



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:14 AM UTC

PDB ID : 8KEG / pdb_00008keg
EMDB ID : EMD-37155
Title : Cyanophage A-1(L) neck/gp5-neck fiber
Authors : Yu, R.C.; Li, Q.; Zhou, C.Z.
Deposited on : 2023-08-11
Resolution : 3.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

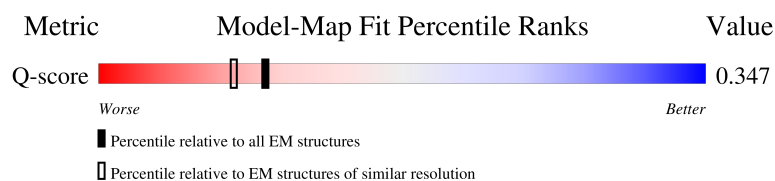
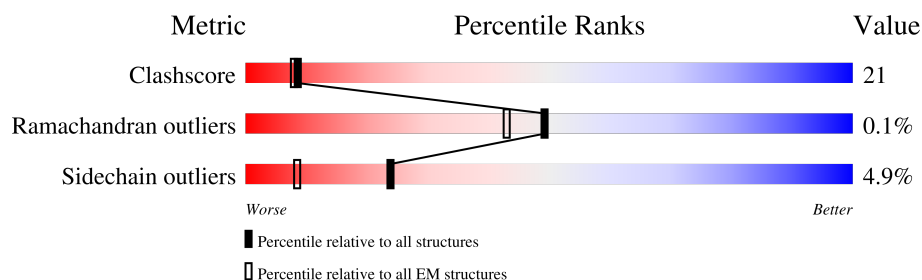
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.66 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.



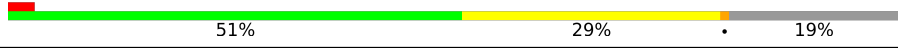
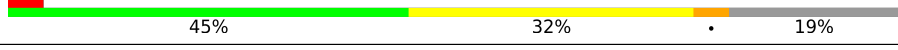
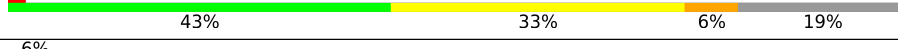
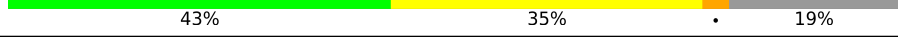
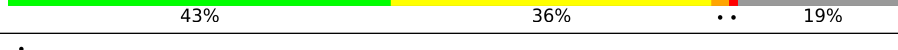
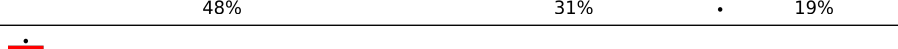
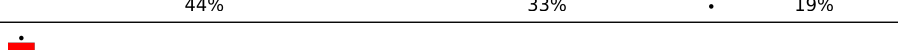
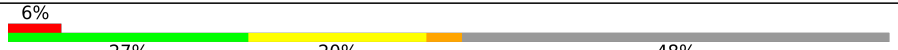
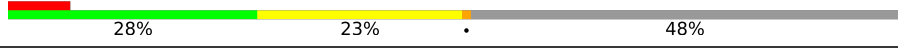
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11491 (3.16 - 4.16)

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	162	 41% 38% 19%
1	B	162	 5% 44% 33% 19%
1	C	162	 46% 31% 19%
1	D	162	 5% 52% 25% 5% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	162	
1	F	162	
1	G	162	
1	H	162	
1	I	162	
1	J	162	
1	K	162	
1	L	162	
1	M	162	
1	N	162	
1	O	162	
2	a	241	
2	b	241	
2	c	241	
2	d	241	
2	e	241	
2	f	241	
2	g	241	
2	h	241	
2	i	241	
2	j	241	
2	k	241	
2	l	241	
2	m	241	
2	n	241	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	o	241	6%27%23%48%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30930 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.

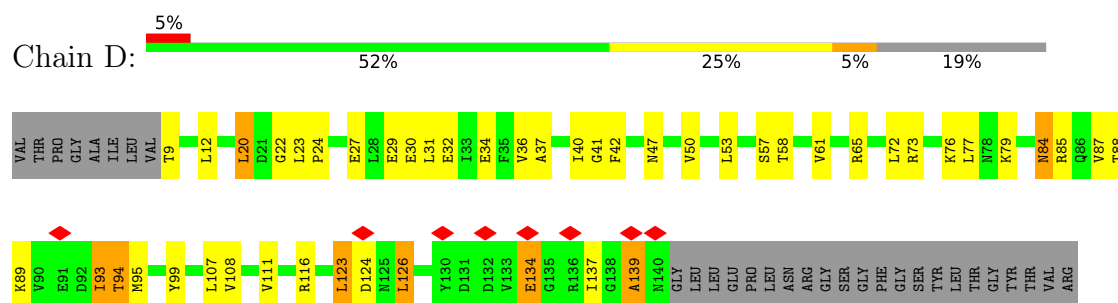
- Molecule 1 is a protein called Neck gp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	B	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	C	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	D	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	E	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	F	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	G	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	H	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	I	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	J	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	K	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	L	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	M	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	N	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		
1	O	132	Total	C	N	O	S	0	0
			1066	677	173	212	4		

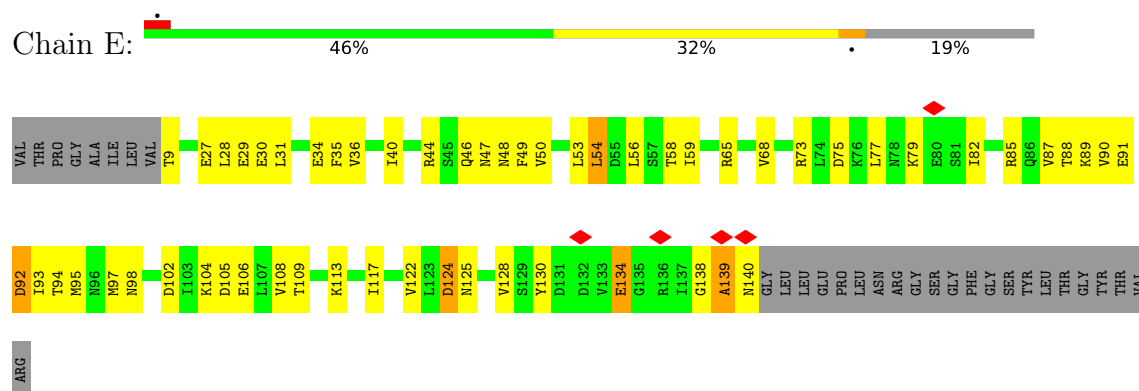
- Molecule 2 is a protein called neck fiber gp82N.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	b	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	c	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	d	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	e	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	f	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	g	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	h	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	i	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	j	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	k	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	l	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	m	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	n	125	Total 996	C 631	N 165	O 199	S 1	0	0
2	o	125	Total 996	C 631	N 165	O 199	S 1	0	0

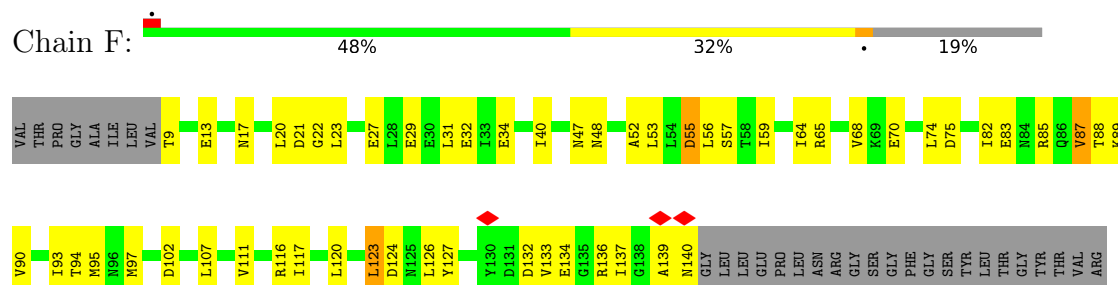
- Molecule 1: Neck gp5



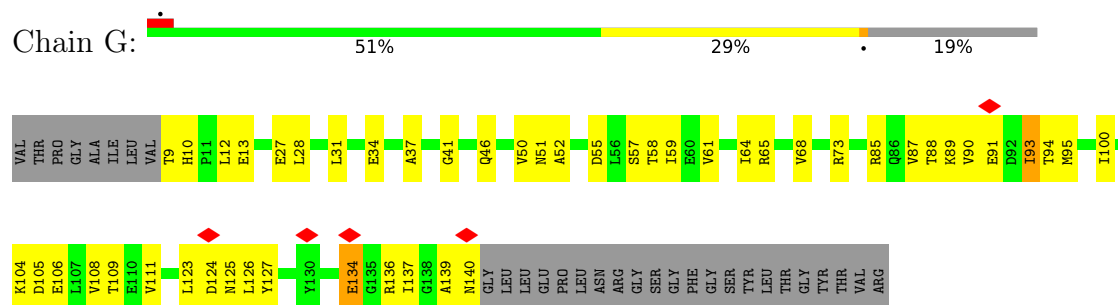
- Molecule 1: Neck gp5



- Molecule 1: Neck gp5

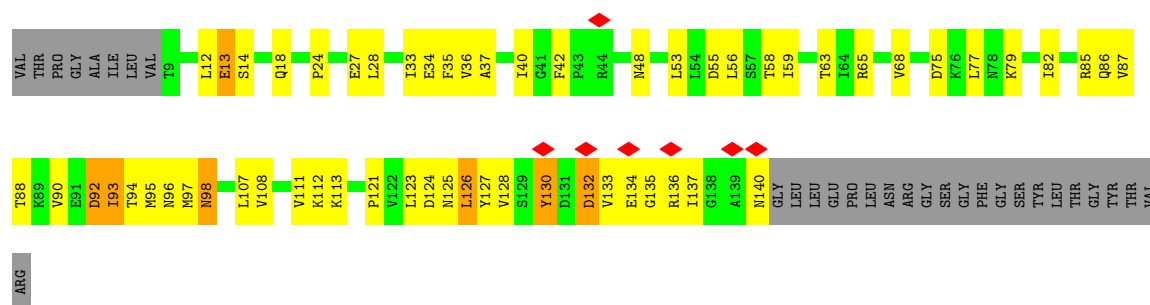


- Molecule 1: Neck gp5

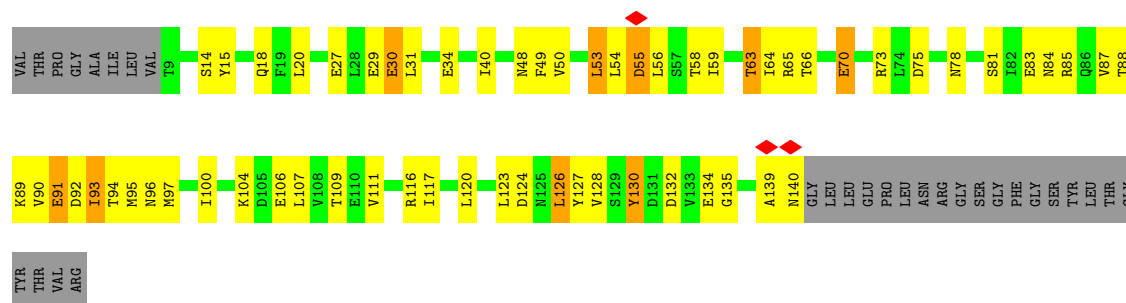


- Molecule 1: Neck gp5

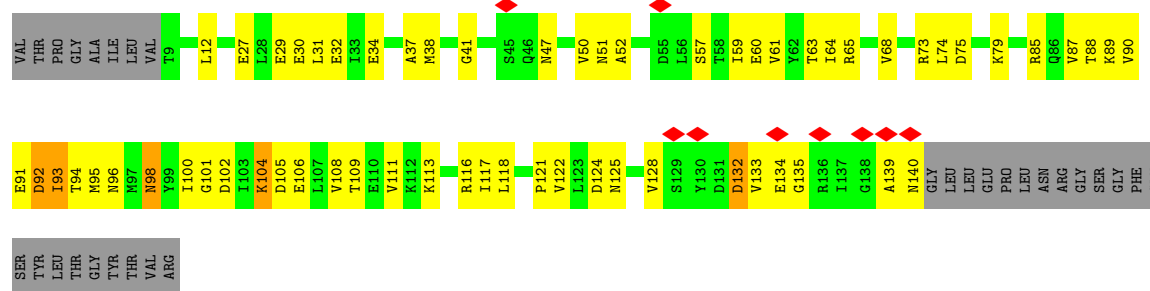
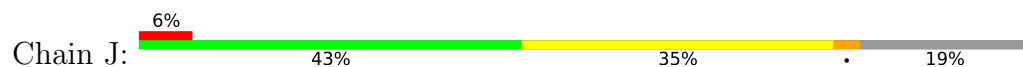




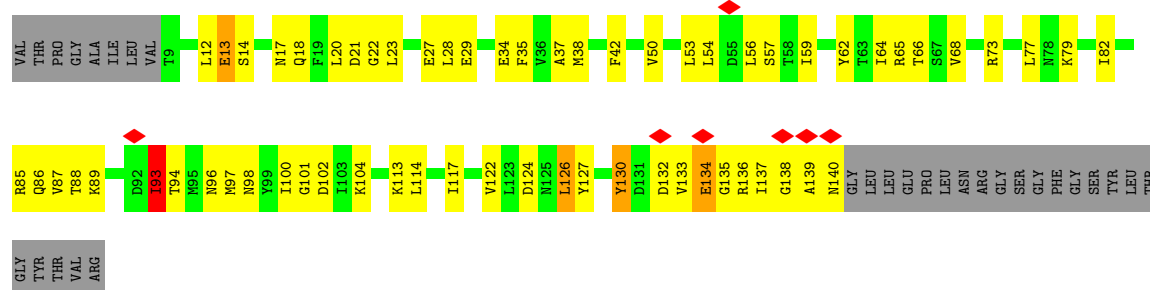
• Molecule 1: Neck gp5



• Molecule 1: Neck gp5

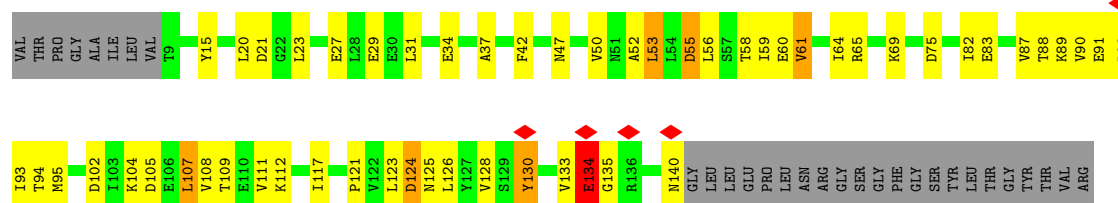


• Molecule 1: Neck gp5



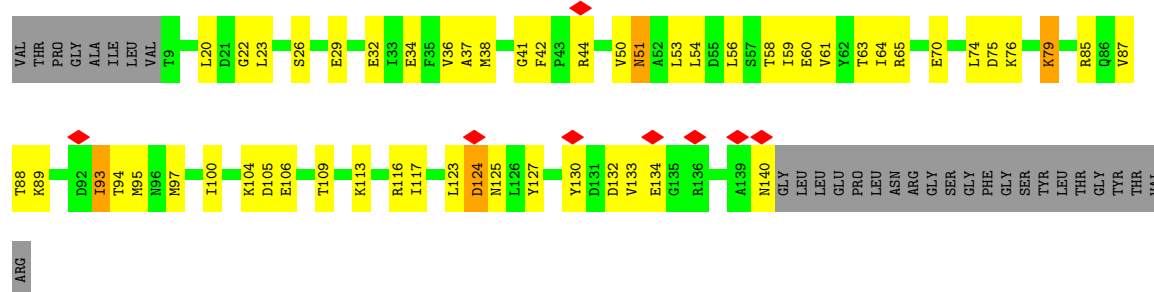
- Molecule 1: Neck gp5

Chain L: 



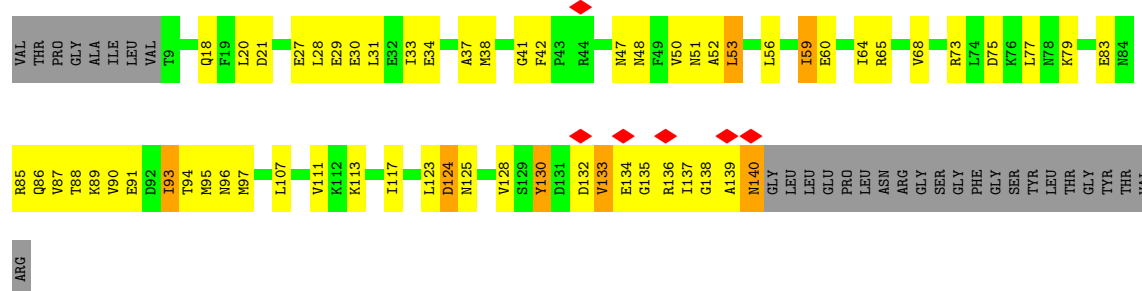
- Molecule 1: Neck gp5

Chain M: 



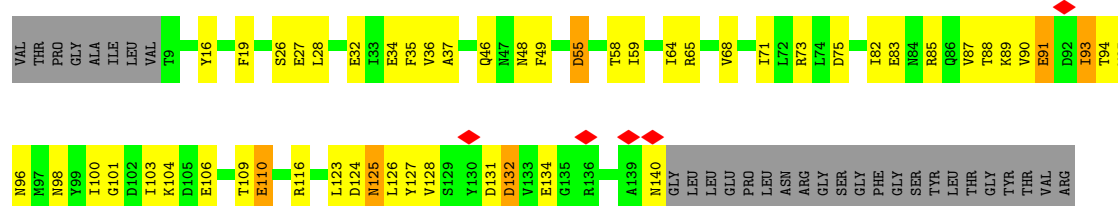
- Molecule 1: Neck gp5

Chain N: 



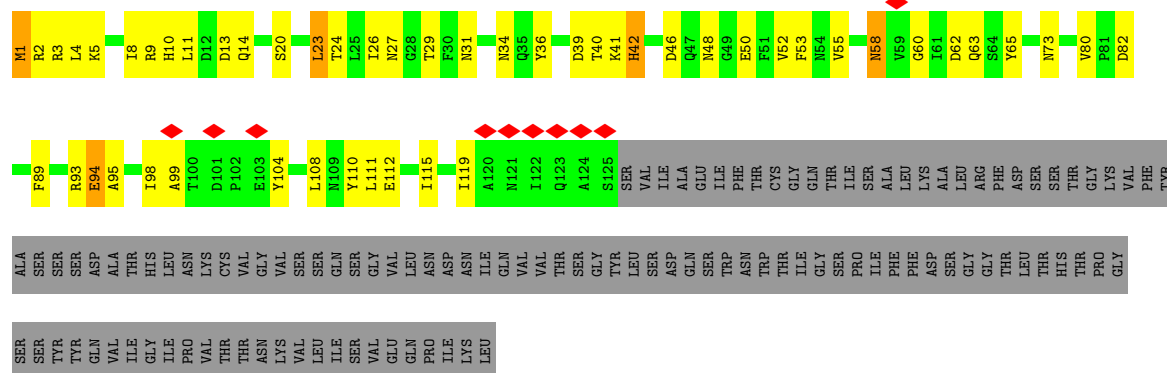
- Molecule 1: Neck gp5

Chain O: 



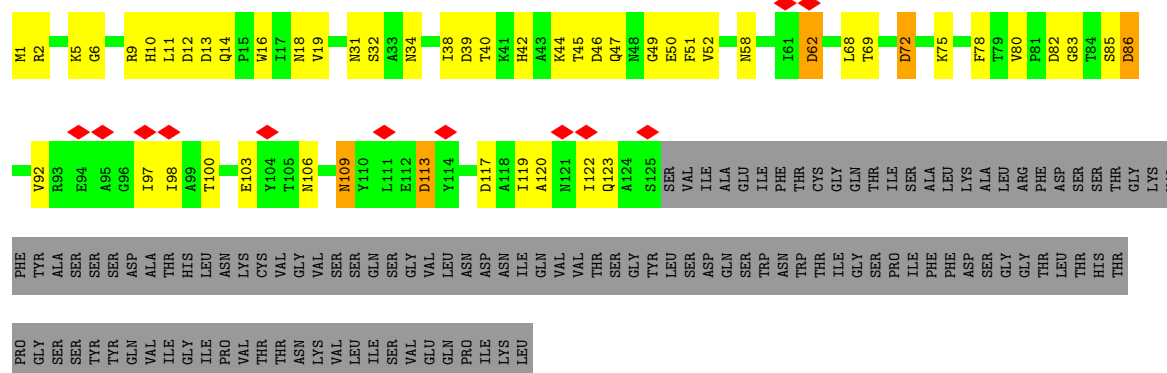
- Molecule 2: neck fiber gp82N

Chain a: 



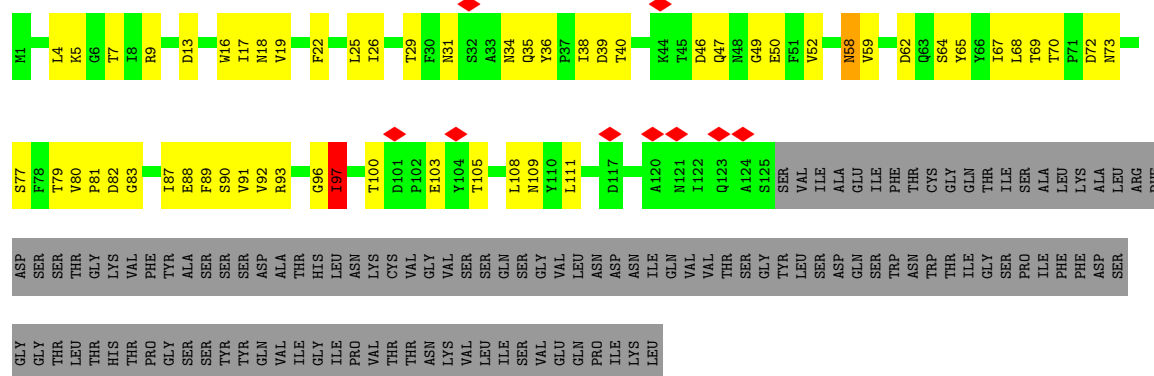
• Molecule 2: neck fiber gp82N

Chain b: 



• Molecule 2: neck fiber gp82N

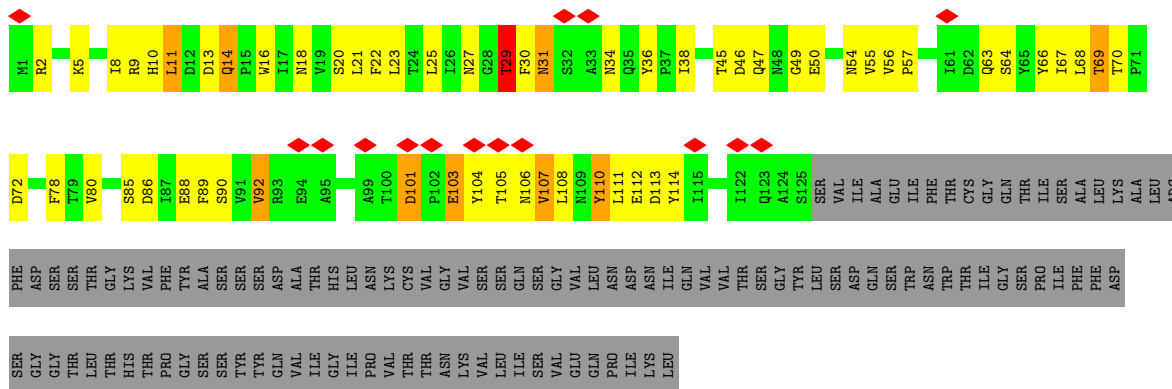
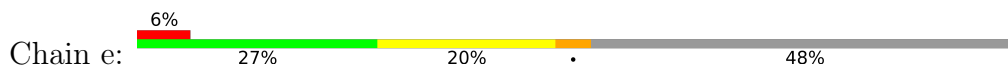
Chain c: 



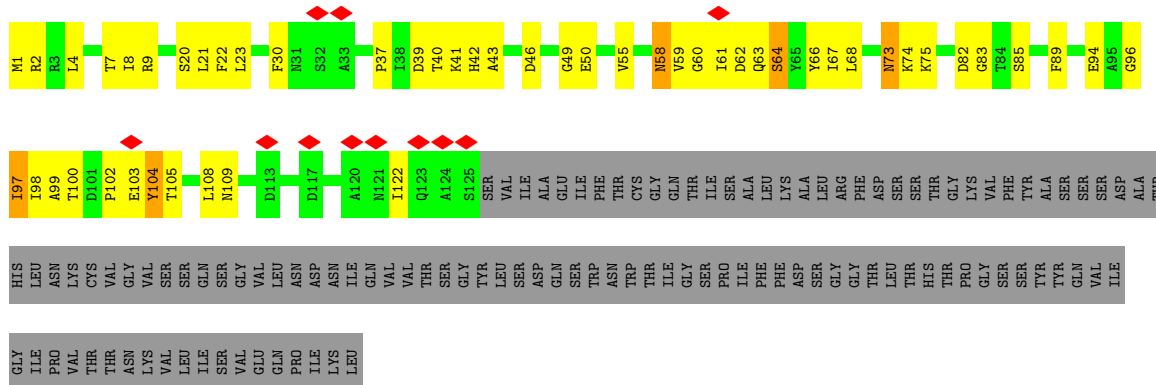
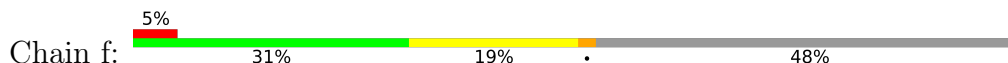
• Molecule 2: neck fiber gp82N

