



## Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 04:15 am BST

PDB ID : 6TSU  
EMDB ID : EMD-10565  
Title : Capsid of empty GTA particle computed with C5 symmetry  
Authors : Bardy, P.; Fuzik, T.; Hrebik, D.; Pantucek, R.; Beatty, J.T.; Plevka, P.  
Deposited on : 2019-12-21  
Resolution : 3.42 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

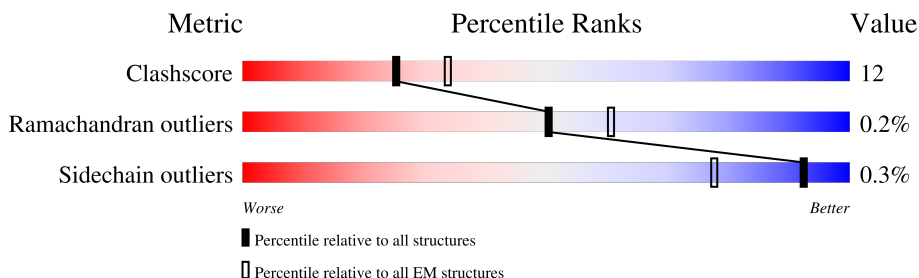
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 Å.

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





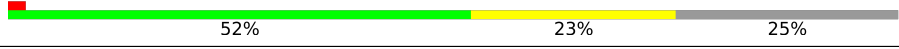

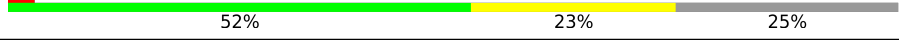

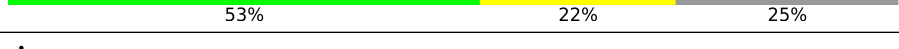
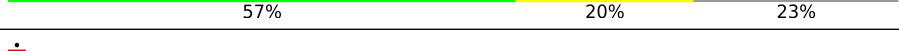
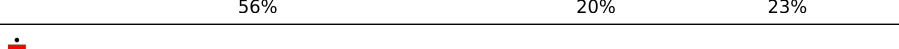
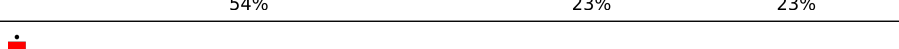
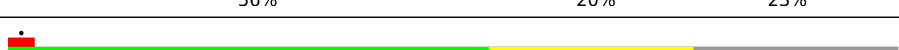

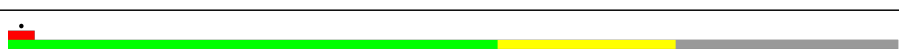
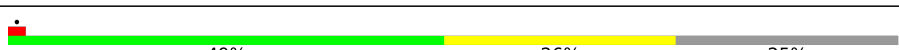
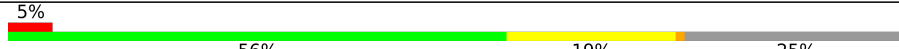





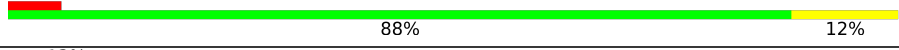
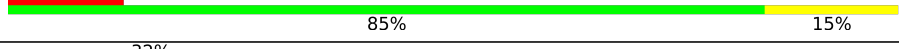



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	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	
1	G4	386	
1	H4	386	
1	I4	386	
1	J4	386	
1	K4	386	
1	L4	386	
1	M4	386	
1	N4	386	
1	O4	386	
1	P4	386	
1	Q4	386	
1	R4	386	
1	S4	386	
1	T4	386	
1	U4	386	
1	V4	386	
1	W4	386	
1	X4	386	
1	Y4	386	
1	Z4	386	
2	A1	84	
2	A2	84	
2	A3	84	
2	B2	84	

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Mol	Chain	Length	Quality of chain
2	B3	84	
2	C2	84	
2	C3	84	
2	D2	84	
2	D3	84	
2	E2	84	
2	E3	84	
3	F2	325	
3	F3	325	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 70607 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
1	C5	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	X4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Y4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Z4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	A5	294	Total	C	N	O	S	0	0
			2184	1385	373	420	6		
1	B5	270	Total	C	N	O	S	0	0
			2012	1281	344	381	6		
1	N4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	R4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	M4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Q4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	O4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	P4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	W4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	U4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	T4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	S4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	K4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		

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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 Uncharacterized protein.

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		
2	E2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	E3	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D3	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	A3	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		

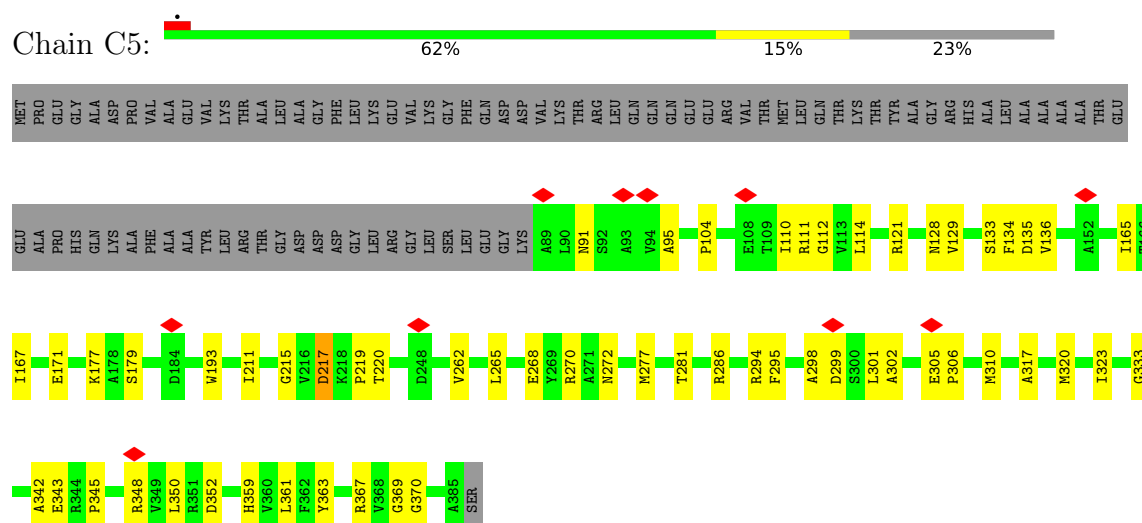
- Molecule 3 is a protein called Uncharacterized protein.

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

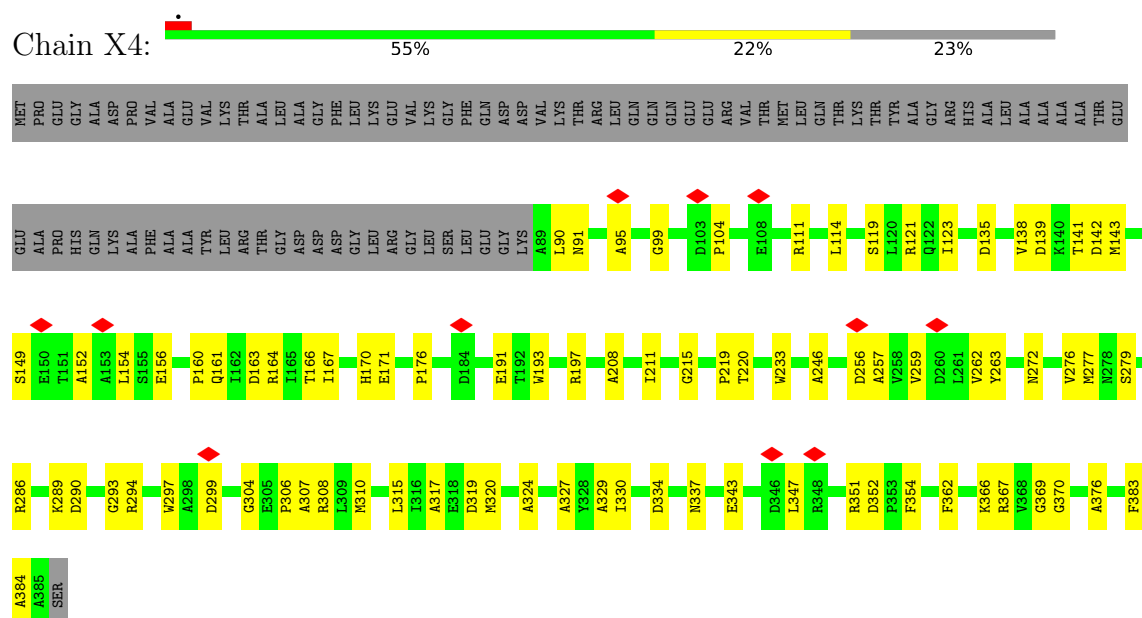
### 3 Residue-property plots

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

#### • Molecule 1: Major capsid protein Rcc01687

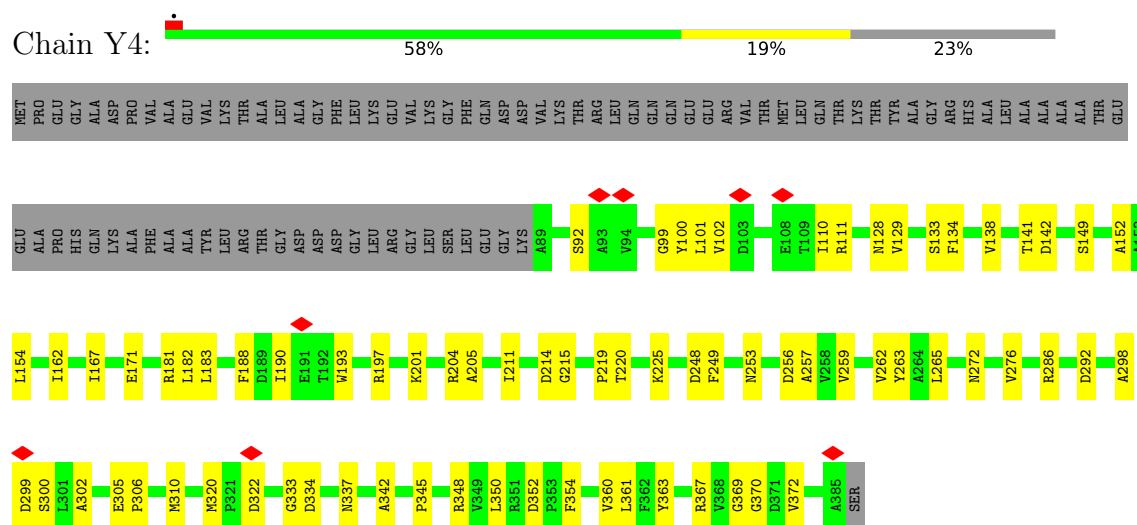


#### • Molecule 1: Major capsid protein Rcc01687

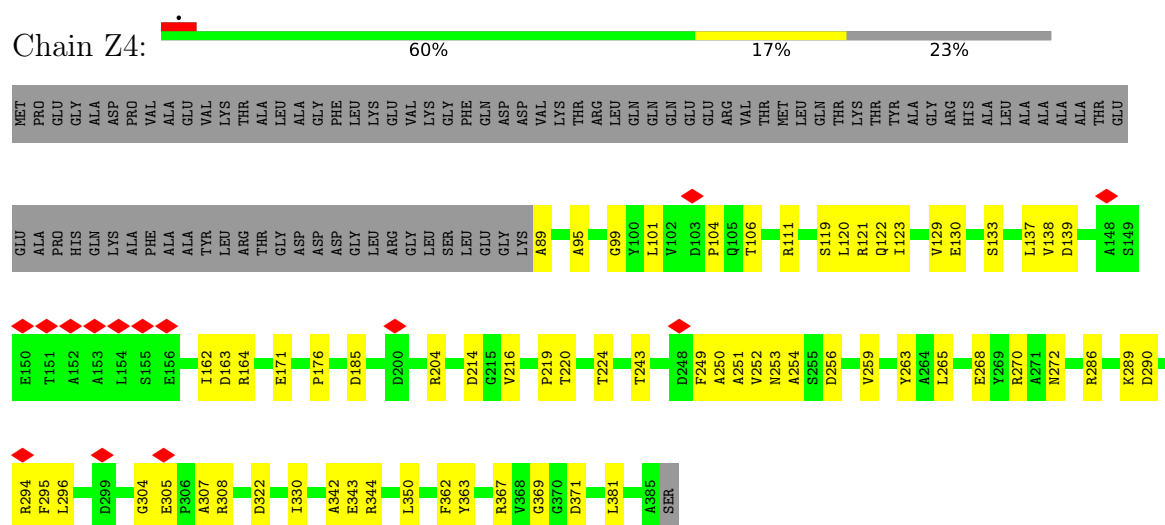




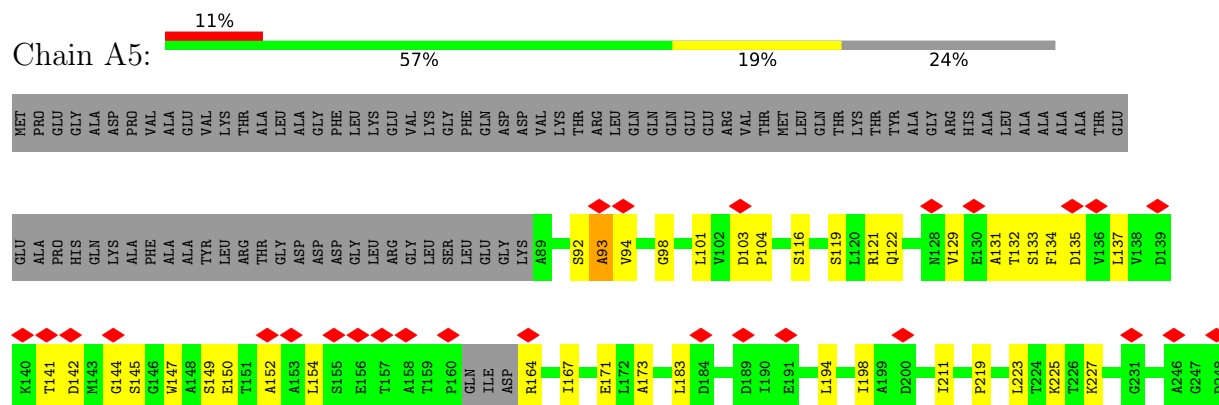
- Molecule 1: Major capsid protein Rcc01687

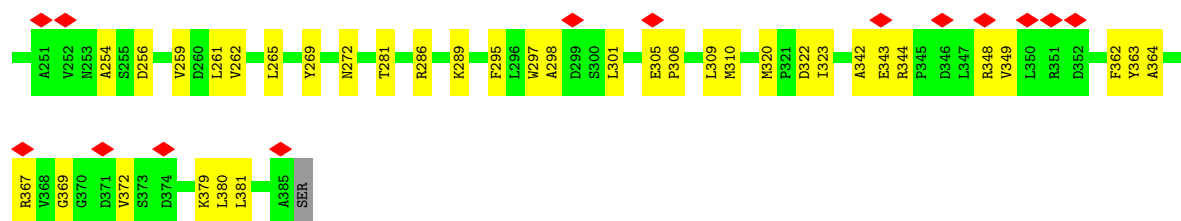


- Molecule 1: Major capsid protein Rcc01687

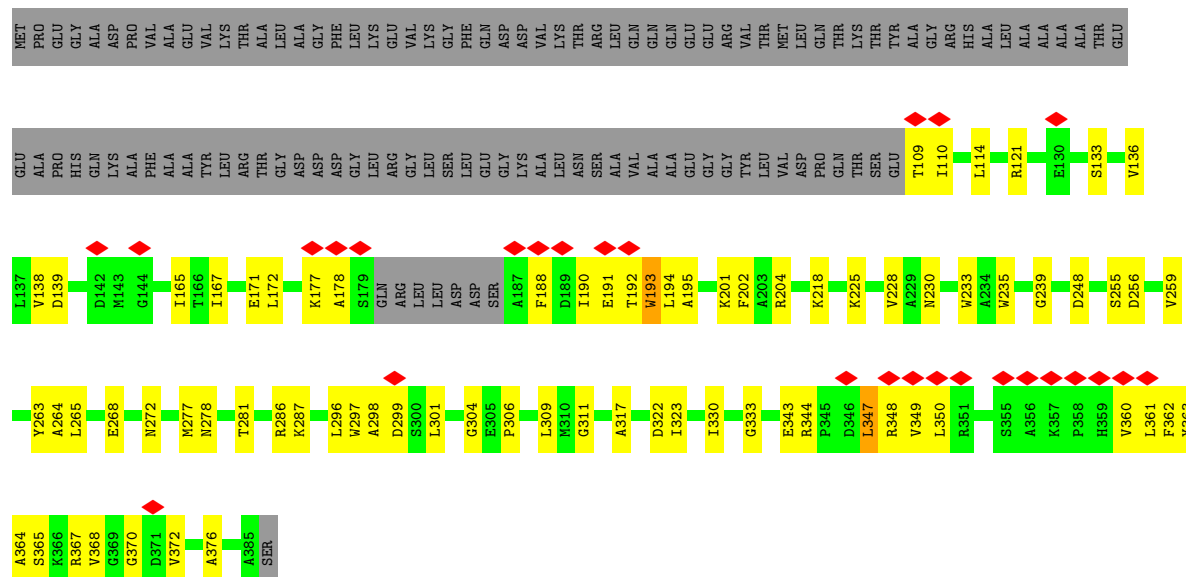


- Molecule 1: Major capsid protein Rcc01687

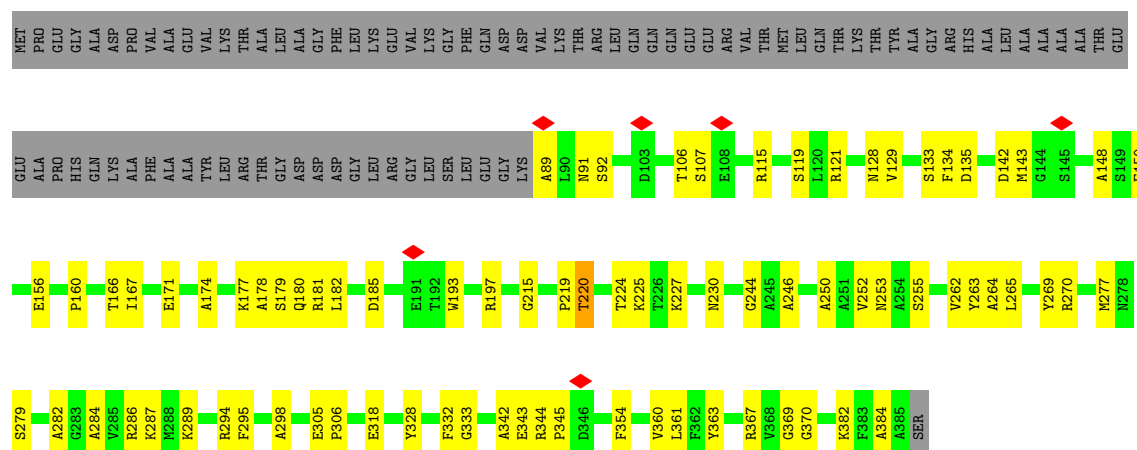




• Molecule 1: Major capsid protein Rcc01687

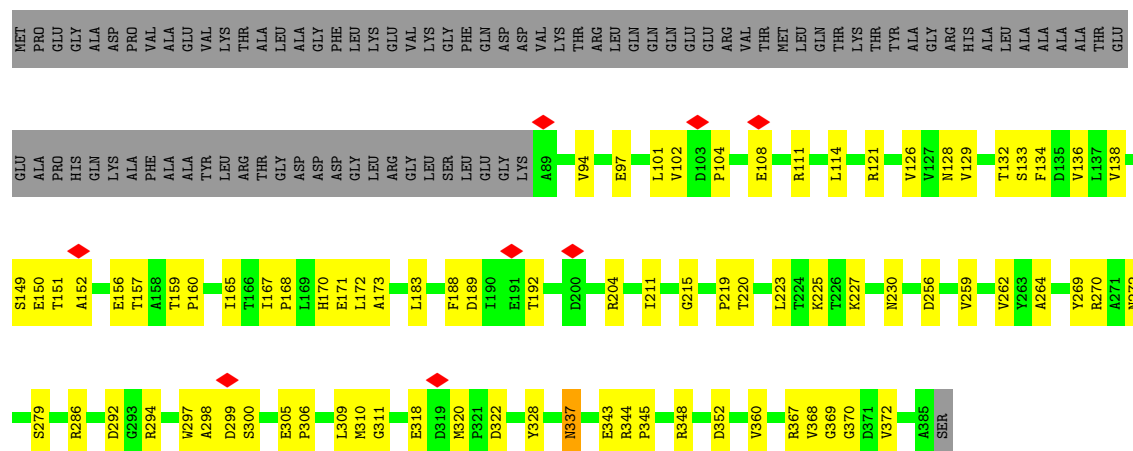


• Molecule 1: Major capsid protein Rcc01687



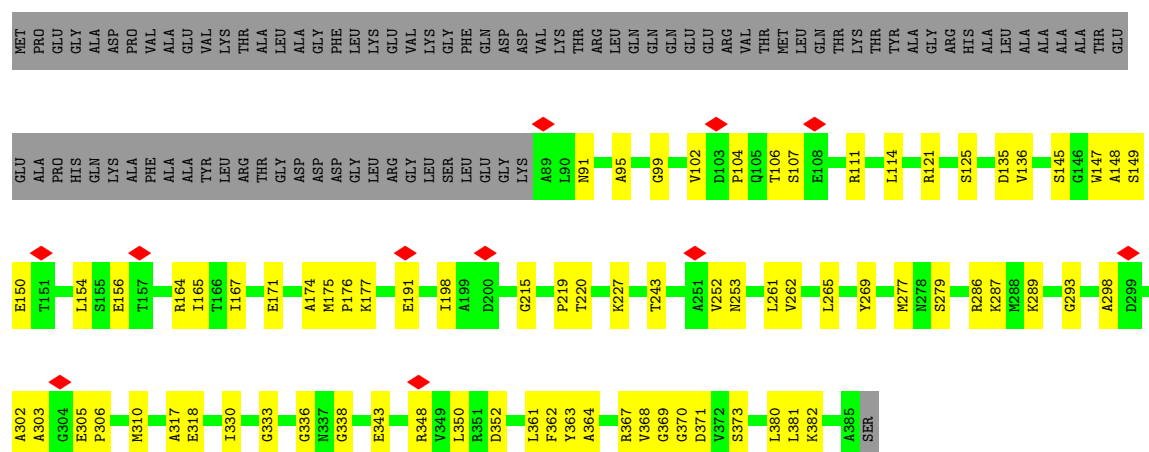
• Molecule 1: Major capsid protein Rcc01687





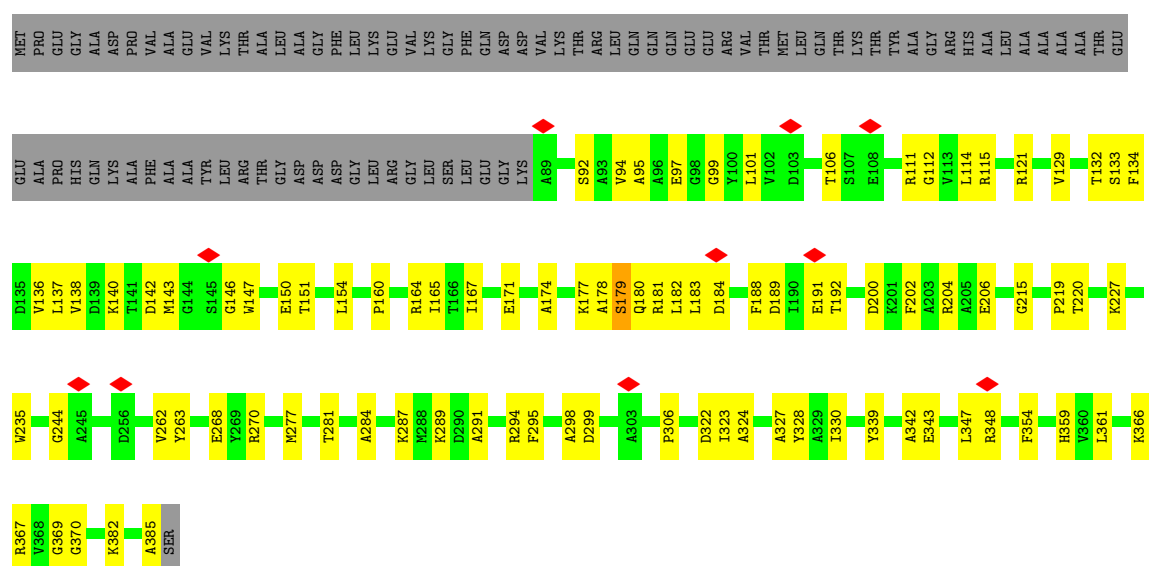
• Molecule 1: Major capsid protein Rcc01687

Chain M4: 57% 20% 23%

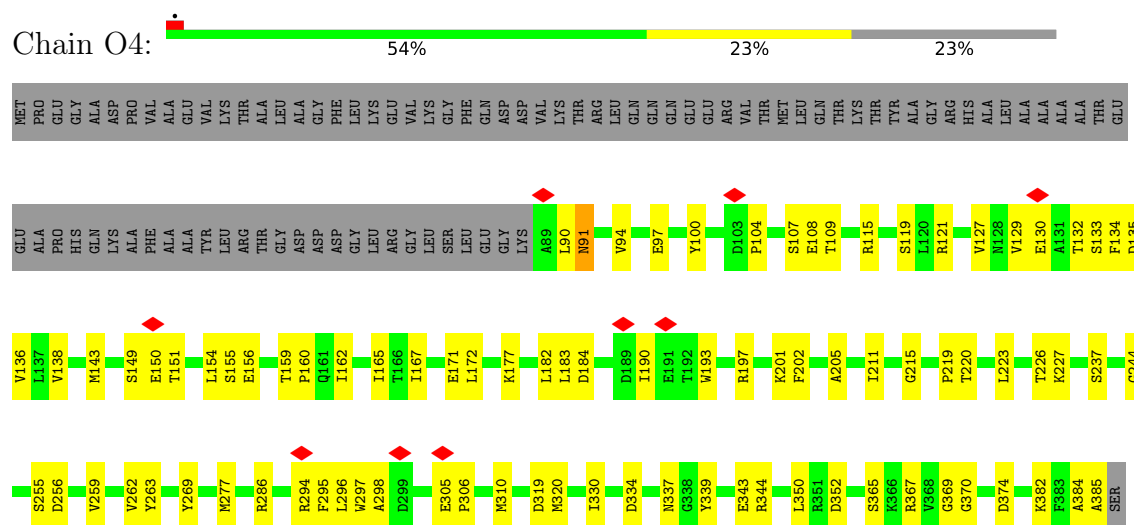


• Molecule 1: Major capsid protein Rcc01687

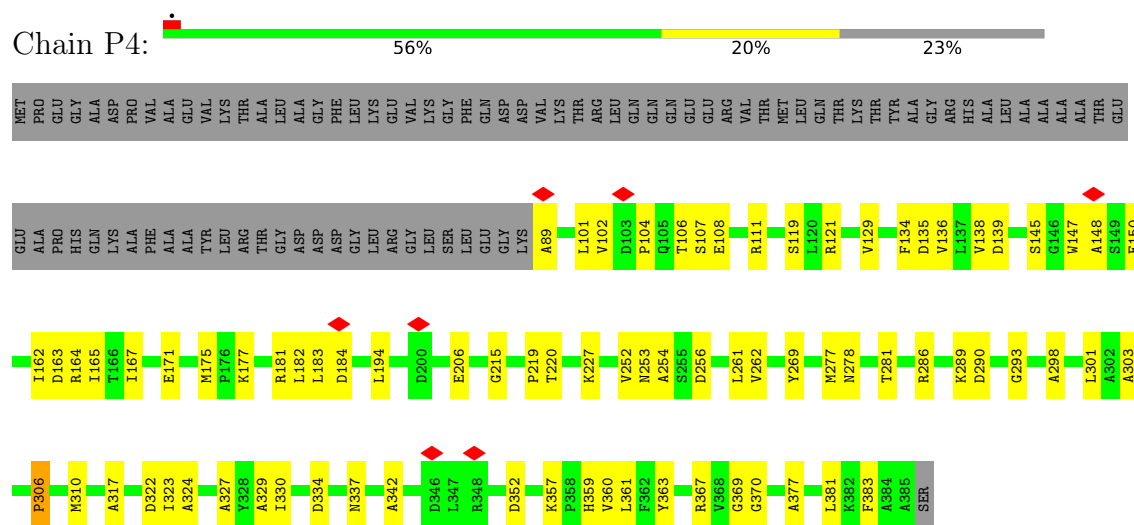
Chain Q4: 54% 23% 23%



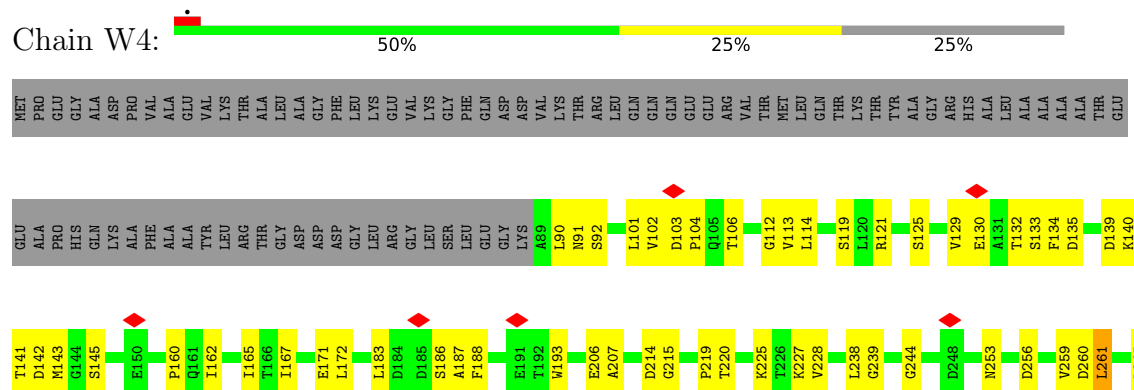
- Molecule 1: Major capsid protein Rcc01687



