



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 07:01 pm GMT

PDB ID : 6TB9
EMDB ID : EMD-10442
Title : Capsid of native GTA particle computed with C5 symmetry
Authors : Bardy, P.; Fuzik, T.; Hrebik, D.; Pantucek, R.; Beatty, J.T.; Plevka, P.
Deposited on : 2019-11-01
Resolution : 3.56 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

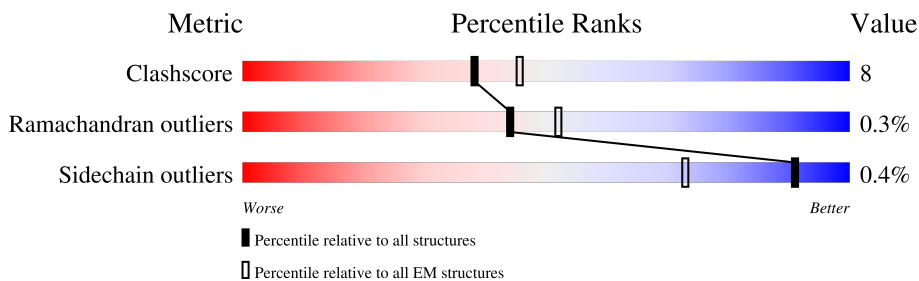
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A4	386	
1	A5	386	
1	B4	386	
1	B5	386	
1	C4	386	
1	C5	386	
1	D4	386	
1	E4	386	

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Mol	Chain	Length	Quality of chain
1	F4	386	 62% 15% 23%
1	G4	386	 65% 12% 23%
1	H4	386	 5% 63% 12% 25%
1	I4	386	 5% 60% 15% 25%
1	J4	386	 5% 59% 16% 25%
1	K4	386	 5% 59% 16% 25%
1	L4	386	 5% 59% 16% 25%
1	M4	386	 5% 63% 13% 23%
1	N4	386	 5% 62% 15% 23%
1	O4	386	 5% 61% 16% 23%
1	P4	386	 5% 63% 13% 23%
1	Q4	386	 5% 61% 15% 23%
1	R4	386	 5% 66% 11% 23%
1	S4	386	 6% 60% 15% 25%
1	T4	386	 5% 61% 14% 25%
1	U4	386	 5% 62% 13% 25%
1	V4	386	 5% 61% 14% 25%
1	W4	386	 6% 59% 16% 25%
1	X4	386	 5% 67% 10% 23%
1	Y4	386	 5% 65% 12% 23%
1	Z4	386	 5% 63% 14% 23%
2	A1	84	 7% 74% 26%
2	A2	84	 17% 64% 36%
2	A3	84	 23% 68% 32%
2	B2	84	 23% 65% 35%

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Mol	Chain	Length	Quality of chain
2	B3	84	<p>19% 65% 35%</p>
2	C2	84	<p>27% 68% 32%</p>
2	C3	84	<p>26% 68% 32%</p>
2	D2	84	<p>24% 69% 31%</p>
2	D3	84	<p>21% 67% 33%</p>
2	E2	84	<p>26% 71% 29%</p>
2	E3	84	<p>15% 69% 31%</p>
3	F2	325	<p>97%</p>
3	F3	325	<p>97%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 70638 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 Major capsid protein Rcc01687.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C5	297	2209	1400	377	426	6	0	0
1	X4	297	2209	1400	377	426	6	0	0
1	Y4	297	2209	1400	377	426	6	0	0
1	Z4	297	2209	1400	377	426	6	0	0
1	A5	297	2209	1400	377	426	6	0	0
1	B5	271	2018	1284	345	383	6	0	0
1	N4	297	2209	1400	377	426	6	0	0
1	R4	297	2209	1400	377	426	6	0	0
1	M4	297	2209	1400	377	426	6	0	0
1	Q4	297	2209	1400	377	426	6	0	0
1	O4	297	2209	1400	377	426	6	0	0
1	P4	297	2209	1400	377	426	6	0	0
1	W4	291	2173	1379	371	417	6	0	0
1	U4	291	2173	1379	371	417	6	0	0
1	T4	291	2173	1379	371	417	6	0	0
1	S4	291	2173	1379	371	417	6	0	0
1	K4	291	2173	1379	371	417	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	V4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	L4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	H4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	I4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	A4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	D4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	E4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	F4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	G4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	B4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	C4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		

- Molecule 2 is a protein called Head spike base Rcc01079.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	D3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	C3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	B3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A1	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	E2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	C2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	B2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		

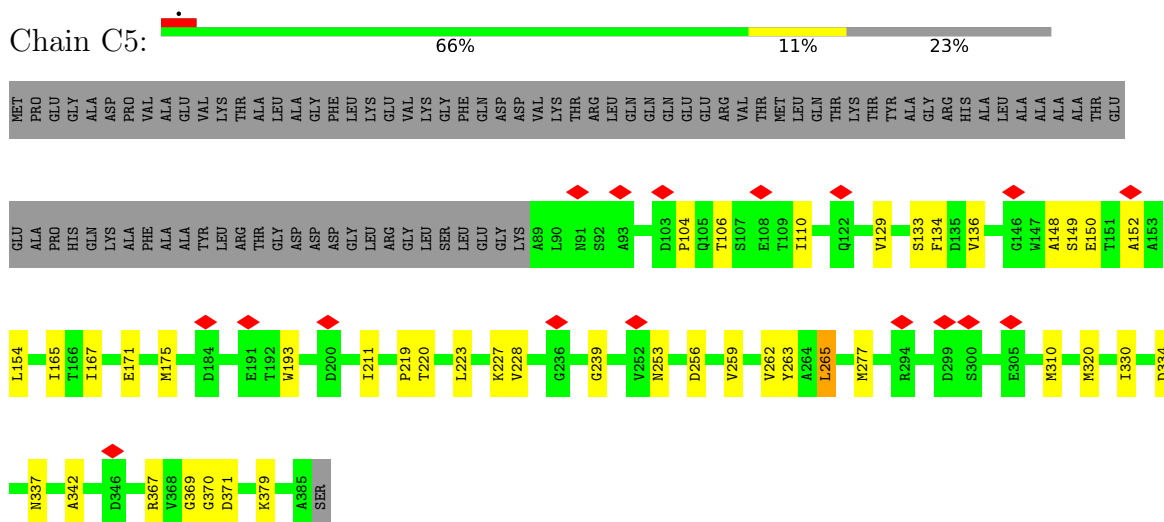
- Molecule 3 is a protein called Head spike fiber Rcc01080.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F3	10	Total	C	N	O	0	0
			62	42	10	10		
3	F2	10	Total	C	N	O	0	0
			62	42	10	10		

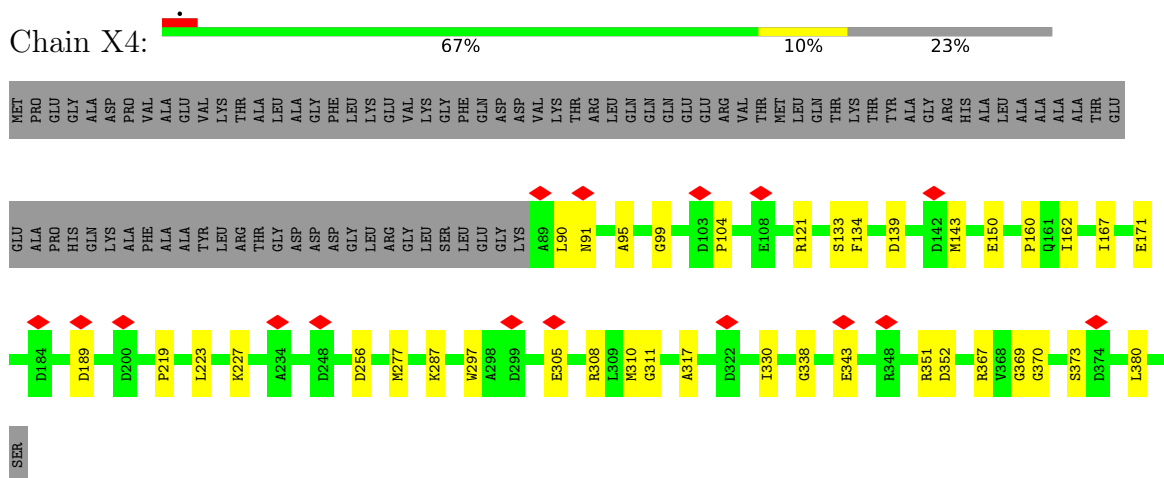
3 Residue-property plots [i](#)

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

- Molecule 1: Major capsid protein Rcc01687

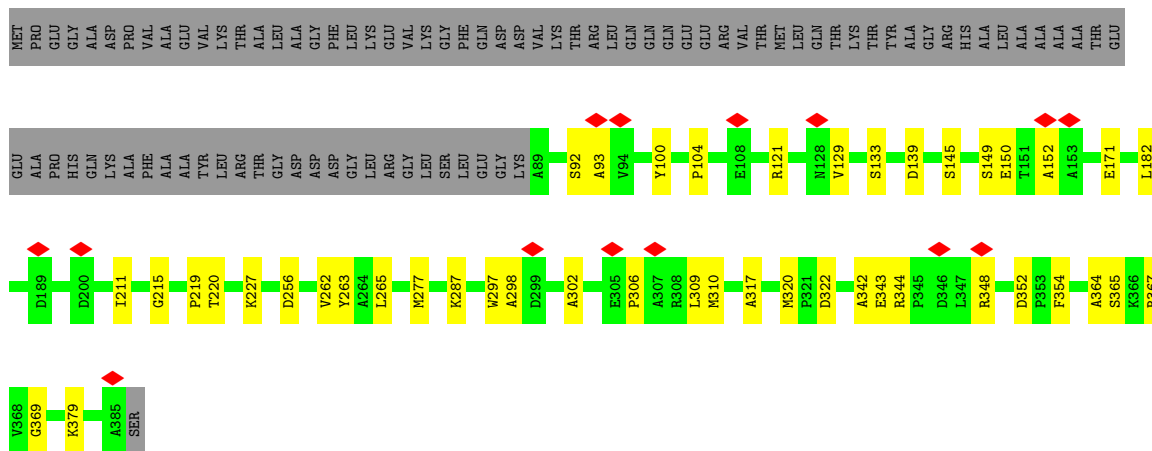


- Molecule 1: Major capsid protein Rcc01687

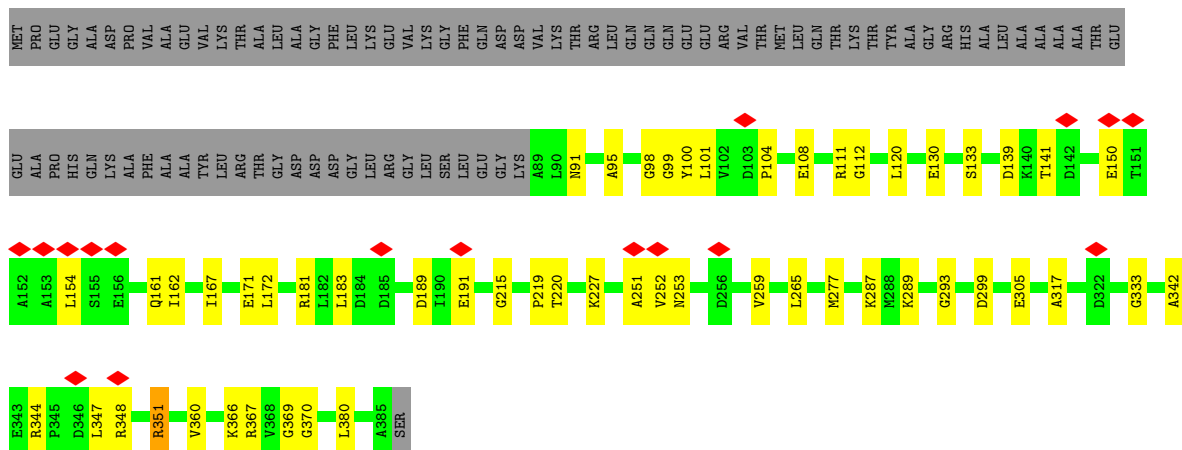


- Molecule 1: Major capsid protein Rcc01687

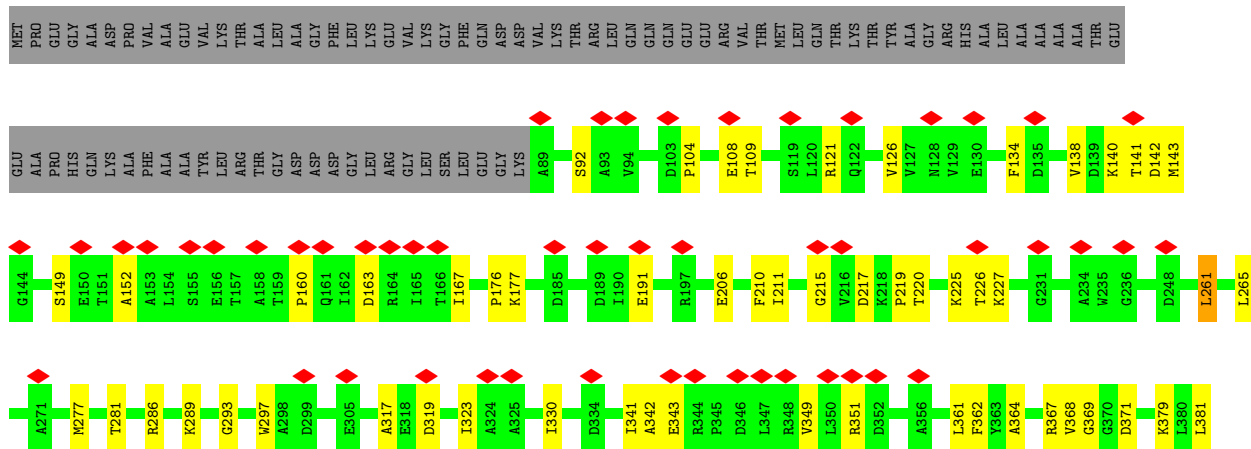


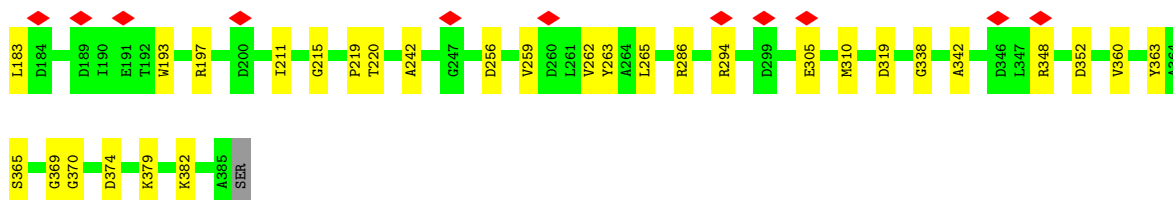


• Molecule 1: Major capsid protein Rcc01687



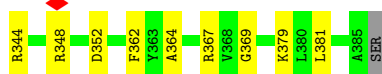
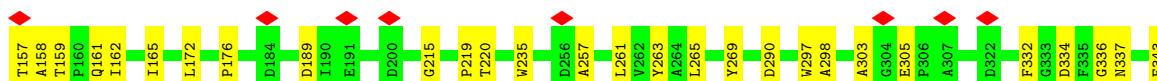
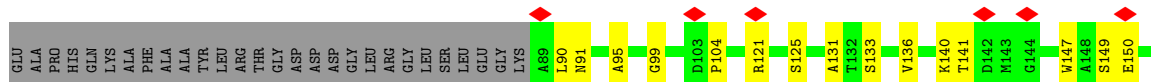
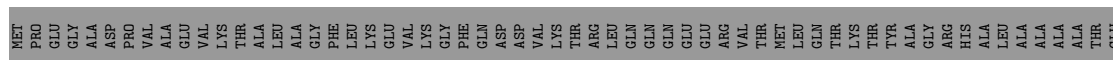
• Molecule 1: Major capsid protein Rcc01687





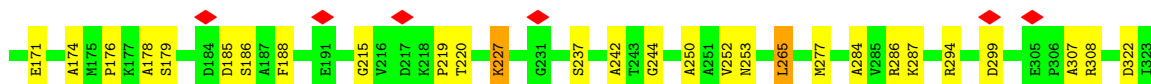
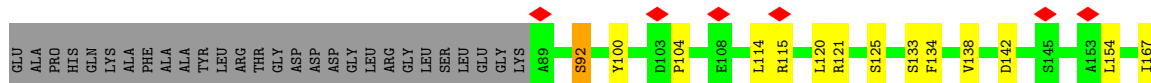
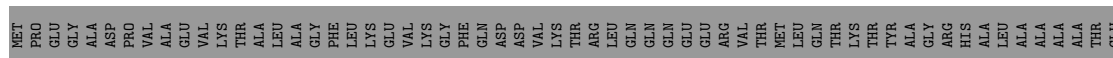
- Molecule 1: Major capsid protein Rcc01687

Chain M4: 63% 13% 23%



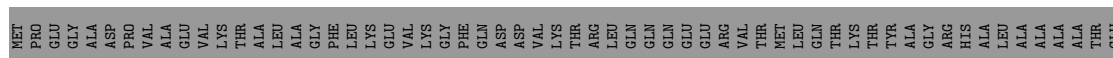
- Molecule 1: Major capsid protein Rcc01687

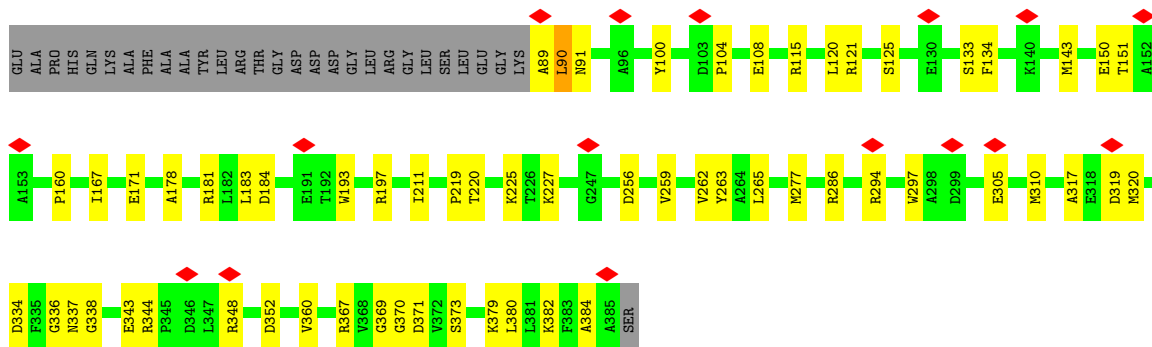
Chain Q4: 61% 15% 23%



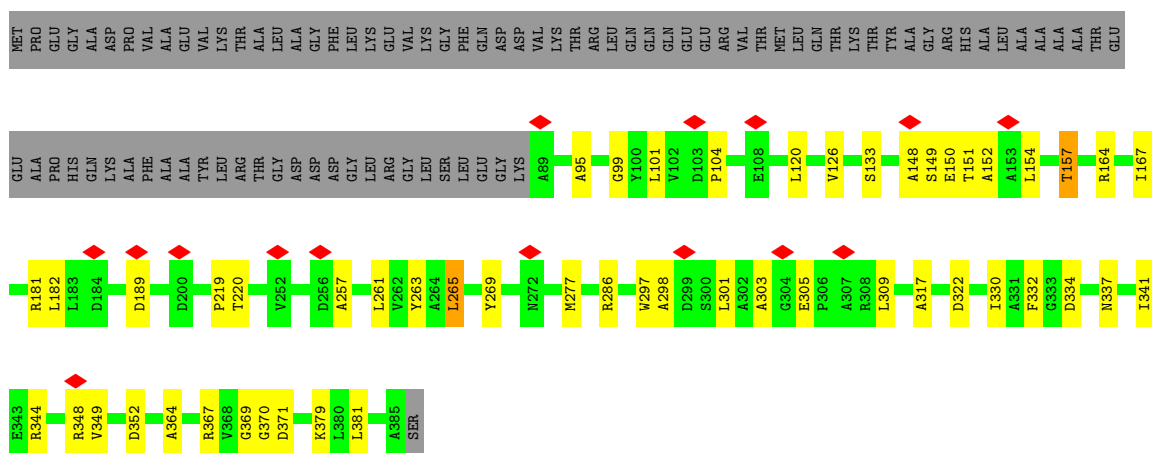
- Molecule 1: Major capsid protein Rcc01687

Chain O4: 61% 16% 23%

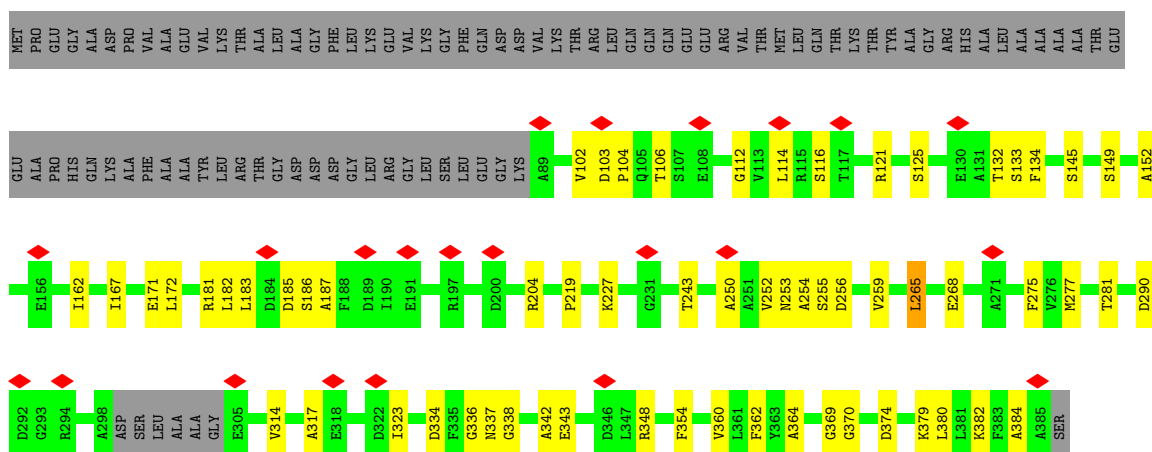




• Molecule 1: Major capsid protein Rcc01687

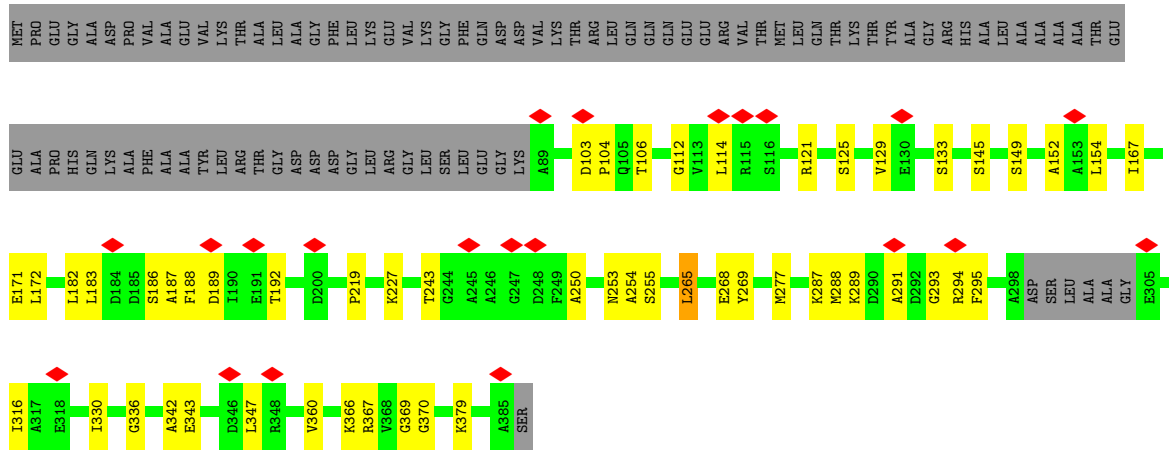


• Molecule 1: Major capsid protein Rcc01687

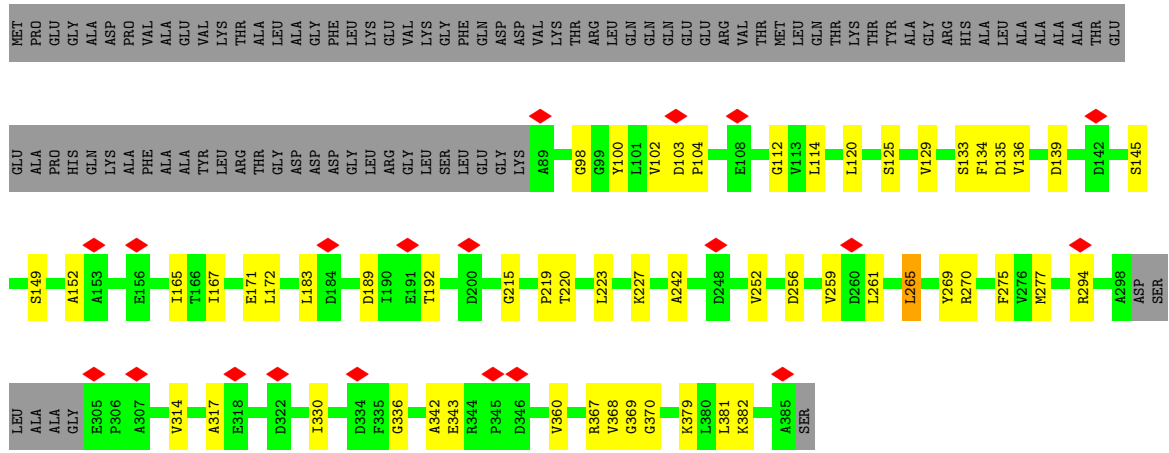


• Molecule 1: Major capsid protein Rcc01687

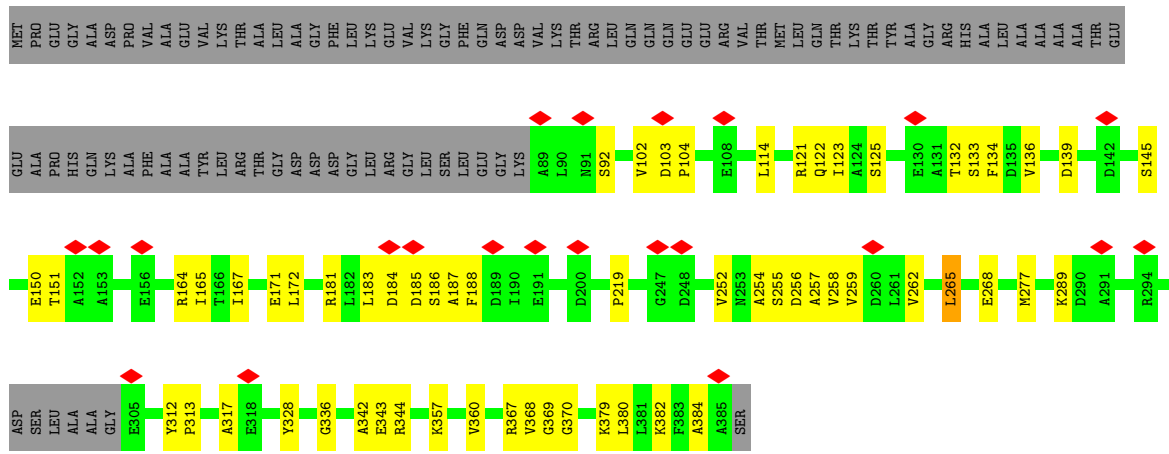




• Molecule 1: Major capsid protein Rcc01687



• Molecule 1: Major capsid protein Rcc01687



• Molecule 1: Major capsid protein Rcc01687

Chain K4:



MET PRO GLU GLY ALA ASP PRO VAL ASP THR LYS VAL THR ALA LEU ASP PHE LEU LYS VAL GLY ASP ASP VAL THR ARG LEU GLN ASP VAL LYS ARG LEU THR ARG GLN GLN GLN GLU ARG VAL MET LEU THR LYS THR THR ALA GLY ARG HIS ALA LEU ALA ALA ALA THR GLU

GLU ALA PRO HIS GLN LYS ALA PHE ALA VAL TYR ARG THR GLY ASP ASP GLY ARG VAL GLY ASP ASP VAL THR MET LEU THR LYS THR TYR ALA GLY ARG HIS ALA LEU ALA ALA THR GLU

A152 A153 L154 R164 I167 E171 R181 L182 L183 D184 S186 A187 F188 D189 I190 E191 G215 P219 T220 L223 K227 D248 A251 A254 S255 D256 V259 D260 L261 L265 E268 F275 V276 M277 T281 M288 A291 R294 A298

ASP SER ALA ALA GLY E305 A307 R308 G311 V314 A317 E318 I323 A324 A327 G336 T340 I341 E342 E343 R348 V360 Y363 R367 V368 G369 G370 K379 A385 SER

- Molecule 1: Major capsid protein Rcc01687

Chain J4:



MET PRO GLU GLY ALA ASP PRO VAL ASP THR LYS VAL THR ALA LEU ASP PHE LEU LYS VAL GLY ASP ASP VAL THR ARG LEU GLN ASP VAL LYS ARG LEU THR ARG GLN GLN GLN GLU ARG VAL MET LEU THR LYS THR THR ALA GLY ARG HIS ALA LEU ALA ALA THR GLU

GLU ALA PRO HIS GLN LYS ALA PHE ALA VAL TYR ARG THR GLY ASP ASP GLY ARG VAL GLY ASP ASP VAL THR MET LEU THR LYS THR TYR ALA GLY ARG HIS ALA LEU ALA ALA THR GLU

L164 I162 D163 R164 I167 E171 L172 L183 D184 S186 A187 F188 E191 D200 P219 A242 A245 D248 V252 N253 A254 S255 D256 A257 V258 V259 D260 L265 M277 V285 M288 K289 G293 R294 A298 SER A131 L132 S133 F134 D135

R308 L309 M310 G311 I316 A317 A324 A327 G336 R337 G338 Y339 T340 T341 E342 E343 R344 F345 D346 V360 R367 V368 G369 G370 D374 K379 K382 A385 SER

- Molecule 1: Major capsid protein Rcc01687

Chain V4:



MET PRO GLU GLY ALA ASP PRO VAL ASP THR LYS VAL THR ALA LEU ASP PHE LEU LYS VAL GLY ASP ASP VAL THR ARG LEU GLN ASP VAL LYS ARG LEU THR ARG GLN GLN GLN GLU ARG VAL MET LEU THR LYS THR THR ALA GLY ARG HIS ALA LEU ALA ALA THR GLU

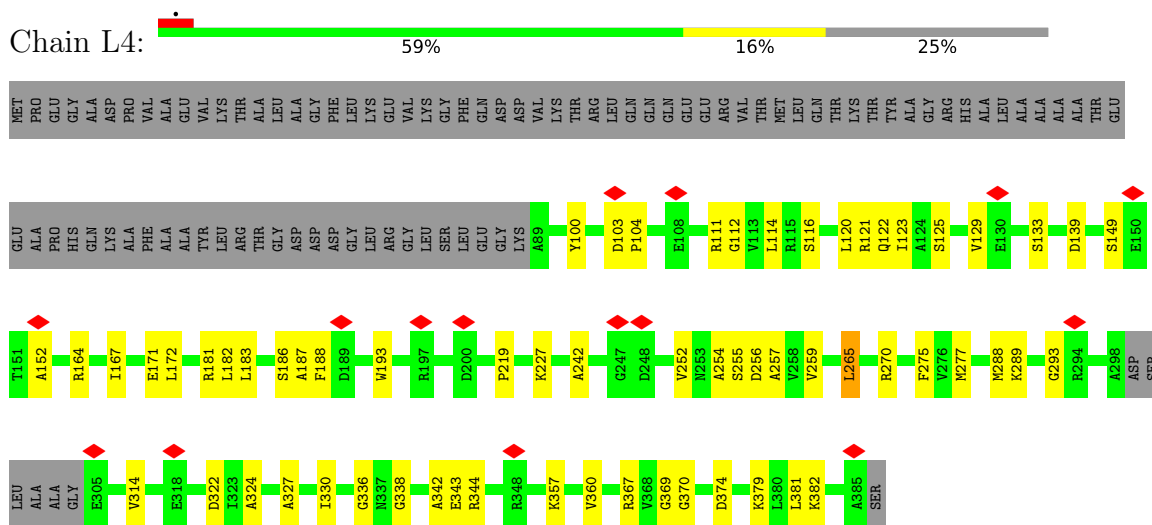
GLU ALA PRO HIS GLN LYS ALA PHE ALA VAL TYR ARG THR GLY ASP ASP GLY ARG VAL GLY ASP ASP VAL THR MET LEU THR LYS THR TYR ALA GLY ARG HIS ALA LEU ALA ALA THR GLU

L183 D184 D185 S186 A187 F188 D189 I190 E191 D200 P219 L223 K227 G236 D248 A254 S255 L265 E268 Y269 F275 V276 M277 M288 K289 R294 A298 SER ASP LEU ALA ALA GLY E305 R308 G311 V314 A317 E318 D322 I323

A324 A327 Y328 G336 A342 E343 R348 V360 Y363 A364 R367 V368 G369 G370 D374 K379 L380 L381 K382 F383 A384 A385 SER

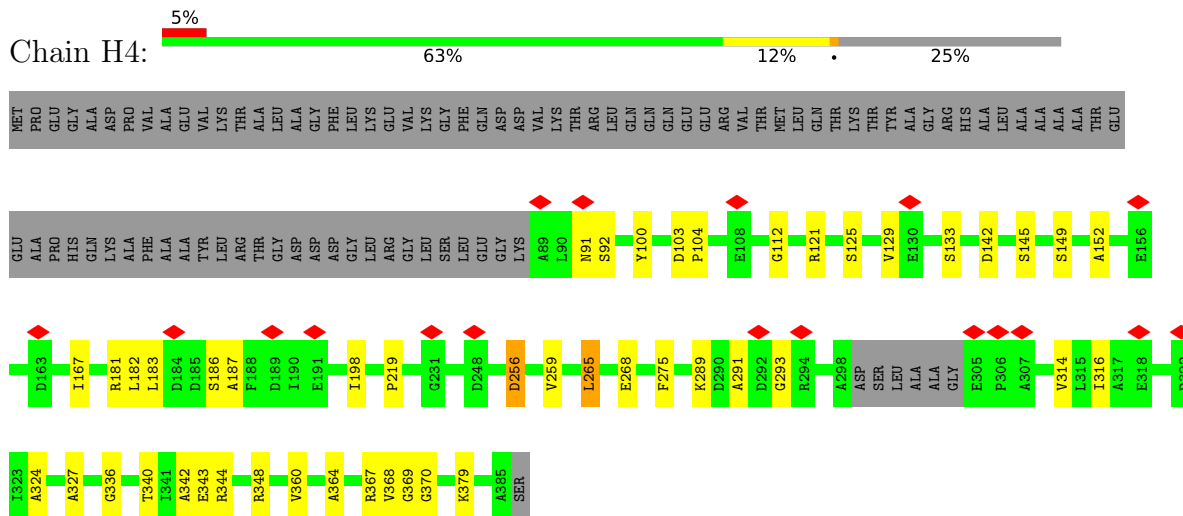
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Chain L4:



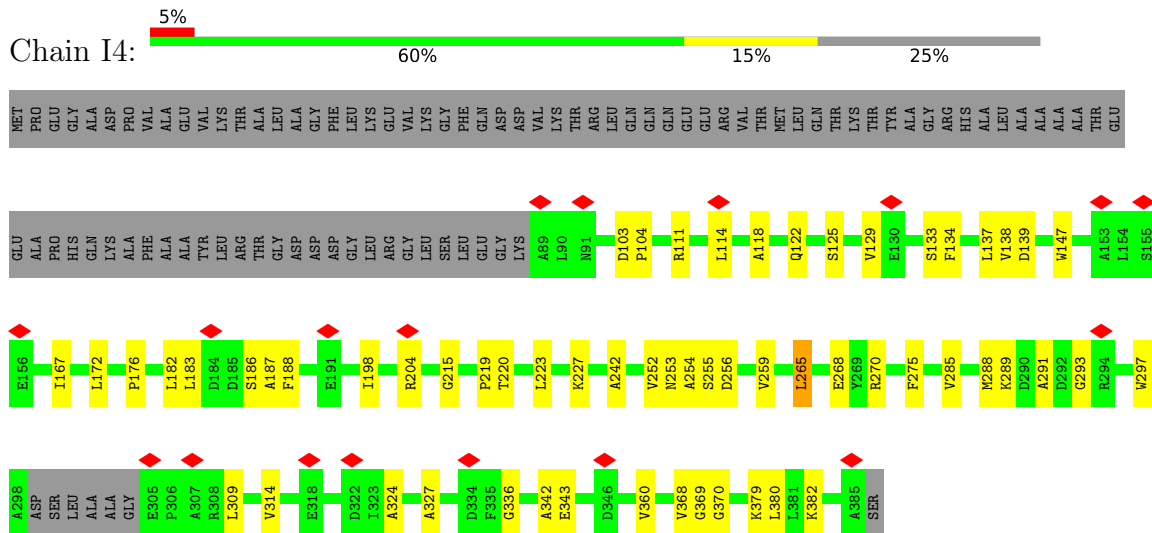
• Molecule 1: Major capsid protein Rcc01687

Chain H4:

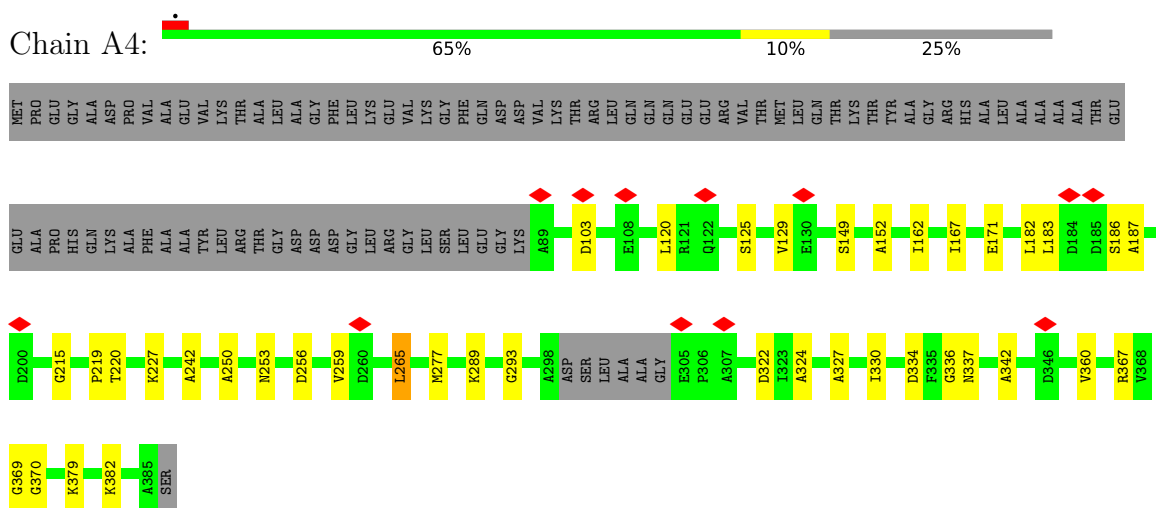


• Molecule 1: Major capsid protein Rcc01687

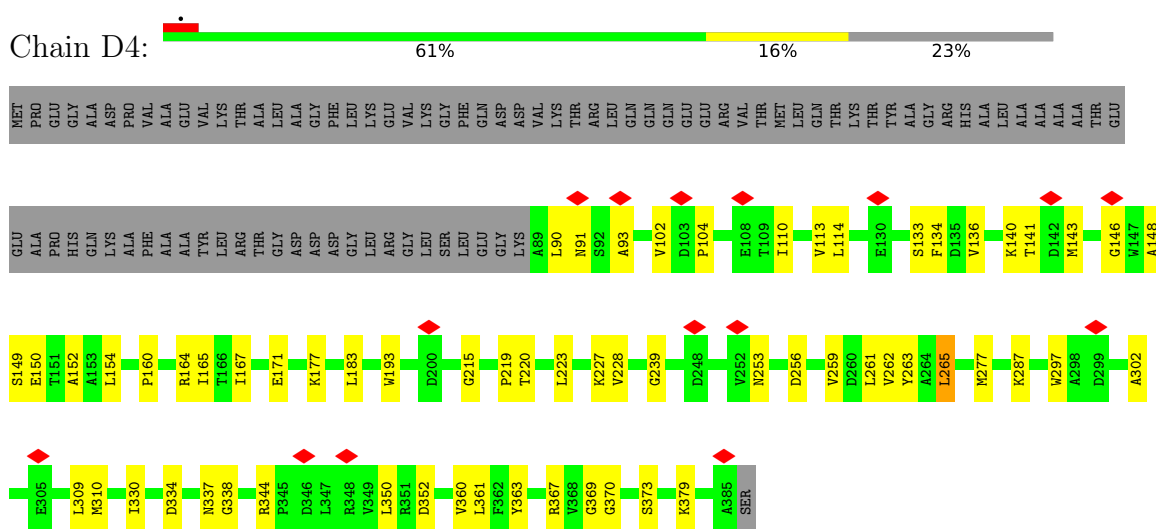
Chain I4:



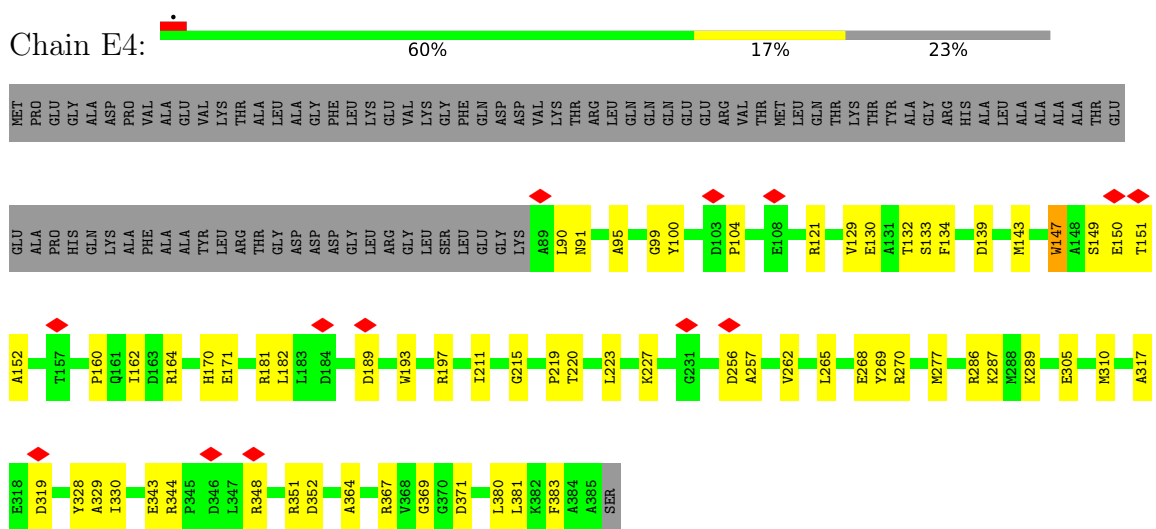
• Molecule 1: Major capsid protein Rcc01687



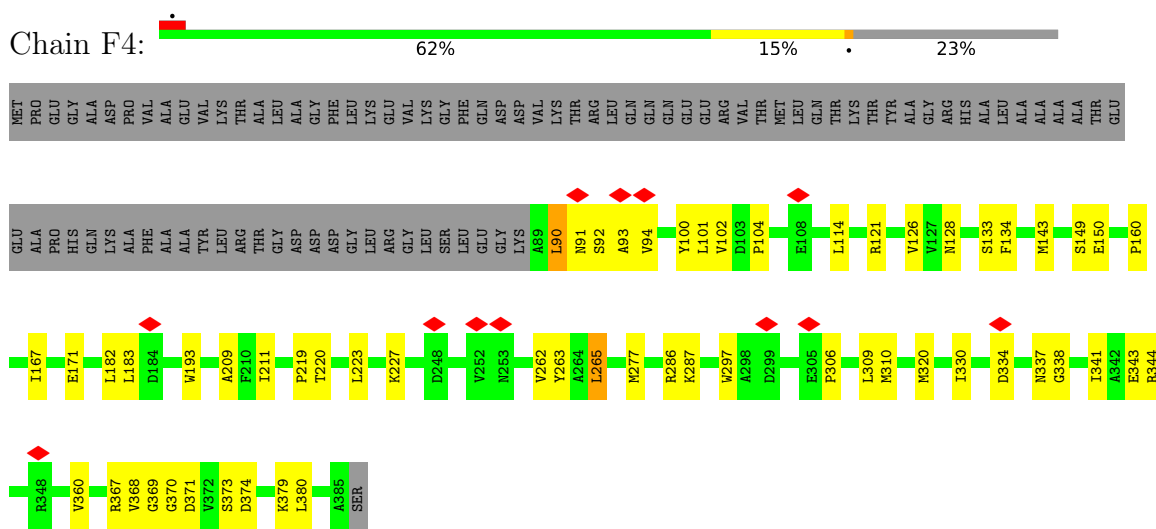
• Molecule 1: Major capsid protein Rcc01687



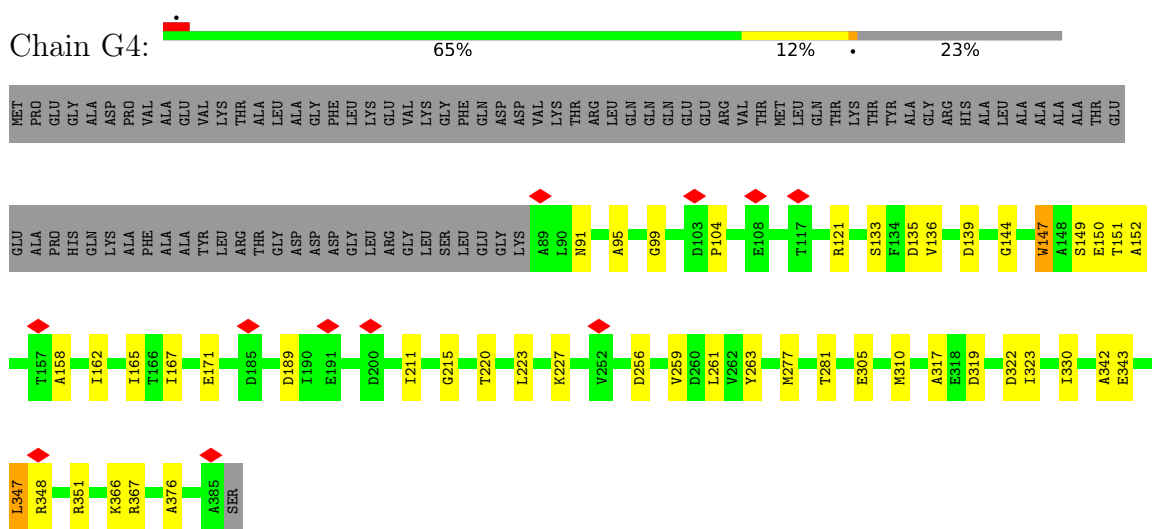
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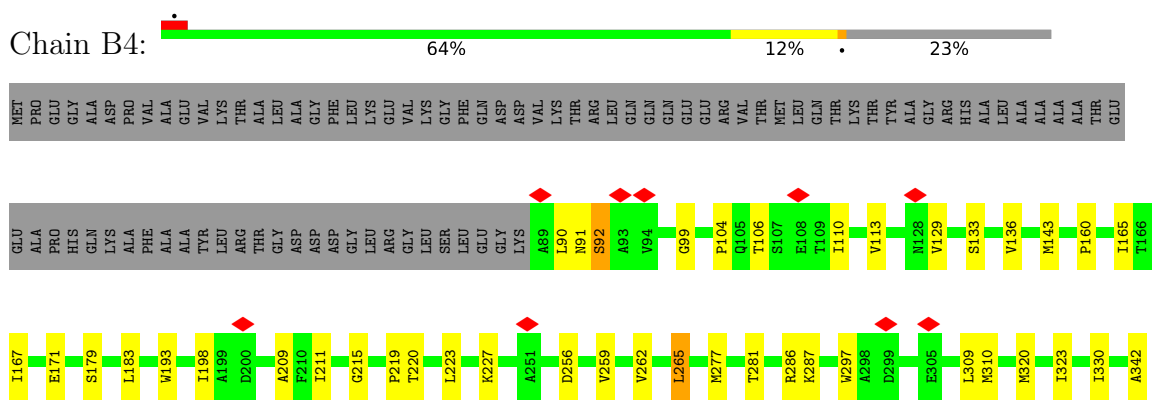
• Molecule 1: Major capsid protein Rcc01687

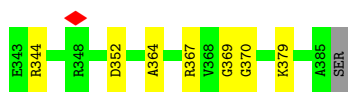


• Molecule 1: Major capsid protein Rcc01687

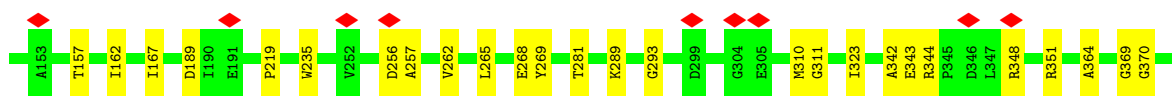
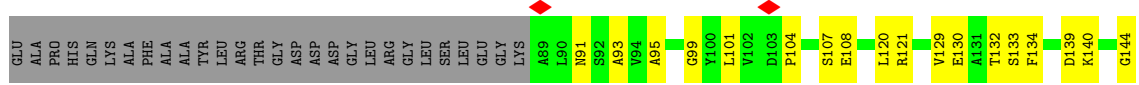
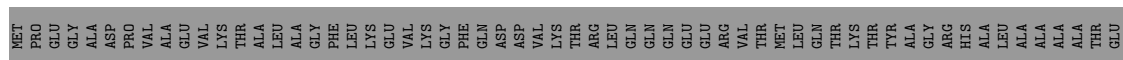


• Molecule 1: Major capsid protein Rcc01687





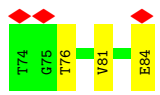
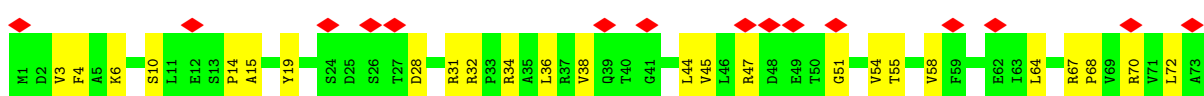
• Molecule 1: Major capsid protein Rcc01687