Chain d: 

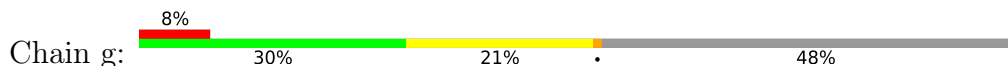
- Molecule 2: neck fiber gp82N

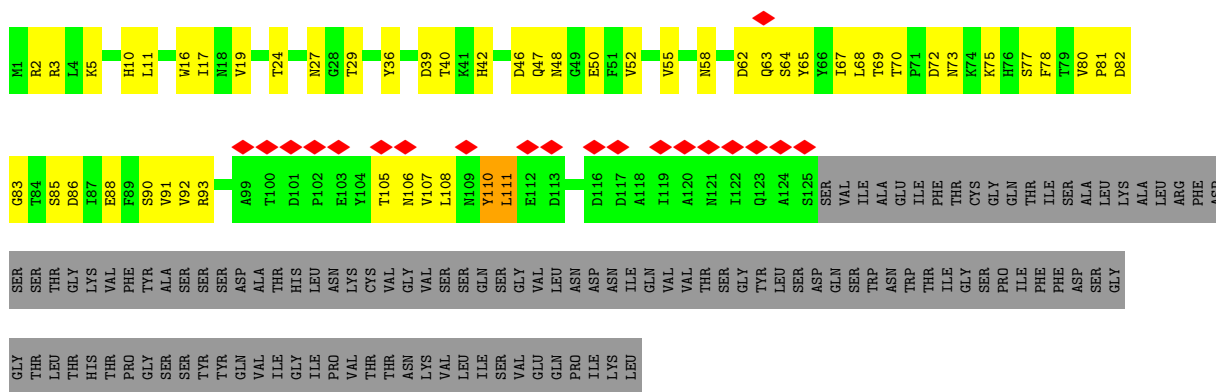


- Molecule 2: neck fiber gp82N

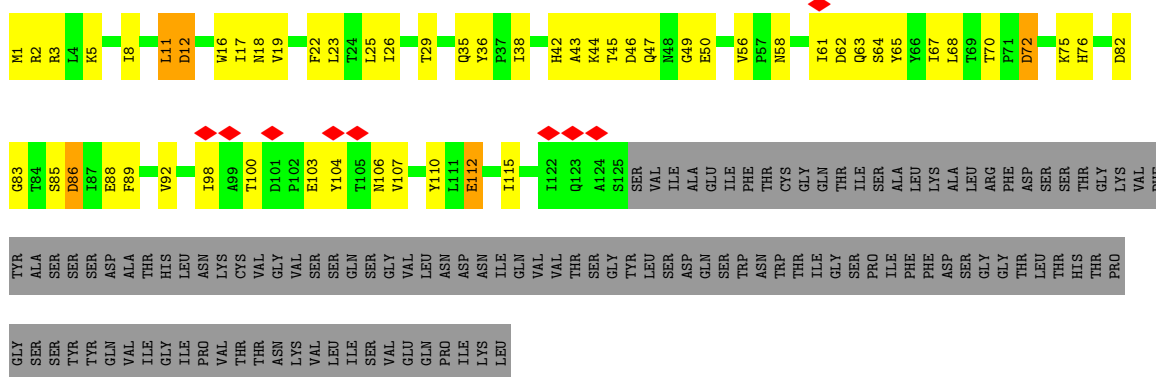
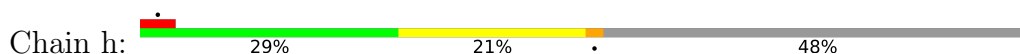


- Molecule 2: neck fiber gp82N

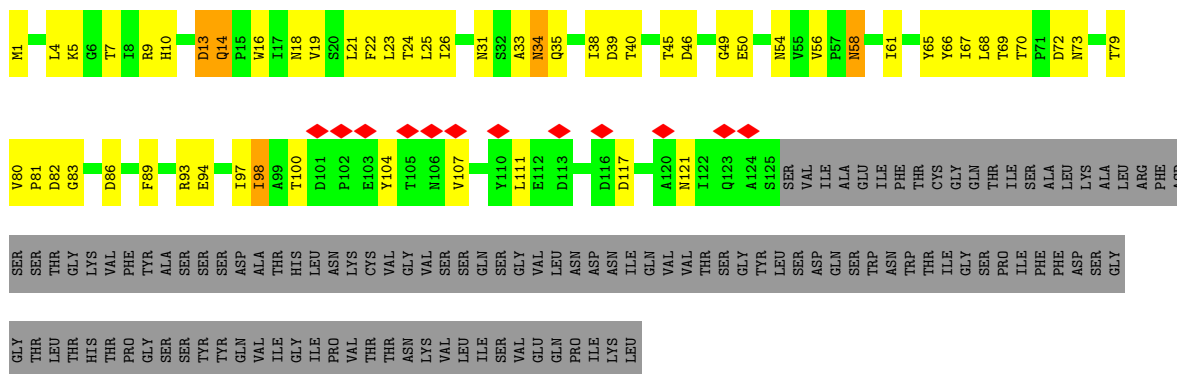
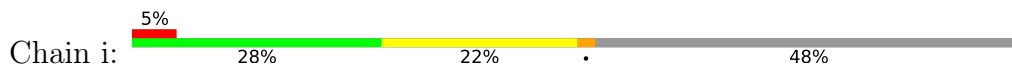




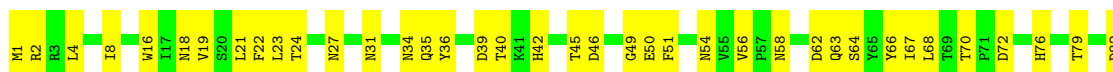
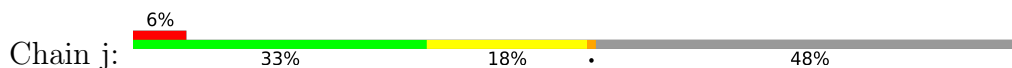
- Molecule 2: neck fiber gp82N

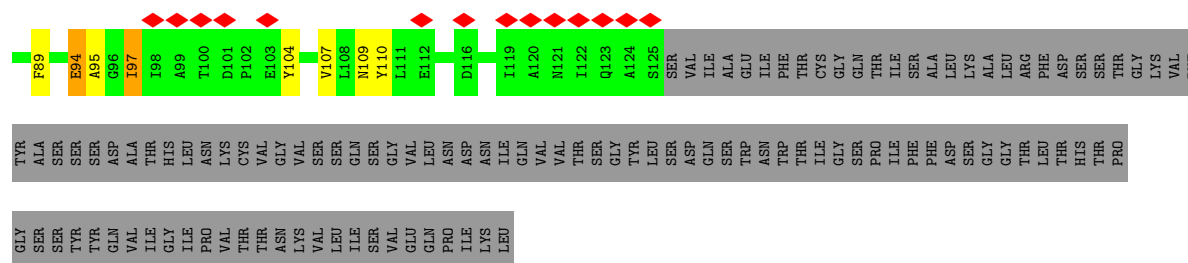


- Molecule 2: neck fiber gp82N

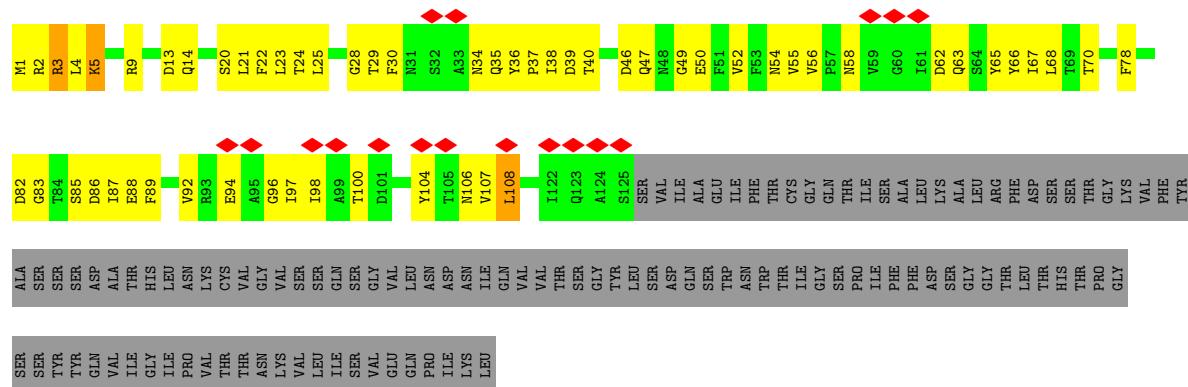
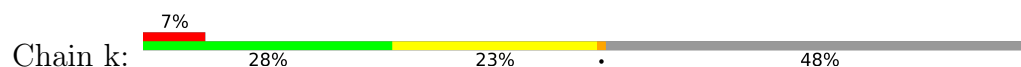


- Molecule 2: neck fiber gp82N

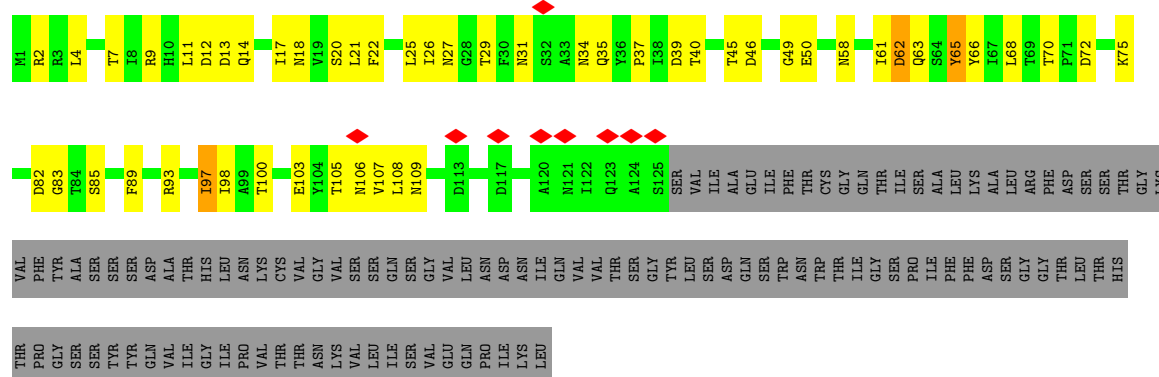
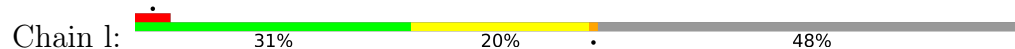




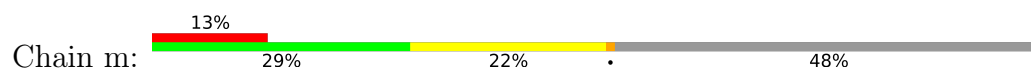
• Molecule 2: neck fiber gp82N



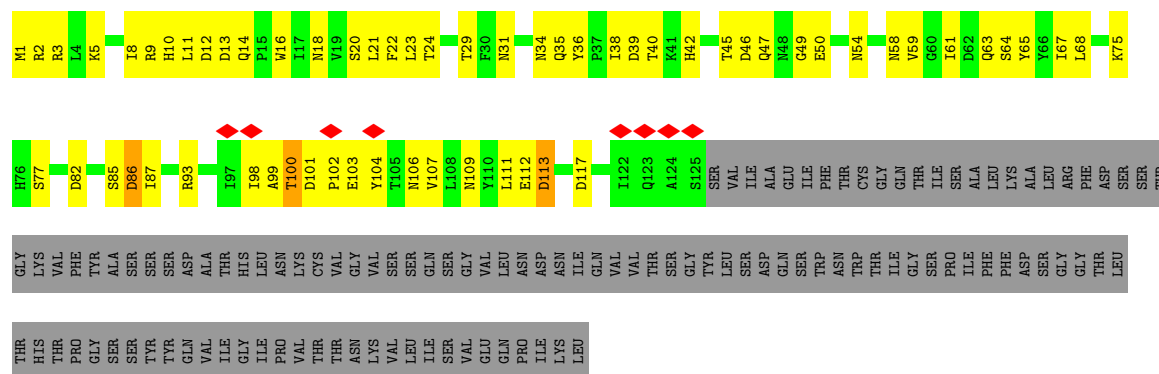
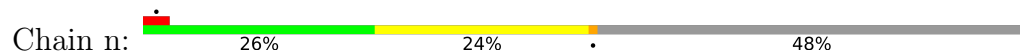
• Molecule 2: neck fiber gp82N



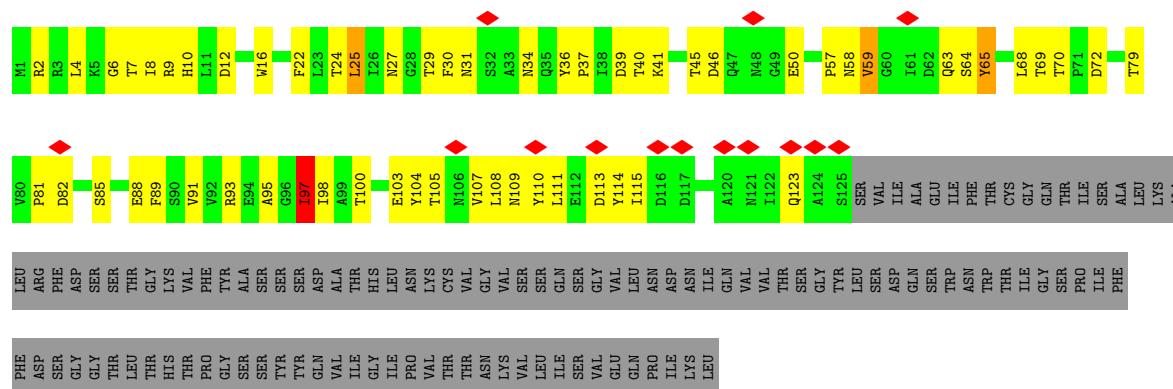
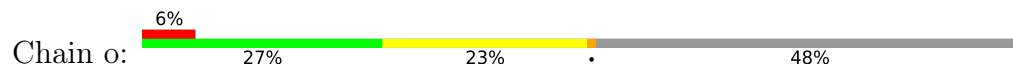
• Molecule 2: neck fiber gp82N



- Molecule 2: neck fiber gp82N



- Molecule 2: neck fiber gp82N



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36158	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.013	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size ($\text{\AA}$)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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	0.16	0/1080	0.65	5/1462 (0.3%)
1	B	0.16	0/1080	0.65	5/1462 (0.3%)
1	C	0.15	0/1080	0.52	2/1462 (0.1%)
1	D	0.16	0/1080	0.63	4/1462 (0.3%)
1	E	0.15	0/1080	0.60	4/1462 (0.3%)
1	F	0.18	0/1080	0.56	2/1462 (0.1%)
1	G	0.15	0/1080	0.60	4/1462 (0.3%)
1	H	0.15	0/1080	0.57	2/1462 (0.1%)
1	I	0.15	0/1080	0.50	3/1462 (0.2%)
1	J	0.15	0/1080	0.53	3/1462 (0.2%)
1	K	0.15	0/1080	0.66	5/1462 (0.3%)
1	L	0.15	0/1080	0.65	4/1462 (0.3%)
1	M	0.16	0/1080	0.67	5/1462 (0.3%)
1	N	0.16	0/1080	0.59	4/1462 (0.3%)
1	O	0.16	0/1080	0.52	2/1462 (0.1%)
2	a	0.15	0/1018	0.37	0/1390
2	b	0.17	0/1018	0.48	2/1390 (0.1%)
2	c	0.17	0/1018	0.42	1/1390 (0.1%)
2	d	0.15	0/1018	0.57	3/1390 (0.2%)
2	e	0.16	0/1018	0.62	4/1390 (0.3%)
2	f	0.17	0/1018	0.44	1/1390 (0.1%)
2	g	0.17	0/1018	0.43	0/1390
2	h	0.15	0/1018	0.54	3/1390 (0.2%)
2	i	0.17	0/1018	0.44	0/1390
2	j	0.15	0/1018	0.37	0/1390
2	k	0.15	0/1018	0.35	0/1390
2	l	0.16	0/1018	0.53	3/1390 (0.2%)
2	m	0.15	0/1018	0.36	0/1390
2	n	0.17	0/1018	0.86	8/1390 (0.6%)
2	o	0.17	0/1018	0.66	3/1390 (0.2%)
All	All	0.16	0/31470	0.56	82/42780 (0.2%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	93	ARG	CA-C-N	11.69	141.60	121.14
2	n	93	ARG	C-N-CA	11.69	141.60	121.14
2	o	57	PRO	CA-C-N	11.63	139.21	120.60
2	o	57	PRO	C-N-CA	11.63	139.21	120.60
1	H	124	ASP	CA-C-N	11.09	139.75	122.11
1	H	124	ASP	C-N-CA	11.09	139.75	122.11
1	L	134	GLU	CA-C-N	11.01	142.99	121.41
1	L	134	GLU	C-N-CA	11.01	142.99	121.41
2	d	95	ALA	CA-C-N	10.66	142.30	121.41
2	d	95	ALA	C-N-CA	10.66	142.30	121.41
2	n	99	ALA	CA-C-N	10.44	143.01	122.03
2	n	99	ALA	C-N-CA	10.44	143.01	122.03
2	e	107	VAL	CA-C-N	10.15	138.00	122.37
2	e	107	VAL	C-N-CA	10.15	138.00	122.37
2	n	100	THR	CA-C-N	9.93	137.65	121.57
2	n	100	THR	C-N-CA	9.93	137.65	121.57
1	K	134	GLU	CA-C-N	9.86	140.73	121.41
1	K	134	GLU	C-N-CA	9.86	140.73	121.41
1	D	134	GLU	CA-C-N	9.79	140.60	121.41
1	D	134	GLU	C-N-CA	9.79	140.60	121.41
1	G	134	GLU	CA-C-N	9.76	140.53	121.41
1	G	134	GLU	C-N-CA	9.76	140.53	121.41
1	K	124	ASP	CA-C-N	9.72	140.10	121.54
1	K	124	ASP	C-N-CA	9.72	140.10	121.54
1	A	134	GLU	CA-C-N	9.65	140.33	121.41
1	A	134	GLU	C-N-CA	9.65	140.33	121.41
1	B	134	GLU	CA-C-N	9.56	140.14	121.41
1	B	134	GLU	C-N-CA	9.56	140.14	121.41
1	M	124	ASP	CA-C-N	9.29	139.65	123.03
1	M	124	ASP	C-N-CA	9.29	139.65	123.03
1	F	124	ASP	CA-C-N	9.24	138.34	122.82
1	F	124	ASP	C-N-CA	9.24	138.34	122.82
1	O	124	ASP	CA-C-N	9.21	138.30	122.82
1	O	124	ASP	C-N-CA	9.21	138.30	122.82
1	B	124	ASP	CA-C-N	9.19	138.27	122.82
1	B	124	ASP	C-N-CA	9.19	138.27	122.82
1	C	124	ASP	CA-C-N	9.14	136.95	122.59
1	C	124	ASP	C-N-CA	9.14	136.95	122.59
1	L	124	ASP	CA-C-N	9.08	136.89	122.36
1	L	124	ASP	C-N-CA	9.08	136.89	122.36
2	h	104	TYR	CA-C-N	9.02	136.48	122.49
2	h	104	TYR	C-N-CA	9.02	136.48	122.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	124	ASP	CA-C-N	8.98	137.90	122.82
1	J	124	ASP	C-N-CA	8.98	137.90	122.82
1	M	44	ARG	CA-C-N	8.97	135.03	121.40
1	M	44	ARG	C-N-CA	8.97	135.03	121.40
2	n	102	PRO	CA-C-N	8.90	137.54	120.99
2	n	102	PRO	C-N-CA	8.90	137.54	120.99
1	A	124	ASP	CA-C-N	8.89	136.59	122.36
1	A	124	ASP	C-N-CA	8.89	136.59	122.36
1	E	134	GLU	CA-C-N	8.88	134.37	120.07
1	E	134	GLU	C-N-CA	8.88	134.37	120.07
2	l	65	TYR	CA-C-N	8.69	137.32	122.37
2	l	65	TYR	C-N-CA	8.69	137.32	122.37
1	D	124	ASP	CA-C-N	8.68	136.27	122.21
1	D	124	ASP	C-N-CA	8.68	136.27	122.21
1	I	124	ASP	CA-C-N	8.52	137.14	122.82
1	I	124	ASP	C-N-CA	8.52	137.14	122.82
1	E	124	ASP	CA-C-N	8.25	137.29	121.54
1	E	124	ASP	C-N-CA	8.25	137.29	121.54
1	N	124	ASP	CA-C-N	8.22	137.08	122.45
1	N	124	ASP	C-N-CA	8.22	137.08	122.45
1	G	124	ASP	CA-C-N	7.30	135.49	121.54
1	G	124	ASP	C-N-CA	7.30	135.49	121.54
1	N	133	VAL	CA-C-N	6.76	136.91	125.02
1	N	133	VAL	C-N-CA	6.76	136.91	125.02
2	e	29	THR	OG1-CB-CG2	5.82	120.94	109.30
2	b	100	THR	OG1-CB-CG2	5.72	120.75	109.30
2	h	100	THR	OG1-CB-CG2	5.66	120.63	109.30
2	e	107	VAL	CG1-CB-CG2	5.20	122.23	110.80
2	f	97	ILE	CG1-CB-CG2	5.16	126.17	110.70
1	K	93	ILE	CG1-CB-CG2	5.15	126.15	110.70
2	b	98	ILE	CG1-CB-CG2	5.14	126.12	110.70
2	c	97	ILE	CG1-CB-CG2	5.12	126.05	110.70
2	l	97	ILE	CG1-CB-CG2	5.10	126.00	110.70
2	o	97	ILE	CG1-CB-CG2	5.09	125.97	110.70
1	A	93	ILE	CG1-CB-CG2	5.09	125.96	110.70
1	J	93	ILE	CG1-CB-CG2	5.08	125.93	110.70
2	d	97	ILE	CG1-CB-CG2	5.06	125.89	110.70
1	B	93	ILE	CG1-CB-CG2	5.06	125.87	110.70
1	M	93	ILE	CG1-CB-CG2	5.04	125.81	110.70
1	I	93	ILE	CG1-CB-CG2	5.03	125.78	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1066	0	1075	55	0
1	B	1066	0	1075	62	0
1	C	1066	0	1075	49	0
1	D	1066	0	1075	41	0
1	E	1066	0	1075	59	0
1	F	1066	0	1075	58	0
1	G	1066	0	1075	48	0
1	H	1066	0	1075	56	0
1	I	1066	0	1075	54	0
1	J	1066	0	1075	54	0
1	K	1066	0	1075	56	0
1	L	1066	0	1075	56	0
1	M	1066	0	1075	62	0
1	N	1066	0	1075	70	0
1	O	1066	0	1075	52	0
2	a	996	0	959	46	0
2	b	996	0	959	40	0
2	c	996	0	959	59	0
2	d	996	0	959	48	0
2	e	996	0	959	41	0
2	f	996	0	959	41	0
2	g	996	0	959	41	0
2	h	996	0	959	47	0
2	i	996	0	959	45	0
2	j	996	0	959	35	0
2	k	996	0	959	43	0
2	l	996	0	959	34	0
2	m	996	0	959	43	0
2	n	996	0	959	45	0
2	o	996	0	959	47	0
All	All	30930	0	30510	1309	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 21.

