



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 04:13 AM JST

PDB ID : 7E8T  
EMDB ID : EMD-31022  
Title : Monomer of Ypt32-TRAPP1I  
Authors : Mi, C.C.; Sui, S.F.  
Deposited on : 2021-03-02  
Resolution : 3.80 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](mailto: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>.

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

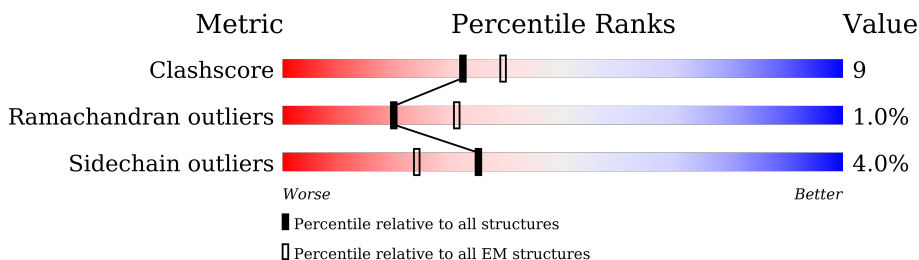
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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.



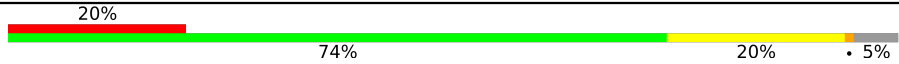



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	L	222	
2	I	1102	
3	J	1289	
4	K	560	
5	B	268	
6	G	283	
7	E	219	
8	H	175	

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Mol	Chain	Length	Quality of chain
9	A	152	 20% 74% 20% • 5%
10	D	159	 67% 28% • •
11	C	193	 81% 13% • •
11	F	193	 79% 14% • 5%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 24894 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 GTP-binding protein YPT32/YPT11.

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

- Molecule 2 is a protein called Trafficking protein particle complex II-specific subunit 130.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Trafficking protein particle complex II-specific subunit 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	882	6452	4114	1113	1206	19	0	0

- Molecule 4 is a protein called Trafficking protein particle complex II-specific subunit 65.

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

- Molecule 5 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	197	1590	1027	268	287	8	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	163	Total	C	N	O	S	0	0
			1317	851	210	246	10		

- Molecule 8 is a protein called Trafficking protein particle complex subunit 20.

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

- Molecule 9 is a protein called TRAPP-associated protein TCA17.

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

- Molecule 10 is a protein called Trafficking protein particle complex subunit BET5.

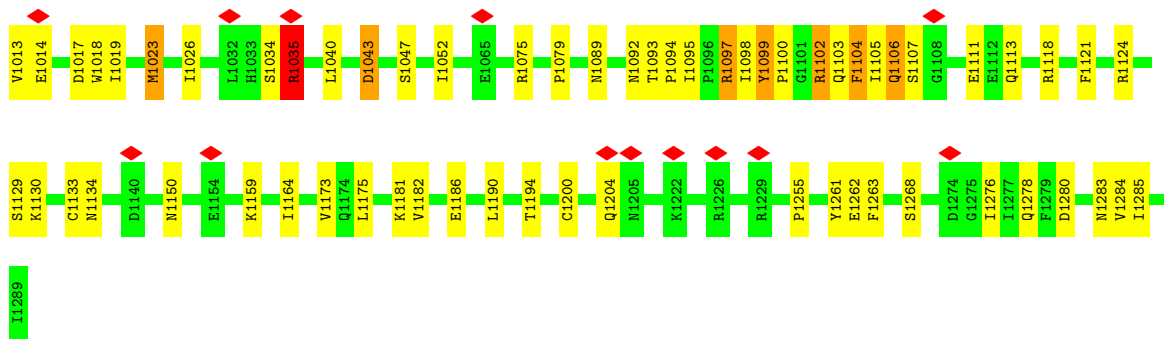
Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	156	Total	C	N	O	S	0	0
			1273	813	216	238	6		

- Molecule 11 is a protein called Trafficking protein particle complex subunit BET3.

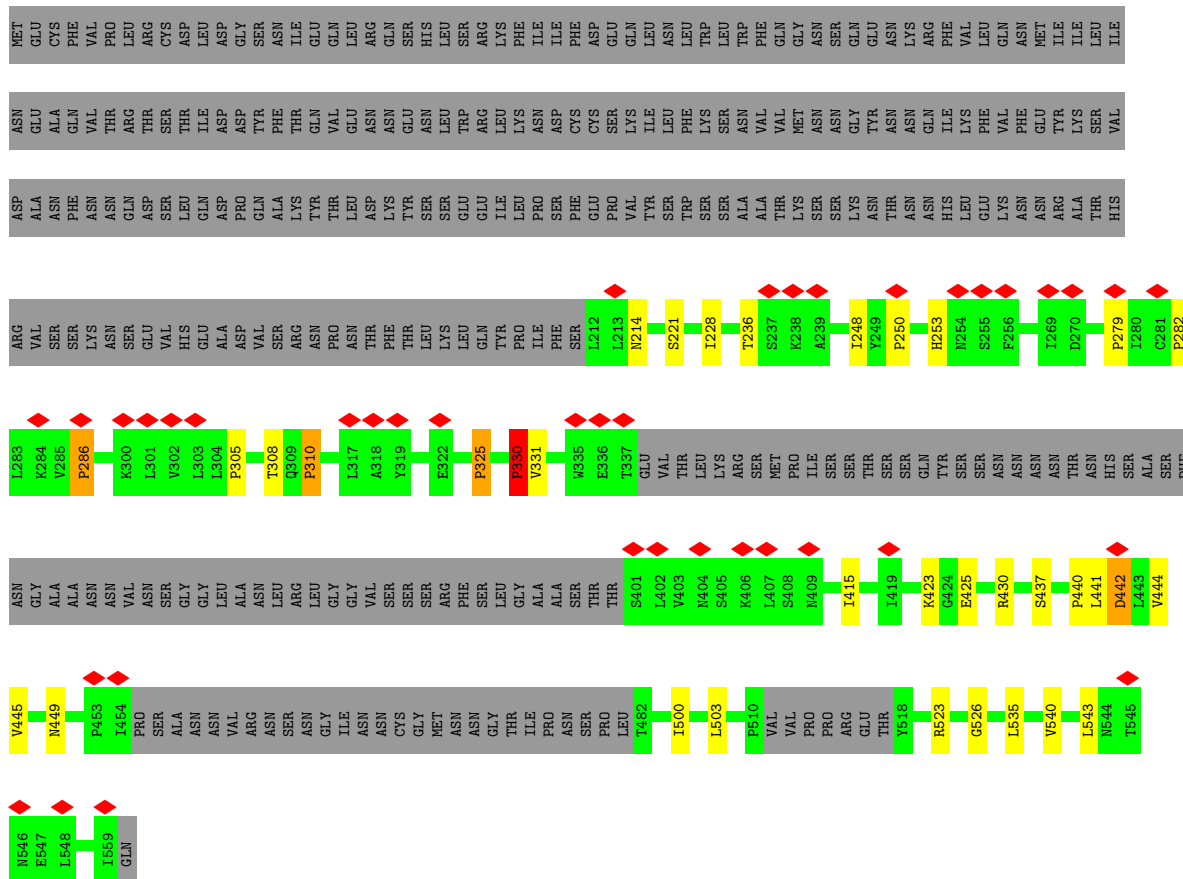
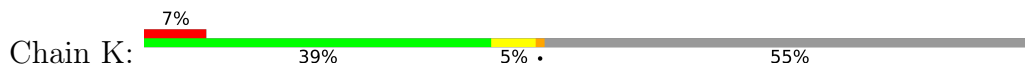
Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	183	Total	C	N	O	S	0	0
			1478	945	243	279	11		
11	C	185	Total	C	N	O	S	0	0
			1488	950	242	285	11		



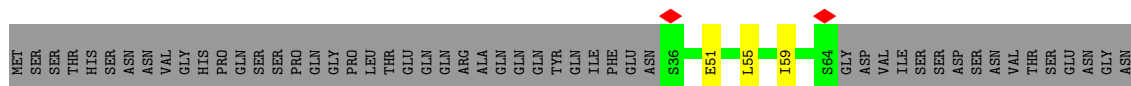




• Molecule 4: Trafficking protein particle complex II-specific subunit 65

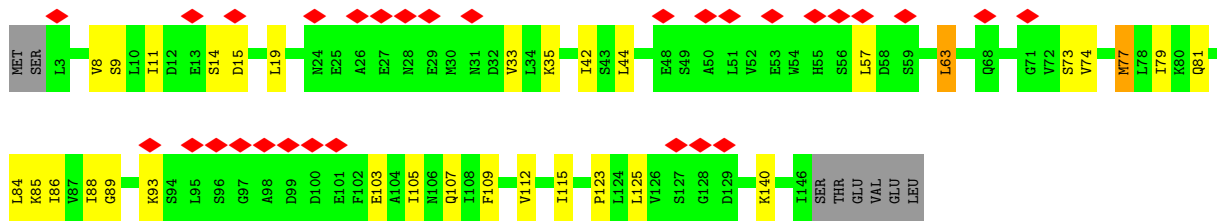


• Molecule 5: Trafficking protein particle complex subunit 33





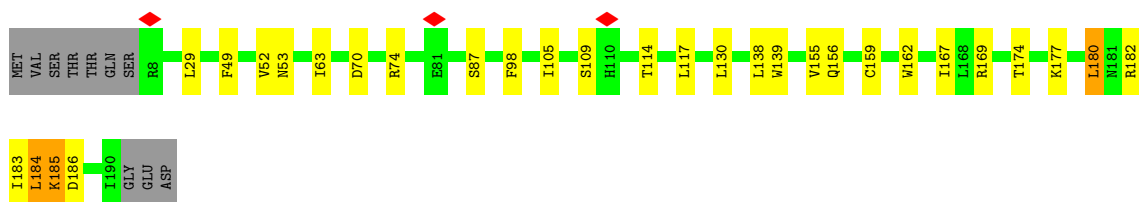
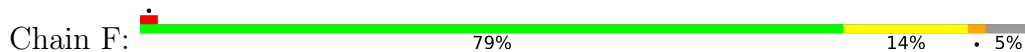