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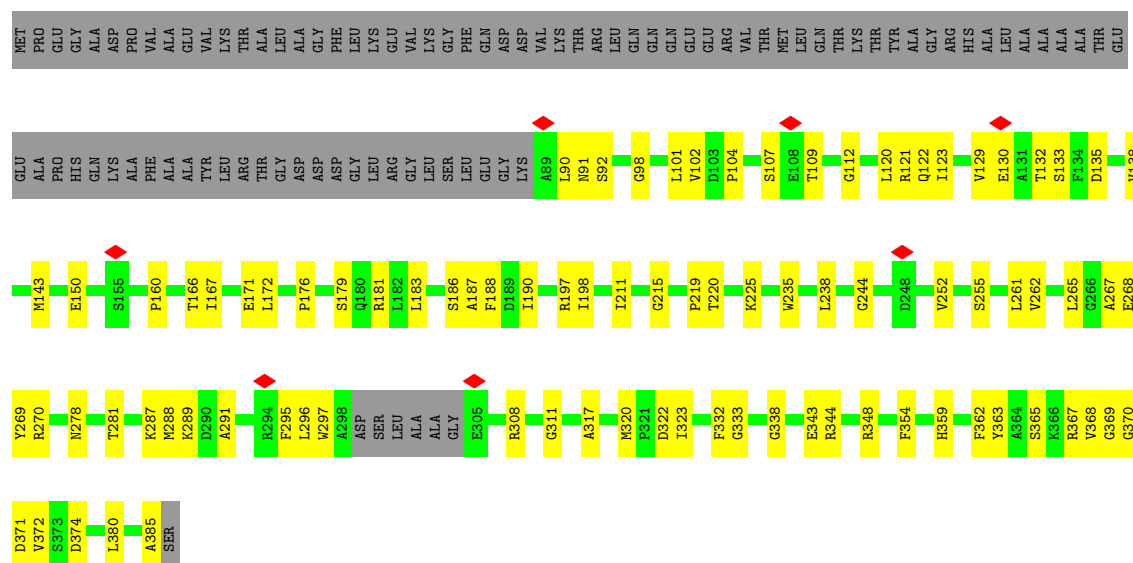






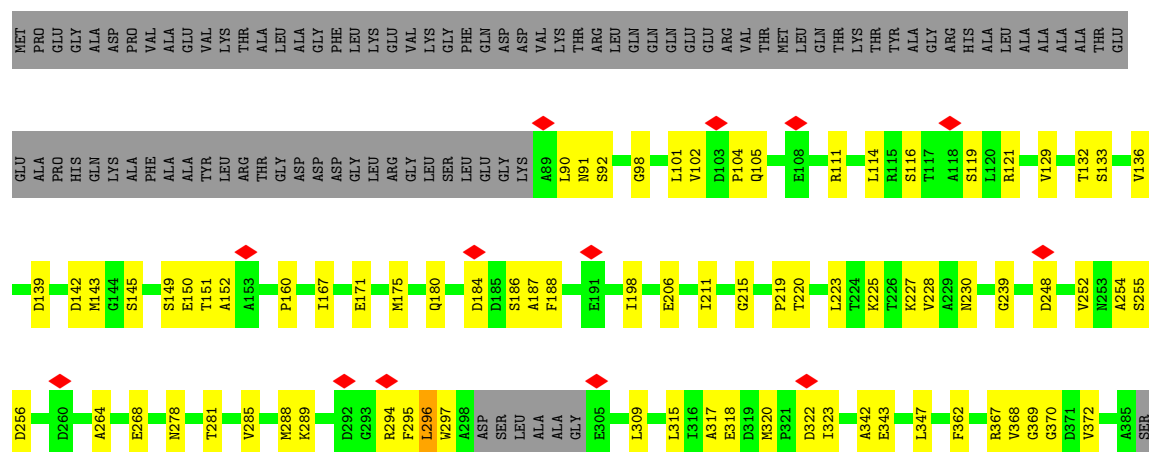


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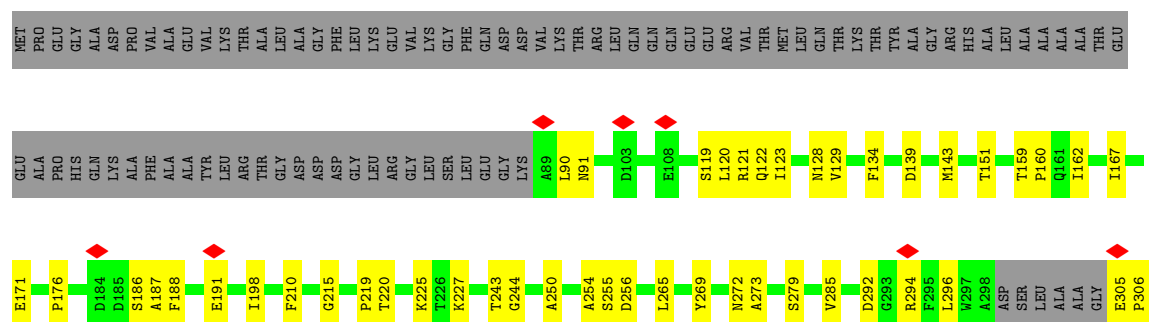
• Molecule 1: Major capsid protein Rcc01687

Chain I4: 



• Molecule 1: Major capsid protein Rcc01687

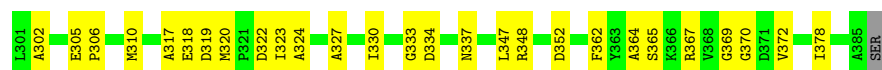
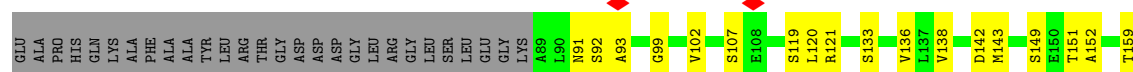
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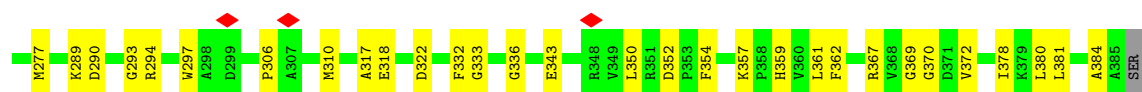
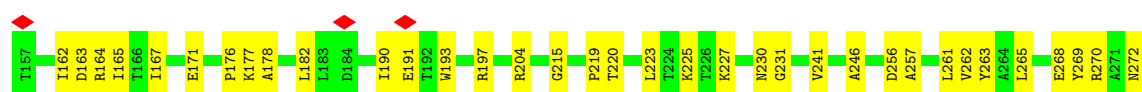




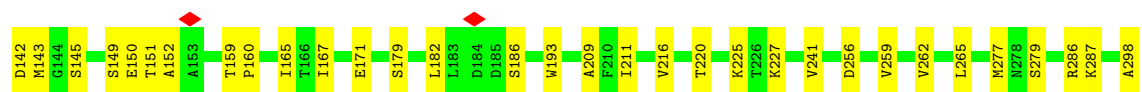
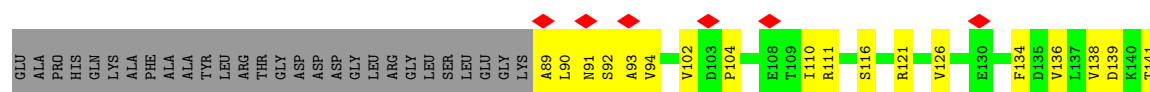
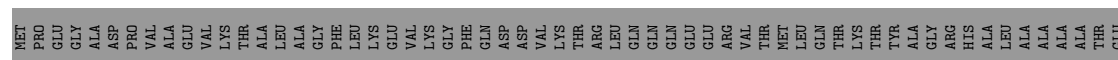
• Molecule 1: Major capsid protein Rcc01687



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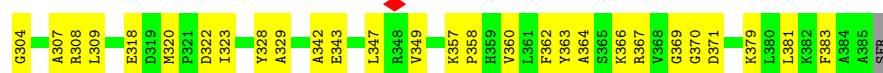
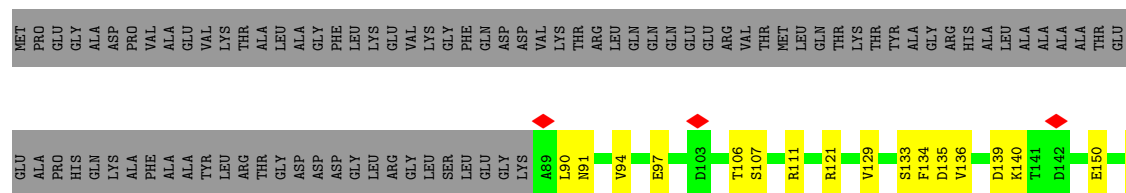
• Molecule 1: Major capsid protein Rcc01687





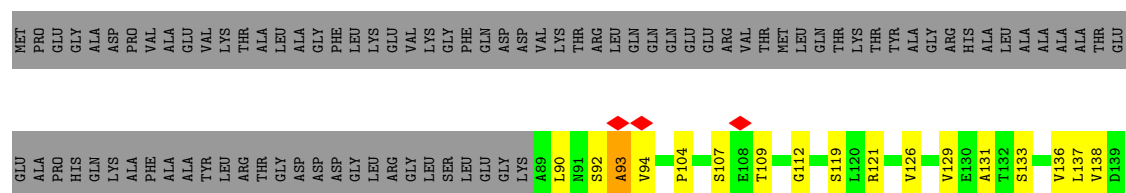
• Molecule 1: Major capsid protein Rcc01687

Chain G4: 56% 20% 23%



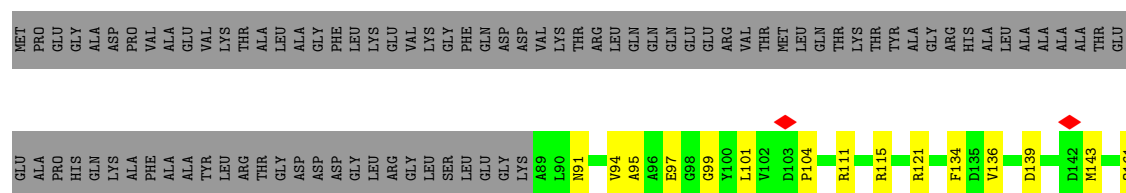
• Molecule 1: Major capsid protein Rcc01687

Chain B4: 59% 18% 23%



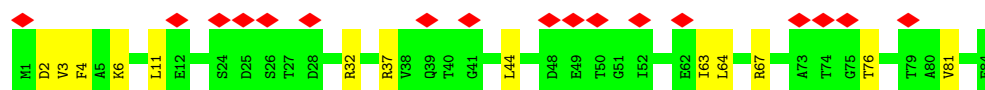
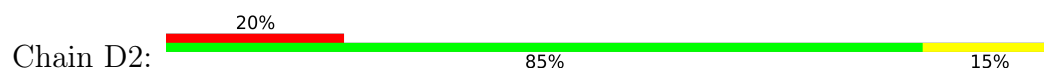
• Molecule 1: Major capsid protein Rcc01687

Chain C4: 59% 18% 23%

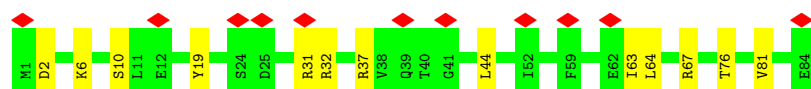
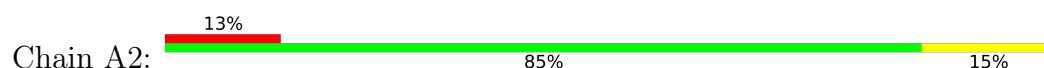




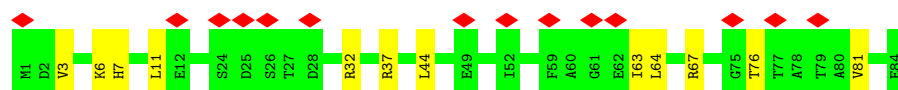
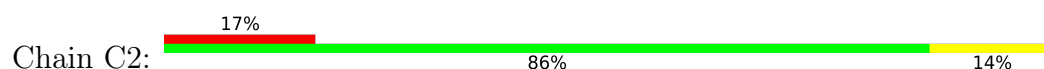
- Molecule 2: Uncharacterized protein



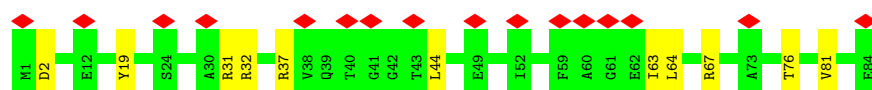
- Molecule 2: Uncharacterized protein



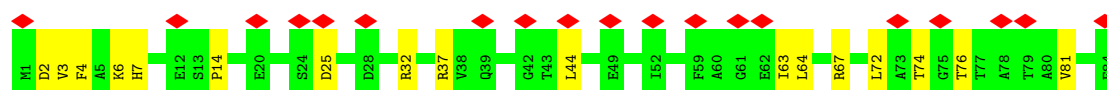
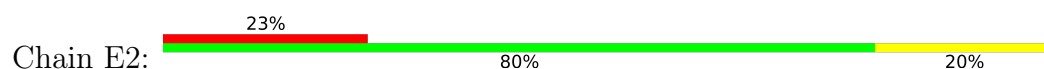
- Molecule 2: Uncharacterized protein



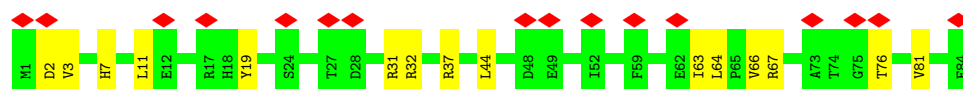
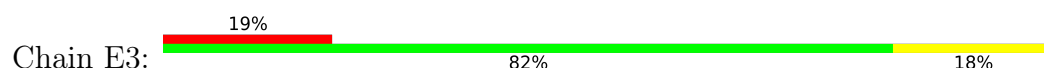
- Molecule 2: Uncharacterized protein



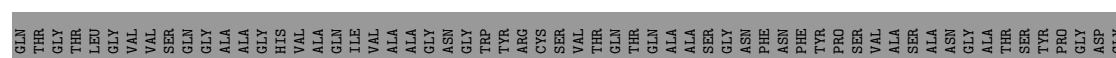
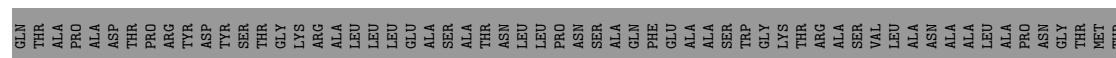
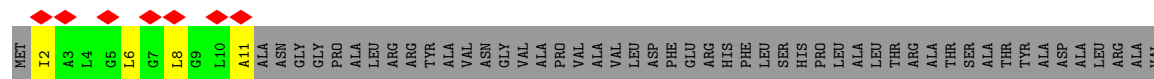
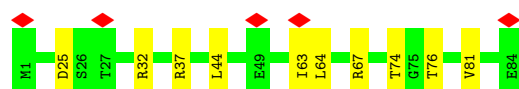
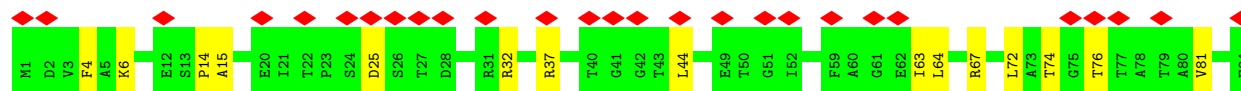
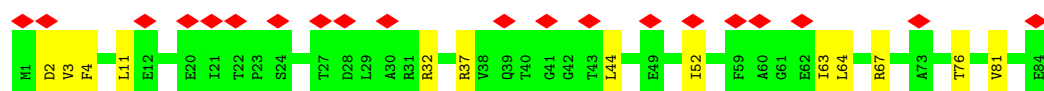
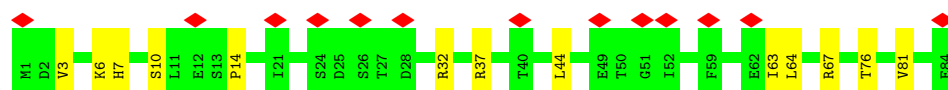
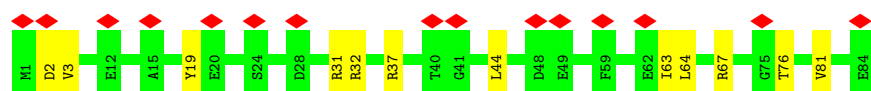
- Molecule 2: Uncharacterized protein



- Molecule 2: Uncharacterized protein



- Molecule 2: Uncharacterized protein



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- Molecule 3: Uncharacterized protein

Chain F3:  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	47071	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	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.560	Depositor
Minimum map value	-0.341	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.113	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	0.47	0/2216	0.59	0/3012
1	A5	0.40	0/2227	0.55	0/3027
1	B4	0.48	0/2253	0.56	0/3064
1	B5	0.45	0/2053	0.61	0/2789
1	C4	0.46	0/2253	0.53	0/3064
1	C5	0.45	0/2253	0.54	0/3064
1	D4	0.45	0/2253	0.53	0/3064
1	E4	0.45	0/2253	0.52	0/3064
1	F4	0.46	0/2253	0.54	0/3064
1	G4	0.47	0/2253	0.58	0/3064
1	H4	0.45	0/2216	0.52	0/3012
1	I4	0.45	0/2216	0.59	1/3012 (0.0%)
1	J4	0.43	0/2216	0.52	0/3012
1	K4	0.43	0/2216	0.52	0/3012
1	L4	0.43	0/2216	0.52	0/3012
1	M4	0.44	0/2253	0.54	0/3064
1	N4	0.44	0/2253	0.55	0/3064
1	O4	0.43	0/2253	0.53	0/3064
1	P4	0.45	0/2253	0.53	0/3064
1	Q4	0.45	0/2253	0.53	0/3064
1	R4	0.44	0/2253	0.55	0/3064
1	S4	0.42	0/2216	0.53	0/3012
1	T4	0.45	0/2216	0.52	0/3012
1	U4	0.44	0/2216	0.58	1/3012 (0.0%)
1	V4	0.42	0/2216	0.53	0/3012
1	W4	0.43	0/2216	0.53	0/3012
1	X4	0.44	0/2253	0.53	0/3064
1	Y4	0.44	0/2253	0.53	0/3064
1	Z4	0.43	0/2253	0.59	0/3064
2	A1	0.43	0/652	0.68	1/892 (0.1%)
2	A2	0.43	0/652	0.68	1/892 (0.1%)
2	A3	0.43	0/652	0.68	1/892 (0.1%)
2	B2	0.43	0/652	0.68	1/892 (0.1%)
2	B3	0.43	0/652	0.68	1/892 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	C2	0.43	0/652	0.68	1/892 (0.1%)
2	C3	0.43	0/652	0.68	1/892 (0.1%)
2	D2	0.43	0/652	0.68	1/892 (0.1%)
2	D3	0.43	0/652	0.68	1/892 (0.1%)
2	E2	0.43	0/652	0.68	1/892 (0.1%)
2	E3	0.43	0/652	0.68	1/892 (0.1%)
3	F2	0.40	0/61	1.46	2/81 (2.5%)
3	F3	0.40	0/61	1.46	2/81 (2.5%)
All	All	0.44	0/71998	0.56	17/97946 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F3	8	LEU	CA-CB-CG	6.74	130.81	115.30
3	F2	8	LEU	CA-CB-CG	6.73	130.78	115.30
1	I4	296	LEU	CA-CB-CG	6.57	130.41	115.30
3	F3	6	LEU	CA-CB-CG	5.99	129.08	115.30
3	F2	6	LEU	CA-CB-CG	5.97	129.03	115.30
2	C3	64	LEU	CA-CB-CG	5.57	128.10	115.30
2	B2	64	LEU	CA-CB-CG	5.55	128.07	115.30
2	D3	64	LEU	CA-CB-CG	5.55	128.06	115.30
2	A2	64	LEU	CA-CB-CG	5.54	128.05	115.30
2	E3	64	LEU	CA-CB-CG	5.54	128.05	115.30
2	D2	64	LEU	CA-CB-CG	5.54	128.03	115.30
2	C2	64	LEU	CA-CB-CG	5.54	128.03	115.30
2	A3	64	LEU	CA-CB-CG	5.53	128.02	115.30
2	E2	64	LEU	CA-CB-CG	5.53	128.02	115.30
2	B3	64	LEU	CA-CB-CG	5.53	128.01	115.30
2	A1	64	LEU	CA-CB-CG	5.52	128.00	115.30
1	U4	296	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A4	2173	0	2142	37	0
1	A5	2184	0	2152	65	0
1	B4	2209	0	2176	48	0
1	B5	2012	0	1990	70	0
1	C4	2209	0	2176	50	0
1	C5	2209	0	2176	46	0
1	D4	2209	0	2176	57	0
1	E4	2209	0	2176	64	0
1	F4	2209	0	2176	64	0
1	G4	2209	0	2176	50	0
1	H4	2173	0	2142	71	0
1	I4	2173	0	2142	68	0
1	J4	2173	0	2142	70	0
1	K4	2173	0	2142	63	0
1	L4	2173	0	2142	67	0
1	M4	2209	0	2176	61	0
1	N4	2209	0	2176	67	0
1	O4	2209	0	2176	67	0
1	P4	2209	0	2176	74	0
1	Q4	2209	0	2176	74	0
1	R4	2209	0	2176	60	0
1	S4	2173	0	2142	65	0
1	T4	2173	0	2142	77	0
1	U4	2173	0	2142	66	0
1	V4	2173	0	2142	69	0
1	W4	2173	0	2142	77	0
1	X4	2209	0	2176	61	0
1	Y4	2209	0	2176	60	0
1	Z4	2209	0	2176	58	0
2	A1	640	0	653	7	0
2	A2	640	0	653	12	0
2	A3	640	0	653	13	0
2	B2	640	0	653	8	0
2	B3	640	0	653	11	0
2	C2	640	0	653	14	0
2	C3	640	0	653	11	0
2	D2	640	0	653	15	0
2	D3	640	0	653	14	0
2	E2	640	0	653	16	0
2	E3	640	0	653	14	0
3	F2	62	0	73	1	0
3	F3	62	0	73	1	0
All	All	70607	0	69849	1615	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 12.

All (1615) 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:J4:102:VAL:HB	1:I4:132:THR:HG21	1.47	0.94
1:Q4:179:SER:HA	1:Q4:359:HIS:HA	1.49	0.93
1:P4:286:ARG:HH11	1:P4:303:ALA:HB1	1.35	0.90
1:B5:348:ARG:HA	1:B5:348:ARG:NE	1.86	0.89
1:O4:296:LEU:HB3	1:P4:301:LEU:HG	1.55	0.89
1:Z4:290:ASP:HB3	1:Z4:296:LEU:HD11	1.55	0.89
1:F4:220:THR:HG23	1:F4:371:ASP:HB3	1.53	0.88
1:G4:150:GLU:HG3	1:C4:91:ASN:HB2	1.57	0.85
1:Z4:289:LYS:HA	1:Z4:295:PHE:HA	1.59	0.83
1:B5:348:ARG:HA	1:B5:348:ARG:CZ	2.08	0.82
1:O4:286:ARG:HH12	1:O4:305:GLU:HA	1.44	0.82
1:U4:102:VAL:HB	1:T4:132:THR:HG21	1.61	0.81
1:U4:294:ARG:HE	1:V4:294:ARG:HH12	1.28	0.80
1:C4:215:GLY:HA2	1:C4:220:THR:HG22	1.64	0.80
1:H4:215:GLY:HA2	1:H4:220:THR:HG22	1.63	0.79
1:E4:215:GLY:HA2	1:E4:220:THR:HG22	1.66	0.78
1:Y4:101:LEU:HD23	1:Q4:188:PHE:HE2	1.47	0.78
1:B5:286:ARG:HH12	1:B5:304:GLY:H	1.32	0.77
1:E4:265:LEU:HD21	1:E4:269:TYR:HB2	1.63	0.77
1:U4:116:SER:HA	1:T4:268:GLU:HB2	1.66	0.77
1:Y4:100:TYR:HB2	1:P4:162:ILE:HD11	1.67	0.77
1:B4:140:LYS:HE3	1:B4:163:ASP:HB2	1.67	0.76
1:H4:143:MET:HG2	1:H4:160:PRO:HD3	1.67	0.76
1:L4:219:PRO:HG3	1:L4:369:GLY:HA2	1.67	0.76
1:O4:143:MET:HG2	1:O4:160:PRO:HD3	1.67	0.76
1:D4:143:MET:HG2	1:D4:160:PRO:HD3	1.65	0.76
1:A5:309:LEU:HD23	1:A5:310:MET:HG2	1.66	0.75
1:L4:265:LEU:HD11	1:L4:333:GLY:HA2	1.66	0.75
1:T4:143:MET:HG2	1:T4:160:PRO:HD3	1.67	0.75
1:W4:143:MET:HG2	1:W4:160:PRO:HD3	1.69	0.75
1:W4:102:VAL:HB	1:V4:132:THR:HG21	1.66	0.75
1:H4:268:GLU:HB2	1:I4:116:SER:HA	1.69	0.74
1:R4:149:SER:HB3	1:R4:152:ALA:HB2	1.67	0.74
1:H4:261:LEU:HD21	1:H4:332:PHE:HB3	1.68	0.74
1:J4:141:THR:HG22	1:J4:142:ASP:H	1.52	0.74
1:J4:180:GLN:NE2	1:J4:184:ASP:OD1	2.21	0.74
1:U4:149:SER:HB3	1:U4:152:ALA:HB2	1.70	0.73