All (1309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:VAL:O	1:M:116:ARG:NH2	1.99	0.95
1:K:27:GLU:O	1:K:65:ARG:NH2	2.02	0.93
1:I:128:VAL:O	1:J:116:ARG:NH2	2.05	0.89
1:N:27:GLU:O	1:N:65:ARG:NH2	2.06	0.89
1:B:27:GLU:O	1:B:65:ARG:NH2	2.05	0.88
2:m:39:ASP:OD2	2:m:41:LYS:NZ	2.05	0.88
2:g:70:THR:OG1	2:g:72:ASP:OD1	1.92	0.87
1:J:27:GLU:O	1:J:65:ARG:NH2	2.07	0.86
2:k:3:ARG:O	2:k:5:LYS:NZ	2.07	0.86
1:E:27:GLU:O	1:E:65:ARG:NH2	2.08	0.85
2:c:97:ILE:O	2:c:100:THR:OG1	1.95	0.85
2:e:70:THR:OG1	2:e:72:ASP:OD1	1.95	0.85
1:D:27:GLU:O	1:D:65:ARG:NH2	2.09	0.85
1:H:27:GLU:O	1:H:65:ARG:NH2	2.10	0.85
1:M:85:ARG:NH1	1:M:97:MET:O	2.10	0.84
1:N:75:ASP:O	1:N:79:LYS:NZ	2.10	0.84
1:M:51:ASN:HA	1:M:54:LEU:HD12	1.61	0.83
1:I:29:GLU:N	1:I:29:GLU:OE1	2.11	0.83
1:F:27:GLU:O	1:F:65:ARG:NH2	2.12	0.83
2:i:70:THR:OG1	2:i:72:ASP:OD1	1.97	0.82
2:i:58:ASN:ND2	2:i:80:VAL:O	2.12	0.82
1:H:88:THR:O	1:I:94:THR:OG1	1.96	0.82
1:N:75:ASP:OD1	1:N:79:LYS:NZ	2.11	0.82
1:N:128:VAL:O	1:O:116:ARG:NH2	2.12	0.82
2:d:103:GLU:OE2	2:d:105:THR:OG1	1.99	0.81
2:i:97:ILE:O	2:i:100:THR:OG1	1.97	0.81
1:L:29:GLU:N	1:L:29:GLU:OE1	2.13	0.80
1:E:87:VAL:HA	1:F:95:MET:HA	1.63	0.80
2:h:58:ASN:ND2	2:h:64:SER:O	2.15	0.80
1:C:27:GLU:O	1:C:65:ARG:NH2	2.15	0.80
2:i:31:ASN:OD1	2:i:34:ASN:N	2.15	0.80
2:d:14:GLN:N	2:d:14:GLN:OE1	2.16	0.79
2:g:65:TYR:OH	2:g:77:SER:OG	1.99	0.79
2:m:31:ASN:OD1	2:m:34:ASN:N	2.15	0.79
1:I:27:GLU:O	1:I:65:ARG:NH2	2.14	0.79
2:h:18:ASN:OD1	2:h:44:LYS:NZ	2.12	0.79
1:L:27:GLU:O	1:L:65:ARG:NH2	2.15	0.79
2:o:31:ASN:OD1	2:o:34:ASN:N	2.16	0.79
1:F:29:GLU:OE1	1:F:29:GLU:N	2.16	0.79
2:h:3:ARG:NH1	2:h:86:ASP:OD2	2.16	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:35:GLN:OE1	2:c:36:TYR:N	2.16	0.78
2:c:70:THR:OG1	2:c:72:ASP:OD1	2.01	0.78
1:C:29:GLU:OE1	1:C:29:GLU:N	2.17	0.78
2:a:31:ASN:OD1	2:a:34:ASN:N	2.15	0.78
2:c:105:THR:O	2:c:109:ASN:ND2	2.17	0.78
2:j:31:ASN:OD1	2:j:34:ASN:N	2.17	0.77
2:l:14:GLN:N	2:l:14:GLN:OE1	2.17	0.77
1:K:88:THR:HB	1:L:94:THR:HG23	1.64	0.77
1:O:27:GLU:O	1:O:65:ARG:NH2	2.17	0.77
2:b:18:ASN:OD1	2:b:44:LYS:NZ	2.17	0.77
2:l:29:THR:O	2:l:35:GLN:NE2	2.18	0.77
1:N:123:LEU:O	1:N:125:ASN:ND2	2.18	0.77
1:F:9:THR:OG1	1:F:13:GLU:OE1	2.02	0.77
1:I:87:VAL:HG11	1:I:90:VAL:HG22	1.66	0.77
2:l:46:ASP:OD1	2:l:50:GLU:N	2.18	0.77
2:a:31:ASN:ND2	2:a:36:TYR:OH	2.18	0.76
2:d:31:ASN:OD1	2:d:34:ASN:N	2.17	0.76
1:M:75:ASP:OD1	1:M:76:LYS:N	2.18	0.76
1:A:134:GLU:OE1	1:A:139:ALA:N	2.19	0.76
1:K:87:VAL:HA	1:L:95:MET:HA	1.68	0.76
1:N:83:GLU:OE2	1:O:73:ARG:NH1	2.19	0.76
2:b:31:ASN:OD1	2:b:34:ASN:N	2.19	0.76
2:o:88:GLU:OE1	2:o:88:GLU:N	2.18	0.76
2:g:27:ASN:ND2	2:g:63:GLN:O	2.20	0.75
2:g:58:ASN:ND2	2:g:80:VAL:O	2.19	0.75
2:d:27:ASN:ND2	2:d:62:ASP:OD1	2.20	0.75
2:m:2:ARG:NH1	2:m:82:ASP:O	2.20	0.75
1:G:88:THR:HA	1:G:95:MET:SD	2.28	0.74
1:I:83:GLU:OE2	1:J:73:ARG:NH1	2.20	0.74
1:O:26:SER:OG	1:O:27:GLU:OE1	2.04	0.74
2:j:39:ASP:OD1	2:j:40:THR:N	2.20	0.74
2:k:3:ARG:HE	2:k:52:VAL:HG11	1.52	0.74
1:F:87:VAL:HG11	1:F:90:VAL:HG22	1.70	0.74
1:H:123:LEU:O	1:H:125:ASN:ND2	2.19	0.74
2:e:14:GLN:N	2:e:14:GLN:OE1	2.20	0.74
2:n:31:ASN:OD1	2:n:34:ASN:N	2.20	0.74
1:I:87:VAL:HG13	1:J:93:ILE:HG23	1.69	0.74
2:l:97:ILE:O	2:l:100:THR:OG1	2.05	0.74
1:K:29:GLU:OE1	1:K:29:GLU:N	2.20	0.74
2:l:7:THR:OG1	2:l:50:GLU:OE1	2.03	0.73
2:m:39:ASP:OD1	2:m:40:THR:N	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:31:ASN:OD1	2:c:34:ASN:N	2.19	0.73
1:O:88:THR:HA	1:O:95:MET:HE1	1.70	0.73
2:h:46:ASP:OD1	2:h:50:GLU:N	2.20	0.73
1:E:29:GLU:N	1:E:29:GLU:OE1	2.20	0.73
1:G:9:THR:OG1	1:G:13:GLU:OE1	2.06	0.73
2:d:2:ARG:NH2	2:d:85:SER:OG	2.21	0.73
2:o:27:ASN:ND2	2:o:63:GLN:OE1	2.21	0.73
2:a:23:LEU:HD11	2:a:53:PHE:CE1	2.24	0.73
2:a:62:ASP:OD1	2:a:63:GLN:N	2.22	0.73
1:L:88:THR:HA	1:L:95:MET:SD	2.29	0.72
2:e:38:ILE:N	2:m:72:ASP:OD2	2.22	0.72
2:j:58:ASN:OD1	2:j:64:SER:OG	2.01	0.72
2:k:63:GLN:N	2:k:63:GLN:OE1	2.23	0.72
2:e:88:GLU:OE1	2:e:89:PHE:N	2.21	0.72
1:L:95:MET:SD	1:L:95:MET:N	2.61	0.72
2:o:7:THR:OG1	2:o:50:GLU:OE1	2.07	0.72
1:D:89:LYS:HA	1:D:93:ILE:O	1.87	0.72
2:i:58:ASN:OD1	2:i:79:THR:OG1	2.07	0.72
2:n:2:ARG:NH2	2:n:85:SER:OG	2.23	0.72
1:A:73:ARG:NH1	1:O:83:GLU:OE2	2.22	0.72
2:l:11:LEU:HD23	2:l:11:LEU:O	1.90	0.72
1:G:88:THR:HB	1:H:94:THR:HG23	1.71	0.72
2:c:58:ASN:ND2	2:c:80:VAL:O	2.23	0.72
2:o:70:THR:OG1	2:o:72:ASP:OD1	2.02	0.72
1:M:88:THR:HA	1:M:95:MET:HE2	1.71	0.72
2:c:88:GLU:N	2:c:88:GLU:OE1	2.22	0.72
2:d:39:ASP:OD1	2:d:40:THR:N	2.23	0.72
2:k:22:PHE:O	2:k:68:LEU:HD12	1.89	0.72
2:d:115:ILE:HG21	2:f:122:ILE:HD13	1.72	0.71
1:K:88:THR:N	1:L:94:THR:O	2.23	0.71
2:n:101:ASP:O	2:n:103:GLU:N	2.20	0.71
1:A:34:GLU:OE2	1:B:59:ILE:N	2.23	0.71
1:E:88:THR:HB	1:F:94:THR:HG23	1.71	0.71
2:e:63:GLN:OE1	2:e:63:GLN:N	2.22	0.71
2:k:88:GLU:OE1	2:k:89:PHE:N	2.23	0.71
1:K:89:LYS:HA	1:K:93:ILE:O	1.91	0.71
1:O:46:GLN:OE1	1:O:48:ASN:N	2.24	0.71
2:l:31:ASN:OD1	2:l:34:ASN:N	2.23	0.71
2:n:46:ASP:OD1	2:n:50:GLU:N	2.23	0.71
2:o:46:ASP:OD1	2:o:50:GLU:N	2.23	0.70
1:I:15:TYR:OH	1:I:29:GLU:OE2	2.09	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:134:GLU:C	1:L:140:ASN:HA	2.16	0.70
2:a:46:ASP:OD1	2:a:50:GLU:N	2.25	0.70
1:E:79:LYS:O	1:E:82:ILE:HG22	1.92	0.70
2:a:50:GLU:N	2:a:50:GLU:OE1	2.25	0.70
2:o:6:GLY:N	2:o:50:GLU:OE2	2.23	0.70
1:A:94:THR:OG1	1:O:88:THR:HB	1.92	0.70
1:N:30:GLU:OE1	1:N:30:GLU:N	2.24	0.70
2:b:9:ARG:NH2	2:b:13:ASP:O	2.24	0.70
1:B:32:GLU:OE1	1:B:32:GLU:N	2.24	0.70
1:E:89:LYS:HA	1:E:93:ILE:O	1.91	0.70
1:G:27:GLU:O	1:G:65:ARG:NH2	2.25	0.70
1:I:88:THR:HB	1:J:94:THR:HG23	1.74	0.70
2:c:25:LEU:HD12	2:c:65:TYR:O	1.92	0.69
2:i:93:ARG:O	2:i:97:ILE:HB	1.91	0.69
2:n:47:GLN:OE1	2:n:47:GLN:N	2.24	0.69
1:B:134:GLU:OE1	1:B:139:ALA:N	2.24	0.69
2:k:47:GLN:N	2:k:47:GLN:OE1	2.24	0.69
2:b:39:ASP:OD1	2:b:40:THR:N	2.25	0.69
2:e:47:GLN:N	2:e:47:GLN:OE1	2.25	0.69
2:f:1:MET:N	2:f:55:VAL:O	2.25	0.69
2:j:62:ASP:OD1	2:j:63:GLN:N	2.25	0.69
2:n:22:PHE:O	2:n:68:LEU:HD12	1.93	0.69
2:b:47:GLN:OE1	2:b:47:GLN:N	2.25	0.69
1:J:89:LYS:HA	1:J:93:ILE:O	1.93	0.69
2:b:46:ASP:OD1	2:b:50:GLU:N	2.26	0.69
2:k:56:VAL:O	2:k:66:TYR:OH	2.09	0.69
1:N:27:GLU:N	1:N:27:GLU:OE1	2.26	0.69
2:k:82:ASP:OD1	2:k:83:GLY:N	2.25	0.69
2:n:9:ARG:NH2	2:n:13:ASP:O	2.24	0.69
1:F:88:THR:HA	1:F:95:MET:SD	2.33	0.68
1:E:134:GLU:OE1	1:E:139:ALA:N	2.26	0.68
2:d:31:ASN:ND2	2:d:36:TYR:OH	2.26	0.68
1:H:125:ASN:OD1	1:H:128:VAL:HG12	1.93	0.68
2:c:88:GLU:O	2:c:91:VAL:HG12	1.92	0.68
2:k:1:MET:N	2:k:55:VAL:O	2.26	0.68
1:A:93:ILE:HG22	1:O:87:VAL:HB	1.76	0.68
1:F:88:THR:HB	1:G:94:THR:HG23	1.75	0.68
1:L:91:GLU:N	1:L:91:GLU:OE1	2.26	0.68
2:g:46:ASP:OD1	2:g:50:GLU:N	2.26	0.68
1:C:132:ASP:N	1:C:132:ASP:OD1	2.25	0.68
1:E:75:ASP:OD1	1:E:79:LYS:NZ	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HA	1:A:93:ILE:O	1.93	0.68
1:B:123:LEU:O	1:B:125:ASN:ND2	2.26	0.68
1:J:75:ASP:OD2	1:J:79:LYS:NZ	2.27	0.68
2:c:26:ILE:HD11	2:c:67:ILE:HG12	1.75	0.68
2:e:110:TYR:O	2:e:114:TYR:N	2.27	0.67
2:m:2:ARG:NH2	2:m:85:SER:OG	2.27	0.67
2:e:5:LYS:O	2:e:89:PHE:N	2.25	0.67
1:B:25:THR:HG23	1:B:61:VAL:HB	1.75	0.67
2:a:39:ASP:OD1	2:a:40:THR:N	2.26	0.67
2:d:66:TYR:C	2:d:67:ILE:HD12	2.19	0.67
2:f:2:ARG:NH2	2:f:85:SER:OG	2.27	0.67
1:L:15:TYR:OH	1:L:29:GLU:OE2	2.11	0.67
2:m:69:THR:OG1	2:m:75:LYS:NZ	2.28	0.67
1:N:125:ASN:OD1	1:N:128:VAL:HG12	1.95	0.67
2:g:39:ASP:OD1	2:g:40:THR:N	2.28	0.67
2:g:88:GLU:OE1	2:g:90:SER:N	2.27	0.67
2:h:47:GLN:N	2:h:47:GLN:OE1	2.28	0.67
2:e:31:ASN:ND2	2:e:34:ASN:O	2.27	0.67
2:o:16:TRP:O	2:o:45:THR:OG1	2.12	0.67
1:C:15:TYR:OH	1:C:29:GLU:OE2	2.13	0.67
1:N:88:THR:N	1:O:94:THR:O	2.27	0.67
2:i:46:ASP:OD1	2:i:50:GLU:N	2.28	0.67
1:B:125:ASN:OD1	1:B:128:VAL:HG12	1.95	0.67
1:C:83:GLU:OE2	1:D:73:ARG:NH1	2.26	0.67
1:I:50:VAL:O	1:I:54:LEU:HD22	1.94	0.67
1:L:20:LEU:HD12	1:L:21:ASP:N	2.10	0.67
1:F:52:ALA:CB	1:F:120:LEU:HD11	2.25	0.66
1:N:123:LEU:HD22	1:N:135:GLY:O	1.95	0.66
2:i:5:LYS:NZ	2:i:86:ASP:OD2	2.26	0.66
2:a:2:ARG:NH1	2:a:82:ASP:O	2.27	0.66
1:A:88:THR:O	1:B:94:THR:HG22	1.95	0.66
1:O:64:ILE:O	1:O:68:VAL:HG23	1.95	0.66
2:h:12:ASP:N	2:h:12:ASP:OD1	2.26	0.66
2:n:39:ASP:OD1	2:n:40:THR:N	2.29	0.66
1:B:87:VAL:HA	1:C:95:MET:HA	1.78	0.66
1:C:134:GLU:HA	1:C:139:ALA:HA	1.78	0.66
1:D:87:VAL:HG12	1:E:95:MET:SD	2.35	0.66
1:H:24:PRO:O	1:H:65:ARG:NH1	2.28	0.66
1:K:64:ILE:HG23	1:K:114:LEU:HD21	1.78	0.66
2:m:65:TYR:CZ	2:m:67:ILE:HD11	2.30	0.66
2:n:8:ILE:HG23	2:o:37:PRO:HG3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:VAL:HB	1:I:93:ILE:HG23	1.78	0.66
1:C:83:GLU:OE1	1:C:83:GLU:N	2.29	0.65
2:i:1:MET:CE	2:i:56:VAL:HG22	2.26	0.65
1:K:135:GLY:N	1:K:139:ALA:O	2.28	0.65
1:H:13:GLU:OE1	1:H:14:SER:N	2.29	0.65
1:K:20:LEU:HD12	1:K:21:ASP:N	2.12	0.65
1:A:93:ILE:HG23	1:O:90:VAL:HA	1.78	0.65
1:M:60:GLU:O	1:M:63:THR:OG1	2.12	0.65
2:j:27:ASN:ND2	2:j:63:GLN:O	2.30	0.65
1:L:134:GLU:OE1	1:L:135:GLY:N	2.29	0.65
2:f:46:ASP:OD1	2:f:50:GLU:N	2.30	0.65
1:A:88:THR:HB	1:B:94:THR:CG2	2.28	0.64
1:F:13:GLU:O	1:F:17:ASN:ND2	2.28	0.64
2:k:3:ARG:NH1	2:k:86:ASP:OD2	2.31	0.64
2:k:96:GLY:O	2:k:97:ILE:HD13	1.97	0.64
1:F:95:MET:SD	1:F:95:MET:N	2.69	0.64
2:j:70:THR:OG1	2:j:72:ASP:OD1	2.14	0.64
1:F:107:LEU:O	1:F:111:VAL:HG23	1.97	0.64
2:g:2:ARG:NH2	2:g:85:SER:OG	2.29	0.64
1:H:34:GLU:OE2	1:I:59:ILE:N	2.31	0.64
1:I:30:GLU:OE1	1:I:30:GLU:N	2.31	0.64
1:N:90:VAL:HG23	1:N:91:GLU:H	1.60	0.64
2:g:50:GLU:N	2:g:50:GLU:OE1	2.30	0.64
1:L:34:GLU:OE2	1:M:58:THR:N	2.31	0.64
2:g:47:GLN:OE1	2:g:47:GLN:N	2.30	0.64
2:i:1:MET:HE2	2:i:56:VAL:HG22	1.80	0.64
1:B:75:ASP:OD1	1:B:79:LYS:NZ	2.30	0.64
1:G:105:ASP:O	1:G:109:THR:HG23	1.98	0.64
1:K:140:ASN:O	1:K:140:ASN:ND2	2.31	0.64
1:C:91:GLU:N	1:C:91:GLU:OE1	2.31	0.64
1:N:134:GLU:OE1	1:N:139:ALA:HA	1.98	0.64
1:H:14:SER:O	1:H:18:GLN:NE2	2.30	0.64
1:N:37:ALA:HB1	1:N:42:PHE:O	1.98	0.64
1:L:104:LYS:O	1:L:108:VAL:HG23	1.98	0.63
1:L:134:GLU:CA	1:L:140:ASN:HA	2.29	0.63
1:B:106:GLU:O	1:B:109:THR:OG1	2.16	0.63
2:i:39:ASP:OD1	2:i:40:THR:N	2.31	0.63
2:l:62:ASP:OD1	2:l:62:ASP:N	2.29	0.63
1:B:25:THR:HG22	1:B:25:THR:O	1.98	0.63
1:K:22:GLY:C	1:K:23:LEU:HD12	2.24	0.63
1:L:88:THR:HB	1:M:94:THR:OG1	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:39:ASP:OD2	2:a:41:LYS:NZ	2.25	0.63
2:l:39:ASP:OD1	2:l:40:THR:N	2.31	0.63
2:a:27:ASN:ND2	2:a:62:ASP:OD1	2.31	0.63
2:h:107:VAL:HG22	2:h:110:TYR:CE2	2.33	0.63
2:k:9:ARG:NH2	2:k:13:ASP:O	2.32	0.63
2:l:82:ASP:OD1	2:l:83:GLY:N	2.32	0.63
2:a:63:GLN:N	2:a:63:GLN:OE1	2.30	0.63
2:b:120:ALA:O	2:b:123:GLN:NE2	2.32	0.63
2:k:78:PHE:HB2	2:k:92:VAL:HG22	1.81	0.63
2:l:26:ILE:HD13	2:l:65:TYR:CG	2.33	0.63
2:b:106:ASN:ND2	2:c:79:THR:O	2.31	0.63
1:B:25:THR:HG21	1:B:58:THR:HA	1.79	0.63
1:C:20:LEU:HD23	1:C:21:ASP:N	2.13	0.63
1:F:34:GLU:OE2	1:G:59:ILE:N	2.31	0.63
2:n:63:GLN:N	2:n:63:GLN:OE1	2.30	0.63
1:A:47:ASN:HA	1:A:50:VAL:HG22	1.81	0.62
1:B:34:GLU:OE2	1:C:59:ILE:N	2.29	0.62
2:g:5:LYS:NZ	2:g:86:ASP:OD2	2.31	0.62
2:i:26:ILE:HG22	2:i:65:TYR:O	1.99	0.62
1:B:18:GLN:OE1	1:B:18:GLN:N	2.31	0.62
1:E:85:ARG:NH1	1:E:97:MET:O	2.32	0.62
1:K:38:MET:HE1	1:L:59:ILE:HG22	1.80	0.62
1:L:89:LYS:HA	1:L:93:ILE:O	1.99	0.62
2:b:39:ASP:OD2	2:g:10:HIS:ND1	2.32	0.62
2:m:93:ARG:O	2:m:93:ARG:NE	2.32	0.62
1:M:105:ASP:O	1:M:109:THR:HG23	2.00	0.62
1:B:105:ASP:O	1:B:109:THR:HG23	1.99	0.62
2:g:93:ARG:O	2:g:93:ARG:NH1	2.32	0.62
2:h:5:LYS:NZ	2:h:50:GLU:OE1	2.31	0.62
1:I:70:GLU:OE1	1:I:73:ARG:NH1	2.32	0.62
1:N:29:GLU:O	1:N:33:ILE:HD12	1.99	0.62
2:a:10:HIS:N	2:a:14:GLN:O	2.29	0.62
2:i:26:ILE:HG21	2:i:65:TYR:CD2	2.34	0.62
1:B:79:LYS:O	1:B:82:ILE:HG22	1.98	0.62
1:I:85:ARG:NH1	1:I:97:MET:O	2.33	0.62
1:L:34:GLU:OE2	1:M:59:ILE:N	2.32	0.62
2:c:58:ASN:OD1	2:c:79:THR:OG1	2.16	0.62
2:d:61:ILE:HD11	2:d:103:GLU:O	2.00	0.62
2:h:88:GLU:OE1	2:h:89:PHE:N	2.32	0.62
2:n:20:SER:C	2:n:21:LEU:HD12	2.24	0.62
1:C:87:VAL:HG11	1:C:90:VAL:HG22	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:GLU:N	1:E:140:ASN:HB2	2.14	0.62
1:F:134:GLU:CD	1:F:139:ALA:HA	2.25	0.62
1:D:34:GLU:OE2	1:E:59:ILE:N	2.30	0.61
2:i:82:ASP:OD1	2:i:83:GLY:N	2.32	0.61
2:k:2:ARG:NH2	2:k:85:SER:OG	2.33	0.61
1:F:29:GLU:N	1:F:32:GLU:OE1	2.30	0.61
2:c:82:ASP:OD1	2:c:83:GLY:N	2.33	0.61
1:B:31:LEU:HD22	1:C:59:ILE:HD11	1.82	0.61
1:C:51:ASN:OD1	1:C:52:ALA:N	2.33	0.61
2:d:23:LEU:O	2:d:40:THR:OG1	2.11	0.61
2:d:65:TYR:CZ	2:d:67:ILE:HD11	2.36	0.61
2:h:62:ASP:OD1	2:h:63:GLN:N	2.33	0.61
1:A:79:LYS:O	1:B:73:ARG:NH2	2.33	0.61
1:H:35:PHE:CE2	1:H:68:VAL:HG13	2.36	0.61
1:I:88:THR:N	1:J:94:THR:O	2.28	0.61
2:b:82:ASP:OD1	2:b:83:GLY:N	2.33	0.61
1:B:64:ILE:HD11	1:B:117:ILE:HG21	1.82	0.61
2:m:10:HIS:N	2:m:14:GLN:O	2.33	0.61
2:c:46:ASP:OD1	2:c:50:GLU:N	2.33	0.61
2:c:68:LEU:HD23	2:c:89:PHE:CZ	2.35	0.61
2:h:35:GLN:OE1	2:h:35:GLN:N	2.34	0.61
1:E:87:VAL:HB	1:F:93:ILE:HG23	1.82	0.61
1:H:37:ALA:HB1	1:H:42:PHE:O	2.01	0.61
1:H:79:LYS:O	1:I:73:ARG:NH2	2.31	0.61
2:e:110:TYR:O	2:e:113:ASP:N	2.34	0.61
1:J:132:ASP:N	1:J:132:ASP:OD1	2.32	0.61
2:d:10:HIS:N	2:d:14:GLN:O	2.34	0.60
1:H:134:GLU:N	1:H:140:ASN:HB3	2.16	0.60
2:a:1:MET:HE2	2:c:13:ASP:CG	2.27	0.60
2:h:5:LYS:O	2:h:89:PHE:N	2.34	0.60
1:D:24:PRO:O	1:D:65:ARG:NH1	2.34	0.60
1:K:86:GLN:O	1:K:86:GLN:NE2	2.34	0.60
1:N:51:ASN:OD1	1:N:52:ALA:N	2.35	0.60
2:a:55:VAL:HG21	2:a:80:VAL:HG11	1.83	0.60
2:e:104:TYR:HD1	2:e:105:THR:HG23	1.67	0.60
2:f:30:PHE:N	2:f:62:ASP:OD2	2.29	0.60
1:E:48:ASN:OD1	1:E:49:PHE:N	2.35	0.60
1:O:88:THR:HA	1:O:95:MET:CE	2.30	0.60
2:e:20:SER:C	2:e:21:LEU:HD22	2.26	0.60
1:F:34:GLU:OE2	1:G:58:THR:N	2.35	0.60
2:d:27:ASN:ND2	2:d:63:GLN:O	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:105:ASP:O	1:J:109:THR:HG23	2.01	0.60
2:f:97:ILE:O	2:f:100:THR:OG1	2.18	0.60
1:K:85:ARG:NE	1:L:102:ASP:OD2	2.30	0.60
1:M:26:SER:O	1:M:65:ARG:NH2	2.35	0.60
1:N:89:LYS:HA	1:N:93:ILE:O	2.01	0.60
2:a:23:LEU:HD21	2:a:53:PHE:CG	2.36	0.60
1:H:18:GLN:OE1	2:h:26:ILE:HD11	2.02	0.60
2:b:58:ASN:OD1	2:b:80:VAL:N	2.30	0.60
2:o:22:PHE:O	2:o:68:LEU:HD12	2.02	0.60
1:B:24:PRO:O	1:B:65:ARG:NH1	2.34	0.60
1:C:34:GLU:OE2	1:D:58:THR:N	2.35	0.60
1:N:34:GLU:OE2	1:O:59:ILE:N	2.34	0.60
2:g:82:ASP:OD1	2:g:83:GLY:N	2.33	0.60
1:G:89:LYS:HA	1:G:93:ILE:O	2.02	0.60
2:k:34:ASN:OD1	2:k:35:GLN:N	2.35	0.60
2:m:46:ASP:OD1	2:m:49:GLY:N	2.35	0.59
2:n:5:LYS:NZ	2:n:86:ASP:OD2	2.35	0.59
2:c:22:PHE:O	2:c:68:LEU:HD12	2.01	0.59
2:d:106:ASN:ND2	2:f:94:GLU:OE1	2.35	0.59
2:n:98:ILE:HG21	2:o:63:GLN:OE1	2.01	0.59
2:n:106:ASN:ND2	2:o:79:THR:O	2.35	0.59
1:D:88:THR:HA	1:D:95:MET:CE	2.32	0.59
1:L:82:ILE:HD12	1:M:106:GLU:OE2	2.03	0.59
2:h:2:ARG:NH2	2:h:85:SER:OG	2.35	0.59
1:E:105:ASP:O	1:E:109:THR:HG23	2.02	0.59
1:K:37:ALA:HB1	1:K:42:PHE:O	2.02	0.59
1:M:100:ILE:HG22	1:M:104:LYS:HZ2	1.67	0.59
2:o:97:ILE:O	2:o:100:THR:HG22	2.02	0.59
1:J:64:ILE:O	1:J:68:VAL:HG23	2.02	0.59
1:J:90:VAL:HG13	1:J:91:GLU:H	1.68	0.59
2:a:13:ASP:OD1	2:k:36:TYR:OH	2.21	0.59
2:f:96:GLY:O	2:f:99:ALA:HB3	2.02	0.59
2:m:106:ASN:OD1	2:m:107:VAL:HG23	2.03	0.59
1:C:32:GLU:O	1:C:36:VAL:HG23	2.02	0.59
2:a:8:ILE:HD11	2:k:37:PRO:HB3	1.83	0.59
2:m:4:LEU:HD11	2:m:89:PHE:HB2	1.85	0.59
1:C:37:ALA:HB1	1:C:42:PHE:O	2.02	0.59
1:K:34:GLU:OE2	1:L:59:ILE:N	2.34	0.59
2:h:22:PHE:O	2:h:68:LEU:HD12	2.03	0.59
2:n:59:VAL:HG11	2:n:82:ASP:CG	2.28	0.59
1:G:90:VAL:HG23	1:G:91:GLU:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:29:GLU:O	1:M:32:GLU:N	2.36	0.58
1:A:85:ARG:NH2	1:A:97:MET:O	2.34	0.58
1:G:88:THR:HB	1:H:94:THR:CG2	2.33	0.58
2:d:29:THR:O	2:d:35:GLN:NE2	2.37	0.58
1:M:79:LYS:O	1:N:73:ARG:NH2	2.36	0.58
2:e:46:ASP:OD1	2:e:50:GLU:N	2.36	0.58
2:f:63:GLN:NE2	2:f:64:SER:O	2.36	0.58
2:l:106:ASN:OD1	2:l:107:VAL:N	2.36	0.58
1:A:9:THR:OG1	1:A:10:HIS:N	2.36	0.58
1:E:34:GLU:OE2	1:F:59:ILE:N	2.35	0.58
2:i:23:LEU:HD12	2:i:67:ILE:O	2.03	0.58
2:j:67:ILE:HD12	2:j:76:HIS:O	2.04	0.58
1:E:50:VAL:O	1:E:54:LEU:HD22	2.03	0.58
1:L:105:ASP:O	1:L:109:THR:HG23	2.03	0.58
2:d:34:ASN:OD1	2:f:9:ARG:NH1	2.37	0.58
1:D:29:GLU:OE1	1:D:31:LEU:N	2.36	0.58
1:J:106:GLU:O	1:J:109:THR:OG1	2.18	0.58
1:K:18:GLN:N	1:K:18:GLN:OE1	2.36	0.58
2:a:111:LEU:CD1	2:c:111:LEU:HD12	2.33	0.58
1:G:57:SER:O	1:G:61:VAL:HG23	2.03	0.58
1:N:86:GLN:N	1:N:86:GLN:OE1	2.37	0.58
2:e:25:LEU:O	2:e:38:ILE:HG23	2.04	0.58
2:f:7:THR:OG1	2:f:50:GLU:OE1	2.12	0.58
2:i:14:GLN:N	2:i:14:GLN:OE1	2.37	0.58
1:H:132:ASP:N	1:H:132:ASP:OD1	2.33	0.58
1:J:30:GLU:OE2	2:g:42:HIS:ND1	2.37	0.58
2:a:48:ASN:ND2	2:a:50:GLU:OE2	2.37	0.58
2:e:23:LEU:HD12	2:e:67:ILE:O	2.03	0.58
1:N:87:VAL:HA	1:O:95:MET:HA	1.86	0.57
2:e:10:HIS:N	2:e:14:GLN:O	2.35	0.57
1:J:125:ASN:ND2	1:J:128:VAL:HG22	2.19	0.57
2:e:8:ILE:HD11	2:f:37:PRO:HG3	1.86	0.57
2:f:97:ILE:O	2:f:104:TYR:OH	2.19	0.57
1:F:53:LEU:O	1:F:56:LEU:HD23	2.05	0.57
1:J:37:ALA:O	1:J:41:GLY:N	2.36	0.57
2:c:108:LEU:H	2:c:108:LEU:HD12	1.68	0.57
2:f:74:LYS:NZ	2:f:75:LYS:O	2.38	0.57
2:m:63:GLN:N	2:m:63:GLN:OE1	2.37	0.57
2:a:34:ASN:OD1	2:c:9:ARG:NE	2.35	0.57
1:K:62:TYR:O	1:K:66:THR:HG23	2.04	0.57
1:N:123:LEU:HA	1:N:132:ASP:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:1:MET:HE2	2:j:56:VAL:HG13	1.85	0.57
1:J:135:GLY:HA3	1:J:139:ALA:HB3	1.85	0.57
2:c:93:ARG:O	2:c:97:ILE:HB	2.05	0.57
1:I:30:GLU:OE1	1:I:31:LEU:N	2.36	0.57
1:K:50:VAL:O	1:K:54:LEU:HD22	2.04	0.57
2:f:98:ILE:O	2:f:98:ILE:HG22	2.04	0.57
1:A:105:ASP:O	1:A:109:THR:HG23	2.04	0.57
2:b:46:ASP:OD1	2:b:49:GLY:N	2.37	0.57
2:e:23:LEU:HD11	2:e:66:TYR:HB3	1.86	0.57
2:h:67:ILE:HD12	2:h:76:HIS:O	2.05	0.57
2:c:39:ASP:OD1	2:c:40:THR:N	2.38	0.57
2:d:46:ASP:OD1	2:d:50:GLU:N	2.38	0.57
1:F:89:LYS:HA	1:F:93:ILE:O	2.04	0.56
1:H:85:ARG:NH1	1:H:97:MET:O	2.38	0.56
1:N:31:LEU:CD1	1:O:59:ILE:HD11	2.35	0.56
2:e:22:PHE:O	2:e:68:LEU:HD12	2.05	0.56
1:G:9:THR:OG1	1:G:10:HIS:N	2.37	0.56
2:g:24:THR:HG23	2:g:40:THR:HG22	1.86	0.56
2:m:1:MET:O	2:m:3:ARG:NH1	2.38	0.56
1:A:37:ALA:O	1:A:41:GLY:N	2.38	0.56
1:J:88:THR:HB	1:K:94:THR:OG1	2.04	0.56
2:e:11:LEU:C	2:e:11:LEU:HD12	2.31	0.56
2:j:8:ILE:HD11	2:j:51:PHE:CE2	2.40	0.56
2:m:34:ASN:OD1	2:o:9:ARG:NE	2.38	0.56
2:n:29:THR:O	2:n:35:GLN:NE2	2.37	0.56
1:H:87:VAL:HG21	1:H:90:VAL:HG22	1.86	0.56
2:m:106:ASN:OD1	2:m:107:VAL:N	2.38	0.56
1:E:35:PHE:CE2	1:E:68:VAL:HG13	2.40	0.56
1:G:95:MET:SD	1:G:95:MET:N	2.78	0.56
2:i:4:LEU:HD11	2:i:89:PHE:HA	1.88	0.56
2:m:66:TYR:C	2:m:67:ILE:HD12	2.31	0.56
2:k:20:SER:C	2:k:21:LEU:HD12	2.31	0.56
1:A:29:GLU:O	1:A:33:ILE:HD12	2.05	0.56
1:A:95:MET:HA	1:O:87:VAL:HA	1.88	0.56
1:D:88:THR:HA	1:D:95:MET:HE1	1.88	0.56
1:M:23:LEU:O	2:c:73:ASN:ND2	2.38	0.56
1:M:51:ASN:HA	1:M:54:LEU:CD1	2.35	0.56
2:m:25:LEU:O	2:m:38:ILE:HG23	2.06	0.56
1:K:87:VAL:HG22	1:K:88:THR:H	1.71	0.56
2:c:4:LEU:HD11	2:c:89:PHE:HB2	1.87	0.56
2:f:46:ASP:OD1	2:f:49:GLY:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:123:GLN:O	2:o:123:GLN:NE2	2.39	0.56
1:B:37:ALA:HB1	1:B:42:PHE:O	2.06	0.56
1:E:88:THR:N	1:F:94:THR:O	2.38	0.56
1:F:22:GLY:O	1:F:23:LEU:HD23	2.06	0.56
1:G:134:GLU:HA	1:G:139:ALA:HA	1.88	0.56
1:M:88:THR:HA	1:M:95:MET:CE	2.36	0.55
2:e:27:ASN:OD1	2:e:63:GLN:NE2	2.39	0.55
2:k:108:LEU:HD12	2:k:108:LEU:C	2.31	0.55
1:C:58:THR:O	1:C:61:VAL:HG22	2.06	0.55
1:O:89:LYS:HA	1:O:93:ILE:O	2.05	0.55
2:h:2:ARG:NE	2:h:85:SER:O	2.38	0.55
1:D:88:THR:N	1:E:94:THR:O	2.39	0.55
1:L:64:ILE:HD11	1:L:117:ILE:HG21	1.87	0.55
1:K:85:ARG:NH1	1:K:97:MET:O	2.38	0.55
1:M:51:ASN:CA	1:M:54:LEU:HD12	2.35	0.55
2:m:31:ASN:ND2	2:m:36:TYR:OH	2.40	0.55
1:A:29:GLU:OE1	1:A:30:GLU:N	2.39	0.55
1:E:27:GLU:N	1:E:27:GLU:OE1	2.39	0.55
1:E:47:ASN:OD1	1:E:48:ASN:N	2.40	0.55
2:a:94:GLU:OE1	2:a:95:ALA:N	2.40	0.55
2:b:2:ARG:NH2	2:b:85:SER:OG	2.39	0.55
2:n:98:ILE:HG22	2:n:100:THR:HG23	1.88	0.55
1:L:64:ILE:HD11	1:L:117:ILE:CG2	2.37	0.55
2:m:27:ASN:ND2	2:m:63:GLN:O	2.39	0.55
1:A:102:ASP:OD2	1:O:85:ARG:NH2	2.39	0.55
1:B:88:THR:HB	1:C:94:THR:HG23	1.89	0.55
1:E:75:ASP:O	1:E:79:LYS:NZ	2.39	0.55
1:G:87:VAL:HG21	1:G:90:VAL:HG12	1.89	0.55
1:N:93:ILE:HD12	1:N:93:ILE:N	2.22	0.55
2:e:11:LEU:HD21	2:f:41:LYS:HG2	1.89	0.55
1:H:93:ILE:N	1:H:93:ILE:HD12	2.21	0.55
1:L:53:LEU:O	1:L:56:LEU:HD13	2.07	0.55
1:B:137:ILE:O	1:B:137:ILE:HG22	2.07	0.55
1:J:64:ILE:HD11	1:J:117:ILE:HG21	1.89	0.55
1:K:85:ARG:NH2	1:K:97:MET:O	2.38	0.55
1:N:136:ARG:CZ	1:N:137:ILE:HD12	2.36	0.55
2:e:2:ARG:NH2	2:e:85:SER:OG	2.40	0.55
2:h:67:ILE:HD11	2:h:75:LYS:HB3	1.88	0.55
2:j:2:ARG:NH1	2:j:82:ASP:O	2.40	0.55
2:n:46:ASP:OD1	2:n:49:GLY:N	2.40	0.55
1:F:93:ILE:H	1:F:93:ILE:HD12	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:GLU:OE1	1:I:92:ASP:N	2.39	0.55
1:G:134:GLU:HA	1:G:140:ASN:H	1.71	0.54
1:M:34:GLU:OE2	1:N:59:ILE:N	2.34	0.54
2:h:23:LEU:HD12	2:h:67:ILE:O	2.07	0.54
1:E:92:ASP:N	1:E:92:ASP:OD1	2.39	0.54
1:N:28:LEU:O	1:N:33:ILE:HD11	2.07	0.54
2:h:106:ASN:OD1	2:h:106:ASN:N	2.40	0.54
2:k:46:ASP:OD1	2:k:50:GLU:N	2.36	0.54
2:i:7:THR:OG1	2:i:50:GLU:OE1	2.21	0.54
2:m:16:TRP:O	2:m:45:THR:OG1	2.15	0.54
2:a:98:ILE:HG23	2:a:99:ALA:H	1.72	0.54
2:f:22:PHE:O	2:f:68:LEU:HD12	2.07	0.54
2:j:104:TYR:HB3	2:j:107:VAL:HG22	1.89	0.54
1:A:122:VAL:O	1:A:133:VAL:N	2.41	0.54
1:B:93:ILE:HD12	1:B:93:ILE:N	2.22	0.54
1:L:90:VAL:HA	1:M:93:ILE:HG23	1.88	0.54
2:g:62:ASP:OD1	2:g:63:GLN:N	2.40	0.54
2:i:23:LEU:HD11	2:i:66:TYR:HB3	1.90	0.54
2:j:22:PHE:O	2:j:68:LEU:HD12	2.06	0.54
2:l:4:LEU:HD11	2:l:89:PHE:HB2	1.89	0.54
1:B:29:GLU:O	1:B:33:ILE:HD12	2.07	0.54
1:I:135:GLY:N	1:I:139:ALA:HB3	2.23	0.54
1:M:51:ASN:HB3	1:M:54:LEU:HD12	1.90	0.54
1:I:64:ILE:HD11	1:I:117:ILE:CG2	2.38	0.54
1:O:83:GLU:N	1:O:83:GLU:OE1	2.36	0.54
2:d:46:ASP:OD1	2:d:49:GLY:N	2.41	0.54
2:e:112:GLU:OE1	2:e:112:GLU:N	2.37	0.54
1:B:25:THR:HG23	1:B:61:VAL:CB	2.38	0.54
1:H:107:LEU:O	1:H:111:VAL:HG23	2.08	0.54
2:e:8:ILE:HD11	2:f:37:PRO:CG	2.37	0.54
2:o:105:THR:O	2:o:109:ASN:N	2.37	0.54
1:M:89:LYS:HA	1:M:93:ILE:O	2.08	0.54
2:l:103:GLU:N	2:l:103:GLU:OE1	2.39	0.54
2:m:31:ASN:HB3	2:m:59:VAL:HG21	1.90	0.54
1:G:64:ILE:O	1:G:68:VAL:HG23	2.08	0.54
1:H:18:GLN:CD	2:h:26:ILE:HD11	2.33	0.54
2:g:105:THR:HA	2:g:108:LEU:HD21	1.90	0.54
1:N:42:PHE:HE1	1:N:123:LEU:HD21	1.72	0.53
2:h:11:LEU:C	2:h:11:LEU:HD23	2.33	0.53
2:k:94:GLU:HA	2:k:97:ILE:HD11	1.91	0.53
1:A:137:ILE:HG22	1:A:137:ILE:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:VAL:HB	1:E:93:ILE:HG23	1.89	0.53
1:E:106:GLU:OE1	1:E:109:THR:OG1	2.22	0.53
1:M:87:VAL:HG12	1:N:95:MET:SD	2.49	0.53
2:l:108:LEU:HD23	2:l:108:LEU:O	2.08	0.53
1:B:36:VAL:O	1:B:40:ILE:HD12	2.07	0.53
1:J:85:ARG:NH2	1:K:102:ASP:OD2	2.39	0.53
1:J:134:GLU:H	1:J:140:ASN:HB3	1.74	0.53
1:K:93:ILE:HD12	1:K:93:ILE:H	1.73	0.53
1:M:123:LEU:HD23	1:M:134:GLU:CD	2.32	0.53
1:D:37:ALA:HB1	1:D:42:PHE:O	2.08	0.53
1:F:82:ILE:HD12	1:G:106:GLU:OE2	2.08	0.53
1:H:123:LEU:HA	1:H:132:ASP:HB2	1.90	0.53
1:J:12:LEU:HD21	1:J:31:LEU:HB3	1.90	0.53
2:c:58:ASN:O	2:c:64:SER:OG	2.12	0.53
2:b:5:LYS:HD3	2:b:52:VAL:HG22	1.89	0.53
1:A:106:GLU:OE2	1:O:82:ILE:HD12	2.09	0.53
2:b:62:ASP:OD1	2:b:62:ASP:N	2.37	0.53
1:N:107:LEU:O	1:N:111:VAL:HG23	2.08	0.53
2:b:11:LEU:HD12	2:b:11:LEU:C	2.34	0.53
2:g:88:GLU:O	2:g:91:VAL:HG22	2.07	0.53
1:I:18:GLN:OE1	2:i:26:ILE:HD13	2.09	0.53
1:J:47:ASN:HA	1:J:50:VAL:HG22	1.91	0.53
1:B:75:ASP:O	1:B:79:LYS:NZ	2.42	0.53
1:J:57:SER:N	1:J:60:GLU:OE1	2.38	0.53
2:a:29:THR:O	2:a:36:TYR:N	2.35	0.53
2:b:12:ASP:OD1	2:b:12:ASP:N	2.42	0.53
1:I:64:ILE:HD11	1:I:117:ILE:HG21	1.90	0.52
1:O:16:TYR:O	1:O:19:PHE:N	2.41	0.52
1:F:134:GLU:HA	1:F:140:ASN:HA	1.91	0.52
1:G:37:ALA:O	1:G:41:GLY:N	2.42	0.52
1:H:126:LEU:HD23	1:I:117:ILE:HD11	1.92	0.52
1:J:96:ASN:OD1	1:J:98:ASN:ND2	2.40	0.52
2:b:113:ASP:OD1	2:b:113:ASP:N	2.41	0.52
2:c:92:VAL:O	2:c:96:GLY:N	2.41	0.52
2:l:98:ILE:HG21	2:l:107:VAL:HG11	1.91	0.52
2:n:65:TYR:OH	2:n:77:SER:OG	2.08	0.52
2:o:68:LEU:HD23	2:o:89:PHE:CZ	2.44	0.52
1:F:64:ILE:O	1:F:68:VAL:HG23	2.09	0.52
2:b:103:GLU:OE1	2:b:103:GLU:N	2.37	0.52
2:g:108:LEU:HD23	2:g:108:LEU:H	1.74	0.52
1:B:89:LYS:HD2	1:B:92:ASP:HA	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:THR:N	1:D:94:THR:O	2.37	0.52
2:d:106:ASN:OD1	2:d:107:VAL:N	2.39	0.52
2:j:24:THR:HG23	2:j:40:THR:HG22	1.90	0.52
2:b:6:GLY:N	2:b:50:GLU:OE2	2.42	0.52
2:h:16:TRP:CE3	2:h:19:VAL:HG11	2.44	0.52
2:n:67:ILE:HD11	2:n:75:LYS:HB3	1.91	0.52
1:E:106:GLU:O	1:E:109:THR:OG1	2.27	0.52
1:J:12:LEU:HD21	1:J:31:LEU:CB	2.39	0.52
2:e:106:ASN:OD1	2:e:107:VAL:HG23	2.09	0.52
2:h:82:ASP:OD1	2:h:83:GLY:N	2.41	0.52
2:j:4:LEU:HD11	2:j:89:PHE:HA	1.90	0.52
1:C:78:ASN:HB2	1:C:103:ILE:HD12	1.90	0.52
1:G:136:ARG:C	1:G:137:ILE:HD12	2.35	0.52
2:a:1:MET:HE3	2:a:3:ARG:HH22	1.75	0.52
2:g:78:PHE:HB2	2:g:92:VAL:HG22	1.91	0.52
2:h:25:LEU:HD21	2:h:29:THR:HG22	1.92	0.52
2:j:23:LEU:HD23	2:j:24:THR:N	2.23	0.52
1:J:34:GLU:OE2	1:K:57:SER:OG	2.24	0.52
1:N:89:LYS:NZ	1:N:94:THR:OG1	2.29	0.52
2:e:55:VAL:HG21	2:e:80:VAL:HG21	1.91	0.52
1:J:64:ILE:HD13	1:J:117:ILE:HD13	1.91	0.52
2:g:58:ASN:OD1	2:g:64:SER:OG	2.25	0.52
2:l:26:ILE:N	2:l:26:ILE:HD12	2.24	0.52
1:O:93:ILE:O	1:O:93:ILE:HG22	2.09	0.51
1:C:93:ILE:HG22	1:C:93:ILE:O	2.11	0.51
1:G:136:ARG:NH1	1:G:137:ILE:HD13	2.25	0.51
1:C:128:VAL:O	1:D:116:ARG:NH1	2.43	0.51
1:H:121:PRO:CB	1:H:133:VAL:HG23	2.39	0.51
2:c:105:THR:H	2:c:108:LEU:HD13	1.75	0.51
2:d:68:LEU:HD23	2:d:69:THR:N	2.25	0.51
2:f:103:GLU:OE1	2:f:103:GLU:HA	2.10	0.51
2:l:22:PHE:O	2:l:68:LEU:HD12	2.09	0.51
1:A:70:GLU:O	1:A:74:LEU:HD23	2.11	0.51
1:D:84:ASN:OD1	1:D:84:ASN:N	2.44	0.51
1:N:37:ALA:O	1:N:41:GLY:N	2.41	0.51
2:h:36:TYR:CE1	2:h:56:VAL:HG21	2.45	0.51
1:K:132:ASP:OD1	1:K:132:ASP:N	2.40	0.51
1:O:93:ILE:N	1:O:93:ILE:HD12	2.26	0.51
2:c:29:THR:O	2:c:36:TYR:N	2.39	0.51
2:d:63:GLN:N	2:d:63:GLN:OE1	2.44	0.51
2:h:86:ASP:N	2:h:86:ASP:OD1	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HG22	1:B:40:ILE:O	2.10	0.51
1:H:79:LYS:O	1:H:82:ILE:HG22	2.11	0.51
2:c:17:ILE:O	2:c:19:VAL:HG13	2.11	0.51
2:g:65:TYR:CZ	2:g:67:ILE:HD11	2.46	0.51
1:B:28:LEU:O	1:B:33:ILE:HD11	2.11	0.51
1:H:53:LEU:O	1:H:56:LEU:HD23	2.11	0.51
1:I:87:VAL:CG1	1:J:93:ILE:HG23	2.39	0.51
1:L:52:ALA:O	1:L:56:LEU:HD11	2.11	0.51
1:L:124:ASP:OD1	1:M:116:ARG:NE	2.44	0.51
2:e:9:ARG:NH2	2:e:13:ASP:O	2.43	0.51
2:g:11:LEU:C	2:g:11:LEU:HD23	2.36	0.51
2:l:105:THR:O	2:l:109:ASN:N	2.40	0.51
1:F:136:ARG:NH1	1:F:137:ILE:HD12	2.26	0.51
2:o:59:VAL:HG11	2:o:82:ASP:HB2	1.93	0.51
1:B:33:ILE:HD12	1:B:33:ILE:H	1.75	0.51
1:C:47:ASN:HA	1:C:50:VAL:HG22	1.93	0.51
1:I:107:LEU:O	1:I:111:VAL:HG23	2.11	0.51
1:O:98:ASN:O	1:O:101:GLY:N	2.44	0.51
2:a:23:LEU:HD21	2:a:53:PHE:CD1	2.46	0.51
2:d:9:ARG:NH2	2:d:48:ASN:O	2.44	0.51
2:h:98:ILE:HD12	2:h:98:ILE:H	1.76	0.51
2:o:7:THR:C	2:o:8:ILE:HD13	2.35	0.51
2:o:95:ALA:O	2:o:98:ILE:HD13	2.11	0.51
2:a:98:ILE:HG23	2:a:99:ALA:N	2.26	0.50
2:f:105:THR:CG2	2:f:108:LEU:HD11	2.41	0.50
1:A:28:LEU:HD11	1:A:61:VAL:HG22	1.93	0.50
1:E:77:LEU:C	1:E:77:LEU:HD23	2.37	0.50
1:I:116:ARG:NH1	1:I:120:LEU:O	2.44	0.50
1:A:88:THR:HB	1:B:94:THR:HG21	1.92	0.50
1:E:90:VAL:HG23	1:E:91:GLU:H	1.75	0.50
1:J:79:LYS:O	1:K:73:ARG:NH2	2.44	0.50
1:N:53:LEU:O	1:N:56:LEU:HD23	2.11	0.50
2:o:4:LEU:HD23	2:o:4:LEU:C	2.36	0.50
1:M:89:LYS:O	1:M:89:LYS:HG3	2.11	0.50
2:b:10:HIS:ND1	2:c:39:ASP:OD2	2.32	0.50
2:g:17:ILE:HD12	2:g:17:ILE:N	2.26	0.50
2:k:66:TYR:C	2:k:67:ILE:HD12	2.36	0.50
2:f:108:LEU:HD12	2:f:109:ASN:N	2.27	0.50
2:h:8:ILE:HG22	2:h:16:TRP:CD1	2.46	0.50
2:j:27:ASN:ND2	2:j:62:ASP:OD1	2.45	0.50
1:E:53:LEU:O	1:E:56:LEU:HD23	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:VAL:HA	1:G:95:MET:HA	1.93	0.50
1:K:28:LEU:HD22	1:K:28:LEU:N	2.27	0.50
1:N:123:LEU:HD23	1:N:133:VAL:O	2.11	0.50
2:d:58:ASN:ND2	2:d:62:ASP:O	2.45	0.50
2:f:61:ILE:HD12	2:f:62:ASP:OD1	2.11	0.50
2:n:59:VAL:HG21	2:n:82:ASP:OD1	2.12	0.50
2:n:107:VAL:HG22	2:o:81:PRO:HA	1.92	0.50
1:C:87:VAL:HG11	1:C:90:VAL:CG2	2.42	0.50
1:F:134:GLU:OE2	1:F:139:ALA:HA	2.11	0.50
1:H:93:ILE:HG22	1:H:93:ILE:O	2.12	0.50
1:L:121:PRO:CB	1:L:133:VAL:HG23	2.42	0.50
1:E:85:ARG:NH2	1:F:102:ASP:OD2	2.45	0.50
1:F:88:THR:HB	1:G:94:THR:CG2	2.42	0.50
1:N:83:GLU:N	1:N:83:GLU:OE1	2.44	0.50
2:b:119:ILE:HG23	2:b:122:ILE:HD12	1.93	0.50
2:h:89:PHE:HA	2:h:92:VAL:HG22	1.94	0.50
1:E:125:ASN:ND2	1:E:128:VAL:HG12	2.26	0.50
2:h:72:ASP:OD2	2:i:38:ILE:N	2.37	0.50
2:n:107:VAL:HG12	2:n:111:LEU:HD23	1.93	0.50
1:L:121:PRO:HB2	1:L:133:VAL:HG23	1.93	0.49
2:h:46:ASP:OD1	2:h:49:GLY:N	2.45	0.49
