



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 10:27 AM UTC

PDB ID : 7Z4A / pdb_00007z4a
EMDB ID : EMD-14489
Title : Bacteriophage SU10 tail and bottom part of the capsid (C1)
Authors : Siborova, M.; Fuzik, T.; Prochazkova, M.; Novacek, J.; Plevka, P.
Deposited on : 2022-03-03
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

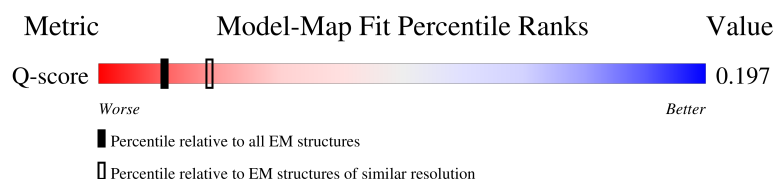
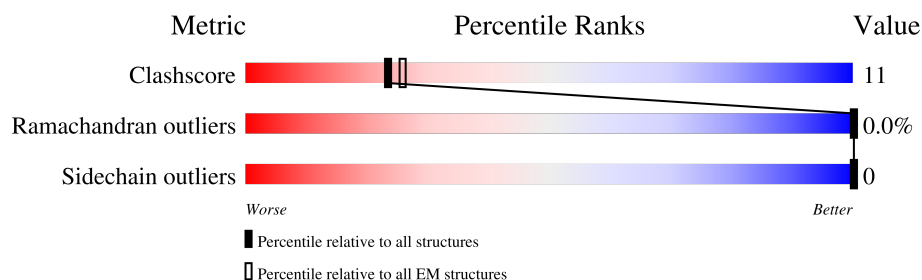
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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.



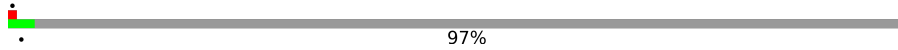
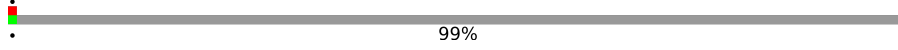
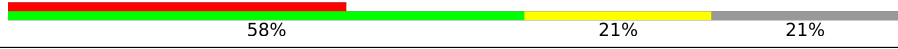
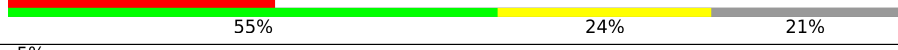
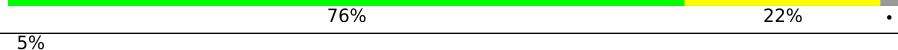
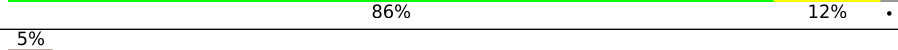
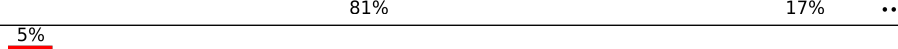
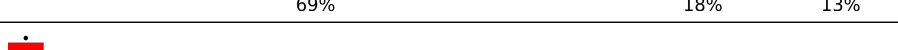
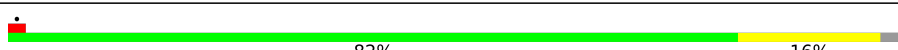
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	250	16% 75% 16% 9%
1	N	250	17% 77% 14% 9%
2	V	1005	8% 78% 12% 9%
3	O	786	96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	R	786	
3	S	786	
4	J	747	
4	K	747	
5	B	352	
5	C	352	
5	D	352	
5	E	352	
5	F	352	
5	G	352	
5	H	352	
5	I	352	
5	L	352	
5	M	352	
5	P	352	
5	Q	352	
5	T	352	
5	U	352	
5	X	352	
5	Y	352	
5	b	352	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65632 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 Adaptor protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	227	Total	C	N	O	S	0	0
			1852	1192	300	354	6		
1	N	228	Total	C	N	O	S	0	0
			1858	1195	301	356	6		

- Molecule 2 is a protein called Surface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	912	Total	C	N	O	S	0	0
			7079	4475	1180	1408	16		

- Molecule 3 is a protein called Putative tail fiber.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	29	Total	C	N	O	0	0
			213	132	37	44		
3	R	25	Total	C	N	O	0	0
			177	110	30	37		
3	S	8	Total	C	N	O	0	0
			58	37	10	11		

- Molecule 4 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	589	Total	C	N	O	S	0	0
			4727	2971	815	919	22		
4	K	589	Total	C	N	O	S	0	0
			4727	2971	815	919	22		

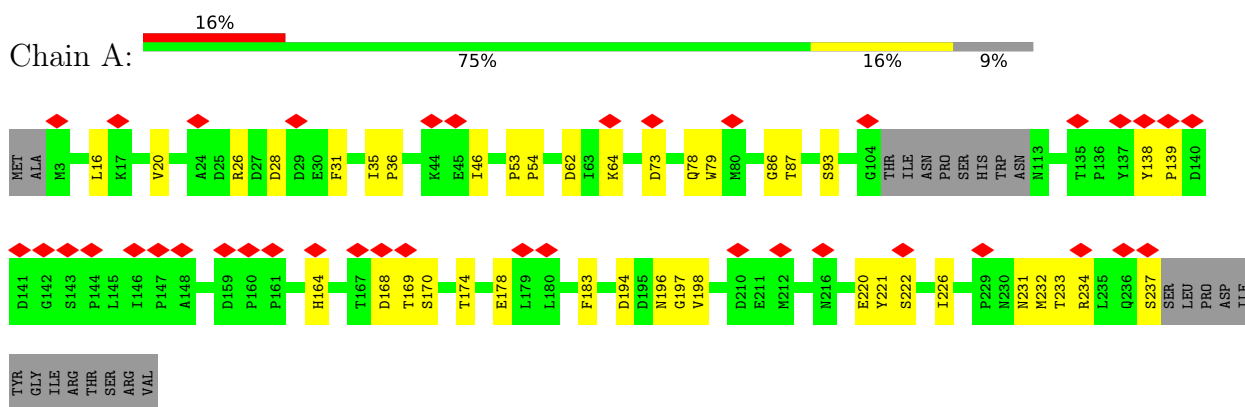
- Molecule 5 is a protein called Major head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	346	Total	C	N	O	S	0	0
			2677	1680	468	519	10		
5	C	316	Total	C	N	O	S	0	0
			2446	1535	432	469	10		
5	G	306	Total	C	N	O	S	0	0
			2383	1497	419	458	9		
5	D	346	Total	C	N	O	S	0	0
			2677	1680	468	519	10		
5	E	346	Total	C	N	O	S	0	0
			2676	1678	468	520	10		
5	F	347	Total	C	N	O	S	0	0
			2685	1684	470	521	10		
5	H	343	Total	C	N	O	S	0	0
			2657	1668	465	514	10		
5	I	346	Total	C	N	O	S	0	0
			2676	1678	468	520	10		
5	L	347	Total	C	N	O	S	0	0
			2685	1684	470	521	10		
5	M	346	Total	C	N	O	S	0	0
			2676	1678	468	520	10		
5	P	343	Total	C	N	O	S	0	0
			2654	1665	464	515	10		
5	Q	346	Total	C	N	O	S	0	0
			2676	1678	468	520	10		
5	T	345	Total	C	N	O	S	0	0
			2668	1674	466	518	10		
5	U	346	Total	C	N	O	S	0	0
			2676	1678	468	520	10		
5	X	346	Total	C	N	O	S	0	0
			2677	1680	468	519	10		
5	Y	346	Total	C	N	O	S	0	0
			2676	1678	468	520	10		
5	b	346	Total	C	N	O	S	0	0
			2676	1678	468	520	10		

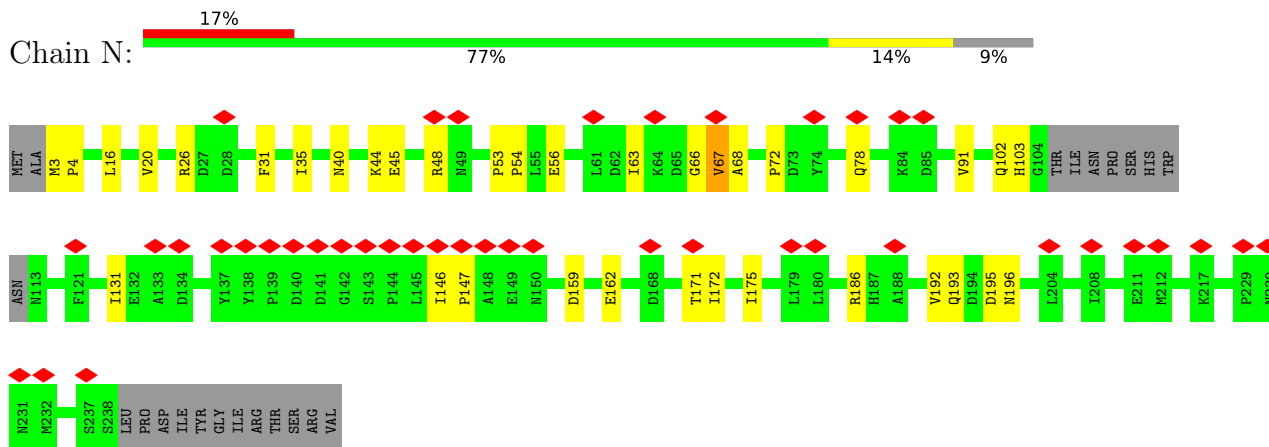
3 Residue-property plots

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

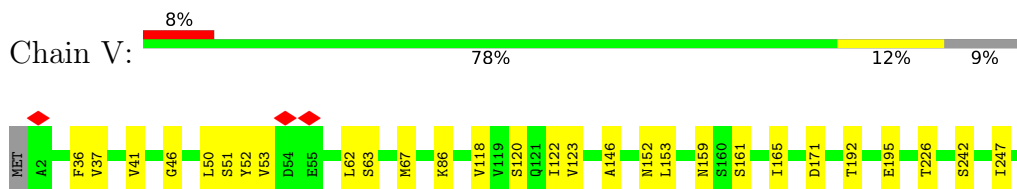
• Molecule 1: Adaptor protein

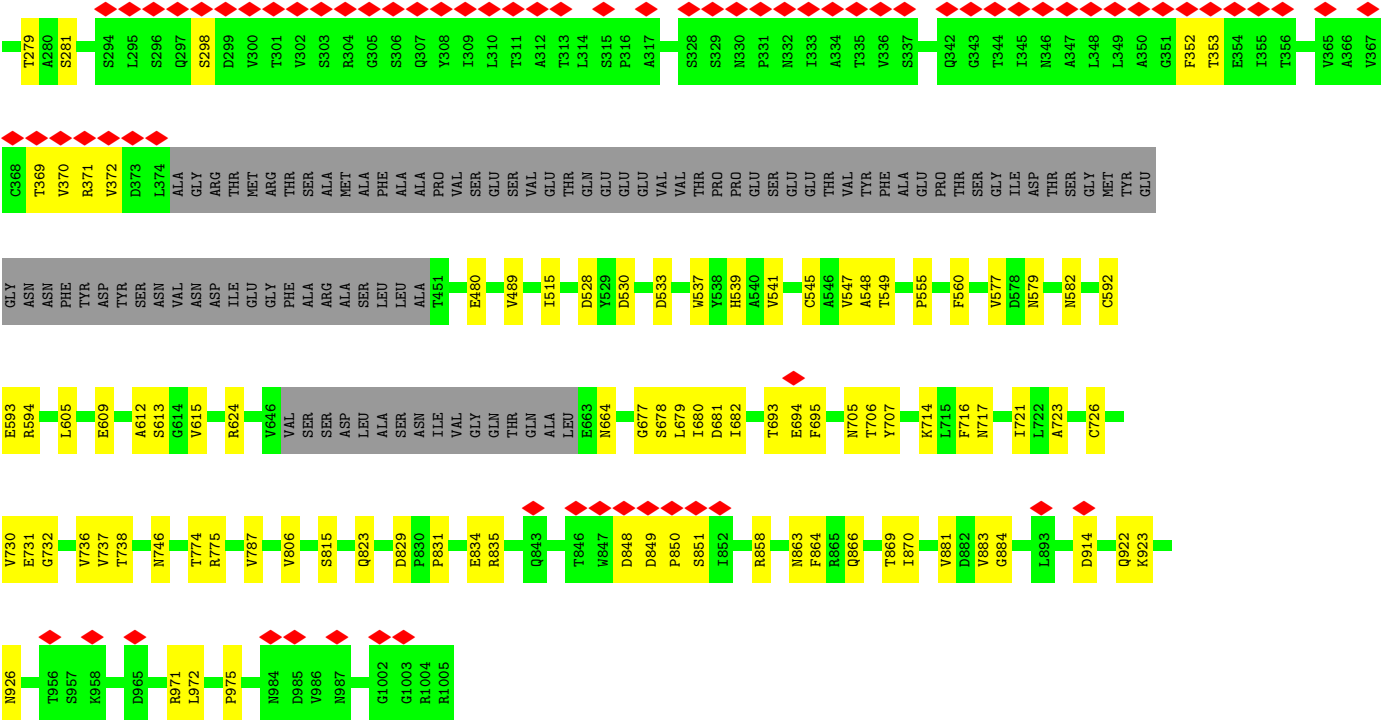


• Molecule 1: Adaptor protein

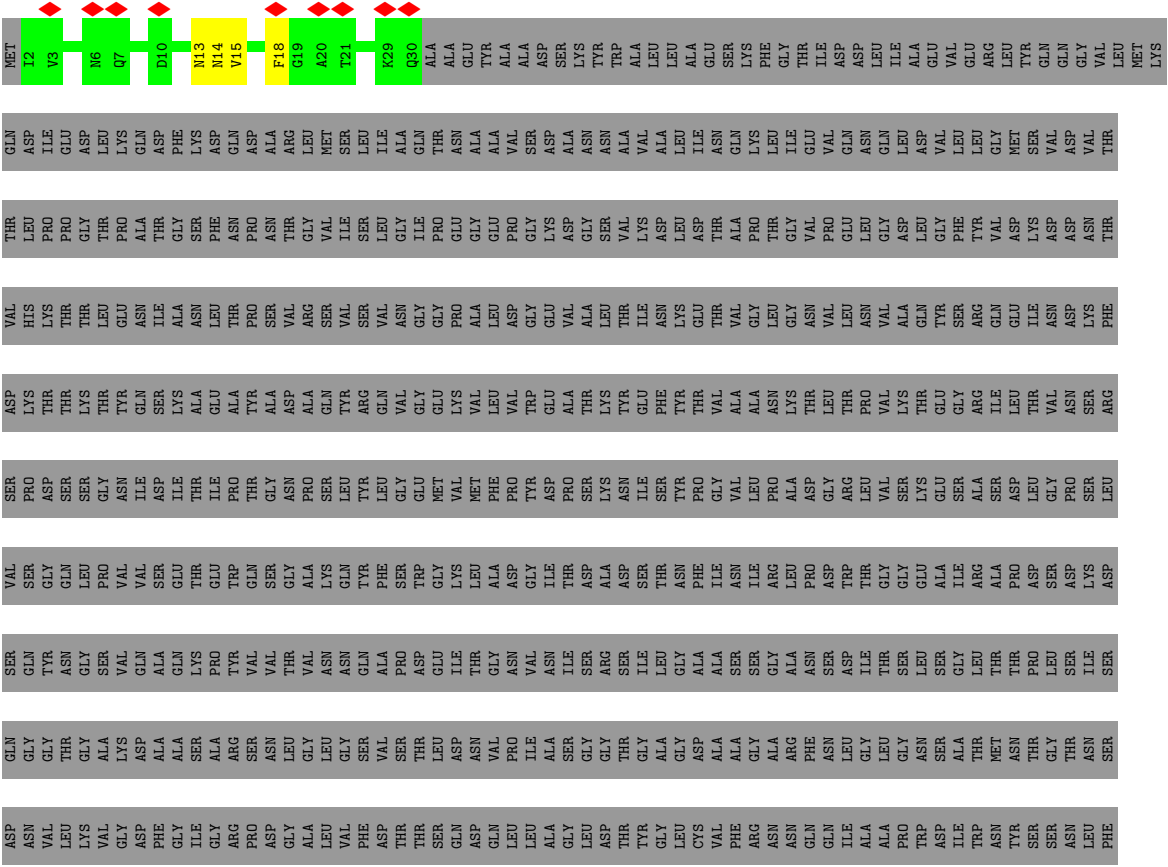


• Molecule 2: Surface protein





● Molecule 3: Putative tail fiber



ASP	TYR	GLU	VAL	LYS	GLU	ASP	GLY	SER	LEU	LEU	ILE	LYS	THR	TYR	HIS	ARG	THR	HIS	SER	THR	SER	PRO	ALA	ALA	ALA	ARG	ASN	GLU	GLU	LEU	GLU	PHE	GLY	SER	ASP	GLY	ASP	PRO	VAL	ASP	ASP	ILE	PRO	LYS	ASP	ALA	ALA	PHE	ILE	SER	VAL	ARG	VAL	GLU	GLU	PRO	PRO	SER	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: Putative tail fiber

Chain R:  97%

THR	LEU	PRO	PRO	PRO	GLY	THR	PRO	ALA	THR	GLY	SER	PHE	ASN	ASN	PRO	THR	GLY	VAL	ILE	ILE	LEU	GLY	GLY	PRO	LYS	ASP	GLY	GLY	SER	VAL	VAL	LYS	ASP	LEU	LEU	THR	THR	ALA	PRO	PRO	THR	THR	GLY	VAL	VAL	PHE	THR	TYR	THR	VAL	VAL	ASP	ASP	LYS	LYS	ASN	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

VAL	GLY	GLY	GLN	LEU	PRO	VAL	VAL	SER	SER	THR	THR	TRP	GLN	GLY	ALA	LYS	GLN	PHE	SER	TRP	GLY	LYS	LEU	ALA	ASP	GLY	ILE	THR	THR	SER	THR	ASN	ASN	PHE	ILE	ILE	ILE	ARG	LEU	PRO	PRO	ASP	ASP	ASP	LYS	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

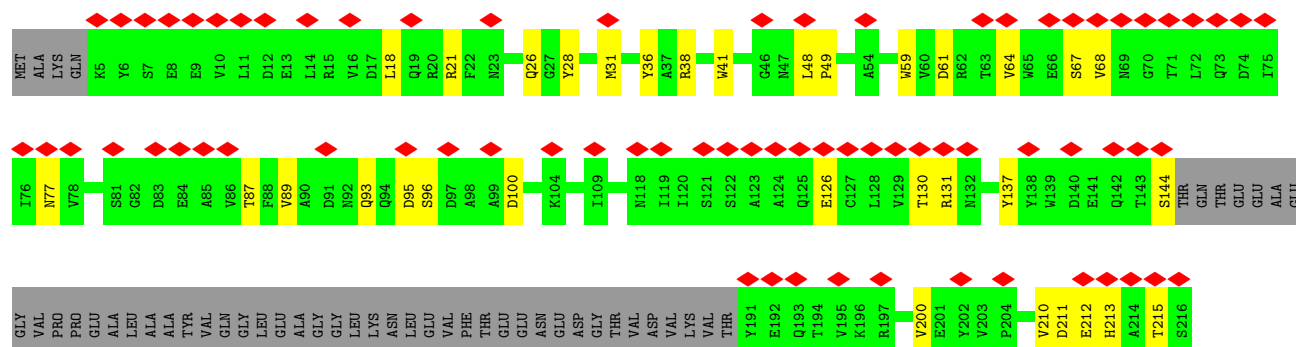
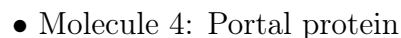
GLN	GLY	GLY	THR	GLY	ALA	LYS	ASP	ALA	ALA	ALA	SER	ALA	ARG	SER	ASN	LEU	GLY	LEU	GLY	SER	VAL	SER	THR	LEU	ASP	ASN	ASN	VAL	PRO	ILE	ALA	SER	GLY	GLY	THR	GLY	ALA	GLY	ASP	ALA	ALA	ALA	ALA	LEU	ASN	ASP	PHE	ARG	ALA	ALA	GLY	GLY	THR	THR	THR	THR	ASN	SER	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

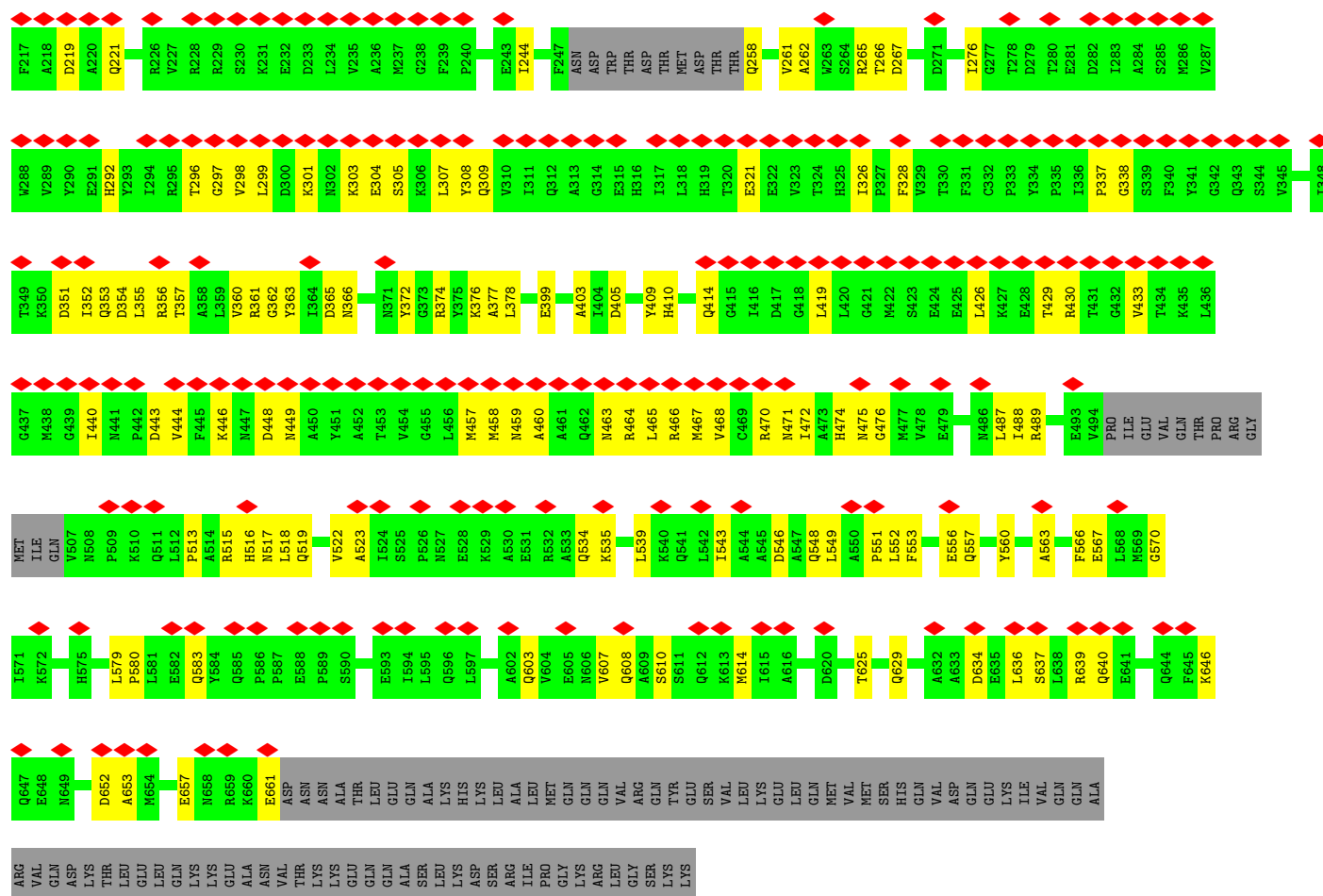
PHE ARG ALA GLY ASP THR TYR SER MET ILE ILE ILE PRO PHE GLU SER SER ALA ALA GLY LYS ILE ILE LYS VAL PHE PHE GLY GLY ALA SER SER SER GLY TRP LYS THR THR ARG ARG VAL VAL ASP ASP THR THR VAL VAL ASN ASN THR THR VAL VAL ASP ASP VAL VAL ASN GLY PHE ILE ILE LYS LYS ALA ALA SER SER PRO ILE ILE VAL VAL LYS VAL

ASP	TYR	GLU	VAL	LYS	ASP	GLU	GLY	SER	LEU	ILE	LYS	THR	TYR	HIS	ARG	THR	SER	SER	PRO	ALA	PHE	ALA	ALA	ARG	ASN	GLU	GLU	GLU	GLY	PHE	SER	ASP	GLY	ASP	PRO	VAL	ILE	PRO	LYS	ASP	ALA	PHE	ILE	SER	VAL	ARG	GLU	MET	PRO	SER	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

