



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:54 AM UTC

PDB ID : 8FJK / pdb_00008fjk
EMDB ID : EMD-29243
Title : Golden Shiner Reovirus Core Polar Vertex
Authors : Stevens, A.S.; Zhou, Z.H.
Deposited on : 2022-12-19
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

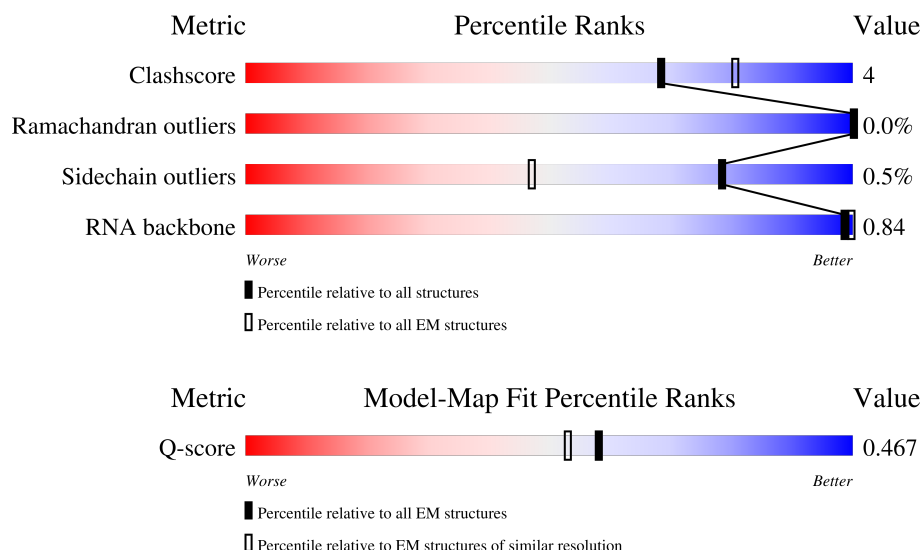
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



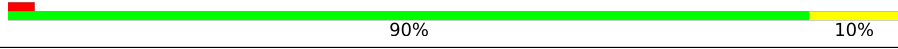
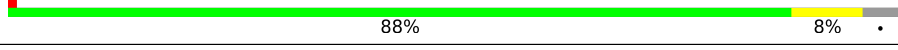
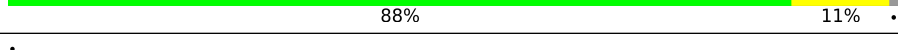
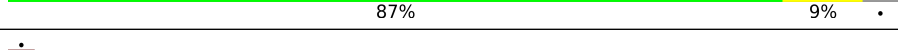
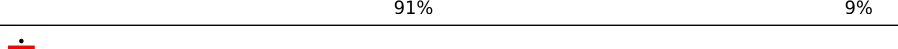
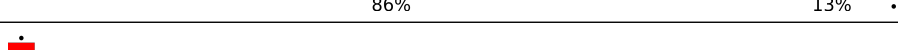
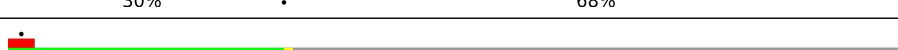
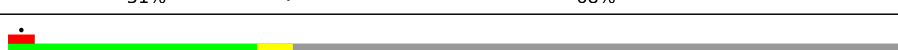
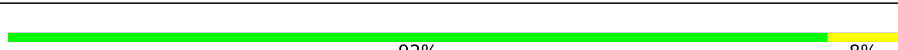
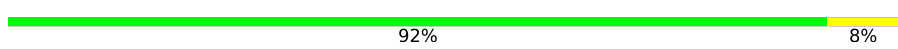
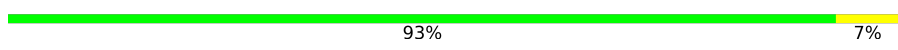
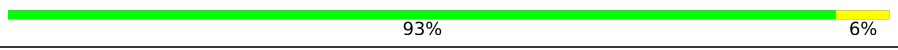
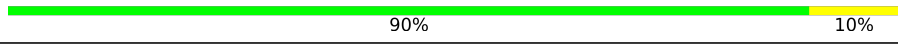
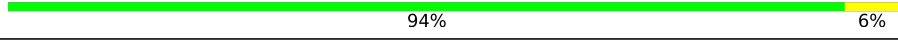
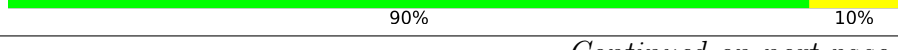
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1273	
2	B	718	
3	C	1138	

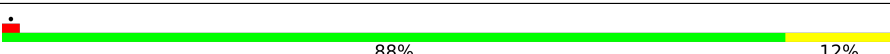
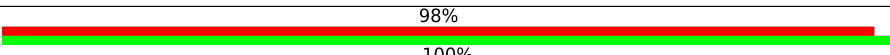
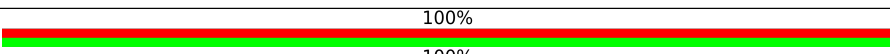
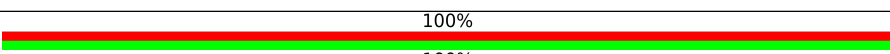
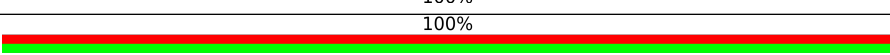
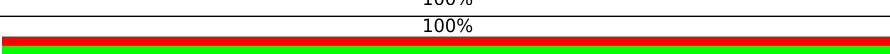
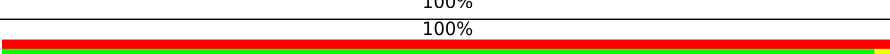
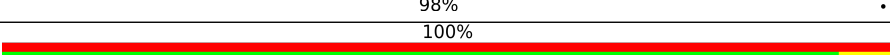
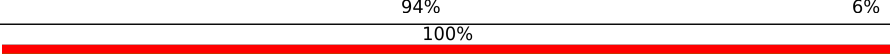
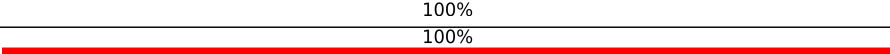
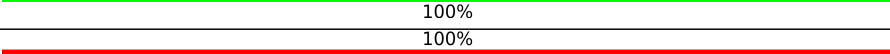
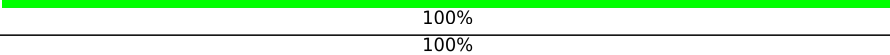
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Mol	Chain	Length	Quality of chain
3	D	1138	
3	E	1138	
3	F	1138	
3	G	1138	
3	H	1138	
3	I	1138	
3	J	1138	
3	K	1138	
3	L	1138	
4	M	94	
4	N	94	
4	k	94	
4	l	94	
4	m	94	
5	V	411	
5	W	411	
5	X	411	
5	a	411	
5	b	411	
5	d	411	
5	e	411	
5	g	411	
5	h	411	
5	n	411	
6	Y	1297	

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Mol	Chain	Length	Quality of chain
6	Z	1297	 88%11%
6	c	1297	 89%11%
6	f	1297	 89%11%
6	i	1297	 88%12%
7	a1	52	 98%100%
7	b1	52	 100%100%
8	a2	60	 100%100%
8	b2	60	 100%100%
9	a3	40	 100%100%
9	b3	40	 98%100%
10	a4	18	 94%6%100%
10	b4	18	 100%100%
11	a5	38	 100%100%
11	b5	38	 100%100%
12	a6	30	 100%100%
12	b6	30	 100%100%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 193908 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 RNA-directed RNA polymerase VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1273	Total	C	N	O	S	0	0
			9978	6375	1736	1822	45		

- Molecule 2 is a protein called Microtubule-associated protein VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	718	Total	C	N	O	S	0	0
			5593	3588	971	1016	18		

- Molecule 3 is a protein called Major inner capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1075	Total	C	N	O	S	0	0
			8300	5296	1421	1534	49		
3	D	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		
3	E	1106	Total	C	N	O	S	0	0
			8534	5440	1463	1579	52		
3	F	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		
3	G	1098	Total	C	N	O	S	0	0
			8477	5403	1454	1568	52		
3	H	1130	Total	C	N	O	S	0	0
			8699	5540	1491	1615	53		
3	I	1065	Total	C	N	O	S	0	0
			8226	5244	1412	1519	51		
3	J	1130	Total	C	N	O	S	0	0
			8699	5540	1491	1615	53		
3	K	1098	Total	C	N	O	S	0	0
			8477	5403	1454	1568	52		
3	L	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		

- Molecule 4 is a protein called Major inner capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	94	Total	C	N	O	S	0	0
			640	377	113	149	1		
4	N	30	Total	C	N	O	S	0	0
			210	128	36	45	1		
4	k	30	Total	C	N	O	S	0	0
			211	128	36	46	1		
4	l	30	Total	C	N	O	S	0	0
			211	128	36	46	1		
4	m	30	Total	C	N	O	S	0	0
			211	128	36	46	1		

- Molecule 5 is a protein called Clamp protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	W	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	X	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	a	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	b	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	d	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	e	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	g	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	h	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
5	n	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		

- Molecule 6 is a protein called Outer capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
6	Z	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
6	c	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
6	i	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		

- Molecule 7 is a RNA chain called RNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a1	52	Total	C	N	O	P	0	0
			1089	494	182	362	51		
7	b1	52	Total	C	N	O	P	0	0
			1089	494	182	362	51		

- Molecule 8 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a2	60	Total	C	N	O	P	0	0
			1257	570	210	418	59		
8	b2	60	Total	C	N	O	P	0	0
			1257	570	210	418	59		

- Molecule 9 is a RNA chain called RNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a3	40	Total	C	N	O	P	0	0
			837	380	140	278	39		
9	b3	40	Total	C	N	O	P	0	0
			837	380	140	278	39		

- Molecule 10 is a RNA chain called RNA (18-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a4	18	Total	C	N	O	P	0	0
			375	171	63	124	17		
10	b4	18	Total	C	N	O	P	0	0
			375	171	63	124	17		

- Molecule 11 is a RNA chain called RNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a5	38	Total	C	N	O	P	0	0
			795	361	133	264	37		
11	b5	38	Total	C	N	O	P	0	0
			795	361	133	264	37		

- Molecule 12 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a6	30	Total	C	N	O	P	0	0
			627	285	105	208	29		
12	b6	30	Total	C	N	O	P	0	0
			627	285	105	208	29		

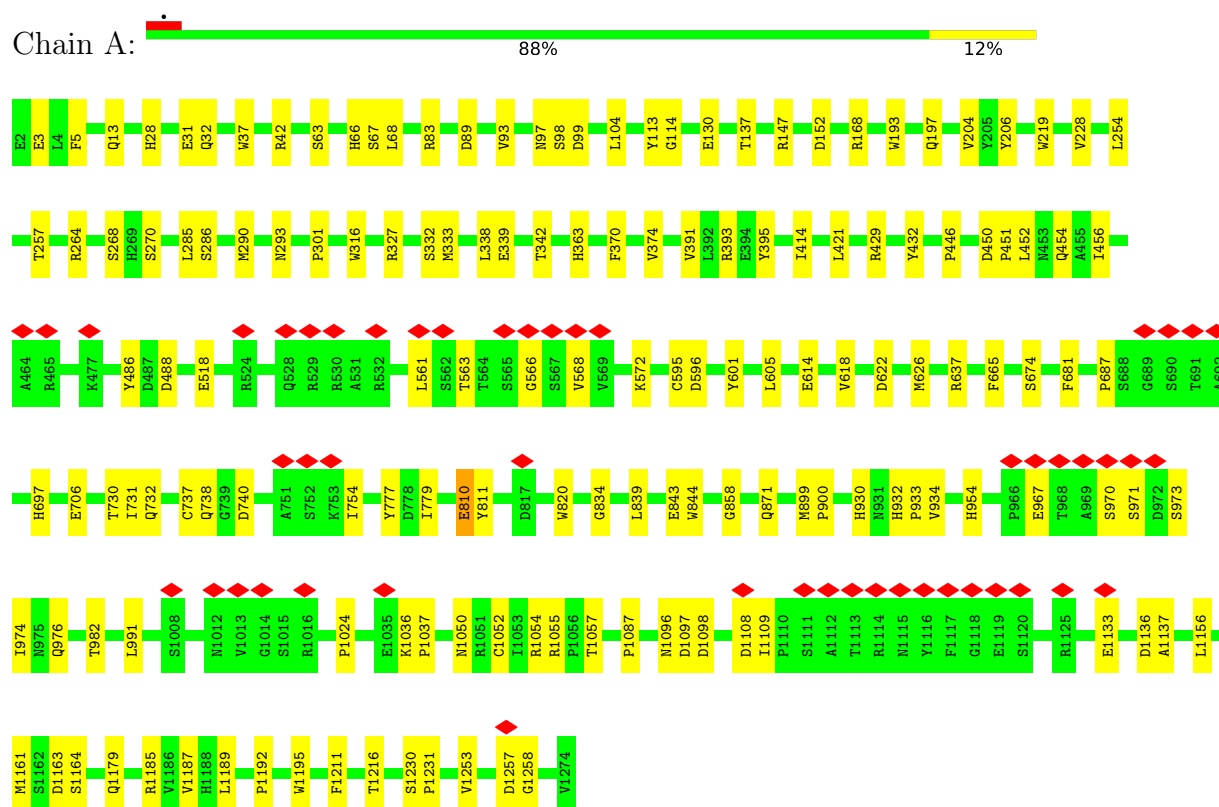
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	E	1	Total	Zn	0
			1	1	
13	G	1	Total	Zn	0
			1	1	
13	I	1	Total	Zn	0
			1	1	
13	K	1	Total	Zn	0
			1	1	

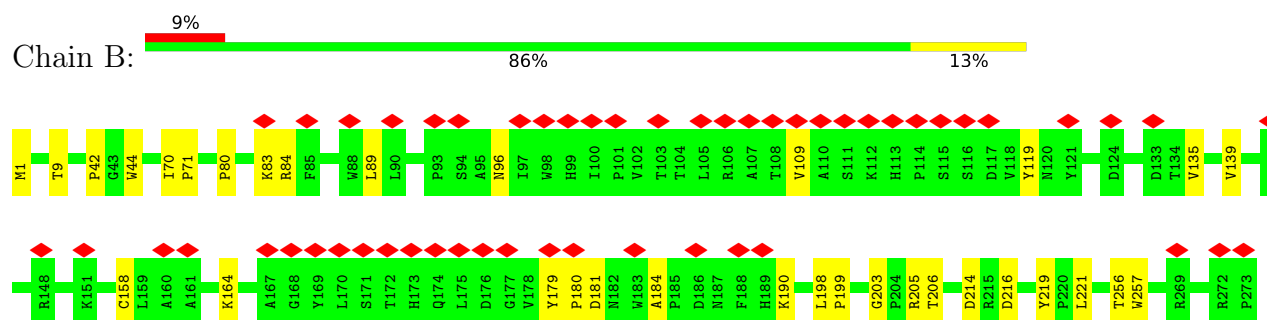
3 Residue-property plots

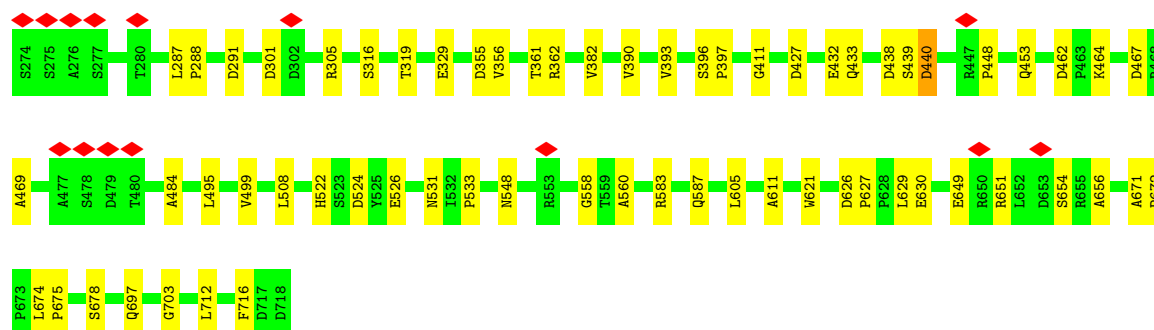
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA-directed RNA polymerase VP2

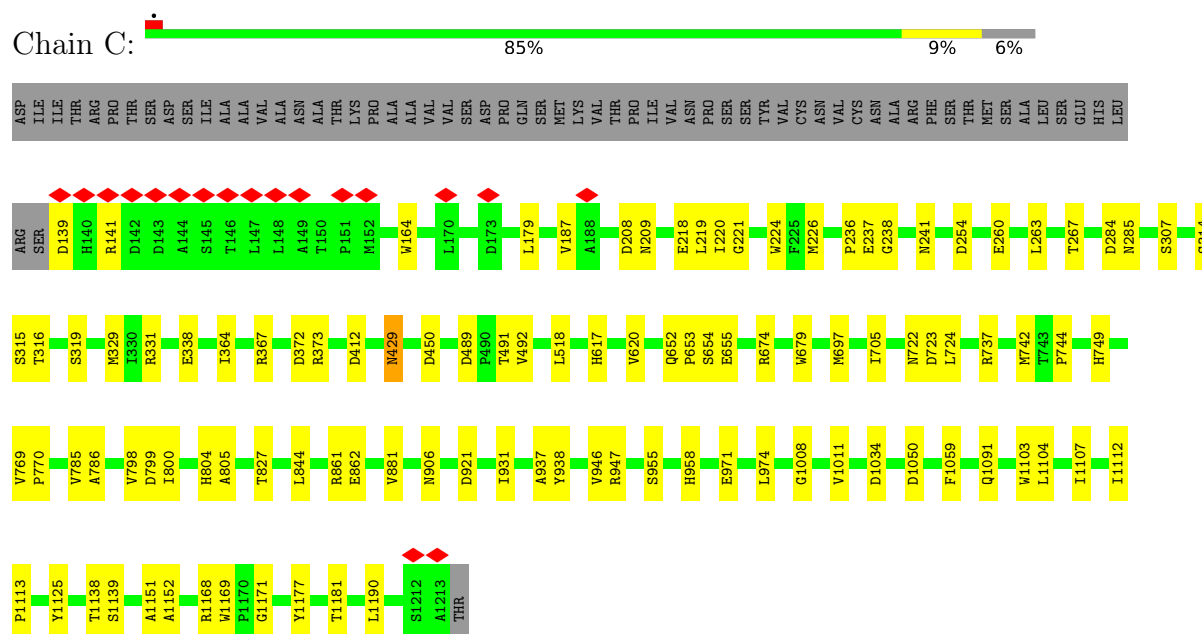


• Molecule 2: Microtubule-associated protein VP5

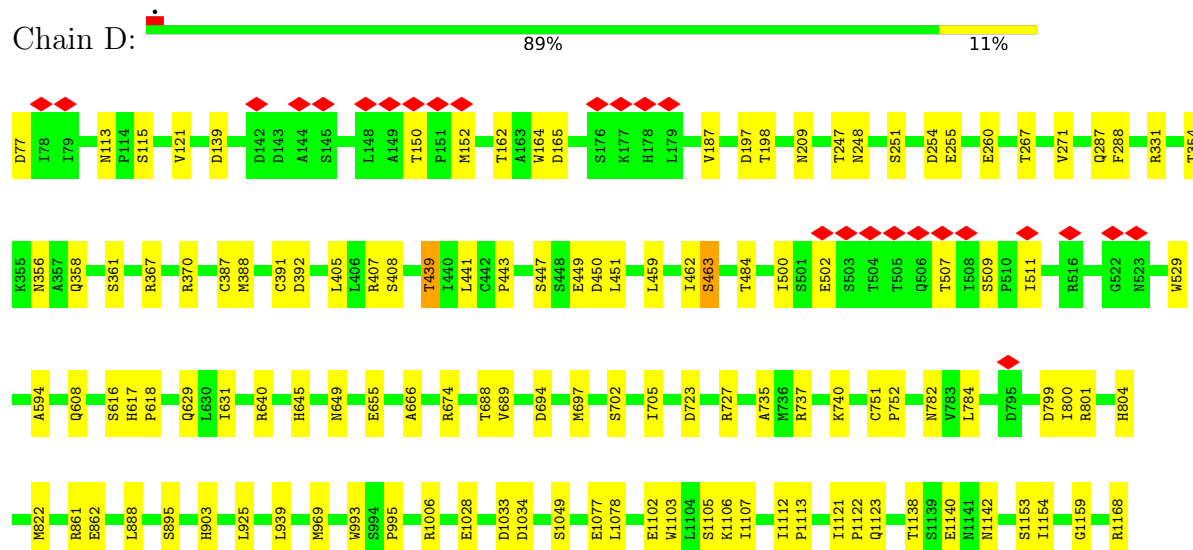


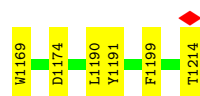


• Molecule 3: Major inner capsid protein VP3



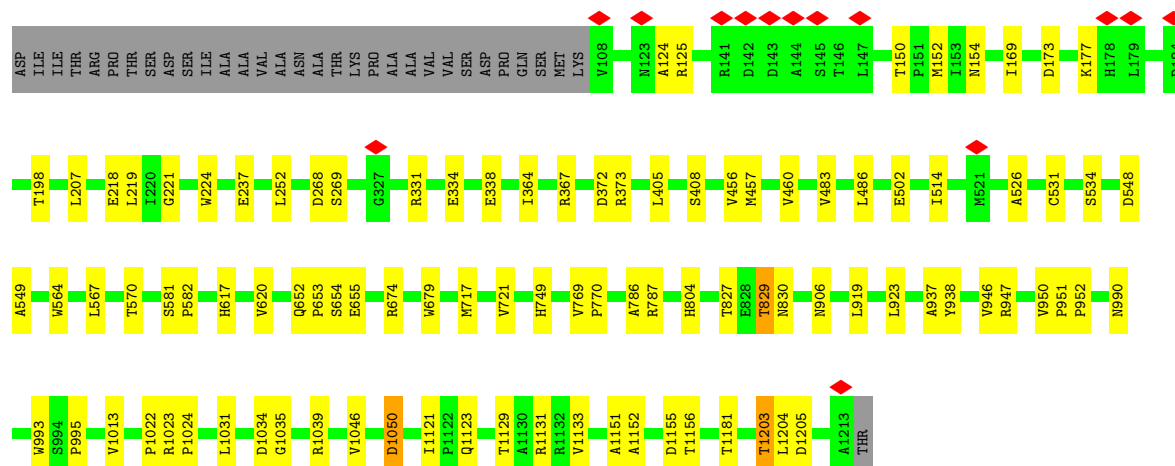
• Molecule 3: Major inner capsid protein VP3





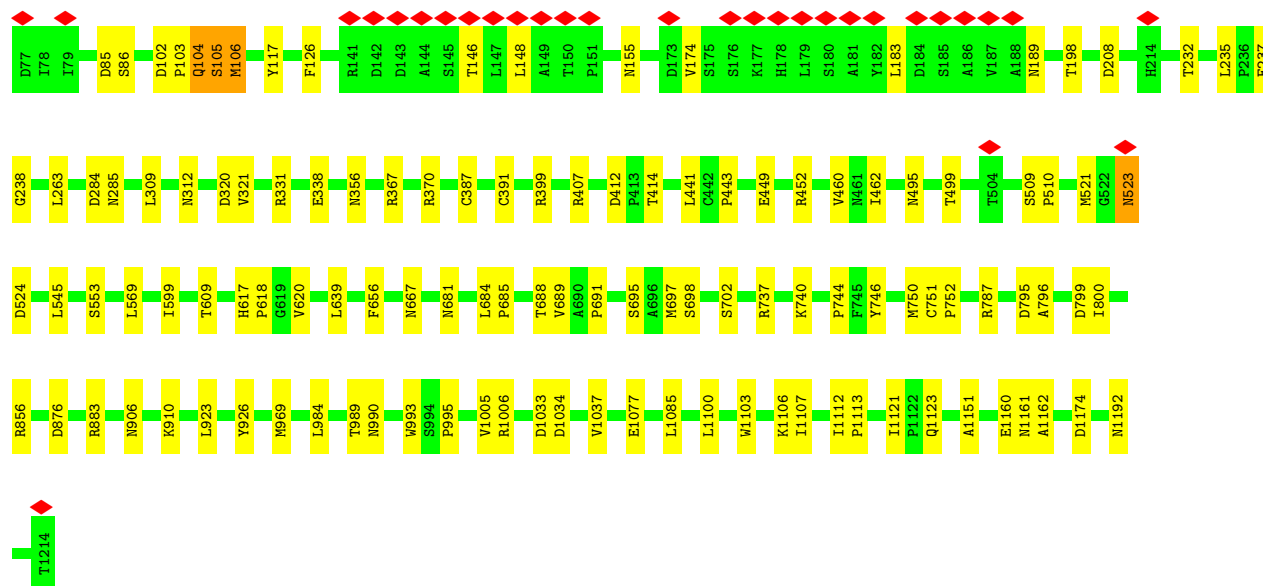
• Molecule 3: Major inner capsid protein VP3

Chain E: 88% 8%



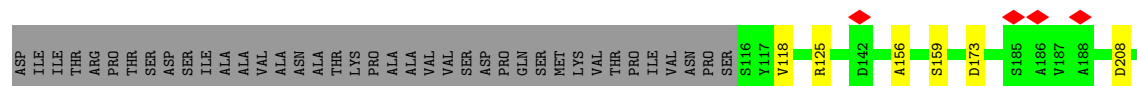
• Molecule 3: Major inner capsid protein VP3

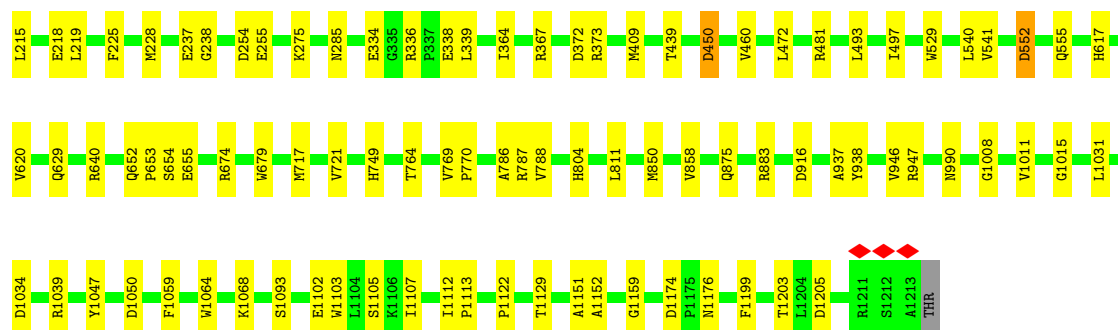
Chain F: 90% 10%



• Molecule 3: Major inner capsid protein VP3

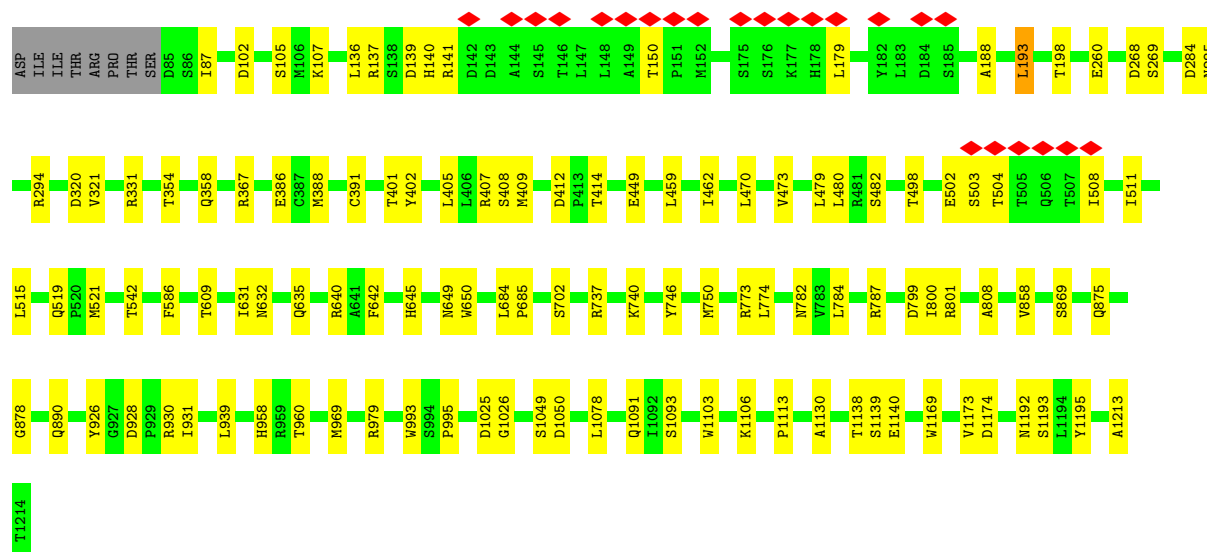
Chain G: 88% 8%





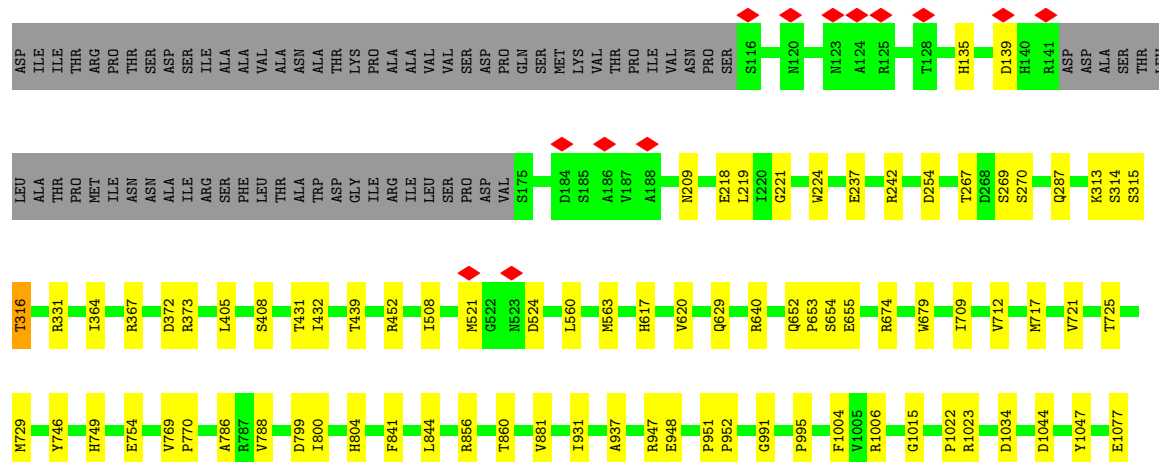
• Molecule 3: Major inner capsid protein VP3

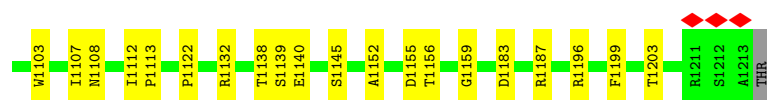
Chain H: 89% 10% .