2:k:97:ILE:O	2:k:98:ILE:HG23	2.12	0.49
1:N:64:ILE:HD11	1:N:117:ILE:HG21	1.94	0.49
2:k:24:THR:HG23	2:k:40:THR:HG22	1.95	0.49
2:m:72:ASP:OD1	2:m:72:ASP:N	2.42	0.49
1:E:77:LEU:HD23	1:E:77:LEU:O	2.12	0.49
1:M:87:VAL:HB	1:N:94:THR:O	2.12	0.49
2:l:20:SER:C	2:l:21:LEU:HD22	2.37	0.49
1:F:52:ALA:HB3	1:F:120:LEU:HD11	1.93	0.49
1:I:93:ILE:HD12	1:I:93:ILE:H	1.78	0.49
1:N:90:VAL:HG23	1:N:91:GLU:N	2.27	0.49
2:a:93:ARG:NH2	2:k:28:GLY:O	2.46	0.49
2:c:26:ILE:N	2:c:26:ILE:HD12	2.26	0.49
2:d:61:ILE:HD12	2:d:102:PRO:HA	1.93	0.49
2:j:104:TYR:CB	2:j:107:VAL:HG22	2.43	0.49
1:E:87:VAL:HG21	1:E:90:VAL:CG1	2.42	0.49
1:K:77:LEU:O	1:K:77:LEU:HD23	2.13	0.49
1:N:28:LEU:N	1:N:28:LEU:HD22	2.27	0.49
2:k:55:VAL:HG12	2:k:56:VAL:N	2.27	0.49
2:o:93:ARG:O	2:o:97:ILE:HD13	2.12	0.49
1:E:138:GLY:O	1:E:139:ALA:HB2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:35:GLN:N	2:i:35:GLN:OE1	2.45	0.49
2:j:50:GLU:OE1	2:j:50:GLU:N	2.46	0.49
1:G:87:VAL:HG21	1:G:90:VAL:CG1	2.43	0.49
1:J:122:VAL:O	1:J:122:VAL:HG13	2.12	0.49
2:c:93:ARG:O	2:c:97:ILE:HD13	2.13	0.49
2:g:80:VAL:HG12	2:g:81:PRO:O	2.13	0.49
2:i:33:ALA:O	2:i:34:ASN:ND2	2.43	0.49
1:A:29:GLU:O	1:A:32:GLU:N	2.46	0.49
1:B:32:GLU:O	1:B:36:VAL:HG23	2.13	0.49
1:D:47:ASN:HA	1:D:50:VAL:HG22	1.94	0.49
1:N:134:GLU:HA	1:N:139:ALA:HA	1.94	0.49
1:D:57:SER:O	1:D:61:VAL:HG23	2.12	0.49
1:I:85:ARG:NH2	1:J:102:ASP:OD2	2.39	0.49
2:b:1:MET:SD	2:b:2:ARG:N	2.86	0.49
2:b:16:TRP:HE3	2:b:19:VAL:HG11	1.77	0.49
2:j:35:GLN:OE1	2:j:36:TYR:N	2.45	0.49
1:N:48:ASN:OD1	1:N:48:ASN:N	2.46	0.49
1:C:30:GLU:HA	1:C:33:ILE:HD12	1.95	0.48
1:J:95:MET:SD	1:J:95:MET:N	2.86	0.48
2:e:46:ASP:OD1	2:e:49:GLY:N	2.46	0.48
2:k:25:LEU:O	2:k:38:ILE:HG23	2.13	0.48
1:N:125:ASN:O	1:O:116:ARG:NE	2.46	0.48
2:n:3:ARG:NH2	2:n:86:ASP:OD2	2.45	0.48
1:B:85:ARG:NH1	1:B:97:MET:O	2.44	0.48
1:D:20:LEU:N	1:D:20:LEU:HD22	2.26	0.48
1:I:134:GLU:C	1:I:139:ALA:HB3	2.37	0.48
2:f:39:ASP:OD1	2:f:40:THR:N	2.45	0.48
2:g:11:LEU:HD23	2:g:11:LEU:O	2.12	0.48
2:g:16:TRP:C	2:g:17:ILE:HD12	2.38	0.48
2:l:65:TYR:HD1	2:l:66:TYR:H	1.61	0.48
2:m:62:ASP:OD1	2:m:62:ASP:N	2.43	0.48
1:J:98:ASN:O	1:J:101:GLY:N	2.46	0.48
1:N:18:GLN:OE1	1:N:18:GLN:N	2.46	0.48
2:n:64:SER:OG	2:n:65:TYR:N	2.46	0.48
2:o:39:ASP:OD1	2:o:40:THR:N	2.45	0.48
1:H:136:ARG:HE	1:H:137:ILE:HG22	1.79	0.48
1:L:87:VAL:HA	1:M:94:THR:O	2.13	0.48
2:d:115:ILE:HG21	2:f:122:ILE:CD1	2.43	0.48
2:g:17:ILE:O	2:g:19:VAL:HG13	2.13	0.48
2:k:29:THR:O	2:k:35:GLN:NE2	2.47	0.48
2:l:70:THR:OG1	2:l:72:ASP:OD1	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:61:ILE:HD11	2:m:103:GLU:O	2.14	0.48
2:n:86:ASP:OD1	2:n:86:ASP:N	2.45	0.48
1:O:88:THR:CA	1:O:95:MET:HE1	2.42	0.48
2:h:11:LEU:O	2:i:56:VAL:HG23	2.14	0.48
2:n:61:ILE:HD12	2:n:61:ILE:H	1.79	0.48
1:B:25:THR:O	1:B:25:THR:CG2	2.62	0.48
1:N:29:GLU:OE1	1:N:29:GLU:N	2.44	0.48
2:d:24:THR:HG23	2:d:40:THR:HB	1.95	0.48
2:g:29:THR:O	2:g:36:TYR:N	2.40	0.48
1:G:87:VAL:HB	1:H:93:ILE:HG23	1.96	0.48
1:I:93:ILE:HD12	1:I:93:ILE:N	2.29	0.48
1:K:53:LEU:O	1:K:56:LEU:HD23	2.14	0.48
1:L:23:LEU:HD21	1:L:69:LYS:HE2	1.95	0.48
2:d:82:ASP:OD1	2:d:82:ASP:N	2.46	0.48
2:f:20:SER:C	2:f:21:LEU:HD22	2.39	0.48
2:o:4:LEU:HD23	2:o:4:LEU:O	2.14	0.48
1:L:55:ASP:N	1:L:55:ASP:OD1	2.47	0.48
1:M:20:LEU:N	1:M:20:LEU:HD22	2.29	0.48
2:j:31:ASN:ND2	2:j:36:TYR:OH	2.47	0.48
1:H:135:GLY:HA3	1:H:140:ASN:HA	1.96	0.48
1:I:89:LYS:HA	1:I:93:ILE:O	2.13	0.48
1:J:51:ASN:OD1	1:J:52:ALA:N	2.47	0.48
1:K:35:PHE:CE1	1:K:68:VAL:HG13	2.49	0.48
1:M:53:LEU:O	1:M:56:LEU:HD13	2.13	0.48
1:N:64:ILE:HD11	1:N:117:ILE:CG2	2.43	0.48
2:o:111:LEU:O	2:o:115:ILE:HG12	2.14	0.48
1:A:50:VAL:O	1:A:54:LEU:HD22	2.14	0.47
1:N:47:ASN:HA	1:N:50:VAL:HG22	1.95	0.47
2:o:114:TYR:CD2	2:o:115:ILE:HD13	2.49	0.47
1:D:137:ILE:O	1:D:137:ILE:HG22	2.14	0.47
1:G:88:THR:O	1:H:94:THR:HG22	2.14	0.47
1:G:90:VAL:HG23	1:G:91:GLU:N	2.29	0.47
1:N:125:ASN:O	1:O:116:ARG:NH2	2.47	0.47
2:k:4:LEU:HD11	2:k:89:PHE:HB2	1.96	0.47
1:F:64:ILE:HD11	1:F:117:ILE:HG21	1.97	0.47
1:H:48:ASN:OD1	1:H:48:ASN:N	2.46	0.47
1:O:90:VAL:HG12	1:O:91:GLU:OE1	2.15	0.47
2:a:24:THR:HB	2:a:40:THR:HG22	1.96	0.47
2:c:90:SER:OG	2:c:93:ARG:NH2	2.47	0.47
1:F:133:VAL:HG12	1:F:134:GLU:H	1.78	0.47
1:M:113:LYS:O	1:M:117:ILE:HG22	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:23:LEU:N	2:a:23:LEU:HD12	2.29	0.47
2:c:4:LEU:HD11	2:c:89:PHE:HA	1.95	0.47
2:c:105:THR:OG1	2:c:109:ASN:ND2	2.47	0.47
2:e:18:ASN:N	2:e:45:THR:OG1	2.47	0.47
2:i:9:ARG:NH1	2:i:13:ASP:O	2.42	0.47
2:k:23:LEU:HD11	2:k:66:TYR:HB3	1.94	0.47
1:G:126:LEU:C	1:G:126:LEU:HD23	2.39	0.47
1:H:92:ASP:N	1:H:92:ASP:OD1	2.47	0.47
1:K:93:ILE:HD12	1:K:93:ILE:N	2.30	0.47
2:c:73:ASN:OD1	2:c:73:ASN:C	2.58	0.47
2:g:65:TYR:CE2	2:g:67:ILE:HD11	2.50	0.47
1:A:106:GLU:O	1:A:109:THR:OG1	2.24	0.47
1:B:53:LEU:O	1:B:56:LEU:HD23	2.14	0.47
1:E:134:GLU:H	1:E:140:ASN:HB2	1.80	0.47
1:G:27:GLU:OE1	1:G:28:LEU:N	2.48	0.47
1:J:92:ASP:N	1:J:92:ASP:OD1	2.48	0.47
1:K:98:ASN:O	1:K:101:GLY:N	2.47	0.47
1:M:125:ASN:OD1	1:M:127:TYR:N	2.45	0.47
2:c:4:LEU:HD11	2:c:89:PHE:CA	2.44	0.47
2:c:16:TRP:HB3	2:c:19:VAL:HG11	1.97	0.47
2:c:26:ILE:HD13	2:c:65:TYR:CG	2.49	0.47
2:d:65:TYR:CE2	2:d:67:ILE:HD11	2.50	0.47
2:j:94:GLU:OE1	2:j:95:ALA:N	2.47	0.47
1:F:83:GLU:OE1	1:F:83:GLU:N	2.44	0.47
2:m:88:GLU:OE1	2:m:89:PHE:N	2.43	0.47
1:F:88:THR:N	1:G:94:THR:O	2.39	0.47
1:M:51:ASN:OD1	1:M:51:ASN:N	2.42	0.47
2:h:12:ASP:HB3	2:i:54:ASN:O	2.15	0.47
2:o:29:THR:HG22	2:o:30:PHE:N	2.29	0.47
2:o:58:ASN:O	2:o:64:SER:OG	2.33	0.47
1:G:46:GLN:O	1:G:50:VAL:HG23	2.15	0.47
1:O:28:LEU:N	1:O:28:LEU:HD22	2.30	0.47
2:d:2:ARG:NH1	2:d:82:ASP:O	2.48	0.47
2:d:4:LEU:HD11	2:d:89:PHE:HB2	1.96	0.47
2:j:109:ASN:OD1	2:j:110:TYR:N	2.48	0.47
2:n:1:MET:SD	2:n:54:ASN:ND2	2.88	0.47
1:D:32:GLU:O	1:D:36:VAL:HG23	2.15	0.46
1:F:133:VAL:HG12	1:F:134:GLU:N	2.30	0.46
2:h:25:LEU:HD12	2:h:65:TYR:O	2.16	0.46
2:j:8:ILE:HD11	2:j:51:PHE:CD2	2.49	0.46
2:n:8:ILE:HG22	2:n:16:TRP:CD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD12	1:A:28:LEU:H	1.80	0.46
1:K:13:GLU:OE1	1:K:14:SER:N	2.48	0.46
1:M:88:THR:HG22	1:M:97:MET:CE	2.45	0.46
1:E:90:VAL:HG23	1:E:91:GLU:N	2.30	0.46
2:f:7:THR:O	2:f:8:ILE:HD13	2.14	0.46
2:m:65:TYR:CE2	2:m:67:ILE:HD11	2.50	0.46
2:n:10:HIS:N	2:n:14:GLN:O	2.38	0.46
1:A:53:LEU:O	1:A:56:LEU:HD11	2.15	0.46
1:D:85:ARG:NH2	1:E:102:ASP:OD2	2.47	0.46
1:F:31:LEU:HD21	2:f:22:PHE:CE1	2.49	0.46
1:G:9:THR:HG1	1:G:10:HIS:H	1.62	0.46
1:G:12:LEU:HD21	1:G:31:LEU:HB3	1.97	0.46
1:G:126:LEU:HD21	1:H:113:LYS:HD3	1.98	0.46
1:H:108:VAL:HG22	1:H:112:LYS:NZ	2.31	0.46
1:L:126:LEU:H	1:L:126:LEU:HD23	1.81	0.46
2:m:17:ILE:O	2:m:18:ASN:ND2	2.48	0.46
1:I:34:GLU:OE2	1:J:59:ILE:N	2.45	0.46
1:J:34:GLU:OE2	1:K:59:ILE:N	2.44	0.46
1:N:77:LEU:HD23	1:N:77:LEU:C	2.41	0.46
2:m:46:ASP:OD1	2:m:50:GLU:N	2.46	0.46
1:H:75:ASP:OD2	1:H:127:TYR:OH	2.29	0.46
2:b:78:PHE:HB2	2:b:92:VAL:HG22	1.98	0.46
2:d:100:THR:HG22	2:d:101:ASP:N	2.30	0.46
2:g:106:ASN:OD1	2:g:107:VAL:N	2.48	0.46
2:n:23:LEU:HD12	2:n:67:ILE:O	2.16	0.46
1:C:107:LEU:O	1:C:111:VAL:HG23	2.16	0.46
2:i:22:PHE:HB2	2:i:69:THR:OG1	2.16	0.46
2:j:34:ASN:OD1	2:l:9:ARG:NH2	2.49	0.46
2:k:1:MET:O	2:k:54:ASN:ND2	2.48	0.46
1:M:22:GLY:C	1:M:23:LEU:HD12	2.41	0.46
1:N:133:VAL:HG12	1:N:134:GLU:HG2	1.98	0.46
2:h:18:ASN:N	2:h:45:THR:OG1	2.48	0.46
2:k:106:ASN:ND2	2:k:107:VAL:HG23	2.30	0.46
1:B:30:GLU:O	1:B:44:ARG:NH2	2.48	0.46
1:C:58:THR:HG23	1:C:59:ILE:N	2.31	0.46
1:M:50:VAL:O	1:M:54:LEU:N	2.49	0.46
1:M:53:LEU:HD13	1:M:56:LEU:HD11	1.98	0.46
2:d:107:VAL:HG23	2:f:94:GLU:OE2	2.16	0.46
2:i:25:LEU:O	2:i:38:ILE:HG23	2.16	0.46
2:k:28:GLY:N	2:k:38:ILE:HD11	2.31	0.46
1:A:59:ILE:HG22	1:O:34:GLU:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ILE:O	1:D:123:LEU:HD12	2.16	0.45
1:I:100:ILE:O	1:I:104:LYS:HG2	2.16	0.45
1:J:57:SER:O	1:J:61:VAL:HG23	2.15	0.45
1:J:90:VAL:HG13	1:J:91:GLU:N	2.30	0.45
1:K:87:VAL:HG22	1:K:88:THR:N	2.31	0.45
1:K:122:VAL:O	1:K:122:VAL:HG13	2.16	0.45
1:N:134:GLU:O	1:N:138:GLY:O	2.34	0.45
2:d:20:SER:OG	2:d:42:HIS:ND1	2.49	0.45
2:d:24:THR:HG1	2:d:40:THR:CB	2.22	0.45
1:B:85:ARG:O	1:C:96:ASN:HB3	2.17	0.45
1:C:55:ASP:N	1:C:55:ASP:OD1	2.48	0.45
1:E:28:LEU:N	1:E:28:LEU:HD22	2.32	0.45
1:G:87:VAL:HG12	1:H:95:MET:SD	2.56	0.45
1:H:59:ILE:O	1:H:63:THR:HG23	2.16	0.45
1:I:14:SER:O	1:I:18:GLN:NE2	2.42	0.45
2:f:42:HIS:CG	2:f:43:ALA:N	2.85	0.45
2:j:1:MET:SD	2:j:54:ASN:ND2	2.89	0.45
2:j:16:TRP:HE3	2:j:19:VAL:HG11	1.80	0.45
2:j:23:LEU:HD21	2:j:66:TYR:HD2	1.81	0.45
2:l:46:ASP:OD1	2:l:49:GLY:N	2.49	0.45
2:m:65:TYR:CE1	2:m:67:ILE:HD11	2.52	0.45
2:o:103:GLU:HA	2:o:103:GLU:OE1	2.16	0.45
1:D:37:ALA:O	1:D:41:GLY:N	2.46	0.45
1:F:83:GLU:OE2	1:G:73:ARG:NH1	2.49	0.45
2:i:73:ASN:C	2:i:73:ASN:OD1	2.59	0.45
1:B:88:THR:N	1:C:94:THR:O	2.41	0.45
1:D:12:LEU:HD21	1:D:31:LEU:HB3	1.98	0.45
1:E:87:VAL:HG21	1:E:90:VAL:HG12	1.98	0.45
1:L:58:THR:HG23	1:L:59:ILE:N	2.31	0.45
1:M:26:SER:O	1:M:61:VAL:HG21	2.17	0.45
2:a:26:ILE:HG22	2:a:26:ILE:O	2.16	0.45
2:k:25:LEU:HD12	2:k:65:TYR:O	2.17	0.45
2:n:101:ASP:CG	2:o:65:TYR:HH	2.22	0.45
1:E:93:ILE:N	1:E:93:ILE:HD12	2.32	0.45
1:J:118:LEU:HD12	1:J:118:LEU:N	2.32	0.45
1:A:82:ILE:N	1:A:82:ILE:HD12	2.32	0.45
1:C:29:GLU:O	1:C:32:GLU:N	2.49	0.45
1:F:55:ASP:OD1	1:F:55:ASP:N	2.49	0.45
1:H:135:GLY:N	1:H:140:ASN:HA	2.32	0.45
1:K:14:SER:O	1:K:18:GLN:NE2	2.46	0.45
2:e:22:PHE:HD2	2:e:69:THR:HG23	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:48:ASN:ND2	2:g:50:GLU:OE2	2.49	0.45
1:A:86:GLN:HG3	1:A:87:VAL:HG13	1.98	0.45
1:A:107:LEU:O	1:A:111:VAL:HG23	2.17	0.45
1:D:126:LEU:HD23	1:E:117:ILE:HD11	1.99	0.45
1:E:46:GLN:OE1	1:E:47:ASN:N	2.49	0.45
1:L:42:PHE:N	1:L:123:LEU:HD21	2.31	0.45
2:b:97:ILE:HD12	2:b:97:ILE:C	2.42	0.45
2:d:104:TYR:O	2:d:107:VAL:N	2.50	0.45
2:e:88:GLU:OE1	2:e:90:SER:N	2.42	0.45
2:i:68:LEU:C	2:i:68:LEU:HD23	2.42	0.45
2:l:17:ILE:O	2:l:18:ASN:OD1	2.35	0.45
1:J:109:THR:O	1:J:113:LYS:HG3	2.17	0.45
1:L:134:GLU:HA	1:L:140:ASN:HA	1.99	0.45
1:O:37:ALA:HB2	1:O:49:PHE:HE2	1.82	0.45
2:f:94:GLU:O	2:f:97:ILE:HB	2.17	0.45
1:C:87:VAL:CG1	1:C:88:THR:N	2.79	0.45
1:C:123:LEU:HD12	1:C:123:LEU:C	2.41	0.45
1:E:30:GLU:O	1:E:44:ARG:NH2	2.50	0.45
1:O:58:THR:HG23	1:O:59:ILE:N	2.31	0.45
2:h:26:ILE:O	2:h:38:ILE:HD12	2.17	0.45
2:h:107:VAL:HG11	2:i:81:PRO:HA	1.99	0.45
2:n:2:ARG:HD3	2:n:87:ILE:HD11	1.97	0.45
1:E:113:LYS:O	1:E:117:ILE:HG12	2.17	0.44
1:L:60:GLU:O	1:L:64:ILE:HG12	2.17	0.44
1:N:60:GLU:O	1:N:64:ILE:HG12	2.17	0.44
1:N:140:ASN:OD1	1:N:140:ASN:N	2.48	0.44
2:f:73:ASN:O	2:f:73:ASN:CG	2.60	0.44
2:g:73:ASN:O	2:g:75:LYS:NZ	2.47	0.44
1:K:93:ILE:O	1:K:93:ILE:HG22	2.17	0.44
1:K:136:ARG:O	1:K:137:ILE:HD13	2.18	0.44
1:O:71:ILE:HD11	1:O:110:GLU:HB2	1.99	0.44
2:a:80:VAL:O	2:a:80:VAL:HG23	2.17	0.44
2:i:93:ARG:O	2:i:97:ILE:HD13	2.17	0.44
2:j:24:THR:HB	2:j:67:ILE:HG23	2.00	0.44
1:O:55:ASP:N	1:O:55:ASP:OD1	2.47	0.44
2:i:18:ASN:N	2:i:45:THR:O	2.45	0.44
1:A:51:ASN:OD1	1:A:52:ALA:N	2.51	0.44
1:B:34:GLU:OE2	1:C:57:SER:OG	2.34	0.44
1:C:20:LEU:HD23	1:C:20:LEU:C	2.41	0.44
1:E:104:LYS:O	1:E:108:VAL:HG23	2.17	0.44
1:J:38:MET:SD	1:K:117:ILE:HD12	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:124:ASP:N	1:M:132:ASP:OD2	2.51	0.44
1:M:133:VAL:HG12	1:M:140:ASN:HD21	1.82	0.44
2:a:20:SER:OG	2:a:42:HIS:ND1	2.50	0.44
2:a:24:THR:CB	2:a:40:THR:HG22	2.47	0.44
2:e:108:LEU:HD22	2:e:111:LEU:HG	1.98	0.44
2:j:8:ILE:HD12	2:j:8:ILE:N	2.32	0.44
2:o:108:LEU:C	2:o:108:LEU:HD23	2.43	0.44
1:A:52:ALA:O	1:A:56:LEU:HD21	2.18	0.44
1:A:64:ILE:HD11	1:A:117:ILE:HG21	1.98	0.44
1:B:25:THR:O	1:B:26:SER:C	2.60	0.44
1:H:135:GLY:CA	1:H:140:ASN:HA	2.47	0.44
1:L:31:LEU:HD11	1:M:59:ILE:HD13	1.99	0.44
2:c:46:ASP:OD1	2:c:49:GLY:N	2.50	0.44
2:f:66:TYR:O	2:f:67:ILE:HD13	2.17	0.44
2:h:11:LEU:HD23	2:h:11:LEU:O	2.18	0.44
2:k:68:LEU:HD23	2:k:89:PHE:CZ	2.52	0.44
1:H:77:LEU:C	1:H:77:LEU:HD23	2.42	0.44
1:J:87:VAL:HB	1:K:94:THR:O	2.18	0.44
1:J:100:ILE:HG22	1:J:104:LYS:HZ2	1.83	0.44
1:M:64:ILE:CD1	1:M:117:ILE:HD13	2.47	0.44
1:O:132:ASP:OD1	1:O:132:ASP:N	2.49	0.44
2:c:4:LEU:HD11	2:c:89:PHE:CB	2.48	0.44
2:e:108:LEU:O	2:e:111:LEU:HD23	2.18	0.44
2:l:61:ILE:HD12	2:l:61:ILE:N	2.32	0.44
1:A:60:GLU:O	1:A:64:ILE:HG12	2.17	0.44
1:F:123:LEU:HA	1:F:132:ASP:OD1	2.17	0.44
1:M:23:LEU:HD12	1:M:23:LEU:N	2.32	0.44
1:M:51:ASN:CB	1:M:54:LEU:HD12	2.46	0.44
1:N:85:ARG:NH2	1:N:97:MET:O	2.49	0.44
1:N:124:ASP:N	1:N:132:ASP:OD1	2.51	0.44
2:a:110:TYR:CG	2:c:91:VAL:HG21	2.53	0.44
2:c:17:ILE:HD12	2:c:47:GLN:HA	2.00	0.44
2:c:68:LEU:HD23	2:c:89:PHE:CE2	2.53	0.44
2:h:110:TYR:N	2:h:110:TYR:CD1	2.83	0.44
2:i:10:HIS:N	2:i:14:GLN:O	2.44	0.44
2:n:104:TYR:CE1	2:o:59:VAL:HG23	2.52	0.44
1:N:31:LEU:HD11	1:O:59:ILE:HD11	1.99	0.44
1:A:23:LEU:HD12	1:A:23:LEU:N	2.33	0.44
1:C:105:ASP:O	1:C:109:THR:HG23	2.17	0.44
1:C:116:ARG:NH1	1:C:120:LEU:O	2.49	0.44
2:b:113:ASP:O	2:b:117:ASP:N	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:98:ILE:HG22	2:l:98:ILE:O	2.18	0.44
2:m:82:ASP:OD1	2:m:82:ASP:N	2.51	0.44
1:A:34:GLU:OE2	1:B:58:THR:N	2.50	0.43
1:B:85:ARG:NE	1:C:102:ASP:OD2	2.48	0.43
1:B:124:ASP:OD2	1:C:116:ARG:NE	2.50	0.43
1:B:138:GLY:O	1:B:139:ALA:HB2	2.18	0.43
1:D:22:GLY:C	1:D:23:LEU:HD22	2.43	0.43
1:F:87:VAL:CG1	1:F:88:THR:N	2.80	0.43
1:F:94:THR:HG23	1:F:94:THR:O	2.18	0.43
1:M:38:MET:SD	1:N:117:ILE:HD12	2.57	0.43
2:b:32:SER:O	2:g:90:SER:OG	2.36	0.43
2:e:56:VAL:HG12	2:e:57:PRO:O	2.17	0.43
2:g:3:ARG:NH2	2:g:52:VAL:HG11	2.33	0.43
2:n:18:ASN:N	2:n:45:THR:OG1	2.51	0.43
2:o:2:ARG:NH2	2:o:85:SER:OG	2.46	0.43
1:A:84:ASN:O	1:A:85:ARG:HB3	2.18	0.43
1:B:37:ALA:O	1:B:41:GLY:N	2.51	0.43
1:C:100:ILE:O	1:C:104:LYS:HG2	2.18	0.43
1:J:60:GLU:O	1:J:64:ILE:HG12	2.18	0.43
2:b:86:ASP:OD1	2:b:86:ASP:N	2.49	0.43
2:c:59:VAL:HG13	2:c:59:VAL:O	2.19	0.43
2:j:23:LEU:HD21	2:j:66:TYR:CD2	2.53	0.43
1:J:64:ILE:HD11	1:J:117:ILE:CG2	2.48	0.43
1:M:37:ALA:HB1	1:M:42:PHE:O	2.18	0.43
1:N:20:LEU:HD12	1:N:20:LEU:N	2.34	0.43
2:d:93:ARG:HD2	2:d:93:ARG:O	2.18	0.43
2:i:21:LEU:HD23	2:i:70:THR:HA	2.00	0.43
2:l:12:ASP:O	2:l:13:ASP:HB2	2.18	0.43
2:o:31:ASN:ND2	2:o:36:TYR:OH	2.51	0.43
1:C:116:ARG:NE	1:C:116:ARG:HA	2.33	0.43
1:D:9:THR:HG23	1:D:9:THR:O	2.18	0.43
1:D:34:GLU:OE2	1:E:58:THR:N	2.50	0.43
1:F:34:GLU:HG2	1:G:59:ILE:HG22	2.01	0.43
1:G:126:LEU:HD22	1:G:127:TYR:CZ	2.53	0.43
1:K:89:LYS:HA	1:K:93:ILE:C	2.43	0.43
1:L:83:GLU:OE1	1:L:83:GLU:N	2.45	0.43
1:O:134:GLU:HA	1:O:140:ASN:HA	2.00	0.43
2:i:16:TRP:HB3	2:i:19:VAL:HG11	2.00	0.43
2:i:107:VAL:O	2:i:111:LEU:HG	2.18	0.43
2:j:46:ASP:OD1	2:j:49:GLY:N	2.51	0.43
1:B:60:GLU:O	1:B:64:ILE:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ASP:OD1	1:F:116:ARG:NE	2.49	0.43
1:N:64:ILE:O	1:N:68:VAL:HG23	2.18	0.43
1:O:125:ASN:OD1	1:O:127:TYR:N	2.49	0.43
2:e:101:ASP:OD2	2:e:104:TYR:N	2.52	0.43
2:i:67:ILE:N	2:i:67:ILE:HD12	2.33	0.43
1:B:81:SER:OG	1:B:100:ILE:HD11	2.17	0.43
1:K:136:ARG:HG3	1:K:137:ILE:H	1.82	0.43
1:L:89:LYS:O	1:L:89:LYS:HG3	2.18	0.43
1:M:85:ARG:O	1:N:96:ASN:HB3	2.18	0.43
1:N:77:LEU:HD23	1:N:77:LEU:O	2.17	0.43
2:a:5:LYS:CD	2:a:52:VAL:HG23	2.49	0.43
2:n:24:THR:HG23	2:n:40:THR:HG22	2.00	0.43
1:A:49:PHE:CE1	1:A:53:LEU:HD11	2.54	0.43
1:B:64:ILE:HD11	1:B:117:ILE:CG2	2.49	0.43
1:D:77:LEU:HD23	1:D:77:LEU:C	2.44	0.43
1:D:77:LEU:HD21	1:D:99:TYR:HE2	1.84	0.43
1:M:75:ASP:OD1	1:M:75:ASP:C	2.61	0.43
2:b:69:THR:HG22	2:b:75:LYS:HD2	2.01	0.43
2:d:61:ILE:O	2:d:100:THR:HG21	2.19	0.43
2:g:110:TYR:CD2	2:g:111:LEU:HD22	2.54	0.43
2:j:1:MET:CE	2:j:56:VAL:HG13	2.47	0.43
2:l:63:GLN:OE1	2:l:65:TYR:HB2	2.18	0.43
2:n:112:GLU:OE1	2:n:113:ASP:N	2.52	0.43
1:B:130:TYR:O	1:B:130:TYR:CG	2.72	0.43
1:D:53:LEU:HD12	1:D:53:LEU:O	2.19	0.43
1:E:98:ASN:ND2	1:E:102:ASP:OD1	2.50	0.43
1:F:40:ILE:O	1:F:40:ILE:HG22	2.19	0.43
1:G:34:GLU:OE2	1:H:58:THR:N	2.52	0.43
1:I:81:SER:O	1:I:84:ASN:N	2.49	0.43
1:I:126:LEU:HD11	1:I:127:TYR:CZ	2.53	0.43
1:J:121:PRO:HB2	1:J:133:VAL:HG23	2.01	0.43
1:K:17:ASN:N	1:K:17:ASN:OD1	2.50	0.43
1:K:100:ILE:O	1:K:104:LYS:HG2	2.19	0.43
1:L:123:LEU:HB3	1:L:134:GLU:HB3	2.01	0.43
1:M:130:TYR:O	1:M:130:TYR:CG	2.71	0.43
2:d:29:THR:HG22	2:d:30:PHE:N	2.34	0.43
2:l:93:ARG:O	2:l:97:ILE:HD13	2.19	0.43
2:m:9:ARG:NH1	2:m:13:ASP:O	2.52	0.43
1:A:58:THR:N	1:O:34:GLU:OE2	2.52	0.43
1:F:20:LEU:HD12	1:F:21:ASP:N	2.34	0.43
1:H:12:LEU:HD11	1:H:35:PHE:CB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:ALA:O	1:I:140:ASN:C	2.62	0.43
1:L:58:THR:O	1:L:61:VAL:HG22	2.19	0.43
1:N:130:TYR:O	1:N:130:TYR:CG	2.72	0.43
2:b:109:ASN:OD1	2:b:109:ASN:N	2.52	0.43
1:A:22:GLY:C	1:A:23:LEU:HD12	2.44	0.43
1:D:30:GLU:OE1	2:m:42:HIS:ND1	2.52	0.43
1:E:89:LYS:HA	1:E:93:ILE:C	2.44	0.43
1:L:108:VAL:HG12	1:L:112:LYS:NZ	2.33	0.43
1:N:21:ASP:OD1	1:N:21:ASP:N	2.50	0.43
2:b:19:VAL:N	2:b:45:THR:OG1	2.41	0.43
2:c:80:VAL:HG12	2:c:81:PRO:O	2.19	0.43
2:f:105:THR:HG23	2:f:108:LEU:HD11	1.99	0.43
2:h:61:ILE:N	2:h:61:ILE:HD12	2.34	0.43
2:k:46:ASP:OD1	2:k:49:GLY:N	2.52	0.43
2:n:11:LEU:HD21	2:o:41:LYS:CG	2.49	0.43
1:A:123:LEU:HA	1:A:132:ASP:HB3	2.00	0.42
1:D:88:THR:HB	1:E:94:THR:OG1	2.19	0.42
1:F:40:ILE:O	1:F:123:LEU:HD12	2.19	0.42
1:N:21:ASP:O	2:a:73:ASN:OD1	2.37	0.42
1:O:16:TYR:OH	1:O:32:GLU:OE2	2.25	0.42
2:c:4:LEU:HD12	2:c:87:ILE:O	2.18	0.42
2:h:98:ILE:HD12	2:h:98:ILE:N	2.33	0.42
2:n:98:ILE:HD13	2:o:63:GLN:H	1.84	0.42
1:B:122:VAL:O	1:B:133:VAL:N	2.47	0.42
1:F:53:LEU:C	1:F:56:LEU:HD23	2.43	0.42
1:H:130:TYR:O	1:H:130:TYR:CG	2.72	0.42
1:H:136:ARG:HG3	1:H:137:ILE:H	1.84	0.42
1:K:134:GLU:O	1:K:138:GLY:N	2.52	0.42
2:f:59:VAL:HG22	2:f:60:GLY:N	2.34	0.42
2:k:23:LEU:HD12	2:k:24:THR:H	1.83	0.42
1:B:89:LYS:HA	1:B:93:ILE:O	2.18	0.42
1:D:89:LYS:HG3	1:D:89:LYS:O	2.19	0.42
1:E:31:LEU:CD1	1:F:59:ILE:HD11	2.49	0.42
1:K:113:LYS:O	1:K:117:ILE:HG12	2.19	0.42
1:L:125:ASN:O	1:M:116:ARG:NH2	2.44	0.42
1:N:134:GLU:CD	1:N:139:ALA:HA	2.44	0.42
2:b:68:LEU:HD23	2:b:69:THR:N	2.34	0.42
2:c:62:ASP:OD1	2:c:62:ASP:N	2.52	0.42
2:f:58:ASN:CG	2:f:64:SER:HG	2.20	0.42
2:j:18:ASN:N	2:j:45:THR:O	2.43	0.42
2:n:8:ILE:HG23	2:o:37:PRO:CG	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:TYR:O	1:I:130:TYR:CG	2.72	0.42
1:O:106:GLU:O	1:O:109:THR:OG1	2.30	0.42
2:b:72:ASP:OD1	2:c:38:ILE:HD12	2.20	0.42
2:h:112:GLU:HA	2:h:115:ILE:HG12	2.02	0.42
2:m:21:LEU:HD23	2:m:71:PRO:HD3	2.01	0.42
1:B:48:ASN:OD1	1:B:49:PHE:N	2.53	0.42
1:H:85:ARG:O	1:I:96:ASN:HB3	2.19	0.42
1:H:98:ASN:OD1	1:H:98:ASN:N	2.52	0.42
1:J:85:ARG:O	1:K:96:ASN:HB3	2.19	0.42
1:J:121:PRO:CB	1:J:133:VAL:HG23	2.49	0.42
1:L:34:GLU:HG2	1:M:59:ILE:HG22	2.00	0.42
1:M:64:ILE:CD1	1:M:117:ILE:HG21	2.50	0.42
2:a:9:ARG:O	2:k:37:PRO:HD2	2.19	0.42
2:b:50:GLU:OE1	2:b:51:PHE:N	2.51	0.42
2:k:9:ARG:O	2:l:37:PRO:HD2	2.19	0.42
2:m:29:THR:HG22	2:m:30:PHE:H	1.85	0.42
1:L:93:ILE:O	1:L:95:MET:HE1	2.18	0.42
1:O:134:GLU:HA	1:O:140:ASN:H	1.85	0.42
2:a:58:ASN:ND2	2:a:60:GLY:O	2.53	0.42
2:g:55:VAL:HG21	2:g:80:VAL:HG21	2.01	0.42
2:h:42:HIS:CG	2:h:43:ALA:N	2.87	0.42
1:C:134:GLU:O	1:C:135:GLY:C	2.63	0.42
1:D:87:VAL:HG23	1:D:95:MET:HE1	2.02	0.42
1:F:126:LEU:HD11	1:F:127:TYR:CZ	2.54	0.42
1:G:108:VAL:HA	1:G:111:VAL:HG22	2.02	0.42
1:H:28:LEU:O	1:H:33:ILE:HD11	2.19	0.42
2:d:16:TRP:CE3	2:d:19:VAL:HG11	2.54	0.42
2:f:82:ASP:OD1	2:f:83:GLY:N	2.49	0.42
2:l:25:LEU:HD21	2:l:27:ASN:O	2.19	0.42
2:n:29:THR:HG21	2:n:64:SER:HB2	2.01	0.42
1:C:130:TYR:O	1:C:130:TYR:CG	2.73	0.42
1:I:58:THR:HG23	1:I:59:ILE:N	2.34	0.42
2:c:17:ILE:O	2:c:18:ASN:OD1	2.37	0.42
2:m:111:LEU:O	2:m:115:ILE:HG12	2.19	0.42
1:A:85:ARG:NE	1:A:100:ILE:HD12	2.35	0.42
1:A:136:ARG:HG3	1:A:137:ILE:N	2.34	0.42
1:B:35:PHE:CE2	1:B:68:VAL:HG13	2.55	0.42
1:I:134:GLU:O	1:I:135:GLY:C	2.63	0.42
2:c:7:THR:OG1	2:c:50:GLU:OE1	2.36	0.42
2:m:87:ILE:HG22	2:m:88:GLU:N	2.35	0.42
1:A:100:ILE:O	1:A:104:LYS:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD12	1:B:40:ILE:N	2.35	0.42
1:D:134:GLU:HA	1:D:139:ALA:H	1.83	0.42
1:G:41:GLY:HA3	1:G:123:LEU:HD11	2.02	0.42
1:L:37:ALA:HB1	1:L:42:PHE:O	2.20	0.42
1:L:130:TYR:O	1:L:130:TYR:CG	2.71	0.42
1:M:100:ILE:HG22	1:M:104:LYS:NZ	2.34	0.42
1:N:38:MET:HE1	1:O:59:ILE:HG22	2.02	0.42
2:a:11:LEU:O	2:k:36:TYR:OH	2.31	0.42
2:a:115:ILE:O	2:a:119:ILE:HG12	2.20	0.42
2:c:103:GLU:HA	2:c:103:GLU:OE1	2.20	0.42
1:E:36:VAL:O	1:E:40:ILE:HG12	2.20	0.41
1:G:85:ARG:O	1:H:96:ASN:HB3	2.19	0.41
1:H:75:ASP:O	1:H:79:LYS:HG2	2.19	0.41
1:I:63:THR:HA	1:I:66:THR:HG22	2.02	0.41
2:b:38:ILE:HD12	2:g:72:ASP:OD2	2.20	0.41
2:m:24:THR:CB	2:m:40:THR:HG1	2.26	0.41
2:o:93:ARG:O	2:o:97:ILE:HB	2.20	0.41
1:A:36:VAL:O	1:A:40:ILE:HG12	2.20	0.41
1:A:59:ILE:HD11	1:O:35:PHE:HD1	1.85	0.41
1:I:40:ILE:HG22	1:I:40:ILE:O	2.20	0.41
1:L:88:THR:HB	1:M:94:THR:HG1	1.85	0.41
1:O:93:ILE:HD12	1:O:93:ILE:H	1.84	0.41
2:c:59:VAL:HG11	2:c:82:ASP:OD2	2.20	0.41
2:c:67:ILE:HD13	2:c:77:SER:HA	2.02	0.41
2:f:104:TYR:CD1	2:f:104:TYR:N	2.88	0.41
2:i:46:ASP:OD1	2:i:49:GLY:N	2.52	0.41
1:K:12:LEU:HD21	1:L:59:ILE:HD13	2.00	0.41
1:M:70:GLU:O	1:M:74:LEU:HD23	2.19	0.41
1:N:85:ARG:NH1	1:N:97:MET:O	2.51	0.41
2:a:23:LEU:HD12	2:a:23:LEU:H	1.85	0.41
2:a:104:TYR:O	2:a:108:LEU:N	2.36	0.41
2:b:68:LEU:HD23	2:b:68:LEU:C	2.45	0.41
2:d:68:LEU:HD23	2:d:68:LEU:C	2.45	0.41
2:m:29:THR:HG22	2:m:30:PHE:N	2.35	0.41
2:o:24:THR:HG22	2:o:25:LEU:O	2.21	0.41
1:C:18:GLN:N	1:C:18:GLN:OE1	2.54	0.41
1:F:47:ASN:O	1:F:48:ASN:C	2.64	0.41
1:I:64:ILE:CD1	1:I:117:ILE:HG21	2.50	0.41
1:I:106:GLU:O	1:I:109:THR:OG1	2.31	0.41
1:N:33:ILE:HD12	1:N:33:ILE:H	1.85	0.41
2:c:91:VAL:HG13	2:c:92:VAL:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:17:ILE:HG22	2:h:47:GLN:O	2.20	0.41
2:h:61:ILE:HD12	2:h:61:ILE:H	1.84	0.41
2:l:18:ASN:N	2:l:45:THR:O	2.47	0.41
1:C:9:THR:OG1	1:C:10:HIS:N	2.52	0.41
1:E:31:LEU:HD12	1:F:59:ILE:HD11	2.02	0.41
1:E:53:LEU:C	1:E:56:LEU:HD23	2.45	0.41
1:H:53:LEU:C	1:H:56:LEU:HD23	2.45	0.41
1:M:41:GLY:HA3	1:M:123:LEU:HD11	2.03	0.41
1:M:61:VAL:CG2	1:M:65:ARG:HE	2.33	0.41
2:b:10:HIS:N	2:b:14:GLN:O	2.34	0.41
2:d:42:HIS:CG	2:d:43:ALA:N	2.86	0.41
2:d:55:VAL:HG21	2:d:80:VAL:HG11	2.03	0.41
2:f:23:LEU:HD12	2:f:67:ILE:O	2.21	0.41
2:f:98:ILE:O	2:f:102:PRO:HA	2.20	0.41
1:B:105:ASP:O	1:B:108:VAL:HG22	2.21	0.41
1:D:72:LEU:O	1:D:76:LYS:HG2	2.20	0.41
1:G:123:LEU:O	1:G:125:ASN:ND2	2.53	0.41
1:I:53:LEU:O	1:I:56:LEU:HD22	2.20	0.41
1:K:126:LEU:HD11	1:K:127:TYR:CE2	2.55	0.41
1:N:113:LYS:O	1:N:117:ILE:HG12	2.20	0.41
1:O:123:LEU:C	1:O:123:LEU:HD12	2.45	0.41
2:c:5:LYS:HG2	2:c:52:VAL:HG22	2.03	0.41
2:f:4:LEU:HD11	2:f:89:PHE:HB2	2.01	0.41
2:i:97:ILE:O	2:i:97:ILE:HG23	2.20	0.41
2:j:79:THR:OG1	2:j:97:ILE:HA	2.20	0.41
2:n:11:LEU:HD23	2:n:12:ASP:H	1.84	0.41
2:o:58:ASN:HB3	2:o:79:THR:HG23	2.03	0.41
1:B:85:ARG:NH2	1:C:102:ASP:OD2	2.52	0.41
1:I:55:ASP:OD1	1:I:55:ASP:N	2.53	0.41
1:I:116:ARG:NE	1:I:116:ARG:HA	2.36	0.41
2:d:62:ASP:OD1	2:d:63:GLN:N	2.53	0.41
2:e:78:PHE:HB2	2:e:92:VAL:HG22	2.01	0.41
2:e:86:ASP:OD1	2:e:86:ASP:N	2.54	0.41
2:g:68:LEU:HD23	2:g:69:THR:N	2.35	0.41
2:i:66:TYR:C	2:i:67:ILE:HD12	2.46	0.41
2:m:1:MET:SD	2:m:2:ARG:N	2.88	0.41
2:m:92:VAL:O	2:m:92:VAL:HG22	2.20	0.41
2:o:110:TYR:HA	2:o:113:ASP:OD2	2.21	0.41
1:I:20:LEU:H	1:I:20:LEU:HD23	1.86	0.41
1:I:48:ASN:OD1	1:I:49:PHE:N	2.53	0.41
1:L:107:LEU:O	1:L:111:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:MET:HE1	1:N:117:ILE:HD12	2.02	0.41
2:c:58:ASN:HB2	2:c:64:SER:HB2	2.02	0.41
2:e:103:GLU:O	2:e:103:GLU:HG3	2.20	0.41
2:k:62:ASP:OD1	2:k:62:ASP:N	2.52	0.41
1:A:64:ILE:HD13	1:A:117:ILE:HD13	2.01	0.41
1:A:98:ASN:O	1:A:101:GLY:N	2.53	0.41
1:A:134:GLU:O	1:A:139:ALA:N	2.52	0.41
1:E:34:GLU:OE2	1:F:57:SER:OG	2.26	0.41
1:E:93:ILE:O	1:E:93:ILE:HG22	2.20	0.41
1:F:70:GLU:O	1:F:74:LEU:HD23	2.20	0.41
1:F:87:VAL:HG11	1:G:93:ILE:HG22	2.03	0.41
1:F:133:VAL:O	1:F:134:GLU:C	2.63	0.41
1:G:100:ILE:O	1:G:104:LYS:HG2	2.21	0.41
1:H:88:THR:HB	1:I:94:THR:OG1	2.21	0.41
1:H:135:GLY:N	1:H:140:ASN:HB3	2.35	0.41
1:L:47:ASN:O	1:L:50:VAL:HG22	2.20	0.41
1:N:85:ARG:O	1:O:96:ASN:HB3	2.21	0.41
2:e:54:ASN:ND2	2:m:13:ASP:OD2	2.54	0.41
2:i:61:ILE:HD12	2:i:61:ILE:N	2.36	0.41
2:k:21:LEU:HD12	2:k:21:LEU:N	2.36	0.41
2:n:29:THR:N	2:n:36:TYR:O	2.54	0.41
2:o:88:GLU:O	2:o:91:VAL:HG12	2.20	0.41
1:B:88:THR:HG22	1:B:89:LYS:N	2.36	0.41
1:C:31:LEU:HD11	2:o:22:PHE:CZ	2.56	0.41
1:D:108:VAL:HA	1:D:111:VAL:HG22	2.02	0.41
1:E:122:VAL:HG13	1:E:122:VAL:O	2.21	0.41
1:F:85:ARG:NH1	1:F:97:MET:O	2.42	0.41
1:H:92:ASP:H	1:H:93:ILE:HD12	1.86	0.41
1:J:29:GLU:O	1:J:32:GLU:N	2.54	0.41
1:M:133:VAL:HG12	1:M:133:VAL:O	2.21	0.41
1:O:100:ILE:O	1:O:104:LYS:HG2	2.21	0.41
2:a:9:ARG:NH1	2:a:13:ASP:O	2.45	0.41
2:d:58:ASN:OD1	2:d:100:THR:HG23	2.21	0.41
1:C:85:ARG:NH1	1:C:97:MET:O	2.44	0.40
1:G:51:ASN:OD1	1:G:52:ALA:N	2.54	0.40
1:L:123:LEU:H	1:L:123:LEU:HD23	1.85	0.40
1:M:64:ILE:HD13	1:M:117:ILE:HD13	2.03	0.40
1:O:32:GLU:O	1:O:36:VAL:HG23	2.20	0.40
1:O:128:VAL:HG22	1:O:131:ASP:OD1	2.21	0.40
2:a:4:LEU:HD11	2:a:89:PHE:HB2	2.03	0.40
2:d:20:SER:C	2:d:21:LEU:HD22	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:111:LEU:O	2:d:115:ILE:HG12	2.21	0.40
2:h:63:GLN:OE1	2:h:64:SER:N	2.55	0.40
2:j:21:LEU:HD13	2:j:70:THR:HA	2.03	0.40
1:H:36:VAL:O	1:H:40:ILE:HG12	2.21	0.40
1:K:79:LYS:O	1:K:82:ILE:HG22	2.22	0.40
2:b:106:ASN:HB3	2:c:79:THR:CG2	2.51	0.40
2:l:2:ARG:NH2	2:l:85:SER:OG	2.55	0.40
2:n:11:LEU:HD23	2:n:12:ASP:N	2.37	0.40
1:B:53:LEU:C	1:B:56:LEU:HD23	2.46	0.40
1:I:123:LEU:HD12	1:I:123:LEU:C	2.46	0.40
1:J:60:GLU:O	1:J:63:THR:OG1	2.34	0.40
1:J:89:LYS:HA	1:J:93:ILE:C	2.45	0.40
1:J:108:VAL:HA	1:J:111:VAL:HG22	2.03	0.40
1:K:130:TYR:O	1:K:130:TYR:CG	2.75	0.40
2:c:58:ASN:O	2:c:58:ASN:CG	2.64	0.40
2:i:23:LEU:HD12	2:i:24:THR:H	1.87	0.40
2:o:97:ILE:O	2:o:97:ILE:HG23	2.21	0.40
1:A:20:LEU:N	1:A:20:LEU:HD22	2.36	0.40
1:D:79:LYS:O	1:E:73:ARG:NH2	2.54	0.40
1:D:88:THR:HA	1:D:95:MET:HE2	2.04	0.40
1:I:88:THR:HA	1:I:95:MET:HG2	2.04	0.40
1:K:126:LEU:HD11	1:K:127:TYR:CZ	2.56	0.40
1:K:133:VAL:HG23	1:K:133:VAL:O	2.20	0.40
1:M:32:GLU:O	1:M:36:VAL:HG13	2.21	0.40
1:O:100:ILE:O	1:O:103:ILE:HG12	2.22	0.40
2:b:2:ARG:NH1	2:b:82:ASP:O	2.54	0.40
2:i:94:GLU:O	2:i:98:ILE:HG23	2.20	0.40
2:k:39:ASP:CG	2:k:40:THR:N	2.79	0.40
2:n:106:ASN:HA	2:n:109:ASN:OD1	2.20	0.40
2:o:107:VAL:O	2:o:111:LEU:HG	2.21	0.40
1:A:92:ASP:N	1:A:92:ASP:OD1	2.55	0.40
1:G:105:ASP:O	1:G:108:VAL:HG22	2.22	0.40
2:a:8:ILE:HD12	2:a:8:ILE:HA	2.00	0.40
2:a:23:LEU:HD12	2:a:41:LYS:O	2.20	0.40
2:d:121:ASN:O	2:d:125:SER:N	2.55	0.40
2:e:29:THR:N	2:e:36:TYR:O	2.50	0.40
2:g:106:ASN:OD1	2:g:107:VAL:HG23	2.21	0.40
2:i:25:LEU:HD12	2:i:65:TYR:O	2.21	0.40
2:o:10:HIS:HB2	2:o:12:ASP:OD1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	130/162 (80%)	120 (92%)	9 (7%)	1 (1%)	16	45
1	B	130/162 (80%)	118 (91%)	11 (8%)	1 (1%)	16	45
1	C	130/162 (80%)	117 (90%)	13 (10%)	0	100	100
1	D	130/162 (80%)	115 (88%)	14 (11%)	1 (1%)	16	45
1	E	130/162 (80%)	116 (89%)	13 (10%)	1 (1%)	16	45
1	F	130/162 (80%)	118 (91%)	12 (9%)	0	100	100
1	G	130/162 (80%)	119 (92%)	11 (8%)	0	100	100
1	H	130/162 (80%)	118 (91%)	12 (9%)	0	100	100
1	I	130/162 (80%)	119 (92%)	11 (8%)	0	100	100
1	J	130/162 (80%)	119 (92%)	11 (8%)	0	100	100
1	K	130/162 (80%)	118 (91%)	12 (9%)	0	100	100
1	L	130/162 (80%)	120 (92%)	10 (8%)	0	100	100
1	M	130/162 (80%)	117 (90%)	13 (10%)	0	100	100
1	N	130/162 (80%)	117 (90%)	13 (10%)	0	100	100
1	O	130/162 (80%)	119 (92%)	11 (8%)	0	100	100
2	a	123/241 (51%)	111 (90%)	12 (10%)	0	100	100
2	b	123/241 (51%)	114 (93%)	9 (7%)	0	100	100
2	c	123/241 (51%)	112 (91%)	11 (9%)	0	100	100
2	d	123/241 (51%)	116 (94%)	7 (6%)	0	100	100
2	e	123/241 (51%)	112 (91%)	11 (9%)	0	100	100
2	f	123/241 (51%)	113 (92%)	10 (8%)	0	100	100
2	g	123/241 (51%)	110 (89%)	13 (11%)	0	100	100
2	h	123/241 (51%)	113 (92%)	10 (8%)	0	100	100
2	i	123/241 (51%)	111 (90%)	12 (10%)	0	100	100
2	j	123/241 (51%)	112 (91%)	10 (8%)	1 (1%)	16	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	k	123/241 (51%)	112 (91%)	11 (9%)	0	100	100
2	l	123/241 (51%)	110 (89%)	13 (11%)	0	100	100
2	m	123/241 (51%)	111 (90%)	12 (10%)	0	100	100
2	n	123/241 (51%)	114 (93%)	9 (7%)	0	100	100
2	o	123/241 (51%)	114 (93%)	9 (7%)	0	100	100
All	All	3795/6045 (63%)	3455 (91%)	335 (9%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	139	ALA
1	E	139	ALA
1	A	139	ALA
1	B	139	ALA
2	j	97	ILE

