



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:07 AM UTC

PDB ID : 8FQC / pdb_00008fqc
EMDB ID : EMD-29383
Title : Structure of baseplate with receptor binding complex of Agrobacterium phage Milano
Authors : Sonani, R.R.; Leiman, P.G.; Wang, F.; Kreutzberger, M.A.B.; Sebastian, A.; Esteves, N.C.; Kelly, R.J.; Scharf, B.; Egelman, E.H.
Deposited on : 2023-01-05
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

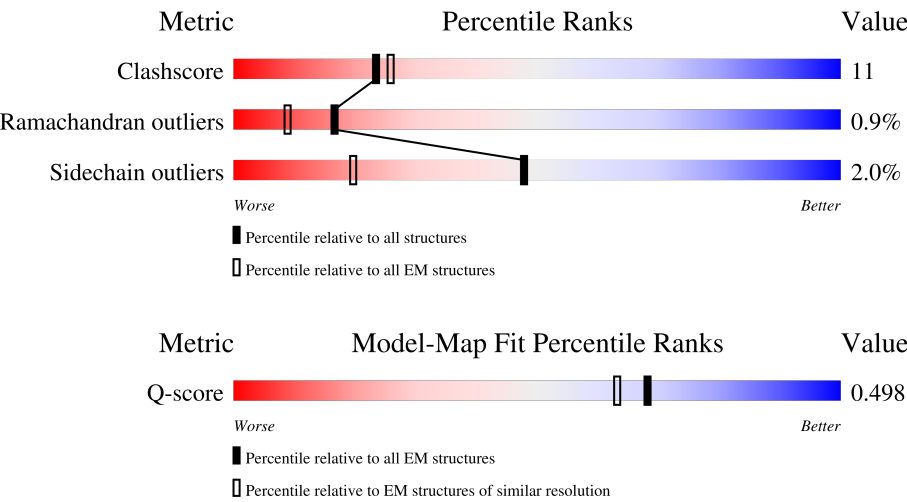
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



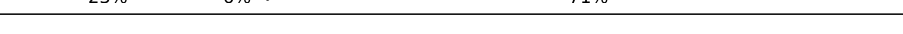
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	C1	457	
2	E1	136	
2	a1	136	
2	f1	136	

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Mol	Chain	Length	Quality of chain
2	g1	136	 82% 15% .
3	F1	396	 84% 14% ..
3	G1	396	 77% 20% ...
3	h1	396	 86% 12% ..
3	i1	396	 77% 21% ..
4	H1	178	 78% 21% .
4	j1	178	 78% 20% ..
5	I1	503	 77% 21% ..
5	K1	503	 74% 22% ..
5	k1	503	 74% 24% ..
5	m1	503	 72% 24% . .
6	J1	286	 74% 22% .
6	l1	286	 79% 18% .
7	P1	587	 22% 6% 72%
7	Q1	587	 23% 6% . 71%
7	R1	587	 22% 6% . 71%
7	r1	587	 21% 6% 72%
7	s1	587	 23% 5% . 71%
7	t1	587	 22% 7% 71%
8	S1	300	 28% 12% 60%
8	T1	300	 24% 16% 60%
8	V1	300	 26% 14% 60%
8	W1	300	 28% 12% 60%
8	X1	300	 28% 11% 60%
8	Y1	300	 30% 10% 60%

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Mol	Chain	Length	Quality of chain
8	u1	300	28%11%60%
8	v1	300	21%18%60%
8	w1	300	28%11%60%
8	x1	300	25%14%60%
8	y1	300	27%13%60%
8	z1	300	29%10%60%
9	U1	398	85%13%...
9	e1	398	81%16%..
10	A	188	64%15%8%•11%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 66089 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 Baseplate hub protein, gp26.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	326	Total	C	N	O	S	0	0
			2551	1610	434	500	7		

- Molecule 2 is a protein called Tail-tube, gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	a1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	f1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		
2	g1	131	Total	C	N	O	S	0	0
			995	617	165	206	7		

- Molecule 3 is a protein called Baseplate Wedge 2 protein, gp29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	G1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	h1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		
3	i1	393	Total	C	N	O	S	0	0
			3016	1900	515	580	21		

- Molecule 4 is a protein called Baseplate wedge 1, gp28.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	j1	176	Total	C	N	O	S	0	0
			1334	817	244	264	9		

- Molecule 5 is a protein called Tail sheath protein, gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	K1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		
5	k1	498	Total	C	N	O	S	0	0
			3739	2342	633	742	22		
5	m1	494	Total	C	N	O	S	0	0
			3706	2322	628	735	21		

- Molecule 6 is a protein called Baseplate Wedge 3 protein, gp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		
6	l1	285	Total	C	N	O	S	0	0
			2185	1390	355	420	20		

- Molecule 7 is a protein called Tail Spike protein, gp124.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	Q1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	R1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	r1	162	Total	C	N	O	S	0	0
			1227	782	194	248	3		
7	s1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		
7	t1	173	Total	C	N	O	S	0	0
			1308	835	210	260	3		

- Molecule 8 is a protein called Short Tail Fibers, gp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	T1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	V1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	W1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	X1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	Y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	v1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	w1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	x1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	y1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	u1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		
8	z1	119	Total	C	N	O	S	0	0
			878	545	150	174	9		

- Molecule 9 is a protein called Baseplate Centerpiece, gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		
9	e1	394	Total	C	N	O	S	0	0
			3027	1910	522	590	5		

- Molecule 10 is a protein called Baseplate Central Spike, gp27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	168	Total	C	N	O	S	0	0
			1289	799	223	264	3		

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total 1	Fe 1	0

Chain f1:  80% 16%



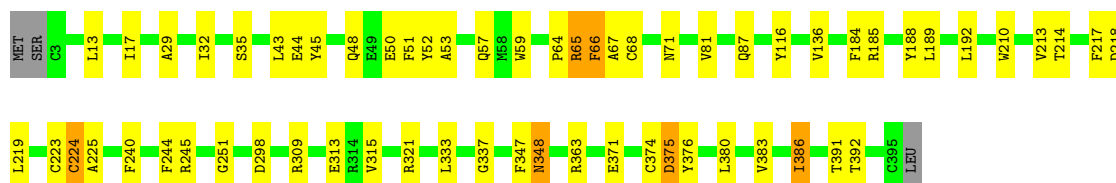
- Molecule 2: Tail-tube, gp21

Chain g1:  82% 15%



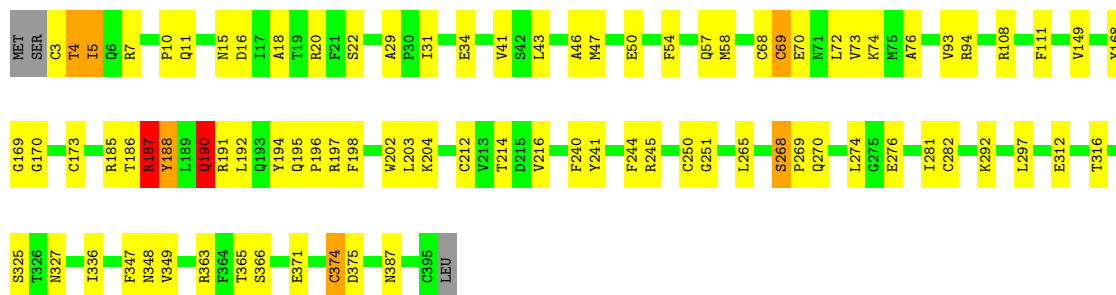
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain F1:  84% 14%



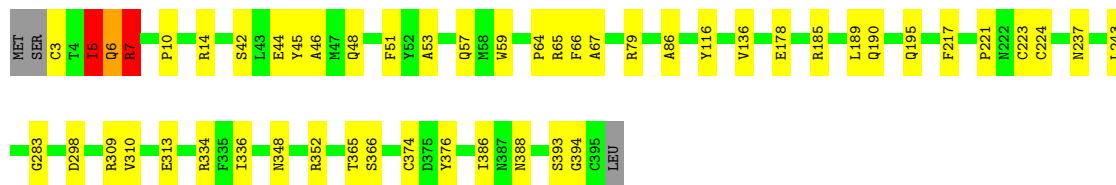
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain G1:  77% 20%



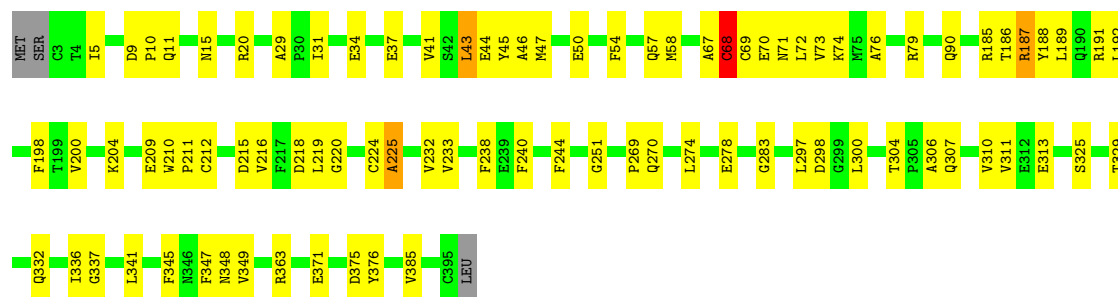
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain h1:  86% 12%



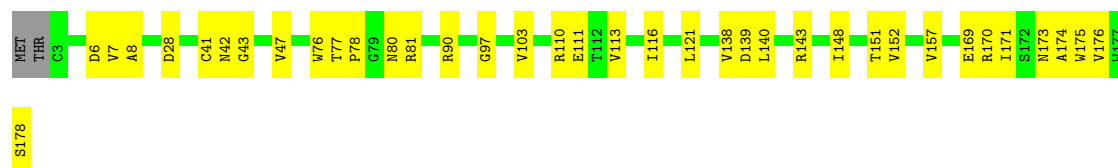
- Molecule 3: Baseplate Wedge 2 protein, gp29

Chain i1:  77% 21%



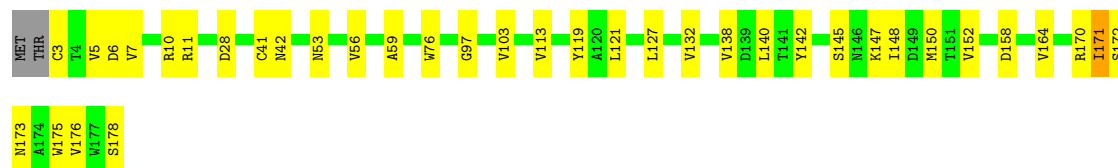
- Molecule 4: Baseplate wedge 1, gp28

Chain H1:  78% 21%



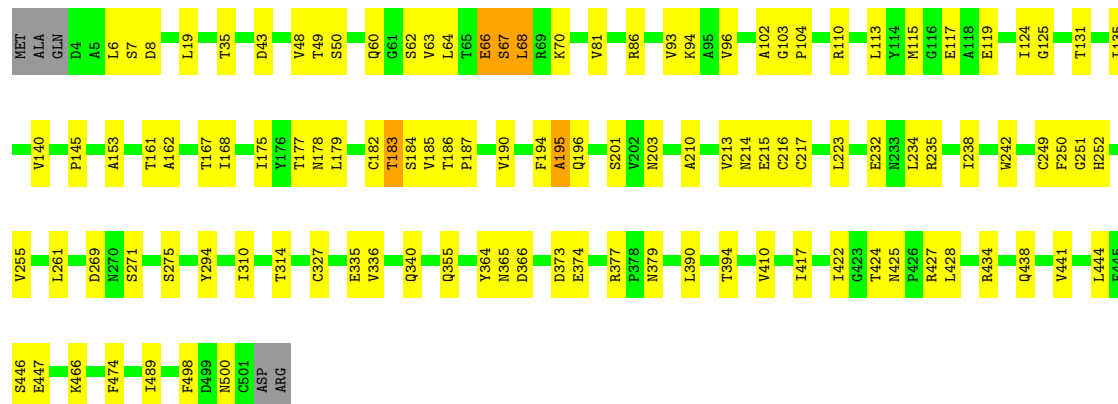
- Molecule 4: Baseplate wedge 1, gp28

Chain j1:  78% 20%



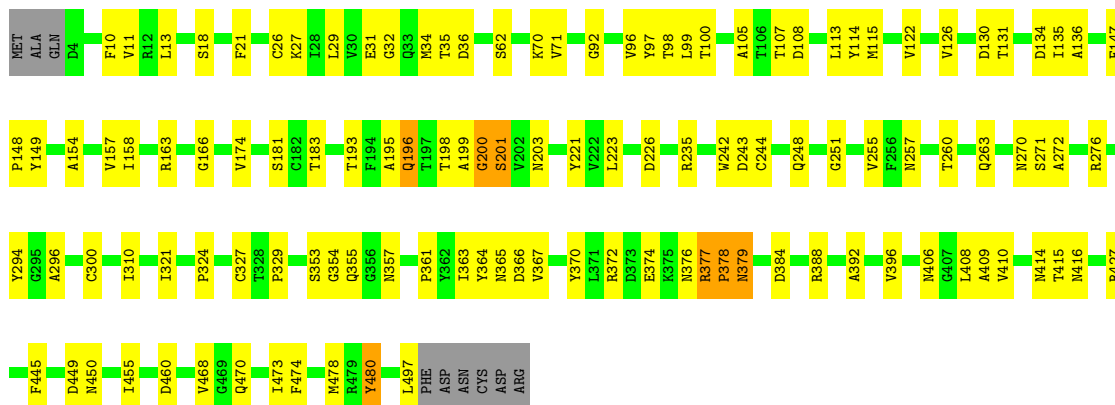
- Molecule 5: Tail sheath protein, gp20

Chain I1:  77% 21%



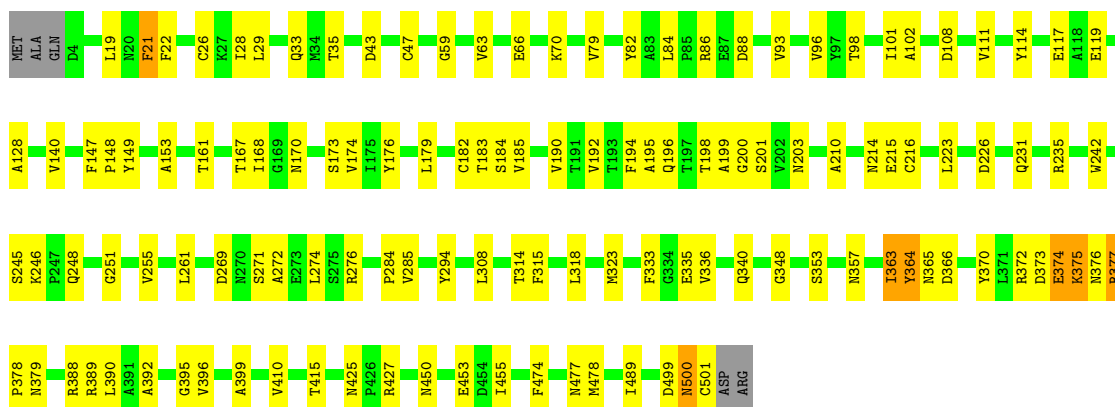
- Molecule 5: Tail sheath protein, gp20

Chain K1:  74% 22%



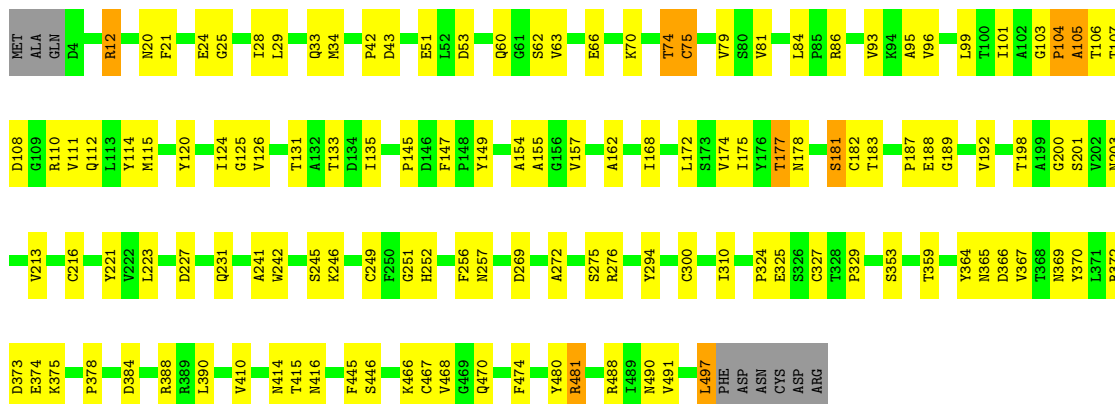
• Molecule 5: Tail sheath protein, gp20

Chain k1: 74% 24% ..



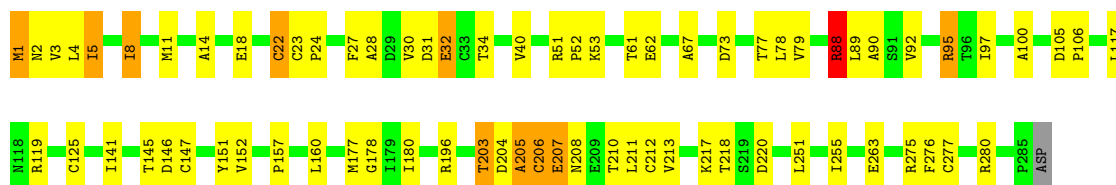
• Molecule 5: Tail sheath protein, gp20

Chain m1: 72% 24% ..



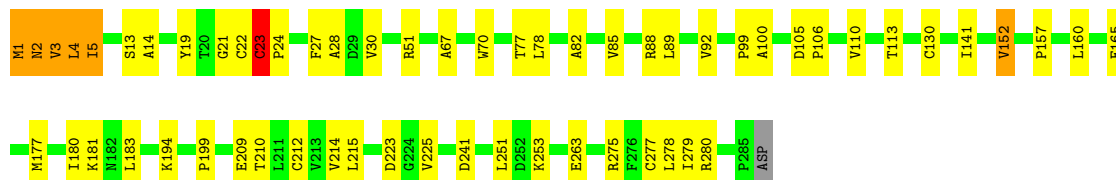
• Molecule 6: Baseplate Wedge 3 protein, gp30

Chain J1: 74% 22% .



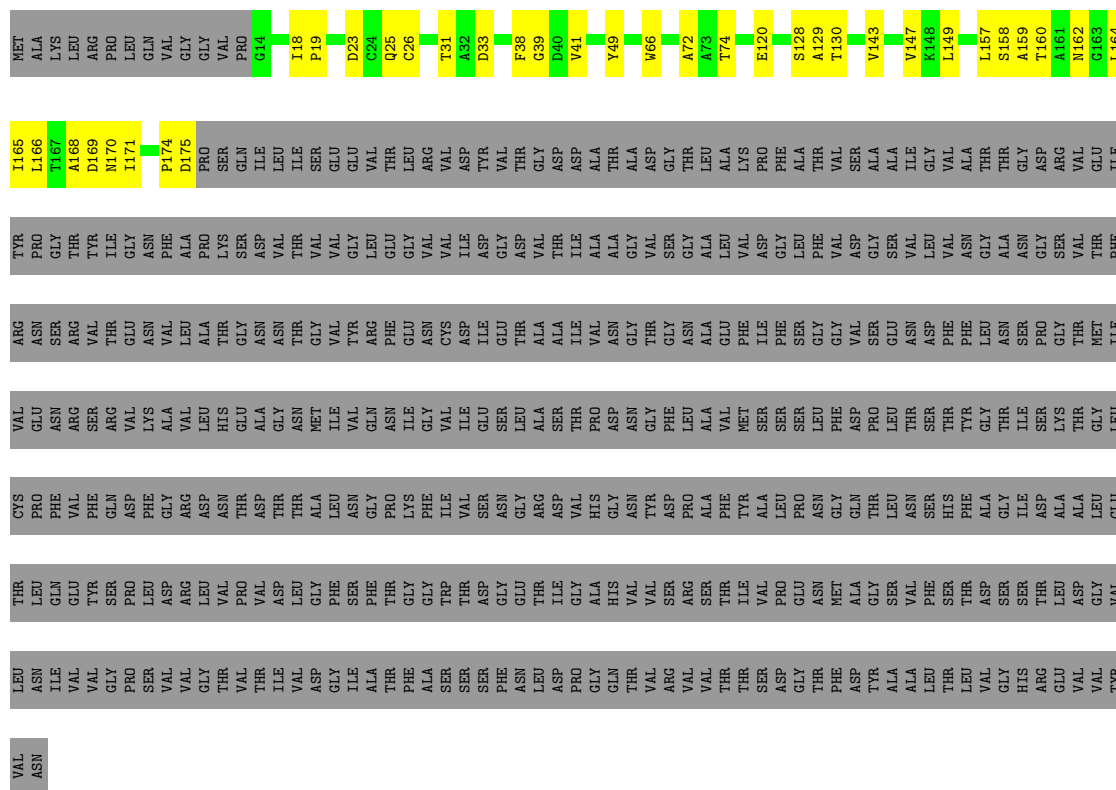
• Molecule 6: Baseplate Wedge 3 protein, gp30

Chain 11: 79% 18%



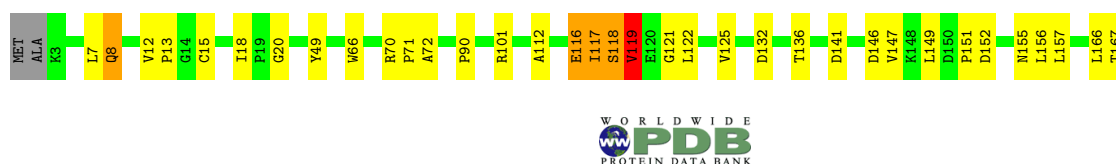
• Molecule 7: Tail Spike protein, gp124

Chain P1: 22% 6% 72%



• Molecule 7: Tail Spike protein, gp124

Chain Q1: 23% 6% 71%



A168	D169	M170	I171	D175	PRO	SER	GLN	SER	ILE	ASP	LEU	THR	LEU	SER	GLU	VAL	THR	LEU	ARG	VAL	VAL	ASP	THR	GLY	THR	THR	ALA	LEU	VAL	LYS	PRO	PHE	ALA	THR	THR	GLY	ASP	ARG	VAL	VAL	GLU	ILE	TYR	PRO	GLY	THR		
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR
					PRO	SER	GLY	ASN	VAL	THR	VAL	VAL	VAL	GLY	THR	ARG	PHE	GLY	ASN	CYS	VAL	ILE	THR	ASP	THR	ALA	LEU	VAL	LYS	PRO	PHE	GLY	LEU	ASN	GLY	VAL	VAL	LEU	ASN	GLY	THR	ARG	VAL	VAL	LEU	ASN	GLY	THR

● Molecule 7: Tail Spike protein, gp124

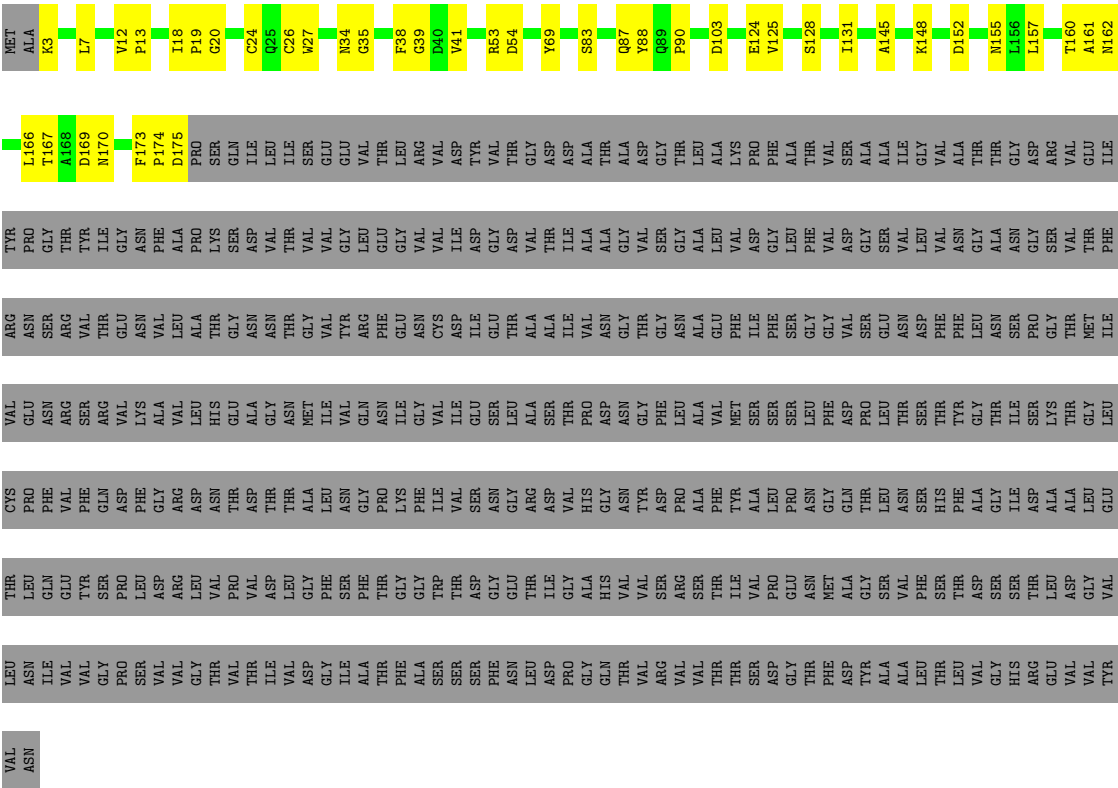
Chain R1:

<

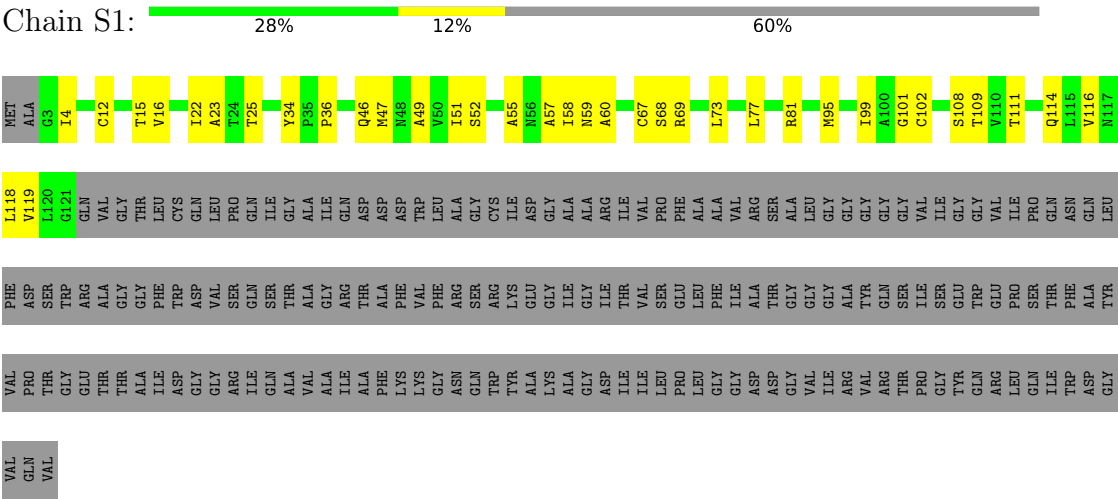
● Molecule 7: Tail Spike protein, gp124

Chain r1: 21% 6% 72%

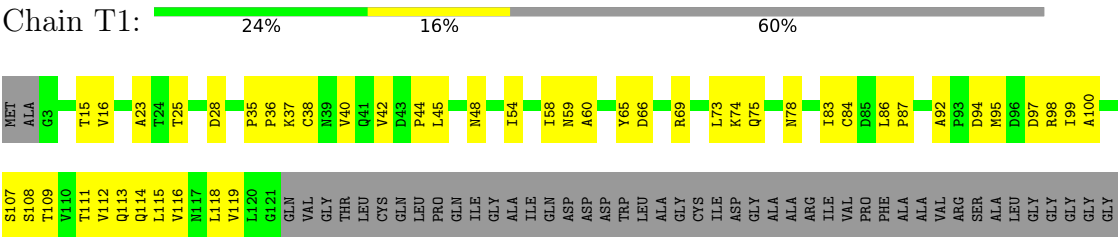
MET	ALA	LYS	LEU	ARG	PRO	PRO	LEU	GLN	VAL	GLY	GLY	VAL	VAL	PRO	PRO	G14	M17	I18	P19	E22	D23	C24	Q25	C26	F38	G39	Y49	R53	D65	W66	A72	A73	T74	S83	T84	Y85	P90	L104	N113	V119	E120	G121	S128	I131	V143	V147		
GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR



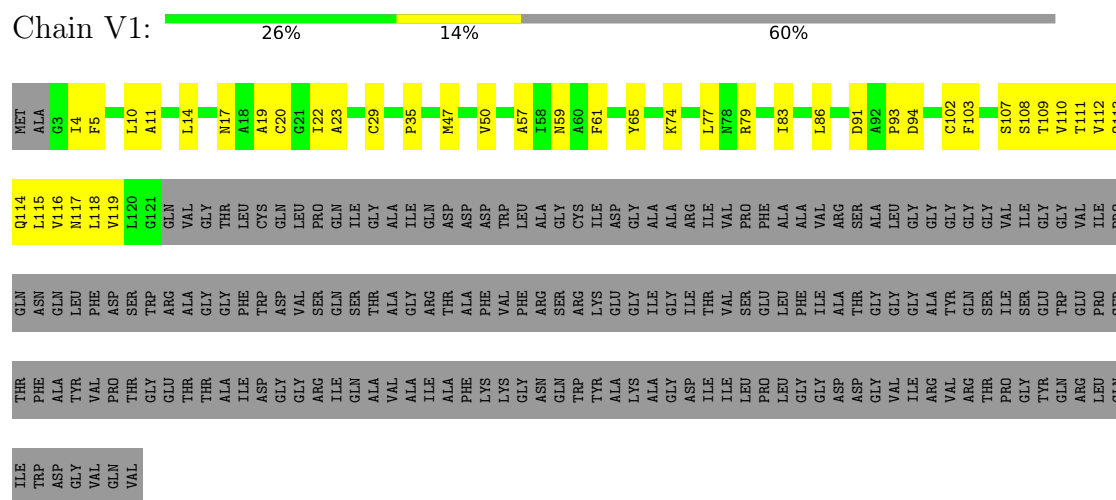
• Molecule 8: Short Tail Fibers, gp31



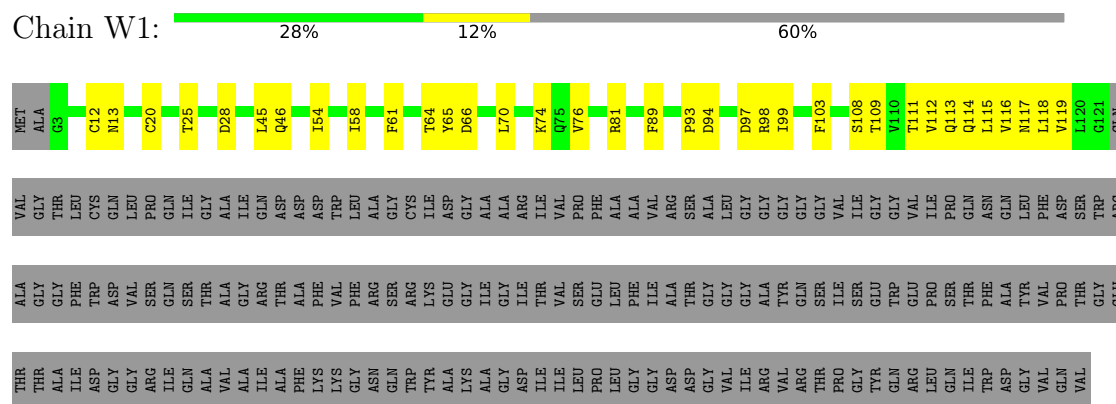
• Molecule 8: Short Tail Fibers, gp31



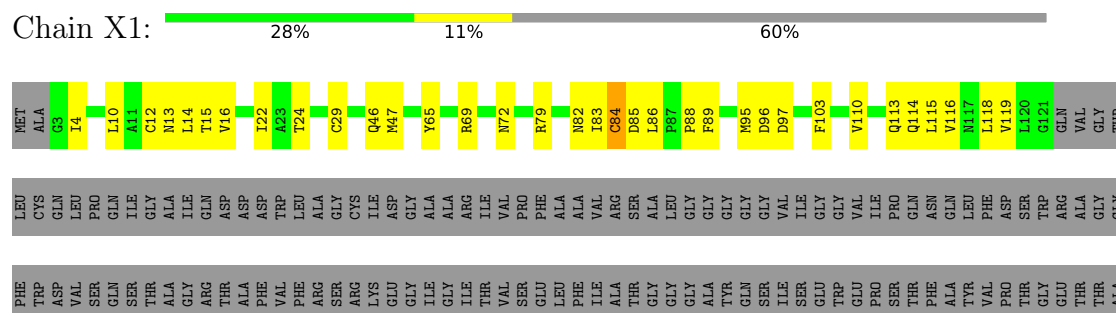
- Molecule 8: Short Tail Fibers, gp31

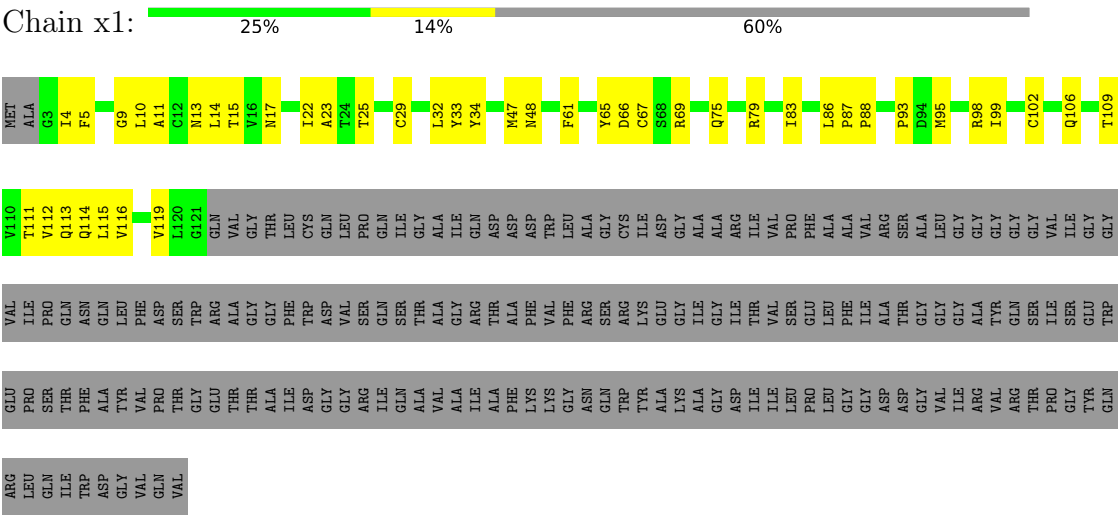


- Molecule 8: Short Tail Fibers, gp31

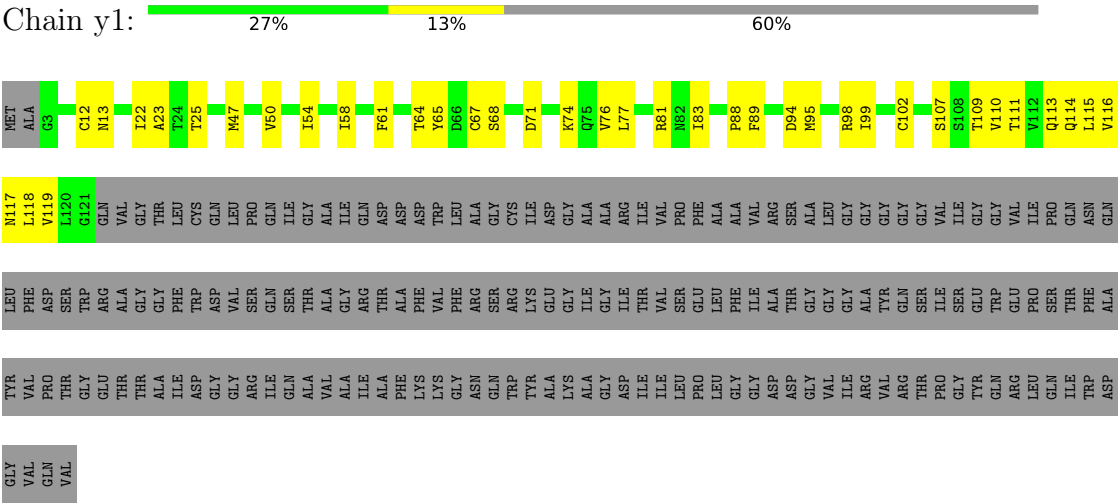


- Molecule 8: Short Tail Fibers, gp31

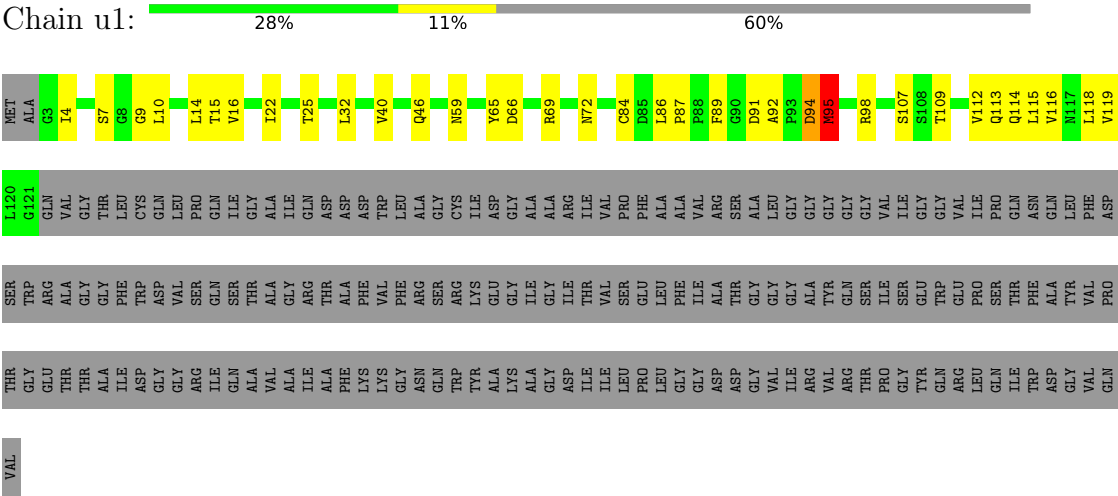




• Molecule 8: Short Tail Fibers, gp31



• Molecule 8: Short Tail Fibers, gp31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14856	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.478	Depositor
Minimum map value	-0.780	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	624.24005, 624.24005, 624.24005	wwPDB
Map dimensions	578, 578, 578	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: FE