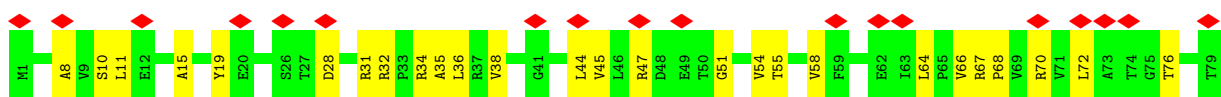
• Molecule 2: Head spike base Rcc01079



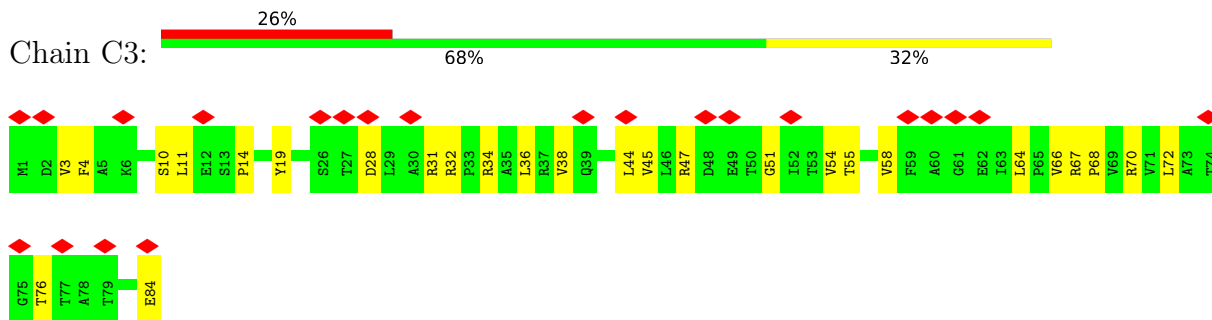
• Molecule 2: Head spike base Rcc01079



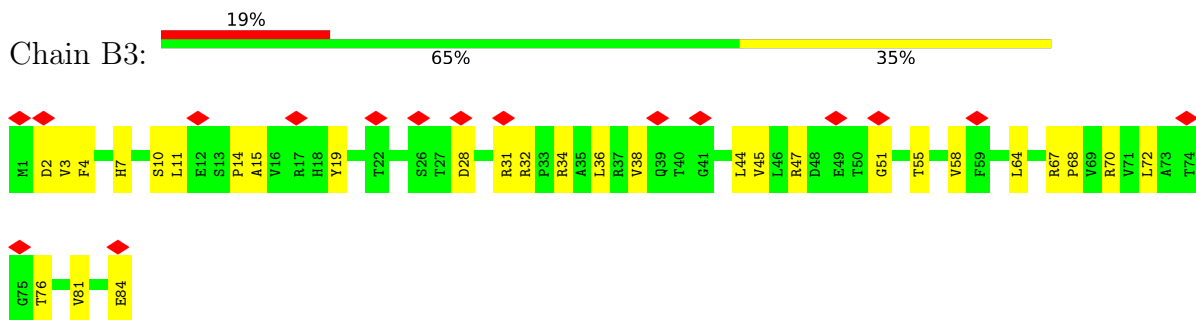
• Molecule 2: Head spike base Rcc01079



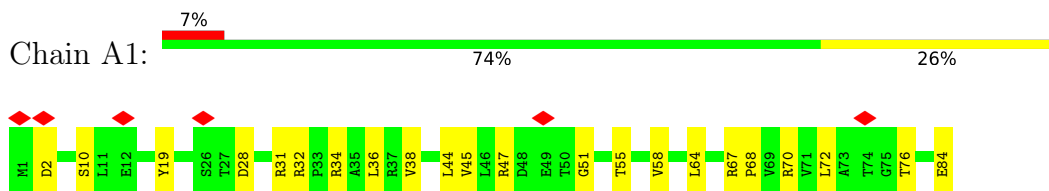
• Molecule 2: Head spike base Rcc01079



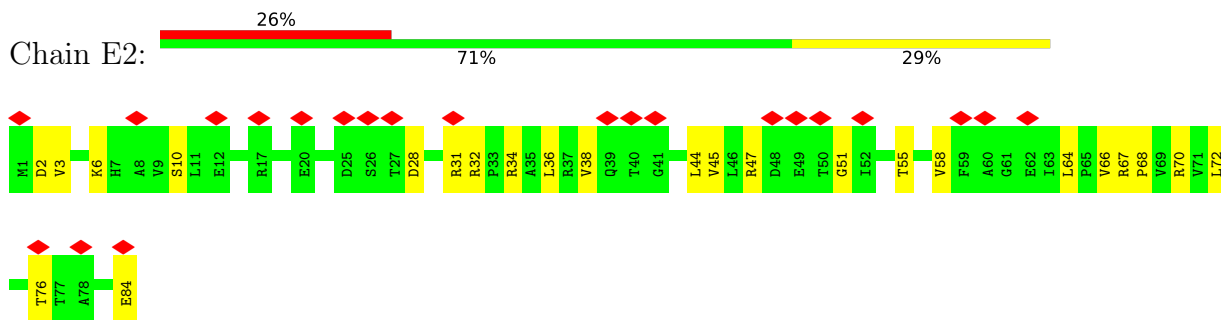
• Molecule 2: Head spike base Rcc01079



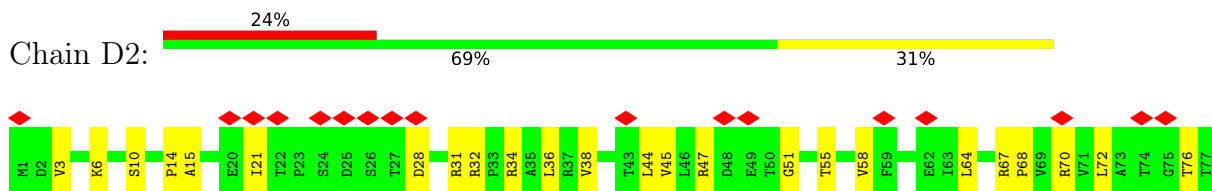
• Molecule 2: Head spike base Rcc01079



• Molecule 2: Head spike base Rcc01079




• Molecule 2: Head spike base Rcc01079



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• Molecule 3: Head spike fiber Rcc01080

Chain F2:  97%


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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	39403	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 ($e^-/\text{\AA}^2$)	42.75	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.491	Depositor
Minimum map value	-0.292	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.103	Depositor
Map size (Å)	544.256, 544.256, 544.256	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A4	0.44	0/2216	0.67	3/3012 (0.1%)
1	A5	0.38	0/2253	0.67	1/3064 (0.0%)
1	B4	0.42	0/2253	0.66	1/3064 (0.0%)
1	B5	0.43	0/2059	0.66	1/2797 (0.0%)
1	C4	0.43	0/2253	0.65	1/3064 (0.0%)
1	C5	0.40	0/2253	0.67	1/3064 (0.0%)
1	D4	0.43	0/2253	0.68	1/3064 (0.0%)
1	E4	0.43	0/2253	0.65	1/3064 (0.0%)
1	F4	0.42	0/2253	0.66	2/3064 (0.1%)
1	G4	0.42	0/2253	0.65	1/3064 (0.0%)
1	H4	0.42	0/2216	0.65	2/3012 (0.1%)
1	I4	0.41	0/2216	0.66	2/3012 (0.1%)
1	J4	0.41	0/2216	0.65	2/3012 (0.1%)
1	K4	0.42	1/2216 (0.0%)	0.66	2/3012 (0.1%)
1	L4	0.42	0/2216	0.67	3/3012 (0.1%)
1	M4	0.41	0/2253	0.67	0/3064
1	N4	0.42	0/2253	0.69	1/3064 (0.0%)
1	O4	0.42	0/2253	0.68	2/3064 (0.1%)
1	P4	0.40	0/2253	0.70	2/3064 (0.1%)
1	Q4	0.42	0/2253	0.71	3/3064 (0.1%)
1	R4	0.42	0/2253	0.66	0/3064
1	S4	0.41	0/2216	0.68	2/3012 (0.1%)
1	T4	0.41	0/2216	0.65	3/3012 (0.1%)
1	U4	0.41	0/2216	0.66	2/3012 (0.1%)
1	V4	0.41	0/2216	0.66	2/3012 (0.1%)
1	W4	0.41	0/2216	0.66	2/3012 (0.1%)
1	X4	0.40	0/2253	0.64	0/3064
1	Y4	0.40	0/2253	0.65	0/3064
1	Z4	0.39	0/2253	0.65	1/3064 (0.0%)
2	A1	0.43	0/652	0.65	1/892 (0.1%)
2	A2	0.43	0/652	0.65	1/892 (0.1%)
2	A3	0.43	0/652	0.65	1/892 (0.1%)
2	B2	0.43	0/652	0.65	1/892 (0.1%)
2	B3	0.43	0/652	0.65	1/892 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C2	0.43	0/652	0.65	1/892 (0.1%)
2	C3	0.43	0/652	0.65	1/892 (0.1%)
2	D2	0.43	0/652	0.65	1/892 (0.1%)
2	D3	0.43	0/652	0.65	1/892 (0.1%)
2	E2	0.43	0/652	0.65	1/892 (0.1%)
2	E3	0.43	0/652	0.65	1/892 (0.1%)
3	F2	0.40	0/61	1.43	2/81 (2.5%)
3	F3	0.41	0/61	1.42	2/81 (2.5%)
All	All	0.42	1/72030 (0.0%)	0.67	59/97991 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K4	251	ALA	C-N	-5.36	1.21	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A5	217	ASP	CB-CG-OD1	8.07	125.56	118.30
1	L4	265	LEU	CA-CB-CG	7.04	131.50	115.30
3	F2	8	LEU	CA-CB-CG	6.92	131.20	115.30
3	F3	8	LEU	CA-CB-CG	6.91	131.20	115.30
1	S4	265	LEU	CA-CB-CG	6.88	131.12	115.30
1	U4	265	LEU	CA-CB-CG	6.79	130.92	115.30
1	F4	90	LEU	CA-CB-CG	6.63	130.55	115.30
1	I4	265	LEU	CA-CB-CG	6.58	130.43	115.30
1	K4	265	LEU	CA-CB-CG	6.55	130.37	115.30
1	H4	103	ASP	CB-CG-OD1	6.48	124.13	118.30
1	W4	265	LEU	CA-CB-CG	6.41	130.05	115.30
1	K4	103	ASP	CB-CG-OD1	6.37	124.04	118.30
1	J4	265	LEU	CA-CB-CG	6.26	129.70	115.30
1	H4	265	LEU	CA-CB-CG	6.24	129.66	115.30
1	L4	103	ASP	CB-CG-OD1	6.24	123.92	118.30
1	V4	103	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D4	265	LEU	CA-CB-CG	6.17	129.49	115.30
1	C5	265	LEU	CA-CB-CG	6.15	129.44	115.30
1	T4	103	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A4	265	LEU	CA-CB-CG	6.09	129.30	115.30
1	E4	371	ASP	CB-CG-OD1	6.08	123.78	118.30
1	P4	120	LEU	CA-CB-CG	6.01	129.13	115.30
1	N4	265	LEU	CA-CB-CG	5.95	128.98	115.30
1	J4	103	ASP	CB-CG-OD1	5.92	123.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q4	361	LEU	CA-CB-CG	5.89	128.85	115.30
1	T4	265	LEU	CA-CB-CG	5.87	128.81	115.30
1	V4	265	LEU	CA-CB-CG	5.82	128.68	115.30
2	A2	64	LEU	CA-CB-CG	5.79	128.62	115.30
1	S4	103	ASP	CB-CG-OD1	5.79	123.51	118.30
2	A3	64	LEU	CA-CB-CG	5.79	128.61	115.30
2	A1	64	LEU	CA-CB-CG	5.76	128.56	115.30
2	D2	64	LEU	CA-CB-CG	5.76	128.55	115.30
2	B3	64	LEU	CA-CB-CG	5.76	128.54	115.30
2	E3	64	LEU	CA-CB-CG	5.75	128.53	115.30
2	D3	64	LEU	CA-CB-CG	5.75	128.53	115.30
1	Q4	265	LEU	CA-CB-CG	5.75	128.52	115.30
2	E2	64	LEU	CA-CB-CG	5.75	128.52	115.30
2	C2	64	LEU	CA-CB-CG	5.75	128.52	115.30
2	B2	64	LEU	CA-CB-CG	5.75	128.51	115.30
2	C3	64	LEU	CA-CB-CG	5.74	128.50	115.30
1	A4	103	ASP	CB-CG-OD1	5.68	123.41	118.30
1	Z4	120	LEU	CA-CB-CG	5.66	128.32	115.30
1	B4	265	LEU	CA-CB-CG	5.64	128.28	115.30
1	Q4	120	LEU	CA-CB-CG	5.60	128.18	115.30
1	F4	265	LEU	CA-CB-CG	5.59	128.16	115.30
1	U4	103	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A4	120	LEU	CA-CB-CG	5.55	128.06	115.30
3	F3	6	LEU	CA-CB-CG	5.54	128.03	115.30
3	F2	6	LEU	CA-CB-CG	5.54	128.03	115.30
1	I4	103	ASP	CB-CG-OD1	5.52	123.27	118.30
1	W4	103	ASP	CB-CG-OD1	5.46	123.22	118.30
1	C4	120	LEU	CA-CB-CG	5.44	127.81	115.30
1	B5	120	LEU	CA-CB-CG	5.40	127.71	115.30
1	T4	120	LEU	CA-CB-CG	5.32	127.53	115.30
1	O4	120	LEU	CA-CB-CG	5.22	127.31	115.30
1	G4	347	LEU	CA-CB-CG	5.17	127.20	115.30
1	P4	265	LEU	CA-CB-CG	5.14	127.13	115.30
1	O4	90	LEU	CA-CB-CG	5.13	127.09	115.30
1	L4	120	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A4	2173	0	2142	23	0
1	A5	2209	0	2176	41	0
1	B4	2209	0	2176	31	0
1	B5	2018	0	1995	48	0
1	C4	2209	0	2176	33	0
1	C5	2209	0	2176	30	0
1	D4	2209	0	2176	46	0
1	E4	2209	0	2176	56	0
1	F4	2209	0	2176	50	0
1	G4	2209	0	2176	39	0
1	H4	2173	0	2142	32	0
1	I4	2173	0	2142	45	0
1	J4	2173	0	2142	45	0
1	K4	2173	0	2142	46	0
1	L4	2173	0	2142	50	0
1	M4	2209	0	2176	37	0
1	N4	2209	0	2176	45	0
1	O4	2209	0	2176	46	0
1	P4	2209	0	2176	40	0
1	Q4	2209	0	2176	42	0
1	R4	2209	0	2176	29	0
1	S4	2173	0	2142	46	0
1	T4	2173	0	2142	39	0
1	U4	2173	0	2142	35	0
1	V4	2173	0	2142	40	0
1	W4	2173	0	2142	49	0
1	X4	2209	0	2176	30	0
1	Y4	2209	0	2176	35	0
1	Z4	2209	0	2176	40	0
2	A1	640	0	653	13	0
2	A2	640	0	653	24	0
2	A3	640	0	653	20	0
2	B2	640	0	653	24	0
2	B3	640	0	653	23	0
2	C2	640	0	653	18	0
2	C3	640	0	653	20	0
2	D2	640	0	653	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D3	640	0	653	23	0
2	E2	640	0	653	17	0
2	E3	640	0	653	17	0
3	F2	62	0	73	1	0
3	F3	62	0	73	1	0
All	All	70638	0	69878	1120	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 8.