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R4:104:PRO:HB3	1:Q4:133:SER:HB2	1.67	0.73
1:B5:191:GLU:HG2	1:B5:362:PHE:HZ	1.53	0.73
1:Z4:139:ASP:OD1	1:Z4:139:ASP:O	2.07	0.73
1:A4:162:ILE:HD13	1:C4:101:LEU:HD21	1.70	0.72
1:D4:265:LEU:HD11	1:D4:333:GLY:HA2	1.71	0.72
1:W4:145:SER:HB2	1:S4:172:LEU:HD11	1.72	0.72
1:O4:219:PRO:HG3	1:O4:369:GLY:HA2	1.71	0.72
1:C5:265:LEU:HD11	1:C5:333:GLY:HA2	1.71	0.72
1:B5:265:LEU:HD11	1:B5:333:GLY:HA2	1.72	0.72
1:U4:286:ARG:NH1	1:T4:263:TYR:OH	2.23	0.72
1:B4:265:LEU:HD11	1:B4:333:GLY:HA2	1.70	0.72
1:Y4:265:LEU:HD11	1:Y4:333:GLY:HA2	1.72	0.71
1:N4:215:GLY:HA2	1:N4:220:THR:HG22	1.71	0.71
1:U4:133:SER:HB2	1:V4:104:PRO:HB3	1.73	0.71
1:T4:219:PRO:HG3	1:T4:369:GLY:HA2	1.73	0.71
1:S4:265:LEU:HD11	1:S4:333:GLY:HA2	1.73	0.71
1:S4:334:ASP:OD2	1:S4:337:ASN:ND2	2.24	0.70
1:Q4:284:ALA:HA	1:Q4:287:LYS:HD3	1.73	0.70
1:V4:265:LEU:HD11	1:V4:333:GLY:HA2	1.72	0.70
1:O4:184:ASP:OD2	1:K4:348:ARG:NH2	2.24	0.70
1:Y4:162:ILE:HD13	1:W4:101:LEU:HD11	1.74	0.70
1:J4:265:LEU:HD11	1:J4:333:GLY:HA2	1.74	0.70
1:B5:191:GLU:HG2	1:B5:362:PHE:CZ	2.27	0.70
1:N4:133:SER:HB2	1:O4:104:PRO:HB3	1.74	0.70
1:L4:132:THR:HG21	1:H4:102:VAL:HB	1.75	0.69
1:F4:143:MET:HG2	1:F4:160:PRO:HD3	1.73	0.69
1:X4:263:TYR:OH	1:Y4:286:ARG:NH1	2.25	0.69
1:P4:181:ARG:HH21	1:W4:171:GLU:HG2	1.58	0.69
1:W4:106:THR:HA	1:V4:135:ASP:HB2	1.74	0.69
1:A4:279:SER:HB2	1:A4:318:GLU:OE2	1.92	0.69
1:P4:121:ARG:NH2	1:P4:206:GLU:OE2	2.26	0.69
1:K4:215:GLY:HA2	1:K4:220:THR:HG22	1.73	0.69
1:E4:223:LEU:O	1:E4:227:LYS:NZ	2.22	0.69
1:F4:150:GLU:HG3	1:F4:151:THR:HG23	1.74	0.69
1:Y4:182:LEU:HB2	1:Q4:92:SER:HB3	1.75	0.69
1:O4:150:GLU:HG3	1:O4:151:THR:HG23	1.74	0.69
1:Z4:256:ASP:HA	1:Z4:259:VAL:HG12	1.75	0.69
1:J4:256:ASP:HA	1:J4:259:VAL:HG12	1.74	0.68
1:J4:143:MET:HG2	1:J4:160:PRO:HD3	1.73	0.68
1:B4:279:SER:HB2	1:B4:318:GLU:OE2	1.92	0.68
1:S4:261:LEU:HD21	1:S4:332:PHE:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J4:183:LEU:HD22	1:J4:360:VAL:HG21	1.74	0.68
1:Z4:121:ARG:NH1	1:Z4:343:GLU:OE1	2.27	0.68
1:C5:286:ARG:NH1	1:C5:305:GLU:OE2	2.27	0.68
1:F4:265:LEU:HD11	1:F4:333:GLY:HA2	1.76	0.68
1:J4:275:PHE:HB2	1:J4:314:VAL:HG22	1.75	0.68
1:D4:171:GLU:HA	1:D4:367:ARG:HA	1.76	0.68
1:K4:149:SER:HB3	1:K4:152:ALA:HB2	1.76	0.68
1:D4:142:ASP:OD2	1:E4:204:ARG:NH2	2.28	0.67
1:R4:294:ARG:HH21	1:Q4:294:ARG:HD3	1.58	0.67
1:Q4:219:PRO:HG3	1:Q4:369:GLY:HA2	1.76	0.67
1:T4:265:LEU:HD11	1:T4:333:GLY:HA2	1.76	0.67
1:V4:289:LYS:HA	1:V4:295:PHE:HA	1.76	0.67
1:R4:204:ARG:NH2	1:Q4:142:ASP:OD1	2.28	0.67
1:K4:145:SER:HB3	1:L4:172:LEU:HD11	1.75	0.67
1:C4:262:VAL:HG21	1:C4:310:MET:HG2	1.77	0.67
1:V4:219:PRO:HG3	1:V4:369:GLY:HA2	1.77	0.67
1:U4:279:SER:HB2	1:U4:318:GLU:OE1	1.95	0.67
1:J4:289:LYS:HA	1:J4:295:PHE:HA	1.77	0.67
1:H4:262:VAL:HG12	1:H4:270:ARG:HD3	1.75	0.67
1:G4:223:LEU:O	1:G4:227:LYS:NZ	2.22	0.67
1:L4:145:SER:HB2	1:H4:172:LEU:HD11	1.77	0.66
1:G4:220:THR:HB	1:G4:371:ASP:OD2	1.94	0.66
1:Y4:286:ARG:NH1	1:Y4:305:GLU:OE1	2.28	0.66
1:R4:223:LEU:O	1:R4:227:LYS:NZ	2.22	0.66
1:A5:121:ARG:NH1	1:A5:343:GLU:OE2	2.28	0.66
1:V4:215:GLY:HA2	1:V4:220:THR:HG22	1.77	0.66
1:F4:211:ILE:HD12	1:F4:319:ASP:HB2	1.78	0.66
1:U4:171:GLU:HA	1:U4:367:ARG:HA	1.76	0.66
1:F4:298:ALA:HB2	1:F4:306:PRO:HD3	1.78	0.66
1:W4:265:LEU:HD11	1:W4:333:GLY:HA2	1.75	0.66
1:H4:132:THR:HG21	1:I4:102:VAL:HB	1.78	0.66
1:U4:256:ASP:HA	1:U4:259:VAL:HG12	1.77	0.66
1:D4:149:SER:HB3	1:D4:152:ALA:HB2	1.78	0.66
1:T4:172:LEU:HD11	1:S4:145:SER:HB3	1.77	0.66
1:Y4:215:GLY:HA2	1:Y4:220:THR:HG22	1.76	0.66
1:B4:256:ASP:HA	1:B4:259:VAL:HG12	1.77	0.65
1:C5:270:ARG:NH1	1:X4:279:SER:OG	2.29	0.65
1:M4:106:THR:HG23	1:M4:107:SER:H	1.61	0.65
1:K4:104:PRO:HB3	1:J4:133:SER:HB2	1.77	0.65
1:K4:289:LYS:HA	1:K4:295:PHE:HA	1.78	0.65
1:A5:149:SER:HB3	1:A5:152:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N4:284:ALA:HA	1:N4:287:LYS:HD3	1.79	0.65
1:A5:297:TRP:HB2	1:B5:301:LEU:HD12	1.77	0.65
1:U4:172:LEU:HD11	1:T4:145:SER:HB3	1.79	0.65
1:C5:302:ALA:O	1:B5:311:GLY:N	2.29	0.65
1:A5:141:THR:HG22	1:A5:142:ASP:H	1.61	0.65
1:O4:215:GLY:HA2	1:O4:220:THR:HG22	1.79	0.65
1:H4:133:SER:HB3	1:I4:104:PRO:HB3	1.78	0.65
1:Y4:133:SER:HB3	1:Z4:104:PRO:HB3	1.79	0.65
1:B4:219:PRO:HG3	1:B4:369:GLY:HA2	1.78	0.65
1:Z4:344:ARG:HE	1:Z4:367:ARG:HD3	1.62	0.65
1:V4:141:THR:HG22	1:V4:142:ASP:H	1.62	0.65
1:L4:163:ASP:OD2	1:L4:235:TRP:NE1	2.29	0.65
1:W4:141:THR:HG22	1:W4:142:ASP:H	1.62	0.65
1:J4:227:LYS:HE2	1:J4:227:LYS:H	1.61	0.65
1:L4:143:MET:HG2	1:L4:160:PRO:HD3	1.77	0.65
1:X4:352:ASP:HB3	1:Q4:354:PHE:HD1	1.62	0.64
1:C4:94:VAL:HG13	1:C4:97:GLU:HB2	1.79	0.64
1:N4:178:ALA:HB3	1:N4:360:VAL:HB	1.80	0.64
1:R4:219:PRO:HG3	1:R4:369:GLY:HA2	1.80	0.64
1:Q4:227:LYS:HD2	1:Q4:328:TYR:CZ	2.32	0.64
1:D4:279:SER:OG	1:C4:270:ARG:NH1	2.30	0.64
1:N4:150:GLU:OE1	1:S4:181:ARG:HD2	1.97	0.64
1:R4:286:ARG:NH1	1:Q4:263:TYR:OH	2.25	0.64
1:R4:286:ARG:HH12	1:R4:305:GLU:HA	1.63	0.64
1:U4:294:ARG:HE	1:V4:294:ARG:NH1	1.93	0.64
1:F4:121:ARG:NH1	1:F4:343:GLU:OE1	2.31	0.64
1:G4:286:ARG:HH12	1:G4:304:GLY:H	1.45	0.64
1:R4:298:ALA:HB2	1:R4:306:PRO:HD3	1.78	0.64
1:M4:219:PRO:HG3	1:M4:369:GLY:HA2	1.79	0.64
1:B4:215:GLY:HA2	1:B4:220:THR:HG22	1.79	0.64
1:Z4:253:ASN:HB3	1:Z4:256:ASP:OD2	1.98	0.64
1:C4:167:ILE:HG23	1:C4:370:GLY:HA2	1.80	0.64
1:U4:215:GLY:HA2	1:U4:220:THR:HG22	1.78	0.64
1:Z4:219:PRO:HG3	1:Z4:369:GLY:HA2	1.80	0.64
1:X4:219:PRO:HG3	1:X4:369:GLY:HA2	1.79	0.63
1:T4:100:TYR:O	1:J4:164:ARG:NH1	2.31	0.63
1:S4:143:MET:HG2	1:S4:160:PRO:HD3	1.78	0.63
1:K4:265:LEU:HD11	1:K4:333:GLY:HA2	1.79	0.63
1:O4:298:ALA:HB2	1:O4:306:PRO:HD3	1.79	0.63
1:I4:281:THR:HG23	1:I4:323:ILE:HD11	1.80	0.63
1:B4:121:ARG:NH1	1:B4:343:GLU:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N4:244:GLY:HA3	1:N4:250:ALA:HB2	1.80	0.63
1:V4:186:SER:O	1:V4:188:PHE:N	2.32	0.63
1:C5:215:GLY:HA2	1:C5:220:THR:HG22	1.80	0.63
1:X4:95:ALA:HA	1:X4:99:GLY:HA3	1.81	0.63
1:R4:94:VAL:HG23	1:R4:97:GLU:HB2	1.80	0.63
1:Q4:324:ALA:HB3	1:Q4:327:ALA:HB2	1.81	0.63
1:W4:215:GLY:HA2	1:W4:220:THR:HG22	1.79	0.63
1:B5:281:THR:HG23	1:B5:323:ILE:HD11	1.81	0.63
1:E4:219:PRO:HG3	1:E4:369:GLY:HA2	1.80	0.63
1:Q4:281:THR:HG23	1:Q4:323:ILE:HD11	1.80	0.63
1:L4:186:SER:O	1:L4:188:PHE:N	2.31	0.63
1:I4:219:PRO:HG3	1:I4:369:GLY:HA2	1.79	0.63
1:F4:149:SER:HB2	1:F4:152:ALA:HB2	1.80	0.63
1:A5:281:THR:HG23	1:A5:323:ILE:HD11	1.81	0.63
1:D4:171:GLU:OE1	1:D4:348:ARG:NH1	2.30	0.63
1:U4:252:VAL:HG21	2:E3:3:VAL:HG21	1.80	0.62
1:J4:121:ARG:NH1	1:J4:343:GLU:OE2	2.32	0.62
1:N4:142:ASP:HB3	1:O4:115:ARG:HH12	1.62	0.62
1:O4:171:GLU:HA	1:O4:367:ARG:HA	1.81	0.62
1:V4:159:THR:HG22	1:V4:160:PRO:HD2	1.81	0.62
1:V4:268:GLU:OE1	1:V4:268:GLU:N	2.29	0.62
1:S4:215:GLY:HA2	1:S4:220:THR:HG22	1.80	0.62
1:D4:302:ALA:O	1:C4:311:GLY:N	2.32	0.62
1:U4:294:ARG:NE	1:V4:294:ARG:HH12	1.95	0.62
1:C5:298:ALA:HB2	1:C5:306:PRO:HD3	1.80	0.62
1:T4:238:LEU:HD23	1:T4:380:LEU:HD11	1.80	0.62
1:F4:344:ARG:HE	1:F4:367:ARG:HD3	1.65	0.62
1:X4:171:GLU:HA	1:X4:367:ARG:HA	1.81	0.62
1:M4:215:GLY:HA2	1:M4:220:THR:HG22	1.82	0.62
1:U4:132:THR:HG21	1:V4:102:VAL:HB	1.82	0.62
1:J4:204:ARG:NH2	1:I4:142:ASP:OD1	2.32	0.62
1:G4:176:PRO:HD2	1:G4:362:PHE:O	1.99	0.62
1:A5:298:ALA:HB2	1:A5:306:PRO:HD3	1.81	0.62
1:R4:256:ASP:HA	1:R4:259:VAL:HG12	1.82	0.62
1:Q4:206:GLU:OE1	1:Q4:366:LYS:NZ	2.25	0.62
1:P4:136:VAL:HG22	1:P4:165:ILE:HB	1.80	0.62
1:L4:171:GLU:HA	1:L4:367:ARG:HA	1.79	0.62
1:M4:352:ASP:HB3	1:F4:354:PHE:HD1	1.64	0.62
1:U4:279:SER:OG	1:T4:270:ARG:NH1	2.33	0.62
1:S4:289:LYS:HA	1:S4:295:PHE:HA	1.82	0.61
1:B5:178:ALA:HB3	1:B5:360:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J4:186:SER:O	1:J4:188:PHE:N	2.33	0.61
1:R4:102:VAL:HB	1:Q4:132:THR:HG21	1.82	0.61
1:C5:121:ARG:NH1	1:C5:343:GLU:OE1	2.32	0.61
1:Y4:141:THR:HG22	1:Y4:142:ASP:H	1.65	0.61
1:N4:180:GLN:HB2	1:N4:360:VAL:HG23	1.83	0.61
1:R4:149:SER:OG	1:R4:150:GLU:N	2.33	0.61
1:P4:182:LEU:HB2	1:S4:92:SER:HB3	1.83	0.61
1:G4:129:VAL:HG11	1:G4:342:ALA:HB1	1.83	0.61
1:R4:171:GLU:HA	1:R4:367:ARG:HA	1.83	0.61
1:T4:159:THR:HG22	1:T4:160:PRO:HD2	1.82	0.61
1:L4:154:LEU:HD13	1:H4:363:TYR:HE1	1.64	0.61
1:I4:98:GLY:HA2	1:I4:101:LEU:HD13	1.83	0.61
1:C4:256:ASP:HA	1:C4:259:VAL:HG12	1.83	0.61
1:N4:121:ARG:NH1	1:N4:343:GLU:OE2	2.34	0.61
1:M4:298:ALA:HB1	1:M4:303:ALA:HB1	1.81	0.61
1:K4:132:THR:HG21	1:L4:102:VAL:HB	1.82	0.61
1:B4:223:LEU:O	1:B4:227:LYS:NZ	2.28	0.61
1:T4:102:VAL:HB	1:S4:132:THR:HG21	1.81	0.61
1:P4:89:ALA:HB2	1:S4:193:TRP:HZ3	1.66	0.61
1:H4:98:GLY:HA2	1:D4:162:ILE:HD12	1.83	0.61
1:D4:133:SER:HB2	1:E4:104:PRO:HB3	1.83	0.61
1:B5:256:ASP:HA	1:B5:259:VAL:HG12	1.83	0.60
1:Q4:143:MET:HG2	1:Q4:160:PRO:HD3	1.81	0.60
1:T4:287:LYS:O	1:T4:289:LYS:NZ	2.34	0.60
1:U4:204:ARG:NH2	1:T4:142:ASP:OD2	2.33	0.60
1:S4:281:THR:HG23	1:S4:323:ILE:HD11	1.83	0.60
1:I4:288:MET:HG2	2:C2:6:LYS:HD2	1.84	0.60
1:D4:262:VAL:HG21	1:D4:310:MET:HG2	1.83	0.60
1:N4:106:THR:HG23	1:N4:107:SER:H	1.66	0.60
1:N4:265:LEU:HD11	1:N4:333:GLY:HA2	1.83	0.60
1:Q4:106:THR:HA	1:P4:135:ASP:HB2	1.82	0.60
1:N4:344:ARG:NH1	1:L4:185:ASP:OD1	2.34	0.60
1:K4:183:LEU:HD22	1:K4:360:VAL:HG21	1.83	0.60
1:A5:219:PRO:HG3	1:A5:369:GLY:HA2	1.82	0.60
1:V4:275:PHE:HB2	1:V4:314:VAL:HG22	1.82	0.60
1:H4:308:ARG:NH2	1:H4:311:GLY:O	2.35	0.60
1:P4:286:ARG:NH1	1:P4:303:ALA:HB1	2.12	0.60
1:W4:104:PRO:HB3	1:V4:133:SER:HB2	1.84	0.60
1:K4:263:TYR:OH	1:L4:286:ARG:NH1	2.35	0.60
1:Z4:171:GLU:HA	1:Z4:367:ARG:HA	1.83	0.60
1:N4:129:VAL:HG11	1:N4:342:ALA:HB1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y4:211:ILE:HG21	1:Y4:320:MET:HG2	1.82	0.60
1:Z4:286:ARG:HH12	1:Z4:304:GLY:H	1.47	0.60
1:C5:268:GLU:HG2	1:X4:114:LEU:HB3	1.82	0.60
1:A4:198:ILE:HG22	1:A4:347:LEU:HD11	1.83	0.60
1:C4:223:LEU:O	1:C4:227:LYS:NZ	2.27	0.60
1:M4:154:LEU:HD23	1:L4:357:LYS:HB3	1.84	0.59
1:S4:238:LEU:HD23	1:S4:380:LEU:HD11	1.84	0.59
1:Y4:256:ASP:HA	1:Y4:259:VAL:HG12	1.84	0.59
1:O4:132:THR:HG21	1:P4:102:VAL:HB	1.84	0.59
1:H4:265:LEU:HD11	1:H4:333:GLY:HA2	1.83	0.59
1:A5:92:SER:O	1:A5:94:VAL:N	2.35	0.59
1:Y4:171:GLU:HA	1:Y4:367:ARG:HA	1.83	0.59
1:M4:287:LYS:O	1:M4:289:LYS:NZ	2.28	0.59
1:S4:219:PRO:HG3	1:S4:369:GLY:HA2	1.83	0.59
1:A4:215:GLY:HA2	1:A4:220:THR:HG22	1.84	0.59
1:G4:281:THR:HG23	1:G4:323:ILE:HD11	1.83	0.59
1:W4:129:VAL:HG11	1:W4:342:ALA:HB1	1.85	0.59
1:T4:252:VAL:HG11	2:D3:3:VAL:HG11	1.83	0.59
1:E4:265:LEU:HD22	1:E4:270:ARG:HG3	1.83	0.59
1:B4:136:VAL:HG22	1:B4:165:ILE:HB	1.84	0.59
1:F4:159:THR:HG22	1:F4:160:PRO:HD2	1.83	0.59
1:O4:334:ASP:OD2	1:O4:337:ASN:ND2	2.35	0.59
1:V4:183:LEU:HD21	1:V4:362:PHE:HZ	1.68	0.59
1:L4:150:GLU:HG2	1:I4:91:ASN:HB2	1.85	0.59
1:I4:186:SER:O	1:I4:188:PHE:N	2.36	0.59
1:O4:159:THR:HG21	1:S4:90:LEU:HB2	1.84	0.59
1:U4:248:ASP:OD1	1:U4:249:PHE:N	2.36	0.59
1:A4:285:VAL:HG11	1:A4:309:LEU:HD11	1.84	0.59
1:W4:186:SER:O	1:W4:188:PHE:N	2.35	0.59
1:T4:278:ASN:OD1	1:T4:278:ASN:N	2.36	0.59
1:K4:275:PHE:HB2	1:K4:314:VAL:HG22	1.84	0.58
1:G4:106:THR:OG1	1:G4:107:SER:N	2.33	0.58
1:Z4:130:GLU:OE2	1:Z4:344:ARG:NH2	2.35	0.58
1:N4:182:LEU:HB2	1:F4:92:SER:CB	2.32	0.58
1:X4:352:ASP:HB3	1:Q4:354:PHE:CD1	2.38	0.58
1:A5:344:ARG:HG3	1:A5:367:ARG:HB2	1.85	0.58
1:F4:171:GLU:HA	1:F4:367:ARG:HA	1.83	0.58
1:X4:142:ASP:OD2	1:Y4:204:ARG:NH2	2.37	0.58
1:R4:215:GLY:HA2	1:R4:220:THR:HG22	1.85	0.58
1:W4:219:PRO:HG3	1:W4:369:GLY:HA2	1.84	0.58
1:S4:256:ASP:HA	1:S4:259:VAL:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X4:121:ARG:NH1	1:X4:343:GLU:OE2	2.33	0.58
1:O4:286:ARG:NH2	1:O4:305:GLU:H	2.01	0.58
1:E4:139:ASP:HA	1:E4:162:ILE:HA	1.84	0.58
1:C5:286:ARG:NH2	1:C5:305:GLU:H	2.02	0.58
1:N4:289:LYS:HZ2	1:N4:295:PHE:HE1	1.52	0.58
1:M4:171:GLU:HA	1:M4:367:ARG:HA	1.85	0.58
1:W4:119:SER:HB2	1:W4:207:ALA:HB2	1.85	0.58
1:U4:223:LEU:O	1:U4:227:LYS:NZ	2.29	0.58
1:K4:143:MET:HG2	1:K4:160:PRO:HD3	1.84	0.58
1:W4:125:SER:OG	1:W4:336:GLY:O	2.22	0.58
1:W4:256:ASP:HA	1:W4:259:VAL:HG22	1.85	0.58
1:A4:186:SER:O	1:A4:188:PHE:N	2.37	0.58
1:C5:136:VAL:HG22	1:C5:165:ILE:HB	1.86	0.58
1:S4:183:LEU:HD22	1:S4:360:VAL:HG21	1.86	0.58
1:H4:181:ARG:HG3	1:D4:367:ARG:HH12	1.69	0.58
1:H4:219:PRO:HG3	1:H4:369:GLY:HA2	1.86	0.58
1:K4:134:PHE:HB3	1:K4:167:ILE:HB	1.86	0.58
1:K4:324:ALA:HB3	1:K4:327:ALA:HB2	1.86	0.58
1:P4:261:LEU:HD22	1:P4:381:LEU:HB2	1.86	0.57
1:L4:149:SER:HB3	1:L4:152:ALA:HB2	1.84	0.57
1:D4:256:ASP:HA	1:D4:259:VAL:HG12	1.86	0.57
1:B4:136:VAL:HG12	1:C4:111:ARG:HH21	1.70	0.57
1:C5:286:ARG:NH1	1:B5:263:TYR:OH	2.36	0.57
1:P4:281:THR:HG23	1:P4:323:ILE:HD11	1.86	0.57
1:I4:215:GLY:HA2	1:I4:220:THR:HG22	1.85	0.57
1:E4:133:SER:HB2	1:F4:104:PRO:HB3	1.86	0.57
1:E4:171:GLU:HA	1:E4:367:ARG:HA	1.85	0.57
1:C5:281:THR:HG23	1:C5:323:ILE:HD11	1.86	0.57
1:W4:133:SER:HB3	1:S4:104:PRO:HB3	1.86	0.57
1:W4:253:ASN:ND2	2:B3:3:VAL:O	2.34	0.57
1:D4:219:PRO:HG3	1:D4:369:GLY:HA2	1.85	0.57
1:A5:286:ARG:NH2	1:A5:305:GLU:H	2.03	0.57
1:P4:171:GLU:HA	1:P4:367:ARG:HA	1.86	0.57
1:K4:286:ARG:NH1	1:J4:263:TYR:OH	2.37	0.57
1:F4:286:ARG:HH22	1:F4:305:GLU:H	1.52	0.57
1:X4:141:THR:HG22	1:X4:161:GLN:HG2	1.86	0.57
1:V4:334:ASP:OD2	1:V4:337:ASN:ND2	2.38	0.57
1:H4:354:PHE:CD1	1:D4:352:ASP:HB3	2.40	0.57
1:G4:289:LYS:HA	1:G4:295:PHE:HA	1.87	0.57
1:C4:95:ALA:HA	1:C4:99:GLY:HA3	1.86	0.57
1:C5:171:GLU:HA	1:C5:367:ARG:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P4:101:LEU:HD21	1:W4:162:ILE:HD13	1.86	0.57
1:P4:106:THR:HG23	1:P4:107:SER:H	1.70	0.57
1:T4:171:GLU:HG3	1:T4:367:ARG:HG2	1.86	0.57
1:L4:215:GLY:HA2	1:L4:220:THR:HG22	1.87	0.57
1:T4:89:ALA:HB2	1:K4:193:TRP:HZ3	1.70	0.57
1:A5:269:TYR:CE1	1:B5:114:LEU:HB2	2.39	0.57
1:P4:359:HIS:HE1	1:V4:151:THR:HG22	1.69	0.57
1:K4:305:GLU:HG3	1:K4:306:PRO:HD3	1.86	0.57
1:J4:159:THR:HG22	1:J4:160:PRO:HD2	1.85	0.57
1:C4:281:THR:HG23	1:C4:323:ILE:HD11	1.86	0.57
1:F4:90:LEU:HD23	1:F4:90:LEU:O	2.04	0.57
1:Y4:352:ASP:HB3	1:W4:354:PHE:CD1	2.40	0.57
1:A5:223:LEU:C	1:A5:223:LEU:HD23	2.25	0.57
1:Q4:328:TYR:OH	1:Q4:382:LYS:NZ	2.37	0.57
1:U4:107:SER:OG	1:T4:136:VAL:HA	2.05	0.57
1:Y4:262:VAL:HG21	1:Y4:310:MET:HG2	1.87	0.56
1:E4:246:ALA:HA	1:E4:384:ALA:HA	1.87	0.56
1:B4:298:ALA:HB2	1:B4:306:PRO:HD3	1.87	0.56
1:W4:132:THR:HG21	1:S4:102:VAL:HB	1.87	0.56
1:D4:167:ILE:HG23	1:D4:370:GLY:HA2	1.87	0.56
1:D4:286:ARG:HH12	1:D4:305:GLU:HA	1.70	0.56
1:C4:176:PRO:HD2	1:C4:362:PHE:O	2.04	0.56
1:C5:219:PRO:HG3	1:C5:369:GLY:HA2	1.88	0.56
1:A5:142:ASP:OD2	1:B5:204:ARG:NH2	2.38	0.56
1:R4:286:ARG:NH2	1:R4:305:GLU:H	2.03	0.56
1:T4:279:SER:OG	1:S4:270:ARG:NH1	2.38	0.56
1:L4:261:LEU:HD21	1:L4:332:PHE:HB3	1.87	0.56
1:I4:318:GLU:HA	1:I4:318:GLU:OE1	2.04	0.56
1:K4:167:ILE:HG23	1:K4:370:GLY:HA2	1.88	0.56
1:J4:116:SER:HA	1:I4:268:GLU:HB2	1.88	0.56
1:H4:289:LYS:HA	1:H4:295:PHE:HA	1.86	0.56
1:X4:256:ASP:HA	1:X4:259:VAL:HG12	1.86	0.56
1:Y4:138:VAL:HA	1:Z4:111:ARG:O	2.05	0.56
1:P4:277:MET:HG2	1:P4:330:ILE:HG12	1.87	0.56
1:T4:349:VAL:HG12	1:T4:364:ALA:HB2	1.86	0.56
1:V4:305:GLU:HB2	1:V4:306:PRO:HD3	1.88	0.56
1:G4:94:VAL:HG23	1:G4:97:GLU:HB2	1.87	0.56
1:Y4:101:LEU:HD23	1:Q4:188:PHE:CE2	2.34	0.56
1:R4:129:VAL:HG11	1:R4:134:PHE:CD1	2.40	0.56
1:I4:278:ASN:ND2	1:I4:322:ASP:OD1	2.39	0.56
1:C5:167:ILE:HG23	1:C5:370:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P4:262:VAL:HG21	1:P4:310:MET:HG2	1.87	0.56
1:X4:286:ARG:HH12	1:X4:304:GLY:H	1.52	0.56
1:N4:182:LEU:HD22	1:F4:92:SER:HA	1.85	0.56
1:M4:289:LYS:HD3	1:M4:293:GLY:HA2	1.88	0.56
1:O4:167:ILE:HG23	1:O4:370:GLY:HA2	1.87	0.56
1:T4:359:HIS:HE1	1:I4:151:THR:HG22	1.70	0.56
1:J4:129:VAL:HG11	1:J4:134:PHE:CD1	2.40	0.56
1:F4:145:SER:HB3	1:G4:172:LEU:HD11	1.88	0.56
1:O4:211:ILE:HD13	1:O4:320:MET:HG2	1.87	0.56
1:T4:193:TRP:HZ3	1:K4:89:ALA:HB2	1.69	0.56
1:X4:170:HIS:HA	1:Q4:181:ARG:NH2	2.20	0.56
1:J4:253:ASN:ND2	2:E2:3:VAL:O	2.39	0.56
1:I4:288:MET:HB3	1:I4:296:LEU:HD21	1.87	0.56
1:B4:286:ARG:NH1	1:B4:305:GLU:HA	2.20	0.56
1:J4:149:SER:OG	1:J4:150:GLU:N	2.39	0.55
1:L4:275:PHE:HB2	1:L4:314:VAL:HG22	1.87	0.55
1:H4:255:SER:OG	1:H4:255:SER:O	2.23	0.55
1:G4:219:PRO:HG3	1:G4:369:GLY:HA2	1.88	0.55
1:Z4:243:THR:O	1:Z4:250:ALA:HB2	2.06	0.55
1:A5:286:ARG:HH12	1:A5:305:GLU:HA	1.71	0.55
1:N4:179:SER:O	1:N4:181:ARG:N	2.36	0.55
1:K4:91:ASN:HB2	1:I4:150:GLU:HG2	1.87	0.55
1:I4:129:VAL:HG11	1:I4:342:ALA:HB1	1.88	0.55
1:I4:294:ARG:HG3	1:I4:295:PHE:N	2.20	0.55
1:R4:337:ASN:N	1:R4:337:ASN:HD22	2.05	0.55
1:V4:121:ARG:NH1	1:V4:343:GLU:OE2	2.39	0.55
1:C5:134:PHE:O	1:C5:167:ILE:N	2.39	0.55
1:M4:135:ASP:OD2	1:M4:164:ARG:NE	2.39	0.55
1:V4:149:SER:HB2	1:V4:152:ALA:HB2	1.87	0.55
1:C4:121:ARG:NH1	1:C4:343:GLU:OE2	2.37	0.55
1:A5:137:LEU:HD13	1:B5:188:PHE:CE1	2.42	0.55
1:W4:227:LYS:HG2	1:W4:380:LEU:HD22	1.88	0.55
1:W4:260:ASP:OD1	1:W4:261:LEU:N	2.40	0.55
1:T4:190:ILE:HD11	1:K4:101:LEU:HD23	1.89	0.55
1:T4:275:PHE:HB2	1:T4:314:VAL:HG22	1.89	0.55
1:L4:238:LEU:HD23	1:L4:380:LEU:HD11	1.89	0.55
1:N4:367:ARG:NH2	1:L4:181:ARG:HG3	2.21	0.55
1:P4:334:ASP:OD2	1:P4:337:ASN:ND2	2.36	0.55
1:J4:114:LEU:HG	1:I4:268:GLU:HG3	1.87	0.55
1:J4:252:VAL:HG13	1:J4:253:ASN:H	1.70	0.55
1:O4:223:LEU:O	1:O4:227:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G4:171:GLU:HA	1:G4:367:ARG:HA	1.89	0.55
1:C5:136:VAL:HG12	1:X4:111:ARG:HH21	1.72	0.55
1:Q4:150:GLU:HG3	1:Q4:151:THR:HG23	1.88	0.55
1:O4:149:SER:OG	1:O4:150:GLU:N	2.40	0.55
1:A4:171:GLU:HA	1:A4:367:ARG:HA	1.89	0.55
1:E4:167:ILE:HG23	1:E4:370:GLY:HA2	1.89	0.55
1:R4:211:ILE:HG21	1:R4:320:MET:HG2	1.87	0.54
1:Q4:138:VAL:HG11	1:Q4:235:TRP:CH2	2.42	0.54
1:C5:348:ARG:HH12	1:C5:367:ARG:HD3	1.72	0.54
1:A5:135:ASP:OD2	1:A5:164:ARG:NH1	2.40	0.54
1:W4:296:LEU:HB2	1:S4:294:ARG:HG3	1.89	0.54
1:U4:159:THR:HG22	1:U4:160:PRO:HD2	1.88	0.54
1:U4:183:LEU:HD22	1:U4:360:VAL:HG21	1.89	0.54
1:T4:182:LEU:HD13	1:K4:92:SER:HB2	1.87	0.54
1:H4:176:PRO:HG3	1:H4:198:ILE:HD11	1.89	0.54
1:A4:322:ASP:OD1	1:A4:322:ASP:N	2.39	0.54
1:A5:154:LEU:HD11	1:B5:363:TYR:HE1	1.71	0.54
1:B5:278:ASN:ND2	1:B5:322:ASP:OD1	2.39	0.54
1:B5:344:ARG:NH1	1:B5:367:ARG:HH11	2.04	0.54
1:O4:262:VAL:HG21	1:O4:310:MET:HG2	1.89	0.54
1:X4:154:LEU:HD21	1:Y4:363:TYR:HE1	1.73	0.54
1:U4:94:VAL:HG13	1:U4:97:GLU:HB2	1.89	0.54
1:A4:129:VAL:HG11	1:A4:134:PHE:CD1	2.42	0.54
1:D4:322:ASP:N	1:D4:322:ASP:OD1	2.40	0.54
1:X4:143:MET:HG2	1:X4:160:PRO:HD3	1.90	0.54
1:R4:111:ARG:O	1:Q4:138:VAL:HA	2.08	0.54
1:P4:298:ALA:HB2	1:P4:306:PRO:CG	2.37	0.54
1:T4:101:LEU:HD23	1:K4:190:ILE:HD11	1.88	0.54
1:B4:171:GLU:HA	1:B4:367:ARG:HA	1.89	0.54
1:A5:223:LEU:HD23	1:A5:223:LEU:O	2.07	0.54
1:Q4:179:SER:CA	1:Q4:359:HIS:HA	2.32	0.54
1:O4:352:ASP:N	1:O4:352:ASP:OD1	2.39	0.54
1:T4:181:ARG:NH2	1:J4:171:GLU:OE2	2.39	0.54
1:E4:134:PHE:HB3	1:E4:167:ILE:HB	1.89	0.54
1:C4:246:ALA:HA	1:C4:384:ALA:HA	1.90	0.54
2:A2:32:ARG:NH2	2:A2:67:ARG:O	2.40	0.54
1:C5:91:ASN:HB3	1:C5:95:ALA:HB2	1.90	0.54
1:K4:102:VAL:HB	1:J4:132:THR:HG21	1.90	0.54
1:J4:252:VAL:HG11	2:E2:3:VAL:HG21	1.89	0.54
1:I4:252:VAL:HG21	2:D2:3:VAL:HG21	1.87	0.54
1:Z4:101:LEU:HD21	1:V4:162:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z4:139:ASP:HA	1:Z4:162:ILE:HA	1.88	0.54
1:G4:135:ASP:OD1	1:G4:166:THR:HG22	2.08	0.54
1:M4:125:SER:OG	1:M4:336:GLY:O	2.25	0.54
1:P4:289:LYS:HD3	1:P4:293:GLY:HA2	1.89	0.54
1:W4:171:GLU:HA	1:W4:367:ARG:HA	1.89	0.54
1:T4:167:ILE:HG23	1:T4:370:GLY:HA2	1.89	0.54
1:V4:134:PHE:HB3	1:V4:167:ILE:HB	1.90	0.54
1:O4:297:TRP:HB2	1:P4:301:LEU:HD12	1.90	0.53
1:P4:286:ARG:HH11	1:P4:303:ALA:CB	2.15	0.53
1:P4:329:ALA:HB3	1:P4:383:PHE:HE2	1.71	0.53
1:J4:305:GLU:HG2	1:J4:306:PRO:HD3	1.89	0.53
1:V4:183:LEU:HD22	1:V4:360:VAL:HG21	1.89	0.53
1:H4:92:SER:HB2	1:E4:182:LEU:HB2	1.90	0.53
1:H4:287:LYS:O	1:H4:289:LYS:NZ	2.40	0.53
1:W4:288:MET:HA	2:A3:6:LYS:HB3	1.90	0.53
1:J4:171:GLU:HA	1:J4:367:ARG:HA	1.90	0.53
1:J4:262:VAL:O	1:J4:270:ARG:HD3	2.06	0.53
1:I4:175:MET:HG3	1:I4:362:PHE:O	2.09	0.53
1:D4:298:ALA:HB2	1:D4:306:PRO:HD3	1.89	0.53
1:E4:263:TYR:OH	1:F4:286:ARG:NH1	2.25	0.53
2:D2:32:ARG:NH2	2:D2:67:ARG:O	2.40	0.53
1:R4:132:THR:HG21	1:M4:102:VAL:HB	1.90	0.53
1:J4:281:THR:HG23	1:J4:323:ILE:HD11	1.90	0.53
1:M4:175:MET:HG3	1:M4:363:TYR:HD1	1.73	0.53
1:U4:288:MET:HB3	1:U4:296:LEU:HD21	1.89	0.53
1:V4:167:ILE:HD12	1:V4:370:GLY:HA2	1.90	0.53
1:I4:285:VAL:HG11	1:I4:309:LEU:HD11	1.90	0.53
1:D4:215:GLY:HA2	1:D4:220:THR:HG22	1.91	0.53
1:N4:354:PHE:CD1	1:E4:352:ASP:HB3	2.43	0.53
1:P4:139:ASP:HA	1:P4:162:ILE:HA	1.90	0.53
1:L4:288:MET:HE2	1:L4:297:TRP:HE1	1.73	0.53
1:E4:354:PHE:O	1:E4:357:LYS:NZ	2.33	0.53
1:F4:225:LYS:HE2	1:F4:372:VAL:HG22	1.90	0.53
1:G4:349:VAL:HG23	1:G4:364:ALA:HB2	1.91	0.53
1:B4:262:VAL:HG21	1:B4:310:MET:HG2	1.91	0.53
1:N4:227:LYS:HD2	1:N4:328:TYR:CZ	2.44	0.53
1:U4:125:SER:OG	1:U4:336:GLY:O	2.22	0.53
1:K4:308:ARG:NH2	1:K4:311:GLY:O	2.42	0.53
1:J4:104:PRO:HB3	1:I4:133:SER:HB2	1.90	0.53
2:D3:32:ARG:NH2	2:D3:67:ARG:O	2.40	0.53
1:Y4:181:ARG:HB3	1:O4:150:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z4:296:LEU:HD23	1:A5:295:PHE:CE2	2.44	0.53
1:O4:352:ASP:HB3	1:S4:354:PHE:CD1	2.44	0.53
1:X4:294:ARG:NH2	1:X4:299:ASP:OD2	2.42	0.53
1:N4:182:LEU:HB2	1:F4:92:SER:HB2	1.89	0.53
1:O4:182:LEU:HB2	1:L4:92:SER:HB3	1.91	0.53
1:W4:183:LEU:HD21	1:W4:362:PHE:HZ	1.74	0.53
1:W4:278:ASN:HA	1:W4:317:ALA:O	2.09	0.53
1:U4:285:VAL:HG11	1:U4:309:LEU:HD11	1.91	0.53
1:T4:359:HIS:CE1	1:I4:151:THR:HG22	2.44	0.53
1:K4:279:SER:OG	1:J4:270:ARG:NH1	2.41	0.53
1:L4:256:ASP:OD1	1:L4:257:ALA:N	2.41	0.53
1:H4:181:ARG:HH21	1:D4:171:GLU:HG2	1.74	0.53
1:F4:299:ASP:OD1	1:F4:300:SER:N	2.36	0.53
1:A4:90:LEU:HG	1:A4:91:ASN:H	1.74	0.53
1:A5:265:LEU:HD12	1:A5:379:LYS:HG2	1.90	0.52
1:N4:363:TYR:CE1	1:M4:154:LEU:HD21	2.44	0.52
1:O4:138:VAL:HA	1:P4:111:ARG:O	2.08	0.52
1:P4:177:LYS:HE3	1:P4:361:LEU:HD11	1.90	0.52
1:U4:343:GLU:HB3	1:U4:368:VAL:HG23	1.91	0.52
1:X4:191:GLU:OE2	1:X4:351:ARG:NH1	2.42	0.52
1:Y4:322:ASP:OD1	1:Y4:322:ASP:N	2.41	0.52
1:L4:256:ASP:HA	1:L4:259:VAL:HG12	1.90	0.52
1:I4:121:ARG:NH1	1:I4:343:GLU:OE1	2.43	0.52
1:E4:116:SER:HB3	1:E4:318:GLU:HG3	1.90	0.52
1:B4:92:SER:OG	1:B4:93:ALA:N	2.42	0.52
1:C4:139:ASP:HA	1:C4:162:ILE:HA	1.91	0.52
2:C3:32:ARG:NH2	2:C3:67:ARG:O	2.40	0.52
1:O4:133:SER:HB3	1:P4:104:PRO:HB3	1.91	0.52
1:C5:104:PRO:HB3	1:B5:133:SER:HB2	1.90	0.52
1:M4:148:ALA:O	1:M4:149:SER:HB3	2.09	0.52
1:P4:219:PRO:HG3	1:P4:369:GLY:HA2	1.92	0.52
1:U4:167:ILE:HG23	1:U4:370:GLY:HA2	1.91	0.52
1:T4:382:LYS:HE2	1:T4:384:ALA:HB2	1.89	0.52
1:C4:277:MET:O	1:C4:317:ALA:N	2.43	0.52
1:M4:191:GLU:HG3	1:M4:362:PHE:CE1	2.45	0.52
1:S4:107:SER:OG	1:S4:109:THR:O	2.22	0.52
1:K4:149:SER:OG	1:K4:150:GLU:N	2.42	0.52
1:L4:278:ASN:HA	1:L4:317:ALA:O	2.10	0.52
1:H4:281:THR:HA	1:H4:323:ILE:HD11	1.90	0.52
1:Q4:134:PHE:HB3	1:Q4:167:ILE:HB	1.91	0.52
1:T4:111:ARG:NH1	1:S4:340:THR:OG1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H4:121:ARG:NH1	1:H4:343:GLU:OE2	2.43	0.52
1:I4:230:ASN:ND2	1:I4:264:ALA:HB1	2.25	0.52
1:F4:110:ILE:HD11	1:F4:193:TRP:CE2	2.45	0.52
1:C5:134:PHE:HB3	1:C5:167:ILE:HB	1.91	0.52
1:C5:211:ILE:HG21	1:C5:320:MET:HG2	1.90	0.52
1:X4:211:ILE:HD12	1:X4:319:ASP:HB2	1.90	0.52
1:Z4:120:LEU:HD12	1:Z4:123:ILE:HD11	1.91	0.52
1:J4:155:SER:OG	1:J4:156:GLU:N	2.43	0.52
1:D4:107:SER:OG	1:C4:136:VAL:HA	2.09	0.52
1:D4:277:MET:HG2	1:D4:330:ILE:HG12	1.91	0.52
1:A5:227:LYS:HG2	1:A5:380:LEU:HD12	1.91	0.52
1:N4:106:THR:HA	1:M4:135:ASP:HB2	1.91	0.52
1:N4:185:ASP:OD1	1:N4:185:ASP:N	2.42	0.52
1:M4:262:VAL:HG21	1:M4:310:MET:HG3	1.92	0.52
1:T4:215:GLY:HA2	1:T4:220:THR:HG22	1.90	0.52
1:D4:223:LEU:O	1:D4:227:LYS:NZ	2.29	0.52
1:E4:227:LYS:HG2	1:E4:380:LEU:HD22	1.91	0.52
2:D3:63:ILE:O	2:D3:63:ILE:HG13	2.10	0.52
2:A1:63:ILE:O	2:A1:63:ILE:HG13	2.10	0.52
1:K4:186:SER:O	1:K4:188:PHE:N	2.43	0.52
1:I4:255:SER:HB3	1:I4:296:LEU:HD11	1.91	0.52
1:E4:163:ASP:OD1	1:E4:164:ARG:N	2.43	0.52
2:C2:63:ILE:HG13	2:C2:63:ILE:O	2.10	0.52
1:X4:289:LYS:HD3	1:X4:293:GLY:HA2	1.91	0.51
1:A5:147:TRP:CD1	1:B5:218:LYS:HE3	2.45	0.51
1:B5:298:ALA:HB2	1:B5:306:PRO:HD3	1.91	0.51
1:U4:111:ARG:O	1:T4:138:VAL:HA	2.10	0.51
1:U4:135:ASP:OD2	1:U4:164:ARG:NH2	2.43	0.51
2:E2:63:ILE:O	2:E2:63:ILE:HG13	2.10	0.51
2:A3:63:ILE:HG13	2:A3:63:ILE:O	2.10	0.51
1:C5:305:GLU:OE2	1:B5:263:TYR:OH	2.27	0.51
1:X4:149:SER:HB2	1:X4:152:ALA:HB2	1.91	0.51
1:B5:139:ASP:OD2	1:B5:139:ASP:N	2.42	0.51
1:R4:128:ASN:ND2	1:R4:345:PRO:HG3	2.24	0.51
1:T4:151:THR:O	1:T4:151:THR:OG1	2.25	0.51
1:I4:288:MET:HA	2:C2:6:LYS:HB3	1.91	0.51
1:D4:159:THR:HG22	1:D4:160:PRO:HD2	1.92	0.51
1:G4:220:THR:HB	1:G4:371:ASP:CG	2.29	0.51
1:B5:347:LEU:HD13	1:B5:347:LEU:O	2.10	0.51
1:K4:288:MET:HA	2:E2:6:LYS:HB3	1.92	0.51
1:K4:338:GLY:O	1:K4:373:SER:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:343:GLU:HB3	1:L4:368:VAL:HG23	1.92	0.51
2:A1:32:ARG:NH2	2:A1:67:ARG:O	2.40	0.51
1:X4:290:ASP:OD1	1:X4:290:ASP:N	2.43	0.51
1:Y4:219:PRO:HG3	1:Y4:369:GLY:HA2	1.92	0.51
1:R4:133:SER:HB2	1:M4:104:PRO:HB3	1.91	0.51