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	C1	0.42	1/2598 (0.0%)	0.61	3/3525 (0.1%)
2	E1	0.43	0/1011	0.46	0/1382
2	a1	0.32	0/1011	0.46	1/1382 (0.1%)
2	f1	0.31	0/1011	0.39	0/1382
2	g1	0.33	0/1011	0.43	0/1382
3	F1	0.40	0/3085	0.47	1/4207 (0.0%)
3	G1	0.50	1/3085 (0.0%)	0.62	5/4207 (0.1%)
3	h1	0.41	0/3085	0.48	1/4207 (0.0%)
3	i1	0.51	0/3085	0.56	0/4207
4	H1	0.34	0/1353	0.47	0/1831
4	j1	0.30	0/1353	0.48	0/1831
5	I1	0.40	0/3815	0.50	3/5211 (0.1%)
5	K1	0.38	1/3781 (0.0%)	0.53	3/5165 (0.1%)
5	k1	0.38	0/3815	0.50	1/5211 (0.0%)
5	m1	0.34	0/3781	0.50	0/5165
6	J1	0.50	1/2237 (0.0%)	0.56	2/3063 (0.1%)
6	l1	0.43	0/2237	0.52	0/3063
7	P1	0.21	0/1269	0.36	0/1755
7	Q1	0.29	0/1352	0.46	0/1868
7	R1	0.19	0/1352	0.38	1/1868 (0.1%)
7	r1	0.22	0/1269	0.37	0/1755
7	s1	0.28	0/1352	0.43	0/1868
7	t1	0.20	0/1352	0.39	0/1868
8	S1	0.16	0/892	0.35	0/1217
8	T1	0.17	0/892	0.38	0/1217
8	V1	0.17	0/892	0.41	0/1217
8	W1	0.23	0/892	0.37	0/1217
8	X1	0.22	0/892	0.40	0/1217
8	Y1	0.19	0/892	0.36	0/1217
8	u1	0.20	0/892	0.41	0/1217
8	v1	0.21	0/892	0.38	0/1217
8	w1	0.16	0/892	0.36	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	x1	0.16	0/892	0.36	0/1217
8	y1	0.21	0/892	0.38	0/1217
8	z1	0.23	0/892	0.39	0/1217
9	U1	0.40	0/3093	0.50	4/4214 (0.1%)
9	e1	0.41	0/3093	0.47	1/4214 (0.0%)
10	A	0.81	0/1320	1.28	13/1791 (0.7%)
All	All	0.38	4/67510 (0.0%)	0.51	39/92226 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G1	188	TYR	CA-C	-7.62	1.45	1.52
6	J1	88	ARG	CA-C	-5.74	1.45	1.52
1	C1	59	VAL	CA-C	-5.62	1.48	1.53
5	K1	357	ASN	CA-C	-5.06	1.50	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	73	SER	N-CA-C	-10.78	97.64	112.30
10	A	39	GLY	N-CA-C	-10.73	101.79	115.42
10	A	44	GLU	N-CA-C	-9.42	101.04	112.54
3	h1	336	ILE	N-CA-C	-8.12	101.07	113.16
3	G1	187	ARG	N-CA-C	-8.01	101.33	113.51
3	G1	188	TYR	N-CA-C	-7.77	101.71	112.12
3	G1	191	ARG	N-CA-C	-7.45	104.08	113.02
5	I1	67	SER	N-CA-C	-7.33	99.68	111.04
5	k1	363	ILE	N-CA-C	6.92	117.86	108.17
3	G1	187	ARG	CB-CA-C	6.88	116.64	109.83
9	U1	199	TRP	N-CA-C	-6.71	105.22	113.41
10	A	170	GLN	OE1-CD-NE2	-6.70	115.90	122.60
10	A	116	ILE	N-CA-C	-6.64	95.53	109.34
3	G1	197	ARG	N-CA-C	6.50	122.94	114.75
10	A	117	TRP	N-CA-C	6.45	118.79	108.41
1	C1	56	GLU	N-CA-C	6.42	124.49	110.80
10	A	48	PRO	CB-CA-C	-6.25	101.25	111.56
9	U1	139	VAL	N-CA-C	-6.17	106.49	112.29
10	A	72	GLY	N-CA-C	-6.09	100.25	111.34
9	U1	138	LEU	CA-C-N	-5.82	114.01	122.28
9	U1	138	LEU	C-N-CA	-5.82	114.01	122.28
6	J1	8	ILE	N-CA-C	-5.77	105.77	112.98
5	K1	201	SER	CB-CA-C	-5.76	108.94	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	47	VAL	CA-C-N	-5.70	112.71	119.84
10	A	47	VAL	C-N-CA	-5.70	112.71	119.84
1	C1	57	ILE	N-CA-C	5.66	116.86	108.65
1	C1	130	LEU	N-CA-C	-5.63	105.51	112.38
5	I1	183	THR	N-CA-C	-5.62	103.07	110.43
9	e1	198	LYS	N-CA-C	-5.52	105.18	111.14
5	K1	357	ASN	CB-CA-C	-5.45	109.23	117.07
3	F1	65	ARG	O-C-N	-5.37	116.29	122.09
10	A	47	VAL	N-CA-C	5.36	120.45	108.88
2	a1	20	ASP	N-CA-C	-5.33	107.44	114.04
5	I1	195	ALA	N-CA-C	5.32	122.13	110.80
10	A	31	THR	N-CA-C	-5.30	104.82	113.19
7	R1	20	GLY	N-CA-C	5.26	117.92	111.45
6	J1	22	CYS	N-CA-C	5.20	117.09	108.20
10	A	48	PRO	N-CA-C	5.13	123.03	112.47
5	K1	357	ASN	N-CA-C	5.04	112.91	108.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	2551	0	2522	127	0
2	E1	995	0	968	10	0
2	a1	995	0	968	19	0
2	f1	995	0	969	18	0
2	g1	995	0	968	13	0
3	F1	3016	0	2903	47	0
3	G1	3016	0	2901	66	0
3	h1	3016	0	2902	36	0
3	i1	3016	0	2905	58	0
4	H1	1334	0	1308	30	0
4	j1	1334	0	1307	30	0
5	I1	3739	0	3607	84	0
5	K1	3706	0	3585	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	k1	3739	0	3606	85	0
5	m1	3706	0	3586	91	0
6	J1	2185	0	2140	53	0
6	l1	2185	0	2140	46	0
7	P1	1227	0	1119	33	0
7	Q1	1308	0	1213	31	0
7	R1	1308	0	1214	42	0
7	r1	1227	0	1118	31	0
7	s1	1308	0	1212	29	0
7	t1	1308	0	1212	33	0
8	S1	878	0	844	41	0
8	T1	878	0	844	50	0
8	V1	878	0	844	37	0
8	W1	878	0	844	36	0
8	X1	878	0	845	29	0
8	Y1	878	0	845	31	0
8	u1	878	0	844	31	0
8	v1	878	0	845	51	0
8	w1	878	0	844	34	0
8	x1	878	0	844	44	0
8	y1	878	0	844	39	0
8	z1	878	0	844	29	0
9	U1	3027	0	2908	46	0
9	e1	3027	0	2906	59	0
10	A	1289	0	1201	55	0
11	A	1	0	0	0	0
All	All	66089	0	63519	1421	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1421) 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:G1:269:PRO:HD2	3:G1:274:LEU:HD12	1.36	1.04
7:R1:24:CYS:SG	7:R1:24:CYS:O	2.16	1.04
3:G1:68:CYS:O	3:G1:68:CYS:SG	2.16	1.04
6:l1:5:ILE:HD11	6:l1:14:ALA:HB2	1.43	0.99
3:G1:268:SER:HB2	3:G1:269:PRO:HD3	1.46	0.96
5:I1:498:PHE:HE2	5:I1:500:ASN:OD1	1.52	0.91
10:A:43:GLN:HG2	10:A:46:ASP:HA	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:69:GLY:HA2	1:C1:126:ARG:HG3	1.52	0.90
8:x1:95:MET:HG3	8:x1:113:GLN:CG	2.03	0.87
1:C1:9:ILE:HA	1:C1:57:ILE:HG22	1.56	0.87
3:h1:224:CYS:HB2	8:v1:38:CYS:SG	2.15	0.85
3:F1:224:CYS:SG	3:F1:225:ALA:N	2.50	0.84
5:k1:63:VAL:HG21	5:k1:168:ILE:HD12	1.59	0.84
3:h1:224:CYS:CB	8:v1:38:CYS:SG	2.66	0.83
1:C1:251:GLY:O	10:A:31:THR:HG21	1.82	0.80
7:R1:26:CYS:HG	7:R1:27:TRP:CD1	1.99	0.80
5:K1:296:ALA:O	5:K1:300:CYS:HB2	1.82	0.80
8:x1:95:MET:HG3	8:x1:113:GLN:HG3	1.63	0.80
8:w1:45:LEU:HA	8:w1:48:ASN:HD22	1.47	0.79
5:I1:498:PHE:CE2	5:I1:500:ASN:OD1	2.34	0.79
7:s1:168:ALA:HA	7:s1:171:ILE:HD12	1.64	0.78
8:X1:116:VAL:HA	8:X1:119:VAL:HG22	1.66	0.78
8:X1:22:ILE:HG23	8:Y1:59:ASN:HD21	1.49	0.77
3:F1:65:ARG:HD2	3:F1:66:PHE:CZ	2.19	0.77
8:y1:23:ALA:H	8:u1:59:ASN:HD21	1.31	0.77
8:T1:45:LEU:HA	8:T1:48:ASN:HD22	1.50	0.76
7:R1:27:TRP:HE3	7:R1:41:VAL:HG11	1.51	0.76
1:C1:141:PHE:CZ	10:A:43:GLN:HG3	2.21	0.75
5:m1:445:PHE:HD1	5:m1:480:TYR:HB2	1.52	0.75
4:j1:173:ASN:HD22	4:j1:175:TRP:HE1	1.34	0.75
7:R1:26:CYS:HG	7:R1:27:TRP:CG	2.04	0.74
8:y1:74:LYS:HG3	8:z1:60:ALA:HB2	1.69	0.74
5:k1:196:GLN:NE2	5:k1:198:THR:O	2.20	0.74
3:i1:79:ARG:HD3	6:l1:177:MET:HE1	1.69	0.74
8:S1:15:THR:HG22	8:S1:16:VAL:H	1.52	0.74
8:x1:95:MET:HG3	8:x1:113:GLN:HG2	1.68	0.74
6:J1:263:GLU:OE1	6:J1:280:ARG:NH2	2.21	0.73
8:v1:63:ASN:HD22	8:v1:79:ARG:HH12	1.37	0.73
7:s1:167:THR:HG22	7:s1:169:ASP:H	1.52	0.73
3:h1:65:ARG:HD2	3:h1:66:PHE:CZ	2.23	0.73
5:I1:63:VAL:HG21	5:I1:168:ILE:HD12	1.68	0.73
7:Q1:167:THR:HG22	7:Q1:169:ASP:H	1.52	0.72
5:m1:446:SER:HB3	5:m1:481:ARG:HG3	1.69	0.72
10:A:38:LYS:C	10:A:40:SER:H	1.95	0.72
3:i1:188:TYR:O	3:i1:191:ARG:HB3	1.90	0.72
1:C1:39:LEU:HD13	1:C1:119:VAL:HG21	1.72	0.72
3:G1:198:PHE:HB2	6:J1:180:ILE:HD11	1.70	0.72
5:K1:154:ALA:HB3	5:K1:157:VAL:HB	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P1:38:PHE:O	7:Q1:70:ARG:NH1	2.23	0.71
8:S1:119:VAL:HG23	8:T1:116:VAL:HG13	1.72	0.71
3:G1:268:SER:HB2	3:G1:269:PRO:CD	2.21	0.71
5:I1:213:VAL:HG23	5:I1:216:CYS:HB3	1.73	0.71
3:F1:71:ASN:ND2	3:G1:3:CYS:SG	2.64	0.70
7:r1:174:PRO:HD2	7:t1:174:PRO:HD2	1.74	0.70
2:f1:79:TYR:HB3	2:f1:115:VAL:HG11	1.73	0.70
8:u1:66:ASP:OD2	8:u1:69:ARG:NH1	2.25	0.70
5:K1:410:VAL:HG11	5:K1:474:PHE:HZ	1.58	0.69
7:P1:174:PRO:HD2	7:R1:174:PRO:HD2	1.75	0.69
8:W1:74:LYS:HG3	8:Y1:60:ALA:HB2	1.74	0.69
8:u1:10:LEU:HD23	8:u1:14:LEU:HB3	1.73	0.69
2:a1:84:GLN:HE21	2:a1:101:GLU:HA	1.56	0.69
8:u1:22:ILE:HG23	8:z1:59:ASN:HD21	1.58	0.69
10:A:48:PRO:HG2	10:A:80:ALA:H	1.57	0.69
3:F1:374:CYS:O	3:F1:376:TYR:HD2	1.76	0.69
3:h1:67:ALA:O	3:h1:185:ARG:NH2	2.26	0.69
1:C1:25:THR:HG22	1:C1:27:LYS:H	1.58	0.68
5:K1:97:TYR:HA	5:K1:196:GLN:HA	1.76	0.68
8:v1:49:ALA:HB2	8:x1:17:ASN:HD22	1.58	0.68
10:A:47:VAL:HB	10:A:48:PRO:HD3	1.75	0.68
1:C1:221:LEU:HD22	1:C1:332:ILE:HG23	1.73	0.68
8:S1:49:ALA:HB2	8:V1:17:ASN:HD22	1.59	0.68
10:A:48:PRO:CG	10:A:79:PHE:HA	2.23	0.68
5:K1:455:ILE:HG12	5:K1:478:MET:HG3	1.74	0.68
5:k1:183:THR:HG22	7:t1:3:LYS:HB3	1.74	0.68
5:m1:99:LEU:HD11	5:m1:192:VAL:HB	1.76	0.68
8:S1:116:VAL:HG12	8:V1:119:VAL:HG23	1.76	0.68
8:T1:86:LEU:HD12	8:T1:87:PRO:HD2	1.75	0.68
3:i1:363:ARG:NH2	3:i1:371:GLU:OE1	2.26	0.68
3:F1:17:ILE:HD13	3:F1:44:GLU:HG2	1.76	0.68
1:C1:2:ILE:HG23	1:C1:313:HIS:CE1	2.29	0.68
6:l1:77:THR:HG22	6:l1:78:LEU:H	1.58	0.68
8:w1:42:VAL:HG21	8:x1:47:MET:HG3	1.75	0.68
1:C1:192:GLN:HE22	1:C1:281:TYR:HB2	1.59	0.67
5:m1:325:GLU:CD	5:m1:353:SER:H	2.03	0.67
8:u1:69:ARG:O	8:u1:72:ASN:ND2	2.28	0.67
5:k1:198:THR:HG22	5:k1:199:ALA:H	1.59	0.67
8:v1:86:LEU:HD12	8:v1:87:PRO:HD2	1.76	0.67
1:C1:4:PRO:HB3	1:C1:314:VAL:HG21	1.76	0.67
1:C1:279:GLN:NE2	1:C1:281:TYR:OH	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P1:168:ALA:HA	7:P1:171:ILE:HD12	1.77	0.67
1:C1:142:PHE:HB2	1:C1:174:VAL:HB	1.77	0.67
5:I1:410:VAL:HG21	5:I1:474:PHE:HZ	1.60	0.67
5:I1:424:THR:HG22	5:I1:425:ASN:H	1.60	0.67
1:C1:141:PHE:CE1	10:A:43:GLN:HA	2.29	0.66
6:J1:208:ASN:O	6:J1:275:ARG:NH1	2.27	0.66
5:m1:364:TYR:HB2	5:m1:365:ASN:HD22	1.60	0.66
1:C1:12:GLU:HB3	9:e1:134:LEU:HB3	1.75	0.66
3:F1:57:GLN:OE1	3:G1:5:ILE:HG13	1.95	0.66
5:I1:70:LYS:NZ	5:I1:117:GLU:OE1	2.28	0.66
3:F1:298:ASP:HB2	3:F1:386:ILE:HD11	1.77	0.66
6:I1:5:ILE:HD11	6:I1:14:ALA:CB	2.21	0.66
7:t1:18:ILE:HD12	7:t1:19:PRO:HD2	1.76	0.66
1:C1:287:GLU:O	1:C1:291:ARG:HG3	1.96	0.66
5:m1:96:VAL:N	5:m1:198:THR:OG1	2.23	0.66
3:F1:87:GLN:OE1	9:e1:206:ARG:NH1	2.28	0.66
8:W1:111:THR:HG22	8:W1:113:GLN:H	1.61	0.66
7:t1:18:ILE:HG13	7:t1:20:GLY:H	1.60	0.66
5:k1:336:VAL:O	5:k1:340:GLN:HG2	1.95	0.66
5:m1:24:GLU:HG2	5:m1:25:GLY:H	1.61	0.66
10:A:75:ALA:O	10:A:76:SER:C	2.39	0.66
3:i1:198:PHE:HB2	6:I1:180:ILE:HD11	1.77	0.66
3:i1:68:CYS:SG	6:I1:23:CYS:HA	2.36	0.65
10:A:74:ASP:O	10:A:75:ALA:C	2.39	0.65
9:e1:299:GLN:OE1	9:e1:341:ARG:NH2	2.29	0.65
3:h1:14:ARG:NH2	3:h1:42:SER:OG	2.29	0.65
3:G1:269:PRO:CD	3:G1:274:LEU:HD12	2.19	0.65
8:W1:99:ILE:HA	8:Y1:101:GLY:HA3	1.79	0.65
5:k1:235:ARG:HG3	5:k1:271:SER:HB2	1.79	0.65
8:v1:15:THR:HG22	8:v1:16:VAL:H	1.60	0.65
3:G1:250:CYS:SG	3:G1:292:LYS:NZ	2.70	0.65
10:A:22:VAL:HG22	10:A:23:PHE:H	1.61	0.65
7:P1:160:THR:HG23	7:P1:162:ASN:H	1.60	0.65
5:m1:133:THR:HG22	5:m1:155:ALA:HB1	1.78	0.65
3:G1:268:SER:CB	3:G1:269:PRO:HD3	2.25	0.65
2:a1:70:ARG:NH2	2:f1:126:GLU:OE2	2.29	0.65
1:C1:2:ILE:HG23	1:C1:313:HIS:HE1	1.61	0.65
7:s1:25:GLN:NE2	7:s1:29:GLU:HG2	2.12	0.65
8:X1:69:ARG:O	8:X1:72:ASN:ND2	2.29	0.65
5:m1:445:PHE:CD1	5:m1:480:TYR:HB2	2.32	0.65
3:F1:59:TRP:HB2	6:J1:100:ALA:HB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G1:325:SER:HB2	3:G1:374:CYS:HB2	1.78	0.64
8:v1:101:GLY:HA3	8:w1:99:ILE:HD12	1.79	0.64
5:I1:377:ARG:HH21	5:K1:497:LEU:HD11	1.61	0.64
1:C1:141:PHE:CE2	10:A:43:GLN:HG3	2.32	0.64
6:J1:217:LYS:NZ	6:J1:220:ASP:OD1	2.25	0.64
6:l1:209:GLU:HG2	6:l1:210:THR:HG23	1.80	0.64
3:G1:173:CYS:SG	3:G1:212:CYS:N	2.71	0.64
7:R1:18:ILE:HD12	7:R1:19:PRO:HD2	1.79	0.64
5:k1:33:GLN:NE2	5:k1:88:ASP:OD2	2.31	0.64
9:U1:27:SER:HB3	9:U1:90:HIS:CE1	2.33	0.63
8:v1:110:VAL:HG21	8:w1:93:PRO:HG3	1.79	0.63
2:a1:70:ARG:HH22	2:f1:128:LEU:HD21	1.62	0.63
9:e1:349:ILE:HD11	9:e1:395:ARG:HG3	1.80	0.63
4:j1:113:VAL:HG13	4:j1:140:LEU:HD22	1.80	0.63
5:k1:111:VAL:HG22	5:k1:179:LEU:HD21	1.81	0.63
5:m1:43:ASP:OD1	5:m1:86:ARG:NH1	2.32	0.63
7:r1:119:VAL:HG13	7:s1:117:ILE:HB	1.80	0.63
8:S1:51:ILE:HD11	8:V1:5:PHE:H	1.64	0.63
9:U1:380:ASN:HD21	9:U1:392:ILE:H	1.46	0.63
3:h1:57:GLN:HE22	3:i1:5:ILE:HG13	1.64	0.63
5:I1:43:ASP:OD1	5:I1:86:ARG:NH1	2.32	0.62
8:S1:99:ILE:HG12	8:T1:99:ILE:HD11	1.81	0.62
8:T1:35:PRO:HD2	8:T1:40:VAL:HG21	1.81	0.62
9:e1:175:MET:HE2	9:e1:221:ALA:HB1	1.81	0.62
9:e1:321:ASN:ND2	3:h1:53:ALA:O	2.32	0.62
3:h1:86:ALA:HB2	3:h1:178:GLU:HG2	1.80	0.62
1:C1:218:ASP:O	1:C1:220:ILE:HD12	1.99	0.62
8:V1:61:PHE:O	8:V1:79:ARG:NH2	2.33	0.62
4:j1:3:CYS:O	4:j1:6:ASP:N	2.32	0.62
8:y1:111:THR:HG22	8:y1:113:GLN:H	1.62	0.62
7:r1:38:PHE:O	7:s1:70:ARG:NH1	2.32	0.62
10:A:48:PRO:HG3	10:A:79:PHE:CD1	2.34	0.62
6:J1:88:ARG:HG3	6:J1:88:ARG:HH11	1.65	0.62
8:v1:52:SER:HB3	8:w1:70:LEU:HD12	1.80	0.62
7:R1:157:LEU:HA	7:R1:166:LEU:HD21	1.81	0.62
8:V1:111:THR:HG23	8:V1:114:GLN:H	1.65	0.62
3:i1:31:ILE:HD13	3:i1:41:VAL:HG21	1.82	0.62
7:r1:160:THR:HG23	7:r1:162:ASN:H	1.64	0.62
1:C1:280:HIS:CD2	1:C1:282:GLY:H	2.18	0.62
5:K1:414:ASN:O	5:K1:416:ASN:N	2.33	0.62
1:C1:278:ILE:HG13	1:C1:296:GLU:OE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:j1:41:CYS:SG	4:j1:42:ASN:N	2.72	0.61
5:I1:115:MET:HG3	5:I1:175:ILE:HD12	1.82	0.61
1:C1:305:LYS:HD3	1:C1:365:PRO:HD2	1.81	0.61
5:I1:498:PHE:HE2	5:I1:500:ASN:CG	2.07	0.61
8:S1:81:ARG:NH1	8:V1:79:ARG:O	2.33	0.61
4:j1:158:ASP:O	4:j1:170:ARG:NH2	2.24	0.61
8:S1:59:ASN:HD21	8:V1:23:ALA:H	1.49	0.61
9:U1:175:MET:HE2	9:U1:221:ALA:HB1	1.82	0.61
5:m1:154:ALA:HB3	5:m1:157:VAL:HB	1.83	0.61
9:U1:163:ILE:HD11	9:U1:168:THR:HA	1.81	0.61
8:w1:98:ARG:HA	8:w1:111:THR:HA	1.83	0.61
5:K1:468:VAL:O	5:K1:470:GLN:NE2	2.33	0.61
3:i1:57:GLN:HE21	6:l1:24:PRO:HB3	1.64	0.61
3:i1:47:MET:HG3	6:l1:89:LEU:HB2	1.83	0.61
7:t1:128:SER:O	7:t1:148:LYS:NZ	2.33	0.61
5:I1:67:SER:O	5:I1:68:LEU:C	2.44	0.61
5:K1:372:ARG:HD3	5:K1:376:ASN:HA	1.83	0.61
7:R1:81:GLU:HG2	7:R1:108:PRO:HA	1.82	0.61
3:i1:90:GLN:OE1	3:i1:211:PRO:HG2	2.00	0.61
9:U1:137:ASN:C	9:U1:139:VAL:H	2.09	0.60
3:G1:72:LEU:HD22	3:G1:185:ARG:HE	1.65	0.60
4:H1:173:ASN:HD22	4:H1:175:TRP:HE1	1.47	0.60
8:S1:34:TYR:HB2	8:T1:48:ASN:HD21	1.66	0.60
5:m1:60:GLN:NE2	5:m1:145:PRO:O	2.34	0.60
7:Q1:156:LEU:HD22	7:Q1:171:ILE:HD13	1.82	0.60
5:m1:115:MET:HG2	5:m1:174:VAL:HG12	1.84	0.60
9:e1:27:SER:HB3	9:e1:90:HIS:CE1	2.37	0.60
9:e1:288:THR:O	9:e1:341:ARG:NH1	2.34	0.60
5:k1:140:VAL:HG21	5:k1:153:ALA:HB2	1.82	0.60
1:C1:135:GLN:HE21	1:C1:179:GLY:H	1.49	0.60
2:g1:9:VAL:HG23	2:g1:37:LEU:HD22	1.83	0.60
5:m1:231:GLN:OE1	5:m1:276:ARG:NH1	2.35	0.60
3:i1:46:ALA:O	3:i1:50:GLU:HG2	2.02	0.60
5:I1:336:VAL:O	5:I1:340:GLN:HG2	2.01	0.60
5:I1:379:ASN:OD1	5:K1:497:LEU:HG	2.02	0.60
8:X1:82:ASN:HD21	8:X1:84:CYS:HB2	1.65	0.60
5:m1:242:TRP:HE1	5:m1:251:GLY:H	1.49	0.60
3:F1:52:TYR:HE2	6:J1:95:ARG:HH21	1.47	0.60
1:C1:141:PHE:CD1	10:A:43:GLN:HA	2.37	0.60
3:F1:50:GLU:OE2	3:G1:20:ARG:NH2	2.35	0.60
7:R1:157:LEU:HD23	7:R1:166:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:43:GLN:HG2	10:A:46:ASP:CA	2.28	0.60
1:C1:142:PHE:HB3	1:C1:145:THR:HG21	1.83	0.60
1:C1:238:ASN:HD22	1:C1:300:ARG:NE	2.00	0.60
8:S1:118:LEU:HD21	8:T1:92:ALA:HB1	1.84	0.60
3:G1:204:LYS:HG2	3:G1:216:VAL:HG13	1.83	0.59
4:H1:113:VAL:HG13	4:H1:140:LEU:HD22	1.84	0.59
10:A:48:PRO:HG3	10:A:79:PHE:HA	1.83	0.59
7:R1:130:THR:HG23	7:R1:131:ILE:HG12	1.84	0.59
8:X1:4:ILE:O	8:X1:46:GLN:NE2	2.33	0.59
3:h1:224:CYS:CB	8:v1:38:CYS:HG	2.10	0.59
1:C1:56:GLU:HG2	1:C1:56:GLU:O	2.02	0.59
7:R1:53:ARG:NH1	7:R1:54:ASP:O	2.36	0.59
7:R1:18:ILE:HG13	7:R1:20:GLY:H	1.66	0.59
1:C1:181:ARG:HE	1:C1:184:ASN:ND2	2.01	0.59
9:e1:349:ILE:HD11	9:e1:395:ARG:HD2	1.84	0.59
3:i1:270:GLN:NE2	3:i1:283:GLY:O	2.35	0.59
3:G1:31:ILE:HD13	3:G1:41:VAL:HG21	1.82	0.59
9:U1:349:ILE:HD11	9:U1:395:ARG:HG3	1.85	0.59
7:P1:39:GLY:HA2	7:Q1:72:ALA:HB3	1.85	0.59
7:Q1:90:PRO:HD2	7:R1:74:THR:HG23	1.85	0.59
5:k1:47:CYS:HA	5:k1:82:TYR:HA	1.84	0.59
8:y1:98:ARG:NH2	8:u1:84:CYS:SG	2.75	0.59
5:K1:243:ASP:OD1	5:K1:244:CYS:N	2.35	0.59
8:y1:61:PHE:HE2	8:y1:76:VAL:HG13	1.68	0.59
5:K1:107:THR:HG22	5:K1:108:ASP:H	1.68	0.59
5:k1:98:THR:HB	5:k1:195:ALA:HB3	1.85	0.59
8:W1:70:LEU:O	8:Y1:56:ASN:ND2	2.36	0.59
3:F1:13:LEU:HD23	3:F1:45:TYR:HE2	1.68	0.58
4:H1:41:CYS:SG	4:H1:42:ASN:N	2.76	0.58
5:I1:215:GLU:HG3	5:K1:329:PRO:HG3	1.83	0.58
7:r1:24:CYS:SG	7:t1:24:CYS:HB2	2.43	0.58
10:A:49:VAL:O	10:A:50:ILE:C	2.45	0.58
3:G1:202:TRP:HE3	3:G1:203:LEU:HD22	1.69	0.58
7:r1:24:CYS:SG	7:t1:24:CYS:CB	2.91	0.58
8:w1:103:PHE:CE2	8:w1:110:VAL:HG23	2.38	0.58
4:H1:111:GLU:HG2	9:U1:10:ALA:HB2	1.86	0.58
10:A:35:VAL:HG12	10:A:46:ASP:HB3	1.85	0.58
1:C1:12:GLU:HB3	9:e1:134:LEU:HD22	1.85	0.58
3:F1:380:LEU:HD11	3:F1:383:VAL:HG23	1.84	0.58
8:W1:93:PRO:HG2	8:Y1:118:LEU:HD22	1.86	0.58
7:t1:38:PHE:N	7:t1:54:ASP:OD1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f1:4:ASN:OD1	2:f1:5:LYS:HG3	2.04	0.58
5:m1:103:GLY:O	5:m1:104:PRO:C	2.47	0.58
9:e1:143:LEU:HD22	9:e1:279:ALA:HB1	1.85	0.58
5:k1:96:VAL:HG22	5:k1:161:THR:HG23	1.85	0.58
9:U1:288:THR:O	9:U1:341:ARG:NH1	2.37	0.58
6:l1:263:GLU:OE1	6:l1:280:ARG:NH2	2.33	0.58
5:K1:223:LEU:HB3	5:K1:255:VAL:HG12	1.84	0.57
10:A:35:VAL:HG22	10:A:36:SER:H	1.69	0.57
10:A:110:GLN:HE21	10:A:112:ASP:CG	2.12	0.57
4:H1:116:ILE:HD13	5:I1:489:ILE:HD11	1.86	0.57
8:X1:10:LEU:HD23	8:X1:14:LEU:HB3	1.84	0.57
6:l1:141:ILE:O	6:l1:152:VAL:HG12	2.04	0.57
5:K1:408:LEU:O	5:K1:409:ALA:C	2.46	0.57
6:J1:31:ASP:HB3	6:J1:34:THR:HG22	1.85	0.57
3:G1:214:THR:HG21	3:G1:245:ARG:HB2	1.85	0.57
4:H1:77:THR:H	5:I1:314:THR:HG22	1.70	0.57
2:a1:18:ASP:OD1	2:a1:20:ASP:N	2.36	0.57
2:a1:47:ASN:HB3	2:a1:55:VAL:HG21	1.86	0.57
7:r1:22:GLU:O	7:r1:23:ASP:C	2.47	0.57
7:Q1:101:ARG:NH1	7:Q1:112:ALA:O	2.38	0.57
5:k1:117:GLU:HG3	5:k1:119:GLU:H	1.69	0.57
8:x1:61:PHE:O	8:x1:79:ARG:NH2	2.38	0.57
1:C1:69:GLY:CA	1:C1:126:ARG:HG3	2.31	0.57
5:I1:194:PHE:HD2	7:R1:9:VAL:HA	1.70	0.57
5:K1:115:MET:HG2	5:K1:174:VAL:HG22	1.87	0.57
5:K1:445:PHE:CD1	5:K1:480:TYR:HB2	2.40	0.57
7:s1:101:ARG:NH1	7:s1:112:ALA:O	2.38	0.57
8:v1:99:ILE:HD11	8:v1:112:VAL:HG22	1.85	0.57
2:E1:42:ASN:HD21	2:E1:97:MET:HE1	1.69	0.57
5:I1:210:ALA:O	5:I1:214:ASN:HB3	2.04	0.57
8:T1:98:ARG:HA	8:T1:111:THR:HA	1.87	0.57
5:k1:174:VAL:HG11	5:k1:284:PRO:HA	1.87	0.57
5:m1:410:VAL:HG21	5:m1:474:PHE:HZ	1.69	0.57
5:I1:60:GLN:NE2	5:I1:145:PRO:HB2	2.20	0.56
5:I1:294:TYR:OH	5:I1:366:ASP:OD1	2.23	0.56
8:y1:83:ILE:HD11	8:z1:86:LEU:HD13	1.87	0.56
1:C1:238:ASN:HD22	1:C1:300:ARG:HE	1.52	0.56
3:G1:363:ARG:NH2	3:G1:371:GLU:OE1	2.36	0.56
5:m1:468:VAL:O	5:m1:470:GLN:NE2	2.37	0.56
8:v1:81:ARG:NH1	8:x1:79:ARG:O	2.37	0.56
2:E1:21:THR:HG23	2:E1:23:GLU:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G1:74:LYS:C	3:G1:76:ALA:H	2.12	0.56
9:U1:33:ARG:NH1	9:U1:52:GLY:O	2.38	0.56
2:f1:41:LYS:NZ	2:f1:43:CYS:O	2.39	0.56
5:k1:415:THR:HB	5:k1:425:ASN:HD22	1.71	0.56
5:m1:93:VAL:HG22	5:m1:201:SER:HB3	1.87	0.56
5:K1:203:ASN:OD1	5:K1:203:ASN:N	2.36	0.56
7:Q1:125:VAL:HG12	7:R1:143:VAL:HB	1.88	0.56
5:k1:43:ASP:OD1	5:k1:86:ARG:NH1	2.38	0.56
5:k1:410:VAL:HG11	5:k1:474:PHE:HZ	1.71	0.56
3:G1:297:LEU:HD23	3:G1:349:VAL:HG22	1.87	0.56
8:v1:59:ASN:HD21	8:x1:23:ALA:H	1.54	0.56
3:h1:59:TRP:HB2	6:l1:100:ALA:HB1	1.88	0.56
5:m1:34:MET:HA	5:m1:62:SER:HB2	1.88	0.56
1:C1:169:ILE:CD1	1:C1:193:ASN:HB3	2.36	0.56
4:H1:6:ASP:O	4:H1:8:ALA:N	2.39	0.56
8:S1:116:VAL:HA	8:S1:119:VAL:HG12	1.87	0.56
5:I1:261:LEU:HD22	5:I1:335:GLU:HG2	1.88	0.56
5:k1:261:LEU:HD22	5:k1:335:GLU:HG2	1.86	0.56
8:X1:95:MET:SD	8:X1:96:ASP:N	2.80	0.55
5:m1:325:GLU:OE1	5:m1:359:THR:HG21	2.05	0.55
3:F1:53:ALA:O	9:U1:321:ASN:ND2	2.40	0.55
3:G1:46:ALA:O	3:G1:50:GLU:HG2	2.06	0.55
7:Q1:116:GLU:CD	7:Q1:116:GLU:H	2.13	0.55
8:T1:15:THR:HG23	8:T1:36:PRO:HD3	1.87	0.55
6:l1:3:VAL:O	6:l1:4:LEU:HB2	2.07	0.55
6:l1:22:CYS:O	6:l1:23:CYS:HB2	2.04	0.55
7:t1:103:ASP:OD1	7:t1:103:ASP:N	2.40	0.55
8:v1:19:ALA:O	8:v1:33:TYR:OH	2.22	0.55
8:v1:48:ASN:HD21	8:x1:34:TYR:H	1.52	0.55
1:C1:214:THR:O	1:C1:326:THR:HG23	2.06	0.55
5:I1:117:GLU:HG3	5:I1:119:GLU:H	1.70	0.55
5:I1:140:VAL:HG21	5:I1:153:ALA:HB2	1.87	0.55
3:i1:278:GLU:HG3	6:l1:181:LYS:HB2	1.88	0.55
5:k1:500:ASN:O	5:k1:501:CYS:SG	2.65	0.55
1:C1:302:ALA:HA	1:C1:364:PRO:CD	2.37	0.55
9:U1:308:GLU:OE1	9:U1:328:ARG:NH1	2.30	0.55
3:i1:11:GLN:NE2	3:i1:15:ASN:OD1	2.39	0.55
5:k1:373:ASP:CG	5:k1:374:GLU:H	2.14	0.55
7:r1:143:VAL:HB	7:t1:125:VAL:HG12	1.89	0.55
1:C1:151:ILE:HG12	1:C1:186:ILE:HG12	1.89	0.55
1:C1:263:GLN:HG3	1:C1:290:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T1:115:LEU:O	8:T1:119:VAL:HG23	2.06	0.55
6:l1:214:VAL:HG12	6:l1:279:ILE:HB	1.89	0.55
7:P1:143:VAL:HB	7:R1:125:VAL:HG12	1.89	0.55
5:k1:348:GLY:HA3	5:k1:364:TYR:OH	2.07	0.55
3:F1:64:PRO:HB2	3:F1:189:LEU:HD21	1.88	0.55
8:W1:116:VAL:HG23	8:Y1:119:VAL:HG23	1.89	0.55
8:Y1:116:VAL:HA	8:Y1:119:VAL:HG12	1.89	0.55
5:k1:455:ILE:HG12	5:k1:478:MET:HG3	1.89	0.55
1:C1:244:LYS:HG3	1:C1:245:GLY:H	1.72	0.55
6:l1:241:ASP:OD1	6:l1:253:LYS:NZ	2.37	0.55
5:m1:111:VAL:HB	5:m1:124:ILE:HG13	1.89	0.55
1:C1:302:ALA:HA	1:C1:364:PRO:HD2	1.89	0.54
7:R1:103:ASP:OD1	7:R1:103:ASP:N	2.40	0.54
8:S1:52:SER:HB2	8:V1:19:ALA:HB2	1.87	0.54
2:g1:51:THR:HG22	2:g1:52:ASN:H	1.72	0.54
6:l1:27:PHE:O	6:l1:30:VAL:HG12	2.06	0.54
1:C1:5:MET:O	1:C1:6:ARG:HG3	2.07	0.54
5:K1:97:TYR:CD1	5:K1:196:GLN:HB2	2.42	0.54
9:e1:132:PHE:O	9:e1:133:GLY:C	2.51	0.54
2:g1:99:LEU:HD12	2:g1:124:ILE:HG12	1.89	0.54
10:A:38:LYS:C	10:A:40:SER:N	2.61	0.54
7:R1:25:GLN:CD	7:R1:26:CYS:H	2.15	0.54
9:U1:73:THR:O	9:U1:77:ILE:HG12	2.07	0.54
8:u1:119:VAL:HG12	8:z1:116:VAL:HG12	1.88	0.54
5:l1:48:VAL:HB	5:l1:81:VAL:HG23	1.88	0.54
5:l1:93:VAL:H	5:l1:201:SER:HB2	1.71	0.54
5:K1:126:VAL:HG22	5:K1:135:ILE:HD12	1.90	0.54
3:h1:48:GLN:HE21	6:l1:88:ARG:HD2	1.72	0.54
6:l1:152:VAL:HG11	6:l1:251:LEU:HD11	1.89	0.54
5:m1:110:ARG:HE	5:m1:125:GLY:HA2	1.72	0.54
5:K1:92:GLY:HA2	5:K1:201:SER:OG	2.08	0.54
9:U1:143:LEU:HD22	9:U1:279:ALA:HB1	1.89	0.54
7:t1:7:LEU:HD12	7:t1:13:PRO:HB3	1.88	0.54
9:U1:61:ARG:NH1	9:U1:119:GLU:OE2	2.41	0.54
8:W1:98:ARG:O	8:Y1:102:CYS:N	2.40	0.54
9:e1:380:ASN:HD21	9:e1:391:ILE:HA	1.73	0.54
6:J1:18:GLU:H	6:J1:18:GLU:CD	2.16	0.54
7:Q1:7:LEU:HD21	7:Q1:15:CYS:HB2	1.90	0.54
9:U1:81:GLU:O	9:e1:33:ARG:NH2	2.41	0.54
9:e1:297:LEU:HD13	4:j1:10:ARG:HH11	1.72	0.54
5:m1:93:VAL:N	5:m1:201:SER:OG	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R1:26:CYS:SG	7:R1:27:TRP:N	2.79	0.54
8:W1:114:GLN:HA	8:W1:117:ASN:HD22	1.73	0.54
5:k1:379:ASN:ND2	5:m1:497:LEU:HD12	2.23	0.54
3:F1:13:LEU:HD23	3:F1:45:TYR:CE2	2.43	0.53
5:I1:373:ASP:OD2	5:I1:374:GLU:N	2.37	0.53
5:K1:96:VAL:H	5:K1:198:THR:HG1	1.53	0.53
5:I1:182:CYS:O	6:J1:28:ALA:HB1	2.08	0.53
5:K1:272:ALA:O	5:K1:388:ARG:NH2	2.41	0.53
8:V1:113:GLN:HE21	8:V1:117:ASN:HD21	1.57	0.53
5:m1:367:VAL:HA	5:m1:384:ASP:HA	1.89	0.53
7:t1:167:THR:OG1	7:t1:170:ASN:OD1	2.23	0.53
2:E1:90:GLU:HG3	2:E1:96:VAL:HG22	1.91	0.53
8:S1:101:GLY:HA3	8:T1:99:ILE:HD12	1.91	0.53
9:e1:349:ILE:HD11	9:e1:395:ARG:CD	2.38	0.53
3:i1:31:ILE:HG23	3:i1:37:GLU:HG3	1.90	0.53
8:X1:82:ASN:HD22	8:X1:85:ASP:H	1.55	0.53
9:e1:349:ILE:HD11	9:e1:395:ARG:CG	2.39	0.53
3:i1:269:PRO:HD2	3:i1:274:LEU:HD12	1.90	0.53
7:r1:39:GLY:HA2	7:s1:72:ALA:HB3	1.90	0.53
8:v1:51:ILE:HD11	8:x1:5:PHE:H	1.72	0.53
8:y1:102:CYS:SG	8:y1:107:SER:HB3	2.48	0.53
1:C1:141:PHE:CB	10:A:43:GLN:H	2.22	0.53
5:m1:488:ARG:NH1	5:m1:490:ASN:HD21	2.06	0.53
8:v1:35:PRO:HG2	8:v1:40:VAL:HG21	1.90	0.53
5:K1:97:TYR:CZ	5:K1:196:GLN:HG3	2.43	0.53
8:v1:116:VAL:HA	8:v1:119:VAL:HG22	1.90	0.53
8:x1:116:VAL:HA	8:x1:119:VAL:HG12	1.91	0.53
8:u1:86:LEU:HD12	8:u1:87:PRO:HD2	1.89	0.53
10:A:71:ASP:O	10:A:72:GLY:C	2.48	0.53
10:A:115:SER:OG	10:A:117:TRP:HB2	2.07	0.53
8:T1:108:SER:OG	8:T1:109:THR:N	2.42	0.53
8:X1:24:THR:HG21	8:X1:29:CYS:O	2.08	0.53
5:m1:103:GLY:HA3	5:m1:189:GLY:O	2.08	0.53
8:u1:40:VAL:HG23	8:z1:44:PRO:HG2	1.90	0.53
1:C1:12:GLU:HG2	9:e1:134:LEU:HB3	1.90	0.53
3:i1:74:LYS:C	3:i1:76:ALA:H	2.16	0.53
1:C1:251:GLY:HA2	10:A:31:THR:HG21	1.91	0.53
7:Q1:121:GLY:O	7:Q1:122:LEU:HD22	2.09	0.53
2:f1:17:THR:HG23	2:f1:84:GLN:HB3	1.90	0.53
6:l1:215:LEU:HD12	6:l1:278:LEU:HD21	1.91	0.53
7:Q1:116:GLU:HG2	7:Q1:117:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T1:74:LYS:O	8:T1:78:ASN:ND2	2.41	0.53
9:e1:85:PRO:HB3	9:e1:99:ALA:HB2	1.90	0.53
3:i1:232:VAL:HG22	3:i1:233:VAL:H	1.73	0.53
8:v1:59:ASN:ND2	8:x1:23:ALA:H	2.07	0.53
8:x1:83:ILE:HA	8:x1:86:LEU:HD23	1.91	0.53