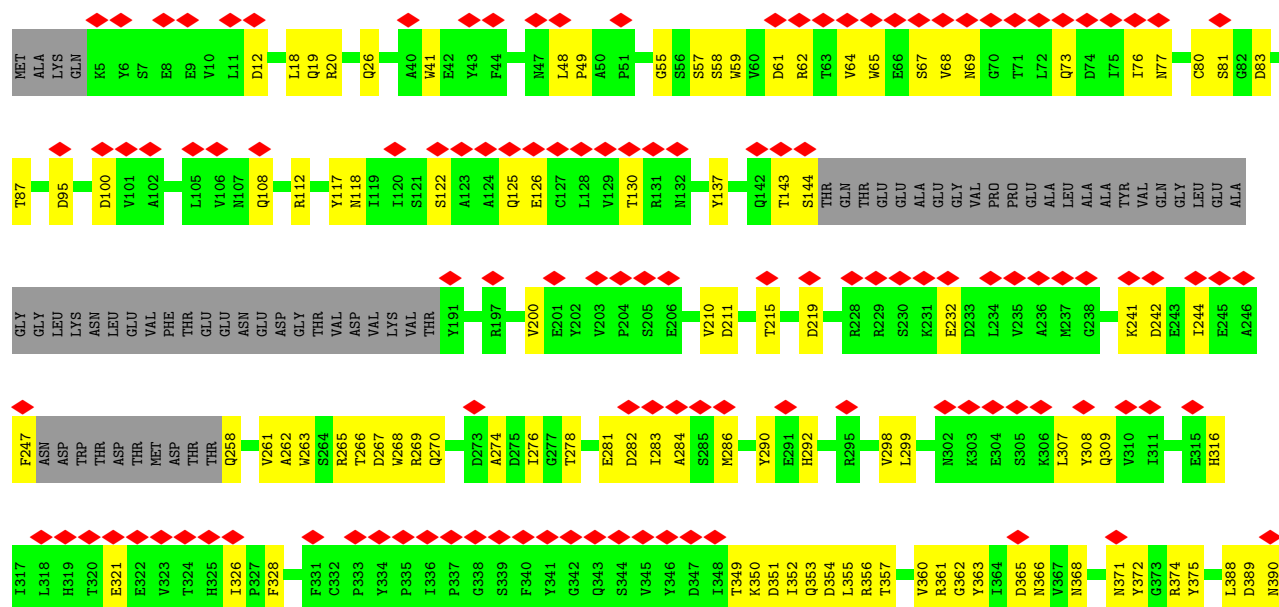
- Molecule 3: Putative tail fiber

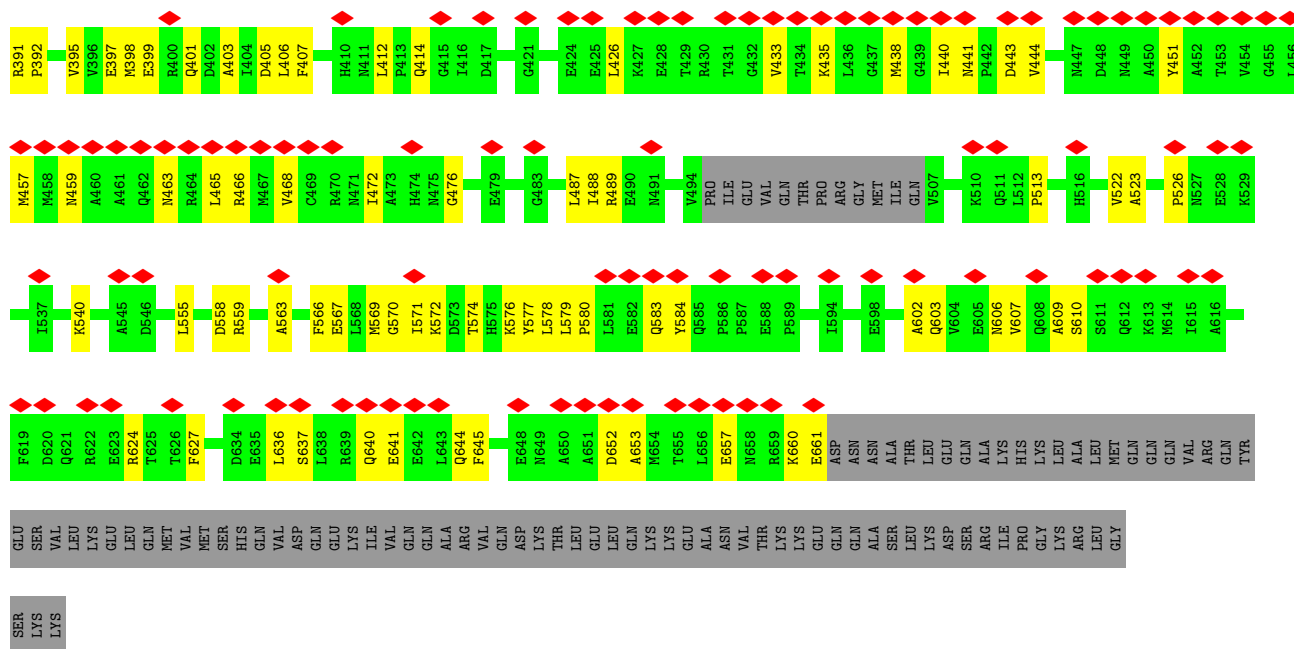
Chain S: 99%



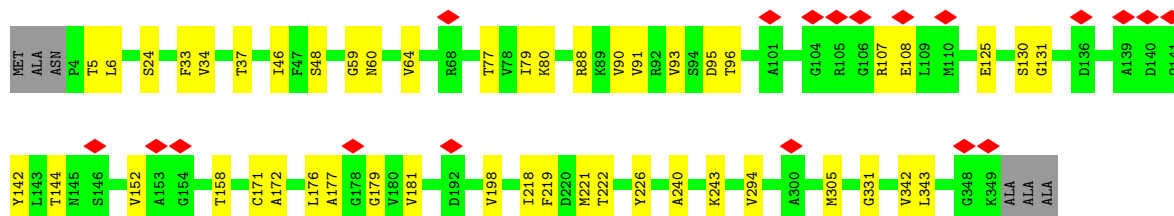
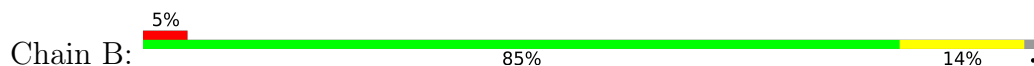


• Molecule 4: Portal protein

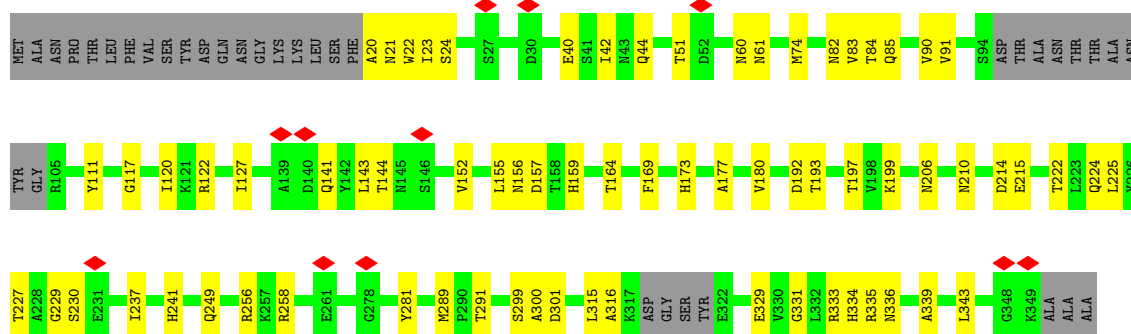




• Molecule 5: Major head protein

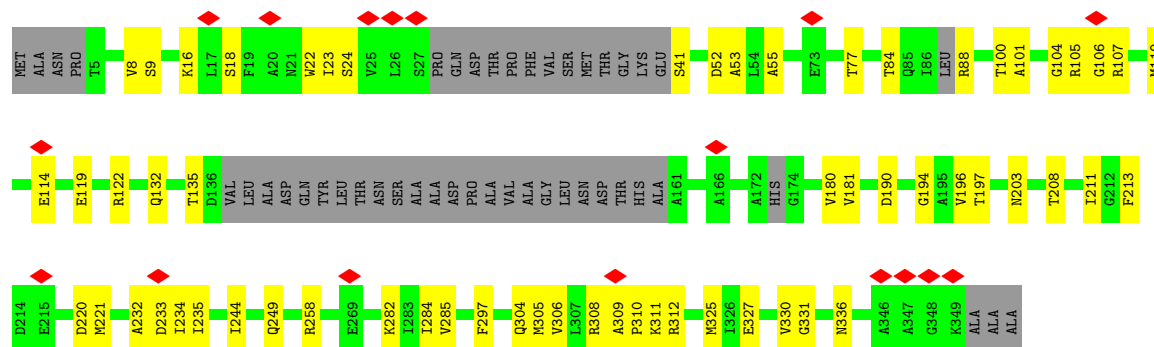


• Molecule 5: Major head protein

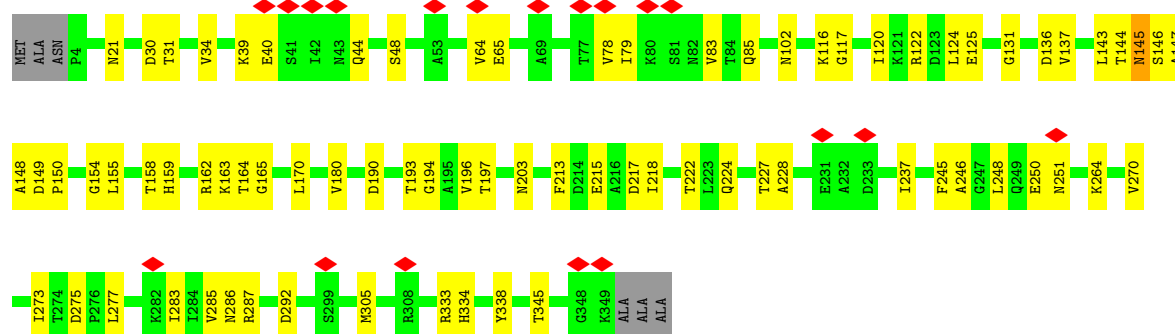
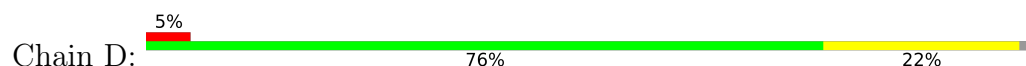


• Molecule 5: Major head protein

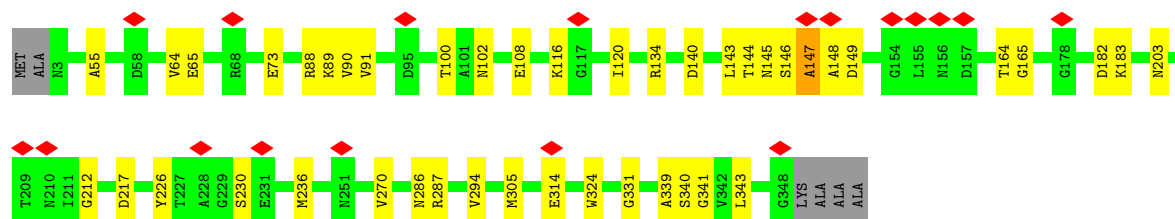
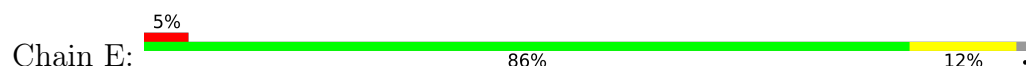




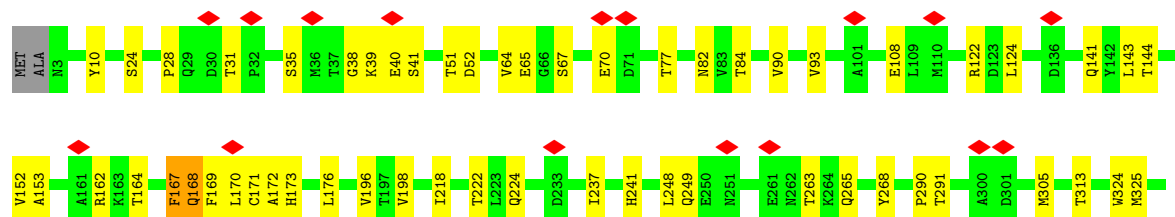
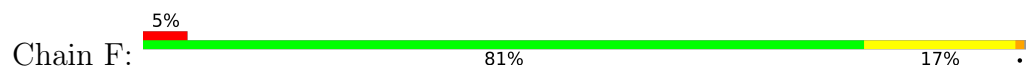
• Molecule 5: Major head protein

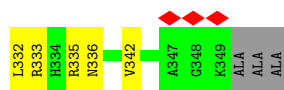


• Molecule 5: Major head protein



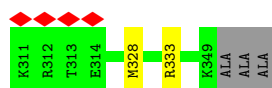
• Molecule 5: Major head protein





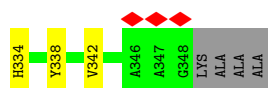
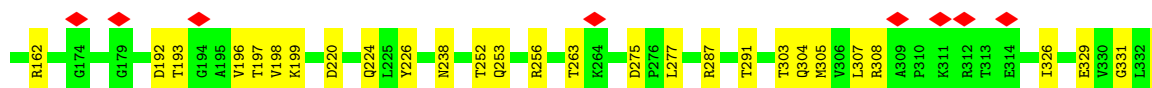
- Molecule 5: Major head protein

Chain H: 81% 16%



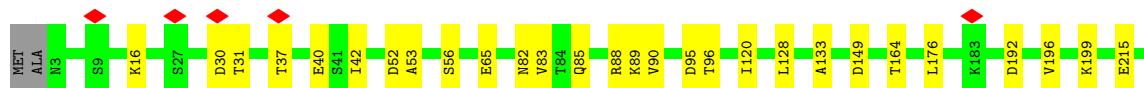
- Molecule 5: Major head protein

Chain I: 5% 82% 16%



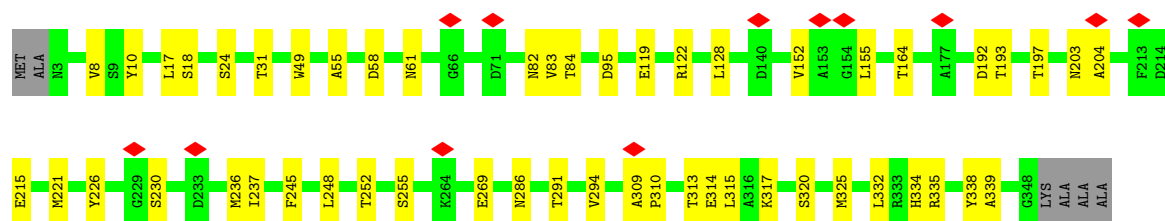
- Molecule 5: Major head protein

Chain L: 85% 14%

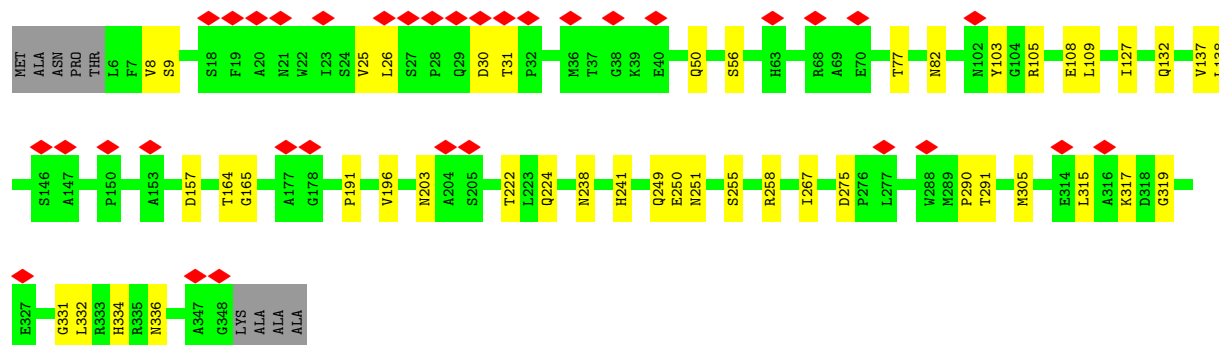
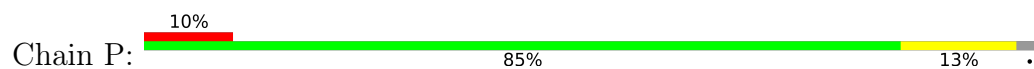


- Molecule 5: Major head protein

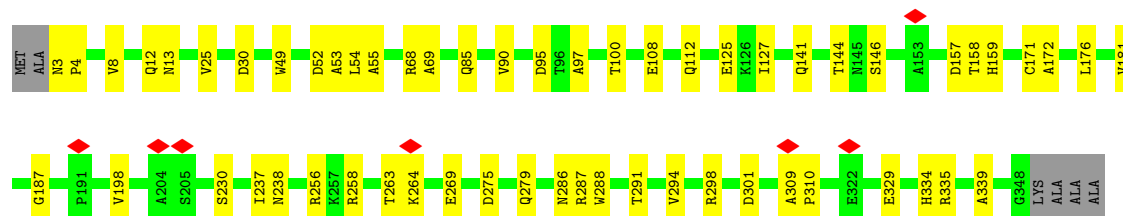
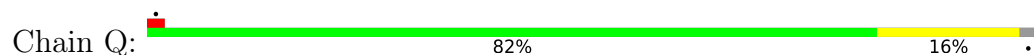
Chain M: 84% 15%



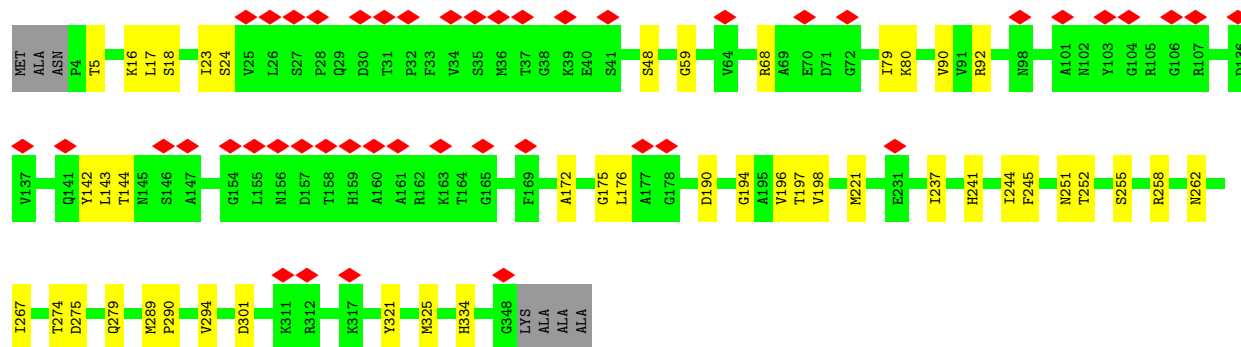
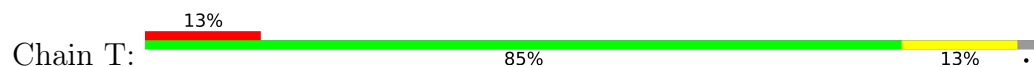
- Molecule 5: Major head protein



- Molecule 5: Major head protein

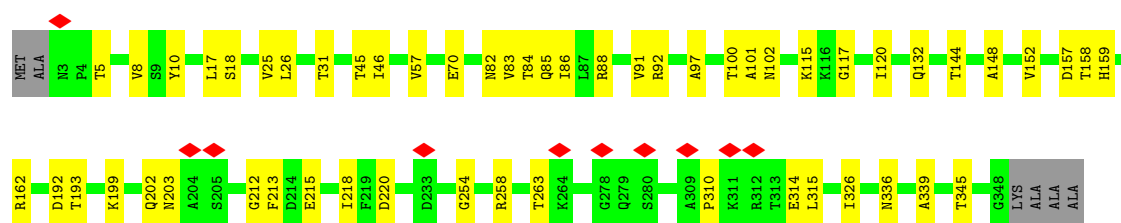


- Molecule 5: Major head protein



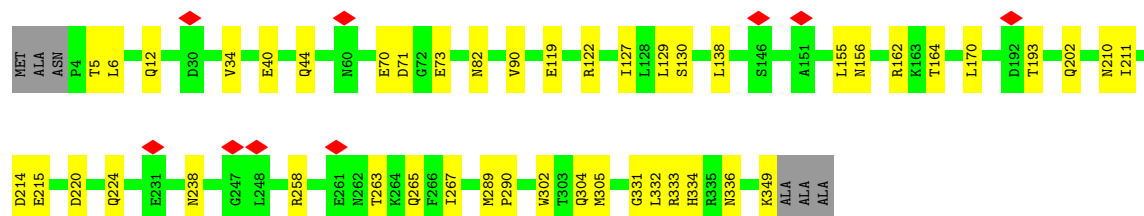
- Molecule 5: Major head protein

Chain U:  83% 16%



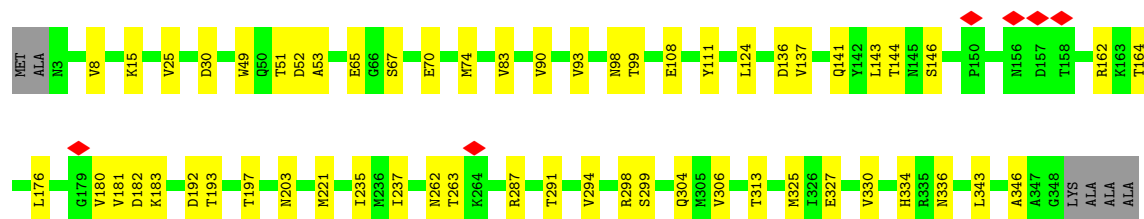
• Molecule 5: Major head protein

Chain X:  85% 13%



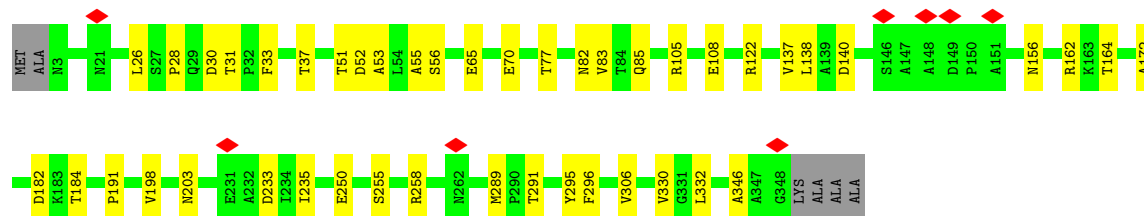
• Molecule 5: Major head protein

Chain Y:  82% 16%



• Molecule 5: Major head protein

Chain b:  86% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	552.0, 552.0, 552.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/1905	0.38	0/2597
1	N	0.14	0/1911	0.34	0/2605
2	V	0.12	0/7231	0.31	1/9874 (0.0%)
3	O	0.11	0/216	0.24	0/293
3	R	0.18	0/179	0.24	0/241
3	S	0.10	0/58	0.18	0/76
4	J	0.13	0/4817	0.33	0/6524
4	K	0.13	0/4817	0.33	0/6524
5	B	0.13	0/2728	0.34	0/3694
5	C	0.13	0/2489	0.34	0/3366
5	D	0.14	0/2728	0.39	0/3694
5	E	0.13	0/2727	0.35	0/3695
5	F	0.14	0/2736	0.40	0/3706
5	G	0.14	0/2422	0.35	0/3266
5	H	0.13	0/2706	0.34	0/3661
5	I	0.13	0/2727	0.33	0/3695
5	L	0.13	0/2736	0.31	0/3706
5	M	0.13	0/2727	0.33	0/3695
5	P	0.13	0/2704	0.36	0/3662
5	Q	0.13	0/2727	0.31	0/3695
5	T	0.13	0/2719	0.35	0/3683
5	U	0.12	0/2727	0.31	0/3695
5	X	0.13	0/2728	0.34	0/3694
5	Y	0.12	0/2727	0.31	0/3695
5	b	0.13	0/2727	0.30	0/3695
All	All	0.13	0/66919	0.34	1/90731 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
-----	-------	---------------------	---------------------

Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	247	ILE	N-CA-C	-5.86	108.14	113.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	167	PHE	Peptide
5	F	168	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1852	0	1776	69	0
1	N	1858	0	1781	27	0
2	V	7079	0	6910	78	0
3	O	213	0	197	4	0
3	R	177	0	162	2	0
3	S	58	0	58	0	0
4	J	4727	0	4570	570	0
4	K	4727	0	4571	615	0
5	B	2677	0	2646	33	0
5	C	2446	0	2433	79	0
5	D	2677	0	2646	53	0
5	E	2676	0	2638	28	0
5	F	2685	0	2651	42	0
5	G	2383	0	2360	99	0
5	H	2657	0	2629	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	2676	0	2638	39	0
5	L	2685	0	2651	35	0
5	M	2676	0	2638	37	0
5	P	2654	0	2618	32	0
5	Q	2676	0	2638	39	0
5	T	2668	0	2633	32	0
5	U	2676	0	2638	43	0
5	X	2677	0	2646	35	0
5	Y	2676	0	2638	44	0
5	b	2676	0	2638	33	0
All	All	65632	0	64404	1426	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 11.