1:L4:288:MET:HG2	2:A2:6:LYS:HD2	1.91	0.51
1:F4:167:ILE:HG23	1:F4:370:GLY:HA2	1.92	0.51
2:C3:63:ILE:HG13	2:C3:63:ILE:O	2.10	0.51
1:U4:136:VAL:HA	1:V4:107:SER:OG	2.11	0.51
1:S4:308:ARG:NH2	1:S4:311:GLY:O	2.43	0.51
2:B2:63:ILE:HG13	2:B2:63:ILE:O	2.10	0.51
2:E3:63:ILE:O	2:E3:63:ILE:HG13	2.10	0.51
1:Y4:354:PHE:CD1	1:P4:352:ASP:HB3	2.45	0.51
1:R4:134:PHE:HB3	1:R4:167:ILE:HB	1.93	0.51
1:R4:159:THR:HG22	1:R4:160:PRO:HD2	1.92	0.51
1:T4:255:SER:HB2	1:T4:297:TRP:CZ2	2.46	0.51
2:D2:63:ILE:HG13	2:D2:63:ILE:O	2.10	0.51
1:N4:171:GLU:HG2	1:L4:181:ARG:HH21	1.75	0.51
1:N4:265:LEU:CD1	1:N4:333:GLY:HA2	2.41	0.51
1:M4:348:ARG:O	1:M4:364:ALA:HA	2.10	0.51
1:M4:352:ASP:HB3	1:F4:354:PHE:CD1	2.46	0.51
1:Q4:121:ARG:NH2	1:Q4:343:GLU:OE1	2.34	0.51
1:Q4:277:MET:HG2	1:Q4:330:ILE:HG12	1.91	0.51
1:O4:162:ILE:HD13	1:S4:101:LEU:HD11	1.93	0.51
1:W4:92:SER:O	1:W4:92:SER:OG	2.28	0.51
1:S4:260:ASP:OD1	1:S4:261:LEU:N	2.44	0.51
1:E4:150:GLU:HG3	1:G4:91:ASN:HB2	1.93	0.51
1:K4:191:GLU:OE1	1:K4:351:ARG:NE	2.44	0.51
1:J4:326:ASN:HB3	1:J4:382:LYS:HE2	1.93	0.51
1:V4:135:ASP:OD1	1:V4:166:THR:HG22	2.11	0.51
1:A4:292:ASP:OD2	1:A4:294:ARG:NH1	2.43	0.51
1:C4:277:MET:HE3	1:C4:282:ALA:HB2	1.93	0.51
2:A2:63:ILE:HG13	2:A2:63:ILE:O	2.10	0.51
2:C2:32:ARG:NH2	2:C2:67:ARG:O	2.40	0.51
2:E3:32:ARG:NH2	2:E3:67:ARG:O	2.40	0.51
1:B5:177:LYS:HA	1:B5:361:LEU:HA	1.92	0.51
1:B5:190:ILE:HG13	1:B5:193:TRP:CE3	2.46	0.51
1:N4:142:ASP:HB3	1:O4:115:ARG:NH1	2.26	0.51
1:H4:252:VAL:HG11	2:C2:3:VAL:HG13	1.92	0.51
1:D4:120:LEU:HD23	1:D4:210:PHE:HB3	1.93	0.51
2:B3:63:ILE:HG13	2:B3:63:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X4:154:LEU:HD21	1:Y4:363:TYR:CE1	2.46	0.51
1:O4:190:ILE:HD11	1:L4:101:LEU:HD23	1.91	0.51
1:T4:321:PRO:HB2	1:T4:327:ALA:HB1	1.93	0.51
1:K4:219:PRO:HG3	1:K4:369:GLY:HA2	1.93	0.51
1:I4:198:ILE:HG22	1:I4:347:LEU:HD11	1.92	0.51
1:C4:171:GLU:HA	1:C4:367:ARG:HA	1.93	0.51
2:B2:32:ARG:NH2	2:B2:67:ARG:O	2.40	0.51
1:A5:121:ARG:NH2	1:A5:343:GLU:OE1	2.41	0.50
1:O4:263:TYR:HE2	1:P4:286:ARG:HD3	1.76	0.50
1:S4:186:SER:O	1:S4:188:PHE:N	2.44	0.50
1:K4:265:LEU:HD13	1:K4:332:PHE:CD2	2.46	0.50
1:Z4:220:THR:HB	1:Z4:371:ASP:HB3	1.94	0.50
1:R4:299:ASP:OD1	1:R4:300:SER:N	2.44	0.50
1:W4:112:GLY:HA2	1:V4:139:ASP:H	1.76	0.50
1:U4:121:ARG:NH1	1:U4:343:GLU:OE2	2.44	0.50
1:J4:107:SER:OG	1:I4:136:VAL:HA	2.11	0.50
1:L4:128:ASN:OD1	1:L4:345:PRO:HG3	2.10	0.50
1:H4:107:SER:OG	1:H4:109:THR:O	2.23	0.50
1:H4:269:TYR:CZ	1:I4:114:LEU:HB2	2.46	0.50
1:H4:288:MET:HE1	1:H4:297:TRP:HE1	1.76	0.50
2:E3:44:LEU:HA	2:E3:76:THR:HA	1.94	0.50
2:B3:44:LEU:HA	2:B3:76:THR:HA	1.94	0.50
1:M4:265:LEU:HD11	1:M4:333:GLY:HA2	1.92	0.50
1:P4:134:PHE:HB3	1:P4:167:ILE:HB	1.94	0.50
1:V4:167:ILE:HG23	1:V4:370:GLY:HA2	1.93	0.50
1:B4:322:ASP:OD1	1:B4:322:ASP:N	2.40	0.50
1:C4:248:ASP:OD1	1:C4:249:PHE:N	2.43	0.50
1:P4:298:ALA:HB2	1:P4:306:PRO:CD	2.41	0.50
1:J4:277:MET:HG2	1:J4:330:ILE:HG12	1.92	0.50
1:X4:156:GLU:HG2	1:Y4:361:LEU:HD11	1.93	0.50
1:Y4:110:ILE:HD11	1:Y4:193:TRP:CE2	2.46	0.50
1:A5:183:LEU:HD21	1:A5:362:PHE:HZ	1.76	0.50
1:O4:119:SER:O	1:O4:119:SER:OG	2.29	0.50
1:U4:113:VAL:HG23	1:T4:139:ASP:O	2.12	0.50
1:H4:211:ILE:HG21	1:H4:320:MET:HG2	1.93	0.50
1:F4:256:ASP:HA	1:F4:259:VAL:HG12	1.92	0.50
2:B2:44:LEU:HA	2:B2:76:THR:HA	1.94	0.50
3:F3:2:ILE:HG13	3:F3:11:ALA:HB1	1.94	0.50
2:B3:32:ARG:NH2	2:B3:67:ARG:O	2.40	0.50
1:R4:279:SER:OG	1:R4:318:GLU:OE2	2.24	0.50
1:Q4:215:GLY:HA2	1:Q4:220:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K4:309:LEU:HD23	1:K4:310:MET:HB2	1.94	0.50
1:J4:261:LEU:HD21	1:J4:332:PHE:HB3	1.93	0.50
1:D4:347:LEU:HD21	1:D4:364:ALA:HB1	1.93	0.50
1:F4:138:VAL:HG12	1:F4:139:ASP:H	1.77	0.50
2:E2:44:LEU:HA	2:E2:76:THR:HA	1.94	0.50
1:Z4:176:PRO:HD2	1:Z4:362:PHE:O	2.12	0.50
1:Z4:322:ASP:OD1	1:Z4:322:ASP:N	2.39	0.50
1:A5:98:GLY:HA2	1:A5:101:LEU:HD12	1.93	0.50
1:A5:261:LEU:CD1	1:A5:381:LEU:HB2	2.41	0.50
1:N4:219:PRO:HG3	1:N4:369:GLY:HA2	1.94	0.50
1:O4:286:ARG:HH22	1:O4:305:GLU:H	1.59	0.50
1:V4:343:GLU:HB3	1:V4:368:VAL:HG23	1.94	0.50
1:L4:154:LEU:HD13	1:H4:363:TYR:CE1	2.46	0.50
1:B4:129:VAL:HG13	1:B4:169:LEU:HD22	1.93	0.50
1:C4:219:PRO:HG3	1:C4:369:GLY:HA2	1.93	0.50
3:F2:2:ILE:HG13	3:F2:11:ALA:HB1	1.94	0.50
2:A1:25:ASP:OD1	2:A1:74:THR:HG23	2.12	0.50
1:U4:214:ASP:OD2	1:U4:214:ASP:N	2.32	0.50
1:E4:262:VAL:HG21	1:E4:310:MET:HG2	1.92	0.50
1:C5:301:LEU:HD11	1:B5:255:SER:HB2	1.94	0.50
1:L4:162:ILE:HD13	1:E4:101:LEU:HD21	1.94	0.50
1:I4:92:SER:O	1:I4:92:SER:OG	2.26	0.50
1:D4:352:ASP:OD1	1:D4:352:ASP:N	2.45	0.50
2:A2:44:LEU:HA	2:A2:76:THR:HA	1.94	0.50
2:C2:44:LEU:HA	2:C2:76:THR:HA	1.94	0.50
1:X4:352:ASP:OD1	1:X4:352:ASP:N	2.43	0.49
1:A5:134:PHE:HD2	1:A5:167:ILE:HD12	1.77	0.49
1:R4:157:THR:HG21	1:M4:174:ALA:HA	1.93	0.49
1:R4:167:ILE:HG23	1:R4:370:GLY:HA2	1.94	0.49
1:U4:111:ARG:NH1	1:T4:340:THR:OG1	2.38	0.49
1:A4:167:ILE:HG23	1:A4:370:GLY:HA2	1.94	0.49
2:D2:44:LEU:HA	2:D2:76:THR:HA	1.94	0.49
1:Q4:167:ILE:HG23	1:Q4:370:GLY:HA2	1.95	0.49
1:L4:244:GLY:O	1:L4:385:ALA:HA	2.12	0.49
1:E4:139:ASP:N	1:E4:139:ASP:OD1	2.45	0.49
1:B4:159:THR:HG22	1:B4:160:PRO:HD2	1.94	0.49
1:C4:136:VAL:HG22	1:C4:165:ILE:HB	1.94	0.49
1:N4:277:MET:HE3	1:N4:282:ALA:HB2	1.93	0.49
1:H4:90:LEU:HG	1:H4:91:ASN:H	1.77	0.49
1:D4:238:LEU:HD11	1:D4:372:VAL:HG11	1.94	0.49
1:D4:334:ASP:OD2	1:D4:337:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E4:95:ALA:HA	1:E4:99:GLY:HA3	1.94	0.49
1:Y4:286:ARG:NH2	1:Y4:305:GLU:H	2.10	0.49
1:B5:248:ASP:N	1:B5:248:ASP:OD1	2.46	0.49
1:M4:305:GLU:OE2	1:M4:305:GLU:HA	2.12	0.49
1:Q4:177:LYS:HG2	1:Q4:361:LEU:HD13	1.94	0.49
1:K4:227:LYS:HG2	1:K4:380:LEU:HD22	1.92	0.49
1:K4:262:VAL:HG12	1:K4:270:ARG:HD3	1.94	0.49
1:I4:167:ILE:HG23	1:I4:370:GLY:HA2	1.93	0.49
2:A3:25:ASP:OD1	2:A3:74:THR:HG23	2.12	0.49
2:A1:44:LEU:HA	2:A1:76:THR:HA	1.94	0.49
1:X4:290:ASP:HB2	1:Y4:292:ASP:O	2.12	0.49
1:Z4:290:ASP:HB3	1:Z4:296:LEU:CD1	2.35	0.49
1:A5:171:GLU:OE2	1:A5:173:ALA:HB2	2.11	0.49
1:B5:349:VAL:HA	1:B5:364:ALA:HA	1.93	0.49
1:Q4:184:ASP:OD1	1:Q4:184:ASP:N	2.42	0.49
1:V4:324:ALA:HB3	1:V4:327:ALA:HB2	1.94	0.49
1:H4:343:GLU:HB3	1:H4:368:VAL:HG23	1.95	0.49
1:H4:348:ARG:NH1	1:H4:365:SER:O	2.46	0.49
1:X4:193:TRP:HE1	1:X4:197:ARG:NH1	2.10	0.49
1:Q4:95:ALA:HA	1:Q4:99:GLY:HA3	1.95	0.49
1:P4:277:MET:O	1:P4:317:ALA:N	2.44	0.49
1:T4:121:ARG:NH1	1:T4:343:GLU:OE2	2.45	0.49
1:K4:112:GLY:HA2	1:J4:139:ASP:H	1.78	0.49
2:E2:25:ASP:OD1	2:E2:74:THR:HG23	2.12	0.49
2:A3:44:LEU:HA	2:A3:76:THR:HA	1.93	0.49
1:M4:265:LEU:CD1	1:M4:333:GLY:HA2	2.43	0.49
1:I4:149:SER:OG	1:I4:150:GLU:N	2.46	0.49
1:D4:286:ARG:NH1	1:C4:263:TYR:OH	2.45	0.49
1:F4:286:ARG:HH12	1:F4:305:GLU:H	1.61	0.49
1:B5:297:TRP:CE2	1:B5:309:LEU:HD13	2.47	0.49
1:O4:156:GLU:OE1	1:P4:177:LYS:HD2	2.11	0.49
1:P4:184:ASP:O	1:W4:344:ARG:NH1	2.46	0.49
1:S4:167:ILE:HD12	1:S4:370:GLY:HA2	1.95	0.49
1:S4:183:LEU:HD21	1:S4:362:PHE:HZ	1.78	0.49
1:V4:308:ARG:NH2	1:V4:311:GLY:O	2.43	0.49
2:E2:32:ARG:NH2	2:E2:67:ARG:O	2.40	0.49
1:A5:342:ALA:O	1:A5:369:GLY:N	2.43	0.49
1:R4:136:VAL:HG22	1:R4:165:ILE:HB	1.95	0.49
1:R4:344:ARG:HE	1:R4:367:ARG:HD3	1.78	0.49
1:Q4:167:ILE:HD12	1:Q4:370:GLY:HA2	1.95	0.49
1:W4:113:VAL:HG23	1:V4:139:ASP:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K4:176:PRO:HG3	1:K4:198:ILE:HD11	1.95	0.49
1:L4:186:SER:O	1:L4:186:SER:OG	2.30	0.49
1:E4:322:ASP:OD1	1:E4:322:ASP:N	2.45	0.49
2:C3:44:LEU:HA	2:C3:76:THR:HA	1.94	0.49
1:N4:148:ALA:O	1:S4:181:ARG:NH2	2.46	0.49
1:R4:188:PHE:CZ	1:Q4:137:LEU:HD12	2.48	0.49
1:M4:121:ARG:NH1	1:M4:343:GLU:OE2	2.39	0.49
1:M4:277:MET:O	1:M4:317:ALA:N	2.46	0.49
1:O4:121:ARG:NH2	1:O4:343:GLU:OE1	2.28	0.49
1:P4:107:SER:OG	1:P4:108:GLU:N	2.45	0.49
1:W4:90:LEU:HG	1:W4:91:ASN:H	1.77	0.49
1:J4:288:MET:HG2	2:D2:6:LYS:HD2	1.95	0.49
1:Y4:298:ALA:HB2	1:Y4:306:PRO:HD3	1.94	0.48
1:Z4:344:ARG:NE	1:Z4:367:ARG:HD3	2.28	0.48
1:N4:382:LYS:HE2	1:N4:384:ALA:HB2	1.95	0.48
1:M4:121:ARG:HH12	1:M4:343:GLU:CD	2.17	0.48
1:U4:296:LEU:HA	1:V4:294:ARG:CD	2.43	0.48
1:V4:289:LYS:O	2:E3:7:HIS:HA	2.13	0.48
1:H4:179:SER:HA	1:H4:359:HIS:HA	1.94	0.48
1:H4:278:ASN:ND2	1:H4:322:ASP:OD1	2.44	0.48
1:T4:305:GLU:HG2	1:T4:306:PRO:HD3	1.94	0.48
1:S4:277:MET:O	1:S4:317:ALA:N	2.46	0.48
1:J4:294:ARG:NH1	1:I4:294:ARG:HG2	2.28	0.48
1:A4:143:MET:HG3	1:A4:160:PRO:HD3	1.94	0.48
1:D4:211:ILE:HD12	1:D4:319:ASP:HB2	1.95	0.48
1:E4:121:ARG:NH1	1:E4:343:GLU:OE1	2.45	0.48
1:C5:295:PHE:CE2	1:C5:301:LEU:HD12	2.48	0.48
1:B5:350:LEU:N	1:B5:363:TYR:O	2.36	0.48
1:O4:134:PHE:HB3	1:O4:167:ILE:HB	1.95	0.48
1:T4:98:GLY:HA2	1:J4:162:ILE:HD12	1.96	0.48
1:S4:90:LEU:HG	1:S4:91:ASN:H	1.77	0.48
1:K4:130:GLU:N	1:K4:130:GLU:OE1	2.45	0.48
1:J4:215:GLY:HA2	1:J4:220:THR:HG22	1.95	0.48
1:I4:143:MET:HG2	1:I4:160:PRO:HD3	1.96	0.48
1:D4:119:SER:C	1:D4:121:ARG:H	2.17	0.48
1:C4:289:LYS:HD3	1:C4:293:GLY:HA2	1.95	0.48
1:C5:111:ARG:O	1:B5:138:VAL:HA	2.14	0.48
1:Z4:119:SER:H	1:Z4:122:GLN:HE22	1.62	0.48
1:Q4:200:ASP:OD2	1:Q4:204:ARG:NH1	2.47	0.48
1:W4:134:PHE:HB3	1:W4:167:ILE:HB	1.95	0.48
1:K4:296:LEU:HD23	1:K4:296:LEU:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H4:138:VAL:HA	1:I4:111:ARG:O	2.13	0.48
1:A4:225:LYS:HE2	1:A4:372:VAL:HG22	1.95	0.48
1:Z4:286:ARG:HH12	1:Z4:304:GLY:N	2.10	0.48
1:O4:244:GLY:O	1:O4:385:ALA:HA	2.13	0.48
1:I4:180:GLN:NE2	1:I4:184:ASP:OD1	2.46	0.48
1:D4:151:THR:O	1:D4:151:THR:OG1	2.31	0.48
1:G4:307:ALA:O	1:G4:308:ARG:HG2	2.12	0.48
2:D3:44:LEU:HA	2:D3:76:THR:HA	1.94	0.48
1:C5:133:SER:HB2	1:X4:104:PRO:HB3	1.95	0.48
1:P4:183:LEU:HD12	1:P4:360:VAL:HG21	1.95	0.48
1:S4:159:THR:HG22	1:S4:160:PRO:HD2	1.95	0.48
1:V4:225:LYS:HE2	1:V4:372:VAL:HG22	1.94	0.48
1:L4:141:THR:OG1	1:L4:161:GLN:HG2	2.14	0.48
1:L4:214:ASP:OD2	1:L4:216:VAL:HG22	2.13	0.48
1:B4:357:LYS:HB3	1:B4:358:PRO:HD3	1.95	0.48
2:A3:32:ARG:NH2	2:A3:67:ARG:O	2.40	0.48
1:Z4:307:ALA:O	1:Z4:308:ARG:HG2	2.14	0.48
1:B4:107:SER:OG	1:B4:109:THR:O	2.27	0.48
1:C4:322:ASP:OD1	1:C4:322:ASP:N	2.38	0.48
1:C5:112:GLY:HA2	1:B5:139:ASP:OD2	2.14	0.48
1:A5:348:ARG:HA	1:A5:348:ARG:NE	2.28	0.48
1:R4:227:LYS:HE3	1:R4:328:TYR:CE2	2.49	0.48
1:M4:121:ARG:NH2	1:M4:343:GLU:OE1	2.38	0.48
1:S4:253:ASN:ND2	2:C3:3:VAL:O	2.46	0.48
1:E4:268:GLU:HG2	1:F4:116:SER:HA	1.95	0.48
1:C4:258:VAL:O	1:C4:262:VAL:HG23	2.14	0.48
1:X4:289:LYS:HB2	1:X4:293:GLY:HA2	1.96	0.48
1:M4:265:LEU:HD21	1:M4:269:TYR:HB2	1.96	0.48
1:O4:382:LYS:HE2	1:O4:384:ALA:HB2	1.95	0.48
1:T4:209:ALA:HB1	1:T4:219:PRO:HD2	1.95	0.48
1:J4:334:ASP:OD2	1:J4:337:ASN:ND2	2.45	0.48
1:H4:338:GLY:HA2	1:H4:374:ASP:HB3	1.96	0.48
1:D4:348:ARG:HG2	1:D4:365:SER:O	2.13	0.48
1:B4:92:SER:O	1:B4:94:VAL:N	2.46	0.48
1:C4:193:TRP:HE1	1:C4:197:ARG:HH11	1.62	0.48
1:X4:208:ALA:HB2	1:X4:319:ASP:OD2	2.14	0.48
1:B5:190:ILE:HG13	1:B5:193:TRP:CZ3	2.48	0.48
1:M4:305:GLU:OE2	1:M4:305:GLU:CA	2.61	0.48
1:M4:305:GLU:O	1:M4:305:GLU:HG3	2.13	0.48
1:V4:289:LYS:HD3	1:V4:293:GLY:HA2	1.95	0.48
1:L4:305:GLU:HB2	1:L4:306:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H4:92:SER:O	1:H4:92:SER:OG	2.28	0.48
1:Y4:142:ASP:OD2	1:Z4:204:ARG:NH2	2.45	0.47
1:Z4:119:SER:N	1:Z4:122:GLN:HE22	2.12	0.47
1:R4:297:TRP:CE2	1:R4:309:LEU:HD13	2.49	0.47
1:P4:129:VAL:HG11	1:P4:342:ALA:HB1	1.96	0.47
1:V4:136:VAL:HG11	1:V4:373:SER:HB2	1.96	0.47
1:A4:255:SER:HB3	1:A4:296:LEU:HD21	1.96	0.47
1:D4:92:SER:OG	1:D4:93:ALA:N	2.47	0.47
1:F4:286:ARG:HH12	1:F4:305:GLU:N	2.12	0.47
1:C5:129:VAL:HG11	1:C5:342:ALA:HB1	1.96	0.47
1:N4:134:PHE:HB3	1:N4:167:ILE:HB	1.95	0.47
1:J4:278:ASN:HA	1:J4:317:ALA:O	2.14	0.47
1:Y4:134:PHE:HB3	1:Y4:167:ILE:HB	1.96	0.47
1:Y4:167:ILE:HG23	1:Y4:370:GLY:HA2	1.96	0.47
1:W4:193:TRP:CH2	1:V4:162:ILE:HD11	2.49	0.47
1:B5:121:ARG:NH1	1:B5:343:GLU:OE2	2.47	0.47
1:V4:268:GLU:H	1:V4:268:GLU:CD	2.09	0.47
1:L4:176:PRO:HG3	1:L4:198:ILE:HD11	1.96	0.47
1:C5:177:LYS:HB2	1:C5:361:LEU:HD13	1.97	0.47
1:Y4:92:SER:HA	1:Q4:182:LEU:HD13	1.96	0.47
1:B5:167:ILE:HG23	1:B5:370:GLY:HA2	1.96	0.47
1:B5:202:PHE:HD2	1:B5:347:LEU:HD21	1.79	0.47
1:R4:225:LYS:HE2	1:R4:372:VAL:HG22	1.96	0.47
1:Q4:298:ALA:HB2	1:Q4:306:PRO:HD3	1.95	0.47
1:W4:347:LEU:HD23	1:W4:349:VAL:HG23	1.97	0.47
1:T4:278:ASN:HA	1:T4:317:ALA:O	2.14	0.47
1:C5:128:ASN:ND2	1:C5:345:PRO:HG3	2.30	0.47
1:R4:156:GLU:HG2	1:M4:177:LYS:HD2	1.95	0.47
1:I4:211:ILE:HG21	1:I4:320:MET:HG2	1.95	0.47
1:A4:159:THR:HG22	1:A4:160:PRO:HD2	1.97	0.47
1:Z4:137:LEU:HD23	1:Z4:164:ARG:HB2	1.95	0.47
1:N4:167:ILE:HD12	1:N4:370:GLY:HA2	1.97	0.47
1:Q4:136:VAL:HG22	1:Q4:165:ILE:HB	1.96	0.47
1:O4:256:ASP:HA	1:O4:259:VAL:HG12	1.97	0.47
1:T4:289:LYS:HA	1:T4:295:PHE:HA	1.96	0.47
1:K4:150:GLU:HG2	1:H4:91:ASN:HB2	1.97	0.47
1:L4:94:VAL:HG13	1:L4:97:GLU:HB2	1.97	0.47
1:I4:343:GLU:HB3	1:I4:368:VAL:HG23	1.95	0.47
1:D4:194:LEU:HD23	1:C4:143:MET:HE1	1.97	0.47
1:D4:286:ARG:NH2	1:D4:305:GLU:H	2.13	0.47
2:A2:32:ARG:HG2	2:B2:2:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z4:163:ASP:OD1	1:Z4:164:ARG:N	2.48	0.47
1:A5:256:ASP:OD1	1:B5:287:LYS:HE3	2.15	0.47
1:O4:269:TYR:OH	1:O4:374:ASP:OD2	2.24	0.47
1:P4:119:SER:O	1:P4:119:SER:OG	2.30	0.47
1:E4:277:MET:O	1:E4:317:ALA:N	2.47	0.47
1:B4:126:VAL:HG12	1:B4:341:ILE:HB	1.97	0.47
1:A5:137:LEU:CD1	1:B5:188:PHE:CE1	2.98	0.47
1:A5:144:GLY:HA2	1:B5:201:LYS:NZ	2.30	0.47
1:N4:91:ASN:H	1:F4:179:SER:HB2	1.79	0.47
1:N4:181:ARG:HG3	1:E4:367:ARG:HH22	1.79	0.47
1:Q4:348:ARG:HH12	1:Q4:367:ARG:HD2	1.79	0.47
1:P4:181:ARG:NH2	1:W4:171:GLU:HG2	2.26	0.47
1:W4:281:THR:HG23	1:W4:323:ILE:HD11	1.96	0.47
1:U4:172:LEU:HD21	1:U4:205:ALA:HB3	1.97	0.47
1:T4:140:LYS:HG3	1:T4:161:GLN:HG3	1.96	0.47
1:K4:130:GLU:O	1:K4:130:GLU:HG2	2.14	0.47
1:K4:281:THR:HG23	1:K4:323:ILE:HD11	1.96	0.47
1:H4:167:ILE:HG23	1:H4:370:GLY:HA2	1.96	0.47
1:G4:279:SER:HB2	1:G4:318:GLU:OE2	2.15	0.47
1:B4:121:ARG:NH2	1:B4:206:GLU:OE2	2.48	0.47
1:Y4:334:ASP:OD2	1:Y4:337:ASN:ND2	2.47	0.47
1:B5:121:ARG:NH2	1:B5:343:GLU:OE1	2.48	0.47
1:M4:338:GLY:O	1:M4:373:SER:N	2.46	0.47
1:W4:244:GLY:O	1:W4:385:ALA:HA	2.15	0.47
1:U4:252:VAL:CG2	2:E3:3:VAL:HG21	2.45	0.47
1:T4:280:LYS:HB2	1:T4:280:LYS:HE2	1.69	0.47
1:T4:292:ASP:OD2	1:T4:294:ARG:NH2	2.35	0.47
1:X4:246:ALA:HA	1:X4:384:ALA:HA	1.97	0.46
1:A5:145:SER:HG	1:B5:202:PHE:HE1	1.62	0.46
1:S4:134:PHE:HB3	1:S4:167:ILE:HB	1.96	0.46
1:K4:147:TRP:H	1:L4:172:LEU:HD12	1.79	0.46
1:J4:252:VAL:HG13	1:J4:253:ASN:N	2.29	0.46
1:A4:129:VAL:HG11	1:A4:134:PHE:HD1	1.81	0.46
1:A4:244:GLY:O	1:A4:385:ALA:HA	2.14	0.46
1:F4:138:VAL:HA	1:G4:111:ARG:O	2.15	0.46
1:F4:142:ASP:OD2	1:G4:204:ARG:NH2	2.47	0.46
1:B5:343:GLU:HB3	1:B5:368:VAL:HG23	1.96	0.46
1:A4:119:SER:C	1:A4:121:ARG:H	2.19	0.46
1:B4:167:ILE:HG23	1:B4:370:GLY:HA2	1.97	0.46
1:B5:228:VAL:O	1:B5:239:GLY:HA2	2.15	0.46
1:B5:348:ARG:CZ	1:B5:348:ARG:CA	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O4:136:VAL:HG22	1:O4:165:ILE:HB	1.97	0.46
1:P4:101:LEU:HG	1:S4:190:ILE:HD11	1.97	0.46
1:U4:148:ALA:HB2	1:U4:154:LEU:HD13	1.96	0.46
1:T4:265:LEU:HD13	1:T4:332:PHE:CD2	2.51	0.46
1:V4:278:ASN:ND2	1:V4:322:ASP:OD1	2.47	0.46
1:H4:278:ASN:HA	1:H4:317:ALA:O	2.15	0.46
1:I4:248:ASP:OD1	1:I4:323:ILE:HG21	2.15	0.46
1:F4:211:ILE:HG21	1:F4:320:MET:HG2	1.97	0.46
2:B3:32:ARG:HG2	2:C3:2:ASP:HB3	1.97	0.46
1:C5:179:SER:HA	1:C5:359:HIS:HA	1.96	0.46
1:Z4:296:LEU:HB3	1:A5:301:LEU:HB2	1.97	0.46
1:W4:343:GLU:HB3	1:W4:368:VAL:HG23	1.97	0.46
1:S4:265:LEU:HD13	1:S4:332:PHE:CD2	2.50	0.46
1:J4:112:GLY:HA2	1:I4:139:ASP:H	1.80	0.46
1:G4:140:LYS:HG3	1:G4:235:TRP:CD1	2.51	0.46
1:G4:150:GLU:HA	1:G4:150:GLU:OE1	2.16	0.46
1:G4:168:PRO:HB2	1:G4:170:HIS:CE1	2.51	0.46
1:C5:217:ASP:OD1	1:C5:217:ASP:N	2.47	0.46
1:A5:322:ASP:OD1	1:A5:322:ASP:N	2.37	0.46
1:N4:128:ASN:ND2	1:N4:345:PRO:HG3	2.31	0.46
1:S4:227:LYS:HE3	1:S4:328:TYR:CE2	2.50	0.46
1:H4:186:SER:OG	1:E4:101:LEU:HB3	2.14	0.46
1:B4:211:ILE:HG21	1:B4:320:MET:HG2	1.96	0.46
1:C4:201:LYS:NZ	1:C4:205:ALA:HB2	2.31	0.46
1:Y4:183:LEU:HD13	1:Y4:360:VAL:HG21	1.96	0.46
1:N4:224:THR:O	1:N4:225:LYS:HD2	2.16	0.46
1:S4:278:ASN:HA	1:S4:317:ALA:O	2.15	0.46
1:H4:171:GLU:HA	1:H4:367:ARG:HA	1.96	0.46
1:A4:120:LEU:HD12	1:A4:123:ILE:HD11	1.98	0.46
1:A4:128:ASN:ND2	1:A4:345:PRO:HG3	2.30	0.46
1:X4:310:MET:H	1:Y4:302:ALA:HA	1.81	0.46
1:A5:225:LYS:HE3	1:A5:372:VAL:HG22	1.98	0.46
1:A5:262:VAL:HG21	1:A5:310:MET:HG3	1.98	0.46
1:P4:167:ILE:HG23	1:P4:370:GLY:HA2	1.97	0.46
1:W4:348:ARG:HH11	1:W4:367:ARG:HG3	1.79	0.46
1:T4:176:PRO:HG3	1:T4:198:ILE:HD11	1.96	0.46
1:T4:183:LEU:HD22	1:T4:360:VAL:HG21	1.97	0.46
1:H4:269:TYR:CE1	1:I4:114:LEU:HB2	2.51	0.46
1:A4:305:GLU:HB3	1:A4:306:PRO:HD3	1.98	0.46
1:D4:93:ALA:HB2	1:D4:102:VAL:HG21	1.97	0.46
1:E4:176:PRO:HD2	1:E4:362:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:103:ASP:N	1:A5:103:ASP:OD2	2.49	0.46
1:U4:219:PRO:HG3	1:U4:369:GLY:HA2	1.98	0.46
1:T4:244:GLY:O	1:T4:385:ALA:HA	2.16	0.46
1:E4:256:ASP:OD2	1:E4:257:ALA:N	2.48	0.46
1:G4:129:VAL:HG13	1:G4:169:LEU:HD22	1.98	0.46
1:G4:167:ILE:HG23	1:G4:370:GLY:HA2	1.98	0.46
1:X4:176:PRO:HD2	1:X4:362:PHE:O	2.16	0.46
1:B5:230:ASN:ND2	1:B5:264:ALA:HB1	2.31	0.46
1:W4:265:LEU:HD12	1:W4:379:LYS:HG2	1.97	0.46
1:E4:156:GLU:HG2	1:F4:361:LEU:HD11	1.97	0.46
1:E4:263:TYR:O	1:F4:279:SER:OG	2.34	0.46
1:F4:91:ASN:HD21	1:F4:94:VAL:HB	1.81	0.46
2:A3:37:ARG:HD2	2:A3:63:ILE:HG22	1.98	0.46
1:Y4:263:TYR:OH	1:Z4:305:GLU:OE1	2.31	0.46
1:R4:150:GLU:HG3	1:R4:151:THR:HG23	1.98	0.46
1:O4:255:SER:HB2	1:P4:301:LEU:HD21	1.97	0.46
1:O4:277:MET:HG2	1:O4:330:ILE:HG12	1.98	0.46
1:W4:277:MET:HG2	1:W4:330:ILE:HG12	1.96	0.46
1:W4:305:GLU:HB2	1:W4:306:PRO:HD3	1.97	0.46
1:T4:265:LEU:HD12	1:T4:379:LYS:HG2	1.97	0.46
1:T4:352:ASP:OD2	1:T4:355:SER:OG	2.26	0.46
1:V4:211:ILE:HG21	1:V4:320:MET:HG2	1.98	0.46
1:H4:225:LYS:HE2	1:H4:372:VAL:HG22	1.97	0.46
1:E4:225:LYS:HE2	1:E4:372:VAL:HG22	1.98	0.46
1:X4:277:MET:HG2	1:X4:330:ILE:HG12	1.97	0.45
1:A5:92:SER:OG	1:A5:93:ALA:N	2.47	0.45
1:N4:255:SER:OG	1:O4:295:PHE:HZ	2.00	0.45
1:Q4:112:GLY:HA2	1:P4:138:VAL:HG23	1.98	0.45
1:O4:201:LYS:O	1:O4:205:ALA:N	2.47	0.45
1:W4:133:SER:OG	1:W4:167:ILE:O	2.30	0.45
1:U4:315:LEU:HD23	1:U4:317:ALA:HB2	1.98	0.45
1:S4:296:LEU:H	1:S4:296:LEU:HD23	1.80	0.45
1:H4:130:GLU:OE1	1:H4:344:ARG:NH2	2.48	0.45
1:H4:188:PHE:O	1:H4:190:ILE:N	2.48	0.45
1:A4:219:PRO:HG3	1:A4:369:GLY:HA2	1.96	0.45
1:D4:324:ALA:HB3	1:D4:327:ALA:HB2	1.98	0.45
1:E4:297:TRP:CE2	1:E4:306:PRO:HG2	2.51	0.45
1:G4:201:LYS:HZ3	1:G4:205:ALA:HB2	1.81	0.45
1:A5:131:ALA:O	1:A5:133:SER:N	2.49	0.45
1:A5:348:ARG:O	1:A5:364:ALA:HA	2.16	0.45
1:R4:311:GLY:N	1:M4:302:ALA:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q4:121:ARG:NH1	1:Q4:343:GLU:OE2	2.44	0.45
1:A4:265:LEU:HG	1:A4:269:TYR:HB2	1.98	0.45
1:F4:277:MET:O	1:F4:317:ALA:N	2.49	0.45
1:B4:225:LYS:HE2	1:B4:372:VAL:HG22	1.98	0.45
2:D3:37:ARG:HD2	2:D3:63:ILE:HG22	1.98	0.45
2:D3:37:ARG:HB3	2:D3:81:VAL:HG13	1.99	0.45
1:Y4:225:LYS:HE2	1:Y4:372:VAL:HG22	1.98	0.45
1:Z4:251:ALA:O	1:Z4:252:VAL:HG22	2.16	0.45
1:Z4:272:ASN:N	1:Z4:272:ASN:OD1	2.49	0.45
1:A5:147:TRP:CZ3	1:B5:172:LEU:HB2	2.51	0.45
1:M4:167:ILE:HG23	1:M4:370:GLY:HA2	1.98	0.45
1:M4:350:LEU:HD11	1:F4:354:PHE:CE1	2.51	0.45
1:S4:357:LYS:HE2	1:S4:357:LYS:HB2	1.71	0.45
1:K4:268:GLU:HG2	1:L4:114:LEU:HG	1.98	0.45
1:G4:175:MET:HG3	1:G4:363:TYR:HB2	1.98	0.45
2:D2:37:ARG:HB3	2:D2:81:VAL:HG13	1.99	0.45
2:B2:37:ARG:HD2	2:B2:63:ILE:HG22	1.98	0.45
2:E2:32:ARG:HE	2:E2:67:ARG:HG2	1.82	0.45
2:E2:37:ARG:HB3	2:E2:81:VAL:HG13	1.99	0.45
1:X4:324:ALA:HB3	1:X4:327:ALA:HB2	1.99	0.45
1:R4:292:ASP:O	1:Q4:291:ALA:HB3	2.17	0.45
1:Q4:178:ALA:HB1	1:Q4:183:LEU:HD21	1.97	0.45
1:T4:106:THR:HA	1:S4:135:ASP:HB2	1.99	0.45
1:S4:382:LYS:HE2	1:S4:384:ALA:HB2	1.98	0.45
1:E4:230:ASN:OD1	1:E4:231:GLY:N	2.49	0.45
1:B4:129:VAL:HG11	1:B4:342:ALA:HB1	1.99	0.45
2:A2:37:ARG:HD2	2:A2:63:ILE:HG22	1.98	0.45
1:X4:139:ASP:OD1	1:X4:139:ASP:N	2.37	0.45
1:X4:347:LEU:HD13	1:X4:366:LYS:HB2	1.98	0.45
1:Z4:119:SER:H	1:Z4:122:GLN:NE2	2.15	0.45
1:O4:339:TYR:OH	1:O4:370:GLY:O	2.27	0.45
1:W4:268:GLU:HG2	1:S4:114:LEU:HG	1.98	0.45
1:J4:165:ILE:HD12	1:J4:373:SER:HA	1.99	0.45
1:I4:119:SER:C	1:I4:121:ARG:H	2.20	0.45
1:A4:343:GLU:HB3	1:A4:368:VAL:HG23	1.97	0.45
1:G4:90:LEU:HB3	1:G4:91:ASN:H	1.65	0.45
2:D2:37:ARG:HD2	2:D2:63:ILE:HG22	1.98	0.45
2:B2:32:ARG:HE	2:B2:67:ARG:HG2	1.82	0.45
2:E2:37:ARG:HD2	2:E2:63:ILE:HG22	1.98	0.45
2:E3:32:ARG:HE	2:E3:67:ARG:HG2	1.82	0.45
2:C3:32:ARG:HE	2:C3:67:ARG:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C3:37:ARG:HB3	2:C3:81:VAL:HG13	1.99	0.45
2:A3:37:ARG:HB3	2:A3:81:VAL:HG13	1.99	0.45
1:C5:294:ARG:HH12	1:B5:296:LEU:HA	1.81	0.45
1:Y4:128:ASN:ND2	1:Y4:345:PRO:HG3	2.30	0.45
1:Y4:201:LYS:HZ2	1:Y4:205:ALA:HB2	1.81	0.45
1:A5:171:GLU:HB2	1:A5:367:ARG:NE	2.32	0.45
1:R4:134:PHE:O	1:R4:167:ILE:N	2.44	0.45
1:M4:95:ALA:HA	1:M4:99:GLY:HA3	1.98	0.45
1:Q4:121:ARG:HH12	1:Q4:343:GLU:CD	2.20	0.45
1:W4:225:LYS:HE2	1:W4:372:VAL:HG22	1.98	0.45
1:W4:294:ARG:HH12	1:V4:294:ARG:HG3	1.81	0.45
1:K4:343:GLU:HB3	1:K4:368:VAL:HG23	1.98	0.45
1:J4:265:LEU:HD13	1:J4:332:PHE:CD2	2.52	0.45
1:A4:139:ASP:HB2	1:A4:160:PRO:HB2	1.99	0.45
1:A4:191:GLU:HG2	1:A4:362:PHE:CZ	2.51	0.45
2:D2:32:ARG:HE	2:D2:67:ARG:HG2	1.82	0.45
2:A2:37:ARG:HB3	2:A2:81:VAL:HG13	1.99	0.45
2:C2:37:ARG:HB3	2:C2:81:VAL:HG13	1.99	0.45
1:X4:143:MET:HE3	1:Y4:197:ARG:HB2	1.99	0.45
1:A5:137:LEU:O	1:B5:110:ILE:HG13	2.16	0.45
1:M4:277:MET:HG2	1:M4:330:ILE:HG12	1.99	0.45
1:Q4:137:LEU:HD21	1:Q4:164:ARG:HB2	1.99	0.45
1:T4:226:THR:O	1:T4:237:SER:HB2	2.17	0.45
1:L4:150:GLU:CG	1:I4:91:ASN:HB2	2.46	0.45
1:I4:171:GLU:HA	1:I4:367:ARG:HA	1.99	0.45
2:C2:37:ARG:HD2	2:C2:63:ILE:HG22	1.98	0.45
2:B3:37:ARG:HB3	2:B3:81:VAL:HG13	1.99	0.45
2:A1:32:ARG:HE	2:A1:67:ARG:HG2	1.82	0.45
1:Z4:220:THR:HG23	1:Z4:224:THR:HG23	1.99	0.45
1:P4:106:THR:HG23	1:P4:107:SER:N	2.31	0.45
1:W4:238:LEU:HD23	1:W4:380:LEU:HD11	1.99	0.45
1:J4:194:LEU:HD22	1:I4:143:MET:CE	2.47	0.45
1:H4:288:MET:CE	1:H4:297:TRP:HE1	2.30	0.45
1:D4:138:VAL:HG23	1:D4:163:ASP:HB3	1.98	0.45
1:E4:177:LYS:HD2	1:E4:359:HIS:CD2	2.52	0.45
2:B3:32:ARG:HE	2:B3:67:ARG:HG2	1.82	0.45
1:Z4:294:ARG:O	1:Z4:295:PHE:HB2	2.17	0.45
1:B5:172:LEU:O	1:B5:365:SER:HA	2.16	0.45
1:N4:106:THR:HG23	1:N4:107:SER:N	2.30	0.45
1:N4:135:ASP:OD1	1:N4:166:THR:HG22	2.16	0.45
1:M4:136:VAL:CG2	1:M4:165:ILE:HB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M4:279:SER:HB2	1:M4:318:GLU:OE2	2.17	0.45
1:A4:243:THR:O	1:A4:250:ALA:HB2	2.17	0.45
1:E4:136:VAL:CG2	1:E4:165:ILE:HB	2.46	0.45
1:E4:191:GLU:HG3	1:E4:362:PHE:CE1	2.52	0.45
1:B4:133:SER:HB2	1:C4:104:PRO:HB3	1.98	0.45
1:B4:140:LYS:HE2	1:B4:235:TRP:CD1	2.51	0.45
2:B2:37:ARG:HB3	2:B2:81:VAL:HG13	1.99	0.45
1:Y4:256:ASP:OD2	1:Y4:257:ALA:N	2.49	0.45
1:B5:225:LYS:HE2	1:B5:372:VAL:HG22	1.98	0.45
1:R4:230:ASN:ND2	1:R4:264:ALA:HB1	2.32	0.45
1:M4:261:LEU:HD22	1:M4:381:LEU:HB2	1.99	0.45
1:H4:183:LEU:HD21	1:H4:362:PHE:HZ	1.82	0.45
1:I4:121:ARG:NH2	1:I4:206:GLU:OE2	2.50	0.45
1:I4:228:VAL:O	1:I4:239:GLY:HA2	2.16	0.45
1:B4:119:SER:C	1:B4:121:ARG:H	2.20	0.45
2:A3:32:ARG:HE	2:A3:67:ARG:HG2	1.82	0.45
2:A3:72:LEU:O	2:A3:76:THR:OG1	2.29	0.45
1:X4:262:VAL:HG21	1:X4:310:MET:HG2	1.98	0.44
1:B5:171:GLU:HA	1:B5:367:ARG:HA	1.98	0.44
1:W4:261:LEU:HD13	1:W4:381:LEU:HB2	1.99	0.44
1:T4:150:GLU:HG2	1:V4:91:ASN:HB2	2.00	0.44
1:H4:138:VAL:HG21	1:H4:235:TRP:HZ2	1.81	0.44
1:G4:133:SER:HB3	1:B4:104:PRO:HB3	1.99	0.44
1:B4:138:VAL:HG23	1:B4:163:ASP:HB3	1.99	0.44
1:Y4:214:ASP:OD1	1:Y4:214:ASP:N	2.33	0.44
1:B5:348:ARG:NE	1:B5:348:ARG:CA	2.66	0.44
1:N4:265:LEU:HD13	1:N4:332:PHE:CD2	2.53	0.44
1:N4:294:ARG:HD3	1:O4:294:ARG:NH2	2.32	0.44
1:M4:136:VAL:HG23	1:M4:165:ILE:HB	1.99	0.44
1:Q4:189:ASP:HB3	1:Q4:192:THR:HG22	1.99	0.44
1:P4:167:ILE:HD12	1:P4:370:GLY:HA2	1.98	0.44
1:S4:95:ALA:HA	1:S4:99:GLY:HA3	1.99	0.44
1:K4:261:LEU:HD22	1:K4:381:LEU:HB2	1.99	0.44
1:V4:291:ALA:O	2:D3:10:SER:HB2	2.17	0.44
1:H4:269:TYR:OH	1:H4:374:ASP:OD2	2.20	0.44
1:I4:90:LEU:HG	1:I4:91:ASN:H	1.82	0.44
1:I4:289:LYS:O	2:C2:7:HIS:HA	2.17	0.44
1:D4:333:GLY:HA3	1:D4:378:ILE:HA	1.99	0.44
1:G4:255:SER:HB3	1:G4:296:LEU:HD13	1.99	0.44
1:B4:136:VAL:O	1:B4:164:ARG:HA	2.17	0.44
2:A1:37:ARG:HD2	2:A1:63:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A1:37:ARG:HB3	2:A1:81:VAL:HG13	1.99	0.44
1:J4:219:PRO:HG3	1:J4:369:GLY:HA2	1.99	0.44
1:J4:227:LYS:H	1:J4:227:LYS:CE	2.26	0.44
1:V4:183:LEU:HD21	1:V4:362:PHE:CZ	2.52	0.44
1:E4:256:ASP:HB2	1:F4:287:LYS:HE3	1.98	0.44
1:E4:265:LEU:HD11	1:E4:333:GLY:HA2	2.00	0.44
1:F4:182:LEU:O	1:F4:186:SER:OG	2.22	0.44
2:B3:37:ARG:HD2	2:B3:63:ILE:HG22	1.98	0.44
1:C5:277:MET:O	1:C5:317:ALA:N	2.50	0.44
1:X4:277:MET:O	1:X4:317:ALA:N	2.49	0.44
1:Z4:129:VAL:HG11	1:Z4:342:ALA:HB1	1.98	0.44
1:R4:172:LEU:HA	1:Q4:147:TRP:H	1.82	0.44
1:O4:226:THR:O	1:O4:237:SER:HB2	2.17	0.44
1:K4:117:THR:HG22	1:J4:268:GLU:OE1	2.17	0.44
1:V4:214:ASP:OD1	1:V4:214:ASP:N	2.44	0.44
1:A4:273:ALA:O	1:A4:313:PRO:HD2	2.18	0.44
1:C4:121:ARG:HH12	1:C4:343:GLU:CD	2.19	0.44