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	123/146 (84%)	118 (96%)	5 (4%)	27	50
1	B	123/146 (84%)	120 (98%)	3 (2%)	43	60
1	C	123/146 (84%)	116 (94%)	7 (6%)	18	43
1	D	123/146 (84%)	116 (94%)	7 (6%)	18	43
1	E	123/146 (84%)	119 (97%)	4 (3%)	33	54
1	F	123/146 (84%)	119 (97%)	4 (3%)	33	54
1	G	123/146 (84%)	121 (98%)	2 (2%)	55	66
1	H	123/146 (84%)	114 (93%)	9 (7%)	13	38
1	I	123/146 (84%)	112 (91%)	11 (9%)	9	31
1	J	123/146 (84%)	118 (96%)	5 (4%)	27	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	123/146 (84%)	119 (97%)	4 (3%)	33	54
1	L	123/146 (84%)	115 (94%)	8 (6%)	15	40
1	M	123/146 (84%)	121 (98%)	2 (2%)	55	66
1	N	123/146 (84%)	118 (96%)	5 (4%)	27	50
1	O	123/146 (84%)	115 (94%)	8 (6%)	15	40
2	a	112/213 (53%)	105 (94%)	7 (6%)	16	41
2	b	112/213 (53%)	106 (95%)	6 (5%)	20	45
2	c	112/213 (53%)	109 (97%)	3 (3%)	39	57
2	d	112/213 (53%)	105 (94%)	7 (6%)	16	41
2	e	112/213 (53%)	100 (89%)	12 (11%)	6	26
2	f	112/213 (53%)	108 (96%)	4 (4%)	31	53
2	g	112/213 (53%)	110 (98%)	2 (2%)	51	65
2	h	112/213 (53%)	104 (93%)	8 (7%)	13	38
2	i	112/213 (53%)	104 (93%)	8 (7%)	13	38
2	j	112/213 (53%)	110 (98%)	2 (2%)	51	65
2	k	112/213 (53%)	102 (91%)	10 (9%)	9	31
2	l	112/213 (53%)	109 (97%)	3 (3%)	39	57
2	m	112/213 (53%)	107 (96%)	5 (4%)	24	48
2	n	112/213 (53%)	106 (95%)	6 (5%)	20	45
2	o	112/213 (53%)	106 (95%)	6 (5%)	20	45
All	All	3525/5385 (66%)	3352 (95%)	173 (5%)	24	47