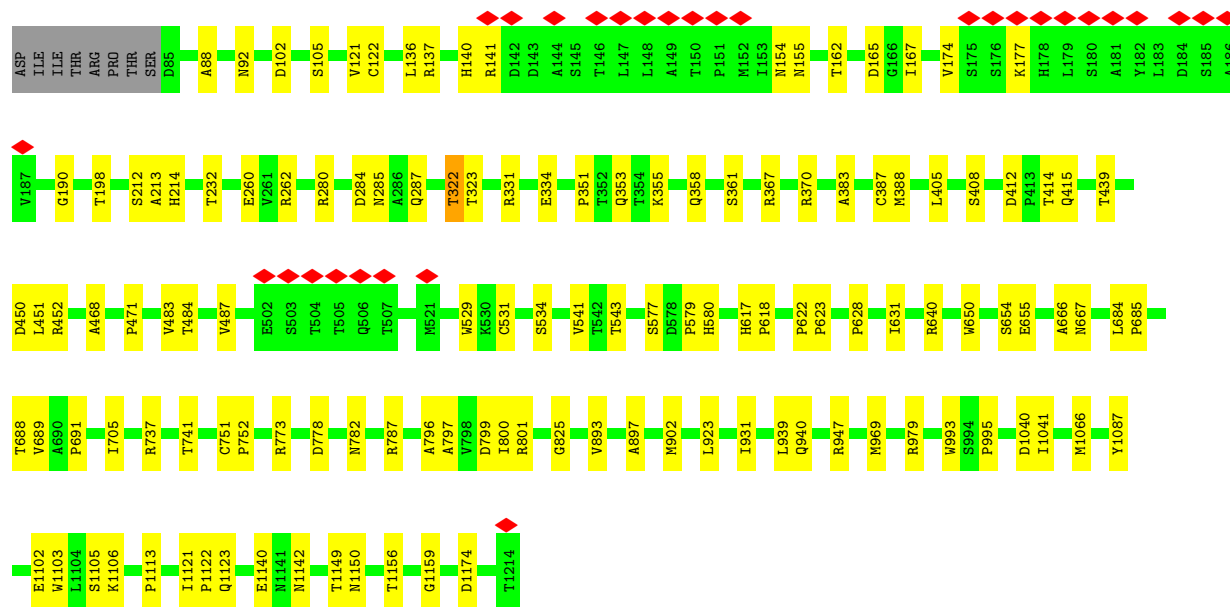
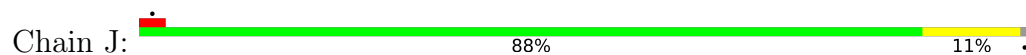
• Molecule 3: Major inner capsid protein VP3

Chain I: 85% 9% 6%

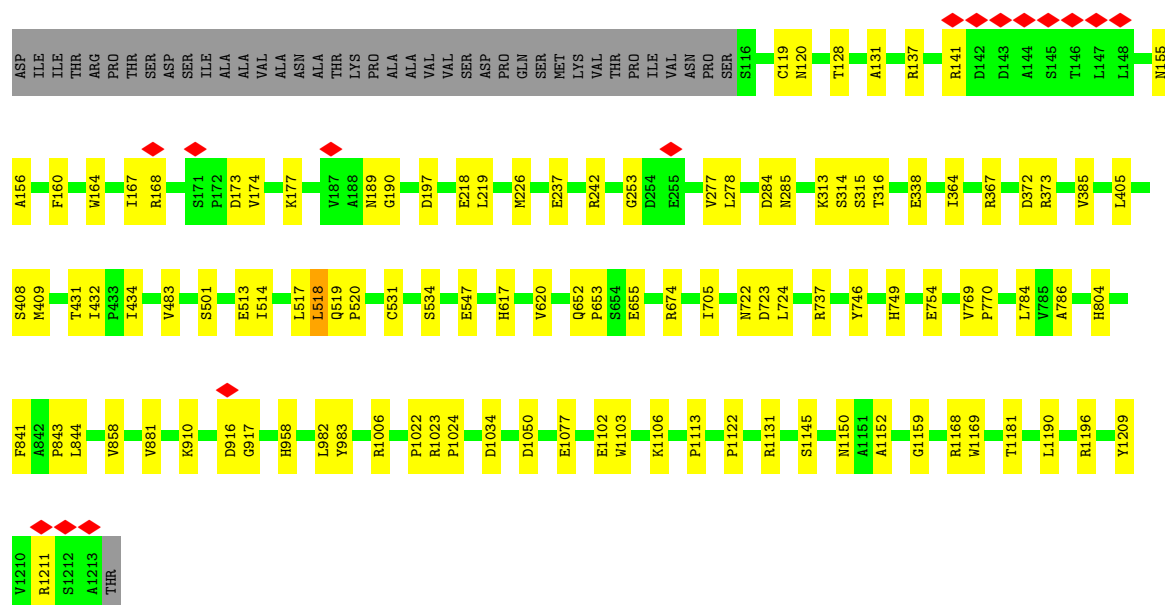




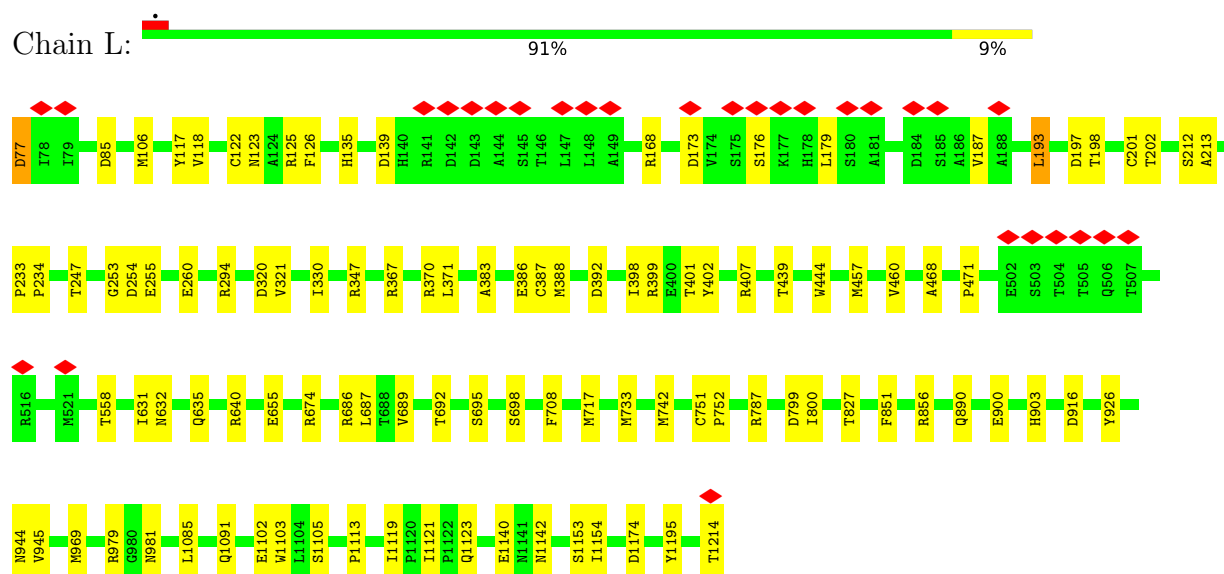
• Molecule 3: Major inner capsid protein VP3



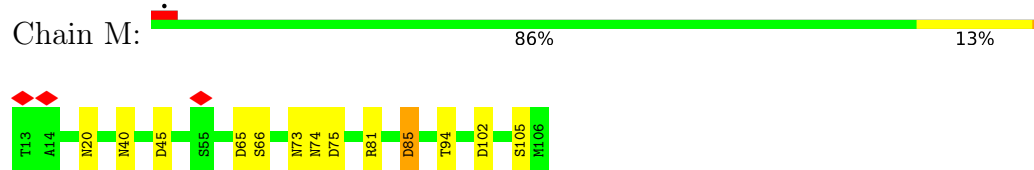
• Molecule 3: Major inner capsid protein VP3



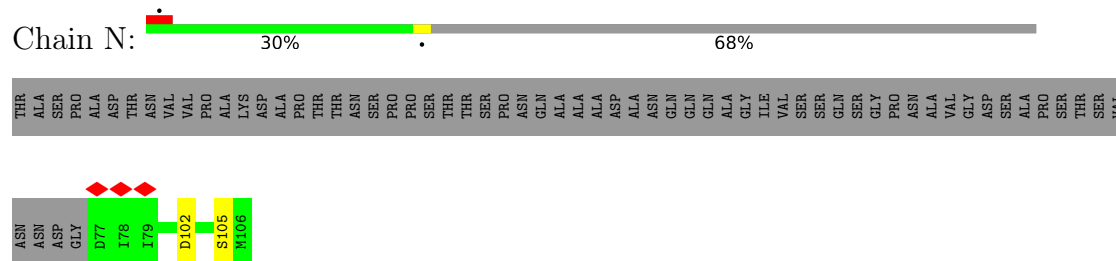
• Molecule 3: Major inner capsid protein VP3



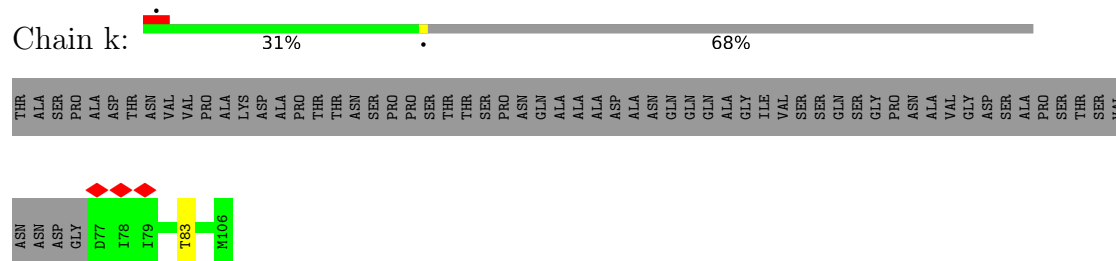
- Molecule 4: Major inner capsid protein VP3



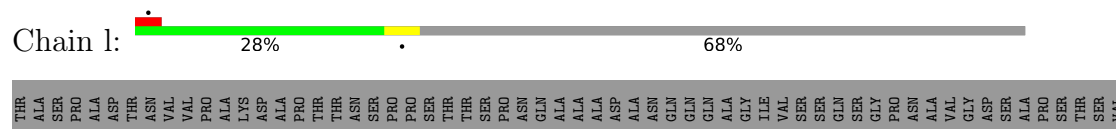
- Molecule 4: Major inner capsid protein VP3

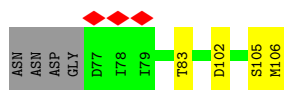


- Molecule 4: Major inner capsid protein VP3

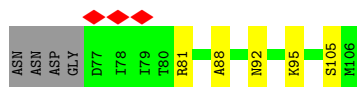
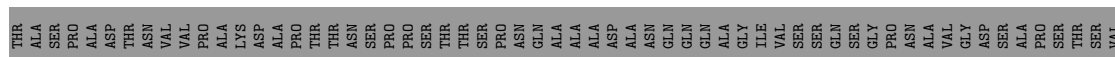


- Molecule 4: Major inner capsid protein VP3

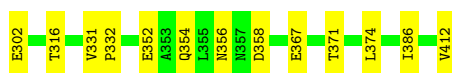
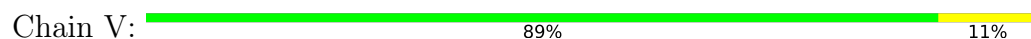




- Molecule 4: Major inner capsid protein VP3



- Molecule 5: Clamp protein VP6



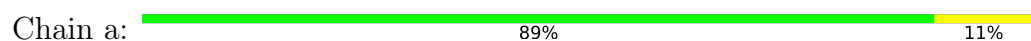
- Molecule 5: Clamp protein VP6

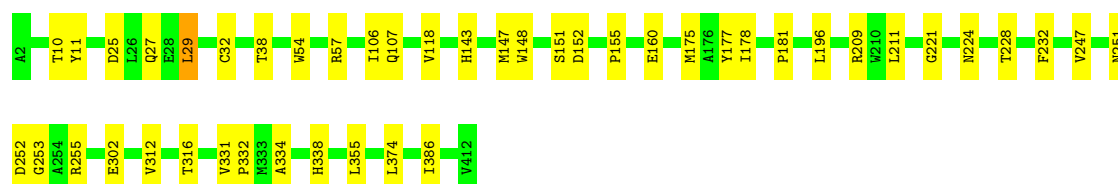


- Molecule 5: Clamp protein VP6



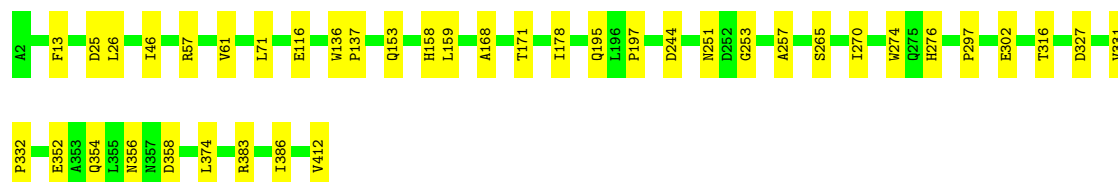
- Molecule 5: Clamp protein VP6





• Molecule 5: Clamp protein VP6

Chain b: 90% 10%



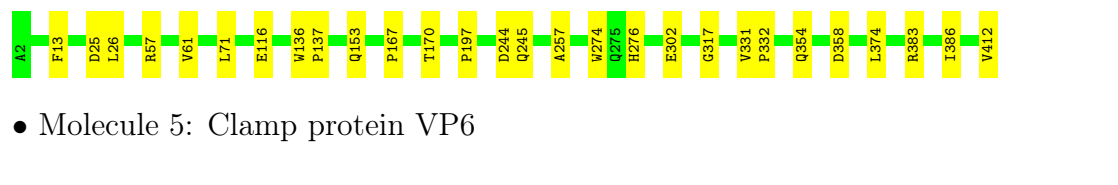
• Molecule 5: Clamp protein VP6

Chain d: 92% 8%



• Molecule 5: Clamp protein VP6

Chain e: 93% 7%



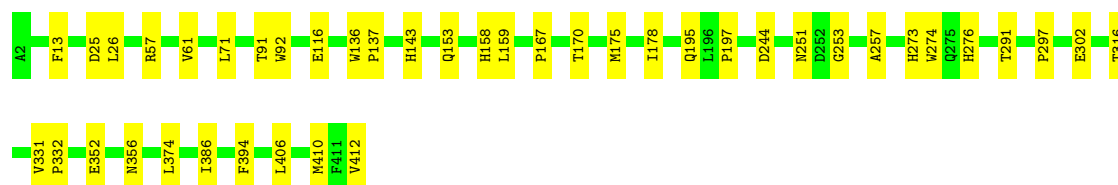
• Molecule 5: Clamp protein VP6

Chain g: 93% 6%

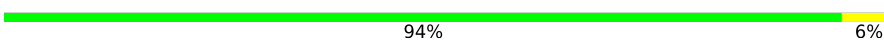


• Molecule 5: Clamp protein VP6

Chain h: 90% 10%



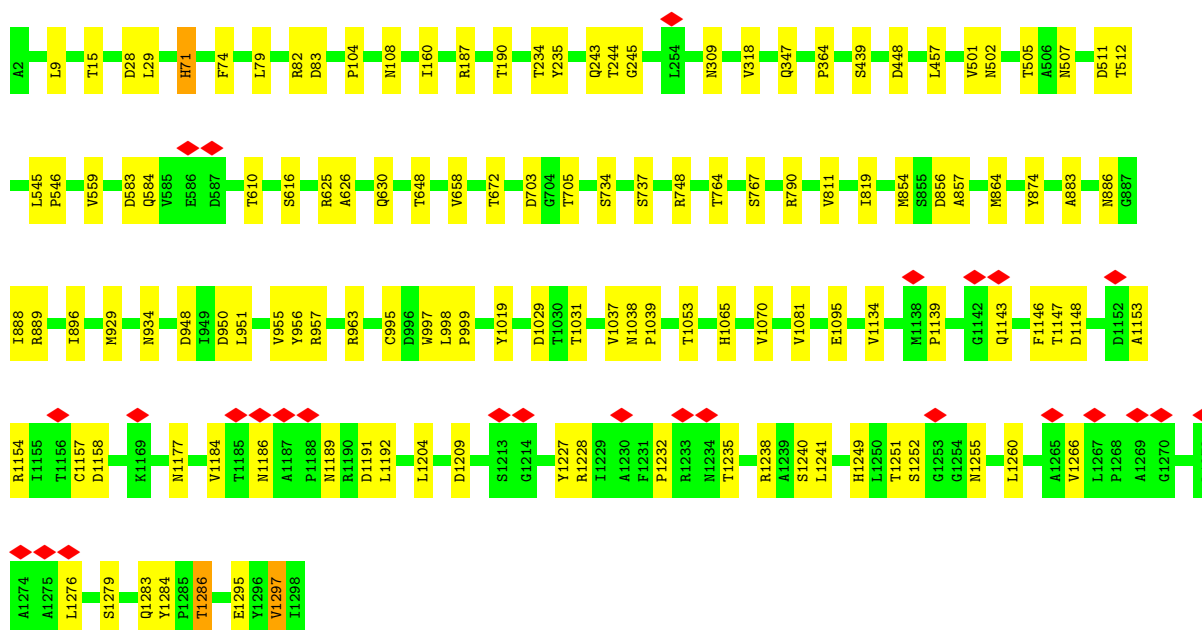
- Molecule 5: Clamp protein VP6

Chain n:  94% 6%



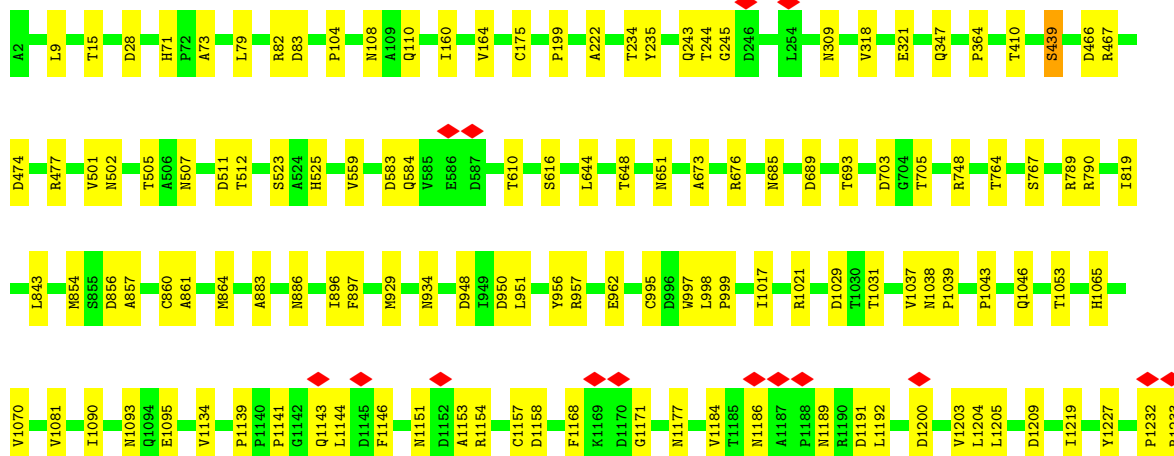
- Molecule 6: Outer capsid protein VP1

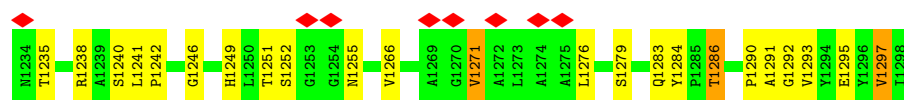
Chain Y:  90% 10%



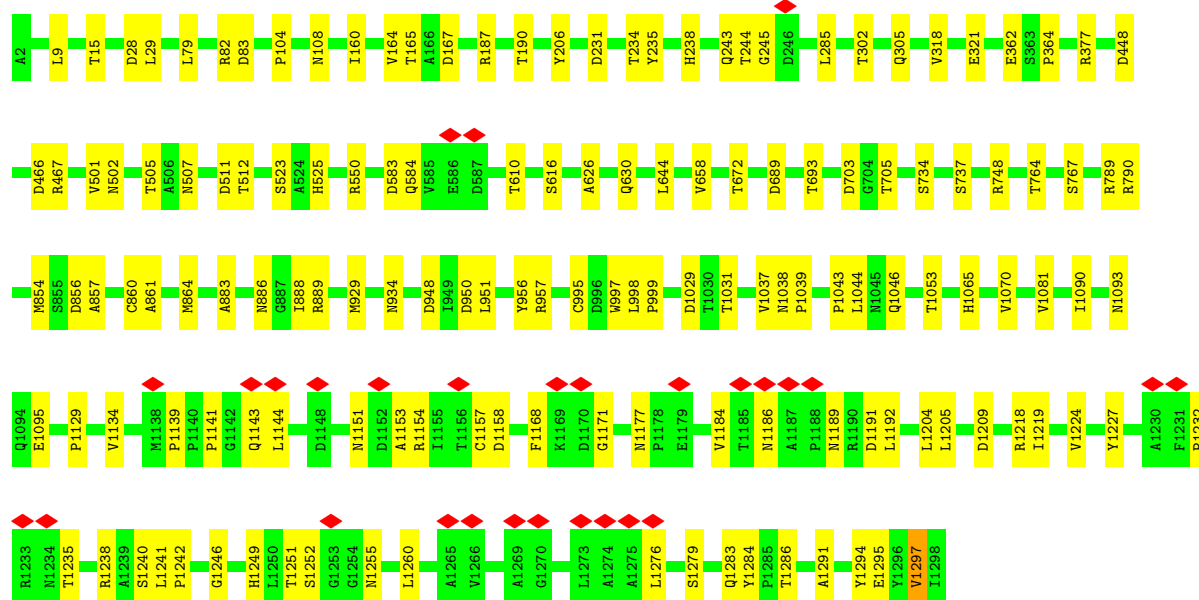
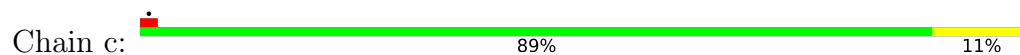
- Molecule 6: Outer capsid protein VP1

Chain Z:  88% 11%

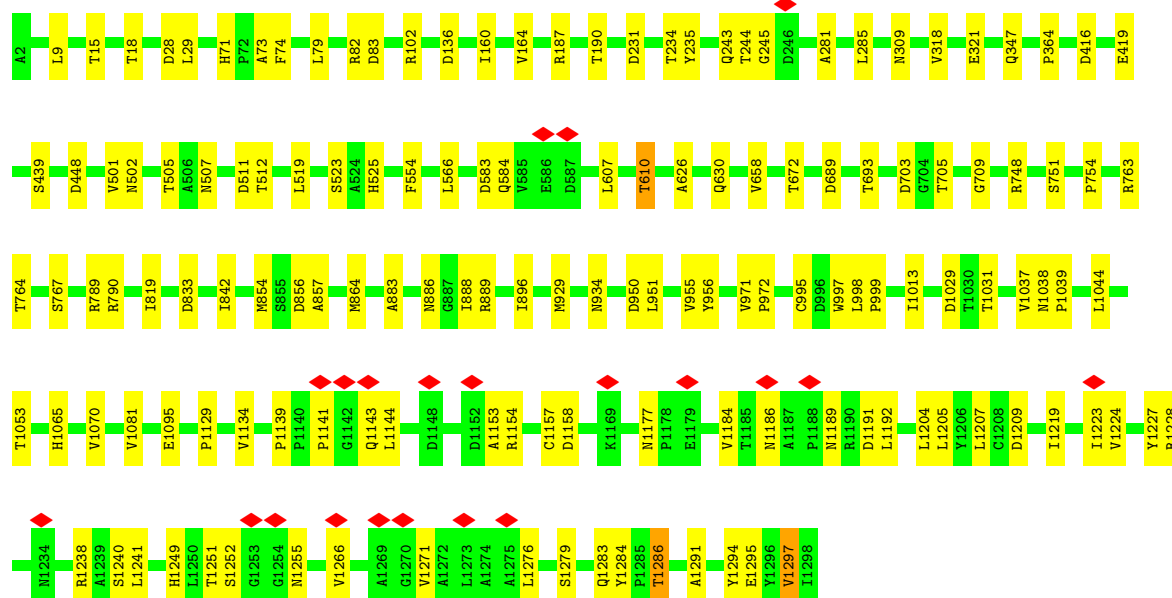
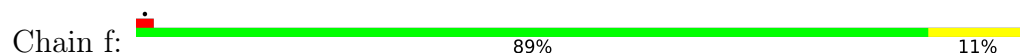




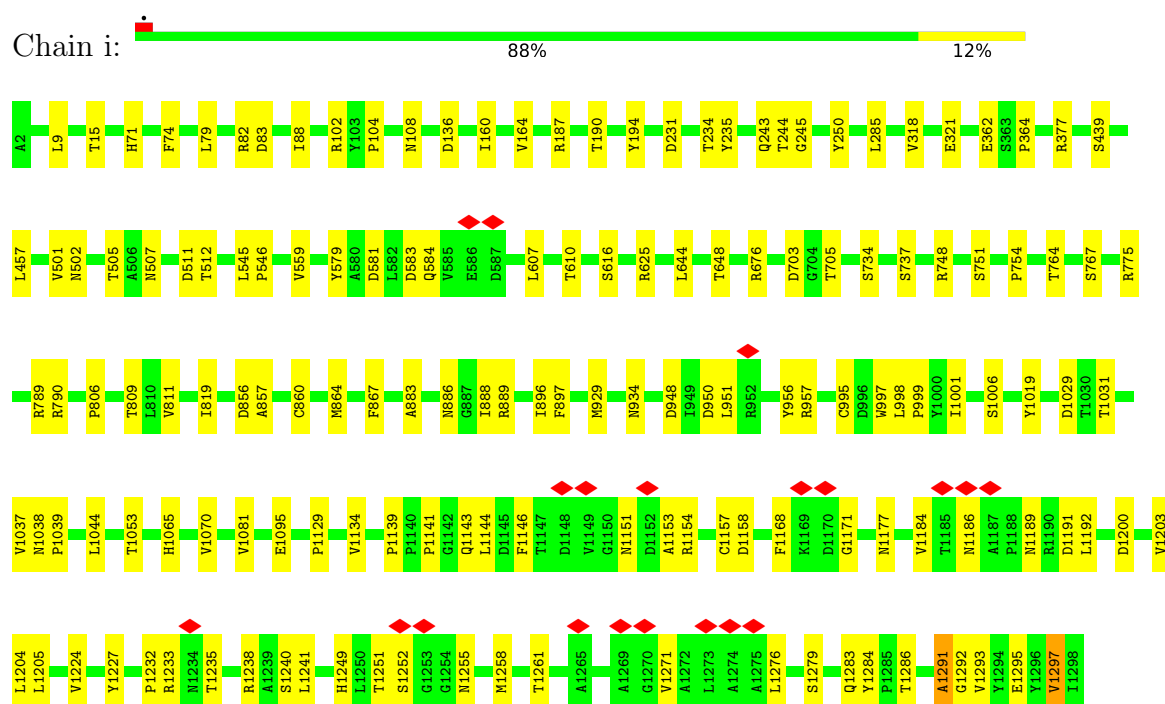
• Molecule 6: Outer capsid protein VP1



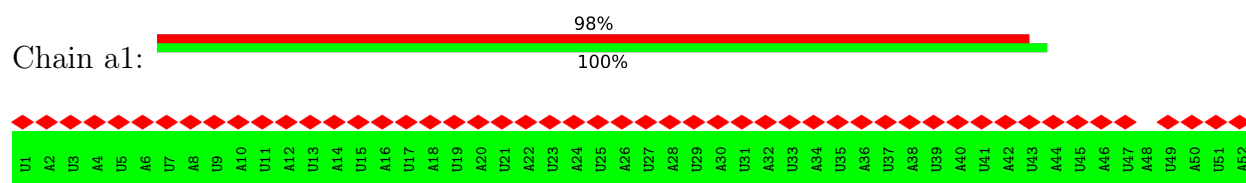
• Molecule 6: Outer capsid protein VP1



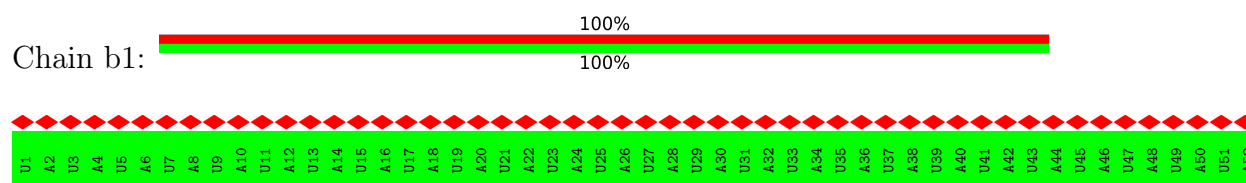
• Molecule 6: Outer capsid protein VP1



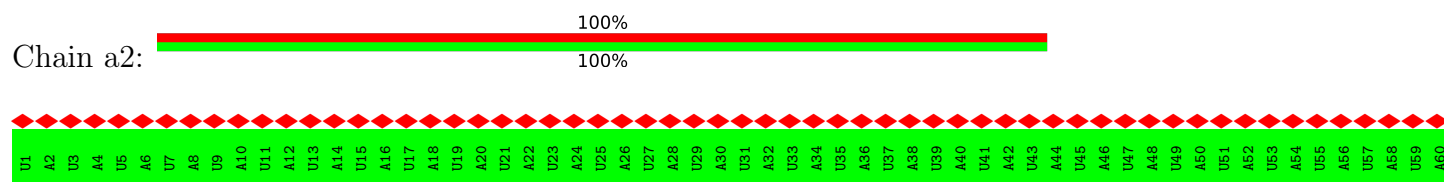
• Molecule 7: RNA (52-MER)