All (1120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K4:305:GLU:HB2	1:K4:306:PRO:HD3	1.47	0.94
1:L4:252:VAL:HG11	2:B2:3:VAL:HG13	1.59	0.84
1:B5:357:LYS:HE2	1:B5:357:LYS:HA	1.60	0.83
1:N4:182:LEU:HB2	1:F4:92:SER:HB2	1.61	0.83
1:B5:177:LYS:HB2	1:B5:359:HIS:HB3	1.59	0.82
1:G4:149:SER:HB3	1:G4:152:ALA:HB2	1.62	0.81
1:Q4:174:ALA:HA	1:P4:157:THR:HG21	1.62	0.81
1:Z4:251:ALA:O	1:Z4:252:VAL:HG22	1.81	0.80
1:E4:150:GLU:HG3	1:G4:91:ASN:HB2	1.61	0.80
1:M4:348:ARG:O	1:M4:364:ALA:HA	1.80	0.80
1:B5:357:LYS:N	1:B5:358:PRO:HD2	1.98	0.79
1:L4:256:ASP:HA	1:L4:259:VAL:HG12	1.65	0.78
1:A5:177:LYS:HG3	1:A5:361:LEU:HD13	1.64	0.78
1:T4:252:VAL:HG11	2:D3:3:VAL:CG1	2.15	0.76
1:P4:348:ARG:O	1:P4:364:ALA:HA	1.87	0.75
1:B5:357:LYS:HE2	1:B5:357:LYS:CA	2.18	0.73
1:T4:252:VAL:HG11	2:D3:3:VAL:HG13	1.72	0.70
1:B4:90:LEU:HD13	1:B4:91:ASN:HB2	1.72	0.70
1:G4:150:GLU:HG3	1:C4:91:ASN:HB2	1.73	0.70
1:C5:220:THR:HB	1:C5:371:ASP:HB3	1.73	0.69
1:J4:256:ASP:HA	1:J4:259:VAL:HG12	1.75	0.68
1:J4:252:VAL:HG11	2:E2:3:VAL:CG1	2.23	0.68
1:J4:252:VAL:HG11	2:E2:3:VAL:HG13	1.75	0.68
1:E4:348:ARG:O	1:E4:364:ALA:HA	1.93	0.68
1:A5:289:LYS:HB2	1:A5:289:LYS:NZ	2.08	0.67
1:U4:291:ALA:O	2:C3:10:SER:HB2	1.94	0.67
1:M4:157:THR:HG23	1:M4:158:ALA:H	1.58	0.67
1:F4:101:LEU:N	1:F4:101:LEU:HD12	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N4:367:ARG:HH22	1:L4:181:ARG:HG3	1.60	0.67
1:C4:348:ARG:O	1:C4:364:ALA:HA	1.94	0.66
1:W4:252:VAL:HG11	2:B3:3:VAL:CG1	2.25	0.66
1:R4:91:ASN:HB2	1:P4:150:GLU:OE1	1.95	0.66
1:B5:177:LYS:HB2	1:B5:359:HIS:CB	2.25	0.65
1:R4:104:PRO:HB3	1:Q4:133:SER:HB2	1.78	0.65
1:I4:254:ALA:O	1:I4:255:SER:OG	2.13	0.65
1:L4:289:LYS:HD2	2:A2:7:HIS:CE1	2.31	0.65
1:I4:252:VAL:HG11	2:D2:3:VAL:HG13	1.77	0.65
1:E4:149:SER:HB3	1:E4:152:ALA:HB2	1.78	0.65
1:C5:175:MET:CE	1:B5:155:SER:HA	2.27	0.65
1:U4:253:ASN:OD1	1:U4:253:ASN:O	2.15	0.65
1:A5:141:THR:HG22	1:A5:142:ASP:N	2.11	0.65
1:I4:256:ASP:HA	1:I4:259:VAL:HG12	1.79	0.64
1:S4:252:VAL:HG11	2:C3:3:VAL:HG13	1.78	0.64
1:Z4:150:GLU:HG2	1:Z4:154:LEU:HD23	1.80	0.64
1:R4:115:ARG:HH12	1:Q4:142:ASP:HB3	1.63	0.64
1:Q4:171:GLU:HG3	1:P4:148:ALA:HB3	1.80	0.64
1:D4:133:SER:HB2	1:E4:104:PRO:HB3	1.80	0.64
1:K4:167:ILE:HD12	1:K4:370:GLY:HA2	1.80	0.64
1:Z4:139:ASP:HA	1:Z4:162:ILE:HA	1.80	0.64
1:Z4:219:PRO:HG3	1:Z4:369:GLY:HA2	1.80	0.63
1:S4:150:GLU:HG3	1:S4:151:THR:HG23	1.81	0.63
1:R4:215:GLY:HA2	1:R4:220:THR:HG22	1.80	0.63
1:Y4:367:ARG:HH22	1:W4:181:ARG:HG3	1.64	0.63
1:T4:275:PHE:HB2	1:T4:314:VAL:HG22	1.81	0.62
1:A5:219:PRO:HG3	1:A5:368:VAL:O	2.00	0.62
1:L4:265:LEU:HD23	1:L4:379:LYS:HG2	1.82	0.62
1:A5:149:SER:HB3	1:A5:152:ALA:HB2	1.81	0.62
1:Q4:286:ARG:NH1	1:P4:263:TYR:OH	2.32	0.62
1:V4:254:ALA:O	1:V4:255:SER:OG	2.15	0.62
1:A4:265:LEU:HD23	1:A4:379:LYS:HG2	1.82	0.62
1:G4:147:TRP:HZ2	1:B4:209:ALA:HB2	1.65	0.62
1:S4:256:ASP:HA	1:S4:259:VAL:HG12	1.82	0.62
1:G4:139:ASP:HA	1:G4:162:ILE:HA	1.82	0.61
1:Z4:133:SER:HB2	1:A5:104:PRO:HB3	1.82	0.61
1:P4:219:PRO:HG3	1:P4:369:GLY:HA2	1.82	0.61
1:C5:219:PRO:HG3	1:C5:369:GLY:HA2	1.81	0.61
1:B5:350:LEU:HB2	1:B5:363:TYR:HB3	1.82	0.61
1:N4:133:SER:HB2	1:O4:104:PRO:HB3	1.82	0.61
1:N4:286:ARG:NH1	1:M4:263:TYR:OH	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:149:SER:HB2	1:L4:152:ALA:HB2	1.83	0.61
1:R4:219:PRO:HG3	1:R4:369:GLY:HA2	1.83	0.61
1:K4:102:VAL:HB	1:J4:132:THR:HG21	1.82	0.61
1:N4:182:LEU:HB2	1:F4:92:SER:CB	2.29	0.61
1:W4:256:ASP:HA	1:W4:259:VAL:HG12	1.83	0.61
1:T4:219:PRO:HG3	1:T4:369:GLY:HA2	1.82	0.61
1:K4:305:GLU:HB2	1:K4:306:PRO:CD	2.26	0.61
1:Q4:178:ALA:HB3	1:Q4:360:VAL:HB	1.83	0.61
1:W4:254:ALA:O	1:W4:255:SER:OG	2.14	0.61
1:L4:219:PRO:HG3	1:L4:369:GLY:HA2	1.83	0.61
1:H4:167:ILE:HD12	1:H4:370:GLY:HA2	1.83	0.61
1:Q4:284:ALA:HA	1:Q4:287:LYS:HD3	1.84	0.60
1:L4:252:VAL:HG11	2:B2:3:VAL:CG1	2.31	0.60
1:Y4:133:SER:HB2	1:Z4:104:PRO:HB3	1.83	0.60
1:N4:179:SER:HB2	1:D4:150:GLU:OE2	2.01	0.60
1:O4:344:ARG:NH1	1:S4:185:ASP:OD1	2.34	0.60
1:U4:145:SER:HB3	1:V4:172:LEU:HD11	1.82	0.60
1:R4:133:SER:HB2	1:M4:104:PRO:HB3	1.84	0.60
1:Z4:251:ALA:O	1:Z4:252:VAL:CG2	2.49	0.60
1:E4:132:THR:CG2	1:F4:102:VAL:HG22	2.31	0.60
1:W4:219:PRO:HG3	1:W4:369:GLY:HA2	1.82	0.60
1:V4:219:PRO:HG3	1:V4:369:GLY:HA2	1.84	0.60
1:K4:265:LEU:HD23	1:K4:379:LYS:HG2	1.82	0.60
1:W4:133:SER:HB2	1:S4:104:PRO:HB3	1.82	0.60
1:U4:133:SER:HB2	1:V4:104:PRO:HB3	1.83	0.59
1:K4:305:GLU:CB	1:K4:306:PRO:HD3	2.28	0.59
1:J4:167:ILE:HD12	1:J4:370:GLY:HA2	1.84	0.59
1:D4:223:LEU:O	1:D4:227:LYS:NZ	2.32	0.59
1:Z4:167:ILE:HD12	1:Z4:370:GLY:HA2	1.83	0.59
1:K4:219:PRO:HG3	1:K4:369:GLY:HA2	1.84	0.59
1:C5:175:MET:HE2	1:B5:155:SER:HA	1.83	0.59
1:Y4:344:ARG:HE	1:Y4:367:ARG:HD3	1.68	0.59
1:O4:219:PRO:HG3	1:O4:369:GLY:HA2	1.83	0.59
1:O4:352:ASP:OD2	1:S4:357:LYS:NZ	2.35	0.59
1:P4:349:VAL:O	1:P4:349:VAL:HG13	2.03	0.59
1:U4:104:PRO:HB3	1:T4:133:SER:HB2	1.83	0.59
1:S4:252:VAL:HG11	2:C3:3:VAL:CG1	2.32	0.59
1:G4:133:SER:HB2	1:B4:104:PRO:HB3	1.85	0.59
1:R4:178:ALA:HB3	1:R4:360:VAL:HB	1.82	0.59
1:X4:139:ASP:HA	1:X4:162:ILE:HA	1.85	0.59
1:B5:200:ASP:OD2	1:B5:204:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R4:262:VAL:HG21	1:R4:310:MET:HG2	1.84	0.59
1:M4:219:PRO:HG3	1:M4:369:GLY:HA2	1.85	0.59
1:O4:367:ARG:HH22	1:S4:181:ARG:HG3	1.67	0.59
1:P4:182:LEU:HB2	1:S4:92:SER:HB2	1.85	0.59
1:L4:256:ASP:CA	1:L4:259:VAL:HG12	2.31	0.59
1:I4:252:VAL:HG12	1:I4:253:ASN:HD22	1.67	0.58
1:F4:223:LEU:O	1:F4:227:LYS:NZ	2.33	0.58
1:C4:219:PRO:HG3	1:C4:369:GLY:HA2	1.85	0.58
1:C5:262:VAL:HG21	1:C5:310:MET:HG2	1.85	0.58
1:H4:275:PHE:HB2	1:H4:314:VAL:HG22	1.85	0.58
1:X4:133:SER:HB2	1:Y4:104:PRO:HB3	1.84	0.58
1:O4:178:ALA:HB3	1:O4:360:VAL:HB	1.84	0.58
2:D3:31:ARG:NH1	2:D3:84:GLU:OE1	2.37	0.58
2:A3:31:ARG:NH1	2:A3:84:GLU:OE1	2.37	0.58
1:R4:145:SER:HB3	1:M4:172:LEU:HD11	1.85	0.58
1:M4:261:LEU:HD22	1:M4:332:PHE:HB3	1.85	0.58
1:E4:147:TRP:CZ2	1:F4:209:ALA:HB2	2.37	0.58
2:D2:31:ARG:NH1	2:D2:84:GLU:OE1	2.37	0.58
1:T4:252:VAL:HG11	2:D3:3:VAL:HG11	1.84	0.58
1:S4:254:ALA:O	1:S4:255:SER:OG	2.18	0.58
2:E2:31:ARG:NH1	2:E2:84:GLU:OE1	2.37	0.58
1:J4:254:ALA:O	1:J4:255:SER:OG	2.21	0.58
2:C3:28:ASP:OD1	2:C3:70:ARG:NH1	2.37	0.58
2:B3:31:ARG:NH1	2:B3:84:GLU:OE1	2.37	0.58
2:A1:31:ARG:NH1	2:A1:84:GLU:OE1	2.37	0.58
1:R4:265:LEU:HD23	1:R4:379:LYS:HG2	1.86	0.58
2:E3:31:ARG:NH1	2:E3:84:GLU:OE1	2.37	0.58
2:D3:28:ASP:OD1	2:D3:70:ARG:NH1	2.37	0.58
2:C3:31:ARG:NH1	2:C3:84:GLU:OE1	2.37	0.58
2:A2:31:ARG:NH1	2:A2:84:GLU:OE1	2.37	0.58
2:C2:31:ARG:NH1	2:C2:84:GLU:OE1	2.37	0.58
2:A3:28:ASP:OD1	2:A3:70:ARG:NH1	2.37	0.58
1:Q4:171:GLU:CG	1:P4:148:ALA:HB3	2.34	0.57
1:M4:159:THR:HG21	1:F4:90:LEU:H	1.69	0.57
1:O4:171:GLU:HG2	1:S4:181:ARG:HH21	1.69	0.57
1:A4:167:ILE:HD12	1:A4:370:GLY:HA2	1.85	0.57
1:E4:149:SER:HB3	1:E4:152:ALA:CB	2.33	0.57
2:E2:28:ASP:OD1	2:E2:70:ARG:NH1	2.37	0.57
2:B2:28:ASP:OD1	2:B2:70:ARG:NH1	2.37	0.57
1:O4:184:ASP:OD2	1:K4:348:ARG:NH2	2.38	0.57
1:I4:167:ILE:HD12	1:I4:370:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D4:265:LEU:HD23	1:D4:379:LYS:HG2	1.86	0.57
1:F4:102:VAL:HG13	1:F4:102:VAL:O	2.05	0.57
1:X4:150:GLU:HG3	1:Z4:91:ASN:HB2	1.86	0.57
1:N4:244:GLY:HA3	1:N4:250:ALA:HB2	1.87	0.57
1:W4:252:VAL:HG11	2:B3:3:VAL:HG11	1.85	0.57
1:W4:334:ASP:OD2	1:W4:337:ASN:ND2	2.38	0.57
1:A4:219:PRO:HG3	1:A4:369:GLY:HA2	1.87	0.57
2:C2:28:ASP:OD1	2:C2:70:ARG:NH1	2.37	0.57
1:A5:191:GLU:OE1	1:A5:351:ARG:NH2	2.38	0.57
1:B5:154:LEU:HD13	1:B5:154:LEU:O	2.05	0.57
1:R4:286:ARG:HH12	1:R4:305:GLU:HA	1.69	0.57
1:E4:219:PRO:HG3	1:E4:369:GLY:HA2	1.87	0.57
1:B4:265:LEU:HD23	1:B4:379:LYS:HG2	1.86	0.57
2:A1:28:ASP:OD1	2:A1:70:ARG:NH1	2.37	0.57
1:N4:219:PRO:HG3	1:N4:369:GLY:HA2	1.86	0.57
2:D2:28:ASP:OD1	2:D2:70:ARG:NH1	2.37	0.57
1:V4:223:LEU:O	1:V4:227:LYS:NZ	2.34	0.57
2:B2:31:ARG:NH1	2:B2:84:GLU:OE1	2.37	0.57
1:C5:134:PHE:HB3	1:C5:167:ILE:HB	1.86	0.57
1:M4:176:PRO:HG2	1:M4:362:PHE:HB2	1.86	0.57
1:S4:219:PRO:HG3	1:S4:369:GLY:HA2	1.86	0.57
1:G4:223:LEU:O	1:G4:227:LYS:NZ	2.33	0.57
1:C4:130:GLU:O	1:C4:344:ARG:NH1	2.37	0.57
2:A2:28:ASP:OD1	2:A2:70:ARG:NH1	2.37	0.57
1:U4:289:LYS:HD3	1:U4:293:GLY:HA2	1.86	0.57
2:E3:28:ASP:OD1	2:E3:70:ARG:NH1	2.37	0.57
2:B3:28:ASP:OD1	2:B3:70:ARG:NH1	2.37	0.57
1:U4:149:SER:HB2	1:U4:152:ALA:HB2	1.85	0.56
1:S4:125:SER:OG	1:S4:336:GLY:O	2.22	0.56
1:J4:308:ARG:NH2	1:J4:311:GLY:O	2.38	0.56
1:A5:289:LYS:HB2	1:A5:289:LYS:HZ2	1.69	0.56
1:B5:257:ALA:HB1	1:B5:381:LEU:HD11	1.87	0.56
1:N4:177:LYS:HB2	1:F4:90:LEU:HD23	1.87	0.56
1:Q4:244:GLY:HA3	1:Q4:250:ALA:HB2	1.88	0.56
1:O4:256:ASP:HA	1:O4:259:VAL:HG12	1.87	0.56
1:A4:256:ASP:HA	1:A4:259:VAL:HG12	1.86	0.56
1:A5:261:LEU:HD13	1:A5:381:LEU:HD12	1.87	0.56
1:B5:167:ILE:HD12	1:B5:370:GLY:HA2	1.87	0.56
1:H4:181:ARG:HG3	1:D4:367:ARG:HH22	1.71	0.56
1:H4:265:LEU:HD23	1:H4:379:LYS:HG2	1.88	0.56
1:C5:256:ASP:HA	1:C5:259:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y4:171:GLU:OE1	1:Y4:348:ARG:NH1	2.39	0.56
1:C5:104:PRO:HB3	1:B5:133:SER:HB2	1.87	0.56
1:J4:288:MET:HA	2:D2:6:LYS:HB3	1.88	0.56
1:H4:219:PRO:HG3	1:H4:369:GLY:HA2	1.87	0.56
1:D4:136:VAL:HG22	1:D4:165:ILE:HB	1.88	0.56
1:O4:334:ASP:OD2	1:O4:337:ASN:ND2	2.39	0.56
1:X4:310:MET:H	1:Y4:302:ALA:HA	1.71	0.56
1:Q4:265:LEU:HD23	1:Q4:379:LYS:HG2	1.88	0.56
1:W4:102:VAL:HB	1:V4:132:THR:HG21	1.87	0.56
1:U4:219:PRO:HG3	1:U4:369:GLY:HA2	1.88	0.56
1:A5:289:LYS:HD2	1:A5:293:GLY:O	2.06	0.56
1:S4:164:ARG:NH1	1:K4:100:TYR:O	2.39	0.56
1:D4:215:GLY:HA2	1:D4:220:THR:HG22	1.88	0.56
1:C5:167:ILE:HD12	1:C5:370:GLY:HA2	1.88	0.56
1:E4:150:GLU:OE1	1:E4:150:GLU:HA	2.05	0.56
1:B4:219:PRO:HG3	1:B4:369:GLY:HA2	1.87	0.56
1:X4:121:ARG:NH1	1:X4:343:GLU:OE1	2.36	0.55
1:P4:261:LEU:HD22	1:P4:332:PHE:HB3	1.88	0.55
1:A5:215:GLY:HA2	1:A5:220:THR:HB	1.88	0.55
1:T4:172:LEU:HD11	1:S4:145:SER:HB3	1.89	0.55
1:U4:254:ALA:O	1:U4:255:SER:HB3	2.05	0.55
1:E4:133:SER:HB2	1:F4:104:PRO:HB3	1.88	0.55
1:B5:167:ILE:HG21	1:B5:342:ALA:HB3	1.87	0.55
1:N4:142:ASP:HB3	1:O4:115:ARG:HH12	1.71	0.55
1:O4:181:ARG:HH21	1:K4:171:GLU:HG2	1.72	0.55
1:U4:265:LEU:HD23	1:U4:379:LYS:HG2	1.87	0.55
1:F4:220:THR:HB	1:F4:371:ASP:HB3	1.87	0.55
1:W4:252:VAL:HG12	1:W4:253:ASN:HD22	1.72	0.55
1:S4:344:ARG:NH1	1:K4:185:ASP:OD1	2.39	0.55
1:Y4:262:VAL:HG21	1:Y4:310:MET:HG2	1.88	0.55
1:C4:265:LEU:HD21	1:C4:269:TYR:HB2	1.87	0.55
1:J4:183:LEU:HD22	1:J4:360:VAL:HG21	1.89	0.55
1:C5:334:ASP:OD2	1:C5:337:ASN:ND2	2.38	0.55
1:J4:256:ASP:CA	1:J4:259:VAL:HG12	2.37	0.55
1:R4:338:GLY:HA2	1:R4:374:ASP:HB3	1.88	0.55
1:T4:167:ILE:HD12	1:T4:370:GLY:HA2	1.88	0.55
1:U4:167:ILE:HD12	1:U4:370:GLY:HA2	1.88	0.54
1:N4:284:ALA:HA	1:N4:287:LYS:HD3	1.89	0.54
1:N4:334:ASP:OD2	1:N4:337:ASN:ND2	2.40	0.54
1:T4:102:VAL:HB	1:S4:132:THR:HG21	1.88	0.54
1:T4:134:PHE:HB3	1:T4:167:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S4:367:ARG:HH22	1:K4:181:ARG:HG3	1.71	0.54
1:J4:344:ARG:HE	1:J4:367:ARG:HD3	1.72	0.54
1:D4:219:PRO:HG3	1:D4:369:GLY:HA2	1.90	0.54
1:F4:265:LEU:HD23	1:F4:379:LYS:HG2	1.88	0.54
1:F4:334:ASP:OD2	1:F4:337:ASN:ND2	2.40	0.54
1:B4:133:SER:HB2	1:C4:104:PRO:HB3	1.88	0.54
1:T4:149:SER:HB2	1:T4:152:ALA:HB2	1.89	0.54
1:K4:254:ALA:O	1:K4:255:SER:HB3	2.08	0.54
1:J4:219:PRO:HG3	1:J4:369:GLY:HA2	1.89	0.54
1:F4:133:SER:HB2	1:G4:104:PRO:HB3	1.89	0.54
1:S4:265:LEU:HD23	1:S4:379:LYS:HG2	1.88	0.54
1:V4:288:MET:HA	2:E3:6:LYS:HB3	1.88	0.54
1:F4:92:SER:O	1:F4:94:VAL:N	2.40	0.54
1:W4:112:GLY:HA2	1:V4:139:ASP:H	1.71	0.54
1:Y4:211:ILE:HG21	1:Y4:320:MET:HG2	1.89	0.54
1:Z4:130:GLU:OE1	1:Z4:344:ARG:NH2	2.41	0.54
1:O4:262:VAL:HG21	1:O4:310:MET:HG2	1.88	0.54
1:I4:252:VAL:HG11	2:D2:3:VAL:CG1	2.37	0.54
1:R4:193:TRP:HE1	1:R4:197:ARG:HE	1.56	0.54
1:Q4:219:PRO:HG3	1:Q4:369:GLY:HA2	1.90	0.54
1:I4:125:SER:OG	1:I4:336:GLY:O	2.26	0.54
2:A1:32:ARG:NH2	2:A1:67:ARG:O	2.41	0.54
1:X4:308:ARG:NH1	1:X4:311:GLY:O	2.41	0.54
1:Y4:100:TYR:O	1:P4:164:ARG:NH1	2.41	0.54
1:K4:133:SER:HB2	1:L4:104:PRO:HB3	1.88	0.54
1:K4:308:ARG:NH2	1:K4:311:GLY:O	2.39	0.54
1:H4:340:THR:OG1	1:I4:111:ARG:NH1	2.39	0.54
1:E4:277:MET:HG2	1:E4:330:ILE:HG12	1.89	0.54
2:A3:32:ARG:NH2	2:A3:67:ARG:O	2.41	0.54
1:Y4:256:ASP:HB2	1:Z4:287:LYS:HE2	1.90	0.54
1:R4:167:ILE:HD12	1:R4:370:GLY:HA2	1.88	0.54
1:W4:252:VAL:HG11	2:B3:3:VAL:HG13	1.90	0.54
1:K4:148:ALA:O	1:E4:181:ARG:NH2	2.41	0.54
1:I4:265:LEU:HD23	1:I4:379:LYS:HG2	1.89	0.54
2:E3:32:ARG:NH2	2:E3:67:ARG:O	2.41	0.54
1:V4:183:LEU:HD22	1:V4:360:VAL:HG21	1.90	0.54
1:T4:223:LEU:O	1:T4:227:LYS:NZ	2.31	0.53
1:H4:142:ASP:OD2	1:I4:204:ARG:NH2	2.41	0.53
1:G4:147:TRP:CZ2	1:B4:209:ALA:HB2	2.44	0.53
1:Z4:259:VAL:HG23	1:A5:286:ARG:HD2	1.90	0.53
1:N4:354:PHE:HD1	1:E4:352:ASP:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q4:252:VAL:O	1:Q4:253:ASN:OD1	2.27	0.53
1:J4:265:LEU:HD23	1:J4:379:LYS:HG2	1.91	0.53
1:L4:182:LEU:O	1:L4:186:SER:CB	2.57	0.53
1:I4:183:LEU:HD22	1:I4:360:VAL:HG21	1.89	0.53
1:W4:116:SER:HA	1:V4:268:GLU:HB2	1.91	0.53
1:I4:219:PRO:HG3	1:I4:369:GLY:HA2	1.89	0.53
1:E4:147:TRP:HZ2	1:F4:209:ALA:HB2	1.73	0.53
1:F4:219:PRO:HG3	1:F4:369:GLY:HA2	1.89	0.53
1:B4:129:VAL:HG11	1:B4:342:ALA:HB1	1.90	0.53
1:A5:330:ILE:HB	1:A5:381:LEU:HD13	1.91	0.53
1:T4:256:ASP:HA	1:T4:259:VAL:HG12	1.89	0.53
1:W4:125:SER:OG	1:W4:336:GLY:O	2.26	0.53
1:L4:133:SER:HB2	1:H4:104:PRO:HB3	1.90	0.53
1:B4:167:ILE:HD12	1:B4:370:GLY:HA2	1.91	0.53
1:W4:104:PRO:HB3	1:V4:133:SER:HB2	1.91	0.53
1:W4:265:LEU:HD23	1:W4:379:LYS:HG2	1.89	0.53
1:T4:136:VAL:HG23	1:T4:165:ILE:HB	1.91	0.53
1:T4:215:GLY:HA2	1:T4:220:THR:HG22	1.90	0.53
1:S4:167:ILE:HD12	1:S4:370:GLY:HA2	1.90	0.53
1:P4:344:ARG:HE	1:P4:367:ARG:HD3	1.73	0.53
1:A4:125:SER:OG	1:A4:336:GLY:O	2.27	0.53
1:D4:102:VAL:HG22	1:D4:102:VAL:O	2.09	0.53
1:D4:183:LEU:HD13	1:D4:360:VAL:HG21	1.91	0.53
1:A5:141:THR:CG2	1:A5:142:ASP:N	2.71	0.53
2:B3:32:ARG:NH2	2:B3:67:ARG:O	2.41	0.53
1:R4:263:TYR:OH	1:M4:305:GLU:OE1	2.27	0.52
1:O4:263:TYR:OH	1:P4:305:GLU:OE1	2.26	0.52
1:B4:215:GLY:HA2	1:B4:220:THR:HG22	1.90	0.52
1:X4:91:ASN:HD22	1:B5:151:THR:HB	1.74	0.52
1:A5:167:ILE:HG21	1:A5:342:ALA:HB3	1.91	0.52
1:Q4:185:ASP:N	1:Q4:185:ASP:OD1	2.42	0.52
1:J4:104:PRO:HB3	1:I4:133:SER:HB2	1.90	0.52
1:H4:125:SER:OG	1:H4:336:GLY:O	2.28	0.52
1:F4:262:VAL:HG21	1:F4:310:MET:HG2	1.91	0.52
2:B2:32:ARG:NH2	2:B2:67:ARG:O	2.41	0.52
1:Y4:219:PRO:HG3	1:Y4:369:GLY:HA2	1.90	0.52
1:W4:149:SER:HB2	1:W4:152:ALA:HB2	1.90	0.52
1:V4:167:ILE:HD12	1:V4:370:GLY:HA2	1.90	0.52
1:E4:215:GLY:HA2	1:E4:220:THR:HG22	1.90	0.52
1:Y4:129:VAL:HG11	1:Y4:342:ALA:HB1	1.91	0.52
1:P4:95:ALA:HA	1:P4:99:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W4:167:ILE:HD12	1:W4:370:GLY:HA2	1.91	0.52
1:G4:259:VAL:HG22	1:G4:310:MET:CE	2.40	0.52
2:D3:32:ARG:NH2	2:D3:67:ARG:O	2.41	0.52
1:O4:133:SER:HB2	1:P4:104:PRO:HB3	1.90	0.52
1:L4:289:LYS:HD3	1:L4:293:GLY:HA2	1.90	0.52
1:A4:334:ASP:OD2	1:A4:337:ASN:ND2	2.40	0.52
1:C4:167:ILE:HD12	1:C4:370:GLY:HA2	1.91	0.52
1:Z4:98:GLY:HA2	1:Z4:101:LEU:HD23	1.91	0.52
1:O4:193:TRP:HE1	1:O4:197:ARG:HE	1.58	0.52
1:C4:139:ASP:HA	1:C4:162:ILE:HA	1.92	0.52
1:B5:219:PRO:HG3	1:B5:369:GLY:HA2	1.91	0.52
1:R4:294:ARG:HH21	1:Q4:294:ARG:HD3	1.74	0.52
1:K4:171:GLU:HA	1:K4:367:ARG:HA	1.92	0.52
1:J4:125:SER:OG	1:J4:336:GLY:O	2.26	0.52
1:L4:125:SER:OG	1:L4:336:GLY:O	2.25	0.52
1:W4:243:THR:O	1:W4:250:ALA:HB2	2.10	0.52
1:L4:182:LEU:O	1:L4:186:SER:HB3	2.10	0.52
1:A4:215:GLY:HA2	1:A4:220:THR:HG22	1.92	0.52
1:C4:257:ALA:HB1	1:C4:381:LEU:HD11	1.91	0.52
1:Y4:139:ASP:H	1:Z4:112:GLY:HA2	1.75	0.52
1:M4:334:ASP:OD2	1:M4:337:ASN:ND2	2.43	0.52
1:O4:167:ILE:HD12	1:O4:370:GLY:HA2	1.92	0.52
1:F4:167:ILE:HD12	1:F4:370:GLY:HA2	1.92	0.52
1:B5:143:MET:O	1:B5:158:ALA:HB3	2.10	0.51
1:U4:106:THR:HA	1:T4:135:ASP:HB2	1.91	0.51
1:L4:139:ASP:H	1:H4:112:GLY:HA2	1.75	0.51
1:L4:254:ALA:O	1:L4:255:SER:OG	2.21	0.51
1:I4:291:ALA:O	2:B2:10:SER:HB2	2.10	0.51
1:G4:121:ARG:NH2	1:G4:343:GLU:OE1	2.40	0.51
1:Q4:167:ILE:HG21	1:Q4:342:ALA:HB3	1.93	0.51
1:H4:181:ARG:HH21	1:D4:171:GLU:HG2	1.75	0.51
1:X4:223:LEU:O	1:X4:227:LYS:NZ	2.34	0.51
1:Q4:121:ARG:NH1	1:Q4:343:GLU:OE2	2.44	0.51
1:A4:149:SER:HB2	1:A4:152:ALA:HB2	1.92	0.51
2:C3:32:ARG:NH2	2:C3:67:ARG:O	2.41	0.51
1:Y4:298:ALA:HB2	1:Y4:306:PRO:HD3	1.92	0.51
1:B5:121:ARG:NH1	1:B5:343:GLU:OE2	2.43	0.51
1:P4:167:ILE:HD12	1:P4:370:GLY:HA2	1.92	0.51
1:V4:348:ARG:O	1:V4:364:ALA:HA	2.11	0.51
1:L4:167:ILE:HD12	1:L4:370:GLY:HA2	1.93	0.51
1:L4:183:LEU:HD22	1:L4:360:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N4:167:ILE:HD12	1:N4:370:GLY:HA2	1.92	0.51
1:P4:181:ARG:HH21	1:W4:171:GLU:HG2	1.74	0.51
1:H4:344:ARG:HE	1:H4:367:ARG:HD3	1.76	0.51
1:D4:228:VAL:O	1:D4:239:GLY:HA2	2.11	0.51
1:E4:132:THR:HB	1:F4:102:VAL:CG2	2.41	0.51
1:C4:95:ALA:HA	1:C4:99:GLY:HA3	1.93	0.51
1:X4:227:LYS:HG2	1:X4:380:LEU:HD22	1.93	0.51
1:R4:286:ARG:HH22	1:R4:305:GLU:H	1.59	0.51
1:Q4:125:SER:OG	1:Q4:336:GLY:O	2.26	0.51
1:T4:125:SER:OG	1:T4:336:GLY:O	2.28	0.51
1:L4:275:PHE:HB2	1:L4:314:VAL:HG22	1.93	0.51
1:C4:134:PHE:HB3	1:C4:167:ILE:HB	1.92	0.51
1:B5:130:GLU:OE1	1:B5:344:ARG:NH2	2.44	0.51
1:L4:344:ARG:HE	1:L4:367:ARG:HD3	1.76	0.51
1:E4:262:VAL:HG21	1:E4:310:MET:HG2	1.92	0.51
1:Z4:289:LYS:HD3	1:Z4:293:GLY:HA2	1.93	0.51
1:B5:171:GLU:HA	1:B5:367:ARG:HA	1.92	0.51
1:M4:125:SER:OG	1:M4:336:GLY:O	2.27	0.51
1:O4:150:GLU:HG3	1:O4:151:THR:HG23	1.91	0.51
1:P4:257:ALA:HB1	1:P4:381:LEU:HD11	1.92	0.51
1:G4:95:ALA:HA	1:G4:99:GLY:HA3	1.92	0.51
1:C5:265:LEU:HD23	1:C5:379:LYS:HG2	1.93	0.51
1:Q4:227:LYS:HA	1:Q4:237:SER:HB2	1.93	0.51
1:U4:121:ARG:NH1	1:U4:343:GLU:OE2	2.44	0.51
1:K4:125:SER:OG	1:K4:336:GLY:O	2.28	0.51
1:H4:100:TYR:O	1:D4:164:ARG:NH1	2.43	0.51
1:N4:185:ASP:O	1:F4:102:VAL:HG23	2.10	0.50
1:H4:133:SER:HB2	1:I4:104:PRO:HB3	1.93	0.50
1:I4:182:LEU:O	1:I4:186:SER:CB	2.58	0.50
2:D2:32:ARG:NH2	2:D2:67:ARG:O	2.41	0.50
1:A5:211:ILE:HD12	1:A5:319:ASP:HB2	1.93	0.50
1:D4:263:TYR:OH	1:E4:305:GLU:OE1	2.26	0.50
1:B4:90:LEU:HD13	1:B4:90:LEU:C	2.32	0.50
1:B4:223:LEU:O	1:B4:227:LYS:NZ	2.34	0.50
1:C4:144:GLY:O	1:C4:157:THR:OG1	2.29	0.50
1:B5:177:LYS:HA	1:B5:361:LEU:HA	1.93	0.50
1:W4:275:PHE:HB2	1:W4:314:VAL:HG22	1.92	0.50
1:J4:338:GLY:HA2	1:J4:374:ASP:HB3	1.92	0.50
1:B4:136:VAL:HG22	1:B4:165:ILE:HB	1.93	0.50
1:Y4:348:ARG:HE	1:Y4:365:SER:HG	1.58	0.50
1:N4:294:ARG:HD3	1:O4:294:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R4:256:ASP:HA	1:R4:259:VAL:HG12	1.93	0.50
1:A4:183:LEU:HD22	1:A4:360:VAL:HG21	1.93	0.50
1:Z4:344:ARG:HE	1:Z4:367:ARG:HD3	1.77	0.50
1:N4:164:ARG:NH1	1:L4:100:TYR:O	2.45	0.50
1:P4:149:SER:C	1:P4:151:THR:N	2.65	0.50
1:U4:129:VAL:HG11	1:U4:342:ALA:HB1	1.93	0.50
1:D4:350:LEU:O	1:D4:363:TYR:HB3	2.11	0.50
1:G4:376:ALA:HB3	1:B4:113:VAL:HG23	1.94	0.50
2:A2:32:ARG:NH2	2:A2:67:ARG:O	2.41	0.50
1:M4:162:ILE:HD13	1:F4:100:TYR:HB2	1.92	0.50
1:A4:182:LEU:O	1:A4:186:SER:CB	2.60	0.50
1:N4:178:ALA:HB3	1:N4:360:VAL:HB	1.94	0.50
1:T4:104:PRO:HB3	1:S4:133:SER:HB2	1.92	0.50
1:S4:183:LEU:HD22	1:S4:360:VAL:HG21	1.94	0.50
1:V4:125:SER:OG	1:V4:336:GLY:O	2.25	0.50
1:I4:289:LYS:HD3	1:I4:293:GLY:HA2	1.94	0.50
1:E4:150:GLU:HG3	1:G4:91:ASN:CB	2.35	0.50
1:R4:183:LEU:HD13	1:R4:360:VAL:HG21	1.92	0.50
1:Q4:242:ALA:HA	1:Q4:382:LYS:O	2.12	0.50
1:V4:382:LYS:HE2	1:V4:384:ALA:HB3	1.93	0.50
1:A5:289:LYS:NZ	1:A5:289:LYS:CB	2.73	0.50
1:N4:89:ALA:HB2	1:F4:193:TRP:HZ3	1.75	0.50
1:N4:171:GLU:HG2	1:L4:181:ARG:HH21	1.76	0.50
1:N4:182:LEU:HD13	1:N4:182:LEU:C	2.32	0.50
1:V4:308:ARG:NH2	1:V4:311:GLY:O	2.38	0.50
1:I4:242:ALA:HA	1:I4:382:LYS:O	2.12	0.50
2:E2:32:ARG:NH2	2:E2:67:ARG:O	2.41	0.50
1:C5:256:ASP:HB2	1:X4:287:LYS:HE2	1.93	0.49
1:C5:277:MET:HG2	1:C5:330:ILE:HG12	1.94	0.49
1:X4:95:ALA:HA	1:X4:99:GLY:HA3	1.92	0.49
1:A5:121:ARG:NH2	1:A5:343:GLU:OE1	2.43	0.49
1:N4:181:ARG:HH22	1:E4:170:HIS:HA	1.77	0.49
1:M4:141:THR:HG22	1:M4:161:GLN:HG2	1.95	0.49
1:S4:258:VAL:O	1:S4:262:VAL:HG23	2.12	0.49
1:V4:324:ALA:HB3	1:V4:327:ALA:HB2	1.94	0.49
1:I4:134:PHE:HB3	1:I4:167:ILE:HB	1.93	0.49
1:D4:148:ALA:HB2	1:D4:154:LEU:HD22	1.93	0.49
1:G4:139:ASP:N	1:G4:139:ASP:OD1	2.43	0.49
1:C4:262:VAL:HG21	1:C4:310:MET:HG2	1.94	0.49
1:K4:167:ILE:HG21	1:K4:342:ALA:HB3	1.94	0.49
1:K4:343:GLU:HB3	1:K4:368:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:171:GLU:HA	1:L4:367:ARG:HA	1.94	0.49
1:D4:113:VAL:HG22	1:C4:235:TRP:HZ3	1.76	0.49
1:Z4:191:GLU:OE2	1:Z4:351:ARG:NH1	2.45	0.49
1:U4:125:SER:OG	1:U4:336:GLY:O	2.29	0.49
1:F4:183:LEU:HD13	1:F4:360:VAL:HG21	1.94	0.49
1:C4:167:ILE:HG21	1:C4:342:ALA:HB3	1.94	0.49
1:X4:143:MET:HG2	1:X4:160:PRO:HD3	1.95	0.49
1:B5:357:LYS:N	1:B5:358:PRO:CD	2.71	0.49
1:T4:98:GLY:HA2	1:J4:162:ILE:HD12	1.93	0.49
1:K4:268:GLU:HB2	1:L4:116:SER:HA	1.94	0.49
1:V4:275:PHE:HB2	1:V4:314:VAL:HG22	1.92	0.49
1:D4:334:ASP:OD2	1:D4:337:ASN:ND2	2.45	0.49
1:W4:281:THR:HA	1:W4:323:ILE:HD11	1.94	0.49
1:G4:151:THR:HG23	1:G4:151:THR:O	2.12	0.49
1:Y4:182:LEU:HB2	1:Q4:92:SER:HB3	1.94	0.49
1:B5:284:ALA:HA	1:B5:287:LYS:HD3	1.94	0.49
1:N4:167:ILE:HG21	1:N4:342:ALA:HB3	1.94	0.49
1:S4:256:ASP:OD1	1:S4:257:ALA:N	2.46	0.49
1:K4:275:PHE:HB2	1:K4:314:VAL:HG22	1.95	0.49
1:V4:265:LEU:HD23	1:V4:379:LYS:HG2	1.95	0.49
1:N4:121:ARG:NH2	1:N4:343:GLU:OE1	2.42	0.49
1:W4:338:GLY:HA2	1:W4:374:ASP:HB3	1.93	0.49
1:K4:121:ARG:NH1	1:K4:343:GLU:OE2	2.46	0.49
1:B5:215:GLY:HA2	1:B5:220:THR:HG22	1.95	0.49
1:N4:179:SER:HA	1:N4:359:HIS:HA	1.94	0.49
1:M4:189:ASP:OD1	1:M4:189:ASP:N	2.44	0.49
1:P4:334:ASP:OD2	1:P4:337:ASN:ND2	2.45	0.49
1:T4:129:VAL:HG11	1:T4:342:ALA:HB1	1.95	0.49
1:J4:121:ARG:NH1	1:J4:343:GLU:OE2	2.45	0.49
1:V4:129:VAL:HG11	1:V4:342:ALA:HB1	1.95	0.49
1:H4:348:ARG:O	1:H4:364:ALA:HA	2.13	0.49
2:A1:19:TYR:OH	2:A1:31:ARG:O	2.23	0.49
1:X4:139:ASP:OD1	1:X4:139:ASP:N	2.43	0.49
1:A5:134:PHE:HD2	1:A5:167:ILE:HD13	1.78	0.49
1:Q4:134:PHE:HB3	1:Q4:167:ILE:HB	1.95	0.49
1:P4:352:ASP:OD1	1:P4:352:ASP:N	2.45	0.49
1:W4:183:LEU:HD22	1:W4:360:VAL:HG21	1.95	0.49
1:D4:262:VAL:HG21	1:D4:310:MET:HG2	1.94	0.49
2:C2:32:ARG:NH2	2:C2:67:ARG:O	2.41	0.49
1:Q4:171:GLU:OE2	1:P4:148:ALA:HB3	2.13	0.48
1:O4:143:MET:HG2	1:O4:160:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I4:223:LEU:O	1:I4:227:LYS:NZ	2.31	0.48
1:O4:125:SER:OG	1:O4:336:GLY:O	2.26	0.48
1:U4:112:GLY:HA2	1:T4:139:ASP:H	1.77	0.48
1:J4:129:VAL:HG11	1:J4:342:ALA:HB1	1.95	0.48
1:E4:193:TRP:HE1	1:E4:197:ARG:HH11	1.62	0.48
1:C4:121:ARG:NH2	1:C4:343:GLU:OE1	2.39	0.48
1:X4:189:ASP:OD1	1:X4:189:ASP:N	2.47	0.48
1:M4:157:THR:HG23	1:M4:158:ALA:N	2.26	0.48
1:B4:344:ARG:HE	1:B4:367:ARG:HD3	1.77	0.48
1:C5:133:SER:HB2	1:X4:104:PRO:HB3	1.94	0.48
1:C5:175:MET:HE1	1:B5:155:SER:HA	1.95	0.48
1:C4:129:VAL:HG21	1:C4:134:PHE:HB2	1.93	0.48
1:Z4:259:VAL:CG2	1:A5:286:ARG:HD2	2.43	0.48
1:D4:302:ALA:O	1:C4:311:GLY:N	2.46	0.48
1:E4:130:GLU:O	1:E4:344:ARG:NH1	2.44	0.48
1:B4:256:ASP:HA	1:B4:259:VAL:HG12	1.94	0.48
2:E3:19:TYR:OH	2:E3:31:ARG:O	2.23	0.48
1:P4:189:ASP:OD1	1:P4:189:ASP:N	2.47	0.48
1:W4:121:ARG:NH1	1:W4:343:GLU:OE2	2.47	0.48
1:W4:132:THR:HG21	1:S4:102:VAL:HB	1.96	0.48
1:J4:172:LEU:HD12	1:I4:147:TRP:H	1.78	0.48
1:D4:104:PRO:HB3	1:C4:133:SER:HB2	1.95	0.48
1:M4:162:ILE:HD12	1:F4:100:TYR:HD2	1.79	0.48
1:O4:265:LEU:HD23	1:O4:379:LYS:HG2	1.95	0.48
1:O4:286:ARG:HH12	1:O4:305:GLU:HA	1.77	0.48
1:P4:220:THR:HB	1:P4:371:ASP:HB3	1.95	0.48
1:U4:171:GLU:HA	1:U4:367:ARG:HA	1.96	0.48
1:U4:183:LEU:HD22	1:U4:360:VAL:HG21	1.95	0.48
1:L4:121:ARG:NH1	1:L4:343:GLU:OE2	2.47	0.48
1:E4:95:ALA:HA	1:E4:99:GLY:HA3	1.96	0.48
1:B4:262:VAL:HG21	1:B4:310:MET:HG2	1.96	0.48
1:B4:281:THR:HA	1:B4:323:ILE:HD11	1.96	0.48
1:T4:277:MET:O	1:T4:317:ALA:N	2.46	0.48
1:L4:322:ASP:OD1	1:L4:322:ASP:N	2.46	0.48
1:D4:287:LYS:HE3	1:C4:256:ASP:HB2	1.96	0.48
1:F4:344:ARG:HE	1:F4:367:ARG:HD3	1.78	0.48
1:Y4:171:GLU:HG2	1:W4:181:ARG:HH21	1.78	0.48
1:Z4:167:ILE:HG21	1:Z4:342:ALA:HB3	1.95	0.48
1:Q4:167:ILE:HD12	1:Q4:370:GLY:HA2	1.96	0.48
1:V4:134:PHE:HB3	1:V4:167:ILE:HB	1.96	0.48
2:C3:4:PHE:HB2	2:B3:67:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F4:126:VAL:HA	1:F4:341:ILE:O	2.12	0.47
1:O4:134:PHE:HB3	1:O4:167:ILE:HB	1.95	0.47
1:T4:189:ASP:HB3	1:T4:192:THR:HG22	1.96	0.47
1:S4:121:ARG:NH1	1:S4:343:GLU:OE2	2.47	0.47
1:I4:182:LEU:O	1:I4:186:SER:HB3	2.14	0.47
1:D4:90:LEU:HD13	1:D4:91:ASN:HB2	1.96	0.47
1:E4:189:ASP:N	1:E4:189:ASP:OD1	2.47	0.47
1:E4:211:ILE:HD12	1:E4:319:ASP:HB2	1.95	0.47
1:Z4:189:ASP:OD1	1:Z4:189:ASP:N	2.47	0.47
1:Q4:186:SER:OG	1:Q4:188:PHE:O	2.31	0.47
1:O4:89:ALA:HB2	1:L4:193:TRP:HZ3	1.80	0.47
1:G4:171:GLU:HA	1:G4:367:ARG:HA	1.96	0.47
1:Z4:100:TYR:O	1:V4:164:ARG:NH1	2.47	0.47
1:W4:182:LEU:O	1:W4:186:SER:CB	2.63	0.47
1:H4:149:SER:HB2	1:H4:152:ALA:HB2	1.96	0.47
1:C5:228:VAL:O	1:C5:239:GLY:HA2	2.14	0.47
1:A5:265:LEU:HD23	1:A5:379:LYS:HG2	1.95	0.47
1:O4:227:LYS:HB2	1:O4:227:LYS:HE2	1.77	0.47
1:I4:275:PHE:HB2	1:I4:314:VAL:HG22	1.97	0.47
1:N4:125:SER:OG	1:N4:336:GLY:O	2.25	0.47
1:N4:324:ALA:HB3	1:N4:327:ALA:HB2	1.96	0.47
1:J4:112:GLY:HA2	1:I4:139:ASP:H	1.78	0.47
1:J4:252:VAL:HG11	2:E2:3:VAL:HG11	1.96	0.47
1:L4:182:LEU:O	1:L4:186:SER:OG	2.29	0.47
2:C2:4:PHE:HB2	2:B2:67:ARG:NH2	2.29	0.47
1:Z4:95:ALA:HA	1:Z4:99:GLY:HA3	1.96	0.47
1:R4:111:ARG:HG3	1:Q4:138:VAL:HG12	1.97	0.47
1:Q4:322:ASP:OD1	1:Q4:322:ASP:N	2.45	0.47
1:W4:204:ARG:NH2	1:V4:142:ASP:OD2	2.48	0.47
1:U4:294:ARG:HH12	1:T4:294:ARG:HE	1.62	0.47
1:T4:265:LEU:HD23	1:T4:379:LYS:HG2	1.96	0.47
1:K4:215:GLY:HA2	1:K4:220:THR:HG22	1.96	0.47
1:J4:289:LYS:HD3	1:J4:293:GLY:HA2	1.95	0.47
1:L4:242:ALA:HA	1:L4:382:LYS:O	2.13	0.47
1:A4:289:LYS:HD3	1:A4:293:GLY:HA2	1.97	0.47
1:C4:139:ASP:N	1:C4:139:ASP:OD1	2.48	0.47
1:Y4:149:SER:HB3	1:Y4:152:ALA:HB2	1.95	0.47
1:N4:104:PRO:HA	1:M4:131:ALA:HB1	1.97	0.47
1:P4:297:TRP:CE2	1:P4:309:LEU:HD23	2.49	0.47
1:H4:289:LYS:HD3	1:H4:293:GLY:HA2	1.95	0.47
1:I4:129:VAL:HG11	1:I4:342:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E4:257:ALA:HB1	1:E4:381:LEU:HD11	1.97	0.47
1:F4:121:ARG:NH1	1:F4:343:GLU:OE2	2.48	0.47
1:A5:277:MET:O	1:A5:317:ALA:N	2.46	0.47
1:H4:92:SER:HB2	1:E4:182:LEU:HB2	1.96	0.47
1:E4:139:ASP:HA	1:E4:162:ILE:HA	1.97	0.47
1:C4:121:ARG:NH1	1:C4:343:GLU:OE2	2.48	0.47
1:B5:157:THR:O	1:B5:158:ALA:HB2	2.15	0.47
1:M4:215:GLY:HA2	1:M4:220:THR:HG22	1.96	0.47
1:P4:298:ALA:HB1	1:P4:303:ALA:HB1	1.96	0.47
1:U4:289:LYS:HA	1:U4:295:PHE:HA	1.96	0.47
1:S4:256:ASP:CA	1:S4:259:VAL:HG12	2.44	0.47
1:K4:111:ARG:NH1	1:J4:340:THR:OG1	2.43	0.47
1:J4:277:MET:O	1:J4:317:ALA:N	2.41	0.47
1:L4:167:ILE:HG21	1:L4:342:ALA:HB3	1.97	0.47
1:A4:162:ILE:HD13	1:C4:101:LEU:HD21	1.97	0.47
1:O4:220:THR:HG22	1:O4:225:LYS:HD3	1.96	0.46
1:P4:167:ILE:HG21	1:P4:342:ALA:HB3	1.97	0.46
1:L4:252:VAL:HA	2:A2:9:VAL:HB	1.96	0.46
1:E4:256:ASP:HB2	1:F4:287:LYS:HE3	1.97	0.46
1:O4:367:ARG:HH12	1:S4:181:ARG:HG3	1.81	0.46
1:H4:291:ALA:O	2:A2:10:SER:HB2	2.14	0.46