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	57	SER
1	A	60	GLU
1	A	93	ILE
1	A	110	GLU
1	B	53	LEU
1	B	92	ASP
1	B	93	ILE
1	C	20	LEU
1	C	55	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	123	LEU
1	C	130	TYR
1	C	132	ASP
1	C	133	VAL
1	C	134	GLU
1	D	20	LEU
1	D	84	ASN
1	D	93	ILE
1	D	94	THR
1	D	107	LEU
1	D	123	LEU
1	D	126	LEU
1	E	9	THR
1	E	54	LEU
1	E	92	ASP
1	E	130	TYR
1	F	55	ASP
1	F	75	ASP
1	F	87	VAL
1	F	123	LEU
1	G	55	ASP
1	G	93	ILE
1	H	13	GLU
1	H	55	ASP
1	H	86	GLN
1	H	92	ASP
1	H	93	ILE
1	H	98	ASN
1	H	126	LEU
1	H	130	TYR
1	H	132	ASP
1	I	30	GLU
1	I	53	LEU
1	I	55	ASP
1	I	63	THR
1	I	70	GLU
1	I	75	ASP
1	I	78	ASN
1	I	91	GLU
1	I	126	LEU
1	I	130	TYR
1	I	132	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	74	LEU
1	J	92	ASP
1	J	98	ASN
1	J	104	LYS
1	J	132	ASP
1	K	13	GLU
1	K	93	ILE
1	K	126	LEU
1	K	130	TYR
1	L	53	LEU
1	L	55	ASP
1	L	61	VAL
1	L	75	ASP
1	L	92	ASP
1	L	107	LEU
1	L	130	TYR
1	L	134	GLU
1	M	51	ASN
1	M	79	LYS
1	N	53	LEU
1	N	59	ILE
1	N	93	ILE
1	N	130	TYR
1	N	140	ASN
1	O	55	ASP
1	O	75	ASP
1	O	91	GLU
1	O	93	ILE
1	O	110	GLU
1	O	125	ASN
1	O	126	LEU
1	O	132	ASP
2	a	1	MET
2	a	23	LEU
2	a	42	HIS
2	a	58	ASN
2	a	65	TYR
2	a	94	GLU
2	a	112	GLU
2	b	42	HIS
2	b	62	ASP
2	b	72	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	86	ASP
2	b	109	ASN
2	b	113	ASP
2	c	58	ASN
2	c	69	THR
2	c	97	ILE
2	d	1	MET
2	d	42	HIS
2	d	64	SER
2	d	82	ASP
2	d	94	GLU
2	d	110	TYR
2	d	121	ASN
2	e	11	LEU
2	e	14	GLN
2	e	16	TRP
2	e	29	THR
2	e	30	PHE
2	e	31	ASN
2	e	64	SER
2	e	69	THR
2	e	92	VAL
2	e	101	ASP
2	e	103	GLU
2	e	110	TYR
2	f	58	ASN
2	f	64	SER
2	f	73	ASN
2	f	104	TYR
2	g	110	TYR
2	g	111	LEU
2	h	1	MET
2	h	11	LEU
2	h	12	ASP
2	h	70	THR
2	h	72	ASP
2	h	86	ASP
2	h	103	GLU
2	h	112	GLU
2	i	13	ASP
2	i	14	GLN
2	i	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	i	58	ASN
2	i	98	ILE
2	i	104	TYR
2	i	117	ASP
2	i	121	ASN
2	j	42	HIS
2	j	94	GLU
2	k	3	ARG
2	k	5	LYS
2	k	14	GLN
2	k	30	PHE
2	k	58	ASN
2	k	70	THR
2	k	87	ILE
2	k	100	THR
2	k	104	TYR
2	k	108	LEU
2	l	58	ASN
2	l	62	ASP
2	l	75	LYS
2	m	72	ASP
2	m	73	ASN
2	m	75	LYS
2	m	79	THR
2	m	110	TYR
2	n	38	ILE
2	n	42	HIS
2	n	58	ASN
2	n	86	ASP
2	n	113	ASP
2	n	117	ASP
2	o	25	LEU
2	o	59	VAL
2	o	65	TYR
2	o	69	THR
2	o	97	ILE
2	o	104	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	86	GLN
1	D	18	GLN
1	F	84	ASN
1	F	86	GLN
1	G	18	GLN
1	G	46	GLN
1	G	98	ASN
1	K	96	ASN
1	L	47	ASN
1	M	47	ASN
1	N	98	ASN
2	a	10	HIS
2	b	34	ASN
2	b	73	ASN
2	c	58	ASN
2	c	109	ASN
2	e	42	HIS
2	g	18	ASN
2	g	48	ASN
2	h	31	ASN
2	i	10	HIS
2	k	18	ASN
2	k	109	ASN
2	n	48	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