All (1426) 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)
4:K:268:TRP:CH2	5:G:311:LYS:HE2	1.30	1.64
4:J:374:ARG:CZ	4:K:390:ASN:HA	1.12	1.53
4:J:552:LEU:HD11	4:K:579:LEU:CB	1.28	1.53
4:J:614:MET:CE	4:K:609:ALA:HB3	1.32	1.53
4:J:552:LEU:CD1	4:K:579:LEU:HB3	1.26	1.52
1:A:233:THR:CG2	4:K:368:ASN:ND2	1.73	1.52
4:J:560:TYR:CB	4:K:576:LYS:HG3	1.17	1.46
4:J:614:MET:CE	4:K:609:ALA:CB	1.89	1.46
4:J:337:PRO:HD3	4:K:125:GLN:CD	1.35	1.45
4:J:213:HIS:CB	4:K:276:ILE:HD11	1.45	1.44
4:J:337:PRO:CD	4:K:125:GLN:CD	1.91	1.43
4:J:625:THR:HG22	4:K:624:ARG:NH2	1.29	1.43
4:J:38:ARG:NH2	5:C:21:ASN:H	1.08	1.42
4:J:374:ARG:HH12	4:K:390:ASN:N	1.06	1.42
4:J:213:HIS:HB2	4:K:276:ILE:CD1	1.47	1.41
4:J:337:PRO:CD	4:K:125:GLN:OE1	1.68	1.41
4:K:268:TRP:CZ3	5:G:308:ARG:HD2	1.54	1.41
4:J:625:THR:CG2	4:K:624:ARG:HH22	1.34	1.41
1:A:234:ARG:NH1	4:J:361:ARG:HH12	1.16	1.40
4:J:337:PRO:CG	4:K:125:GLN:OE1	1.66	1.40
4:J:374:ARG:CD	4:K:395:VAL:CG2	2.00	1.39
4:J:548:GLN:O	4:K:555:LEU:CD1	1.68	1.38
4:J:430:ARG:NH2	4:K:62:ARG:HB2	1.30	1.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:551:PRO:CB	4:K:584:TYR:OH	1.71	1.36
4:J:374:ARG:HH11	4:K:390:ASN:C	1.31	1.35
1:A:233:THR:HG21	4:K:368:ASN:ND2	1.04	1.34
4:J:557:GLN:O	4:K:576:LYS:HG2	1.27	1.33
4:J:338:GLY:HA3	4:K:263:TRP:CH2	1.64	1.33
4:J:31:MET:HE3	5:G:304:GLN:O	1.16	1.32
4:J:374:ARG:NH1	4:K:390:ASN:CB	1.92	1.32
4:J:475:ASN:ND2	4:K:118:ASN:OD1	1.59	1.32
4:J:471:ASN:HA	4:K:117:TYR:OH	1.27	1.31
4:J:614:MET:HE3	4:K:609:ALA:CB	1.55	1.31
4:J:560:TYR:HB3	4:K:576:LYS:CG	0.93	1.30
4:J:552:LEU:HD21	4:K:579:LEU:O	1.17	1.30
4:J:430:ARG:HH22	4:K:62:ARG:CB	1.44	1.29
4:J:374:ARG:NH1	4:K:390:ASN:C	1.85	1.28
4:J:470:ARG:NH1	4:K:81:SER:CA	1.96	1.28
4:J:470:ARG:NH1	4:K:81:SER:HA	1.48	1.28
4:J:338:GLY:O	4:K:263:TRP:HZ2	1.15	1.26
4:J:213:HIS:H	4:K:276:ILE:CD1	1.49	1.25
1:A:233:THR:CB	4:K:368:ASN:HD21	1.49	1.25
4:J:337:PRO:CG	4:K:125:GLN:CD	2.08	1.23
4:J:265:ARG:HD2	5:C:21:ASN:O	1.38	1.23
4:J:374:ARG:HD3	4:K:395:VAL:CG2	1.62	1.22
4:J:516:HIS:HB3	4:K:108:GLN:OE1	1.38	1.21
4:J:38:ARG:HH22	5:C:21:ASN:N	1.37	1.20
4:J:213:HIS:N	4:K:276:ILE:HD11	1.54	1.20
4:J:552:LEU:CD2	4:K:579:LEU:O	1.86	1.20
4:J:551:PRO:HB3	4:K:584:TYR:OH	1.30	1.20
4:J:213:HIS:CA	4:K:276:ILE:HD11	1.70	1.19
1:A:231:ASN:O	4:K:55:GLY:HA3	1.38	1.19
4:K:268:TRP:CH2	5:G:311:LYS:CE	2.25	1.19
4:J:338:GLY:O	4:K:263:TRP:CZ2	1.96	1.18
4:J:374:ARG:HB3	4:K:395:VAL:CG2	1.72	1.18
1:A:237:SER:OG	4:K:57:SER:C	1.87	1.18
4:J:305:SER:OG	4:K:284:ALA:HB2	1.42	1.18
4:J:337:PRO:HG2	4:K:125:GLN:CG	1.75	1.15
4:J:372:TYR:O	4:K:392:PRO:HB3	1.46	1.15
4:J:38:ARG:NH2	5:C:21:ASN:N	1.92	1.15
4:J:213:HIS:HB2	4:K:276:ILE:HD12	1.17	1.15
4:J:374:ARG:HD3	4:K:395:VAL:HG22	1.24	1.15
1:A:234:ARG:NH1	4:J:361:ARG:NH1	1.95	1.14
4:J:265:ARG:CD	5:C:21:ASN:O	1.93	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:374:ARG:NH1	4:K:390:ASN:N	1.73	1.14
4:J:552:LEU:HG	4:K:579:LEU:H	1.13	1.14
1:A:93:SER:CB	4:K:388:LEU:HD12	1.77	1.14
4:J:213:HIS:CB	4:K:276:ILE:CD1	2.13	1.13
4:J:337:PRO:HD3	4:K:125:GLN:OE1	1.34	1.13
4:J:548:GLN:O	4:K:555:LEU:HD13	1.26	1.12
4:J:552:LEU:HD11	4:K:579:LEU:CA	1.79	1.12
4:J:471:ASN:CA	4:K:117:TYR:OH	1.89	1.12
4:K:268:TRP:CZ3	5:G:308:ARG:CD	2.31	1.12
4:J:614:MET:HE3	4:K:609:ALA:HB1	1.19	1.12
4:J:372:TYR:HA	4:K:392:PRO:HG3	1.29	1.11
1:A:237:SER:CB	4:K:57:SER:HA	1.80	1.11
4:J:551:PRO:HB2	4:K:584:TYR:OH	1.49	1.11
4:J:546:ASP:OD2	4:K:558:ASP:OD2	1.64	1.11
4:J:337:PRO:HG3	4:K:125:GLN:OE1	1.24	1.10
4:J:337:PRO:CG	4:K:125:GLN:CG	2.30	1.09
1:A:93:SER:HB3	4:K:388:LEU:HD12	1.08	1.08
4:J:301:LYS:HG3	4:K:283:ILE:HB	1.20	1.08
4:J:515:ARG:O	4:K:112:ARG:NE	1.86	1.08
4:J:614:MET:HE1	4:K:609:ALA:CB	1.63	1.08
4:K:268:TRP:CZ3	5:G:311:LYS:HG3	1.88	1.07
4:J:458:MET:HB3	4:K:438:MET:HG2	1.34	1.07
4:J:21:ARG:HH11	4:K:278:THR:HA	1.09	1.07
4:J:471:ASN:HA	4:K:117:TYR:CZ	1.88	1.07
4:J:475:ASN:ND2	4:K:118:ASN:CG	2.12	1.07
4:J:301:LYS:HG3	4:K:283:ILE:CB	1.65	1.06
4:J:21:ARG:NH1	4:K:278:THR:HA	1.71	1.06
4:J:657:GLU:O	4:J:661:GLU:CG	2.04	1.06
4:K:268:TRP:HZ3	5:G:311:LYS:HG3	1.20	1.05
4:J:552:LEU:CG	4:K:579:LEU:H	1.68	1.05
4:J:337:PRO:HD3	4:K:125:GLN:NE2	1.71	1.05
4:J:265:ARG:HE	5:C:22:TRP:CA	1.70	1.05
4:K:657:GLU:O	4:K:661:GLU:CG	2.04	1.05
4:J:374:ARG:HB3	4:K:395:VAL:HG21	1.36	1.04
1:A:237:SER:HA	4:K:57:SER:CB	1.87	1.03
4:J:549:LEU:HD11	4:K:558:ASP:CG	1.83	1.03
4:K:268:TRP:CZ2	5:G:311:LYS:HE2	1.92	1.03
4:J:374:ARG:HD2	4:K:395:VAL:CG2	1.88	1.03
4:J:374:ARG:CB	4:K:395:VAL:HG21	1.89	1.03
4:J:430:ARG:CZ	4:K:62:ARG:HB2	1.88	1.03
4:J:516:HIS:CB	4:K:108:GLN:OE1	2.06	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:376:LYS:HG2	4:K:401:GLN:HE21	1.24	1.02
4:J:560:TYR:CB	4:K:576:LYS:CG	1.87	1.02
4:J:516:HIS:CD2	4:K:108:GLN:OE1	2.13	1.02
4:J:560:TYR:HB2	4:K:576:LYS:HG3	1.38	1.01
1:A:231:ASN:O	4:K:55:GLY:CA	2.08	1.01
4:J:31:MET:HE3	5:G:304:GLN:C	1.78	1.01
4:J:338:GLY:HA3	4:K:263:TRP:HH2	1.01	1.01
4:J:372:TYR:CD2	4:K:390:ASN:OD1	2.14	1.01
4:J:372:TYR:O	4:K:392:PRO:CB	2.09	1.00
4:K:316:HIS:HE1	5:G:22:TRP:CZ2	1.79	1.00
4:J:557:GLN:O	4:K:576:LYS:CG	2.09	1.00
4:J:458:MET:HB3	4:K:438:MET:CG	1.69	0.99
4:J:374:ARG:CB	4:K:395:VAL:CG2	2.40	0.98
4:J:131:ARG:CZ	4:K:269:ARG:NH1	2.25	0.98
4:J:374:ARG:CD	4:K:395:VAL:HG21	1.90	0.98
4:J:551:PRO:HB2	4:K:584:TYR:CZ	1.98	0.98
1:A:237:SER:OG	4:K:58:SER:N	1.96	0.98
4:J:376:LYS:HG2	4:K:401:GLN:NE2	1.78	0.97
4:K:657:GLU:O	4:K:661:GLU:HG2	1.63	0.97
1:A:237:SER:OG	4:K:57:SER:CA	2.10	0.97
4:J:31:MET:CE	5:G:304:GLN:O	2.12	0.97
4:J:36:TYR:OH	5:G:41:SER:HB3	1.63	0.97
4:J:305:SER:OG	4:K:284:ALA:CB	2.12	0.97
4:J:213:HIS:CE1	4:K:274:ALA:O	2.17	0.96
4:J:448:ASP:OD2	4:K:441:ASN:OD1	1.80	0.96
4:J:301:LYS:O	4:K:283:ILE:CD1	2.13	0.96
4:K:268:TRP:CE3	5:G:308:ARG:CD	2.49	0.96
4:J:614:MET:CE	4:K:609:ALA:HB1	1.77	0.96
4:J:625:THR:CG2	4:K:624:ARG:NH2	2.06	0.96
1:A:234:ARG:CZ	4:J:361:ARG:NH1	2.28	0.96
4:J:372:TYR:HA	4:K:392:PRO:CG	1.95	0.95
1:A:234:ARG:CZ	4:J:361:ARG:HH12	1.79	0.95
1:A:237:SER:OG	4:K:57:SER:HA	1.65	0.95
4:J:265:ARG:HE	5:C:22:TRP:HA	1.30	0.95
4:J:31:MET:O	5:G:41:SER:N	1.99	0.95
4:J:213:HIS:N	4:K:276:ILE:CD1	2.18	0.95
4:J:552:LEU:CD1	4:K:579:LEU:CB	2.07	0.95
4:J:89:VAL:CG2	4:K:571:ILE:HD11	1.97	0.95
4:J:657:GLU:O	4:J:661:GLU:HG2	1.63	0.95
4:K:268:TRP:CZ3	5:G:311:LYS:HE2	2.02	0.94
4:J:376:LYS:CB	4:K:397:GLU:OE1	2.09	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:430:ARG:NH2	4:K:62:ARG:CB	2.15	0.94
4:J:549:LEU:HD11	4:K:558:ASP:OD1	1.67	0.94
4:J:548:GLN:O	4:K:555:LEU:HD11	1.64	0.93
4:J:213:HIS:CG	4:K:276:ILE:HD11	2.02	0.93
4:J:467:MET:HE2	4:K:73:GLN:HB3	1.49	0.93
4:J:557:GLN:C	4:K:576:LYS:HG2	1.94	0.92
4:J:470:ARG:CZ	4:K:81:SER:HA	1.98	0.92
4:J:548:GLN:HG2	4:K:555:LEU:HD12	1.51	0.92
4:J:470:ARG:NH1	4:K:81:SER:C	2.28	0.92
4:J:470:ARG:HH22	4:K:80:CYS:C	1.66	0.92
4:J:374:ARG:CD	4:K:395:VAL:HG23	1.99	0.92
4:J:516:HIS:HB3	4:K:108:GLN:CD	1.94	0.92
4:J:338:GLY:CA	4:K:263:TRP:CH2	2.52	0.91
4:J:374:ARG:HD2	4:K:395:VAL:HG21	1.44	0.91
4:J:430:ARG:HH22	4:K:62:ARG:HB2	0.75	0.91
4:J:560:TYR:HB3	4:K:576:LYS:CB	2.01	0.90
4:J:374:ARG:CG	4:K:395:VAL:CG2	2.49	0.90
4:J:516:HIS:CG	4:K:108:GLN:OE1	2.24	0.90
4:J:552:LEU:HD21	4:K:579:LEU:C	1.97	0.89
1:A:237:SER:HA	4:K:57:SER:HB3	1.53	0.89
4:J:265:ARG:NE	5:C:22:TRP:HB3	1.86	0.89
4:J:374:ARG:CD	4:K:395:VAL:HG22	1.84	0.89
4:J:557:GLN:HG2	4:K:576:LYS:O	1.45	0.89
1:A:233:THR:HB	4:K:368:ASN:HD21	1.36	0.89
4:J:448:ASP:OD2	4:K:441:ASN:ND2	2.06	0.89
4:J:448:ASP:OD2	4:K:441:ASN:CG	2.15	0.89
4:J:464:ARG:NH1	4:K:69:ASN:OD1	1.94	0.89
4:J:372:TYR:O	4:K:392:PRO:CA	2.21	0.88
4:K:268:TRP:CZ3	5:G:311:LYS:CG	2.55	0.88
4:J:301:LYS:O	4:K:283:ILE:HD12	1.71	0.88
4:J:374:ARG:HH11	4:K:390:ASN:CB	1.72	0.88
4:K:19:GLN:NE2	5:G:106:GLY:HA3	1.87	0.88
4:J:552:LEU:HD12	4:K:579:LEU:HB3	1.51	0.88
4:J:607:VAL:CG1	4:K:606:ASN:ND2	2.37	0.88
4:J:657:GLU:O	4:J:661:GLU:HG3	1.74	0.87
1:A:233:THR:HA	4:K:372:TYR:OH	1.73	0.87
4:K:247:PHE:CD2	5:G:114:GLU:OE1	2.08	0.87
1:A:234:ARG:HH12	4:J:361:ARG:HH12	1.22	0.87
4:J:374:ARG:CG	4:K:395:VAL:HG23	2.04	0.87
5:F:51:THR:O	5:F:77:THR:OG1	1.92	0.87
4:J:661:GLU:HB2	4:K:660:LYS:NZ	1.90	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:464:ARG:NH1	4:K:65:TRP:CZ2	2.42	0.86
4:K:261:VAL:HG23	5:G:312:ARG:NE	1.90	0.86
4:K:657:GLU:O	4:K:661:GLU:HG3	1.74	0.86
1:A:233:THR:CG2	4:K:368:ASN:HD21	1.55	0.86
4:J:301:LYS:O	4:K:283:ILE:HB	1.75	0.86
4:J:337:PRO:HG2	4:K:125:GLN:HG3	1.54	0.86
4:J:517:ASN:C	4:K:112:ARG:HH22	1.84	0.86
4:J:301:LYS:CG	4:K:283:ILE:HB	2.05	0.86
4:J:517:ASN:CA	4:K:112:ARG:NH2	2.39	0.86
5:M:230:SER:OG	5:M:339:ALA:O	1.94	0.86
4:J:414:GLN:NE2	4:K:412:LEU:HB2	1.89	0.85
4:J:607:VAL:HG13	4:K:606:ASN:ND2	1.91	0.85
4:J:458:MET:O	4:K:438:MET:HA	1.77	0.85
4:J:376:LYS:HB3	4:K:397:GLU:OE1	1.75	0.85
4:J:265:ARG:HE	5:C:22:TRP:CB	1.89	0.85
4:J:460:ALA:CB	4:K:435:LYS:O	2.25	0.85
4:J:539:LEU:HD13	4:K:566:PHE:CE1	2.12	0.84
4:K:316:HIS:HE1	5:G:22:TRP:HZ2	1.20	0.84
5:M:58:ASP:O	5:M:61:ASN:ND2	2.10	0.84
4:J:470:ARG:HH22	4:K:80:CYS:CB	1.90	0.84
5:G:18:SER:OG	5:G:104:GLY:O	1.94	0.84
4:J:372:TYR:HD2	4:K:390:ASN:OD1	1.60	0.84
4:J:265:ARG:NE	5:C:22:TRP:HA	1.92	0.83
1:A:233:THR:CB	4:K:368:ASN:ND2	2.25	0.83
4:J:474:HIS:HB2	4:K:117:TYR:CD2	2.13	0.83
4:K:268:TRP:CZ3	5:G:311:LYS:CD	2.60	0.83
4:J:475:ASN:OD1	4:K:117:TYR:CE2	2.32	0.83
4:J:374:ARG:HD3	4:K:395:VAL:HG23	1.54	0.83
4:J:517:ASN:HA	4:K:112:ARG:NH2	1.93	0.83
4:J:470:ARG:HH22	4:K:80:CYS:HB3	1.42	0.83
4:J:460:ALA:HB3	4:K:435:LYS:O	1.78	0.82
4:J:265:ARG:NE	5:C:21:ASN:O	2.10	0.82
4:J:89:VAL:HG22	4:K:571:ILE:HD11	1.58	0.82
4:J:374:ARG:NH1	4:K:390:ASN:CA	0.68	0.82
4:J:475:ASN:ND2	4:K:118:ASN:ND2	2.26	0.82
4:K:20:ARG:HE	5:G:101:ALA:HB2	1.43	0.82
4:K:20:ARG:HH11	5:G:101:ALA:CB	1.93	0.82
4:J:338:GLY:CA	4:K:263:TRP:HH2	1.87	0.82
4:J:338:GLY:HA3	4:K:263:TRP:CZ2	2.13	0.82
4:J:372:TYR:CE2	4:K:390:ASN:OD1	2.33	0.82
4:J:374:ARG:HH12	4:K:389:ASP:C	1.87	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:374:ARG:NH1	4:K:389:ASP:C	2.36	0.82
5:E:236:MET:SD	5:E:286:ASN:ND2	2.53	0.82
4:K:316:HIS:CE1	5:G:22:TRP:CZ2	2.67	0.82
5:P:238:ASN:ND2	5:P:290:PRO:O	2.13	0.82
4:J:337:PRO:HG2	4:K:125:GLN:HG2	1.60	0.81
4:J:475:ASN:OD1	4:K:117:TYR:HE2	1.62	0.81
5:C:51:THR:OG1	5:F:24:SER:O	1.97	0.81
4:J:474:HIS:CB	4:K:117:TYR:CD2	2.64	0.81
5:D:287:ARG:NH1	5:E:226:TYR:O	2.13	0.81
4:J:517:ASN:CA	4:K:112:ARG:HH22	1.94	0.81
4:J:301:LYS:O	4:K:283:ILE:CB	2.29	0.81
5:P:317:LYS:NZ	5:P:319:GLY:O	2.12	0.80
4:J:96:SER:OG	4:K:572:LYS:HD3	1.79	0.80
4:J:372:TYR:C	4:K:392:PRO:HB3	2.06	0.80
4:J:372:TYR:CD1	4:K:392:PRO:HG3	2.15	0.80
4:J:607:VAL:CG1	4:K:602:ALA:HB1	2.11	0.80
5:C:84:THR:OG1	5:C:329:GLU:OE2	1.99	0.80
4:J:131:ARG:CZ	4:K:269:ARG:HH12	1.94	0.80
4:J:372:TYR:CA	4:K:392:PRO:HG3	2.11	0.80
4:J:539:LEU:HD13	4:K:566:PHE:HE1	1.45	0.80
4:J:566:PHE:O	4:J:570:GLY:N	2.15	0.80
4:K:566:PHE:O	4:K:570:GLY:N	2.15	0.80
5:Y:30:ASP:OD2	5:Y:287:ARG:NH2	2.14	0.80
4:J:265:ARG:NE	5:C:22:TRP:CB	2.45	0.80
4:J:517:ASN:HA	4:K:112:ARG:HH22	1.46	0.80
5:X:202:GLN:O	5:X:349:LYS:NZ	2.14	0.80
4:J:517:ASN:N	4:K:112:ARG:NH1	2.22	0.79
4:J:131:ARG:NH2	4:K:269:ARG:NH1	2.30	0.79
4:J:89:VAL:CG2	4:K:571:ILE:CD1	2.60	0.79
4:J:305:SER:CB	4:K:284:ALA:HB2	2.13	0.79
4:J:464:ARG:NH1	4:K:65:TRP:CH2	2.50	0.79
4:J:430:ARG:HH22	4:K:62:ARG:CG	1.96	0.79
4:K:20:ARG:NE	5:G:101:ALA:HB2	1.97	0.79
4:J:657:GLU:CB	4:J:661:GLU:OE2	2.31	0.79
4:J:77:ASN:ND2	4:J:440:ILE:O	2.16	0.79
4:J:131:ARG:HD3	4:K:269:ARG:HH12	1.47	0.79
4:J:372:TYR:O	4:K:392:PRO:HA	1.82	0.79
4:K:657:GLU:CB	4:K:661:GLU:OE2	2.31	0.79
4:J:338:GLY:C	4:K:263:TRP:CZ2	2.60	0.79
4:J:378:LEU:HA	4:K:398:MET:HG3	1.64	0.79
4:J:430:ARG:NH1	4:K:62:ARG:O	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:625:THR:HG23	4:K:624:ARG:HH22	1.47	0.79
1:A:237:SER:C	4:K:57:SER:HB3	2.08	0.78
5:D:203:ASN:ND2	5:D:213:PHE:O	2.17	0.78
4:J:374:ARG:HB3	4:K:395:VAL:HG23	1.63	0.78
5:E:203:ASN:ND2	5:E:212:GLY:O	2.16	0.78
4:J:213:HIS:H	4:K:276:ILE:HD11	1.12	0.78
5:U:101:ALA:O	5:X:44:GLN:NE2	2.16	0.78
4:J:297:GLY:N	4:K:282:ASP:OD1	2.15	0.78
4:J:552:LEU:HG	4:K:579:LEU:N	1.96	0.78
4:K:77:ASN:ND2	4:K:440:ILE:O	2.16	0.78
5:F:52:ASP:OD2	5:F:336:ASN:ND2	2.17	0.78
4:J:475:ASN:CG	4:K:118:ASN:OD1	2.27	0.77
4:J:646:LYS:HZ1	4:K:645:PHE:N	1.82	0.77
4:J:338:GLY:C	4:K:263:TRP:HZ2	1.91	0.77
1:A:93:SER:HB3	4:K:388:LEU:CD1	2.04	0.77
4:J:337:PRO:HG3	4:K:125:GLN:CD	1.94	0.76
4:J:515:ARG:O	4:K:112:ARG:CZ	2.33	0.76
4:J:551:PRO:C	4:K:584:TYR:HE1	1.93	0.76
4:J:458:MET:C	4:K:438:MET:HA	2.00	0.76
4:J:126:GLU:O	4:J:130:THR:OG1	2.01	0.76
4:J:470:ARG:NH2	4:K:80:CYS:HB3	2.00	0.76
4:J:517:ASN:N	4:K:112:ARG:CZ	2.49	0.76
4:J:89:VAL:HG23	4:K:571:ILE:CD1	2.16	0.75
4:J:28:TYR:HE1	4:K:269:ARG:O	1.69	0.75
4:J:374:ARG:HH12	4:K:390:ASN:CA	0.78	0.75
5:T:258:ARG:NH1	5:T:267:ILE:O	2.19	0.75
4:K:316:HIS:CE1	5:G:22:TRP:CH2	2.74	0.75
1:A:237:SER:CA	4:K:57:SER:HB3	2.17	0.75
5:M:82:ASN:ND2	5:M:332:LEU:O	2.18	0.75
4:J:548:GLN:HG2	4:K:555:LEU:CD1	2.16	0.75
5:C:241:HIS:NE2	5:C:291:THR:O	2.16	0.75
4:J:471:ASN:HA	4:K:117:TYR:CE2	2.22	0.75
5:U:199:LYS:NZ	5:U:220:ASP:OD2	2.20	0.74
1:A:237:SER:HB2	4:K:57:SER:HA	1.66	0.74
4:J:516:HIS:C	4:K:112:ARG:CZ	2.60	0.74
5:F:82:ASN:ND2	5:F:332:LEU:O	2.19	0.74
4:J:464:ARG:N	4:K:73:GLN:OE1	2.21	0.74
5:G:249:GLN:OE1	5:G:258:ARG:NH1	2.21	0.74
5:H:61:ASN:O	5:L:85:GLN:NE2	2.19	0.74
4:J:372:TYR:HA	4:K:392:PRO:CB	2.17	0.74
4:J:470:ARG:NH2	4:K:80:CYS:C	2.27	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:95:ASP:OD1	5:M:320:SER:OG	2.04	0.74
2:V:52:TYR:OH	2:V:829:ASP:O	2.06	0.74
4:K:268:TRP:HZ3	5:G:308:ARG:HD2	1.48	0.74
4:K:126:GLU:O	4:K:130:THR:OG1	2.01	0.73
2:V:537:TRP:CZ3	2:V:548:ALA:HB1	2.23	0.73
5:P:305:MET:N	5:P:331:GLY:O	2.21	0.73
4:J:36:TYR:CZ	5:G:41:SER:HB3	2.23	0.73
5:C:206:ASN:ND2	5:C:210:ASN:OD1	2.21	0.73
5:H:44:GLN:NE2	5:L:16:LYS:O	2.22	0.73
5:H:236:MET:SD	5:H:286:ASN:ND2	2.62	0.73
1:A:237:SER:CA	4:K:57:SER:CB	2.66	0.73
1:A:237:SER:CB	4:K:57:SER:CA	2.63	0.72
4:J:131:ARG:CD	4:K:269:ARG:HH12	2.02	0.72
4:J:474:HIS:CE1	4:K:80:CYS:SG	2.82	0.72
4:J:517:ASN:C	4:K:112:ARG:NH2	2.35	0.72
4:J:213:HIS:CG	4:K:276:ILE:CD1	2.67	0.72
5:C:24:SER:OG	5:G:336:ASN:OD1	2.01	0.72
4:J:414:GLN:HE22	4:K:412:LEU:HB2	1.52	0.72
4:J:374:ARG:HH12	4:K:390:ASN:CB	1.77	0.72
5:Y:203:ASN:ND2	5:Y:346:ALA:O	2.23	0.72
4:J:430:ARG:NH1	4:K:62:ARG:HB2	2.05	0.71
4:K:242:ASP:OD1	5:D:40:GLU:HG2	1.90	0.71
5:C:141:GLN:O	5:C:144:THR:HG23	1.89	0.71
4:J:338:GLY:CA	4:K:263:TRP:CZ2	2.72	0.71
4:J:657:GLU:CA	4:J:661:GLU:OE2	2.39	0.71
4:K:657:GLU:CA	4:K:661:GLU:OE2	2.38	0.71
4:K:20:ARG:HH11	5:G:101:ALA:HB3	1.55	0.71
4:J:657:GLU:HA	4:J:661:GLU:OE2	1.89	0.71
5:I:47:PHE:O	5:I:81:SER:OG	2.04	0.71
5:L:40:GLU:OE1	5:L:333:ARG:NH1	2.24	0.71
4:J:374:ARG:CZ	4:K:390:ASN:CA	1.99	0.71
5:C:156:ASN:O	5:C:159:HIS:NE2	2.23	0.71
4:J:607:VAL:HG12	4:K:606:ASN:HD21	1.56	0.71
4:K:268:TRP:CE3	5:G:308:ARG:HD3	2.24	0.71
4:J:614:MET:HE1	4:K:609:ALA:HB3	0.73	0.71
5:M:252:THR:OG1	5:M:255:SER:OG	2.09	0.71
4:J:337:PRO:HG3	4:K:122:SER:HA	1.73	0.71
1:A:233:THR:HG21	4:K:368:ASN:HD22	0.88	0.70
4:J:516:HIS:HD2	4:K:108:GLN:OE1	1.69	0.70
5:L:253:GLN:N	5:L:253:GLN:OE1	2.25	0.70
5:B:33:PHE:O	5:B:37:THR:HG23	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:44:LYS:NZ	3:O:14:ASN:O	2.24	0.70
4:J:410:HIS:N	4:K:406:LEU:HD12	2.06	0.70
5:D:193:THR:OG1	5:D:227:THR:O	2.05	0.70
4:K:414:GLN:OE1	4:K:414:GLN:N	2.24	0.70
1:N:56:GLU:OE2	1:N:78:GLN:NE2	2.25	0.70
4:K:657:GLU:HA	4:K:661:GLU:OE2	1.89	0.70
4:J:374:ARG:NH1	4:K:391:ARG:N	2.40	0.70
4:K:242:ASP:OD1	5:D:40:GLU:CG	2.40	0.70
1:A:237:SER:HA	4:K:57:SER:OG	1.91	0.69
4:J:474:HIS:HB2	4:K:117:TYR:CE2	2.27	0.69
5:D:155:LEU:O	5:D:158:THR:OG1	2.09	0.69
4:J:374:ARG:CB	4:K:395:VAL:HG23	2.15	0.69
4:J:552:LEU:HD11	4:K:579:LEU:C	2.16	0.69
5:D:154:GLY:O	5:D:159:HIS:NE2	2.25	0.69
4:J:552:LEU:CG	4:K:579:LEU:N	2.50	0.69
4:J:557:GLN:OE1	4:K:578:LEU:C	2.21	0.69
5:F:82:ASN:OD1	5:F:164:THR:OG1	2.08	0.69
4:J:265:ARG:HH11	5:C:22:TRP:CA	2.05	0.69
5:G:88:ARG:NH2	5:G:327:GLU:OE2	2.25	0.69
1:N:102:GLN:HG3	1:N:103:HIS:HD2	1.58	0.69
4:J:337:PRO:CG	4:K:125:GLN:HG2	2.16	0.69
5:U:45:THR:HG23	5:U:46:ILE:HD12	1.74	0.69
5:b:250:GLU:OE2	5:b:258:ARG:NH2	2.25	0.69
2:V:714:LYS:NZ	2:V:716:PHE:O	2.25	0.69
4:J:265:ARG:NH1	5:C:22:TRP:HB2	2.07	0.68
4:K:261:VAL:CG1	5:G:312:ARG:O	2.41	0.68
5:L:65:GLU:OE2	5:b:162:ARG:NH1	2.26	0.68
5:I:119:GLU:OE2	5:M:55:ALA:N	2.26	0.68
4:J:414:GLN:N	4:J:414:GLN:OE1	2.24	0.68
4:J:607:VAL:CG1	4:K:606:ASN:HD21	2.04	0.68
4:J:552:LEU:HD12	4:K:579:LEU:CB	2.16	0.68
4:J:607:VAL:HG11	4:K:602:ALA:HB1	1.74	0.68
5:Q:238:ASN:ND2	5:Q:291:THR:OG1	2.27	0.68
5:X:238:ASN:ND2	5:X:290:PRO:O	2.26	0.68
2:V:120:SER:OG	2:V:146:ALA:O	2.11	0.68
4:J:474:HIS:HE1	4:K:80:CYS:SG	2.16	0.68
5:C:256:ARG:NH2	5:F:268:TYR:OH	2.27	0.68
5:D:143:LEU:O	5:D:144:THR:OG1	2.11	0.68
5:F:38:GLY:O	5:F:39:LYS:NZ	2.27	0.68
5:L:220:ASP:O	5:L:224:GLN:NE2	2.26	0.68
4:J:429:THR:OG1	4:K:435:LYS:HE2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:470:ARG:HH11	4:K:81:SER:C	1.99	0.68
4:K:268:TRP:CZ3	5:G:311:LYS:CE	2.67	0.68
4:K:657:GLU:HB3	4:K:661:GLU:OE2	1.94	0.68
2:V:272:THR:HG22	2:V:281:SER:HA	1.75	0.67
5:X:5:THR:C	5:X:6:LEU:HD23	2.19	0.67
4:J:467:MET:SD	4:K:73:GLN:HA	2.35	0.67
4:K:265:ARG:HA	5:G:311:LYS:HZ2	1.58	0.67
5:E:146:SER:O	5:E:149:ASP:N	2.25	0.67
4:J:474:HIS:HB3	4:K:117:TYR:CD2	2.29	0.67
5:U:192:ASP:OD1	5:U:193:THR:N	2.27	0.67
4:J:515:ARG:O	4:K:112:ARG:NH1	2.28	0.67
4:K:309:GLN:NE2	4:K:321:GLU:OE2	2.28	0.67
4:J:446:LYS:O	4:K:526:PRO:HG2	1.95	0.67
4:J:552:LEU:HD22	4:K:579:LEU:O	1.94	0.67
4:J:38:ARG:HH22	5:C:21:ASN:H	0.67	0.67
4:J:305:SER:OG	4:K:284:ALA:CA	2.42	0.67
4:J:131:ARG:NH2	4:K:269:ARG:HH12	1.87	0.67
4:J:607:VAL:HG12	4:K:606:ASN:ND2	2.08	0.66
5:D:170:LEU:O	5:D:334:HIS:ND1	2.28	0.66
4:J:265:ARG:HE	5:C:22:TRP:HB3	1.51	0.66
5:B:88:ARG:NH2	5:F:67:SER:O	2.28	0.66
4:J:131:ARG:NE	4:K:269:ARG:NH1	2.43	0.66
4:J:657:GLU:HB3	4:J:661:GLU:OE2	1.95	0.66
5:I:49:TRP:NE1	5:I:334:HIS:O	2.28	0.66
2:V:971:ARG:C	2:V:972:LEU:HD12	2.20	0.66
5:C:334:HIS:NE2	5:C:336:ASN:O	2.28	0.66
1:A:233:THR:HA	4:K:372:TYR:HH	1.57	0.66
2:V:677:GLY:O	2:V:693:THR:OG1	2.13	0.66
4:J:301:LYS:HG2	4:K:281:GLU:O	1.95	0.66
4:J:475:ASN:ND2	4:K:118:ASN:HD21	1.93	0.66
4:K:19:GLN:NE2	5:G:105:ARG:O	2.26	0.66
5:L:234:ILE:HG23	5:L:284:ILE:HD12	1.77	0.66
5:L:251:ASN:OD1	5:L:254:GLY:N	2.29	0.66
4:J:309:GLN:NE2	4:J:321:GLU:OE2	2.28	0.66
4:J:548:GLN:CG	4:K:555:LEU:HA	2.26	0.66
4:J:551:PRO:O	4:K:584:TYR:HE1	1.79	0.66
5:H:236:MET:O	5:H:294:VAL:HG13	1.95	0.66
4:J:429:THR:HG21	4:K:435:LYS:HE3	1.77	0.66
4:J:657:GLU:C	4:J:661:GLU:HG2	2.21	0.66
4:K:657:GLU:C	4:K:661:GLU:HG2	2.21	0.66
2:V:36:PHE:CD1	2:V:41:VAL:HG22	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:213:HIS:HE1	4:K:274:ALA:O	1.75	0.65
4:J:414:GLN:NE2	4:K:412:LEU:CB	2.58	0.65
4:J:551:PRO:CB	4:K:584:TYR:CZ	2.63	0.65
4:J:608:GLN:OE1	4:K:602:ALA:HB2	1.97	0.65
2:V:270:THR:O	2:V:272:THR:HG23	1.96	0.65
4:K:19:GLN:HE21	5:G:106:GLY:HA3	1.59	0.65
5:E:144:THR:O	5:E:145:ASN:ND2	2.30	0.65
4:K:261:VAL:HG23	5:G:312:ARG:HE	1.61	0.65
2:V:537:TRP:CE3	2:V:548:ALA:HB1	2.32	0.65
4:J:560:TYR:CD2	4:K:576:LYS:HD2	2.32	0.65
5:C:249:GLN:OE1	5:C:258:ARG:NH2	2.29	0.65
4:J:374:ARG:HG2	4:K:391:ARG:O	1.96	0.65
4:K:268:TRP:HZ3	5:G:311:LYS:CG	1.98	0.65
5:I:253:GLN:N	5:I:253:GLN:OE1	2.28	0.65
4:J:374:ARG:HH11	4:K:390:ASN:CA	0.81	0.65
1:N:26:ARG:NH2	2:V:926:ASN:O	2.30	0.65
2:V:594:ARG:NE	2:V:680:ILE:O	2.28	0.65
5:G:132:GLN:OE1	5:G:132:GLN:N	2.30	0.65
5:H:192:ASP:OD1	5:H:193:THR:N	2.30	0.65
4:J:467:MET:HE1	4:K:69:ASN:O	1.97	0.64
4:J:519:GLN:NE2	4:K:83:ASP:HB2	2.13	0.64
4:K:262:ALA:O	4:K:266:THR:HG23	1.97	0.64
4:J:89:VAL:HG23	4:K:571:ILE:HD12	1.80	0.64
4:J:298:VAL:HG13	4:J:299:LEU:HD12	1.78	0.64
4:J:376:LYS:C	4:K:401:GLN:HE22	2.05	0.64
4:K:298:VAL:HG13	4:K:299:LEU:HD12	1.78	0.64
4:J:608:GLN:OE1	4:K:602:ALA:CB	2.46	0.64
5:I:27:SER:O	5:I:29:GLN:NE2	2.30	0.64
5:U:115:LYS:NZ	5:Y:52:ASP:OD2	2.30	0.64
2:V:51:SER:OG	2:V:53:VAL:O	2.14	0.64
4:J:460:ALA:HB2	4:K:435:LYS:O	1.96	0.64
4:J:551:PRO:C	4:K:584:TYR:CE1	2.75	0.64
4:J:262:ALA:O	4:J:266:THR:HG23	1.97	0.64
4:J:31:MET:CE	5:G:304:GLN:C	2.56	0.64
2:V:883:VAL:HG22	2:V:884:GLY:H	1.62	0.64
4:J:337:PRO:HB3	4:K:122:SER:HB3	1.78	0.64
4:J:552:LEU:CD2	4:K:579:LEU:H	2.11	0.64
4:J:265:ARG:NH1	5:C:22:TRP:CB	2.61	0.64
4:J:304:GLU:HG3	4:K:232:GLU:OE2	1.97	0.64
5:P:127:ILE:HD11	5:T:59:GLY:HA2	1.78	0.64
1:A:178:GLU:OE2	1:N:48:ARG:NH1	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:265:ARG:HH11	5:C:22:TRP:CB	2.11	0.63
5:D:116:LYS:NZ	5:E:73:GLU:O	2.16	0.63
4:J:372:TYR:HA	4:K:392:PRO:HB3	1.81	0.63
4:J:372:TYR:HD1	4:K:392:PRO:HG3	1.60	0.63
4:J:646:LYS:NZ	4:K:645:PHE:N	2.47	0.63
4:J:96:SER:OG	4:K:572:LYS:CD	2.47	0.63
4:J:213:HIS:H	4:K:276:ILE:CG1	2.11	0.63
4:J:470:ARG:HH11	4:K:81:SER:CA	2.08	0.63