1:C4:329:ALA:HB3	1:C4:383:PHE:CE2	2.52	0.44
1:C5:352:ASP:OD1	1:C5:352:ASP:N	2.46	0.44
1:Q4:262:VAL:HG12	1:Q4:270:ARG:HD3	2.00	0.44
1:W4:139:ASP:H	1:S4:112:GLY:HA2	1.82	0.44
1:T4:127:VAL:HG11	1:T4:134:PHE:CE2	2.52	0.44
1:K4:191:GLU:HG2	1:K4:362:PHE:CZ	2.53	0.44
1:G4:178:ALA:O	1:G4:360:VAL:HG22	2.17	0.44
2:A2:32:ARG:HE	2:A2:67:ARG:HG2	1.82	0.44
2:E3:19:TYR:OH	2:E3:31:ARG:O	2.30	0.44
2:E3:37:ARG:HD2	2:E3:63:ILE:HG22	1.98	0.44
1:X4:272:ASN:OD1	1:X4:272:ASN:N	2.50	0.44
1:Y4:190:ILE:HD11	1:Q4:101:LEU:HD13	1.99	0.44
1:B5:138:VAL:HG21	1:B5:235:TRP:HZ2	1.83	0.44
1:R4:322:ASP:OD1	1:R4:322:ASP:N	2.39	0.44
1:W4:121:ARG:NH2	1:W4:206:GLU:OE2	2.50	0.44
1:U4:136:VAL:HG22	1:U4:165:ILE:HB	2.00	0.44
1:U4:227:LYS:HG2	1:U4:380:LEU:HD22	1.99	0.44
1:U4:288:MET:HA	2:D3:6:LYS:HB3	1.98	0.44
1:L4:288:MET:HA	2:A2:6:LYS:HB3	1.99	0.44
1:I4:315:LEU:HD23	1:I4:317:ALA:HB2	1.99	0.44
1:D4:277:MET:O	1:D4:317:ALA:N	2.50	0.44
1:F4:134:PHE:HB3	1:F4:167:ILE:HB	2.00	0.44
1:G4:272:ASN:OD1	1:G4:272:ASN:N	2.51	0.44
1:C4:134:PHE:HB3	1:C4:167:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E2:72:LEU:O	2:E2:76:THR:OG1	2.30	0.44
2:D3:32:ARG:HE	2:D3:67:ARG:HG2	1.82	0.44
1:R4:272:ASN:N	1:R4:272:ASN:OD1	2.50	0.44
1:R4:343:GLU:HB3	1:R4:368:VAL:HG23	1.98	0.44
1:O4:91:ASN:N	1:O4:91:ASN:ND2	2.64	0.44
1:S4:186:SER:O	1:S4:186:SER:OG	2.30	0.44
1:V4:227:LYS:HG2	1:V4:380:LEU:HD22	1.99	0.44
1:I4:223:LEU:O	1:I4:227:LYS:NZ	2.28	0.44
1:A4:151:THR:O	1:A4:151:THR:OG1	2.33	0.44
2:C2:32:ARG:HE	2:C2:67:ARG:HG2	1.82	0.44
1:C5:272:ASN:N	1:C5:272:ASN:OD1	2.51	0.44
1:A5:254:ALA:C	1:A5:256:ASP:H	2.20	0.44
1:A5:269:TYR:CZ	1:B5:114:LEU:HB2	2.53	0.44
1:N4:252:VAL:HG23	1:N4:253:ASN:H	1.81	0.44
1:R4:114:LEU:HD23	1:Q4:268:GLU:HG3	2.00	0.44
1:R4:189:ASP:HB3	1:R4:192:THR:HG22	1.98	0.44
1:O4:94:VAL:HG23	1:O4:97:GLU:HB2	2.00	0.44
1:H4:122:GLN:HG2	1:H4:123:ILE:HG23	1.99	0.44
1:A4:254:ALA:C	1:A4:256:ASP:H	2.20	0.44
1:A5:149:SER:OG	1:A5:150:GLU:N	2.50	0.44
1:A5:194:LEU:O	1:A5:198:ILE:HG12	2.17	0.44
1:A5:289:LYS:HZ2	1:A5:295:PHE:HE1	1.61	0.44
1:N4:89:ALA:HB2	1:F4:193:TRP:HZ3	1.83	0.44
1:N4:177:LYS:HG2	1:N4:361:LEU:HD13	2.00	0.44
1:N4:286:ARG:NH1	1:N4:305:GLU:H	2.15	0.44
1:Q4:111:ARG:O	1:P4:138:VAL:HA	2.18	0.44
1:Q4:289:LYS:HZ1	1:Q4:295:PHE:HE1	1.65	0.44
1:T4:307:ALA:O	1:T4:314:VAL:HB	2.16	0.44
1:J4:288:MET:HA	2:D2:6:LYS:HB3	1.99	0.44
1:H4:238:LEU:HD23	1:H4:380:LEU:HD11	1.99	0.44
1:F4:141:THR:HG22	1:F4:142:ASP:N	2.32	0.44
1:G4:347:LEU:HB3	1:G4:366:LYS:HB2	1.99	0.44
1:P4:194:LEU:HD21	1:S4:89:ALA:HB2	1.99	0.43
1:U4:119:SER:C	1:U4:121:ARG:H	2.22	0.43
1:U4:183:LEU:HD21	1:U4:362:PHE:HZ	1.83	0.43
1:T4:243:THR:HG23	1:T4:382:LYS:O	2.18	0.43
1:L4:209:ALA:HA	1:L4:213:GLY:HA3	2.00	0.43
1:I4:252:VAL:CG2	2:D2:3:VAL:HG21	2.48	0.43
1:E4:178:ALA:HB3	1:E4:362:PHE:HE2	1.82	0.43
1:F4:136:VAL:HG22	1:F4:165:ILE:HB	2.00	0.43
1:G4:243:THR:O	1:G4:250:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G4:357:LYS:HB2	1:G4:358:PRO:HD3	2.00	0.43
2:C3:37:ARG:HD2	2:C3:63:ILE:HG22	1.98	0.43
1:X4:90:LEU:HB3	1:X4:91:ASN:H	1.71	0.43
1:Z4:119:SER:C	1:Z4:121:ARG:H	2.21	0.43
1:Z4:268:GLU:HG2	1:A5:116:SER:HA	1.99	0.43
1:N4:167:ILE:HG21	1:N4:342:ALA:HB3	2.00	0.43
1:R4:183:LEU:HD12	1:R4:360:VAL:HG21	1.98	0.43
1:W4:167:ILE:HD12	1:W4:370:GLY:HA2	1.99	0.43
1:U4:270:ARG:NH1	1:V4:279:SER:OG	2.51	0.43
1:Y4:182:LEU:HD11	1:Q4:101:LEU:HD11	2.00	0.43
1:A5:141:THR:HG22	1:A5:142:ASP:N	2.31	0.43
1:M4:227:LYS:HG2	1:M4:380:LEU:HD22	1.99	0.43
1:O4:90:LEU:HD23	1:K4:159:THR:OG1	2.17	0.43
1:O4:211:ILE:HD12	1:O4:319:ASP:HB2	2.00	0.43
1:V4:142:ASP:OD1	1:V4:142:ASP:N	2.50	0.43
1:E4:265:LEU:HD21	1:E4:269:TYR:CB	2.43	0.43
1:G4:220:THR:CB	1:G4:371:ASP:OD2	2.65	0.43
1:G4:261:LEU:HD22	1:G4:381:LEU:HB2	1.99	0.43
1:Y4:99:GLY:O	1:Y4:102:VAL:HG22	2.19	0.43
1:B5:347:LEU:HD12	1:B5:349:VAL:HG12	2.01	0.43
1:T4:281:THR:HA	1:T4:323:ILE:HD11	2.00	0.43
1:K4:289:LYS:HD2	2:E2:7:HIS:CE1	2.54	0.43
1:F4:110:ILE:HD13	1:F4:110:ILE:HG21	1.80	0.43
1:C4:286:ARG:HH12	1:C4:304:GLY:H	1.66	0.43
2:E3:37:ARG:HB3	2:E3:81:VAL:HG13	1.99	0.43
1:X4:276:VAL:HG12	1:X4:320:MET:HG3	2.00	0.43
1:N4:171:GLU:HG2	1:L4:181:ARG:NH2	2.33	0.43
1:O4:183:LEU:HD12	1:O4:190:ILE:HB	2.00	0.43
1:P4:278:ASN:HD21	1:P4:322:ASP:HB3	1.84	0.43
1:U4:357:LYS:HB2	1:U4:357:LYS:HE2	1.74	0.43
1:J4:348:ARG:HH11	1:J4:367:ARG:HG3	1.84	0.43
1:H4:267:ALA:HB3	1:I4:116:SER:HB2	1.99	0.43
1:F4:141:THR:HG22	1:F4:142:ASP:H	1.84	0.43
1:F4:351:ARG:HH21	1:F4:360:VAL:HG21	1.83	0.43
1:Z4:101:LEU:HD21	1:V4:162:ILE:CD1	2.47	0.43
1:A5:256:ASP:HA	1:A5:259:VAL:HG22	2.00	0.43
1:B5:272:ASN:OD1	1:B5:272:ASN:N	2.51	0.43
1:R4:121:ARG:NH2	1:R4:343:GLU:OE1	2.50	0.43
1:M4:343:GLU:HB3	1:M4:368:VAL:HG23	2.01	0.43
1:W4:130:GLU:OE2	1:W4:344:ARG:NH2	2.52	0.43
1:J4:114:LEU:HG	1:I4:268:GLU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:277:MET:HG2	1:L4:330:ILE:HG12	1.99	0.43
1:A4:272:ASN:N	1:A4:272:ASN:OD1	2.49	0.43
1:G4:329:ALA:HB3	1:G4:383:PHE:CE2	2.54	0.43
1:M4:243:THR:HG23	1:M4:382:LYS:O	2.18	0.43
1:W4:308:ARG:NH2	1:W4:311:GLY:O	2.51	0.43
1:S4:136:VAL:HG11	1:S4:373:SER:HB2	2.00	0.43
1:V4:286:ARG:HA	1:V4:286:ARG:HD3	1.87	0.43
1:L4:289:LYS:HD3	1:L4:293:GLY:HA2	2.01	0.43
1:I4:254:ALA:C	1:I4:256:ASP:H	2.22	0.43
1:D4:93:ALA:HA	1:D4:99:GLY:HA3	2.00	0.43
1:Q4:244:GLY:O	1:Q4:385:ALA:HA	2.18	0.43
1:Q4:322:ASP:OD1	1:Q4:322:ASP:N	2.40	0.43
1:P4:290:ASP:OD1	1:P4:290:ASP:N	2.42	0.43
1:P4:324:ALA:HB3	1:P4:327:ALA:HB2	2.01	0.43
1:U4:138:VAL:HG21	1:U4:235:TRP:HZ2	1.84	0.43
1:T4:193:TRP:CZ3	1:K4:89:ALA:HB2	2.52	0.43
1:T4:324:ALA:HB3	1:T4:327:ALA:HB2	2.01	0.43
1:K4:227:LYS:HE2	1:K4:227:LYS:HB2	1.81	0.43
1:L4:265:LEU:HD12	1:L4:379:LYS:HG2	1.99	0.43
1:I4:225:LYS:HE2	1:I4:372:VAL:HG22	1.99	0.43
1:D4:228:VAL:O	1:D4:239:GLY:HA2	2.18	0.43
1:F4:241:VAL:O	1:F4:381:LEU:HD12	2.19	0.43
1:X4:329:ALA:HB3	1:X4:383:PHE:CE2	2.54	0.43
1:Z4:214:ASP:OD1	1:Z4:214:ASP:N	2.42	0.43
1:A5:131:ALA:C	1:A5:133:SER:H	2.21	0.43
1:N4:156:GLU:HG2	1:O4:177:LYS:HE3	2.00	0.43
1:J4:285:VAL:HG11	1:J4:309:LEU:HD11	2.01	0.43
1:V4:277:MET:HG2	1:V4:330:ILE:HG12	2.01	0.43
1:B4:156:GLU:OE1	1:C4:177:LYS:HE2	2.18	0.43
1:C5:350:LEU:HB3	1:C5:363:TYR:HD2	1.84	0.43
1:T4:348:ARG:NH1	1:T4:367:ARG:HG3	2.33	0.43
1:K4:92:SER:O	1:K4:92:SER:OG	2.25	0.43
1:K4:243:THR:O	1:K4:250:ALA:HB2	2.19	0.43
1:K4:357:LYS:HD3	1:K4:357:LYS:HA	1.80	0.43
1:J4:91:ASN:HB2	1:H4:150:GLU:HG2	2.01	0.43
1:L4:162:ILE:HD13	1:E4:101:LEU:CD2	2.49	0.43
1:E4:138:VAL:HG12	1:F4:111:ARG:HG3	2.01	0.43
1:B4:272:ASN:OD1	1:B4:272:ASN:N	2.52	0.43
1:X4:233:TRP:CH2	1:X4:376:ALA:HB2	2.54	0.42
1:Y4:350:LEU:HD11	1:W4:354:PHE:HE1	1.83	0.42
1:B5:299:ASP:OD1	1:B5:299:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R4:102:VAL:HB	1:Q4:132:THR:CG2	2.49	0.42
1:R4:352:ASP:OD1	1:R4:352:ASP:N	2.51	0.42
1:W4:214:ASP:OD1	1:W4:214:ASP:N	2.44	0.42
1:B4:343:GLU:HB3	1:B4:368:VAL:HG23	2.01	0.42
1:X4:119:SER:O	1:X4:119:SER:OG	2.29	0.42
1:Y4:129:VAL:HG11	1:Y4:342:ALA:HB1	2.01	0.42
1:N4:174:ALA:HB2	1:M4:145:SER:HB2	2.00	0.42
1:M4:352:ASP:OD1	1:M4:352:ASP:N	2.52	0.42
1:Q4:180:GLN:OE1	1:Q4:180:GLN:HA	2.19	0.42
1:Q4:202:PHE:HD2	1:Q4:347:LEU:HD11	1.84	0.42
1:O4:90:LEU:HD22	1:L4:177:LYS:O	2.19	0.42
1:O4:154:LEU:HG	1:O4:155:SER:O	2.19	0.42
1:W4:228:VAL:O	1:W4:239:GLY:HA2	2.19	0.42
1:T4:255:SER:O	1:T4:259:VAL:HG13	2.20	0.42
1:V4:296:LEU:HD23	1:V4:296:LEU:H	1.84	0.42
1:L4:261:LEU:HD21	1:L4:332:PHE:CB	2.48	0.42
1:H4:296:LEU:HD23	1:H4:296:LEU:H	1.83	0.42
1:I4:143:MET:CG	1:I4:160:PRO:HD3	2.48	0.42
1:D4:289:LYS:NZ	1:C4:253:ASN:HD21	2.17	0.42
1:E4:147:TRP:CZ2	1:F4:209:ALA:HB2	2.54	0.42
1:B4:90:LEU:HD23	1:B4:90:LEU:O	2.19	0.42
1:C5:262:VAL:HG21	1:C5:310:MET:HG2	2.01	0.42
1:Q4:140:LYS:HE3	1:Q4:235:TRP:HB3	2.00	0.42
1:Q4:154:LEU:HD23	1:Q4:154:LEU:H	1.84	0.42
1:Q4:339:TYR:OH	1:Q4:370:GLY:O	2.36	0.42
1:P4:357:LYS:NZ	1:W4:352:ASP:OD2	2.40	0.42
1:K4:256:ASP:HA	1:K4:259:VAL:HG12	2.01	0.42
1:H4:101:LEU:HD23	1:E4:190:ILE:HD11	2.00	0.42
1:H4:186:SER:O	1:H4:188:PHE:N	2.52	0.42
1:H4:197:ARG:HD3	1:H4:197:ARG:HA	1.85	0.42
1:I4:149:SER:HB3	1:I4:152:ALA:HB2	2.01	0.42
1:D4:227:LYS:HB3	1:D4:240:TYR:HD1	1.84	0.42
1:B4:297:TRP:CE2	1:B4:309:LEU:HD13	2.54	0.42
1:B5:192:THR:O	1:B5:195:ALA:N	2.51	0.42
1:N4:177:LYS:HD2	1:M4:156:GLU:HG2	2.00	0.42
1:P4:334:ASP:N	1:P4:377:ALA:O	2.51	0.42
1:W4:349:VAL:HG22	1:W4:364:ALA:HB2	2.00	0.42
1:U4:289:LYS:HD2	2:D3:7:HIS:CE1	2.54	0.42
1:U4:315:LEU:CD2	1:U4:317:ALA:HB2	2.49	0.42
1:S4:223:LEU:O	1:S4:227:LYS:NZ	2.26	0.42
1:K4:139:ASP:H	1:L4:112:GLY:HA2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V4:328:TYR:CE1	1:V4:382:LYS:HB2	2.54	0.42
1:H4:167:ILE:HD12	1:H4:370:GLY:HA2	2.01	0.42
1:H4:252:VAL:HG11	2:C2:3:VAL:CG1	2.48	0.42
1:A4:176:PRO:HD2	1:A4:362:PHE:O	2.19	0.42
1:D4:281:THR:HG23	1:D4:323:ILE:HD11	2.01	0.42
1:E4:290:ASP:OD1	1:E4:290:ASP:N	2.46	0.42
1:X4:138:VAL:HA	1:Y4:111:ARG:O	2.20	0.42
1:X4:167:ILE:HG23	1:X4:370:GLY:HA2	2.01	0.42
1:Y4:248:ASP:CG	1:Y4:249:PHE:H	2.22	0.42
1:Z4:350:LEU:N	1:Z4:363:TYR:O	2.44	0.42
1:B5:109:THR:O	1:B5:109:THR:OG1	2.37	0.42
1:B5:194:LEU:HA	1:B5:194:LEU:HD23	1.72	0.42
1:B5:233:TRP:CH2	1:B5:376:ALA:HB2	2.54	0.42
1:N4:143:MET:HG2	1:N4:160:PRO:HD3	2.01	0.42
1:N4:246:ALA:HA	1:N4:384:ALA:O	2.19	0.42
1:N4:279:SER:HG	1:N4:318:GLU:CD	2.23	0.42
1:M4:298:ALA:HB2	1:M4:306:PRO:HD3	2.00	0.42
1:U4:211:ILE:HG21	1:U4:320:MET:HG2	2.01	0.42
1:A4:227:LYS:HE2	1:A4:227:LYS:HB2	1.87	0.42
1:E4:147:TRP:CH2	1:F4:209:ALA:HB2	2.54	0.42
1:E4:289:LYS:HE3	1:E4:289:LYS:HB3	1.85	0.42
1:F4:92:SER:OG	1:F4:93:ALA:N	2.53	0.42
1:Y4:299:ASP:OD1	1:Y4:300:SER:N	2.52	0.42
1:Z4:95:ALA:HA	1:Z4:99:GLY:HA3	2.01	0.42
1:A5:310:MET:HE1	1:B5:301:LEU:HD22	2.00	0.42
1:A5:310:MET:HA	1:B5:301:LEU:O	2.18	0.42
1:O4:172:LEU:HD21	1:O4:202:PHE:HA	2.02	0.42
1:P4:329:ALA:HB3	1:P4:383:PHE:CE2	2.52	0.42
1:W4:276:VAL:HG12	1:W4:320:MET:SD	2.59	0.42
1:V4:262:VAL:HG12	1:V4:270:ARG:HD3	2.01	0.42
1:L4:138:VAL:HG23	1:L4:163:ASP:HB3	2.02	0.42
2:B3:19:TYR:OH	2:B3:31:ARG:O	2.31	0.42
1:X4:161:GLN:HG2	1:X4:161:GLN:H	1.71	0.42
1:N4:182:LEU:HD21	1:F4:89:ALA:N	2.35	0.42
1:P4:252:VAL:HG13	1:P4:253:ASN:N	2.35	0.42
1:W4:172:LEU:HD11	1:V4:145:SER:HB3	2.00	0.42
1:U4:288:MET:CE	1:U4:297:TRP:HE1	2.32	0.42
1:D4:318:GLU:O	1:D4:318:GLU:HG3	2.19	0.42
1:G4:297:TRP:CE2	1:G4:309:LEU:HD13	2.54	0.42
1:B4:168:PRO:HB2	1:B4:170:HIS:CE1	2.55	0.42
1:C4:269:TYR:OH	1:C4:374:ASP:OD2	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X4:163:ASP:OD1	1:X4:164:ARG:N	2.52	0.42
1:Y4:350:LEU:HD11	1:W4:354:PHE:CE1	2.54	0.42
1:A5:211:ILE:HG21	1:A5:320:MET:HG2	2.00	0.42
1:B5:136:VAL:CG2	1:B5:165:ILE:HB	2.50	0.42
1:B5:277:MET:HG2	1:B5:330:ILE:HG12	2.02	0.42
1:N4:167:ILE:HG23	1:N4:370:GLY:HA2	2.01	0.42
1:Q4:106:THR:HG22	1:P4:164:ARG:HH11	1.84	0.42
1:W4:270:ARG:NH1	1:S4:279:SER:OG	2.53	0.42
1:W4:366:LYS:HB2	1:W4:366:LYS:HE2	1.87	0.42
1:K4:280:LYS:HE3	1:K4:322:ASP:OD2	2.20	0.42
1:J4:175:MET:HA	1:J4:362:PHE:O	2.20	0.42
1:H4:220:THR:OG1	1:H4:371:ASP:HB3	2.19	0.42
1:I4:254:ALA:O	1:I4:255:SER:OG	2.31	0.42
1:D4:211:ILE:HG21	1:D4:320:MET:HG2	2.01	0.42
1:D4:290:ASP:OD2	1:E4:294:ARG:HD3	2.18	0.42
1:E4:193:TRP:HE1	1:E4:197:ARG:NH1	2.17	0.42
1:Z4:133:SER:HB2	1:A5:104:PRO:HB3	2.01	0.42
1:A5:272:ASN:OD1	1:A5:272:ASN:N	2.52	0.42
1:A5:349:VAL:HA	1:A5:363:TYR:O	2.20	0.42
1:N4:119:SER:O	1:N4:119:SER:OG	2.38	0.42
1:N4:180:GLN:HB2	1:N4:360:VAL:CG2	2.50	0.42
1:Q4:299:ASP:OD1	1:Q4:299:ASP:N	2.52	0.42
1:W4:288:MET:CE	1:W4:297:TRP:HE1	2.33	0.42
1:J4:346:ASP:OD2	1:J4:346:ASP:N	2.52	0.42
1:G4:121:ARG:HH12	1:G4:343:GLU:CD	2.24	0.42
1:B4:286:ARG:HH21	1:B4:286:ARG:HG3	1.84	0.42
1:C4:226:THR:O	1:C4:237:SER:HB2	2.20	0.42
1:X4:215:GLY:HA2	1:X4:220:THR:HG22	2.01	0.42
1:Z4:263:TYR:HE2	1:A5:286:ARG:HE	1.67	0.42
1:B5:277:MET:O	1:B5:317:ALA:N	2.52	0.42
1:N4:230:ASN:ND2	1:N4:264:ALA:HB1	2.34	0.42
1:O4:227:LYS:HB2	1:O4:227:LYS:HE2	1.84	0.42
1:P4:163:ASP:OD1	1:P4:164:ARG:N	2.53	0.42
1:U4:136:VAL:CG2	1:U4:165:ILE:HB	2.50	0.42
1:T4:191:GLU:OE2	1:T4:351:ARG:NE	2.53	0.42
1:A4:367:ARG:NH1	1:C4:181:ARG:HD3	2.35	0.42
1:E4:289:LYS:HB2	1:E4:293:GLY:HA2	2.01	0.42
1:F4:262:VAL:HG21	1:F4:310:MET:HG3	2.02	0.42
1:B4:137:LEU:O	1:C4:111:ARG:N	2.51	0.42
1:B4:142:ASP:HB3	1:C4:115:ARG:NH2	2.35	0.42
2:B2:19:TYR:OH	2:B2:31:ARG:O	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X4:135:ASP:OD2	1:X4:166:THR:HG22	2.20	0.41
1:Z4:265:LEU:HB3	1:Z4:270:ARG:HG3	2.02	0.41
1:R4:269:TYR:CE1	1:M4:114:LEU:HB2	2.55	0.41
1:Q4:94:VAL:HB	1:Q4:97:GLU:OE2	2.20	0.41
1:Q4:137:LEU:HD23	1:Q4:137:LEU:HA	1.69	0.41
1:T4:252:VAL:HG11	2:D3:3:VAL:CG1	2.50	0.41
1:S4:330:ILE:HD12	1:S4:381:LEU:HD23	2.02	0.41
1:J4:172:LEU:HD11	1:I4:145:SER:HB3	2.01	0.41
1:F4:227:LYS:HG2	1:F4:380:LEU:HD22	2.01	0.41
1:G4:227:LYS:HE3	1:G4:328:TYR:CE2	2.55	0.41
1:C4:136:VAL:CG2	1:C4:165:ILE:HB	2.49	0.41
2:D2:11:LEU:HD23	2:E2:14:PRO:HD2	2.02	0.41
1:X4:334:ASP:OD2	1:X4:337:ASN:ND2	2.53	0.41
1:Y4:276:VAL:HG12	1:Y4:320:MET:SD	2.60	0.41
1:Q4:183:LEU:HD13	1:Q4:191:GLU:OE2	2.20	0.41
1:P4:177:LYS:HE2	1:P4:359:HIS:CD2	2.55	0.41
1:T4:220:THR:OG1	1:T4:371:ASP:HB3	2.20	0.41
1:L4:227:LYS:HE2	1:L4:227:LYS:HB2	1.90	0.41
1:H4:135:ASP:OD1	1:H4:166:THR:HG22	2.20	0.41
1:H4:265:LEU:HD13	1:H4:332:PHE:CE2	2.55	0.41
1:E4:294:ARG:HD2	1:E4:294:ARG:HA	1.84	0.41
1:F4:277:MET:HG2	1:F4:330:ILE:HG12	2.02	0.41
1:G4:255:SER:HB2	1:B4:295:PHE:HZ	1.86	0.41
2:A2:19:TYR:OH	2:A2:31:ARG:O	2.31	0.41
2:B3:2:ASP:HB3	2:A3:32:ARG:HG2	2.02	0.41
1:Y4:272:ASN:OD1	1:Y4:272:ASN:N	2.52	0.41
1:B5:202:PHE:CE2	1:B5:347:LEU:HD11	2.55	0.41
1:N4:354:PHE:CE1	1:E4:350:LEU:HD11	2.55	0.41
1:R4:348:ARG:H	1:R4:348:ARG:HG2	1.71	0.41
1:R4:348:ARG:NH1	1:R4:367:ARG:HD2	2.36	0.41
1:P4:147:TRP:O	1:P4:148:ALA:HB3	2.20	0.41
1:P4:301:LEU:HD23	1:P4:301:LEU:HA	1.76	0.41
1:K4:277:MET:HG2	1:K4:330:ILE:HG12	2.01	0.41
1:H4:244:GLY:O	1:H4:385:ALA:HA	2.20	0.41
1:A4:143:MET:CG	1:A4:160:PRO:HD3	2.50	0.41
1:E4:241:VAL:HG23	1:E4:381:LEU:HD12	2.02	0.41
1:C4:167:ILE:HD12	1:C4:370:GLY:HA2	2.02	0.41
1:X4:256:ASP:OD2	1:X4:257:ALA:N	2.53	0.41
1:A5:183:LEU:HD21	1:A5:362:PHE:CZ	2.55	0.41
1:O4:135:ASP:HB2	1:P4:106:THR:O	2.21	0.41
1:P4:227:LYS:H	1:P4:227:LYS:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W4:268:GLU:HB2	1:S4:116:SER:HA	2.02	0.41
1:U4:159:THR:CG2	1:U4:160:PRO:HD2	2.49	0.41
1:U4:167:ILE:HD13	1:U4:371:ASP:OD1	2.21	0.41
1:U4:269:TYR:CE1	1:V4:114:LEU:HB2	2.56	0.41
1:K4:114:LEU:HG	1:J4:268:GLU:HG2	2.01	0.41
1:E4:177:LYS:HD3	1:E4:361:LEU:HD11	2.01	0.41
1:E4:265:LEU:HD13	1:E4:332:PHE:CE2	2.56	0.41
1:E4:272:ASN:OD1	1:E4:272:ASN:N	2.53	0.41
1:E4:333:GLY:HA3	1:E4:378:ILE:HA	2.03	0.41
2:D2:67:ARG:NH2	2:E2:4:PHE:HB2	2.35	0.41
1:Y4:149:SER:OG	1:Y4:152:ALA:HB2	2.20	0.41
1:Y4:154:LEU:HD11	1:Z4:363:TYR:HE1	1.85	0.41
1:Z4:138:VAL:O	1:Z4:138:VAL:HG23	2.20	0.41
1:B5:136:VAL:HG22	1:B5:165:ILE:HB	2.03	0.41
1:P4:101:LEU:HD11	1:S4:110:ILE:HD12	2.02	0.41
1:S4:248:ASP:OD2	1:S4:248:ASP:N	2.44	0.41
1:V4:122:GLN:HG2	1:V4:123:ILE:HG23	2.02	0.41
1:L4:358:PRO:HG2	1:L4:359:HIS:CD2	2.56	0.41
1:H4:167:ILE:HD13	1:H4:371:ASP:OD1	2.20	0.41
1:D4:136:VAL:CG2	1:D4:165:ILE:HB	2.50	0.41
1:G4:265:LEU:HG	1:G4:269:TYR:HB2	2.03	0.41
1:B4:149:SER:HB2	1:B4:152:ALA:HB2	2.02	0.41
1:C4:297:TRP:CZ2	1:C4:309:LEU:HB2	2.56	0.41
1:C4:297:TRP:NE1	1:C4:306:PRO:HG2	2.35	0.41
1:X4:352:ASP:C	1:X4:354:PHE:H	2.24	0.41
1:Z4:330:ILE:HD12	1:Z4:381:LEU:HD23	2.02	0.41
1:R4:168:PRO:HB2	1:R4:170:HIS:CE1	2.56	0.41
1:R4:173:ALA:H	1:Q4:146:GLY:HA3	1.85	0.41
1:M4:176:PRO:HG3	1:M4:198:ILE:HD11	2.03	0.41
1:Q4:114:LEU:HB2	1:P4:269:TYR:CZ	2.56	0.41
1:U4:361:LEU:HD12	1:U4:361:LEU:HA	1.89	0.41
1:J4:134:PHE:HB3	1:J4:167:ILE:HB	2.02	0.41
1:J4:216:VAL:HG23	1:J4:216:VAL:O	2.20	0.41
1:V4:127:VAL:HG11	1:V4:134:PHE:CZ	2.54	0.41
1:V4:227:LYS:HE2	1:V4:227:LYS:HB2	1.87	0.41
1:L4:322:ASP:N	1:L4:322:ASP:OD1	2.51	0.41
1:D4:286:ARG:NH1	1:D4:305:GLU:HA	2.33	0.41
1:B4:136:VAL:CG1	1:C4:111:ARG:HH21	2.31	0.41
2:D3:14:PRO:HD2	2:C3:11:LEU:HD23	2.03	0.41
1:Z4:89:ALA:HA	1:V4:159:THR:HG21	2.03	0.41
1:Z4:123:ILE:H	1:Z4:123:ILE:HG12	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z4:249:PHE:HB3	1:Z4:254:ALA:HB1	2.02	0.41
1:Z4:251:ALA:O	1:Z4:253:ASN:N	2.54	0.41
1:N4:262:VAL:HG12	1:N4:270:ARG:HD3	2.01	0.41
1:N4:298:ALA:HB2	1:N4:306:PRO:HD3	2.03	0.41
1:R4:262:VAL:HG21	1:R4:310:MET:HG2	2.03	0.41
1:Q4:174:ALA:HB2	1:P4:145:SER:HB3	2.02	0.41
1:O4:365:SER:O	1:O4:365:SER:OG	2.33	0.41
1:W4:135:ASP:HA	1:W4:165:ILE:O	2.21	0.41
1:L4:133:SER:HB2	1:H4:104:PRO:HB3	2.02	0.41
1:L4:139:ASP:H	1:H4:112:GLY:HA2	1.85	0.41
1:L4:265:LEU:HD13	1:L4:332:PHE:CD2	2.55	0.41
1:L4:361:LEU:HD12	1:L4:361:LEU:HA	1.87	0.41
1:H4:120:LEU:HD23	1:H4:120:LEU:O	2.20	0.41
1:H4:129:VAL:HG23	1:I4:105:GLN:CD	2.41	0.41
1:I4:289:LYS:HD2	2:C2:7:HIS:CE1	2.56	0.41
1:G4:276:VAL:HG12	1:G4:320:MET:SD	2.60	0.41
1:B4:299:ASP:OD1	1:B4:299:ASP:N	2.53	0.41
1:U4:126:VAL:HG13	1:U4:343:GLU:HG2	2.02	0.41
1:T4:272:ASN:OD1	1:T4:272:ASN:N	2.54	0.41
1:T4:294:ARG:NH2	1:S4:292:ASP:OD2	2.54	0.41
1:K4:265:LEU:HD12	1:K4:379:LYS:HG2	2.01	0.41
1:F4:167:ILE:HD12	1:F4:370:GLY:HA2	2.02	0.41
1:G4:133:SER:OG	1:G4:134:PHE:N	2.54	0.41
1:G4:230:ASN:ND2	1:G4:379:LYS:HD2	2.35	0.41
2:D2:4:PHE:HB3	2:C2:11:LEU:HD11	2.03	0.41
2:E3:2:ASP:HB3	2:D3:32:ARG:HG2	2.03	0.41
1:C5:114:LEU:HB3	1:B5:268:GLU:HG2	2.03	0.41
1:X4:286:ARG:NH1	1:X4:304:GLY:H	2.15	0.41
1:X4:307:ALA:O	1:X4:308:ARG:HD2	2.20	0.41
1:Z4:216:VAL:HG23	1:Z4:216:VAL:O	2.21	0.41
1:N4:185:ASP:O	1:F4:102:VAL:HG12	2.20	0.41
1:N4:193:TRP:O	1:N4:197:ARG:HG2	2.21	0.41
1:N4:263:TYR:OH	1:O4:286:ARG:NH1	2.54	0.41
1:M4:177:LYS:HG3	1:M4:361:LEU:HD12	2.02	0.41
1:M4:220:THR:OG1	1:M4:371:ASP:HB2	2.21	0.41
1:O4:107:SER:O	1:O4:109:THR:N	2.54	0.41
1:O4:127:VAL:O	1:O4:129:VAL:HG23	2.21	0.41
1:P4:181:ARG:HD3	1:W4:367:ARG:NH1	2.36	0.41
1:P4:254:ALA:C	1:P4:256:ASP:H	2.23	0.41
1:U4:163:ASP:OD1	1:U4:164:ARG:N	2.54	0.41
1:U4:289:LYS:CD	2:D3:7:HIS:CE1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T4:228:VAL:O	1:T4:239:GLY:HA2	2.20	0.41
1:S4:128:ASN:OD1	1:S4:128:ASN:C	2.58	0.41
1:S4:167:ILE:HG23	1:S4:370:GLY:HA2	2.03	0.41
1:J4:228:VAL:O	1:J4:239:GLY:HA2	2.21	0.41
1:J4:309:LEU:HD23	1:J4:310:MET:HB2	2.01	0.41
1:J4:324:ALA:HB3	1:J4:327:ALA:HB2	2.02	0.41
1:V4:119:SER:O	1:V4:119:SER:OG	2.35	0.41
1:V4:265:LEU:HD13	1:V4:332:PHE:CD2	2.55	0.41
1:L4:214:ASP:OD2	1:L4:215:GLY:N	2.54	0.41
1:H4:291:ALA:O	2:A2:10:SER:HB2	2.21	0.41
1:I4:223:LEU:HD23	1:I4:223:LEU:HA	1.92	0.41
1:D4:272:ASN:OD1	1:D4:272:ASN:N	2.54	0.41
1:F4:126:VAL:HG12	1:F4:341:ILE:HB	2.03	0.41
1:F4:216:VAL:O	1:F4:216:VAL:HG23	2.21	0.41
1:F4:352:ASP:OD1	1:F4:352:ASP:N	2.51	0.41
1:G4:139:ASP:OD1	1:B4:112:GLY:HA2	2.21	0.41
1:B4:131:ALA:O	1:B4:169:LEU:HD23	2.21	0.41
1:C4:277:MET:HG2	1:C4:330:ILE:HG12	2.03	0.41
2:D2:2:ASP:HB3	2:C2:32:ARG:HG2	2.03	0.41
2:A2:2:ASP:HB3	2:E2:32:ARG:HG2	2.03	0.41
2:E3:66:VAL:HA	2:A3:15:ALA:HB3	2.03	0.41
1:C5:220:THR:O	1:C5:220:THR:OG1	2.36	0.41
1:C5:299:ASP:OD1	1:C5:299:ASP:N	2.53	0.41
1:Z4:185:ASP:HB3	1:V4:132:THR:HB	2.02	0.41
1:R4:138:VAL:HA	1:M4:111:ARG:O	2.20	0.41
1:R4:270:ARG:NH1	1:M4:279:SER:OG	2.53	0.41
1:M4:286:ARG:NH1	1:M4:305:GLU:H	2.19	0.41
1:Q4:129:VAL:HG11	1:Q4:342:ALA:HB1	2.03	0.41
1:O4:193:TRP:HE1	1:O4:197:ARG:HE	1.68	0.41
1:W4:114:LEU:HD23	1:W4:114:LEU:HA	1.97	0.41
1:W4:382:LYS:HE2	1:W4:384:ALA:HB2	2.03	0.41
1:U4:138:VAL:HA	1:V4:111:ARG:O	2.21	0.41
1:T4:123:ILE:HD13	1:T4:315:LEU:HD13	2.03	0.41
1:L4:329:ALA:HB3	1:L4:383:PHE:CE2	2.56	0.41
1:A4:120:LEU:HD23	1:A4:210:PHE:HB3	2.02	0.41
1:F4:286:ARG:NH1	1:F4:305:GLU:HG2	2.36	0.41
2:E3:67:ARG:NH2	2:A3:4:PHE:HB2	2.35	0.41
1:X4:297:TRP:CE2	1:X4:306:PRO:HG2	2.56	0.40
1:Y4:171:GLU:OE1	1:Y4:348:ARG:NH1	2.53	0.40
1:Y4:181:ARG:NH1	1:P4:171:GLU:HG2	2.36	0.40
1:Z4:252:VAL:HG23	1:Z4:253:ASN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N4:171:GLU:HA	1:N4:367:ARG:HA	2.03	0.40
1:W4:268:GLU:CG	1:S4:114:LEU:HG	2.51	0.40
1:J4:305:GLU:N	1:J4:305:GLU:OE1	2.54	0.40
1:V4:285:VAL:HG11	1:V4:309:LEU:HD11	2.02	0.40
1:F4:324:ALA:HB3	1:F4:327:ALA:HB2	2.03	0.40
1:G4:322:ASP:N	1:G4:322:ASP:OD1	2.37	0.40
1:Y4:188:PHE:HD2	1:Q4:101:LEU:HB2	1.86	0.40
1:M4:147:TRP:H	1:M4:147:TRP:HE3	1.67	0.40
1:O4:130:GLU:OE2	1:O4:344:ARG:NH2	2.54	0.40
1:P4:215:GLY:HA2	1:P4:220:THR:HG22	2.02	0.40
1:U4:227:LYS:HE3	1:U4:328:TYR:CE2	2.56	0.40
1:T4:256:ASP:HA	1:T4:259:VAL:HG22	2.04	0.40
1:J4:142:ASP:N	1:J4:142:ASP:OD1	2.54	0.40
1:D4:175:MET:HA	1:D4:362:PHE:O	2.22	0.40
1:C5:110:ILE:HD11	1:C5:193:TRP:CE2	2.56	0.40
1:C5:135:ASP:HA	1:C5:165:ILE:O	2.21	0.40
1:C5:136:VAL:CG1	1:X4:111:ARG:HH21	2.32	0.40
1:Y4:352:ASP:OD1	1:Y4:352:ASP:N	2.54	0.40
1:M4:91:ASN:HB3	1:Q4:151:THR:CG2	2.51	0.40
1:M4:176:PRO:HD2	1:M4:362:PHE:O	2.21	0.40
1:Q4:171:GLU:HA	1:Q4:367:ARG:HA	2.03	0.40
1:O4:90:LEU:O	1:L4:182:LEU:HD22	2.21	0.40
1:O4:350:LEU:HD11	1:S4:354:PHE:HE1	1.86	0.40
1:P4:175:MET:HE3	1:P4:363:TYR:HB2	2.02	0.40
1:W4:186:SER:O	1:W4:186:SER:OG	2.26	0.40
1:S4:227:LYS:HE2	1:S4:227:LYS:HB2	1.91	0.40
1:L4:179:SER:O	1:L4:183:LEU:HD13	2.21	0.40
1:I4:288:MET:CE	1:I4:297:TRP:HE1	2.35	0.40
1:D4:213:GLY:O	1:D4:220:THR:HA	2.21	0.40
1:E4:125:SER:HB2	1:E4:336:GLY:O	2.21	0.40
1:G4:136:VAL:CG2	1:G4:165:ILE:HB	2.51	0.40
2:C3:52:ILE:H	2:C3:52:ILE:HG13	1.72	0.40
1:A5:129:VAL:HG21	1:A5:134:PHE:HD1	1.85	0.40
1:R4:126:VAL:HG13	1:R4:343:GLU:HG2	2.03	0.40
1:M4:252:VAL:HG13	1:M4:253:ASN:N	2.36	0.40
1:W4:143:MET:CE	1:S4:194:LEU:HD22	2.51	0.40
1:U4:172:LEU:HD12	1:T4:147:TRP:H	1.85	0.40
1:U4:186:SER:O	1:U4:188:PHE:N	2.55	0.40
1:T4:136:VAL:HG13	1:T4:165:ILE:HB	2.03	0.40
1:T4:308:ARG:NH2	1:T4:311:GLY:O	2.54	0.40
1:K4:243:THR:HG23	1:K4:382:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L4:136:VAL:HG22	1:L4:165:ILE:HB	2.03	0.40
1:L4:241:VAL:HG21	1:L4:261:LEU:HB2	2.04	0.40
1:E4:261:LEU:HD22	1:E4:381:LEU:HB2	2.03	0.40
2:E3:11:LEU:HD23	2:A3:14:PRO:HD2	2.02	0.40
2:B3:67:ARG:NH2	2:C3:4:PHE:HB2	2.37	0.40
1:C5:136:VAL:CG2	1:C5:165:ILE:HB	2.51	0.40
1:X4:123:ILE:HD13	1:X4:315:LEU:HD22	2.03	0.40
1:Z4:106:THR:OG1	1:W4:103:ASP:OD1	2.28	0.40
1:A5:119:SER:C	1:A5:121:ARG:H	2.25	0.40
1:N4:265:LEU:HD21	1:N4:269:TYR:HB2	2.03	0.40
1:P4:298:ALA:HB2	1:P4:306:PRO:HG2	2.03	0.40
1:P4:357:LYS:HD3	1:P4:357:LYS:HA	1.97	0.40
1:W4:140:LYS:HB2	1:W4:140:LYS:HE3	1.92	0.40
1:W4:162:ILE:HD11	1:S4:193:TRP:CH2	2.56	0.40
1:U4:141:THR:HG23	1:U4:160:PRO:HA	2.02	0.40
1:J4:149:SER:H	1:J4:152:ALA:HB2	1.86	0.40
1:J4:272:ASN:OD1	1:J4:272:ASN:N	2.54	0.40
1:D4:299:ASP:OD1	1:D4:300:SER:N	2.55	0.40
1:C4:248:ASP:CG	1:C4:249:PHE:H	2.24	0.40
2:D2:32:ARG:HG2	2:E2:2:ASP:HB3	2.04	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	290/386 (75%)	259 (89%)	29 (10%)	2 (1%)	22	58
1	B4	295/386 (76%)	260 (88%)	34 (12%)	1 (0%)	41	74
1	B5	266/386 (69%)	227 (85%)	38 (14%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C4	295/386 (76%)	262 (89%)	33 (11%)	0	100	100
1	C5	295/386 (76%)	265 (90%)	30 (10%)	0	100	100
1	D4	295/386 (76%)	264 (90%)	30 (10%)	1 (0%)	41	74
1	E4	295/386 (76%)	266 (90%)	29 (10%)	0	100	100
1	F4	295/386 (76%)	265 (90%)	30 (10%)	0	100	100
1	G4	295/386 (76%)	259 (88%)	35 (12%)	1 (0%)	41	74
1	H4	287/386 (74%)	254 (88%)	32 (11%)	1 (0%)	41	74
1	I4	287/386 (74%)	261 (91%)	25 (9%)	1 (0%)	41	74
1	J4	287/386 (74%)	249 (87%)	37 (13%)	1 (0%)	41	74
1	K4	287/386 (74%)	257 (90%)	29 (10%)	1 (0%)	41	74
1	L4	287/386 (74%)	256 (89%)	30 (10%)	1 (0%)	41	74
1	M4	295/386 (76%)	257 (87%)	38 (13%)	0	100	100
1	N4	295/386 (76%)	259 (88%)	35 (12%)	1 (0%)	41	74
1	O4	295/386 (76%)	256 (87%)	38 (13%)	1 (0%)	41	74
1	P4	295/386 (76%)	250 (85%)	44 (15%)	1 (0%)	41	74
1	Q4	295/386 (76%)	259 (88%)	35 (12%)	1 (0%)	41	74
1	R4	295/386 (76%)	254 (86%)	40 (14%)	1 (0%)	41	74
1	S4	287/386 (74%)	254 (88%)	32 (11%)	1 (0%)	41	74
1	T4	287/386 (74%)	261 (91%)	26 (9%)	0	100	100
1	U4	287/386 (74%)	257 (90%)	29 (10%)	1 (0%)	41	74
1	V4	287/386 (74%)	256 (89%)	30 (10%)	1 (0%)	41	74
1	W4	287/386 (74%)	254 (88%)	32 (11%)	1 (0%)	41	74
1	X4	295/386 (76%)	265 (90%)	30 (10%)	0	100	100
1	Y4	295/386 (76%)	265 (90%)	30 (10%)	0	100	100
1	Z4	295/386 (76%)	257 (87%)	38 (13%)	0	100	100
2	A1	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	A2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	A3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	B2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	B3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	C2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	D2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	D3	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	E2	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
2	E3	82/84 (98%)	76 (93%)	6 (7%)	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	9351/12768 (73%)	8312 (89%)	1018 (11%)	21 (0%)	50	80

