



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:52 PM UTC

PDB ID : 8K39 / pdb_00008k39
EMDB ID : EMD-36848
Title : Structure of the bacteriophage lambda portal vertex
Authors : Xiao, H.; Tan, L.; Cheng, L.P.; Liu, H.R.
Deposited on : 2023-07-14
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

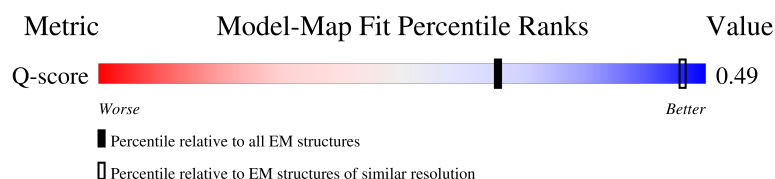
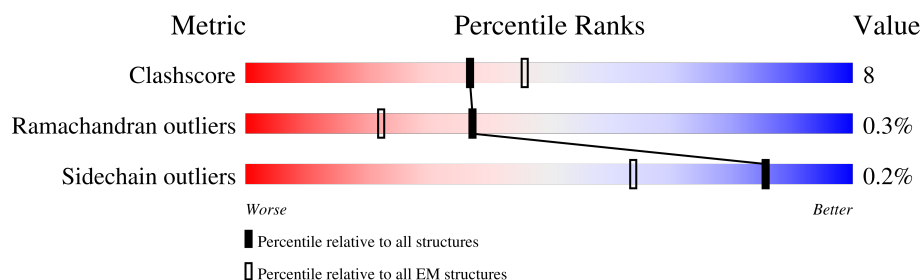
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



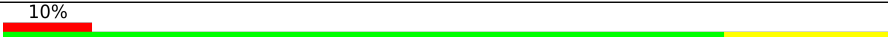
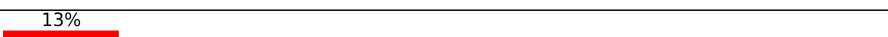
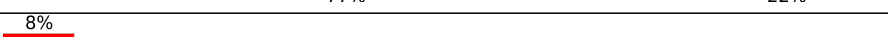
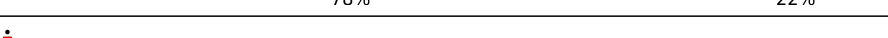
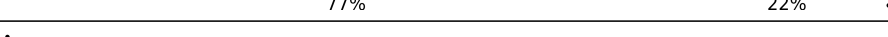
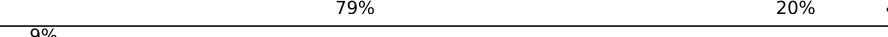
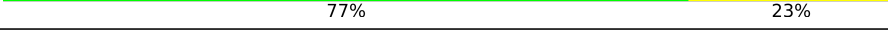
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	0	341	74% 25% .
1	1	341	80% 20% .
1	2	341	82% 17% .
1	3	341	79% 19% .

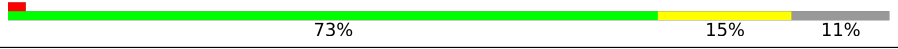
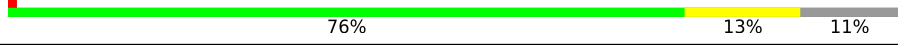
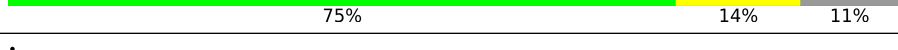
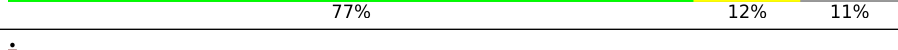
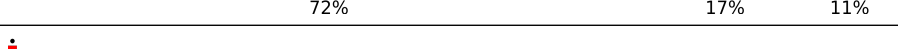
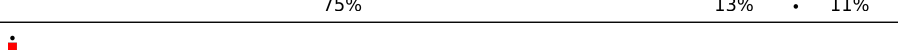
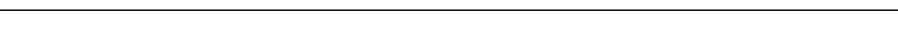
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Mol	Chain	Length	Quality of chain
1	4	341	
1	5	341	
1	6	341	
1	7	341	
1	A	341	
1	B	341	
1	C	341	
1	D	341	
1	E	341	
1	F	341	
1	G	341	
1	H	341	
1	I	341	
1	J	341	
1	K	341	
1	L	341	
1	M	341	
1	N	341	
1	O	341	
1	P	341	
1	Q	341	
1	R	341	
1	S	341	
1	T	341	
1	g	341	

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Mol	Chain	Length	Quality of chain
1	h	341	
2	U	533	
2	V	533	
2	W	533	
2	X	533	
2	Y	533	
2	Z	533	
2	a	533	
2	b	533	
2	c	533	
2	d	533	
2	e	533	
2	f	533	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 124618 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	1	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	2	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	3	337	Total	C	N	O	S	0	0
			2649	1668	455	514	12		
1	4	337	Total	C	N	O	S	0	0
			2649	1668	455	514	12		
1	5	337	Total	C	N	O	S	0	0
			2649	1668	455	514	12		
1	6	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	7	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	A	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	B	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	C	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	D	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	E	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	F	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	G	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	H	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	I	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	K	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	L	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	M	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	N	337	Total	C	N	O	S	0	0
			2649	1668	455	514	12		
1	O	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	P	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	Q	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	R	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	S	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	T	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	g	340	Total	C	N	O	S	0	0
			2675	1685	458	519	13		
1	h	337	Total	C	N	O	S	0	0
			2649	1668	455	514	12		

- Molecule 2 is a protein called Portal protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	468	Total	C	N	O	S	0	0
			3675	2294	663	695	23		
2	V	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	W	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	X	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	Y	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	Z	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		

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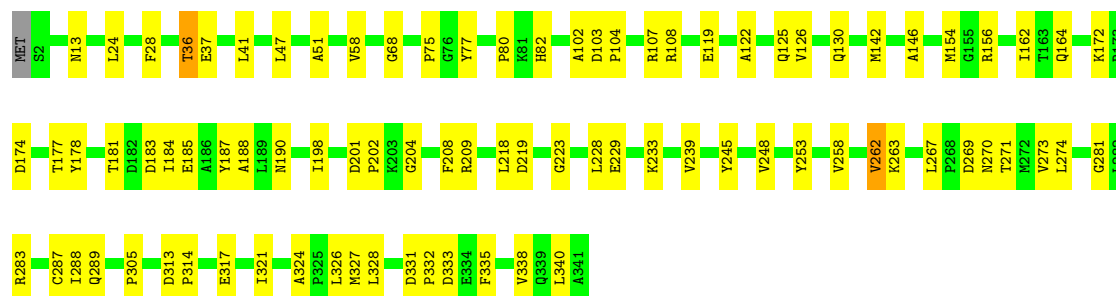
Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	476	Total	C	N	O	S	0	0
			3743	2339	673	707	24		
2	b	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	c	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	d	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	e	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		
2	f	472	Total	C	N	O	S	0	0
			3708	2317	668	699	24		

3 Residue-property plots

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

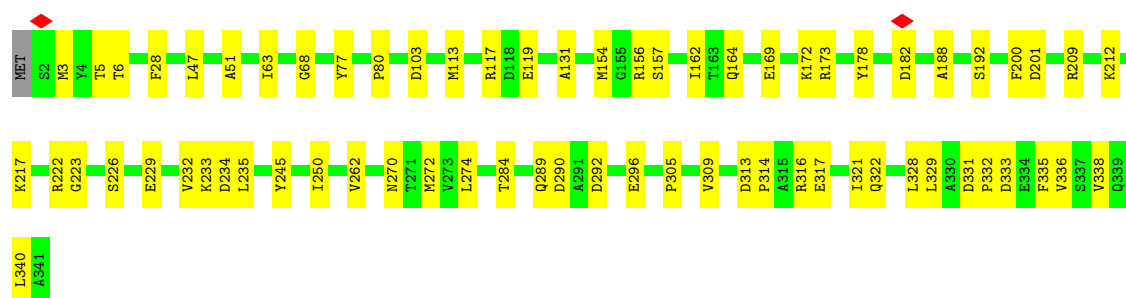
- Molecule 1: Major capsid protein

Chain 0: 



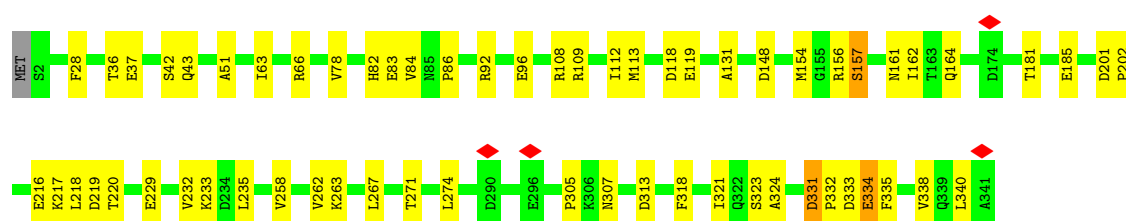
- Molecule 1: Major capsid protein

Chain 1: 

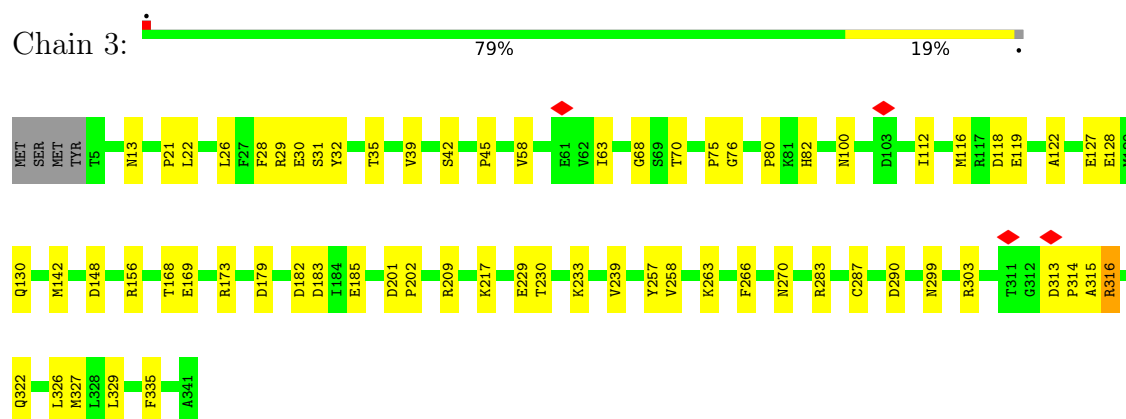


- Molecule 1: Major capsid protein

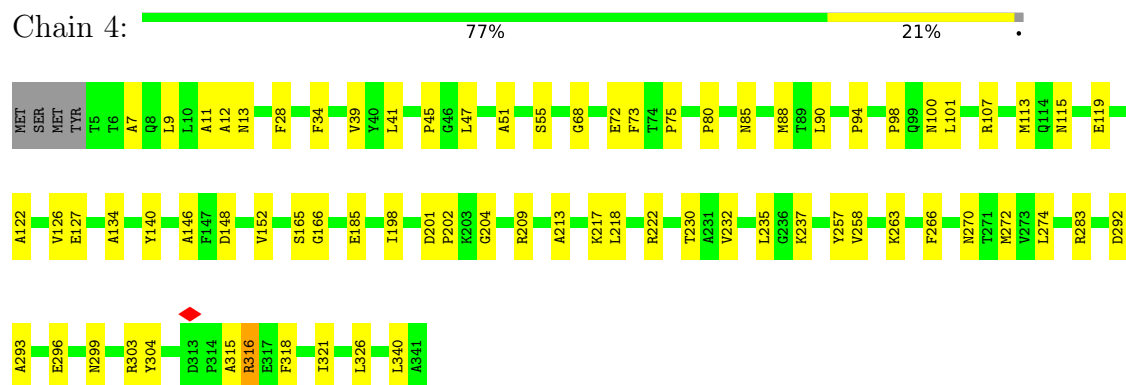
Chain 2: 



- Molecule 1: Major capsid protein



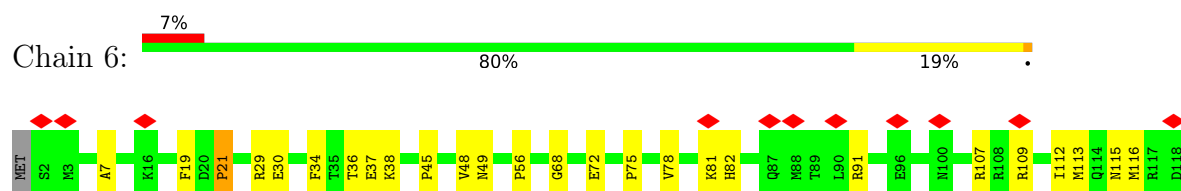
- Molecule 1: Major capsid protein

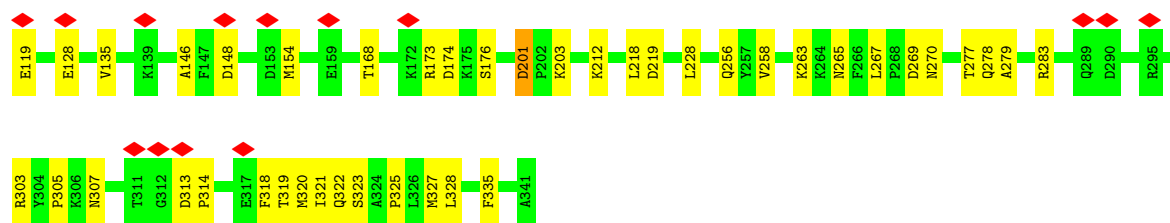


- Molecule 1: Major capsid protein

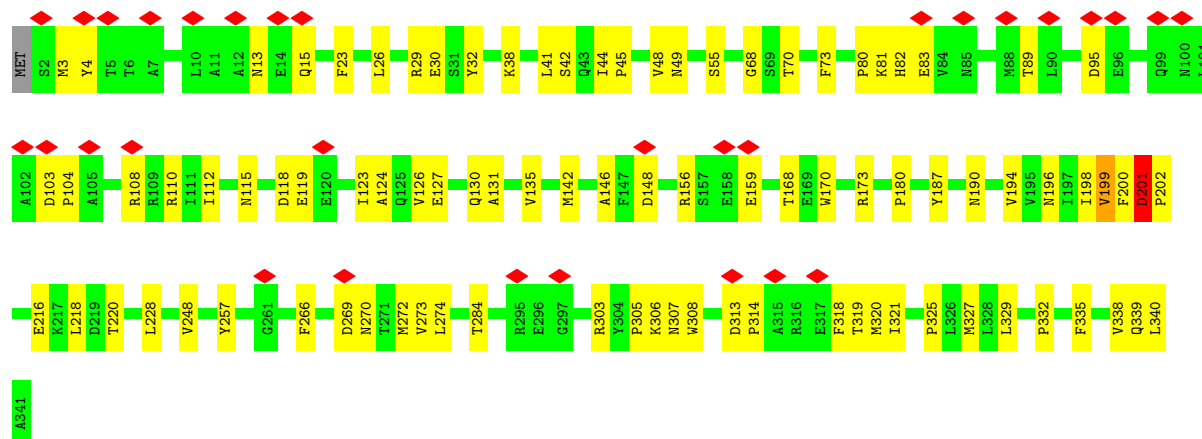
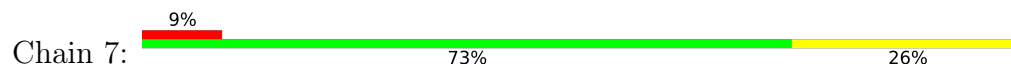


- Molecule 1: Major capsid protein

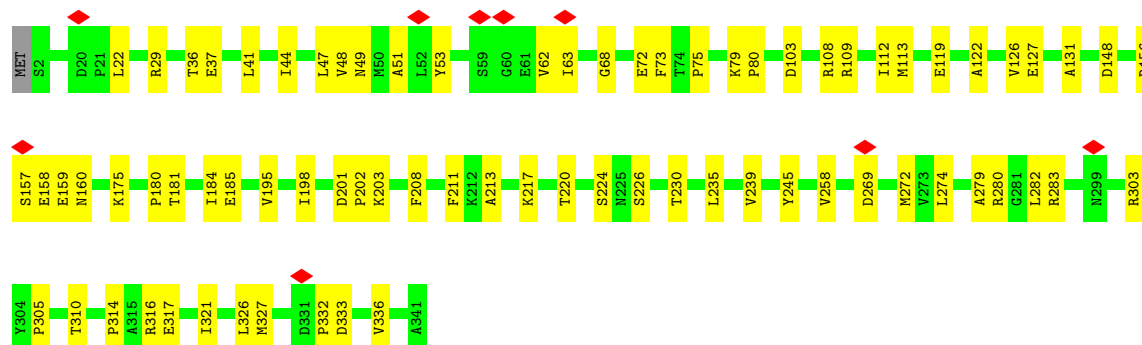
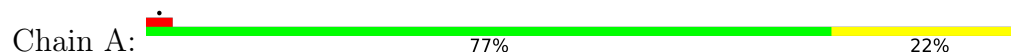




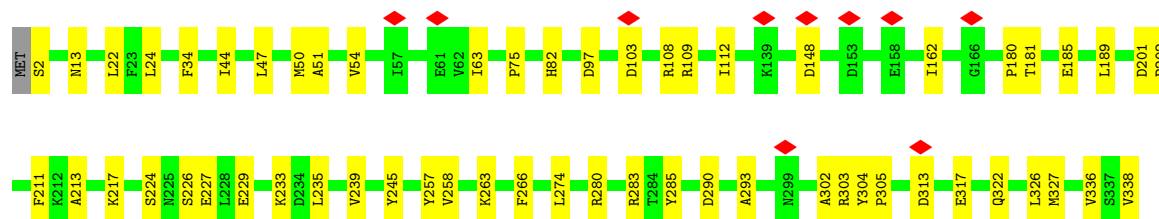
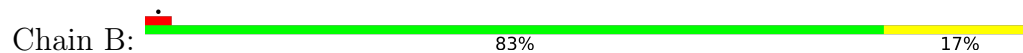
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



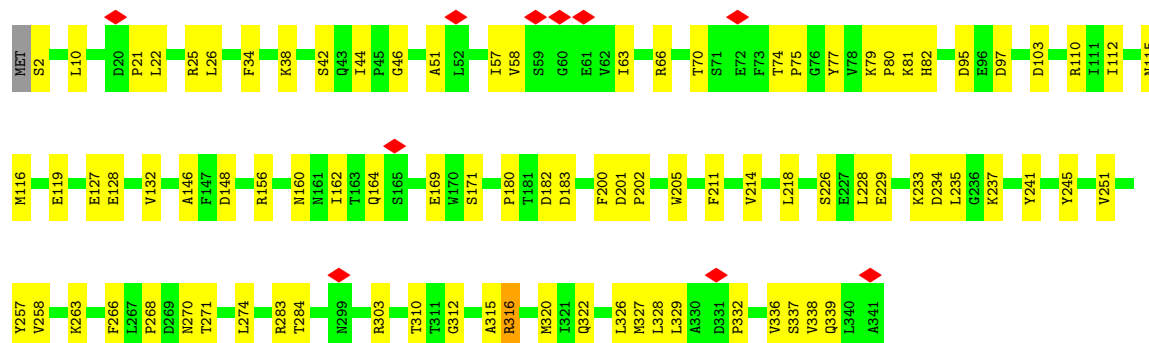
• Molecule 1: Major capsid protein





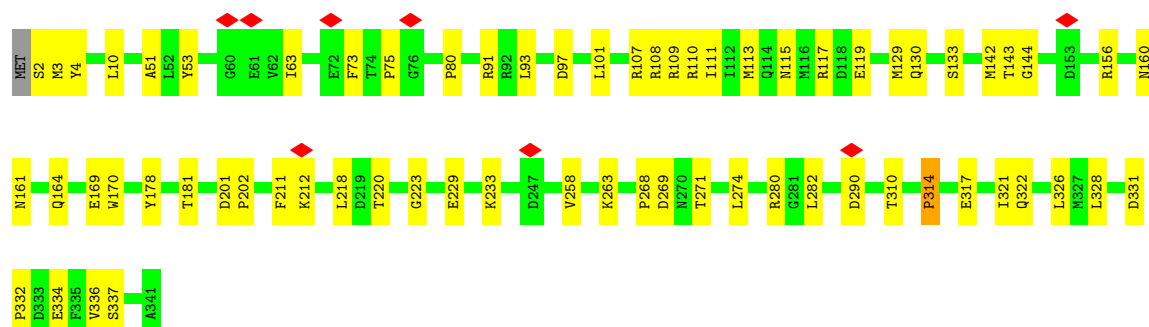
- Molecule 1: Major capsid protein

Chain C: 74% 26%



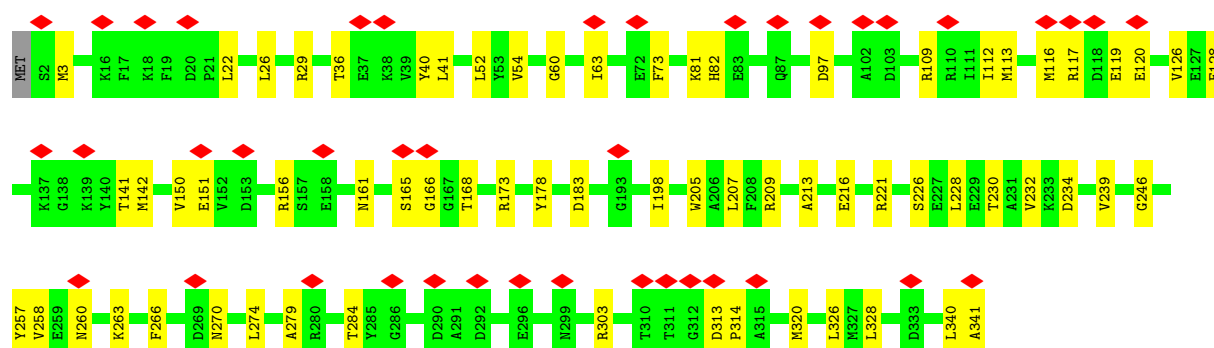
- Molecule 1: Major capsid protein

Chain D: 80% 19%



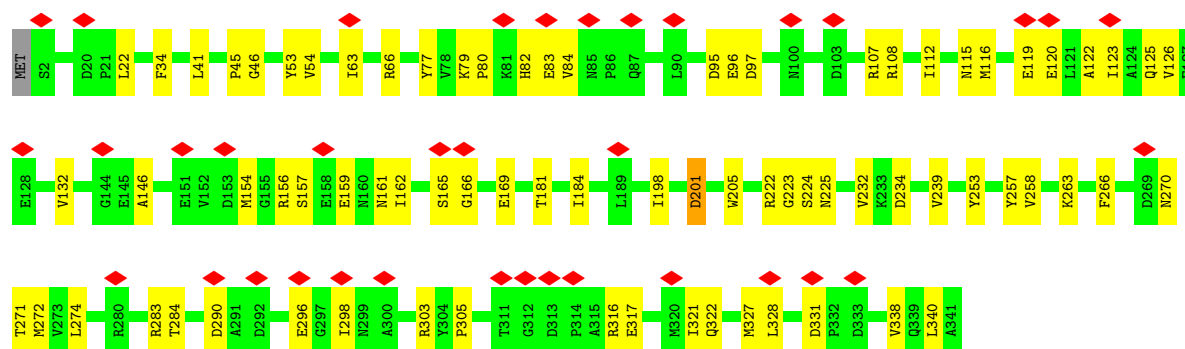
- Molecule 1: Major capsid protein

Chain E: 12% 80% 20%

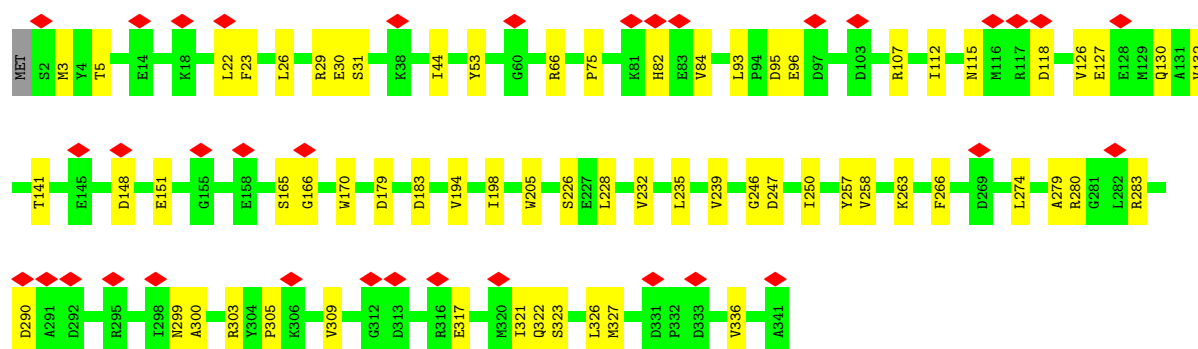
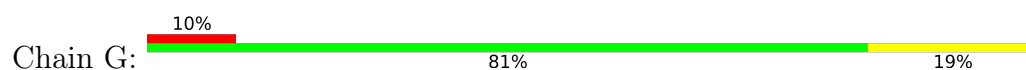