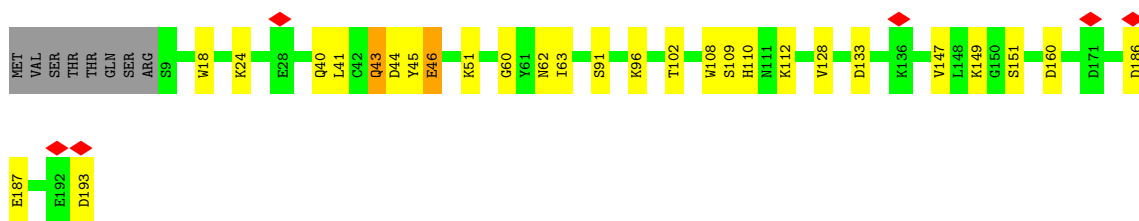
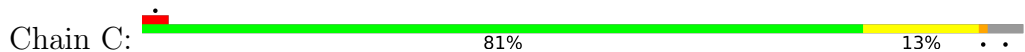
• Molecule 10: Trafficking protein particle complex subunit BET5



• Molecule 11: Trafficking protein particle complex subunit BET3



• Molecule 11: Trafficking protein particle complex subunit BET3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81870	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	0.048	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	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	L	0.56	0/1507	0.78	3/2038 (0.1%)
2	I	0.32	0/4219	0.65	14/5852 (0.2%)
3	J	0.45	2/6562 (0.0%)	0.86	28/8927 (0.3%)
4	K	0.34	0/1663	0.83	11/2268 (0.5%)
5	B	0.43	0/1617	0.91	7/2174 (0.3%)
6	G	0.45	0/1658	0.82	3/2236 (0.1%)
7	E	0.49	0/1341	0.79	1/1807 (0.1%)
8	H	0.48	0/1211	0.95	5/1643 (0.3%)
9	A	0.39	0/1180	0.87	4/1592 (0.3%)
10	D	0.50	0/1302	0.76	2/1758 (0.1%)
11	C	0.47	0/1515	0.81	1/2049 (0.0%)
11	F	0.45	0/1505	0.80	4/2035 (0.2%)
All	All	0.44	2/25280 (0.0%)	0.81	83/34379 (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
11	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1100	PRO	N-CD	-10.29	1.33	1.47
3	J	738	PRO	N-CD	-7.32	1.37	1.47

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	46	ASP	CB-CG-OD1	10.25	127.53	118.30
11	C	186	ASP	CB-CG-OD1	9.62	126.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	783	LEU	CA-CB-CG	8.98	135.96	115.30
3	J	815	ILE	CG1-CB-CG2	-8.86	91.90	111.40
10	D	119	LEU	CA-CB-CG	7.96	133.62	115.30
3	J	592	LEU	CA-CB-CG	7.96	133.60	115.30
3	J	631	LEU	CA-CB-CG	7.91	133.49	115.30
4	K	442	ASP	CB-CG-OD1	7.62	125.16	118.30
3	J	806	LEU	CA-CB-CG	7.59	132.77	115.30
2	I	346	PRO	N-CA-CB	7.53	112.33	103.30
4	K	535	LEU	CA-CB-CG	7.22	131.92	115.30
7	E	50	LEU	CA-CB-CG	7.13	131.71	115.30
5	B	188	ASP	CB-CG-OD1	7.03	124.63	118.30
4	K	325	PRO	N-CA-CB	7.03	111.73	103.30
3	J	466	ASP	CB-CG-OD1	7.00	124.60	118.30
2	I	483	PRO	N-CA-CB	6.96	111.65	103.30
9	A	33	VAL	CA-CB-CG1	6.88	121.22	110.90
3	J	783	LEU	CB-CG-CD1	6.83	122.62	111.00
4	K	330	PRO	N-CA-CB	6.79	111.44	103.30
1	L	199	PRO	N-CA-CB	6.73	111.38	103.30
5	B	132	LEU	CA-CB-CG	6.65	130.60	115.30
3	J	481	ASN	C-N-CA	-6.58	105.24	121.70
3	J	1100	PRO	CA-N-CD	6.45	120.73	111.70
4	K	310	PRO	N-CA-CB	6.41	110.99	103.30
3	J	1175	LEU	CA-CB-CG	6.35	129.91	115.30
4	K	286	PRO	N-CA-CB	6.30	110.86	103.30
5	B	190	ASP	CB-CG-OD1	6.28	123.95	118.30
2	I	649	PRO	N-CA-CB	6.24	110.78	103.30
2	I	976	PRO	N-CA-CB	6.24	110.78	103.30
2	I	1067	PRO	N-CA-CB	6.22	110.77	103.30
3	J	909	MET	CA-CB-CG	6.21	123.86	113.30
2	I	1076	PRO	N-CA-CB	6.21	110.75	103.30
8	H	46	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	I	639	PRO	N-CA-CB	6.19	110.72	103.30
2	I	704	PRO	N-CA-CB	6.18	110.72	103.30
2	I	252	PRO	N-CA-CB	6.14	110.67	103.30
4	K	282	PRO	N-CA-CB	6.14	110.67	103.30
2	I	572	PRO	N-CA-CB	6.14	110.67	103.30
2	I	970	PRO	N-CA-CB	6.14	110.67	103.30
3	J	398	PRO	N-CA-CB	6.13	110.66	103.30
3	J	1043	ASP	CB-CG-OD1	6.06	123.76	118.30
3	J	1255	PRO	N-CA-CB	6.01	110.52	103.30
11	F	155	VAL	CA-CB-CG1	5.98	119.87	110.90
6	G	66	PHE	CB-CG-CD1	5.97	124.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	305	PRO	N-CA-CB	5.96	110.45	103.30
3	J	956	PRO	N-CA-CB	5.89	110.36	103.30
4	K	441	LEU	CA-CB-CG	5.88	128.82	115.30
4	K	279	PRO	N-CA-CB	5.87	110.35	103.30
3	J	1023	MET	CG-SD-CE	5.86	109.57	100.20
5	B	87	ARG	NE-CZ-NH1	5.84	123.22	120.30
11	F	180	LEU	CA-CB-CG	5.80	128.65	115.30
3	J	436	PRO	N-CA-CB	5.80	110.26	103.30
4	K	250	PRO	N-CA-CB	5.79	110.25	103.30
2	I	721	PRO	N-CA-CB	5.79	110.24	103.30
3	J	388	PRO	N-CA-CB	5.78	110.23	103.30
9	A	44	LEU	CA-CB-CG	5.74	128.50	115.30
3	J	673	PRO	N-CA-CB	5.72	110.17	103.30
3	J	410	PRO	N-CA-CB	5.62	110.04	103.30
9	A	63	LEU	CA-CB-CG	5.60	128.17	115.30
3	J	667	PRO	N-CA-CB	5.58	110.00	103.30
2	I	799	LEU	CB-CG-CD1	-5.58	101.51	111.00
3	J	1035	ARG	CA-CB-CG	5.56	125.63	113.40
8	H	26	PRO	N-CA-CB	5.56	109.97	103.30
5	B	108	LEU	CA-CB-CG	5.53	128.01	115.30
1	L	9	ASP	CB-CG-OD1	5.49	123.24	118.30
6	G	267	LEU	CA-CB-CG	5.48	127.91	115.30
2	I	980	PRO	N-CA-CB	5.47	109.86	103.30
3	J	1052	ILE	CG1-CB-CG2	-5.43	99.45	111.40
5	B	150	GLU	CA-CB-CG	5.43	125.34	113.40
10	D	63	VAL	CG1-CB-CG2	-5.37	102.31	110.90
3	J	614	ILE	CG1-CB-CG2	-5.35	99.62	111.40
3	J	1040	LEU	CA-CB-CG	5.35	127.59	115.30
3	J	654	LEU	CA-CB-CG	5.34	127.59	115.30
8	H	131	ARG	NE-CZ-NH1	5.29	122.95	120.30
3	J	1190	LEU	CA-CB-CG	5.24	127.35	115.30
9	A	125	LEU	CB-CG-CD1	5.22	119.88	111.00
1	L	111	LEU	CB-CG-CD2	-5.20	102.17	111.00
11	F	117	LEU	CA-CB-CG	5.17	127.19	115.30
5	B	142	ASN	C-N-CA	5.08	134.40	121.70
6	G	169	MET	CB-CG-SD	5.05	127.54	112.40
8	H	168	LEU	CB-CG-CD2	-5.03	102.44	111.00
3	J	738	PRO	N-CA-CB	-5.02	97.07	102.60
11	F	130	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	C	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	L	1484	0	1410	44	0
2	I	4199	0	2172	26	0
3	J	6452	0	5798	224	0
4	K	1649	0	1338	21	0
5	B	1590	0	1612	27	0
6	G	1624	0	1601	16	0
7	E	1317	0	1323	24	0
8	H	1180	0	1132	15	0
9	A	1160	0	1184	20	0
10	D	1273	0	1245	23	0
11	C	1488	0	1487	24	0
11	F	1478	0	1487	20	0
All	All	24894	0	21789	436	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 9.

