M:184:PHE:HD1	2:M:184:PHE:N	2.05	0.54
4:D:103:LEU:HD23	4:D:106:ILE:HD11	1.90	0.54
3:F:26:ASN:ND2	3:F:28:GLU:OE2	2.41	0.54
9:J:638:PRO:HA	9:J:641:THR:HG22	1.90	0.54
9:J:1008:LEU:O	9:J:1023:MET:SD	2.66	0.54
3:Q:26:ASN:ND2	3:Q:28:GLU:OE2	2.41	0.54
2:M:238:CYS:SG	2:M:239:LEU:N	2.78	0.54
1:A:80:LYS:O	1:A:80:LYS:HG2	2.08	0.53
3:Q:82:ASN:OD1	3:Q:85:LYS:N	2.41	0.53
2:B:187:LEU:CD2	2:B:187:LEU:H	2.22	0.53
4:D:92:SER:OG	4:D:93:ASP:N	2.40	0.53
6:G:250:VAL:HG13	6:G:268:ILE:HG22	1.89	0.53
4:O:92:SER:OG	4:O:93:ASP:N	2.40	0.53
2:B:177:LYS:C	2:B:185:TYR:CE1	2.86	0.53
9:J:1017:ASP:N	9:J:1017:ASP:OD1	2.40	0.53
1:L:54:TRP:CZ2	1:L:78:LEU:HD12	2.43	0.53
2:M:187:LEU:CD2	2:M:187:LEU:H	2.22	0.53
4:O:114:TYR:O	4:O:118:ASN:ND2	2.41	0.53
9:U:1203:LYS:HG2	9:U:1205:ASN:H	1.73	0.53
1:A:61:PRO:HB2	1:A:79:ILE:CD1	2.28	0.53
3:F:71:PHE:O	3:F:75:THR:OG1	2.25	0.53
6:G:94:ILE:HA	6:G:97:ARG:HD3	1.90	0.53
4:D:114:TYR:O	4:D:118:ASN:ND2	2.41	0.53
5:E:20:ASN:HB2	5:E:23:ASN:HD21	1.73	0.53
9:J:735:VAL:O	9:J:736:GLN:NE2	2.41	0.53
2:M:177:LYS:HB3	2:M:185:TYR:CE1	2.43	0.53
3:Q:49:PHE:O	3:Q:53:ASN:ND2	2.41	0.53
6:R:94:ILE:HA	6:R:97:ARG:HD3	1.90	0.53
9:U:735:VAL:O	9:U:736:GLN:NE2	2.41	0.53
7:H:37:ASN:OD1	7:H:38:PRO:HD3	2.08	0.53
2:M:177:LYS:C	2:M:185:TYR:CE1	2.86	0.53
5:P:190:VAL:HG21	5:P:202:ILE:HG23	1.90	0.53
3:C:48:ASP:OD1	3:C:48:ASP:N	2.38	0.53
6:R:250:VAL:HG13	6:R:268:ILE:HG22	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:638:PRO:HA	9:U:641:THR:HG22	1.90	0.53
1:A:54:TRP:CZ2	1:A:78:LEU:HD12	2.43	0.53
3:C:186:ASP:OD1	4:D:133:ARG:NH1	2.42	0.53
3:N:186:ASP:OD1	4:O:133:ARG:NH1	2.42	0.53
4:O:103:LEU:HD23	4:O:106:ILE:HD11	1.90	0.53
9:U:479:ILE:C	9:U:481:ASN:N	2.56	0.53
3:F:49:PHE:O	3:F:53:ASN:ND2	2.41	0.52
9:J:474:ARG:HH12	9:J:491:TYR:HA	1.75	0.52
9:J:1203:LYS:HG2	9:J:1205:ASN:H	1.73	0.52
1:L:10:LEU:HA	1:L:86:ILE:HG22	1.92	0.52
2:B:187:LEU:CD2	2:B:187:LEU:N	2.73	0.52
3:C:161:VAL:HG12	3:C:178:VAL:HG13	1.91	0.52
6:G:168:LYS:HD2	6:G:170:ARG:NH1	2.14	0.52
9:U:481:ASN:HB3	9:U:484:MET:CG	2.34	0.52
1:A:10:LEU:HA	1:A:86:ILE:HG22	1.92	0.52
2:B:185:TYR:HB3	2:B:261:HIS:HA	1.92	0.52
6:G:89:ASP:N	6:G:89:ASP:OD1	2.42	0.52
9:J:1006:ASN:ND2	10:K:498:GLU:OE2	2.43	0.52
3:N:161:VAL:HG12	3:N:178:VAL:HG13	1.91	0.52
3:C:86:THR:HA	3:C:89:VAL:HG12	1.92	0.52
6:R:89:ASP:OD1	6:R:89:ASP:N	2.42	0.52
7:H:2:PRO:CB	7:H:29:PHE:CE1	2.92	0.52
1:L:61:PRO:CD	1:L:79:ILE:CD1	2.85	0.52
2:M:187:LEU:HD23	2:M:187:LEU:C	2.31	0.52
7:S:2:PRO:CB	7:S:29:PHE:CE1	2.92	0.52
3:N:8:ARG:HE	3:N:10:LEU:H	1.57	0.51
5:P:20:ASN:HB2	5:P:23:ASN:HD21	1.74	0.51
9:U:737:ASN:C	9:U:737:ASN:OD1	2.51	0.51
5:E:137:GLY:O	5:E:139:LYS:NZ	2.44	0.51
3:F:53:ASN:HD21	3:F:138:LEU:HA	1.76	0.51
1:L:61:PRO:CB	1:L:79:ILE:CD1	2.87	0.51
2:M:187:LEU:CD2	2:M:187:LEU:N	2.73	0.51
1:L:42:ILE:O	1:L:46:TYR:CB	2.59	0.51
3:N:132:MET:HA	3:N:135:MET:HB2	1.92	0.51
1:A:42:ILE:O	1:A:46:TYR:CB	2.59	0.51
1:A:61:PRO:CD	1:A:79:ILE:CD1	2.85	0.51
2:B:181:ARG:CA	2:B:184:PHE:HE1	2.23	0.51
7:H:31:GLN:NE2	7:H:31:GLN:CA	2.73	0.51
5:P:113:ASN:ND2	5:P:115:ASN:OD1	2.43	0.51
3:Q:49:PHE:HB3	3:Q:138:LEU:HB2	1.92	0.51
9:U:1006:ASN:ND2	10:V:498:GLU:OE2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:ARG:HG2	4:D:85:GLY:HA3	1.93	0.51
2:M:181:ARG:CA	2:M:184:PHE:HE1	2.23	0.51
7:S:31:GLN:NE2	7:S:31:GLN:CA	2.73	0.51
9:J:1000:MET:HE1	9:J:1040:LEU:HD12	1.92	0.51
9:J:1034:SER:OG	9:J:1035:ARG:N	2.44	0.51
2:M:186:LEU:O	2:M:260:PHE:HB2	2.11	0.51
3:C:8:ARG:HE	3:C:10:LEU:H	1.57	0.51
5:E:113:ASN:ND2	5:E:115:ASN:OD1	2.43	0.51
9:U:1000:MET:HE1	9:U:1040:LEU:HD12	1.92	0.51
5:P:137:GLY:O	5:P:139:LYS:NZ	2.44	0.51
1:A:100:ASP:O	1:A:104:ALA:HB2	2.11	0.51
5:E:115:ASN:HA	5:E:133:GLN:HE21	1.75	0.51
6:R:167:THR:O	7:S:131:ARG:NH2	2.42	0.51
9:U:474:ARG:HH12	9:U:491:TYR:HA	1.75	0.51
9:U:633:LYS:HA	9:U:636:ILE:HG12	1.93	0.51
2:B:144:PRO:HD2	2:B:147:LYS:HB3	1.93	0.50
3:C:53:ASN:ND2	3:C:139:TRP:O	2.42	0.50
9:J:1272:ASN:ND2	9:J:1273:GLN:O	2.44	0.50
2:M:139:ILE:HG22	2:M:147:LYS:HB2	1.92	0.50
9:U:1272:ASN:ND2	9:U:1273:GLN:O	2.44	0.50
2:M:178:THR:OG1	2:M:184:PHE:CD1	2.52	0.50
3:N:147:VAL:O	3:N:151:SER:HB3	2.10	0.50
9:U:735:VAL:HG13	9:U:827:GLU:HG3	1.94	0.50
2:B:135:SER:HB2	2:B:149:LYS:HE2	1.92	0.50
2:B:139:ILE:HG22	2:B:147:LYS:HB2	1.92	0.50
10:K:401:SER:O	10:K:553:ASN:ND2	2.44	0.50
2:M:181:ARG:CA	2:M:184:PHE:CE1	2.92	0.50
3:N:86:THR:HA	3:N:89:VAL:HG12	1.92	0.50
3:Q:53:ASN:HD21	3:Q:138:LEU:HA	1.76	0.50
7:S:37:ASN:OD1	7:S:38:PRO:HD3	2.08	0.50
10:V:401:SER:O	10:V:553:ASN:ND2	2.44	0.50
2:B:177:LYS:HB3	2:B:185:TYR:CE1	2.43	0.50
2:B:186:LEU:O	2:B:260:PHE:HB2	2.11	0.50
9:J:818:ASP:HB3	9:J:820:ARG:HG3	1.94	0.50
9:J:1268:SER:HA	9:J:1276:ILE:HA	1.94	0.50
2:M:55:LEU:HD11	3:N:41:LEU:HD21	1.94	0.50
2:M:124:ARG:NH1	2:M:216:GLU:OE2	2.45	0.50
3:N:53:ASN:ND2	3:N:139:TRP:O	2.42	0.50
8:T:994:GLU:CB	8:T:1030:ASP:HA	2.42	0.50
2:B:184:PHE:N	2:B:184:PHE:CD1	2.76	0.50
5:E:2:ALA:N	5:E:219:GLN:OE1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:37:ASN:O	7:S:41:LEU:CG	2.49	0.50
9:U:481:ASN:CB	9:U:484:MET:CE	2.81	0.50
9:U:1268:SER:HA	9:U:1276:ILE:HA	1.94	0.50
2:B:184:PHE:O	2:B:262:VAL:HG12	2.11	0.50
3:C:132:MET:HA	3:C:135:MET:HB2	1.92	0.50
3:C:147:VAL:O	3:C:151:SER:HB3	2.11	0.50
3:F:82:ASN:OD1	3:F:85:LYS:N	2.41	0.50
9:J:735:VAL:HG13	9:J:827:GLU:HG3	1.94	0.50
2:M:184:PHE:O	2:M:262:VAL:HG12	2.11	0.50
5:P:115:ASN:HA	5:P:133:GLN:HE21	1.75	0.50
9:U:1014:GLU:OE2	9:U:1027:ARG:NH1	2.45	0.50
1:L:100:ASP:O	1:L:104:ALA:HB2	2.11	0.50
4:O:113:LYS:HA	4:O:117:ASN:HD22	1.77	0.50
2:B:124:ARG:NH1	2:B:216:GLU:OE2	2.45	0.50
2:B:181:ARG:CA	2:B:184:PHE:CE1	2.92	0.50
3:F:49:PHE:HB3	3:F:138:LEU:HB2	1.92	0.50
6:G:97:ARG:NH2	7:H:145:LEU:O	2.45	0.50
9:J:565:LEU:HB2	9:J:567:ILE:HG12	1.94	0.50
9:J:633:LYS:HA	9:J:636:ILE:HG12	1.93	0.50
9:U:818:ASP:HB3	9:U:820:ARG:HG3	1.94	0.50
2:B:154:LEU:O	2:B:184:PHE:CE2	2.65	0.50
8:I:994:GLU:CB	8:I:1030:ASP:HA	2.41	0.50
2:M:137:LEU:HD13	2:M:140:PHE:HD2	1.76	0.50
2:M:154:LEU:O	2:M:184:PHE:CE2	2.65	0.50
3:N:48:ASP:OD1	3:N:48:ASP:N	2.38	0.50
6:R:97:ARG:NH2	7:S:145:LEU:O	2.45	0.50
5:E:8:VAL:HG23	5:E:16:ILE:HB	1.94	0.49
9:J:1014:GLU:OE2	9:J:1027:ARG:NH1	2.45	0.49
2:M:185:TYR:HB3	2:M:261:HIS:HA	1.92	0.49
3:N:17:ILE:HA	3:N:20:ASN:HB2	1.94	0.49
9:U:735:VAL:O	9:U:736:GLN:HG2	2.13	0.49
4:D:113:LYS:HA	4:D:117:ASN:HD22	1.77	0.49
9:J:1222:LYS:NZ	9:J:1223:ILE:O	2.42	0.49
9:J:968:TYR:HA	9:J:984:SER:HA	1.95	0.49
4:O:11:ARG:HG2	4:O:85:GLY:HA3	1.93	0.49
5:P:8:VAL:HG23	5:P:16:ILE:HB	1.94	0.49
3:Q:144:LEU:HA	3:Q:147:VAL:HG12	1.95	0.49
9:J:735:VAL:O	9:J:736:GLN:HG2	2.13	0.49
5:P:2:ALA:N	5:P:219:GLN:OE1	2.45	0.49