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P4	306	PRO
1	J4	187	ALA
1	V4	187	ALA
1	L4	187	ALA
1	A5	132	THR
1	Q4	179	SER
1	W4	187	ALA
1	U4	187	ALA
1	S4	187	ALA
1	K4	187	ALA
1	H4	187	ALA
1	I4	187	ALA
1	A4	187	ALA
1	G4	295	PHE
1	A5	93	ALA
1	B5	193	TRP
1	N4	92	SER
1	R4	108	GLU
1	O4	108	GLU
1	D4	91	ASN
1	B4	93	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A4	215/285 (75%)	214 (100%)	1 (0%)	88	95
1	A5	215/285 (75%)	214 (100%)	1 (0%)	88	95
1	B4	218/285 (76%)	217 (100%)	1 (0%)	88	95
1	B5	197/285 (69%)	196 (100%)	1 (0%)	88	95
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%)	218 (100%)	0	100	100
1	E4	218/285 (76%)	218 (100%)	0	100	100
1	F4	218/285 (76%)	218 (100%)	0	100	100
1	G4	218/285 (76%)	217 (100%)	1 (0%)	88	95
1	H4	215/285 (75%)	215 (100%)	0	100	100
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%)	215 (100%)	0	100	100
1	L4	215/285 (75%)	214 (100%)	1 (0%)	88	95
1	M4	218/285 (76%)	217 (100%)	1 (0%)	88	95
1	N4	218/285 (76%)	216 (99%)	2 (1%)	78	90
1	O4	218/285 (76%)	216 (99%)	2 (1%)	78	90
1	P4	218/285 (76%)	217 (100%)	1 (0%)	88	95
1	Q4	218/285 (76%)	217 (100%)	1 (0%)	88	95
1	R4	218/285 (76%)	216 (99%)	2 (1%)	78	90
1	S4	215/285 (75%)	215 (100%)	0	100	100
1	T4	215/285 (75%)	214 (100%)	1 (0%)	88	95
1	U4	215/285 (75%)	213 (99%)	2 (1%)	78	90
1	V4	215/285 (75%)	215 (100%)	0	100	100
1	W4	215/285 (75%)	214 (100%)	1 (0%)	88	95
1	X4	218/285 (76%)	218 (100%)	0	100	100
1	Y4	218/285 (76%)	217 (100%)	1 (0%)	88	95
1	Z4	218/285 (76%)	218 (100%)	0	100	100
2	A1	69/69 (100%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	7034/9472 (74%)	7012 (100%)	22 (0%)	92	97