- Molecule 1: Major capsid protein

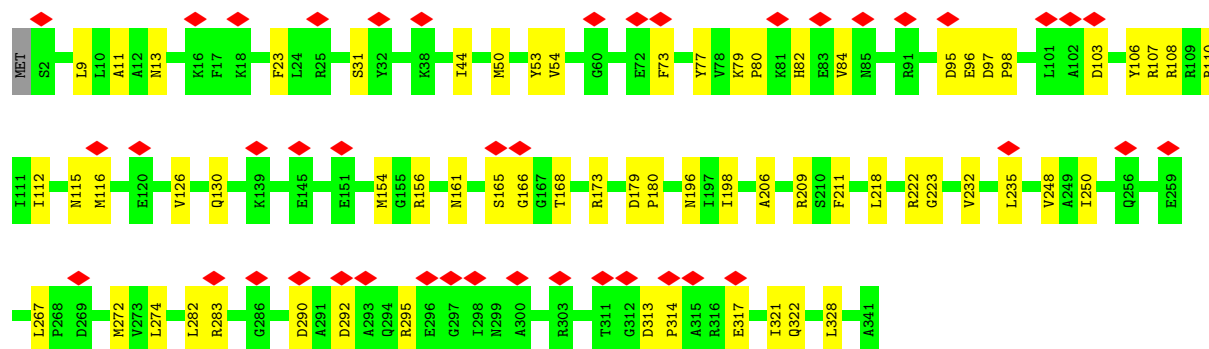
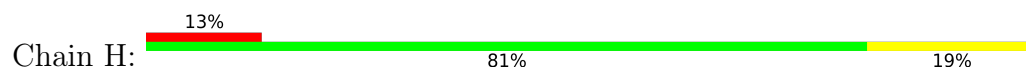
Chain F: 11% 77% 22%



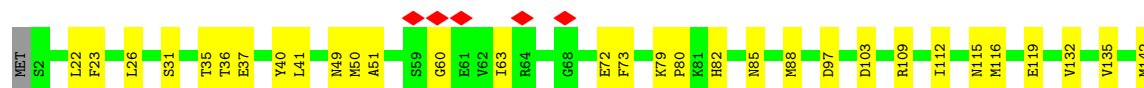
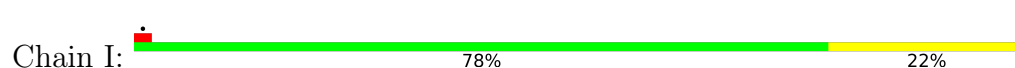
• Molecule 1: Major capsid protein

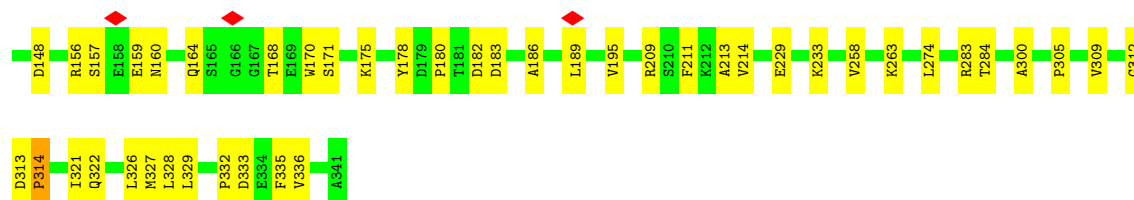


• Molecule 1: Major capsid protein

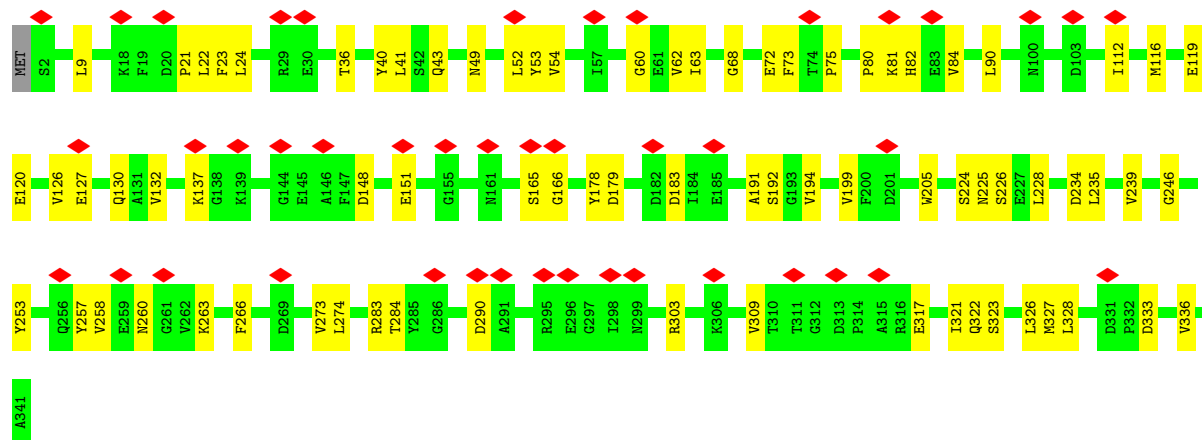
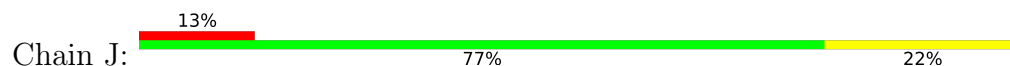


• Molecule 1: Major capsid protein

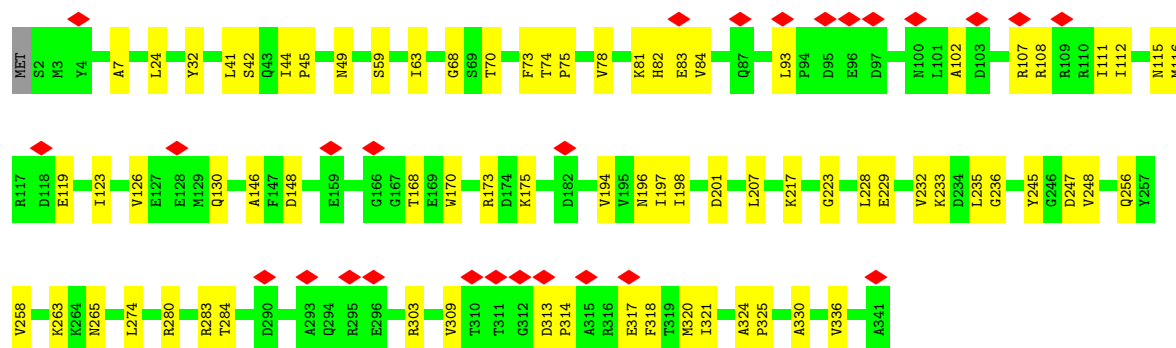
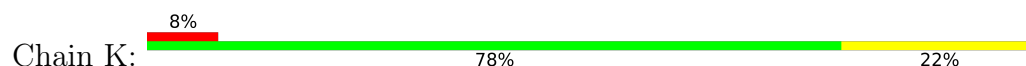




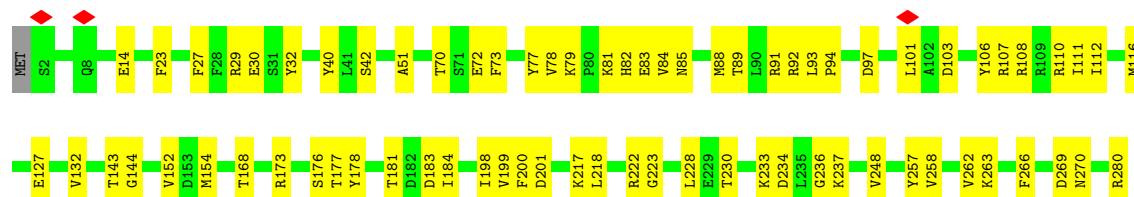
• Molecule 1: Major capsid protein

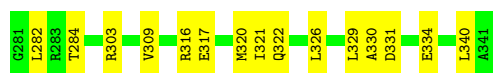


• Molecule 1: Major capsid protein



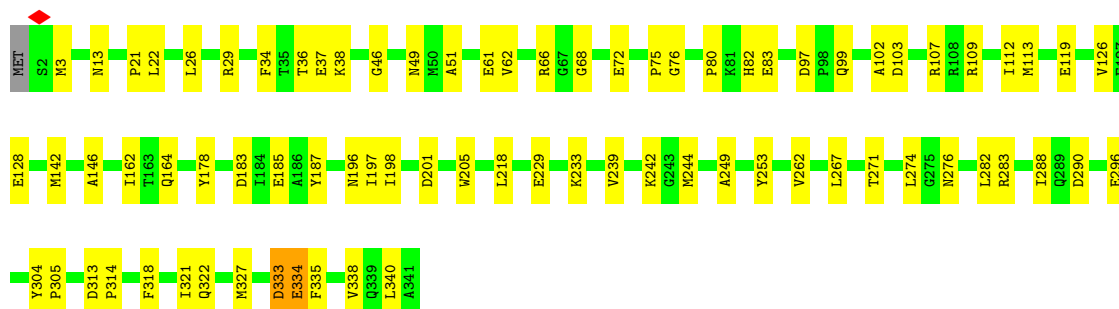
• Molecule 1: Major capsid protein





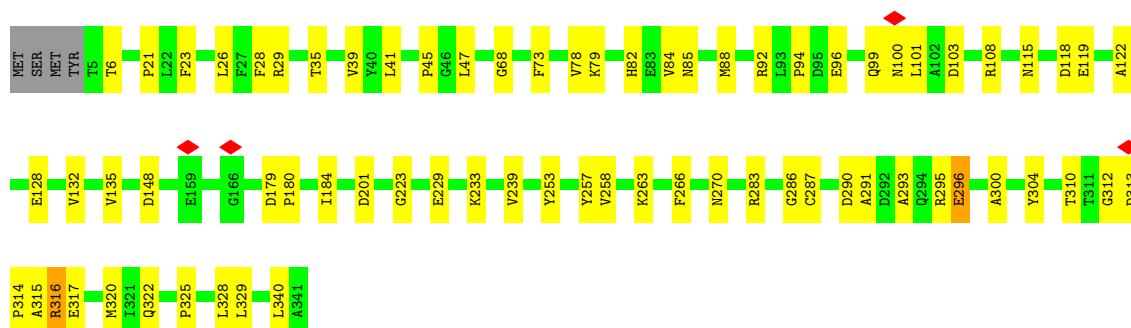
- Molecule 1: Major capsid protein

Chain M: 77% 22%



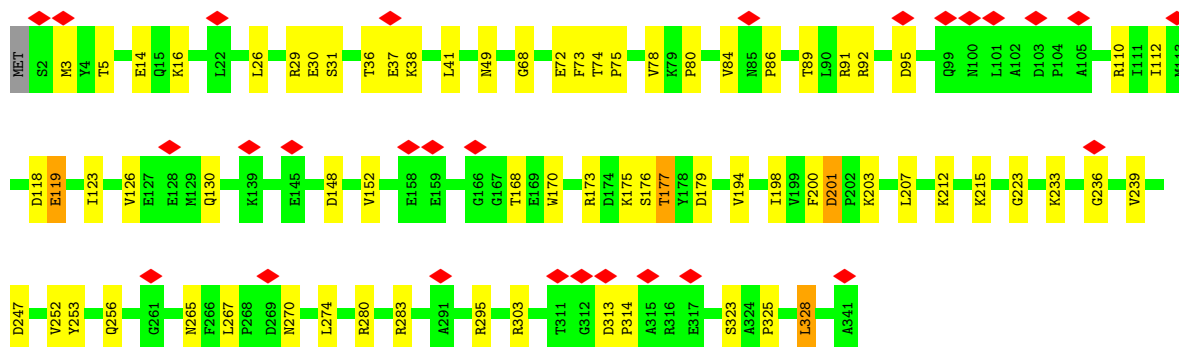
- Molecule 1: Major capsid protein

Chain N: 78% 21%



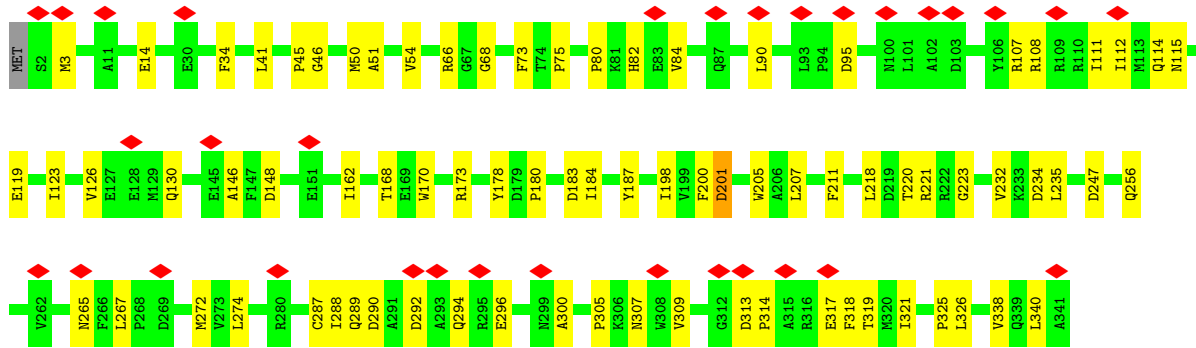
- Molecule 1: Major capsid protein

Chain O: 8% 79% 20%

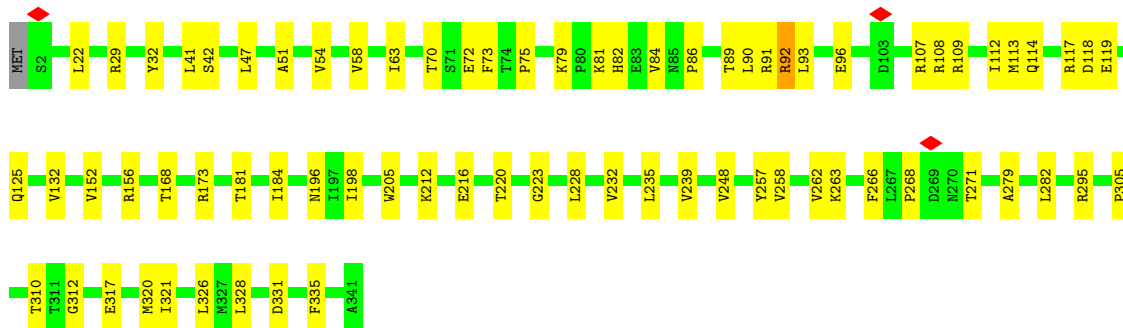


- Molecule 1: Major capsid protein

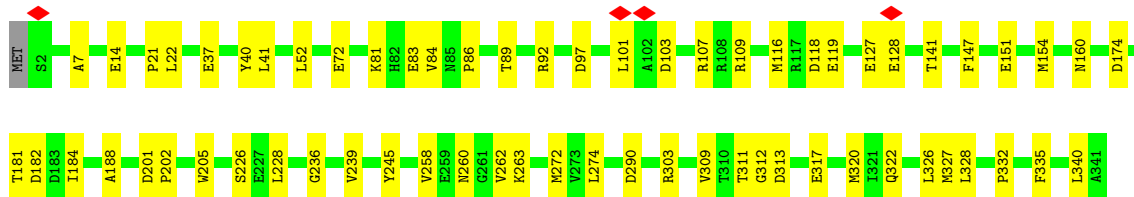
Chain P: 9% 77% 23%



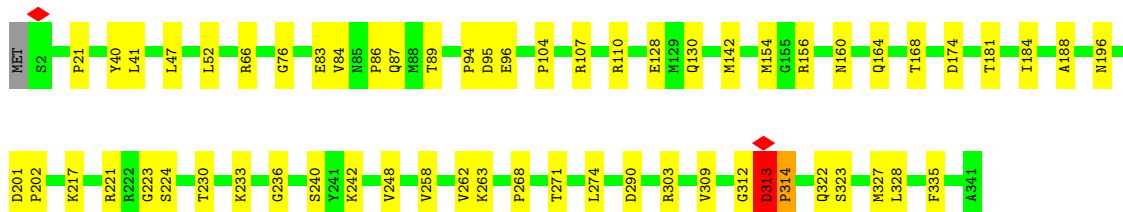
Chain Q: 78% 21%



Chain R: 81% 19%



Chain S: 82% 17%

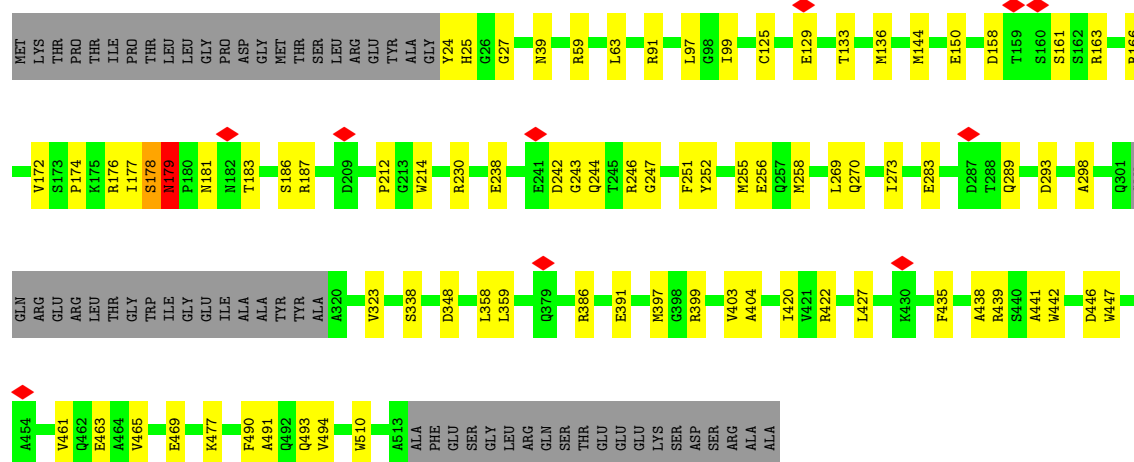


Chain T: 81% 17%



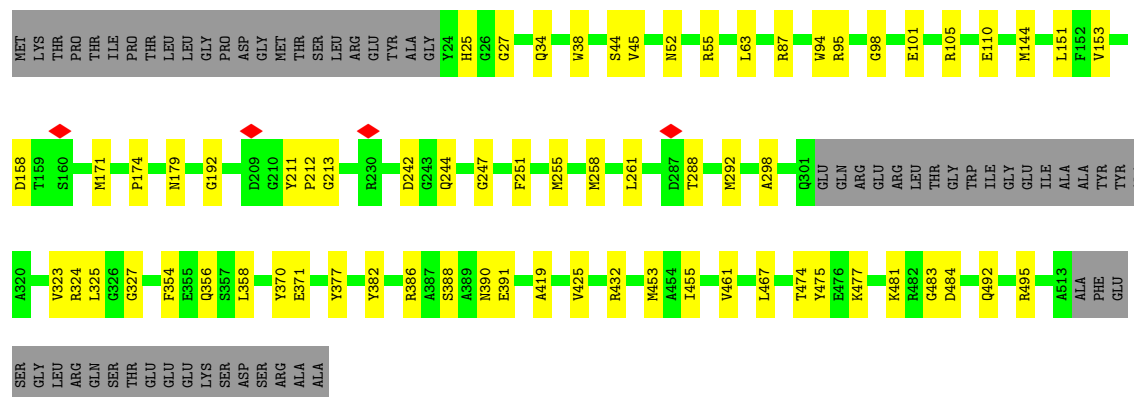
• Molecule 2: Portal protein B

Chain V: 73% 15% 11%



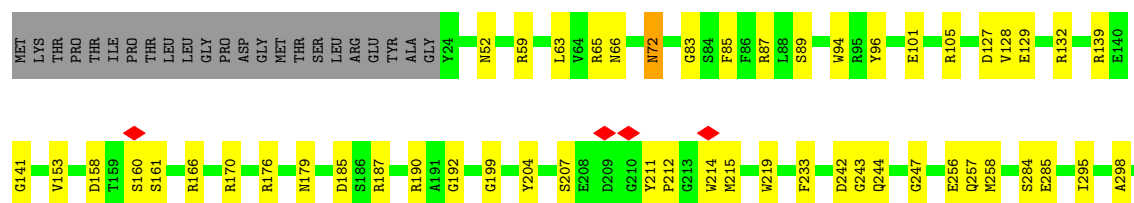
• Molecule 2: Portal protein B

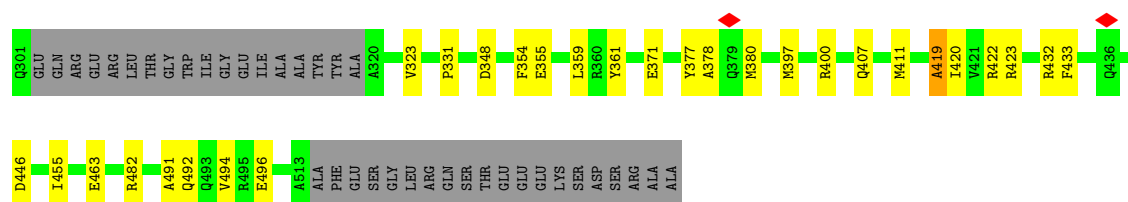
Chain W: 76% 13% 11%



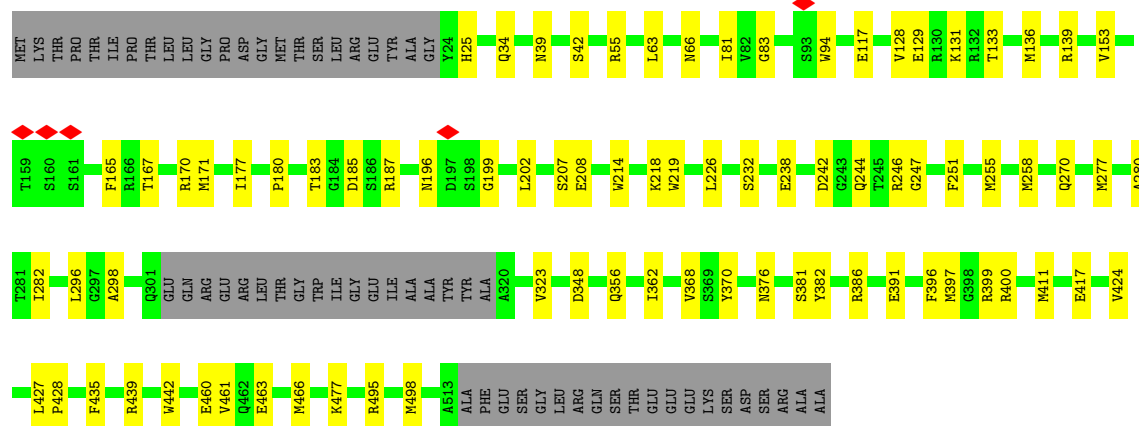
• Molecule 2: Portal protein B

Chain X: 73% 15% 11%

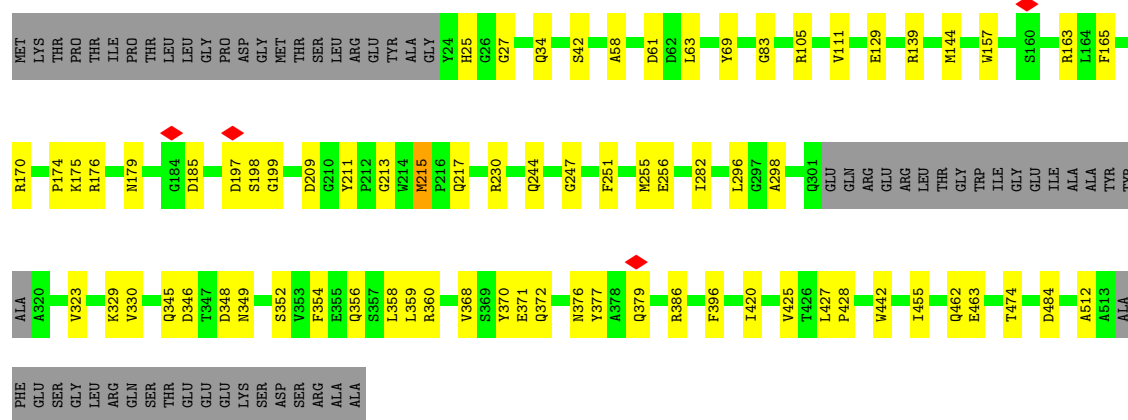
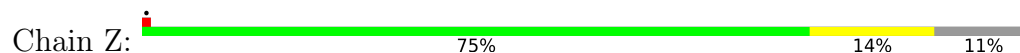