7:S:2:PRO:CB	7:S:29:PHE:HE1	2.26	0.49
3:F:96:LYS:HG2	3:F:100:ASN:HD22	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:69:SER:OG	5:P:123:CYS:SG	2.66	0.49
2:M:135:SER:HB2	2:M:149:LYS:HE2	1.92	0.49
2:M:144:PRO:HD2	2:M:147:LYS:HB3	1.93	0.49
9:U:565:LEU:HB2	9:U:567:ILE:HG12	1.94	0.49
2:B:55:LEU:HD11	3:C:41:LEU:HD21	1.94	0.49
2:B:137:LEU:HD13	2:B:140:PHE:HD2	1.76	0.49
9:J:735:VAL:O	9:J:735:VAL:CG2	2.60	0.49
4:O:99:TYR:HB3	4:O:102:VAL:HB	1.95	0.49
6:R:172:ARG:NH2	7:S:86:ASN:O	2.46	0.49
7:S:36:LEU:C	7:S:36:LEU:CD1	2.85	0.49
4:D:71:SER:HB2	5:E:121:GLN:HG2	1.93	0.49
4:O:71:SER:HB2	5:P:121:GLN:HG2	1.93	0.49
3:F:144:LEU:HA	3:F:147:VAL:HG12	1.94	0.49
1:L:37:ASN:O	1:L:41:ASN:ND2	2.45	0.49
7:H:31:GLN:NE2	7:H:31:GLN:N	2.61	0.48
7:H:157:ARG:NH1	7:H:162:ASP:OD2	2.46	0.48
7:S:31:GLN:NE2	7:S:31:GLN:N	2.61	0.48
7:S:157:ARG:NH1	7:S:162:ASP:OD2	2.46	0.48
3:C:17:ILE:HA	3:C:20:ASN:HB2	1.94	0.48
4:D:99:TYR:HB3	4:D:102:VAL:HB	1.95	0.48
9:U:762:ARG:HE	9:U:791:THR:HG21	1.79	0.48
9:U:968:TYR:HA	9:U:984:SER:HA	1.95	0.48
3:F:53:ASN:ND2	3:F:137:SER:O	2.47	0.48
9:J:762:ARG:HE	9:J:791:THR:HG21	1.79	0.48
9:J:1021:TYR:HD2	9:J:1079:PRO:HG2	1.79	0.48
6:G:275:LEU:O	6:G:279:GLY:N	2.45	0.48
7:H:36:LEU:C	7:H:36:LEU:CD1	2.85	0.48
10:V:542:ASP:HB3	10:V:547:GLU:HB3	1.96	0.48
1:A:63:LEU:HA	1:A:77:MET:SD	2.53	0.48
3:N:138:LEU:O	3:N:169:ARG:NH1	2.40	0.48
2:B:223:ARG:HE	2:B:235:GLU:HB3	1.79	0.48
6:G:172:ARG:NH2	7:H:86:ASN:O	2.46	0.48
7:H:2:PRO:CB	7:H:29:PHE:HE1	2.26	0.48
10:K:542:ASP:HB3	10:K:547:GLU:HB3	1.96	0.48
9:U:1034:SER:OG	9:U:1035:ARG:N	2.44	0.48
9:J:1094:PRO:HD3	9:J:1122:TRP:HE1	1.78	0.48
9:U:1094:PRO:HD3	9:U:1122:TRP:HE1	1.78	0.48
4:D:17:PHE:CZ	4:D:20:GLU:HA	2.48	0.48
9:J:481:ASN:HD22	9:J:484:MET:HE2	1.70	0.47
2:M:127:GLY:HA2	2:M:130:ILE:HD12	1.96	0.47
8:T:989:GLN:N	8:T:1082:ASN:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:182:ARG:NH1	3:F:183:ILE:O	2.47	0.47
7:H:38:PRO:HB3	9:J:584:TRP:CH2	2.49	0.47
3:Q:53:ASN:ND2	3:Q:137:SER:O	2.46	0.47
1:A:37:ASN:O	1:A:41:ASN:ND2	2.45	0.47
2:B:186:LEU:HD12	2:B:186:LEU:HA	1.78	0.47
4:D:67:ILE:HA	5:E:124:THR:HG22	1.96	0.47
4:D:69:SER:OG	5:E:123:CYS:SG	2.66	0.47
9:J:393:MET:O	9:J:397:ALA:CB	2.62	0.47
9:J:479:ILE:HD11	9:J:485:PHE:HB2	1.97	0.47
10:K:500:ILE:HG22	10:K:526:GLY:HA2	1.96	0.47
3:Q:182:ARG:NH1	3:Q:183:ILE:O	2.47	0.47
9:U:481:ASN:HB2	9:U:484:MET:CE	2.44	0.47
1:L:61:PRO:HB2	1:L:79:ILE:CD1	2.28	0.47
6:R:201:LYS:NZ	6:R:206:ASP:OD1	2.46	0.47
10:V:500:ILE:HG22	10:V:526:GLY:HA2	1.96	0.47
2:B:127:GLY:HA2	2:B:130:ILE:HD12	1.96	0.47
2:B:226:LEU:O	2:B:230:GLY:N	2.47	0.47
6:R:275:LEU:O	6:R:279:GLY:N	2.46	0.47
3:F:82:ASN:O	3:F:86:THR:OG1	2.33	0.47
6:G:201:LYS:NZ	6:G:206:ASP:OD1	2.46	0.47
9:J:482:SER:HB3	9:J:483:PRO:HD3	1.76	0.47
1:L:63:LEU:HA	1:L:77:MET:SD	2.53	0.47
4:O:17:PHE:CZ	4:O:20:GLU:HA	2.48	0.47
4:O:67:ILE:HA	5:P:124:THR:HG22	1.96	0.47
8:I:676:LEU:HA	8:I:689:VAL:HA	1.97	0.47
2:M:223:ARG:HE	2:M:235:GLU:HB3	1.79	0.47
2:M:226:LEU:O	2:M:230:GLY:N	2.47	0.47
3:Q:96:LYS:HG2	3:Q:100:ASN:HD22	1.78	0.47
9:U:393:MET:O	9:U:397:ALA:CB	2.62	0.47
9:U:483:PRO:O	9:U:486:PRO:HG3	2.15	0.47
9:J:479:ILE:CG1	9:J:484:MET:O	2.63	0.47
3:Q:71:PHE:O	3:Q:75:THR:OG1	2.25	0.47
7:S:157:ARG:HA	7:S:157:ARG:HD2	1.74	0.47
9:U:1021:TYR:HD2	9:U:1079:PRO:HG2	1.78	0.47
9:J:747:ASP:OD1	9:J:747:ASP:N	2.44	0.47
7:S:32:ASP:HA	7:S:35:GLU:OE2	2.15	0.47
10:V:218:ARG:HA	10:V:232:LEU:HA	1.97	0.47
2:B:60:GLU:OE1	2:B:61:ARG:NH2	2.48	0.46
7:H:38:PRO:HB3	9:J:584:TRP:CE2	2.50	0.46
8:I:598:ASP:HA	8:I:603:LYS:HA	1.97	0.46
6:R:171:ARG:NH2	7:S:84:THR:O	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:967:GLU:N	9:U:985:ILE:O	2.45	0.46
2:M:110:LYS:O	2:M:209:LYS:NZ	2.44	0.46
6:R:171:ARG:HD3	7:S:86:ASN:HB2	1.96	0.46
6:R:180:LEU:HD12	6:R:199:LEU:HD12	1.98	0.46
7:S:38:PRO:HB3	9:U:584:TRP:CH2	2.50	0.46
7:H:32:ASP:HA	7:H:35:GLU:OE2	2.15	0.46
9:J:1197:THR:OG1	9:J:1198:SER:N	2.48	0.46
1:L:80:LYS:HB3	1:L:80:LYS:HE3	1.43	0.46
6:G:172:ARG:HH12	7:H:104:ILE:HG22	1.81	0.46
8:I:860:ASN:ND2	8:I:966:ARG:O	2.49	0.46
9:J:1056:VAL:O	9:J:1063:SER:OG	2.32	0.46
1:L:79:ILE:CG2	1:L:81:GLN:CB	2.88	0.46
2:M:60:GLU:OE1	2:M:61:ARG:NH2	2.48	0.46
2:B:110:LYS:O	2:B:209:LYS:NZ	2.44	0.46
3:C:138:LEU:O	3:C:169:ARG:NH1	2.40	0.46
9:J:1092:ASN:O	9:J:1122:TRP:NE1	2.49	0.46
4:O:20:GLU:HB2	4:O:24:ALA:HB3	1.97	0.46
5:P:32:GLU:HA	5:P:35:ILE:HD12	1.98	0.46
8:T:598:ASP:HA	8:T:603:LYS:HA	1.98	0.46
8:T:860:ASN:ND2	8:T:966:ARG:O	2.49	0.46
1:A:79:ILE:CG2	1:A:81:GLN:CB	2.88	0.46
6:G:197:ASP:OD2	6:G:214:ASN:ND2	2.49	0.46
8:I:590:ASP:H	8:I:613:ARG:HA	1.81	0.46
9:J:1119:GLN:OE1	9:J:1168:ARG:NH1	2.49	0.46
1:L:61:PRO:CG	1:L:79:ILE:HD13	2.42	0.46
1:A:61:PRO:CB	1:A:79:ILE:CD1	2.86	0.46
6:R:172:ARG:HH12	7:S:104:ILE:HG22	1.81	0.46
7:S:32:ASP:OD1	7:S:36:LEU:CD2	2.39	0.46
9:U:1056:VAL:O	9:U:1063:SER:OG	2.32	0.46
6:G:167:THR:O	7:H:131:ARG:NH2	2.42	0.46
6:G:180:LEU:HD12	6:G:199:LEU:HD12	1.98	0.46
2:M:185:TYR:HB2	2:M:260:PHE:O	2.16	0.46
3:Q:90:LEU:O	3:Q:94:ALA:CB	2.64	0.46
9:U:1197:THR:OG1	9:U:1198:SER:N	2.49	0.46
2:B:174:ASP:O	2:B:187:LEU:O	2.34	0.46
3:F:85:LYS:HA	3:F:88:GLU:HG2	1.98	0.46
9:J:903:PRO:HA	9:J:906:TRP:HB3	1.98	0.46
3:Q:82:ASN:O	3:Q:86:THR:OG1	2.33	0.46
8:T:940:LEU:O	8:T:944:LEU:N	2.47	0.46
8:I:793:ARG:NH2	8:I:831:GLY:O	2.49	0.46
9:J:1095:ILE:O	9:J:1097:ARG:NH1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:218:ARG:HA	10:K:232:LEU:HA	1.97	0.46
3:N:8:ARG:HG3	3:N:11:LYS:H	1.81	0.46
6:R:197:ASP:OD2	6:R:214:ASN:ND2	2.49	0.46
9:U:628:GLN:O	9:U:632:PHE:CB	2.63	0.46
6:R:184:HIS:NE2	6:R:196:SER:O	2.49	0.45
1:A:42:ILE:O	1:A:46:TYR:HB3	2.16	0.45
2:B:178:THR:OG1	2:B:184:PHE:CE1	2.65	0.45
6:G:171:ARG:HD3	7:H:86:ASN:HB2	1.96	0.45
1:A:24:ASN:ND2	1:A:28:ASN:OD1	2.50	0.45
7:H:31:GLN:N	7:H:31:GLN:HE21	2.14	0.45
7:S:31:GLN:N	7:S:31:GLN:HE21	2.14	0.45
7:S:38:PRO:HB3	9:U:584:TRP:CE2	2.49	0.45
7:S:165:VAL:O	7:S:169:ALA:N	2.48	0.45
9:U:1092:ASN:O	9:U:1122:TRP:NE1	2.49	0.45
9:U:1222:LYS:NZ	9:U:1223:ILE:O	2.42	0.45
3:C:8:ARG:HG3	3:C:11:LYS:H	1.81	0.45
4:D:7:TRP:HA	4:D:17:PHE:HB2	1.99	0.45
9:J:967:GLU:N	9:J:985:ILE:O	2.45	0.45
7:S:29:PHE:CD2	7:S:36:LEU:CD2	3.00	0.45
8:I:989:GLN:N	8:I:1082:ASN:O	2.47	0.45
9:J:625:GLN:NE2	9:J:747:ASP:O	2.48	0.45
3:N:144:LEU:HA	3:N:147:VAL:HG22	1.99	0.45
8:T:676:LEU:HA	8:T:689:VAL:HA	1.97	0.45
3:C:144:LEU:HA	3:C:147:VAL:HG22	1.99	0.45
5:E:32:GLU:HA	5:E:35:ILE:HD12	1.98	0.45
3:F:119:LEU:O	3:F:174:THR:OG1	2.35	0.45
9:U:757:PHE:HA	9:U:766:SER:HB3	1.98	0.45
9:U:1119:GLN:OE1	9:U:1168:ARG:NH1	2.49	0.45
6:G:167:THR:OG1	6:G:168:LYS:N	2.50	0.45
9:J:628:GLN:O	9:J:632:PHE:CB	2.63	0.45