1:C1:162:LEU:HD21	1:C1:164:TRP:HE3	1.73	0.52
5:K1:166:GLY:O	5:K1:200:GLY:HA3	2.09	0.52
3:i1:44:GLU:O	3:i1:45:TYR:C	2.49	0.52
3:i1:72:LEU:HD22	3:i1:185:ARG:HE	1.73	0.52
8:u1:116:VAL:HA	8:u1:119:VAL:HG22	1.91	0.52
10:A:74:ASP:OD1	10:A:74:ASP:N	2.42	0.52
1:C1:137:HIS:CD2	1:C1:138:PRO:HD2	2.43	0.52
3:F1:374:CYS:O	3:F1:376:TYR:CD2	2.59	0.52
8:W1:89:PHE:HB3	8:Y1:110:VAL:HG12	1.91	0.52
3:h1:44:GLU:O	3:h1:45:TYR:C	2.51	0.52
5:K1:377:ARG:O	5:K1:378:PRO:C	2.52	0.52
7:P1:72:ALA:HB3	7:R1:39:GLY:HA2	1.91	0.52
9:e1:322:GLU:O	9:e1:326:GLN:HG2	2.09	0.52
1:C1:58:LEU:HD12	1:C1:60:TYR:CE2	2.45	0.52
3:G1:203:LEU:HB3	3:G1:240:PHE:HZ	1.74	0.52
6:J1:77:THR:HG22	6:J1:78:LEU:H	1.75	0.52
7:R1:164:LEU:H	7:R1:164:LEU:HD12	1.75	0.52
5:k1:242:TRP:HE1	5:k1:251:GLY:H	1.56	0.52
3:F1:391:THR:OG1	3:F1:392:THR:N	2.43	0.52
5:I1:110:ARG:HE	5:I1:125:GLY:HA2	1.74	0.52
5:K1:294:TYR:OH	5:K1:366:ASP:OD1	2.25	0.52
5:K1:310:ILE:O	5:K1:366:ASP:HB2	2.10	0.52
9:e1:128:VAL:HG12	9:e1:129:LEU:H	1.75	0.52
5:k1:215:GLU:HG3	5:m1:329:PRO:HG3	1.91	0.52
5:m1:488:ARG:HH12	5:m1:490:ASN:HD21	1.55	0.52
8:v1:116:VAL:HG12	8:x1:119:VAL:HG23	1.90	0.52
5:I1:67:SER:O	5:I1:70:LYS:N	2.40	0.52
7:P1:160:THR:HB	7:P1:165:ILE:HD13	1.90	0.52
9:e1:33:ARG:NH1	9:e1:52:GLY:O	2.41	0.52
5:m1:213:VAL:HG23	5:m1:216:CYS:HB2	1.91	0.52
3:G1:241:TYR:OH	3:G1:375:ASP:OD1	2.27	0.52
8:T1:60:ALA:HB2	8:V1:74:LYS:HG3	1.90	0.52
4:j1:76:TRP:HE3	5:k1:314:THR:HG21	1.73	0.52
2:a1:84:GLN:NE2	2:a1:101:GLU:HA	2.25	0.52
2:f1:57:ARG:HD2	2:g1:6:GLN:NE2	2.25	0.52
5:m1:53:ASP:OD1	5:m1:53:ASP:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:y1:88:PRO:HG3	8:z1:98:ARG:HH22	1.74	0.52
6:J1:32:GLU:HG3	6:J1:90:ALA:HB3	1.92	0.52
5:k1:174:VAL:CG1	5:k1:284:PRO:HA	2.40	0.52
5:I1:394:THR:HG22	5:I1:444:LEU:HB3	1.90	0.52
5:K1:242:TRP:HE1	5:K1:251:GLY:H	1.58	0.52
7:P1:26:CYS:SG	7:R1:26:CYS:SG	3.01	0.52
9:U1:63:ARG:NH2	2:g1:51:THR:OG1	2.43	0.52
2:a1:17:THR:HG23	2:a1:84:GLN:HB3	1.92	0.52
7:s1:174:PRO:O	7:s1:175:ASP:C	2.53	0.52
1:C1:181:ARG:HE	1:C1:184:ASN:HD21	1.58	0.51
1:C1:194:CYS:HB2	1:C1:295:PHE:HB2	1.93	0.51
8:T1:118:LEU:HD11	8:V1:93:PRO:HG2	1.91	0.51
8:u1:4:ILE:O	8:u1:46:GLN:NE2	2.40	0.51
1:C1:192:GLN:NE2	1:C1:281:TYR:HB2	2.24	0.51
7:P1:165:ILE:HA	7:R1:155:ASN:HD21	1.74	0.51
8:v1:108:SER:OG	8:v1:109:THR:N	2.43	0.51
4:H1:157:VAL:CG2	4:H1:171:ILE:HD11	2.40	0.51
8:z1:108:SER:OG	8:z1:109:THR:N	2.42	0.51
7:Q1:149:LEU:HD11	7:Q1:157:LEU:HB3	1.93	0.51
8:X1:82:ASN:ND2	8:X1:85:ASP:H	2.08	0.51
3:i1:58:MET:HG2	6:l1:27:PHE:CE1	2.45	0.51
5:k1:294:TYR:OH	5:k1:366:ASP:OD1	2.26	0.51
4:H1:148:ILE:HG22	5:I1:489:ILE:HG23	1.93	0.51
8:T1:97:ASP:O	8:T1:112:VAL:HG23	2.11	0.51
2:a1:60:SER:OG	2:a1:61:ASN:N	2.42	0.51
3:i1:187:ARG:O	3:i1:187:ARG:HG3	2.10	0.51
5:m1:106:THR:OG1	5:m1:188:GLU:HB2	2.10	0.51
8:v1:12:CYS:SG	8:v1:13:ASN:N	2.83	0.51
1:C1:4:PRO:O	1:C1:62:MET:N	2.44	0.51
3:G1:47:MET:HG3	6:J1:89:LEU:HB2	1.93	0.51
9:e1:261:GLU:H	9:e1:261:GLU:CD	2.17	0.51
4:H1:171:ILE:HG13	4:H1:174:ALA:HB2	1.93	0.51
8:V1:11:ALA:HB3	8:V1:14:LEU:HD13	1.92	0.51
2:g1:12:ILE:HG12	2:g1:89:VAL:HG22	1.93	0.51
5:k1:101:ILE:HG12	5:k1:192:VAL:HG12	1.93	0.51
8:v1:111:THR:HG22	8:v1:114:GLN:OE1	2.11	0.51
1:C1:33:LEU:HD23	1:C1:57:ILE:HD11	1.91	0.51
3:G1:186:THR:O	3:G1:187:ARG:HB3	2.11	0.51
5:K1:11:VAL:HG11	5:k1:399:ALA:HB1	1.91	0.51
5:K1:310:ILE:O	5:K1:363:ILE:HD11	2.11	0.51
8:T1:42:VAL:HG21	8:V1:47:MET:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W1:115:LEU:O	8:W1:118:LEU:HG	2.10	0.51
3:i1:224:CYS:O	3:i1:225:ALA:HB3	2.10	0.51
5:m1:272:ALA:HB2	5:m1:370:TYR:HD1	1.74	0.51
8:x1:11:ALA:H	8:x1:14:LEU:HD13	1.76	0.51
5:K1:147:PHE:CE2	5:K1:149:TYR:HB2	2.46	0.51
8:T1:23:ALA:H	8:V1:59:ASN:ND2	2.09	0.51
8:v1:113:GLN:HE22	8:v1:117:ASN:HD21	1.59	0.51
8:w1:28:ASP:OD1	8:w1:28:ASP:N	2.44	0.51
8:u1:9:GLY:HA3	8:u1:32:LEU:HB3	1.91	0.51
1:C1:344:VAL:N	1:C1:361:GLU:O	2.43	0.50
4:H1:78:PRO:HG3	4:j1:164:VAL:HG23	1.92	0.50
6:J1:23:CYS:O	6:J1:24:PRO:C	2.54	0.50
7:R1:124:GLU:N	7:R1:124:GLU:OE1	2.44	0.50
7:r1:128:SER:HG	7:s1:144:SER:HG	1.50	0.50
7:t1:167:THR:OG1	7:t1:169:ASP:OD1	2.28	0.50
8:v1:73:LEU:HA	8:v1:76:VAL:HG12	1.93	0.50
10:A:18:PHE:CZ	10:A:67:PHE:HB3	2.46	0.50
1:C1:192:GLN:HB3	1:C1:280:HIS:CE1	2.46	0.50
3:G1:297:LEU:HD22	3:G1:347:PHE:CE2	2.46	0.50
4:H1:176:VAL:HG23	4:H1:178:SER:H	1.77	0.50
8:y1:114:GLN:HA	8:y1:117:ASN:HD22	1.75	0.50
7:P1:128:SER:OG	7:P1:129:ALA:N	2.43	0.50
7:Q1:12:VAL:O	7:Q1:13:PRO:C	2.55	0.50
3:h1:309:ARG:O	3:h1:313:GLU:HG3	2.11	0.50
3:h1:352:ARG:NH2	8:u1:7:SER:O	2.39	0.50
5:m1:269:ASP:O	5:m1:369:ASN:ND2	2.44	0.50
7:r1:19:PRO:HB3	7:s1:18:ILE:HD12	1.93	0.50
1:C1:296:GLU:O	1:C1:300:ARG:HG3	2.10	0.50
7:R1:80:ASN:OD1	7:R1:81:GLU:N	2.45	0.50
9:U1:137:ASN:C	9:U1:139:VAL:N	2.68	0.50
8:W1:113:GLN:O	8:W1:116:VAL:HG12	2.12	0.50
4:H1:121:LEU:HD13	4:H1:138:VAL:HG22	1.94	0.50
7:P1:25:GLN:NE2	7:P1:26:CYS:H	2.10	0.50
9:U1:63:ARG:NH2	9:U1:65:GLN:OE1	2.44	0.50
6:l1:67:ALA:HB3	7:r1:18:ILE:HD11	1.94	0.50
7:r1:49:TYR:HB3	7:r1:66:TRP:HB3	1.92	0.50
8:x1:9:GLY:HA3	8:x1:32:LEU:HB3	1.93	0.50
8:x1:95:MET:CG	8:x1:113:GLN:HG2	2.37	0.50
8:y1:102:CYS:HA	8:y1:107:SER:HA	1.92	0.50
8:y1:115:LEU:O	8:y1:118:LEU:HG	2.10	0.50
3:G1:11:GLN:NE2	3:G1:15:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H1:80:ASN:HD22	5:I1:314:THR:HG23	1.77	0.50
5:K1:34:MET:HA	5:K1:62:SER:HB2	1.93	0.50
2:a1:70:ARG:HD2	2:a1:76:LEU:HD13	1.92	0.50
7:s1:23:ASP:N	7:s1:23:ASP:OD2	2.45	0.50
8:X1:103:PHE:CE2	8:X1:110:VAL:HG13	2.46	0.50
5:k1:29:LEU:HD12	5:k1:82:TYR:O	2.12	0.50
6:l1:4:LEU:HD23	6:l1:13:SER:HB3	1.94	0.50
2:E1:99:LEU:HD12	2:E1:124:ILE:HG12	1.93	0.50
5:K1:367:VAL:HA	5:K1:384:ASP:HA	1.93	0.50
8:S1:51:ILE:HD11	8:V1:4:ILE:HB	1.94	0.50
9:e1:320:ASP:N	9:e1:320:ASP:OD1	2.44	0.50
5:k1:272:ALA:O	5:k1:388:ARG:NH2	2.45	0.50
5:m1:414:ASN:O	5:m1:416:ASN:N	2.44	0.50
8:v1:34:TYR:HB2	8:w1:48:ASN:HD21	1.77	0.50
5:K1:31:GLU:OE1	5:K1:32:GLY:N	2.45	0.50
8:S1:111:THR:HG22	8:S1:114:GLN:HG2	1.93	0.50
2:g1:105:VAL:HG13	2:g1:106:GLU:HG2	1.93	0.50
8:z1:61:PHE:HE2	8:z1:80:ALA:HB2	1.76	0.50
1:C1:364:PRO:O	1:C1:366:PRO:HD3	2.11	0.49
7:P1:120:GLU:HB3	7:Q1:118:SER:O	2.12	0.49
8:T1:100:ALA:HB2	8:V1:83:ILE:HG12	1.94	0.49
8:w1:116:VAL:HA	8:w1:119:VAL:HG22	1.94	0.49
1:C1:25:THR:HG22	1:C1:27:LYS:N	2.24	0.49
1:C1:239:SER:HA	1:C1:270:VAL:HG21	1.95	0.49
5:K1:408:LEU:O	5:K1:410:VAL:HG23	2.12	0.49
8:T1:15:THR:HG22	8:T1:16:VAL:H	1.77	0.49
8:T1:95:MET:HE1	8:T1:116:VAL:HB	1.94	0.49
2:a1:87:VAL:HG21	2:a1:119:ILE:HD13	1.93	0.49
3:h1:44:GLU:C	3:h1:46:ALA:N	2.70	0.49
6:l1:19:TYR:CE1	6:l1:21:GLY:HA2	2.47	0.49
7:s1:169:ASP:OD1	7:s1:170:ASN:N	2.44	0.49
1:C1:217:GLU:HG3	9:U1:134:LEU:HG	1.94	0.49
1:C1:251:GLY:CA	10:A:31:THR:HG21	2.42	0.49
2:a1:26:GLY:HA2	2:a1:28:ILE:HG13	1.93	0.49
3:h1:237:ASN:HB3	3:h1:283:GLY:HA2	1.95	0.49
1:C1:61:ILE:N	1:C1:64:GLU:O	2.46	0.49
4:H1:138:VAL:HG12	4:H1:152:VAL:HG22	1.95	0.49
5:I1:390:LEU:O	5:I1:394:THR:HG23	2.12	0.49
7:P1:165:ILE:HA	7:R1:155:ASN:ND2	2.28	0.49
9:U1:285:TYR:CD2	9:U1:303:ILE:HD11	2.47	0.49
2:g1:51:THR:O	2:g1:53:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:m1:95:ALA:O	5:m1:162:ALA:N	2.43	0.49
7:s1:25:GLN:HE22	7:s1:29:GLU:HG2	1.76	0.49
8:y1:99:ILE:N	8:y1:110:VAL:O	2.40	0.49
2:E1:12:ILE:HG12	2:E1:89:VAL:HG22	1.94	0.49
4:H1:76:TRP:HE3	5:I1:314:THR:HG21	1.78	0.49
6:J1:203:THR:O	6:J1:204:ASP:C	2.52	0.49
3:i1:341:LEU:HD13	3:i1:345:PHE:CD1	2.47	0.49
5:m1:149:TYR:CZ	5:m1:172:LEU:HD22	2.48	0.49
10:A:18:PHE:CE2	10:A:67:PHE:HB3	2.47	0.49
5:I1:364:TYR:HB2	5:I1:365:ASN:HD22	1.78	0.49
5:K1:29:LEU:HD23	5:K1:221:TYR:HD1	1.78	0.49
7:R1:27:TRP:CE3	7:R1:41:VAL:HG11	2.40	0.49
2:a1:30:HIS:NE2	2:a1:79:TYR:OH	2.25	0.49
3:h1:116:TYR:HB3	3:h1:136:VAL:CG1	2.43	0.49
1:C1:322:TRP:HH2	9:U1:131:GLY:CA	2.26	0.49
3:F1:363:ARG:NH2	3:F1:371:GLU:OE1	2.46	0.49
5:K1:71:VAL:HG22	5:K1:296:ALA:HB2	1.94	0.49
8:S1:15:THR:HG22	8:S1:16:VAL:N	2.25	0.49
8:S1:55:ALA:O	8:S1:58:ILE:HG22	2.13	0.49
8:W1:103:PHE:HB3	8:X1:89:PHE:CZ	2.48	0.49
8:v1:15:THR:HG22	8:v1:16:VAL:N	2.26	0.49
3:G1:268:SER:CB	3:G1:269:PRO:CD	2.89	0.49
5:I1:310:ILE:O	5:I1:366:ASP:HB2	2.13	0.49
8:S1:4:ILE:O	8:S1:46:GLN:NE2	2.35	0.49
8:S1:108:SER:OG	8:S1:109:THR:N	2.46	0.49
3:i1:297:LEU:HD22	3:i1:347:PHE:CE2	2.48	0.49
7:s1:8:GLN:O	7:s1:9:VAL:C	2.54	0.49
7:t1:157:LEU:HD23	7:t1:166:LEU:HD11	1.95	0.49
3:F1:188:TYR:CZ	3:F1:192:LEU:HD11	2.48	0.49
5:K1:148:PRO:HA	5:K1:163:ARG:HD2	1.95	0.49
8:X1:113:GLN:HA	8:X1:116:VAL:HG22	1.93	0.49
9:e1:68:ASP:OD1	9:e1:68:ASP:N	2.46	0.49
8:v1:115:LEU:O	8:v1:118:LEU:HG	2.12	0.49
8:u1:46:GLN:HE22	8:z1:51:ILE:HD11	1.78	0.49
1:C1:141:PHE:CE2	10:A:43:GLN:CD	2.91	0.48
3:F1:32:ILE:O	3:F1:35:SER:OG	2.27	0.48
5:I1:327:CYS:SG	5:I1:355:GLN:NE2	2.86	0.48
3:h1:388:ASN:OD1	3:h1:388:ASN:N	2.45	0.48
7:r1:147:VAL:HG13	7:t1:131:ILE:HD11	1.93	0.48
10:A:33:ALA:O	10:A:48:PRO:HA	2.12	0.48
4:H1:157:VAL:HG22	4:H1:171:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J1:147:CYS:HB3	8:T1:37:LYS:HZ1	1.78	0.48
7:Q1:7:LEU:O	7:Q1:8:GLN:HB2	2.14	0.48
7:r1:119:VAL:CG1	7:s1:117:ILE:HB	2.41	0.48
8:x1:95:MET:HE1	8:x1:116:VAL:HG21	1.95	0.48
7:R1:38:PHE:N	7:R1:54:ASP:OD1	2.45	0.48
8:T1:23:ALA:H	8:V1:59:ASN:HD22	1.61	0.48
8:Y1:108:SER:OG	8:Y1:109:THR:N	2.45	0.48
2:a1:47:ASN:HB3	2:a1:55:VAL:CG2	2.43	0.48
3:i1:218:ASP:OD2	3:i1:219:LEU:N	2.42	0.48
3:F1:48:GLN:HE21	6:J1:88:ARG:CD	2.26	0.48
5:K1:181:SER:HA	5:K1:355:GLN:CG	2.43	0.48
7:P1:157:LEU:HD23	7:P1:166:LEU:HD13	1.95	0.48
1:C1:323:ASP:HA	1:C1:326:THR:OG1	2.13	0.48
3:G1:57:GLN:HE21	6:J1:24:PRO:HB3	1.79	0.48
4:H1:169:GLU:O	4:H1:170:ARG:C	2.55	0.48
5:I1:70:LYS:HA	5:I1:70:LYS:HD3	1.54	0.48
5:K1:449:ASP:OD1	5:K1:450:ASN:N	2.46	0.48
7:s1:11:GLY:O	7:s1:12:VAL:HB	2.13	0.48
8:v1:51:ILE:HD11	8:x1:4:ILE:HB	1.96	0.48
2:E1:90:GLU:HB2	5:I1:428:LEU:HD11	1.95	0.48
6:J1:205:ALA:O	6:J1:206:CYS:C	2.55	0.48
5:K1:257:ASN:OD1	5:K1:276:ARG:HD2	2.14	0.48
5:K1:392:ALA:O	5:K1:396:VAL:HG23	2.13	0.48
9:U1:98:ALA:HB1	9:U1:122:PHE:HB3	1.94	0.48
3:h1:51:PHE:HD2	6:l1:92:VAL:HG21	1.78	0.48
5:m1:223:LEU:HD23	5:m1:231:GLN:HG2	1.94	0.48
7:t1:26:CYS:O	7:t1:27:TRP:C	2.56	0.48
1:C1:276:LEU:HD21	1:C1:278:ILE:HG12	1.95	0.48
3:G1:58:MET:HE3	6:J1:27:PHE:CE2	2.49	0.48
5:K1:18:SER:O	5:K1:18:SER:OG	2.30	0.48
7:Q1:118:SER:O	7:Q1:119:VAL:HG22	2.14	0.48
8:S1:25:THR:HG23	8:T1:65:TYR:O	2.14	0.48
5:k1:66:GLU:OE1	5:k1:148:PRO:HG3	2.13	0.48
5:m1:126:VAL:HG22	5:m1:135:ILE:HD12	1.96	0.48
5:m1:252:HIS:HE2	5:m1:275:SER:HG	1.61	0.48
7:r1:167:THR:OG1	7:r1:169:ASP:OD1	2.29	0.48
8:w1:71:ASP:OD1	8:w1:71:ASP:N	2.46	0.48
10:A:110:GLN:HG2	10:A:112:ASP:OD2	2.14	0.48
1:C1:305:LYS:HB3	1:C1:364:PRO:HG3	1.95	0.48
1:C1:311:VAL:HG22	1:C1:358:THR:HB	1.95	0.48
5:I1:167:THR:OG1	5:I1:203:ASN:ND2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I1:195:ALA:O	5:I1:196:GLN:HB3	2.14	0.48
8:S1:34:TYR:N	8:T1:48:ASN:OD1	2.40	0.48
8:Y1:24:THR:OG1	8:Y1:25:THR:N	2.47	0.48
9:e1:213:PHE:CZ	3:h1:310:VAL:HG11	2.49	0.48
3:i1:220:GLY:HA3	3:i1:325:SER:OG	2.13	0.48
5:m1:410:VAL:HG21	5:m1:474:PHE:CZ	2.48	0.48
1:C1:128:LYS:O	1:C1:131:ILE:N	2.39	0.48
7:R1:160:THR:HG23	7:R1:162:ASN:H	1.78	0.48
8:W1:98:ARG:HD2	8:W1:109:THR:OG1	2.14	0.48
5:k1:93:VAL:H	5:k1:201:SER:CB	2.27	0.48
8:w1:71:ASP:OD2	8:w1:75:GLN:NE2	2.43	0.48
8:y1:23:ALA:N	8:u1:59:ASN:HD21	2.08	0.48
5:I1:217:CYS:HB3	5:I1:249:CYS:HB3	1.64	0.48
9:U1:27:SER:HB3	9:U1:90:HIS:HE1	1.76	0.48
3:F1:374:CYS:O	3:F1:376:TYR:N	2.47	0.47
5:I1:35:THR:HG23	5:I1:62:SER:HB3	1.95	0.47
9:U1:320:ASP:OD1	9:U1:320:ASP:N	2.44	0.47
3:i1:68:CYS:HB2	3:i1:71:ASN:HB2	1.96	0.47
3:i1:69:CYS:O	3:i1:73:VAL:HG13	2.14	0.47
4:j1:53:ASN:HB3	4:j1:56:VAL:HG12	1.96	0.47
10:A:115:SER:O	10:A:117:TRP:N	2.47	0.47
1:C1:198:TYR:CZ	1:C1:206:LEU:HD23	2.49	0.47
2:E1:79:TYR:HB3	2:E1:115:VAL:HG11	1.96	0.47
3:G1:188:TYR:C	3:G1:190:GLN:H	2.21	0.47
5:I1:364:TYR:HB2	5:I1:365:ASN:ND2	2.29	0.47
3:i1:300:LEU:HB2	3:i1:385:VAL:HG13	1.96	0.47
4:j1:176:VAL:HG23	4:j1:178:SER:H	1.79	0.47
5:k1:274:LEU:HD12	5:k1:276:ARG:HH12	1.80	0.47
8:y1:116:VAL:HA	8:y1:119:VAL:HG12	1.96	0.47
1:C1:218:ASP:CG	1:C1:329:TYR:HB3	2.39	0.47
9:e1:23:ASP:OD1	9:e1:23:ASP:N	2.39	0.47
6:l1:113:THR:OG1	6:l1:165:GLU:OE2	2.26	0.47
5:m1:28:ILE:HG22	5:m1:81:VAL:HA	1.96	0.47
7:r1:104:LEU:HD22	7:r1:113:ASN:HB3	1.96	0.47
2:E1:93:ASP:OD1	2:E1:93:ASP:N	2.36	0.47
3:G1:186:THR:O	3:G1:187:ARG:CB	2.62	0.47
6:J1:145:THR:HG22	6:J1:146:ASP:OD2	2.13	0.47
5:m1:70:LYS:HA	5:m1:70:LYS:HD3	1.62	0.47
8:y1:67:CYS:HB2	8:z1:3:GLY:HA3	1.96	0.47
4:j1:138:VAL:HG12	4:j1:152:VAL:HG22	1.95	0.47
8:v1:33:TYR:HB3	8:w1:48:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:141:PHE:CE2	10:A:43:GLN:CG	2.98	0.47
1:C1:342:GLU:HB3	1:C1:363:ALA:HB3	1.97	0.47
6:J1:1:MET:HE3	6:J1:1:MET:HB2	1.78	0.47
7:s1:12:VAL:HB	7:s1:13:PRO:HD3	1.96	0.47
1:C1:323:ASP:O	1:C1:343:CYS:HB2	2.15	0.47
3:F1:245:ARG:HH12	3:F1:321:ARG:HE	1.62	0.47
3:F1:374:CYS:O	3:F1:375:ASP:C	2.57	0.47
5:I1:498:PHE:CE2	5:I1:500:ASN:CG	2.90	0.47
8:Y1:95:MET:HG3	8:Y1:113:GLN:OE1	2.14	0.47
5:k1:114:TYR:HB3	5:k1:176:TYR:HB2	1.96	0.47
5:k1:182:CYS:O	6:l1:28:ALA:HB1	2.14	0.47
6:l1:5:ILE:CD1	6:l1:14:ALA:CB	2.91	0.47
8:x1:66:ASP:OD1	8:x1:67:CYS:N	2.47	0.47
8:x1:112:VAL:O	8:x1:116:VAL:HG23	2.15	0.47
8:y1:95:MET:HE2	8:y1:113:GLN:HA	1.96	0.47
8:u1:113:GLN:HA	8:u1:116:VAL:HG22	1.95	0.47
10:A:40:SER:O	10:A:41:GLY:C	2.56	0.47
5:I1:252:HIS:HE2	5:I1:275:SER:HG	1.63	0.47
7:s1:157:LEU:HD21	7:t1:166:LEU:HD12	1.97	0.47
3:F1:52:TYR:CE2	6:J1:95:ARG:NH2	2.81	0.47
3:G1:34:GLU:OE2	4:H1:97:GLY:N	2.47	0.47
5:I1:102:ALA:O	5:I1:190:VAL:HA	2.15	0.47
7:P1:147:VAL:HG12	7:R1:130:THR:HG21	1.97	0.47
8:S1:59:ASN:HD21	8:V1:22:ILE:HA	1.79	0.47
8:T1:28:ASP:OD1	8:T1:28:ASP:N	2.47	0.47
9:e1:297:LEU:HD12	4:j1:10:ARG:HD3	1.96	0.47
2:f1:30:HIS:NE2	2:f1:79:TYR:OH	2.39	0.47
3:h1:5:ILE:O	3:h1:6:GLN:HB2	2.15	0.47
3:i1:200:VAL:HG23	3:i1:238:PHE:CZ	2.49	0.47
8:w1:97:ASP:O	8:w1:112:VAL:HG23	2.15	0.47
5:K1:460:ASP:HB2	5:K1:473:ILE:HB	1.96	0.47
8:T1:15:THR:HG22	8:T1:16:VAL:N	2.30	0.47
8:V1:10:LEU:HD11	8:V1:35:PRO:HB3	1.97	0.47
8:V1:108:SER:OG	8:V1:109:THR:N	2.48	0.47
8:W1:103:PHE:HE2	8:W1:108:SER:C	2.23	0.47
9:e1:138:LEU:O	9:e1:138:LEU:HD23	2.15	0.47
3:h1:65:ARG:HD2	3:h1:66:PHE:CE2	2.49	0.47
3:i1:189:LEU:HA	3:i1:192:LEU:HG	1.97	0.47
6:l1:212:CYS:HA	6:l1:277:CYS:HB3	1.97	0.47
5:m1:131:THR:O	5:m1:135:ILE:HG12	2.15	0.47
8:v1:94:ASP:N	8:v1:97:ASP:OD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:y1:64:THR:OG1	8:z1:25:THR:HG22	2.15	0.47
2:E1:64:MET:HE2	2:E1:66:LEU:HD13	1.96	0.46
3:F1:244:PHE:O	3:F1:251:GLY:HA2	2.15	0.46
3:G1:70:GLU:HA	3:G1:73:VAL:HG22	1.97	0.46
8:S1:47:MET:HE1	8:V1:50:VAL:HG21	1.97	0.46
8:W1:116:VAL:HA	8:W1:119:VAL:HG12	1.96	0.46
5:k1:216:CYS:HB2	5:m1:327:CYS:HB3	1.64	0.46
5:k1:308:LEU:O	5:k1:389:ARG:NH2	2.48	0.46
5:m1:110:ARG:NE	5:m1:125:GLY:HA2	2.30	0.46
8:y1:111:THR:H	8:y1:114:GLN:NE2	2.12	0.46
8:z1:116:VAL:O	8:z1:119:VAL:HG12	2.14	0.46
1:C1:161:VAL:HG13	1:C1:204:LYS:HG2	1.96	0.46
1:C1:255:ASN:HA	1:C1:259:VAL:HG23	1.97	0.46
1:C1:355:THR:HB	1:C1:356:LEU:H	1.34	0.46
9:U1:303:ILE:HD12	9:U1:338:MET:HE2	1.97	0.46
2:a1:79:TYR:HB3	2:a1:115:VAL:HG11	1.97	0.46
5:m1:272:ALA:O	5:m1:388:ARG:NH2	2.48	0.46
1:C1:141:PHE:CZ	10:A:43:GLN:HA	2.50	0.46
3:G1:94:ARG:HB2	3:G1:168:TYR:HE1	1.79	0.46
4:H1:173:ASN:O	4:H1:176:VAL:HG22	2.15	0.46
7:r1:25:GLN:O	7:r1:26:CYS:C	2.58	0.46
1:C1:12:GLU:CB	9:e1:134:LEU:HD22	2.45	0.46
3:F1:309:ARG:HG2	3:F1:313:GLU:OE2	2.16	0.46
6:J1:141:ILE:HG22	6:J1:255:ILE:HD13	1.97	0.46
8:W1:12:CYS:HB3	8:W1:20:CYS:HB3	1.74	0.46
5:k1:29:LEU:HD11	5:k1:84:LEU:HB2	1.98	0.46
5:k1:392:ALA:O	5:k1:396:VAL:HG23	2.16	0.46
5:m1:66:GLU:OE1	5:m1:120:TYR:OH	2.29	0.46
7:r1:149:LEU:HD23	7:r1:149:LEU:H	1.80	0.46
8:x1:15:THR:HG21	8:x1:33:TYR:HB2	1.96	0.46
8:y1:88:PRO:HB3	8:z1:98:ARG:HH12	1.78	0.46
8:u1:15:THR:OG1	8:u1:16:VAL:N	2.48	0.46
1:C1:302:ALA:HA	1:C1:364:PRO:HG2	1.97	0.46
2:E1:31:GLU:OE1	2:f1:52:ASN:ND2	2.49	0.46
6:J1:51:ARG:HB3	6:J1:52:PRO:HD3	1.97	0.46
4:j1:142:TYR:HE2	4:j1:147:LYS:HE2	1.80	0.46
5:k1:210:ALA:O	5:k1:214:ASN:HB3	2.15	0.46
5:k1:378:PRO:O	5:k1:379:ASN:ND2	2.48	0.46
5:I1:64:LEU:C	5:I1:66:GLU:H	2.23	0.46
8:X1:83:ILE:N	8:Y1:107:SER:OG	2.48	0.46
7:s1:131:ILE:HG21	7:t1:145:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:x1:69:ARG:HH22	8:x1:75:GLN:HG3	1.79	0.46
3:G1:195:GLN:HG2	6:J1:178:GLY:HA3	1.98	0.46
4:H1:103:VAL:HG11	4:H1:116:ILE:HG12	1.98	0.46
6:J1:147:CYS:HB3	8:T1:37:LYS:NZ	2.31	0.46
8:S1:60:ALA:HA	8:T1:74:LYS:NZ	2.31	0.46
3:h1:57:GLN:NE2	3:i1:5:ILE:HG13	2.28	0.46
4:j1:171:ILE:HG13	4:j1:172:SER:H	1.80	0.46
7:s1:116:GLU:CD	7:s1:116:GLU:H	2.23	0.46
8:y1:99:ILE:HB	8:y1:110:VAL:HG13	1.97	0.46
5:I1:178:ASN:OD1	5:I1:183:THR:HG21	2.16	0.46
3:h1:217:PHE:HE2	3:h1:243:LEU:HD12	1.81	0.46
3:i1:298:ASP:HB3	3:i1:348:ASN:ND2	2.30	0.46
8:T1:84:CYS:HB3	8:V1:102:CYS:HB3	1.71	0.46
2:a1:104:VAL:O	2:f1:47:ASN:ND2	2.49	0.46
5:m1:107:THR:OG1	5:m1:108:ASP:N	2.49	0.46
10:A:33:ALA:HB3	10:A:49:VAL:HG11	1.98	0.46
3:G1:74:LYS:C	3:G1:76:ALA:N	2.73	0.46
5:I1:49:THR:OG1	5:I1:50:SER:N	2.49	0.46
5:K1:181:SER:O	5:K1:183:THR:N	2.49	0.46
8:S1:22:ILE:HG23	8:T1:59:ASN:HD21	1.81	0.46
8:Y1:116:VAL:O	8:Y1:120:LEU:HG	2.17	0.46
9:e1:393:SER:OG	9:e1:394:GLU:N	2.38	0.46
3:i1:204:LYS:HG2	3:i1:216:VAL:HG13	1.97	0.46
3:F1:218:ASP:OD2	3:F1:219:LEU:N	2.49	0.45
7:Q1:169:ASP:OD1	7:Q1:170:ASN:N	2.48	0.45
9:U1:110:VAL:HG22	9:e1:25:ASP:OD1	2.17	0.45
9:e1:261:GLU:OE2	9:e1:261:GLU:N	2.39	0.45
5:k1:19:LEU:HD23	5:k1:19:LEU:H	1.81	0.45
8:v1:25:THR:HG22	8:w1:65:TYR:O	2.15	0.45
8:y1:12:CYS:SG	8:y1:13:ASN:N	2.89	0.45
1:C1:127:THR:OG1	1:C1:199:GLU:OE2	2.31	0.45
3:G1:387:ASN:ND2	6:l1:130:CYS:HB3	2.31	0.45
5:I1:438:GLN:HA	5:I1:441:VAL:HG23	1.98	0.45
5:K1:10:PHE:O	5:m1:488:ARG:HA	2.16	0.45
7:R1:128:SER:O	7:R1:148:LYS:NZ	2.41	0.45
9:U1:315:LYS:HE2	9:U1:315:LYS:HB3	1.70	0.45
7:t1:12:VAL:HG13	7:t1:13:PRO:HD2	1.98	0.45
1:C1:135:GLN:HG3	1:C1:179:GLY:HA2	1.98	0.45
3:F1:65:ARG:NH1	6:J1:119:ARG:HB2	2.31	0.45
3:F1:67:ALA:O	3:F1:185:ARG:NH2	2.49	0.45
3:G1:93:VAL:HG12	3:G1:94:ARG:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I1:446:SER:OG	5:I1:447:GLU:N	2.50	0.45
7:P1:19:PRO:HG2	7:Q1:20:GLY:HA2	1.98	0.45
8:T1:75:GLN:HA	8:T1:78:ASN:HD22	1.81	0.45
9:U1:198:LYS:HD3	9:U1:199:TRP:CZ3	2.51	0.45
8:W1:12:CYS:SG	8:W1:13:ASN:N	2.89	0.45
8:X1:15:THR:OG1	8:X1:16:VAL:N	2.49	0.45
8:X1:114:GLN:NE2	8:Y1:93:PRO:HD3	2.31	0.45
2:g1:79:TYR:HB3	2:g1:115:VAL:HG11	1.99	0.45
3:i1:209:GLU:O	3:i1:210:TRP:C	2.59	0.45
5:k1:21:PHE:CG	5:k1:22:PHE:N	2.83	0.45
5:k1:269:ASP:N	5:k1:269:ASP:OD1	2.48	0.45
8:w1:54:ILE:O	8:w1:58:ILE:HG12	2.16	0.45
1:C1:272:ALA:O	1:C1:274:ILE:HD12	2.17	0.45
3:G1:54:PHE:CD2	3:G1:58:MET:HE1	2.52	0.45
3:G1:58:MET:HE2	3:G1:58:MET:HB2	1.62	0.45
4:H1:110:ARG:HG3	4:H1:143:ARG:HH11	1.81	0.45
5:I1:6:LEU:HD23	5:k1:333:PHE:CE1	2.51	0.45
6:J1:141:ILE:O	6:J1:152:VAL:HG12	2.16	0.45
5:K1:200:GLY:O	5:K1:201:SER:C	2.59	0.45
8:S1:58:ILE:HD12	8:S1:58:ILE:HA	1.84	0.45
9:e1:68:ASP:O	9:e1:72:GLN:HG2	2.16	0.45
4:j1:145:SER:H	4:j1:147:LYS:NZ	2.14	0.45
5:k1:35:THR:OG1	5:k1:59:GLY:HA3	2.16	0.45
6:l1:180:ILE:HD12	6:l1:180:ILE:HA	1.88	0.45
1:C1:5:MET:HA	1:C1:60:TYR:O	2.17	0.45
1:C1:251:GLY:C	10:A:31:THR:HG21	2.40	0.45
8:W1:45:LEU:HD22	8:Y1:16:VAL:HG22	1.99	0.45
2:a1:128:LEU:HD23	2:a1:128:LEU:HA	1.80	0.45
5:k1:26:CYS:CB	5:k1:79:VAL:HG12	2.47	0.45
5:k1:353:SER:HB3	5:k1:357:ASN:HB3	1.98	0.45
5:k1:373:ASP:CG	5:k1:374:GLU:N	2.75	0.45
5:m1:310:ILE:O	5:m1:366:ASP:HB2	2.16	0.45
5:m1:325:GLU:OE2	5:m1:353:SER:HB3	2.17	0.45
10:A:24:LYS:HB3	10:A:24:LYS:HE2	1.68	0.45
1:C1:12:GLU:CB	9:e1:134:LEU:HB3	2.47	0.45
1:C1:12:GLU:CG	9:e1:134:LEU:HD13	2.47	0.45
3:F1:81:VAL:HG12	3:F1:184:PHE:HE2	1.80	0.45
5:K1:130:ASP:HB3	5:K1:135:ILE:HD11	1.99	0.45
7:Q1:141:ASP:OD1	7:Q1:141:ASP:N	2.49	0.45
7:R1:167:THR:OG1	7:R1:169:ASP:OD2	2.23	0.45
8:S1:73:LEU:HB3	8:V1:57:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:m1:203:ASN:HD21	5:m1:227:ASP:HB2	1.81	0.45
8:v1:98:ARG:HB2	8:x1:102:CYS:HB3	1.98	0.45
1:C1:220:ILE:HG13	1:C1:331:GLU:HB3	1.99	0.45
5:I1:179:LEU:HD12	5:I1:190:VAL:HG23	1.99	0.45
5:I1:424:THR:HG22	5:I1:425:ASN:N	2.30	0.45
7:P1:26:CYS:SG	7:R1:26:CYS:HB2	2.56	0.45
3:h1:221:PRO:C	3:h1:223:CYS:H	2.24	0.45
6:l1:194:LYS:NZ	6:l1:223:ASP:OD2	2.47	0.45
8:v1:102:CYS:N	8:w1:98:ARG:O	2.50	0.45
8:y1:77:LEU:HG	8:z1:61:PHE:CZ	2.52	0.45
3:G1:365:THR:HG22	3:G1:366:SER:H	1.82	0.45
5:K1:70:LYS:HD3	5:K1:70:LYS:HA	1.66	0.45
5:K1:260:THR:HG22	5:K1:263:GLN:OE1	2.16	0.45
7:P1:158:SER:OG	7:P1:159:ALA:N	2.49	0.45
9:e1:329:ALA:O	9:e1:332:VAL:HG12	2.17	0.45
3:i1:186:THR:O	3:i1:187:ARG:CB	2.64	0.45
4:j1:173:ASN:HD22	4:j1:175:TRP:NE1	2.07	0.45
5:m1:93:VAL:HG22	5:m1:201:SER:CB	2.47	0.45
8:w1:118:LEU:HD11	8:x1:93:PRO:HG2	1.99	0.45
8:z1:12:CYS:SG	8:z1:13:ASN:N	2.90	0.45
1:C1:44:THR:HG23	1:C1:45:LYS:HD3	1.99	0.45
1:C1:190:CYS:HB2	1:C1:195:HIS:HB2	1.98	0.45
3:G1:387:ASN:HD22	6:l1:130:CYS:HB3	1.82	0.45
7:Q1:151:PRO:HD2	7:R1:162:ASN:HD21	1.82	0.45
8:W1:46:GLN:HE22	8:X1:47:MET:HE3	1.81	0.45
8:X1:12:CYS:SG	8:X1:13:ASN:N	2.90	0.45
2:a1:99:LEU:HD12	2:a1:124:ILE:HG12	1.98	0.45
9:e1:73:THR:O	9:e1:77:ILE:HG12	2.17	0.45
3:h1:190:GLN:HG2	3:h1:195:GLN:NE2	2.32	0.45
3:i1:45:TYR:O	3:i1:46:ALA:C	2.57	0.45
5:m1:104:PRO:O	5:m1:105:ALA:HB2	2.17	0.45
5:m1:147:PHE:CE2	5:m1:149:TYR:HB2	2.52	0.45
7:t1:53:ARG:NH1	7:t1:54:ASP:O	2.50	0.45
8:v1:65:TYR:O	8:x1:25:THR:HG23	2.17	0.45
8:w1:112:VAL:O	8:w1:116:VAL:HG23	2.16	0.45
3:F1:43:LEU:O	3:F1:44:GLU:C	2.59	0.45
5:K1:136:ALA:HB1	5:K1:158:ILE:HD11	1.99	0.45
4:j1:148:ILE:HB	5:k1:489:ILE:HG22	1.99	0.45
5:m1:114:TYR:CZ	5:m1:324:PRO:HD3	2.52	0.45
8:y1:89:PHE:HB3	8:z1:110:VAL:HG22	1.97	0.45
10:A:23:PHE:CE1	10:A:58:PRO:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:154:LEU:HD21	1:C1:176:LEU:HD13	1.99	0.44
5:K1:166:GLY:HA2	5:K1:200:GLY:O	2.16	0.44
7:P1:130:THR:OG1	7:Q1:147:VAL:HG12	2.16	0.44
8:S1:15:THR:HG21	8:S1:34:TYR:O	2.17	0.44
8:T1:95:MET:HG3	8:T1:113:GLN:HG3	1.99	0.44
5:m1:272:ALA:HB2	5:m1:370:TYR:CD1	2.52	0.44
5:m1:497:LEU:HD13	5:m1:497:LEU:H	1.82	0.44
7:r1:157:LEU:HD23	7:r1:166:LEU:HD13	1.99	0.44
7:t1:124:GLU:N	7:t1:124:GLU:OE1	2.50	0.44
8:y1:23:ALA:H	8:u1:59:ASN:ND2	2.09	0.44
8:z1:115:LEU:O	8:z1:118:LEU:HG	2.17	0.44
10:A:20:ARG:HH11	10:A:20:ARG:HB3	1.82	0.44
1:C1:342:GLU:O	1:C1:363:ALA:N	2.50	0.44
3:G1:18:ALA:HB1	3:G1:31:ILE:HD12	1.98	0.44
8:W1:58:ILE:HG21	8:W1:65:TYR:HB2	1.98	0.44
3:i1:212:CYS:O	3:i1:244:PHE:HD1	2.01	0.44
6:l1:4:LEU:CD2	6:l1:13:SER:HB3	2.48	0.44
5:m1:34:MET:HE2	5:m1:42:PRO:HG3	2.00	0.44
8:x1:112:VAL:O	8:x1:115:LEU:HG	2.18	0.44
8:z1:48:ASN:HA	8:z1:51:ILE:HD12	2.00	0.44
8:z1:113:GLN:O	8:z1:117:ASN:ND2	2.49	0.44
6:J1:61:THR:OG1	6:J1:62:GLU:OE2	2.35	0.44
3:h1:298:ASP:OD1	3:h1:386:ILE:HB	2.18	0.44
4:j1:173:ASN:O	4:j1:176:VAL:HG22	2.17	0.44
6:l1:1:MET:HE3	6:l1:1:MET:HB3	1.62	0.44
4:H1:139:ASP:HB2	4:H1:151:THR:HG23	1.99	0.44
6:J1:40:VAL:HG12	6:J1:53:LYS:HG2	2.00	0.44
8:S1:68:SER:OG	8:S1:69:ARG:N	2.51	0.44
8:T1:44:PRO:O	8:T1:48:ASN:ND2	2.50	0.44
8:V1:83:ILE:HA	8:V1:86:LEU:HD23	2.00	0.44
8:V1:112:VAL:O	8:V1:115:LEU:HG	2.17	0.44
8:W1:64:THR:OG1	8:Y1:25:THR:HG22	2.17	0.44
8:X1:83:ILE:O	8:X1:84:CYS:C	2.60	0.44
3:i1:34:GLU:OE2	4:j1:97:GLY:N	2.51	0.44
7:r1:83:SER:HB2	7:r1:85:TYR:CZ	2.53	0.44
10:A:22:VAL:HG13	10:A:23:PHE:N	2.31	0.44
3:G1:94:ARG:HB2	3:G1:168:TYR:CE1	2.52	0.44