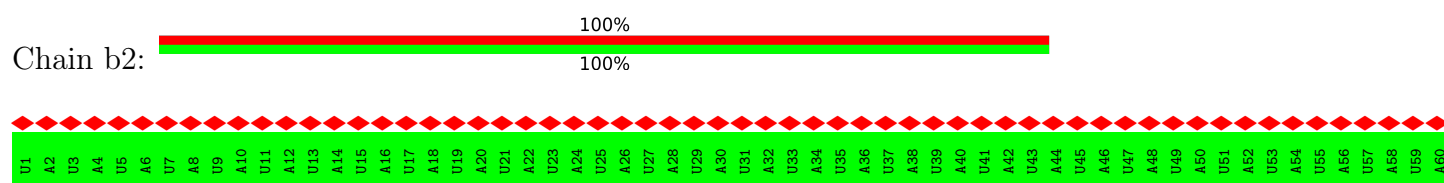
• Molecule 7: RNA (52-MER)



• Molecule 8: RNA (60-MER)

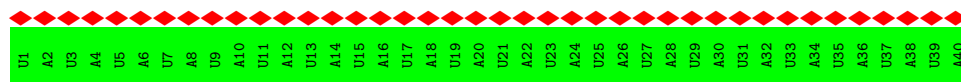


• Molecule 8: RNA (60-MER)



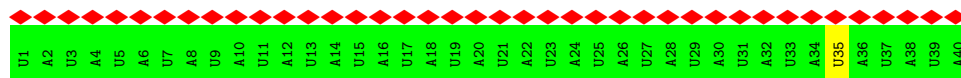
● Molecule 9: RNA (40-MER)

Chain a3:  100%
100%



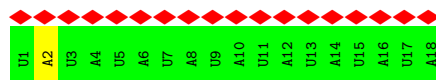
● Molecule 9: RNA (40-MER)

Chain b3:  100%
98%



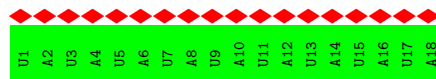
● Molecule 10: RNA (18-MER)

Chain a4:  100%
94% 6%



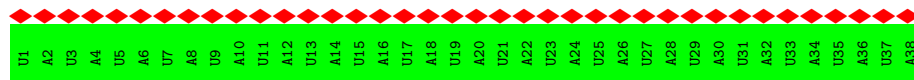
● Molecule 10: RNA (18-MER)

Chain b4:  100%
100%



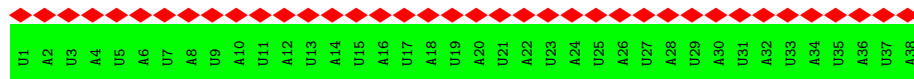
● Molecule 11: RNA (38-MER)

Chain a5:  100%
100%



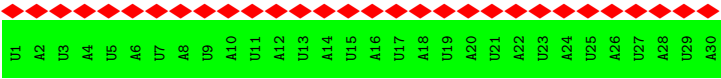
● Molecule 11: RNA (38-MER)

Chain b5:  100%
100%

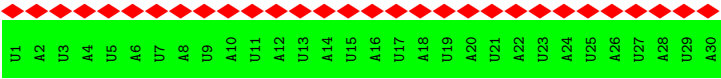


● Molecule 12: RNA (30-MER)

Chain a6:  100%
100%



● Molecule 12: RNA (30-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119182	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.039	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00665	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/10261	0.36	2/14016 (0.0%)
2	B	0.21	0/5734	0.34	0/7849
3	C	0.25	0/8516	0.30	0/11674
3	D	0.24	0/8985	0.32	1/12316 (0.0%)
3	E	0.24	0/8755	0.31	0/12001
3	F	0.25	0/8985	0.33	0/12316
3	G	0.24	0/8696	0.30	0/11917
3	H	0.24	0/8922	0.30	0/12229
3	I	0.25	0/8439	0.30	0/11562
3	J	0.24	0/8922	0.32	0/12229
3	K	0.25	0/8696	0.31	0/11917
3	L	0.24	0/8985	0.31	0/12316
4	M	0.20	0/650	0.29	0/898
4	N	0.23	0/212	0.29	0/291
4	k	0.28	0/213	0.32	0/291
4	l	0.20	0/213	0.25	0/291
4	m	0.19	0/213	0.27	0/291
5	V	0.23	0/3234	0.30	0/4444
5	W	0.24	0/3234	0.31	0/4444
5	X	0.23	0/3234	0.30	0/4444
5	a	0.24	0/3234	0.31	0/4444
5	b	0.23	0/3234	0.30	0/4444
5	d	0.24	0/3234	0.31	0/4444
5	e	0.23	0/3234	0.30	0/4444
5	g	0.24	0/3234	0.32	0/4444
5	h	0.23	0/3234	0.30	0/4444
5	n	0.24	0/3234	0.32	0/4444
6	Y	0.20	0/10233	0.31	0/14057
6	Z	0.21	0/10233	0.32	0/14057
6	c	0.20	0/10233	0.32	0/14057
6	f	0.20	0/10233	0.32	0/14057
6	i	0.21	0/10233	0.32	0/14057

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	a1	0.09	0/1218	0.21	0/1890
7	b1	0.09	0/1218	0.21	0/1890
8	a2	0.09	0/1406	0.21	0/2182
8	b2	0.09	0/1406	0.22	0/2182
9	a3	0.09	0/936	0.22	0/1452
9	b3	0.09	0/936	0.21	0/1452
10	a4	0.09	0/419	0.22	0/649
10	b4	0.09	0/419	0.21	0/649
11	a5	0.09	0/889	0.21	0/1379
11	b5	0.09	0/889	0.21	0/1379
12	a6	0.09	0/701	0.21	0/1087
12	b6	0.09	0/701	0.21	0/1087
All	All	0.23	0/200040	0.31	3/276407 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	GLY	N-CA-C	-6.15	105.13	113.37
1	A	568	VAL	N-CA-C	5.43	115.63	110.42
3	D	463	SER	CB-CA-C	-5.29	110.45	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9978	0	9895	92	0
2	B	5593	0	5692	65	0
3	C	8300	0	8262	66	0
3	D	8761	0	8726	76	0
3	E	8534	0	8491	64	0
3	F	8761	0	8726	70	0
3	G	8477	0	8430	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	8699	0	8661	73	0
3	I	8226	0	8177	58	0
3	J	8699	0	8661	79	0
3	K	8477	0	8430	69	0
3	L	8761	0	8726	57	0
4	M	640	0	605	9	0
4	N	210	0	212	1	0
4	k	211	0	212	0	0
4	l	211	0	212	3	0
4	m	211	0	212	4	0
5	V	3138	0	3059	27	0
5	W	3138	0	3059	19	0
5	X	3138	0	3059	18	0
5	a	3138	0	3059	27	0
5	b	3138	0	3059	24	0
5	d	3138	0	3059	21	0
5	e	3138	0	3059	16	0
5	g	3138	0	3059	16	0
5	h	3138	0	3059	23	0
5	n	3138	0	3059	14	0
6	Y	9963	0	9899	68	0
6	Z	9963	0	9899	88	0
6	c	9963	0	9899	84	0
6	f	9963	0	9899	80	0
6	i	9963	0	9899	86	0
7	a1	1089	0	548	0	0
7	b1	1089	0	548	0	0
8	a2	1257	0	632	0	0
8	b2	1257	0	632	0	0
9	a3	837	0	422	0	0
9	b3	837	0	422	1	0
10	a4	375	0	191	1	0
10	b4	375	0	191	0	0
11	a5	795	0	401	0	0
11	b5	795	0	401	0	0
12	a6	627	0	317	0	0
12	b6	627	0	317	0	0
13	E	1	0	0	0	0
13	G	1	0	0	0	0
13	I	1	0	0	0	0
13	K	1	0	0	0	0
All	All	193908	0	187437	1393	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 4.