1:Z4:183:LEU:HD22	1:Z4:360:VAL:HG21	1.97	0.46
1:M4:298:ALA:HB1	1:M4:303:ALA:HB1	1.97	0.46
1:O4:220:THR:CG2	1:O4:225:LYS:HD3	2.46	0.46
1:T4:183:LEU:HD22	1:T4:360:VAL:HG21	1.97	0.46
1:J4:285:VAL:HG11	1:J4:309:LEU:HD11	1.98	0.46
1:L4:129:VAL:HG11	1:L4:342:ALA:HB1	1.95	0.46
1:B4:277:MET:HG2	1:B4:330:ILE:HG12	1.97	0.46
1:C4:189:ASP:OD1	1:C4:189:ASP:N	2.48	0.46
1:Y4:145:SER:HB3	1:Z4:172:LEU:HD11	1.98	0.46
1:A5:210:PHE:HZ	1:A5:368:VAL:HG21	1.79	0.46
1:M4:257:ALA:HB1	1:M4:381:LEU:HD11	1.97	0.46
1:W4:167:ILE:HG21	1:W4:342:ALA:HB3	1.97	0.46
1:K4:183:LEU:HD22	1:K4:360:VAL:HG21	1.98	0.46
2:A2:32:ARG:HG2	2:B2:2:ASP:HB3	1.97	0.46
1:V4:289:LYS:HD2	2:E3:7:HIS:CE1	2.50	0.46
1:V4:328:TYR:HB3	1:V4:380:LEU:HD23	1.97	0.46
1:L4:338:GLY:HA2	1:L4:374:ASP:HB3	1.97	0.46
2:A3:32:ARG:HG2	2:B3:2:ASP:HB3	1.97	0.46
1:R4:352:ASP:OD1	1:R4:352:ASP:N	2.49	0.46
1:O4:100:TYR:O	1:K4:164:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U4:243:THR:O	1:U4:250:ALA:HB2	2.15	0.46
1:K4:281:THR:HA	1:K4:323:ILE:HD11	1.98	0.46
1:B5:151:THR:HG23	1:B5:151:THR:O	2.15	0.46
1:N4:265:LEU:HD23	1:N4:379:LYS:HG2	1.97	0.46
1:W4:348:ARG:O	1:W4:364:ALA:HA	2.15	0.46
1:J4:343:GLU:HB3	1:J4:368:VAL:HG23	1.97	0.46
2:B3:19:TYR:OH	2:B3:31:ARG:O	2.23	0.46
1:T4:100:TYR:O	1:J4:164:ARG:NH1	2.49	0.46
1:F4:149:SER:OG	1:F4:150:GLU:N	2.49	0.46
1:F4:211:ILE:HG21	1:F4:320:MET:HG2	1.97	0.46
2:E2:44:LEU:HA	2:E2:76:THR:HA	1.98	0.46
2:D2:44:LEU:HA	2:D2:76:THR:HA	1.98	0.46
1:X4:338:GLY:O	1:X4:373:SER:N	2.49	0.46
1:Z4:181:ARG:HH21	1:V4:171:GLU:HG2	1.81	0.46
1:M4:95:ALA:HA	1:M4:99:GLY:HA3	1.98	0.46
1:M4:121:ARG:NH2	1:M4:343:GLU:OE1	2.49	0.46
1:V4:121:ARG:NH1	1:V4:343:GLU:OE2	2.48	0.46
1:V4:171:GLU:HA	1:V4:367:ARG:HA	1.97	0.46
1:A4:324:ALA:HB3	1:A4:327:ALA:HB2	1.97	0.46
1:D4:110:ILE:HD11	1:D4:193:TRP:CE2	2.51	0.46
1:B4:110:ILE:HD11	1:B4:193:TRP:CE2	2.51	0.46
1:B4:352:ASP:OD1	1:B4:352:ASP:N	2.49	0.46
1:C4:281:THR:HG23	1:C4:323:ILE:HD11	1.98	0.46
2:B2:44:LEU:HA	2:B2:76:THR:HA	1.98	0.46
1:Z4:227:LYS:HG2	1:Z4:380:LEU:HD22	1.97	0.46
1:Z4:347:LEU:HB3	1:Z4:366:LYS:HB2	1.97	0.46
1:M4:344:ARG:HE	1:M4:367:ARG:HD3	1.81	0.46
1:O4:183:LEU:HD13	1:O4:360:VAL:HG21	1.97	0.46
1:K4:340:THR:OG1	1:L4:111:ARG:NH1	2.46	0.46
1:L4:288:MET:HA	2:A2:6:LYS:HB3	1.98	0.46
2:A3:35:ALA:HB2	3:F3:6:LEU:HD13	1.97	0.46
2:C2:44:LEU:HA	2:C2:76:THR:HA	1.98	0.46
1:B5:154:LEU:O	1:B5:154:LEU:CD1	2.64	0.45
1:N4:347:LEU:HD12	1:N4:366:LYS:HD2	1.98	0.45
1:E4:90:LEU:HB3	1:E4:91:ASN:H	1.62	0.45
1:F4:227:LYS:HE2	1:F4:227:LYS:HB2	1.80	0.45
1:G4:135:ASP:HB2	1:B4:106:THR:HG22	1.97	0.45
2:D3:10:SER:O	2:D3:34:ARG:NH2	2.50	0.45
2:D2:10:SER:O	2:D2:34:ARG:NH2	2.49	0.45
1:X4:162:ILE:H	1:X4:162:ILE:HG13	1.57	0.45
1:Y4:215:GLY:HA2	1:Y4:220:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P4:101:LEU:HD21	1:W4:162:ILE:HD13	1.98	0.45
1:L4:270:ARG:HH12	1:H4:316:ILE:HG21	1.82	0.45
1:C4:289:LYS:HD3	1:C4:293:GLY:HA2	1.97	0.45
2:E3:10:SER:O	2:E3:34:ARG:NH2	2.49	0.45
2:C3:44:LEU:HA	2:C3:76:THR:HA	1.98	0.45
2:A2:35:ALA:HB2	3:F2:6:LEU:HD13	1.97	0.45
2:C2:10:SER:O	2:C2:34:ARG:NH2	2.49	0.45
1:C5:211:ILE:HG21	1:C5:320:MET:HG2	1.97	0.45
1:Z4:108:GLU:OE2	1:Z4:111:ARG:NH1	2.48	0.45
1:N4:181:ARG:NH2	1:E4:170:HIS:HA	2.31	0.45
1:K4:104:PRO:HB3	1:J4:133:SER:HB2	1.99	0.45
1:K4:223:LEU:O	1:K4:227:LYS:NZ	2.32	0.45
1:K4:288:MET:HA	2:E2:6:LYS:HB3	1.98	0.45
1:J4:256:ASP:OD1	1:J4:257:ALA:N	2.50	0.45
1:H4:129:VAL:HG11	1:H4:342:ALA:HB1	1.98	0.45
1:H4:256:ASP:HA	1:H4:259:VAL:HG12	1.97	0.45
1:H4:268:GLU:HG2	1:I4:114:LEU:HG	1.98	0.45
1:F4:263:TYR:OH	1:G4:305:GLU:OE1	2.26	0.45
2:A3:10:SER:O	2:A3:34:ARG:NH2	2.49	0.45
2:E2:2:ASP:HB3	2:D2:32:ARG:HG2	1.99	0.45
2:E2:47:ARG:NH2	2:E2:51:GLY:O	2.50	0.45
1:X4:134:PHE:HB3	1:X4:167:ILE:HB	1.98	0.45
1:X4:256:ASP:HB2	1:Y4:287:LYS:HE3	1.98	0.45
1:Z4:215:GLY:HA2	1:Z4:220:THR:HG22	1.99	0.45
1:Z4:265:LEU:HD11	1:Z4:333:GLY:HA2	1.98	0.45
1:S4:382:LYS:HE2	1:S4:384:ALA:HB2	1.98	0.45
1:A4:250:ALA:HB3	1:A4:253:ASN:O	2.16	0.45
1:F4:338:GLY:HA2	1:F4:374:ASP:HB3	1.99	0.45
2:E3:44:LEU:HA	2:E3:76:THR:HA	1.98	0.45
2:B2:10:SER:O	2:B2:34:ARG:NH2	2.49	0.45
2:B2:19:TYR:OH	2:B2:31:ARG:O	2.23	0.45
2:B2:47:ARG:NH2	2:B2:51:GLY:O	2.50	0.45
1:N4:137:LEU:HD21	1:N4:164:ARG:HE	1.81	0.45
1:Q4:338:GLY:O	1:Q4:373:SER:N	2.42	0.45
1:O4:348:ARG:NH2	1:S4:184:ASP:OD2	2.50	0.45
1:J4:122:GLN:HG2	1:J4:123:ILE:HG23	1.97	0.45
1:A4:129:VAL:HG11	1:A4:342:ALA:HB1	1.99	0.45
1:D4:310:MET:SD	1:E4:286:ARG:NH1	2.89	0.45
2:E3:47:ARG:NH2	2:E3:51:GLY:O	2.50	0.45
2:A1:44:LEU:HA	2:A1:76:THR:HA	1.98	0.45
2:D2:47:ARG:NH2	2:D2:51:GLY:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:10:SER:O	2:A2:34:ARG:NH2	2.50	0.45
1:O4:277:MET:O	1:O4:317:ALA:N	2.45	0.45
1:H4:324:ALA:HB3	1:H4:327:ALA:HB2	1.98	0.45
1:E4:162:ILE:H	1:E4:162:ILE:HG13	1.56	0.45
1:G4:136:VAL:HG22	1:G4:165:ILE:HB	1.99	0.45
1:G4:144:GLY:H	1:G4:158:ALA:HB3	1.80	0.45
1:B4:211:ILE:HG21	1:B4:320:MET:HG2	1.98	0.45
1:X4:171:GLU:HA	1:X4:367:ARG:HA	1.97	0.45
1:Y4:352:ASP:HB3	1:W4:354:PHE:HD1	1.81	0.45
1:R4:242:ALA:HA	1:R4:382:LYS:O	2.17	0.45
1:O4:90:LEU:HB3	1:O4:91:ASN:H	1.58	0.45
1:O4:121:ARG:NH2	1:O4:343:GLU:OE1	2.41	0.45
1:O4:211:ILE:HG21	1:O4:320:MET:HG2	1.98	0.45
1:A4:182:LEU:O	1:A4:186:SER:HB3	2.17	0.45
1:E4:277:MET:O	1:E4:317:ALA:N	2.44	0.45
1:F4:126:VAL:HG12	1:F4:341:ILE:HB	1.99	0.45
2:C3:19:TYR:OH	2:C3:31:ARG:O	2.23	0.45
2:B3:47:ARG:NH2	2:B3:51:GLY:O	2.50	0.45
2:A1:10:SER:O	2:A1:34:ARG:NH2	2.49	0.45
2:A1:47:ARG:NH2	2:A1:51:GLY:O	2.50	0.45
2:E2:66:VAL:HA	2:A2:15:ALA:HB3	1.99	0.45
2:A2:44:LEU:HA	2:A2:76:THR:HA	1.98	0.45
1:P4:265:LEU:HA	1:P4:379:LYS:HG3	1.98	0.45
1:K4:256:ASP:HA	1:K4:259:VAL:HG12	1.99	0.45
1:D4:277:MET:HG2	1:D4:330:ILE:HG12	1.98	0.45
2:D3:44:LEU:HA	2:D3:76:THR:HA	1.98	0.45
2:D3:47:ARG:NH2	2:D3:51:GLY:O	2.50	0.45
2:C3:10:SER:O	2:C3:34:ARG:NH2	2.49	0.45
1:Y4:297:TRP:CE2	1:Y4:309:LEU:HD23	2.51	0.45
1:Y4:322:ASP:OD1	1:Y4:322:ASP:N	2.49	0.45
1:Z4:139:ASP:HB3	1:Z4:162:ILE:HG22	1.99	0.45
1:A5:281:THR:HG23	1:A5:323:ILE:HD11	1.99	0.45
1:N4:352:ASP:OD2	1:L4:357:LYS:NZ	2.39	0.45
1:D4:256:ASP:HA	1:D4:259:VAL:HG12	1.97	0.45
1:E4:143:MET:HG2	1:E4:160:PRO:HD3	1.98	0.45
1:F4:134:PHE:HB3	1:F4:167:ILE:HB	1.98	0.45
2:A3:44:LEU:HA	2:A3:76:THR:HA	1.98	0.45
2:B3:10:SER:O	2:B3:34:ARG:NH2	2.49	0.45
1:Y4:121:ARG:NH1	1:Y4:343:GLU:OE2	2.50	0.45
1:Y4:344:ARG:NH1	1:W4:185:ASP:OD1	2.49	0.45
1:N4:104:PRO:HB3	1:M4:133:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S4:289:LYS:HD2	2:B3:7:HIS:CE1	2.52	0.45
1:F4:297:TRP:CE2	1:F4:309:LEU:HD23	2.52	0.45
1:G4:215:GLY:HA2	1:G4:220:THR:HG22	1.98	0.45
2:C2:47:ARG:NH2	2:C2:51:GLY:O	2.50	0.45
1:X4:219:PRO:HG3	1:X4:369:GLY:HA2	1.99	0.44
1:A5:176:PRO:HG2	1:A5:362:PHE:HB2	1.98	0.44
1:B5:272:ASN:OD1	1:B5:272:ASN:N	2.50	0.44
1:R4:211:ILE:HD12	1:R4:319:ASP:HB2	1.99	0.44
1:Q4:324:ALA:HB3	1:Q4:327:ALA:HB2	1.98	0.44
1:I4:227:LYS:HG2	1:I4:380:LEU:HD22	2.00	0.44
1:D4:143:MET:HG2	1:D4:160:PRO:HD3	1.99	0.44
1:D4:352:ASP:OD1	1:D4:352:ASP:N	2.50	0.44
1:E4:151:THR:HB	1:G4:91:ASN:HD22	1.82	0.44
1:F4:277:MET:HG2	1:F4:330:ILE:HG12	1.99	0.44
2:E3:2:ASP:HB3	2:D3:32:ARG:HG2	1.99	0.44
2:A3:47:ARG:NH2	2:A3:51:GLY:O	2.50	0.44
2:C3:47:ARG:NH2	2:C3:51:GLY:O	2.50	0.44
2:B3:44:LEU:HA	2:B3:76:THR:HA	1.98	0.44
2:E2:10:SER:O	2:E2:34:ARG:NH2	2.50	0.44
1:L4:164:ARG:NH1	1:E4:100:TYR:O	2.51	0.44
1:F4:167:ILE:HG23	1:F4:370:GLY:HA2	1.98	0.44
1:F4:286:ARG:HH12	1:F4:306:PRO:HD2	1.81	0.44
1:G4:167:ILE:HG21	1:G4:342:ALA:HB3	1.97	0.44
2:B3:32:ARG:HE	2:B3:67:ARG:HG2	1.83	0.44
2:E2:32:ARG:HE	2:E2:67:ARG:HG2	1.83	0.44
2:A2:47:ARG:NH2	2:A2:51:GLY:O	2.50	0.44
2:B2:32:ARG:HE	2:B2:67:ARG:HG2	1.83	0.44
1:Z4:171:GLU:HA	1:Z4:367:ARG:HA	1.99	0.44
1:A5:143:MET:O	1:B5:201:LYS:NZ	2.49	0.44
1:T4:171:GLU:HA	1:T4:367:ARG:HA	1.98	0.44
1:E4:121:ARG:NH2	1:E4:343:GLU:OE1	2.44	0.44
1:Q4:176:PRO:O	1:Q4:361:LEU:HA	2.17	0.44
1:H4:121:ARG:NH1	1:H4:343:GLU:OE2	2.50	0.44
1:B4:171:GLU:HA	1:B4:367:ARG:HA	1.98	0.44
1:M4:136:VAL:HG23	1:M4:165:ILE:HB	1.99	0.44
1:Q4:277:MET:HG2	1:Q4:330:ILE:HG12	2.00	0.44
1:U4:172:LEU:HD11	1:T4:145:SER:HB3	1.99	0.44
1:I4:343:GLU:HB3	1:I4:368:VAL:HG23	2.00	0.44
1:E4:329:ALA:HB3	1:E4:383:PHE:HE2	1.82	0.44
1:G4:277:MET:O	1:G4:317:ALA:N	2.45	0.44
2:E3:32:ARG:HE	2:E3:67:ARG:HG2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C5:136:VAL:HG22	1:C5:165:ILE:HB	1.98	0.44
1:B5:177:LYS:HD2	1:B5:359:HIS:CG	2.52	0.44
1:B5:357:LYS:HE2	1:B5:357:LYS:N	2.33	0.44
1:U4:268:GLU:HG2	1:V4:114:LEU:HG	1.99	0.44
1:L4:252:VAL:HG13	2:B2:4:PHE:CE1	2.52	0.44
1:E4:265:LEU:HD22	1:E4:270:ARG:HG3	1.98	0.44
2:D2:32:ARG:HE	2:D2:67:ARG:HG2	1.83	0.44
1:C5:263:TYR:OH	1:X4:305:GLU:OE1	2.25	0.44
1:Y4:265:LEU:HD23	1:Y4:379:LYS:HG2	2.00	0.44
1:Z4:139:ASP:N	1:Z4:139:ASP:OD1	2.45	0.44
1:A5:297:TRP:HB2	1:B5:301:LEU:HD12	2.00	0.44
1:B5:139:ASP:HA	1:B5:162:ILE:HA	2.00	0.44
2:A3:32:ARG:HE	2:A3:67:ARG:HG2	1.83	0.44
1:Z4:150:GLU:HA	1:Z4:154:LEU:HB3	1.99	0.44
1:W4:227:LYS:HE2	1:W4:227:LYS:HB2	1.88	0.44
1:H4:343:GLU:HB3	1:H4:368:VAL:HG23	1.99	0.44
1:D4:114:LEU:HB3	1:C4:268:GLU:HG2	1.99	0.44
1:E4:132:THR:HG21	1:F4:102:VAL:HG22	1.99	0.44
2:A3:11:LEU:HD23	2:B3:14:PRO:HD2	2.00	0.44
2:A3:19:TYR:OH	2:A3:31:ARG:O	2.23	0.44
2:A3:67:ARG:NH2	2:B3:4:PHE:HB2	2.33	0.44
2:A2:11:LEU:HD23	2:B2:14:PRO:HD2	2.00	0.44
2:A2:19:TYR:OH	2:A2:31:ARG:O	2.23	0.44
1:A5:177:LYS:HG3	1:A5:361:LEU:CD1	2.42	0.44
1:N4:215:GLY:HA2	1:N4:220:THR:HG22	1.98	0.44
1:R4:363:TYR:HE1	1:Q4:154:LEU:HD11	1.83	0.44
1:M4:140:LYS:HG3	1:M4:235:TRP:CD1	2.52	0.44
1:J4:116:SER:HA	1:I4:268:GLU:HB2	2.00	0.44
1:J4:242:ALA:HA	1:J4:382:LYS:O	2.18	0.44
1:L4:171:GLU:HG2	1:E4:181:ARG:HH21	1.82	0.44
1:I4:255:SER:HB2	1:I4:297:TRP:CZ2	2.53	0.44
1:X4:352:ASP:HB3	1:Q4:354:PHE:CD1	2.53	0.43
1:Y4:92:SER:OG	1:Y4:93:ALA:N	2.49	0.43
1:P4:277:MET:O	1:P4:317:ALA:N	2.47	0.43
1:U4:347:LEU:HD23	1:U4:366:LYS:HB3	1.99	0.43
1:T4:114:LEU:HG	1:S4:268:GLU:HG2	2.00	0.43
1:K4:149:SER:HB2	1:K4:152:ALA:HB2	1.99	0.43
1:D4:338:GLY:O	1:D4:373:SER:N	2.48	0.43
2:C2:32:ARG:HE	2:C2:67:ARG:HG2	1.83	0.43
1:Z4:162:ILE:H	1:Z4:162:ILE:HG13	1.71	0.43
1:N4:277:MET:HG2	1:N4:330:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U4:227:LYS:HE2	1:U4:227:LYS:HB2	1.87	0.43
1:U4:288:MET:HA	2:D3:6:LYS:HB3	2.00	0.43
1:S4:167:ILE:HG21	1:S4:342:ALA:HB3	2.00	0.43
1:E4:227:LYS:HG2	1:E4:380:LEU:HD22	2.00	0.43
2:C3:32:ARG:HE	2:C3:67:ARG:HG2	1.83	0.43
1:A5:349:VAL:HG23	1:A5:364:ALA:HB2	2.01	0.43
1:P4:149:SER:C	1:P4:151:THR:H	2.19	0.43
1:U4:182:LEU:O	1:U4:186:SER:CB	2.66	0.43
1:K4:106:THR:HA	1:J4:135:ASP:HB2	2.00	0.43
1:J4:134:PHE:HB3	1:J4:167:ILE:HB	2.00	0.43
1:J4:171:GLU:HA	1:J4:367:ARG:HA	2.00	0.43
1:L4:186:SER:O	1:L4:188:PHE:N	2.52	0.43
1:H4:183:LEU:HD22	1:H4:360:VAL:HG21	1.98	0.43
1:D4:256:ASP:HB2	1:E4:287:LYS:HE2	2.00	0.43
1:G4:347:LEU:HB3	1:G4:366:LYS:HB2	2.00	0.43
2:D3:32:ARG:HE	2:D3:67:ARG:HG2	1.83	0.43
2:A1:32:ARG:HE	2:A1:67:ARG:HG2	1.82	0.43
1:N4:263:TYR:OH	1:O4:286:ARG:NH1	2.51	0.43
1:Q4:179:SER:HA	1:Q4:359:HIS:HA	2.00	0.43
1:K4:145:SER:HB3	1:L4:172:LEU:HD11	2.00	0.43
1:L4:122:GLN:HG2	1:L4:123:ILE:HG23	2.01	0.43
1:D4:177:LYS:HA	1:D4:361:LEU:HA	2.00	0.43
1:E4:129:VAL:HG21	1:E4:134:PHE:HB2	2.00	0.43
2:A2:32:ARG:HE	2:A2:67:ARG:HG2	1.83	0.43
1:C5:129:VAL:HG11	1:C5:342:ALA:HB1	1.98	0.43
1:O4:263:TYR:OH	1:P4:286:ARG:NH2	2.47	0.43
1:P4:126:VAL:HA	1:P4:341:ILE:O	2.18	0.43
2:D3:36:LEU:HD11	2:D3:68:PRO:HG2	2.01	0.43
2:A3:36:LEU:HD11	2:A3:68:PRO:HG2	2.01	0.43
2:C3:14:PRO:HD2	2:B3:11:LEU:HD23	2.00	0.43
1:A5:108:GLU:HG3	1:A5:109:THR:HG23	2.00	0.43
1:A5:138:VAL:HG23	1:A5:163:ASP:HB3	2.00	0.43
1:B5:261:LEU:HD13	1:B5:381:LEU:HB2	2.01	0.43
1:Q4:294:ARG:HH21	1:Q4:299:ASP:HB2	1.84	0.43
1:W4:172:LEU:HD12	1:V4:147:TRP:H	1.83	0.43
1:D4:102:VAL:HG22	1:C4:132:THR:HB	2.01	0.43
1:D4:253:ASN:HD21	1:E4:289:LYS:HD2	1.84	0.43
2:A2:67:ARG:NH2	2:B2:4:PHE:HB2	2.33	0.43
1:Y4:277:MET:O	1:Y4:317:ALA:N	2.50	0.43
1:N4:281:THR:HA	1:N4:323:ILE:HD11	2.01	0.43
1:O4:211:ILE:HD12	1:O4:319:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I4:289:LYS:HD2	2:C2:7:HIS:CE1	2.54	0.43
1:E4:171:GLU:HA	1:E4:367:ARG:HA	2.00	0.43
1:E4:265:LEU:HD21	1:E4:269:TYR:HB2	1.99	0.43
2:E3:66:VAL:HA	2:A3:15:ALA:HB3	1.99	0.43
2:A2:66:VAL:HA	2:B2:15:ALA:HB3	2.00	0.43
1:P4:277:MET:HG2	1:P4:330:ILE:HG12	2.00	0.43
1:U4:316:ILE:HG21	1:T4:270:ARG:HH12	1.83	0.43
1:T4:242:ALA:HA	1:T4:382:LYS:O	2.19	0.43
1:D4:167:ILE:HD12	1:D4:370:GLY:HA2	2.00	0.43
2:E3:45:VAL:HG12	2:E3:55:THR:HG22	2.01	0.43
2:D3:19:TYR:OH	2:D3:31:ARG:O	2.23	0.43
2:A1:36:LEU:HD11	2:A1:68:PRO:HG2	2.01	0.43
2:A2:54:VAL:HG21	2:B2:81:VAL:HG21	2.01	0.43
1:Y4:348:ARG:O	1:Y4:364:ALA:HA	2.19	0.43
1:Q4:104:PRO:HB3	1:P4:133:SER:HB2	2.00	0.43
2:B2:36:LEU:HD11	2:B2:68:PRO:HG2	2.01	0.43
1:C5:110:ILE:HD11	1:C5:193:TRP:CE2	2.54	0.43
1:R4:167:ILE:HG21	1:R4:342:ALA:HB3	2.01	0.43
1:Q4:344:ARG:HE	1:Q4:367:ARG:HD3	1.84	0.43
2:A2:45:VAL:HG12	2:A2:55:THR:HG22	2.01	0.43
1:C5:227:LYS:HE2	1:C5:227:LYS:HB2	1.86	0.42
1:B5:162:ILE:H	1:B5:162:ILE:HG13	1.71	0.42
1:B5:265:LEU:HD21	1:B5:269:TYR:HB2	2.01	0.42
1:N4:301:LEU:HD12	1:M4:297:TRP:HB2	1.99	0.42
1:N4:328:TYR:HB3	1:N4:380:LEU:HD23	2.00	0.42
1:M4:265:LEU:HA	1:M4:379:LYS:HG3	2.01	0.42
1:P4:149:SER:HB3	1:P4:152:ALA:HB2	2.01	0.42
1:V4:343:GLU:HB3	1:V4:368:VAL:HG23	2.01	0.42
1:I4:227:LYS:HB2	1:I4:227:LYS:HE2	1.86	0.42
1:I4:324:ALA:HB3	1:I4:327:ALA:HB2	2.00	0.42
1:X4:90:LEU:HB3	1:X4:91:ASN:H	1.63	0.42
1:N4:92:SER:HB3	1:F4:182:LEU:HB2	2.02	0.42
1:T4:343:GLU:HB3	1:T4:368:VAL:HG23	2.01	0.42
1:S4:328:TYR:HB3	1:S4:380:LEU:HD23	2.00	0.42
1:K4:324:ALA:HB3	1:K4:327:ALA:HB2	2.01	0.42
1:I4:215:GLY:HA2	1:I4:220:THR:HG22	2.00	0.42
1:A4:182:LEU:O	1:A4:186:SER:OG	2.29	0.42
1:A4:227:LYS:HB2	1:A4:227:LYS:HE2	1.89	0.42
1:D4:134:PHE:HB3	1:D4:167:ILE:HB	2.00	0.42
2:B3:45:VAL:HG12	2:B3:55:THR:HG22	2.01	0.42
2:A1:45:VAL:HG12	2:A1:55:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:47:ARG:HE	2:A1:72:LEU:HD11	1.85	0.42
2:E2:36:LEU:HD11	2:E2:68:PRO:HG2	2.01	0.42
1:C5:171:GLU:HA	1:C5:367:ARG:HA	2.01	0.42
1:A5:134:PHE:HB3	1:A5:167:ILE:HB	2.01	0.42
1:O4:297:TRP:HB2	1:P4:301:LEU:HD12	2.00	0.42
1:W4:227:LYS:HG2	1:W4:380:LEU:HD22	2.01	0.42
1:W4:382:LYS:HE2	1:W4:384:ALA:HB2	2.00	0.42
1:T4:252:VAL:HG13	2:D3:4:PHE:CZ	2.53	0.42
1:S4:277:MET:O	1:S4:317:ALA:N	2.49	0.42
1:I4:288:MET:HA	2:C2:6:LYS:HB3	2.01	0.42
1:F4:101:LEU:N	1:F4:101:LEU:CD1	2.79	0.42
1:G4:150:GLU:HB3	1:C4:93:ALA:HB2	2.00	0.42
1:G4:259:VAL:HG22	1:G4:310:MET:HE3	2.00	0.42
2:A3:66:VAL:HA	2:B3:15:ALA:HB3	2.00	0.42
2:D2:38:VAL:HG21	2:D2:58:VAL:HG21	2.02	0.42
2:D2:81:VAL:HG21	2:C2:54:VAL:HG21	2.01	0.42
2:A2:36:LEU:HD11	2:A2:68:PRO:HG2	2.01	0.42
2:C2:45:VAL:HG12	2:C2:55:THR:HG22	2.01	0.42
1:A5:219:PRO:CG	1:A5:368:VAL:O	2.66	0.42
1:B5:357:LYS:CA	1:B5:357:LYS:CE	2.92	0.42
1:M4:157:THR:CG2	1:M4:158:ALA:H	2.30	0.42
1:Q4:114:LEU:HB2	1:P4:269:TYR:CZ	2.54	0.42
1:O4:227:LYS:HG2	1:O4:380:LEU:HD22	2.01	0.42
1:O4:382:LYS:HE2	1:O4:384:ALA:HB2	1.99	0.42
1:S4:343:GLU:HB3	1:S4:368:VAL:HG23	2.00	0.42
1:K4:277:MET:O	1:K4:317:ALA:N	2.49	0.42
1:H4:182:LEU:O	1:H4:186:SER:CB	2.68	0.42
1:F4:143:MET:HG2	1:F4:160:PRO:HD3	2.01	0.42
1:F4:227:LYS:HG2	1:F4:380:LEU:HD22	2.00	0.42
2:D3:14:PRO:HD2	2:C3:11:LEU:HD23	2.02	0.42
2:C3:38:VAL:HG21	2:C3:58:VAL:HG21	2.02	0.42
2:C3:47:ARG:HE	2:C3:72:LEU:HD11	1.85	0.42
2:B3:38:VAL:HG21	2:B3:58:VAL:HG21	2.02	0.42
1:W4:277:MET:O	1:W4:317:ALA:N	2.51	0.42
1:J4:316:ILE:HG21	1:I4:270:ARG:HH12	1.85	0.42
1:A4:277:MET:HG2	1:A4:330:ILE:HG12	2.02	0.42
1:D4:93:ALA:HB2	1:D4:102:VAL:HG11	2.02	0.42
2:B3:47:ARG:HE	2:B3:72:LEU:HD11	1.85	0.42
2:C2:14:PRO:HD2	2:B2:11:LEU:HD23	2.00	0.42
1:Z4:277:MET:O	1:Z4:317:ALA:N	2.49	0.42
1:R4:348:ARG:HE	1:R4:365:SER:HG	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W4:106:THR:HA	1:V4:135:ASP:HB2	2.01	0.42
1:W4:145:SER:HB3	1:S4:172:LEU:HD11	2.00	0.42
1:U4:154:LEU:HD23	1:V4:363:TYR:HE1	1.85	0.42
1:K4:129:VAL:HG11	1:K4:342:ALA:HB1	2.02	0.42
1:K4:363:TYR:HE1	1:J4:154:LEU:HD22	1.84	0.42
1:J4:90:LEU:HB3	1:J4:91:ASN:H	1.62	0.42
1:E4:328:TYR:HB3	1:E4:380:LEU:HD23	2.00	0.42
1:F4:338:GLY:O	1:F4:373:SER:N	2.49	0.42
1:G4:91:ASN:OD1	1:G4:91:ASN:N	2.53	0.42
2:D3:81:VAL:HG21	2:C3:54:VAL:HG21	2.01	0.42
2:C3:45:VAL:HG12	2:C3:55:THR:HG22	2.01	0.42
2:B2:45:VAL:HG12	2:B2:55:THR:HG22	2.01	0.42
1:Y4:263:TYR:OH	1:Z4:305:GLU:OE1	2.28	0.42
1:A5:206:GLU:OE1	1:A5:368:VAL:HG11	2.19	0.42
1:S4:134:PHE:HB3	1:S4:167:ILE:HB	2.02	0.42
1:K4:291:ALA:O	2:D2:10:SER:HB2	2.19	0.42
1:J4:255:SER:O	1:J4:258:VAL:HG12	2.20	0.42
1:A4:322:ASP:N	1:A4:322:ASP:OD1	2.47	0.42
1:D4:149:SER:HB3	1:D4:152:ALA:HB2	2.01	0.42
2:D3:45:VAL:HG12	2:D3:55:THR:HG22	2.01	0.42
2:A3:38:VAL:HG21	2:A3:58:VAL:HG21	2.02	0.42
2:D2:47:ARG:HE	2:D2:72:LEU:HD11	1.85	0.42
1:A5:126:VAL:HG12	1:A5:341:ILE:HB	2.01	0.42
1:O4:220:THR:HB	1:O4:371:ASP:HB3	2.02	0.42
1:W4:134:PHE:HB3	1:W4:167:ILE:HB	2.01	0.42
1:K4:227:LYS:HE2	1:K4:227:LYS:HB2	1.78	0.42
1:A4:171:GLU:HA	1:A4:367:ARG:HA	2.01	0.42
1:D4:113:VAL:CG2	1:C4:235:TRP:CZ3	3.03	0.42
1:D4:297:TRP:CE2	1:D4:309:LEU:HD23	2.55	0.42
1:G4:281:THR:HG23	1:G4:323:ILE:HD11	2.01	0.42
2:E3:36:LEU:HD11	2:E3:68:PRO:HG2	2.01	0.42
2:C3:36:LEU:HD11	2:C3:68:PRO:HG2	2.01	0.42
2:E2:47:ARG:HE	2:E2:72:LEU:HD11	1.85	0.42
2:C2:36:LEU:HD11	2:C2:68:PRO:HG2	2.01	0.42
1:C5:223:LEU:O	1:C5:227:LYS:NZ	2.36	0.42
1:X4:227:LYS:HE2	1:X4:227:LYS:HB2	1.91	0.42
1:B5:290:ASP:OD1	1:B5:294:ARG:N	2.49	0.42
1:M4:290:ASP:OD1	1:M4:290:ASP:N	2.49	0.42
1:U4:189:ASP:HB3	1:U4:192:THR:HG22	2.01	0.42
1:U4:277:MET:HG2	1:U4:330:ILE:HG12	2.02	0.42
1:E4:139:ASP:N	1:E4:139:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E3:47:ARG:HE	2:E3:72:LEU:HD11	1.84	0.42
2:A3:54:VAL:HG21	2:B3:81:VAL:HG21	2.01	0.42
2:D2:36:LEU:HD11	2:D2:68:PRO:HG2	2.01	0.42
2:D2:45:VAL:HG12	2:D2:55:THR:HG22	2.01	0.42
2:A2:47:ARG:HE	2:A2:72:LEU:HD11	1.85	0.42
2:B2:38:VAL:HG21	2:B2:58:VAL:HG21	2.02	0.42
1:C5:148:ALA:HB2	1:C5:154:LEU:HD22	2.01	0.42
1:A5:225:LYS:HZ1	1:A5:371:ASP:HB2	1.85	0.42
1:W4:290:ASP:HA	2:A3:8:ALA:HB3	2.01	0.42
2:D3:38:VAL:HG21	2:D3:58:VAL:HG21	2.02	0.42
2:A3:47:ARG:HE	2:A3:72:LEU:HD11	1.84	0.42
2:B3:36:LEU:HD11	2:B3:68:PRO:HG2	2.01	0.42
2:A2:38:VAL:HG21	2:A2:58:VAL:HG21	2.02	0.42
1:C5:149:SER:HB3	1:C5:152:ALA:HB2	2.02	0.41
1:X4:277:MET:HG2	1:X4:330:ILE:HG12	2.02	0.41
1:Z4:253:ASN:ND2	1:A5:289:LYS:HE3	2.34	0.41
1:B5:343:GLU:HB3	1:B5:368:VAL:HG23	2.02	0.41
1:T4:227:LYS:HB2	1:T4:227:LYS:HE2	1.81	0.41
1:V4:167:ILE:HG21	1:V4:342:ALA:HB3	2.02	0.41
1:D4:140:LYS:HG3	1:D4:141:THR:HG23	2.01	0.41
1:G4:189:ASP:OD1	1:G4:189:ASP:N	2.53	0.41
2:E2:38:VAL:HG21	2:E2:58:VAL:HG21	2.02	0.41
2:D2:21:ILE:H	2:D2:21:ILE:HG13	1.79	0.41
1:A5:143:MET:HB3	1:A5:160:PRO:HD3	2.02	0.41
1:M4:352:ASP:OD1	1:M4:352:ASP:N	2.51	0.41
1:W4:114:LEU:HB3	1:V4:269:TYR:HE1	1.85	0.41
1:T4:261:LEU:HD13	1:T4:381:LEU:HB2	2.02	0.41
1:E4:223:LEU:O	1:E4:227:LYS:NZ	2.33	0.41
1:G4:322:ASP:OD1	1:G4:322:ASP:N	2.50	0.41
1:B4:198:ILE:HG21	1:B4:364:ALA:HB3	2.01	0.41
2:A3:45:VAL:HG12	2:A3:55:THR:HG22	2.01	0.41
2:C2:47:ARG:HE	2:C2:72:LEU:HD11	1.85	0.41
1:C5:175:MET:HE2	1:B5:156:GLU:H	1.86	0.41
1:A5:219:PRO:HG3	1:A5:369:GLY:HA2	2.02	0.41
1:B5:130:GLU:O	1:B5:344:ARG:NH1	2.48	0.41
1:R4:90:LEU:HB3	1:R4:91:ASN:H	1.65	0.41
1:I4:285:VAL:HG11	1:I4:309:LEU:HD11	2.02	0.41
2:D3:47:ARG:HE	2:D3:72:LEU:HD11	1.85	0.41
2:D2:14:PRO:HD2	2:C2:11:LEU:HD23	2.02	0.41
2:C2:38:VAL:HG21	2:C2:58:VAL:HG21	2.02	0.41
2:B2:47:ARG:HE	2:B2:72:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R4:286:ARG:NH2	1:R4:305:GLU:H	2.18	0.41
1:J4:114:LEU:HG	1:I4:268:GLU:HG2	2.02	0.41
1:H4:182:LEU:O	1:H4:186:SER:OG	2.30	0.41
1:F4:171:GLU:HA	1:F4:367:ARG:HA	2.02	0.41
1:G4:277:MET:HG2	1:G4:330:ILE:HG12	2.01	0.41
2:E2:45:VAL:HG12	2:E2:55:THR:HG22	2.01	0.41
1:N4:114:LEU:HB2	1:M4:269:TYR:CZ	2.56	0.41
1:Q4:215:GLY:HA2	1:Q4:220:THR:HG22	2.02	0.41
1:A4:289:LYS:HE3	1:A4:289:LYS:HB3	1.91	0.41
1:E4:268:GLU:HG3	1:F4:114:LEU:HD23	2.03	0.41
1:E4:269:TYR:CZ	1:F4:114:LEU:HB2	2.56	0.41
2:E3:38:VAL:HG21	2:E3:58:VAL:HG21	2.02	0.41
1:B5:289:LYS:HB2	1:B5:293:GLY:HA2	2.02	0.41
1:Q4:307:ALA:O	1:Q4:308:ARG:NE	2.46	0.41
1:O4:352:ASP:N	1:O4:352:ASP:OD1	2.54	0.41
1:W4:182:LEU:O	1:W4:186:SER:OG	2.29	0.41
1:V4:277:MET:O	1:V4:317:ALA:N	2.50	0.41
1:L4:324:ALA:HB3	1:L4:327:ALA:HB2	2.03	0.41
1:G4:263:TYR:OH	1:B4:286:ARG:NH1	2.53	0.41
2:A1:38:VAL:HG21	2:A1:58:VAL:HG21	2.02	0.41
1:X4:277:MET:O	1:X4:317:ALA:N	2.50	0.41
1:X4:297:TRP:CD1	1:Y4:302:ALA:HB2	2.56	0.41
1:Y4:150:GLU:OE1	1:A5:92:SER:OG	2.36	0.41
1:B5:262:VAL:HG21	1:B5:310:MET:HG2	2.03	0.41
1:N4:100:TYR:O	1:E4:164:ARG:NH1	2.53	0.41
1:M4:147:TRP:H	1:M4:147:TRP:HE3	1.68	0.41
1:M4:150:GLU:OE1	1:O4:91:ASN:HB2	2.20	0.41
1:Q4:338:GLY:HA2	1:Q4:374:ASP:HB3	2.03	0.41
1:W4:114:LEU:HB3	1:V4:269:TYR:CE1	2.55	0.41
1:U4:287:LYS:O	2:D3:6:LYS:HB3	2.20	0.41
1:G4:149:SER:C	1:G4:151:THR:N	2.73	0.41
1:B5:175:MET:HG2	1:B5:361:LEU:HD11	2.02	0.41
1:S4:312:TYR:HA	1:S4:313:PRO:HD3	1.96	0.41
1:D4:90:LEU:HD13	1:D4:90:LEU:C	2.40	0.41
1:G4:162:ILE:H	1:G4:162:ILE:HG13	1.50	0.41
1:C4:140:LYS:HG3	1:C4:235:TRP:CD1	2.56	0.41
1:N4:167:ILE:HG23	1:N4:370:GLY:HA2	2.03	0.41
1:M4:149:SER:O	1:M4:150:GLU:C	2.58	0.41
1:O4:338:GLY:O	1:O4:373:SER:N	2.49	0.41
1:P4:322:ASP:OD1	1:P4:322:ASP:N	2.53	0.41
1:U4:269:TYR:CE1	1:V4:114:LEU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K4:139:ASP:H	1:L4:112:GLY:HA2	1.86	0.41
1:J4:111:ARG:N	1:I4:137:LEU:O	2.53	0.41
1:V4:186:SER:O	1:V4:188:PHE:N	2.53	0.41
1:H4:145:SER:HB3	1:I4:172:LEU:HD11	2.02	0.41
1:I4:118:ALA:HA	1:I4:122:GLN:HE22	1.85	0.41
1:I4:186:SER:O	1:I4:188:PHE:N	2.54	0.41
1:E4:227:LYS:HB2	1:E4:227:LYS:HE2	1.88	0.41
1:G4:211:ILE:HD12	1:G4:319:ASP:HB2	2.02	0.41
1:B4:92:SER:O	1:B4:99:GLY:HA3	2.20	0.41
1:B4:143:MET:HG2	1:B4:160:PRO:HD3	2.02	0.41
2:A2:21:ILE:H	2:A2:21:ILE:HG13	1.79	0.41
1:X4:162:ILE:HD13	1:Q4:100:TYR:HB2	2.03	0.41
1:Y4:227:LYS:HB2	1:Y4:227:LYS:HE2	1.85	0.41
1:W4:183:LEU:HD21	1:W4:362:PHE:HZ	1.86	0.41
1:B4:179:SER:O	1:B4:183:LEU:HB2	2.21	0.41
2:A1:2:ASP:OD1	2:A1:2:ASP:N	2.51	0.41
2:D2:15:ALA:HB3	2:C2:66:VAL:HA	2.03	0.41
1:C5:106:THR:HG22	1:B5:135:ASP:HB2	2.02	0.40
1:B5:344:ARG:HE	1:B5:367:ARG:HD3	1.85	0.40
1:R4:149:SER:OG	1:R4:150:GLU:N	2.53	0.40
1:T4:112:GLY:HA2	1:S4:139:ASP:H	1.86	0.40
1:T4:330:ILE:HD12	1:T4:381:LEU:HD23	2.02	0.40
1:K4:268:GLU:HG2	1:L4:114:LEU:HG	2.02	0.40
1:A4:242:ALA:HA	1:A4:382:LYS:O	2.21	0.40
1:D4:146:GLY:HA3	1:D4:154:LEU:HD21	2.03	0.40
1:D4:344:ARG:HE	1:D4:367:ARG:HD3	1.85	0.40
1:F4:343:GLU:HB3	1:F4:368:VAL:HG23	2.03	0.40
1:G4:256:ASP:HB2	1:B4:287:LYS:HE3	2.03	0.40
1:Y4:354:PHE:CD1	1:P4:352:ASP:HB3	2.56	0.40
1:Z4:299:ASP:OD1	1:Z4:299:ASP:N	2.52	0.40
1:B5:277:MET:HG2	1:B5:330:ILE:HG12	2.03	0.40
1:W4:182:LEU:O	1:W4:186:SER:HB3	2.21	0.40
1:U4:114:LEU:HB3	1:T4:269:TYR:HE1	1.87	0.40
1:J4:111:ARG:HB2	1:I4:138:VAL:HG12	2.04	0.40
1:J4:324:ALA:HB3	1:J4:327:ALA:HB2	2.03	0.40
1:L4:277:MET:HG2	1:L4:330:ILE:HG12	2.04	0.40
1:H4:198:ILE:HG21	1:H4:364:ALA:HB3	2.03	0.40
1:B4:297:TRP:CE2	1:B4:309:LEU:HD23	2.56	0.40
2:E3:18:HIS:CD2	2:D3:54:VAL:HG22	2.57	0.40
2:D3:15:ALA:HB3	2:C3:66:VAL:HA	2.03	0.40
1:C5:149:SER:OG	1:C5:150:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X4:167:ILE:HD12	1:X4:370:GLY:HA2	2.02	0.40
1:A5:141:THR:CG2	1:A5:142:ASP:H	2.35	0.40
1:U4:186:SER:O	1:U4:188:PHE:N	2.55	0.40
1:V4:227:LYS:HE2	1:V4:227:LYS:HB2	1.89	0.40
1:L4:227:LYS:HE2	1:L4:227:LYS:HB2	1.87	0.40
1:I4:176:PRO:HG3	1:I4:198:ILE:HD11	2.03	0.40
1:I4:182:LEU:O	1:I4:186:SER:OG	2.27	0.40
1:Z4:141:THR:HG22	1:Z4:161:GLN:HG2	2.03	0.40
1:N4:309:LEU:HD22	1:N4:309:LEU:HA	1.96	0.40
1:M4:90:LEU:HB3	1:M4:91:ASN:H	1.75	0.40
1:Q4:358:PRO:HG2	1:Q4:359:HIS:CD2	2.56	0.40
1:W4:268:GLU:HG2	1:S4:114:LEU:HG	2.03	0.40
1:S4:122:GLN:HG2	1:S4:123:ILE:HG23	2.02	0.40
1:S4:171:GLU:HG2	1:K4:181:ARG:HH21	1.85	0.40
1:S4:186:SER:O	1:S4:188:PHE:N	2.54	0.40
1:S4:256:ASP:OD1	1:S4:256:ASP:C	2.59	0.40
1:K4:150:GLU:HG2	1:H4:91:ASN:HB2	2.04	0.40
1:J4:186:SER:O	1:J4:188:PHE:N	2.54	0.40
1:L4:257:ALA:HB1	1:L4:381:LEU:HD11	2.04	0.40
1:D4:90:LEU:HD13	1:D4:91:ASN:N	2.36	0.40
1:E4:130:GLU:OE1	1:E4:344:ARG:NH2	2.54	0.40
1:G4:150:GLU:HG3	1:C4:91:ASN:CB	2.45	0.40
2:B2:21:ILE:H	2:B2:21:ILE:HG13	1.79	0.40
1:C5:167:ILE:HG23	1:C5:370:GLY:HA2	2.04	0.40
1:S4:136:VAL:HG23	1:S4:165:ILE:HB	2.04	0.40
1:C4:107:SER:OG	1:C4:108:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A4	287/386 (74%)	258 (90%)	28 (10%)	1 (0%)	41	74
1	A5	295/386 (76%)	273 (92%)	21 (7%)	1 (0%)	41	74
1	B4	295/386 (76%)	264 (90%)	30 (10%)	1 (0%)	41	74
1	B5	267/386 (69%)	242 (91%)	22 (8%)	3 (1%)	14	54
1	C4	295/386 (76%)	266 (90%)	29 (10%)	0	100	100
1	C5	295/386 (76%)	264 (90%)	31 (10%)	0	100	100
1	D4	295/386 (76%)	264 (90%)	31 (10%)	0	100	100
1	E4	295/386 (76%)	258 (88%)	36 (12%)	1 (0%)	41	74
1	F4	295/386 (76%)	264 (90%)	29 (10%)	2 (1%)	22	62
1	G4	295/386 (76%)	263 (89%)	31 (10%)	1 (0%)	41	74
1	H4	287/386 (74%)	252 (88%)	34 (12%)	1 (0%)	41	74
1	I4	287/386 (74%)	251 (88%)	35 (12%)	1 (0%)	41	74
1	J4	287/386 (74%)	256 (89%)	29 (10%)	2 (1%)	22	62
1	K4	287/386 (74%)	246 (86%)	40 (14%)	1 (0%)	41	74
1	L4	287/386 (74%)	255 (89%)	31 (11%)	1 (0%)	41	74
1	M4	295/386 (76%)	254 (86%)	41 (14%)	0	100	100
1	N4	295/386 (76%)	264 (90%)	30 (10%)	1 (0%)	41	74
1	O4	295/386 (76%)	257 (87%)	37 (12%)	1 (0%)	41	74
1	P4	295/386 (76%)	256 (87%)	38 (13%)	1 (0%)	41	74
1	Q4	295/386 (76%)	260 (88%)	34 (12%)	1 (0%)	41	74
1	R4	295/386 (76%)	261 (88%)	33 (11%)	1 (0%)	41	74
1	S4	287/386 (74%)	257 (90%)	29 (10%)	1 (0%)	41	74
1	T4	287/386 (74%)	255 (89%)	32 (11%)	0	100	100
1	U4	287/386 (74%)	253 (88%)	33 (12%)	1 (0%)	41	74
1	V4	287/386 (74%)	258 (90%)	28 (10%)	1 (0%)	41	74
1	W4	287/386 (74%)	251 (88%)	35 (12%)	1 (0%)	41	74
1	X4	295/386 (76%)	259 (88%)	36 (12%)	0	100	100
1	Y4	295/386 (76%)	264 (90%)	31 (10%)	0	100	100
1	Z4	295/386 (76%)	269 (91%)	26 (9%)	0	100	100
2	A1	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	A2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	A3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	B3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	C2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	C3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	D2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	D3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	E2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	E3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
3	F2	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	F3	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
All	All	9357/12768 (73%)	8351 (89%)	981 (10%)	25 (0%)	44	74