5:L:305:MET:O	5:L:331:GLY:N	2.30	0.63
1:A:174:THR:O	1:N:44:LYS:NZ	2.31	0.63
4:K:636:LEU:O	4:K:640:GLN:NE2	2.31	0.63
4:J:131:ARG:NE	4:K:269:ARG:HH12	1.96	0.63
4:J:560:TYR:HD2	4:K:576:LYS:HB2	1.63	0.63
1:A:237:SER:HG	4:K:58:SER:N	1.95	0.62
4:J:213:HIS:H	4:K:276:ILE:HD13	1.58	0.62
4:K:20:ARG:NH1	5:G:101:ALA:CB	2.61	0.62
5:H:289:MET:HE1	5:H:295:TYR:CD2	2.34	0.62
4:J:517:ASN:CA	4:K:112:ARG:CZ	2.61	0.62
4:J:374:ARG:CG	4:K:395:VAL:HG21	2.24	0.62
4:J:636:LEU:O	4:J:640:GLN:NE2	2.31	0.62
2:V:86:LYS:NZ	2:V:528:ASP:OD1	2.25	0.62
5:E:134:ARG:NH2	5:E:140:ASP:OD1	2.32	0.62
5:M:24:SER:OG	5:Q:335:ARG:O	2.09	0.62
5:U:82:ASN:OD1	5:U:83:VAL:N	2.33	0.62
4:J:213:HIS:CA	4:K:276:ILE:CD1	2.54	0.62
4:J:265:ARG:HH11	5:C:22:TRP:HB2	1.62	0.62
4:J:470:ARG:HH22	4:K:80:CYS:CA	2.11	0.62
4:J:548:GLN:HG2	4:K:555:LEU:HA	1.82	0.62
5:Q:298:ARG:NH1	5:Q:301:ASP:OD1	2.32	0.62
4:J:41:TRP:CD1	4:J:266:THR:HG22	2.35	0.62
5:D:122:ARG:NH1	5:E:55:ALA:O	2.33	0.62
5:H:68:ARG:O	5:L:88:ARG:NH2	2.32	0.62
5:Y:49:TRP:NE1	5:Y:334:HIS:O	2.32	0.62
4:K:41:TRP:CD1	4:K:266:THR:HG22	2.35	0.62
5:E:305:MET:O	5:E:331:GLY:N	2.32	0.62
4:J:304:GLU:OE1	4:K:143:THR:O	2.18	0.61
5:Q:230:SER:OG	5:Q:339:ALA:O	2.07	0.61
2:V:923:LYS:NZ	2:V:975:PRO:O	2.32	0.61
4:J:557:GLN:CG	4:K:576:LYS:O	2.36	0.61
5:D:222:THR:HG21	5:D:275:ASP:OD2	2.00	0.61
5:b:83:VAL:O	5:b:164:THR:HG22	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:38:ARG:HH12	5:C:20:ALA:HA	1.66	0.61
5:L:255:SER:OG	5:b:250:GLU:OE1	2.15	0.61
5:T:92:ARG:NH2	5:T:321:TYR:O	2.33	0.61
5:D:190:ASP:O	5:D:194:GLY:N	2.33	0.61
5:X:40:GLU:OE2	5:X:333:ARG:NH1	2.33	0.61
5:L:298:ARG:NH1	5:L:301:ASP:OD1	2.32	0.61
5:T:143:LEU:O	5:T:144:THR:OG1	2.16	0.61
5:B:64:VAL:O	5:E:88:ARG:NH1	2.33	0.61
4:K:258:GLN:OE1	5:G:110:MET:HE1	2.01	0.61
5:I:143:LEU:O	5:I:143:LEU:HD23	2.00	0.61
5:b:56:SER:OG	5:b:191:PRO:O	2.18	0.61
5:C:177:ALA:N	5:C:180:VAL:O	2.33	0.61
5:H:133:ALA:N	5:H:179:GLY:O	2.30	0.61
4:J:553:PHE:CD1	4:K:577:TYR:HB2	2.36	0.61
5:U:91:VAL:HG23	5:Y:74:MET:HE2	1.81	0.61
4:J:429:THR:CB	4:K:435:LYS:CE	2.79	0.60
5:P:249:GLN:OE1	5:P:258:ARG:NH1	2.34	0.60
5:L:85:GLN:HB2	5:L:164:THR:HG23	1.84	0.60
3:O:13:ASN:ND2	3:O:18:PHE:O	2.32	0.60
5:Q:97:ALA:O	5:Q:100:THR:OG1	2.19	0.60
5:D:48:SER:HB3	5:D:79:ILE:HD12	1.83	0.60
5:b:28:PRO:O	5:b:122:ARG:NH2	2.35	0.60
1:N:66:GLY:O	1:N:68:ALA:N	2.34	0.60
5:Y:313:THR:OG1	5:Y:325:MET:O	2.18	0.60
4:K:443:ASP:OD1	4:K:444:VAL:N	2.34	0.60
1:A:232:MET:HE2	4:K:374:ARG:HH12	1.67	0.60
4:K:522:VAL:HG12	4:K:523:ALA:H	1.65	0.60
4:J:372:TYR:CA	4:K:392:PRO:HB3	2.32	0.60
4:J:522:VAL:HG12	4:J:523:ALA:H	1.66	0.60
5:P:8:VAL:O	5:P:9:SER:OG	2.17	0.60
4:J:361:ARG:NH2	4:K:371:ASN:ND2	2.50	0.60
4:J:430:ARG:HH12	4:K:62:ARG:N	2.00	0.60
4:J:443:ASP:OD1	4:J:444:VAL:N	2.34	0.60
4:J:548:GLN:C	4:K:555:LEU:CD1	2.68	0.60
5:I:24:SER:OG	5:M:335:ARG:NE	2.35	0.59
5:I:52:ASP:OD2	5:Y:111:TYR:OH	2.20	0.59
5:M:192:ASP:OD1	5:M:193:THR:N	2.35	0.59
5:b:52:ASP:OD1	5:b:53:ALA:N	2.34	0.59
4:J:21:ARG:CZ	4:K:278:THR:HA	2.16	0.59
5:D:305:MET:HE3	5:D:333:ARG:HB2	1.83	0.59
1:N:31:PHE:CE2	1:N:35:ILE:HD11	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:467:MET:CE	4:K:73:GLN:HB3	2.27	0.59
4:K:20:ARG:NH1	5:G:101:ALA:HB2	2.18	0.59
4:K:20:ARG:CZ	5:G:101:ALA:HB2	2.32	0.59
5:C:122:ARG:NH1	5:G:55:ALA:O	2.35	0.59
5:F:143:LEU:O	5:F:144:THR:OG1	2.13	0.59
4:J:552:LEU:HD11	4:K:579:LEU:HB3	0.67	0.59
5:P:56:SER:OG	5:P:191:PRO:O	2.17	0.59
4:J:614:MET:SD	4:K:609:ALA:C	2.85	0.59
5:b:182:ASP:OD1	5:b:184:THR:OG1	2.17	0.59
4:J:18:LEU:HD11	4:J:292:HIS:CG	2.38	0.59
5:G:305:MET:O	5:G:331:GLY:N	2.36	0.59
5:I:45:THR:OG1	5:I:162:ARG:NH2	2.35	0.59
4:J:470:ARG:HH11	4:K:81:SER:HA	1.59	0.59
4:K:265:ARG:HA	5:G:311:LYS:NZ	2.17	0.59
5:M:122:ARG:HH21	5:Q:54:LEU:HD12	1.68	0.59
5:T:5:THR:OG1	5:X:156:ASN:ND2	2.35	0.59
4:J:265:ARG:HH11	5:C:23:ILE:H	1.49	0.58
4:K:261:VAL:HG11	5:G:312:ARG:O	2.03	0.58
5:F:263:THR:OG1	5:F:265:GLN:OE1	2.21	0.58
4:J:409:TYR:HD1	4:K:375:TYR:HH	1.51	0.58
5:B:240:ALA:O	5:B:243:LYS:NZ	2.36	0.58
1:A:233:THR:CG2	4:K:368:ASN:CG	2.70	0.58
1:N:63:ILE:HA	1:N:68:ALA:HB2	1.86	0.58
4:K:18:LEU:HD11	4:K:292:HIS:CG	2.38	0.58
5:B:77:THR:O	5:Q:13:ASN:ND2	2.35	0.58
2:V:858:ARG:NH2	2:V:866:GLN:OE1	2.36	0.58
4:J:457:MET:HE1	4:J:466:ARG:NE	2.19	0.58
4:K:457:MET:HE1	4:K:466:ARG:NE	2.19	0.58
5:M:8:VAL:O	5:M:8:VAL:HG13	2.04	0.58
4:J:661:GLU:HB2	4:K:660:LYS:HZ1	1.63	0.58
4:J:265:ARG:CZ	5:C:22:TRP:HA	2.34	0.58
4:J:372:TYR:CA	4:K:392:PRO:CB	2.82	0.58
4:J:551:PRO:HB2	4:K:584:TYR:CE1	2.38	0.58
5:G:100:THR:HG22	5:G:101:ALA:H	1.69	0.58
4:J:213:HIS:N	4:K:276:ILE:HD13	2.17	0.57
4:J:301:LYS:CG	4:K:283:ILE:CB	2.61	0.57
5:E:90:VAL:O	5:E:116:LYS:NZ	2.36	0.57
5:L:305:MET:N	5:L:331:GLY:O	2.37	0.57
3:R:21:THR:HG23	3:R:21:THR:O	2.04	0.57
4:J:464:ARG:HH12	4:K:69:ASN:ND2	1.84	0.57
4:J:607:VAL:HG11	4:K:602:ALA:CB	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:614:MET:SD	4:K:609:ALA:CB	2.92	0.57
4:J:31:MET:HA	5:G:41:SER:N	2.19	0.57
4:J:374:ARG:CZ	4:K:391:ARG:H	2.18	0.57
4:J:265:ARG:CZ	5:C:22:TRP:CB	2.82	0.57
4:J:307:LEU:HD23	4:J:308:TYR:N	2.20	0.57
5:Y:327:GLU:N	5:Y:327:GLU:OE1	2.37	0.57
5:P:109:LEU:HD23	5:P:109:LEU:O	2.04	0.57
5:I:252:THR:O	5:I:256:ARG:N	2.37	0.57
5:U:17:LEU:HD13	5:Y:143:LEU:CD1	2.35	0.57
1:A:46:ILE:HD11	1:A:183:PHE:CD2	2.40	0.57
2:V:533:ASP:OD2	2:V:823:GLN:NE2	2.37	0.57
5:Y:52:ASP:OD1	5:Y:53:ALA:N	2.38	0.57
4:J:430:ARG:HH12	4:K:62:ARG:CA	2.17	0.57
4:K:307:LEU:HD23	4:K:308:TYR:N	2.20	0.57
5:C:82:ASN:OD1	5:C:83:VAL:N	2.38	0.57
5:H:63:HIS:NE2	5:H:70:GLU:OE1	2.37	0.57
5:Y:8:VAL:HG13	5:Y:8:VAL:O	2.04	0.57
4:K:12:ASP:OD2	5:G:16:LYS:O	2.23	0.57
5:U:97:ALA:O	5:U:100:THR:OG1	2.14	0.57
4:J:326:ILE:HG22	4:J:328:PHE:H	1.70	0.56
4:J:466:ARG:HH12	4:K:77:ASN:CG	2.13	0.56
4:J:28:TYR:CE1	4:K:269:ARG:O	2.54	0.56
4:J:429:THR:OG1	4:K:435:LYS:CE	2.53	0.56
4:J:614:MET:SD	4:K:609:ALA:HB1	2.45	0.56
4:K:326:ILE:HG22	4:K:328:PHE:H	1.70	0.56
5:D:215:GLU:O	5:D:217:ASP:N	2.37	0.56
5:H:186:ASN:OD1	5:H:200:VAL:HG22	2.06	0.56
5:P:82:ASN:ND2	5:P:332:LEU:O	2.38	0.56
4:K:290:TYR:CZ	5:G:107:ARG:NH1	2.72	0.56
5:E:230:SER:OG	5:E:339:ALA:O	2.12	0.56
5:F:84:THR:O	5:F:162:ARG:NH1	2.38	0.56
5:P:334:HIS:NE2	5:P:336:ASN:O	2.38	0.56
4:J:629:GLN:N	4:K:627:PHE:HE2	2.03	0.56
5:I:263:THR:HG22	5:I:263:THR:O	2.06	0.56
4:J:265:ARG:NH1	5:C:22:TRP:HA	2.20	0.56
1:A:196:ASN:OD1	1:A:197:GLY:N	2.37	0.56
4:K:268:TRP:CH2	5:G:308:ARG:HD2	2.31	0.56
4:K:268:TRP:CZ3	5:G:311:LYS:HD3	2.40	0.56
5:C:84:THR:HG22	5:C:331:GLY:HA3	1.88	0.56
5:Q:141:GLN:O	5:Q:144:THR:HG22	2.06	0.56
5:U:25:VAL:HG23	5:U:25:VAL:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:82:ASN:ND2	5:b:332:LEU:O	2.38	0.56
2:V:46:GLY:N	2:V:883:VAL:O	2.38	0.56
4:J:467:MET:HG3	4:K:76:ILE:CD1	2.36	0.56
5:X:6:LEU:HD21	5:b:156:ASN:HA	1.88	0.56
5:b:291:THR:O	5:b:291:THR:HG22	2.05	0.56
5:G:203:ASN:ND2	5:G:211:ILE:O	2.37	0.56
5:M:291:THR:HG22	5:M:291:THR:O	2.06	0.56
4:J:549:LEU:HD21	4:K:559:ARG:HA	1.89	0.55
5:E:314:GLU:OE1	5:E:324:TRP:NE1	2.39	0.55
5:X:82:ASN:HD21	5:X:170:LEU:HD21	1.71	0.55
1:N:3:MET:HB3	1:N:4:PRO:HD3	1.87	0.55
4:J:646:LYS:NZ	4:K:641:GLU:O	2.39	0.55
5:C:111:TYR:OH	5:G:52:ASP:OD2	2.24	0.55
5:M:269:GLU:OE1	5:Q:258:ARG:N	2.38	0.55
5:Q:49:TRP:NE1	5:Q:334:HIS:O	2.39	0.55
5:X:334:HIS:NE2	5:X:336:ASN:O	2.39	0.55
5:Y:298:ARG:O	5:Y:299:SER:OG	2.16	0.55
1:A:237:SER:CA	4:K:57:SER:HA	2.35	0.55
5:P:103:TYR:O	5:P:105:ARG:NH2	2.39	0.55
1:A:93:SER:N	4:K:388:LEU:CD1	2.69	0.55
4:J:471:ASN:N	4:K:117:TYR:OH	2.40	0.55
4:J:265:ARG:HH11	5:C:22:TRP:HA	1.70	0.55
4:J:376:LYS:CG	4:K:401:GLN:NE2	2.63	0.55
4:J:467:MET:HG3	4:K:76:ILE:HD13	1.89	0.55
5:L:56:SER:OG	5:L:192:ASP:O	2.23	0.55
4:J:89:VAL:HG22	4:K:571:ILE:CD1	2.28	0.55
5:M:49:TRP:NE1	5:M:334:HIS:O	2.39	0.55
4:J:374:ARG:CG	4:K:391:ARG:O	2.54	0.55
4:J:535:LYS:HB3	4:K:569:MET:HE2	1.88	0.55
5:B:107:ARG:NH1	5:B:108:GLU:O	2.40	0.55
4:K:268:TRP:CE3	5:G:308:ARG:NE	2.75	0.54
5:X:73:GLU:N	5:X:73:GLU:OE1	2.40	0.54
4:J:31:MET:CA	5:G:41:SER:N	2.71	0.54
5:I:98:ASN:OD1	5:I:107:ARG:NH2	2.36	0.54
5:L:65:GLU:OE1	5:L:65:GLU:N	2.38	0.54
5:L:199:LYS:NZ	5:L:220:ASP:OD2	2.41	0.54
5:T:275:ASP:OD1	5:T:279:GLN:N	2.39	0.54
5:Y:182:ASP:OD1	5:Y:183:LYS:N	2.39	0.54
4:J:303:LYS:O	4:K:283:ILE:HG21	2.08	0.54
5:D:245:PHE:O	5:D:248:LEU:HD22	2.07	0.54
5:D:246:ALA:HA	5:D:270:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:248:LEU:HD12	5:F:249:GLN:N	2.23	0.54
5:H:70:GLU:O	5:L:90:VAL:HG21	2.08	0.54
5:I:196:VAL:O	5:I:224:GLN:NE2	2.41	0.54
5:I:84:THR:OG1	5:I:329:GLU:OE2	2.22	0.54
4:J:296:THR:OG1	4:K:282:ASP:CG	2.51	0.54
4:J:467:MET:SD	4:K:73:GLN:CA	2.95	0.54
4:K:265:ARG:CA	5:G:311:LYS:HZ2	2.19	0.54
4:K:268:TRP:CZ2	5:G:311:LYS:CE	2.75	0.54
5:C:169:PHE:O	5:C:173:HIS:ND1	2.39	0.54
4:J:38:ARG:NH2	5:C:21:ASN:CB	2.70	0.54
5:F:167:PHE:N	5:F:169:PHE:O	2.36	0.54
5:Q:171:CYS:SG	5:Q:172:ALA:N	2.81	0.54
4:J:87:THR:HG23	4:J:87:THR:O	2.08	0.54
4:J:553:PHE:HB2	4:K:578:LEU:CD2	2.38	0.54
4:K:87:THR:HG23	4:K:87:THR:O	2.08	0.54
5:M:31:THR:HG23	5:M:31:THR:O	2.06	0.54
5:Q:269:GLU:OE1	5:U:258:ARG:N	2.41	0.54
5:T:197:THR:O	5:T:221:MET:HE1	2.08	0.54
4:J:560:TYR:HB3	4:K:576:LYS:HG3	0.55	0.54
5:G:208:THR:O	5:G:208:THR:HG22	2.07	0.53
2:V:152:ASN:C	2:V:153:LEU:HD12	2.33	0.53
4:J:552:LEU:CD1	4:K:579:LEU:CA	2.67	0.53
4:J:372:TYR:C	4:K:392:PRO:HA	2.33	0.53
4:J:419:LEU:CD2	4:K:363:TYR:CD1	2.82	0.53
4:J:463:ASN:C	4:K:73:GLN:OE1	2.51	0.53
4:K:316:HIS:CE1	5:G:22:TRP:HZ2	2.12	0.53
5:G:23:ILE:HG22	5:G:24:SER:H	1.73	0.53
5:U:157:ASP:O	5:U:158:THR:OG1	2.21	0.53
5:U:203:ASN:ND2	5:U:212:GLY:O	2.41	0.53
4:J:552:LEU:HD21	4:K:579:LEU:N	2.24	0.53
2:V:863:ASN:OD1	2:V:864:PHE:N	2.42	0.53
4:J:374:ARG:CZ	4:K:391:ARG:N	2.69	0.53
4:J:557:GLN:CA	4:K:576:LYS:HG2	2.39	0.53
5:F:218:ILE:O	5:F:222:THR:HG23	2.09	0.53
5:H:86:ILE:C	5:H:87:LEU:HD12	2.34	0.53
2:V:226:THR:OG1	2:V:261:ILE:O	2.20	0.53
5:I:307:LEU:HD23	5:I:307:LEU:O	2.09	0.53
5:U:215:GLU:N	5:U:215:GLU:OE1	2.42	0.53
2:V:122:ILE:HG22	2:V:123:VAL:H	1.74	0.53
4:J:661:GLU:HB2	4:K:660:LYS:HZ2	1.68	0.53
5:B:46:ILE:HD13	5:B:142:TYR:OH	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:176:LEU:HD11	5:B:179:GLY:O	2.09	0.53
5:B:342:VAL:C	5:B:343:LEU:HD22	2.33	0.53
5:C:215:GLU:OE2	5:C:215:GLU:N	2.41	0.53
4:J:93:GLN:NE2	4:K:574:THR:OG1	2.41	0.53
4:J:557:GLN:OE1	4:K:579:LEU:N	2.41	0.53
5:B:24:SER:OG	5:F:335:ARG:NE	2.41	0.53
5:L:246:ALA:O	5:L:258:ARG:NH1	2.41	0.53
1:N:40:ASN:ND2	1:N:162:GLU:OE2	2.41	0.53
4:J:475:ASN:HD22	4:K:118:ASN:HD21	1.57	0.53
4:J:67:SER:HA	4:J:433:VAL:HG21	1.91	0.53
4:J:458:MET:O	4:K:438:MET:CA	2.54	0.53
5:M:237:ILE:HG22	5:M:294:VAL:CG1	2.39	0.53
5:P:196:VAL:O	5:P:224:GLN:NE2	2.42	0.53
5:U:45:THR:CG2	5:U:46:ILE:HD12	2.38	0.53
2:V:615:VAL:HG13	2:V:615:VAL:O	2.08	0.52
5:P:332:LEU:H	5:P:332:LEU:HD23	1.74	0.52
5:U:5:THR:OG1	5:X:71:ASP:OD1	2.26	0.52
4:J:221:GLN:OE1	4:K:278:THR:HG21	2.08	0.52
4:J:552:LEU:CD2	4:K:579:LEU:N	2.73	0.52
5:E:143:LEU:O	5:E:144:THR:OG1	2.24	0.52
5:Q:291:THR:O	5:Q:291:THR:HG22	2.08	0.52
5:U:31:THR:HG23	5:U:31:THR:O	2.09	0.52
1:A:194:ASP:O	1:A:198:VAL:HG23	2.09	0.52
4:J:36:TYR:OH	5:G:41:SER:CB	2.48	0.52
4:J:38:ARG:NH2	5:C:21:ASN:CA	2.72	0.52
5:Q:256:ARG:NH2	5:U:254:GLY:O	2.42	0.52
2:V:242:SER:OG	2:V:271:ILE:HG12	2.09	0.52
4:J:539:LEU:HD13	4:K:566:PHE:CD1	2.43	0.52
5:X:34:VAL:HG13	5:X:304:GLN:OE1	2.10	0.52
1:N:16:LEU:O	1:N:20:VAL:HG23	2.09	0.52
4:J:31:MET:C	5:G:41:SER:N	2.65	0.52
4:K:67:SER:HA	4:K:433:VAL:HG21	1.92	0.52
5:H:305:MET:HE3	5:H:333:ARG:CZ	2.40	0.52
5:I:198:VAL:HG12	5:I:342:VAL:HG22	1.91	0.52
1:N:102:GLN:HG3	1:N:103:HIS:CD2	2.43	0.52
2:V:548:ALA:HB3	2:V:555:PRO:O	2.10	0.52
4:J:301:LYS:C	4:K:283:ILE:HB	2.34	0.52
5:I:226:TYR:O	5:Y:287:ARG:NE	2.38	0.52
5:X:90:VAL:HG11	5:b:70:GLU:O	2.09	0.52
4:J:38:ARG:NH2	5:C:21:ASN:HB2	2.23	0.52
5:D:136:ASP:OD1	5:D:137:VAL:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:24:SER:OG	3:R:25:ILE:N	2.42	0.52
4:J:607:VAL:HG12	4:K:602:ALA:HB1	1.91	0.52
5:D:21:ASN:O	5:D:21:ASN:ND2	2.43	0.52
5:D:124:LEU:C	5:D:124:LEU:HD23	2.35	0.52
1:A:237:SER:CA	4:K:57:SER:CA	2.87	0.52
4:J:221:GLN:HE21	4:K:286:MET:HE2	1.75	0.52
4:J:377:ALA:N	4:K:401:GLN:HE22	2.08	0.52
1:A:234:ARG:CZ	4:J:361:ARG:HH11	2.21	0.52
2:V:787:VAL:HG13	2:V:787:VAL:O	2.08	0.52
4:J:474:HIS:HD1	4:K:117:TYR:HB2	1.75	0.52
5:B:95:ASP:O	5:B:96:THR:OG1	2.15	0.52
4:J:301:LYS:O	4:K:283:ILE:HD13	2.04	0.51
4:J:474:HIS:CB	4:K:117:TYR:CG	2.93	0.51
5:E:108:GLU:OE1	5:Q:12:GLN:NE2	2.43	0.51
5:I:197:THR:HG21	5:I:338:TYR:HA	1.91	0.51
5:b:85:GLN:HB2	5:b:164:THR:HG23	1.91	0.51
2:V:370:VAL:O	2:V:370:VAL:HG13	2.10	0.51
5:M:83:VAL:O	5:M:164:THR:OG1	2.25	0.51
5:b:140:ASP:OD1	5:b:140:ASP:C	2.52	0.51
1:A:232:MET:HE2	4:K:374:ARG:NH1	2.25	0.51
4:J:261:VAL:HG11	5:C:22:TRP:CD1	2.46	0.51
4:J:376:LYS:CG	4:K:401:GLN:HE21	2.11	0.51
4:K:244:ILE:O	4:K:244:ILE:HG22	2.11	0.51
5:L:37:THR:HG21	5:L:299:SER:O	2.09	0.51
1:A:233:THR:HB	4:K:368:ASN:ND2	2.09	0.51
4:J:646:LYS:HE3	4:K:645:PHE:HA	1.92	0.51
5:C:225:LEU:O	5:C:229:GLY:N	2.42	0.51
4:J:265:ARG:NH1	5:C:22:TRP:CA	2.74	0.51
4:K:316:HIS:CE1	5:G:22:TRP:HH2	2.25	0.51
5:H:34:VAL:O	5:H:34:VAL:HG12	2.11	0.51
5:T:237:ILE:HD11	5:T:241:HIS:CB	2.40	0.51
5:I:84:THR:HG22	5:I:331:GLY:HA3	1.91	0.51
5:L:215:GLU:OE2	5:L:256:ARG:NH1	2.44	0.51
5:U:213:PHE:HD1	5:U:345:THR:HG23	1.75	0.51
4:J:374:ARG:NE	4:K:391:ARG:H	2.09	0.51
5:T:262:ASN:HB3	5:X:267:ILE:HD12	1.92	0.51
1:A:231:ASN:O	4:K:55:GLY:HA2	2.07	0.51
5:D:131:GLY:O	5:D:180:VAL:HG12	2.11	0.51
5:U:8:VAL:O	5:U:8:VAL:HG13	2.09	0.51
5:X:129:LEU:HD12	5:X:289:MET:SD	2.51	0.51
5:Y:306:VAL:HA	5:Y:330:VAL:HG12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:51:THR:O	5:b:77:THR:OG1	2.20	0.51
4:J:467:MET:HA	4:K:76:ILE:HD11	1.93	0.50
5:C:155:LEU:HD12	5:C:157:ASP:H	1.76	0.50
5:I:69:ALA:HB1	5:Y:90:VAL:HG21	1.92	0.50
2:V:579:ASN:O	2:V:582:ASN:ND2	2.42	0.50
5:D:197:THR:HG21	5:D:338:TYR:C	2.36	0.50
5:P:315:LEU:HD21	5:T:68:ARG:NH2	2.26	0.50
5:U:310:PRO:CB	5:U:326:ILE:HD11	2.40	0.50
5:X:210:ASN:OD1	5:X:211:ILE:N	2.43	0.50
4:K:19:GLN:HE22	5:G:106:GLY:HA3	1.70	0.50
4:J:221:GLN:NE2	4:K:286:MET:HE2	2.25	0.50
4:K:137:TYR:HB3	4:K:200:VAL:HG22	1.93	0.50
5:H:290:PRO:O	5:H:291:THR:HG22	2.12	0.50
5:I:275:ASP:OD1	5:I:277:LEU:N	2.42	0.50
5:Y:141:GLN:O	5:Y:144:THR:HG22	2.12	0.50
2:V:62:LEU:O	2:V:63:SER:OG	2.28	0.50
4:J:301:LYS:O	4:K:283:ILE:CG2	2.59	0.50
4:J:410:HIS:CE1	4:K:407:PHE:N	2.80	0.50
5:T:301:ASP:OD2	5:T:334:HIS:NE2	2.45	0.50
5:b:203:ASN:ND2	5:b:346:ALA:O	2.40	0.50
5:b:235:ILE:HG23	5:b:296:PHE:HE1	1.77	0.50
4:J:244:ILE:HG22	4:J:244:ILE:O	2.11	0.50
4:J:629:GLN:HB2	4:K:627:PHE:HZ	1.76	0.50
5:M:315:LEU:O	5:M:317:LYS:NZ	2.37	0.50
5:Q:157:ASP:O	5:Q:158:THR:OG1	2.25	0.50
2:V:592:CYS:SG	2:V:593:GLU:N	2.85	0.50
4:J:374:ARG:HB3	4:K:395:VAL:CB	2.39	0.50
4:J:464:ARG:NH1	4:K:69:ASN:ND2	2.35	0.50
5:D:102:ASN:ND2	5:X:12:GLN:OE1	2.44	0.50
5:b:33:PHE:CZ	5:b:37:THR:HG21	2.47	0.50
5:G:234:ILE:HD11	5:G:284:ILE:HD12	1.93	0.50
5:D:224:GLN:O	5:D:227:THR:OG1	2.30	0.50
5:E:236:MET:O	5:E:294:VAL:HG13	2.10	0.50
4:J:405:ASP:OD1	4:J:405:ASP:N	2.44	0.50
4:J:430:ARG:HH12	4:K:62:ARG:HB2	1.75	0.50
4:J:467:MET:CB	4:K:76:ILE:HD11	2.41	0.50
5:D:83:VAL:HG11	5:D:162:ARG:O	2.12	0.50
5:D:83:VAL:HG12	5:D:164:THR:HA	1.94	0.50
5:I:287:ARG:NH1	5:M:226:TYR:O	2.43	0.50
5:X:155:LEU:O	5:X:156:ASN:OD1	2.30	0.50
4:J:374:ARG:HH11	4:K:390:ASN:CG	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:25:VAL:HG23	5:H:25:VAL:O	2.12	0.49
5:I:34:VAL:HG13	5:I:304:GLN:HE22	1.77	0.49
5:T:190:ASP:O	5:T:194:GLY:N	2.44	0.49
4:J:429:THR:CB	4:K:435:LYS:HE2	2.43	0.49
4:J:467:MET:SD	4:K:73:GLN:N	2.84	0.49
4:K:522:VAL:HG12	4:K:523:ALA:N	2.27	0.49
2:V:122:ILE:HG22	2:V:123:VAL:N	2.27	0.49
4:J:522:VAL:HG12	4:J:523:ALA:N	2.27	0.49
5:B:176:LEU:HD12	5:B:181:VAL:HA	1.93	0.49
5:L:196:VAL:HG23	5:L:196:VAL:O	2.13	0.49
5:U:336:ASN:HB3	5:U:339:ALA:HB2	1.94	0.49
5:Y:83:VAL:O	5:Y:164:THR:OG1	2.30	0.49
1:A:232:MET:CE	4:K:374:ARG:NH1	2.76	0.49
4:J:519:GLN:HE22	4:K:83:ASP:HB2	1.77	0.49
4:K:144:SER:O	4:K:144:SER:OG	2.31	0.49
4:K:261:VAL:CG2	5:G:312:ARG:O	2.60	0.49
5:B:158:THR:HG23	5:B:158:THR:O	2.13	0.49
4:J:560:TYR:CD2	4:K:576:LYS:HB2	2.45	0.49
4:K:351:ASP:N	4:K:351:ASP:OD1	2.44	0.49
4:K:459:ASN:O	4:K:463:ASN:ND2	2.42	0.49
5:B:226:TYR:O	5:E:287:ARG:NH1	2.44	0.49
5:D:292:ASP:OD1	5:D:345:THR:OG1	2.28	0.49
1:A:168:ASP:OD1	1:A:169:THR:N	2.44	0.49
5:C:197:THR:HG22	5:C:197:THR:O	2.12	0.49
4:J:137:TYR:HB3	4:J:200:VAL:HG22	1.93	0.49
4:J:144:SER:O	4:J:144:SER:OG	2.31	0.49
4:J:213:HIS:NE2	4:K:274:ALA:O	2.45	0.49
5:F:176:LEU:HD23	5:F:176:LEU:H	1.78	0.49
5:F:170:LEU:HD12	5:F:172:ALA:H	1.76	0.49
5:Q:187:GLY:H	5:Q:198:VAL:HG13	1.78	0.49
2:V:612:ALA:O	2:V:613:SER:OG	2.23	0.49
4:J:276:ILE:HG22	4:J:276:ILE:O	2.13	0.49
4:K:276:ILE:O	4:K:276:ILE:HG22	2.13	0.49
5:M:197:THR:O	5:M:221:MET:HE1	2.12	0.49
5:P:165:GLY:O	5:P:332:LEU:HD21	2.12	0.49
5:U:162:ARG:NE	5:Y:65:GLU:OE2	2.45	0.49
4:J:131:ARG:CD	4:K:269:ARG:NH1	2.75	0.48
4:J:553:PHE:HB2	4:K:578:LEU:HD21	1.94	0.48
5:B:219:PHE:O	5:B:222:THR:OG1	2.29	0.48
5:E:64:VAL:HG12	5:E:65:GLU:N	2.27	0.48
1:A:233:THR:HG22	4:K:368:ASN:ND2	2.09	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:237:ILE:HD11	5:F:241:HIS:CB	2.43	0.48
5:T:175:GLY:C	5:T:176:LEU:HD12	2.38	0.48
1:A:232:MET:CE	4:K:374:ARG:HH12	2.25	0.48
4:J:212:GLU:H	4:K:276:ILE:HG12	1.77	0.48
4:J:337:PRO:HB3	4:K:122:SER:CB	2.44	0.48
4:J:515:ARG:NH2	4:K:112:ARG:O	2.45	0.48
4:J:652:ASP:OD1	4:J:653:ALA:N	2.46	0.48
5:H:17:LEU:HD12	5:H:19:PHE:CD2	2.49	0.48
5:H:137:VAL:HG23	5:H:138:LEU:HD12	1.95	0.48
5:Q:275:ASP:OD1	5:Q:279:GLN:N	2.46	0.48
2:V:774:THR:O	2:V:775:ARG:NH2	2.46	0.48
4:K:365:ASP:OD1	4:K:366:ASN:N	2.46	0.48
4:K:652:ASP:OD1	4:K:653:ALA:N	2.46	0.48
5:G:306:VAL:HG12	5:G:330:VAL:HG12	1.95	0.48
5:I:82:ASN:OD1	5:I:83:VAL:N	2.46	0.48
5:L:128:LEU:HD22	5:L:332:LEU:HD13	1.96	0.48
5:b:172:ALA:O	5:b:198:VAL:HG21	2.14	0.48
1:A:138:TYR:N	1:A:139:PRO:CD	2.76	0.48
5:B:79:ILE:HD11	5:Q:13:ASN:HB3	1.95	0.48
5:D:64:VAL:HG12	5:D:65:GLU:N	2.28	0.48
1:N:159:ASP:HB2	3:O:15:VAL:HG13	1.95	0.48
2:V:723:ALA:HB3	2:V:726:CYS:SG	2.54	0.48
4:J:351:ASP:OD1	4:J:351:ASP:N	2.44	0.48
4:J:365:ASP:OD1	4:J:366:ASN:N	2.46	0.48
4:J:449:ASN:ND2	4:K:451:TYR:CE2	2.82	0.48
5:U:314:GLU:O	5:U:315:LEU:HD12	2.13	0.48
5:Y:192:ASP:OD1	5:Y:193:THR:N	2.47	0.48
4:J:410:HIS:CE1	4:K:407:PHE:H	2.32	0.48
4:K:405:ASP:OD1	4:K:405:ASP:N	2.44	0.48
5:H:190:ASP:O	5:H:194:GLY:N	2.43	0.48
5:L:30:ASP:O	5:L:31:THR:OG1	2.29	0.48
4:J:61:ASP:OD2	4:J:356:ARG:NE	2.40	0.48
4:J:265:ARG:HH11	5:C:23:ILE:N	2.11	0.48
4:K:489:ARG:NE	4:K:513:PRO:O	2.47	0.48
5:H:234:ILE:HD12	5:H:299:SER:HB3	1.96	0.48
5:Q:125:GLU:OE2	5:Q:286:ASN:ND2	2.39	0.48
5:T:17:LEU:O	5:T:18:SER:OG	2.27	0.48
1:N:45:GLU:OE2	1:N:186:ARG:NH2	2.47	0.48
4:J:337:PRO:CD	4:K:125:GLN:CG	2.77	0.48
4:K:261:VAL:HG13	5:G:312:ARG:O	2.13	0.48
5:G:52:ASP:OD1	5:G:53:ALA:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:337:PRO:CG	4:K:122:SER:HA	2.41	0.48
4:J:557:GLN:O	4:K:576:LYS:CD	2.61	0.48
4:K:268:TRP:CZ3	5:G:308:ARG:NE	2.82	0.48
4:K:579:LEU:HD21	4:K:583:GLN:HB2	1.96	0.47
4:J:374:ARG:NH1	4:K:390:ASN:CG	2.67	0.47
4:J:549:LEU:CD2	4:K:559:ARG:HA	2.43	0.47
5:X:122:ARG:NH1	5:b:55:ALA:O	2.47	0.47
4:J:409:TYR:HA	4:K:375:TYR:OH	2.14	0.47
4:J:470:ARG:NH2	4:K:80:CYS:CB	2.64	0.47
4:J:489:ARG:NE	4:J:513:PRO:O	2.47	0.47
5:T:48:SER:OG	5:T:79:ILE:HD11	2.14	0.47
4:J:610:SER:OG	4:K:606:ASN:OD1	2.29	0.47
5:B:294:VAL:HG12	5:B:294:VAL:O	2.14	0.47
5:X:258:ARG:N	5:b:255:SER:O	2.47	0.47
5:b:235:ILE:HG23	5:b:296:PHE:CE1	2.49	0.47
1:A:16:LEU:O	1:A:20:VAL:HG23	2.14	0.47
4:K:215:THR:HG22	4:K:219:ASP:OD1	2.15	0.47
5:E:89:LYS:HG2	5:E:120:ILE:HD11	1.96	0.47
5:Y:70:GLU:N	5:Y:70:GLU:OE1	2.47	0.47
4:J:414:GLN:HE21	4:K:412:LEU:CB	2.27	0.47
4:J:657:GLU:HA	4:J:661:GLU:CD	2.40	0.47
5:D:218:ILE:O	5:D:222:THR:HG23	2.14	0.47
5:I:305:MET:SD	5:I:333:ARG:NH2	2.88	0.47
2:V:37:VAL:HG23	2:V:37:VAL:O	2.15	0.47
4:J:38:ARG:NH1	5:C:20:ALA:HA	2.30	0.47
4:J:131:ARG:HD3	4:K:269:ARG:NH1	2.23	0.47
4:J:465:LEU:O	4:J:468:VAL:HG12	2.15	0.47
4:K:465:LEU:O	4:K:468:VAL:HG12	2.15	0.47
4:K:657:GLU:HA	4:K:661:GLU:CD	2.40	0.47
5:H:17:LEU:H	5:H:17:LEU:HD23	1.78	0.47
5:L:52:ASP:OD1	5:L:53:ALA:N	2.47	0.47
5:X:127:ILE:O	5:X:130:SER:OG	2.21	0.47
5:G:119:GLU:OE1	5:G:122:ARG:NH1	2.45	0.47
4:J:304:GLU:HG3	4:K:232:GLU:CD	2.40	0.47
4:J:464:ARG:CA	4:K:73:GLN:OE1	2.62	0.47
4:K:268:TRP:CH2	5:G:311:LYS:HG3	2.47	0.47
5:D:83:VAL:HG22	5:D:162:ARG:HD2	1.95	0.47
5:b:233:ASP:N	5:b:233:ASP:OD1	2.46	0.47
1:N:172:ILE:HA	1:N:175:ILE:HG22	1.96	0.47
4:J:457:MET:HE1	4:J:466:ARG:HE	1.80	0.47
4:J:557:GLN:HA	4:K:576:LYS:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:8:VAL:HG23	5:G:9:SER:N	2.30	0.47
5:Q:25:VAL:O	5:Q:25:VAL:HG23	2.14	0.47
5:U:88:ARG:NH1	5:Y:67:SER:OG	2.45	0.47
2:V:545:CYS:SG	2:V:560:PHE:N	2.88	0.46