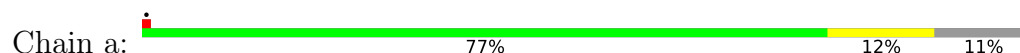
• Molecule 2: Portal protein B

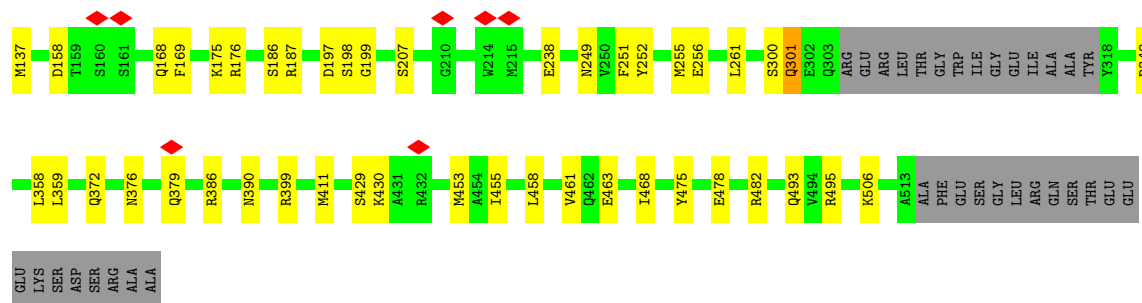


• Molecule 2: Portal protein B



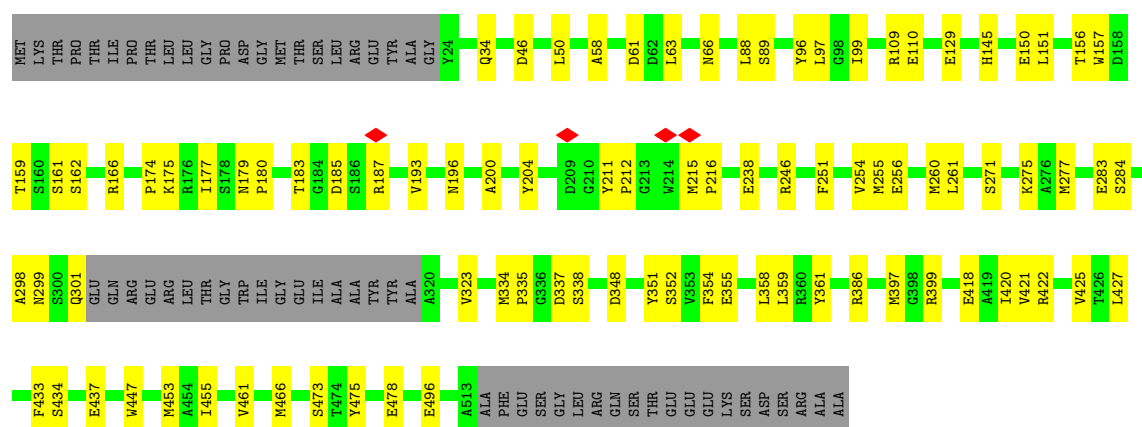
• Molecule 2: Portal protein B





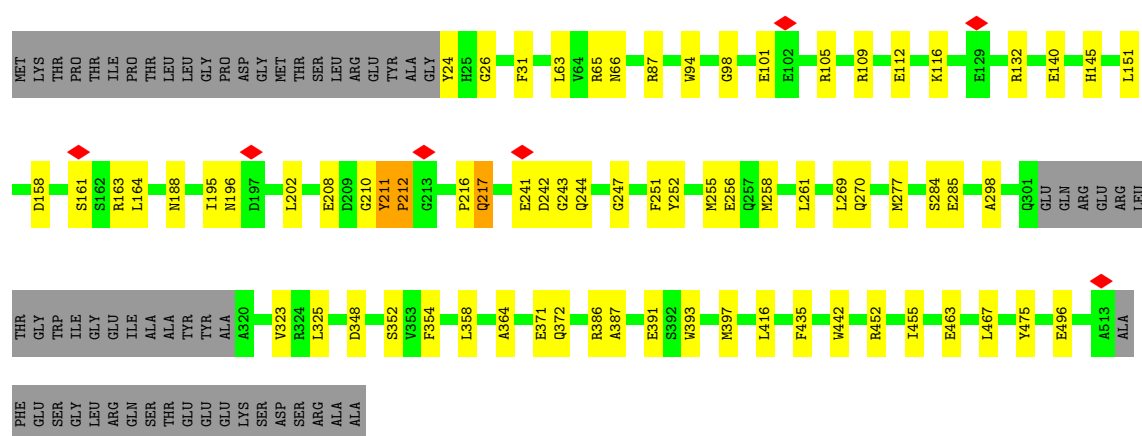
• Molecule 2: Portal protein B

Chain b: 72% 17% 11%



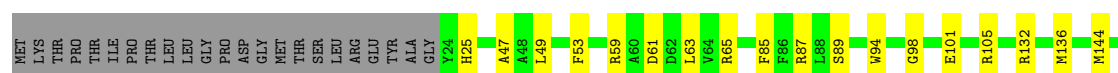
• Molecule 2: Portal protein B

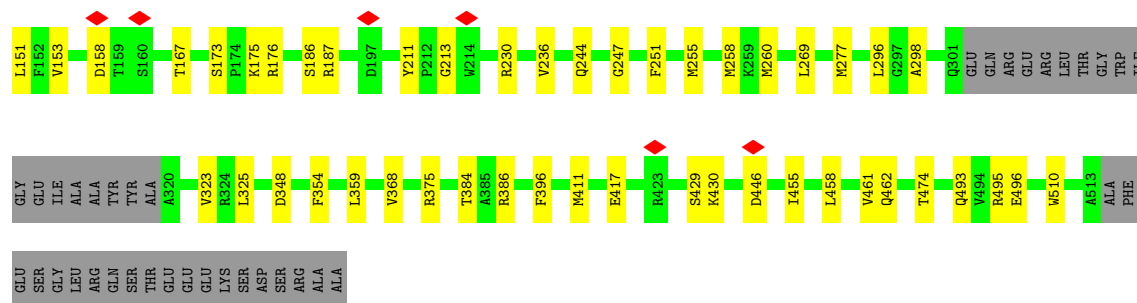
Chain c: 75% 13% 11%



• Molecule 2: Portal protein B

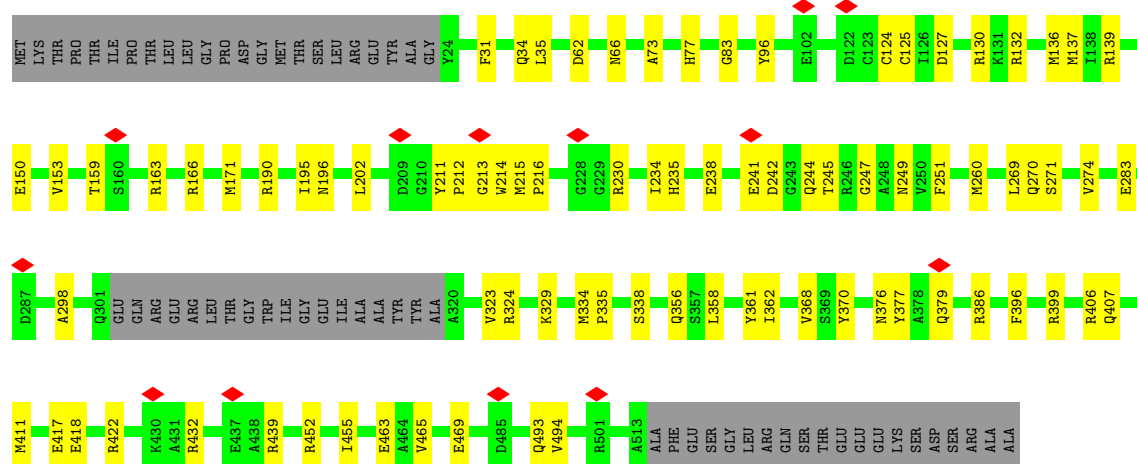
Chain d: 76% 12% 11%





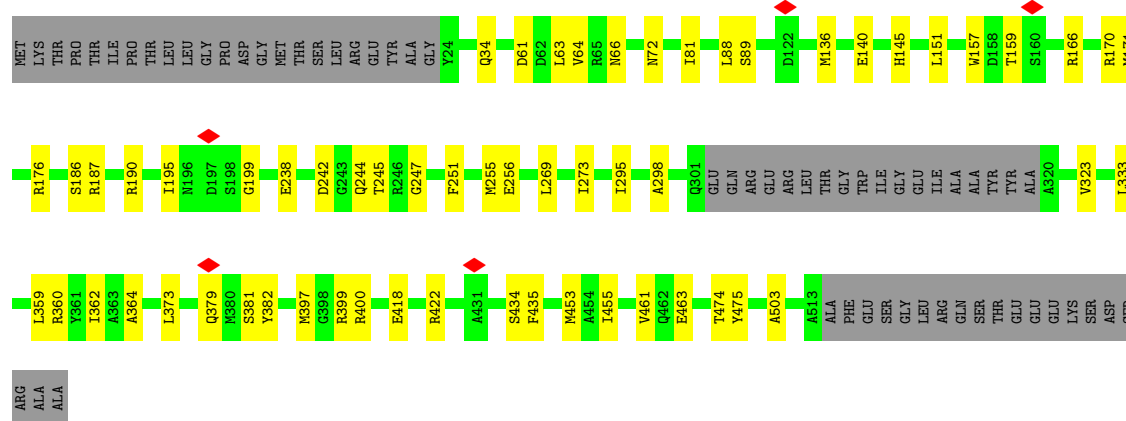
• Molecule 2: Portal protein B

Chain e: 73% 16% 11%



• Molecule 2: Portal protein B

Chain f: 77% 11% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67924	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	43.077	Depositor
Minimum map value	-28.271	Depositor
Average map value	0.003	Depositor
Map value standard deviation	2.155	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.27	0/2728	0.50	2/3693 (0.1%)
1	1	0.21	0/2728	0.37	0/3693
1	2	0.26	0/2728	0.44	3/3693 (0.1%)
1	3	0.20	0/2701	0.38	0/3657
1	4	0.21	0/2701	0.41	0/3657
1	5	0.21	0/2701	0.39	0/3657
1	6	0.26	0/2728	0.45	1/3693 (0.0%)
1	7	0.27	0/2728	0.46	2/3693 (0.1%)
1	A	0.25	0/2728	0.45	0/3693
1	B	0.21	0/2728	0.40	2/3693 (0.1%)
1	C	0.22	0/2728	0.45	3/3693 (0.1%)
1	D	0.23	0/2728	0.41	1/3693 (0.0%)
1	E	0.16	0/2728	0.39	0/3693
1	F	0.24	0/2728	0.38	1/3693 (0.0%)
1	G	0.14	0/2728	0.30	0/3693
1	H	0.14	0/2728	0.32	0/3693
1	I	0.22	0/2728	0.45	1/3693 (0.0%)
1	J	0.14	0/2728	0.31	0/3693
1	K	0.19	0/2728	0.40	2/3693 (0.1%)
1	L	0.32	0/2728	0.52	3/3693 (0.1%)
1	M	0.31	0/2728	0.46	2/3693 (0.1%)
1	N	0.31	0/2701	0.48	2/3657 (0.1%)
1	O	0.33	0/2728	0.50	3/3693 (0.1%)
1	P	0.21	0/2728	0.38	0/3693
1	Q	0.23	0/2728	0.46	2/3693 (0.1%)
1	R	0.21	0/2728	0.45	2/3693 (0.1%)
1	S	0.25	0/2728	0.45	4/3693 (0.1%)
1	T	0.28	0/2728	0.55	6/3693 (0.2%)
1	g	0.40	0/2728	0.48	1/3693 (0.0%)
1	h	0.41	0/2701	0.51	1/3657 (0.0%)
2	U	0.17	0/3755	0.31	0/5072
2	V	0.27	1/3792 (0.0%)	0.36	1/5125 (0.0%)
2	W	0.22	0/3792	0.33	1/5125 (0.0%)
2	X	0.24	1/3792 (0.0%)	0.34	2/5125 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Y	0.29	0/3792	0.39	1/5125 (0.0%)
2	Z	0.22	0/3792	0.32	0/5125
2	a	0.18	0/3828	0.33	0/5174
2	b	0.24	0/3792	0.37	2/5125 (0.0%)
2	c	0.37	2/3792 (0.1%)	0.46	4/5125 (0.1%)
2	d	0.21	0/3792	0.34	0/5125
2	e	0.23	0/3792	0.34	0/5125
2	f	0.17	0/3792	0.32	0/5125
All	All	0.25	4/127208 (0.0%)	0.41	55/172106 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	179	ASN	CA-C	-5.81	1.45	1.52
2	c	208	GLU	CA-C	-5.52	1.46	1.52
2	X	419	ALA	CA-C	-5.48	1.46	1.52
2	c	416	LEU	CA-C	-5.44	1.45	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	91	ARG	N-CA-C	9.60	122.69	109.54
1	L	91	ARG	N-CA-C	9.18	123.64	108.49
1	0	37	GLU	N-CA-C	8.78	120.85	111.28
1	T	95	ASP	N-CA-C	8.69	124.11	113.17
1	O	175	LYS	N-CA-C	-8.39	97.50	110.17
1	7	200	PHE	N-CA-C	8.32	123.52	113.12
1	M	334	GLU	N-CA-C	-8.05	101.35	112.30
1	h	176	SER	N-CA-C	-6.99	98.69	109.52
1	N	179	ASP	CA-C-N	-6.95	112.48	120.89
1	N	179	ASP	C-N-CA	-6.95	112.48	120.89
2	b	162	SER	N-CA-C	-6.91	104.88	113.38
1	0	36	THR	N-CA-C	6.75	118.71	110.41
1	T	98	PRO	N-CA-C	-6.74	104.56	113.65
1	Q	92	ARG	N-CA-C	6.67	120.44	111.24
1	Q	91	ARG	N-CA-C	6.64	121.55	107.67
1	B	313	ASP	CA-C-N	-6.50	111.71	119.84
1	B	313	ASP	C-N-CA	-6.50	111.71	119.84
1	R	311	THR	N-CA-C	6.45	120.85	112.92
1	T	89	THR	N-CA-C	6.42	120.82	112.92
1	F	205	TRP	N-CA-C	-6.41	104.29	111.28
1	R	312	GLY	N-CA-C	6.29	120.28	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	21	PRO	CB-CA-C	-6.26	104.58	113.09
1	M	333	ASP	N-CA-C	6.24	117.34	108.54
1	2	334	GLU	N-CA-C	-5.95	98.13	110.80
1	C	315	ALA	N-CA-C	5.92	123.41	110.80
1	S	314	PRO	N-CA-C	-5.91	100.29	112.47
2	Y	167	THR	N-CA-C	5.88	118.73	109.96
2	W	419	ALA	N-CA-C	-5.79	104.97	111.28
1	O	179	ASP	CA-C-N	-5.73	113.85	120.04
1	O	179	ASP	C-N-CA	-5.73	113.85	120.04
1	I	312	GLY	N-CA-C	-5.72	101.17	110.55
1	L	199	VAL	N-CA-C	5.70	116.01	107.51
1	C	312	GLY	N-CA-C	-5.65	101.19	110.56
1	g	259	GLU	N-CA-C	5.54	120.52	113.55
2	c	208	GLU	N-CA-C	-5.51	100.72	109.59
1	2	331	ASP	CA-C-N	-5.50	114.09	119.64
1	2	331	ASP	C-N-CA	-5.50	114.09	119.64
1	C	316	ARG	N-CA-C	5.48	122.46	110.80
2	c	211	TYR	CA-C-N	-5.43	113.32	118.97
2	c	211	TYR	C-N-CA	-5.43	113.32	118.97
1	L	200	PHE	CB-CA-C	-5.38	100.42	109.50
1	K	324	ALA	CA-C-N	-5.26	113.26	119.84
1	K	324	ALA	C-N-CA	-5.26	113.26	119.84
1	7	202	PRO	N-CA-C	5.20	120.90	113.47
1	D	314	PRO	N-CA-C	-5.16	101.83	112.47
1	T	311	THR	N-CA-C	5.16	119.42	113.18
2	b	159	THR	N-CA-C	5.14	116.88	111.28
1	T	313	ASP	N-CA-C	5.14	119.74	112.75
1	S	313	ASP	CA-C-N	-5.13	113.43	119.84
1	S	313	ASP	C-N-CA	-5.13	113.43	119.84
2	V	178	SER	N-CA-C	5.10	116.68	110.41
1	S	312	GLY	N-CA-C	5.09	125.25	113.18
2	X	419	ALA	CA-C-N	-5.08	113.37	120.53
2	X	419	ALA	C-N-CA	-5.08	113.37	120.53
2	c	212	PRO	N-CA-C	5.00	120.62	113.47