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C5	217	ASP
1	Y4	253	ASN
1	A5	122	GLN
1	B5	347	LEU
1	N4	115	ARG
1	N4	220	THR
1	R4	101	LEU
1	R4	337	ASN
1	M4	150	GLU
1	Q4	115	ARG
1	O4	91	ASN
1	O4	100	TYR
1	P4	150	GLU
1	W4	261	LEU
1	U4	214	ASP
1	U4	256	ASP
1	T4	278	ASN
1	L4	272	ASN
1	A4	122	GLN
1	G4	260	ASP
1	B4	348	ARG

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Mol	Chain	Res	Type
1	C4	161	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C5	196	ASN
1	X4	91	ASN
1	Z4	91	ASN
1	R4	337	ASN
1	Q4	359	HIS
1	O4	91	ASN
1	U4	326	ASN
1	I4	180	GLN
1	A4	337	ASN
1	D4	337	ASN
1	B4	253	ASN
1	C4	196	ASN
1	C4	253	ASN
2	A2	7	HIS
2	B2	7	HIS
2	E2	7	HIS
2	E3	7	HIS
2	D3	7	HIS
2	A3	7	HIS
2	A1	7	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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.

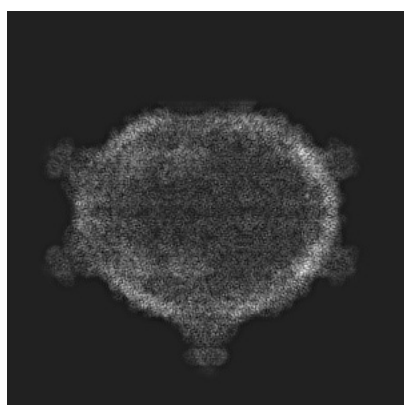
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10565. These allow visual inspection of the internal detail of the map and identification of artifacts.

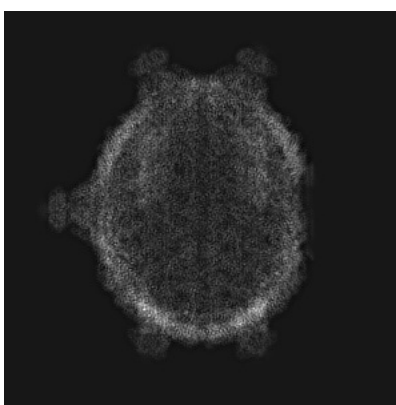
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

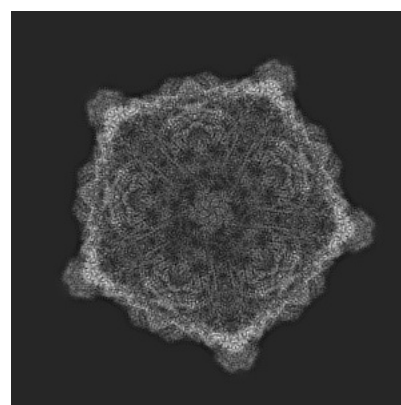
#### 6.1.1 Primary map



X



Y



Z

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

### 6.2 Central slices [i](#)

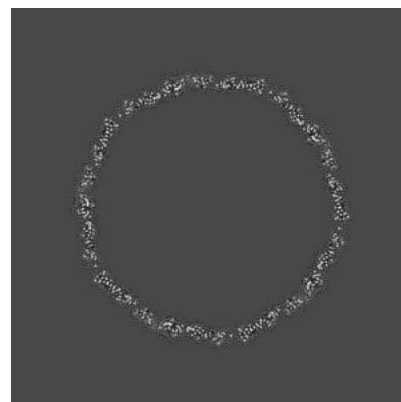
#### 6.2.1 Primary map



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: 345



Y Index: 167

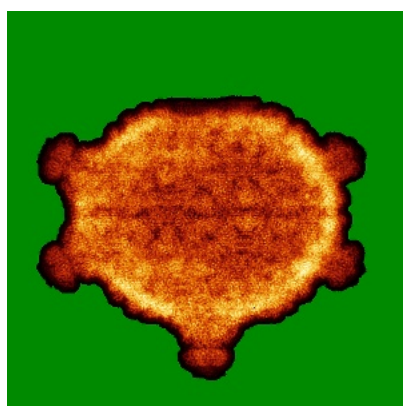


Z Index: 185

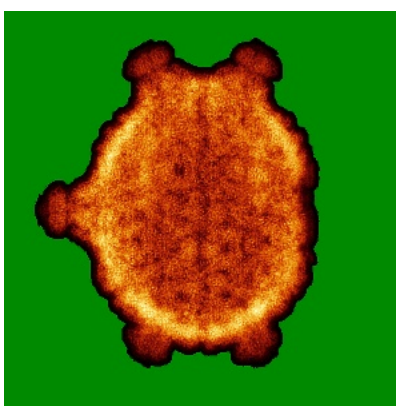
The images above show the largest variance slices of the map in three orthogonal directions.