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E4	147	TRP
1	F4	93	ALA
1	G4	147	TRP
1	N4	179	SER
1	W4	187	ALA
1	U4	187	ALA
1	S4	187	ALA
1	K4	187	ALA
1	J4	187	ALA
1	J4	252	VAL
1	V4	187	ALA
1	L4	187	ALA
1	H4	187	ALA
1	I4	187	ALA
1	A4	187	ALA
1	B5	158	ALA
1	B5	189	ASP
1	P4	157	THR
1	A5	226	THR
1	B4	92	SER
1	O4	108	GLU
1	F4	91	ASN
1	R4	180	GLN

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Mol	Chain	Res	Type
1	Q4	92	SER
1	B5	353	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A4	215/285 (75%)	215 (100%)	0	100 100
1	A5	218/285 (76%)	214 (98%)	4 (2%)	59 81
1	B4	218/285 (76%)	218 (100%)	0	100 100
1	B5	198/285 (70%)	195 (98%)	3 (2%)	65 84
1	C4	218/285 (76%)	217 (100%)	1 (0%)	88 95
1	C5	218/285 (76%)	217 (100%)	1 (0%)	88 95
1	D4	218/285 (76%)	217 (100%)	1 (0%)	88 95
1	E4	218/285 (76%)	217 (100%)	1 (0%)	88 95
1	F4	218/285 (76%)	217 (100%)	1 (0%)	88 95
1	G4	218/285 (76%)	215 (99%)	3 (1%)	67 85
1	H4	215/285 (75%)	214 (100%)	1 (0%)	88 95
1	I4	215/285 (75%)	215 (100%)	0	100 100
1	J4	215/285 (75%)	215 (100%)	0	100 100
1	K4	215/285 (75%)	214 (100%)	1 (0%)	88 95
1	L4	215/285 (75%)	215 (100%)	0	100 100
1	M4	218/285 (76%)	218 (100%)	0	100 100
1	N4	218/285 (76%)	214 (98%)	4 (2%)	59 81
1	O4	218/285 (76%)	218 (100%)	0	100 100
1	P4	218/285 (76%)	217 (100%)	1 (0%)	88 95
1	Q4	218/285 (76%)	215 (99%)	3 (1%)	67 85
1	R4	218/285 (76%)	218 (100%)	0	100 100
1	S4	215/285 (75%)	215 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T4	215/285 (75%)	215 (100%)	0	100	100
1	U4	215/285 (75%)	215 (100%)	0	100	100
1	V4	215/285 (75%)	215 (100%)	0	100	100
1	W4	215/285 (75%)	215 (100%)	0	100	100
1	X4	218/285 (76%)	217 (100%)	1 (0%)	88	95
1	Y4	218/285 (76%)	218 (100%)	0	100	100
1	Z4	218/285 (76%)	216 (99%)	2 (1%)	78	90
2	A1	69/69 (100%)	69 (100%)	0	100	100
2	A2	69/69 (100%)	69 (100%)	0	100	100
2	A3	69/69 (100%)	69 (100%)	0	100	100
2	B2	69/69 (100%)	69 (100%)	0	100	100
2	B3	69/69 (100%)	69 (100%)	0	100	100
2	C2	69/69 (100%)	69 (100%)	0	100	100
2	C3	69/69 (100%)	69 (100%)	0	100	100
2	D2	69/69 (100%)	69 (100%)	0	100	100
2	D3	69/69 (100%)	69 (100%)	0	100	100
2	E2	69/69 (100%)	69 (100%)	0	100	100
2	E3	69/69 (100%)	69 (100%)	0	100	100
3	F2	5/224 (2%)	5 (100%)	0	100	100
3	F3	5/224 (2%)	5 (100%)	0	100	100
All	All	7038/9472 (74%)	7010 (100%)	28 (0%)	91	97