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	0	2675	0	2638	71	0
1	1	2675	0	2638	49	0
1	2	2675	0	2638	43	0
1	3	2649	0	2615	44	0
1	4	2649	0	2615	57	0
1	5	2649	0	2615	58	0
1	6	2675	0	2638	47	0
1	7	2675	0	2638	65	0
1	A	2675	0	2638	52	0
1	B	2675	0	2638	44	0
1	C	2675	0	2638	56	0
1	D	2675	0	2638	46	0
1	E	2675	0	2638	51	0
1	F	2675	0	2638	56	0
1	G	2675	0	2638	49	0
1	H	2675	0	2638	45	0
1	I	2675	0	2638	53	0
1	J	2675	0	2638	60	0
1	K	2675	0	2638	58	0
1	L	2675	0	2638	60	0
1	M	2675	0	2638	53	0
1	N	2649	0	2615	49	0
1	O	2675	0	2638	45	0
1	P	2675	0	2638	58	0
1	Q	2675	0	2638	56	0
1	R	2675	0	2638	41	0
1	S	2675	0	2638	41	0
1	T	2675	0	2638	51	0
1	g	2675	0	2638	38	0
1	h	2649	0	2615	45	0
2	U	3675	0	3524	56	0
2	V	3708	0	3554	61	0
2	W	3708	0	3554	50	0
2	X	3708	0	3554	58	0
2	Y	3708	0	3554	58	0
2	Z	3708	0	3554	57	0
2	a	3743	0	3582	51	0
2	b	3708	0	3554	63	0
2	c	3708	0	3554	57	0
2	d	3708	0	3554	48	0
2	e	3708	0	3554	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	f	3708	0	3554	46	0
All	All	124618	0	121671	1869	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1869) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:SER:N	1:S:40:TYR:HH	1.70	0.87
2:b:187:ARG:HA	2:c:212:PRO:HG3	1.55	0.85
1:C:2:SER:N	1:R:40:TYR:HH	1.76	0.83
1:I:283:ARG:HG2	1:I:327:MET:HE1	1.61	0.82
1:Q:310:THR:HG22	1:Q:312:GLY:H	1.47	0.79
1:Q:125:GLN:HE21	1:Q:257:TYR:HB2	1.47	0.79
1:7:168:THR:HA	1:7:173:ARG:HD2	1.65	0.79
2:V:166:ARG:HE	2:V:422:ARG:HH21	1.30	0.79
1:B:180:PRO:HG3	1:B:211:PHE:HD2	1.47	0.78
1:B:2:SER:N	1:L:40:TYR:HH	1.83	0.77
2:d:260:MET:HE3	2:e:270:GLN:HE22	1.49	0.77
1:3:283:ARG:HG3	1:3:327:MET:HE1	1.66	0.77
1:F:41:LEU:HD11	1:F:328:LEU:HD13	1.67	0.76
1:T:218:LEU:HD21	1:T:228:LEU:HB3	1.67	0.76
2:b:298:ALA:HB2	2:b:323:VAL:HG22	1.67	0.76
1:6:49:ASN:HA	1:Q:258:VAL:HG23	1.67	0.76
1:0:262:VAL:HG12	1:0:263:LYS:H	1.50	0.76
1:5:229:GLU:HG3	1:5:233:LYS:HD2	1.68	0.76
2:e:407:GLN:HG2	2:e:411:MET:HE2	1.66	0.75
2:c:244:GLN:HE21	2:c:247:GLY:HA2	1.52	0.75
1:H:82:HIS:HB2	1:H:115:ASN:HD21	1.51	0.75
2:Z:298:ALA:HB2	2:Z:323:VAL:HG22	1.69	0.74
1:J:75:PRO:HA	1:J:326:LEU:HD12	1.69	0.74
2:a:187:ARG:HG2	2:b:212:PRO:HG3	1.69	0.74
1:E:257:TYR:HB3	1:E:266:PHE:HE2	1.52	0.74
2:V:161:SER:HG	2:V:163:ARG:HE	1.35	0.73
1:5:299:ASN:HD21	1:g:103:ASP:HB2	1.53	0.73
2:Y:196:ASN:HB3	2:Y:202:LEU:HD11	1.69	0.72
1:2:258:VAL:HG12	1:2:263:LYS:HA	1.70	0.72
1:S:313:ASP:HB3	1:S:314:PRO:HD3	1.69	0.72
1:E:120:GLU:HB2	1:E:303:ARG:HH21	1.53	0.72
2:Z:360:ARG:NH1	2:a:376:ASN:OD1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:45:PRO:HD3	1:5:68:GLY:HA2	1.71	0.72
1:J:127:GLU:OE1	1:J:303:ARG:NH2	2.23	0.72
1:M:290:ASP:OD2	1:M:322:GLN:NE2	2.23	0.71
2:W:244:GLN:HE21	2:W:247:GLY:HA2	1.56	0.71
1:6:269:ASP:OD1	1:6:270:ASN:N	2.22	0.71
1:1:154:MET:HE1	1:1:329:LEU:HB2	1.70	0.71
1:D:229:GLU:HG2	1:D:233:LYS:HB2	1.71	0.71
1:I:229:GLU:HG2	1:I:233:LYS:HD3	1.73	0.71
2:X:63:LEU:HD13	2:X:258:MET:HE3	1.73	0.71
1:L:51:ALA:HB2	1:g:122:ALA:HB1	1.71	0.70
1:0:104:PRO:HD2	1:h:299:ASN:HD22	1.54	0.70
1:O:26:LEU:O	1:O:29:ARG:NH1	2.25	0.70
2:a:127:ASP:HB3	2:a:137:MET:HE1	1.73	0.70
2:e:244:GLN:HE21	2:e:247:GLY:HA2	1.56	0.70
2:W:386:ARG:O	2:W:390:ASN:ND2	2.25	0.70
2:c:242:ASP:OD2	2:d:176:ARG:NH1	2.25	0.70
1:S:96:GLU:OE1	1:S:107:ARG:NH1	2.25	0.70
1:7:198:ILE:HG13	1:7:248:VAL:HG21	1.74	0.70
1:T:84:VAL:HG11	1:T:112:ILE:HD11	1.73	0.70
1:g:66:ARG:NH1	1:h:118:ASP:OD2	2.25	0.69
2:W:34:GLN:NE2	2:X:256:GLU:OE2	2.22	0.69
2:e:159:THR:HA	2:e:166:ARG:HH21	1.56	0.69
1:3:179:ASP:OD2	1:3:217:LYS:NZ	2.25	0.69
1:6:203:LYS:HB2	1:6:270:ASN:HB3	1.73	0.69
1:7:269:ASP:OD2	1:7:270:ASN:N	2.26	0.69
2:Y:133:THR:H	2:Y:136:MET:HE3	1.57	0.69
2:X:463:GLU:HG3	2:Y:461:VAL:HG21	1.74	0.69
2:U:176:ARG:NH1	2:f:242:ASP:OD2	2.25	0.69
2:W:382:TYR:OH	2:W:386:ARG:NH1	2.25	0.69
1:P:82:HIS:ND1	1:P:115:ASN:OD1	2.25	0.69
1:I:80:PRO:HG2	1:I:119:GLU:HB2	1.75	0.69
1:Q:258:VAL:HG12	1:Q:263:LYS:HA	1.75	0.69
1:7:81:LYS:HB3	1:7:320:MET:HG3	1.75	0.68
1:Q:86:PRO:HA	1:Q:89:THR:HG22	1.75	0.68
2:Y:282:ILE:HG13	2:Y:296:LEU:HD21	1.74	0.68
1:B:274:LEU:HB2	1:B:336:VAL:HB	1.75	0.68
2:f:244:GLN:HE21	2:f:247:GLY:HA2	1.58	0.68
1:1:156:ARG:NH1	1:1:332:PRO:O	2.26	0.68
1:T:92:ARG:HH21	1:T:97:ASP:C	2.02	0.68
1:M:229:GLU:HG2	1:M:233:LYS:HD3	1.75	0.68
2:W:34:GLN:OE1	2:Y:270:GLN:NE2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:PHE:O	1:N:283:ARG:NH2	2.25	0.68
1:O:270:ASN:HB3	1:O:340:LEU:HB2	1.76	0.68
1:7:156:ARG:HH22	1:7:335:PHE:HB2	1.58	0.68
1:H:31:SER:HA	1:H:283:ARG:HB2	1.75	0.68
1:L:222:ARG:NH2	1:g:220:THR:O	2.27	0.68
1:S:104:PRO:HA	1:S:107:ARG:HD3	1.74	0.68
1:h:258:VAL:HG12	1:h:263:LYS:HA	1.76	0.68
2:e:463:GLU:HG3	2:f:461:VAL:HG21	1.75	0.68
1:G:257:TYR:HB3	1:G:266:PHE:HE1	1.58	0.67
1:N:85:ASN:HB3	1:N:316:ARG:HG3	1.76	0.67
1:B:22:LEU:HD23	1:B:239:VAL:HG12	1.75	0.67
1:G:226:SER:HB3	1:G:246:GLY:H	1.59	0.67
1:Q:96:GLU:OE2	1:Q:107:ARG:NH1	2.27	0.67
1:O:331:ASP:OD1	1:4:13:ASN:ND2	2.27	0.67
1:2:258:VAL:HG11	1:S:47:LEU:HD11	1.76	0.67
1:4:101:LEU:O	2:V:39:ASN:ND2	2.28	0.67
1:5:201:ASP:HB3	1:5:270:ASN:HA	1.76	0.67
1:L:84:VAL:HG11	1:L:112:ILE:HD11	1.76	0.67
1:7:168:THR:H	1:7:173:ARG:HH11	1.43	0.67
1:E:116:MET:HA	1:E:119:GLU:OE1	1.94	0.67
1:R:272:MET:HE3	1:R:340:LEU:HD21	1.75	0.67
1:1:113:MET:HB3	1:1:117:ARG:HH22	1.58	0.67
1:1:305:PRO:HB3	1:1:321:ILE:HG12	1.76	0.67
1:S:87:GLN:N	1:S:87:GLN:OE1	2.28	0.67
2:W:94:TRP:HE1	2:W:95:ARG:HH21	1.43	0.67
1:J:303:ARG:H	1:J:323:SER:HB2	1.60	0.66
1:T:92:ARG:HH21	1:T:98:PRO:N	1.93	0.66
1:T:258:VAL:HG12	1:T:263:LYS:HA	1.76	0.66
2:V:230:ARG:HA	2:V:439:ARG:HH22	1.59	0.66
2:Y:242:ASP:OD2	2:Z:176:ARG:NH1	2.28	0.66
2:Y:244:GLN:HE21	2:Y:247:GLY:HA2	1.60	0.66
2:e:96:TYR:O	2:e:432:ARG:NH1	2.27	0.66
2:e:62:ASP:OD1	2:e:66:ASN:ND2	2.28	0.66
1:O:103:ASP:HB2	1:h:299:ASN:HD21	1.60	0.66
1:B:108:ARG:NH2	1:B:317:GLU:OE2	2.27	0.66
1:D:63:ILE:O	1:H:82:HIS:ND1	2.29	0.66
2:Z:345:GLN:OE1	2:Z:349:ASN:ND2	2.28	0.66
2:a:158:ASP:OD1	2:a:168:GLN:NE2	2.29	0.66
1:A:160:ASN:ND2	1:A:333:ASP:OD1	2.28	0.66
1:O:108:ARG:NH2	1:O:317:GLU:OE2	2.27	0.66
1:M:68:GLY:H	1:N:94:PRO:HG3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:290:ASP:OD2	1:3:322:GLN:NE2	2.21	0.66
1:R:101:LEU:O	1:R:107:ARG:NH2	2.29	0.66
1:O:168:THR:HA	1:O:173:ARG:HE	1.61	0.66
1:M:36:THR:HG1	1:N:6:THR:HG1	1.42	0.66
2:U:129:GLU:HG2	2:f:199:GLY:HA3	1.77	0.66
1:2:84:VAL:HG11	1:2:112:ILE:HD11	1.78	0.65
1:4:272:MET:HE3	1:4:340:LEU:HD11	1.76	0.65
2:c:26:GLY:O	2:d:59:ARG:NH1	2.30	0.65
2:f:269:LEU:O	2:f:273:ILE:HD12	1.95	0.65
1:L:81:LYS:HG3	1:L:320:MET:HE2	1.76	0.65
1:G:141:THR:HG22	1:G:151:GLU:HG3	1.78	0.65
2:c:252:TYR:HA	2:c:255:MET:HE2	1.77	0.65
1:1:209:ARG:NH2	1:R:182:ASP:OD2	2.28	0.65
1:T:168:THR:HA	1:T:173:ARG:HH21	1.62	0.65
2:U:129:GLU:HB3	2:U:131:LYS:HE2	1.77	0.65
1:K:168:THR:H	1:K:173:ARG:HH11	1.45	0.65
2:d:25:HIS:ND1	2:f:66:ASN:OD1	2.29	0.65
2:X:242:ASP:OD1	2:X:243:GLY:N	2.30	0.65
1:E:168:THR:HA	1:E:173:ARG:HH21	1.61	0.64
1:M:66:ARG:NH1	1:N:118:ASP:OD2	2.30	0.64
1:F:154:MET:HE1	1:F:328:LEU:HA	1.79	0.64
2:Y:34:GLN:NE2	2:Z:256:GLU:OE2	2.30	0.64
1:3:229:GLU:HG2	1:3:233:LYS:HB2	1.79	0.64
1:R:290:ASP:OD2	1:R:322:GLN:NE2	2.29	0.64
2:a:34:GLN:OE1	2:c:270:GLN:NE2	2.29	0.64
1:5:258:VAL:HG12	1:5:263:LYS:HA	1.80	0.64
1:Q:132:VAL:HG11	1:Q:266:PHE:HB3	1.80	0.64
2:U:354:PHE:HB2	2:V:348:ASP:HB2	1.78	0.64
2:c:463:GLU:HG3	2:d:461:VAL:HG21	1.79	0.64
1:E:113:MET:HA	1:E:116:MET:SD	2.37	0.64
1:G:127:GLU:OE1	1:G:303:ARG:NH2	2.30	0.64
1:I:22:LEU:O	1:I:26:LEU:HB2	1.97	0.64
2:V:298:ALA:HB2	2:V:323:VAL:HG22	1.78	0.64
2:a:468:ILE:HD11	2:a:478:GLU:HG3	1.77	0.64
1:2:36:THR:HG22	1:2:37:GLU:H	1.62	0.64
2:V:161:SER:O	2:V:166:ARG:NH1	2.31	0.64
2:a:429:SER:OG	2:a:430:LYS:NZ	2.27	0.64
2:V:27:GLY:O	2:W:52:ASN:ND2	2.30	0.64
2:Y:391:GLU:OE2	2:Z:372:GLN:NE2	2.30	0.64
1:g:77:TYR:OH	1:g:289:GLN:N	2.30	0.64
1:G:53:TYR:OH	1:O:130:GLN:NE2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:463:GLU:HG3	2:V:461:VAL:HG21	1.79	0.64
1:C:274:LEU:HB2	1:C:336:VAL:HB	1.80	0.63
1:I:309:VAL:HB	1:Q:295:ARG:HH22	1.62	0.63
1:J:326:LEU:HD22	1:J:328:LEU:HD23	1.79	0.63
1:M:267:LEU:HD12	1:M:271:THR:HG21	1.79	0.63
2:U:334:MET:HG3	2:U:335:PRO:HD2	1.80	0.63
1:h:201:ASP:HB3	1:h:270:ASN:HA	1.78	0.63
1:6:21:PRO:HB3	1:6:128:GLU:CD	2.22	0.63
1:D:108:ARG:NH1	1:D:317:GLU:OE1	2.31	0.63
1:H:196:ASN:HA	1:H:248:VAL:HG12	1.79	0.63
1:J:205:TRP:HH2	1:J:228:LEU:HD13	1.63	0.63
1:3:209:ARG:HD2	1:3:230:THR:HG23	1.80	0.63
1:R:127:GLU:HG3	1:R:303:ARG:HH22	1.64	0.63
1:T:205:TRP:HH2	1:T:228:LEU:HD21	1.62	0.63
2:V:161:SER:OG	2:V:163:ARG:NE	2.25	0.63
1:h:45:PRO:HD3	1:h:68:GLY:HA2	1.79	0.63
1:D:258:VAL:HG22	1:D:263:LYS:HG2	1.79	0.63
1:M:109:ARG:HG2	1:M:113:MET:HE1	1.79	0.63
2:d:101:GLU:OE2	2:d:105:ARG:NH2	2.32	0.63
1:N:108:ARG:NH1	1:N:317:GLU:OE1	2.32	0.63
1:C:229:GLU:HG2	1:C:233:LYS:HB2	1.80	0.63
2:c:101:GLU:OE1	2:d:495:ARG:NH2	2.31	0.63
1:A:203:LYS:HE2	1:A:269:ASP:HB2	1.81	0.63
2:U:298:ALA:HB2	2:U:323:VAL:HG22	1.81	0.63
2:e:241:GLU:HG2	2:e:242:ASP:H	1.63	0.63
1:I:112:ILE:HA	1:I:115:ASN:HD22	1.64	0.62
2:V:133:THR:H	2:V:136:MET:HE2	1.63	0.62
1:C:180:PRO:HG3	1:C:211:PHE:HD2	1.64	0.62
1:K:112:ILE:O	1:K:116:MET:HG2	2.00	0.62
2:Z:170:ARG:HH21	2:Z:176:ARG:HH12	1.47	0.62
1:2:267:LEU:HD12	1:2:271:THR:HG21	1.82	0.62
1:7:82:HIS:ND1	1:F:63:ILE:O	2.25	0.62
1:G:3:MET:HG3	1:G:5:THR:HG22	1.81	0.62
2:V:270:GLN:NE2	2:f:34:GLN:OE1	2.25	0.62
2:Y:25:HIS:ND1	2:a:66:ASN:OD1	2.32	0.62
1:0:122:ALA:HB1	1:Q:51:ALA:HB2	1.81	0.62
2:W:25:HIS:ND1	2:Y:66:ASN:OD1	2.32	0.62
1:6:21:PRO:HB3	1:6:128:GLU:OE2	1.99	0.62
2:e:379:GLN:O	2:f:379:GLN:NE2	2.31	0.62
1:g:229:GLU:HG2	1:g:233:LYS:HD3	1.80	0.62
1:g:331:ASP:OD1	1:h:13:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:229:GLU:HG2	1:2:233:LYS:HD3	1.82	0.62
1:D:223:GLY:HA2	1:H:218:LEU:HD23	1.80	0.62
2:b:271:SER:OG	2:b:275:LYS:NZ	2.33	0.62
1:4:47:LEU:HD22	1:A:258:VAL:HG21	1.82	0.62
1:L:218:LEU:HD21	1:L:228:LEU:HB3	1.81	0.62
2:Z:197:ASP:OD1	2:Z:198:SER:N	2.33	0.62
2:b:238:GLU:OE1	2:b:399:ARG:NH2	2.28	0.62
2:c:112:GLU:O	2:c:116:LYS:HG2	2.00	0.62
1:0:201:ASP:OD2	1:0:202:PRO:HD2	1.98	0.61
1:F:162:ILE:HB	1:F:338:VAL:HG12	1.81	0.61
2:b:354:PHE:HB2	2:c:348:ASP:HB2	1.82	0.61
2:c:298:ALA:HB2	2:c:323:VAL:HG22	1.82	0.61
1:O:194:VAL:HA	1:S:236:GLY:HA3	1.82	0.61
2:a:34:GLN:NE2	2:b:256:GLU:OE2	2.30	0.61
2:d:211:TYR:O	2:d:213:GLY:N	2.33	0.61
2:V:242:ASP:OD1	2:V:243:GLY:N	2.33	0.61
2:Y:417:GLU:OE2	2:Y:439:ARG:NE	2.28	0.61
2:a:42:SER:HB2	2:b:58:ALA:HB2	1.81	0.61
1:4:9:LEU:HD21	1:4:12:ALA:HB2	1.81	0.61
1:P:232:VAL:HG22	1:P:235:LEU:HD11	1.82	0.61
2:U:211:TYR:HB3	2:U:212:PRO:HD3	1.81	0.61
2:b:475:TYR:HB2	2:c:496:GLU:OE2	2.01	0.61
1:g:310:THR:HG22	1:g:311:THR:H	1.65	0.61
1:3:58:VAL:HG21	1:C:146:ALA:HB1	1.82	0.61
2:U:261:LEU:HD13	2:U:358:LEU:HD12	1.81	0.61
1:2:219:ASP:O	1:S:221:ARG:NH1	2.33	0.61
2:U:199:GLY:HA3	2:V:129:GLU:HG2	1.82	0.61
1:F:165:SER:OG	1:F:166:GLY:N	2.33	0.61
1:R:41:LEU:HD11	1:R:328:LEU:HD13	1.82	0.61
2:X:153:VAL:HG11	2:X:411:MET:HE2	1.83	0.61
2:b:196:ASN:HD21	2:b:200:ALA:HB3	1.66	0.61
1:5:313:ASP:CG	1:5:314:PRO:HD3	2.26	0.61
1:0:156:ARG:NH1	1:0:332:PRO:O	2.34	0.61
2:c:387:ALA:O	2:c:391:GLU:HG2	2.01	0.61
1:0:47:LEU:HD11	1:4:258:VAL:HG11	1.81	0.60
1:D:93:LEU:HD12	1:D:110:ARG:HH11	1.65	0.60
1:F:96:GLU:OE2	1:F:107:ARG:NH1	2.34	0.60
1:L:101:LEU:O	1:L:107:ARG:NH2	2.32	0.60
2:W:242:ASP:OD2	2:X:176:ARG:NH1	2.34	0.60
1:N:290:ASP:OD2	1:N:322:GLN:NE2	2.20	0.60
2:U:110:GLU:HG2	2:U:425:VAL:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:238:GLU:OE1	2:Y:399:ARG:NH2	2.32	0.60
2:e:190:ARG:HD2	2:e:245:THR:HG21	1.82	0.60
1:2:232:VAL:HG21	1:S:184:ILE:HD11	1.83	0.60
1:E:26:LEU:O	1:E:29:ARG:NH1	2.34	0.60
2:Y:296:LEU:HD11	2:Z:330:VAL:HG11	1.84	0.60
1:F:82:HIS:HB2	1:F:115:ASN:HD21	1.66	0.60
2:U:461:VAL:HG21	2:f:463:GLU:HG3	1.84	0.60
1:1:290:ASP:OD2	1:1:322:GLN:NE2	2.34	0.60
1:B:229:GLU:HG2	1:B:233:LYS:HD3	1.84	0.60
1:F:77:TYR:HE2	1:F:79:LYS:HD2	1.67	0.60
1:L:184:ILE:HD11	1:g:232:VAL:HG21	1.84	0.60
1:L:234:ASP:OD1	1:L:237:LYS:NZ	2.28	0.60
2:X:298:ALA:HB2	2:X:323:VAL:HG22	1.84	0.60
2:Y:370:TYR:OH	2:Y:376:ASN:ND2	2.33	0.60
1:I:156:ARG:HH21	1:I:335:PHE:HB2	1.67	0.60
2:W:63:LEU:HD13	2:W:258:MET:HE3	1.83	0.60
2:d:474:THR:HG22	2:e:493:GLN:HG3	1.83	0.60
1:G:165:SER:OG	1:G:166:GLY:N	2.35	0.60
1:g:82:HIS:ND1	1:g:119:GLU:OE2	2.35	0.60
1:H:156:ARG:NH1	1:H:161:ASN:OD1	2.35	0.60
1:P:84:VAL:HG11	1:P:112:ILE:HD11	1.83	0.59
2:V:25:HIS:ND1	2:X:66:ASN:OD1	2.35	0.59
2:Z:83:GLY:O	2:Z:139:ARG:NH1	2.34	0.59
1:J:23:PHE:HD2	1:J:132:VAL:HG22	1.67	0.59
1:K:119:GLU:HB2	1:K:321:ILE:HD12	1.83	0.59
1:E:270:ASN:HD21	1:E:341:ALA:HB3	1.68	0.59
1:J:84:VAL:HG11	1:J:112:ILE:HD11	1.84	0.59
1:M:183:ASP:O	1:M:187:TYR:HD2	1.84	0.59
2:f:159:THR:HG22	2:f:166:ARG:HH22	1.67	0.59
1:h:228:LEU:HD21	1:h:245:TYR:HB2	1.85	0.59
1:D:75:PRO:HA	1:D:326:LEU:HD12	1.84	0.59
1:S:86:PRO:HA	1:S:89:THR:HG22	1.85	0.59
1:G:75:PRO:HA	1:G:326:LEU:HD12	1.85	0.59
2:d:85:PHE:HD2	2:d:87:ARG:HG3	1.66	0.59
2:e:125:CYS:SG	2:e:130:ARG:NH1	2.76	0.59
1:G:274:LEU:HB2	1:G:336:VAL:HB	1.85	0.59
1:I:327:MET:HA	1:I:327:MET:HE3	1.84	0.59
1:G:299:ASN:OD1	1:G:300:ALA:N	2.35	0.59
2:c:161:SER:OG	2:c:163:ARG:NH1	2.36	0.59
1:0:258:VAL:HG12	1:0:263:LYS:HA	1.85	0.58
1:0:313:ASP:HB3	1:0:314:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:251:PHE:HB3	2:a:255:MET:HG2	1.84	0.58
2:d:244:GLN:HE21	2:d:247:GLY:HA2	1.68	0.58
2:d:386:ARG:HG2	2:e:455:ILE:O	2.03	0.58
1:B:162:ILE:HB	1:B:338:VAL:HG22	1.83	0.58
1:S:160:ASN:ND2	1:S:335:PHE:O	2.36	0.58
2:U:251:PHE:O	2:U:255:MET:HG3	2.03	0.58
2:a:25:HIS:ND1	2:c:66:ASN:OD1	2.35	0.58
2:b:334:MET:HG3	2:b:335:PRO:HD2	1.84	0.58
1:A:181:THR:HG23	1:E:232:VAL:HG13	1.84	0.58
1:B:180:PRO:HG3	1:B:211:PHE:CD2	2.35	0.58
1:Q:84:VAL:HG11	1:Q:112:ILE:HD11	1.83	0.58
1:1:103:ASP:HB2	1:3:299:ASN:HD21	1.66	0.58
1:K:82:HIS:ND1	1:K:119:GLU:OE2	2.37	0.58
1:2:82:HIS:ND1	1:2:119:GLU:OE2	2.36	0.58
1:6:218:LEU:HD11	1:6:228:LEU:HD23	1.85	0.58