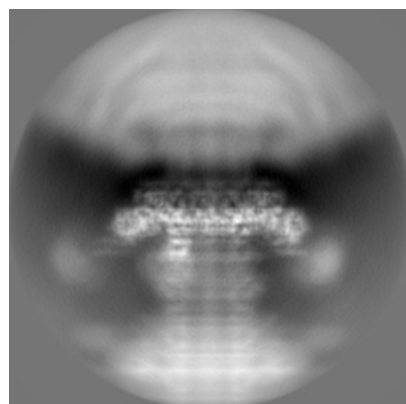
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37155. These allow visual inspection of the internal detail of the map and identification of artifacts.

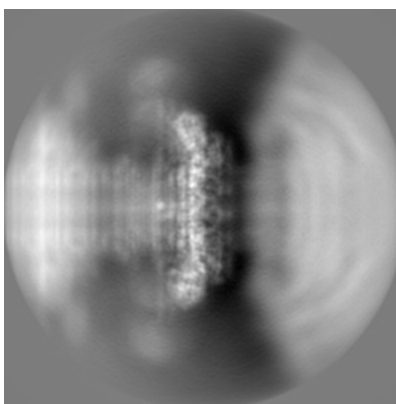
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

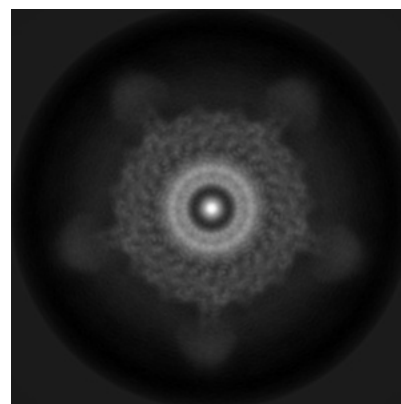
6.1.1 Primary map



X

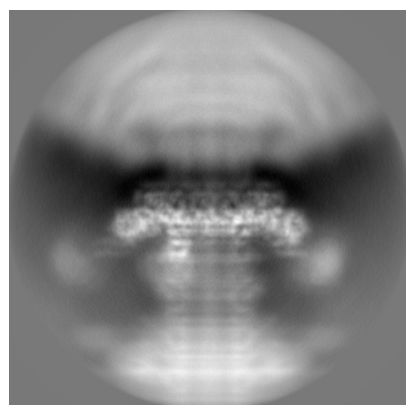


Y

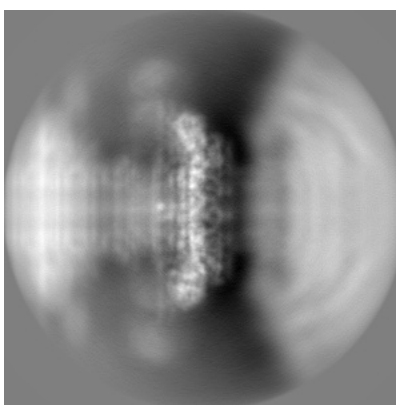


Z

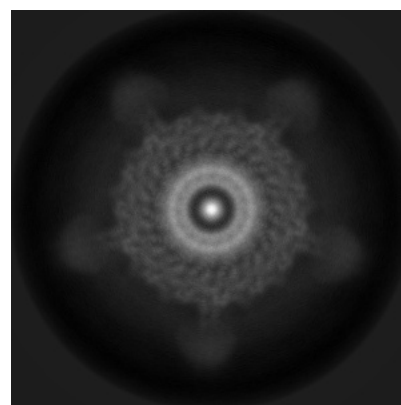
6.1.2 Raw map



X



Y

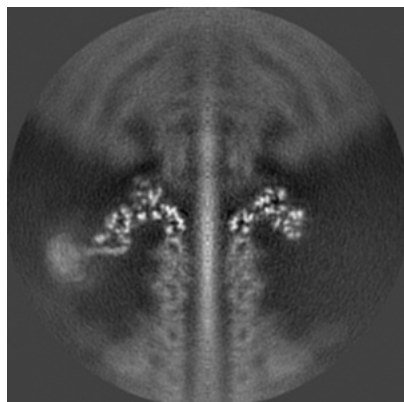


Z

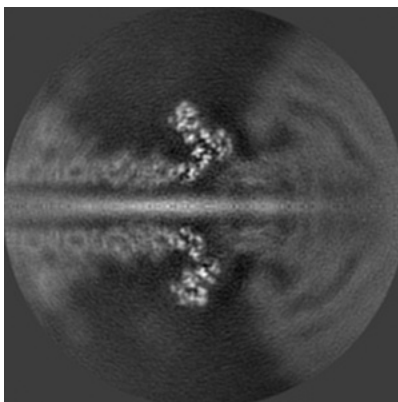
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

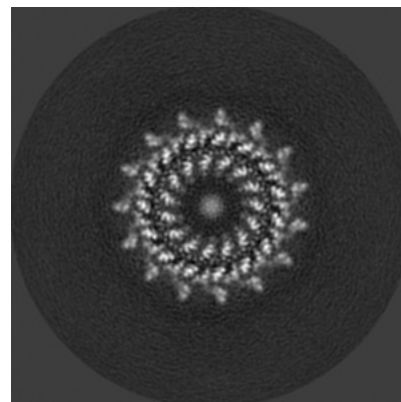
6.2.1 Primary map



X Index: 160

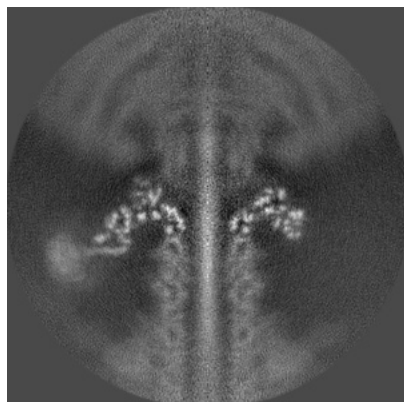


Y Index: 160

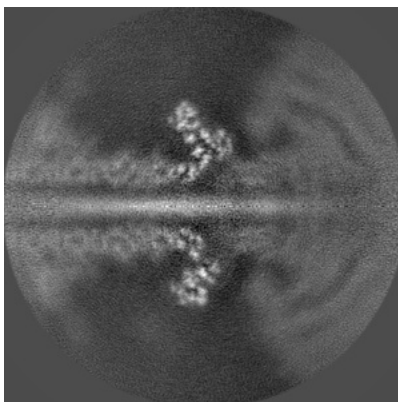


Z Index: 160

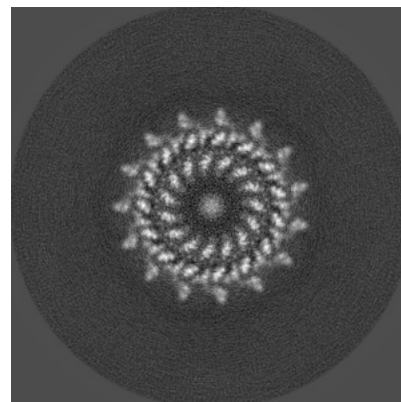
6.2.2 Raw map



X Index: 160



Y Index: 160

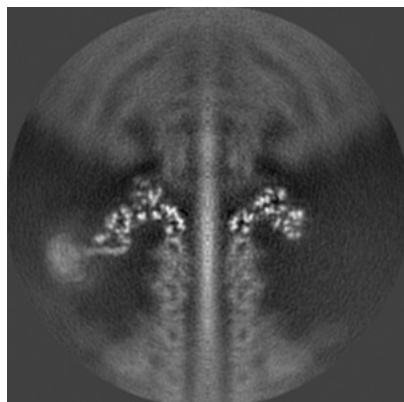


Z Index: 160

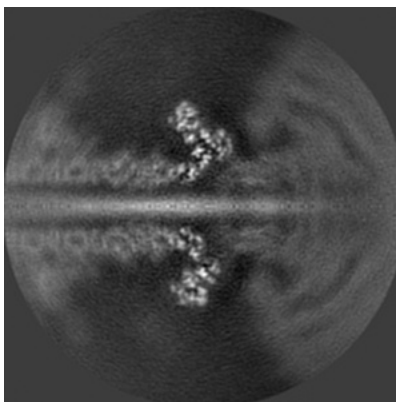
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

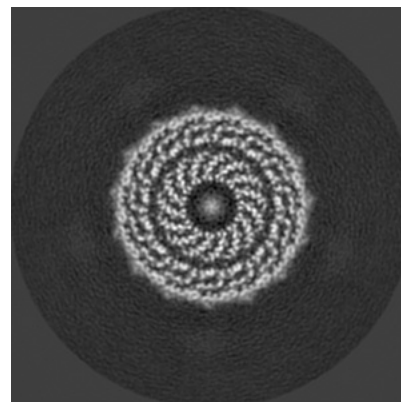
6.3.1 Primary map



X Index: 160

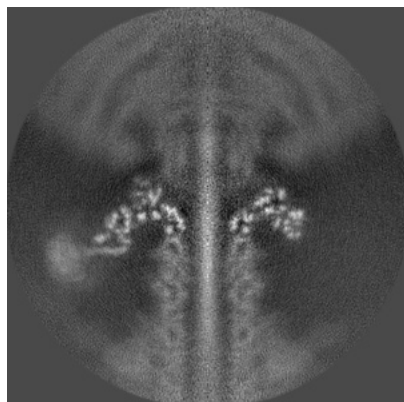


Y Index: 160

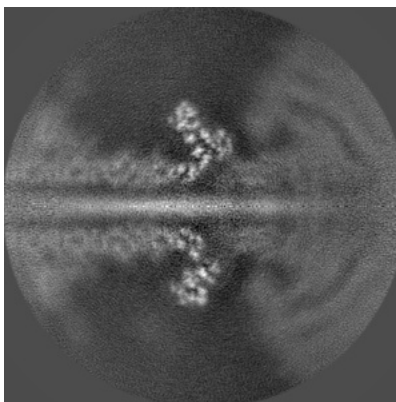


Z Index: 151

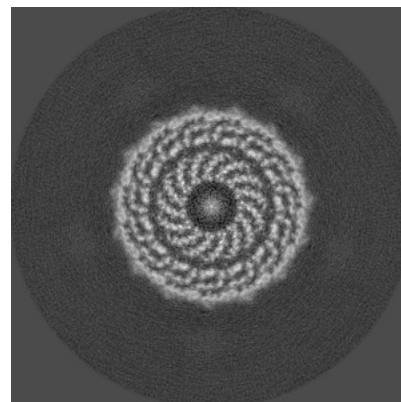
6.3.2 Raw map



X Index: 160



Y Index: 160

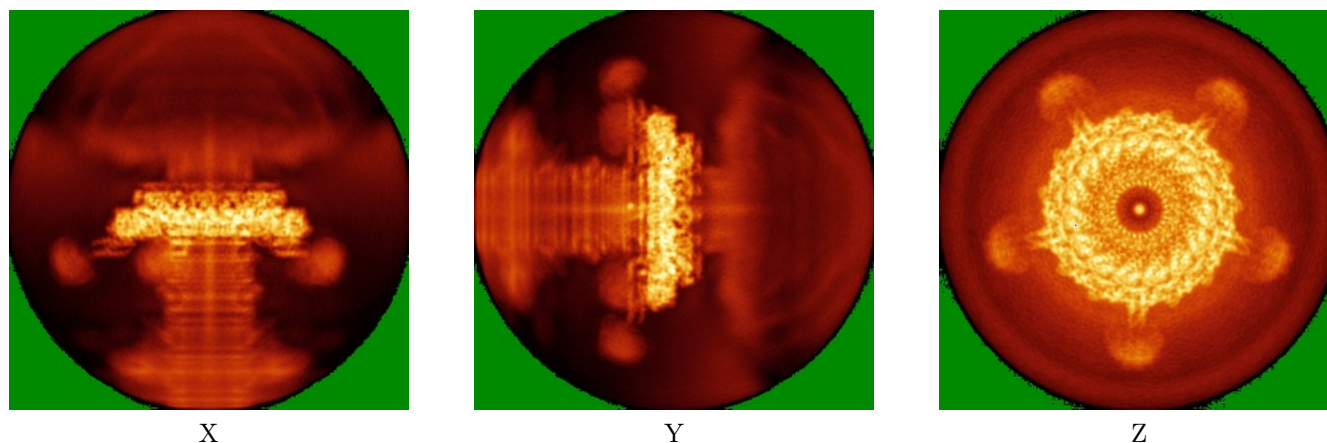


Z Index: 151

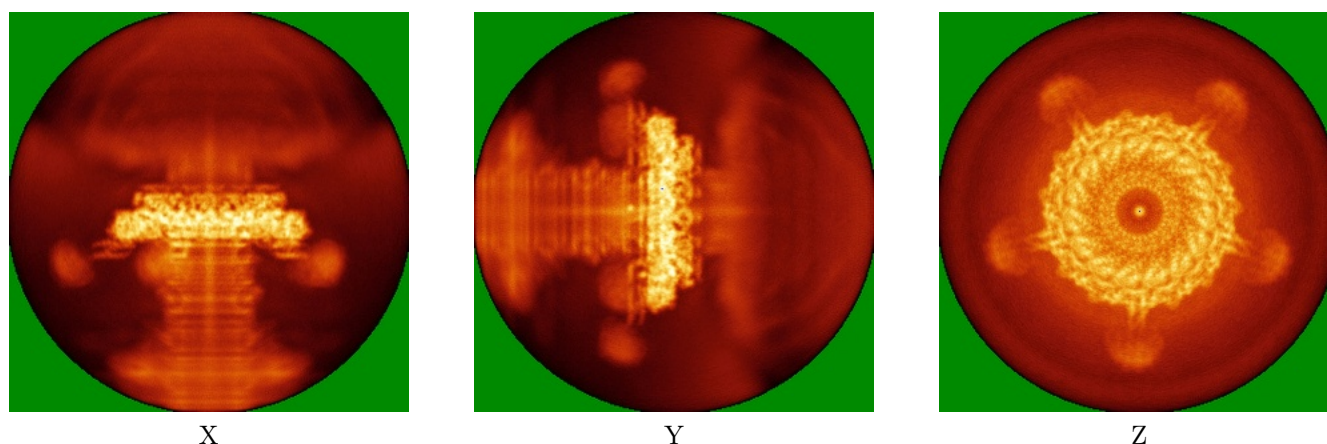
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