All (1393) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:931:ILE:HD11	3:D:689:VAL:HG21	1.67	0.77
3:F:617:HIS:ND1	3:F:618:PRO:O	2.18	0.76
3:I:841:PHE:HA	3:I:844:LEU:HD23	1.70	0.73
1:A:601:TYR:HA	1:A:605:LEU:HB2	1.70	0.73
3:I:237:GLU:HB2	3:I:1152:ALA:HB2	1.71	0.72
3:K:119:CYS:SG	3:K:120:ASN:N	2.62	0.72
3:K:237:GLU:HB2	3:K:1152:ALA:HB2	1.72	0.71
6:Y:626:ALA:O	6:Y:630:GLN:NE2	2.25	0.70
3:J:351:PRO:O	3:J:353:GLN:NE2	2.25	0.69
2:B:656:ALA:HB2	2:B:712:LEU:HD11	1.73	0.68
5:b:158:HIS:CE1	5:b:297:PRO:HG2	2.29	0.68
3:E:1133:VAL:HG13	3:F:106:MET:HE1	1.75	0.68
3:J:484:THR:HG21	3:J:529:TRP:CH2	2.30	0.67
3:J:580:HIS:CE1	3:J:618:PRO:HD3	2.30	0.67
3:H:609:THR:O	3:H:609:THR:HG22	1.95	0.67
3:J:617:HIS:ND1	3:J:618:PRO:HD2	2.08	0.67
4:M:85:ASP:OD1	4:M:85:ASP:N	2.26	0.67
3:L:900:GLU:OE1	3:L:900:GLU:N	2.22	0.66
3:D:391:CYS:SG	3:D:392:ASP:N	2.68	0.66
1:A:67:SER:HB2	1:A:228:VAL:HG22	1.78	0.66
1:A:1179:GLN:N	1:A:1179:GLN:OE1	2.27	0.66
3:F:523:ASN:O	3:F:523:ASN:ND2	2.23	0.66
3:I:313:LYS:O	3:I:1196:ARG:NH1	2.29	0.66
3:E:237:GLU:HB2	3:E:1152:ALA:HB2	1.76	0.66
6:f:626:ALA:O	6:f:630:GLN:NE2	2.28	0.66
2:B:181:ASP:HA	2:B:184:ALA:HB2	1.79	0.65
3:E:1050:ASP:N	3:E:1050:ASP:OD1	2.30	0.65
3:E:655:GLU:OE2	3:E:674:ARG:NE	2.29	0.65
3:H:136:LEU:O	3:H:141:ARG:NH1	2.30	0.65
2:B:611:ALA:N	2:B:629:LEU:O	2.29	0.65
6:i:1065:HIS:HB3	6:i:1070:VAL:HG21	1.79	0.65
3:I:991:GLY:O	3:I:1132:ARG:NH2	2.29	0.64
2:B:630:GLU:N	2:B:630:GLU:OE1	2.30	0.64
3:K:514:ILE:HA	3:K:517:LEU:HD12	1.78	0.64
6:c:1143:GLN:O	6:c:1151:ASN:ND2	2.31	0.64
3:E:268:ASP:OD1	3:E:269:SER:N	2.31	0.64
3:D:705:ILE:HG21	3:D:737:ARG:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:1044:LEU:HD12	6:i:1129:PRO:HA	1.80	0.63
3:D:1121:ILE:O	3:D:1123:GLN:NE2	2.30	0.63
3:H:746:TYR:HD1	3:H:750:MET:HE3	1.62	0.63
1:A:488:ASP:N	1:A:488:ASP:OD1	2.32	0.63
2:B:256:THR:HG22	3:E:252:LEU:HD23	1.81	0.63
3:L:1085:LEU:HD12	3:L:1119:ILE:HD13	1.81	0.63
3:G:118:VAL:HG12	3:G:125:ARG:HG2	1.80	0.63
3:J:787:ARG:HD3	3:J:931:ILE:HG22	1.82	0.62
1:A:3:GLU:OE1	1:A:3:GLU:N	2.32	0.62
1:A:1052:CYS:SG	1:A:1055:ARG:NH2	2.72	0.62
3:J:579:PRO:HG2	3:J:580:HIS:HD2	1.63	0.62
3:L:969:MET:O	3:L:979:ARG:NH2	2.32	0.62
1:A:1211:PHE:HA	1:A:1216:THR:HG21	1.81	0.62
5:b:25:ASP:OD1	5:b:57:ARG:NH2	2.32	0.62
3:J:287:GLN:NE2	3:J:1106:LYS:O	2.32	0.62
5:W:22:ASP:OD1	5:W:23:LEU:N	2.33	0.62
3:C:284:ASP:OD1	3:C:285:ASN:N	2.31	0.61
3:D:1140:GLU:O	3:D:1142:ASN:ND2	2.31	0.61
6:f:1065:HIS:HB3	6:f:1070:VAL:HG21	1.82	0.61
3:E:906:ASN:ND2	3:E:919:LEU:O	2.33	0.61
5:e:25:ASP:OD1	5:e:57:ARG:NH2	2.33	0.61
3:G:338:GLU:OE1	3:G:338:GLU:N	2.31	0.61
6:c:1065:HIS:HB3	6:c:1070:VAL:HG21	1.81	0.61
3:K:1209:TYR:O	3:K:1211:ARG:NE	2.34	0.61
3:F:284:ASP:OD1	3:F:285:ASN:N	2.32	0.61
1:A:971:SER:HA	1:A:974:ILE:HB	1.82	0.60
6:f:1044:LEU:HD12	6:f:1129:PRO:HA	1.83	0.60
3:J:355:LYS:NZ	3:J:1149:THR:O	2.34	0.60
1:A:446:PRO:HG2	3:E:526:ALA:HB2	1.84	0.60
3:I:1006:ARG:NH1	3:I:1077:GLU:OE1	2.35	0.60
6:c:1153:ALA:O	6:c:1192:LEU:N	2.34	0.60
3:E:150:THR:O	3:E:154:ASN:ND2	2.35	0.60
3:K:218:GLU:HG3	3:K:219:LEU:HG	1.83	0.60
3:K:284:ASP:OD1	3:K:285:ASN:N	2.33	0.60
1:A:339:GLU:O	1:A:342:THR:OG1	2.20	0.59
5:X:273:HIS:CE1	5:X:394:PHE:HD1	2.19	0.59
5:V:25:ASP:OD1	5:V:57:ARG:NH2	2.33	0.59
6:c:511:ASP:OD1	6:c:512:THR:N	2.35	0.59
1:A:839:LEU:O	1:A:1096:ASN:ND2	2.33	0.59
3:J:198:THR:O	3:J:331:ARG:NH2	2.34	0.59
3:H:787:ARG:NH2	3:H:926:TYR:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:854:MET:HE3	6:Z:864:MET:HE1	1.84	0.59
6:Y:856:ASP:OD1	6:Y:857:ALA:N	2.36	0.59
6:Z:511:ASP:OD1	6:Z:512:THR:N	2.36	0.59
6:Z:1143:GLN:O	6:Z:1151:ASN:ND2	2.36	0.59
3:E:502:GLU:OE1	3:E:502:GLU:N	2.36	0.59
5:h:25:ASP:OD1	5:h:57:ARG:NH2	2.32	0.59
6:i:748:ARG:NH1	6:i:790:ARG:O	2.36	0.59
3:D:209:ASN:HD21	3:D:267:THR:HG23	1.68	0.58
6:f:1154:ARG:NH2	6:f:1189:ASN:OD1	2.36	0.58
3:H:284:ASP:OD1	3:H:285:ASN:N	2.34	0.58
5:X:153:GLN:O	5:X:274:TRP:NE1	2.35	0.58
6:f:82:ARG:NH1	6:f:83:ASP:OD1	2.36	0.58
3:C:164:TRP:NE1	3:C:518:LEU:O	2.35	0.58
6:Z:1065:HIS:HB3	6:Z:1070:VAL:HG21	1.84	0.58
5:a:334:ALA:O	5:a:338:HIS:HD2	1.85	0.58
3:E:1131:ARG:HB3	3:F:106:MET:HG2	1.83	0.58
3:L:77:ASP:OD1	3:L:77:ASP:N	2.33	0.58
6:Y:1065:HIS:HB3	6:Y:1070:VAL:HG21	1.83	0.58
6:Z:856:ASP:OD1	6:Z:857:ALA:N	2.36	0.58
5:g:160:GLU:OE2	5:g:209:ARG:NE	2.33	0.58
3:F:198:THR:O	3:F:331:ARG:NH2	2.37	0.58
3:H:969:MET:O	3:H:979:ARG:NH2	2.36	0.58
1:A:67:SER:OG	1:A:99:ASP:N	2.37	0.58
3:K:313:LYS:O	3:K:1196:ARG:NH1	2.37	0.58
6:f:854:MET:HE3	6:f:864:MET:HE1	1.85	0.58
3:E:218:GLU:HG3	3:E:219:LEU:HG	1.85	0.57
3:J:969:MET:O	3:J:979:ARG:NH2	2.36	0.57
6:Z:1153:ALA:O	6:Z:1192:LEU:N	2.36	0.57
5:b:354:GLN:NE2	5:b:358:ASP:OD1	2.37	0.57
6:c:626:ALA:O	6:c:630:GLN:NE2	2.36	0.57
2:B:70:ILE:HB	2:B:71:PRO:HD3	1.86	0.57
3:G:237:GLU:HB2	3:G:1152:ALA:HB2	1.84	0.57
3:I:1155:ASP:OD1	3:I:1156:THR:N	2.38	0.57
3:K:910:LYS:NZ	3:K:917:GLY:O	2.37	0.57
6:Y:511:ASP:OD1	6:Y:512:THR:N	2.37	0.57
5:b:374:LEU:HA	5:b:386:ILE:HD11	1.87	0.57
6:i:511:ASP:OD1	6:i:512:THR:N	2.38	0.57
3:C:237:GLU:HB2	3:C:1152:ALA:HB2	1.85	0.57
3:I:135:HIS:ND1	3:I:139:ASP:OD2	2.38	0.57
2:B:671:ALA:HB3	2:B:672:PRO:HD3	1.87	0.57
3:J:947:ARG:NH2	5:d:252:ASP:OD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1040:ASP:OD1	3:J:1041:ILE:N	2.37	0.57
4:N:102:ASP:OD1	4:N:105:SER:OG	2.23	0.57
1:A:1163:ASP:OD1	1:A:1164:SER:N	2.37	0.57
3:E:1155:ASP:OD1	3:E:1156:THR:N	2.37	0.57
5:X:374:LEU:HA	5:X:386:ILE:HD11	1.87	0.57
3:C:372:ASP:OD1	3:C:373:ARG:N	2.37	0.56
3:C:749:HIS:CE1	6:c:160:ILE:HD11	2.40	0.56
3:E:338:GLU:OE1	3:E:338:GLU:N	2.37	0.56
3:F:460:VAL:HG11	3:F:923:LEU:HD12	1.86	0.56
1:A:130:GLU:OE1	1:A:130:GLU:N	2.33	0.56
1:A:954:HIS:ND1	1:A:1057:THR:HG21	2.20	0.56
3:I:218:GLU:HG3	3:I:219:LEU:HG	1.86	0.56
3:L:254:ASP:OD1	3:L:255:GLU:N	2.35	0.56
3:L:689:VAL:O	3:L:692:THR:OG1	2.23	0.56
3:D:358:GLN:O	3:D:361:SER:OG	2.22	0.56
3:H:511:ILE:HG13	3:H:515:LEU:HD23	1.85	0.56
3:H:787:ARG:HB3	3:H:931:ILE:HG22	1.88	0.56
4:M:73:ASN:OD1	4:M:74:ASN:N	2.38	0.56
6:Y:748:ARG:NH1	6:Y:790:ARG:O	2.36	0.56
5:h:374:LEU:HA	5:h:386:ILE:HD11	1.87	0.56
3:D:694:ASP:OD1	3:D:694:ASP:N	2.39	0.56
5:a:25:ASP:OD1	5:a:57:ARG:NH2	2.39	0.56
5:h:153:GLN:O	5:h:274:TRP:NE1	2.39	0.56
2:B:219:TYR:CE2	2:B:221:LEU:HB2	2.41	0.56
3:G:218:GLU:HG3	3:G:219:LEU:HG	1.86	0.56
3:G:254:ASP:OD1	3:G:255:GLU:N	2.39	0.56
6:c:948:ASP:HB2	6:c:957:ARG:HB2	1.87	0.56
5:W:228:THR:OG1	5:W:232:PHE:O	2.22	0.56
6:Y:1154:ARG:NH2	6:Y:1189:ASN:OD1	2.38	0.56
5:e:374:LEU:HA	5:e:386:ILE:HD11	1.87	0.56
6:f:748:ARG:NH1	6:f:790:ARG:O	2.37	0.56
1:A:42:ARG:NH1	1:A:152:ASP:OD2	2.39	0.56
6:f:583:ASP:OD1	6:f:584:GLN:N	2.39	0.56
3:D:631:ILE:O	3:D:640:ARG:NH1	2.39	0.56
6:i:82:ARG:NH1	6:i:83:ASP:OD1	2.39	0.56
3:E:173:ASP:OD1	3:E:173:ASP:N	2.40	0.55
6:Z:1233:ARG:HD3	6:Z:1293:VAL:HG23	1.88	0.55
3:C:906:ASN:ND2	3:C:921:ASP:OD1	2.39	0.55
3:F:367:ARG:NH2	3:F:1174:ASP:O	2.36	0.55
5:V:354:GLN:NE2	5:V:358:ASP:OD1	2.39	0.55
6:i:9:LEU:HD13	6:i:318:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:412:ASP:OD2	3:J:414:THR:OG1	2.20	0.55
6:Y:854:MET:HE3	6:Y:864:MET:HE1	1.87	0.55
6:c:9:LEU:HD13	6:c:318:VAL:HG11	1.88	0.55
3:E:124:ALA:C	3:E:125:ARG:HE	2.15	0.55
3:J:893:VAL:HG23	3:J:897:ALA:HB3	1.88	0.55
4:M:102:ASP:OD1	4:M:105:SER:OG	2.23	0.55
6:c:995:CYS:HB3	6:c:998:LEU:HD23	1.89	0.55
6:i:1070:VAL:HG13	6:i:1081:VAL:HG23	1.87	0.55
6:f:1153:ALA:O	6:f:1192:LEU:N	2.36	0.55
1:A:810:GLU:OE1	1:A:811:TYR:N	2.39	0.55
2:B:411:GLY:O	2:B:548:ASN:ND2	2.39	0.55
3:F:146:THR:HG22	3:F:148:LEU:H	1.71	0.55
3:H:875:GLN:HE21	3:H:878:GLY:HA3	1.70	0.55
5:a:374:LEU:HA	5:a:386:ILE:HD11	1.88	0.55
5:d:374:LEU:HA	5:d:386:ILE:HD11	1.89	0.55
1:A:83:ARG:HG2	1:A:93:VAL:HA	1.89	0.55
1:A:137:THR:HG22	1:A:674:SER:HA	1.88	0.55
3:H:519:GLN:HB3	3:H:521:MET:HE3	1.88	0.55
6:c:1070:VAL:HG13	6:c:1081:VAL:HG23	1.89	0.55
3:F:1103:TRP:CD1	3:F:1113:PRO:HG2	2.42	0.54
3:J:1150:ASN:HD22	3:J:1156:THR:HG22	1.71	0.54
5:n:374:LEU:HA	5:n:386:ILE:HD11	1.89	0.54
6:c:583:ASP:OD1	6:c:584:GLN:N	2.40	0.54
1:A:1216:THR:HG22	1:A:1253:VAL:O	2.07	0.54
6:c:1154:ARG:NH2	6:c:1189:ASN:OD1	2.40	0.54
6:i:1233:ARG:HD3	6:i:1293:VAL:HG23	1.90	0.54
1:A:1187:VAL:HG23	1:A:1189:LEU:HD23	1.89	0.54
2:B:291:ASP:OD1	2:B:316:SER:N	2.40	0.54
3:I:749:HIS:CE1	6:i:160:ILE:HD11	2.42	0.54
3:J:799:ASP:OD1	3:J:800:ILE:N	2.39	0.54
6:c:854:MET:HE3	6:c:864:MET:HE1	1.89	0.54
6:f:1205:LEU:O	6:f:1227:TYR:OH	2.26	0.54
6:c:1044:LEU:HD12	6:c:1129:PRO:HA	1.90	0.54
1:A:967:GLU:HB3	1:A:970:SER:HB3	1.89	0.54
2:B:214:ASP:OD1	2:B:214:ASP:N	2.40	0.54
6:Z:82:ARG:NH1	6:Z:83:ASP:OD1	2.41	0.54
3:J:782:ASN:HB2	3:J:939:LEU:HD13	1.89	0.54
3:L:118:VAL:HA	3:L:125:ARG:HA	1.88	0.54
3:J:631:ILE:O	3:J:640:ARG:NH1	2.41	0.54
5:d:25:ASP:OD1	5:d:57:ARG:NH2	2.41	0.54
6:f:9:LEU:HD13	6:f:318:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:610:THR:HG21	6:i:616:SER:HB3	1.90	0.54
2:B:654:SER:O	2:B:712:LEU:HD13	2.07	0.54
3:J:1121:ILE:O	3:J:1123:GLN:NE2	2.36	0.54
3:K:338:GLU:OE1	3:K:338:GLU:N	2.34	0.54
5:X:257:ALA:HB3	5:X:412:VAL:OXT	2.08	0.54
3:D:509:SER:O	3:D:511:ILE:N	2.41	0.54
3:F:338:GLU:OE1	3:F:338:GLU:N	2.36	0.54
3:J:140:HIS:O	3:J:141:ARG:NE	2.41	0.53
3:K:189:ASN:OD1	3:K:190:GLY:N	2.41	0.53
6:i:1205:LEU:O	6:i:1227:TYR:OH	2.23	0.53
6:i:1224:VAL:HA	6:i:1227:TYR:CD2	2.43	0.53
3:D:451:LEU:HB3	3:D:666:ALA:HB2	1.90	0.53
3:J:1140:GLU:O	3:J:1142:ASN:ND2	2.42	0.53
3:K:372:ASP:OD1	3:K:373:ARG:N	2.41	0.53
6:c:1238:ARG:HH22	6:c:1276:LEU:HB3	1.73	0.53
3:D:113:ASN:ND2	3:D:115:SER:OG	2.40	0.53
3:K:1122:PRO:HA	3:K:1159:GLY:HA3	1.90	0.53
3:L:122:CYS:O	3:L:168:ARG:NH2	2.30	0.53
6:f:1204:LEU:HA	6:f:1227:TYR:CE1	2.43	0.53
6:Y:610:THR:HG21	6:Y:616:SER:HB3	1.91	0.53
6:f:607:LEU:O	6:f:610:THR:OG1	2.26	0.53
2:B:649:GLU:N	2:B:649:GLU:OE1	2.41	0.53
3:F:1160:GLU:OE1	3:F:1161:ASN:N	2.41	0.53
6:Y:448:ASP:OD2	6:Y:672:THR:OG1	2.25	0.53
6:Z:1241:LEU:HD12	6:Z:1284:TYR:CE1	2.43	0.53
5:e:257:ALA:HB3	5:e:412:VAL:OXT	2.08	0.53
3:E:405:LEU:O	3:E:408:SER:OG	2.20	0.53
3:K:1050:ASP:OD2	3:L:1214:THR:OG1	2.26	0.53
5:b:257:ALA:HB3	5:b:412:VAL:OXT	2.09	0.53
1:A:97:ASN:ND2	1:A:268:SER:O	2.42	0.53
3:C:655:GLU:OE2	3:C:674:ARG:NE	2.30	0.53
3:F:85:ASP:OD1	3:F:86:SER:N	2.42	0.53
3:F:1107:ILE:HG23	3:F:1112:ILE:HG22	1.90	0.53
3:K:749:HIS:CE1	6:f:160:ILE:HD11	2.43	0.53
3:C:1091:GLN:OE1	3:C:1125:TYR:OH	2.21	0.53
3:I:372:ASP:OD1	3:I:373:ARG:N	2.42	0.53
3:L:799:ASP:OD1	3:L:800:ILE:N	2.42	0.53
5:V:61:VAL:HG22	5:V:276:HIS:HA	1.89	0.53
6:Y:9:LEU:HD13	6:Y:318:VAL:HG11	1.91	0.53
6:i:1153:ALA:O	6:i:1192:LEU:N	2.39	0.53
3:G:654:SER:OG	3:G:679:TRP:O	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1107:ILE:HG23	3:G:1112:ILE:HG22	1.91	0.53
3:I:655:GLU:OE2	3:I:674:ARG:NE	2.30	0.53
3:K:160:PHE:HE1	3:K:518:LEU:HB3	1.73	0.53
6:f:995:CYS:HB3	6:f:998:LEU:HD23	1.91	0.53
6:f:1238:ARG:HH22	6:f:1276:LEU:HB3	1.73	0.53
6:f:1240:SER:HB2	6:f:1286:THR:HG22	1.91	0.53
1:A:754:ILE:HD12	1:A:754:ILE:H	1.74	0.53
1:A:1257:ASP:OD1	1:A:1258:GLY:N	2.40	0.53
3:G:937:ALA:HB2	3:G:947:ARG:HA	1.90	0.53
5:V:374:LEU:HA	5:V:386:ILE:HD11	1.91	0.53
5:X:354:GLN:NE2	5:X:358:ASP:OD1	2.42	0.53
6:Z:1204:LEU:HA	6:Z:1227:TYR:CE2	2.44	0.53
6:c:764:THR:O	6:c:767:SER:OG	2.24	0.53
6:i:1240:SER:HB2	6:i:1286:THR:HG22	1.91	0.53
3:C:260:GLU:OE1	3:C:307:SER:OG	2.26	0.52
3:G:749:HIS:CE1	6:Y:160:ILE:HD11	2.44	0.52
3:H:869:SER:HB2	3:H:958:HIS:CE1	2.43	0.52
3:J:358:GLN:O	3:J:361:SER:OG	2.23	0.52
6:Y:1029:ASP:OD1	6:Y:1031:THR:HG22	2.09	0.52
5:g:374:LEU:HA	5:g:386:ILE:HD11	1.90	0.52
4:m:88:ALA:O	4:m:92:ASN:ND2	2.42	0.52
1:A:834:GLY:HA3	1:A:844:TRP:CE2	2.44	0.52
2:B:89:LEU:HD22	2:B:96:ASN:HA	1.91	0.52
3:E:993:TRP:CD1	3:E:995:PRO:HD3	2.44	0.52
3:H:1103:TRP:CD1	3:H:1113:PRO:HG2	2.43	0.52
6:c:502:ASN:ND2	6:c:505:THR:OG1	2.39	0.52
6:i:1154:ARG:NH2	6:i:1189:ASN:OD1	2.41	0.52
3:L:632:ASN:OD1	3:L:635:GLN:N	2.37	0.52
5:b:61:VAL:HG22	5:b:276:HIS:HA	1.92	0.52
6:f:1070:VAL:HG13	6:f:1081:VAL:HG23	1.90	0.52
3:J:322:THR:HG22	3:J:323:THR:H	1.75	0.52
6:Z:1238:ARG:HH22	6:Z:1276:LEU:HB3	1.75	0.52
6:i:583:ASP:OD1	6:i:584:GLN:N	2.42	0.52
6:i:1204:LEU:HA	6:i:1227:TYR:CE1	2.44	0.52
6:Y:234:THR:OG1	6:Y:235:TYR:N	2.42	0.52
6:Y:995:CYS:HB3	6:Y:998:LEU:HD23	1.91	0.52
6:Y:1251:THR:HB	6:Y:1295:GLU:HB2	1.92	0.52
3:D:1033:ASP:OD1	3:D:1034:ASP:N	2.43	0.52
3:F:1006:ARG:NH1	3:F:1077:GLU:OE2	2.40	0.52
3:H:869:SER:HB2	3:H:958:HIS:HE1	1.74	0.52
6:f:234:THR:OG1	6:f:235:TYR:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:502:ASN:ND2	6:f:505:THR:OG1	2.40	0.52
2:B:287:LEU:HD12	2:B:288:PRO:HD2	1.92	0.52
3:C:937:ALA:HB2	3:C:947:ARG:HA	1.92	0.52
3:E:1013:VAL:HG12	3:E:1046:VAL:HB	1.91	0.52
3:H:1139:SER:OG	3:H:1140:GLU:OE1	2.27	0.52
3:K:655:GLU:OE2	3:K:674:ARG:NE	2.29	0.52
6:Y:583:ASP:OD1	6:Y:584:GLN:N	2.43	0.52
5:b:158:HIS:HE1	5:b:297:PRO:HG2	1.75	0.52
3:F:237:GLU:HA	3:F:1151:ALA:HB3	1.91	0.52
5:V:153:GLN:O	5:V:274:TRP:NE1	2.42	0.52
6:i:502:ASN:ND2	6:i:505:THR:OG1	2.38	0.52
5:n:25:ASP:OD1	5:n:57:ARG:NH2	2.42	0.52
3:E:652:GLN:HB3	6:Z:244:THR:HG22	1.92	0.52
3:I:654:SER:OG	3:I:679:TRP:O	2.22	0.52
3:J:284:ASP:OD1	3:J:285:ASN:N	2.43	0.52
5:V:257:ALA:HB3	5:V:412:VAL:OXT	2.10	0.52
6:c:104:PRO:O	6:c:108:ASN:ND2	2.37	0.52
6:c:883:ALA:O	6:c:886:ASN:ND2	2.41	0.52
1:A:706:GLU:HB2	1:A:731:ILE:HD13	1.92	0.51
1:A:1156:LEU:HD12	1:A:1161:MET:HG3	1.93	0.51
3:G:552:ASP:OD2	3:G:555:GLN:HG2	2.09	0.51
3:J:136:LEU:HA	3:J:140:HIS:HD1	1.74	0.51
3:D:198:THR:O	3:D:331:ARG:NH2	2.42	0.51
3:D:1153:SER:OG	3:D:1154:ILE:N	2.43	0.51
3:E:937:ALA:HB2	3:E:947:ARG:HA	1.92	0.51
3:J:370:ARG:HA	3:J:387:CYS:HA	1.92	0.51
3:J:580:HIS:HE1	3:J:618:PRO:HD3	1.73	0.51
3:L:85:ASP:OD1	3:L:85:ASP:N	2.37	0.51
5:n:160:GLU:OE2	5:n:209:ARG:NE	2.36	0.51
1:A:596:ASP:N	1:A:596:ASP:OD1	2.41	0.51
3:I:1183:ASP:OD2	3:I:1187:ARG:NH1	2.43	0.51
6:Y:1070:VAL:HG13	6:Y:1081:VAL:HG23	1.91	0.51
6:f:1029:ASP:OD1	6:f:1031:THR:HG22	2.10	0.51
6:i:1029:ASP:OD1	6:i:1031:THR:HG22	2.11	0.51
1:A:293:ASN:O	1:A:327:ARG:NH1	2.41	0.51
3:K:746:TYR:OH	3:K:754:GLU:OE1	2.28	0.51
3:L:193:LEU:O	3:L:402:TYR:OH	2.25	0.51
6:Y:883:ALA:O	6:Y:886:ASN:ND2	2.44	0.51
6:Z:502:ASN:ND2	6:Z:505:THR:OG1	2.41	0.51
6:c:448:ASP:OD2	6:c:672:THR:OG1	2.20	0.51
6:c:1029:ASP:OD1	6:c:1031:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:1291:ALA:O	6:f:1294:TYR:OH	2.20	0.51
6:i:1238:ARG:HH22	6:i:1276:LEU:HB3	1.75	0.51
2:B:329:GLU:HA	2:B:382:VAL:HG23	1.92	0.51
3:C:237:GLU:HA	3:C:1151:ALA:HB3	1.93	0.51
3:F:1033:ASP:OD1	3:F:1034:ASP:N	2.43	0.51
3:K:652:GLN:HB3	6:f:244:THR:HG22	1.92	0.51
3:K:1024:PRO:HB3	5:b:46:ILE:HB	1.93	0.51
3:H:498:THR:O	3:H:503:SER:OG	2.29	0.51
3:I:653:PRO:HD2	6:i:244:THR:HG21	1.93	0.51
3:J:214:HIS:O	3:J:214:HIS:ND1	2.44	0.51
3:L:320:ASP:CG	3:L:347:ARG:HH22	2.18	0.51
3:D:287:GLN:NE2	3:D:1106:LYS:O	2.36	0.51
3:I:521:MET:HE2	3:I:524:ASP:HB2	1.92	0.51
6:Z:995:CYS:HB3	6:Z:998:LEU:HD23	1.93	0.51
5:h:257:ALA:HB3	5:h:412:VAL:OXT	2.11	0.51
2:B:649:GLU:O	2:B:651:ARG:NH1	2.44	0.51
3:J:367:ARG:NH1	3:J:1174:ASP:O	2.41	0.51
5:V:158:HIS:ND1	5:V:159:LEU:N	2.59	0.51
6:Y:764:THR:O	6:Y:767:SER:OG	2.26	0.51
6:i:1235:THR:O	6:i:1291:ALA:HA	2.10	0.51
3:D:784:LEU:HD22	3:D:799:ASP:HB3	1.91	0.51
3:E:237:GLU:HA	3:E:1151:ALA:HB3	1.92	0.51
3:F:407:ARG:HB3	5:V:178:ILE:HB	1.92	0.51
3:L:686:ARG:O	3:L:687:LEU:HB2	2.11	0.51
6:f:1157:CYS:SG	6:f:1158:ASP:N	2.84	0.51
6:i:860:CYS:SG	6:i:864:MET:HE3	2.51	0.51
4:l:102:ASP:OD1	4:l:105:SER:OG	2.28	0.51
3:C:723:ASP:OD1	3:C:724:LEU:N	2.44	0.51
3:C:1050:ASP:OD2	3:D:1214:THR:OG1	2.29	0.51
3:K:1034:ASP:OD1	3:K:1034:ASP:N	2.43	0.51
6:c:1241:LEU:HD12	6:c:1284:TYR:CE1	2.46	0.51
3:C:1103:TRP:CD1	3:C:1113:PRO:HG2	2.45	0.50
3:G:653:PRO:HD2	6:Y:244:THR:HG21	1.93	0.50
3:I:314:SER:HA	3:I:1196:ARG:HD3	1.92	0.50
3:I:1122:PRO:HA	3:I:1159:GLY:HA3	1.93	0.50
1:A:264:ARG:O	1:A:264:ARG:NH1	2.42	0.50
1:A:393:ARG:HA	1:A:393:ARG:HH11	1.76	0.50
3:L:367:ARG:NH1	3:L:1174:ASP:O	2.42	0.50
6:Y:1153:ALA:O	6:Y:1192:LEU:N	2.42	0.50
1:A:681:PHE:HD2	2:B:531:ASN:HB3	1.76	0.50
3:F:787:ARG:NH2	3:F:926:TYR:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:374:LEU:HA	5:W:386:ILE:HD11	1.93	0.50
6:Y:1240:SER:HB2	6:Y:1286:THR:HG22	1.93	0.50
6:Z:748:ARG:NH1	6:Z:790:ARG:O	2.42	0.50
6:Z:1134:VAL:HG23	6:Z:1157:CYS:HB2	1.94	0.50
5:d:160:GLU:OE2	5:d:209:ARG:NE	2.41	0.50
3:C:221:GLY:O	3:C:224:TRP:NE1	2.43	0.50
3:F:370:ARG:HA	3:F:387:CYS:HA	1.94	0.50
3:H:386:GLU:HB2	3:H:1195:TYR:CZ	2.47	0.50
5:X:13:PHE:N	5:X:116:GLU:OE1	2.39	0.50
6:c:748:ARG:NH1	6:c:790:ARG:O	2.42	0.50
6:f:1177:ASN:ND2	6:f:1279:SER:O	2.45	0.50
3:J:121:VAL:HG23	3:J:122:CYS:H	1.76	0.50
3:K:173:ASP:OD1	3:K:174:VAL:N	2.45	0.50
3:L:787:ARG:NH2	3:L:926:TYR:O	2.44	0.50
3:L:1121:ILE:O	3:L:1123:GLN:NE2	2.34	0.50
5:d:331:VAL:HB	5:d:332:PRO:HD3	1.94	0.50
3:E:372:ASP:OD1	3:E:373:ARG:N	2.44	0.50
3:J:177:LYS:HB3	3:J:190:GLY:H	1.77	0.50
5:X:61:VAL:HG22	5:X:276:HIS:HA	1.94	0.50
6:f:1251:THR:HB	6:f:1295:GLU:HB2	1.94	0.50
5:n:151:SER:OG	5:n:268:ARG:NH1	2.44	0.50
3:D:459:LEU:HA	3:D:462:ILE:HG22	1.94	0.50
3:G:617:HIS:O	3:G:620:VAL:HG22	2.11	0.50
3:J:137:ARG:O	3:J:137:ARG:NH1	2.43	0.50
6:Y:439:SER:O	6:Y:648:THR:OG1	2.20	0.50
6:Y:502:ASN:ND2	6:Y:505:THR:OG1	2.38	0.50
6:Z:9:LEU:HD13	6:Z:318:VAL:HG11	1.94	0.50
6:Z:583:ASP:OD1	6:Z:584:GLN:N	2.45	0.50
6:c:856:ASP:OD1	6:c:857:ALA:N	2.45	0.50
6:f:448:ASP:OD2	6:f:672:THR:OG1	2.22	0.50
3:E:1031:LEU:O	3:E:1039:ARG:N	2.44	0.50
3:L:1103:TRP:CD1	3:L:1113:PRO:HG2	2.47	0.50
1:A:930:HIS:CD2	3:C:141:ARG:HE	2.30	0.49
2:B:361:THR:OG1	2:B:362:ARG:N	2.44	0.49
3:C:1107:ILE:HG23	3:C:1112:ILE:HG22	1.93	0.49
3:E:617:HIS:O	3:E:620:VAL:HG22	2.12	0.49
3:H:193:LEU:O	3:H:402:TYR:OH	2.27	0.49
6:Y:71:HIS:CE1	6:Y:74:PHE:HB2	2.47	0.49
6:Z:673:ALA:HA	6:Z:676:ARG:HE	1.77	0.49
6:Z:1233:ARG:HG3	6:Z:1292:GLY:HA2	1.94	0.49
6:f:1134:VAL:HG23	6:f:1157:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:HIS:O	1:A:32:GLN:HG2	2.12	0.49
5:g:25:ASP:OD1	5:g:57:ARG:NH2	2.43	0.49
3:C:218:GLU:HG3	3:C:219:LEU:HG	1.94	0.49
3:D:995:PRO:O	3:D:1138:THR:HG22	2.12	0.49
3:H:198:THR:O	3:H:331:ARG:NH2	2.42	0.49
3:H:367:ARG:NH1	3:H:1174:ASP:O	2.42	0.49
3:H:508:ILE:HD12	3:H:515:LEU:HD21	1.94	0.49
3:I:1103:TRP:CD1	3:I:1113:PRO:HG2	2.48	0.49
3:K:164:TRP:CE2	3:K:520:PRO:HD3	2.47	0.49
3:K:723:ASP:OD1	3:K:724:LEU:N	2.46	0.49
6:Y:1139:PRO:HB2	6:Y:1143:GLN:HB2	1.94	0.49
6:Z:1029:ASP:OD1	6:Z:1031:THR:HG22	2.13	0.49
6:c:1240:SER:HB2	6:c:1286:THR:HG22	1.95	0.49
6:f:929:MET:SD	6:f:929:MET:N	2.85	0.49
2:B:355:ASP:OD1	2:B:356:VAL:N	2.45	0.49
3:F:312:ASN:OD1	3:F:399:ARG:NH1	2.45	0.49
6:Z:309:ASN:OD1	6:Z:347:GLN:HG3	2.11	0.49
6:Z:1070:VAL:HG13	6:Z:1081:VAL:HG23	1.94	0.49
6:f:511:ASP:OD1	6:f:512:THR:N	2.46	0.49
6:f:764:THR:O	6:f:767:SER:OG	2.27	0.49
5:h:13:PHE:N	5:h:116:GLU:OE1	2.43	0.49
6:i:811:VAL:HG21	6:i:1019:TYR:CD1	2.48	0.49
3:D:799:ASP:OD1	3:D:800:ILE:N	2.45	0.49
3:H:928:ASP:CG	3:H:930:ARG:HE	2.21	0.49
3:K:137:ARG:O	3:K:141:ARG:HD3	2.13	0.49
3:K:405:LEU:O	3:K:408:SER:OG	2.21	0.49
3:L:631:ILE:O	3:L:640:ARG:NH1	2.43	0.49
6:Y:1241:LEU:HD12	6:Y:1284:TYR:CE1	2.47	0.49
5:a:331:VAL:HB	5:a:332:PRO:HD3	1.95	0.49
6:f:883:ALA:O	6:f:886:ASN:ND2	2.43	0.49
3:C:881:VAL:O	5:a:27:GLN:NE2	2.45	0.49
3:C:958:HIS:NE2	5:a:32:CYS:SG	2.85	0.49
5:e:61:VAL:HG22	5:e:276:HIS:HA	1.94	0.49
2:B:1:MET:HE2	2:B:190:LYS:HA	1.95	0.49
3:E:198:THR:O	3:E:331:ARG:NH2	2.45	0.49
3:E:990:ASN:O	3:E:1129:THR:OG1	2.27	0.49
3:H:1049:SER:HB2	3:H:1078:LEU:HD23	1.95	0.49
5:e:354:GLN:NE2	5:e:358:ASP:OD1	2.42	0.49
5:g:251:ASN:OD1	5:g:253:GLY:N	2.46	0.49
5:h:158:HIS:ND1	5:h:159:LEU:N	2.60	0.49
6:i:234:THR:OG1	6:i:235:TYR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:SER:HA	1:A:976:GLN:HB2	1.95	0.49
2:B:427:ASP:OD1	2:B:427:ASP:N	2.45	0.49
3:C:697:MET:HE2	3:C:744:PRO:HA	1.95	0.49
3:D:655:GLU:HG3	3:D:674:ARG:HH21	1.77	0.49
3:D:1103:TRP:CD1	3:D:1113:PRO:HG2	2.47	0.49
3:K:1006:ARG:NH1	3:K:1077:GLU:OE1	2.45	0.49
6:Y:309:ASN:OD1	6:Y:347:GLN:HG3	2.13	0.49
6:Z:860:CYS:SG	6:Z:861:ALA:N	2.86	0.49
6:Z:1177:ASN:ND2	6:Z:1279:SER:O	2.45	0.49
5:d:152:ASP:OD1	5:d:152:ASP:N	2.44	0.49
6:f:1241:LEU:HD12	6:f:1284:TYR:CE1	2.48	0.49
2:B:396:SER:OG	2:B:583:ARG:NH2	2.33	0.49
3:D:370:ARG:HA	3:D:387:CYS:HA	1.95	0.49
3:D:1169:TRP:CE3	3:D:1190:LEU:HB2	2.48	0.49
3:I:617:HIS:O	3:I:620:VAL:HG22	2.12	0.49
3:J:102:ASP:O	3:J:105:SER:OG	2.31	0.49
6:c:1134:VAL:HG23	6:c:1157:CYS:HB2	1.95	0.49
5:e:136:TRP:CE2	5:e:197:PRO:HA	2.48	0.49
6:f:1224:VAL:HA	6:f:1227:TYR:CD2	2.47	0.49
6:i:71:HIS:CE1	6:i:74:PHE:HB2	2.48	0.49
6:i:1037:VAL:HG22	6:i:1039:PRO:HD2	1.93	0.49
3:I:315:SER:OG	3:I:316:THR:N	2.46	0.49
3:J:617:HIS:HD2	3:K:434:ILE:HD12	1.78	0.49
6:Z:1154:ARG:NH2	6:Z:1189:ASN:OD1	2.46	0.49
1:A:622:ASP:OD1	1:A:622:ASP:N	2.46	0.48
3:K:843:PRO:HG2	3:K:844:LEU:HD22	1.95	0.48
3:K:1103:TRP:CD1	3:K:1113:PRO:HG2	2.48	0.48
1:A:982:THR:HG22	1:A:1024:PRO:HG2	1.95	0.48
3:F:795:ASP:OD1	3:F:796:ALA:N	2.41	0.48
3:L:903:HIS:HB3	4:m:81:ARG:NH1	2.28	0.48
6:Z:439:SER:O	6:Z:648:THR:OG1	2.28	0.48
6:i:104:PRO:O	6:i:108:ASN:ND2	2.37	0.48
3:D:407:ARG:HB3	5:X:178:ILE:HB	1.95	0.48
3:H:799:ASP:OD2	3:H:801:ARG:NH1	2.47	0.48
5:W:331:VAL:HB	5:W:332:PRO:HD3	1.95	0.48
5:b:136:TRP:CE2	5:b:197:PRO:HA	2.49	0.48
5:d:251:ASN:OD1	5:d:253:GLY:N	2.43	0.48
5:g:331:VAL:HB	5:g:332:PRO:HD3	1.95	0.48
2:B:205:ARG:NE	4:M:45:ASP:OD2	2.41	0.48
3:D:164:TRP:NE1	3:D:165:ASP:OD2	2.46	0.48
3:L:1140:GLU:O	3:L:1142:ASN:ND2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:1134:VAL:HG23	6:i:1157:CYS:HB2	1.95	0.48
6:i:1251:THR:HB	6:i:1295:GLU:HB2	1.95	0.48
3:D:895:SER:HB3	4:M:75:ASP:OD1	2.14	0.48
3:E:749:HIS:CE1	6:Z:160:ILE:HD11	2.47	0.48
3:F:695:SER:O	3:F:698:SER:OG	2.28	0.48
3:G:237:GLU:HA	3:G:1151:ALA:HB3	1.94	0.48
6:Y:929:MET:SD	6:Y:929:MET:N	2.86	0.48
6:f:309:ASN:OD1	6:f:347:GLN:HG3	2.14	0.48
5:n:331:VAL:HB	5:n:332:PRO:HD3	1.94	0.48
3:G:275:LYS:NZ	3:G:285:ASN:O	2.46	0.48
3:H:609:THR:O	3:H:609:THR:CG2	2.60	0.48
3:J:628:PRO:O	3:J:640:ARG:NH1	2.46	0.48
3:L:370:ARG:HA	3:L:387:CYS:HA	1.96	0.48
6:f:1227:TYR:C	6:f:1228:ARG:HE	2.22	0.48
6:i:1143:GLN:HB3	6:i:1151:ASN:ND2	2.29	0.48
5:n:312:VAL:N	5:n:316:THR:OG1	2.46	0.48
3:E:221:GLY:O	3:E:224:TRP:NE1	2.46	0.48
6:Z:234:THR:OG1	6:Z:235:TYR:N	2.46	0.48
2:B:190:LYS:HD2	2:B:190:LYS:N	2.28	0.48
3:D:354:THR:OG1	3:D:356:ASN:OD1	2.21	0.48
3:K:155:ASN:OD1	3:K:156:ALA:N	2.47	0.48
5:e:13:PHE:N	5:e:116:GLU:OE1	2.43	0.48
1:A:68:LEU:O	1:A:98:SER:OG	2.31	0.48
5:b:13:PHE:N	5:b:116:GLU:OE1	2.41	0.48
3:C:179:LEU:HD21	3:C:844:LEU:HD11	1.96	0.48
3:C:254:ASP:OD1	3:C:254:ASP:N	2.45	0.48
3:C:653:PRO:HD2	6:c:244:THR:HG21	1.95	0.48
3:D:1168:ARG:O	3:D:1169:TRP:HD1	1.96	0.48
3:G:541:VAL:HG21	3:G:811:LEU:HD13	1.94	0.48
3:I:439:THR:HG1	3:I:1199:PHE:HA	1.79	0.48
3:I:799:ASP:OD1	3:I:800:ILE:N	2.47	0.48
6:i:607:LEU:O	6:i:610:THR:OG1	2.32	0.48
1:A:113:TYR:HA	1:A:219:TRP:HA	1.94	0.47
3:F:412:ASP:OD2	3:F:414:THR:OG1	2.22	0.47
3:J:367:ARG:HB3	3:J:388:MET:HE3	1.96	0.47
6:Z:1205:LEU:N	6:Z:1227:TYR:OH	2.43	0.47
6:f:71:HIS:CE1	6:f:74:PHE:HB2	2.48	0.47
1:A:730:THR:OG1	1:A:732:GLN:OE1	2.26	0.47
3:G:1102:GLU:O	3:G:1105:SER:OG	2.27	0.47
3:H:412:ASP:OD2	3:H:414:THR:OG1	2.20	0.47
3:I:560:LEU:H	3:I:560:LEU:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:881:VAL:O	5:g:27:GLN:NE2	2.45	0.47
3:J:796:ALA:O	3:J:797:ALA:C	2.56	0.47
3:K:128:THR:HG23	3:K:131:ALA:H	1.80	0.47
3:L:695:SER:O	3:L:698:SER:OG	2.23	0.47
5:V:158:HIS:CD2	5:V:297:PRO:HG2	2.49	0.47
6:c:734:SER:O	6:c:737:SER:OG	2.30	0.47
6:f:15:THR:HG22	6:f:364:PRO:HB2	1.96	0.47
3:C:226:MET:HE2	3:C:226:MET:HA	1.95	0.47
3:F:103:PRO:HB2	3:F:104:GLN:HE21	1.79	0.47
3:H:449:GLU:OE1	3:H:449:GLU:N	2.43	0.47
3:I:242:ARG:NH2	3:I:1145:SER:OG	2.46	0.47
5:X:331:VAL:HB	5:X:332:PRO:HD3	1.96	0.47
6:c:231:ASP:OD2	6:c:285:LEU:N	2.48	0.47
1:A:454:GLN:HG2	1:A:626:MET:HE1	1.95	0.47
2:B:198:LEU:HD23	2:B:199:PRO:HD2	1.96	0.47
3:D:405:LEU:O	3:D:408:SER:OG	2.22	0.47
3:D:439:THR:OG1	3:D:1199:PHE:HA	2.15	0.47
3:E:829:THR:HG23	3:E:830:ASN:H	1.78	0.47
3:G:990:ASN:O	3:G:1129:THR:OG1	2.31	0.47
3:J:741:THR:OG1	3:J:825:GLY:N	2.48	0.47
6:Y:1037:VAL:HG22	6:Y:1039:PRO:HD2	1.95	0.47
6:Z:501:VAL:HG23	6:Z:507:ASN:C	2.40	0.47
6:c:703:ASP:O	6:c:705:THR:N	2.44	0.47
6:c:1177:ASN:ND2	6:c:1279:SER:O	2.47	0.47
6:c:1251:THR:HB	6:c:1295:GLU:HB2	1.96	0.47
6:f:997:TRP:CD1	6:f:997:TRP:H	2.33	0.47
6:i:751:SER:OG	6:i:754:PRO:O	2.29	0.47
6:i:929:MET:SD	6:i:929:MET:N	2.87	0.47
6:i:1241:LEU:HD12	6:i:1284:TYR:CE1	2.50	0.47
1:A:370:PHE:O	1:A:374:VAL:HG12	2.15	0.47
1:A:421:LEU:O	1:A:429:ARG:NH2	2.47	0.47
3:C:786:ALA:HB2	3:C:804:HIS:CG	2.50	0.47
3:H:1025:ASP:OD1	3:H:1026:GLY:N	2.42	0.47
5:a:338:HIS:CE1	5:a:355:LEU:HB3	2.49	0.47
5:e:153:GLN:O	5:e:274:TRP:NE1	2.46	0.47
6:f:1037:VAL:HG22	6:f:1039:PRO:HD2	1.95	0.47
5:g:152:ASP:OD1	5:g:152:ASP:N	2.47	0.47
1:A:563:THR:HB	1:A:737:CYS:H	1.79	0.47
1:A:777:TYR:HB3	1:A:779:ILE:HG23	1.96	0.47
2:B:288:PRO:HA	2:B:390:VAL:HA	1.95	0.47
3:E:653:PRO:HD2	6:Z:244:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1008:GLY:O	3:G:1011:VAL:HG12	2.14	0.47
3:J:1103:TRP:CD1	3:J:1113:PRO:HG2	2.49	0.47
3:K:547:GLU:OE1	3:K:547:GLU:N	2.40	0.47
3:K:617:HIS:O	3:K:620:VAL:HG22	2.13	0.47
3:L:1153:SER:OG	3:L:1154:ILE:N	2.45	0.47
5:W:160:GLU:OE2	5:W:209:ARG:NE	2.36	0.47
5:a:251:ASN:OD1	5:a:253:GLY:N	2.48	0.47
1:A:254:LEU:O	1:A:257:THR:OG1	2.26	0.47
2:B:621:TRP:CG	2:B:703:GLY:H	2.33	0.47
2:B:626:ASP:N	2:B:627:PRO:HD3	2.30	0.47
3:C:489:ASP:O	3:C:492:VAL:HG12	2.14	0.47
3:C:617:HIS:O	3:C:620:VAL:HG22	2.15	0.47
3:C:799:ASP:OD1	3:C:800:ILE:N	2.48	0.47
3:G:1093:SER:HG	3:H:105:SER:H	1.62	0.47
3:H:479:LEU:O	3:H:482:SER:OG	2.32	0.47
3:I:937:ALA:HB2	3:I:947:ARG:HA	1.97	0.47
3:J:162:THR:OG1	3:J:165:ASP:OD1	2.25	0.47
3:J:531:CYS:O	3:J:534:SER:OG	2.31	0.47
3:K:653:PRO:HD2	6:f:244:THR:HG21	1.97	0.47
5:X:136:TRP:CE2	5:X:197:PRO:HA	2.49	0.47
6:c:929:MET:SD	6:c:929:MET:N	2.87	0.47
6:f:1139:PRO:HB2	6:f:1143:GLN:HB2	1.96	0.47
6:f:1141:PRO:HA	6:f:1144:LEU:HD13	1.97	0.47
6:i:948:ASP:HB2	6:i:957:ARG:HB2	1.96	0.47
3:D:77:ASP:N	3:D:77:ASP:OD1	2.47	0.47
3:D:449:GLU:OE1	3:D:449:GLU:N	2.43	0.47
3:J:280:ARG:O	4:l:83:THR:HG23	2.14	0.47
5:W:152:ASP:OD1	5:W:152:ASP:N	2.47	0.47
4:m:105:SER:O	4:m:105:SER:OG	2.24	0.47
3:D:463:SER:O	3:D:801:ARG:NH2	2.48	0.47
3:E:531:CYS:O	3:E:534:SER:OG	2.31	0.47
3:I:1138:THR:OG1	3:I:1139:SER:N	2.48	0.47
6:Y:104:PRO:O	6:Y:108:ASN:ND2	2.36	0.47
6:Z:1240:SER:HB2	6:Z:1286:THR:HG22	1.97	0.47
6:i:1053:THR:HA	6:i:1095:GLU:HG2	1.97	0.47
3:D:502:GLU:OE2	3:D:507:THR:OG1	2.31	0.47
3:F:105:SER:O	3:F:106:MET:C	2.58	0.47
3:K:173:ASP:O	3:K:177:LYS:NZ	2.48	0.47
4:M:40:ASN:HB3	4:M:66:SER:HB2	1.97	0.47
5:a:152:ASP:OD1	5:a:152:ASP:N	2.44	0.47
6:i:362:GLU:OE1	6:i:377:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:447:SER:OG	3:D:449:GLU:OE1	2.33	0.46
3:E:938:TYR:CZ	3:E:946:VAL:HG21	2.50	0.46
6:Y:1184:VAL:HB	6:Y:1191:ASP:HB2	1.97	0.46
6:Z:929:MET:SD	6:Z:929:MET:N	2.88	0.46
6:c:1143:GLN:HB3	6:c:1151:ASN:ND2	2.30	0.46
5:d:10:THR:HG1	5:d:118:VAL:H	1.61	0.46
6:i:1141:PRO:HA	6:i:1144:LEU:HD13	1.97	0.46
1:A:31:GLU:OE1	1:A:871:GLN:NE2	2.45	0.46
3:D:688:THR:OG1	3:D:689:VAL:N	2.47	0.46
3:F:441:LEU:HG	3:F:443:PRO:HD3	1.97	0.46
3:H:87:ILE:HD12	3:H:87:ILE:H	1.80	0.46
3:I:405:LEU:O	3:I:408:SER:OG	2.25	0.46
3:K:982:LEU:HD23	3:K:983:TYR:N	2.30	0.46
6:c:234:THR:OG1	6:c:235:TYR:N	2.49	0.46
6:c:1141:PRO:HA	6:c:1144:LEU:HD13	1.98	0.46
6:f:501:VAL:HG23	6:f:507:ASN:C	2.40	0.46
6:i:819:ILE:HD11	6:i:896:ILE:HG13	1.97	0.46
6:i:856:ASP:OD1	6:i:857:ALA:N	2.48	0.46
2:B:467:ASP:HB3	3:E:152:MET:SD	2.55	0.46
3:C:429:ASN:OD1	3:C:429:ASN:N	2.47	0.46
3:G:225:PHE:O	3:G:228:MET:HG2	2.15	0.46
3:I:652:GLN:HB3	6:i:244:THR:HG22	1.97	0.46
3:J:260:GLU:OE2	3:J:262:ARG:NE	2.37	0.46
3:K:242:ARG:NH1	3:K:1145:SER:OG	2.49	0.46
3:K:841:PHE:HA	3:K:844:LEU:HD23	1.97	0.46
5:W:312:VAL:N	5:W:316:THR:OG1	2.47	0.46
6:Z:1037:VAL:HG22	6:Z:1039:PRO:HD2	1.96	0.46
6:c:466:ASP:OD1	6:c:467:ARG:N	2.48	0.46
6:f:1209:ASP:HB2	6:f:1219:ILE:HG12	1.97	0.46
5:h:26:LEU:HD13	5:h:71:LEU:HD11	1.98	0.46
3:D:740:LYS:HE3	3:D:740:LYS:HB3	1.82	0.46
3:L:212:SER:OG	3:L:213:ALA:N	2.48	0.46
3:L:655:GLU:OE1	3:L:674:ARG:HD2	2.14	0.46
5:W:235:GLU:OE1	5:W:236:PHE:N	2.48	0.46
5:b:158:HIS:HD2	5:b:265:SER:O	1.97	0.46
6:c:1209:ASP:OD1	6:c:1218:ARG:NH2	2.33	0.46
5:d:222:ARG:NH2	5:d:408:GLN:OE1	2.44	0.46
5:h:331:VAL:HB	5:h:332:PRO:HD3	1.98	0.46
1:A:432:TYR:OH	1:A:614:GLU:OE1	2.27	0.46
1:A:740:ASP:OD1	1:A:740:ASP:N	2.46	0.46
3:C:364:ILE:HB	3:C:367:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1047:TYR:HE2	3:G:1059:PHE:CD1	2.34	0.46
3:K:314:SER:HA	3:K:1196:ARG:HD3	1.96	0.46
3:L:247:THR:OG1	3:L:260:GLU:OE1	2.28	0.46
6:f:856:ASP:OD1	6:f:857:ALA:N	2.48	0.46
1:A:316:TRP:HB2	1:A:1109:ILE:HD12	1.97	0.46
2:B:179:TYR:CD2	2:B:180:PRO:HD3	2.50	0.46
2:B:440:ASP:N	2:B:440:ASP:OD1	2.47	0.46
3:H:409:MET:HE2	3:H:858:VAL:HG11	1.97	0.46
3:I:209:ASN:HD21	3:I:267:THR:HG23	1.79	0.46
3:I:315:SER:HB3	3:I:331:ARG:HD2	1.97	0.46
3:K:705:ILE:HG21	3:K:737:ARG:HB2	1.95	0.46
5:a:151:SER:OG	5:a:152:ASP:O	2.33	0.46
5:e:244:ASP:OD1	5:e:244:ASP:N	2.48	0.46
3:C:236:PRO:HG2	3:C:241:ASN:HD22	1.81	0.46
3:I:746:TYR:OH	3:I:754:GLU:OE1	2.32	0.46
3:K:226:MET:HA	3:K:226:MET:HE2	1.98	0.46
3:L:320:ASP:OD1	3:L:321:VAL:N	2.49	0.46
6:Z:644:LEU:HD23	6:Z:644:LEU:HA	1.84	0.46
6:f:934:ASN:HB2	6:f:956:TYR:CE2	2.51	0.46
5:h:136:TRP:CE2	5:h:197:PRO:HA	2.50	0.46
6:i:734:SER:O	6:i:737:SER:OG	2.31	0.46
3:C:769:VAL:HG22	3:C:770:PRO:HD2	1.98	0.46
3:D:804:HIS:CE1	4:M:65:ASP:HB3	2.50	0.46
5:V:352:GLU:O	5:V:356:ASN:ND2	2.43	0.46
5:X:352:GLU:O	5:X:356:ASN:ND2	2.44	0.46
6:Y:1146:PHE:CZ	6:Y:1232:PRO:HD3	2.51	0.46
6:Z:610:THR:HG21	6:Z:616:SER:HB3	1.98	0.46
5:g:10:THR:HG1	5:g:118:VAL:H	1.61	0.46
5:h:91:THR:OG1	5:h:92:TRP:N	2.49	0.46
5:n:152:ASP:OD1	5:n:152:ASP:N	2.45	0.46
1:A:63:SER:HA	1:A:66:HIS:CE1	2.51	0.46
2:B:462:ASP:OD1	2:B:464:LYS:N	2.47	0.46
3:C:654:SER:OG	3:C:679:TRP:O	2.26	0.46
3:E:514:ILE:HD11	3:E:564:TRP:CE3	2.51	0.46
3:E:654:SER:OG	3:E:679:TRP:O	2.21	0.46
3:F:155:ASN:N	3:F:174:VAL:O	2.36	0.46
3:F:989:THR:OG1	3:F:990:ASN:N	2.48	0.46
3:G:364:ILE:HB	3:G:367:ARG:HG3	1.98	0.46
3:G:786:ALA:HB2	3:G:804:HIS:CD2	2.50	0.46
3:H:782:ASN:HB2	3:H:939:LEU:HD13	1.98	0.46
6:f:1205:LEU:HG	6:f:1223:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:938:TYR:CZ	3:C:946:VAL:HG21	2.51	0.46
3:D:1122:PRO:HA	3:D:1159:GLY:HA3	1.98	0.46
3:F:617:HIS:O	3:F:620:VAL:HG22	2.16	0.46
3:I:452:ARG:NH2	3:I:948:GLU:OE2	2.43	0.46
3:I:1004:PHE:CD2	3:I:1044:ASP:HB3	2.51	0.46
3:K:531:CYS:O	3:K:534:SER:OG	2.34	0.46
3:K:1102:GLU:OE2	3:K:1106:LYS:NZ	2.36	0.46
5:V:26:LEU:HD13	5:V:71:LEU:HD11	1.97	0.46
6:Y:1177:ASN:ND2	6:Y:1279:SER:O	2.46	0.46
6:i:457:LEU:O	6:i:625:ARG:NH2	2.41	0.46
3:D:697:MET:HE3	3:D:822:MET:HE3	1.97	0.45
3:D:888:LEU:HD13	3:D:969:MET:HE1	1.98	0.45
3:J:383:ALA:HB1	3:J:439:THR:HG23	1.97	0.45
6:Y:819:ILE:HD11	6:Y:896:ILE:HG13	1.98	0.45
1:A:595:CYS:SG	1:A:697:HIS:ND1	2.81	0.45
3:E:1203:THR:OG1	3:E:1204:LEU:N	2.49	0.45
3:F:1160:GLU:OE1	3:F:1162:ALA:N	2.49	0.45
3:I:1022:PRO:O	3:I:1023:ARG:HD3	2.16	0.45
3:K:373:ARG:HB3	3:K:385:VAL:HG23	1.98	0.45
6:Y:1053:THR:HA	6:Y:1095:GLU:HG2	1.98	0.45
6:c:82:ARG:NH1	6:c:83:ASP:OD1	2.49	0.45
6:c:934:ASN:HB2	6:c:956:TYR:CE2	2.51	0.45
1:A:5:PHE:O	1:A:13:GLN:NE2	2.46	0.45
1:A:1192:PRO:HD2	1:A:1195:TRP:CD2	2.50	0.45
3:C:798:VAL:HG22	3:C:799:ASP:H	1.81	0.45
3:D:254:ASP:OD1	3:D:255:GLU:N	2.44	0.45
3:F:969:MET:HE2	3:F:969:MET:HA	1.99	0.45
3:G:372:ASP:OD1	3:G:373:ARG:N	2.47	0.45
3:J:543:THR:HG23	3:J:577:SER:H	1.80	0.45
3:L:197:ASP:OD1	3:L:198:THR:N	2.49	0.45
5:X:26:LEU:HD13	5:X:71:LEU:HD11	1.97	0.45
6:Z:962:GLU:OE2	6:c:550:ARG:NE	2.49	0.45
6:f:231:ASP:OD2	6:f:285:LEU:N	2.48	0.45
5:h:61:VAL:HG22	5:h:276:HIS:HA	1.98	0.45
1:A:1097:ASP:OD1	1:A:1098:ASP:N	2.49	0.45
3:D:367:ARG:NH1	3:D:1174:ASP:O	2.43	0.45
3:L:981:ASN:N	3:L:981:ASN:OD1	2.49	0.45
6:Z:948:ASP:HB2	6:Z:957:ARG:HB2	1.98	0.45
6:c:243:GLN:CD	6:c:245:GLY:H	2.24	0.45
6:f:523:SER:H	6:f:525:HIS:CE1	2.35	0.45
6:f:998:LEU:N	6:f:999:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:995:CYS:HB3	6:i:998:LEU:HD23	1.98	0.45