5:I1:223:LEU:HB3	5:I1:255:VAL:HG12	1.99	0.44
9:U1:63:ARG:HH21	9:U1:65:GLN:CD	2.26	0.44
9:U1:67:ASN:HD21	9:e1:3:GLY:HA3	1.83	0.44
9:U1:138:LEU:HD11	9:U1:336:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W1:61:PHE:HE2	8:W1:76:VAL:HG13	1.82	0.44
3:h1:393:SER:OG	3:h1:394:GLY:N	2.50	0.44
3:i1:70:GLU:HA	3:i1:73:VAL:HG22	1.98	0.44
3:i1:244:PHE:O	3:i1:251:GLY:HA2	2.18	0.44
5:m1:497:LEU:H	5:m1:497:LEU:HD22	1.81	0.44
8:w1:107:SER:O	8:x1:86:LEU:HD12	2.17	0.44
5:I1:110:ARG:HH21	5:I1:124:ILE:C	2.24	0.44
9:U1:274:ARG:HH12	9:U1:309:GLN:NE2	2.15	0.44
5:m1:245:SER:OG	5:m1:246:LYS:N	2.49	0.44
1:C1:242:THR:HG22	1:C1:264:THR:OG1	2.18	0.44
3:F1:214:THR:HG21	3:F1:245:ARG:HB2	2.00	0.44
3:G1:265:LEU:HD12	3:G1:276:GLU:HB2	1.99	0.44
6:J1:152:VAL:HG11	6:J1:251:LEU:HD11	1.99	0.44
7:Q1:152:ASP:HB3	7:Q1:155:ASN:HB2	1.98	0.44
8:W1:98:ARG:HB2	8:Y1:102:CYS:HB2	2.00	0.44
5:m1:33:GLN:HA	5:m1:86:ARG:O	2.18	0.44
8:u1:114:GLN:HE21	8:z1:93:PRO:HD3	1.83	0.44
1:C1:181:ARG:HD2	1:C1:183:TYR:CE1	2.53	0.44
3:F1:52:TYR:HE2	6:J1:95:ARG:NH2	2.15	0.44
5:I1:269:ASP:N	5:I1:269:ASP:OD1	2.50	0.44
5:K1:376:ASN:C	5:K1:377:ARG:HG2	2.42	0.44
8:T1:112:VAL:O	8:T1:116:VAL:HG23	2.17	0.44
8:X1:13:ASN:N	8:X1:13:ASN:OD1	2.51	0.44
8:X1:83:ILE:HD12	8:Y1:107:SER:HB3	2.00	0.44
8:Y1:112:VAL:O	8:Y1:115:LEU:HG	2.17	0.44
9:e1:17:PHE:CE2	9:e1:18:LYS:HE2	2.53	0.44
3:i1:304:THR:HG22	3:i1:306:ALA:H	1.83	0.44
5:m1:51:GLU:OE1	5:m1:51:GLU:N	2.51	0.44
5:m1:107:THR:HG23	5:m1:187:PRO:HA	2.00	0.44
5:m1:373:ASP:CG	5:m1:374:GLU:H	2.24	0.44
7:t1:166:LEU:HD23	7:t1:166:LEU:HA	1.84	0.44
8:w1:103:PHE:HD2	8:w1:108:SER:HB3	1.82	0.44
8:y1:22:ILE:HA	8:u1:59:ASN:ND2	2.33	0.44
8:y1:25:THR:HG23	8:u1:65:TYR:O	2.17	0.44
3:G1:111:PHE:HB3	3:G1:149:VAL:HG11	1.99	0.44
5:I1:19:LEU:HD23	5:I1:19:LEU:H	1.82	0.44
6:J1:27:PHE:HE2	6:J1:97:ILE:HG22	1.82	0.44
5:K1:131:THR:O	5:K1:135:ILE:HG12	2.18	0.44
5:K1:226:ASP:OD1	5:K1:226:ASP:N	2.48	0.44
9:U1:131:GLY:O	9:U1:132:PHE:C	2.59	0.44
8:W1:81:ARG:HH21	8:Y1:86:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i1:58:MET:HE2	3:i1:58:MET:HB2	1.65	0.44
3:i1:189:LEU:H	3:i1:189:LEU:HD23	1.83	0.44
8:z1:112:VAL:O	8:z1:115:LEU:HG	2.18	0.44
10:A:33:ALA:HB3	10:A:49:VAL:CG1	2.48	0.44
3:G1:198:PHE:CE1	3:G1:203:LEU:HD21	2.53	0.43
8:S1:101:GLY:HA3	8:T1:99:ILE:HA	1.99	0.43
8:W1:65:TYR:O	8:Y1:25:THR:HG23	2.17	0.43
5:k1:108:ASP:OD2	5:k1:128:ALA:N	2.50	0.43
1:C1:141:PHE:HB2	10:A:42:THR:HA	2.00	0.43
5:I1:377:ARG:HH21	5:K1:497:LEU:CD1	2.29	0.43
5:K1:98:THR:HB	5:K1:195:ALA:HB3	1.99	0.43
5:K1:105:ALA:HB2	5:K1:130:ASP:HB2	2.00	0.43
8:S1:102:CYS:O	8:T1:97:ASP:HB3	2.18	0.43
2:g1:90:GLU:HG3	2:g1:96:VAL:HG22	1.99	0.43
5:m1:390:LEU:HD12	5:m1:390:LEU:HA	1.83	0.43
7:r1:160:THR:OG1	7:r1:161:ALA:N	2.50	0.43
8:v1:60:ALA:HA	8:w1:74:LYS:NZ	2.34	0.43
8:y1:83:ILE:HB	8:u1:107:SER:OG	2.18	0.43
8:z1:116:VAL:HA	8:z1:119:VAL:HG12	1.99	0.43
10:A:43:GLN:C	10:A:45:GLU:N	2.70	0.43
3:G1:312:GLU:O	3:G1:316:THR:HG23	2.18	0.43
5:I1:187:PRO:O	5:I1:190:VAL:HG22	2.18	0.43
6:J1:146:ASP:OD2	6:J1:146:ASP:N	2.48	0.43
8:S1:23:ALA:H	8:T1:59:ASN:ND2	2.17	0.43
9:U1:129:LEU:HD22	9:U1:129:LEU:HA	1.74	0.43
8:W1:25:THR:HG23	8:X1:65:TYR:O	2.17	0.43
5:k1:333:PHE:CE1	6:l1:51:ARG:HG3	2.53	0.43
6:l1:157:PRO:HD2	6:l1:160:LEU:HD23	1.99	0.43
5:m1:294:TYR:OH	5:m1:366:ASP:OD1	2.35	0.43
8:x1:69:ARG:NH2	8:x1:75:GLN:HG3	2.33	0.43
1:C1:57:ILE:HD11	1:C1:123:ALA:CB	2.49	0.43
3:F1:29:ALA:HB3	4:H1:47:VAL:HG22	2.00	0.43
3:F1:348:ASN:OD1	3:F1:348:ASN:N	2.52	0.43
3:G1:169:GLY:O	3:G1:170:GLY:C	2.60	0.43
5:I1:93:VAL:H	5:I1:201:SER:CB	2.31	0.43
5:I1:214:ASN:OD1	5:I1:214:ASN:N	2.52	0.43
5:I1:466:LYS:HB2	5:I1:466:LYS:HE2	1.73	0.43
6:J1:22:CYS:O	6:J1:22:CYS:SG	2.77	0.43
8:V1:112:VAL:O	8:V1:116:VAL:HG23	2.18	0.43
3:h1:64:PRO:HB2	3:h1:189:LEU:HD21	2.00	0.43
5:k1:226:ASP:OD1	5:k1:226:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l1:2:ASN:N	6:l1:2:ASN:OD1	2.52	0.43
5:m1:200:GLY:O	5:m1:201:SER:OG	2.35	0.43
7:t1:87:GLN:HG2	7:t1:88:TYR:CD2	2.53	0.43
3:F1:217:PHE:O	3:F1:240:PHE:HB2	2.19	0.43
3:G1:297:LEU:HD22	3:G1:347:PHE:HE2	1.83	0.43
5:l1:196:GLN:O	5:l1:196:GLN:HG3	2.19	0.43
6:j1:67:ALA:HB3	7:P1:18:ILE:HD11	2.01	0.43
7:P1:166:LEU:HB2	7:R1:157:LEU:HD21	2.01	0.43
7:Q1:166:LEU:HD12	7:Q1:166:LEU:HA	1.79	0.43
8:S1:60:ALA:HA	8:T1:74:LYS:HZ2	1.82	0.43
8:X1:84:CYS:C	8:X1:86:LEU:N	2.75	0.43
2:g1:64:MET:HE2	2:g1:66:LEU:HD13	1.99	0.43
4:j1:3:CYS:O	4:j1:5:VAL:N	2.52	0.43
5:k1:167:THR:OG1	5:k1:203:ASN:ND2	2.48	0.43
5:k1:223:LEU:HB3	5:k1:255:VAL:HG12	2.01	0.43
7:s1:149:LEU:H	7:s1:149:LEU:HD23	1.83	0.43
8:v1:89:PHE:HE1	8:x1:106:GLN:HE21	1.66	0.43
1:C1:241:ILE:HG12	1:C1:276:LEU:HD22	1.99	0.43
7:Q1:49:TYR:HB3	7:Q1:66:TRP:HB3	2.00	0.43
8:S1:67:CYS:HB3	8:V1:29:CYS:HB3	1.67	0.43
9:U1:274:ARG:HH12	9:U1:309:GLN:CD	2.26	0.43
8:Y1:61:PHE:HE2	8:Y1:80:ALA:HB2	1.84	0.43
3:h1:6:GLN:O	3:h1:7:ARG:HB2	2.18	0.43
3:h1:374:CYS:O	3:h1:376:TYR:HD2	2.02	0.43
7:r1:160:THR:HB	7:r1:165:ILE:HD13	2.00	0.43
8:y1:113:GLN:NE2	8:y1:117:ASN:HD21	2.17	0.43
1:C1:164:TRP:CZ3	1:C1:207:ILE:HG21	2.54	0.43
3:G1:244:PHE:O	3:G1:251:GLY:HA2	2.19	0.43
5:l1:422:ILE:HG22	5:l1:422:ILE:O	2.19	0.43
5:K1:113:LEU:HB2	5:K1:122:VAL:HG22	2.00	0.43
5:K1:321:ILE:O	5:K1:361:PRO:HD2	2.19	0.43
7:P1:41:VAL:HG12	7:Q1:71:PRO:HG2	2.01	0.43
7:R1:27:TRP:CD1	7:R1:48:LEU:HD21	2.54	0.43
9:U1:105:VAL:HG11	9:e1:93:ARG:NH2	2.34	0.43
8:V1:103:PHE:CE2	8:V1:110:VAL:HG13	2.54	0.43
8:W1:103:PHE:HA	8:X1:97:ASP:CG	2.43	0.43
9:e1:294:ASN:HD22	4:j1:10:ARG:HD2	1.84	0.43
5:k1:379:ASN:HD21	5:m1:497:LEU:HD12	1.81	0.43
7:r1:90:PRO:HD2	7:s1:74:THR:HB	2.01	0.43
7:s1:132:ASP:HB3	7:s1:146:ASP:OD1	2.19	0.43
8:v1:27:ASP:O	8:v1:30:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:v1:67:CYS:HB3	8:x1:29:CYS:HB3	1.67	0.43
8:z1:112:VAL:O	8:z1:116:VAL:HG22	2.19	0.43
1:C1:52:VAL:C	1:C1:54:GLY:N	2.75	0.43
3:F1:65:ARG:HD2	3:F1:66:PHE:CE1	2.54	0.43
6:J1:73:ASP:N	6:J1:73:ASP:OD1	2.51	0.43
7:P1:31:THR:OG1	7:P1:33:ASP:OD2	2.28	0.43
8:S1:22:ILE:HG23	8:T1:59:ASN:ND2	2.34	0.43
8:T1:107:SER:O	8:V1:86:LEU:HD12	2.18	0.43
5:m1:241:ALA:HB1	5:m1:249:CYS:O	2.18	0.43
5:m1:269:ASP:OD1	5:m1:269:ASP:N	2.51	0.43
5:I1:115:MET:HE2	5:I1:115:MET:HB2	1.95	0.43
5:I1:242:TRP:CZ2	5:I1:250:PHE:HB3	2.54	0.43
6:J1:105:ASP:OD2	6:J1:106:PRO:HD2	2.19	0.43
9:e1:198:LYS:HE2	9:e1:199:TRP:HZ3	1.84	0.43
9:e1:315:LYS:HE2	9:e1:315:LYS:HB3	1.86	0.43
7:t1:41:VAL:HG21	7:t1:69:TYR:CD2	2.53	0.43
8:y1:54:ILE:O	8:y1:58:ILE:HG12	2.18	0.43
8:u1:112:VAL:O	8:u1:116:VAL:HG13	2.19	0.43
8:z1:95:MET:HG3	8:z1:113:GLN:OE1	2.19	0.43
1:C1:155:VAL:CG2	1:C1:160:VAL:HB	2.49	0.43
8:S1:34:TYR:HB2	8:T1:48:ASN:ND2	2.33	0.43
8:S1:95:MET:O	8:S1:111:THR:OG1	2.37	0.43
8:V1:102:CYS:HA	8:V1:107:SER:HA	2.00	0.43
8:W1:28:ASP:OD2	8:W1:28:ASP:N	2.47	0.43
4:j1:140:LEU:HD12	4:j1:150:MET:HG3	2.01	0.43
8:y1:47:MET:HA	8:y1:50:VAL:HG12	2.01	0.43
5:I1:43:ASP:OD1	5:I1:86:ARG:HD3	2.19	0.42
5:K1:270:ASN:ND2	5:K1:372:ARG:O	2.40	0.42
5:K1:445:PHE:HD1	5:K1:480:TYR:HB2	1.81	0.42
7:P1:147:VAL:HG11	7:P1:164:LEU:HD21	2.01	0.42
7:Q1:132:ASP:HB3	7:Q1:146:ASP:OD1	2.18	0.42
8:T1:94:ASP:OD1	8:T1:95:MET:N	2.51	0.42
8:Y1:112:VAL:O	8:Y1:116:VAL:HG22	2.19	0.42
5:k1:70:LYS:NZ	5:k1:117:GLU:OE1	2.42	0.42
8:v1:37:LYS:HE3	8:v1:37:LYS:HB3	1.89	0.42
10:A:47:VAL:HG21	10:A:77:ASN:OD1	2.19	0.42
1:C1:61:ILE:HB	1:C1:66:ALA:HB2	2.01	0.42
3:G1:190:GLN:C	3:G1:192:LEU:H	2.27	0.42
6:J1:157:PRO:HD2	6:J1:160:LEU:HD23	2.01	0.42
5:K1:243:ASP:O	5:K1:248:GLN:NE2	2.51	0.42
5:K1:272:ALA:HB2	5:K1:370:TYR:HD1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P1:33:ASP:OD2	7:P1:33:ASP:N	2.51	0.42
9:U1:212:GLU:N	9:U1:212:GLU:OE2	2.50	0.42
8:W1:97:ASP:O	8:W1:112:VAL:HG23	2.19	0.42
4:j1:59:ALA:HB2	4:j1:127:LEU:HD11	2.02	0.42
5:k1:102:ALA:O	5:k1:190:VAL:HA	2.18	0.42
5:m1:75:CYS:SG	5:m1:79:VAL:HB	2.60	0.42
8:u1:9:GLY:C	8:u1:10:LEU:HD12	2.44	0.42
8:u1:89:PHE:CZ	8:u1:91:ASP:HB3	2.53	0.42
1:C1:127:THR:HG22	1:C1:160:VAL:HG11	2.02	0.42
4:H1:42:ASN:OD1	4:H1:43:GLY:N	2.47	0.42
5:I1:234:LEU:O	5:I1:238:ILE:HD12	2.18	0.42
5:K1:364:TYR:HB2	5:K1:365:ASN:HD22	1.84	0.42
9:e1:61:ARG:HD2	9:e1:119:GLU:HG3	2.01	0.42
3:h1:365:THR:O	3:h1:366:SER:C	2.61	0.42
6:l1:99:PRO:O	6:l1:100:ALA:HB3	2.19	0.42
1:C1:222:GLY:HA2	9:e1:41:VAL:O	2.19	0.42
5:K1:100:THR:OG1	5:K1:193:THR:HB	2.20	0.42
7:P1:49:TYR:HB3	7:P1:66:TRP:HB3	2.01	0.42
8:S1:57:ALA:HB2	8:T1:73:LEU:HB3	2.00	0.42
3:i1:297:LEU:HD23	3:i1:349:VAL:HG12	2.02	0.42
5:k1:427:ARG:HA	5:k1:427:ARG:HD2	1.78	0.42
7:t1:173:PHE:O	7:t1:174:PRO:C	2.60	0.42
1:C1:33:LEU:HD23	1:C1:57:ILE:CD1	2.49	0.42
1:C1:312:PHE:O	1:C1:357:GLU:HA	2.20	0.42
3:G1:10:PRO:HD3	9:e1:374:ARG:NH1	2.35	0.42
3:G1:93:VAL:HG12	3:G1:94:ARG:N	2.34	0.42
4:H1:76:TRP:O	4:j1:164:VAL:N	2.39	0.42
5:I1:94:LYS:HD3	5:I1:162:ALA:O	2.20	0.42
6:J1:117:LEU:HD23	6:J1:117:LEU:HA	1.81	0.42
6:J1:196:ARG:HH11	6:J1:218:THR:HG22	1.85	0.42
5:K1:235:ARG:HG3	5:K1:271:SER:OG	2.20	0.42
7:P1:74:THR:HG21	7:R1:74:THR:OG1	2.20	0.42
8:V1:94:ASP:OD1	8:V1:94:ASP:N	2.45	0.42
9:e1:285:TYR:CE2	9:e1:299:GLN:HB3	2.55	0.42
3:i1:307:GLN:O	3:i1:311:VAL:HG23	2.20	0.42
3:i1:329:THR:HG23	3:i1:332:GLN:H	1.84	0.42
5:k1:70:LYS:HA	5:k1:70:LYS:HD3	1.66	0.42
5:m1:372:ARG:HA	5:m1:378:PRO:HA	2.02	0.42
8:v1:48:ASN:ND2	8:x1:34:TYR:H	2.17	0.42
8:y1:77:LEU:HG	8:z1:61:PHE:CE2	2.55	0.42
1:C1:356:LEU:HD12	1:C1:356:LEU:HA	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G1:365:THR:HG22	3:G1:366:SER:N	2.35	0.42
4:H1:6:ASP:C	4:H1:8:ALA:H	2.28	0.42
5:K1:131:THR:HG23	5:K1:134:ASP:H	1.85	0.42
5:K1:248:GLN:OE1	5:K1:248:GLN:N	2.52	0.42
7:R1:167:THR:OG1	7:R1:170:ASN:ND2	2.52	0.42
8:T1:54:ILE:O	8:T1:58:ILE:HG12	2.20	0.42
3:i1:67:ALA:O	3:i1:185:ARG:NH1	2.53	0.42
5:k1:147:PHE:CE2	5:k1:149:TYR:HB2	2.55	0.42
6:l1:183:LEU:HD21	6:l1:199:PRO:HD3	2.01	0.42
7:s1:119:VAL:HG22	7:s1:120:GLU:H	1.84	0.42
8:v1:88:PRO:HB3	8:x1:98:ARG:NH2	2.34	0.42
8:v1:102:CYS:O	8:w1:97:ASP:HB3	2.19	0.42
1:C1:270:VAL:HG23	1:C1:271:GLY:H	1.85	0.42
5:I1:103:GLY:HA3	5:I1:104:PRO:HA	1.90	0.42
8:T1:111:THR:HG22	8:T1:114:GLN:OE1	2.20	0.42
8:V1:113:GLN:HE21	8:V1:117:ASN:ND2	2.17	0.42
3:h1:79:ARG:O	3:h1:79:ARG:HG3	2.20	0.42
5:m1:20:ASN:OD1	5:m1:21:PHE:N	2.52	0.42
7:s1:7:LEU:HD12	7:s1:7:LEU:HA	1.77	0.42
8:v1:56:ASN:ND2	8:w1:70:LEU:O	2.45	0.42
8:w1:33:TYR:HB3	8:x1:48:ASN:OD1	2.19	0.42
8:y1:71:ASP:OD2	8:y1:71:ASP:N	2.51	0.42
1:C1:219:ILE:HG22	1:C1:225:ILE:HG12	2.00	0.42
5:I1:113:LEU:HG	5:I1:177:THR:HG22	2.02	0.42
5:I1:215:GLU:CG	5:K1:329:PRO:HG3	2.49	0.42
5:K1:414:ASN:C	5:K1:416:ASN:H	2.28	0.42
7:Q1:136:THR:OG1	7:Q1:141:ASP:OD2	2.23	0.42
7:R1:160:THR:OG1	7:R1:161:ALA:N	2.53	0.42
8:W1:54:ILE:O	8:W1:58:ILE:HG12	2.18	0.42
3:i1:54:PHE:CD1	3:i1:58:MET:HE1	2.55	0.42
3:i1:375:ASP:O	3:i1:376:TYR:CG	2.72	0.42
4:j1:147:LYS:HE2	4:j1:147:LYS:HB2	1.84	0.42
5:m1:256:PHE:O	5:m1:257:ASN:ND2	2.52	0.42
1:C1:164:TRP:NE1	1:C1:167:GLU:O	2.47	0.42
3:G1:68:CYS:O	3:G1:70:GLU:N	2.50	0.42
4:H1:81:ARG:NH2	9:e1:365:GLU:O	2.53	0.42
8:S1:95:MET:HE3	8:V1:118:LEU:HD11	2.02	0.42
5:k1:375:LYS:O	5:k1:377:ARG:HG3	2.20	0.42
7:t1:53:ARG:HA	7:t1:83:SER:OG	2.19	0.42
7:t1:160:THR:HG23	7:t1:162:ASN:H	1.84	0.42
8:w1:25:THR:HG23	8:x1:65:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:68:THR:HG21	1:C1:202:ASP:O	2.20	0.42
3:F1:51:PHE:HD2	6:J1:92:VAL:HG21	1.84	0.42
7:P1:149:LEU:HD23	7:P1:149:LEU:HA	1.86	0.42
9:U1:285:TYR:CE2	9:U1:299:GLN:HB3	2.55	0.42
2:f1:128:LEU:HD23	2:f1:128:LEU:HA	1.79	0.42
5:k1:147:PHE:HA	5:k1:148:PRO:HD3	1.94	0.42
6:l1:105:ASP:OD1	6:l1:106:PRO:HD2	2.20	0.42
5:m1:29:LEU:HD11	5:m1:84:LEU:HB2	2.02	0.42
7:s1:30:TRP:HB2	7:s1:42:VAL:HG21	2.02	0.42
10:A:38:LYS:HG3	10:A:41:GLY:H	1.85	0.42
10:A:71:ASP:O	10:A:74:ASP:N	2.53	0.42
1:C1:12:GLU:HG2	9:e1:134:LEU:HD13	2.02	0.41
1:C1:150:VAL:HG11	1:C1:174:VAL:HG11	2.02	0.41
1:C1:322:TRP:HH2	9:U1:131:GLY:HA3	1.83	0.41
1:C1:341:LEU:HB3	1:C1:362:LEU:HD22	2.01	0.41
3:F1:68:CYS:CB	3:G1:3:CYS:SG	3.06	0.41
6:J1:40:VAL:HG13	6:J1:79:VAL:HG13	2.02	0.41
5:K1:378:PRO:HB2	5:K1:379:ASN:H	1.71	0.41
7:P1:19:PRO:HG3	7:Q1:18:ILE:HB	2.02	0.41
7:Q1:166:LEU:HD12	7:Q1:170:ASN:HD21	1.84	0.41
8:X1:114:GLN:HE21	8:Y1:93:PRO:HD3	1.85	0.41
2:a1:66:LEU:HD22	2:a1:87:VAL:HG11	2.01	0.41
9:e1:63:ARG:HG2	9:e1:117:TYR:CD1	2.55	0.41
2:f1:96:VAL:HB	2:f1:127:LEU:HB2	2.02	0.41
4:j1:121:LEU:HD12	4:j1:121:LEU:HA	1.86	0.41
5:k1:245:SER:OG	5:k1:246:LYS:N	2.53	0.41
5:k1:248:GLN:OE1	5:k1:248:GLN:N	2.52	0.41
5:k1:340:GLN:OE1	5:k1:365:ASN:ND2	2.53	0.41
5:m1:257:ASN:OD1	5:m1:276:ARG:HD2	2.19	0.41
8:y1:98:ARG:HD2	8:y1:109:THR:OG1	2.19	0.41
1:C1:39:LEU:HD23	1:C1:39:LEU:O	2.20	0.41
1:C1:215:VAL:HG22	1:C1:216:GLY:H	1.85	0.41
3:F1:116:TYR:HB3	3:F1:136:VAL:CG1	2.50	0.41
5:K1:35:THR:OG1	5:K1:36:ASP:N	2.53	0.41
9:U1:137:ASN:O	9:U1:139:VAL:N	2.52	0.41
8:W1:114:GLN:HA	8:W1:117:ASN:ND2	2.33	0.41
9:e1:33:ARG:HD2	9:e1:50:ASP:OD1	2.21	0.41
3:i1:337:GLY:HA3	3:i1:347:PHE:CE1	2.55	0.41
5:k1:272:ALA:HA	5:k1:370:TYR:HB2	2.02	0.41
5:m1:112:GLN:HG3	5:m1:178:ASN:ND2	2.34	0.41
8:w1:37:LYS:HD2	8:w1:37:LYS:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:19:SER:OG	1:C1:36:GLU:HG3	2.20	0.41
1:C1:141:PHE:CG	10:A:43:GLN:N	2.80	0.41
6:J1:5:ILE:HD11	6:J1:14:ALA:HB3	2.02	0.41
6:J1:180:ILE:HD12	6:J1:180:ILE:HA	1.81	0.41
8:W1:66:ASP:HB3	8:Y1:25:THR:HG21	2.02	0.41
2:f1:26:GLY:HA2	2:f1:28:ILE:HG13	2.02	0.41
3:i1:9:ASP:OD2	3:i1:10:PRO:HD2	2.21	0.41
5:k1:173:SER:HA	5:k1:194:PHE:HE2	1.85	0.41
6:l1:82:ALA:HA	6:l1:85:VAL:HG12	2.02	0.41
5:m1:181:SER:C	5:m1:183:THR:H	2.28	0.41
7:r1:131:ILE:HG12	7:r1:147:VAL:HG12	2.01	0.41
7:s1:128:SER:OG	7:s1:129:ALA:N	2.54	0.41
7:t1:152:ASP:OD1	7:t1:155:ASN:HB2	2.19	0.41
8:v1:13:ASN:N	8:v1:13:ASN:OD1	2.50	0.41
8:y1:94:ASP:OD1	8:y1:94:ASP:N	2.54	0.41
1:C1:128:LYS:HB2	1:C1:128:LYS:HE2	1.59	0.41
3:F1:48:GLN:HE21	6:J1:88:ARG:HD3	1.85	0.41
6:J1:147:CYS:HB3	8:T1:38:CYS:HB2	1.73	0.41
8:W1:89:PHE:CZ	8:Y1:103:PHE:HB3	2.55	0.41
8:X1:115:LEU:O	8:X1:118:LEU:HG	2.20	0.41
5:m1:29:LEU:HD23	5:m1:221:TYR:HD1	1.85	0.41
5:m1:466:LYS:NZ	5:m1:467:CYS:H	2.18	0.41
7:r1:120:GLU:HG3	7:r1:121:GLY:H	1.86	0.41
8:w1:114:GLN:O	8:w1:118:LEU:HG	2.20	0.41
8:x1:87:PRO:HA	8:x1:88:PRO:HD3	1.94	0.41
8:x1:111:THR:HG23	8:x1:114:GLN:H	1.84	0.41
6:J1:177:MET:HB2	6:J1:177:MET:HE3	1.83	0.41
3:i1:70:GLU:O	3:i1:74:LYS:NZ	2.51	0.41
5:k1:390:LEU:HD23	5:k1:390:LEU:HA	1.81	0.41
8:v1:70:LEU:HD23	8:v1:70:LEU:HA	1.87	0.41
8:u1:25:THR:HG23	8:z1:65:TYR:O	2.20	0.41
8:u1:115:LEU:O	8:u1:118:LEU:HG	2.21	0.41
10:A:19:GLU:HG2	10:A:68:LEU:HB2	2.01	0.41
1:C1:27:LYS:HD3	1:C1:27:LYS:HA	1.89	0.41
3:F1:337:GLY:HA3	3:F1:347:PHE:CE1	2.56	0.41
5:I1:235:ARG:HG3	5:I1:271:SER:OG	2.20	0.41
5:I1:417:ILE:HD12	5:I1:417:ILE:H	1.86	0.41
6:J1:5:ILE:H	6:J1:5:ILE:HG12	1.43	0.41
6:J1:11:MET:HE3	6:J1:11:MET:HB3	1.81	0.41
6:J1:27:PHE:O	6:J1:30:VAL:HG22	2.20	0.41
7:P1:169:ASP:OD2	7:P1:170:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W1:113:GLN:NE2	8:W1:117:ASN:HD21	2.19	0.41
2:f1:3:CYS:C	2:f1:5:LYS:H	2.28	0.41
5:k1:147:PHE:CD2	5:k1:149:TYR:HB2	2.55	0.41
5:m1:12:ARG:HH11	5:m1:12:ARG:HB3	1.85	0.41
5:m1:497:LEU:HD13	5:m1:497:LEU:N	2.36	0.41
7:r1:72:ALA:HB3	7:t1:39:GLY:HA2	2.03	0.41
8:w1:113:GLN:HE21	8:w1:117:ASN:ND2	2.18	0.41
3:G1:16:ASP:OD1	9:U1:336:ARG:NH2	2.54	0.41
5:I1:7:SER:OG	5:I1:8:ASP:N	2.54	0.41
5:I1:232:GLU:HG3	5:I1:235:ARG:HH21	1.85	0.41
8:Y1:87:PRO:HA	8:Y1:88:PRO:HD3	1.97	0.41
3:i1:212:CYS:O	3:i1:244:PHE:CD1	2.73	0.41
7:r1:53:ARG:NH1	7:r1:65:ASP:OD2	2.54	0.41
8:z1:71:ASP:OD1	8:z1:71:ASP:N	2.52	0.41
10:A:18:PHE:HA	10:A:68:LEU:O	2.21	0.41
1:C1:180:ASN:O	1:C1:181:ARG:HG3	2.21	0.41
3:G1:4:THR:C	3:G1:5:ILE:HG12	2.37	0.41
3:G1:327:ASN:OD1	3:G1:371:GLU:HA	2.21	0.41
8:T1:74:LYS:HG3	8:T1:78:ASN:HD21	1.85	0.41
9:U1:285:TYR:HD2	9:U1:303:ILE:HD11	1.85	0.41
2:f1:4:ASN:OD1	2:f1:4:ASN:C	2.64	0.41
3:h1:10:PRO:HB3	3:h1:45:TYR:OH	2.20	0.41
4:j1:103:VAL:HG22	4:j1:119:TYR:HD2	1.86	0.41
5:k1:450:ASN:ND2	5:k1:453:GLU:OE2	2.54	0.41
8:w1:100:ALA:HB2	8:x1:83:ILE:HD12	2.03	0.41
8:y1:65:TYR:O	8:z1:25:THR:HG23	2.21	0.41
10:A:40:SER:O	10:A:42:THR:N	2.54	0.41
1:C1:33:LEU:HD13	1:C1:59:VAL:HG21	2.02	0.41
1:C1:194:CYS:O	1:C1:195:HIS:ND1	2.54	0.41
1:C1:244:LYS:HG3	1:C1:245:GLY:N	2.36	0.41
3:G1:22:SER:HB2	3:G1:29:ALA:O	2.21	0.41
5:I1:96:VAL:HG22	5:I1:161:THR:HG23	2.02	0.41
5:K1:21:PHE:CZ	5:k1:477:ASN:HB3	2.55	0.41
5:K1:427:ARG:HH21	2:a1:127:LEU:HG	1.85	0.41
9:U1:315:LYS:O	9:U1:315:LYS:HG2	2.20	0.41
8:V1:91:ASP:OD2	8:V1:91:ASP:N	2.53	0.41
8:W1:98:ARG:HH11	8:X1:88:PRO:HG3	1.86	0.41
9:e1:15:ALA:HB2	9:e1:91:PRO:HG3	2.02	0.41
9:e1:256:SER:OG	9:e1:266:GLU:OE1	2.25	0.41
2:f1:34:ASP:OD1	2:f1:34:ASP:N	2.51	0.41
2:g1:51:THR:O	2:g1:52:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h1:65:ARG:HG3	3:h1:66:PHE:H	1.86	0.41
3:h1:65:ARG:HG3	3:h1:66:PHE:N	2.36	0.41
4:j1:28:ASP:OD1	4:j1:28:ASP:C	2.64	0.41
5:k1:314:THR:OG1	5:k1:315:PHE:N	2.53	0.41
5:k1:500:ASN:C	5:k1:501:CYS:SG	3.03	0.41
5:m1:147:PHE:CD2	5:m1:149:TYR:HB2	2.56	0.41
5:m1:175:ILE:HG22	5:m1:177:THR:H	1.86	0.41
5:m1:181:SER:O	5:m1:183:THR:N	2.54	0.41
5:m1:269:ASP:H	5:m1:369:ASN:HD21	1.68	0.41
7:t1:160:THR:OG1	7:t1:161:ALA:N	2.53	0.41
8:v1:12:CYS:HB3	8:v1:20:CYS:HB3	1.68	0.41
8:v1:77:LEU:HA	8:v1:77:LEU:HD12	1.87	0.41
8:w1:111:THR:HG22	8:w1:114:GLN:OE1	2.21	0.41
8:x1:10:LEU:O	8:x1:32:LEU:HA	2.20	0.41
8:y1:81:ARG:HB2	8:z1:61:PHE:CZ	2.55	0.41
8:u1:94:ASP:C	8:u1:95:MET:HG2	2.46	0.41
10:A:110:GLN:NE2	10:A:112:ASP:OD1	2.53	0.41
1:C1:198:TYR:O	1:C1:205:LEU:HD12	2.21	0.41
1:C1:331:GLU:HG2	1:C1:333:PRO:HD3	2.02	0.41
5:K1:96:VAL:N	5:K1:198:THR:OG1	2.40	0.41
5:K1:478:MET:HE2	5:K1:478:MET:HB3	1.89	0.41
9:e1:212:GLU:OE2	9:e1:212:GLU:N	2.54	0.41
9:e1:380:ASN:HD21	9:e1:392:ILE:H	1.69	0.41
3:i1:43:LEU:HD12	3:i1:43:LEU:HA	1.76	0.41
5:k1:375:LYS:HB2	5:k1:377:ARG:HD3	2.03	0.41
5:k1:388:ARG:HA	5:k1:388:ARG:HD3	1.92	0.41
1:C1:52:VAL:HG23	1:C1:53:ARG:H	1.85	0.40
5:I1:242:TRP:HE1	5:I1:251:GLY:H	1.67	0.40
5:K1:13:LEU:HD21	5:k1:395:GLY:CA	2.52	0.40
5:K1:181:SER:C	5:K1:183:THR:H	2.28	0.40
8:T1:25:THR:HG23	8:V1:65:TYR:O	2.20	0.40
9:U1:115:VAL:HB	2:g1:50:LEU:HD21	2.02	0.40
8:W1:94:ASP:OD1	8:W1:94:ASP:N	2.51	0.40
9:e1:98:ALA:HB1	9:e1:122:PHE:HB3	2.03	0.40
3:i1:310:VAL:HA	3:i1:313:GLU:HG2	2.02	0.40
7:r1:74:THR:HG23	7:t1:90:PRO:HD2	2.03	0.40
7:r1:169:ASP:OD1	7:r1:170:ASN:N	2.53	0.40
8:v1:55:ALA:O	8:v1:58:ILE:HG22	2.21	0.40
8:v1:55:ALA:HB1	8:x1:22:ILE:HD12	2.04	0.40
8:w1:15:THR:HG21	8:w1:33:TYR:HB2	2.03	0.40
10:A:28:HIS:CE1	10:A:33:ALA:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:117:TRP:CD1	10:A:117:TRP:C	2.99	0.40
3:F1:315:VAL:HG23	3:F1:333:LEU:HD22	2.02	0.40
7:Q1:118:SER:C	7:Q1:119:VAL:O	2.65	0.40
8:S1:77:LEU:HD21	8:V1:77:LEU:HD23	2.03	0.40
8:V1:116:VAL:HA	8:V1:119:VAL:HG12	2.04	0.40
8:Y1:103:PHE:CZ	8:Y1:110:VAL:HG13	2.57	0.40
3:i1:29:ALA:HB2	4:j1:11:ARG:HB3	2.02	0.40
4:j1:132:VAL:HG13	4:j1:176:VAL:HG21	2.02	0.40
5:k1:170:ASN:HD21	5:k1:200:GLY:HA3	1.86	0.40
8:w1:108:SER:OG	8:w1:109:THR:N	2.54	0.40
8:x1:13:ASN:HB2	8:y1:68:SER:OG	2.21	0.40
8:x1:99:ILE:O	8:x1:109:THR:HA	2.22	0.40
1:C1:12:GLU:CG	9:e1:134:LEU:HB3	2.52	0.40
1:C1:14:LEU:HB3	1:C1:17:TYR:HD1	1.87	0.40
3:F1:50:GLU:CD	9:U1:328:ARG:HG2	2.47	0.40
3:G1:3:CYS:O	3:G1:5:ILE:N	2.55	0.40
3:G1:4:THR:OG1	3:G1:5:ILE:N	2.54	0.40
5:K1:13:LEU:HD21	5:k1:395:GLY:HA3	2.04	0.40
5:K1:99:LEU:HA	5:K1:193:THR:O	2.20	0.40
5:K1:114:TYR:CZ	5:K1:324:PRO:HD3	2.57	0.40
7:P1:26:CYS:HG	7:R1:26:CYS:CB	2.33	0.40
7:R1:7:LEU:HD23	7:R1:8:GLN:O	2.21	0.40
7:R1:167:THR:H	7:R1:170:ASN:ND2	2.19	0.40
8:S1:15:THR:HG23	8:S1:36:PRO:HD3	2.04	0.40
8:X1:79:ARG:O	8:Y1:81:ARG:NH1	2.54	0.40
5:k1:285:VAL:HG23	5:k1:323:MET:HG2	2.04	0.40
5:m1:63:VAL:HG11	5:m1:168:ILE:HD12	2.03	0.40
7:s1:7:LEU:O	7:s1:8:GLN:HB2	2.22	0.40
7:s1:155:ASN:HA	7:t1:166:LEU:O	2.21	0.40
1:C1:279:GLN:HG2	1:C1:281:TYR:CE2	2.57	0.40
3:G1:188:TYR:C	3:G1:190:GLN:N	2.79	0.40
4:H1:28:ASP:OD1	4:H1:28:ASP:C	2.65	0.40
4:H1:90:ARG:H	4:H1:90:ARG:HG2	1.74	0.40
5:I1:131:THR:O	5:I1:135:ILE:HG12	2.22	0.40
5:I1:427:ARG:HD2	5:I1:427:ARG:HA	1.80	0.40
6:J1:30:VAL:HG12	9:e1:385:TRP:HZ2	1.85	0.40
7:P1:157:LEU:HA	7:P1:166:LEU:HD13	2.04	0.40
9:U1:199:TRP:HA	9:U1:199:TRP:HE3	1.87	0.40
5:k1:318:LEU:HD21	5:k1:363:ILE:HD11	2.04	0.40
6:l1:22:CYS:O	6:l1:23:CYS:CB	2.68	0.40
8:y1:114:GLN:HA	8:y1:117:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:u1:91:ASP:OD1	8:u1:92:ALA:N	2.54	0.40
8:u1:98:ARG:NE	8:u1:109:THR:OG1	2.45	0.40
1:C1:280:HIS:HD2	1:C1:282:GLY:H	1.68	0.40
3:F1:210:TRP:HB3	3:F1:213:VAL:HG21	2.03	0.40
5:I1:434:ARG:HH11	5:I1:434:ARG:HD2	1.77	0.40
5:K1:242:TRP:CH2	5:K1:388:ARG:HD2	2.56	0.40
7:Q1:12:VAL:N	7:Q1:13:PRO:HD2	2.36	0.40
8:T1:66:ASP:OD2	8:T1:69:ARG:HG2	2.21	0.40
8:X1:29:CYS:HB3	8:Y1:67:CYS:HB3	1.89	0.40
2:f1:70:ARG:HD2	2:f1:76:LEU:HD13	2.03	0.40
2:f1:127:LEU:HA	2:f1:127:LEU:HD12	1.82	0.40
5:k1:231:GLN:NE2	5:k1:255:VAL:HB	2.37	0.40
5:k1:379:ASN:HD22	5:k1:379:ASN:HA	1.64	0.40
6:l1:70:TRP:HB2	7:r1:17:ASN:HB3	2.03	0.40
6:l1:110:VAL:HG22	6:l1:225:VAL:HB	2.03	0.40
5:m1:353:SER:O	5:m1:353:SER:OG	2.32	0.40
7:t1:34:ASN:OD1	7:t1:35:GLY:N	2.54	0.40
8:v1:48:ASN:HD21	8:x1:34:TYR:HB2	1.86	0.40
8:w1:84:CYS:HA	8:x1:102:CYS:HB2	2.04	0.40
8:y1:83:ILE:HD12	8:u1:107:SER:HB3	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	C1	320/457 (70%)	247 (77%)	65 (20%)	8 (2%)	4	27
2	E1	129/136 (95%)	117 (91%)	12 (9%)	0	100	100
2	a1	129/136 (95%)	117 (91%)	12 (9%)	0	100	100
2	f1	129/136 (95%)	118 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	g1	129/136 (95%)	118 (92%)	10 (8%)	1 (1%)	16	50
3	F1	391/396 (99%)	371 (95%)	19 (5%)	1 (0%)	36	68
3	G1	391/396 (99%)	366 (94%)	21 (5%)	4 (1%)	12	45
3	h1	391/396 (99%)	378 (97%)	10 (3%)	3 (1%)	16	50
3	i1	391/396 (99%)	363 (93%)	26 (7%)	2 (0%)	24	59
4	H1	174/178 (98%)	149 (86%)	24 (14%)	1 (1%)	21	56
4	j1	174/178 (98%)	145 (83%)	27 (16%)	2 (1%)	11	43
5	I1	496/503 (99%)	439 (88%)	56 (11%)	1 (0%)	43	73
5	K1	492/503 (98%)	421 (86%)	64 (13%)	7 (1%)	9	39
5	k1	496/503 (99%)	441 (89%)	53 (11%)	2 (0%)	30	62
5	m1	492/503 (98%)	404 (82%)	80 (16%)	8 (2%)	7	36
6	J1	283/286 (99%)	258 (91%)	20 (7%)	5 (2%)	6	34
6	l1	283/286 (99%)	253 (89%)	27 (10%)	3 (1%)	11	43
7	P1	160/587 (27%)	146 (91%)	13 (8%)	1 (1%)	21	56
7	Q1	171/587 (29%)	155 (91%)	12 (7%)	4 (2%)	5	29
7	R1	171/587 (29%)	158 (92%)	12 (7%)	1 (1%)	21	56
7	r1	160/587 (27%)	147 (92%)	12 (8%)	1 (1%)	21	56
7	s1	171/587 (29%)	158 (92%)	10 (6%)	3 (2%)	6	34
7	t1	171/587 (29%)	156 (91%)	15 (9%)	0	100	100
8	S1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	T1	117/300 (39%)	112 (96%)	4 (3%)	1 (1%)	14	47
8	V1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	W1	117/300 (39%)	109 (93%)	8 (7%)	0	100	100
8	X1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	Y1	117/300 (39%)	111 (95%)	6 (5%)	0	100	100
8	u1	117/300 (39%)	110 (94%)	6 (5%)	1 (1%)	14	47
8	v1	117/300 (39%)	107 (92%)	10 (8%)	0	100	100
8	w1	117/300 (39%)	114 (97%)	3 (3%)	0	100	100
8	x1	117/300 (39%)	105 (90%)	12 (10%)	0	100	100
8	y1	117/300 (39%)	110 (94%)	7 (6%)	0	100	100
8	z1	117/300 (39%)	108 (92%)	7 (6%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	U1	392/398 (98%)	368 (94%)	21 (5%)	3 (1%)	16	50
9	e1	392/398 (98%)	361 (92%)	30 (8%)	1 (0%)	36	68
10	A	166/188 (88%)	142 (86%)	13 (8%)	11 (7%)	1	7
All	All	8648/13631 (63%)	7807 (90%)	764 (9%)	77 (1%)	16	47