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C5	253	ASN
1	X4	351	ARG
1	Z4	348	ARG
1	Z4	351	ARG
1	A5	140	LYS
1	A5	227	LYS
1	A5	261	LEU
1	A5	367	ARG
1	B5	189	ASP
1	B5	190	ILE

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Mol	Chain	Res	Type
1	B5	261	LEU
1	N4	101	LEU
1	N4	115	ARG
1	N4	227	LYS
1	N4	348	ARG
1	Q4	115	ARG
1	Q4	227	LYS
1	Q4	348	ARG
1	P4	154	LEU
1	K4	261	LEU
1	H4	256	ASP
1	D4	261	LEU
1	E4	351	ARG
1	F4	128	ASN
1	G4	261	LEU
1	G4	348	ARG
1	G4	351	ARG
1	C4	351	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B5	337	ASN
1	F4	128	ASN
2	E3	7	HIS
2	E3	39	GLN
2	D3	39	GLN
2	A3	7	HIS
2	A3	39	GLN
2	C3	7	HIS
2	C3	39	GLN
2	B3	7	HIS
2	B3	39	GLN
2	A1	7	HIS
2	E2	7	HIS
2	E2	39	GLN
2	D2	7	HIS
2	D2	39	GLN
2	A2	7	HIS
2	A2	39	GLN
2	C2	7	HIS
2	C2	39	GLN

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Mol	Chain	Res	Type
2	B2	7	HIS
2	B2	39	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

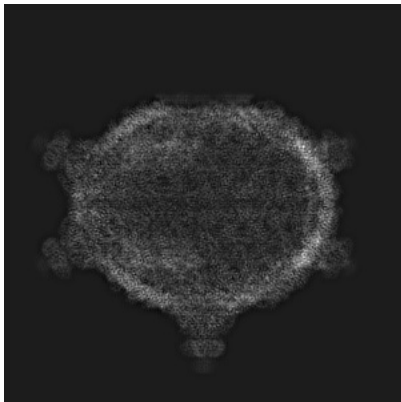
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10442. These allow visual inspection of the internal detail of the map and identification of artifacts.

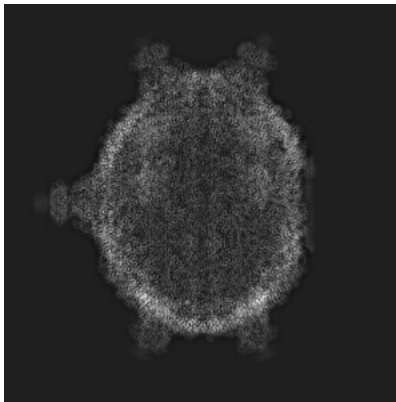
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

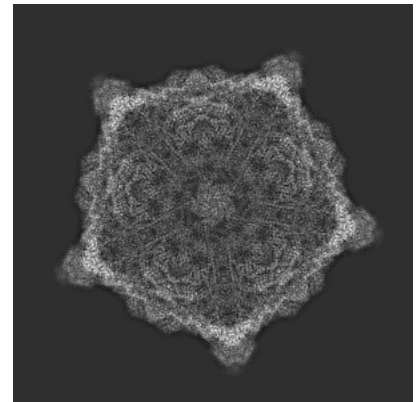
6.1.1 Primary map



X



Y



Z

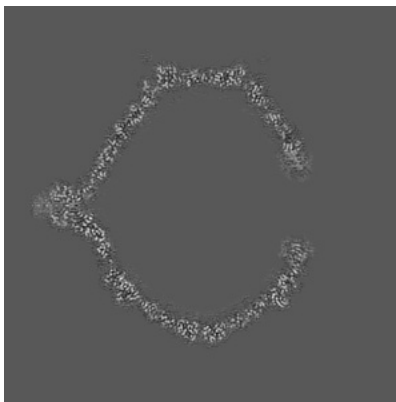
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

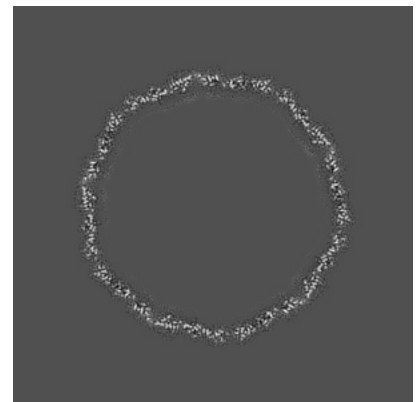
6.2.1 Primary map



X Index: 256



Y Index: 256

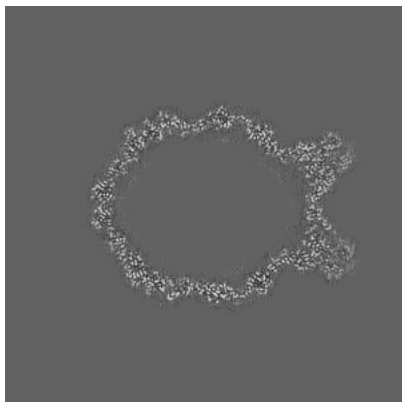


Z Index: 256

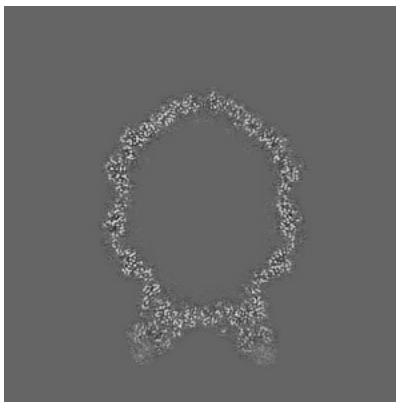
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

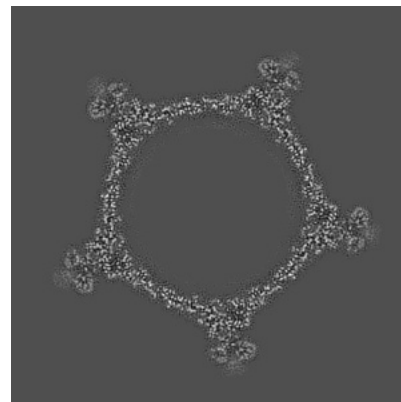
6.3.1 Primary map



X Index: 346



Y Index: 168

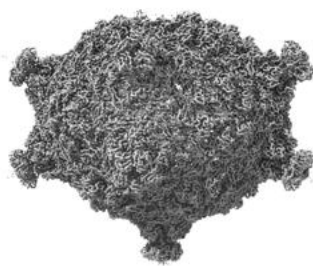


Z Index: 182

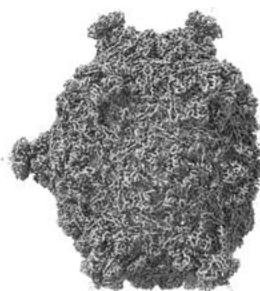
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

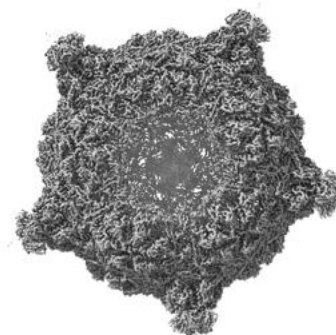
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.103. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