1:D:3:MET:HE3	1:D:4:TYR:H	1.68	0.58
1:G:29:ARG:NH2	1:G:279:ALA:O	2.35	0.58
2:e:358:LEU:O	2:e:362:ILE:HG12	2.02	0.58
1:h:313:ASP:HB3	1:h:314:PRO:HD3	1.85	0.58
1:2:66:ARG:NH2	1:3:118:ASP:OD1	2.29	0.58
1:O:256:GLN:HA	1:O:265:ASN:HA	1.85	0.58
2:V:244:GLN:HE21	2:V:247:GLY:HA2	1.69	0.58
2:V:397:MET:HA	2:V:397:MET:HE3	1.85	0.58
1:2:305:PRO:HB3	1:2:321:ILE:HG22	1.84	0.58
1:B:181:THR:HG23	1:F:232:VAL:HG13	1.85	0.58
1:E:165:SER:OG	1:E:166:GLY:N	2.37	0.58
1:M:313:ASP:HB3	1:M:314:PRO:HD3	1.86	0.58
1:4:85:ASN:HB3	1:4:316:ARG:HG3	1.85	0.58
1:I:135:VAL:O	1:I:156:ARG:NH2	2.34	0.58
1:N:310:THR:HG23	1:N:312:GLY:H	1.69	0.58
2:X:214:TRP:CD1	2:X:215:MET:H	2.21	0.58
2:X:244:GLN:HE21	2:X:247:GLY:HA2	1.69	0.58
2:a:390:ASN:ND2	2:b:453:MET:O	2.37	0.58
1:3:201:ASP:HB3	1:3:270:ASN:HA	1.85	0.57
1:E:156:ARG:NH1	1:E:161:ASN:OD1	2.36	0.57
1:H:84:VAL:HG11	1:H:112:ILE:HD11	1.86	0.57
1:P:66:ARG:NH2	1:T:118:ASP:OD1	2.32	0.57
1:F:112:ILE:O	1:F:116:MET:HG2	2.03	0.57
1:L:30:GLU:OE2	1:L:280:ARG:NH1	2.37	0.57
1:P:50:MET:HE2	1:T:126:VAL:HA	1.86	0.57
1:T:201:ASP:OD1	1:T:202:PRO:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:376:ASN:OD1	2:f:360:ARG:NH1	2.36	0.57
2:Z:420:ILE:HG23	2:Z:427:LEU:HD11	1.85	0.57
1:I:160:ASN:ND2	1:I:333:ASP:OD1	2.36	0.57
2:X:257:GLN:HE21	2:X:361:TYR:HE2	1.51	0.57
2:e:417:GLU:OE1	2:e:439:ARG:NH1	2.37	0.57
1:1:182:ASP:OD1	1:5:209:ARG:NH2	2.38	0.57
2:U:87:ARG:NH2	2:U:483:GLY:O	2.38	0.57
1:1:229:GLU:HG2	1:1:233:LYS:HD3	1.86	0.57
1:L:181:THR:HA	1:L:184:ILE:HG12	1.86	0.57
1:L:258:VAL:HG12	1:L:263:LYS:HA	1.87	0.57
1:O:201:ASP:HB3	1:O:267:LEU:HD22	1.86	0.57
2:d:277:MET:HE3	2:e:329:LYS:HD2	1.87	0.57
1:1:173:ARG:HD2	1:1:178:TYR:CE2	2.40	0.57
1:5:177:THR:H	1:5:212:LYS:NZ	2.02	0.57
1:I:178:TYR:OH	1:I:183:ASP:OD2	2.20	0.57
1:T:81:LYS:HG3	1:T:320:MET:HE2	1.87	0.57
1:K:223:GLY:HA2	1:L:218:LEU:HD23	1.85	0.57
1:L:154:MET:HE3	1:L:329:LEU:HB2	1.86	0.57
1:Q:212:LYS:NZ	1:Q:216:GLU:OE2	2.37	0.57
2:c:261:LEU:HD13	2:c:358:LEU:HD12	1.86	0.57
1:4:45:PRO:HD3	1:4:68:GLY:HA2	1.87	0.57
1:D:331:ASP:OD2	1:H:13:ASN:ND2	2.36	0.57
1:J:63:ILE:HB	1:K:82:HIS:CD2	2.40	0.57
1:0:80:PRO:HB2	1:0:119:GLU:HG3	1.85	0.57
1:E:258:VAL:HA	1:E:263:LYS:HA	1.87	0.57
1:Q:181:THR:HA	1:Q:184:ILE:HG22	1.87	0.57
1:3:30:GLU:HG3	1:3:32:TYR:CE1	2.39	0.57
1:4:90:LEU:O	1:4:107:ARG:NH1	2.38	0.57
1:6:7:ALA:HB1	1:E:40:TYR:HE1	1.69	0.57
1:N:45:PRO:HD3	1:N:68:GLY:HA2	1.86	0.57
1:7:49:ASN:ND2	1:R:260:ASN:O	2.36	0.56
1:F:34:PHE:HE1	1:F:284:THR:HB	1.70	0.56
1:G:82:HIS:HB2	1:G:115:ASN:HD21	1.69	0.56
2:U:417:GLU:HG2	2:U:435:PHE:HE2	1.70	0.56
2:d:493:GLN:HG2	2:d:510:TRP:CE2	2.40	0.56
1:3:258:VAL:HG12	1:3:263:LYS:HA	1.87	0.56
1:H:54:VAL:HG12	1:P:146:ALA:HB3	1.86	0.56
1:0:103:ASP:HB2	1:h:299:ASN:ND2	2.20	0.56
1:2:218:LEU:HD13	1:S:223:GLY:HA2	1.86	0.56
1:D:130:GLN:NE2	1:D:142:MET:SD	2.78	0.56
1:K:256:GLN:HA	1:K:265:ASN:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:83:GLY:O	2:X:139:ARG:NH1	2.38	0.56
2:Y:177:ILE:O	2:Y:246:ARG:NH1	2.29	0.56
2:e:127:ASP:OD2	2:e:130:ARG:N	2.38	0.56
1:5:299:ASN:ND2	1:g:103:ASP:HB2	2.20	0.56
1:M:34:PHE:HZ	1:M:75:PRO:HG3	1.68	0.56
2:W:87:ARG:NH2	2:W:483:GLY:O	2.38	0.56
1:5:41:LEU:HD12	1:5:73:PHE:HE2	1.71	0.56
2:b:277:MET:HE3	2:c:325:LEU:HD12	1.88	0.56
2:e:83:GLY:O	2:e:139:ARG:NH1	2.39	0.56
1:h:28:PHE:HE1	1:h:329:LEU:HD13	1.69	0.56
1:D:181:THR:HG23	1:H:232:VAL:HG13	1.87	0.56
1:L:106:TYR:O	1:L:110:ARG:HG3	2.06	0.56
1:O:68:GLY:H	1:S:94:PRO:HG2	1.71	0.56
1:P:168:THR:HA	1:P:173:ARG:HD2	1.86	0.56
1:P:272:MET:HE2	1:P:340:LEU:HD11	1.87	0.56
1:4:113:MET:HG2	2:W:213:GLY:HA3	1.87	0.56
1:K:198:ILE:HG13	1:K:248:VAL:HG11	1.87	0.56
1:R:309:VAL:HG22	1:R:317:GLU:HB3	1.88	0.56
2:U:270:GLN:NE2	2:e:34:GLN:OE1	2.36	0.56
2:Y:368:VAL:HG12	2:Y:396:PHE:HZ	1.70	0.56
1:g:267:LEU:HD22	1:g:271:THR:HG21	1.87	0.56
1:7:201:ASP:OD1	1:7:270:ASN:HA	2.06	0.56
1:G:30:GLU:OE2	1:G:280:ARG:NH1	2.39	0.56
1:G:258:VAL:HA	1:G:263:LYS:HA	1.87	0.56
2:Z:25:HIS:ND1	2:b:66:ASN:OD1	2.38	0.56
2:a:61:ASP:OD2	2:a:175:LYS:NZ	2.23	0.56
2:X:423:ARG:NH1	2:X:423:ARG:HB2	2.20	0.56
2:Y:251:PHE:O	2:Y:255:MET:HG3	2.06	0.56
1:h:159:GLU:O	1:h:190:ASN:ND2	2.39	0.56
1:4:201:ASP:HB3	1:4:270:ASN:HA	1.86	0.56
1:H:222:ARG:NH2	1:P:220:THR:O	2.39	0.56
1:I:63:ILE:O	1:J:82:HIS:ND1	2.36	0.56
1:K:82:HIS:ND1	1:K:115:ASN:OD1	2.39	0.56
1:L:27:PHE:O	1:L:29:ARG:NH1	2.39	0.56
2:W:144:MET:HE3	2:W:151:LEU:HA	1.87	0.56
2:X:101:GLU:HB3	2:X:105:ARG:NH1	2.21	0.56
1:G:232:VAL:HG22	1:G:235:LEU:HD11	1.88	0.55
1:H:53:TYR:OH	1:P:130:GLN:OE1	2.25	0.55
1:H:165:SER:OG	1:H:166:GLY:N	2.39	0.55
1:J:309:VAL:HG22	1:J:317:GLU:HG2	1.88	0.55
1:E:29:ARG:NH2	1:E:279:ALA:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:201:ASP:HB3	1:N:270:ASN:HA	1.88	0.55
1:6:81:LYS:HB3	1:6:320:MET:HG3	1.88	0.55
1:7:198:ILE:HG12	1:7:274:LEU:HD13	1.88	0.55
1:K:232:VAL:HG22	1:K:235:LEU:HD11	1.88	0.55
1:P:305:PRO:HB3	1:P:321:ILE:HG12	1.89	0.55
2:c:132:ARG:NH1	2:c:140:GLU:OE1	2.38	0.55
1:6:91:ARG:O	1:6:107:ARG:NH1	2.39	0.55
1:A:103:ASP:OD2	1:T:299:ASN:ND2	2.37	0.55
1:G:96:GLU:OE2	1:G:107:ARG:NH1	2.40	0.55
1:Q:220:THR:HG22	1:Q:223:GLY:H	1.70	0.55
2:a:99:ILE:HG13	2:a:100:GLY:N	2.20	0.55
2:c:251:PHE:O	2:c:255:MET:HG3	2.07	0.55
1:4:292:ASP:O	1:4:296:GLU:HG2	2.07	0.55
1:7:32:TYR:HB2	1:7:284:THR:HG22	1.88	0.55
1:O:303:ARG:H	1:O:323:SER:HB2	1.70	0.55
2:X:85:PHE:HD2	2:X:87:ARG:HG3	1.72	0.55
2:X:129:GLU:OE2	2:X:170:ARG:NH1	2.39	0.55
2:Y:153:VAL:HG11	2:Y:411:MET:HE2	1.88	0.55
2:Y:477:LYS:NZ	2:Z:484:ASP:OD2	2.39	0.55
1:D:178:TYR:HD2	1:D:211:PHE:HE2	1.55	0.55
1:H:290:ASP:HB2	1:H:322:GLN:HE22	1.71	0.55
1:J:120:GLU:OE2	1:J:303:ARG:NH1	2.40	0.55
1:T:92:ARG:NH2	1:T:97:ASP:C	2.63	0.55
2:Y:129:GLU:HB3	2:Y:131:LYS:HE3	1.88	0.55
2:Y:187:ARG:NH1	2:Z:209:ASP:O	2.40	0.55
1:O:209:ARG:NH2	1:Q:181:THR:OG1	2.39	0.55
1:E:209:ARG:NH1	1:E:230:THR:O	2.39	0.55
1:K:123:ILE:HG22	1:K:303:ARG:HH21	1.71	0.55
1:M:22:LEU:HD13	1:M:239:VAL:HG11	1.88	0.55
1:h:127:GLU:CD	1:h:303:ARG:HH22	2.15	0.55
1:5:130:GLN:HG3	1:5:327:MET:HG2	1.89	0.55
1:B:290:ASP:OD2	1:B:322:GLN:NE2	2.37	0.55
1:F:290:ASP:OD2	1:F:322:GLN:NE2	2.39	0.55
1:P:187:TYR:CD1	1:P:338:VAL:HG11	2.42	0.55
2:U:354:PHE:HE2	2:V:269:LEU:HD13	1.71	0.55
2:f:72:ASN:ND2	2:f:373:LEU:O	2.39	0.55
1:4:165:SER:OG	1:4:166:GLY:N	2.38	0.55
1:G:290:ASP:OD2	1:G:322:GLN:NE2	2.39	0.55
1:H:232:VAL:HB	1:H:235:LEU:HD11	1.89	0.55
2:V:125:CYS:SG	2:V:163:ARG:NH1	2.80	0.55
2:Y:81:ILE:O	2:Y:400:ARG:NE	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:146:ALA:HB3	1:E:54:VAL:HG12	1.89	0.55
1:M:218:LEU:HD13	1:T:223:GLY:HA2	1.89	0.55
2:V:150:GLU:OE2	2:V:246:ARG:NH2	2.31	0.55
1:7:168:THR:H	1:7:173:ARG:NH1	2.05	0.54
1:A:274:LEU:HB2	1:A:336:VAL:HB	1.89	0.54
1:J:40:TYR:HB3	1:J:72:GLU:HA	1.89	0.54
1:J:192:SER:OG	1:J:333:ASP:O	2.24	0.54
1:K:82:HIS:HB3	1:K:115:ASN:HD21	1.72	0.54
2:U:197:ASP:OD1	2:U:198:SER:N	2.40	0.54
2:X:419:ALA:O	2:X:420:ILE:C	2.50	0.54
1:1:232:VAL:HG13	1:1:235:LEU:HD21	1.88	0.54
1:7:220:THR:O	1:F:222:ARG:NH2	2.39	0.54
1:C:164:GLN:HG2	1:C:169:GLU:HA	1.89	0.54
1:M:146:ALA:HB1	1:T:58:VAL:HG21	1.88	0.54
1:Q:205:TRP:HH2	1:Q:228:LEU:HD21	1.72	0.54
1:4:152:VAL:HG21	1:4:326:LEU:HD11	1.88	0.54
1:I:258:VAL:HG22	1:I:263:LYS:HG2	1.89	0.54
1:J:258:VAL:HA	1:J:263:LYS:HA	1.89	0.54
1:4:198:ILE:HG12	1:4:274:LEU:HD23	1.89	0.54
1:E:112:ILE:HG22	1:E:116:MET:HE1	1.90	0.54
1:K:102:ALA:O	1:K:107:ARG:NH2	2.40	0.54
1:R:326:LEU:HD21	1:R:328:LEU:HD21	1.88	0.54
2:X:161:SER:O	2:X:166:ARG:NH1	2.40	0.54
2:a:261:LEU:HD13	2:a:358:LEU:HD12	1.90	0.54
1:3:22:LEU:HD12	1:3:239:VAL:HG12	1.89	0.54
1:B:44:ILE:HD11	1:F:95:ASP:HB3	1.89	0.54
1:F:119:GLU:O	1:F:123:ILE:HG12	2.07	0.54
2:V:477:LYS:NZ	2:W:484:ASP:OD2	2.40	0.54
2:f:140:GLU:HG2	2:f:171:MET:HE2	1.89	0.54
1:B:181:THR:O	1:B:185:GLU:HG3	2.08	0.54
1:J:165:SER:OG	1:J:166:GLY:N	2.40	0.54
1:N:92:ARG:NH1	1:N:96:GLU:O	2.40	0.54
2:e:260:MET:HE2	2:e:260:MET:HA	1.89	0.54
2:f:170:ARG:HH21	2:f:176:ARG:HH12	1.56	0.54
1:g:22:LEU:HD13	1:g:239:VAL:HG11	1.90	0.54
1:0:283:ARG:HG2	1:0:327:MET:SD	2.48	0.54
1:T:154:MET:HE3	1:T:329:LEU:H	1.73	0.54
2:W:371:GLU:HB3	2:W:377:TYR:CE2	2.43	0.54
1:0:229:GLU:HG2	1:0:233:LYS:HD3	1.88	0.54
1:A:22:LEU:HD23	1:A:239:VAL:HG22	1.90	0.54
1:F:108:ARG:O	1:F:112:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:ILE:HG22	1:M:249:ALA:HB3	1.88	0.54
1:Q:41:LEU:HD11	1:Q:328:LEU:HD13	1.90	0.54
1:0:68:GLY:H	1:4:94:PRO:HG3	1.73	0.54
1:0:164:GLN:NE2	1:0:187:TYR:OH	2.37	0.54
1:2:63:ILE:HB	1:3:82:HIS:CE1	2.42	0.54
1:I:182:ASP:OD1	1:I:183:ASP:N	2.40	0.54
1:L:73:PHE:HD1	1:L:152:VAL:HG23	1.73	0.54
1:L:103:ASP:OD1	1:L:103:ASP:N	2.40	0.54
1:Q:168:THR:HA	1:Q:173:ARG:HE	1.71	0.54
2:c:196:ASN:HB3	2:c:202:LEU:HD11	1.89	0.54
1:H:44:ILE:HB	1:P:14:GLU:HA	1.89	0.53
1:S:196:ASN:HA	1:S:248:VAL:HG12	1.89	0.53
2:d:63:LEU:HD13	2:d:258:MET:HE3	1.90	0.53
1:I:41:LEU:HD11	1:I:328:LEU:HD13	1.89	0.53
1:N:315:ALA:O	1:N:316:ARG:HB2	2.07	0.53
2:b:150:GLU:OE2	2:b:246:ARG:NH2	2.33	0.53
1:4:201:ASP:O	1:4:204:GLY:N	2.41	0.53
1:5:91:ARG:HG3	1:5:92:ARG:H	1.73	0.53
1:Q:156:ARG:HH22	1:Q:335:PHE:HB2	1.73	0.53
1:S:181:THR:HA	1:S:184:ILE:HG12	1.91	0.53
1:J:226:SER:HB3	1:J:246:GLY:H	1.73	0.53
2:Z:215:MET:O	2:Z:217:GLN:NE2	2.39	0.53
2:c:242:ASP:OD1	2:c:243:GLY:N	2.40	0.53
1:0:41:LEU:HD11	1:0:328:LEU:HD13	1.89	0.53
1:1:103:ASP:HB2	1:3:299:ASN:ND2	2.23	0.53
1:G:26:LEU:O	1:G:29:ARG:NH1	2.42	0.53
1:H:95:ASP:HB3	1:H:110:ARG:HH22	1.73	0.53
1:J:239:VAL:HG12	1:J:253:TYR:HD1	1.74	0.53
1:N:115:ASN:O	1:N:119:GLU:HG2	2.08	0.53
1:O:212:LYS:HA	1:O:215:LYS:HD3	1.90	0.53
1:3:182:ASP:OD1	1:3:183:ASP:N	2.42	0.53
1:C:127:GLU:OE1	1:C:303:ARG:NH2	2.41	0.53
1:F:198:ILE:HG12	1:F:274:LEU:HD13	1.91	0.53
1:I:164:GLN:NE2	1:I:168:THR:O	2.38	0.53
1:K:168:THR:H	1:K:173:ARG:NH1	2.05	0.53
1:O:84:VAL:HG11	1:O:112:ILE:HD11	1.90	0.53
2:U:375:ARG:HE	2:f:364:ALA:HA	1.73	0.53
2:W:298:ALA:HB2	2:W:323:VAL:HG22	1.90	0.53
2:W:492:GLN:HE22	2:W:495:ARG:HH21	1.56	0.53
1:h:201:ASP:OD1	1:h:202:PRO:HD2	2.09	0.53
1:7:115:ASN:O	1:7:119:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:229:GLU:OE2	1:K:233:LYS:HD2	2.09	0.53
2:V:463:GLU:HG3	2:W:461:VAL:HG21	1.91	0.53
2:c:354:PHE:HB2	2:d:348:ASP:HB2	1.91	0.53
1:3:63:ILE:HB	1:C:82:HIS:CE1	2.44	0.53
1:5:109:ARG:O	1:5:113:MET:HG3	2.09	0.53
1:3:31:SER:HA	1:3:283:ARG:HB3	1.90	0.53
1:6:109:ARG:O	1:6:113:MET:HG2	2.09	0.53
1:H:9:LEU:HB2	1:H:98:PRO:HD2	1.91	0.53
1:7:95:ASP:OD2	1:7:110:ARG:NH2	2.42	0.53
1:J:22:LEU:HD13	1:J:239:VAL:HG11	1.91	0.53
1:J:290:ASP:OD2	1:J:322:GLN:NE2	2.41	0.53
1:T:127:GLU:OE1	1:T:303:ARG:NH2	2.39	0.53
2:W:354:PHE:HB2	2:X:348:ASP:HB2	1.90	0.53
2:X:397:MET:HE1	2:X:400:ARG:HD2	1.90	0.53
2:f:190:ARG:HD2	2:f:245:THR:HG21	1.90	0.53
1:g:92:ARG:NH1	1:g:96:GLU:O	2.42	0.53
1:4:115:ASN:O	1:4:119:GLU:HG2	2.09	0.52
1:5:120:GLU:OE2	1:5:303:ARG:NH1	2.42	0.52
1:A:80:PRO:HG2	1:A:119:GLU:HB2	1.90	0.52
1:M:46:GLY:HA2	1:M:66:ARG:HE	1.74	0.52
1:N:84:VAL:HA	1:N:88:MET:HE2	1.90	0.52
1:N:313:ASP:HB2	1:N:314:PRO:HD3	1.90	0.52
1:h:293:ALA:HB2	1:h:304:TYR:CE2	2.44	0.52
1:0:262:VAL:O	1:0:263:LYS:HG3	2.09	0.52
1:5:198:ILE:HG12	1:5:274:LEU:HD23	1.89	0.52
1:C:22:LEU:O	1:C:26:LEU:HB2	2.10	0.52
1:C:44:ILE:HD11	1:G:95:ASP:HB3	1.91	0.52
1:I:329:LEU:HD23	1:I:332:PRO:HA	1.92	0.52
1:L:309:VAL:HG22	1:L:317:GLU:HB3	1.91	0.52
1:S:188:ALA:HB2	1:S:274:LEU:HD11	1.92	0.52
2:W:98:GLY:HA3	2:W:432:ARG:HH21	1.74	0.52
2:b:386:ARG:HG2	2:c:455:ILE:O	2.09	0.52
2:U:370:TYR:OH	2:U:376:ASN:ND2	2.43	0.52
2:Z:179:ASN:ND2	2:Z:185:ASP:OD1	2.43	0.52
1:g:41:LEU:HD11	1:g:328:LEU:HD13	1.91	0.52
1:0:75:PRO:HA	1:0:326:LEU:HD12	1.91	0.52
1:I:180:PRO:HG3	1:I:211:PHE:HD2	1.74	0.52
2:U:129:GLU:OE1	2:U:132:ARG:NH2	2.39	0.52
2:b:61:ASP:OD2	2:b:175:LYS:NZ	2.32	0.52
1:G:205:TRP:HH2	1:G:228:LEU:HD13	1.74	0.52
1:P:170:TRP:HB3	1:P:207:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:413:LEU:HD21	2:U:443:GLY:HA3	1.91	0.52
2:b:166:ARG:HE	2:b:422:ARG:HH21	1.58	0.52
2:c:87:ARG:HH21	2:c:116:LYS:NZ	2.08	0.52
2:e:195:ILE:HD11	2:e:245:THR:HG22	1.91	0.52
1:F:83:GLU:OE2	1:F:316:ARG:NH2	2.43	0.52
1:M:178:TYR:OH	1:M:183:ASP:OD2	2.20	0.52
2:Z:463:GLU:OE2	2:a:458:LEU:HA	2.10	0.52
2:c:354:PHE:HE2	2:d:269:LEU:HD13	1.75	0.52
1:1:188:ALA:HB3	1:5:235:LEU:HD12	1.92	0.52
1:1:217:LYS:HE3	1:5:230:THR:HG22	1.90	0.52
1:7:45:PRO:HD3	1:7:68:GLY:HA2	1.91	0.52
1:E:41:LEU:HD12	1:E:73:PHE:HE2	1.74	0.52
1:P:223:GLY:HA2	1:T:218:LEU:HD23	1.90	0.52
1:R:97:ASP:N	1:R:97:ASP:OD1	2.43	0.52
2:b:179:ASN:ND2	2:b:185:ASP:OD1	2.43	0.52
1:2:235:LEU:HD12	1:S:188:ALA:HB3	1.91	0.52
1:5:310:THR:HG23	1:5:312:GLY:H	1.75	0.52
1:D:80:PRO:HG2	1:D:119:GLU:HB2	1.92	0.52
1:J:274:LEU:HB2	1:J:336:VAL:HB	1.91	0.52
1:N:99:GLN:O	1:N:101:LEU:N	2.43	0.52
1:1:47:LEU:HD12	1:5:258:VAL:HG11	1.91	0.52
1:5:232:VAL:HB	1:5:235:LEU:HD21	1.92	0.52
1:A:180:PRO:HG3	1:A:211:PHE:CD2	2.45	0.52
1:B:50:MET:SD	1:F:125:GLN:NE2	2.80	0.52
1:I:186:ALA:HA	1:I:189:LEU:HD13	1.90	0.52
1:K:41:LEU:HD12	1:K:73:PHE:HE2	1.75	0.52
1:K:83:GLU:HA	1:K:318:PHE:HB3	1.92	0.52
2:V:91:ARG:HG3	2:V:91:ARG:O	2.10	0.52
2:X:187:ARG:NE	1:h:296:GLU:OE1	2.31	0.52
2:f:434:SER:OG	2:f:435:PHE:N	2.43	0.52
1:h:198:ILE:HG12	1:h:274:LEU:HD23	1.92	0.52
1:7:339:GLN:NE2	1:7:339:GLN:O	2.39	0.52
1:B:75:PRO:HA	1:B:326:LEU:HD12	1.92	0.52
1:E:205:TRP:HH2	1:E:228:LEU:HD13	1.73	0.52
1:J:60:GLY:O	1:K:81:LYS:NZ	2.32	0.52
1:L:217:LYS:NZ	1:g:231:ALA:HA	2.25	0.52
2:b:177:ILE:O	2:b:246:ARG:NH1	2.37	0.52
1:g:169:GLU:HG3	1:g:172:LYS:HD2	1.92	0.52
1:2:108:ARG:O	1:2:112:ILE:HG12	2.10	0.51
1:4:100:ASN:O	2:V:39:ASN:ND2	2.42	0.51
1:7:130:GLN:NE2	1:F:53:TYR:OH	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:THR:O	1:A:185:GLU:HG3	2.10	0.51
1:M:49:ASN:HA	1:N:258:VAL:HG23	1.92	0.51
1:N:41:LEU:HD12	1:N:73:PHE:HE2	1.74	0.51
1:S:201:ASP:CG	1:S:202:PRO:HD2	2.35	0.51
2:V:289:GLN:O	2:V:293:ASP:HB2	2.10	0.51
2:X:127:ASP:OD2	2:X:132:ARG:NH1	2.42	0.51
2:f:166:ARG:HD3	2:f:422:ARG:NH1	2.25	0.51
1:h:113:MET:O	1:h:116:MET:N	2.42	0.51