3:H:268:ASP:OD1	3:H:269:SER:N	2.48	0.45
3:J:155:ASN:ND2	3:J:174:VAL:O	2.40	0.45
6:Y:811:VAL:HG21	6:Y:1019:TYR:CD1	2.52	0.45
6:Y:948:ASP:HB2	6:Y:957:ARG:HB2	1.97	0.45
6:Z:1143:GLN:HB3	6:Z:1151:ASN:ND2	2.32	0.45
5:b:302:GLU:HG2	5:b:316:THR:HB	1.97	0.45
6:c:998:LEU:N	6:c:999:PRO:HD2	2.32	0.45
3:E:769:VAL:HG22	3:E:770:PRO:HD2	1.98	0.45
3:F:449:GLU:OE1	3:F:449:GLU:N	2.47	0.45
3:F:746:TYR:HD1	3:F:750:MET:HE2	1.81	0.45
3:G:655:GLU:OE2	3:G:674:ARG:NE	2.29	0.45
3:H:995:PRO:O	3:H:1138:THR:HG22	2.17	0.45
6:Y:1249:HIS:HB3	6:Y:1297:VAL:HG13	1.99	0.45
6:Z:1141:PRO:HA	6:Z:1144:LEU:HD13	1.98	0.45
6:c:1209:ASP:HB2	6:c:1219:ILE:HG12	1.99	0.45
6:i:243:GLN:CD	6:i:245:GLY:H	2.24	0.45
3:E:567:LEU:O	3:E:570:THR:OG1	2.28	0.45
3:E:1022:PRO:O	3:E:1023:ARG:HD3	2.16	0.45
3:F:146:THR:HG22	3:F:148:LEU:N	2.31	0.45
3:F:1005:VAL:HG12	3:F:1006:ARG:H	1.81	0.45
3:J:684:LEU:HD12	3:J:685:PRO:HD2	1.98	0.45
3:K:1168:ARG:O	3:K:1169:TRP:CD1	2.70	0.45
3:K:1169:TRP:CE3	3:K:1190:LEU:HB2	2.52	0.45
5:V:91:THR:OG1	5:V:92:TRP:N	2.49	0.45
5:V:175:MET:O	5:V:178:ILE:HG12	2.17	0.45
5:V:331:VAL:HB	5:V:332:PRO:HD3	1.97	0.45
6:Y:501:VAL:HG23	6:Y:507:ASN:C	2.42	0.45
6:Z:883:ALA:O	6:Z:886:ASN:ND2	2.47	0.45
6:c:362:GLU:OE1	6:c:377:ARG:NH1	2.50	0.45
6:c:1143:GLN:HB3	6:c:1151:ASN:HD21	1.81	0.45
6:i:703:ASP:O	6:i:705:THR:N	2.47	0.45
2:B:397:PRO:HD2	2:B:587:GLN:CD	2.42	0.45
3:C:315:SER:OG	3:C:316:THR:N	2.47	0.45
3:D:702:SER:HB3	3:D:737:ARG:NH2	2.32	0.45
3:G:173:ASP:OD1	3:G:173:ASP:N	2.50	0.45
6:Y:545:LEU:HD12	6:Y:546:PRO:HD2	1.98	0.45
5:b:270:ILE:HB	5:b:327:ASP:HB2	1.98	0.45
6:c:1224:VAL:HA	6:c:1227:TYR:CD2	2.51	0.45
3:C:315:SER:HB3	3:C:331:ARG:HD2	1.98	0.45
3:C:1168:ARG:O	3:C:1169:TRP:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:799:ASP:OD1	3:F:800:ILE:N	2.50	0.45
3:H:407:ARG:HB3	5:h:178:ILE:HB	1.98	0.45
3:I:254:ASP:OD1	3:I:254:ASP:N	2.49	0.45
3:J:452:ARG:NH1	3:J:667:ASN:O	2.50	0.45
5:V:158:HIS:HE1	5:V:264:SER:HB2	1.82	0.45
6:Z:466:ASP:OD1	6:Z:467:ARG:N	2.49	0.45
6:Z:998:LEU:N	6:Z:999:PRO:HD2	2.32	0.45
6:c:502:ASN:ND2	6:c:505:THR:H	2.15	0.45
5:g:151:SER:OG	5:g:152:ASP:O	2.35	0.45
6:i:501:VAL:HG23	6:i:507:ASN:C	2.41	0.45
5:n:273:HIS:CE1	5:n:394:PHE:HD1	2.35	0.45
3:H:139:ASP:OD2	3:H:140:HIS:NE2	2.50	0.45
3:J:1066:MET:HE2	4:l:106:MET:HE1	1.98	0.45
3:L:179:LEU:HB2	3:L:187:VAL:O	2.17	0.45
6:Z:764:THR:O	6:Z:767:SER:OG	2.25	0.45
6:c:1249:HIS:HB3	6:c:1297:VAL:HG13	1.99	0.45
6:i:439:SER:O	6:i:648:THR:OG1	2.20	0.45
1:A:113:TYR:CE2	1:A:219:TRP:HB3	2.52	0.44
1:A:595:CYS:HB2	1:A:697:HIS:HD1	1.81	0.44
3:C:338:GLU:OE1	3:C:338:GLU:N	2.39	0.44
3:E:364:ILE:HB	3:E:367:ARG:HG3	1.99	0.44
3:G:336:ARG:HB3	3:G:339:LEU:HD23	1.99	0.44
3:H:401:THR:HG21	3:H:960:THR:HB	1.98	0.44
3:J:787:ARG:NH2	3:J:923:LEU:HA	2.31	0.44
3:K:518:LEU:HD13	3:K:518:LEU:HA	1.80	0.44
6:Y:15:THR:HG22	6:Y:364:PRO:HB2	1.98	0.44
6:c:15:THR:HG22	6:c:364:PRO:HB2	1.98	0.44
6:i:321:GLU:HB2	6:i:789:ARG:HD3	1.99	0.44
6:i:545:LEU:HD12	6:i:546:PRO:HD2	1.99	0.44
6:i:1177:ASN:ND2	6:i:1279:SER:O	2.46	0.44
1:A:518:GLU:OE1	1:A:518:GLU:N	2.46	0.44
3:C:652:GLN:HB3	6:c:244:THR:HG22	1.99	0.44
3:D:645:HIS:ND1	3:D:649:ASN:OD1	2.50	0.44
3:I:629:GLN:HA	3:I:640:ARG:HH12	1.82	0.44
3:J:451:LEU:HB3	3:J:666:ALA:HB2	2.00	0.44
3:J:778:ASP:O	3:J:940:GLN:NE2	2.49	0.44
3:K:164:TRP:O	3:K:167:ILE:HG22	2.18	0.44
3:K:315:SER:OG	3:K:316:THR:N	2.50	0.44
5:V:136:TRP:CE2	5:V:197:PRO:HA	2.52	0.44
6:Z:502:ASN:ND2	6:Z:505:THR:H	2.15	0.44
5:h:244:ASP:OD1	5:h:244:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:352:GLU:O	5:h:356:ASN:ND2	2.44	0.44
1:A:338:LEU:O	1:A:342:THR:HG23	2.17	0.44
2:B:257:TRP:H	2:B:257:TRP:CD1	2.34	0.44
3:G:460:VAL:HG13	3:G:787:ARG:NE	2.32	0.44
3:H:388:MET:SD	3:H:1193:SER:HB3	2.57	0.44
3:H:502:GLU:HG3	3:H:504:THR:H	1.82	0.44
3:J:334:GLU:OE1	3:J:334:GLU:N	2.36	0.44
6:f:819:ILE:HD11	6:f:896:ILE:HG13	1.99	0.44
6:f:1038:ASN:HB2	6:f:1039:PRO:HD3	1.99	0.44
3:C:742:MET:HG2	3:C:827:THR:HG23	1.99	0.44
3:C:1138:THR:OG1	3:C:1139:SER:N	2.50	0.44
3:H:137:ARG:O	3:H:141:ARG:HD2	2.18	0.44
6:Y:1232:PRO:HG2	6:Y:1235:THR:OG1	2.18	0.44
6:c:501:VAL:HG23	6:c:507:ASN:C	2.42	0.44
6:c:860:CYS:SG	6:c:861:ALA:N	2.90	0.44
6:c:1037:VAL:HG22	6:c:1039:PRO:HD2	1.98	0.44
6:i:187:ARG:HB3	6:i:190:THR:HG23	1.99	0.44
6:i:1232:PRO:HG2	6:i:1235:THR:OG1	2.18	0.44
3:G:156:ALA:O	3:G:159:SER:OG	2.30	0.44
3:H:632:ASN:OD1	3:H:635:GLN:N	2.46	0.44
3:L:856:ARG:NH2	3:L:916:ASP:O	2.43	0.44
6:Y:1238:ARG:HH22	6:Y:1276:LEU:HB3	1.82	0.44
6:c:1204:LEU:HA	6:c:1227:TYR:CE1	2.52	0.44
6:c:1205:LEU:O	6:c:1227:TYR:OH	2.21	0.44
6:i:1186:ASN:HB3	6:i:1189:ASN:O	2.17	0.44
6:i:1249:HIS:HB3	6:i:1297:VAL:HG13	1.99	0.44
1:A:452:LEU:O	1:A:456:ILE:HG12	2.17	0.44
1:A:665:PHE:CZ	1:A:687:PRO:HD3	2.52	0.44
2:B:654:SER:HA	2:B:672:PRO:HG2	1.99	0.44
3:F:391:CYS:O	3:F:1192:ASN:ND2	2.36	0.44
3:F:697:MET:HB3	3:F:744:PRO:HB3	2.00	0.44
3:G:450:ASP:OD1	3:G:450:ASP:N	2.48	0.44
3:G:481:ARG:HD3	3:G:529:TRP:CD1	2.52	0.44
3:H:631:ILE:O	3:H:640:ARG:NH1	2.50	0.44
3:J:212:SER:OG	3:J:213:ALA:N	2.51	0.44
3:J:579:PRO:HG2	3:J:580:HIS:CD2	2.48	0.44
3:L:135:HIS:O	3:L:139:ASP:N	2.45	0.44
3:L:294:ARG:HB3	3:L:890:GLN:HB2	1.99	0.44
3:L:468:ALA:O	3:L:471:PRO:HD2	2.17	0.44
6:Y:457:LEU:O	6:Y:625:ARG:NH2	2.44	0.44
6:Y:703:ASP:O	6:Y:705:THR:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:211:LEU:HD23	5:a:211:LEU:HA	1.87	0.44
5:d:181:PRO:HA	5:d:247:VAL:HG12	2.00	0.44
1:A:104:LEU:HD12	1:A:114:GLY:C	2.43	0.44
1:A:450:ASP:O	1:A:454:GLN:HG3	2.18	0.44
2:B:438:ASP:OD1	2:B:439:SER:N	2.49	0.44
3:D:861:ARG:NE	3:D:862:GLU:OE2	2.51	0.44
3:D:1006:ARG:NH1	3:D:1077:GLU:OE2	2.46	0.44
3:E:456:VAL:HG21	3:E:950:VAL:HG21	1.99	0.44
3:E:514:ILE:HD11	3:E:564:TRP:CD2	2.53	0.44
3:G:1064:TRP:NE1	3:G:1068:LYS:HD2	2.33	0.44
3:L:330:ILE:HD13	3:L:347:ARG:NH2	2.32	0.44
6:Z:703:ASP:O	6:Z:705:THR:N	2.44	0.44
6:Z:1242:PRO:HD2	6:Z:1246:GLY:O	2.17	0.44
5:e:25:ASP:OD1	5:e:383:ARG:NH2	2.50	0.44
5:h:143:HIS:NE2	5:h:291:THR:OG1	2.46	0.44
1:A:967:GLU:O	1:A:971:SER:N	2.51	0.44
1:A:1036:LYS:HD2	1:A:1037:PRO:HD2	1.99	0.44
2:B:396:SER:HB3	2:B:397:PRO:HD3	1.98	0.44
3:C:139:ASP:OD1	3:C:139:ASP:N	2.51	0.44
3:D:150:THR:HG23	3:D:152:MET:SD	2.58	0.44
3:E:1121:ILE:O	3:E:1123:GLN:NE2	2.46	0.44
3:F:688:THR:OG1	3:F:689:VAL:N	2.51	0.44
3:F:906:ASN:HD21	3:F:910:LYS:HE2	1.83	0.44
3:G:1050:ASP:OD2	3:H:1213:ALA:N	2.51	0.44
6:Y:998:LEU:N	6:Y:999:PRO:HD2	2.32	0.44
6:Z:1232:PRO:HG2	6:Z:1235:THR:OG1	2.18	0.44
5:b:26:LEU:HD13	5:b:71:LEU:HD11	1.99	0.44
5:e:331:VAL:HB	5:e:332:PRO:HD3	1.99	0.44
6:i:231:ASP:OD2	6:i:285:LEU:N	2.50	0.44
6:i:764:THR:O	6:i:767:SER:OG	2.26	0.44
6:i:1146:PHE:CZ	6:i:1232:PRO:HD3	2.52	0.44
5:n:211:LEU:HD23	5:n:211:LEU:HA	1.87	0.44
2:B:181:ASP:N	2:B:181:ASP:OD1	2.51	0.44
3:C:971:GLU:HB3	3:C:974:LEU:HD23	2.00	0.44
3:G:1122:PRO:HA	3:G:1159:GLY:HA3	1.99	0.44
3:K:1181:THR:HG22	5:d:54:TRP:CZ2	2.53	0.44
3:L:398:ILE:O	3:L:401:THR:OG1	2.28	0.44
6:Z:1251:THR:HB	6:Z:1295:GLU:HB2	2.00	0.44
5:a:10:THR:HG1	5:a:118:VAL:H	1.62	0.44
6:f:1249:HIS:HB3	6:f:1297:VAL:HG13	2.00	0.44
6:i:998:LEU:N	6:i:999:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:1143:GLN:O	6:i:1151:ASN:ND2	2.51	0.44
6:i:1184:VAL:HB	6:i:1191:ASP:HB2	2.00	0.44
3:D:629:GLN:HA	3:D:640:ARG:HH12	1.83	0.43
3:F:684:LEU:HD12	3:F:685:PRO:HD2	2.00	0.43
3:F:993:TRP:CD1	3:F:995:PRO:HD3	2.53	0.43
3:H:102:ASP:OD1	3:H:105:SER:OG	2.36	0.43
5:V:302:GLU:HG2	5:V:316:THR:HB	1.99	0.43
5:W:143:HIS:O	5:W:147:MET:HG2	2.18	0.43
5:b:168:ALA:O	5:b:171:THR:OG1	2.28	0.43
6:f:1184:VAL:HB	6:f:1191:ASP:HB2	2.00	0.43
6:i:934:ASN:HB2	6:i:956:TYR:CE2	2.53	0.43
2:B:432:GLU:N	2:B:432:GLU:OE1	2.51	0.43
3:C:412:ASP:HB3	5:a:177:TYR:CZ	2.53	0.43
3:D:139:ASP:OD1	3:D:139:ASP:N	2.51	0.43
3:H:179:LEU:HD12	3:H:188:ALA:HB1	2.01	0.43
3:J:405:LEU:O	3:J:408:SER:OG	2.24	0.43
3:J:688:THR:HG23	3:J:691:PRO:HD2	1.99	0.43
6:Z:1043:PRO:HB2	6:Z:1046:GLN:NE2	2.33	0.43
5:a:181:PRO:HA	5:a:247:VAL:HG12	2.00	0.43
6:c:187:ARG:HB3	6:c:190:THR:HG23	1.99	0.43
6:c:997:TRP:CD1	6:c:997:TRP:H	2.35	0.43
6:f:1252:SER:N	6:f:1255:ASN:O	2.52	0.43
5:n:29:LEU:HD12	5:n:29:LEU:HA	1.78	0.43
2:B:9:THR:O	2:B:216:ASP:HB2	2.18	0.43
3:D:993:TRP:CD1	3:D:995:PRO:HD3	2.54	0.43
3:F:208:ASP:HB2	3:F:238:GLY:HA3	2.01	0.43
3:F:702:SER:HB3	3:F:737:ARG:NH2	2.33	0.43
3:F:751:CYS:N	3:F:752:PRO:HD2	2.33	0.43
3:G:850:MET:SD	3:G:850:MET:N	2.91	0.43
5:W:151:SER:OG	5:W:152:ASP:O	2.35	0.43
6:Y:950:ASP:OD1	6:Y:951:LEU:N	2.51	0.43
6:Z:15:THR:HG22	6:Z:364:PRO:HB2	2.00	0.43
6:Z:843:LEU:HD11	6:Z:854:MET:HE1	1.99	0.43
5:a:228:THR:OG1	5:a:232:PHE:O	2.24	0.43
6:c:1038:ASN:HB2	6:c:1039:PRO:HD3	2.01	0.43
1:A:572:LYS:HA	1:A:572:LYS:HE2	2.01	0.43
2:B:605:LEU:HD23	2:B:716:PHE:HA	2.00	0.43
3:E:457:MET:SD	3:E:923:LEU:HD11	2.58	0.43
3:I:856:ARG:O	3:I:860:THR:OG1	2.35	0.43
3:J:88:ALA:O	3:J:92:ASN:ND2	2.38	0.43
6:Y:1252:SER:N	6:Y:1255:ASN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:934:ASN:HB2	6:Z:956:TYR:CE2	2.54	0.43
6:c:1291:ALA:O	6:c:1294:TYR:OH	2.20	0.43
6:f:18:THR:HG23	6:f:281:ALA:HA	1.98	0.43
6:f:321:GLU:HB2	6:f:789:ARG:HD3	1.99	0.43
6:f:1053:THR:HA	6:f:1095:GLU:HG2	2.00	0.43
5:h:158:HIS:CD2	5:h:297:PRO:HG2	2.53	0.43
6:i:883:ALA:O	6:i:886:ASN:ND2	2.47	0.43
3:H:799:ASP:OD1	3:H:800:ILE:N	2.52	0.43
3:H:1050:ASP:OD1	3:H:1050:ASP:N	2.51	0.43
5:X:251:ASN:OD1	5:X:253:GLY:N	2.40	0.43
6:Z:1139:PRO:HB2	6:Z:1143:GLN:HB2	2.00	0.43
6:f:187:ARG:HB3	6:f:190:THR:HG23	2.00	0.43
6:f:243:GLN:CD	6:f:245:GLY:H	2.26	0.43
6:i:806:PRO:O	6:i:809:THR:OG1	2.33	0.43
1:A:1230:SER:N	1:A:1231:PRO:HD2	2.34	0.43
3:C:1008:GLY:O	3:C:1011:VAL:HG22	2.19	0.43
3:D:782:ASN:HB2	3:D:939:LEU:HD13	2.00	0.43
3:H:137:ARG:HD2	3:H:137:ARG:HA	1.77	0.43
3:J:654:SER:OG	3:J:655:GLU:N	2.51	0.43
6:c:1232:PRO:HG2	6:c:1235:THR:OG1	2.17	0.43
5:d:312:VAL:H	5:d:316:THR:HG1	1.66	0.43
2:B:84:ARG:NH2	2:B:164:LYS:O	2.51	0.43
3:E:655:GLU:HG3	6:Z:222:ALA:HB3	2.01	0.43
3:F:117:TYR:O	3:F:126:PHE:N	2.52	0.43
3:F:452:ARG:NH1	3:F:667:ASN:O	2.51	0.43
3:F:521:MET:HE1	3:F:524:ASP:HB3	2.01	0.43
3:H:784:LEU:HD22	3:H:799:ASP:HB3	2.01	0.43
3:I:1140:GLU:OE1	3:I:1140:GLU:N	2.51	0.43
6:Y:864:MET:HE3	6:Y:874:TYR:HB2	2.01	0.43
6:Y:1157:CYS:SG	6:Y:1158:ASP:N	2.92	0.43
6:i:1038:ASN:HB2	6:i:1039:PRO:HD3	2.00	0.43
5:n:302:GLU:HG2	5:n:316:THR:HB	2.01	0.43
2:B:558:GLY:C	2:B:560:ALA:H	2.27	0.43
3:C:722:ASN:OD1	3:C:723:ASP:N	2.52	0.43
3:D:751:CYS:N	3:D:752:PRO:HD2	2.34	0.43
3:D:1102:GLU:O	3:D:1105:SER:OG	2.26	0.43
3:E:334:GLU:OE2	4:M:81:ARG:NE	2.44	0.43
3:E:786:ALA:HB2	3:E:804:HIS:CG	2.54	0.43
3:F:545:LEU:HD13	3:F:569:LEU:HD11	2.00	0.43
3:G:1015:GLY:HA2	3:G:1034:ASP:HA	2.01	0.43
3:G:1103:TRP:CD1	3:G:1113:PRO:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:459:LEU:HA	3:H:462:ILE:HG12	2.00	0.43
6:Y:82:ARG:NH1	6:Y:83:ASP:OD1	2.52	0.43
6:Z:1271:VAL:HG12	6:Z:1290:PRO:HD2	2.01	0.43
10:a:4:2:A:O4'	9:b:3:35:U:OP1	2.37	0.43
5:d:312:VAL:N	5:d:316:THR:OG1	2.49	0.43
2:B:203:GLY:N	2:B:206:THR:OG1	2.52	0.43
3:D:450:ASP:OD1	3:D:861:ARG:HD3	2.18	0.43
3:G:493:LEU:O	3:G:497:ILE:HG12	2.18	0.43
3:G:629:GLN:HA	3:G:640:ARG:HH12	1.82	0.43
3:H:107:LYS:HE3	3:H:107:LYS:HB3	1.85	0.43
3:J:165:ASP:CG	3:J:167:ILE:HG12	2.43	0.43
3:L:197:ASP:OD1	3:L:253:GLY:N	2.47	0.43
5:a:106:ILE:HG22	5:a:107:GLN:HG2	2.00	0.43
5:a:175:MET:HA	5:a:178:ILE:HD11	2.01	0.43
6:c:523:SER:H	6:c:525:HIS:CE1	2.36	0.43
6:c:1043:PRO:HB2	6:c:1046:GLN:NE2	2.34	0.43
6:c:1090:ILE:HG13	6:c:1093:ASN:H	1.83	0.43
5:h:175:MET:O	5:h:178:ILE:HG12	2.19	0.43
3:D:271:VAL:HG23	3:D:288:PHE:HB3	2.01	0.43
3:D:500:ILE:HD12	3:D:735:ALA:HB2	2.00	0.43
3:G:652:GLN:HB3	6:Y:244:THR:HG22	1.99	0.43
3:G:938:TYR:CZ	3:G:946:VAL:HG21	2.53	0.43
3:I:508:ILE:HB	3:K:501:SER:OG	2.18	0.43
6:Y:187:ARG:HB3	6:Y:190:THR:HG23	2.00	0.43
6:Y:502:ASN:ND2	6:Y:505:THR:H	2.16	0.43
6:Z:1249:HIS:HB3	6:Z:1297:VAL:HG13	2.00	0.43
6:f:888:ILE:O	6:f:889:ARG:HD2	2.19	0.43
5:h:406:LEU:O	5:h:410:MET:N	2.51	0.43
6:i:194:TYR:N	6:i:250:TYR:OH	2.49	0.43
6:i:1139:PRO:HB2	6:i:1143:GLN:HB2	2.01	0.43
3:F:320:ASP:OD1	3:F:321:VAL:N	2.52	0.42
3:H:645:HIS:ND1	3:H:649:ASN:OD1	2.50	0.42
3:I:269:SER:OG	3:I:270:SER:N	2.51	0.42
3:K:1131:ARG:HD2	3:L:106:MET:HG3	2.00	0.42
6:Z:997:TRP:CD1	6:Z:997:TRP:H	2.35	0.42
5:b:25:ASP:OD1	5:b:383:ARG:NH2	2.51	0.42
5:d:273:HIS:CE1	5:d:394:PHE:HD1	2.37	0.42
5:h:302:GLU:HG2	5:h:316:THR:HB	2.01	0.42
3:F:509:SER:OG	3:F:510:PRO:HD3	2.19	0.42
3:F:876:ASP:HA	3:F:883:ARG:NH2	2.34	0.42
3:G:439:THR:OG1	3:G:1199:PHE:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:563:MET:HE3	3:I:563:MET:HB3	1.90	0.42
3:I:717:MET:HE3	3:I:721:VAL:HG21	2.01	0.42
3:L:173:ASP:OD2	3:L:176:SER:OG	2.37	0.42
3:L:407:ARG:HB3	5:b:178:ILE:HB	2.01	0.42
5:W:181:PRO:HA	5:W:247:VAL:HG12	2.01	0.42
5:W:302:GLU:HG3	5:W:317:GLY:O	2.19	0.42
6:Y:243:GLN:CD	6:Y:245:GLY:H	2.27	0.42
6:Y:997:TRP:CD1	6:Y:997:TRP:H	2.35	0.42
5:b:153:GLN:O	5:b:274:TRP:NE1	2.52	0.42
6:i:502:ASN:ND2	6:i:505:THR:H	2.16	0.42
1:A:168:ARG:NH1	1:A:843:GLU:OE2	2.47	0.42
2:B:158:CYS:HB3	2:B:181:ASP:C	2.44	0.42
3:D:187:VAL:HG13	4:M:20:ASN:HB2	2.01	0.42
3:F:599:ILE:HD13	3:F:639:LEU:HD23	2.01	0.42
3:J:1087:TYR:HB3	3:J:1121:ILE:HG12	2.01	0.42
3:K:364:ILE:HB	3:K:367:ARG:HG3	2.01	0.42
6:Z:1186:ASN:HB3	6:Z:1189:ASN:O	2.20	0.42
6:i:1001:ILE:O	6:i:1006:SER:OG	2.36	0.42
2:B:288:PRO:O	2:B:319:THR:HG22	2.18	0.42
2:B:393:VAL:CG1	2:B:587:GLN:HA	2.49	0.42
3:F:309:LEU:O	3:F:309:LEU:HD12	2.20	0.42
3:F:656:PHE:HB3	3:F:681:ASN:HD21	1.84	0.42
3:J:799:ASP:OD2	3:J:801:ARG:HD3	2.19	0.42
3:K:431:THR:OG1	3:K:432:ILE:N	2.51	0.42
3:K:722:ASN:OD1	3:K:723:ASP:N	2.52	0.42
5:b:158:HIS:CD2	5:b:159:LEU:N	2.87	0.42
5:b:251:ASN:OD1	5:b:253:GLY:N	2.42	0.42
6:f:751:SER:OG	6:f:754:PRO:O	2.30	0.42
5:h:136:TRP:N	5:h:137:PRO:HD2	2.35	0.42
6:i:676:ARG:NH1	6:i:1081:VAL:O	2.51	0.42
6:i:1200:ASP:HA	6:i:1203:VAL:HG22	2.01	0.42
1:A:414:ILE:HD11	1:A:637:ARG:HG3	2.01	0.42
1:A:970:SER:O	1:A:974:ILE:N	2.48	0.42
3:D:248:ASN:HB3	3:D:251:SER:HB2	2.00	0.42
3:I:221:GLY:O	3:I:224:TRP:NE1	2.52	0.42
6:Y:1186:ASN:HB3	6:Y:1189:ASN:O	2.19	0.42
6:Z:819:ILE:HD11	6:Z:896:ILE:HG13	2.01	0.42
6:Z:1157:CYS:SG	6:Z:1158:ASP:N	2.93	0.42
5:b:331:VAL:HB	5:b:332:PRO:HD3	2.00	0.42
6:c:610:THR:HG21	6:c:616:SER:HB3	2.01	0.42
5:g:181:PRO:HA	5:g:247:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:644:LEU:HD23	6:i:644:LEU:HA	1.81	0.42
6:i:888:ILE:O	6:i:889:ARG:HD2	2.19	0.42
1:A:363:HIS:HE1	1:A:1087:PRO:HG2	1.84	0.42
1:A:391:VAL:HG23	1:A:395:TYR:CE2	2.55	0.42
1:A:451:PRO:HB2	1:A:991:LEU:HD23	2.02	0.42
1:A:932:HIS:CG	1:A:933:PRO:HD2	2.55	0.42
2:B:433:GLN:N	2:B:433:GLN:OE1	2.52	0.42
3:E:177:LYS:HE2	3:E:177:LYS:HB2	1.89	0.42
3:E:252:LEU:HD12	3:E:252:LEU:HA	1.89	0.42
3:F:263:LEU:HD23	3:F:263:LEU:HA	1.87	0.42
3:G:1031:LEU:O	3:G:1039:ARG:N	2.51	0.42
3:H:480:LEU:HD23	3:H:480:LEU:HA	1.93	0.42
3:H:702:SER:HB3	3:H:737:ARG:NH2	2.35	0.42
3:J:468:ALA:O	3:J:471:PRO:HD2	2.20	0.42
3:J:1102:GLU:O	3:J:1105:SER:OG	2.31	0.42
3:K:189:ASN:ND2	3:K:916:ASP:OD1	2.53	0.42
6:Z:175:CYS:SG	6:Z:199:PRO:HA	2.60	0.42
6:Z:1252:SER:N	6:Z:1255:ASN:O	2.51	0.42
6:f:1186:ASN:HB3	6:f:1189:ASN:O	2.19	0.42
6:i:15:THR:HG22	6:i:364:PRO:HB2	2.01	0.42
6:i:950:ASP:OD1	6:i:951:LEU:N	2.51	0.42
6:i:1168:PHE:CZ	6:i:1171:GLY:HA2	2.55	0.42
1:A:147:ARG:HD2	1:A:147:ARG:HA	1.82	0.42
1:A:193:TRP:O	1:A:197:GLN:HG2	2.20	0.42
3:C:705:ILE:HG21	3:C:737:ARG:HB2	2.02	0.42
3:D:1028:GLU:OE1	3:D:1028:GLU:N	2.46	0.42
3:F:183:LEU:HD21	3:F:462:ILE:HG12	2.01	0.42
3:G:472:LEU:HD11	3:G:764:THR:HB	2.01	0.42
3:H:260:GLU:N	3:H:260:GLU:OE1	2.52	0.42
6:Z:104:PRO:O	6:Z:108:ASN:ND2	2.38	0.42
6:c:1139:PRO:HB2	6:c:1143:GLN:HB2	2.01	0.42
5:e:26:LEU:HD13	5:e:71:LEU:HD11	2.02	0.42
6:i:896:ILE:HG22	6:i:897:PHE:CD2	2.54	0.42
6:i:997:TRP:CD1	6:i:997:TRP:H	2.37	0.42
6:i:1252:SER:N	6:i:1255:ASN:O	2.53	0.42
1:A:204:VAL:HG11	1:A:206:TYR:CZ	2.55	0.42
3:G:208:ASP:OD1	3:G:238:GLY:HA3	2.20	0.42
3:J:355:LYS:HZ1	3:J:1156:THR:HG23	1.85	0.42
3:K:881:VAL:O	5:d:27:GLN:NE2	2.43	0.42
3:K:958:HIS:NE2	5:d:32:CYS:SG	2.92	0.42
6:Z:1038:ASN:HB2	6:Z:1039:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:255:ARG:HD2	5:d:255:ARG:N	2.35	0.42
5:n:196:LEU:HD12	5:n:196:LEU:HA	1.96	0.42
1:A:286:SER:O	1:A:290:MET:HG2	2.20	0.42
2:B:621:TRP:CD1	2:B:703:GLY:H	2.37	0.42
3:G:334:GLU:OE1	3:G:334:GLU:N	2.52	0.42
3:J:650:TRP:O	3:J:773:ARG:NH2	2.42	0.42
3:J:688:THR:OG1	3:J:689:VAL:N	2.53	0.42
5:V:244:ASP:OD1	5:V:244:ASP:N	2.51	0.42
6:Y:1227:TYR:C	6:Y:1228:ARG:HE	2.28	0.42
6:Z:28:ASP:OD1	6:Z:28:ASP:N	2.52	0.42
6:c:1260:LEU:HD12	6:c:1260:LEU:HA	1.90	0.42
5:h:273:HIS:CE1	5:h:394:PHE:HD1	2.37	0.42
1:A:899:MET:HG2	1:A:900:PRO:HD2	2.02	0.42
2:B:674:LEU:HD12	2:B:675:PRO:HD2	2.02	0.42
3:C:209:ASN:HD21	3:C:267:THR:HG23	1.85	0.42
3:C:450:ASP:OD1	3:C:861:ARG:HD3	2.20	0.42
3:C:1034:ASP:OD1	3:C:1034:ASP:N	2.51	0.42
3:F:740:LYS:HE3	3:F:740:LYS:HB3	1.87	0.42
3:K:197:ASP:HA	3:K:253:GLY:HA3	2.02	0.42
3:K:786:ALA:HB2	3:K:804:HIS:CD2	2.54	0.42
5:W:273:HIS:CE1	5:W:394:PHE:HD1	2.38	0.42
6:Z:950:ASP:OD1	6:Z:951:LEU:N	2.53	0.42
5:a:196:LEU:HD12	5:a:196:LEU:HA	1.96	0.42
5:a:255:ARG:HD2	5:a:255:ARG:N	2.35	0.42
5:g:231:GLY:O	5:g:250:TRP:HA	2.20	0.42
2:B:508:LEU:HD11	2:B:533:PRO:HD2	2.01	0.41
3:D:617:HIS:CG	3:D:618:PRO:HD2	2.55	0.41
3:D:1107:ILE:HG23	3:D:1112:ILE:HG22	2.01	0.41
3:H:650:TRP:O	3:H:773:ARG:NH2	2.37	0.41
3:I:995:PRO:O	3:I:1138:THR:HG22	2.20	0.41
3:J:415:GLN:HE21	5:e:245:GLN:NE2	2.18	0.41
3:J:1122:PRO:HA	3:J:1159:GLY:HA3	2.02	0.41
3:L:457:MET:HA	3:L:460:VAL:HG12	2.01	0.41
6:Z:1143:GLN:HB3	6:Z:1151:ASN:HD21	1.84	0.41
6:c:165:THR:OG1	6:c:167:ASP:OD1	2.34	0.41
6:f:703:ASP:O	6:f:705:THR:N	2.46	0.41
6:f:1207:LEU:HG	6:f:1223:ILE:HD11	2.02	0.41
5:h:167:PRO:O	5:h:170:THR:OG1	2.34	0.41
6:i:579:TYR:CE2	6:i:581:ASP:HB2	2.54	0.41
6:i:1157:CYS:SG	6:i:1158:ASP:N	2.93	0.41
6:i:1233:ARG:HG3	6:i:1292:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:n:251:ASN:OD1	5:n:253:GLY:N	2.52	0.41
1:A:1136:ASP:OD1	1:A:1137:ALA:N	2.53	0.41
2:B:495:LEU:O	2:B:499:VAL:HG12	2.20	0.41
3:C:1169:TRP:CE3	3:C:1190:LEU:HB2	2.55	0.41
3:D:484:THR:HG21	3:D:529:TRP:CH2	2.55	0.41
3:E:207:LEU:HD12	3:E:207:LEU:HA	1.79	0.41
3:E:460:VAL:O	3:E:787:ARG:NH2	2.53	0.41
3:F:189:ASN:O	3:F:856:ARG:NH1	2.53	0.41
3:F:235:LEU:HB2	3:F:356:ASN:HD22	1.84	0.41
3:I:709:ILE:O	3:I:712:VAL:HG12	2.21	0.41
3:L:708:PHE:HB3	3:L:733:MET:HE1	2.02	0.41
5:V:231:GLY:O	5:V:251:ASN:N	2.50	0.41
6:Z:1184:VAL:HB	6:Z:1191:ASP:HB2	2.03	0.41
6:Z:1209:ASP:HB2	6:Z:1219:ILE:HG12	2.02	0.41
6:c:321:GLU:HB2	6:c:789:ARG:HD3	2.01	0.41
6:c:1252:SER:N	6:c:1255:ASN:O	2.53	0.41
3:C:314:SER:OG	3:C:315:SER:N	2.54	0.41
3:E:786:ALA:HB2	3:E:804:HIS:CD2	2.55	0.41
3:E:951:PRO:HA	3:E:952:PRO:HD3	1.97	0.41
3:F:553:SER:OG	3:F:609:THR:O	2.35	0.41
3:J:902:MET:HE3	3:J:902:MET:HB2	1.98	0.41
3:K:513:GLU:HG3	3:K:517:LEU:HD11	2.01	0.41
3:L:944:ASN:OD1	3:L:945:VAL:N	2.53	0.41
6:Z:321:GLU:HB2	6:Z:789:ARG:HD3	2.01	0.41
6:c:888:ILE:O	6:c:889:ARG:HD2	2.20	0.41
6:c:1184:VAL:HB	6:c:1191:ASP:HB2	2.02	0.41
1:A:595:CYS:CB	1:A:697:HIS:HD1	2.34	0.41
3:C:1181:THR:HG22	5:a:54:TRP:CZ2	2.55	0.41
3:D:388:MET:HE3	3:D:1191:TYR:CE2	2.55	0.41
3:D:441:LEU:HG	3:D:443:PRO:HD3	2.02	0.41
3:D:594:ALA:HA	3:D:608:GLN:NE2	2.35	0.41
3:D:616:SER:OG	3:D:617:HIS:N	2.54	0.41
3:E:1205:ASP:OD1	3:E:1205:ASP:N	2.49	0.41
3:F:984:LEU:HD23	3:F:984:LEU:HA	1.90	0.41
3:H:405:LEU:O	3:H:408:SER:OG	2.26	0.41
3:I:786:ALA:HB2	3:I:804:HIS:CG	2.56	0.41
3:J:580:HIS:HE1	3:J:617:HIS:CA	2.33	0.41
3:J:993:TRP:CD1	3:J:995:PRO:HD3	2.55	0.41
3:K:1022:PRO:O	3:K:1023:ARG:HD3	2.20	0.41
3:L:1102:GLU:O	3:L:1105:SER:OG	2.31	0.41
5:X:136:TRP:N	5:X:137:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:28:ASP:OD1	6:Y:29:LEU:N	2.52	0.41
6:c:28:ASP:OD1	6:c:29:LEU:N	2.54	0.41
5:d:29:LEU:HD12	5:d:29:LEU:HA	1.84	0.41
6:f:971:VAL:HB	6:f:972:PRO:HD3	2.02	0.41
2:B:89:LEU:HB3	2:B:96:ASN:HB2	2.02	0.41
3:C:208:ASP:OD1	3:C:238:GLY:HA3	2.21	0.41
3:C:862:GLU:OE1	3:C:955:SER:OG	2.31	0.41
3:F:235:LEU:HB2	3:F:356:ASN:ND2	2.35	0.41
3:F:1100:LEU:HD13	3:F:1100:LEU:HA	1.96	0.41
3:G:769:VAL:HG22	3:G:770:PRO:HD2	2.03	0.41
3:H:1106:LYS:O	3:H:1113:PRO:HD3	2.21	0.41
3:J:355:LYS:NZ	3:J:1156:THR:HG23	2.35	0.41
5:V:13:PHE:N	5:V:116:GLU:OE1	2.50	0.41
5:W:29:LEU:HD12	5:W:29:LEU:HA	1.84	0.41
6:Y:734:SER:O	6:Y:737:SER:OG	2.35	0.41
5:a:160:GLU:OE2	5:a:209:ARG:NE	2.42	0.41
5:a:312:VAL:N	5:a:316:THR:OG1	2.53	0.41
1:A:932:HIS:CE1	1:A:934:VAL:HG12	2.55	0.41
2:B:675:PRO:O	2:B:678:SER:OG	2.25	0.41
3:E:581:SER:OG	3:E:582:PRO:HD3	2.21	0.41
3:H:740:LYS:HE3	3:H:740:LYS:HB3	1.87	0.41
3:I:364:ILE:HB	3:I:367:ARG:HG3	2.03	0.41
3:J:617:HIS:HD2	3:K:434:ILE:CD1	2.34	0.41
3:J:1150:ASN:ND2	3:J:1156:THR:HG22	2.35	0.41
3:L:371:LEU:HD11	3:L:388:MET:HE2	2.02	0.41
6:Y:1260:LEU:HD12	6:Y:1260:LEU:HA	1.93	0.41
6:Z:71:HIS:CE1	6:Z:73:ALA:HB3	2.55	0.41
6:Z:689:ASP:O	6:Z:693:THR:HG23	2.20	0.41
6:Z:1017:ILE:O	6:Z:1021:ARG:HG2	2.21	0.41
6:Z:1146:PHE:CZ	6:Z:1232:PRO:HD3	2.55	0.41
5:a:148:TRP:CD1	5:a:155:PRO:HB3	2.56	0.41
6:c:1186:ASN:HB3	6:c:1189:ASN:O	2.21	0.41
5:e:136:TRP:N	5:e:137:PRO:HD2	2.36	0.41
1:A:1133:GLU:HG3	1:A:1185:ARG:NH1	2.36	0.41
2:B:42:PRO:HB2	2:B:44:TRP:CD1	2.56	0.41
3:C:1059:PHE:HE2	3:C:1104:LEU:HD21	1.84	0.41
3:F:102:ASP:O	3:F:103:PRO:C	2.62	0.41
3:G:1205:ASP:OD1	3:G:1205:ASP:N	2.51	0.41
3:H:1169:TRP:O	3:H:1173:VAL:HG22	2.21	0.41
3:I:1107:ILE:HG23	3:I:1112:ILE:HG22	2.02	0.41
3:K:784:LEU:HB3	3:K:804:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:233:PRO:HA	3:L:234:PRO:HD3	1.93	0.41
5:V:158:HIS:CE1	5:V:159:LEU:O	2.74	0.41
6:Z:474:ASP:OD1	6:Z:477:ARG:NH1	2.54	0.41
6:f:28:ASP:OD1	6:f:29:LEU:N	2.52	0.41
5:g:143:HIS:O	5:g:147:MET:HG2	2.21	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.95	0.41
2:B:135:VAL:O	2:B:139:VAL:HG23	2.21	0.41
3:C:319:SER:HB3	3:C:329:MET:HG2	2.03	0.41
3:D:1049:SER:HB3	3:D:1078:LEU:HD23	2.03	0.41
3:E:938:TYR:CE2	3:E:946:VAL:HG21	2.56	0.41
3:E:1034:ASP:OD1	3:E:1035:GLY:N	2.53	0.41
5:W:302:GLU:HG2	5:W:316:THR:HB	2.02	0.41
6:Z:1090:ILE:HG13	6:Z:1093:ASN:H	1.85	0.41
5:a:302:GLU:HG2	5:a:316:THR:HB	2.03	0.41
5:b:136:TRP:N	5:b:137:PRO:HD2	2.35	0.41
5:e:302:GLU:HG3	5:e:317:GLY:O	2.21	0.41
6:f:71:HIS:NE2	6:f:73:ALA:HB3	2.35	0.41
6:f:833:ASP:OD2	6:f:842:ILE:HG13	2.20	0.41
6:f:1205:LEU:HD21	6:f:1223:ILE:HB	2.02	0.41
2:B:83:LYS:NZ	2:B:109:VAL:O	2.48	0.41
2:B:469:ALA:HB2	2:B:484:ALA:HB1	2.03	0.41
2:B:697:GLN:OE1	2:B:697:GLN:N	2.41	0.41
3:C:263:LEU:HD23	3:C:263:LEU:HA	1.93	0.41
3:D:162:THR:OG1	3:D:165:ASP:OD1	2.38	0.41
3:D:247:THR:OG1	3:D:260:GLU:OE1	2.37	0.41
3:D:925:LEU:HD23	3:D:925:LEU:HA	1.93	0.41
3:F:1121:ILE:O	3:F:1123:GLN:NE2	2.47	0.41
3:G:460:VAL:HG13	3:G:787:ARG:HE	1.85	0.41
3:H:320:ASP:OD1	3:H:321:VAL:N	2.53	0.41
3:K:277:VAL:HG22	3:K:278:LEU:HG	2.01	0.41
5:V:148:TRP:CD1	5:V:155:PRO:HB3	2.56	0.41
5:V:167:PRO:O	5:V:170:THR:OG1	2.35	0.41
5:V:270:ILE:HD12	5:V:270:ILE:HA	1.83	0.41
5:W:10:THR:OG1	5:W:118:VAL:N	2.36	0.41
6:Y:1038:ASN:HB2	6:Y:1039:PRO:HD3	2.01	0.41
6:Y:1134:VAL:HG23	6:Y:1157:CYS:HB2	2.03	0.41
6:Y:1204:LEU:HD11	6:Z:1266:VAL:HG23	2.02	0.41
6:Z:110:GLN:OE1	6:Z:110:GLN:N	2.44	0.41
5:b:244:ASP:OD1	5:b:244:ASP:N	2.54	0.41
5:b:352:GLU:O	5:b:356:ASN:ND2	2.50	0.41
6:c:1205:LEU:H	6:c:1227:TYR:HE1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:211:LEU:HA	5:d:211:LEU:HD23	1.84	0.41
6:f:439:SER:HB2	6:f:1013:ILE:HD12	2.01	0.41
5:g:29:LEU:HA	5:g:29:LEU:HD12	1.77	0.41
5:g:211:LEU:HA	5:g:211:LEU:HD23	1.86	0.41
5:g:255:ARG:N	5:g:255:ARG:HD2	2.36	0.41
5:n:231:GLY:O	5:n:250:TRP:HA	2.20	0.41
1:A:930:HIS:CG	3:C:141:ARG:HE	2.38	0.41
1:A:1050:ASN:O	1:A:1054:ARG:HD3	2.21	0.41
2:B:524:ASP:N	2:B:524:ASP:OD1	2.53	0.41
3:F:495:ASN:O	3:F:499:THR:HG23	2.21	0.41
3:H:294:ARG:HB3	3:H:890:GLN:HB2	2.02	0.41
3:I:1139:SER:OG	3:I:1140:GLU:OE1	2.28	0.41
3:K:769:VAL:HG22	3:K:770:PRO:HD2	2.03	0.41
3:L:742:MET:HG3	3:L:827:THR:HG23	2.01	0.41
5:V:367:GLU:O	5:V:371:THR:HG22	2.21	0.41
6:Y:888:ILE:O	6:Y:889:ARG:HD2	2.21	0.41
5:a:143:HIS:O	5:a:147:MET:HG2	2.21	0.41
6:c:950:ASP:OD1	6:c:951:LEU:N	2.54	0.41
6:c:1157:CYS:SG	6:c:1158:ASP:N	2.94	0.41
5:d:175:MET:HA	5:d:178:ILE:HD11	2.03	0.41
1:A:301:PRO:HB3	1:A:316:TRP:CZ3	2.55	0.40
1:A:332:SER:OG	1:A:333:MET:N	2.54	0.40
1:A:1108:ASP:OD1	1:A:1109:ILE:N	2.53	0.40
3:C:1171:GLY:HA2	3:C:1177:TYR:CG	2.57	0.40
3:D:197:ASP:OD1	3:D:198:THR:N	2.54	0.40
3:E:169:ILE:HD12	3:E:169:ILE:H	1.86	0.40
3:E:486:LEU:HA	3:E:827:THR:HG22	2.02	0.40
3:G:215:LEU:HD13	3:G:219:LEU:HB2	2.02	0.40
3:G:409:MET:HE1	3:G:858:VAL:HG11	2.02	0.40
3:G:717:MET:HE3	3:G:721:VAL:HG21	2.03	0.40
3:G:1174:ASP:OD1	3:G:1176:ASN:N	2.43	0.40
3:H:479:LEU:HD23	3:H:479:LEU:HA	1.92	0.40
3:H:586:PHE:HA	3:H:642:PHE:HE2	1.83	0.40
3:H:1093:SER:OG	3:H:1130:ALA:HB1	2.21	0.40
3:I:655:GLU:CD	3:I:674:ARG:HH21	2.26	0.40
3:I:769:VAL:HG22	3:I:770:PRO:HD2	2.03	0.40
3:J:154:ASN:HB3	3:J:174:VAL:HG12	2.03	0.40
3:J:622:PRO:HA	3:J:623:PRO:HD3	2.00	0.40
3:K:784:LEU:HB3	3:K:804:HIS:CB	2.50	0.40
3:L:201:CYS:SG	3:L:399:ARG:HD2	2.61	0.40
3:L:386:GLU:HB2	3:L:1195:TYR:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:444:TRP:HB3	3:L:851:PHE:CD1	2.56	0.40
5:X:367:GLU:O	5:X:371:THR:HG22	2.21	0.40
6:Y:934:ASN:HB2	6:Y:956:TYR:CE2	2.56	0.40
6:Y:1147:THR:OG1	6:Y:1148:ASP:N	2.54	0.40
6:Z:243:GLN:CD	6:Z:245:GLY:H	2.29	0.40
6:Z:1200:ASP:HA	6:Z:1203:VAL:HG22	2.02	0.40
5:a:221:GLY:O	5:a:224:ASN:ND2	2.51	0.40
6:f:519:LEU:HD12	6:f:554:PHE:HB2	2.03	0.40
1:A:97:ASN:OD1	1:A:270:SER:N	2.54	0.40
1:A:820:TRP:CE2	1:A:858:GLY:HA3	2.56	0.40
2:B:448:PRO:HG2	2:B:453:GLN:NE2	2.36	0.40
3:C:489:ASP:OD1	3:C:491:THR:OG1	2.28	0.40
3:G:875:GLN:O	3:G:883:ARG:NH2	2.42	0.40
3:J:751:CYS:N	3:J:752:PRO:HD2	2.36	0.40
3:K:409:MET:HE1	3:K:858:VAL:HG11	2.04	0.40
3:L:117:TYR:O	3:L:126:PHE:N	2.46	0.40
3:L:751:CYS:N	3:L:752:PRO:HD2	2.37	0.40
6:Z:1053:THR:HA	6:Z:1095:GLU:HG2	2.01	0.40
6:Z:1233:ARG:O	6:Z:1291:ALA:HB1	2.21	0.40
6:c:206:TYR:CD2	6:c:238:HIS:HB3	2.56	0.40
6:c:644:LEU:HD23	6:c:644:LEU:HA	1.83	0.40
6:c:1053:THR:HA	6:c:1095:GLU:HG2	2.02	0.40
5:d:143:HIS:O	5:d:147:MET:HG2	2.21	0.40
6:i:88:ILE:HD13	6:i:88:ILE:HA	1.98	0.40
3:E:1024:PRO:HB3	5:V:46:ILE:HB	2.03	0.40
3:E:1181:THR:HG22	5:W:54:TRP:CZ2	2.57	0.40
3:H:542:THR:HG23	3:H:808:ALA:HB3	2.02	0.40
3:H:746:TYR:CD1	3:H:750:MET:HE3	2.51	0.40
3:H:773:ARG:HG2	3:H:774:LEU:HG	2.02	0.40
3:I:431:THR:OG1	3:I:432:ILE:N	2.54	0.40
3:I:788:VAL:HG13	3:I:931:ILE:HB	2.03	0.40
3:J:705:ILE:HG21	3:J:737:ARG:HB2	2.03	0.40
3:L:202:THR:HA	3:L:392:ASP:OD1	2.20	0.40
5:V:136:TRP:N	5:V:137:PRO:HD2	2.36	0.40
5:X:91:THR:OG1	5:X:92:TRP:N	2.54	0.40
6:Z:896:ILE:HG22	6:Z:897:PHE:CD2	2.56	0.40
6:Z:1168:PHE:CZ	6:Z:1171:GLY:HA2	2.56	0.40
6:f:416:ASP:HA	6:f:419:GLU:HG2	2.03	0.40
5:g:273:HIS:CE1	5:g:394:PHE:HD1	2.39	0.40
5:h:251:ASN:OD1	5:h:253:GLY:N	2.50	0.40
6:i:775:ARG:HD2	6:i:867:PHE:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ASP:OD1	2:B:305:ARG:N	2.54	0.40
2:B:522:HIS:N	2:B:526:GLU:OE1	2.52	0.40
3:C:220:ILE:HD12	3:C:220:ILE:H	1.86	0.40
3:C:785:VAL:O	3:C:805:ALA:N	2.55	0.40
3:D:1168:ARG:O	3:D:1169:TRP:CD1	2.74	0.40
3:E:548:ASP:OD1	3:E:549:ALA:N	2.54	0.40
3:E:717:MET:HE3	3:E:721:VAL:HG21	2.02	0.40
3:F:1106:LYS:O	3:F:1113:PRO:HD3	2.22	0.40
3:G:916:ASP:OD1	3:G:916:ASP:N	2.49	0.40
3:H:354:THR:O	3:H:358:GLN:HG3	2.21	0.40
3:H:470:LEU:O	3:H:473:VAL:HG22	2.21	0.40
3:H:684:LEU:HD12	3:H:685:PRO:HD2	2.03	0.40
3:H:993:TRP:CD1	3:H:995:PRO:HD3	2.57	0.40
3:I:1015:GLY:HA2	3:I:1034:ASP:HA	2.03	0.40
3:K:1150:ASN:O	3:K:1150:ASN:ND2	2.55	0.40
3:L:383:ALA:HB1	3:L:439:THR:HG23	2.03	0.40
5:X:290:VAL:O	5:X:294:THR:HG22	2.22	0.40
6:Z:523:SER:H	6:Z:525:HIS:CE1	2.39	0.40
6:Z:651:ASN:OD1	6:Z:685:ASN:ND2	2.54	0.40
5:a:29:LEU:HA	5:a:29:LEU:HD12	1.78	0.40
6:c:689:ASP:O	6:c:693:THR:HG23	2.22	0.40
6:c:1242:PRO:HD2	6:c:1246:GLY:O	2.22	0.40
5:e:167:PRO:O	5:e:170:THR:OG1	2.32	0.40
6:f:71:HIS:HE1	6:f:74:PHE:HB2	1.86	0.40
6:f:502:ASN:ND2	6:f:505:THR:H	2.18	0.40
6:f:950:ASP:OD1	6:f:951:LEU:N	2.55	0.40
6:i:102:ARG:NH1	6:i:136:ASP:OD1	2.47	0.40
2:B:80:PRO:O	2:B:119:TYR:OH	2.39	0.40
3:D:723:ASP:OD1	3:D:727:ARG:NE	2.50	0.40
3:F:688:THR:HG23	3:F:691:PRO:HD2	2.03	0.40
3:H:391:CYS:O	3:H:1192:ASN:ND2	2.43	0.40
3:I:287:GLN:HE22	3:I:1108:ASN:CG	2.30	0.40
3:I:725:THR:O	3:I:729:MET:HG3	2.21	0.40
3:I:951:PRO:HA	3:I:952:PRO:HD3	1.98	0.40
3:L:558:THR:HA	3:L:717:MET:HE1	2.04	0.40
5:W:106:ILE:HG22	5:W:107:GLN:HG2	2.03	0.40
5:W:153:GLN:N	5:W:387:GLN:OE1	2.47	0.40
5:X:231:GLY:O	5:X:251:ASN:N	2.53	0.40
6:c:302:THR:HG22	6:c:305:GLN:CD	2.46	0.40
6:c:1168:PHE:CZ	6:c:1171:GLY:HA2	2.56	0.40
6:f:102:ARG:NH1	6:f:136:ASP:OD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:689:ASP:O	6:f:693:THR:HG23	2.22	0.40
6:f:709:GLY:HA3	6:f:763:ARG:CZ	2.51	0.40
4:m:92:ASN:HA	4:m:95:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1271/1273 (100%)	1212 (95%)	59 (5%)	0	100	100
2	B	716/718 (100%)	688 (96%)	28 (4%)	0	100	100
3	C	1073/1138 (94%)	1026 (96%)	47 (4%)	0	100	100
3	D	1136/1138 (100%)	1097 (97%)	39 (3%)	0	100	100
3	E	1104/1138 (97%)	1064 (96%)	40 (4%)	0	100	100
3	F	1136/1138 (100%)	1094 (96%)	42 (4%)	0	100	100
3	G	1096/1138 (96%)	1056 (96%)	40 (4%)	0	100	100
3	H	1128/1138 (99%)	1070 (95%)	58 (5%)	0	100	100
3	I	1061/1138 (93%)	1022 (96%)	39 (4%)	0	100	100
3	J	1128/1138 (99%)	1075 (95%)	53 (5%)	0	100	100
3	K	1096/1138 (96%)	1047 (96%)	49 (4%)	0	100	100
3	L	1136/1138 (100%)	1083 (95%)	53 (5%)	0	100	100
4	M	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
4	N	28/94 (30%)	28 (100%)	0	0	100	100
4	k	28/94 (30%)	26 (93%)	2 (7%)	0	100	100
4	l	28/94 (30%)	27 (96%)	1 (4%)	0	100	100
4	m	28/94 (30%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	V	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
5	W	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
5	X	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
5	a	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
5	b	409/411 (100%)	402 (98%)	7 (2%)	0	100	100
5	d	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
5	e	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
5	g	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
5	h	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
5	n	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
6	Y	1295/1297 (100%)	1254 (97%)	41 (3%)	0	100	100
6	Z	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
6	c	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
6	f	1295/1297 (100%)	1253 (97%)	42 (3%)	0	100	100
6	i	1295/1297 (100%)	1255 (97%)	39 (3%)	1 (0%)	48	75
All	All	23850/24436 (98%)	23009 (96%)	840 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	i	1291	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1092/1092 (100%)	1085 (99%)	7 (1%)	78	81
2	B	619/619 (100%)	618 (100%)	1 (0%)	87	88
3	C	917/972 (94%)	915 (100%)	2 (0%)	87	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	972/972 (100%)	969 (100%)	3 (0%)	86	86
3	E	946/972 (97%)	942 (100%)	4 (0%)	84	84
3	F	972/972 (100%)	965 (99%)	7 (1%)	76	80
3	G	938/972 (96%)	933 (100%)	5 (0%)	81	83
3	H	964/972 (99%)	961 (100%)	3 (0%)	86	86
3	I	910/972 (94%)	907 (100%)	3 (0%)	86	86
3	J	964/972 (99%)	958 (99%)	6 (1%)	78	81
3	K	938/972 (96%)	934 (100%)	4 (0%)	84	84
3	L	972/972 (100%)	968 (100%)	4 (0%)	84	84
4	M	73/73 (100%)	71 (97%)	2 (3%)	39	63
4	N	24/73 (33%)	24 (100%)	0	100	100
4	k	24/73 (33%)	23 (96%)	1 (4%)	26	55
4	l	24/73 (33%)	24 (100%)	0	100	100
4	m	24/73 (33%)	24 (100%)	0	100	100
5	V	325/325 (100%)	325 (100%)	0	100	100
5	W	325/325 (100%)	323 (99%)	2 (1%)	78	81
5	X	325/325 (100%)	324 (100%)	1 (0%)	86	86
5	a	325/325 (100%)	321 (99%)	4 (1%)	63	75
5	b	325/325 (100%)	324 (100%)	1 (0%)	86	86
5	d	325/325 (100%)	324 (100%)	1 (0%)	86	86
5	e	325/325 (100%)	325 (100%)	0	100	100
5	g	325/325 (100%)	323 (99%)	2 (1%)	78	81
5	h	325/325 (100%)	324 (100%)	1 (0%)	86	86
5	n	325/325 (100%)	325 (100%)	0	100	100
6	Y	1089/1089 (100%)	1078 (99%)	11 (1%)	68	76
6	Z	1089/1089 (100%)	1080 (99%)	9 (1%)	73	79
6	c	1089/1089 (100%)	1084 (100%)	5 (0%)	81	83
6	f	1089/1089 (100%)	1078 (99%)	11 (1%)	68	76
6	i	1089/1089 (100%)	1081 (99%)	8 (1%)	76	80
All	All	20068/20491 (98%)	19960 (100%)	108 (0%)	78	83