4:J:551:PRO:CB	4:K:584:TYR:CE1	2.98	0.46
5:G:135:THR:HG23	5:G:135:THR:O	2.15	0.46
1:A:86:GLY:O	1:A:87:THR:OG1	2.27	0.46
1:N:63:ILE:HG21	1:N:131:ILE:HB	1.97	0.46
4:J:475:ASN:OD1	4:K:117:TYR:CD2	2.68	0.46
4:J:579:LEU:HD21	4:J:583:GLN:HB2	1.97	0.46
5:C:299:SER:OG	5:C:300:ALA:N	2.48	0.46
5:G:88:ARG:NH2	5:G:325:MET:SD	2.88	0.46
5:D:78:VAL:HG12	5:D:78:VAL:O	2.15	0.46
5:F:90:VAL:HG12	5:F:324:TRP:O	2.15	0.46
5:Q:95:ASP:N	5:Q:95:ASP:OD1	2.48	0.46
5:X:305:MET:O	5:X:331:GLY:N	2.49	0.46
1:N:171:THR:O	1:N:175:ILE:HG22	2.16	0.46
2:V:352:PHE:CZ	2:V:372:VAL:HG13	2.51	0.46
4:J:215:THR:HG22	4:J:219:ASP:OD1	2.15	0.46
4:K:457:MET:HE1	4:K:466:ARG:HE	1.80	0.46
5:B:152:VAL:HG23	5:B:152:VAL:O	2.15	0.46
5:P:267:ILE:HG23	5:T:274:THR:HB	1.97	0.46
2:V:678:SER:O	2:V:679:LEU:C	2.58	0.46
4:J:301:LYS:O	4:K:283:ILE:HG21	2.15	0.46
4:J:429:THR:CG2	4:K:435:LYS:HE3	2.44	0.46
4:K:298:VAL:HG13	4:K:299:LEU:CD1	2.46	0.46
5:G:220:ASP:OD1	5:G:221:MET:N	2.48	0.46
5:F:290:PRO:O	5:F:291:THR:HG22	2.14	0.46
5:M:10:TYR:HH	5:Q:159:HIS:CG	2.30	0.46
5:Q:329:GLU:OE1	5:Q:329:GLU:N	2.49	0.46
4:J:301:LYS:O	4:K:283:ILE:CG1	2.63	0.46
4:J:474:HIS:HB3	4:K:117:TYR:CG	2.49	0.46
4:J:543:ILE:HD11	4:K:578:LEU:HD21	1.97	0.46
4:K:579:LEU:HD23	4:K:580:PRO:O	2.15	0.46
5:B:130:SER:OG	5:B:131:GLY:N	2.49	0.46
5:D:193:THR:HG21	5:D:228:ALA:HA	1.97	0.46
5:I:238:ASN:HD22	5:I:291:THR:HG23	1.80	0.46
5:Q:30:ASP:OD2	5:Q:287:ARG:NH2	2.48	0.46
4:J:459:ASN:O	4:J:463:ASN:ND2	2.42	0.46
5:B:198:VAL:HG12	5:B:198:VAL:O	2.16	0.46
5:D:44:GLN:NE2	5:D:305:MET:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:238:ASN:OD1	5:H:241:HIS:ND1	2.49	0.46
5:X:302:TRP:HZ3	5:X:332:LEU:HD21	1.80	0.46
5:H:237:ILE:HD11	5:H:241:HIS:HB3	1.97	0.46
5:M:236:MET:HE3	5:M:286:ASN:OD1	2.15	0.46
5:U:117:GLY:O	5:U:120:ILE:HG22	2.15	0.46
4:J:267:ASP:OD1	4:J:267:ASP:N	2.49	0.46
4:J:405:ASP:OD1	4:K:401:GLN:NE2	2.49	0.46
4:J:470:ARG:CZ	4:K:81:SER:CA	2.74	0.46
5:E:146:SER:O	5:E:148:ALA:N	2.49	0.46
5:P:25:VAL:C	5:P:26:LEU:HD22	2.41	0.46
5:Y:98:ASN:OD1	5:Y:99:THR:HG23	2.16	0.46
5:Y:291:THR:HG22	5:Y:291:THR:O	2.16	0.46
1:A:73:ASP:OD1	1:A:73:ASP:N	2.49	0.46
4:J:261:VAL:CG1	5:C:22:TRP:CD1	2.98	0.46
4:J:448:ASP:CG	4:K:441:ASN:OD1	2.56	0.46
4:K:290:TYR:CE2	5:G:107:ARG:NH1	2.80	0.46
2:V:732:GLY:O	2:V:746:ASN:ND2	2.49	0.46
5:B:5:THR:HG22	5:B:6:LEU:N	2.31	0.46
5:L:42:ILE:CG2	5:L:305:MET:HE3	2.46	0.46
5:Y:124:LEU:HD21	5:Y:304:GLN:OE1	2.16	0.46
5:D:30:ASP:O	5:D:31:THR:OG1	2.32	0.45
5:F:70:GLU:OE2	5:F:70:GLU:N	2.49	0.45
5:F:196:VAL:N	5:F:224:GLN:OE1	2.49	0.45
5:I:8:VAL:HG13	5:I:8:VAL:O	2.16	0.45
5:I:31:THR:HG23	5:I:31:THR:O	2.15	0.45
5:P:222:THR:OG1	5:P:275:ASP:OD2	2.15	0.45
1:N:192:VAL:HG22	1:N:193:GLN:H	1.80	0.45
4:K:241:LYS:HD3	5:D:39:LYS:O	2.16	0.45
5:B:90:VAL:HG12	5:B:91:VAL:N	2.31	0.45
5:H:236:MET:SD	5:H:284:ILE:HG23	2.57	0.45
5:Q:85:GLN:HE22	5:Q:127:ILE:HG21	1.80	0.45
5:T:90:VAL:HG12	5:T:325:MET:HB3	1.97	0.45
5:F:31:THR:O	5:F:35:SER:OG	2.30	0.45
5:F:124:LEU:C	5:F:124:LEU:HD23	2.42	0.45
5:I:326:ILE:HG23	5:I:326:ILE:O	2.16	0.45
1:N:53:PRO:N	1:N:54:PRO:HD2	2.31	0.45
1:N:67:VAL:O	1:N:68:ALA:C	2.60	0.45
2:V:273:ALA:O	2:V:279:THR:HG23	2.16	0.45
5:F:173:HIS:HA	5:F:198:VAL:HG11	1.99	0.45
5:I:303:THR:OG1	5:I:333:ARG:NE	2.50	0.45
4:J:376:LYS:HG3	4:K:397:GLU:H	1.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:579:LEU:HD23	4:J:580:PRO:O	2.15	0.45
5:T:237:ILE:HD12	5:T:294:VAL:HG22	1.98	0.45
5:U:92:ARG:O	5:Y:74:MET:HE1	2.17	0.45
1:A:164:HIS:O	1:A:164:HIS:ND1	2.49	0.45
1:A:226:ILE:HG13	1:A:226:ILE:O	2.16	0.45
2:V:530:ASP:N	2:V:530:ASP:OD1	2.48	0.45
2:V:730:VAL:HG13	2:V:731:GLU:H	1.81	0.45
4:J:212:GLU:HG3	4:K:270:GLN:HG3	1.98	0.45
4:J:557:GLN:HG3	4:K:577:TYR:HA	0.80	0.45
4:K:210:VAL:HG12	4:K:211:ASP:N	2.32	0.45
4:J:352:ILE:HD11	4:J:426:LEU:CD2	2.47	0.45
4:J:552:LEU:CD1	4:K:579:LEU:N	2.79	0.45
5:Q:8:VAL:HG11	5:U:159:HIS:CE1	2.51	0.45
5:X:70:GLU:O	5:X:71:ASP:OD1	2.35	0.45
2:V:605:LEU:HD11	2:V:682:ILE:HG22	1.98	0.45
4:J:210:VAL:HG12	4:J:211:ASP:N	2.32	0.45
4:K:20:ARG:NH1	5:G:101:ALA:HB3	2.24	0.45
5:C:85:GLN:HE22	5:C:127:ILE:HG21	1.82	0.45
5:Q:52:ASP:OD1	5:Q:53:ALA:N	2.44	0.45
2:V:171:ASP:OD1	2:V:171:ASP:N	2.49	0.45
4:J:26:GLN:OE1	4:J:258:GLN:NE2	2.50	0.45
5:B:171:CYS:SG	5:B:172:ALA:N	2.90	0.45
5:I:192:ASP:OD1	5:I:193:THR:N	2.50	0.45
5:T:237:ILE:HD11	5:T:241:HIS:HB2	1.97	0.45
5:Y:98:ASN:OD1	5:Y:99:THR:N	2.50	0.45
4:J:546:ASP:OD2	4:K:540:LYS:NZ	2.50	0.45
4:J:552:LEU:CD1	4:K:579:LEU:HB2	2.31	0.45
5:H:177:ALA:N	5:H:180:VAL:O	2.42	0.45
5:M:128:LEU:HD22	5:M:332:LEU:HB2	1.98	0.45
5:Q:108:GLU:OE2	5:Q:112:GLN:NE2	2.49	0.45
1:A:53:PRO:N	1:A:54:PRO:HD2	2.31	0.44
4:J:560:TYR:HD2	4:K:576:LYS:HD2	1.81	0.44
4:K:26:GLN:OE1	4:K:258:GLN:NE2	2.50	0.44
5:C:230:SER:OG	5:C:339:ALA:O	2.31	0.44
5:G:213:PHE:CD2	5:G:244:ILE:HG21	2.52	0.44
5:Y:176:LEU:HD23	5:Y:181:VAL:HA	1.99	0.44
2:V:609:GLU:OE1	2:V:624:ARG:NH2	2.50	0.44
2:V:736:VAL:HG12	2:V:737:VAL:N	2.33	0.44
4:J:410:HIS:HE1	4:K:407:PHE:N	2.14	0.44
4:J:429:THR:CB	4:K:435:LYS:HE3	2.47	0.44
5:D:237:ILE:HG13	5:D:283:ILE:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:THR:OG1	5:E:102:ASN:ND2	2.50	0.44
4:J:516:HIS:CB	4:K:108:GLN:CD	2.75	0.44
4:J:552:LEU:CD1	4:K:579:LEU:H	2.28	0.44
5:C:24:SER:HG	5:G:336:ASN:CG	2.09	0.44
5:H:82:ASN:ND2	5:H:83:VAL:O	2.51	0.44
5:I:308:ARG:HG2	5:I:329:GLU:HB2	1.98	0.44
5:L:95:ASP:OD1	5:L:96:THR:N	2.50	0.44
5:X:162:ARG:NH1	5:b:65:GLU:OE1	2.50	0.44
5:Y:51:THR:OG1	5:Y:336:ASN:ND2	2.51	0.44
2:V:489:VAL:HG23	2:V:515:ILE:HD11	1.98	0.44
4:J:21:ARG:NH1	4:K:278:THR:CA	2.63	0.44
5:C:83:VAL:O	5:C:164:THR:OG1	2.36	0.44
5:C:224:GLN:O	5:C:227:THR:OG1	2.31	0.44
5:G:77:THR:HG23	5:G:77:THR:O	2.18	0.44
5:F:141:GLN:N	5:F:141:GLN:OE1	2.50	0.44
2:V:577:VAL:HG23	2:V:577:VAL:O	2.18	0.44
4:J:18:LEU:HD11	4:J:292:HIS:CD2	2.53	0.44
4:J:212:GLU:CG	4:K:270:GLN:HG3	2.48	0.44
4:J:362:GLY:O	4:J:363:TYR:C	2.60	0.44
5:C:315:LEU:HG	5:C:316:ALA:H	1.83	0.44
5:G:235:ILE:N	5:G:282:LYS:O	2.49	0.44
5:M:152:VAL:HG12	5:M:152:VAL:O	2.17	0.44
5:U:148:ALA:O	5:U:152:VAL:HG22	2.17	0.44
5:U:202:GLN:O	5:U:203:ASN:OD1	2.36	0.44
4:J:100:ASP:OD1	4:J:100:ASP:N	2.49	0.44
4:J:429:THR:HB	4:K:435:LYS:CE	2.46	0.44
4:J:548:GLN:CG	4:K:555:LEU:CD1	2.93	0.44
4:K:657:GLU:HG2	4:K:661:GLU:OE2	2.18	0.44
5:D:264:LYS:C	5:E:270:VAL:HG23	2.42	0.44
5:H:120:ILE:HD12	5:H:328:MET:HE2	1.99	0.44
5:M:309:ALA:O	5:M:310:PRO:C	2.61	0.44
5:T:16:LYS:NZ	5:U:102:ASN:O	2.51	0.44
5:U:85:GLN:NE2	5:U:132:GLN:OE1	2.50	0.44
5:U:144:THR:HG22	5:U:144:THR:O	2.17	0.44
5:b:33:PHE:O	5:b:37:THR:HG23	2.17	0.44
4:J:64:VAL:O	4:J:68:VAL:HG23	2.17	0.44
4:J:305:SER:OG	4:K:284:ALA:HA	2.15	0.44
4:J:361:ARG:HH21	4:K:371:ASN:ND2	2.16	0.44
4:K:59:TRP:CE3	4:K:360:VAL:HG11	2.53	0.44
5:B:221:MET:HG2	5:B:343:LEU:HD21	1.98	0.44
5:M:237:ILE:HG22	5:M:294:VAL:HG12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:68:ARG:O	5:Q:69:ALA:C	2.61	0.44
4:J:59:TRP:CE3	4:J:360:VAL:HG11	2.53	0.44
4:K:18:LEU:HD11	4:K:292:HIS:CD2	2.52	0.44
5:E:182:ASP:OD1	5:E:183:LYS:N	2.51	0.44
5:Q:144:THR:HG23	5:Q:146:SER:H	1.82	0.44
5:Y:144:THR:HG23	5:Y:146:SER:H	1.83	0.44
5:T:79:ILE:HD12	5:T:80:LYS:H	1.83	0.44
1:A:26:ARG:NH2	2:V:922:GLN:OE1	2.51	0.43
2:V:50:LEU:HD22	2:V:870:ILE:CD1	2.48	0.43
2:V:680:ILE:HD11	2:V:721:ILE:HG23	1.99	0.43
2:V:694:GLU:O	2:V:695:PHE:CG	2.71	0.43
4:J:304:GLU:HA	4:K:232:GLU:CD	2.43	0.43
4:K:61:ASP:OD2	4:K:356:ARG:NE	2.40	0.43
4:K:362:GLY:O	4:K:363:TYR:C	2.60	0.43
5:D:163:LYS:O	5:D:165:GLY:N	2.51	0.43
5:D:286:ASN:O	5:D:287:ARG:C	2.61	0.43
5:H:127:ILE:O	5:H:130:SER:OG	2.17	0.43
5:P:251:ASN:O	5:T:255:SER:OG	2.35	0.43
4:J:535:LYS:HB3	4:K:569:MET:CE	2.48	0.43
4:K:64:VAL:O	4:K:68:VAL:HG23	2.17	0.43
5:B:34:VAL:HG23	5:B:125:GLU:OE2	2.18	0.43
4:K:352:ILE:HD11	4:K:426:LEU:CD2	2.47	0.43
5:C:117:GLY:O	5:C:120:ILE:HG22	2.18	0.43
5:b:105:ARG:NH2	5:b:108:GLU:OE1	2.51	0.43
5:B:48:SER:OG	5:B:80:LYS:O	2.26	0.43
5:F:152:VAL:HG22	5:F:153:ALA:N	2.33	0.43
5:F:313:THR:OG1	5:F:325:MET:SD	2.76	0.43
5:M:152:VAL:HG12	5:M:155:LEU:HB3	2.01	0.43
5:Q:237:ILE:HG22	5:Q:294:VAL:HG12	2.00	0.43
5:U:86:ILE:HD12	5:Y:65:GLU:OE2	2.18	0.43
5:X:214:ASP:OD1	5:X:215:GLU:N	2.50	0.43
5:X:263:THR:HG22	5:X:265:GLN:H	1.83	0.43
5:G:196:VAL:O	5:G:196:VAL:HG13	2.19	0.43
5:H:250:GLU:O	5:P:255:SER:OG	2.26	0.43
5:P:250:GLU:OE2	5:P:258:ARG:NH2	2.51	0.43
4:J:372:TYR:CA	4:K:392:PRO:CG	2.82	0.43
4:J:657:GLU:CG	4:J:661:GLU:OE2	2.67	0.43
4:K:258:GLN:CD	5:G:110:MET:HE1	2.43	0.43
5:I:47:PHE:CG	5:I:305:MET:HE1	2.53	0.43
5:T:90:VAL:HG12	5:T:325:MET:CB	2.49	0.43
5:Y:25:VAL:HG23	5:Y:25:VAL:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:730:VAL:HG13	2:V:731:GLU:N	2.33	0.43
4:J:21:ARG:CZ	4:K:278:THR:CA	2.90	0.43
4:J:646:LYS:NZ	4:K:644:GLN:HB3	2.33	0.43
5:B:88:ARG:NH1	5:F:64:VAL:O	2.52	0.43
5:C:193:THR:HG21	5:F:28:PRO:HG2	2.00	0.43
5:D:245:PHE:CE1	5:D:283:ILE:HD12	2.53	0.43
5:H:82:ASN:HD21	5:H:164:THR:HG23	1.83	0.43
5:M:237:ILE:HG21	5:M:245:PHE:HE2	1.83	0.43
5:Q:263:THR:O	5:Q:264:LYS:HB3	2.19	0.43
5:U:314:GLU:C	5:U:315:LEU:HD12	2.44	0.43
5:Y:180:VAL:HG22	5:Y:181:VAL:N	2.33	0.43
1:A:221:TYR:HD2	1:N:91:VAL:HG22	1.83	0.43
2:V:714:LYS:NZ	2:V:717:ASN:OD1	2.40	0.43
2:V:806:VAL:N	2:V:815:SER:O	2.52	0.43
5:F:237:ILE:HD11	5:F:241:HIS:HB3	2.00	0.43
5:b:30:ASP:O	5:b:31:THR:OG1	2.28	0.43
2:V:680:ILE:HG13	2:V:681:ASP:N	2.33	0.43
4:J:301:LYS:CG	4:K:281:GLU:O	2.65	0.43
4:J:657:GLU:HG2	4:J:661:GLU:OE2	2.18	0.43
5:B:93:VAL:O	5:B:93:VAL:HG13	2.19	0.43
5:C:222:THR:HG22	5:C:281:TYR:CE2	2.54	0.43
5:T:244:ILE:HG23	5:T:245:PHE:N	2.33	0.43
1:N:146:ILE:O	1:N:147:PRO:C	2.61	0.43
2:V:848:ASP:O	2:V:849:ASP:OD1	2.36	0.43
4:J:467:MET:CG	4:K:76:ILE:CD1	2.97	0.43
4:J:603:GLN:O	4:J:607:VAL:HG23	2.19	0.43
5:C:301:ASP:OD1	5:C:335:ARG:NH2	2.52	0.43
5:D:117:GLY:O	5:D:120:ILE:HG22	2.19	0.43
5:Q:90:VAL:HG11	5:U:70:GLU:O	2.19	0.43
1:N:195:ASP:OD1	1:N:196:ASN:N	2.52	0.42
4:J:265:ARG:HE	5:C:21:ASN:C	2.27	0.42
4:J:518:LEU:C	4:K:112:ARG:CZ	2.89	0.42
4:K:100:ASP:N	4:K:100:ASP:OD1	2.49	0.42
4:K:657:GLU:CG	4:K:661:GLU:OE2	2.67	0.42
5:C:42:ILE:HD12	5:C:44:GLN:O	2.20	0.42
5:C:237:ILE:HA	5:C:289:MET:HE1	2.01	0.42
5:G:180:VAL:HG22	5:G:181:VAL:N	2.33	0.42
5:P:132:GLN:NE2	5:P:164:THR:O	2.52	0.42
5:b:138:LEU:N	5:b:138:LEU:HD12	2.34	0.42
2:V:50:LEU:HD22	2:V:870:ILE:HD11	2.00	0.42
2:V:67:MET:HE1	2:V:541:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:738:THR:HG23	2:V:738:THR:O	2.18	0.42
4:J:475:ASN:HD22	4:K:118:ASN:ND2	2.08	0.42
4:J:552:LEU:HD11	4:K:579:LEU:N	2.31	0.42
4:K:265:ARG:HE	5:G:311:LYS:HB3	1.75	0.42
4:K:603:GLN:O	4:K:607:VAL:HG23	2.19	0.42
5:C:40:GLU:OE1	5:C:333:ARG:NH1	2.52	0.42
5:D:149:ASP:N	5:D:150:PRO:CD	2.82	0.42
5:H:105:ARG:HH22	5:P:77:THR:HG21	1.84	0.42
5:H:143:LEU:C	5:H:143:LEU:HD23	2.44	0.42
5:P:203:ASN:O	5:P:203:ASN:ND2	2.52	0.42
5:T:237:ILE:HD11	5:T:241:HIS:HB3	2.00	0.42
4:J:516:HIS:O	4:K:112:ARG:NH2	2.52	0.42
4:J:614:MET:SD	4:K:610:SER:N	2.93	0.42
4:J:629:GLN:HB2	4:K:627:PHE:CZ	2.54	0.42
5:C:83:VAL:HG12	5:C:84:THR:N	2.34	0.42
5:C:90:VAL:HG12	5:C:91:VAL:N	2.33	0.42
5:G:84:THR:OG1	5:G:330:VAL:O	2.23	0.42
5:H:105:ARG:NH2	5:P:50:GLN:OE1	2.52	0.42
5:I:145:ASN:ND2	5:Y:15:LYS:O	2.52	0.42
5:M:197:THR:HG21	5:M:338:TYR:O	2.19	0.42
5:Q:3:ASN:N	5:Q:4:PRO:CD	2.83	0.42
5:X:138:LEU:N	5:X:138:LEU:HD12	2.34	0.42
5:b:26:LEU:H	5:b:26:LEU:HD23	1.85	0.42
1:N:3:MET:HB3	1:N:4:PRO:CD	2.47	0.42
4:K:399:GLU:OE1	4:K:403:ALA:HB2	2.20	0.42
5:B:218:ILE:O	5:B:222:THR:HG23	2.20	0.42
5:L:85:GLN:CB	5:L:164:THR:HG23	2.48	0.42
5:M:215:GLU:HG2	5:M:248:LEU:HD13	2.01	0.42
5:P:332:LEU:HD23	5:P:332:LEU:N	2.35	0.42
5:U:218:ILE:HD12	5:U:218:ILE:H	1.83	0.42
1:A:78:GLN:O	1:A:79:TRP:C	2.61	0.42
2:V:850:PRO:O	2:V:851:SER:OG	2.29	0.42
4:J:338:GLY:C	4:K:263:TRP:CH2	2.94	0.42
4:J:409:TYR:HD1	4:K:375:TYR:OH	2.00	0.42
4:J:430:ARG:HH22	4:K:62:ARG:HG3	1.79	0.42
5:B:59:GLY:O	5:B:60:ASN:C	2.62	0.42
5:D:85:GLN:OE1	5:D:85:GLN:N	2.52	0.42
5:E:217:ASP:OD2	5:E:343:LEU:HD11	2.20	0.42
5:T:23:ILE:HG22	5:T:24:SER:N	2.35	0.42
1:A:220:GLU:O	1:A:222:SER:N	2.52	0.42
1:N:159:ASP:N	1:N:159:ASP:OD1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:298:SER:HA	2:V:369:THR:HG23	2.01	0.42
2:V:353:THR:HB	2:V:371:ARG:HD3	2.01	0.42
4:J:399:GLU:OE1	4:J:403:ALA:HB2	2.19	0.42
5:C:143:LEU:O	5:C:144:THR:C	2.63	0.42
5:F:167:PHE:N	5:F:167:PHE:CD1	2.87	0.42
5:F:198:VAL:HG23	5:F:342:VAL:HG23	2.01	0.42
5:H:86:ILE:O	5:H:87:LEU:HD12	2.20	0.42
5:I:52:ASP:OD1	5:I:53:ALA:N	2.51	0.42
5:P:137:VAL:HG13	5:P:138:LEU:HD12	2.02	0.42
5:X:193:THR:O	5:X:193:THR:HG22	2.19	0.42
5:b:306:VAL:HG23	5:b:330:VAL:HG12	2.02	0.42
4:J:296:THR:OG1	4:K:282:ASP:OD1	2.33	0.42
4:J:639:ARG:NH2	4:K:637:SER:OG	2.53	0.42
5:E:164:THR:HG22	5:E:165:GLY:N	2.35	0.42
5:F:64:VAL:HG12	5:F:65:GLU:N	2.35	0.42
5:I:13:ASN:OD1	5:I:14:GLY:N	2.53	0.42
5:M:83:VAL:HG12	5:M:84:THR:N	2.35	0.42
5:T:262:ASN:ND2	5:X:263:THR:HG21	2.34	0.42
5:T:289:MET:HE3	5:T:290:PRO:HD2	2.02	0.42
5:X:5:THR:O	5:X:6:LEU:HD23	2.19	0.42
5:Y:263:THR:O	5:Y:263:THR:HG22	2.19	0.42
2:V:539:HIS:HA	2:V:547:VAL:O	2.19	0.42
4:J:298:VAL:HG13	4:J:299:LEU:CD1	2.46	0.42
5:B:144:THR:HG22	5:B:144:THR:O	2.20	0.42
5:E:91:VAL:O	5:E:91:VAL:HG13	2.19	0.42
5:E:146:SER:O	5:E:147:ALA:C	2.62	0.42
5:M:237:ILE:HG21	5:M:245:PHE:CE2	2.55	0.42
5:Y:197:THR:O	5:Y:221:MET:HE1	2.20	0.42
5:b:137:VAL:C	5:b:138:LEU:HD12	2.45	0.42
1:A:35:ILE:N	1:A:36:PRO:CD	2.83	0.42
2:V:192:THR:HG21	2:V:195:GLU:HB2	2.02	0.42
4:J:356:ARG:O	4:J:357:THR:C	2.63	0.42
4:J:360:VAL:O	4:J:361:ARG:C	2.63	0.42
4:J:372:TYR:CB	4:K:392:PRO:HG3	2.49	0.42
4:J:374:ARG:NE	4:K:391:ARG:N	2.67	0.42
4:J:556:GLU:C	4:K:577:TYR:CZ	2.71	0.42
5:G:196:VAL:O	5:G:197:THR:C	2.63	0.42
5:D:34:VAL:HG13	5:D:125:GLU:OE1	2.20	0.42
5:H:30:ASP:OD1	5:H:30:ASP:N	2.52	0.42
5:L:83:VAL:O	5:L:164:THR:HG22	2.20	0.42
5:Y:93:VAL:HG11	5:Y:98:ASN:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:661:GLU:OE1	4:K:660:LYS:HE3	2.19	0.42
4:K:48:LEU:HB3	4:K:49:PRO:HD3	2.02	0.42
4:K:360:VAL:O	4:K:361:ARG:C	2.63	0.42
5:L:303:THR:HG21	5:L:333:ARG:NH1	2.35	0.42
5:b:289:MET:HE3	5:b:295:TYR:CD2	2.55	0.42
1:A:28:ASP:OD1	1:A:31:PHE:N	2.52	0.41
1:A:93:SER:N	4:K:388:LEU:HD12	2.34	0.41
2:V:831:PRO:O	2:V:835:ARG:N	2.53	0.41
4:K:472:ILE:O	4:K:476:GLY:N	2.53	0.41
5:U:17:LEU:O	5:U:18:SER:C	2.63	0.41
2:V:159:ASN:OD1	2:V:161:SER:OG	2.37	0.41
4:J:48:LEU:HB3	4:J:49:PRO:HD3	2.01	0.41
4:J:351:ASP:O	4:J:352:ILE:C	2.63	0.41
4:J:430:ARG:HH12	4:K:62:ARG:CB	2.32	0.41
5:F:40:GLU:O	5:F:41:SER:C	2.63	0.41
5:Q:176:LEU:HD23	5:Q:181:VAL:HA	2.03	0.41
5:T:196:VAL:O	5:T:196:VAL:HG23	2.19	0.41
5:U:26:LEU:HD22	5:Y:336:ASN:CG	2.45	0.41
5:U:45:THR:OG1	5:U:84:THR:OG1	2.35	0.41
1:A:169:THR:OG1	1:A:170:SER:N	2.53	0.41
2:V:165:ILE:O	2:V:165:ILE:HG13	2.21	0.41
4:J:466:ARG:HH12	4:K:77:ASN:ND2	2.18	0.41
5:C:155:LEU:HD12	5:C:156:ASN:N	2.36	0.41
5:G:309:ALA:HB1	5:G:310:PRO:HD2	2.02	0.41
5:P:108:GLU:OE1	5:P:108:GLU:N	2.53	0.41
5:D:144:THR:O	5:D:145:ASN:CB	2.68	0.41
5:L:133:ALA:HB2	5:L:176:LEU:HD22	2.01	0.41
5:M:17:LEU:O	5:M:18:SER:C	2.62	0.41
5:Y:235:ILE:HG22	5:Y:237:ILE:HG23	2.03	0.41
4:K:95:ASP:OD1	4:K:95:ASP:N	2.53	0.41
4:K:352:ILE:O	4:K:353:GLN:C	2.63	0.41
5:G:232:ALA:HB1	5:G:297:PHE:O	2.21	0.41
5:M:315:LEU:HD11	5:M:325:MET:SD	2.61	0.41
4:J:131:ARG:CZ	4:K:269:ARG:HH11	2.23	0.41
4:J:372:TYR:C	4:K:392:PRO:CB	2.77	0.41
4:J:449:ASN:OD1	4:K:441:ASN:ND2	2.54	0.41
4:J:472:ILE:O	4:J:476:GLY:N	2.53	0.41
4:K:356:ARG:O	4:K:357:THR:C	2.63	0.41
5:C:214:ASP:OD1	5:C:215:GLU:N	2.52	0.41
5:G:233:ASP:N	5:G:233:ASP:OD1	2.52	0.41
5:H:168:GLN:OE1	5:H:295:TYR:OH	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:313:THR:HG22	5:M:314:GLU:N	2.35	0.41
5:P:241:HIS:NE2	5:P:291:THR:O	2.53	0.41
1:A:62:ASP:O	1:A:64:LYS:HD3	2.21	0.41
2:V:869:THR:OG1	2:V:881:VAL:HG12	2.21	0.41
5:D:146:SER:O	5:D:147:ALA:HB3	2.21	0.41
5:F:170:LEU:HD12	5:F:171:CYS:N	2.36	0.41
5:F:237:ILE:HD11	5:F:241:HIS:HB2	2.03	0.41
5:L:82:ASN:ND2	5:L:332:LEU:O	2.50	0.41
5:P:30:ASP:O	5:P:31:THR:OG1	2.33	0.41
5:Y:136:ASP:OD1	5:Y:137:VAL:N	2.53	0.41
1:A:231:ASN:HB3	4:K:55:GLY:C	2.45	0.41
2:V:480:GLU:OE1	2:V:480:GLU:N	2.46	0.41
2:V:547:VAL:HG12	2:V:548:ALA:N	2.36	0.41
4:J:403:ALA:O	4:K:401:GLN:OE1	2.39	0.41
4:J:634:ASP:O	4:J:637:SER:OG	2.39	0.41
5:B:305:MET:O	5:B:331:GLY:N	2.45	0.41
5:C:74:MET:CE	5:F:93:VAL:HG21	2.51	0.41
5:C:152:VAL:HG21	5:F:10:TYR:HB2	2.03	0.41
5:I:25:VAL:HG23	5:I:25:VAL:O	2.21	0.41
5:L:89:LYS:HG2	5:L:120:ILE:HD12	2.02	0.41
5:U:263:THR:O	5:U:263:THR:HG22	2.20	0.41
5:X:220:ASP:O	5:X:224:GLN:HG2	2.21	0.41
1:N:72:PRO:O	3:O:13:ASN:ND2	2.54	0.41
2:V:664:ASN:OD1	2:V:705:ASN:ND2	2.54	0.41
2:V:914:ASP:OD1	2:V:914:ASP:N	2.53	0.41
4:J:352:ILE:O	4:J:353:GLN:C	2.63	0.41
4:J:354:ASP:O	4:J:355:LEU:C	2.64	0.41
4:J:410:HIS:NE2	4:K:374:ARG:O	2.43	0.41
4:J:646:LYS:HZ1	4:K:644:GLN:C	2.28	0.41
4:J:661:GLU:HB2	4:K:660:LYS:CE	2.49	0.41
4:K:354:ASP:O	4:K:355:LEU:C	2.64	0.41
5:C:60:ASN:O	5:C:61:ASN:ND2	2.53	0.41
5:D:147:ALA:O	5:D:148:ALA:C	2.63	0.41
5:D:237:ILE:HG21	5:D:285:VAL:HG13	2.02	0.41
5:L:289:MET:HE1	5:L:295:TYR:CD1	2.56	0.41
5:M:119:GLU:OE2	5:Q:55:ALA:HB3	2.21	0.41
5:P:30:ASP:OD1	5:P:30:ASP:N	2.54	0.41
5:P:157:ASP:N	5:P:157:ASP:OD1	2.52	0.41
5:Q:288:TRP:CZ3	5:U:57:VAL:HG21	2.56	0.41
5:Q:309:ALA:O	5:Q:310:PRO:C	2.64	0.41
5:T:142:TYR:O	5:T:143:LEU:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:10:TYR:OH	5:Y:162:ARG:NE	2.54	0.41
5:Y:262:ASN:OD1	5:Y:263:THR:N	2.53	0.41
1:A:233:THR:O	1:A:234:ARG:HG3	2.21	0.41
4:J:38:ARG:HH21	5:C:21:ASN:CB	2.34	0.41
4:J:376:LYS:HG3	4:K:397:GLU:N	1.88	0.41
4:J:516:HIS:O	4:K:112:ARG:CZ	2.69	0.41
4:K:267:ASP:OD1	4:K:267:ASP:N	2.49	0.41
5:G:190:ASP:O	5:G:194:GLY:N	2.54	0.41
5:I:199:LYS:NZ	5:I:220:ASP:OD1	2.54	0.41
2:V:834:GLU:N	2:V:834:GLU:OE1	2.54	0.40
4:J:95:ASP:OD1	4:J:95:ASP:N	2.53	0.40
4:J:448:ASP:CG	4:K:441:ASN:ND2	2.78	0.40
4:J:474:HIS:ND1	4:K:117:TYR:CD1	2.87	0.40
4:K:563:ALA:O	4:K:567:GLU:HG2	2.21	0.40
4:K:657:GLU:HA	4:K:661:GLU:HG2	2.03	0.40
5:E:340:SER:OG	5:E:341:GLY:N	2.54	0.40
5:H:210:ASN:O	5:H:211:ILE:C	2.64	0.40
5:X:119:GLU:OE2	5:b:55:ALA:N	2.44	0.40
5:Y:294:VAL:HG22	5:Y:343:LEU:HB2	2.03	0.40
2:V:118:VAL:HG22	2:V:118:VAL:O	2.22	0.40
4:J:353:GLN:O	4:J:354:ASP:C	2.64	0.40
4:J:563:ALA:O	4:J:567:GLU:HG2	2.21	0.40
5:C:192:ASP:OD1	5:F:122:ARG:NH1	2.51	0.40
5:F:305:MET:HE1	5:F:333:ARG:HD3	2.03	0.40
5:H:304:GLN:O	5:H:306:VAL:HG13	2.21	0.40
5:M:203:ASN:OD1	5:M:204:ALA:N	2.48	0.40
2:V:706:THR:OG1	2:V:707:TYR:N	2.55	0.40
5:G:285:VAL:HG11	5:D:277:LEU:HD22	2.03	0.40
5:D:245:PHE:CZ	5:D:273:ILE:HD11	2.56	0.40
5:D:250:GLU:O	5:D:251:ASN:HB2	2.21	0.40
5:H:83:VAL:HG22	5:H:84:THR:N	2.36	0.40
5:T:251:ASN:OD1	5:T:252:THR:N	2.55	0.40
5:X:164:THR:O	5:X:164:THR:HG22	2.20	0.40
5:Y:108:GLU:OE1	5:Y:108:GLU:N	2.54	0.40
4:J:467:MET:CG	4:K:76:ILE:HD11	2.51	0.40
4:J:487:LEU:HD23	4:J:488:ILE:N	2.37	0.40
4:J:534:GLN:O	4:J:535:LYS:C	2.63	0.40
5:X:71:ASP:OD1	5:X:71:ASP:C	2.64	0.40
2:V:549:THR:HG22	2:V:549:THR:O	2.22	0.40
4:J:377:ALA:H	4:K:397:GLU:H	1.69	0.40
4:K:349:THR:O	4:K:350:LYS:C	2.63	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:487:LEU:HD23	4:K:488:ILE:N	2.37	0.40
5:B:177:ALA:O	5:B:179:GLY:N	2.50	0.40
5:C:199:LYS:O	5:C:343:LEU:HD12	2.22	0.40
5:D:196:VAL:O	5:D:196:VAL:HG23	2.22	0.40
5:F:108:GLU:HG2	5:F:108:GLU:O	2.22	0.40
5:H:51:THR:HG23	5:H:78:VAL:HB	2.03	0.40
5:I:117:GLY:O	5:I:120:ILE:HG22	2.22	0.40
5:L:149:ASP:OD1	5:L:149:ASP:N	2.54	0.40
5:T:172:ALA:O	5:T:198:VAL:HG21	2.22	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	223/250 (89%)	200 (90%)	23 (10%)	0	100	100
1	N	224/250 (90%)	198 (88%)	25 (11%)	1 (0%)	30	67
2	V	906/1005 (90%)	819 (90%)	87 (10%)	0	100	100
3	O	27/786 (3%)	27 (100%)	0	0	100	100
3	R	23/786 (3%)	22 (96%)	1 (4%)	0	100	100
3	S	6/786 (1%)	6 (100%)	0	0	100	100
4	J	581/747 (78%)	547 (94%)	34 (6%)	0	100	100
4	K	581/747 (78%)	546 (94%)	35 (6%)	0	100	100
5	B	344/352 (98%)	288 (84%)	56 (16%)	0	100	100
5	C	310/352 (88%)	281 (91%)	29 (9%)	0	100	100
5	D	344/352 (98%)	283 (82%)	60 (17%)	1 (0%)	36	71
5	E	344/352 (98%)	302 (88%)	41 (12%)	1 (0%)	36	71
5	F	345/352 (98%)	294 (85%)	50 (14%)	1 (0%)	36	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	296/352 (84%)	268 (90%)	28 (10%)	0	100	100
5	H	339/352 (96%)	300 (88%)	39 (12%)	0	100	100
5	I	344/352 (98%)	321 (93%)	23 (7%)	0	100	100
5	L	345/352 (98%)	320 (93%)	25 (7%)	0	100	100
5	M	344/352 (98%)	323 (94%)	21 (6%)	0	100	100
5	P	341/352 (97%)	312 (92%)	29 (8%)	0	100	100
5	Q	344/352 (98%)	322 (94%)	22 (6%)	0	100	100
5	T	343/352 (97%)	311 (91%)	32 (9%)	0	100	100
5	U	344/352 (98%)	311 (90%)	33 (10%)	0	100	100
5	X	344/352 (98%)	313 (91%)	31 (9%)	0	100	100
5	Y	344/352 (98%)	320 (93%)	24 (7%)	0	100	100
5	b	344/352 (98%)	322 (94%)	22 (6%)	0	100	100
All	All	8330/11341 (74%)	7556 (91%)	770 (9%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	67	VAL
5	D	145	ASN
5	F	168	GLN
5	E	147	ALA