1:5:177:THR:H	1:5:212:LYS:HZ2	1.57	0.51
1:C:80:PRO:HG2	1:C:119:GLU:HB2	1.93	0.51
1:O:95:ASP:OD2	1:O:110:ARG:NH1	2.44	0.51
1:T:21:PRO:HA	1:T:128:GLU:OE2	2.10	0.51
2:Z:348:ASP:OD2	2:Z:352:SER:OG	2.27	0.51
1:h:148:ASP:N	1:h:148:ASP:OD1	2.43	0.51
1:1:284:THR:HG21	1:1:328:LEU:HD12	1.92	0.51
1:B:24:LEU:HD11	1:B:327:MET:HE3	1.92	0.51
1:I:305:PRO:HB3	1:I:321:ILE:HG12	1.93	0.51
1:J:62:VAL:HG21	1:K:83:GLU:HB3	1.92	0.51
1:K:68:GLY:H	1:L:94:PRO:HG3	1.76	0.51
1:4:185:GLU:HG2	1:A:235:LEU:HD21	1.92	0.51
1:7:218:LEU:HD21	1:7:228:LEU:HD23	1.92	0.51
1:A:49:ASN:OD1	1:E:260:ASN:N	2.44	0.51
1:D:161:ASN:HD22	1:D:337:SER:HB3	1.75	0.51
1:E:156:ARG:HG2	1:E:161:ASN:HD21	1.74	0.51
1:G:305:PRO:HA	1:G:321:ILE:HG22	1.91	0.51
1:I:51:ALA:HB3	1:J:126:VAL:HG21	1.92	0.51
1:K:63:ILE:HB	1:L:82:HIS:CD2	2.45	0.51
1:P:34:PHE:HZ	1:P:75:PRO:HG3	1.75	0.51
2:V:144:MET:HE3	2:V:174:PRO:HD3	1.91	0.51
2:c:241:GLU:OE2	2:d:175:LYS:NZ	2.43	0.51
1:h:159:GLU:HB3	1:h:190:ASN:HD21	1.75	0.51
1:O:28:PHE:HD1	1:O:281:GLY:HA3	1.75	0.51
1:F:201:ASP:CG	1:F:271:THR:H	2.18	0.51
1:M:51:ALA:HB2	1:N:122:ALA:HB1	1.92	0.51
1:N:28:PHE:HE1	1:N:329:LEU:HD13	1.76	0.51
2:Y:55:ARG:NH1	1:h:103:ASP:OD2	2.43	0.51
2:a:463:GLU:OE2	2:b:461:VAL:HG21	2.11	0.51
1:7:82:HIS:CE1	1:F:63:ILE:HB	2.45	0.51
1:I:164:GLN:HE22	1:I:170:TRP:CD1	2.29	0.51
1:M:290:ASP:CG	1:M:322:GLN:HE22	2.17	0.51
1:S:217:LYS:O	1:S:224:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:89:SER:OG	2:U:446:ASP:O	2.24	0.51
1:7:83:GLU:HA	1:7:318:PHE:HB3	1.92	0.51
1:A:131:ALA:HB2	1:A:327:MET:HG3	1.93	0.51
1:K:148:ASP:N	1:K:148:ASP:OD1	2.44	0.51
1:Q:125:GLN:NE2	1:Q:258:VAL:H	2.07	0.51
1:S:83:GLU:HG2	1:S:84:VAL:N	2.26	0.51
2:U:400:ARG:NH2	2:U:450:SER:O	2.36	0.51
2:V:273:ILE:HG21	2:W:325:LEU:HD13	1.91	0.51
2:Z:512:ALA:HB2	2:a:506:LYS:HA	1.92	0.51
2:d:458:LEU:HG	2:d:462:GLN:HE22	1.75	0.51
1:g:80:PRO:HB2	1:g:119:GLU:HG3	1.91	0.51
1:h:116:MET:SD	1:h:319:THR:HG21	2.50	0.51
1:0:77:TYR:OH	1:0:287:CYS:O	2.22	0.51
1:4:315:ALA:O	1:4:316:ARG:HB2	2.10	0.51
1:5:222:ARG:HD2	1:B:227:GLU:OE2	2.11	0.51
1:7:272:MET:HE2	1:7:340:LEU:HD11	1.92	0.51
1:G:303:ARG:H	1:G:323:SER:HB2	1.76	0.51
1:K:228:LEU:HD13	1:K:245:TYR:HD1	1.76	0.51
1:M:97:ASP:HB3	1:M:99:GLN:O	2.10	0.51
1:S:268:PRO:HG2	1:S:271:THR:HB	1.91	0.51
2:W:110:GLU:HG2	2:W:425:VAL:HG12	1.93	0.51
2:b:187:ARG:HH12	2:c:210:GLY:HA3	1.76	0.51
1:h:309:VAL:HG12	1:h:317:GLU:HB3	1.93	0.51
1:1:235:LEU:HD12	1:R:188:ALA:HB3	1.93	0.51
1:E:116:MET:O	1:E:120:GLU:OE1	2.29	0.51
1:M:37:GLU:OE1	1:M:38:LYS:HG3	2.11	0.51
1:P:221:ARG:HH22	1:T:221:ARG:CZ	2.24	0.51
1:R:226:SER:HB2	1:R:245:TYR:HA	1.93	0.51
2:d:151:LEU:HD21	2:d:236:VAL:HB	1.91	0.51
1:h:315:ALA:O	1:h:316:ARG:HB2	2.09	0.51
1:P:41:LEU:HD12	1:P:73:PHE:HE2	1.76	0.51
1:P:201:ASP:HB3	1:P:267:LEU:HD22	1.93	0.51
1:g:66:ARG:HH12	1:h:118:ASP:CG	2.19	0.51
1:S:174:ASP:N	1:S:174:ASP:OD1	2.45	0.50
2:U:327:GLY:H	2:c:31:PHE:HE2	1.59	0.50
2:U:493:GLN:HG3	2:f:474:THR:HG22	1.92	0.50
2:Y:280:ALA:HB3	2:Z:330:VAL:HG13	1.92	0.50
2:b:157:TRP:HA	2:b:166:ARG:O	2.11	0.50
2:b:354:PHE:HE2	2:c:269:LEU:HD13	1.74	0.50
1:0:146:ALA:HB1	1:Q:58:VAL:HG21	1.93	0.50
1:0:162:ILE:O	1:0:338:VAL:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:331:ASP:OD1	1:3:13:ASN:ND2	2.44	0.50
1:6:112:ILE:HG22	1:6:116:MET:HE2	1.93	0.50
1:H:73:PHE:HZ	1:H:154:MET:HA	1.77	0.50
1:L:154:MET:N	1:L:154:MET:SD	2.84	0.50
1:N:148:ASP:OD1	1:N:148:ASP:N	2.44	0.50
2:Z:379:GLN:C	2:a:379:GLN:HE21	2.17	0.50
2:f:88:LEU:HD23	2:f:89:SER:N	2.26	0.50
1:2:232:VAL:HG12	1:2:235:LEU:HD21	1.93	0.50
1:3:315:ALA:O	1:3:316:ARG:HB2	2.11	0.50
1:6:29:ARG:NH2	1:6:279:ALA:O	2.40	0.50
1:C:51:ALA:HB3	1:G:126:VAL:HG21	1.93	0.50
2:b:348:ASP:OD1	2:b:351:TYR:HB3	2.11	0.50
2:e:361:TYR:HD2	2:e:362:ILE:HD13	1.75	0.50
1:A:217:LYS:O	1:A:224:SER:OG	2.29	0.50
1:C:284:THR:HG23	1:C:326:LEU:HB3	1.94	0.50
1:H:97:ASP:N	1:H:97:ASP:OD1	2.40	0.50
1:J:284:THR:OG1	1:J:326:LEU:HB3	2.12	0.50
1:K:194:VAL:HA	1:L:236:GLY:HA3	1.94	0.50
1:O:198:ILE:HG12	1:O:274:LEU:HD13	1.94	0.50
1:Q:29:ARG:NH2	1:Q:279:ALA:O	2.41	0.50
1:R:258:VAL:HG12	1:R:263:LYS:HA	1.94	0.50
2:V:24:TYR:CE1	2:X:65:ARG:HG2	2.46	0.50
2:Y:466:MET:HE1	2:Z:462:GLN:HG3	1.94	0.50
1:h:233:LYS:NZ	1:h:241:TYR:O	2.41	0.50
1:7:44:ILE:HD12	1:R:14:GLU:HG3	1.94	0.50
1:A:109:ARG:O	1:A:113:MET:HG2	2.11	0.50
1:A:198:ILE:HG12	1:A:274:LEU:HD13	1.94	0.50
1:B:54:VAL:HG12	1:F:146:ALA:HB3	1.94	0.50
1:C:63:ILE:HB	1:G:82:HIS:CE1	2.47	0.50
1:C:329:LEU:HD23	1:C:332:PRO:HA	1.92	0.50
1:K:45:PRO:HD3	1:K:68:GLY:HA2	1.92	0.50
2:X:199:GLY:HA3	2:Y:129:GLU:HG2	1.93	0.50
1:0:218:LEU:HD11	1:0:228:LEU:HD12	1.93	0.50
1:7:26:LEU:O	1:7:29:ARG:NH1	2.45	0.50
1:7:82:HIS:HB2	1:7:115:ASN:ND2	2.27	0.50
1:7:272:MET:HE3	1:7:338:VAL:HG21	1.94	0.50
1:C:63:ILE:O	1:G:82:HIS:ND1	2.44	0.50
1:F:22:LEU:HD13	1:F:239:VAL:HG11	1.93	0.50
2:b:46:ASP:HA	2:b:50:LEU:HD23	1.94	0.50
1:g:313:ASP:HB2	1:g:314:PRO:HD3	1.92	0.50
1:7:306:LYS:HE3	1:7:308:TRP:CZ3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ALA:O	1:B:217:LYS:HG2	2.12	0.50
1:E:3:MET:HA	1:E:3:MET:HE3	1.92	0.50
1:H:112:ILE:HG22	1:H:116:MET:HE2	1.93	0.50
1:I:85:ASN:OD1	1:I:88:MET:HG3	2.12	0.50
1:L:92:ARG:H	1:L:107:ARG:NH1	2.10	0.50
2:V:212:PRO:HB2	2:V:214:TRP:CD1	2.46	0.50
2:d:187:ARG:CZ	2:e:214:TRP:HD1	2.24	0.50
1:4:55:SER:O	1:A:79:LYS:NZ	2.45	0.50
1:5:63:ILE:HB	1:B:82:HIS:CD2	2.47	0.50
1:E:22:LEU:HD13	1:E:239:VAL:HG11	1.94	0.50
1:G:29:ARG:HG3	1:G:29:ARG:HH11	1.76	0.50
1:O:3:MET:HG3	1:O:5:THR:HG22	1.94	0.50
1:T:42:SER:HB3	1:T:70:THR:HG22	1.94	0.50
2:c:393:TRP:CZ2	2:c:397:MET:HE3	2.46	0.50
1:1:209:ARG:HG2	1:1:209:ARG:O	2.11	0.50
1:3:21:PRO:HA	1:3:128:GLU:OE2	2.12	0.50
1:A:195:VAL:HG11	1:A:274:LEU:HD12	1.93	0.50
1:M:201:ASP:N	1:M:201:ASP:OD1	2.43	0.50
1:P:50:MET:HG3	1:T:126:VAL:HG22	1.92	0.50
2:Z:244:GLN:HE21	2:Z:247:GLY:HA2	1.77	0.50
2:a:238:GLU:OE2	2:a:399:ARG:NH1	2.45	0.50
2:e:298:ALA:HB2	2:e:323:VAL:HG22	1.93	0.50
1:0:58:VAL:HG21	1:4:146:ALA:HB1	1.94	0.49
1:0:184:ILE:HD11	1:0:208:PHE:HE1	1.77	0.49
1:H:206:ALA:HA	1:H:209:ARG:NH1	2.27	0.49
2:W:386:ARG:HG3	2:W:390:ASN:HD21	1.76	0.49
2:e:238:GLU:OE1	2:e:399:ARG:NH1	2.44	0.49
2:e:249:ASN:HD22	2:e:251:PHE:HB2	1.77	0.49
2:f:157:TRP:HE3	2:f:166:ARG:HH21	1.60	0.49
1:7:42:SER:HB3	1:7:70:THR:HG22	1.95	0.49
1:E:234:ASP:N	1:E:234:ASP:OD1	2.45	0.49
1:F:296:GLU:OE2	1:F:298:ILE:HG13	2.11	0.49
1:H:198:ILE:HB	1:H:250:ILE:HD13	1.94	0.49
1:O:86:PRO:HA	1:O:89:THR:HG22	1.93	0.49
2:e:214:TRP:NE1	2:e:216:PRO:HG3	2.27	0.49
1:0:77:TYR:OH	1:0:289:GLN:HG3	2.11	0.49
1:0:198:ILE:HG12	1:0:274:LEU:HD23	1.95	0.49
1:D:280:ARG:HH12	1:H:11:ALA:HB1	1.76	0.49
1:F:46:GLY:HA2	1:F:66:ARG:HE	1.78	0.49
1:F:80:PRO:HD2	1:F:321:ILE:O	2.13	0.49
1:P:3:MET:HE2	1:P:3:MET:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:290:ASP:OD2	1:S:322:GLN:NE2	2.24	0.49
2:U:83:GLY:O	2:U:139:ARG:NH1	2.45	0.49
2:Y:397:MET:HA	2:Y:397:MET:HE3	1.93	0.49
2:c:24:TYR:HE2	2:d:49:LEU:HB2	1.76	0.49
1:7:146:ALA:HB3	1:F:54:VAL:HG12	1.94	0.49
1:A:53:TYR:CE1	1:E:142:MET:HG3	2.48	0.49
1:A:108:ARG:NH1	1:A:317:GLU:OE2	2.36	0.49
1:B:280:ARG:HG3	1:B:280:ARG:HH11	1.78	0.49
1:N:41:LEU:HD11	1:N:328:LEU:HD13	1.95	0.49
1:O:78:VAL:HG22	1:O:80:PRO:HD3	1.93	0.49
2:Y:199:GLY:HA3	2:Z:129:GLU:HG2	1.93	0.49
1:1:200:PHE:CZ	1:1:272:MET:HE2	2.47	0.49
1:3:127:GLU:OE2	1:3:303:ARG:NH2	2.30	0.49
1:3:156:ARG:NH2	1:3:335:PHE:HB2	2.27	0.49
1:I:313:ASP:HB3	1:I:314:PRO:HD3	1.94	0.49
1:K:59:SER:OG	1:L:81:LYS:NZ	2.46	0.49
1:2:148:ASP:N	1:2:148:ASP:OD1	2.45	0.49
1:3:169:GLU:N	1:3:169:GLU:OE1	2.46	0.49
1:4:299:ASN:ND2	1:M:103:ASP:HB2	2.28	0.49
1:B:226:SER:HB3	1:B:245:TYR:HA	1.94	0.49
1:M:13:ASN:HD22	1:T:331:ASP:HB3	1.77	0.49
1:N:78:VAL:HG12	1:N:325:PRO:HD3	1.93	0.49
1:O:176:SER:O	1:O:177:THR:HB	2.12	0.49
2:U:88:LEU:HD23	2:U:89:SER:N	2.28	0.49
2:c:65:ARG:O	2:c:66:ASN:ND2	2.43	0.49
2:c:393:TRP:CE2	2:c:397:MET:HE3	2.48	0.49
1:0:267:LEU:HD22	1:0:271:THR:HG21	1.93	0.49
1:2:28:PHE:HE2	1:2:131:ALA:HB1	1.78	0.49
1:2:42:SER:OG	1:2:43:GLN:N	2.45	0.49
1:7:199:VAL:HG23	1:7:273:VAL:HB	1.94	0.49
1:M:102:ALA:O	1:M:107:ARG:NH1	2.45	0.49
1:M:198:ILE:HG12	1:M:274:LEU:HD13	1.95	0.49
1:N:258:VAL:HG12	1:N:263:LYS:HA	1.95	0.49
1:P:292:ASP:O	1:P:296:GLU:HG2	2.13	0.49
1:R:109:ARG:HH11	1:R:109:ARG:HG3	1.78	0.49
2:Y:196:ASN:HB3	2:Y:202:LEU:CD1	2.42	0.49
2:a:300:SER:O	2:a:301:GLN:HG2	2.12	0.49
1:5:257:TYR:HB3	1:5:266:PHE:CZ	2.47	0.49
1:G:44:ILE:HB	1:O:14:GLU:HA	1.95	0.49
1:G:309:VAL:HG22	1:G:317:GLU:HG2	1.94	0.49
1:L:97:ASP:OD1	1:L:97:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:239:VAL:HG12	1:O:253:TYR:HD1	1.78	0.49
2:Y:83:GLY:O	2:Y:139:ARG:NH1	2.46	0.49
2:a:197:ASP:OD2	2:a:198:SER:N	2.46	0.49
2:c:435:PHE:HA	2:c:442:TRP:CD1	2.47	0.49
1:O:24:LEU:HD23	1:O:28:PHE:HD2	1.78	0.49
1:2:307:ASN:ND2	1:2:318:PHE:O	2.46	0.49
1:7:38:LYS:HG3	1:R:7:ALA:HB2	1.95	0.49
1:C:182:ASP:OD1	1:C:183:ASP:N	2.45	0.49
1:G:84:VAL:HG11	1:G:112:ILE:HD11	1.95	0.49
1:H:23:PHE:HE2	1:H:267:LEU:HD11	1.78	0.49
1:P:54:VAL:HG23	1:T:146:ALA:HB3	1.94	0.49
1:Q:108:ARG:NH2	1:Q:317:GLU:OE2	2.26	0.49
2:U:371:GLU:HB3	2:U:377:TYR:CE1	2.48	0.49
2:Y:386:ARG:HG2	2:Z:455:ILE:O	2.12	0.49
2:c:284:SER:OG	2:c:285:GLU:N	2.46	0.49
1:5:42:SER:HB3	1:5:70:THR:HG22	1.95	0.49
1:H:50:MET:HE3	1:P:126:VAL:HA	1.93	0.49
1:I:73:PHE:HE2	1:I:328:LEU:HD11	1.78	0.49
1:L:89:THR:HG22	1:L:111:ILE:HD12	1.95	0.49
1:O:200:PHE:HB2	1:O:252:VAL:HG22	1.95	0.49
1:S:21:PRO:HA	1:S:128:GLU:OE1	2.12	0.49
2:U:26:GLY:O	2:V:59:ARG:NH1	2.45	0.49
2:Y:277:MET:HE2	2:Z:329:LYS:HE2	1.93	0.49
2:d:251:PHE:O	2:d:255:MET:HG3	2.13	0.49
1:5:268:PRO:HG2	1:5:271:THR:HG21	1.95	0.48
1:5:315:ALA:O	1:5:316:ARG:HB2	2.13	0.48
1:A:29:ARG:NH2	1:A:279:ALA:O	2.37	0.48
1:K:63:ILE:HB	1:L:82:HIS:HD2	1.78	0.48
1:R:86:PRO:HA	1:R:89:THR:HG22	1.94	0.48
1:R:188:ALA:HB2	1:R:274:LEU:HD11	1.94	0.48
2:W:251:PHE:O	2:W:255:MET:HG3	2.13	0.48
2:b:34:GLN:NE2	2:c:256:GLU:OE2	2.45	0.48
1:1:223:GLY:HA2	1:5:218:LEU:HD13	1.94	0.48
1:1:270:ASN:HB3	1:1:340:LEU:HB2	1.94	0.48
1:2:92:ARG:NH1	1:2:96:GLU:O	2.46	0.48
1:3:26:LEU:O	1:3:29:ARG:NH1	2.47	0.48
1:3:31:SER:HB3	1:3:283:ARG:HD2	1.93	0.48
1:F:156:ARG:NH1	1:F:161:ASN:OD1	2.46	0.48
1:H:272:MET:HE2	1:H:274:LEU:HD21	1.95	0.48
1:I:156:ARG:HD3	1:I:160:ASN:HB2	1.95	0.48
2:U:94:TRP:H	2:U:94:TRP:CD1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:97:LEU:HB3	2:V:99:ILE:HG23	1.94	0.48
2:e:386:ARG:HG2	2:f:455:ILE:O	2.14	0.48
2:e:418:GLU:OE2	2:e:422:ARG:HD2	2.12	0.48
1:5:162:ILE:O	1:5:338:VAL:HA	2.13	0.48
1:7:156:ARG:NH2	1:7:332:PRO:O	2.43	0.48
1:7:187:TYR:CD2	1:7:338:VAL:HG11	2.48	0.48
1:G:194:VAL:HA	1:O:236:GLY:HA3	1.93	0.48
1:P:75:PRO:HB3	1:P:326:LEU:HD22	1.94	0.48
1:3:76:GLY:H	1:3:142:MET:HE1	1.77	0.48
1:3:112:ILE:O	1:3:116:MET:HG3	2.13	0.48
1:5:28:PHE:HE1	1:5:329:LEU:HD13	1.77	0.48
1:5:310:THR:HG21	1:5:316:ARG:HH21	1.78	0.48
1:I:180:PRO:HG3	1:I:211:PHE:CD2	2.48	0.48
1:M:26:LEU:O	1:M:29:ARG:NH2	2.46	0.48
2:V:399:ARG:O	2:V:403:VAL:HG22	2.13	0.48
2:e:230:ARG:HH21	2:e:417:GLU:HG2	1.77	0.48
2:e:283:GLU:HB2	2:e:338:SER:OG	2.14	0.48
2:e:494:VAL:HG11	2:f:503:ALA:HB1	1.96	0.48
1:1:313:ASP:HB2	1:1:314:PRO:HD3	1.95	0.48
1:4:222:ARG:NH2	1:A:220:THR:O	2.46	0.48
1:7:194:VAL:HA	1:R:236:GLY:HA3	1.93	0.48
1:H:223:GLY:HA2	1:P:218:LEU:HD13	1.94	0.48
1:L:127:GLU:OE1	1:L:303:ARG:NH2	2.46	0.48
1:N:21:PRO:HA	1:N:128:GLU:OE2	2.13	0.48
1:Q:268:PRO:HG2	1:Q:271:THR:HB	1.94	0.48
2:V:391:GLU:HG3	2:W:377:TYR:OH	2.13	0.48
1:6:307:ASN:HB3	1:6:319:THR:HG22	1.95	0.48
1:7:48:VAL:HG21	1:R:118:ASP:OD1	2.14	0.48
2:Y:128:VAL:HG21	2:Y:170:ARG:HD2	1.96	0.48
2:a:176:ARG:O	2:a:207:SER:OG	2.28	0.48
2:c:277:MET:HE1	2:d:325:LEU:HA	1.95	0.48
2:f:295:ILE:HG23	2:f:333:LEU:HD21	1.96	0.48
1:1:80:PRO:HB2	1:1:119:GLU:HG2	1.95	0.48
1:1:292:ASP:O	1:1:296:GLU:HG2	2.14	0.48
1:6:313:ASP:HB3	1:6:314:PRO:HD3	1.96	0.48
1:B:34:PHE:HZ	1:B:75:PRO:HG3	1.77	0.48
1:g:68:GLY:H	1:h:94:PRO:HG3	1.78	0.48
1:g:198:ILE:HG12	1:g:274:LEU:HD13	1.96	0.48
1:g:305:PRO:HB3	1:g:321:ILE:HG22	1.96	0.48
1:0:269:ASP:OD1	1:0:270:ASN:N	2.46	0.48
1:5:31:SER:HA	1:5:283:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:TYR:CD2	1:B:302:ALA:HB2	2.48	0.48
1:Q:92:ARG:O	1:Q:93:LEU:C	2.54	0.48
1:T:110:ARG:HA	1:T:113:MET:HG2	1.95	0.48
2:W:179:ASN:OD1	2:W:192:GLY:N	2.47	0.48
2:b:473:SER:OG	2:b:478:GLU:OE2	2.31	0.48
1:1:51:ALA:HB2	1:5:122:ALA:HB1	1.96	0.48
1:1:309:VAL:HG22	1:1:317:GLU:HG3	1.96	0.48
1:A:47:LEU:HD23	1:E:258:VAL:HG21	1.95	0.48
1:C:337:SER:O	1:C:337:SER:OG	2.32	0.48
1:L:108:ARG:O	1:L:112:ILE:HG12	2.13	0.48
1:P:108:ARG:O	1:P:112:ILE:HG12	2.14	0.48
2:U:34:GLN:NE2	2:V:256:GLU:OE2	2.30	0.48
2:b:434:SER:N	2:b:437:GLU:OE2	2.35	0.48
1:6:303:ARG:O	1:6:305:PRO:HD3	2.14	0.48
1:C:148:ASP:OD1	1:C:148:ASP:N	2.46	0.48
1:C:200:PHE:HB3	1:C:205:TRP:HB2	1.96	0.48
1:P:313:ASP:HB3	1:P:314:PRO:HD3	1.96	0.48
1:Q:22:LEU:HD13	1:Q:239:VAL:HG21	1.96	0.48
1:S:240:SER:OG	1:S:242:LYS:NZ	2.47	0.48
2:e:35:LEU:HD11	2:f:256:GLU:HG3	1.95	0.48
1:0:223:GLY:HA2	1:4:218:LEU:HD13	1.96	0.47
1:1:222:ARG:NH2	1:5:218:LEU:O	2.47	0.47
1:I:49:ASN:ND2	1:J:260:ASN:O	2.35	0.47
1:T:156:ARG:NH1	1:T:332:PRO:O	2.46	0.47
1:h:23:PHE:CZ	1:h:199:VAL:HG11	2.49	0.47
1:6:154:MET:HE1	1:6:328:LEU:HA	1.95	0.47
1:D:53:TYR:OH	1:H:130:GLN:NE2	2.32	0.47
1:E:141:THR:HG22	1:E:151:GLU:HG2	1.94	0.47
1:K:280:ARG:HG3	1:K:330:ALA:HB3	1.95	0.47
1:N:229:GLU:OE1	1:N:233:LYS:HD2	2.14	0.47
1:P:178:TYR:OH	1:P:183:ASP:OD2	2.28	0.47
1:R:52:LEU:HD23	1:R:52:LEU:H	1.80	0.47
1:T:92:ARG:NH2	1:T:96:GLU:O	2.47	0.47
2:U:256:GLU:OE2	2:f:34:GLN:NE2	2.38	0.47
1:g:185:GLU:OE1	1:h:209:ARG:NH2	2.47	0.47
1:4:257:TYR:HB3	1:4:266:PHE:CZ	2.49	0.47
1:C:46:GLY:HA2	1:C:66:ARG:NH1	2.30	0.47
1:H:292:ASP:N	1:H:292:ASP:OD1	2.44	0.47
1:M:72:GLU:OE1	1:M:72:GLU:N	2.46	0.47
1:Q:82:HIS:ND1	1:Q:119:GLU:OE1	2.46	0.47
2:V:420:ILE:HG23	2:V:427:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:76:LEU:HD11	2:a:372:GLN:O	2.14	0.47
2:a:99:ILE:HG13	2:a:100:GLY:H	1.79	0.47