9:J:663:LEU:HA	9:J:734:ARG:HH21	1.82	0.45
9:J:738:PRO:HG2	9:J:784:PRO:HG2	1.98	0.45
8:T:590:ASP:H	8:T:613:ARG:HA	1.81	0.45
2:B:185:TYR:HB2	2:B:260:PHE:O	2.16	0.45
3:F:90:LEU:O	3:F:94:ALA:CB	2.64	0.45
9:J:536:LEU:HA	9:J:539:VAL:HG12	1.99	0.45
9:U:536:LEU:HA	9:U:539:VAL:HG12	1.99	0.45
4:D:20:GLU:HB2	4:D:24:ALA:HB3	1.97	0.45
7:H:165:VAL:O	7:H:169:ALA:N	2.48	0.45
9:J:479:ILE:CG2	9:J:480:PRO:CD	2.83	0.45
4:O:64:LYS:O	5:P:126:GLN:NE2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:793:ARG:NH2	8:T:831:GLY:O	2.49	0.45
2:M:174:ASP:O	2:M:187:LEU:O	2.34	0.45
5:P:53:LYS:HG2	5:P:55:LEU:HB3	1.99	0.45
9:U:663:LEU:HA	9:U:734:ARG:HH21	1.82	0.45
4:D:142:ASN:HB2	4:D:145:PHE:HB3	1.99	0.44
7:H:29:PHE:CD2	7:H:36:LEU:CD2	3.00	0.44
6:G:184:HIS:NE2	6:G:196:SER:O	2.49	0.44
7:H:4:TYR:N	7:H:114:ILE:O	2.49	0.44
1:L:67:PHE:HD2	1:L:74:VAL:HG23	1.83	0.44
5:P:8:VAL:HG22	5:P:17:TYR:HB3	1.99	0.44
9:U:738:PRO:HG2	9:U:784:PRO:HG2	1.98	0.44
9:U:774:LYS:HD3	9:U:775:ALA:H	1.82	0.44
5:E:8:VAL:HG22	5:E:17:TYR:HB3	1.99	0.44
9:U:1115:ILE:HA	9:U:1118:ARG:HB3	1.98	0.44
2:B:191:TYR:HD2	2:B:194:ILE:HG12	1.83	0.44
5:E:53:LYS:HG2	5:E:55:LEU:HB3	1.99	0.44
9:U:903:PRO:HA	9:U:906:TRP:HB3	1.98	0.44
1:A:61:PRO:HG2	1:A:79:ILE:O	2.18	0.44
4:D:64:LYS:O	5:E:126:GLN:NE2	2.50	0.44
9:J:757:PHE:HA	9:J:766:SER:HB3	1.98	0.44
9:J:758:CYS:HA	9:J:801:LEU:HB2	1.99	0.44
6:G:246:PHE:HA	6:G:274:VAL:HG11	2.00	0.44
7:H:31:GLN:NE2	7:H:31:GLN:HA	2.29	0.44
3:N:34:TYR:OH	3:N:140:TYR:O	2.34	0.44
3:Q:85:LYS:HA	3:Q:88:GLU:HG2	1.98	0.44
6:R:254:ARG:HD3	6:R:262:GLN:HA	2.00	0.44
1:A:10:LEU:O	1:A:18:ILE:N	2.47	0.44
9:J:774:LYS:HD3	9:J:775:ALA:H	1.82	0.44
10:K:499:GLY:O	10:K:527:ILE:N	2.51	0.44
1:L:42:ILE:O	1:L:46:TYR:HB3	2.16	0.44
6:R:167:THR:OG1	6:R:168:LYS:N	2.50	0.44
9:U:1177:LEU:HD13	9:U:1284:VAL:HG11	2.00	0.44
1:A:80:LYS:HE3	1:A:80:LYS:HB3	1.43	0.44
8:I:940:LEU:O	8:I:944:LEU:N	2.47	0.44
4:O:7:TRP:HA	4:O:17:PHE:HB2	1.99	0.44
10:V:499:GLY:O	10:V:527:ILE:N	2.51	0.44
1:A:67:PHE:HD2	1:A:74:VAL:HG23	1.83	0.44
3:C:11:LYS:HD2	3:C:92:LYS:HE3	2.00	0.44
7:H:93:ASP:HB2	7:H:100:ILE:HD11	2.00	0.44
9:J:1115:ILE:HA	9:J:1118:ARG:HB3	1.98	0.44
9:J:1177:LEU:HD13	9:J:1284:VAL:HG11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:267:LYS:H	10:K:273:SER:HA	1.83	0.44
1:L:17:PRO:HB3	1:L:20:ILE:HD11	2.00	0.44
1:L:30:MET:SD	1:L:30:MET:N	2.85	0.44
3:N:11:LYS:HD2	3:N:92:LYS:HE3	2.00	0.44
5:P:130:PHE:N	5:P:142:ALA:O	2.50	0.44
6:R:246:PHE:HA	6:R:274:VAL:HG11	2.00	0.44
7:S:171:LYS:HE3	7:S:171:LYS:HB3	1.90	0.44
1:L:24:ASN:ND2	1:L:28:ASN:OD1	2.50	0.43
3:Q:26:ASN:OD1	3:Q:26:ASN:N	2.50	0.43
3:Q:119:LEU:O	3:Q:174:THR:OG1	2.35	0.43
8:T:795:GLU:HA	8:T:796:PRO:HD3	1.86	0.43
9:U:458:SER:O	9:U:461:SER:OG	2.35	0.43
8:I:399:GLU:O	8:I:403:GLN:N	2.51	0.43
8:I:583:SER:HA	8:I:617:TYR:HA	2.01	0.43
9:J:758:CYS:SG	9:J:759:GLU:N	2.91	0.43
8:T:803:GLU:O	8:T:856:LYS:N	2.52	0.43
6:G:171:ARG:NH2	7:H:84:THR:O	2.46	0.43
7:H:5:PHE:HB3	7:H:18:ILE:HG22	1.99	0.43
1:L:61:PRO:HG2	1:L:79:ILE:O	2.18	0.43
2:M:191:TYR:HD2	2:M:194:ILE:HG12	1.83	0.43
4:O:110:ILE:HD11	4:O:148:VAL:HG13	2.00	0.43
4:O:142:ASN:HB2	4:O:145:PHE:HB3	1.99	0.43
7:S:5:PHE:HB3	7:S:18:ILE:HG22	1.99	0.43
9:U:758:CYS:SG	9:U:759:GLU:N	2.91	0.43
9:U:758:CYS:HA	9:U:801:LEU:HB2	1.99	0.43
10:V:267:LYS:H	10:V:273:SER:HA	1.83	0.43
1:A:129:ASP:OD1	1:A:129:ASP:N	2.50	0.43
4:D:17:PHE:CE2	4:D:20:GLU:HA	2.53	0.43
9:J:481:ASN:ND2	9:J:484:MET:CE	2.74	0.43
9:U:469:VAL:O	9:U:473:HIS:ND1	2.52	0.43
5:E:115:ASN:HB2	5:E:120:ARG:CZ	2.48	0.43
2:M:143:ASN:HA	2:M:147:LYS:HD3	2.00	0.43
5:P:115:ASN:HB2	5:P:120:ARG:CZ	2.48	0.43
8:T:399:GLU:O	8:T:403:GLN:N	2.51	0.43
9:U:465:LEU:HA	9:U:468:ILE:HG22	2.01	0.43
9:U:1086:LYS:HA	9:U:1086:LYS:HD3	1.74	0.43
5:E:130:PHE:N	5:E:142:ALA:O	2.50	0.43
2:M:162:ARG:O	2:M:166:LYS:NZ	2.42	0.43
8:T:583:SER:HA	8:T:617:TYR:HA	2.01	0.43
9:U:735:VAL:O	9:U:735:VAL:CG2	2.60	0.43
9:U:1184:VAL:HG13	9:U:1257:GLU:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:129:ASP:OD1	1:L:129:ASP:N	2.50	0.43
8:T:853:PHE:O	8:T:974:THR:N	2.51	0.43
9:U:544:THR:HG22	9:U:546:ASN:H	1.83	0.43
10:V:306:LYS:HA	10:V:332:ARG:HA	2.01	0.43
1:A:17:PRO:HB3	1:A:20:ILE:HD11	2.00	0.43
8:I:675:GLU:O	8:I:690:GLU:N	2.52	0.43
7:S:31:GLN:NE2	7:S:31:GLN:HA	2.29	0.43
4:D:10:ASP:HA	4:D:86:LEU:HD13	2.01	0.43
4:O:17:PHE:CE2	4:O:20:GLU:HA	2.54	0.43
8:T:675:GLU:O	8:T:690:GLU:N	2.52	0.43
1:L:42:ILE:O	1:L:46:TYR:HB2	2.19	0.43
2:M:128:PHE:O	2:M:132:LEU:N	2.47	0.43
5:P:9:ILE:HB	5:P:139:LYS:HB2	2.01	0.43
7:S:93:ASP:HB2	7:S:100:ILE:HD11	2.00	0.43
9:U:629:ASP:HA	9:U:632:PHE:HB3	2.01	0.43
4:D:48:ILE:O	4:D:52:ARG:N	2.52	0.42
3:F:166:ASP:OD1	3:F:169:ARG:N	2.45	0.42
9:J:544:THR:HG22	9:J:546:ASN:H	1.83	0.42
4:O:10:ASP:HA	4:O:86:LEU:HD13	2.01	0.42
1:A:41:ASN:HA	1:A:44:LEU:HB2	2.01	0.42
3:C:109:SER:OG	3:C:111:ASN:OD1	2.29	0.42
5:E:112:THR:OG1	5:E:113:ASN:N	2.50	0.42
9:J:737:ASN:OD1	9:J:738:PRO:N	2.52	0.42
9:J:1069:GLU:OE1	9:U:1069:GLU:CD	2.58	0.42
3:N:177:LYS:HE2	3:N:177:LYS:HB3	1.89	0.42
8:T:770:SER:N	8:T:789:ASN:O	2.52	0.42
9:U:767:TYR:HB2	9:U:787:ILE:HD11	2.02	0.42
8:I:770:SER:N	8:I:789:ASN:O	2.52	0.42
9:J:594:LEU:HD23	9:J:594:LEU:HA	1.91	0.42
9:J:910:PRO:HA	9:J:911:PRO:HD3	1.79	0.42
3:Q:90:LEU:O	3:Q:94:ALA:HB2	2.19	0.42
8:T:889:TRP:O	8:T:893:TRP:N	2.48	0.42
9:U:908:LYS:HD2	9:U:908:LYS:HA	1.83	0.42
4:D:110:ILE:HD11	4:D:148:VAL:HG13	2.00	0.42
3:F:90:LEU:O	3:F:94:ALA:HB2	2.19	0.42
6:G:254:ARG:HD3	6:G:262:GLN:HA	2.00	0.42
8:I:748:LYS:N	8:I:755:PHE:O	2.49	0.42
8:I:979:LEU:O	8:I:1075:PHE:N	2.52	0.42
9:J:735:VAL:HA	9:J:788:LYS:HD2	2.01	0.42
9:U:737:ASN:OD1	9:U:738:PRO:N	2.52	0.42
8:I:853:PHE:O	8:I:974:THR:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:482:SER:HB3	9:U:483:PRO:HD2	1.67	0.42
9:U:625:GLN:NE2	9:U:747:ASP:O	2.48	0.42
2:B:143:ASN:HA	2:B:147:LYS:HD3	2.00	0.42
3:F:101:ILE:HD12	3:F:101:ILE:HA	1.89	0.42
1:L:43:SER:HA	1:L:46:TYR:HB3	2.01	0.42
3:N:188:ILE:HG23	4:O:133:ARG:HG2	2.02	0.42
9:U:800:CYS:HB3	9:U:812:LYS:HB3	2.02	0.42
1:A:117:ILE:HD12	1:A:117:ILE:HA	1.94	0.42
2:B:137:LEU:HD12	3:C:28:GLU:HG3	2.02	0.42
2:B:178:THR:OG1	2:B:184:PHE:CD1	2.52	0.42
8:I:803:GLU:O	8:I:856:LYS:N	2.51	0.42
6:R:86:LYS:HA	6:R:86:LYS:HD3	1.87	0.42
9:U:735:VAL:HA	9:U:788:LYS:HD2	2.00	0.42
8:I:989:GLN:HA	8:I:1034:TYR:HA	2.02	0.42
9:J:1086:LYS:HA	9:J:1086:LYS:HD3	1.74	0.42
9:U:1025:LYS:HD2	9:U:1025:LYS:HA	1.91	0.42
9:U:1038:ILE:HD11	9:U:1164:ILE:HD12	2.02	0.42
3:F:20:ASN:HB3	3:F:21:LYS:H	1.67	0.42
9:J:469:VAL:O	9:J:473:HIS:ND1	2.52	0.42
9:J:1018:TRP:HB2	9:J:1079:PRO:HG3	2.01	0.42
9:J:1184:VAL:HG13	9:J:1257:GLU:H	1.84	0.42