All (436) 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)
3:J:903:PRO:HB3	3:J:1098:ILE:CG1	1.13	1.58
3:J:903:PRO:CA	3:J:1098:ILE:HG21	1.37	1.50
3:J:915:TYR:H	3:J:1102:ARG:NH2	1.09	1.45
3:J:903:PRO:CB	3:J:1098:ILE:HG12	1.44	1.44
3:J:915:TYR:N	3:J:1102:ARG:HH22	1.07	1.39
3:J:916:ILE:N	3:J:1102:ARG:HH12	1.21	1.36
3:J:1098:ILE:HD11	3:J:1099:TYR:CE2	1.66	1.30
3:J:903:PRO:HA	3:J:1098:ILE:CG2	1.62	1.28
3:J:907:LYS:NZ	3:J:1098:ILE:HG13	1.49	1.26
3:J:1098:ILE:HD11	3:J:1099:TYR:CD2	1.77	1.20
1:L:129:ASP:OD1	1:L:158:LEU:HD23	1.41	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:903:PRO:CA	3:J:1098:ILE:CG2	2.19	1.18
3:J:903:PRO:CB	3:J:1098:ILE:CG1	2.06	1.17
3:J:1094:PRO:HG3	3:J:1118:ARG:CZ	1.74	1.17
3:J:916:ILE:N	3:J:1102:ARG:NH1	1.93	1.16
3:J:1098:ILE:CD1	3:J:1099:TYR:CD2	2.33	1.12
3:J:1094:PRO:HG3	3:J:1118:ARG:NE	1.64	1.12
3:J:481:ASN:OD1	3:J:483:PRO:HD2	1.49	1.11
3:J:903:PRO:HG3	3:J:1098:ILE:HB	1.25	1.10
3:J:1094:PRO:HG3	3:J:1118:ARG:NH2	1.66	1.10
3:J:1094:PRO:HB3	3:J:1118:ARG:CG	1.81	1.09
3:J:903:PRO:HB3	3:J:1098:ILE:CD1	1.84	1.07
3:J:1094:PRO:HB3	3:J:1118:ARG:HG2	1.28	1.07
3:J:907:LYS:HZ1	3:J:1098:ILE:HG13	0.91	1.07
3:J:910:PRO:HD3	3:J:1095:ILE:HG21	1.31	1.06
3:J:903:PRO:HG3	3:J:1098:ILE:CB	1.84	1.06
11:F:182:ARG:HD3	11:F:184:LEU:HD13	1.33	1.06
3:J:903:PRO:HA	3:J:1098:ILE:HG21	1.19	1.04
3:J:907:LYS:NZ	3:J:1098:ILE:CG1	2.19	1.04
3:J:903:PRO:N	3:J:1098:ILE:HG21	1.71	1.03
3:J:916:ILE:H	3:J:1102:ARG:NH1	1.47	1.03
11:F:182:ARG:HD3	11:F:184:LEU:CD1	1.89	1.02
3:J:903:PRO:CB	3:J:1098:ILE:HG21	1.90	1.01
3:J:800:CYS:SG	3:J:814:ASP:HA	2.01	1.00
3:J:907:LYS:HZ1	3:J:1098:ILE:CG1	1.74	0.97
3:J:907:LYS:HD2	3:J:1097:ARG:HG3	1.46	0.96
3:J:915:TYR:C	3:J:1102:ARG:HH12	1.69	0.96
3:J:1094:PRO:CG	3:J:1118:ARG:CZ	2.44	0.96
3:J:903:PRO:HA	3:J:1098:ILE:HG23	1.47	0.95
3:J:1094:PRO:CG	3:J:1118:ARG:NE	2.31	0.92
3:J:915:TYR:N	3:J:1102:ARG:NH2	1.82	0.92
3:J:914:LEU:C	3:J:1102:ARG:HH22	1.72	0.92
3:J:907:LYS:HZ2	3:J:1098:ILE:H	1.04	0.92
3:J:1094:PRO:CG	3:J:1118:ARG:NH2	2.33	0.91
3:J:914:LEU:CB	3:J:1102:ARG:NH2	2.34	0.91
3:J:903:PRO:CG	3:J:1098:ILE:HG21	2.01	0.91
3:J:801:LEU:O	3:J:803:ILE:HD12	1.71	0.91
1:L:156:SER:OG	1:L:158:LEU:HG	1.71	0.91
3:J:500:LEU:HD12	3:J:502:LEU:HG	1.53	0.90
3:J:907:LYS:NZ	3:J:1098:ILE:H	1.68	0.90
9:A:77:MET:SD	9:A:109:PHE:CD2	2.65	0.90
3:J:1094:PRO:HG3	3:J:1118:ARG:HE	1.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:907:LYS:HZ2	3:J:1098:ILE:N	1.71	0.89
3:J:801:LEU:HD23	3:J:801:LEU:H	1.38	0.89
3:J:916:ILE:H	3:J:1102:ARG:HH12	0.95	0.89
1:L:172:VAL:CG1	3:J:703:LYS:HE3	2.01	0.89
3:J:903:PRO:CG	3:J:1098:ILE:CB	2.52	0.88
3:J:903:PRO:HB3	3:J:1098:ILE:CB	2.04	0.86
1:L:129:ASP:OD1	1:L:158:LEU:CD2	2.23	0.86
3:J:903:PRO:CB	3:J:1098:ILE:CB	2.53	0.86
3:J:1094:PRO:CB	3:J:1118:ARG:HG2	2.05	0.86
3:J:1013:VAL:HG23	4:K:425:GLU:CD	1.97	0.85
3:J:1098:ILE:HD12	3:J:1099:TYR:CD2	2.12	0.84
3:J:903:PRO:CB	3:J:1098:ILE:CG2	2.53	0.84
1:L:172:VAL:HG12	3:J:703:LYS:CE	2.07	0.84
3:J:1094:PRO:HG3	3:J:1118:ARG:HH21	1.38	0.84
11:C:45:TYR:O	11:C:46:GLU:OE1	1.96	0.83
3:J:909:MET:HE2	3:J:1121:PHE:HB2	1.60	0.82
9:A:77:MET:HG3	9:A:86:ILE:HG23	1.60	0.82
3:J:1094:PRO:HB3	3:J:1118:ARG:CD	2.11	0.81
1:L:169:GLU:OE1	3:J:698:VAL:CG1	2.28	0.81
3:J:915:TYR:H	3:J:1102:ARG:CZ	1.91	0.81
3:J:903:PRO:CG	3:J:1098:ILE:CG2	2.60	0.80
3:J:903:PRO:HG3	3:J:1098:ILE:CG2	2.12	0.80
3:J:800:CYS:SG	3:J:814:ASP:OD1	2.39	0.79
3:J:910:PRO:HD3	3:J:1095:ILE:CG2	2.11	0.79
3:J:481:ASN:OD1	3:J:482:SER:N	2.16	0.79
2:I:459:TYR:O	2:I:464:LYS:HB2	1.84	0.78
3:J:1094:PRO:CB	3:J:1118:ARG:CG	2.61	0.78
3:J:1094:PRO:CD	3:J:1118:ARG:NH2	2.47	0.78
1:L:172:VAL:HG11	3:J:703:LYS:HE3	1.65	0.77
2:I:853:PHE:HB2	2:I:974:THR:O	1.84	0.77
3:J:1094:PRO:HD3	3:J:1118:ARG:CZ	2.14	0.76
3:J:903:PRO:CG	3:J:1098:ILE:HB	2.10	0.76
3:J:910:PRO:CD	3:J:1095:ILE:HG21	2.12	0.76
3:J:1094:PRO:HB3	3:J:1118:ARG:NE	2.00	0.76
1:L:172:VAL:CG1	3:J:703:LYS:CE	2.63	0.75
1:L:133:LEU:HD22	3:J:1106:GLN:HE22	1.49	0.75
3:J:1094:PRO:CB	3:J:1118:ARG:NE	2.48	0.75
1:L:133:LEU:HD23	1:L:133:LEU:N	2.01	0.75
3:J:655:ARG:O	3:J:815:ILE:CG2	2.35	0.74
1:L:169:GLU:OE1	3:J:698:VAL:HG11	1.88	0.74
3:J:801:LEU:O	3:J:803:ILE:CD1	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:SER:O	1:L:135:ALA:HB2	1.88	0.74
3:J:1263:PHE:O	3:J:1283:ASN:HA	1.87	0.73
3:J:500:LEU:CD1	3:J:502:LEU:HG	2.18	0.73
3:J:501:GLN:HB3	3:J:503:LYS:HE3	1.69	0.73
3:J:735:VAL:HG23	3:J:735:VAL:O	1.89	0.73
3:J:655:ARG:HG3	3:J:655:ARG:HH11	1.54	0.72
3:J:1094:PRO:HD3	3:J:1118:ARG:NH2	2.04	0.72
3:J:907:LYS:HZ3	3:J:1098:ILE:CG1	1.98	0.72
3:J:1013:VAL:CG2	4:K:425:GLU:CD	2.57	0.72
3:J:1094:PRO:CD	3:J:1118:ARG:CZ	2.68	0.72
5:B:102:HIS:CD2	10:D:122:PRO:HB3	2.25	0.71
3:J:914:LEU:CA	3:J:1102:ARG:HH22	2.04	0.71
3:J:903:PRO:CA	3:J:1098:ILE:HG12	2.20	0.71
9:A:77:MET:HG3	9:A:86:ILE:CG2	2.19	0.71
3:J:903:PRO:CG	3:J:1098:ILE:HD13	2.20	0.71
3:J:903:PRO:CB	3:J:1098:ILE:CD1	2.53	0.70
3:J:1106:GLN:OE1	3:J:1106:GLN:HA	1.91	0.70
3:J:907:LYS:HD2	3:J:1097:ARG:CG	2.19	0.69
11:C:45:TYR:CE2	11:C:51:LYS:HB3	2.27	0.69
1:L:172:VAL:HG12	3:J:703:LYS:NZ	2.07	0.69
3:J:903:PRO:CG	3:J:1098:ILE:CG1	2.71	0.69
3:J:915:TYR:N	3:J:1102:ARG:CZ	2.54	0.68
4:K:444:VAL:O	4:K:540:VAL:HA	1.93	0.68
3:J:903:PRO:CB	3:J:1098:ILE:HD13	2.23	0.68
3:J:903:PRO:CD	3:J:1098:ILE:HG21	2.24	0.68
3:J:915:TYR:CA	3:J:1102:ARG:HH12	2.06	0.68
7:E:53:LYS:HA	7:E:53:LYS:HZ3	1.58	0.68
11:C:40:GLN:O	11:C:44:ASP:HB2	1.93	0.67
3:J:1261:TYR:O	3:J:1285:ILE:HA	1.95	0.67
2:I:299:PHE:O	2:I:302:ALA:HB3	1.95	0.67
1:L:172:VAL:HG12	3:J:703:LYS:HZ1	1.59	0.67
3:J:801:LEU:HD23	3:J:801:LEU:N	2.09	0.66
3:J:914:LEU:CA	3:J:1102:ARG:NH2	2.59	0.66
3:J:909:MET:CE	3:J:1121:PHE:HB2	2.26	0.65
3:J:501:GLN:HG3	3:J:503:LYS:HE3	1.79	0.63
5:B:184:PHE:H	5:B:262:VAL:HG22	1.63	0.63
3:J:655:ARG:NH1	3:J:816:ILE:CD1	2.62	0.62
11:C:45:TYR:C	11:C:46:GLU:OE1	2.37	0.62
5:B:176:LEU:HA	5:B:185:TYR:O	1.99	0.62
9:A:77:MET:SD	9:A:109:PHE:CG	2.92	0.62
1:L:39:ASN:HB2	7:E:32:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:655:ARG:NH1	3:J:816:ILE:HD13	2.15	0.62
5:B:159:PHE:O	5:B:163:ASP:HB2	2.00	0.61
11:F:182:ARG:HD3	11:F:184:LEU:HD11	1.80	0.61
4:K:445:VAL:HG12	4:K:540:VAL:HG12	1.83	0.61
7:E:52:PRO:O	7:E:54:ALA:N	2.33	0.61
3:J:628:GLN:HA	3:J:631:LEU:HB3	1.83	0.61
5:B:239:LEU:O	5:B:257:GLY:C	2.39	0.60
11:F:182:ARG:CD	11:F:184:LEU:CD1	2.75	0.60
3:J:501:GLN:HB3	3:J:503:LYS:HG3	1.83	0.60
3:J:655:ARG:HG3	3:J:655:ARG:NH1	2.14	0.60
3:J:1094:PRO:CG	3:J:1118:ARG:HE	2.04	0.59
3:J:1095:ILE:HG22	3:J:1095:ILE:O	2.02	0.59
8:H:13:ASN:HD21	8:H:153:THR:HG22	1.65	0.59
3:J:621:HIS:ND1	6:G:30:GLN:OE1	2.35	0.59
7:E:55:LEU:N	7:E:55:LEU:HD22	2.17	0.59
3:J:626:SER:HA	3:J:629:ASP:HB2	1.85	0.59
3:J:903:PRO:HG2	3:J:1098:ILE:HD13	1.83	0.59
3:J:1013:VAL:HG22	4:K:425:GLU:OE1	2.03	0.59
3:J:628:GLN:O	3:J:632:PHE:HB2	2.03	0.59
3:J:903:PRO:HB3	3:J:1098:ILE:HG12	0.60	0.58
2:I:784:PHE:O	2:I:838:CYS:HA	2.04	0.58
3:J:655:ARG:CZ	3:J:816:ILE:HD13	2.32	0.58
5:B:175:ASN:HB3	5:B:187:LEU:HB2	1.85	0.58
5:B:59:ILE:CG1	11:C:44:ASP:OD2	2.51	0.57
1:L:98:SER:HB2	1:L:135:ALA:HB1	1.86	0.57
3:J:1013:VAL:HG13	3:J:1019:ILE:HG21	1.86	0.57
3:J:907:LYS:NZ	3:J:1098:ILE:N	2.42	0.57
10:D:52:ARG:NH1	10:D:66:ASP:OD2	2.37	0.57
3:J:737:ASN:HA	3:J:786:ILE:HG22	1.87	0.56
8:H:117:ASN:HB2	8:H:121:SER:HB3	1.88	0.56
3:J:1103:GLN:CD	3:J:1103:GLN:H	2.08	0.56
3:J:915:TYR:CA	3:J:1102:ARG:NH1	2.68	0.56
3:J:611:PHE:HA	3:J:614:ILE:HG22	1.87	0.56
3:J:907:LYS:CD	3:J:1097:ARG:HG3	2.29	0.56
3:J:909:MET:CB	3:J:1095:ILE:HD12	2.36	0.56
3:J:501:GLN:CB	3:J:503:LYS:HE3	2.36	0.56
3:J:501:GLN:CG	3:J:503:LYS:HE3	2.36	0.56
11:F:138:LEU:O	11:F:169:ARG:NH1	2.39	0.56
3:J:1262:GLU:HA	3:J:1284:VAL:O	2.07	0.55
5:B:55:LEU:HD11	11:C:41:LEU:HD21	1.88	0.55
7:E:8:VAL:HB	7:E:17:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:108:TRP:HE1	11:C:112:LYS:HE2	1.72	0.55
1:L:156:SER:OG	1:L:158:LEU:CG	2.51	0.55
3:J:1103:GLN:H	3:J:1103:GLN:NE2	2.04	0.55
3:J:1043:ASP:HB3	3:J:1075:ARG:HG2	1.90	0.54
5:B:51:GLU:HB3	10:D:119:LEU:HD11	1.90	0.54
11:C:45:TYR:O	11:C:46:GLU:HB2	2.06	0.54
7:E:53:LYS:HZ3	7:E:53:LYS:CA	2.20	0.54
7:E:113:ASN:ND2	7:E:115:ASN:OD1	2.41	0.54
1:L:95:ILE:O	1:L:135:ALA:N	2.26	0.54
4:K:500:ILE:HA	4:K:526:GLY:HA2	1.89	0.54
11:C:18:TRP:NE1	11:C:96:LYS:O	2.35	0.53
1:L:158:LEU:HD12	1:L:158:LEU:C	2.29	0.53
5:B:59:ILE:HG13	11:C:44:ASP:OD2	2.07	0.53
3:J:492:PHE:O	3:J:496:LYS:NZ	2.41	0.53
9:A:63:LEU:HD11	9:A:105:ILE:HG22	1.91	0.53
5:B:233:SER:OG	5:B:234:GLU:N	2.42	0.53
1:L:172:VAL:CG1	3:J:703:LYS:NZ	2.72	0.53
9:A:77:MET:SD	9:A:109:PHE:HB3	2.49	0.53
11:C:109:SER:OG	11:C:110:HIS:N	2.42	0.53
3:J:1034:SER:OG	3:J:1035:ARG:N	2.41	0.52
3:J:1094:PRO:CG	3:J:1118:ARG:HH21	2.08	0.52
5:B:166:LYS:NZ	5:B:172:GLN:OE1	2.37	0.52
3:J:1017:ASP:N	3:J:1017:ASP:OD1	2.42	0.52
11:F:182:ARG:CD	11:F:184:LEU:HD11	2.38	0.52
10:D:6:PHE:O	10:D:18:ASP:HA	2.10	0.52
3:J:909:MET:HB3	3:J:1095:ILE:HD12	1.92	0.52
3:J:522:ARG:HE	3:J:523:LEU:HD22	1.73	0.52
6:G:47:SER:HB2	8:H:164:ARG:HH22	1.75	0.52
11:F:70:ASP:OD1	11:F:74:ARG:NH2	2.43	0.52
10:D:79:THR:HG22	10:D:89:VAL:HG12	1.90	0.52
3:J:1200:CYS:O	3:J:1204:GLN:NE2	2.42	0.52
5:B:146:LEU:O	9:A:81:GLN:NE2	2.42	0.51
7:E:7:LEU:HB3	7:E:141:VAL:HB	1.92	0.51
9:A:115:ILE:HD11	9:A:140:LYS:HB3	1.91	0.51
2:I:529:GLN:O	2:I:551:LYS:N	2.43	0.51
7:E:53:LYS:N	7:E:53:LYS:CE	2.73	0.51
1:L:45:THR:O	10:D:46:GLY:HA3	2.11	0.51
3:J:481:ASN:O	3:J:484:MET:SD	2.68	0.51
11:F:159:CYS:HA	11:F:180:LEU:HA	1.91	0.51
5:B:177:LYS:HB3	5:B:185:TYR:HB2	1.91	0.51
9:A:79:ILE:HG12	9:A:84:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:141:SER:OG	5:B:142:ASN:N	2.44	0.51
5:B:145:ASN:HB3	9:A:57:LEU:HA	1.93	0.51
1:L:43:LYS:HE2	1:L:70:ALA:HB2	1.91	0.51
3:J:915:TYR:C	3:J:1102:ARG:NH1	2.49	0.51
3:J:1098:ILE:HD12	3:J:1099:TYR:CG	2.46	0.51
2:I:776:ILE:HB	2:I:783:PHE:HB2	1.93	0.50
3:J:485:PHE:HB2	3:J:486:PRO:HD3	1.93	0.50