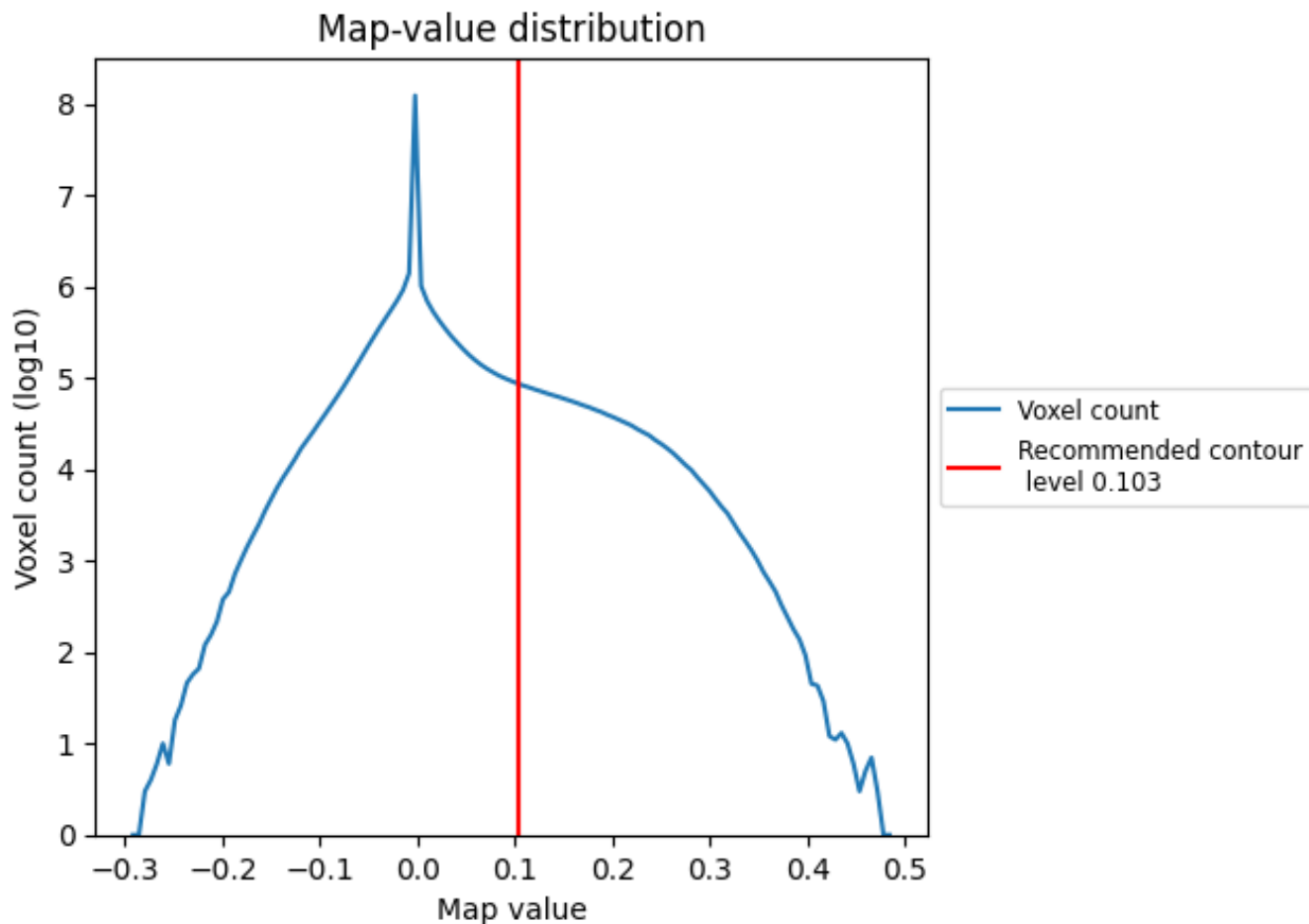
6.5 Mask visualisation

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

7 Map analysis [i](#)

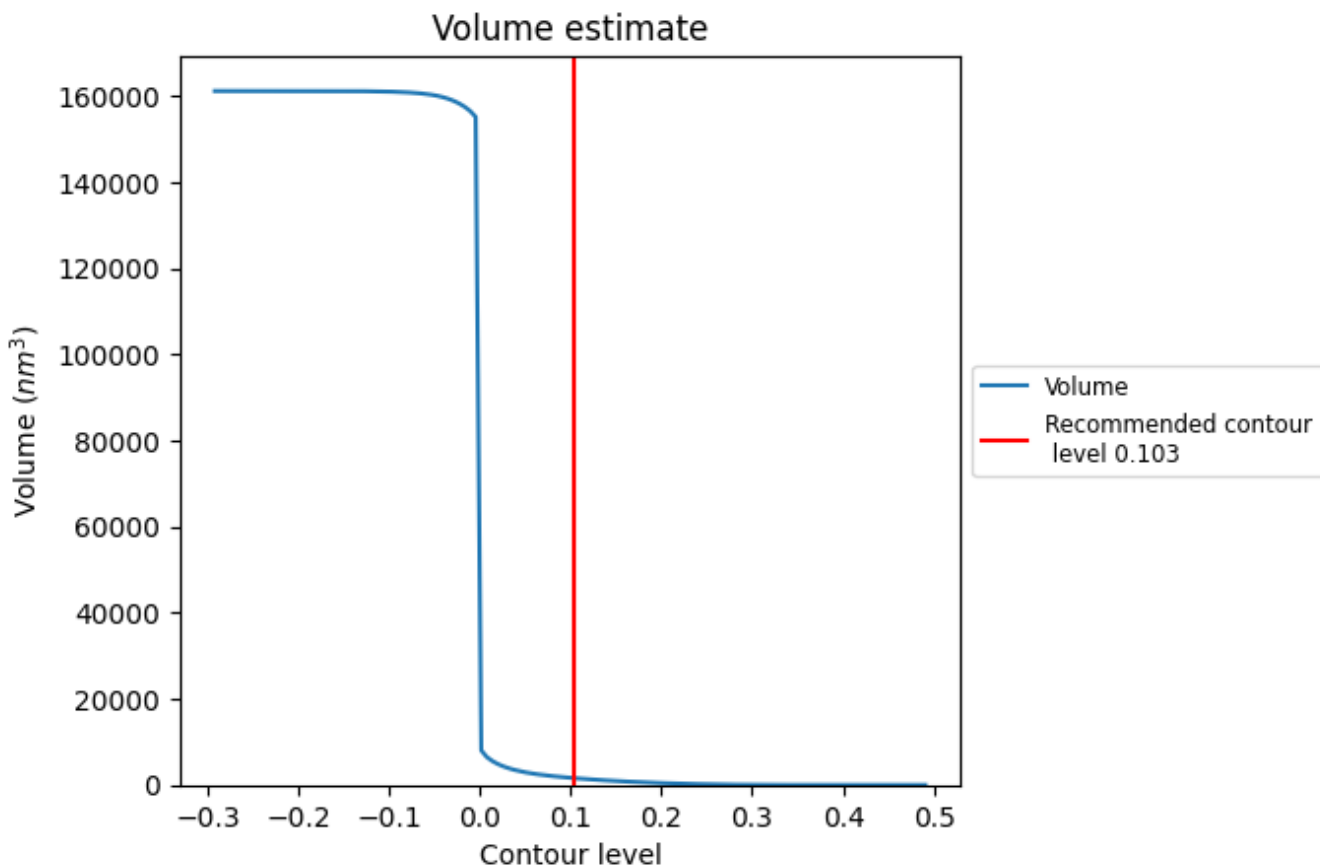
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

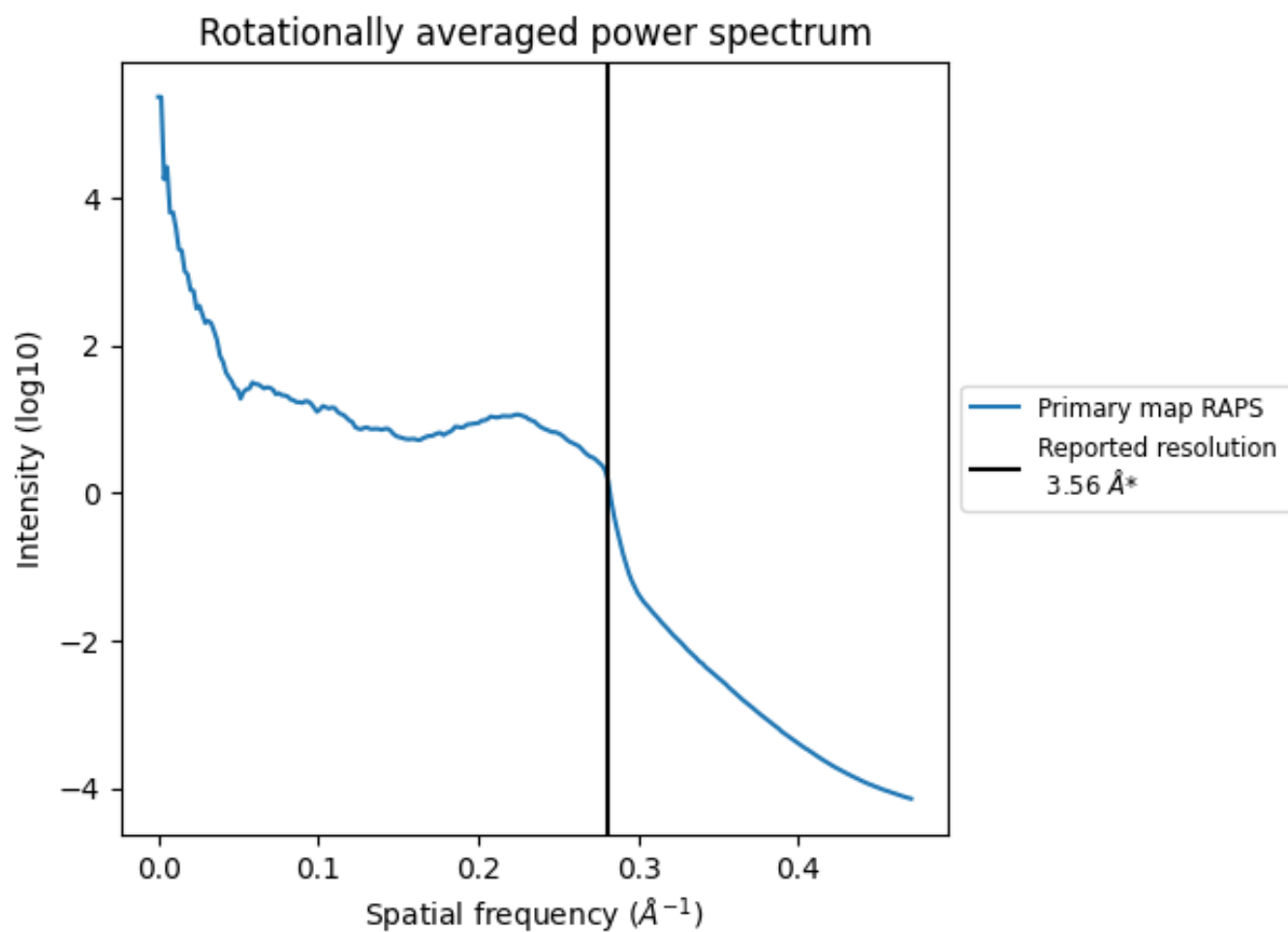
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1599 nm^3 ; this corresponds to an approximate mass of 1444 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

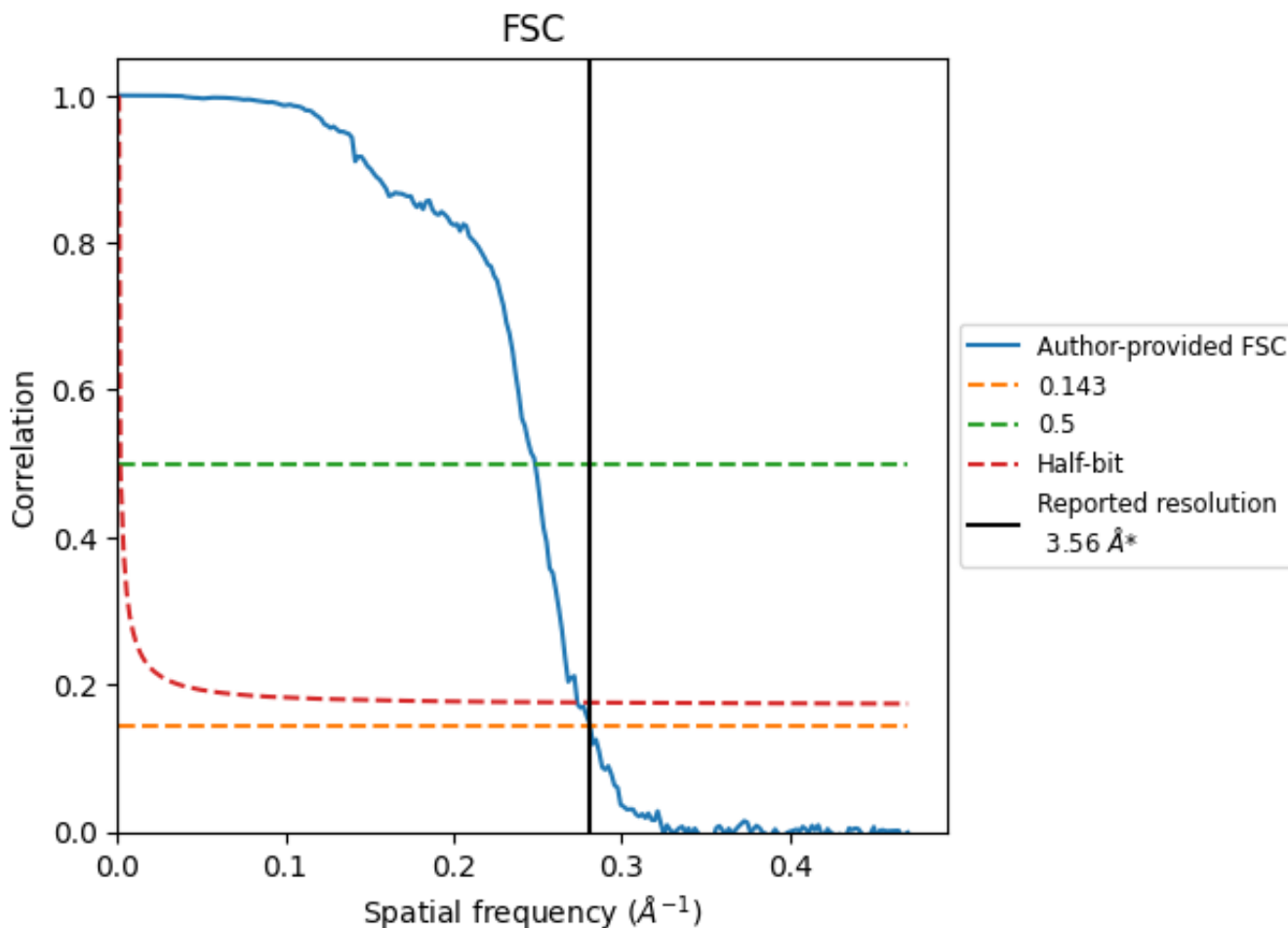


*Reported resolution corresponds to spatial frequency of 0.281\AA^{-1}

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 0.281 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.55	4.02	3.65
Unmasked-calculated*	-	-	-

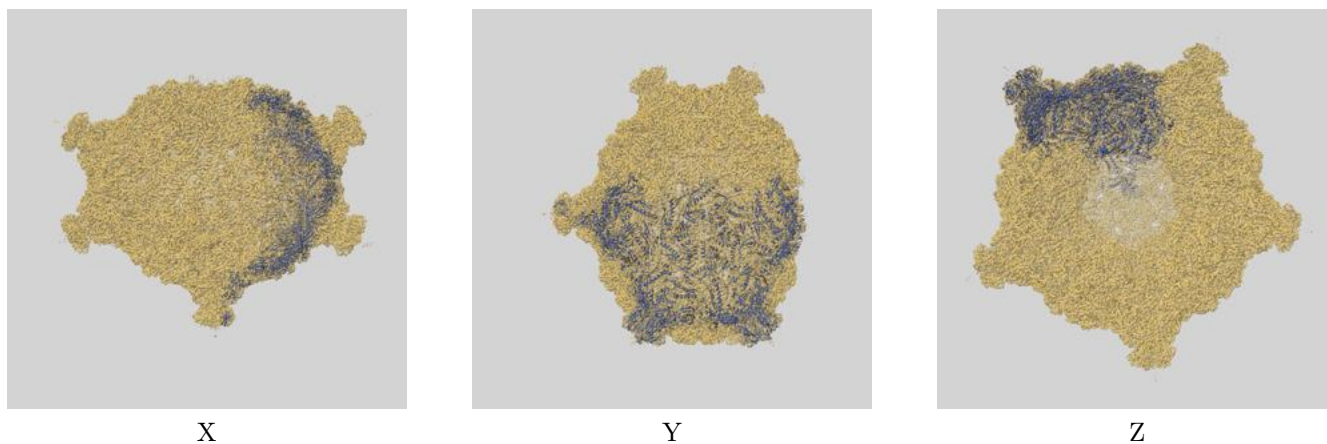
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

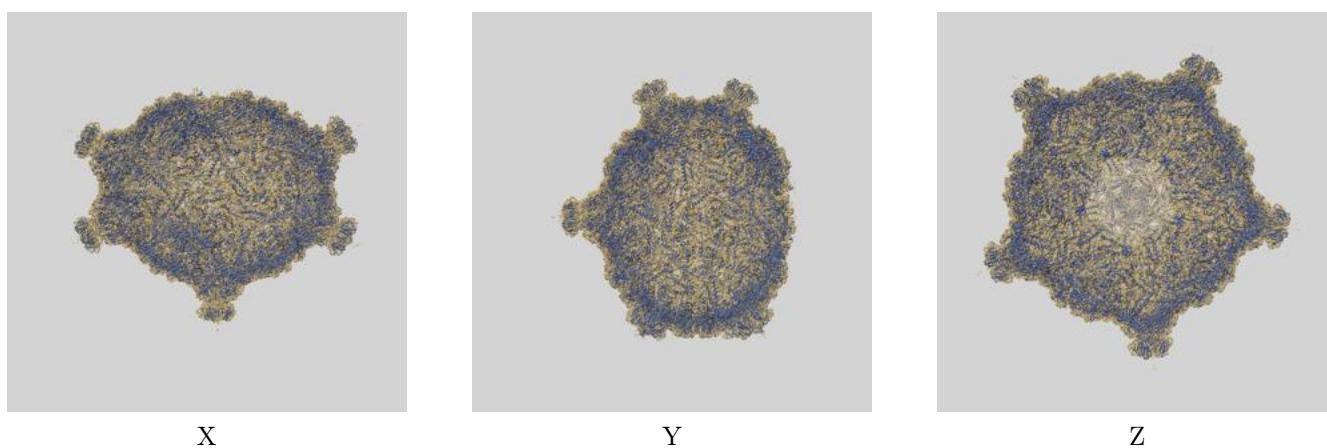
This section contains information regarding the fit between EMDB map EMD-10442 and PDB model 6TB9. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

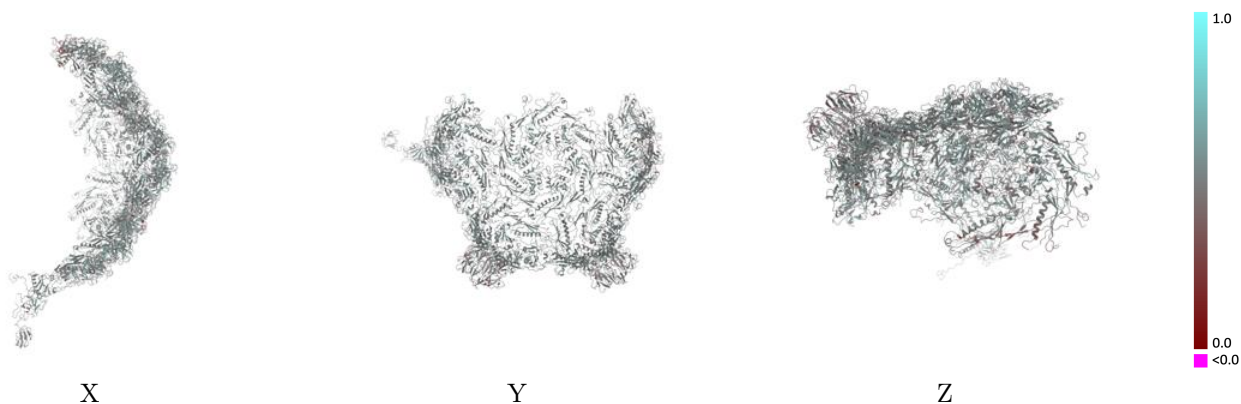


9.1.2 Map-model assembly overlay [i](#)



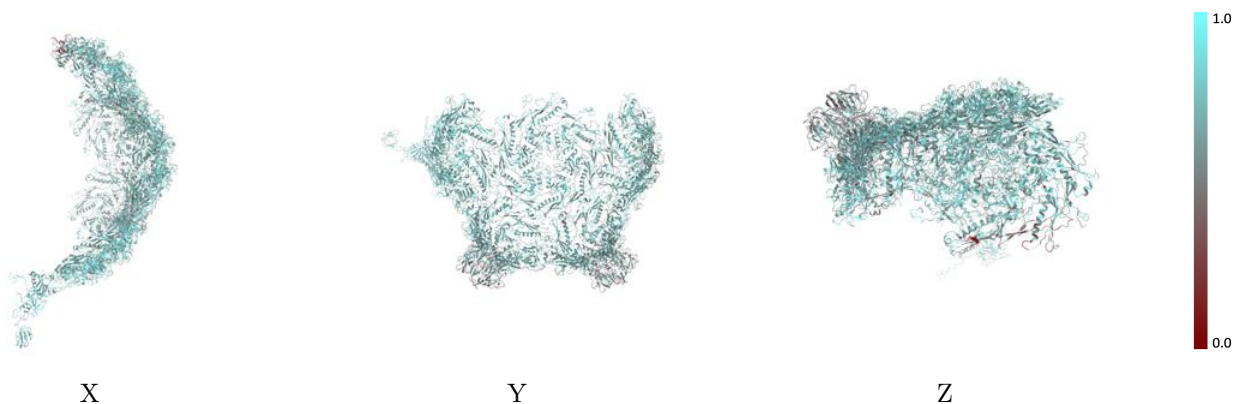
The images above show the 3D surface view of the map at the recommended contour level 0.103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



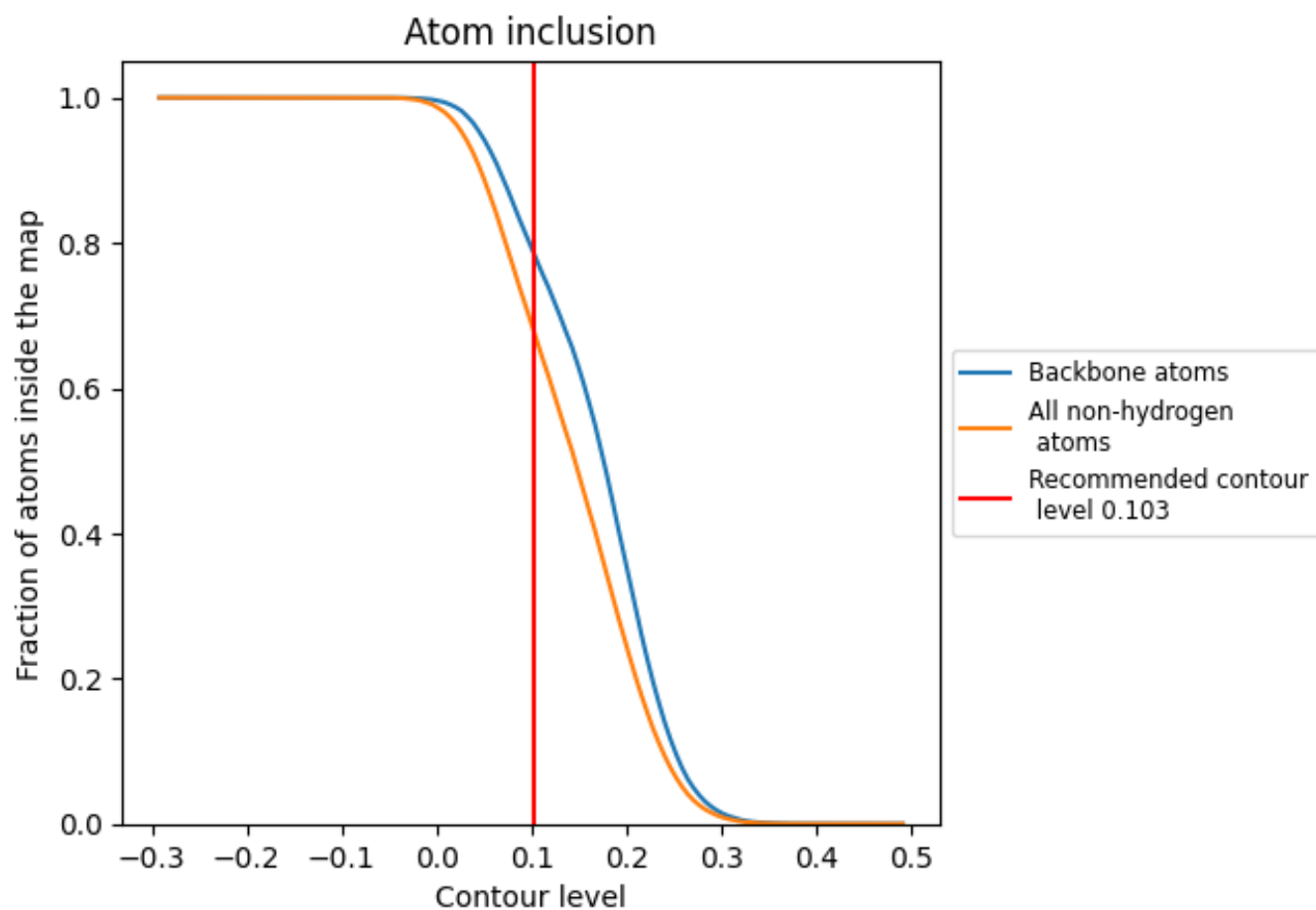
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.103).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6749	 0.4960
A1	 0.6570	 0.4630
A2	 0.5620	 0.4630
A3	 0.5250	 0.4470
A4	 0.7216	 0.5060
A5	 0.6140	 0.4670
B2	 0.5362	 0.4630
B3	 0.5411	 0.4450
B4	 0.7235	 0.5080
B5	 0.6355	 0.4810
C2	 0.5314	 0.4470
C3	 0.5378	 0.4570
C4	 0.7225	 0.5030
C5	 0.6999	 0.5010
D2	 0.5395	 0.4660
D3	 0.5378	 0.4520
D4	 0.7008	 0.5060
E2	 0.5362	 0.4560
E3	 0.5572	 0.4670
E4	 0.7101	 0.5070
F2	 0.3387	 0.4050
F3	 0.2581	 0.3720
F4	 0.7105	 0.5060
G4	 0.7156	 0.5100
H4	 0.6836	 0.4990
I4	 0.6671	 0.4980
J4	 0.6765	 0.5010
K4	 0.6756	 0.4990
L4	 0.6859	 0.5040
M4	 0.6930	 0.5030
N4	 0.6958	 0.4970
O4	 0.7027	 0.5040
P4	 0.6902	 0.5020
Q4	 0.6939	 0.4980
R4	 0.6953	 0.5010



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Chain	Atom inclusion	Q-score
S4	 0.6695	 0.4970
T4	 0.6793	 0.4980
U4	 0.6681	 0.5070
V4	 0.6812	 0.4970
W4	 0.6751	 0.4930
X4	 0.6902	 0.5040
Y4	 0.7054	 0.5050
Z4	 0.6981	 0.5030