2:M:49:LEU:HD23	2:M:52:MET:HE1	2.02	0.42
5:P:112:THR:OG1	5:P:113:ASN:N	2.50	0.42
9:U:1081:LYS:HB3	9:U:1081:LYS:HE2	1.86	0.42
6:G:186:THR:O	6:G:186:THR:OG1	2.35	0.42
8:I:790:SER:O	8:I:793:ARG:NH1	2.45	0.42
1:L:41:ASN:HA	1:L:44:LEU:HB2	2.01	0.42
9:U:655:ARG:HH11	9:U:816:ILE:HG21	1.85	0.42
9:U:1095:ILE:O	9:U:1097:ARG:NH1	2.45	0.42
1:A:42:ILE:O	1:A:46:TYR:HB2	2.19	0.41
1:A:79:ILE:CG2	1:A:81:GLN:CD	2.62	0.41
2:B:187:LEU:H	2:B:187:LEU:HD22	1.85	0.41
4:D:84:SER:O	4:D:84:SER:OG	2.36	0.41
5:E:9:ILE:HB	5:E:139:LYS:HB2	2.01	0.41
7:H:4:TYR:OH	7:H:37:ASN:OD1	2.25	0.41
3:N:141:SER:HB3	3:N:144:LEU:HG	2.02	0.41
4:O:48:ILE:O	4:O:52:ARG:N	2.52	0.41
9:U:512:LYS:HA	9:U:512:LYS:HD2	1.82	0.41
9:U:637:GLN:HA	9:U:640:ILE:HG12	2.02	0.41
9:U:735:VAL:C	9:U:736:GLN:HG2	2.45	0.41
3:C:177:LYS:HE2	3:C:177:LYS:HB3	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:207:ASN:OD1	6:G:207:ASN:N	2.52	0.41
8:I:795:GLU:HA	8:I:796:PRO:HD3	1.86	0.41
9:J:465:LEU:HA	9:J:468:ILE:HG22	2.01	0.41
9:J:479:ILE:HG13	9:J:484:MET:O	2.20	0.41
9:J:637:GLN:HA	9:J:640:ILE:HG12	2.01	0.41
9:J:767:TYR:HB2	9:J:787:ILE:HD11	2.02	0.41
10:K:248:ILE:O	10:K:253:HIS:N	2.53	0.41
10:K:306:LYS:HA	10:K:332:ARG:HA	2.01	0.41
1:L:142:ASP:OD1	1:L:142:ASP:N	2.53	0.41
8:T:979:LEU:O	8:T:1075:PHE:N	2.52	0.41
9:J:629:ASP:HA	9:J:632:PHE:HB3	2.01	0.41
9:J:735:VAL:C	9:J:736:GLN:HG2	2.45	0.41
9:J:1038:ILE:HD11	9:J:1164:ILE:HD12	2.02	0.41
1:L:10:LEU:O	1:L:18:ILE:N	2.47	0.41
3:N:152:LEU:HD22	3:N:157:LEU:HD11	2.03	0.41
5:P:178:PHE:HD2	5:P:179:LEU:HD22	1.85	0.41
8:T:989:GLN:HA	8:T:1034:TYR:HA	2.02	0.41
9:U:747:ASP:OD1	9:U:747:ASP:N	2.44	0.41
1:A:17:PRO:HD2	8:I:464:TRP:HB2	2.01	0.41
2:B:49:LEU:HD23	2:B:52:MET:HE1	2.02	0.41
5:E:135:LEU:HD11	3:F:79:ARG:HE	1.86	0.41
9:J:800:CYS:HB3	9:J:812:LYS:HB3	2.02	0.41
10:V:220:ILE:HA	10:V:230:SER:HA	2.02	0.41
10:K:220:ILE:HA	10:K:230:SER:HA	2.02	0.41
1:L:10:LEU:HB2	1:L:18:ILE:HB	2.03	0.41
4:O:139:LYS:HE2	4:O:139:LYS:HB2	1.92	0.41
6:R:170:ARG:HB3	6:R:171:ARG:H	1.77	0.41
9:U:1018:TRP:HB2	9:U:1079:PRO:HG3	2.01	0.41
9:U:1225:PRO:O	9:U:1233:TYR:OH	2.30	0.41
4:D:110:ILE:HD13	4:D:110:ILE:HG21	1.93	0.41
8:I:320:SER:HA	8:I:324:LEU:H	1.86	0.41
9:J:655:ARG:HH11	9:J:816:ILE:HG21	1.85	0.41
1:A:48:GLU:HB2	1:A:54:TRP:HZ3	1.86	0.41
1:A:132:SER:O	1:A:136:SER:HB3	2.21	0.41
2:B:125:ASN:O	2:B:129:GLN:NE2	2.54	0.41
2:B:203:ALA:HB3	2:B:206:GLU:HG2	2.02	0.41
3:C:188:ILE:HG23	4:D:133:ARG:HG2	2.02	0.41
3:F:26:ASN:OD1	3:F:26:ASN:N	2.50	0.41
9:J:1091:GLU:HA	9:J:1118:ARG:HD3	2.03	0.41
1:L:97:GLY:N	1:L:101:GLU:OE1	2.53	0.41
1:L:132:SER:O	1:L:136:SER:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:125:ASN:O	2:M:129:GLN:NE2	2.54	0.41
9:U:561:ILE:HD13	9:U:561:ILE:HA	1.88	0.41
9:U:735:VAL:O	9:U:736:GLN:CG	2.69	0.41
1:A:10:LEU:HB2	1:A:18:ILE:HB	2.02	0.41
6:G:176:ILE:HG13	6:G:177:LEU:HG	2.03	0.41
9:J:758:CYS:HB3	9:J:765:VAL:HG12	2.03	0.41
9:J:1225:PRO:O	9:J:1233:TYR:OH	2.30	0.41
1:L:17:PRO:HD2	8:T:464:TRP:HB2	2.01	0.41
2:M:137:LEU:HD12	3:N:28:GLU:HG3	2.02	0.41
8:T:748:LYS:N	8:T:755:PHE:O	2.49	0.41
1:A:79:ILE:HG22	1:A:81:GLN:HB2	1.97	0.41
3:C:92:LYS:HE2	3:C:92:LYS:HB2	1.88	0.41
3:C:104:ASN:N	3:C:118:ILE:O	2.48	0.41
5:E:3:ILE:HG12	5:E:144:SER:HB2	2.03	0.41
3:F:28:GLU:H	3:F:28:GLU:HG2	1.58	0.41
8:I:998:ASP:O	8:I:999:ALA:HB3	2.21	0.41
9:J:458:SER:O	9:J:461:SER:OG	2.35	0.41
9:J:511:ILE:HD13	9:J:511:ILE:HA	1.93	0.41
9:J:655:ARG:HA	9:J:655:ARG:HD3	1.91	0.41
9:J:1026:ILE:HD12	9:J:1026:ILE:HA	1.94	0.41
9:J:1193:ILE:HD13	9:J:1193:ILE:HA	1.95	0.41
1:L:117:ILE:HD12	1:L:117:ILE:HA	1.94	0.41
3:N:109:SER:OG	3:N:111:ASN:OD1	2.29	0.41
6:R:172:ARG:HH22	7:S:104:ILE:HB	1.85	0.41
6:R:207:ASN:OD1	6:R:207:ASN:N	2.52	0.41
6:R:225:GLU:HA	6:R:254:ARG:HH22	1.86	0.41
9:U:910:PRO:HA	9:U:911:PRO:HD3	1.79	0.41
9:U:1093:THR:OG1	9:U:1118:ARG:NH2	2.47	0.41
1:A:43:SER:HA	1:A:46:TYR:HB3	2.01	0.41
5:E:23:ASN:OD1	5:E:23:ASN:N	2.54	0.41
6:G:172:ARG:HH22	7:H:104:ILE:HB	1.86	0.41
9:J:512:LYS:HD2	9:J:512:LYS:HA	1.82	0.41
9:J:620:THR:HA	9:J:623:LEU:HD23	2.03	0.41
5:P:23:ASN:OD1	5:P:23:ASN:N	2.54	0.41
9:U:1183:LYS:HE2	9:U:1183:LYS:HB3	1.83	0.41
1:A:11:ILE:HG12	1:A:44:LEU:HD11	2.03	0.40
1:A:13:GLU:HB3	1:A:83:GLY:HA3	2.03	0.40
3:C:26:ASN:OD1	3:C:26:ASN:N	2.54	0.40
6:G:236:ILE:HA	6:G:236:ILE:HD12	1.86	0.40
8:I:517:SER:O	8:I:521:TRP:N	2.54	0.40
9:J:1087:LYS:HE2	9:J:1087:LYS:HB3	1.97	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:320:SER:HA	8:T:324:LEU:H	1.86	0.40
3:C:152:LEU:HD22	3:C:157:LEU:HD11	2.03	0.40
9:J:908:LYS:HD2	9:J:908:LYS:HA	1.83	0.40
9:J:1183:LYS:HB3	9:J:1183:LYS:HE2	1.83	0.40
8:T:790:SER:O	8:T:793:ARG:NH1	2.45	0.40
2:B:128:PHE:O	2:B:132:LEU:N	2.46	0.40
6:G:192:PHE:HB3	6:G:217:THR:HG21	2.03	0.40
9:J:735:VAL:O	9:J:736:GLN:CG	2.69	0.40
1:L:96:SER:OG	1:L:101:GLU:OE1	2.33	0.40
5:P:169:ASN:HB2	5:P:170:LEU:H	1.71	0.40
8:T:802:SER:O	8:T:839:TYR:OH	2.38	0.40
5:E:178:PHE:HD2	5:E:179:LEU:HD22	1.85	0.40
6:G:225:GLU:HA	6:G:254:ARG:HH22	1.86	0.40
6:G:272:ARG:O	6:G:276:ASP:N	2.49	0.40
7:H:108:GLY:O	7:H:110:LYS:NZ	2.55	0.40
8:I:802:SER:O	8:I:839:TYR:OH	2.38	0.40
2:M:203:ALA:HB3	2:M:206:GLU:HG2	2.02	0.40
5:P:135:LEU:HD11	3:Q:79:ARG:HE	1.86	0.40
1:A:142:ASP:OD1	1:A:142:ASP:N	2.53	0.40
3:C:141:SER:HB3	3:C:144:LEU:HG	2.02	0.40
1:L:13:GLU:HB3	1:L:83:GLY:HA3	2.03	0.40
7:S:28:GLY:C	7:S:29:PHE:HD1	2.29	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	148/152 (97%)	129 (87%)	19 (13%)	0	100	100
1	L	148/152 (97%)	129 (87%)	19 (13%)	0	100	100
2	B	189/268 (70%)	165 (87%)	23 (12%)	1 (0%)	24	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	189/268 (70%)	165 (87%)	23 (12%)	1 (0%)	24	63
3	C	182/193 (94%)	169 (93%)	13 (7%)	0	100	100
3	F	180/193 (93%)	164 (91%)	16 (9%)	0	100	100
3	N	182/193 (94%)	169 (93%)	13 (7%)	0	100	100
3	Q	180/193 (93%)	164 (91%)	16 (9%)	0	100	100
4	D	147/159 (92%)	125 (85%)	22 (15%)	0	100	100
4	O	147/159 (92%)	125 (85%)	22 (15%)	0	100	100
5	E	153/219 (70%)	139 (91%)	14 (9%)	0	100	100
5	P	153/219 (70%)	139 (91%)	14 (9%)	0	100	100
6	G	199/283 (70%)	176 (88%)	23 (12%)	0	100	100
6	R	199/283 (70%)	176 (88%)	23 (12%)	0	100	100
7	H	142/175 (81%)	124 (87%)	16 (11%)	2 (1%)	9	40
7	S	142/175 (81%)	124 (87%)	16 (11%)	2 (1%)	9	40
8	I	791/1102 (72%)	649 (82%)	127 (16%)	15 (2%)	6	32
8	T	791/1102 (72%)	649 (82%)	127 (16%)	15 (2%)	6	32
9	J	861/1289 (67%)	693 (80%)	160 (19%)	8 (1%)	14	51
9	U	861/1289 (67%)	692 (80%)	161 (19%)	8 (1%)	14	51
10	K	243/560 (43%)	183 (75%)	55 (23%)	5 (2%)	5	30
10	V	243/560 (43%)	183 (75%)	55 (23%)	5 (2%)	5	30
All	All	6470/9186 (70%)	5431 (84%)	977 (15%)	62 (1%)	15	48