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	202/223 (91%)	202 (100%)	0	100	100
1	N	203/223 (91%)	203 (100%)	0	100	100
2	V	794/870 (91%)	794 (100%)	0	100	100
3	O	21/640 (3%)	21 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	15/640 (2%)	15 (100%)	0	100	100
3	S	5/640 (1%)	5 (100%)	0	100	100
4	J	509/647 (79%)	509 (100%)	0	100	100
4	K	509/647 (79%)	509 (100%)	0	100	100
5	B	285/287 (99%)	285 (100%)	0	100	100
5	C	260/287 (91%)	260 (100%)	0	100	100
5	D	285/287 (99%)	285 (100%)	0	100	100
5	E	285/287 (99%)	285 (100%)	0	100	100
5	F	286/287 (100%)	286 (100%)	0	100	100
5	G	253/287 (88%)	253 (100%)	0	100	100
5	H	283/287 (99%)	283 (100%)	0	100	100
5	I	285/287 (99%)	285 (100%)	0	100	100
5	L	286/287 (100%)	286 (100%)	0	100	100
5	M	285/287 (99%)	285 (100%)	0	100	100
5	P	282/287 (98%)	282 (100%)	0	100	100
5	Q	285/287 (99%)	285 (100%)	0	100	100
5	T	284/287 (99%)	284 (100%)	0	100	100
5	U	285/287 (99%)	285 (100%)	0	100	100
5	X	285/287 (99%)	285 (100%)	0	100	100
5	Y	285/287 (99%)	285 (100%)	0	100	100
5	b	285/287 (99%)	285 (100%)	0	100	100
All	All	7042/9409 (75%)	7042 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	N	37	ASN
1	N	78	GLN
1	N	103	HIS
2	V	47	ASN
2	V	150	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	V	264	ASN
2	V	330	ASN
2	V	332	ASN
2	V	574	GLN
2	V	589	ASN
2	V	627	ASN
2	V	705	ASN
2	V	746	ASN
2	V	880	GLN
2	V	926	ASN
2	V	946	GLN
2	V	989	ASN
4	J	77	ASN
4	J	93	GLN
4	J	142	GLN
4	J	258	GLN
4	J	449	ASN
4	J	471	ASN
4	J	474	HIS
4	J	516	HIS
4	J	519	GLN
4	J	564	GLN
4	J	603	GLN
4	J	630	GLN
4	J	640	GLN
4	K	77	ASN
4	K	142	GLN
4	K	258	GLN
4	K	316	HIS
4	K	368	ASN
4	K	371	ASN
4	K	401	GLN
4	K	441	ASN
4	K	564	GLN
4	K	603	GLN
4	K	630	GLN
4	K	640	GLN
5	B	44	GLN
5	B	60	ASN
5	B	112	GLN
5	B	132	GLN
5	B	279	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	63	HIS
5	C	85	GLN
5	C	168	GLN
5	C	206	ASN
5	C	253	GLN
5	G	60	ASN
5	G	112	GLN
5	D	82	ASN
5	D	202	GLN
5	D	241	HIS
5	E	13	ASN
5	E	102	ASN
5	E	241	HIS
5	E	251	ASN
5	F	85	GLN
5	H	44	GLN
5	H	61	ASN
5	H	82	ASN
5	H	168	GLN
5	H	224	GLN
5	H	265	GLN
5	H	334	HIS
5	H	336	ASN
5	I	210	ASN
5	I	271	ASN
5	I	304	GLN
5	L	21	ASN
5	L	159	HIS
5	L	202	GLN
5	L	210	ASN
5	L	334	HIS
5	M	12	GLN
5	M	29	GLN
5	M	61	ASN
5	M	206	ASN
5	M	224	GLN
5	P	102	ASN
5	P	145	ASN
5	P	156	ASN
5	P	203	ASN
5	Q	12	GLN
5	Q	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Q	60	ASN
5	Q	202	GLN
5	Q	224	GLN
5	Q	238	ASN
5	Q	241	HIS
5	Q	262	ASN
5	T	13	ASN
5	T	50	GLN
5	T	60	ASN
5	T	112	GLN
5	T	241	HIS
5	T	249	GLN
5	T	262	ASN
5	T	279	GLN
5	U	13	ASN
5	U	61	ASN
5	U	85	GLN
5	U	102	ASN
5	U	132	GLN
5	U	168	GLN
5	U	262	ASN
5	U	304	GLN
5	X	132	GLN
5	X	156	ASN
5	X	241	HIS
5	X	279	GLN
5	Y	156	ASN
5	b	21	ASN
5	b	145	ASN
5	b	203	ASN
5	b	206	ASN
5	b	251	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