1:L:26:LYS:HB3	1:L:92:VAL:HG11	1.94	0.50
2:I:1013:TYR:HA	2:I:1064:HIS:HA	1.93	0.50
6:G:163:SER:OG	6:G:164:ASN:N	2.44	0.50
11:C:45:TYR:CD2	11:C:51:LYS:HB3	2.46	0.50
5:B:85:ILE:O	5:B:87:ARG:NH1	2.44	0.50
7:E:66:THR:O	7:E:66:THR:OG1	2.30	0.50
3:J:1013:VAL:HG23	4:K:425:GLU:OE2	2.12	0.50
3:J:483:PRO:C	3:J:484:MET:SD	2.90	0.50
4:K:442:ASP:HB2	4:K:543:LEU:HD12	1.93	0.50
7:E:53:LYS:N	7:E:53:LYS:HE2	2.26	0.50
8:H:11:LYS:O	8:H:11:LYS:HD3	2.11	0.50
3:J:801:LEU:N	3:J:801:LEU:CD2	2.73	0.50
6:G:276:ASP:OD1	6:G:276:ASP:N	2.43	0.50
7:E:53:LYS:N	7:E:53:LYS:NZ	2.60	0.50
3:J:1129:SER:OG	3:J:1130:LYS:NZ	2.43	0.49
9:A:14:SER:OG	9:A:15:ASP:N	2.45	0.49
1:L:136:VAL:HG13	1:L:137:PRO:HD2	1.94	0.49
3:J:1159:LYS:NZ	4:K:449:ASN:O	2.41	0.49
7:E:188:ASP:OD1	7:E:192:LYS:NZ	2.45	0.49
11:C:133:ASP:OD1	11:C:133:ASP:N	2.41	0.49
1:L:175:PHE:O	1:L:179:SER:N	2.43	0.49
3:J:655:ARG:NH1	3:J:816:ILE:HD11	2.27	0.49
3:J:818:ASP:HB3	3:J:820:ARG:HG2	1.93	0.49
6:G:207:ASN:ND2	6:G:270:PHE:O	2.45	0.49
7:E:9:ILE:HA	7:E:15:LEU:HA	1.95	0.49
3:J:779:ARG:NH2	3:J:780:SER:O	2.45	0.49
6:G:227:VAL:HG22	6:G:230:GLU:HB2	1.94	0.49
10:D:2:GLY:N	10:D:93:ASP:OD2	2.46	0.49
2:I:803:GLU:O	2:I:855:LEU:HA	2.12	0.49
4:K:415:ILE:HD13	4:K:430:ARG:HG2	1.95	0.49
5:B:239:LEU:O	5:B:257:GLY:O	2.31	0.49
10:D:19:ARG:HA	10:D:31:THR:HG22	1.95	0.49
1:L:41:GLU:O	1:L:42:SER:HB2	2.12	0.48
3:J:738:PRO:HD3	3:J:786:ILE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:149:LYS:NZ	11:C:160:ASP:OD1	2.44	0.48
1:L:128:SER:OG	1:L:156:SER:HA	2.12	0.48
3:J:907:LYS:NZ	3:J:1098:ILE:HG12	2.21	0.48
3:J:909:MET:HB2	3:J:1095:ILE:HG23	1.96	0.48
5:B:59:ILE:HG12	11:C:44:ASP:OD2	2.12	0.48
9:A:9:SER:HA	9:A:19:LEU:O	2.14	0.48
3:J:478:ASP:OD2	3:J:491:TYR:OH	2.28	0.48
3:J:1013:VAL:HA	4:K:425:GLU:OE2	2.13	0.48
3:J:1092:ASN:N	3:J:1092:ASN:HD22	2.12	0.48
3:J:658:VAL:HG23	3:J:739:PHE:HB3	1.96	0.48
3:J:903:PRO:CG	3:J:1098:ILE:CD1	2.85	0.48
6:G:254:ARG:HG2	6:G:264:THR:HG22	1.96	0.48
1:L:16:ILE:HA	1:L:88:GLY:O	2.13	0.48
11:C:193:ASP:OD1	11:C:193:ASP:N	2.46	0.48
2:I:772:SER:HB3	2:I:787:LEU:HB3	1.96	0.48
3:J:1013:VAL:CG2	4:K:425:GLU:OE1	2.62	0.48
3:J:915:TYR:N	3:J:1102:ARG:NH1	2.62	0.47
4:K:221:SER:O	4:K:228:ILE:HA	2.13	0.47
1:L:89:ALA:HB1	1:L:111:LEU:HD21	1.96	0.47
7:E:55:LEU:N	7:E:55:LEU:CD2	2.77	0.47
3:J:484:MET:SD	3:J:484:MET:N	2.88	0.47
10:D:37:ASN:HD22	10:D:37:ASN:HA	1.47	0.47
11:C:40:GLN:OE1	11:C:43:GLN:NE2	2.40	0.47
3:J:628:GLN:O	3:J:632:PHE:CB	2.62	0.47
11:F:109:SER:HB3	11:F:114:THR:H	1.80	0.47
6:G:191:LEU:HD22	11:F:29:LEU:HD12	1.96	0.47
1:L:171:ILE:HA	1:L:174:ILE:HG22	1.96	0.47
2:I:333:SER:O	2:I:337:TYR:N	2.48	0.47
3:J:907:LYS:HZ3	3:J:1098:ILE:HG12	1.76	0.47
8:H:103:TYR:HB3	8:H:111:PHE:HB2	1.96	0.47
10:D:3:ILE:HD12	10:D:90:LEU:HD11	1.96	0.47
3:J:1018:TRP:HB2	3:J:1079:PRO:HG3	1.97	0.47
3:J:529:LYS:HD2	8:H:43:ALA:HB1	1.96	0.46
9:A:112:VAL:HA	9:A:115:ILE:HG22	1.97	0.46
10:D:7:TRP:HA	10:D:17:PHE:O	2.15	0.46
11:F:156:GLN:HG2	11:F:185:LYS:O	2.15	0.46
3:J:1124:ARG:NH2	3:J:1150:ASN:O	2.48	0.46
3:J:1268:SER:HA	3:J:1276:ILE:HA	1.97	0.46
7:E:16:ILE:HD12	7:E:202:ILE:HD11	1.97	0.46
1:L:46:ILE:HD12	1:L:46:ILE:HA	1.76	0.46
3:J:478:ASP:HB2	3:J:486:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:655:ARG:O	3:J:815:ILE:HG23	2.15	0.46
6:G:38:THR:HA	8:H:170:ARG:HD3	1.98	0.46
6:G:180:LEU:HB3	6:G:199:LEU:HD21	1.96	0.46
3:J:993:ARG:O	3:J:1047:SER:OG	2.33	0.46
6:G:180:LEU:HA	6:G:183:ILE:HG22	1.97	0.46
3:J:754:ILE:O	3:J:804:SER:OG	2.32	0.46
2:I:307:LYS:O	2:I:311:GLU:N	2.47	0.46
3:J:1133:CYS:SG	3:J:1134:ASN:N	2.90	0.45
3:J:590:LYS:NZ	8:H:34:LYS:O	2.42	0.45
3:J:915:TYR:CB	3:J:1102:ARG:NH1	2.79	0.45
2:I:860:ASN:ND2	2:I:966:ARG:O	2.48	0.45
1:L:16:ILE:HG12	1:L:88:GLY:HA3	1.97	0.45
1:L:39:ASN:HB3	10:D:57:LYS:HD3	1.99	0.45
1:L:25:GLY:O	1:L:126:ASN:ND2	2.49	0.45
1:L:76:ARG:HA	1:L:76:ARG:HD3	1.58	0.45
3:J:500:LEU:H	3:J:500:LEU:HG	1.57	0.45
3:J:1104:PHE:HD1	3:J:1104:PHE:O	1.99	0.45
7:E:65:ASN:N	7:E:65:ASN:ND2	2.65	0.45
3:J:1278:GLN:HG2	3:J:1280:ASP:HB2	1.98	0.45
5:B:102:HIS:O	5:B:106:HIS:ND1	2.49	0.45
11:F:167:ILE:HG23	11:F:174:THR:HG23	1.99	0.45
4:K:503:LEU:HB2	4:K:523:ARG:HG3	1.98	0.45
7:E:105:ASP:N	7:E:105:ASP:OD1	2.43	0.45
3:J:481:ASN:OD1	3:J:483:PRO:CD	2.42	0.45
3:J:1089:ASN:ND2	3:J:1092:ASN:ND2	2.64	0.45
3:J:1173:VAL:HG12	3:J:1194:THR:HG23	1.99	0.45
1:L:75:TYR:O	1:L:79:THR:HG23	2.17	0.45
5:B:118:LYS:HE3	5:B:118:LYS:HB2	1.85	0.45
6:G:173:ASP:OD1	6:G:173:ASP:N	2.47	0.44
10:D:5:SER:OG	10:D:7:TRP:NE1	2.46	0.44
10:D:21:TRP:HB3	10:D:24:ALA:HA	1.97	0.44
3:J:907:LYS:HD2	3:J:1097:ARG:CB	2.47	0.44
3:J:535:ARG:HH22	8:H:35:GLU:HB2	1.82	0.44
3:J:914:LEU:CB	3:J:1102:ARG:HH22	2.16	0.44
3:J:652:PHE:HD2	3:J:816:ILE:HG22	1.83	0.44
3:J:1104:PHE:O	3:J:1104:PHE:CD1	2.70	0.44
3:J:1181:LYS:HA	3:J:1181:LYS:HD3	1.80	0.44
5:B:146:LEU:HD22	5:B:156:ILE:HG22	2.00	0.44
1:L:46:ILE:HD11	7:E:43:VAL:HG12	2.00	0.44
2:I:774:GLU:HB3	2:I:785:LYS:HB3	1.99	0.44
3:J:764:ALA:HB1	3:J:786:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:893:PRO:HG2	3:J:953:THR:HA	2.00	0.44
2:I:464:LYS:HD2	2:I:464:LYS:HA	1.49	0.44
10:D:19:ARG:HH11	10:D:31:THR:HG23	1.82	0.44
10:D:44:LEU:HD13	10:D:44:LEU:HA	1.80	0.44
5:B:238:CYS:HB2	5:B:259:SER:HB2	1.99	0.44
7:E:171:ALA:O	7:E:175:ALA:HB2	2.18	0.44
9:A:73:SER:O	9:A:89:GLY:HA2	2.18	0.44
7:E:124:THR:HG22	10:D:67:ILE:HA	1.99	0.43
1:L:89:ALA:HB3	1:L:121:VAL:HG22	2.01	0.43
11:C:147:VAL:O	11:C:151:SER:CB	2.66	0.43
3:J:501:GLN:N	3:J:501:GLN:OE1	2.51	0.43
8:H:88:TYR:OH	8:H:130:MET:SD	2.65	0.43
10:D:115:VAL:HG11	10:D:125:PHE:HZ	1.82	0.43
10:D:127:GLU:O	10:D:128:ASN:HB2	2.18	0.43
9:A:103:GLU:O	9:A:107:GLN:OE1	2.37	0.43
2:I:461:GLN:C	2:I:463:ASN:H	2.22	0.43
2:I:745:SER:HA	2:I:757:GLU:HA	1.99	0.43
3:J:1089:ASN:HB3	3:J:1092:ASN:HD21	1.84	0.43
4:K:308:THR:HA	4:K:330:PRO:HA	2.01	0.43
3:J:517:MET:HA	3:J:520:VAL:HG12	2.00	0.43
2:I:598:ASP:HA	2:I:603:LYS:HA	2.01	0.43
2:I:768:GLN:O	2:I:791:SER:N	2.52	0.43
2:I:1033:GLY:HA2	2:I:1049:GLN:HA	2.01	0.43
4:K:214:ASN:HA	4:K:236:THR:HA	2.01	0.43
1:L:95:ILE:HD11	1:L:128:SER:HA	2.01	0.42
3:J:1099:TYR:HD1	3:J:1099:TYR:O	2.03	0.42
5:B:86:LYS:NZ	5:B:107:GLU:OE2	2.44	0.42
10:D:133:ARG:HG3	11:C:187:GLU:HG3	2.01	0.42
11:C:91:SER:O	11:C:102:THR:OG1	2.34	0.42
1:L:41:GLU:H	1:L:41:GLU:HG3	1.40	0.42
3:J:1182:VAL:HG13	3:J:1186:GLU:HB2	2.01	0.42
11:C:60:GLY:HA2	11:C:63:ILE:HG22	2.01	0.42
1:L:8:TYR:CE1	7:E:30:SER:HB2	2.54	0.42
3:J:972:ALA:HA	3:J:980:LEU:HG	2.01	0.42
5:B:108:LEU:HA	5:B:111:ALA:HB2	2.00	0.42
8:H:4:TYR:HE2	8:H:41:LEU:HD22	1.84	0.42
3:J:1010:SER:OG	4:K:423:LYS:CE	2.67	0.42
3:J:1023:MET:HA	3:J:1026:ILE:HG22	2.01	0.42
9:A:123:PRO:HD2	11:C:128:VAL:HG13	2.01	0.42
11:F:185:LYS:HE2	11:F:185:LYS:HB2	1.67	0.42
11:C:147:VAL:O	11:C:151:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:742:ASP:O	3:J:779:ARG:N	2.52	0.42
11:F:49:PHE:HA	11:F:52:VAL:HG22	2.01	0.42
3:J:501:GLN:N	3:J:501:GLN:CD	2.73	0.42
8:H:40:ILE:O	8:H:44:SER:OG	2.33	0.42
2:I:863:LYS:NZ	2:I:902:LYS:O	2.53	0.42
3:J:1092:ASN:N	3:J:1092:ASN:ND2	2.67	0.42
5:B:200:GLU:HA	10:D:141:THR:O	2.20	0.42
11:F:162:TRP:HE1	11:F:177:LYS:HD2	1.85	0.42
2:I:856:LYS:HE3	2:I:856:LYS:HB3	1.86	0.42
4:K:503:LEU:N	4:K:523:ARG:O	2.46	0.42
4:K:248:ILE:O	4:K:253:HIS:N	2.51	0.42
11:F:87:SER:HB2	11:F:105:ILE:HG12	2.02	0.42
11:F:184:LEU:HB3	11:F:185:LYS:H	1.63	0.42
3:J:510:GLN:HA	3:J:513:ILE:HG22	2.01	0.41
7:E:210:LYS:HA	7:E:210:LYS:HD2	1.88	0.41
1:L:13:LEU:HA	1:L:63:LYS:O	2.21	0.41
3:J:616:ILE:HG22	3:J:619:TYR:HE2	1.85	0.41
3:J:862:SER:HA	3:J:992:ARG:HB2	2.01	0.41
1:L:87:VAL:HG22	1:L:174:ILE:HD11	2.01	0.41
2:I:303:PHE:O	2:I:307:LYS:N	2.47	0.41
3:J:1103:GLN:O	3:J:1104:PHE:HB3	2.21	0.41
5:B:125:ASN:OD1	11:C:40:GLN:NE2	2.39	0.41
9:A:74:VAL:HA	9:A:88:ILE:O	2.21	0.41
10:D:44:LEU:O	10:D:48:ILE:HG12	2.20	0.41
1:L:169:GLU:OE1	3:J:698:VAL:HG12	2.17	0.41
3:J:481:ASN:CG	3:J:482:SER:N	2.72	0.41
3:J:915:TYR:N	3:J:1102:ARG:HH12	2.16	0.41
11:F:74:ARG:HH21	11:F:98:PHE:HE1	1.68	0.41
3:J:655:ARG:HA	3:J:655:ARG:HD2	1.73	0.41
3:J:762:ARG:HB3	3:J:789:LYS:HE3	2.02	0.41
3:J:905:TYR:HA	3:J:908:LYS:HB2	2.02	0.41
6:G:68:GLU:HG3	11:F:63:ILE:HG12	2.03	0.41
3:J:483:PRO:O	3:J:484:MET:SD	2.79	0.41
6:G:100:GLU:OE2	8:H:107:SER:N	2.50	0.41
2:I:332:THR:O	2:I:336:SER:N	2.53	0.41
2:I:982:PHE:HB2	2:I:1075:PHE:HA	2.03	0.41
8:H:5:PHE:HD1	8:H:113:MET:HB2	1.85	0.41
9:A:11:ILE:HB	9:A:85:LYS:HB2	2.02	0.41
9:A:42:ILE:HD12	9:A:42:ILE:HA	1.95	0.41
10:D:127:GLU:HB2	10:D:129:GLU:OE1	2.21	0.41
11:F:53:ASN:HD21	11:F:139:TRP:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:534:LEU:HB3	3:J:561:ILE:HD12	2.03	0.41
3:J:1010:SER:OG	4:K:423:LYS:NZ	2.53	0.41
6:G:53:LYS:HE2	6:G:53:LYS:HB2	1.83	0.41
2:I:273:ASP:O	2:I:277:LEU:N	2.53	0.40
3:J:485:PHE:N	3:J:486:PRO:CD	2.84	0.40
3:J:492:PHE:HE1	3:J:529:LYS:HZ2	1.69	0.40
3:J:1002:ILE:HG12	3:J:1164:ILE:HD11	2.03	0.40
7:E:53:LYS:HZ3	7:E:53:LYS:N	2.19	0.40
4:K:437:SER:HA	4:K:440:PRO:HB3	2.03	0.40
6:G:172:ARG:HH21	8:H:86:ASN:HB3	1.85	0.40
3:J:738:PRO:HG2	3:J:784:PRO:HB2	2.04	0.40
3:J:1098:ILE:CD1	3:J:1099:TYR:CG	2.96	0.40
2:I:336:SER:O	2:I:340:PHE:N	2.54	0.40
3:J:600:ARG:NH1	3:J:603:ASN:OD1	2.45	0.40
9:A:8:VAL:HG12	9:A:88:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	192/222 (86%)	170 (88%)	17 (9%)	5 (3%)	5	36
2	I	782/1102 (71%)	649 (83%)	120 (15%)	13 (2%)	9	43
3	J	868/1289 (67%)	730 (84%)	129 (15%)	9 (1%)	15	52
4	K	243/560 (43%)	205 (84%)	33 (14%)	5 (2%)	7	40
5	B	191/268 (71%)	172 (90%)	19 (10%)	0	100	100
6	G	198/283 (70%)	181 (91%)	17 (9%)	0	100	100
7	E	155/219 (71%)	140 (90%)	13 (8%)	2 (1%)	12	48
8	H	143/175 (82%)	134 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A	142/152 (93%)	131 (92%)	11 (8%)	0	100	100
10	D	154/159 (97%)	139 (90%)	14 (9%)	1 (1%)	25	62
11	C	183/193 (95%)	165 (90%)	17 (9%)	1 (0%)	29	66
11	F	181/193 (94%)	162 (90%)	19 (10%)	0	100	100
All	All	3432/4815 (71%)	2978 (87%)	418 (12%)	36 (1%)	20	52