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	26	PRO
7	H	37	ASN
8	I	252	PRO
8	I	638	PHE
8	I	647	VAL
8	I	976	PRO
8	I	980	PRO
8	I	1067	PRO
8	I	1076	PRO
9	J	482	SER
9	J	667	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	J	1099	PHE
10	K	325	PRO
7	S	26	PRO
7	S	37	ASN
8	T	252	PRO
8	T	638	PHE
8	T	647	VAL
8	T	976	PRO
8	T	980	PRO
8	T	1067	PRO
8	T	1076	PRO
9	U	482	SER
9	U	667	PRO
9	U	1099	PHE
10	V	325	PRO
8	I	639	PRO
8	I	704	PRO
8	I	1054	ILE
10	K	269	ILE
8	T	639	PRO
8	T	704	PRO
8	T	1054	ILE
10	V	269	ILE
8	I	571	PHE
9	J	398	PRO
9	J	672	ILE
10	K	282	PRO
10	K	286	PRO
8	T	571	PHE
9	U	398	PRO
9	U	480	PRO
9	U	672	ILE
10	V	282	PRO
10	V	286	PRO
8	I	1004	ILE
9	J	397	ALA
8	T	1004	ILE
9	U	397	ALA
10	K	281	CYS
10	V	281	CYS
2	B	99	ILE
9	J	955	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	99	ILE
9	U	955	VAL
8	I	1029	ILE
9	J	483	PRO
8	T	1029	ILE
8	I	345	ASN
8	I	483	PRO
8	T	345	ASN
8	T	483	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	140/142 (99%)	137 (98%)	3 (2%)	47	65
1	L	140/142 (99%)	137 (98%)	3 (2%)	47	65
2	B	142/248 (57%)	139 (98%)	3 (2%)	47	65
2	M	142/248 (57%)	139 (98%)	3 (2%)	47	65
3	C	169/178 (95%)	169 (100%)	0	100	100
3	F	168/178 (94%)	168 (100%)	0	100	100
3	N	169/178 (95%)	169 (100%)	0	100	100
3	Q	168/178 (94%)	168 (100%)	0	100	100
4	D	135/145 (93%)	134 (99%)	1 (1%)	76	81
4	O	135/145 (93%)	134 (99%)	1 (1%)	76	81
5	E	145/199 (73%)	145 (100%)	0	100	100
5	P	146/199 (73%)	146 (100%)	0	100	100
6	G	168/249 (68%)	168 (100%)	0	100	100
6	R	168/249 (68%)	168 (100%)	0	100	100
7	H	126/152 (83%)	122 (97%)	4 (3%)	34	56
7	S	126/152 (83%)	122 (97%)	4 (3%)	34	56
8	I	76/1023 (7%)	76 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	T	76/1023 (7%)	76 (100%)	0	100	100
9	J	550/1213 (45%)	545 (99%)	5 (1%)	70	79
9	U	550/1213 (45%)	546 (99%)	4 (1%)	76	81
10	K	93/518 (18%)	93 (100%)	0	100	100
10	V	93/518 (18%)	93 (100%)	0	100	100
All	All	3825/8490 (45%)	3794 (99%)	31 (1%)	70	80