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F1	375	ASP
6	J1	2	ASN
5	K1	378	PRO
7	Q1	117	ILE
7	Q1	119	VAL
9	U1	129	LEU
3	i1	68	CYS
6	l1	23	CYS
5	m1	104	PRO
7	s1	12	VAL
10	A	48	PRO
10	A	49	VAL
10	A	50	ILE
1	C1	353	LYS
3	G1	4	THR
6	J1	207	GLU
5	K1	199	ALA
5	K1	379	ASN
7	Q1	118	SER
9	U1	130	SER
3	h1	5	ILE
3	h1	6	GLN
3	i1	225	ALA
4	j1	171	ILE
5	k1	184	SER
5	m1	74	THR
7	s1	120	GLU
8	z1	36	PRO
10	A	37	VAL
10	A	40	SER
10	A	76	SER
1	C1	355	THR
3	G1	69	CYS

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Mol	Chain	Res	Type
6	J1	205	ALA
5	K1	415	THR
7	P1	23	ASP
9	U1	138	LEU
9	e1	319	HIS
5	m1	105	ALA
8	u1	95	MET
8	z1	37	LYS
10	A	22	VAL
1	C1	4	PRO
1	C1	53	ARG
1	C1	56	GLU
1	C1	352	ALA
3	G1	190	GLN
5	K1	354	GLY
3	h1	7	ARG
5	m1	177	THR
5	m1	181	SER
7	s1	7	LEU
10	A	114	ASP
1	C1	313	HIS
6	J1	3	VAL
5	K1	196	GLN
5	k1	500	ASN
6	l1	4	LEU
5	m1	75	CYS
5	m1	375	LYS
7	r1	23	ASP
1	C1	180	ASN
3	G1	268	SER
5	I1	68	LEU
6	J1	210	THR
7	Q1	8	GLN
2	g1	128	LEU
5	m1	415	THR
10	A	26	ILE
10	A	41	GLY
4	H1	7	VAL
10	A	47	VAL
7	R1	21	GLY
5	K1	200	GLY
8	T1	83	ILE