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	42	SER
1	L	199	PRO
2	I	346	PRO
2	I	483	PRO
2	I	976	PRO
3	J	956	PRO
4	K	325	PRO
4	K	330	PRO
7	E	53	LYS
10	D	128	ASN
11	C	46	GLU
1	L	38	PHE
1	L	179	SER
2	I	252	PRO
2	I	495	VAL
2	I	980	PRO
2	I	1076	PRO
3	J	486	PRO
2	I	343	VAL
2	I	466	SER
2	I	251	VAL
2	I	735	ILE
3	J	409	LEU
4	K	310	PRO
1	L	48	VAL
3	J	666	ASP
3	J	1014	GLU
3	J	1102	ARG
4	K	286	PRO
3	J	672	ILE
3	J	738	PRO
4	K	331	VAL

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Mol	Chain	Res	Type
2	I	1029	ILE
3	J	886	ILE
7	E	68	PRO
2	I	647	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	L	152/189 (80%)	125 (82%)	27 (18%)	2	12
2	I	78/1023 (8%)	77 (99%)	1 (1%)	69	82
3	J	594/1213 (49%)	573 (96%)	21 (4%)	36	64
4	K	121/518 (23%)	121 (100%)	0	100	100
5	B	176/248 (71%)	175 (99%)	1 (1%)	86	92
6	G	179/249 (72%)	179 (100%)	0	100	100
7	E	149/199 (75%)	140 (94%)	9 (6%)	19	50
8	H	127/152 (84%)	125 (98%)	2 (2%)	62	79
9	A	134/142 (94%)	131 (98%)	3 (2%)	52	72
10	D	142/145 (98%)	124 (87%)	18 (13%)	4	23
11	C	170/178 (96%)	168 (99%)	2 (1%)	71	84
11	F	169/178 (95%)	165 (98%)	4 (2%)	49	71
All	All	2191/4434 (49%)	2103 (96%)	88 (4%)	35	59