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	TRP
1	A	89	ASP
1	A	486	TYR
1	A	561	LEU
1	A	618	VAL
1	A	738	GLN
1	A	810	GLU
2	B	440	ASP
3	C	187	VAL
3	C	429	ASN
3	D	121	VAL
3	D	439	THR
3	D	903	HIS
3	E	483	VAL
3	E	829	THR
3	E	1050	ASP
3	E	1203	THR
3	F	104	GLN
3	F	105	SER
3	F	106	MET
3	F	232	THR
3	F	523	ASN
3	F	1037	VAL
3	F	1085	LEU
3	G	450	ASP
3	G	540	LEU
3	G	552	ASP
3	G	788	VAL
3	G	1203	THR
3	H	150	THR
3	H	193	LEU
3	H	1091	GLN
3	I	316	THR
3	I	1047	TYR
3	I	1203	THR
3	J	232	THR
3	J	322	THR
3	J	450	ASP
3	J	483	VAL
3	J	487	VAL
3	J	541	VAL
3	K	168	ARG
3	K	483	VAL

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Mol	Chain	Res	Type
3	K	518	LEU
3	K	519	GLN
3	L	77	ASP
3	L	123	ASN
3	L	193	LEU
3	L	1091	GLN
4	M	85	ASP
4	M	94	THR
5	W	11	TYR
5	W	38	THR
5	X	44	LEU
6	Y	71	HIS
6	Y	79	LEU
6	Y	559	VAL
6	Y	658	VAL
6	Y	955	VAL
6	Y	963	ARG
6	Y	1209	ASP
6	Y	1266	VAL
6	Y	1283	GLN
6	Y	1286	THR
6	Y	1297	VAL
6	Z	79	LEU
6	Z	164	VAL
6	Z	410	THR
6	Z	439	SER
6	Z	559	VAL
6	Z	1271	VAL
6	Z	1283	GLN
6	Z	1286	THR
6	Z	1297	VAL
5	a	11	TYR
5	a	29	LEU
5	a	38	THR
5	a	252	ASP
5	b	195	GLN
6	c	79	LEU
6	c	164	VAL
6	c	658	VAL
6	c	1283	GLN
6	c	1297	VAL
5	d	11	TYR