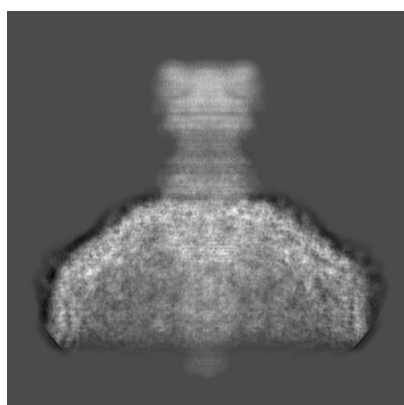
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14489. These allow visual inspection of the internal detail of the map and identification of artifacts.

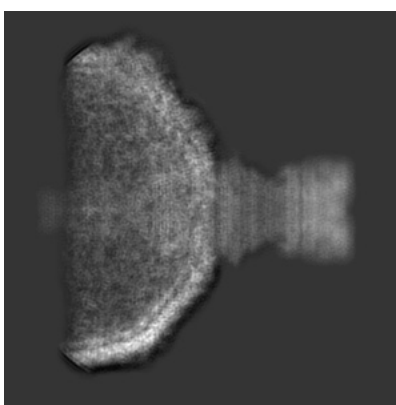
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

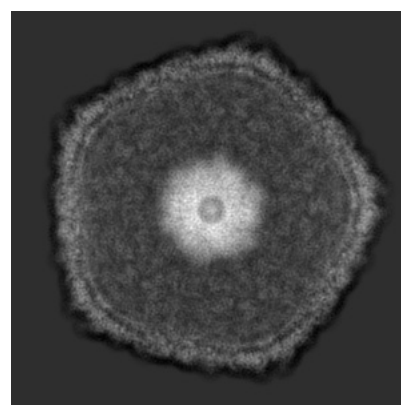
6.1.1 Primary map



X



Y

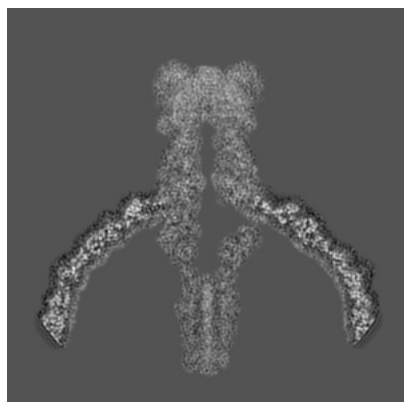


Z

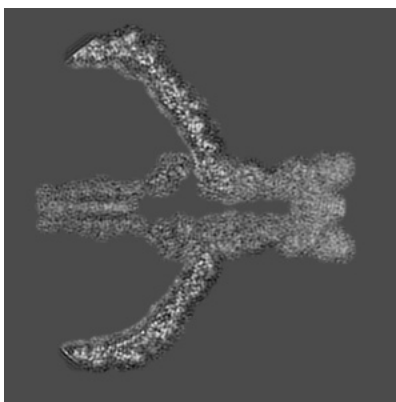
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

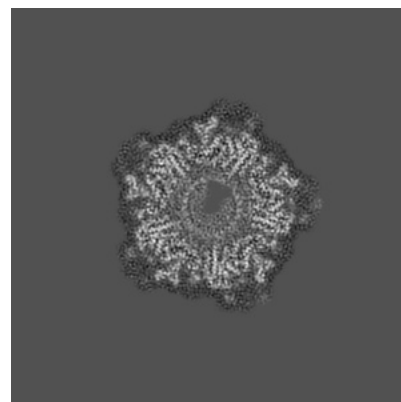
6.2.1 Primary map



X Index: 200



Y Index: 200

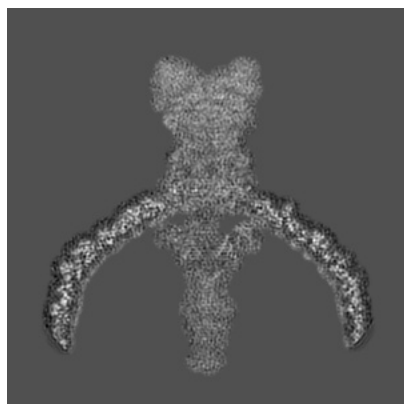


Z Index: 200

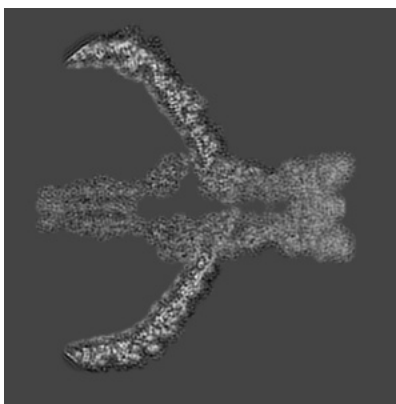
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

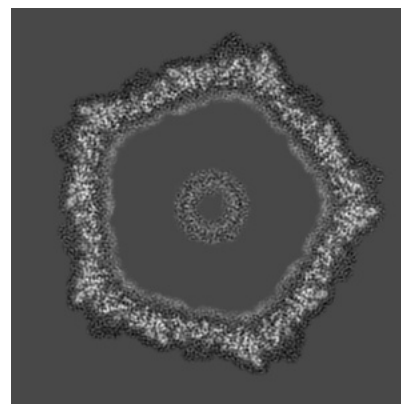
6.3.1 Primary map



X Index: 184



Y Index: 204

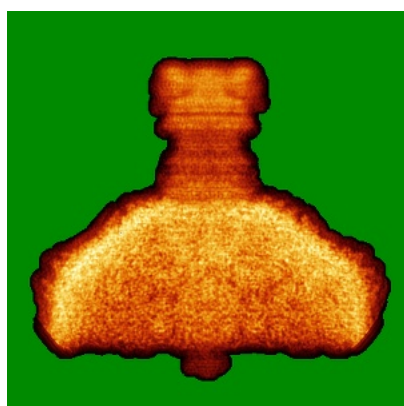


Z Index: 148

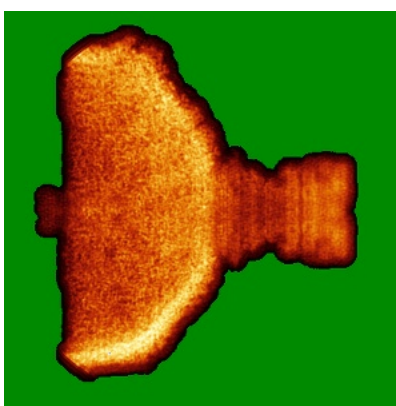
The images above show the largest variance slices of the map in three orthogonal directions.