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

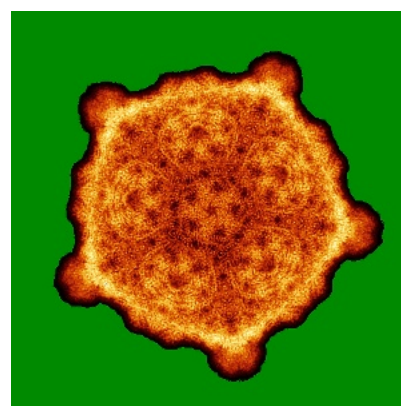
### 6.4.1 Primary map



X



Y

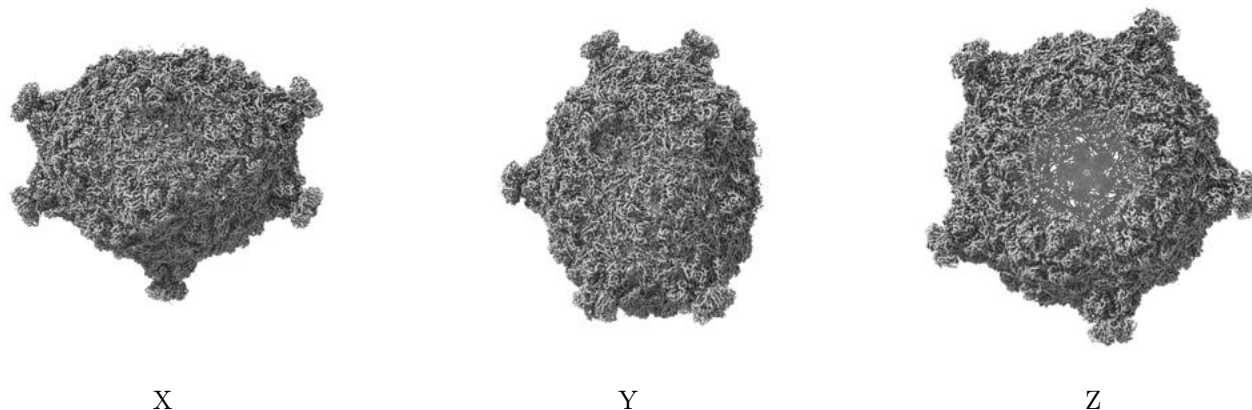


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.113. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

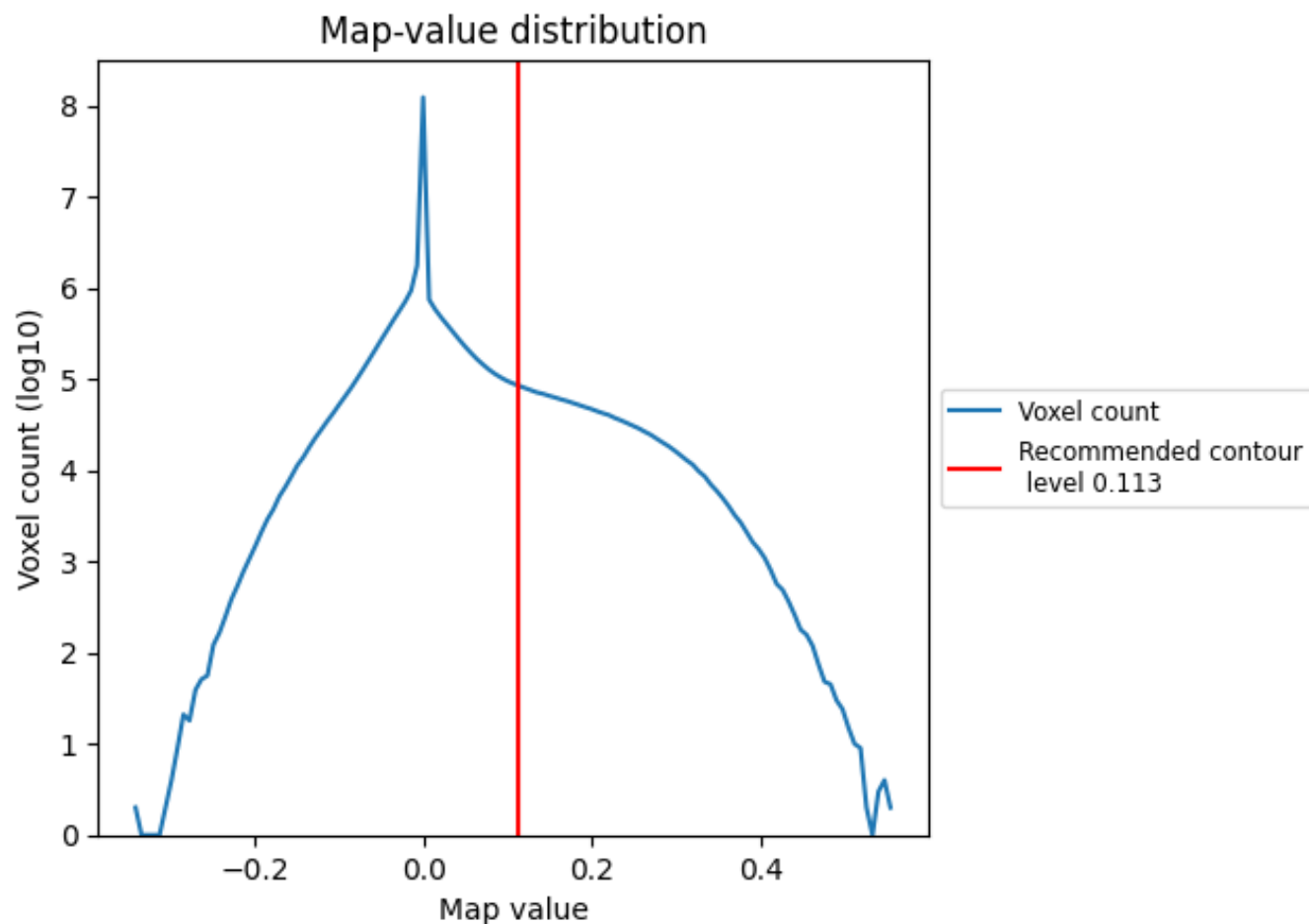
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

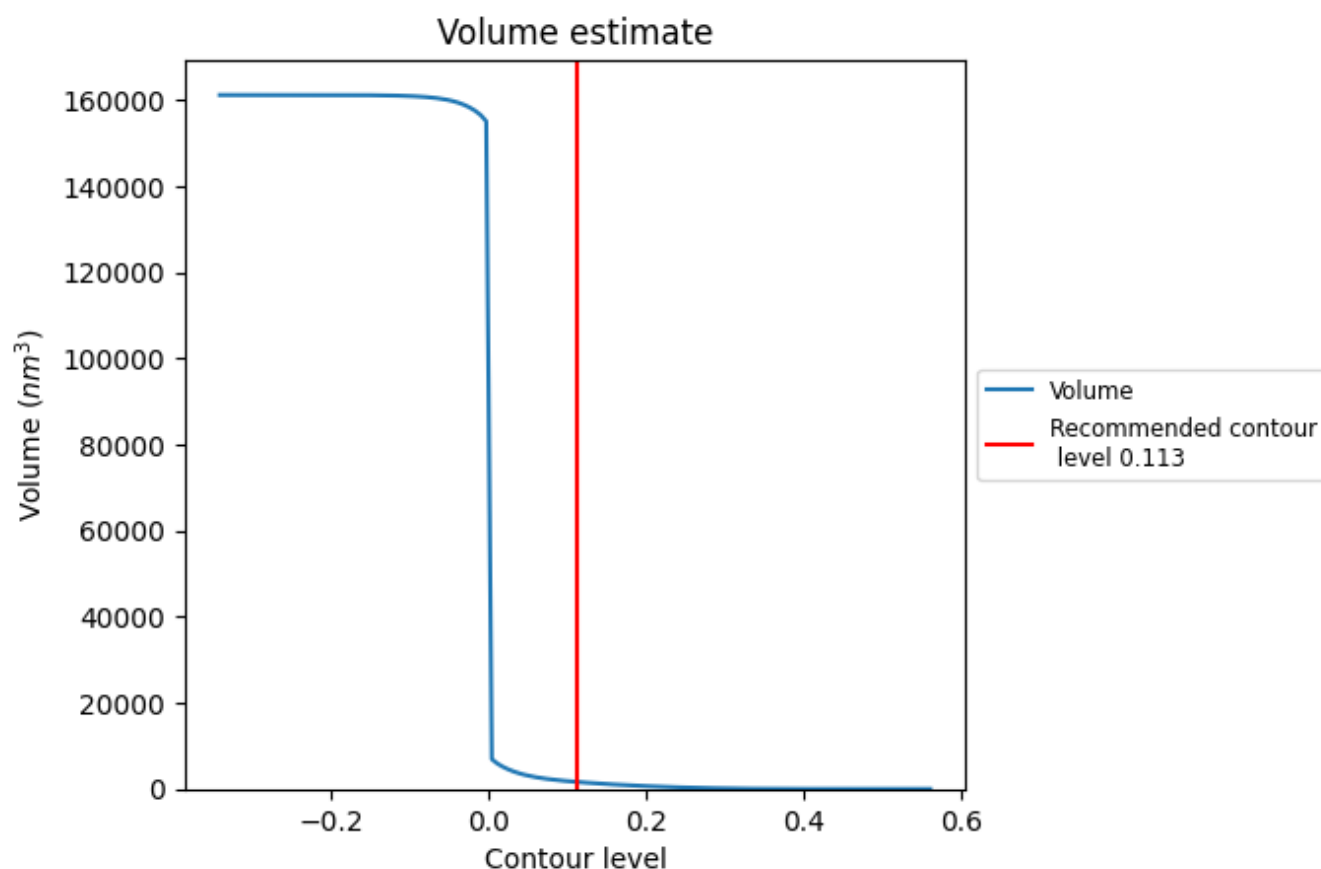
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

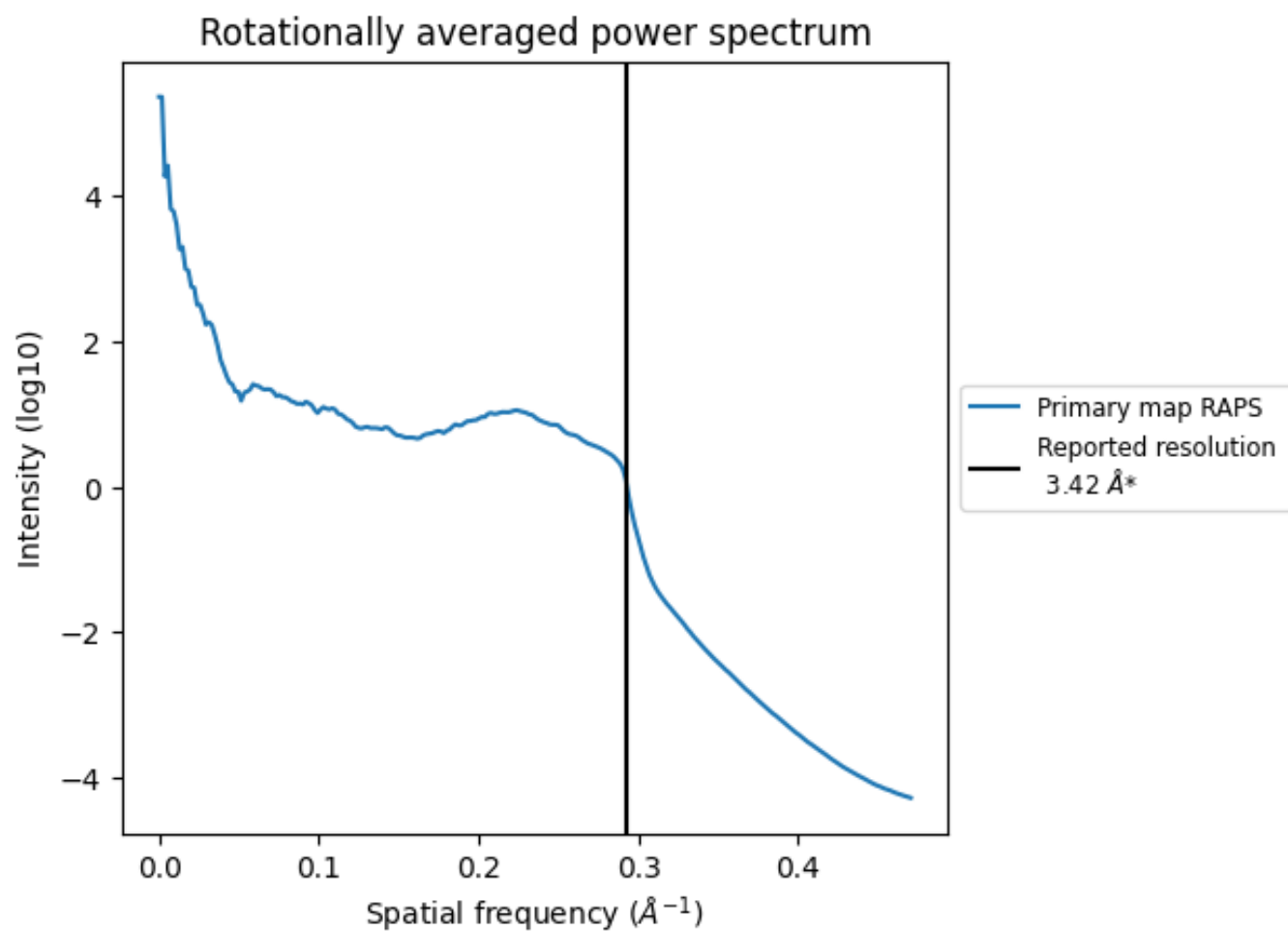
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1618 nm<sup>3</sup>; this corresponds to an approximate mass of 1461 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

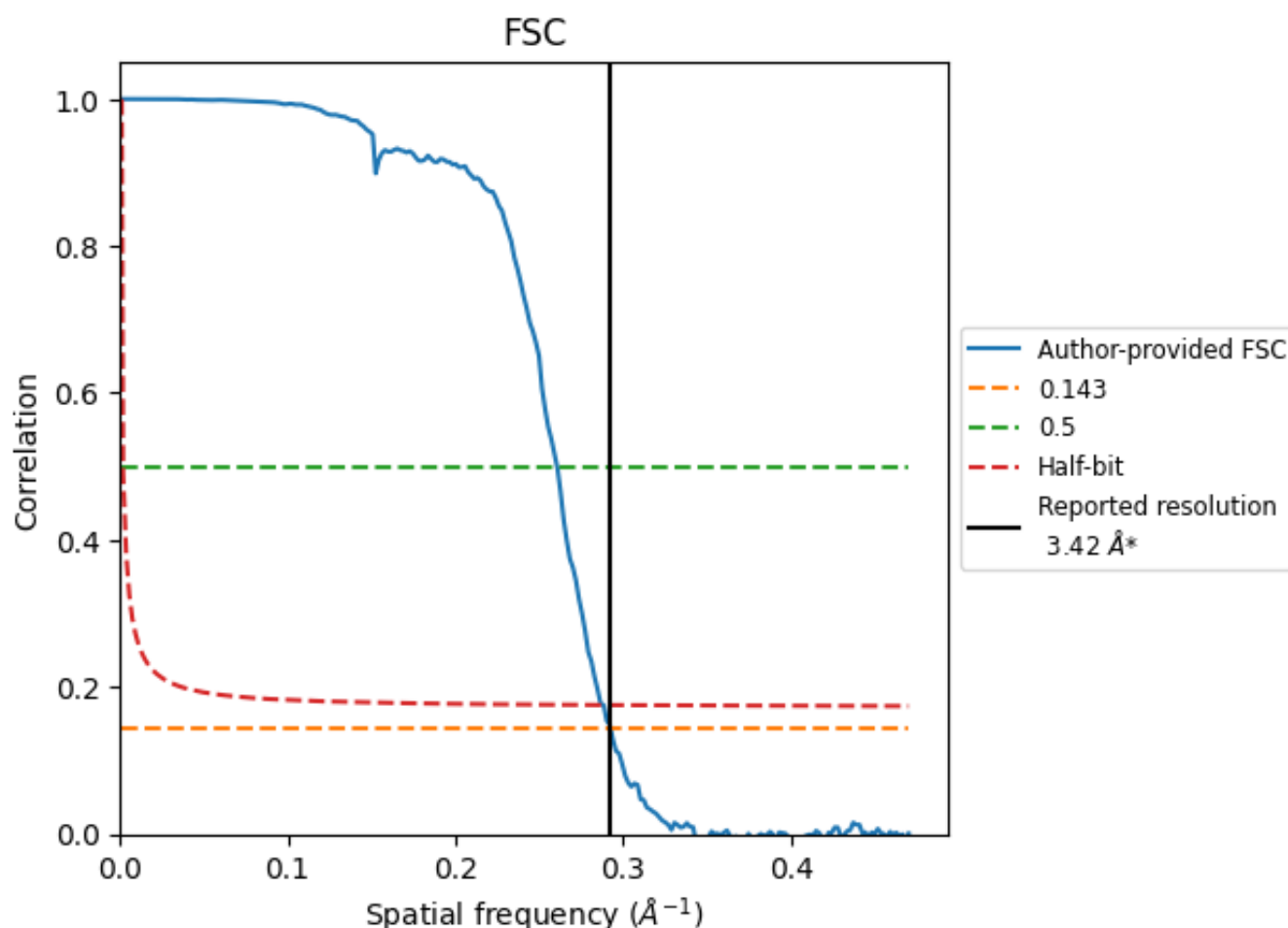


\*Reported resolution corresponds to spatial frequency of 0.292 Å<sup>-1</sup>

## 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 0.292 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.84	3.47
Unmasked-calculated*	-	-	-

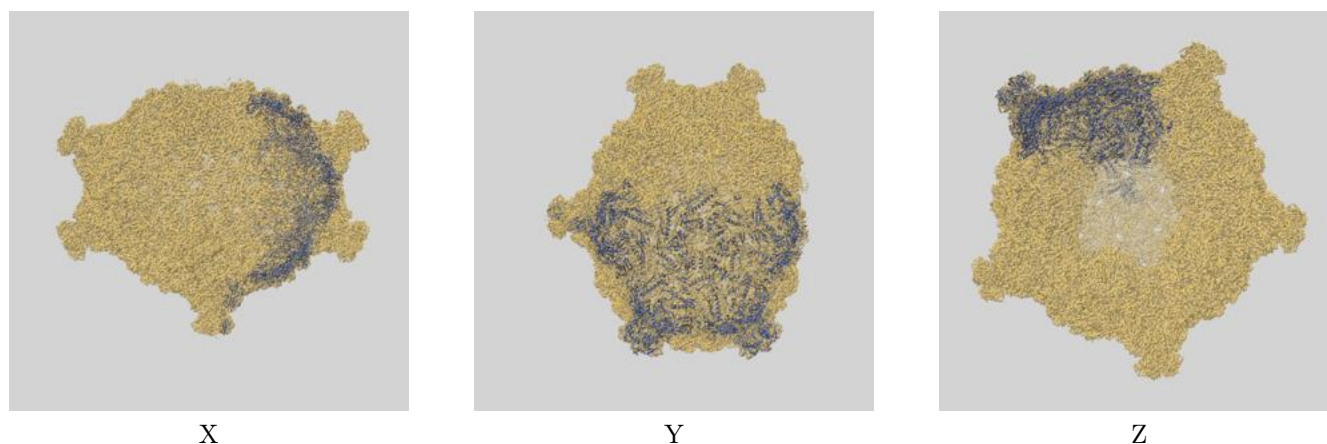
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

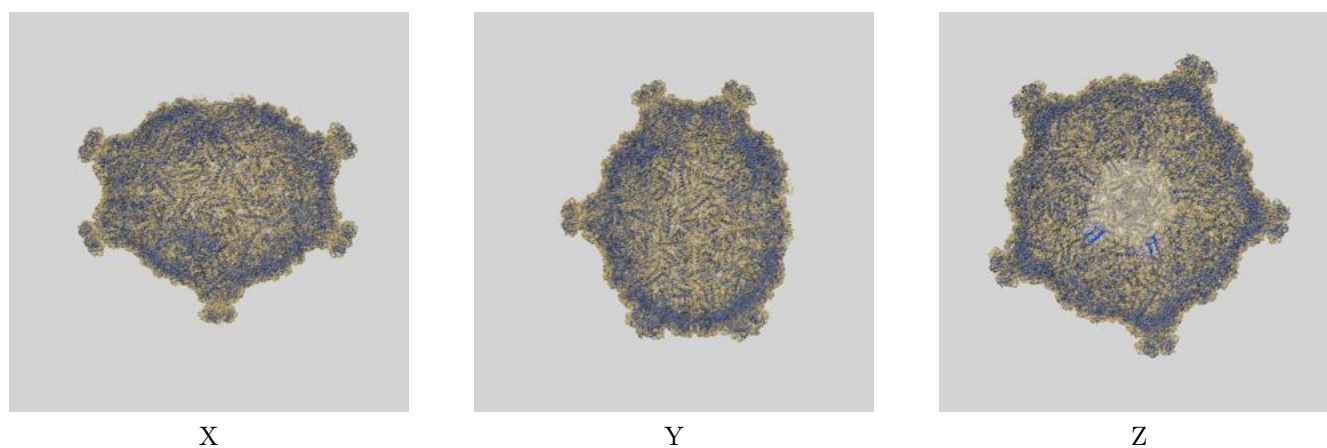
This section contains information regarding the fit between EMDB map EMD-10565 and PDB model 6TSU. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlays

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



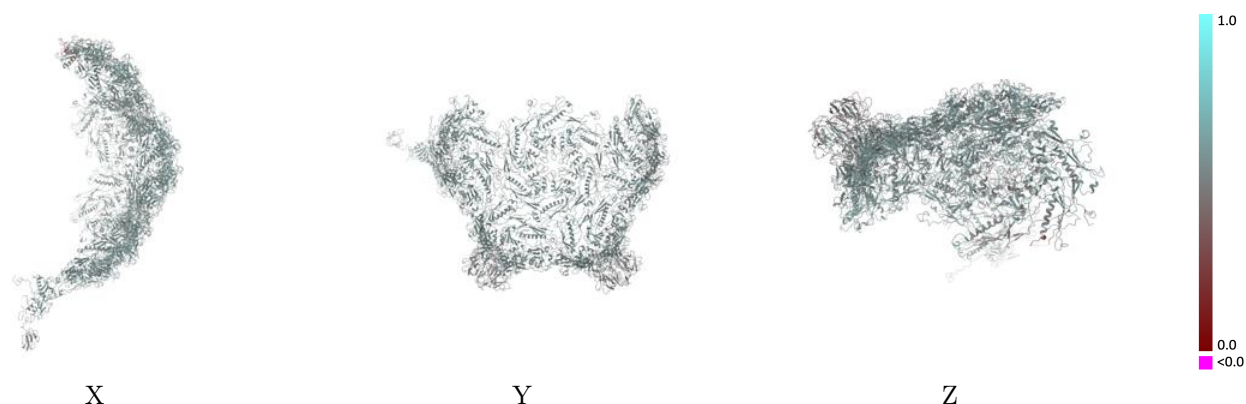
#### 9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.113 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.

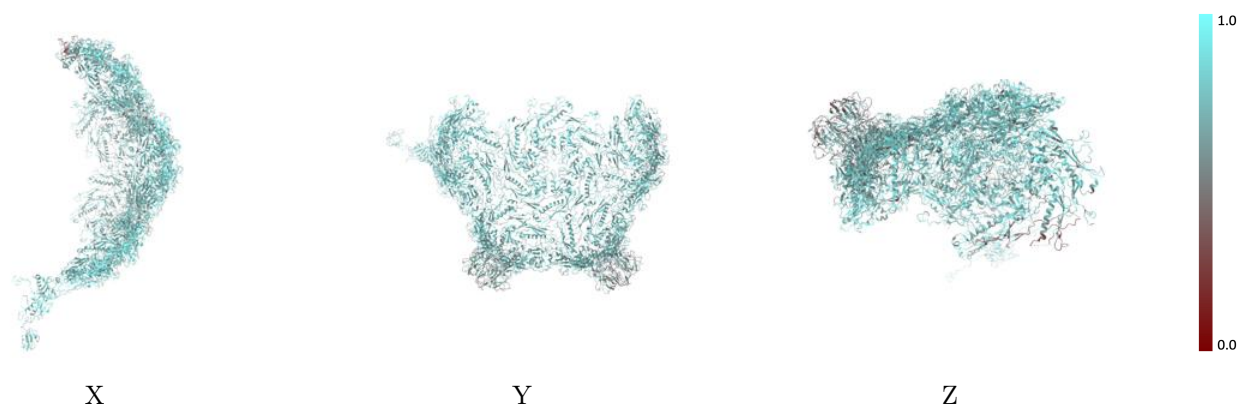


## 9.2 Q-score mapped to coordinate model [i](#)



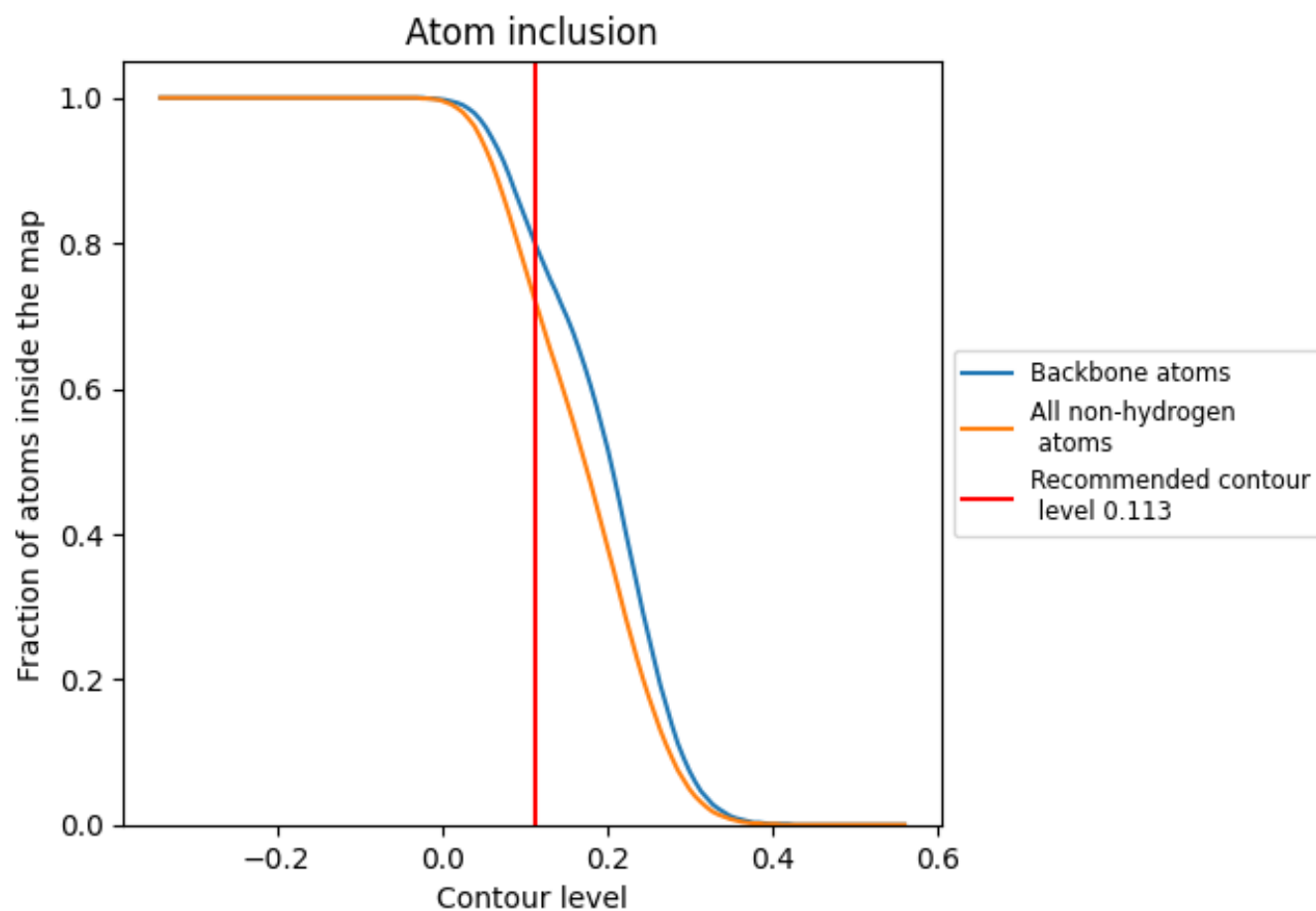
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.113).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.113) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.5320
A1	 0.6750	 0.4910
A2	 0.5940	 0.4770
A3	 0.5200	 0.4670
A4	 0.7650	 0.5410
A5	 0.6610	 0.5090
B2	 0.5510	 0.4800
B3	 0.5800	 0.4690
B4	 0.7760	 0.5420
B5	 0.6740	 0.5080
C2	 0.5680	 0.4840
C3	 0.5620	 0.4820
C4	 0.7750	 0.5460
C5	 0.7400	 0.5350
D2	 0.5570	 0.4700
D3	 0.5890	 0.4680
D4	 0.7640	 0.5490
E2	 0.5540	 0.4690
E3	 0.5590	 0.4700
E4	 0.7670	 0.5430
F2	 0.3060	 0.4300
F3	 0.2740	 0.3970
F4	 0.7630	 0.5440
G4	 0.7580	 0.5390
H4	 0.7430	 0.5410
I4	 0.7210	 0.5350
J4	 0.7210	 0.5430
K4	 0.7220	 0.5400
L4	 0.7400	 0.5460
M4	 0.7390	 0.5400
N4	 0.7470	 0.5420
O4	 0.7420	 0.5400
P4	 0.7440	 0.5410
Q4	 0.7460	 0.5400
R4	 0.7430	 0.5370



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Chain	Atom inclusion	Q-score
S4	 0.7230	 0.5420
T4	 0.7140	 0.5390
U4	 0.7110	 0.5350
V4	 0.7280	 0.5430
W4	 0.7230	 0.5380
X4	 0.7440	 0.5430
Y4	 0.7480	 0.5400
Z4	 0.7130	 0.5270