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Mol	Chain	Res	Type
4	j1	7	VAL
6	l1	3	VAL

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	C1	281/383 (73%)	270 (96%)	11 (4%)	28	62
2	E1	115/116 (99%)	115 (100%)	0	100	100
2	a1	115/116 (99%)	115 (100%)	0	100	100
2	f1	115/116 (99%)	115 (100%)	0	100	100
2	g1	115/116 (99%)	115 (100%)	0	100	100
3	F1	330/333 (99%)	325 (98%)	5 (2%)	57	76
3	G1	330/333 (99%)	315 (96%)	15 (4%)	24	58
3	h1	330/333 (99%)	325 (98%)	5 (2%)	57	76
3	i1	330/333 (99%)	323 (98%)	7 (2%)	47	71
4	H1	145/147 (99%)	145 (100%)	0	100	100
4	j1	145/147 (99%)	145 (100%)	0	100	100
5	I1	404/408 (99%)	400 (99%)	4 (1%)	68	80
5	K1	400/408 (98%)	392 (98%)	8 (2%)	48	72
5	k1	404/408 (99%)	394 (98%)	10 (2%)	42	69
5	m1	400/408 (98%)	392 (98%)	8 (2%)	48	72
6	J1	245/247 (99%)	228 (93%)	17 (7%)	14	45
6	l1	245/247 (99%)	239 (98%)	6 (2%)	43	70
7	P1	129/473 (27%)	128 (99%)	1 (1%)	73	82
7	Q1	138/473 (29%)	136 (99%)	2 (1%)	59	77
7	R1	138/473 (29%)	135 (98%)	3 (2%)	45	71
7	r1	129/473 (27%)	127 (98%)	2 (2%)	55	75
7	s1	138/473 (29%)	135 (98%)	3 (2%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	t1	138/473 (29%)	137 (99%)	1 (1%)	76	83
8	S1	97/229 (42%)	96 (99%)	1 (1%)	68	80
8	T1	97/229 (42%)	97 (100%)	0	100	100
8	V1	97/229 (42%)	96 (99%)	1 (1%)	68	80
8	W1	97/229 (42%)	97 (100%)	0	100	100
8	X1	97/229 (42%)	96 (99%)	1 (1%)	68	80
8	Y1	97/229 (42%)	97 (100%)	0	100	100
8	u1	97/229 (42%)	95 (98%)	2 (2%)	47	71
8	v1	97/229 (42%)	95 (98%)	2 (2%)	47	71
8	w1	97/229 (42%)	97 (100%)	0	100	100
8	x1	97/229 (42%)	97 (100%)	0	100	100
8	y1	97/229 (42%)	97 (100%)	0	100	100
8	z1	97/229 (42%)	94 (97%)	3 (3%)	35	66
9	U1	314/316 (99%)	307 (98%)	7 (2%)	45	71
9	e1	314/316 (99%)	308 (98%)	6 (2%)	50	73
10	A	143/162 (88%)	133 (93%)	10 (7%)	14	45
All	All	7194/10979 (66%)	7053 (98%)	141 (2%)	48	72

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C1	55	LYS
1	C1	56	GLU
1	C1	58	LEU
1	C1	128	LYS
1	C1	132	ASP
1	C1	219	ILE
1	C1	220	ILE
1	C1	311	VAL
1	C1	351	ASP
1	C1	353	LYS
1	C1	355	THR
3	F1	66	PHE
3	F1	223	CYS
3	F1	224	CYS
3	F1	348	ASN

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Mol	Chain	Res	Type
3	F1	386	ILE
3	G1	5	ILE
3	G1	7	ARG
3	G1	43	LEU
3	G1	69	CYS
3	G1	108	ARG
3	G1	187	ARG
3	G1	190	GLN
3	G1	194	TYR
3	G1	196	PRO
3	G1	270	GLN
3	G1	281	ILE
3	G1	282	CYS
3	G1	336	ILE
3	G1	348	ASN
3	G1	374	CYS
5	I1	66	GLU
5	I1	184	SER
5	I1	185	VAL
5	I1	186	THR
6	J1	1	MET
6	J1	4	LEU
6	J1	5	ILE
6	J1	8	ILE
6	J1	32	GLU
6	J1	88	ARG
6	J1	95	ARG
6	J1	125	CYS
6	J1	151	TYR
6	J1	203	THR
6	J1	206	CYS
6	J1	207	GLU
6	J1	211	LEU
6	J1	212	CYS
6	J1	213	VAL
6	J1	276	PHE
6	J1	277	CYS
5	K1	26	CYS
5	K1	27	LYS
5	K1	327	CYS
5	K1	353	SER
5	K1	374	GLU

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Mol	Chain	Res	Type
5	K1	377	ARG
5	K1	406	ASN
5	K1	480	TYR
7	P1	175	ASP
7	Q1	116	GLU
7	Q1	119	VAL
7	R1	23	ASP
7	R1	24	CYS
7	R1	25	GLN
8	S1	12	CYS
9	U1	53	ILE
9	U1	97	PHE
9	U1	128	VAL
9	U1	129	LEU
9	U1	130	SER
9	U1	138	LEU
9	U1	198	LYS
8	V1	20	CYS
8	X1	84	CYS
9	e1	53	ILE
9	e1	97	PHE
9	e1	128	VAL
9	e1	199	TRP
9	e1	319	HIS
9	e1	395	ARG
3	h1	3	CYS
3	h1	5	ILE
3	h1	7	ARG
3	h1	334	ARG
3	h1	348	ASN
3	i1	20	ARG
3	i1	43	LEU
3	i1	68	CYS
3	i1	187	ARG
3	i1	215	ASP
3	i1	240	PHE
3	i1	336	ILE
5	k1	21	PHE
5	k1	28	ILE
5	k1	185	VAL
5	k1	364	TYR
5	k1	372	ARG

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Mol	Chain	Res	Type
5	k1	374	GLU
5	k1	375	LYS
5	k1	376	ASN
5	k1	377	ARG
5	k1	499	ASP
6	l1	1	MET
6	l1	2	ASN
6	l1	5	ILE
6	l1	23	CYS
6	l1	152	VAL
6	l1	275	ARG
5	m1	12	ARG
5	m1	74	THR
5	m1	101	ILE
5	m1	182	CYS
5	m1	300	CYS
5	m1	481	ARG
5	m1	491	VAL
5	m1	497	LEU
7	r1	24	CYS
7	r1	175	ASP
7	s1	7	LEU
7	s1	119	VAL
7	s1	175	ASP
7	t1	175	ASP
8	v1	37	LYS
8	v1	38	CYS
8	u1	94	ASP
8	u1	95	MET
8	z1	37	LYS
8	z1	38	CYS
8	z1	40	VAL
10	A	20	ARG
10	A	36	SER
10	A	38	LYS
10	A	43	GLN
10	A	45	GLU
10	A	73	SER
10	A	74	ASP
10	A	76	SER
10	A	78	LYS
10	A	181	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	C1	135	GLN
1	C1	137	HIS
1	C1	184	ASN
1	C1	192	GLN
1	C1	238	ASN
1	C1	246	HIS
1	C1	255	ASN
1	C1	280	HIS
1	C1	290	GLN
1	C1	313	HIS
2	E1	42	ASN
2	E1	61	ASN
2	E1	84	GLN
3	F1	11	GLN
3	F1	48	GLN
3	F1	195	GLN
3	F1	222	ASN
3	F1	355	ASN
3	F1	359	GLN
3	F1	388	ASN
3	F1	389	ASN
3	G1	11	GLN
3	G1	15	ASN
3	G1	57	GLN
3	G1	105	GLN
3	G1	193	GLN
3	G1	387	ASN
4	H1	80	ASN
4	H1	155	GLN
4	H1	160	ASN
4	H1	173	ASN
5	I1	33	GLN
5	I1	304	ASN
5	I1	355	GLN
5	I1	365	ASN
5	I1	438	GLN
5	I1	450	ASN
5	I1	452	ASN
5	I1	470	GLN
5	K1	178	ASN
5	K1	257	ASN

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Mol	Chain	Res	Type
5	K1	304	ASN
5	K1	313	GLN
5	K1	342	ASN
5	K1	355	GLN
5	K1	365	ASN
5	K1	477	ASN
7	P1	25	GLN
7	Q1	82	ASN
7	R1	34	ASN
7	R1	113	ASN
7	R1	162	ASN
7	R1	170	ASN
8	S1	41	GLN
8	S1	59	ASN
8	S1	75	GLN
8	T1	78	ASN
9	U1	67	ASN
9	U1	90	HIS
9	U1	126	ASN
9	U1	380	ASN
8	V1	17	ASN
8	V1	59	ASN
8	V1	106	GLN
8	V1	113	GLN
8	V1	117	ASN
8	W1	78	ASN
8	W1	82	ASN
8	W1	113	GLN
8	W1	117	ASN
8	X1	75	GLN
8	X1	82	ASN
8	X1	114	GLN
8	X1	117	ASN
8	Y1	41	GLN
8	Y1	59	ASN
8	Y1	117	ASN
2	a1	84	GLN
9	e1	90	HIS
9	e1	126	ASN
9	e1	227	ASN
9	e1	294	ASN
9	e1	358	HIS

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Mol	Chain	Res	Type
9	e1	380	ASN
3	h1	48	GLN
3	h1	195	GLN
3	h1	346	ASN
3	i1	11	GLN
3	i1	15	ASN
3	i1	57	GLN
3	i1	183	GLN
3	i1	193	GLN
3	i1	227	ASN
3	i1	355	ASN
4	j1	80	ASN
4	j1	155	GLN
4	j1	173	ASN
5	k1	33	GLN
5	k1	170	ASN
5	k1	231	GLN
5	k1	342	ASN
5	k1	357	ASN
5	k1	365	ASN
5	k1	379	ASN
5	k1	438	GLN
6	l1	208	ASN
5	m1	33	GLN
5	m1	342	ASN
5	m1	365	ASN
5	m1	369	ASN
5	m1	414	ASN
5	m1	492	ASN
7	r1	34	ASN
7	s1	25	GLN
7	s1	170	ASN
7	t1	94	ASN
8	v1	48	ASN
8	v1	59	ASN
8	v1	75	GLN
8	v1	113	GLN
8	v1	117	ASN
8	w1	41	GLN
8	w1	113	GLN
8	x1	17	ASN
8	x1	106	GLN

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Mol	Chain	Res	Type
8	y1	39	ASN
8	y1	46	GLN
8	y1	72	ASN
8	y1	78	ASN
8	y1	113	GLN
8	y1	117	ASN
8	u1	59	ASN
8	u1	72	ASN
8	u1	75	GLN
8	z1	41	GLN
8	z1	59	ASN
8	z1	117	ASN
10	A	28	HIS
10	A	157	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

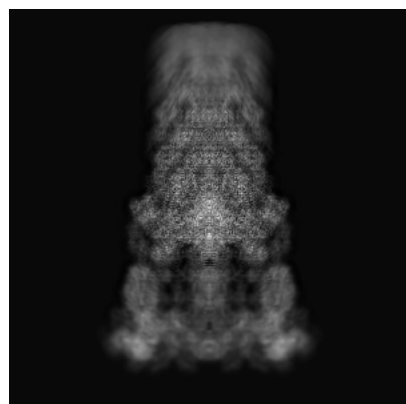
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29383. These allow visual inspection of the internal detail of the map and identification of artifacts.

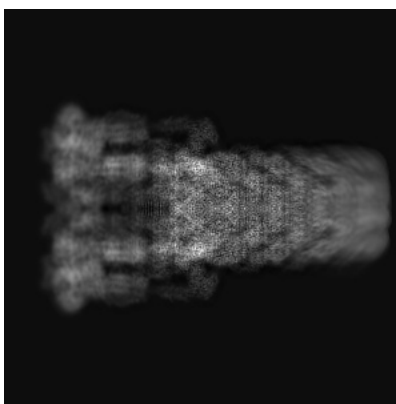
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

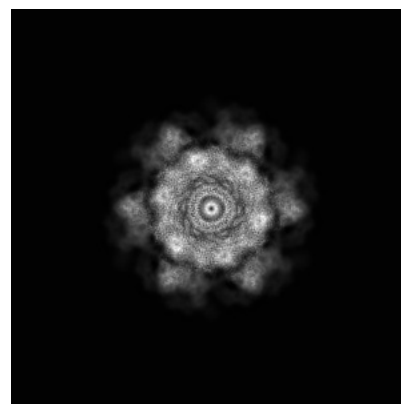
6.1.1 Primary map



X

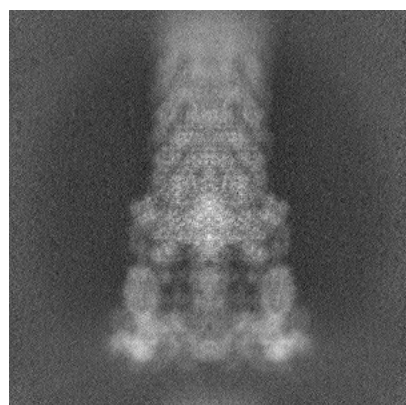


Y

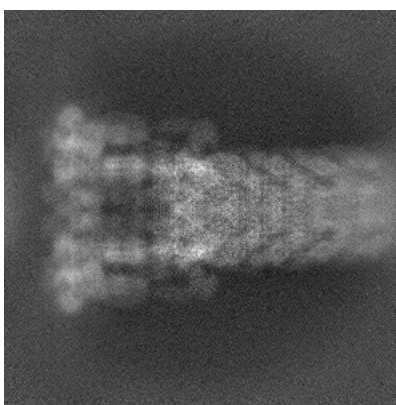


Z

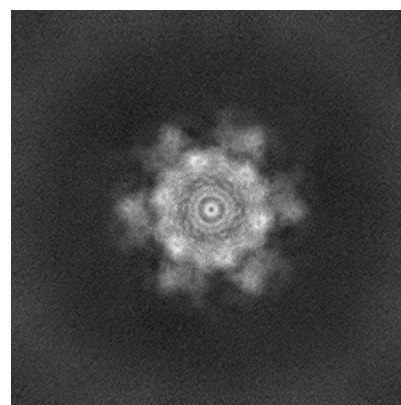
6.1.2 Raw map



X



Y

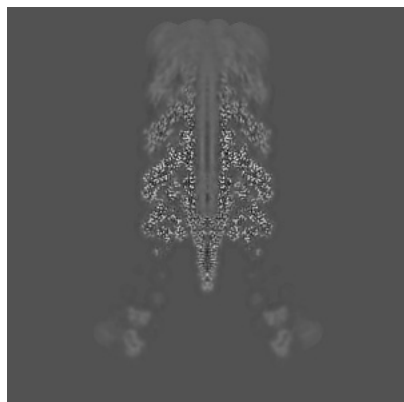


Z

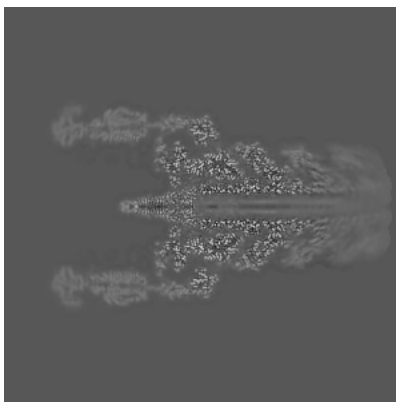
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

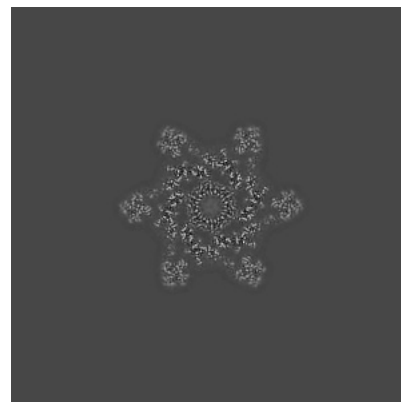
6.2.1 Primary map



X Index: 289

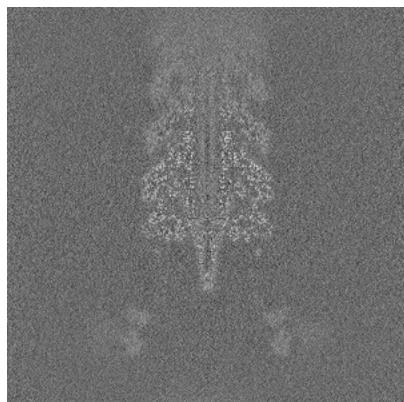


Y Index: 289

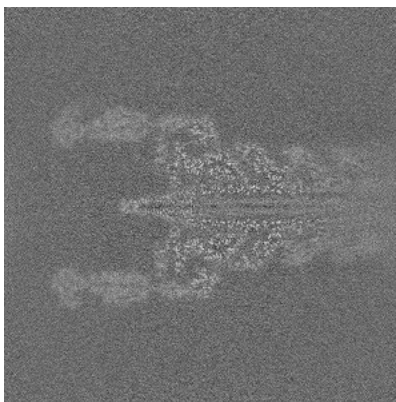


Z Index: 289

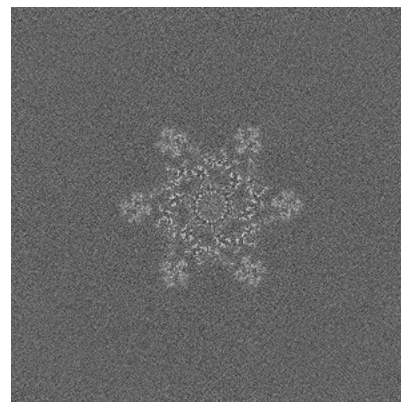
6.2.2 Raw map



X Index: 289



Y Index: 289

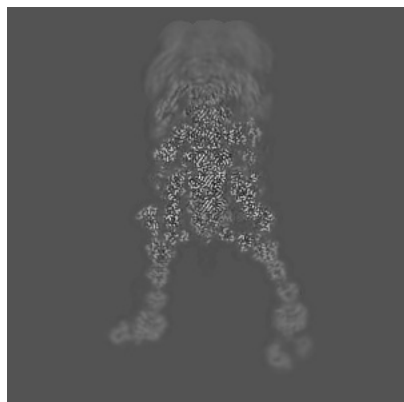


Z Index: 289

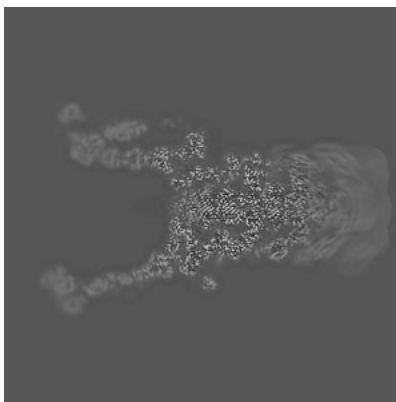
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

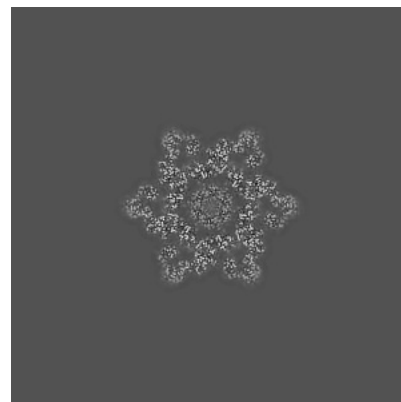
6.3.1 Primary map



X Index: 310

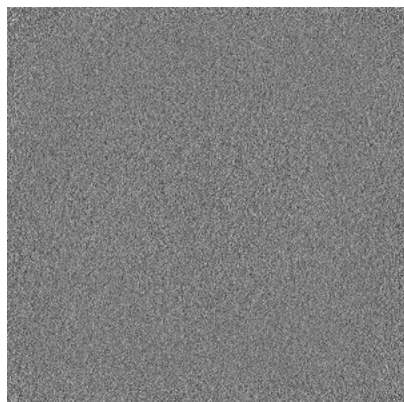


Y Index: 268

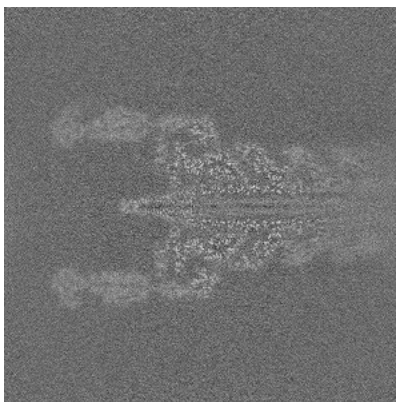


Z Index: 276

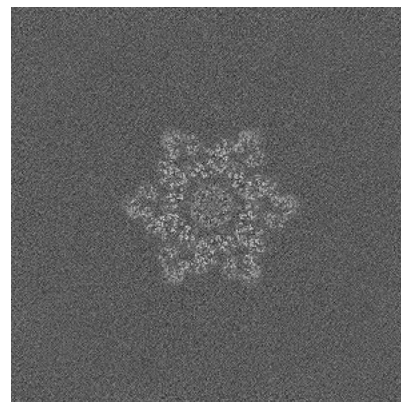
6.3.2 Raw map



X Index: 0



Y Index: 289

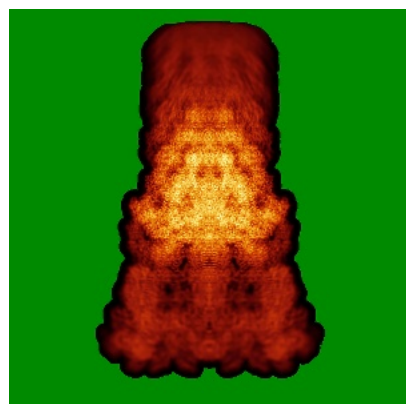


Z Index: 276

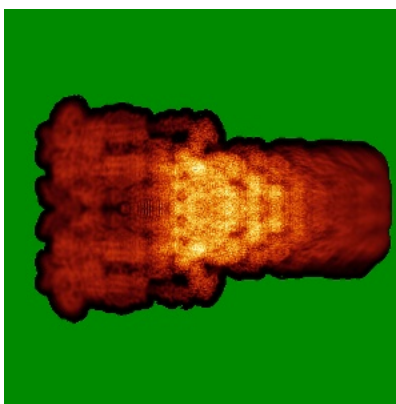
The images above show the largest variance slices of the map in three orthogonal directions.

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

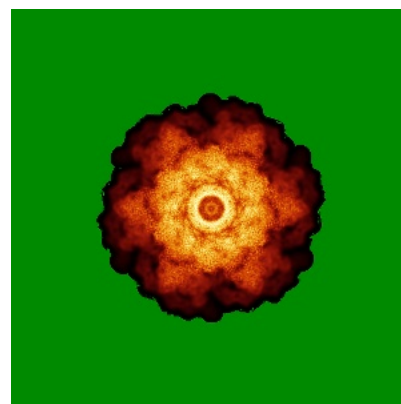
6.4.1 Primary map



X

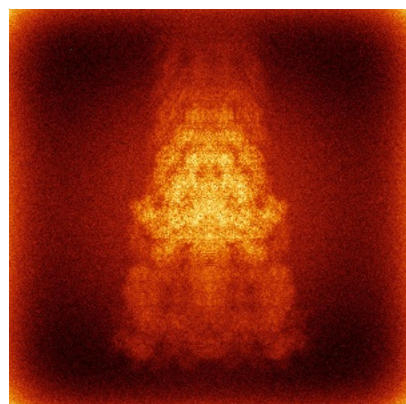


Y

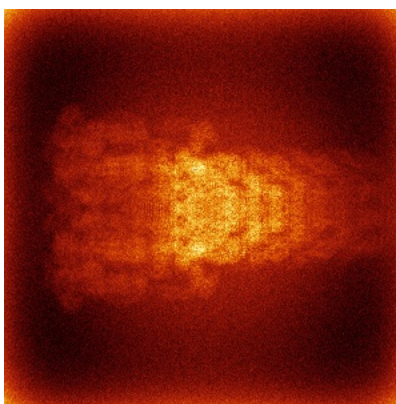


Z

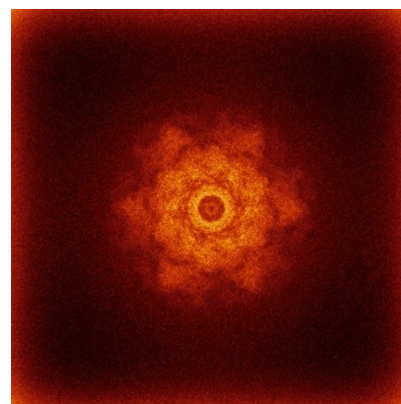
6.4.2 Raw map



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.