1:0:172:LYS:HB3	1:0:172:LYS:HE2	1.74	0.47
1:0:201:ASP:O	1:0:204:GLY:N	2.47	0.47
1:2:162:ILE:O	1:2:338:VAL:HA	2.13	0.47
1:3:168:THR:HA	1:3:173:ARG:NH2	2.29	0.47
1:E:97:ASP:N	1:E:97:ASP:OD1	2.46	0.47
1:J:290:ASP:CG	1:J:322:GLN:HE22	2.21	0.47
2:W:261:LEU:HD13	2:W:358:LEU:HD12	1.97	0.47
2:X:179:ASN:OD1	2:X:192:GLY:N	2.44	0.47
1:0:156:ARG:NH2	1:0:335:PHE:O	2.47	0.47
1:1:226:SER:HB2	1:1:245:TYR:HA	1.96	0.47
1:F:84:VAL:HG11	1:F:112:ILE:HD11	1.97	0.47
1:F:97:ASP:OD1	1:F:97:ASP:N	2.47	0.47
1:I:284:THR:OG1	1:I:326:LEU:O	2.29	0.47
1:J:23:PHE:CD2	1:J:132:VAL:HG22	2.48	0.47
1:J:52:LEU:O	1:K:78:VAL:HG23	2.15	0.47
1:J:130:GLN:HE22	1:J:326:LEU:HA	1.79	0.47
1:J:224:SER:OG	1:J:225:ASN:N	2.48	0.47
1:M:126:VAL:HG21	1:T:51:ALA:HB3	1.97	0.47
1:O:247:ASP:HB2	1:S:233:LYS:HA	1.96	0.47
1:R:103:ASP:OD1	1:R:103:ASP:N	2.45	0.47
1:T:164:GLN:NE2	1:T:168:THR:O	2.48	0.47
1:3:39:VAL:HB	1:C:10:LEU:HD23	1.96	0.47
1:A:156:ARG:HG2	1:A:332:PRO:HB2	1.97	0.47
1:C:112:ILE:HG13	1:C:116:MET:HE3	1.95	0.47
1:M:80:PRO:HB2	1:M:119:GLU:HG3	1.97	0.47
2:V:438:ALA:HB1	2:V:441:ALA:HB3	1.96	0.47
2:X:371:GLU:HB2	2:X:377:TYR:CE2	2.50	0.47
2:c:216:PRO:O	2:c:217:GLN:HB2	2.14	0.47
1:1:331:ASP:OD1	1:5:13:ASN:ND2	2.48	0.47
1:7:307:ASN:HB3	1:7:319:THR:HA	1.97	0.47
1:D:51:ALA:HB3	1:H:126:VAL:HG21	1.97	0.47
1:E:284:THR:OG1	1:E:326:LEU:O	2.30	0.47
1:I:60:GLY:O	1:J:81:LYS:NZ	2.38	0.47
1:J:49:ASN:HA	1:K:258:VAL:HG13	1.96	0.47
1:K:111:ILE:O	1:K:115:ASN:HB2	2.15	0.47
1:L:83:GLU:HG2	1:L:84:VAL:N	2.28	0.47
1:Q:196:ASN:HA	1:Q:248:VAL:HG12	1.96	0.47
2:U:166:ARG:HE	2:U:422:ARG:HH21	1.61	0.47
2:W:467:LEU:HD11	2:X:482:ARG:HH22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:158:ASP:OD1	2:X:160:SER:OG	2.32	0.47
2:X:185:ASP:OD2	2:X:190:ARG:HA	2.14	0.47
2:Y:185:ASP:OD2	2:Z:211:TYR:OH	2.31	0.47
2:Z:27:GLY:O	2:a:52:ASN:ND2	2.48	0.47
2:e:211:TYR:O	2:e:213:GLY:N	2.43	0.47
2:e:334:MET:HG3	2:e:335:PRO:CD	2.45	0.47
1:M:83:GLU:HB3	1:T:62:VAL:HG21	1.97	0.47
1:O:38:LYS:HD3	1:O:72:GLU:HB3	1.97	0.47
1:P:148:ASP:N	1:P:148:ASP:OD1	2.45	0.47
2:W:324:ARG:NE	2:W:324:ARG:HA	2.30	0.47
2:a:461:VAL:HG22	2:a:482:ARG:HH21	1.79	0.47
1:3:257:TYR:HB3	1:3:266:PHE:CZ	2.49	0.47
1:D:93:LEU:HD21	1:D:111:ILE:HD11	1.96	0.47
1:N:229:GLU:CD	1:N:233:LYS:HB2	2.40	0.47
1:S:95:ASP:OD2	1:S:110:ARG:NH2	2.48	0.47
2:Y:435:PHE:HA	2:Y:442:TRP:CD1	2.50	0.47
1:7:119:GLU:HB2	1:7:321:ILE:HD12	1.97	0.47
1:B:217:LYS:O	1:B:224:SER:OG	2.32	0.47
1:F:257:TYR:HB3	1:F:266:PHE:CZ	2.50	0.47
1:J:148:ASP:N	1:J:148:ASP:OD1	2.47	0.47
1:J:151:GLU:N	1:J:151:GLU:OE1	2.48	0.47
1:O:73:PHE:CD1	1:O:152:VAL:HG23	2.50	0.47
1:O:295:ARG:NE	1:O:295:ARG:HA	2.30	0.47
1:S:156:ARG:NH2	1:S:335:PHE:HB2	2.30	0.47
2:c:94:TRP:O	2:c:98:GLY:N	2.44	0.47
2:f:145:HIS:HB2	2:f:151:LEU:HD23	1.97	0.47
1:0:333:ASP:OD1	1:0:333:ASP:N	2.47	0.46
1:C:66:ARG:NH2	1:G:118:ASP:OD1	2.48	0.46
1:D:164:GLN:HG2	1:D:169:GLU:HA	1.96	0.46
1:P:107:ARG:O	1:P:111:ILE:HG12	2.15	0.46
1:Q:32:TYR:HD2	1:Q:282:LEU:HD12	1.80	0.46
1:Q:73:PHE:CD1	1:Q:152:VAL:HG23	2.49	0.46
1:S:41:LEU:HD11	1:S:328:LEU:HD23	1.97	0.46
2:V:252:TYR:HA	2:V:255:MET:HE2	1.96	0.46
2:V:493:GLN:HG2	2:V:510:TRP:CE2	2.51	0.46
2:b:211:TYR:N	2:b:212:PRO:HD2	2.30	0.46
1:g:277:THR:HG23	1:g:278:GLN:OE1	2.14	0.46
1:h:21:PRO:HA	1:h:128:GLU:OE2	2.16	0.46
1:h:42:SER:HB3	1:h:70:THR:HG22	1.97	0.46
1:0:258:VAL:HG11	1:Q:47:LEU:HD11	1.95	0.46
1:2:156:ARG:O	1:2:157:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:168:THR:H	1:6:173:ARG:HH11	1.62	0.46
1:7:23:PHE:CD1	1:7:135:VAL:HG11	2.50	0.46
1:7:148:ASP:N	1:7:148:ASP:OD1	2.46	0.46
1:L:42:SER:HA	1:L:70:THR:HA	1.95	0.46
1:M:283:ARG:HG2	1:M:327:MET:SD	2.55	0.46
1:P:51:ALA:HB3	1:T:126:VAL:HG21	1.97	0.46
2:b:348:ASP:OD2	2:b:352:SER:OG	2.33	0.46
1:5:85:ASN:OD1	1:5:88:MET:HE3	2.16	0.46
1:J:112:ILE:O	1:J:116:MET:HG3	2.15	0.46
1:K:309:VAL:HG22	1:K:317:GLU:HB3	1.98	0.46
1:P:180:PRO:O	1:P:184:ILE:HG12	2.16	0.46
1:R:160:ASN:ND2	1:R:335:PHE:O	2.44	0.46
1:T:96:GLU:H	1:T:96:GLU:HG2	1.41	0.46
2:V:158:ASP:OD1	2:V:158:ASP:N	2.46	0.46
2:b:261:LEU:HD13	2:b:358:LEU:HD12	1.97	0.46
2:c:211:TYR:N	2:c:212:PRO:HD2	2.30	0.46
1:0:162:ILE:HD11	1:0:190:ASN:HD22	1.79	0.46
1:0:274:LEU:O	1:0:335:PHE:HA	2.15	0.46
1:7:82:HIS:HD2	1:7:115:ASN:OD1	1.98	0.46
1:E:81:LYS:HD3	1:E:320:MET:HE2	1.97	0.46
1:M:305:PRO:HB3	1:M:321:ILE:HG22	1.97	0.46
1:T:92:ARG:HH21	1:T:98:PRO:CA	2.28	0.46
2:V:179:ASN:O	2:V:181:ASN:N	2.46	0.46
2:W:38:TRP:O	2:X:59:ARG:NH2	2.48	0.46
2:b:88:LEU:HD12	2:b:89:SER:N	2.31	0.46
2:d:153:VAL:HG11	2:d:411:MET:HE2	1.97	0.46
2:e:153:VAL:HB	2:e:234:ILE:HB	1.96	0.46
1:g:51:ALA:HB2	1:h:122:ALA:HB1	1.98	0.46
1:4:34:PHE:HZ	1:4:75:PRO:HG3	1.81	0.46
1:6:135:VAL:HG13	1:6:335:PHE:CD2	2.50	0.46
1:6:219:ASP:O	1:E:221:ARG:NH1	2.48	0.46
1:D:156:ARG:NH1	1:D:332:PRO:O	2.48	0.46
1:F:224:SER:OG	1:F:225:ASN:N	2.49	0.46
1:G:148:ASP:OD1	1:G:148:ASP:N	2.48	0.46
1:H:168:THR:HA	1:H:173:ARG:HH12	1.80	0.46
1:I:82:HIS:CE1	1:h:63:ILE:HB	2.51	0.46
1:I:97:ASP:OD1	1:I:97:ASP:N	2.48	0.46
1:N:82:HIS:HE1	1:N:118:ASP:HB2	1.81	0.46
1:P:162:ILE:O	1:P:338:VAL:HA	2.15	0.46
1:P:307:ASN:HB3	1:P:319:THR:HG22	1.98	0.46
1:Q:114:GLN:HA	1:Q:117:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:130:GLN:HE21	1:S:327:MET:HG2	1.80	0.46
2:b:284:SER:OG	2:b:337:ASP:OD1	2.28	0.46
1:g:91:ARG:O	1:g:107:ARG:NH1	2.49	0.46
1:0:156:ARG:NH2	1:0:335:PHE:HB2	2.31	0.46
1:F:157:SER:OG	1:F:159:GLU:OE1	2.33	0.46
1:G:31:SER:OG	1:G:283:ARG:O	2.27	0.46
1:G:66:ARG:HH21	1:O:118:ASP:CG	2.22	0.46
1:I:23:PHE:CD2	1:I:132:VAL:HG22	2.50	0.46
1:Q:305:PRO:HB3	1:Q:321:ILE:HG22	1.97	0.46
2:U:261:LEU:HD11	2:U:355:GLU:OE2	2.16	0.46
2:c:386:ARG:HG2	2:d:455:ILE:O	2.16	0.46
1:0:28:PHE:HB3	1:0:283:ARG:HG3	1.98	0.46
1:1:28:PHE:HE2	1:1:131:ALA:HB1	1.81	0.46
1:2:181:THR:O	1:2:185:GLU:HG2	2.15	0.46
1:7:118:ASP:OD2	1:F:66:ARG:NH1	2.49	0.46
1:H:108:ARG:O	1:H:112:ILE:HG12	2.15	0.46
1:K:44:ILE:HD12	1:L:14:GLU:HG3	1.97	0.46
1:O:123:ILE:HG22	1:O:303:ARG:HH21	1.81	0.46
1:g:90:LEU:HD23	1:g:90:LEU:HA	1.79	0.46
1:3:30:GLU:HG3	1:3:32:TYR:HE1	1.79	0.46
1:C:258:VAL:HG22	1:C:263:LYS:HG2	1.97	0.46
1:D:10:LEU:HD23	1:N:39:VAL:HB	1.97	0.46
1:D:101:LEU:HD12	1:D:101:LEU:H	1.81	0.46
1:K:32:TYR:HB2	1:K:284:THR:HG22	1.98	0.46
1:Q:119:GLU:HG3	1:Q:321:ILE:HG12	1.98	0.46
1:R:83:GLU:HG2	1:R:84:VAL:N	2.29	0.46
1:R:205:TRP:HH2	1:R:228:LEU:HD21	1.80	0.46
2:X:355:GLU:O	2:X:359:LEU:HD23	2.16	0.46
2:a:359:LEU:HD23	2:a:359:LEU:HA	1.78	0.46
2:b:215:MET:HB2	2:b:216:PRO:HD3	1.97	0.46
2:b:466:MET:HE3	2:b:466:MET:HB2	1.78	0.46
1:h:115:ASN:O	1:h:119:GLU:HG2	2.16	0.46
1:0:77:TYR:CE1	1:0:324:ALA:HB2	2.51	0.46
1:1:63:ILE:HB	1:5:82:HIS:CD2	2.50	0.46
1:I:171:SER:O	1:I:175:LYS:NZ	2.48	0.46
1:M:103:ASP:N	1:M:103:ASP:OD1	2.48	0.46
2:W:356:GLN:HG2	2:W:370:TYR:OH	2.15	0.46
2:Y:258:MET:HG2	2:Y:362:ILE:HD13	1.97	0.46
1:1:316:ARG:HH11	1:1:316:ARG:HG3	1.80	0.46
1:B:103:ASP:N	1:B:103:ASP:OD1	2.46	0.46
1:K:196:ASN:C	1:K:248:VAL:HG13	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:313:ASP:HB3	1:O:314:PRO:HD3	1.97	0.46
2:X:128:VAL:HG22	2:X:170:ARG:HD3	1.98	0.46
2:b:145:HIS:HB2	2:b:151:LEU:HD23	1.98	0.46
2:d:186:SER:C	2:e:212:PRO:HG2	2.41	0.46
1:O:102:ALA:O	1:O:107:ARG:NH1	2.49	0.45
1:O:125:GLN:HE21	1:O:125:GLN:HB2	1.51	0.45
1:O:239:VAL:HG22	1:O:253:TYR:HD1	1.80	0.45
1:4:213:ALA:O	1:4:217:LYS:HG2	2.15	0.45
1:5:272:MET:HE2	1:5:340:LEU:HD11	1.97	0.45
1:D:331:ASP:HB3	1:D:334:GLU:HG3	1.98	0.45
1:G:29:ARG:NH1	1:G:29:ARG:HG3	2.31	0.45
1:G:82:HIS:HB2	1:G:115:ASN:ND2	2.30	0.45
1:M:164:GLN:HB2	1:M:340:LEU:O	2.15	0.45
1:O:123:ILE:HA	1:O:126:VAL:HG12	1.97	0.45
1:P:247:ASP:HB2	1:T:233:LYS:HA	1.98	0.45
2:U:348:ASP:OD1	2:U:351:TYR:HB3	2.15	0.45
2:Y:214:TRP:NE1	1:h:307:ASN:OD1	2.49	0.45
2:b:299:ASN:HB3	2:b:301:GLN:HG3	1.98	0.45
2:c:188:ASN:O	2:c:195:ILE:N	2.41	0.45
2:f:298:ALA:HB2	2:f:323:VAL:HG22	1.98	0.45
1:A:157:SER:O	1:A:158:GLU:HG3	2.16	0.45
1:I:50:MET:HG2	1:J:258:VAL:O	2.15	0.45
1:I:73:PHE:CE2	1:I:328:LEU:HD21	2.51	0.45
1:N:286:GLY:O	1:N:300:ALA:HA	2.16	0.45
1:S:258:VAL:HG12	1:S:263:LYS:HA	1.97	0.45
1:S:303:ARG:H	1:S:323:SER:HB2	1.82	0.45
2:e:196:ASN:HB3	2:e:202:LEU:HD11	1.99	0.45
1:O:181:THR:O	1:O:185:GLU:OE1	2.34	0.45
1:2:162:ILE:HB	1:2:338:VAL:HG12	1.99	0.45
1:3:313:ASP:HB2	1:3:314:PRO:HD3	1.98	0.45
1:D:109:ARG:O	1:D:113:MET:HG2	2.16	0.45
1:T:92:ARG:NH2	1:T:98:PRO:N	2.62	0.45
2:V:446:ASP:OD1	2:V:447:TRP:N	2.49	0.45
2:X:207:SER:HB3	2:X:219:TRP:CD1	2.51	0.45
2:Y:460:GLU:O	2:Y:463:GLU:HG3	2.17	0.45
1:B:229:GLU:HG2	1:B:233:LYS:HB2	1.97	0.45
1:G:23:PHE:HD2	1:G:132:VAL:HG22	1.81	0.45
1:H:96:GLU:OE2	1:H:107:ARG:NH1	2.50	0.45
1:K:81:LYS:HB3	1:K:320:MET:HG3	1.97	0.45
1:O:16:LYS:HE2	1:O:16:LYS:HB2	1.79	0.45
1:P:256:GLN:HA	1:P:265:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:195:ILE:HD11	2:U:245:THR:HG23	1.97	0.45
2:Y:39:ASN:O	2:Y:39:ASN:ND2	2.49	0.45
2:Y:298:ALA:HB2	2:Y:323:VAL:HG22	1.99	0.45
2:Z:354:PHE:HB2	2:a:348:ASP:HB2	1.98	0.45
2:a:475:TYR:HB2	2:b:496:GLU:CD	2.42	0.45
2:c:105:ARG:O	2:c:109:ARG:HG2	2.16	0.45
1:2:109:ARG:O	1:2:113:MET:HG2	2.16	0.45
1:7:130:GLN:NE2	1:7:142:MET:HE2	2.32	0.45
1:L:112:ILE:O	1:L:116:MET:HG2	2.15	0.45
1:L:269:ASP:OD1	1:L:270:ASN:N	2.44	0.45
2:U:99:ILE:HG13	2:U:100:GLY:N	2.32	0.45
2:U:399:ARG:O	2:U:403:VAL:HG12	2.16	0.45
2:b:355:GLU:O	2:b:359:LEU:HD23	2.17	0.45
2:c:393:TRP:CD1	2:c:452:ARG:HH21	2.35	0.45
2:d:368:VAL:HG12	2:d:396:PHE:HZ	1.81	0.45
2:e:241:GLU:HG2	2:e:242:ASP:N	2.31	0.45
1:1:162:ILE:O	1:1:338:VAL:HA	2.17	0.45
1:4:232:VAL:HB	1:4:235:LEU:HD21	1.98	0.45
1:B:51:ALA:HB2	1:F:122:ALA:HB1	1.98	0.45
1:F:283:ARG:HD2	1:F:327:MET:SD	2.56	0.45
2:d:89:SER:OG	2:d:446:ASP:O	2.26	0.45
2:f:186:SER:OG	2:f:187:ARG:N	2.49	0.45
1:0:188:ALA:HB3	1:4:235:LEU:HD12	1.98	0.45
1:3:130:GLN:HE21	1:3:327:MET:HG2	1.82	0.45
1:4:217:LYS:HD2	1:A:230:THR:HG23	1.98	0.45
1:F:120:GLU:O	1:F:303:ARG:NH2	2.50	0.45
1:F:169:GLU:N	1:F:169:GLU:OE1	2.50	0.45
1:G:257:TYR:HB3	1:G:266:PHE:CE1	2.44	0.45
1:K:123:ILE:HA	1:K:126:VAL:HG12	1.97	0.45
1:M:21:PRO:HA	1:M:128:GLU:OE1	2.17	0.45
1:Q:125:GLN:NE2	1:Q:257:TYR:HB2	2.25	0.45
1:h:103:ASP:N	1:h:103:ASP:OD1	2.46	0.45
1:0:178:TYR:OH	1:0:183:ASP:OD2	2.31	0.45
1:5:78:VAL:HG11	1:5:126:VAL:HG11	1.99	0.45
1:5:299:ASN:HD22	1:g:104:PRO:HD2	1.82	0.45
1:6:81:LYS:NZ	1:E:60:GLY:O	2.37	0.45
1:B:257:TYR:HB3	1:B:266:PHE:CZ	2.52	0.45
1:C:115:ASN:O	1:C:119:GLU:OE1	2.35	0.45
1:K:196:ASN:HA	1:K:248:VAL:HG22	1.98	0.45
1:R:116:MET:O	1:R:119:GLU:HG2	2.17	0.45
2:V:186:SER:OG	2:V:187:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:371:GLU:HG2	2:c:372:GLN:N	2.31	0.45
1:1:164:GLN:HB2	1:1:340:LEU:O	2.17	0.45
1:5:9:LEU:HB3	1:5:97:ASP:OD1	2.16	0.45
1:6:48:VAL:HG11	1:Q:118:ASP:OD1	2.16	0.45
1:B:148:ASP:OD1	1:B:148:ASP:N	2.50	0.45
1:C:169:GLU:HG2	1:C:171:SER:H	1.81	0.45
1:E:142:MET:HB3	1:E:150:VAL:HB	1.99	0.45
1:J:73:PHE:HD2	1:J:328:LEU:HD22	1.81	0.45
1:M:3:MET:HE2	1:M:3:MET:HA	1.98	0.45
1:P:123:ILE:O	1:P:126:VAL:HG12	2.17	0.45
2:b:88:LEU:HB2	2:b:447:TRP:CZ3	2.52	0.45
1:1:338:VAL:HG23	1:1:340:LEU:HD22	1.99	0.45
1:3:35:THR:HA	1:3:287:CYS:SG	2.56	0.45
1:C:226:SER:HB2	1:C:245:TYR:HA	1.98	0.45
1:D:97:ASP:OD1	1:D:97:ASP:N	2.50	0.45
1:L:168:THR:HB	1:L:173:ARG:HH21	1.82	0.45
1:Q:156:ARG:NH2	1:Q:335:PHE:HB2	2.32	0.45
1:R:201:ASP:OD1	1:R:202:PRO:HD2	2.18	0.45
2:U:284:SER:HB2	2:U:337:ASP:OD1	2.17	0.45
2:b:150:GLU:OE2	2:b:174:PRO:HB3	2.16	0.45
2:c:158:ASP:OD2	2:c:161:SER:HB2	2.16	0.45
1:0:41:LEU:HD22	1:4:11:ALA:HB3	1.99	0.44
1:2:323:SER:OG	1:2:324:ALA:N	2.49	0.44
1:6:303:ARG:H	1:6:323:SER:HB2	1.82	0.44
1:A:127:GLU:OE2	1:A:303:ARG:NH2	2.43	0.44
1:C:95:ASP:OD2	1:C:110:ARG:NH2	2.50	0.44
1:E:41:LEU:HD11	1:E:328:LEU:HD13	1.99	0.44
1:H:103:ASP:N	1:H:103:ASP:OD1	2.50	0.44
1:K:93:LEU:HD21	1:K:111:ILE:HD11	1.97	0.44
1:K:247:ASP:HB2	1:L:233:LYS:HA	1.99	0.44
1:L:77:TYR:OH	1:L:322:GLN:OE1	2.35	0.44
1:L:223:GLY:HA2	1:g:218:LEU:HD13	1.98	0.44
1:P:80:PRO:HG2	1:P:119:GLU:HB2	1.99	0.44
1:P:287:CYS:SG	1:P:288:ILE:N	2.90	0.44
1:T:87:GLN:OE1	1:T:87:GLN:N	2.45	0.44
2:U:187:ARG:HG3	2:V:212:PRO:HG3	1.99	0.44
2:U:254:VAL:HG12	2:U:361:TYR:CE2	2.52	0.44
2:U:355:GLU:O	2:U:359:LEU:HD23	2.17	0.44
2:X:354:PHE:HB2	2:Y:348:ASP:HB2	1.98	0.44
2:Z:42:SER:HB2	2:a:58:ALA:HB2	1.98	0.44
2:Z:157:TRP:HE1	2:Z:230:ARG:NH1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:97:LEU:HB3	2:b:99:ILE:HG23	1.97	0.44
2:e:356:GLN:HG3	2:e:370:TYR:OH	2.17	0.44
1:4:134:ALA:HB2	1:4:140:TYR:HE2	1.82	0.44
1:4:258:VAL:HG12	1:4:263:LYS:HA	1.98	0.44
1:5:134:ALA:HB1	1:5:154:MET:HE1	1.99	0.44
1:B:258:VAL:HG22	1:B:263:LYS:HG2	1.99	0.44
1:C:156:ARG:HD3	1:C:160:ASN:HB2	2.00	0.44
1:C:268:PRO:HG2	1:C:271:THR:OG1	2.17	0.44
1:H:80:PRO:HD2	1:H:321:ILE:O	2.17	0.44
1:Q:81:LYS:HA	1:Q:320:MET:HB3	1.99	0.44
2:a:95:ARG:HH12	2:b:109:ARG:HD3	1.82	0.44
2:a:199:GLY:HA3	2:b:129:GLU:HG2	1.99	0.44
2:b:254:VAL:HG12	2:b:361:TYR:HE2	1.82	0.44
1:h:257:TYR:HB3	1:h:266:PHE:CZ	2.52	0.44
1:1:212:LYS:HD3	1:1:212:LYS:HA	1.82	0.44
1:6:82:HIS:CE1	1:E:63:ILE:HB	2.52	0.44
1:7:170:TRP:CZ2	1:7:180:PRO:HB3	2.52	0.44
1:A:310:THR:HG22	1:A:316:ARG:H	1.82	0.44
1:B:185:GLU:O	1:B:189:LEU:HG	2.18	0.44
1:C:205:TRP:HH2	1:C:228:LEU:HD13	1.83	0.44
1:D:229:GLU:HG2	1:D:233:LYS:HD3	1.99	0.44
1:G:3:MET:HE2	1:G:3:MET:HA	1.98	0.44
1:O:36:THR:HG22	1:O:37:GLU:H	1.82	0.44
1:Q:109:ARG:O	1:Q:113:MET:HG3	2.17	0.44
1:Q:232:VAL:HG13	1:Q:235:LEU:HD21	1.99	0.44
2:U:70:ALA:HB2	2:U:258:MET:HE1	1.98	0.44
2:a:186:SER:OG	2:a:187:ARG:N	2.51	0.44
2:f:453:MET:HE2	2:f:453:MET:HB3	1.84	0.44
1:0:51:ALA:HB2	1:4:122:ALA:HB1	1.99	0.44
1:0:245:TYR:O	1:0:248:VAL:HG22	2.18	0.44
1:6:30:GLU:N	1:6:30:GLU:OE1	2.50	0.44
1:7:89:THR:HG22	1:7:104:PRO:HB3	1.98	0.44
1:B:51:ALA:HB3	1:F:126:VAL:HG21	2.00	0.44
1:F:239:VAL:HG12	1:F:253:TYR:HD1	1.81	0.44
1:J:283:ARG:HG3	1:J:327:MET:SD	2.57	0.44
1:K:313:ASP:HB3	1:K:314:PRO:HD3	2.00	0.44
1:P:114:GLN:HG3	1:P:115:ASN:N	2.32	0.44
1:4:41:LEU:HD12	1:4:73:PHE:HE2	1.83	0.44
1:A:148:ASP:OD1	1:A:148:ASP:N	2.46	0.44