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

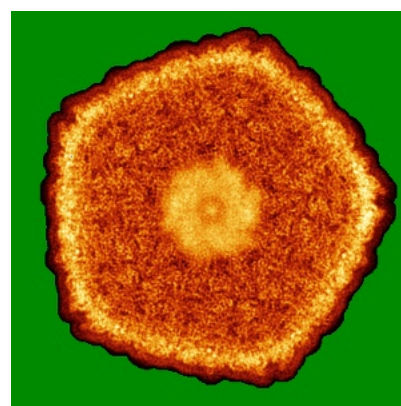
6.4.1 Primary map



X



Y

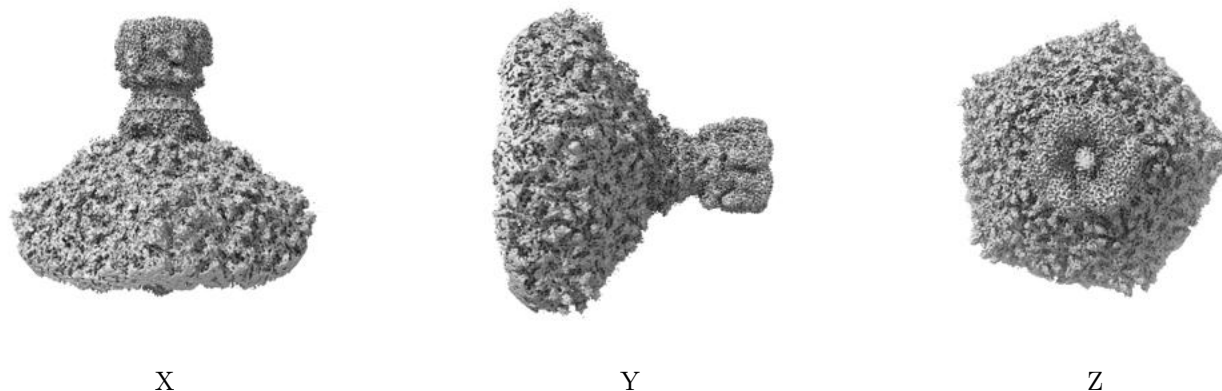


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

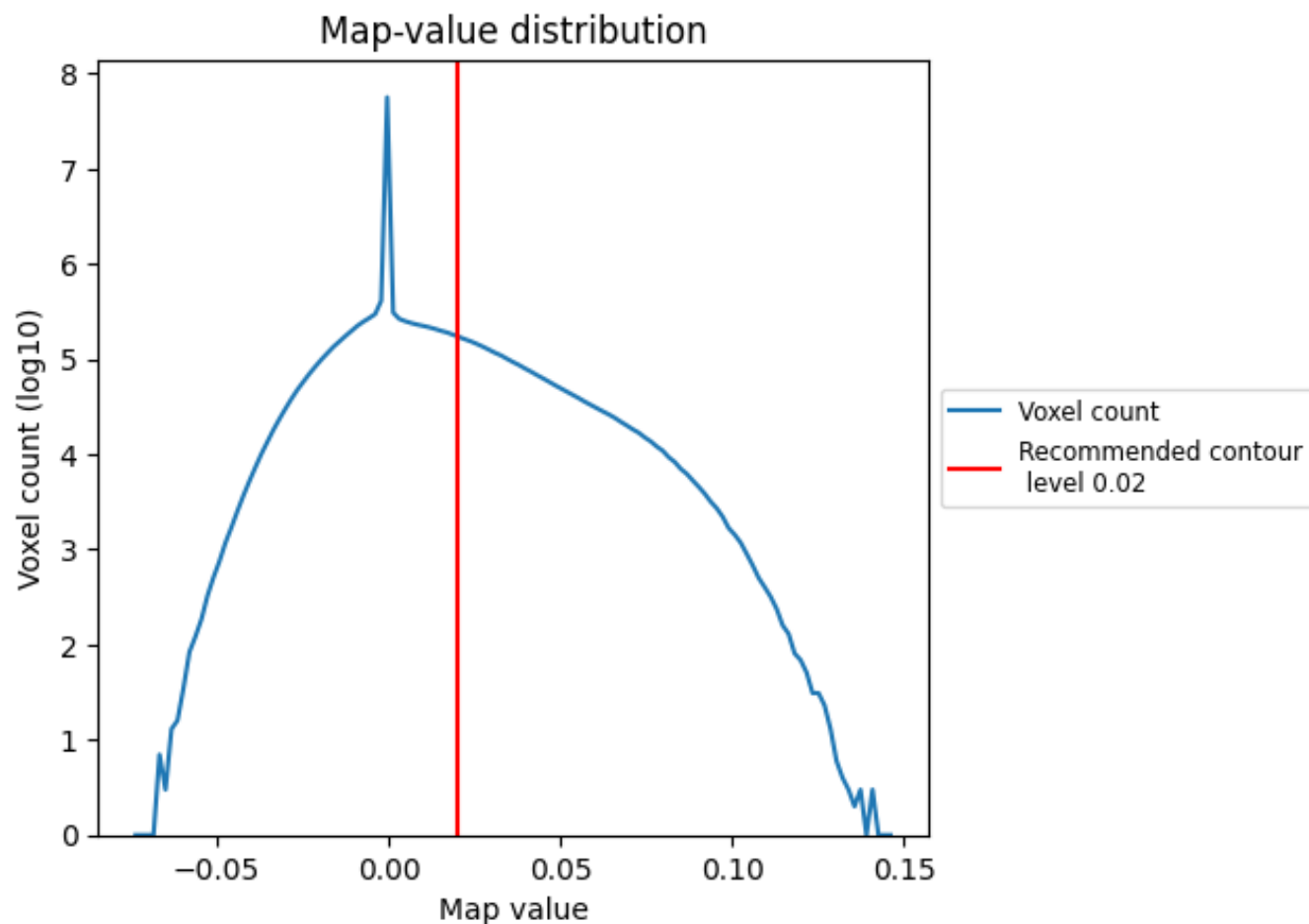
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

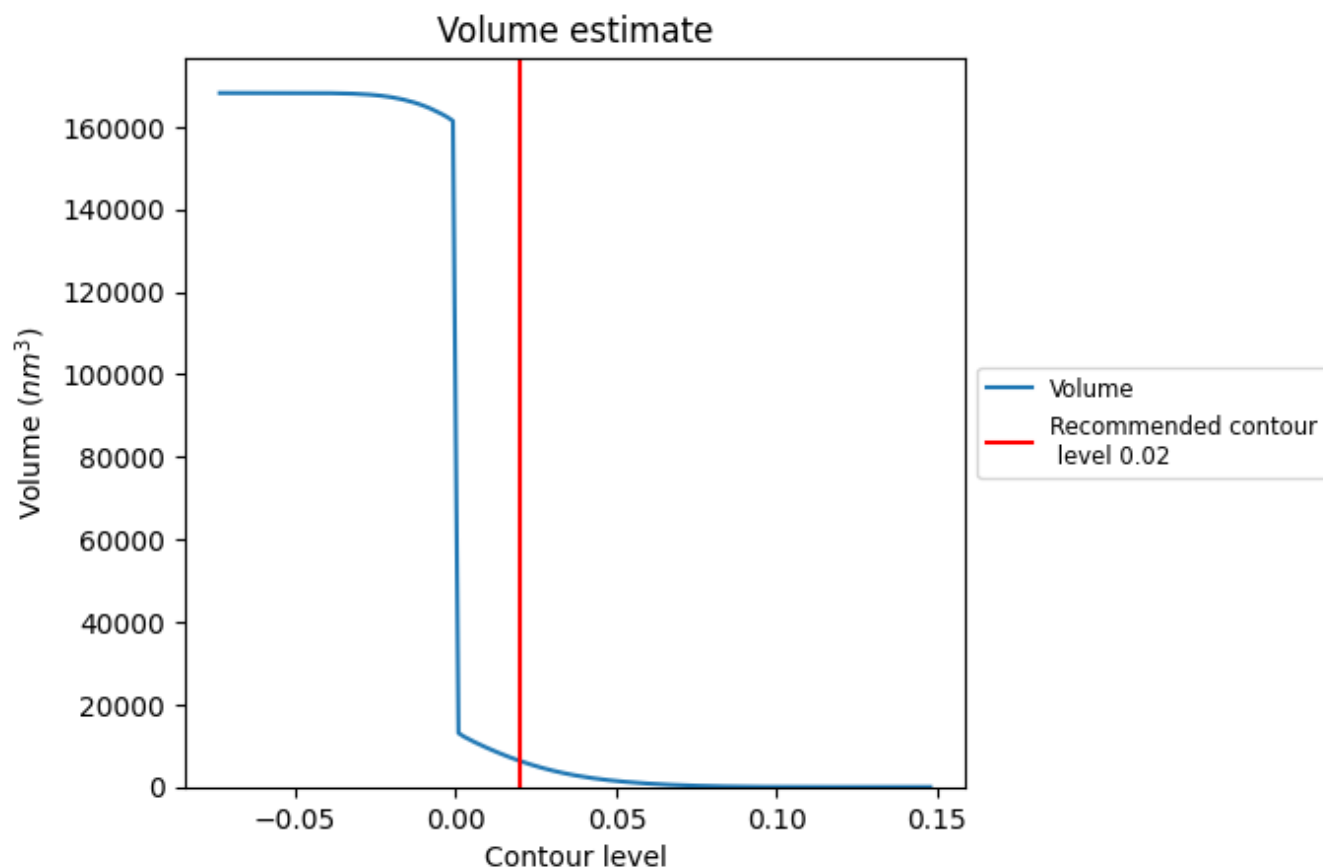
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

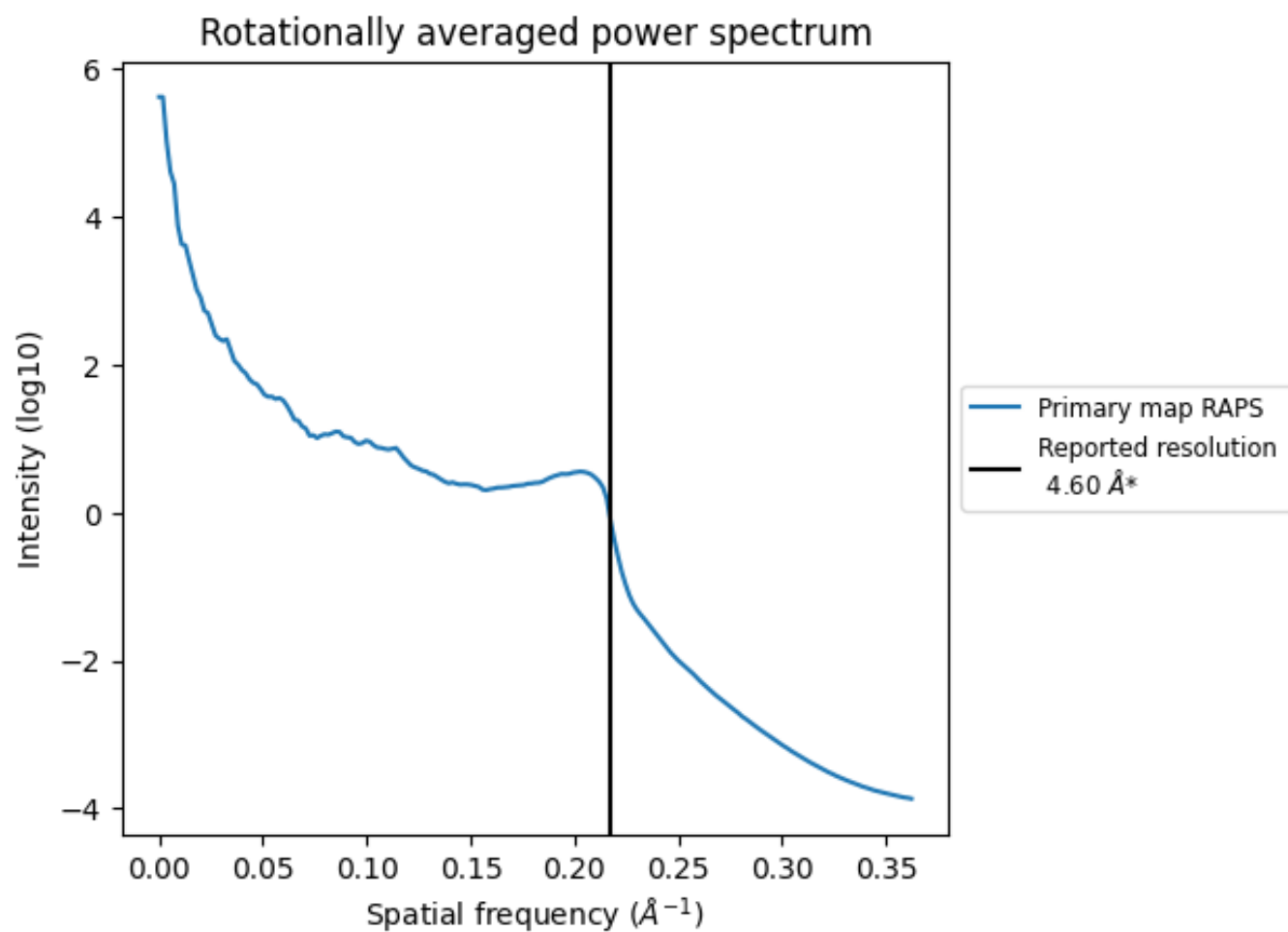
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6302 nm³; this corresponds to an approximate mass of 5692 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 ⓘ

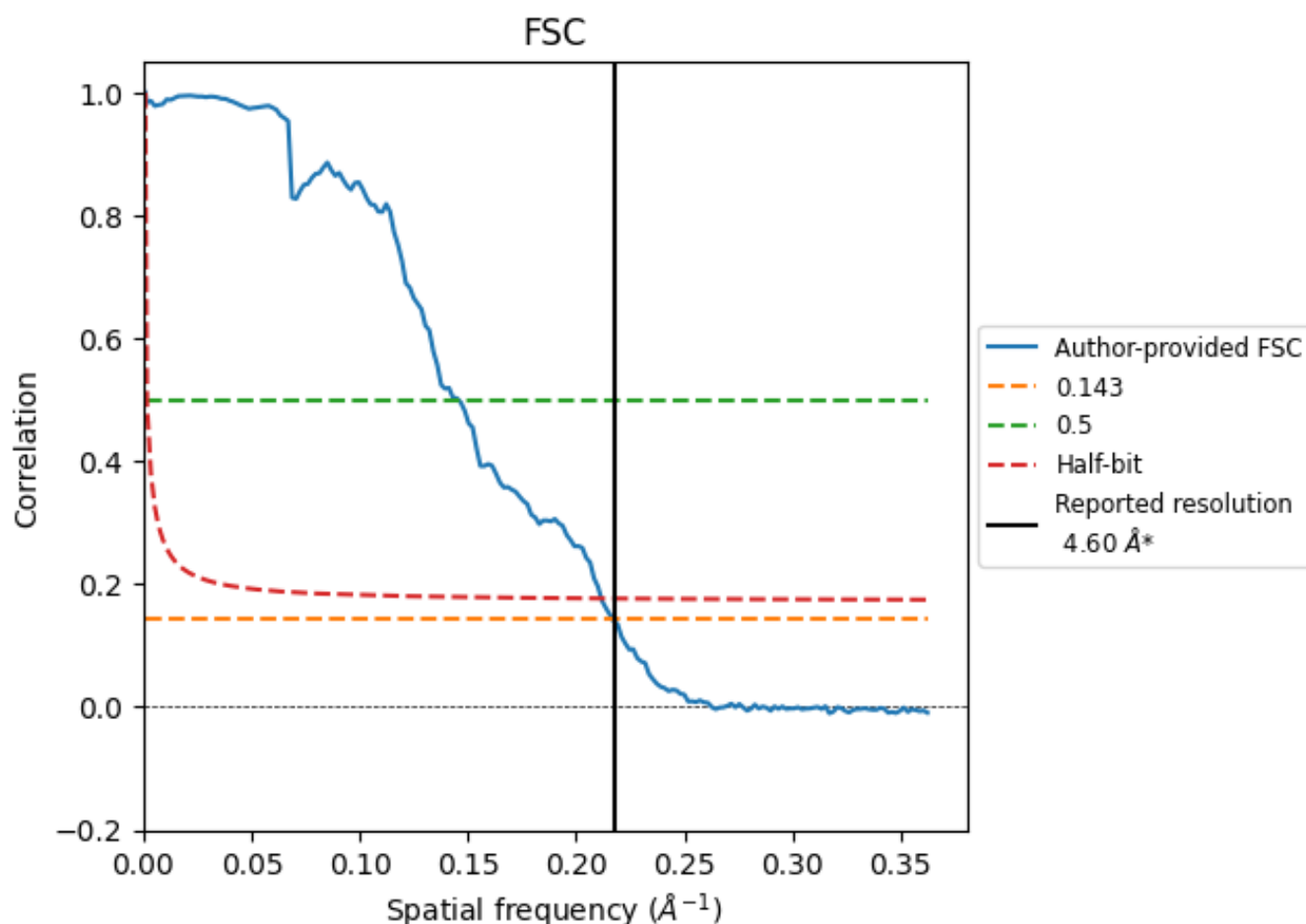


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	6.87	4.73
Unmasked-calculated*	-	-	-

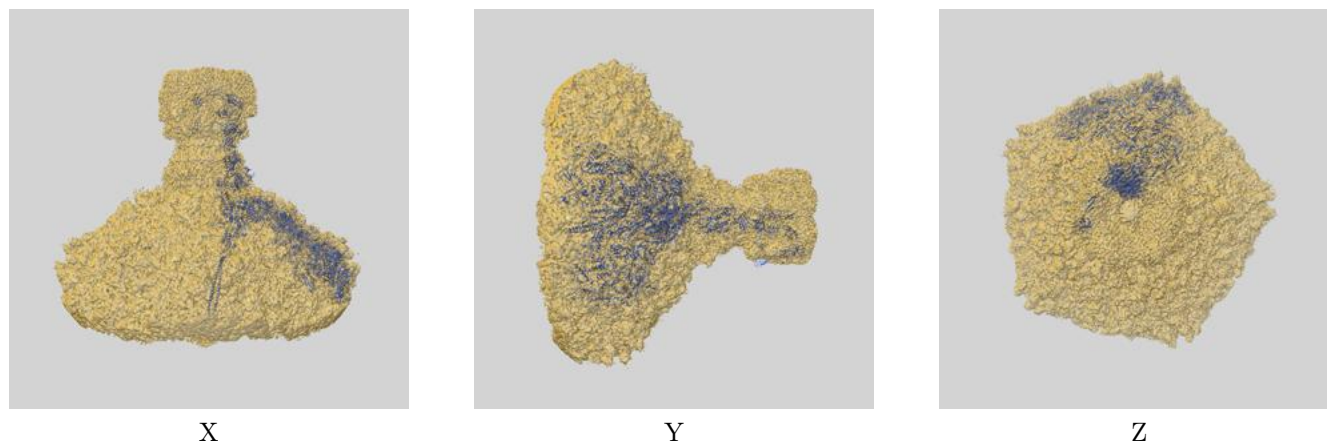
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

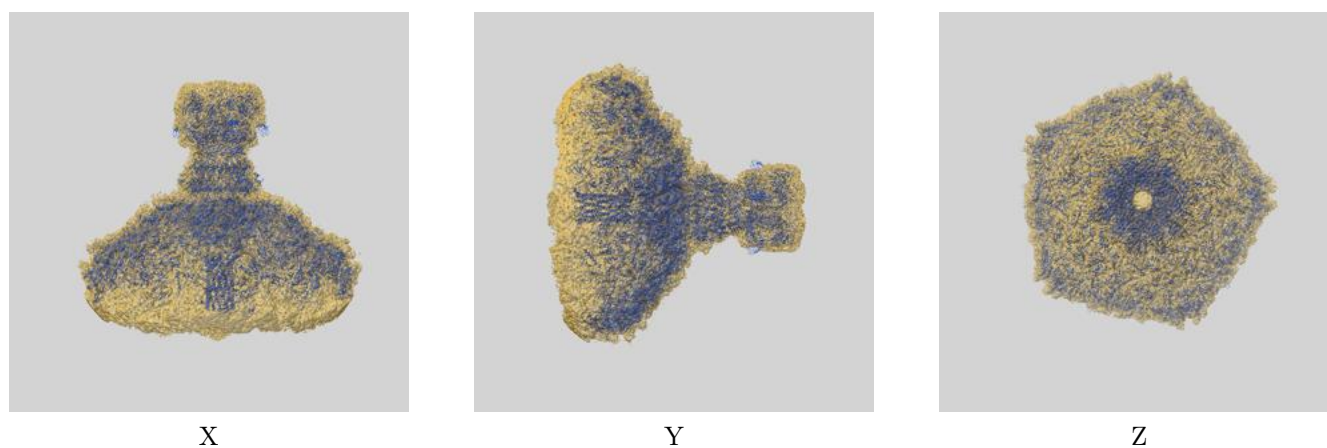
This section contains information regarding the fit between EMDB map EMD-14489 and PDB model 7Z4A. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



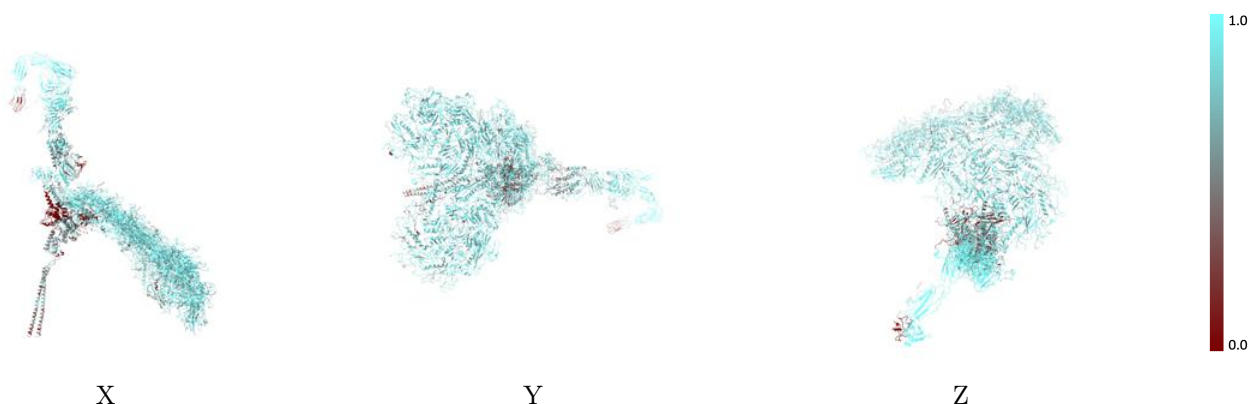
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



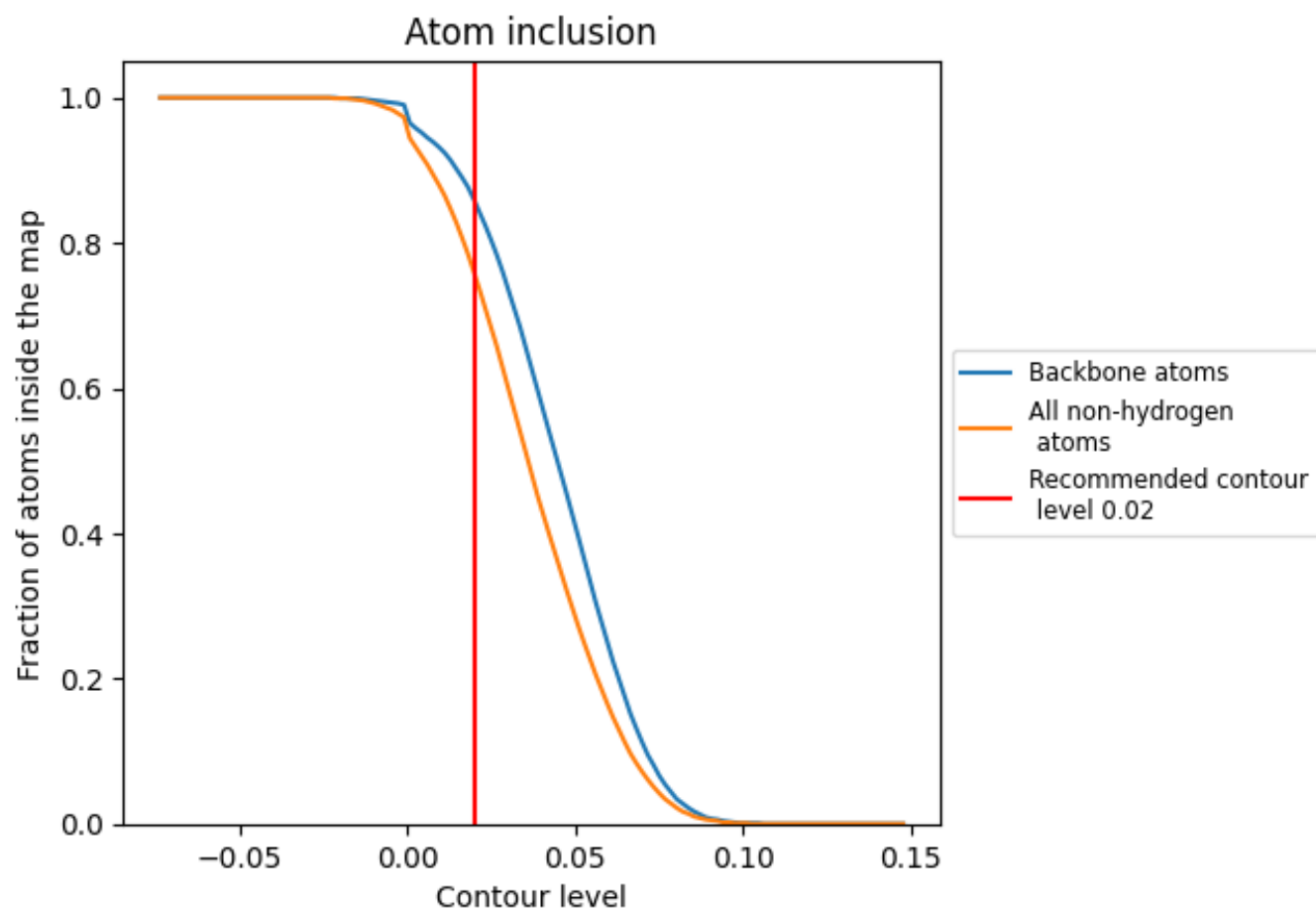
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.1970
A	 0.6610	 0.1460
B	 0.8070	 0.2310
C	 0.8410	 0.2360
D	 0.8040	 0.2350
E	 0.8320	 0.2620
F	 0.8160	 0.2240
G	 0.8350	 0.2360
H	 0.8160	 0.2380
I	 0.7990	 0.2150
J	 0.4270	 0.1130
K	 0.4880	 0.1420
L	 0.8510	 0.2610
M	 0.8180	 0.2220
N	 0.6760	 0.1390
O	 0.5640	 0.1940
P	 0.7710	 0.2150
Q	 0.8340	 0.2270
R	 0.5540	 0.2050
S	 0.4390	 0.1550
T	 0.7390	 0.1860
U	 0.8320	 0.2290
V	 0.8480	 0.1000
X	 0.8360	 0.2410
Y	 0.8240	 0.2280
b	 0.8490	 0.2490