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	79	ILE
1	A	80	LYS
2	B	184	PHE
2	B	186	LEU
2	B	187	LEU
4	D	19	ARG
7	H	29	PHE
7	H	31	GLN
7	H	32	ASP
7	H	40	ILE
9	J	479	ILE
9	J	482	SER
9	J	732	THR
9	J	955	VAL
9	J	1007	GLU
1	L	78	LEU
1	L	79	ILE
1	L	80	LYS
2	M	184	PHE
2	M	186	LEU
2	M	187	LEU
4	O	19	ARG
7	S	29	PHE
7	S	31	GLN
7	S	32	ASP
7	S	40	ILE
9	U	482	SER
9	U	732	THR
9	U	955	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	U	1007	GLU

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

Mol	Chain	Res	Type
2	B	167	GLN
2	B	179	ASN
2	B	261	HIS
2	B	263	GLN
3	C	20	ASN
3	C	104	ASN
3	C	107	ASN
3	C	110	HIS
4	D	36	GLN
4	D	97	GLN
4	D	117	ASN
5	E	29	ASN
3	F	181	ASN
6	G	72	GLN
6	G	257	GLN
7	H	31	GLN
7	H	129	ASN
9	J	471	ASN
9	J	481	ASN
9	J	566	ASN
9	J	593	GLN
9	J	736	GLN
9	J	746	ASN
9	J	772	ASN
9	J	1015	ASN
9	J	1272	ASN
1	L	24	ASN
2	M	167	GLN
2	M	179	ASN
2	M	180	HIS
2	M	261	HIS
2	M	263	GLN
3	N	20	ASN
3	N	104	ASN
3	N	107	ASN
3	N	110	HIS
4	O	14	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	O	36	GLN
4	O	97	GLN
4	O	117	ASN
5	P	29	ASN
3	Q	181	ASN
6	R	72	GLN
6	R	257	GLN
7	S	31	GLN
7	S	129	ASN
9	U	471	ASN
9	U	481	ASN
9	U	566	ASN
9	U	593	GLN
9	U	621	HIS
9	U	736	GLN
9	U	772	ASN
9	U	1015	ASN
9	U	1092	ASN
9	U	1189	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

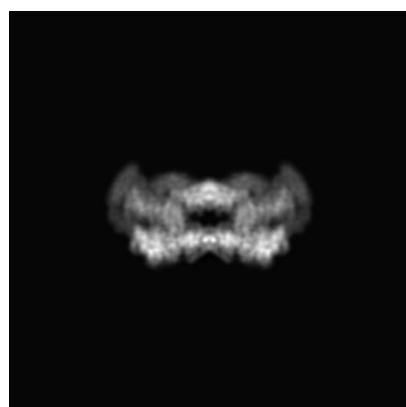
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31027. These allow visual inspection of the internal detail of the map and identification of artifacts.

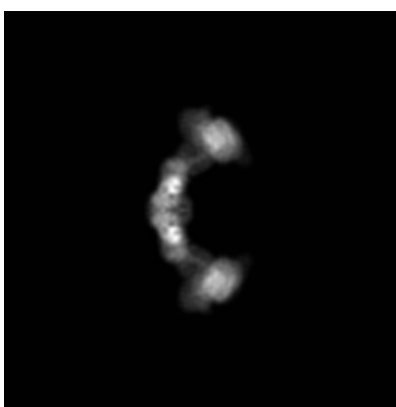
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

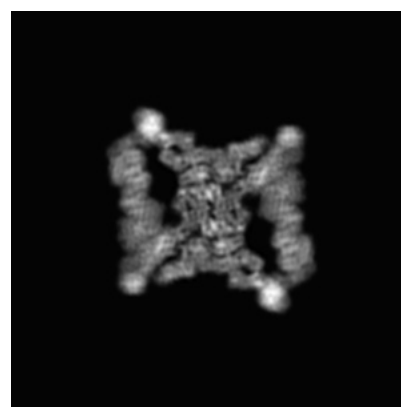
6.1.1 Primary map



X



Y

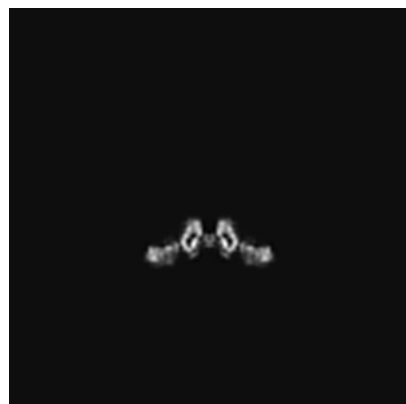


Z

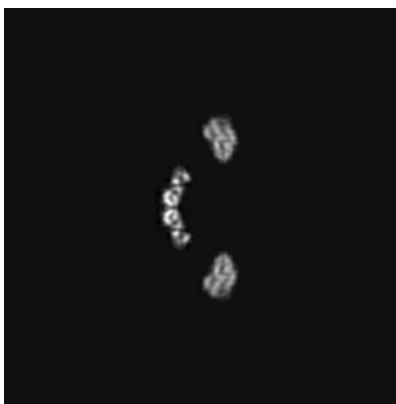
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

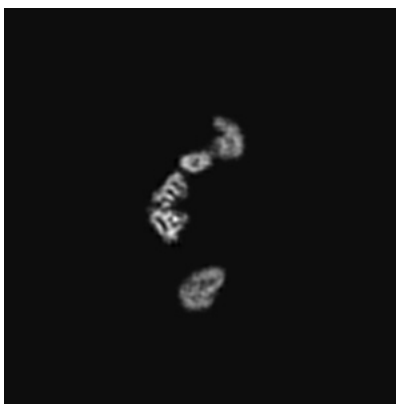
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 328



Y Index: 283

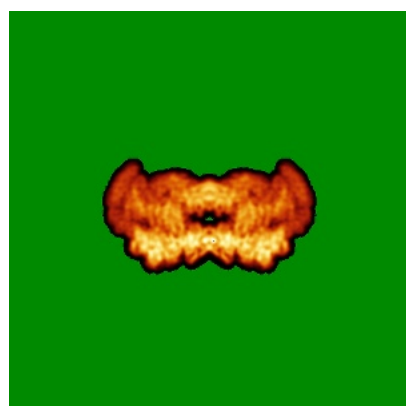


Z Index: 204

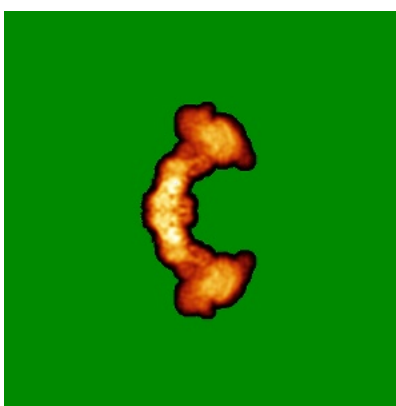
The images above show the largest variance slices of the map in three orthogonal directions.