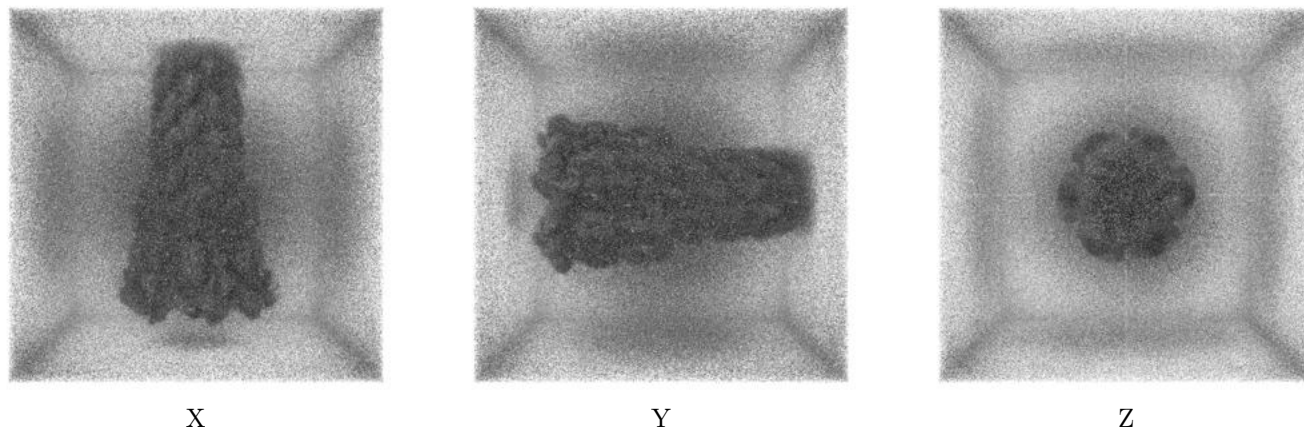
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

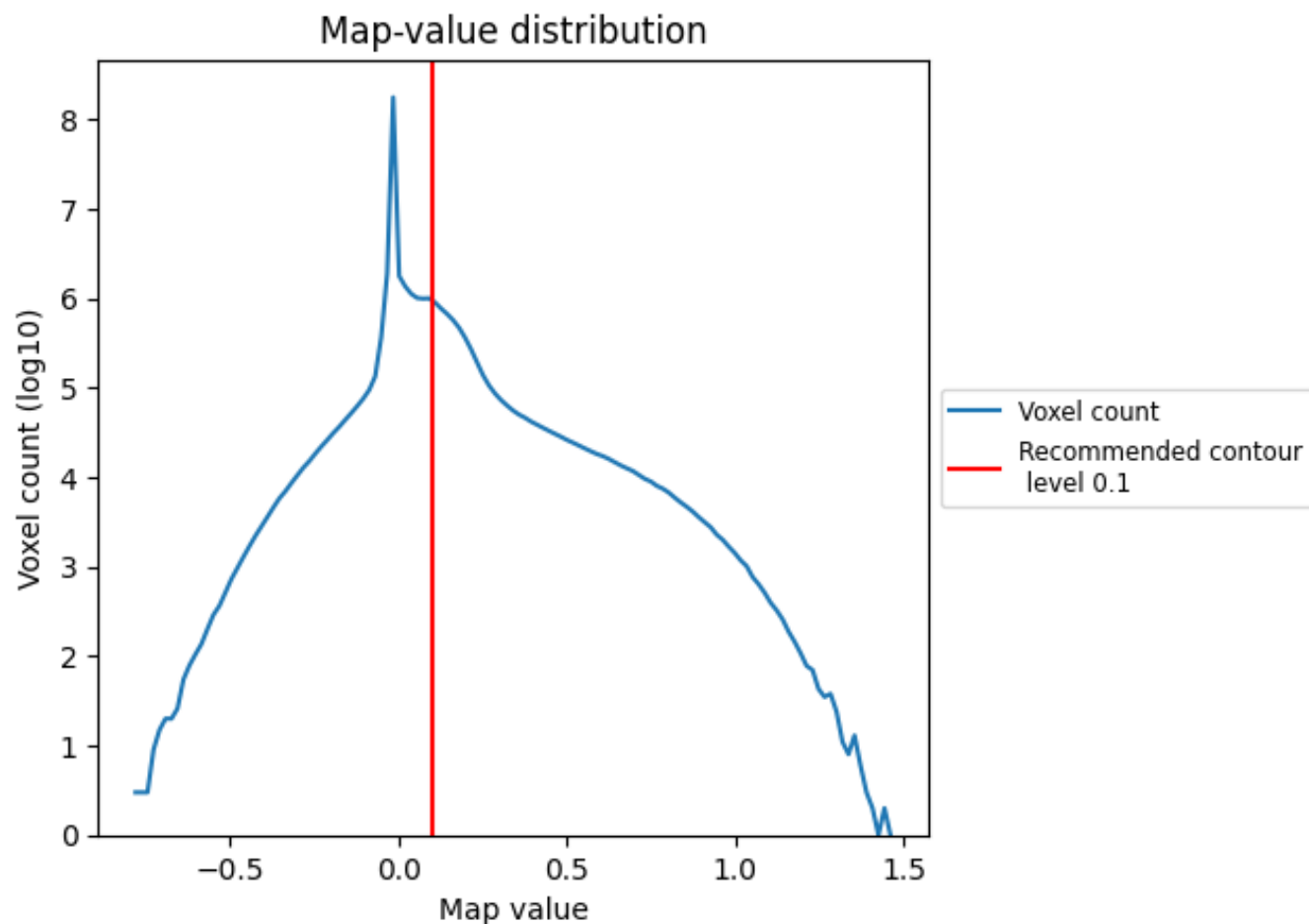
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

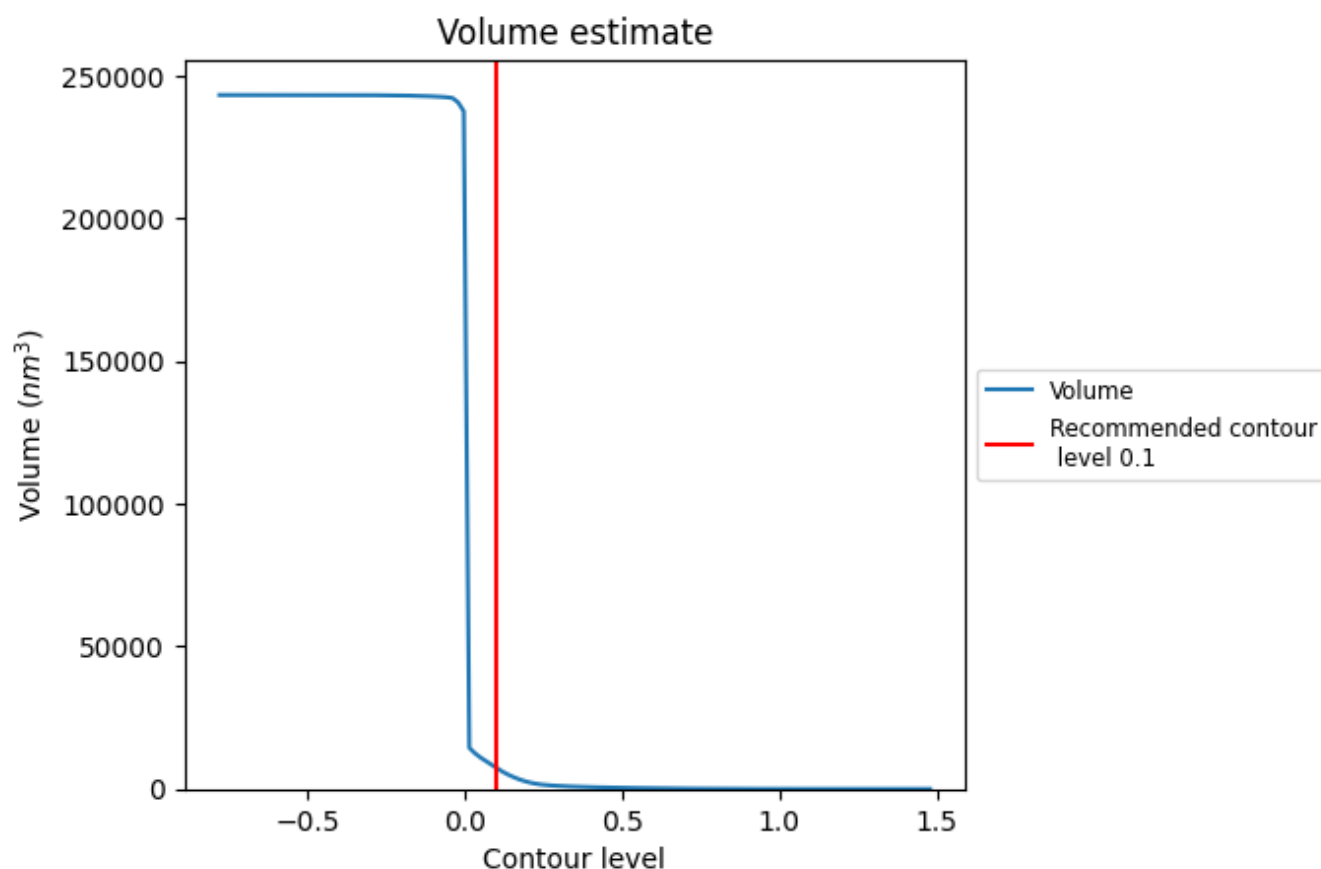
This section contains the results of statistical analysis of the map.

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.

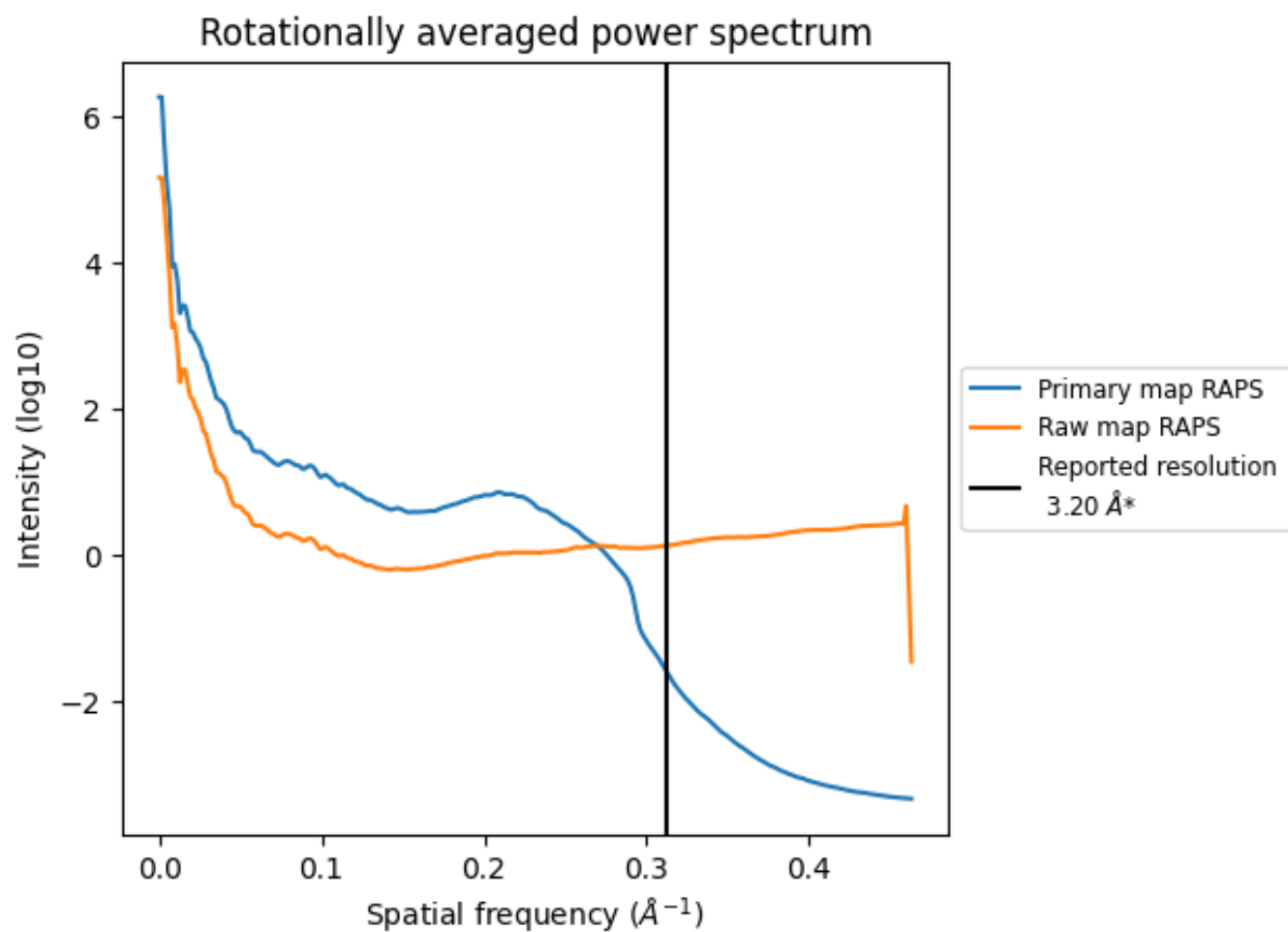
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7391 nm³; this corresponds to an approximate mass of 6676 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 ⓘ

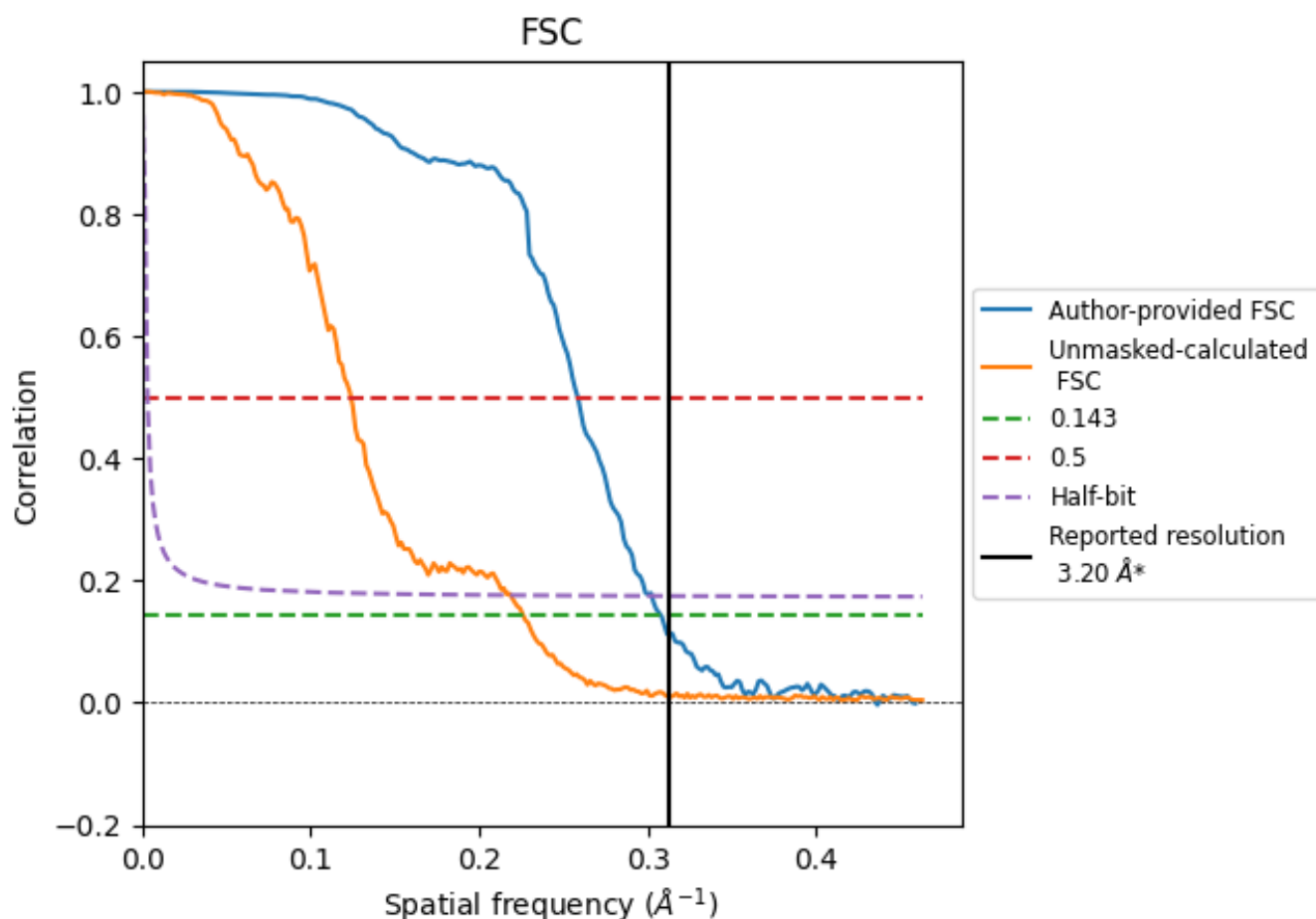


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.25	3.87	3.31
Unmasked-calculated*	4.42	8.07	4.58

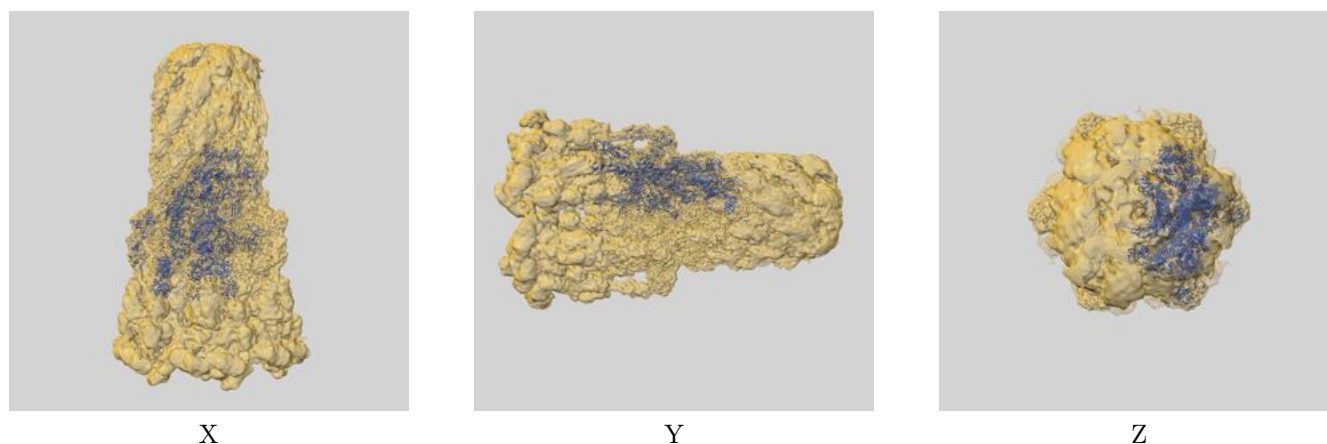
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

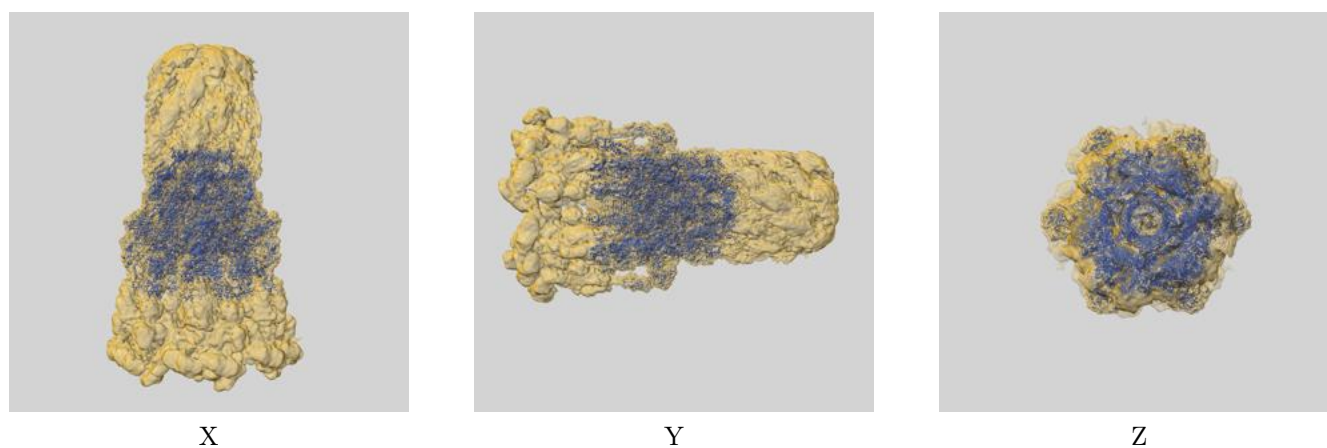
This section contains information regarding the fit between EMDB map EMD-29383 and PDB model 8FQC. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

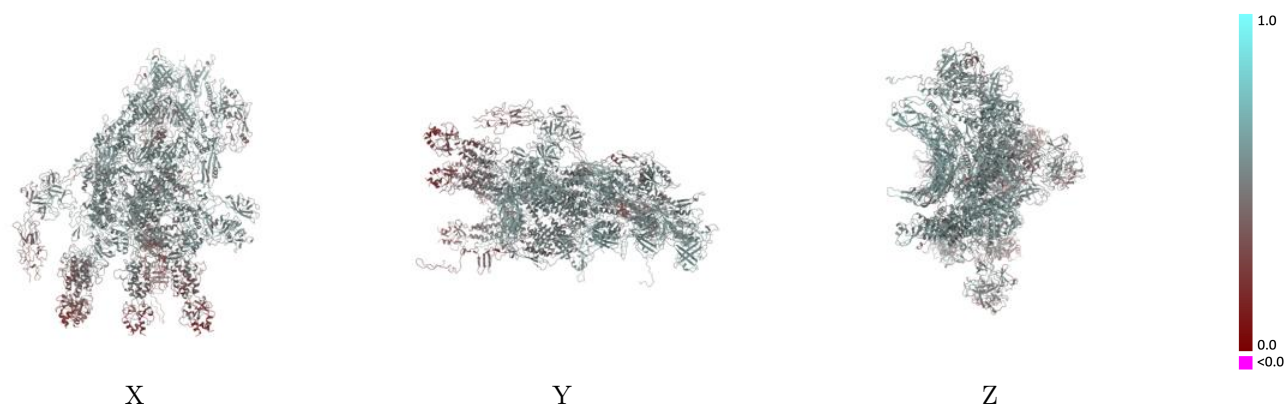


9.1.2 Map-model assembly overlay [i](#)



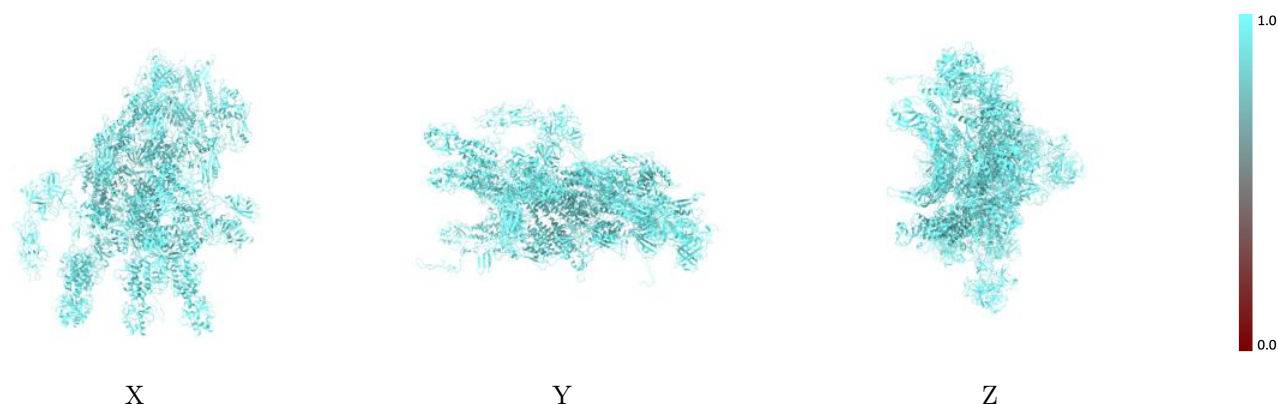
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



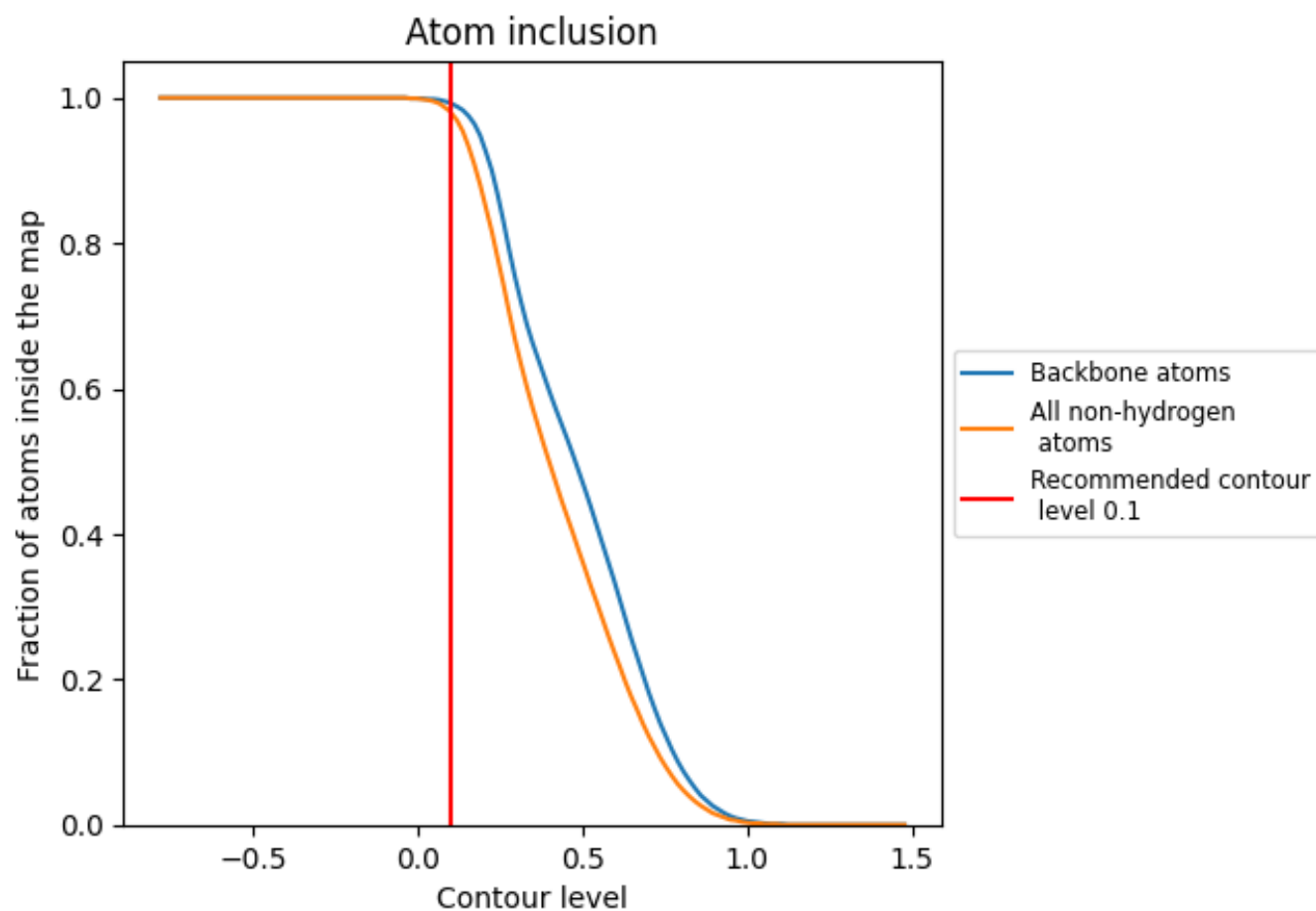
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.4980
A	 0.9070	 0.3820
C1	 0.9400	 0.4770
E1	 0.9870	 0.5640
F1	 0.9840	 0.5370
G1	 0.9880	 0.5390
H1	 0.9770	 0.5290
I1	 0.9860	 0.5410
J1	 0.9880	 0.5400
K1	 0.9790	 0.4980
P1	 0.9880	 0.4520
Q1	 0.9890	 0.4560
R1	 0.9820	 0.4260
S1	 0.9780	 0.3790
T1	 0.9900	 0.3780
U1	 0.9780	 0.5470
V1	 0.9820	 0.3670
W1	 0.9910	 0.4300
X1	 0.9860	 0.4260
Y1	 0.9900	 0.4110
a1	 0.9840	 0.5560
e1	 0.9790	 0.5530
f1	 0.9910	 0.5590
g1	 0.9820	 0.5630
h1	 0.9840	 0.5390
i1	 0.9860	 0.5380
j1	 0.9780	 0.5300
k1	 0.9890	 0.5440
l1	 0.9840	 0.5380
m1	 0.9800	 0.5010
r1	 0.9860	 0.4470
s1	 0.9890	 0.4560
t1	 0.9870	 0.4320
u1	 0.9830	 0.4140
v1	 0.9760	 0.3780



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Chain	Atom inclusion	Q-score
w1	 0.9820	 0.3860
x1	 0.9680	 0.3610
y1	 0.9850	 0.4160
z1	 0.9780	 0.4070