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Mol	Chain	Res	Type
6	f	79	LEU
6	f	164	VAL
6	f	566	LEU
6	f	610	THR
6	f	658	VAL
6	f	955	VAL
6	f	1266	VAL
6	f	1271	VAL
6	f	1283	GLN
6	f	1286	THR
6	f	1297	VAL
5	g	29	LEU
5	g	38	THR
5	h	195	GLN
6	i	79	LEU
6	i	164	VAL
6	i	559	VAL
6	i	1258	MET
6	i	1261	THR
6	i	1271	VAL
6	i	1283	GLN
6	i	1297	VAL
4	k	83	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	A	358	ASN
1	A	425	GLN
1	A	430	HIS
1	A	556	ASN
1	A	560	ASN
1	A	738	GLN
1	A	771	GLN
1	A	895	HIS
1	A	931	ASN
1	A	1206	HIS
2	B	21	ASN
2	B	30	GLN
2	B	513	GLN
2	B	514	GLN

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Mol	Chain	Res	Type
2	B	562	GLN
2	B	705	ASN
3	C	595	GLN
3	C	875	GLN
3	C	973	ASN
3	C	981	ASN
3	D	296	ASN
3	D	358	GLN
3	D	580	HIS
3	D	614	GLN
3	D	663	GLN
3	D	768	GLN
3	D	962	GLN
3	D	963	GLN
3	D	1036	ASN
3	D	1192	ASN
3	E	178	HIS
3	E	209	ASN
3	E	285	ASN
3	E	353	GLN
3	E	506	GLN
3	E	645	HIS
3	E	716	ASN
3	E	962	GLN
3	E	981	ASN
3	F	92	ASN
3	F	104	GLN
3	F	353	GLN
3	F	455	GLN
3	F	458	HIS
3	F	591	ASN
3	F	595	GLN
3	F	667	ASN
3	F	699	ASN
3	F	836	HIS
3	F	903	HIS
3	F	906	ASN
3	F	962	GLN
3	F	963	GLN
3	F	973	ASN
3	F	1010	ASN
3	F	1091	GLN

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Mol	Chain	Res	Type
3	F	1134	HIS
3	G	214	HIS
3	G	308	ASN
3	G	426	ASN
3	G	890	GLN
3	G	903	HIS
3	G	1143	ASN
3	H	135	HIS
3	H	178	HIS
3	H	287	GLN
3	H	353	GLN
3	H	607	HIS
3	H	663	GLN
3	H	768	GLN
3	H	958	HIS
3	H	962	GLN
3	H	1091	GLN
3	I	209	ASN
3	I	287	GLN
3	I	308	ASN
3	I	429	ASN
3	I	645	HIS
3	I	649	ASN
3	I	663	GLN
3	I	748	GLN
3	I	835	HIS
3	I	873	GLN
3	I	906	ASN
3	I	940	GLN
3	I	973	ASN
3	I	1186	ASN
3	J	353	GLN
3	J	411	GLN
3	J	415	GLN
3	J	519	GLN
3	J	580	HIS
3	J	663	GLN
3	J	673	ASN
3	J	713	ASN
3	J	890	GLN
3	J	962	GLN
3	J	1134	HIS

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Mol	Chain	Res	Type
3	K	123	ASN
3	K	230	GLN
3	K	519	GLN
3	K	629	GLN
3	K	635	GLN
3	K	748	GLN
3	K	903	HIS
3	K	906	ASN
3	K	1053	GLN
3	L	123	ASN
3	L	135	HIS
3	L	140	HIS
3	L	353	GLN
3	L	454	GLN
3	L	519	GLN
3	L	555	GLN
3	L	652	GLN
3	L	830	ASN
3	L	1030	GLN
3	L	1036	ASN
3	L	1091	GLN
4	M	92	ASN
5	V	3	GLN
5	V	387	GLN
5	W	87	HIS
5	W	277	GLN
5	X	273	HIS
5	X	387	GLN
6	Y	8	GLN
6	Y	157	GLN
6	Y	825	ASN
6	Y	989	HIS
6	Z	8	GLN
6	Z	685	ASN
6	Z	1046	GLN
6	Z	1065	HIS
6	Z	1151	ASN
6	Z	1201	ASN
5	a	43	HIS
5	a	338	HIS
5	b	158	HIS
5	b	187	GLN

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Mol	Chain	Res	Type
5	b	276	HIS
6	c	8	GLN
6	c	633	ASN
6	c	1046	GLN
6	c	1065	HIS
5	d	5	GLN
5	d	43	HIS
5	d	123	ASN
5	d	277	GLN
5	d	369	HIS
5	e	24	ASN
5	e	153	GLN
5	e	198	GLN
5	e	387	GLN
6	f	8	GLN
5	g	5	GLN
5	g	43	HIS
5	g	87	HIS
5	g	123	ASN
5	g	158	HIS
5	h	198	GLN
5	h	310	GLN
6	i	8	GLN
6	i	309	ASN
6	i	685	ASN
6	i	825	ASN
6	i	989	HIS
6	i	1151	ASN
6	i	1201	ASN
5	n	158	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	a4	17/18 (94%)	0	0
10	b4	17/18 (94%)	0	0
11	a5	37/38 (97%)	0	0
11	b5	37/38 (97%)	0	0
12	a6	29/30 (96%)	0	0
12	b6	29/30 (96%)	0	0
7	a1	51/52 (98%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	b1	51/52 (98%)	0	0
8	a2	59/60 (98%)	0	0
8	b2	59/60 (98%)	0	0
9	a3	39/40 (97%)	0	0
9	b3	39/40 (97%)	0	0
All	All	464/476 (97%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

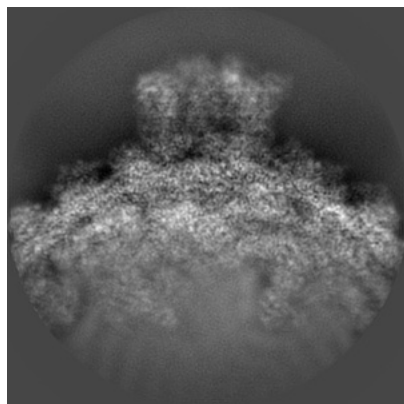
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29243. These allow visual inspection of the internal detail of the map and identification of artifacts.

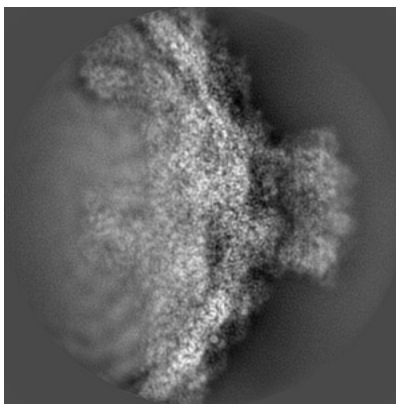
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

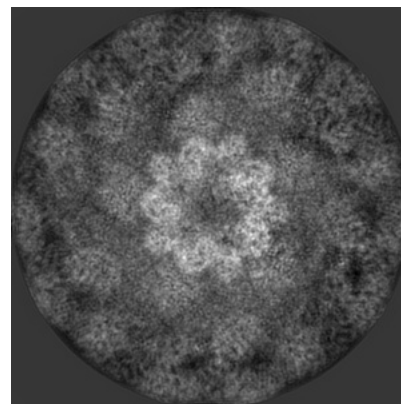
6.1.1 Primary map



X

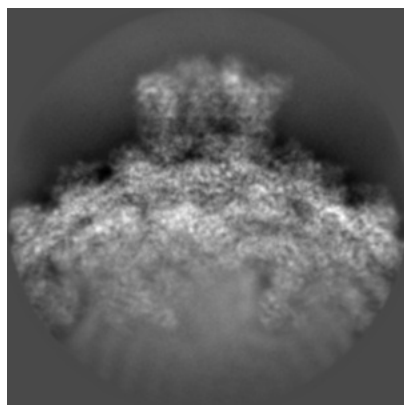


Y

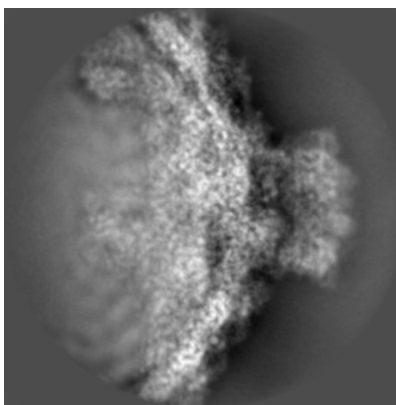


Z

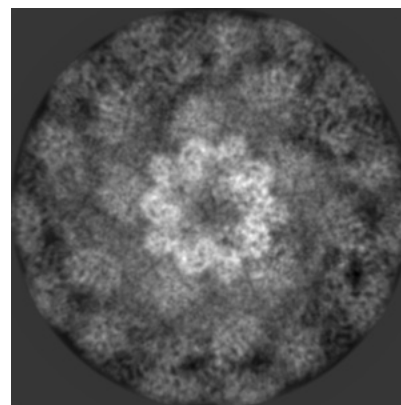
6.1.2 Raw map



X



Y

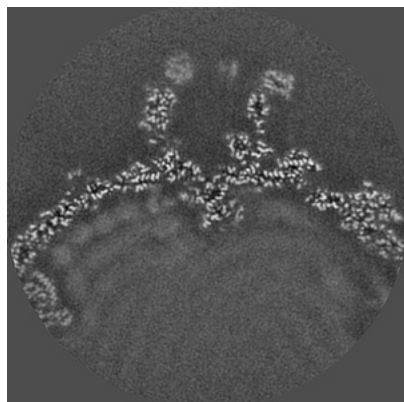


Z

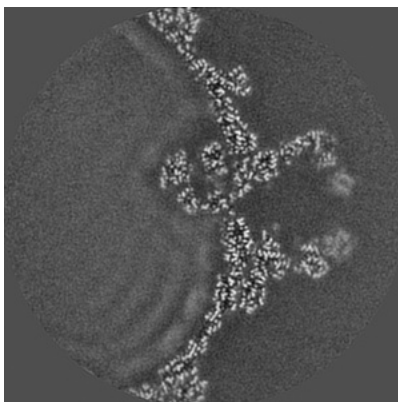
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

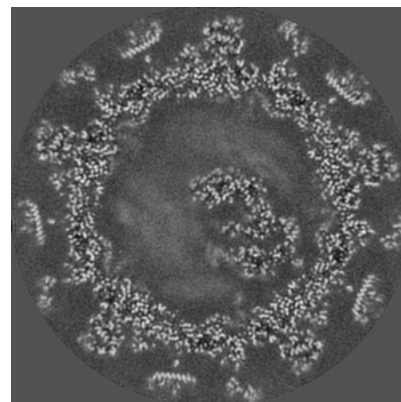
6.2.1 Primary map



X Index: 160

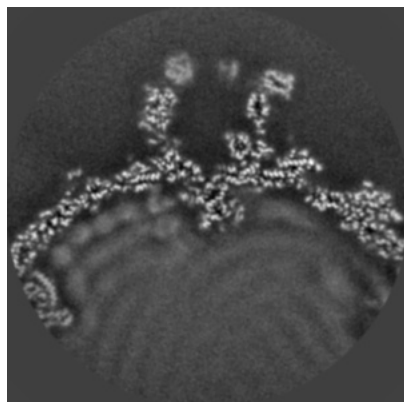


Y Index: 160

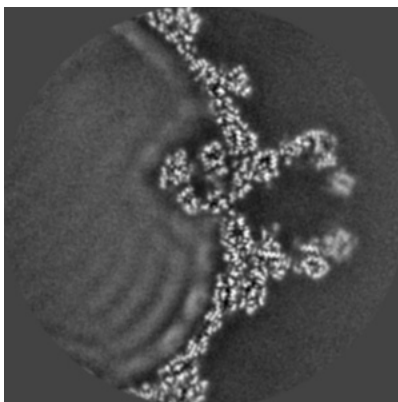


Z Index: 160

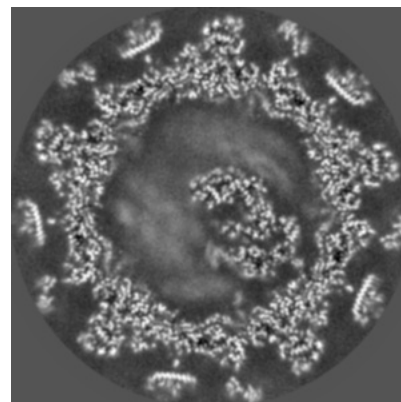
6.2.2 Raw map



X Index: 160



Y Index: 160

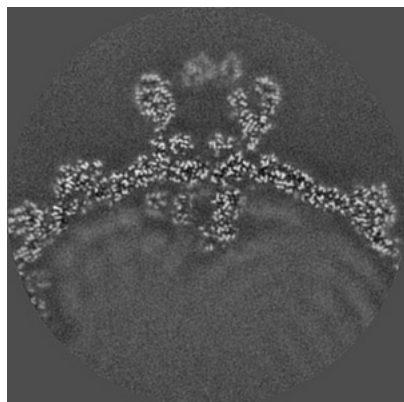


Z Index: 160

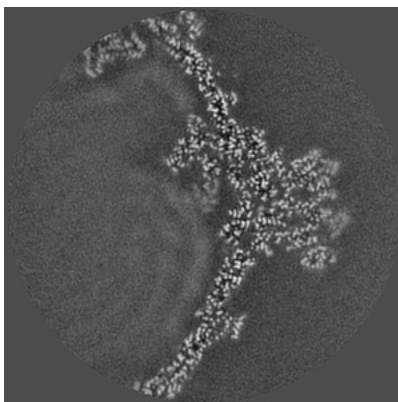
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

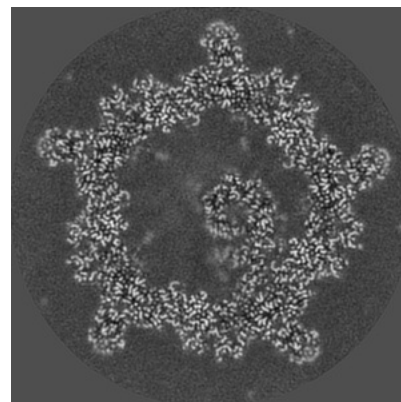
6.3.1 Primary map



X Index: 178

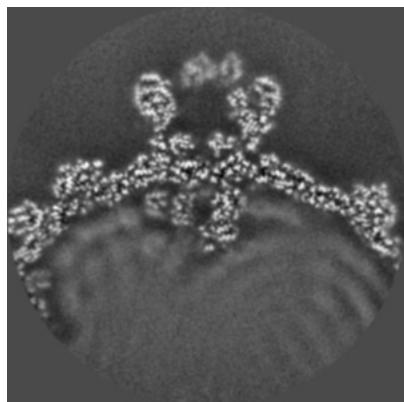


Y Index: 125

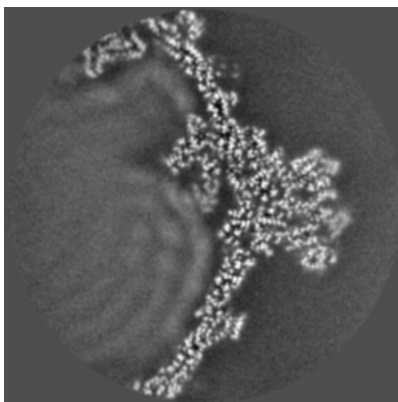


Z Index: 168

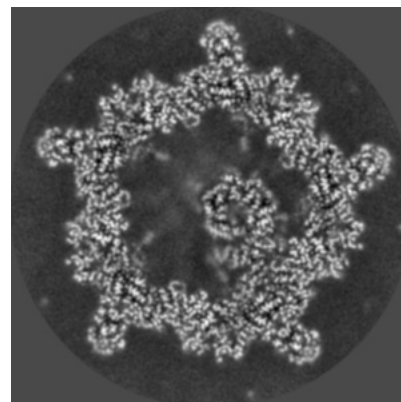
6.3.2 Raw map



X Index: 178



Y Index: 125

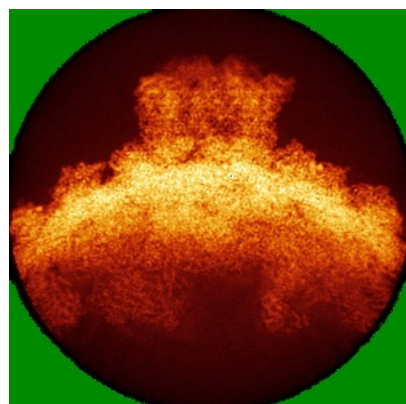


Z Index: 168

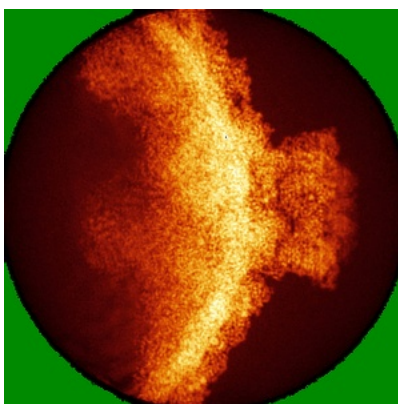
The images above show the largest variance slices of the map in three orthogonal directions.