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

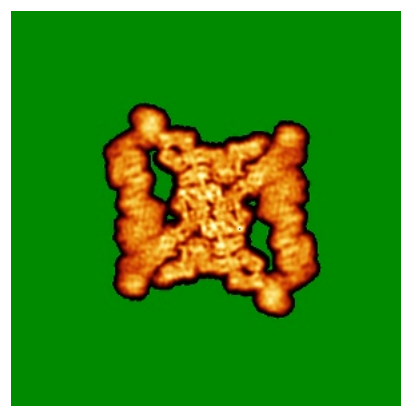
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

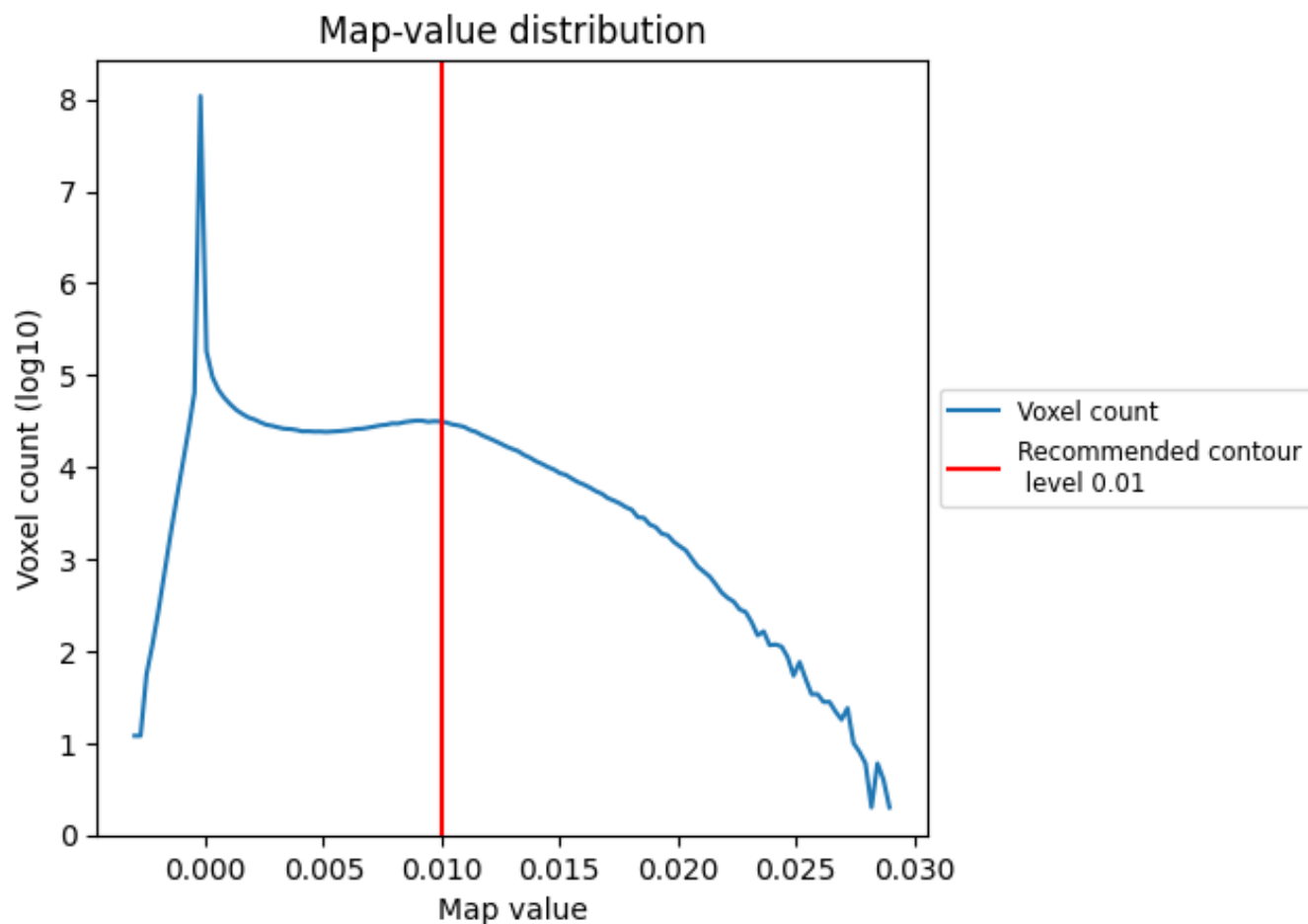
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

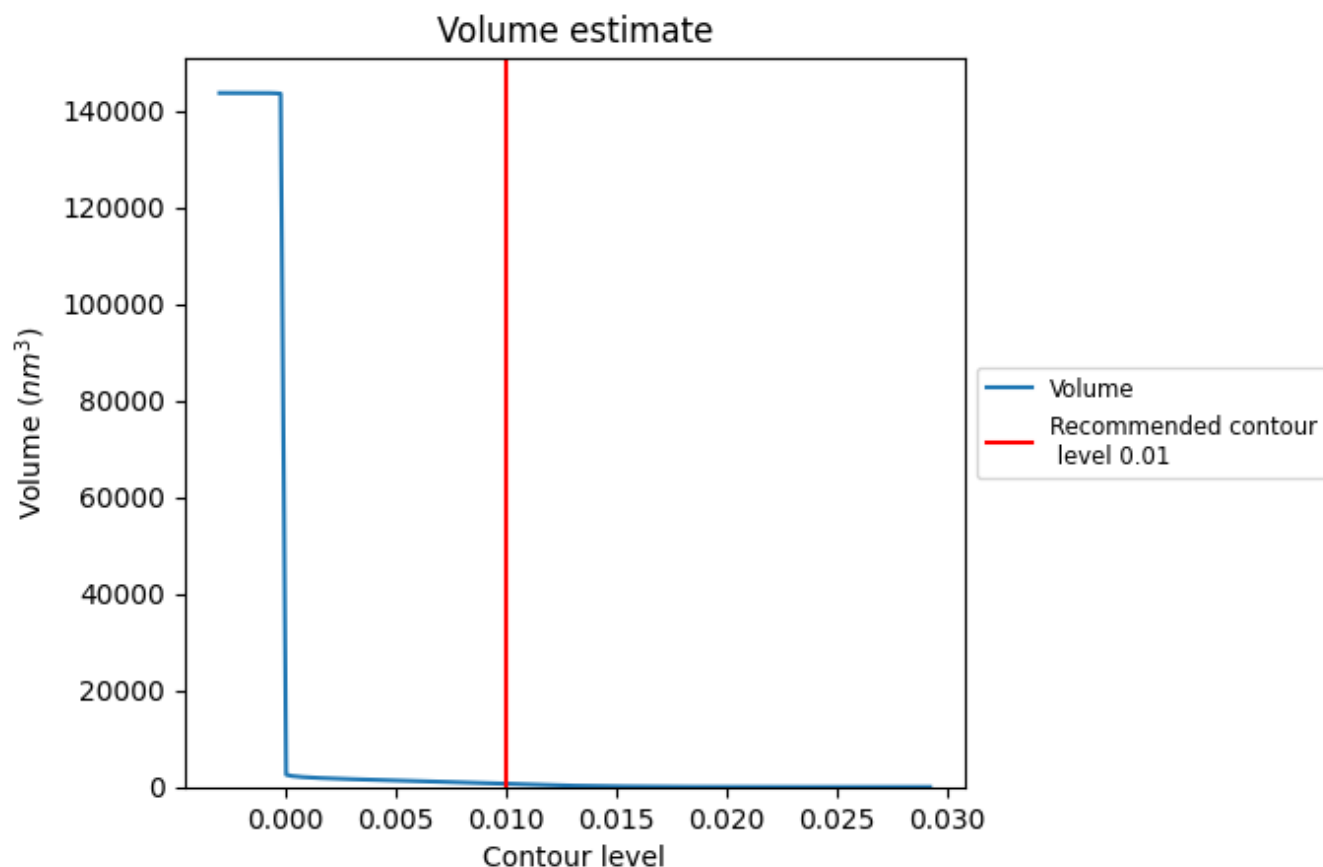
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

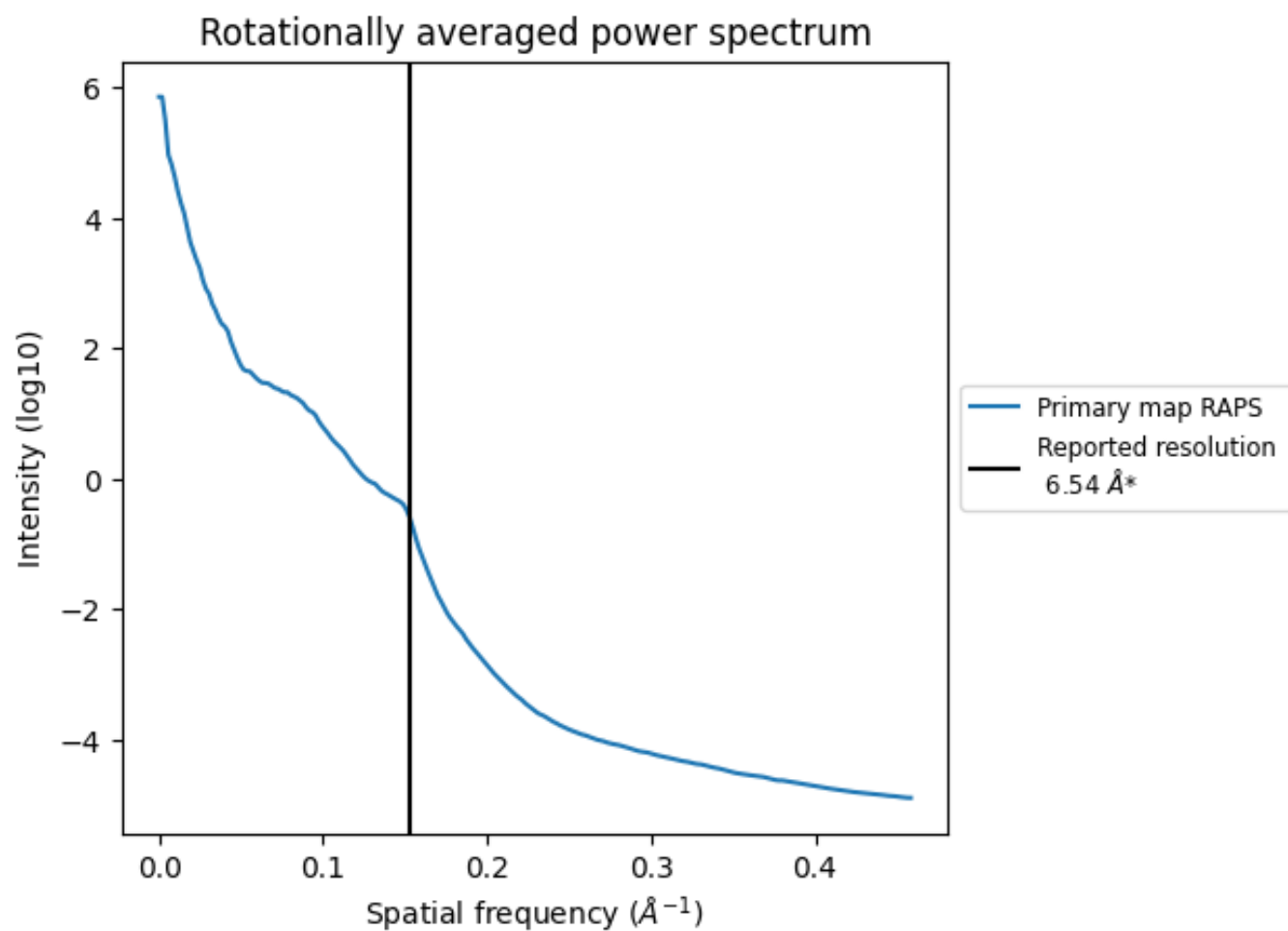
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 631 nm^3 ; this corresponds to an approximate mass of 570 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.153 Å⁻¹