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	38	PHE
1	L	40	ILE
1	L	41	GLU
1	L	42	SER
1	L	44	SER
1	L	45	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	49	GLU
1	L	50	PHE
1	L	54	THR
1	L	61	LYS
1	L	63	LYS
1	L	66	ILE
1	L	69	THR
1	L	73	GLU
1	L	74	ARG
1	L	76	ARG
1	L	105	ASN
1	L	106	HIS
1	L	130	LEU
1	L	132	HIS
1	L	134	ARG
1	L	153	THR
1	L	154	GLU
1	L	160	SER
1	L	176	GLN
1	L	180	LYS
1	L	182	GLN
2	I	464	LYS
3	J	484	MET
3	J	500	LEU
3	J	501	GLN
3	J	655	ARG
3	J	697	GLU
3	J	698	VAL
3	J	699	PHE
3	J	702	PHE
3	J	789	LYS
3	J	1011	SER
3	J	1012	GLN
3	J	1035	ARG
3	J	1093	THR
3	J	1097	ARG
3	J	1099	TYR
3	J	1104	PHE
3	J	1105	ILE
3	J	1106	GLN
3	J	1107	SER
3	J	1111	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	J	1113	GLN
5	B	181	ARG
7	E	22	THR
7	E	25	GLU
7	E	27	LYS
7	E	28	LEU
7	E	29	ASN
7	E	31	ASN
7	E	53	LYS
7	E	56	GLN
7	E	65	ASN
8	H	12	ASP
8	H	91	LYS
9	A	35	LYS
9	A	77	MET
9	A	93	LYS
10	D	20	GLU
10	D	22	THR
10	D	23	LEU
10	D	26	ASN
10	D	29	SER
10	D	33	ASN
10	D	34	SER
10	D	35	LYS
10	D	36	GLN
10	D	37	ASN
10	D	38	GLU
10	D	39	GLU
10	D	43	LEU
10	D	44	LEU
10	D	137	THR
10	D	138	ARG
10	D	139	LYS
10	D	140	ILE
11	F	183	ILE
11	F	184	LEU
11	F	185	LYS
11	F	186	ASP
11	C	24	LYS
11	C	62	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	J	736	GLN
3	J	1092	ASN
3	J	1103	GLN
7	E	65	ASN
7	E	113	ASN
10	D	37	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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.

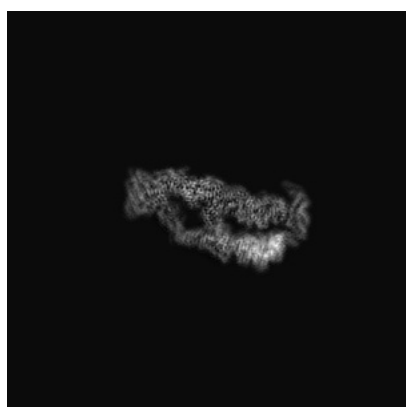
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31022. These allow visual inspection of the internal detail of the map and identification of artifacts.