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

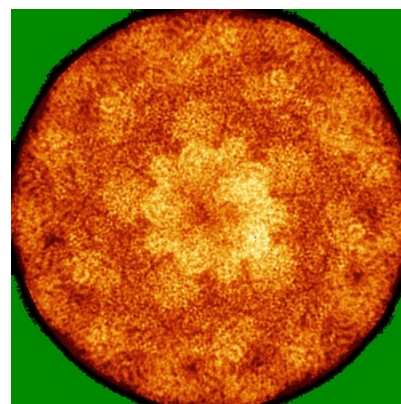
6.4.1 Primary map



X

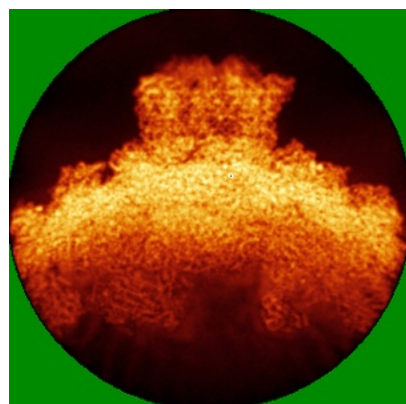


Y

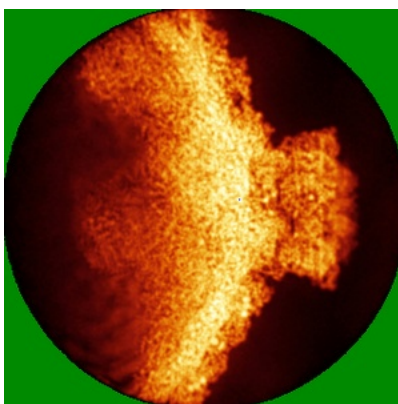


Z

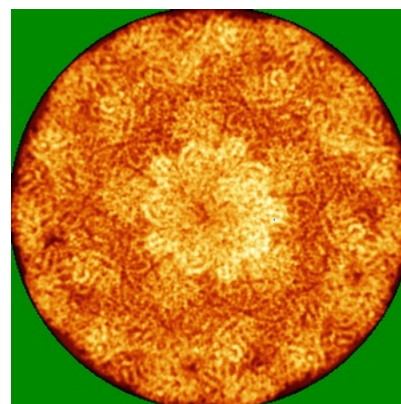
6.4.2 Raw map



X



Y

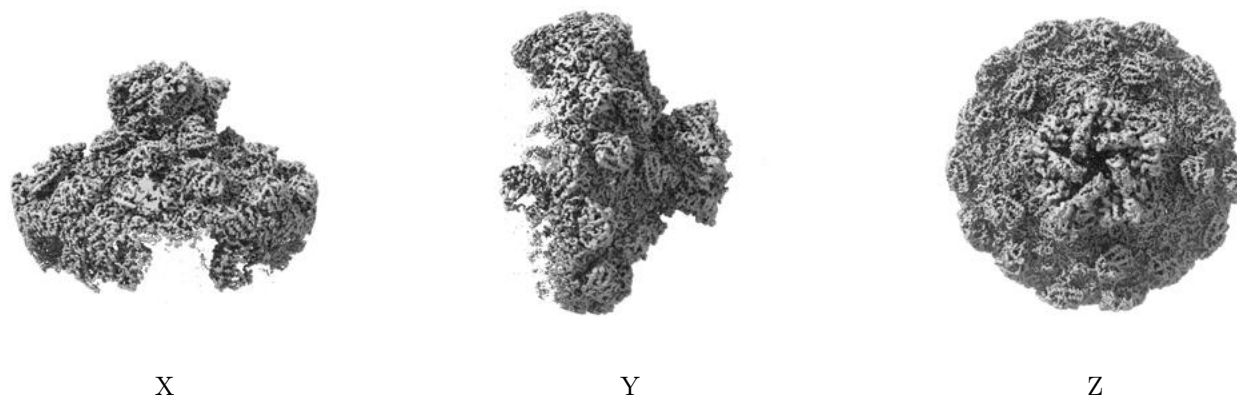


Z

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.

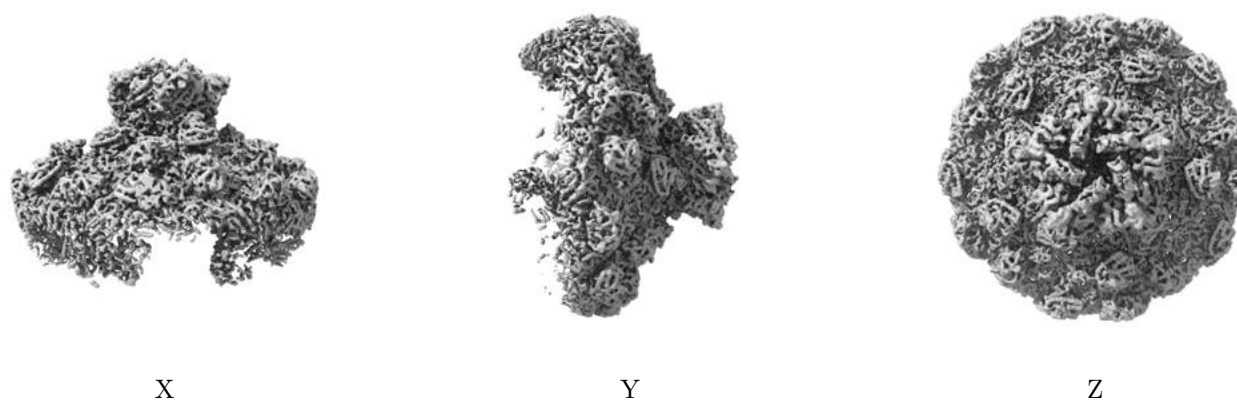
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00665. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

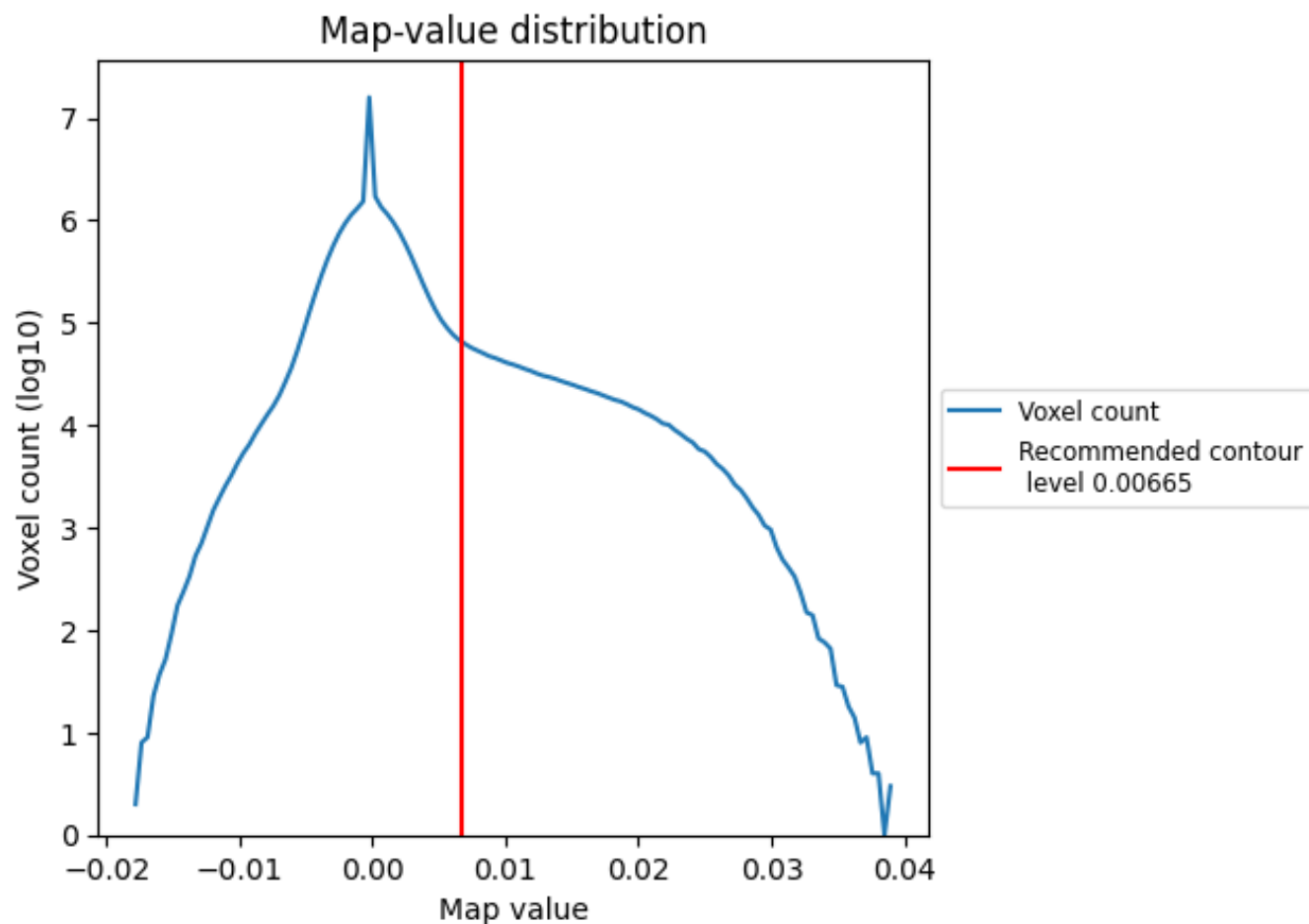
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

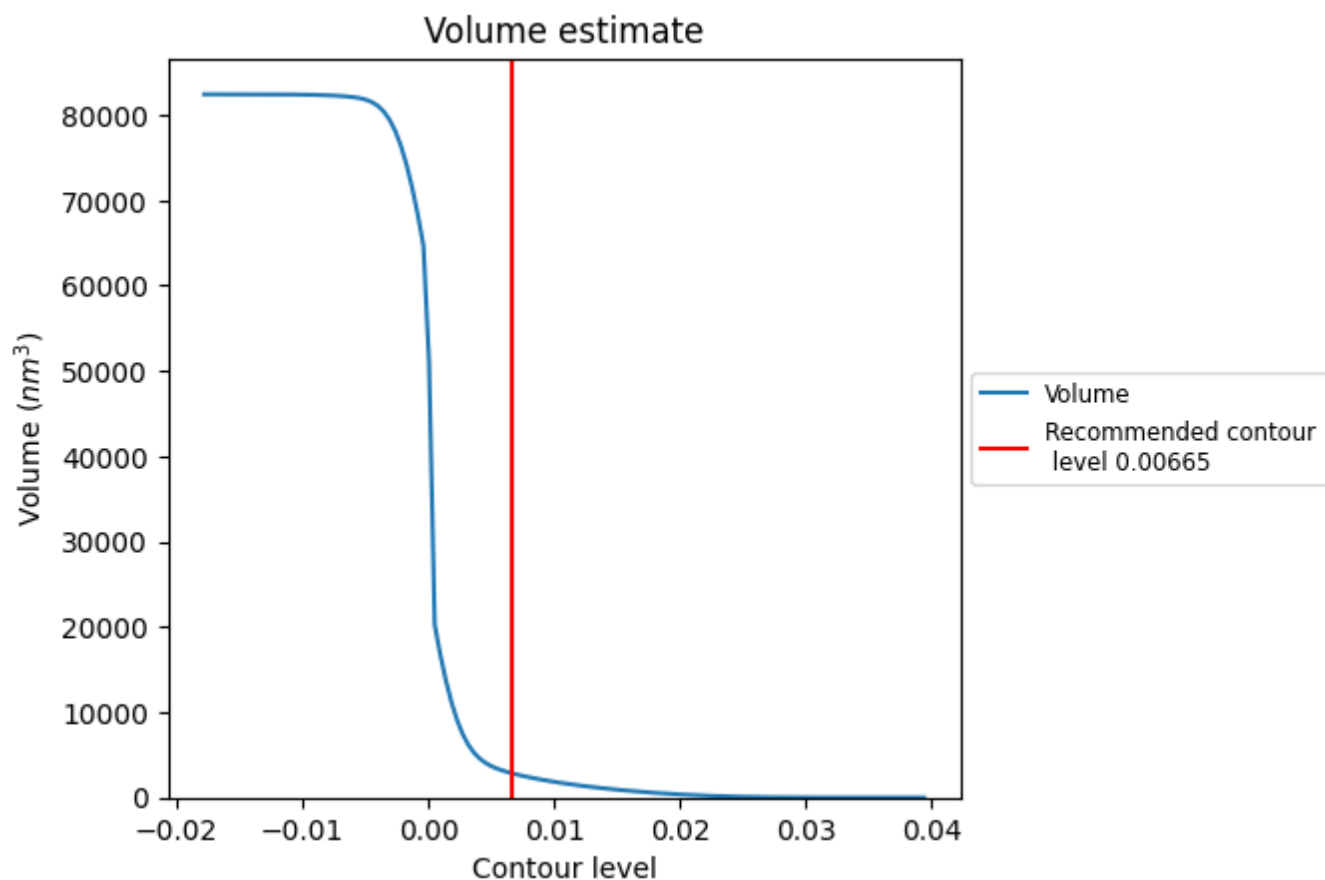
This section contains the results of statistical analysis of the map.

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.

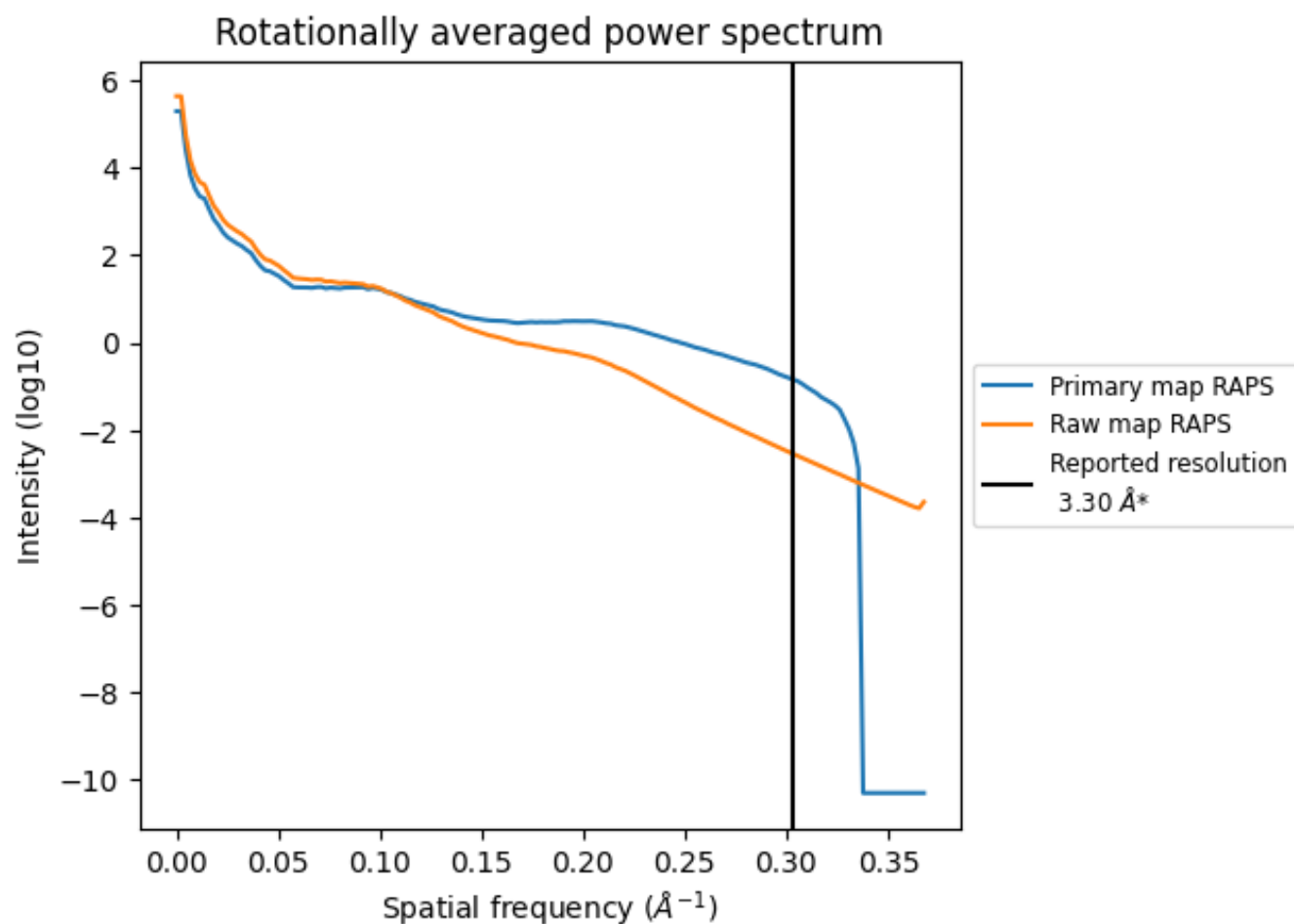
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2845 nm³; this corresponds to an approximate mass of 2570 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 ⓘ

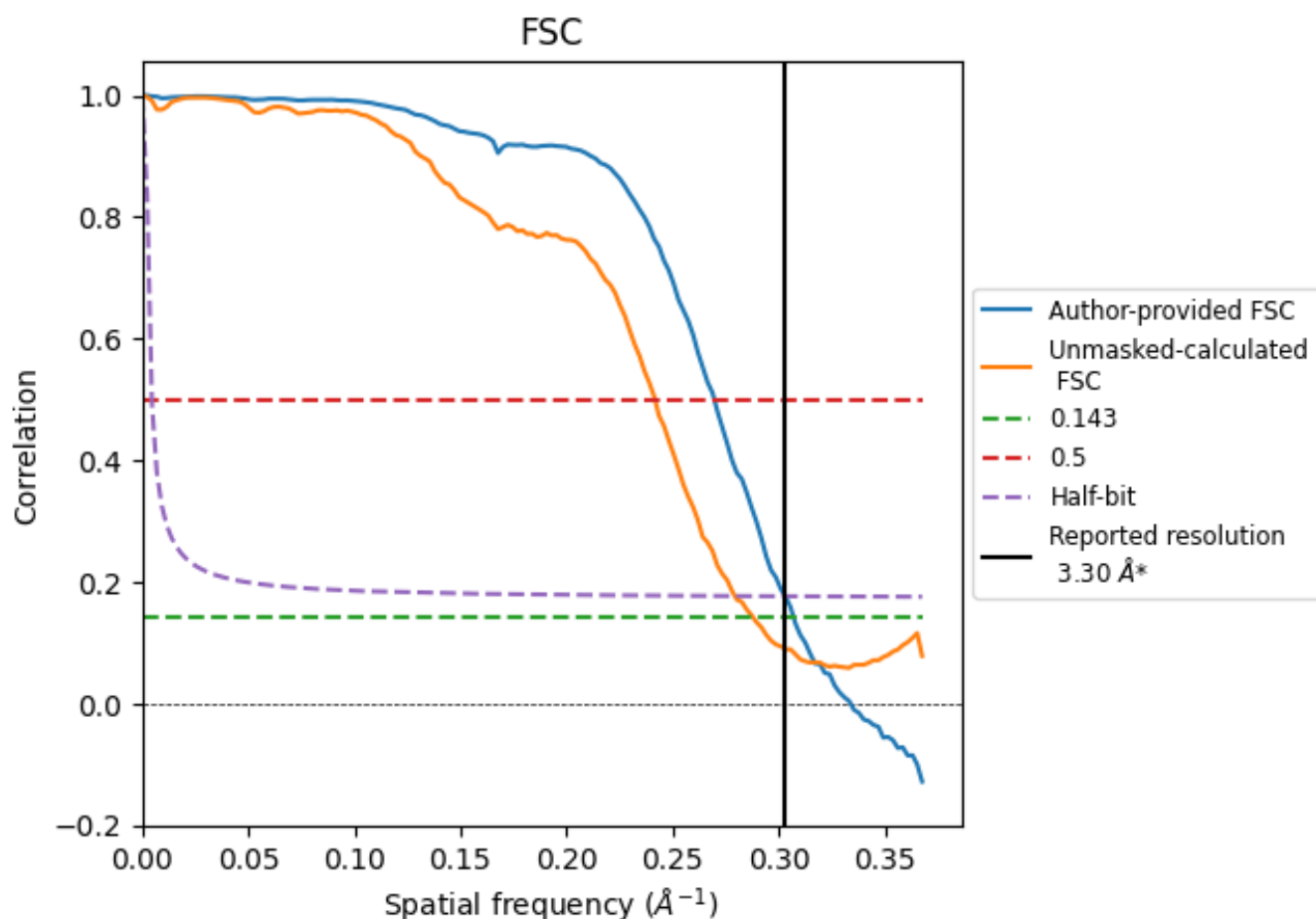


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

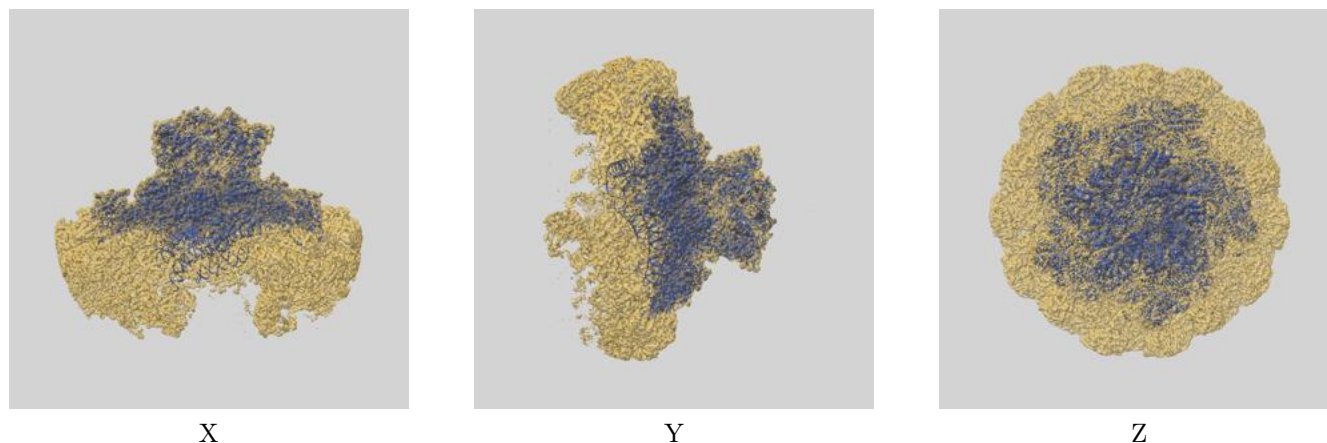
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.71	3.30
Unmasked-calculated*	3.48	4.14	3.58

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

9 Map-model fit [i](#)

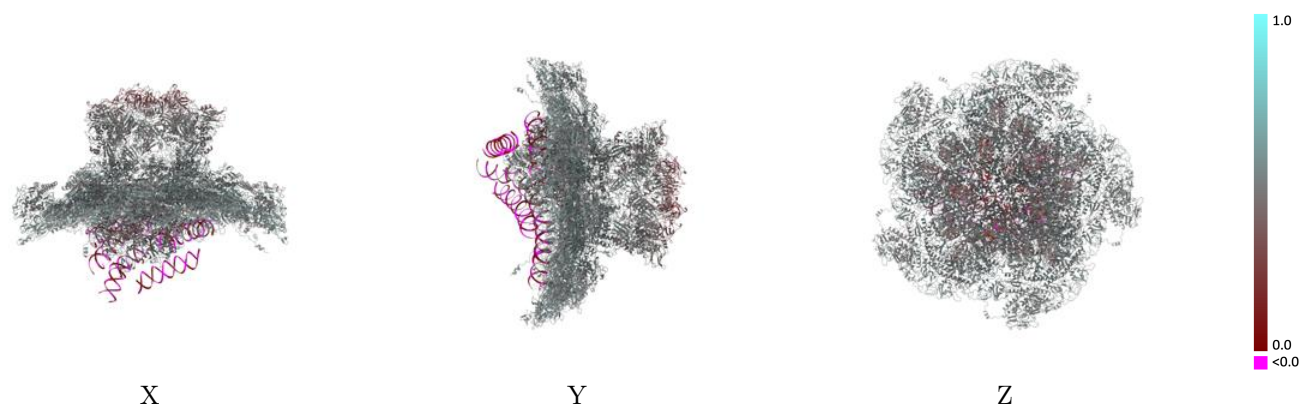
This section contains information regarding the fit between EMDB map EMD-29243 and PDB model 8FJK. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



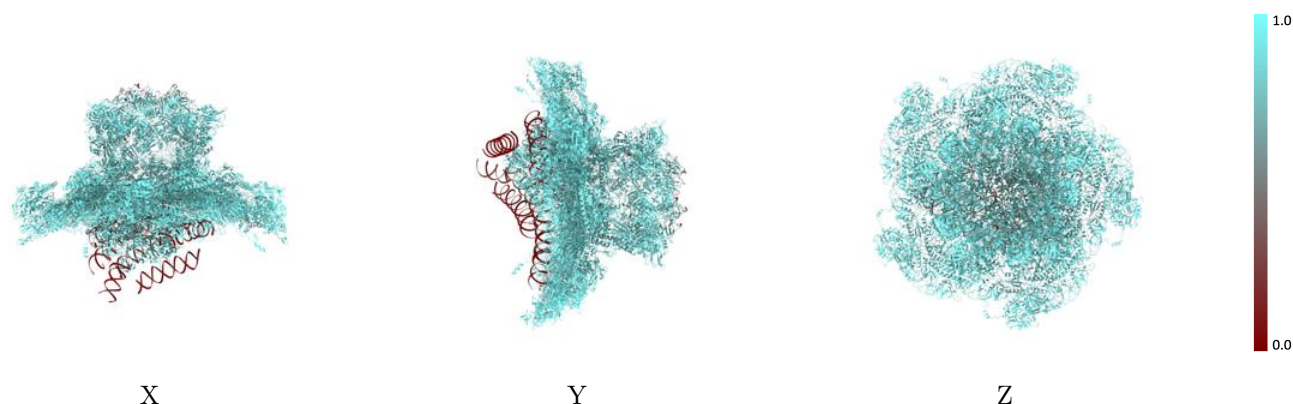
The images above show the 3D surface view of the map at the recommended contour level 0.00665 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



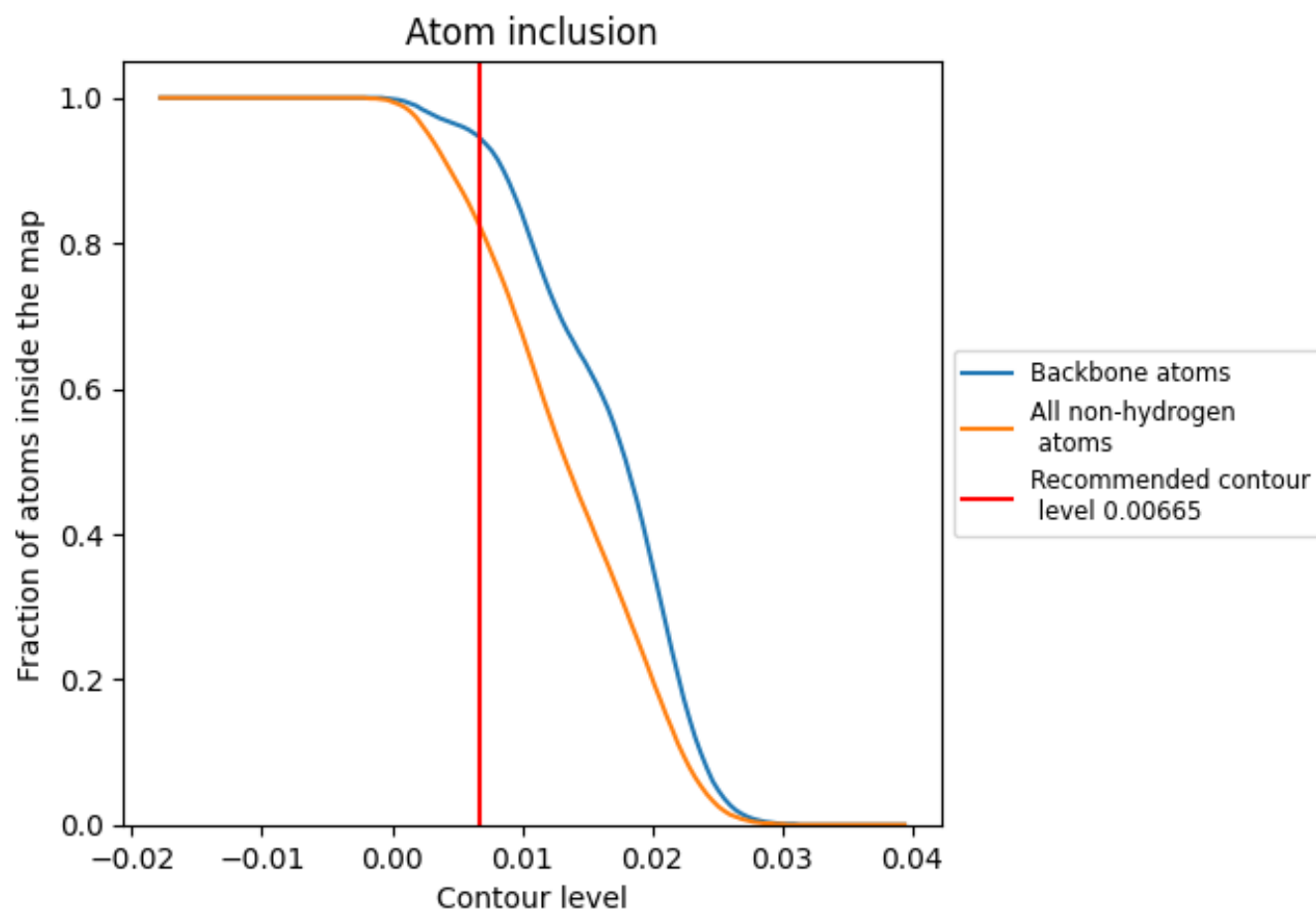
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00665).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 83% 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 (0.00665) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.4670
A	 0.8100	 0.4790
B	 0.7420	 0.4450
C	 0.8750	 0.5130
D	 0.8660	 0.5050
E	 0.8730	 0.5110
F	 0.8680	 0.5070
G	 0.8750	 0.5140
H	 0.8710	 0.5060
I	 0.8750	 0.5150
J	 0.8680	 0.5030
K	 0.8770	 0.5110
L	 0.8750	 0.5060
M	 0.7880	 0.4980
N	 0.7600	 0.4950
V	 0.9110	 0.4990
W	 0.9250	 0.5110
X	 0.9140	 0.4970
Y	 0.8700	 0.4560
Z	 0.8690	 0.4590
a	 0.9230	 0.5120
a1	 0.0540	 0.0240
a2	 0.0350	 0.0340
a3	 0.0000	 0.0060
a4	 0.0030	 0.0280
a5	 0.0110	 0.0020
a6	 0.0000	 0.0230
b	 0.9110	 0.4940
b1	 0.0140	 0.0320
b2	 0.0190	 0.0290
b3	 0.0010	 -0.0000
b4	 0.0000	 0.0310
b5	 0.0200	 0.0340
b6	 0.0000	 0.0220
c	 0.8680	 0.4580



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Chain	Atom inclusion	Q-score
d	 0.9280	 0.5130
e	 0.9090	 0.5020
f	 0.8740	 0.4590
g	 0.9270	 0.5160
h	 0.9190	 0.5020
i	 0.8720	 0.4560
k	 0.8040	 0.5010
l	 0.7890	 0.4830
m	 0.7660	 0.4600
n	 0.9250	 0.5200