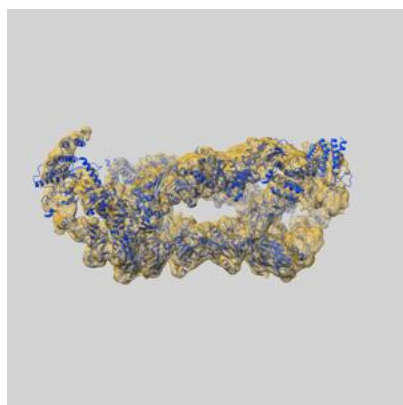
8 Fourier-Shell correlation

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

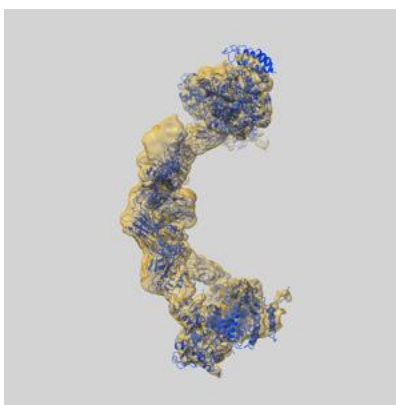
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31027 and PDB model 7E93. Per-residue inclusion information can be found in section [3](#) on page [7](#).

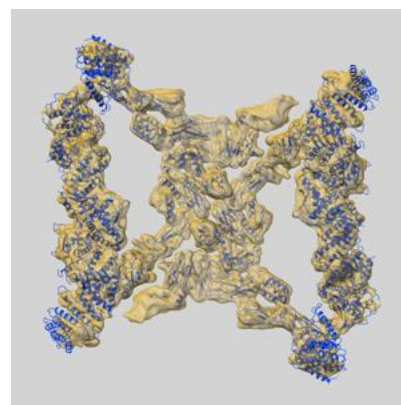
9.1 Map-model overlay [i](#)



X



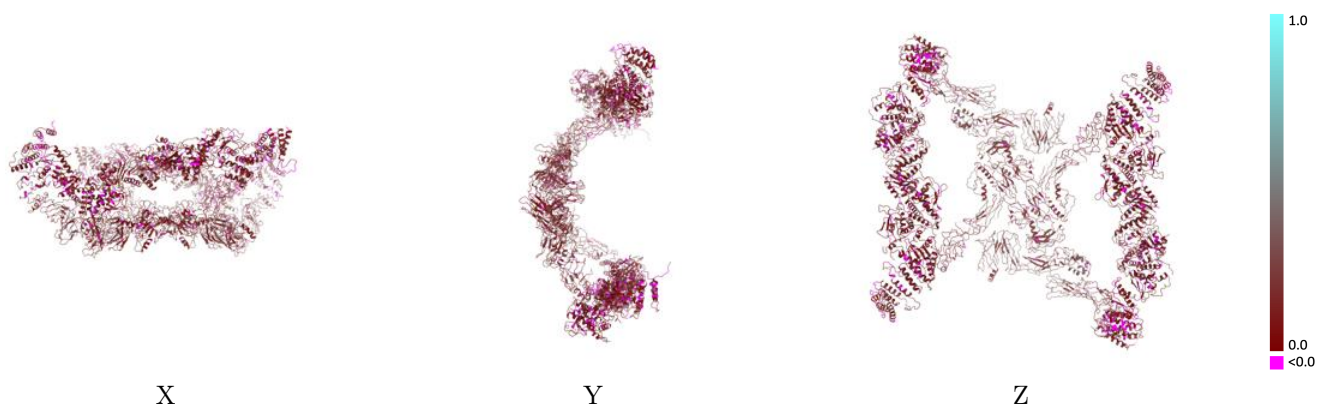
Y



Z

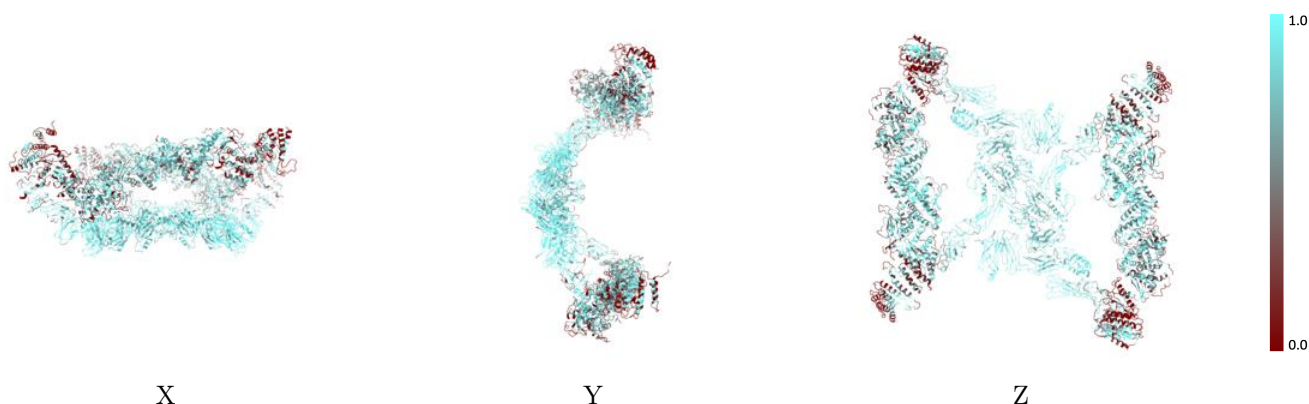
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



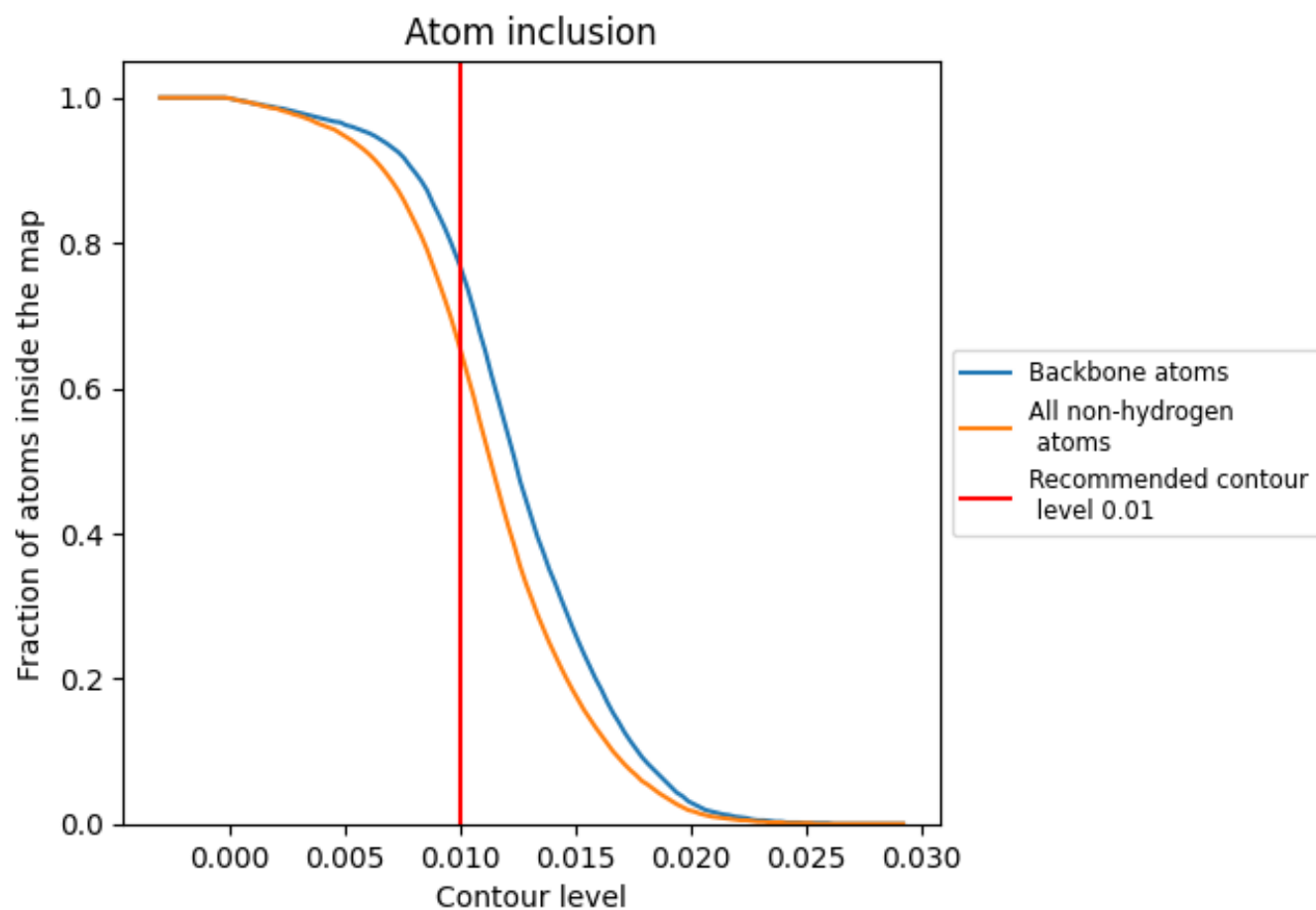
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.1530
A	 0.2520	 0.0920
B	 0.5540	 0.1370
C	 0.4750	 0.1150
D	 0.6930	 0.1440
E	 0.6990	 0.1510
F	 0.7460	 0.1410
G	 0.5860	 0.1330
H	 0.6060	 0.1230
I	 0.7390	 0.1900
J	 0.6900	 0.1630
K	 0.8360	 0.1840
L	 0.2520	 0.0920
M	 0.5560	 0.1380
N	 0.4760	 0.1130
O	 0.6920	 0.1440
P	 0.6980	 0.1520
Q	 0.7460	 0.1430
R	 0.5860	 0.1340
S	 0.6050	 0.1220
T	 0.7390	 0.1890
U	 0.6900	 0.1610
V	 0.8360	 0.1810