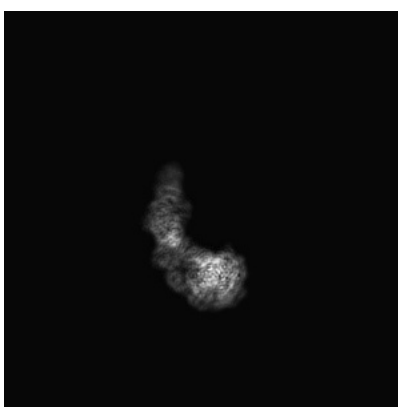
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 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](#)

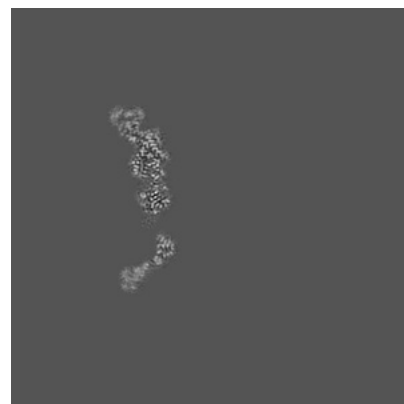
#### 6.2.1 Primary map



X Index: 300



Y Index: 300



Z Index: 300



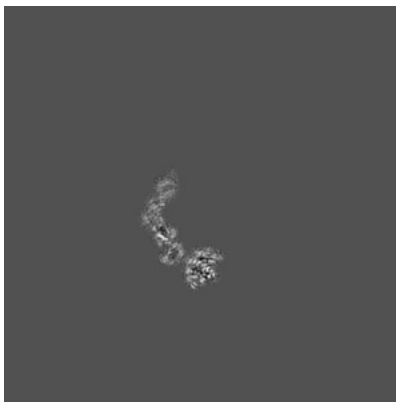
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

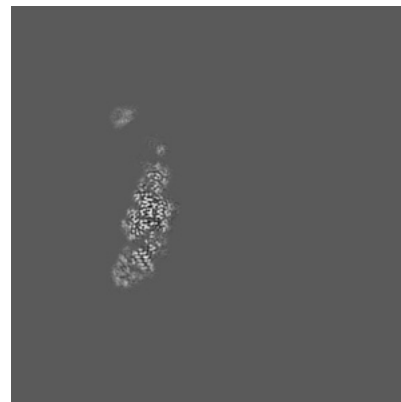
### 6.3.1 Primary map



X Index: 203



Y Index: 378

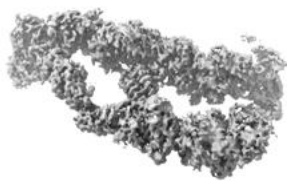


Z Index: 327

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 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

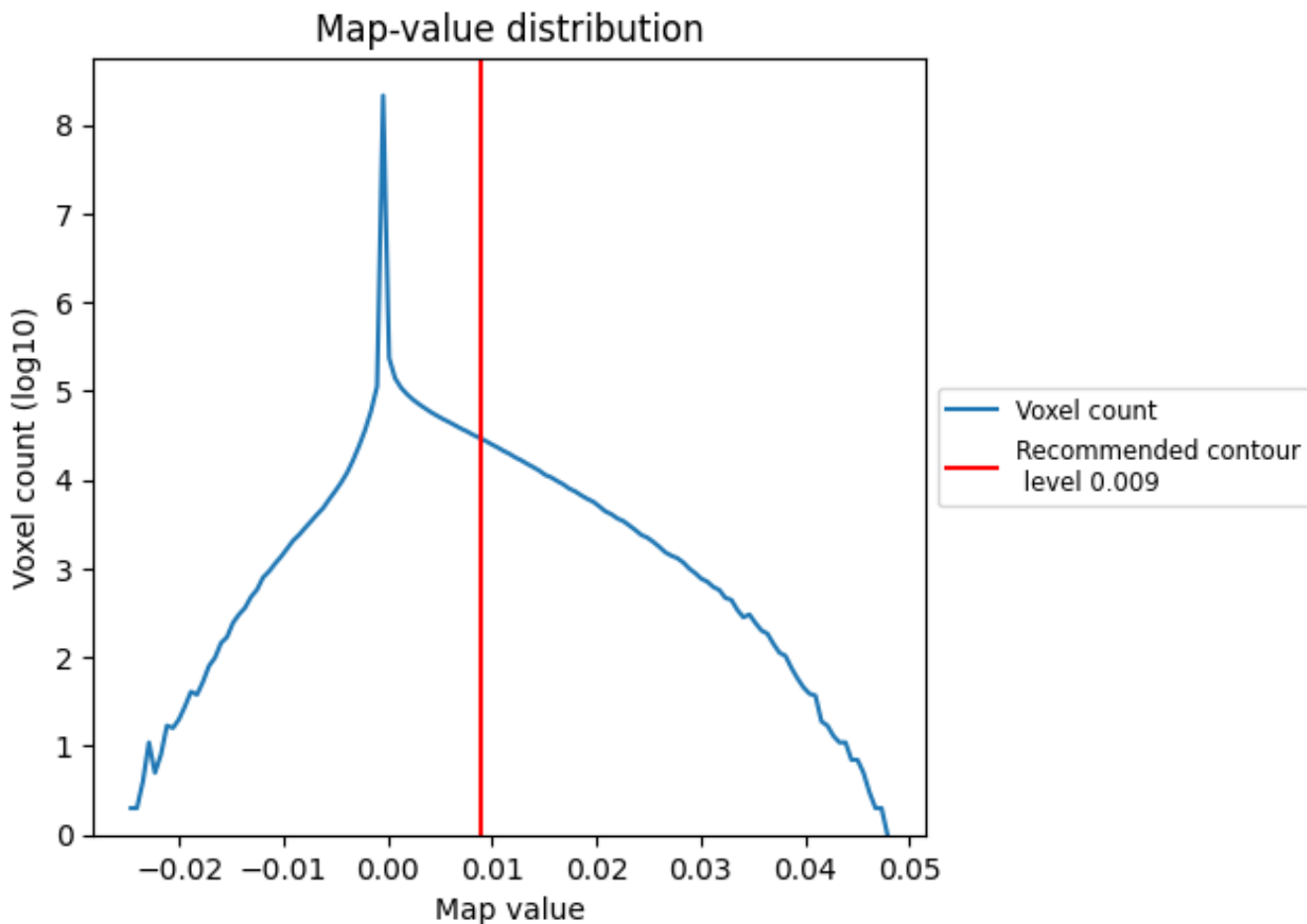
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

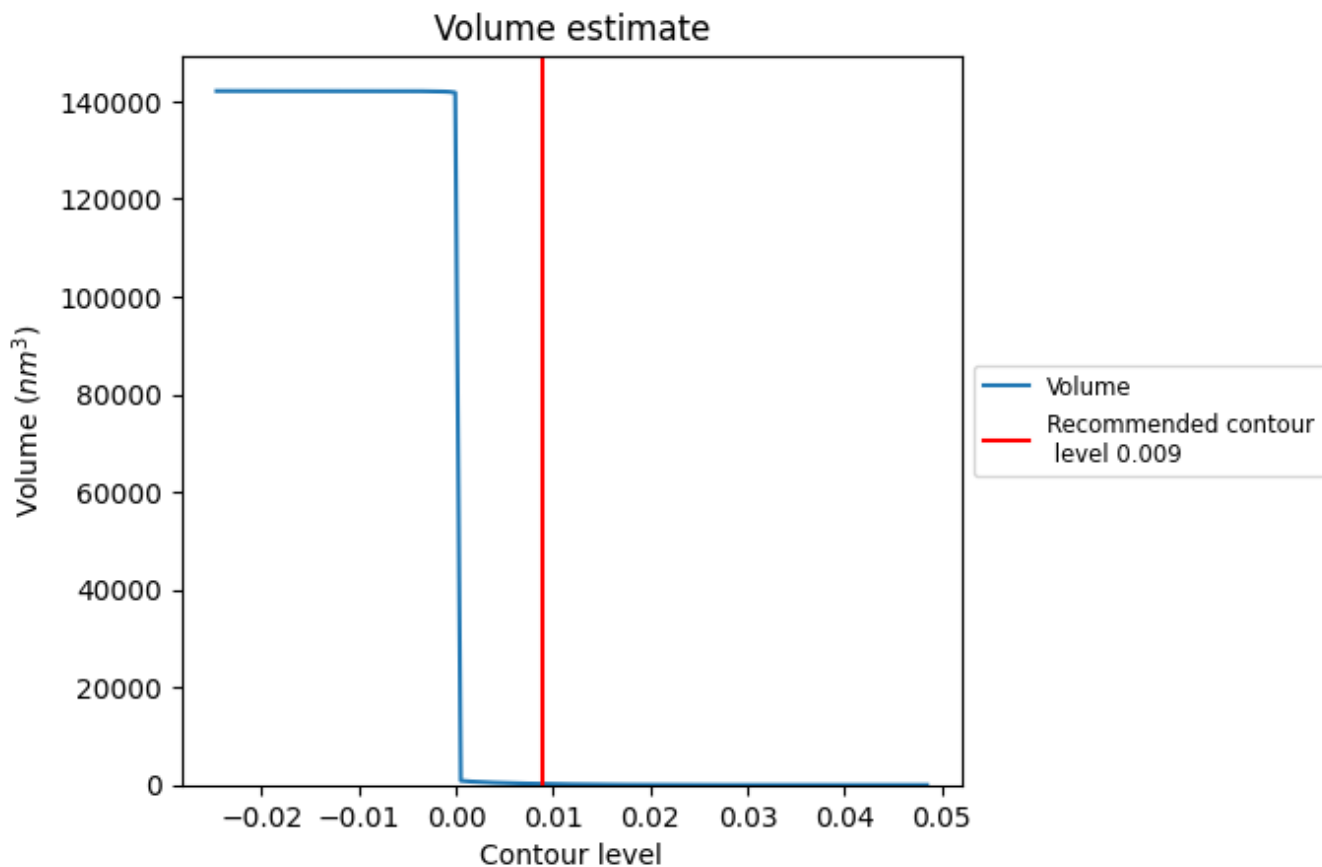
This section contains the results of statistical analysis of the map.