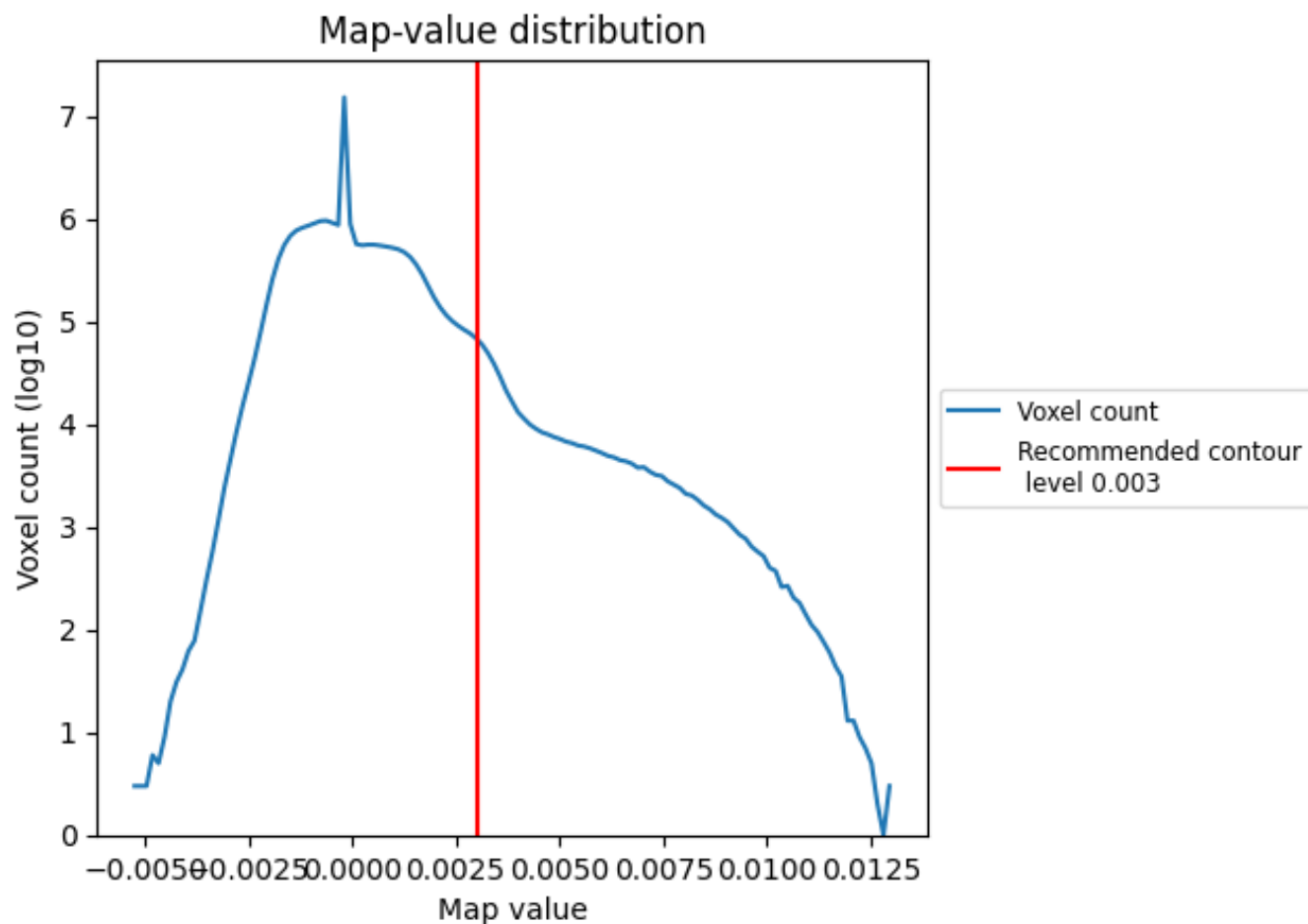
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

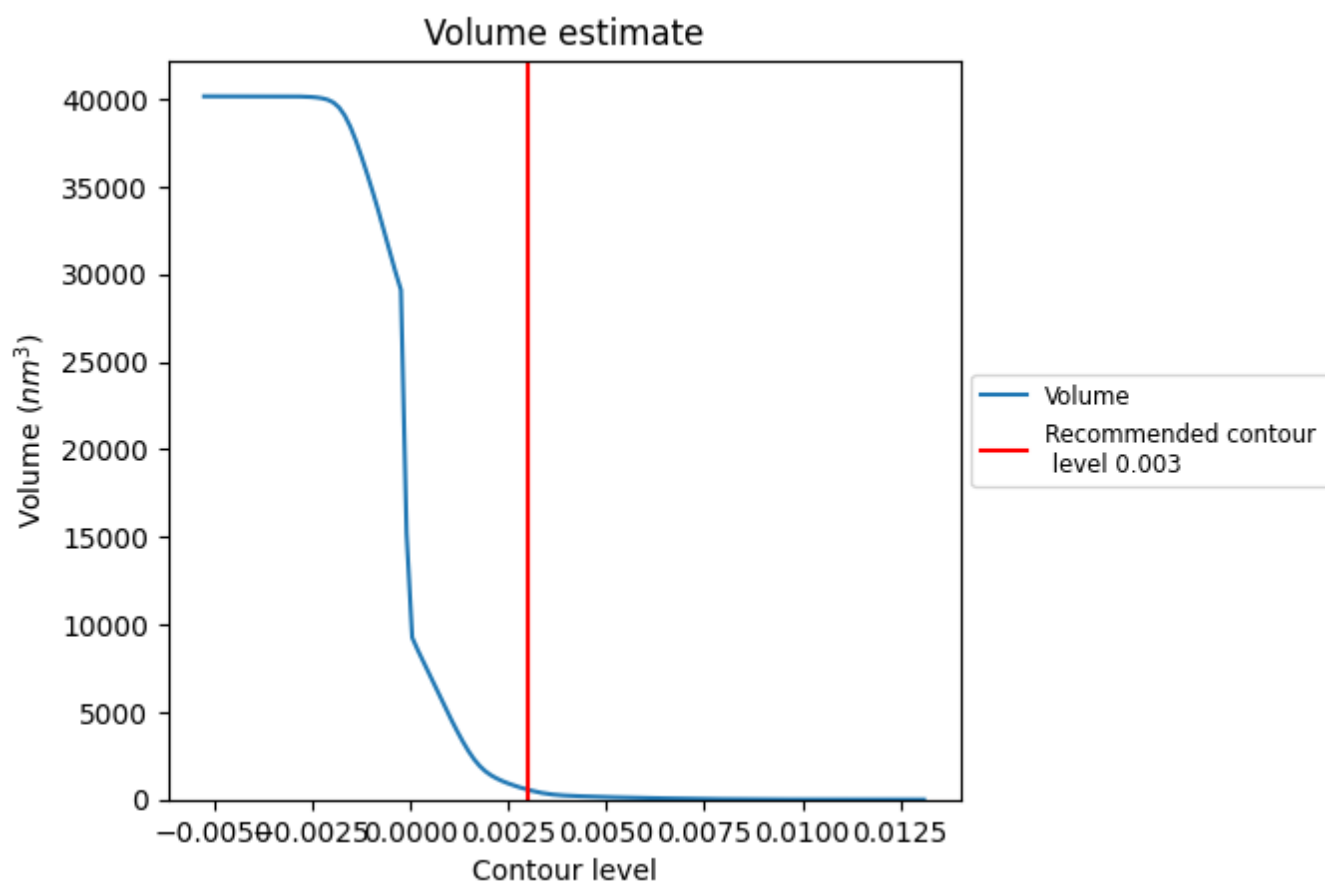
This section contains the results of statistical analysis of the map.

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.

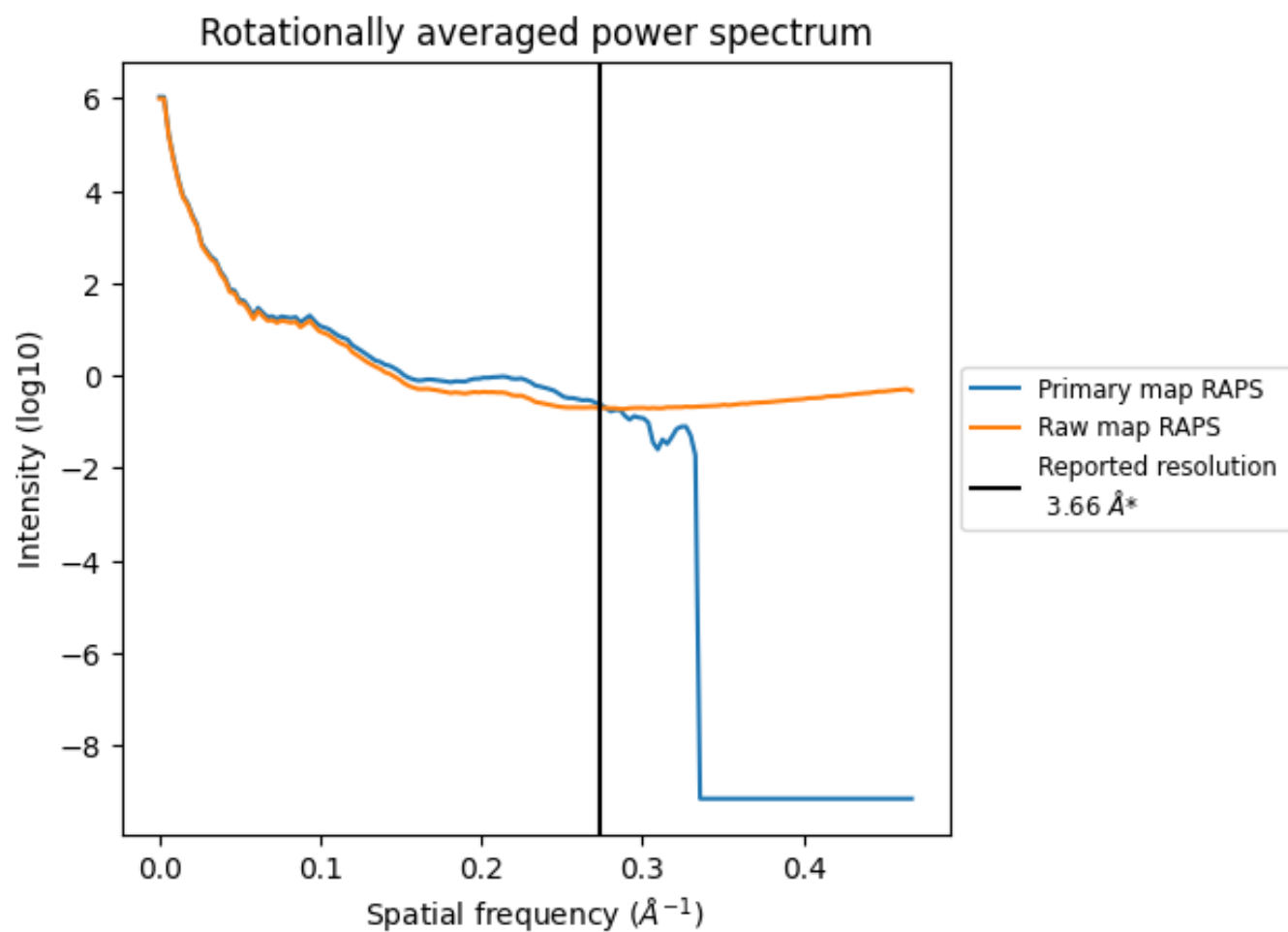
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 566 nm^3 ; this corresponds to an approximate mass of 511 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 ⓘ

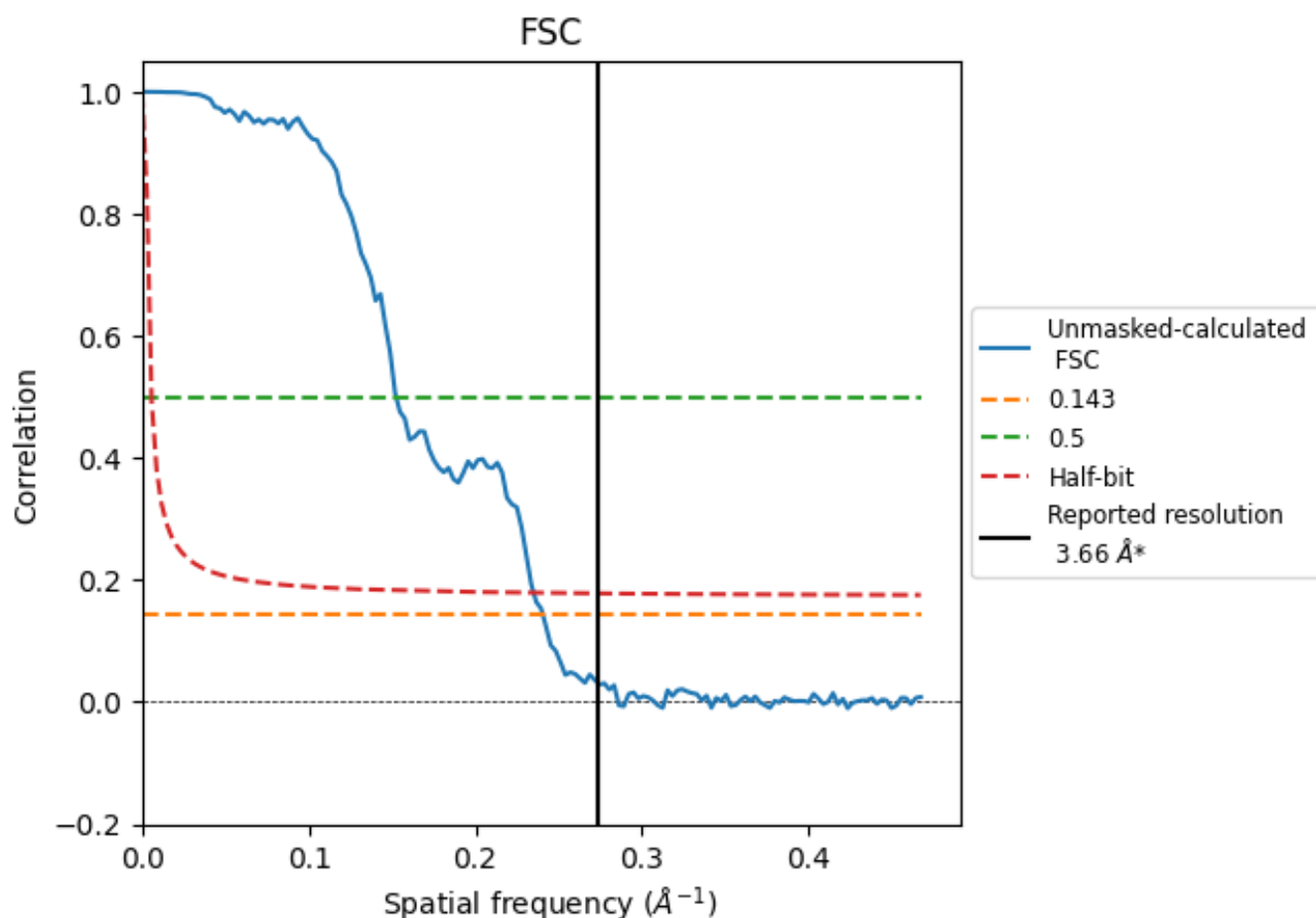


*Reported resolution corresponds to spatial frequency of 0.273 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.273 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	6.56	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.66 by more than 10 %

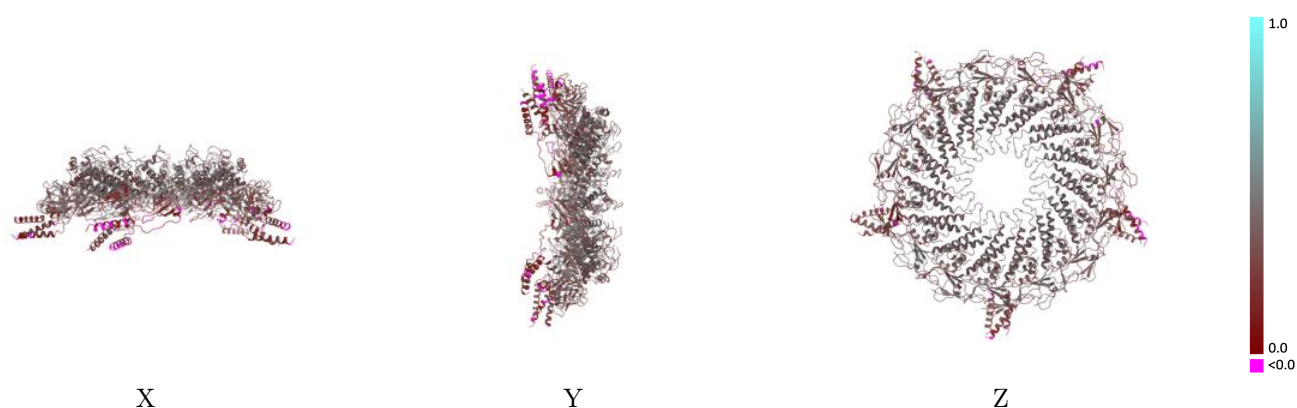
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37155 and PDB model 8KEG. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

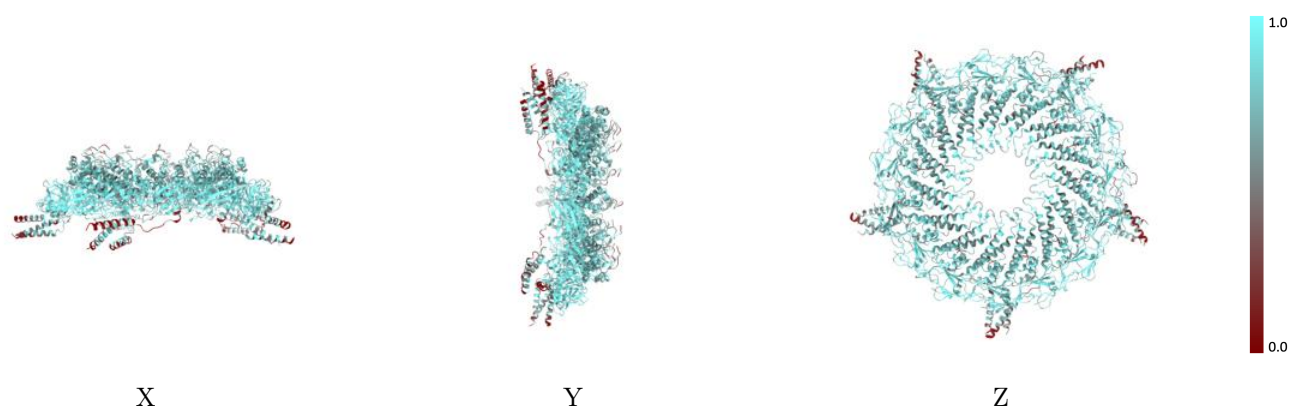
This section was not generated.

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



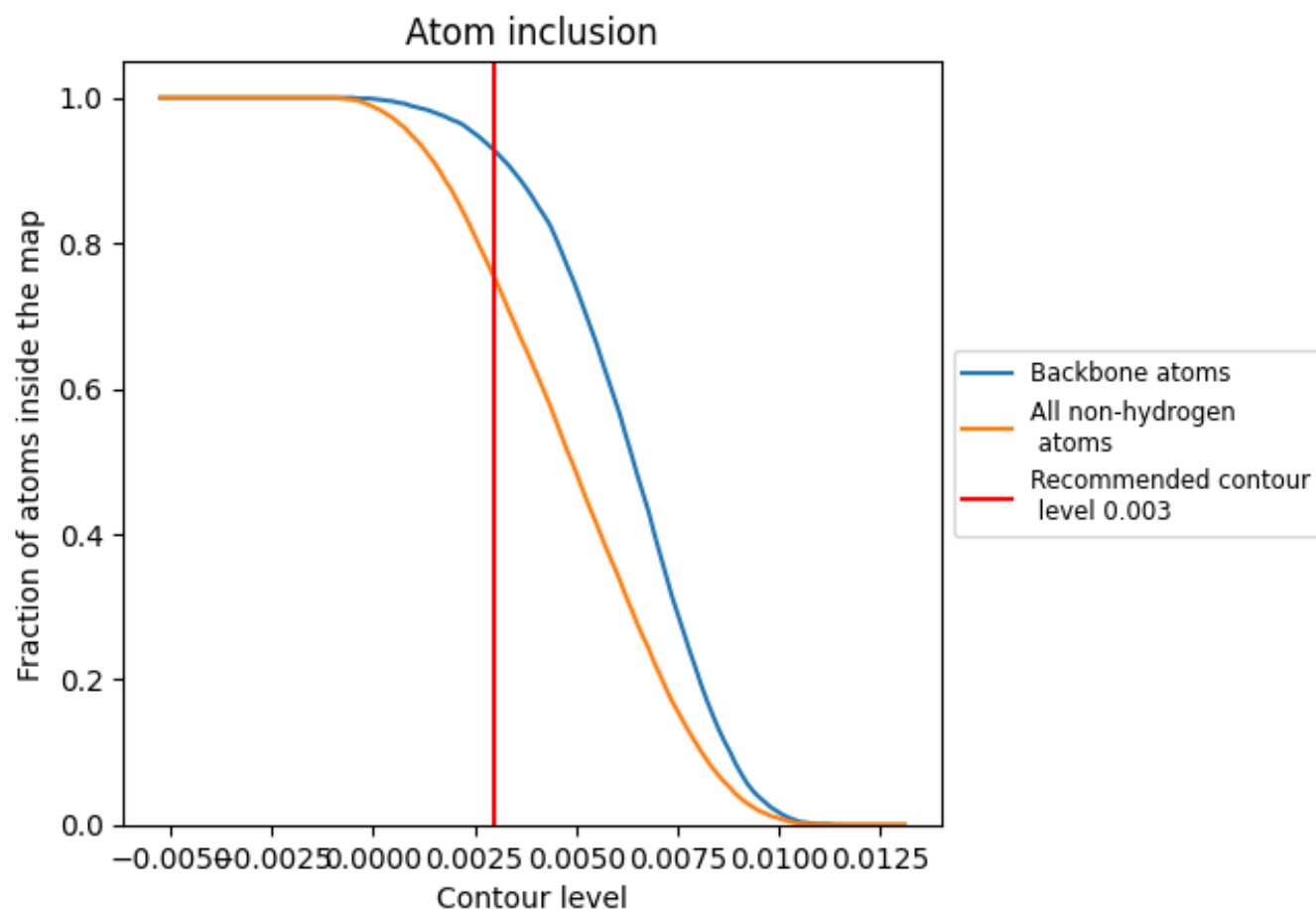
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 75% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7510	 0.3470
A	 0.7280	 0.3820
B	 0.7370	 0.3950
C	 0.7500	 0.4080
D	 0.7320	 0.3990
E	 0.7500	 0.4040
F	 0.7440	 0.4050
G	 0.7410	 0.4000
H	 0.7420	 0.4050
I	 0.7530	 0.4020
J	 0.7230	 0.3960
K	 0.7300	 0.3900
L	 0.7450	 0.4050
M	 0.7390	 0.3910
N	 0.7350	 0.3980
O	 0.7450	 0.4000
a	 0.8170	 0.3690
b	 0.7810	 0.2930
c	 0.7510	 0.2550
d	 0.6970	 0.2330
e	 0.7710	 0.2860
f	 0.7720	 0.2900
g	 0.7370	 0.3000
h	 0.7900	 0.3050
i	 0.7670	 0.3220
j	 0.7760	 0.3220
k	 0.7740	 0.2920
l	 0.7920	 0.3130
m	 0.6670	 0.2170
n	 0.8090	 0.3400
o	 0.7580	 0.2470