### 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.

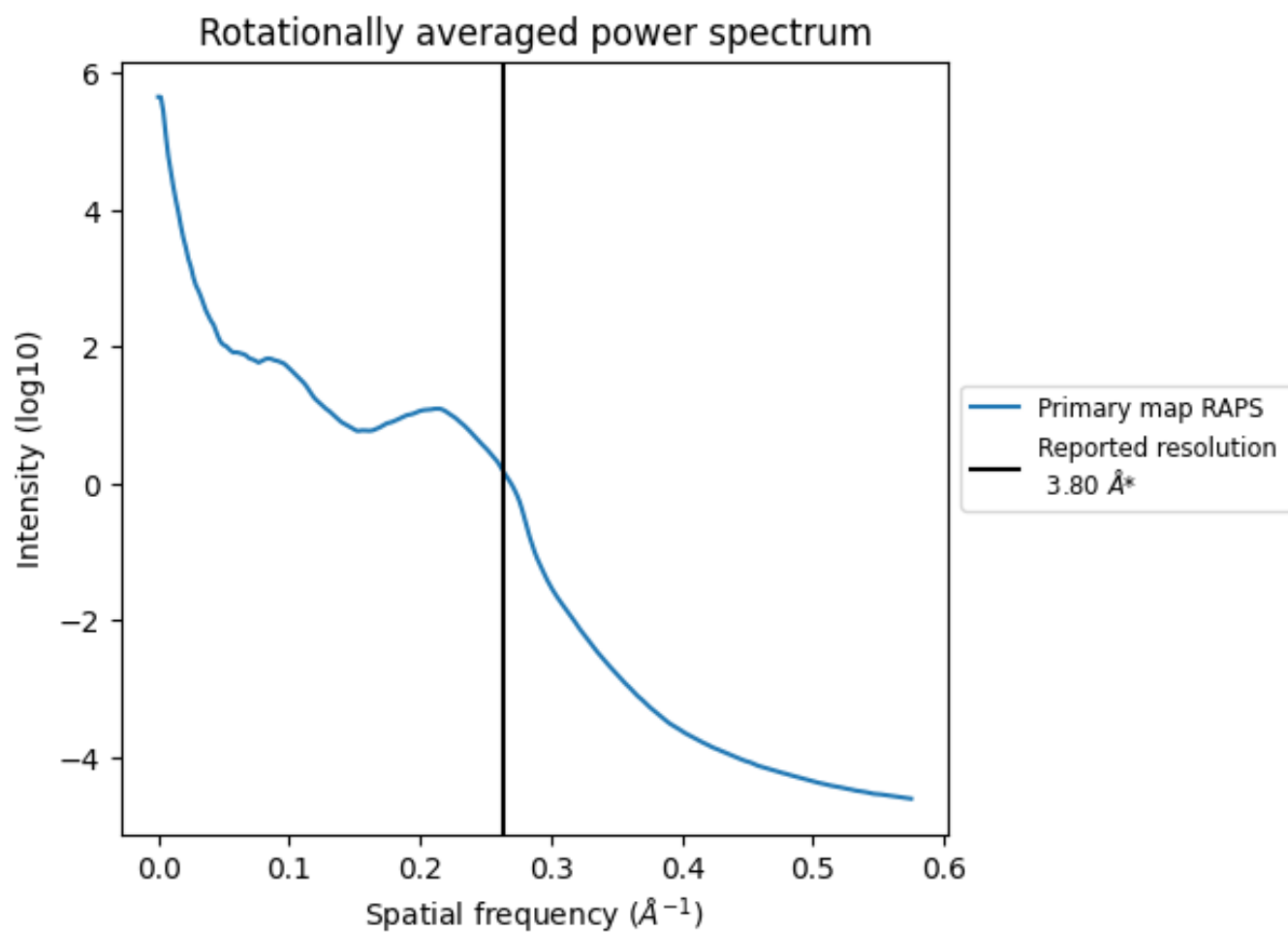
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 220 nm<sup>3</sup>; this corresponds to an approximate mass of 198 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  $0.263 \text{\AA}^{-1}$

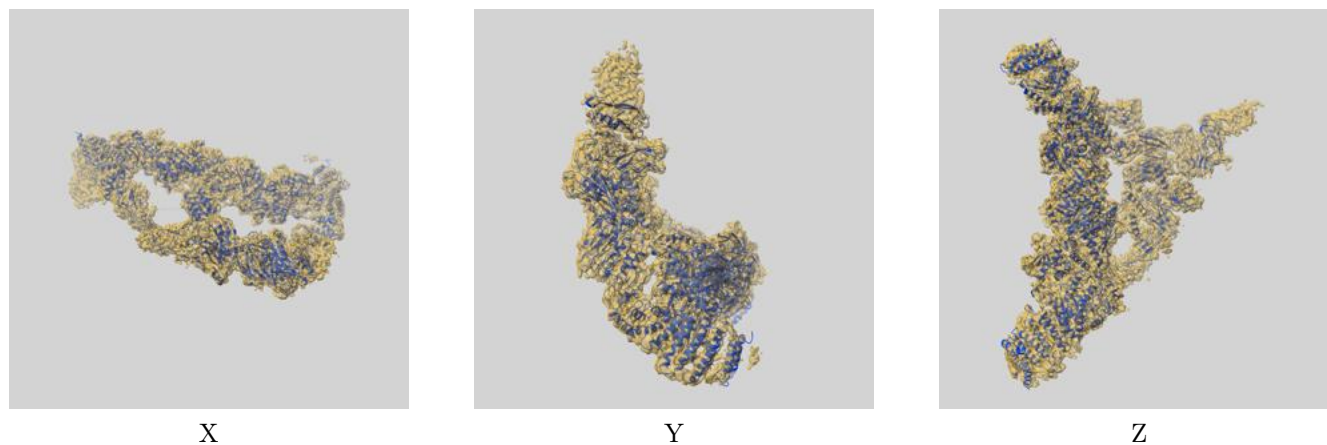
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31022 and PDB model 7E8T. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



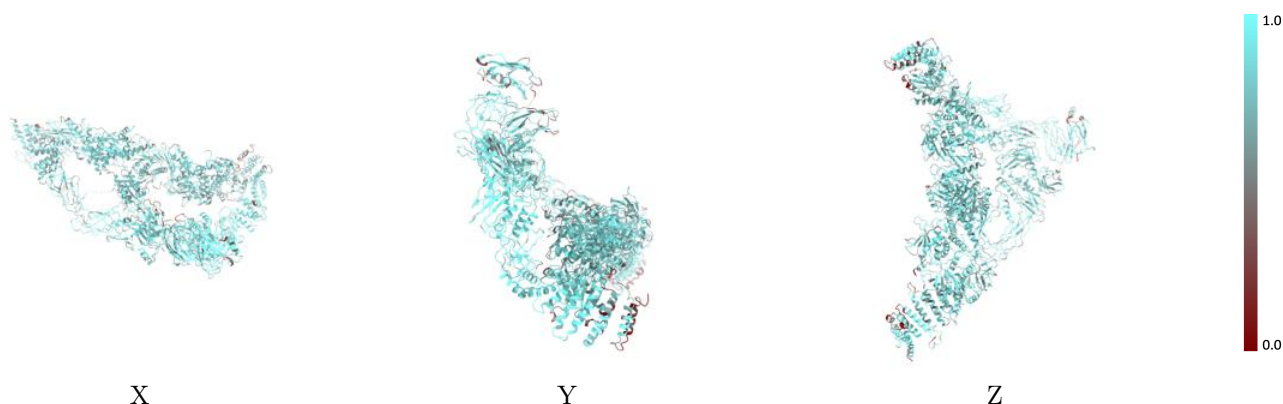
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

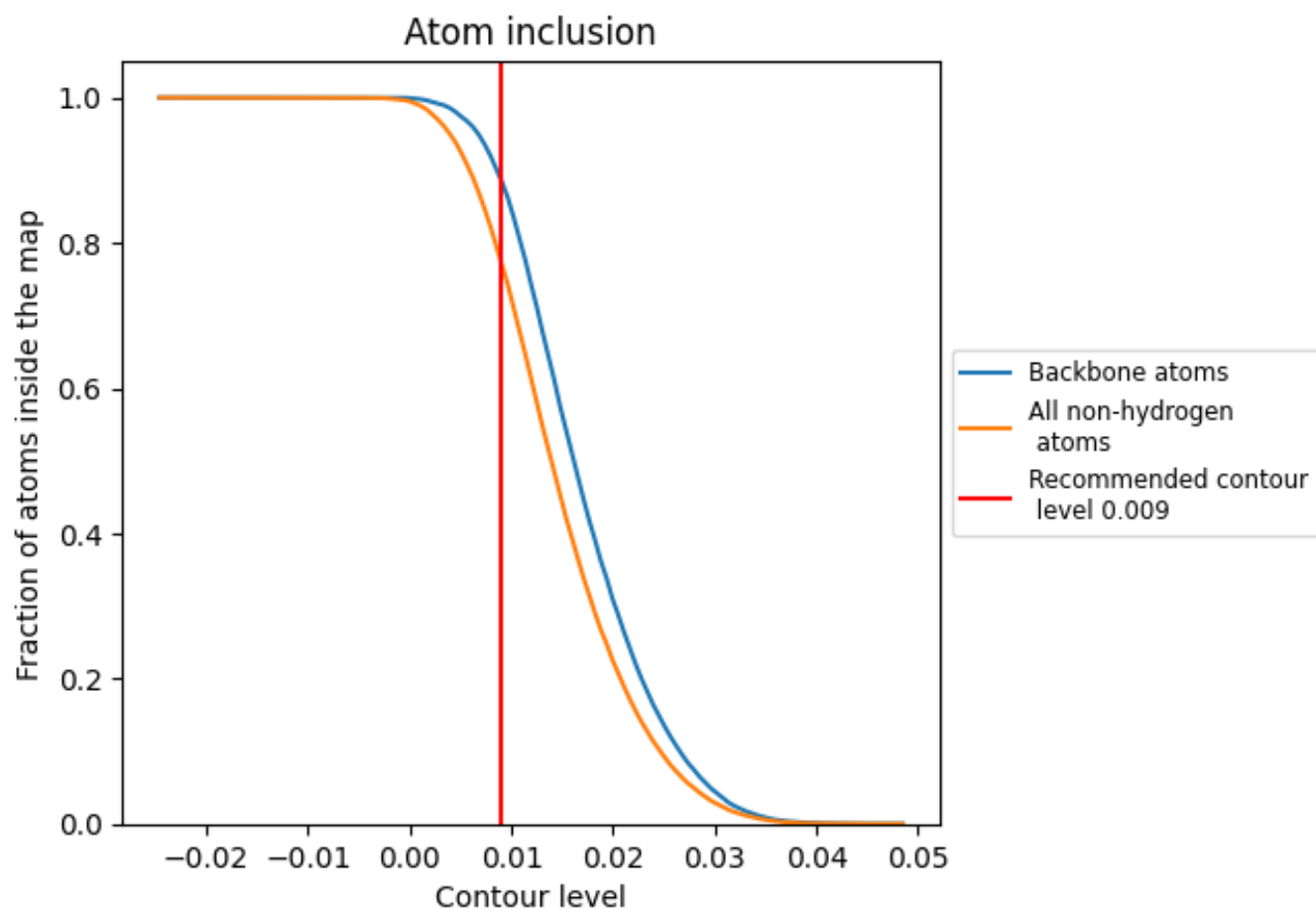
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.009).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 77% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7731	 0.3940
A	 0.6207	 0.3760
B	 0.7399	 0.3940
C	 0.7866	 0.4330
D	 0.8119	 0.4220
E	 0.8114	 0.4520
F	 0.7993	 0.4340
G	 0.8049	 0.4390
H	 0.8034	 0.4210
I	 0.8459	 0.3710
J	 0.7532	 0.3700
K	 0.7052	 0.3390
L	 0.7167	 0.4070