1:C:234:ASP:OD1	1:C:237:LYS:HD3	2.17	0.44
1:E:117:ARG:HA	1:E:120:GLU:CD	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:LEU:HD13	1:G:239:VAL:HG21	2.00	0.44
1:L:198:ILE:HG13	1:L:248:VAL:HG21	2.00	0.44
1:L:280:ARG:HG2	1:L:330:ALA:HB3	1.99	0.44
1:M:239:VAL:HG12	1:M:253:TYR:HD1	1.83	0.44
1:R:174:ASP:OD1	1:R:174:ASP:N	2.47	0.44
1:R:327:MET:O	1:R:328:LEU:HD23	2.18	0.44
2:V:63:LEU:HD23	2:V:63:LEU:HA	1.86	0.44
2:V:238:GLU:OE1	2:V:399:ARG:NH2	2.42	0.44
2:Y:226:LEU:HD13	2:Y:232:SER:HB2	1.98	0.44
2:Z:69:TYR:CE2	2:Z:359:LEU:HD21	2.53	0.44
2:d:132:ARG:HA	2:d:136:MET:HE2	2.00	0.44
1:0:122:ALA:O	1:0:126:VAL:HG23	2.17	0.44
1:5:35:THR:HA	1:5:287:CYS:SG	2.56	0.44
1:6:56:PRO:O	1:Q:79:LYS:NZ	2.47	0.44
1:A:80:PRO:HD2	1:A:321:ILE:O	2.18	0.44
1:C:328:LEU:HD23	1:C:328:LEU:HA	1.79	0.44
1:D:91:ARG:O	1:D:107:ARG:NE	2.51	0.44
1:D:156:ARG:HD3	1:D:160:ASN:HB2	2.00	0.44
1:L:340:LEU:HD23	1:L:340:LEU:HA	1.82	0.44
1:O:73:PHE:HD2	1:O:328:LEU:HD21	1.83	0.44
1:P:289:GLN:OE1	1:P:289:GLN:N	2.50	0.44
1:Q:86:PRO:O	1:Q:89:THR:HG22	2.18	0.44
1:T:274:LEU:HD23	1:T:274:LEU:H	1.82	0.44
2:Z:211:TYR:O	2:Z:213:GLY:N	2.49	0.44
1:0:82:HIS:CD2	1:Q:63:ILE:HB	2.52	0.44
1:4:122:ALA:O	1:4:126:VAL:HG23	2.17	0.44
1:J:80:PRO:HD2	1:J:321:ILE:O	2.17	0.44
1:P:45:PRO:HD3	1:P:68:GLY:HA2	1.99	0.44
1:S:154:MET:N	1:S:154:MET:SD	2.90	0.44
1:T:22:LEU:HD13	1:T:239:VAL:HG21	1.99	0.44
1:T:81:LYS:HA	1:T:320:MET:HB3	1.99	0.44
2:W:251:PHE:CD2	2:W:258:MET:HE1	2.53	0.44
2:Z:251:PHE:HB3	2:Z:255:MET:HG2	2.00	0.44
2:e:171:MET:HE1	2:e:407:GLN:HE22	1.82	0.44
2:e:465:VAL:O	2:e:469:GLU:HG2	2.18	0.44
1:0:305:PRO:HB3	1:0:321:ILE:HG12	1.99	0.44
1:5:178:TYR:OH	1:5:183:ASP:OD2	2.23	0.44
1:5:311:THR:HG22	1:5:311:THR:O	2.16	0.44
1:7:216:GLU:O	1:7:220:THR:OG1	2.35	0.44
1:A:75:PRO:HA	1:A:326:LEU:HD12	1.99	0.44
1:A:109:ARG:O	1:A:112:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TYR:HD2	1:B:322:GLN:HE21	1.66	0.44
1:D:201:ASP:CG	1:D:202:PRO:HD2	2.43	0.44
1:E:128:GLU:HG3	1:E:266:PHE:CE1	2.53	0.44
1:G:130:GLN:HG3	1:G:327:MET:HB2	1.99	0.44
1:I:79:LYS:HB3	1:I:322:GLN:HB3	1.99	0.44
1:I:274:LEU:HB2	1:I:336:VAL:HB	2.00	0.44
1:O:223:GLY:O	1:S:230:THR:HG22	2.17	0.44
2:V:465:VAL:O	2:V:469:GLU:HG2	2.18	0.44
2:W:153:VAL:HG22	2:W:171:MET:SD	2.58	0.44
2:Y:94:TRP:CD1	2:Y:94:TRP:H	2.35	0.44
2:d:230:ARG:HE	2:d:417:GLU:CD	2.25	0.44
2:d:429:SER:HB2	2:d:430:LYS:NZ	2.33	0.44
1:h:41:LEU:O	1:h:71:SER:N	2.51	0.44
1:0:164:GLN:HB2	1:0:340:LEU:O	2.18	0.44
1:1:234:ASP:C	1:1:235:LEU:HD22	2.43	0.44
1:4:51:ALA:HB3	1:A:126:VAL:HG21	1.99	0.44
1:7:3:MET:HE3	1:7:4:TYR:H	1.83	0.44
1:7:313:ASP:HB3	1:7:314:PRO:HD3	1.99	0.44
1:A:63:ILE:HB	1:E:82:HIS:CE1	2.53	0.44
1:J:194:VAL:HG22	1:K:236:GLY:HA3	1.99	0.44
1:K:175:LYS:HB2	1:K:175:LYS:HE2	1.67	0.44
1:P:223:GLY:O	1:T:230:THR:HG22	2.18	0.44
1:Q:93:LEU:HD12	1:Q:93:LEU:HA	1.79	0.44
2:U:493:GLN:O	2:U:497:THR:HG23	2.18	0.44
2:V:283:GLU:O	2:V:338:SER:N	2.50	0.44
2:Y:185:ASP:HB3	2:Z:211:TYR:HE2	1.83	0.44
2:b:110:GLU:HG2	2:b:425:VAL:HG12	1.98	0.44
1:4:80:PRO:HD2	1:4:321:ILE:O	2.18	0.43
1:D:164:GLN:HE22	1:D:170:TRP:CD1	2.34	0.43
1:D:258:VAL:HG11	1:N:47:LEU:HG	2.00	0.43
1:I:35:THR:HG22	1:I:300:ALA:HB3	2.00	0.43
1:J:199:VAL:HB	1:J:273:VAL:HB	1.99	0.43
1:J:257:TYR:HB3	1:J:266:PHE:CZ	2.53	0.43
1:M:296:GLU:OE1	1:M:304:TYR:HE2	2.02	0.43
1:O:49:ASN:HA	1:S:258:VAL:HG23	1.99	0.43
2:V:435:PHE:HA	2:V:442:TRP:CD1	2.53	0.43
2:Y:207:SER:HB3	2:Y:219:TRP:NE1	2.33	0.43
2:b:260:MET:HE2	2:b:260:MET:HA	1.99	0.43
2:f:63:LEU:HD23	2:f:63:LEU:HA	1.74	0.43
1:2:164:GLN:HB2	1:2:340:LEU:O	2.18	0.43
1:2:217:LYS:HE2	1:2:217:LYS:HB2	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:77:TYR:CD2	1:5:324:ALA:HB2	2.53	0.43
1:7:15:GLN:HB2	1:F:45:PRO:O	2.18	0.43
1:C:21:PRO:O	1:C:25:ARG:HG3	2.18	0.43
1:H:292:ASP:HA	1:H:295:ARG:HB2	1.99	0.43
1:Q:42:SER:HA	1:Q:70:THR:HA	1.99	0.43
2:Y:495:ARG:O	2:Y:498:MET:HG3	2.18	0.43
2:Z:61:ASP:OD2	2:Z:175:LYS:NZ	2.46	0.43
2:Z:282:ILE:HD11	2:Z:296:LEU:HG	2.00	0.43
2:d:63:LEU:HD23	2:d:63:LEU:HA	1.82	0.43
2:e:127:ASP:HB3	2:e:137:MET:HE3	1.99	0.43
1:0:146:ALA:HB3	1:Q:54:VAL:HG23	1.99	0.43
1:4:85:ASN:OD1	1:4:88:MET:HE2	2.18	0.43
1:4:293:ALA:HB2	1:4:304:TYR:CE2	2.53	0.43
1:A:305:PRO:HB3	1:A:321:ILE:HG12	2.00	0.43
1:G:93:LEU:HG	1:G:107:ARG:HD3	2.00	0.43
1:I:40:TYR:HE1	1:I:72:GLU:HB3	1.83	0.43
1:M:288:ILE:HG21	1:M:304:TYR:CD1	2.53	0.43
2:X:72:ASN:HD22	2:X:72:ASN:C	2.25	0.43
2:a:56:GLY:HA3	2:a:252:TYR:OH	2.18	0.43
1:7:124:ALA:O	1:7:127:GLU:HG2	2.19	0.43
1:7:218:LEU:HD13	1:F:223:GLY:HA2	1.99	0.43
1:D:80:PRO:HD2	1:D:321:ILE:O	2.18	0.43
1:D:220:THR:HG22	1:D:223:GLY:H	1.83	0.43
1:E:198:ILE:HG12	1:E:274:LEU:HD13	2.00	0.43
1:G:198:ILE:HB	1:G:250:ILE:HD13	2.00	0.43
1:H:313:ASP:HB3	1:H:314:PRO:HD3	2.00	0.43
1:I:142:MET:O	1:I:142:MET:HG2	2.18	0.43
1:R:181:THR:O	1:R:184:ILE:HG22	2.18	0.43
1:T:24:LEU:HD23	1:T:24:LEU:HA	1.86	0.43
2:a:453:MET:HE2	2:a:453:MET:HB3	1.84	0.43
2:c:145:HIS:HB2	2:c:151:LEU:HD23	2.01	0.43
1:3:28:PHE:HE1	1:3:329:LEU:HD13	1.84	0.43
1:4:28:PHE:HB3	1:4:283:ARG:HG3	2.01	0.43
1:6:283:ARG:HG2	1:6:327:MET:HE1	2.00	0.43
1:A:226:SER:HB2	1:A:245:TYR:HA	2.01	0.43
1:B:24:LEU:HG	1:B:283:ARG:HH21	1.83	0.43
1:B:303:ARG:O	1:B:305:PRO:HD3	2.17	0.43
1:C:162:ILE:HD11	1:C:338:VAL:HG22	2.01	0.43
1:M:196:ASN:ND2	1:M:276:ASN:OD1	2.51	0.43
1:M:282:LEU:HD23	1:M:282:LEU:H	1.82	0.43
1:N:257:TYR:HB3	1:N:266:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:72:GLU:OE1	1:Q:72:GLU:N	2.52	0.43
2:W:144:MET:SD	2:W:174:PRO:HD3	2.58	0.43
2:Z:428:PRO:HD2	2:Z:442:TRP:CH2	2.53	0.43
1:6:174:ASP:N	1:6:174:ASP:OD1	2.51	0.43
1:6:258:VAL:HG12	1:6:263:LYS:HA	1.99	0.43
1:6:277:THR:HG23	1:6:278:GLN:HG2	2.00	0.43
1:A:44:ILE:HG22	1:A:68:GLY:HA3	2.00	0.43
1:A:157:SER:O	1:A:159:GLU:N	2.52	0.43
1:C:103:ASP:N	1:C:103:ASP:OD1	2.49	0.43
1:I:209:ARG:HA	1:I:214:VAL:HG21	1.99	0.43
1:K:263:LYS:HB2	1:K:263:LYS:HE2	1.71	0.43
1:L:303:ARG:HB3	1:L:321:ILE:HD11	2.00	0.43
1:P:46:GLY:HA2	1:P:66:ARG:NH1	2.34	0.43
2:V:177:ILE:HB	2:V:246:ARG:HH12	1.83	0.43
2:X:284:SER:OG	2:X:285:GLU:N	2.51	0.43
2:Y:381:SER:OG	2:Y:382:TYR:N	2.50	0.43
2:Z:368:VAL:HG12	2:Z:396:PHE:HZ	1.83	0.43
1:6:176:SER:HA	1:6:212:LYS:HB2	2.01	0.43
1:C:42:SER:HB3	1:C:70:THR:HG22	2.00	0.43
1:E:313:ASP:HB3	1:E:314:PRO:HD3	2.00	0.43
1:F:181:THR:HA	1:F:184:ILE:HD12	2.00	0.43
1:H:77:TYR:HE2	1:H:79:LYS:HE2	1.83	0.43
1:J:54:VAL:HG12	1:K:146:ALA:HB3	2.00	0.43
2:c:24:TYR:CE2	2:d:49:LEU:HB2	2.54	0.43
2:d:359:LEU:HD23	2:d:359:LEU:HA	1.89	0.43
2:f:359:LEU:HA	2:f:359:LEU:HD23	1.80	0.43
1:0:154:MET:HE1	1:0:328:LEU:HA	2.00	0.43
1:0:198:ILE:HA	1:0:273:VAL:O	2.19	0.43
1:6:82:HIS:HD2	1:6:119:GLU:OE2	2.01	0.43
1:7:108:ARG:O	1:7:112:ILE:HG12	2.19	0.43
1:A:48:VAL:O	1:E:258:VAL:HG13	2.18	0.43
1:B:280:ARG:HG3	1:B:280:ARG:NH1	2.34	0.43
1:C:257:TYR:HB3	1:C:266:PHE:CZ	2.53	0.43
1:N:293:ALA:HB2	1:N:304:TYR:CE2	2.54	0.43
1:O:74:THR:HA	1:O:75:PRO:HD3	1.89	0.43
1:O:148:ASP:OD1	1:O:148:ASP:N	2.49	0.43
1:R:21:PRO:HA	1:R:128:GLU:OE2	2.18	0.43
1:S:86:PRO:O	1:S:89:THR:HG22	2.18	0.43
2:X:432:ARG:HH21	2:X:433:PHE:HZ	1.67	0.43
2:b:187:ARG:CA	2:c:212:PRO:HG3	2.38	0.43
2:b:418:GLU:HA	2:b:421:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:132:ARG:HB3	2:e:136:MET:HB2	1.99	0.43
1:6:82:HIS:HB2	1:6:115:ASN:HD21	1.83	0.43
1:J:53:TYR:OH	1:K:130:GLN:NE2	2.46	0.43
1:J:73:PHE:CD2	1:J:328:LEU:HD22	2.53	0.43
2:U:76:LEU:HD23	2:U:76:LEU:HA	1.88	0.43
2:V:251:PHE:O	2:V:255:MET:HG3	2.18	0.43
2:X:491:ALA:HA	2:X:494:VAL:HG12	2.00	0.43
2:Y:165:PHE:HZ	2:Y:424:VAL:HG11	1.82	0.43
2:Y:208:GLU:OE2	2:Y:218:LYS:NZ	2.49	0.43
2:b:193:VAL:HG22	2:b:204:TYR:HD2	1.83	0.43
1:4:296:GLU:OE1	2:V:181:ASN:HB3	2.18	0.43
1:F:132:VAL:HG11	1:F:266:PHE:CD1	2.54	0.43
1:M:185:GLU:HA	1:M:185:GLU:OE1	2.19	0.43
1:M:205:TRP:CE2	1:M:242:LYS:HE2	2.54	0.43
1:N:41:LEU:HD12	1:N:73:PHE:CE2	2.53	0.43
1:Q:184:ILE:HD11	1:Q:198:ILE:HD13	2.00	0.43
2:V:63:LEU:HD13	2:V:258:MET:HE3	2.01	0.43
2:b:420:ILE:HD13	2:b:425:VAL:HG23	2.01	0.43
2:e:73:ALA:O	2:e:77:HIS:ND1	2.44	0.43
1:0:287:CYS:SG	1:0:288:ILE:N	2.92	0.42
1:3:42:SER:OG	1:3:70:THR:HG22	2.19	0.42
1:4:127:GLU:CD	1:4:303:ARG:HH22	2.27	0.42
1:5:293:ALA:HB2	1:5:304:TYR:CE2	2.54	0.42
1:C:38:LYS:HD3	1:C:74:THR:HG22	2.01	0.42
1:I:195:VAL:HB	1:J:235:LEU:HB2	2.01	0.42
1:J:82:HIS:HD2	1:J:119:GLU:OE2	2.02	0.42
1:K:217:LYS:HD2	1:L:230:THR:HG23	2.01	0.42
1:M:162:ILE:O	1:M:338:VAL:HA	2.20	0.42
2:X:141:GLY:HA3	2:X:407:GLN:HE22	1.84	0.42
2:d:94:TRP:O	2:d:98:GLY:N	2.46	0.42
2:f:238:GLU:OE2	2:f:399:ARG:NH2	2.52	0.42
1:4:39:VAL:O	1:4:72:GLU:HA	2.19	0.42
1:5:85:ASN:HB3	1:5:316:ARG:HG2	2.01	0.42
1:7:159:GLU:O	1:7:190:ASN:ND2	2.43	0.42
1:D:290:ASP:CG	1:D:322:GLN:HE22	2.27	0.42
1:F:201:ASP:OD2	1:F:270:ASN:HA	2.19	0.42
1:G:226:SER:CB	1:G:246:GLY:H	2.30	0.42
1:I:103:ASP:OD1	1:I:103:ASP:N	2.49	0.42
1:J:179:ASP:OD1	1:J:179:ASP:N	2.52	0.42
1:M:244:MET:HE3	1:M:244:MET:HB2	1.83	0.42
1:M:274:LEU:O	1:M:335:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:26:LEU:O	1:N:29:ARG:NH1	2.52	0.42
1:N:79:LYS:HD3	1:N:320:MET:CE	2.49	0.42
1:N:340:LEU:HD23	1:N:340:LEU:O	2.19	0.42
1:T:200:PHE:HD2	1:T:205:TRP:HE3	1.66	0.42
1:T:328:LEU:HD23	1:T:328:LEU:HA	1.91	0.42
2:U:393:TRP:NE1	2:U:397:MET:HE3	2.33	0.42
2:X:89:SER:HB3	2:X:446:ASP:O	2.18	0.42
2:X:96:TYR:CE1	2:Y:117:GLU:HG2	2.54	0.42
2:Y:153:VAL:HG22	2:Y:171:MET:SD	2.59	0.42
2:b:63:LEU:HD23	2:b:63:LEU:HA	1.79	0.42
2:d:354:PHE:HE2	2:e:269:LEU:HD13	1.84	0.42
2:e:215:MET:HE2	2:e:215:MET:HB3	1.88	0.42
2:f:190:ARG:HB2	2:f:245:THR:HG21	2.02	0.42
1:3:148:ASP:OD1	1:3:148:ASP:N	2.53	0.42
1:3:329:LEU:HD12	1:3:329:LEU:HA	1.89	0.42
1:7:80:PRO:HD2	1:7:321:ILE:O	2.19	0.42
1:7:218:LEU:HD21	1:7:228:LEU:HB3	2.00	0.42
1:C:97:ASP:OD1	1:C:97:ASP:N	2.48	0.42
1:E:207:LEU:HD23	1:E:340:LEU:HD23	2.01	0.42
1:G:170:TRP:NE1	1:G:183:ASP:OD2	2.45	0.42
1:G:179:ASP:OD1	1:G:179:ASP:N	2.50	0.42
1:H:179:ASP:OD1	1:H:179:ASP:N	2.49	0.42
1:H:282:LEU:HB2	1:H:328:LEU:O	2.19	0.42
1:L:72:GLU:OE1	1:L:72:GLU:N	2.52	0.42
1:P:82:HIS:O	1:P:318:PHE:HB2	2.20	0.42
1:R:154:MET:HB3	1:R:332:PRO:HG3	2.02	0.42
1:1:68:GLY:H	1:5:94:PRO:HG3	1.85	0.42
1:1:113:MET:HB3	1:1:117:ARG:NH2	2.29	0.42
1:5:182:ASP:OD1	1:5:183:ASP:N	2.51	0.42
1:7:30:GLU:OE1	1:7:32:TYR:OH	2.32	0.42
1:7:123:ILE:O	1:7:126:VAL:HG12	2.19	0.42
1:A:62:VAL:HG13	1:E:82:HIS:HA	2.01	0.42
1:A:122:ALA:O	1:A:126:VAL:HG23	2.18	0.42
1:A:213:ALA:O	1:A:217:LYS:HG2	2.19	0.42
1:A:280:ARG:HH12	1:A:282:LEU:HD11	1.84	0.42
1:E:178:TYR:OH	1:E:183:ASP:OD2	2.32	0.42
1:J:191:ALA:HB2	1:J:336:VAL:HG23	2.02	0.42
1:L:32:TYR:CD2	1:L:282:LEU:HD12	2.55	0.42
1:L:143:THR:OG1	1:L:144:GLY:N	2.53	0.42
1:N:128:GLU:OE1	1:N:132:VAL:HG23	2.19	0.42
1:O:31:SER:HA	1:O:283:ARG:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:251:PHE:O	2:f:255:MET:HB2	2.19	0.42
1:g:41:LEU:HD12	1:g:73:PHE:HE2	1.85	0.42
1:1:156:ARG:NH2	1:1:335:PHE:HB2	2.34	0.42
1:2:78:VAL:HG23	1:S:52:LEU:O	2.20	0.42
1:2:216:GLU:O	1:2:220:THR:HG23	2.20	0.42
1:4:148:ASP:OD1	1:4:148:ASP:N	2.50	0.42
1:C:241:TYR:HE1	1:C:251:VAL:HG22	1.83	0.42
1:D:212:LYS:HD2	1:D:212:LYS:HA	1.81	0.42
1:K:170:TRP:HB3	1:K:207:LEU:HD21	2.02	0.42
1:L:23:PHE:CD2	1:L:132:VAL:HG22	2.54	0.42
1:L:284:THR:OG1	1:L:326:LEU:O	2.30	0.42
1:L:331:ASP:O	1:L:334:GLU:HG2	2.20	0.42
1:M:76:GLY:HA3	1:M:142:MET:HE3	2.01	0.42
1:Q:75:PRO:HA	1:Q:326:LEU:HD12	2.02	0.42
1:T:23:PHE:CD2	1:T:132:VAL:HG22	2.54	0.42
2:U:466:MET:HB2	2:U:466:MET:HE3	1.83	0.42
2:U:496:GLU:CD	2:f:475:TYR:HB2	2.45	0.42
2:X:166:ARG:NE	2:X:422:ARG:HH21	2.17	0.42
2:Y:427:LEU:HG	2:Y:428:PRO:HD2	2.01	0.42
2:e:150:GLU:OE1	2:e:235:HIS:NE2	2.47	0.42
2:f:171:MET:HE3	2:f:171:MET:HB3	1.83	0.42
1:h:103:ASP:C	1:h:105:ALA:H	2.28	0.42
1:1:274:LEU:HB2	1:1:336:VAL:HG22	2.01	0.42
1:2:235:LEU:HD12	1:S:188:ALA:CB	2.50	0.42
1:2:313:ASP:OD2	1:N:320:MET:HE1	2.19	0.42
1:5:52:LEU:H	1:5:52:LEU:HD23	1.84	0.42
1:6:78:VAL:HG23	1:E:52:LEU:O	2.20	0.42
1:A:72:GLU:H	1:A:72:GLU:HG3	1.75	0.42
1:B:97:ASP:N	1:B:97:ASP:OD1	2.50	0.42
1:F:258:VAL:HA	1:F:263:LYS:HA	2.02	0.42
1:F:272:MET:HB2	1:F:340:LEU:HD21	2.02	0.42
1:H:106:TYR:O	1:H:110:ARG:HG3	2.19	0.42
1:J:137:LYS:HE3	1:J:137:LYS:HB3	1.77	0.42
1:K:93:LEU:HD13	1:K:107:ARG:HG2	2.01	0.42
1:M:162:ILE:HB	1:M:338:VAL:HG12	2.01	0.42
1:O:41:LEU:HD12	1:O:73:PHE:HE2	1.83	0.42
1:T:331:ASP:OD1	1:T:331:ASP:N	2.52	0.42
2:W:477:LYS:O	2:W:481:LYS:HG2	2.19	0.42
2:X:63:LEU:HD23	2:X:63:LEU:HA	1.83	0.42
2:Z:105:ARG:HH21	2:a:495:ARG:HH21	1.67	0.42
2:b:251:PHE:HB3	2:b:255:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:158:ASP:OD1	2:d:158:ASP:N	2.52	0.42
2:e:271:SER:HA	2:e:274:VAL:HG12	2.00	0.42
1:g:77:TYR:OH	1:g:289:GLN:HG3	2.20	0.42
1:g:164:GLN:HB2	1:g:340:LEU:O	2.19	0.42
1:2:274:LEU:O	1:2:335:PHE:HA	2.20	0.42
1:3:45:PRO:HD3	1:3:68:GLY:HA2	2.00	0.42
1:7:103:ASP:N	1:7:103:ASP:OD1	2.53	0.42
1:C:201:ASP:CG	1:C:202:PRO:HD2	2.45	0.42
1:F:162:ILE:O	1:F:338:VAL:HA	2.20	0.42
1:I:157:SER:C	1:I:159:GLU:H	2.26	0.42
1:L:257:TYR:HB3	1:L:266:PHE:CZ	2.54	0.42
1:O:203:LYS:HB2	1:O:270:ASN:HB3	2.00	0.42
2:U:137:MET:HE1	2:U:169:PHE:HB2	2.02	0.42
2:U:403:VAL:HG13	2:U:404:ALA:N	2.35	0.42
2:Z:111:VAL:HG22	2:Z:425:VAL:HG11	2.00	0.42
2:Z:371:GLU:HB2	2:Z:377:TYR:CE1	2.55	0.42
2:d:61:ASP:OD1	2:d:65:ARG:NE	2.53	0.42
2:d:298:ALA:HB2	2:d:323:VAL:HG22	2.02	0.42
2:e:249:ASN:ND2	2:e:251:PHE:HB2	2.33	0.42
2:f:359:LEU:HD23	2:f:362:ILE:HD12	2.02	0.42
2:f:418:GLU:OE2	2:f:422:ARG:HG3	2.18	0.42
1:O:13:ASN:ND2	1:Q:331:ASP:OD1	2.53	0.42
1:1:3:MET:HG3	1:1:5:THR:HG22	2.02	0.42
1:6:7:ALA:C	1:E:36:THR:HG21	2.45	0.42
1:I:40:TYR:O	1:J:9:LEU:HD12	2.20	0.42
1:K:108:ARG:O	1:K:112:ILE:HG12	2.20	0.42
1:K:274:LEU:HB2	1:K:336:VAL:HB	2.00	0.42
1:L:176:SER:OG	1:L:177:THR:N	2.53	0.42
1:N:79:LYS:HG3	1:N:79:LYS:O	2.19	0.42
1:P:200:PHE:CD2	1:P:205:TRP:HE3	2.37	0.42
2:d:296:LEU:HD23	2:d:296:LEU:HA	1.86	0.42
2:d:384:THR:HG23	2:e:377:TYR:HB3	2.01	0.42
1:O:13:ASN:HD22	1:Q:331:ASP:CG	2.28	0.42
1:1:169:GLU:HG3	1:1:172:LYS:HD2	2.02	0.42
1:1:333:ASP:OD1	1:1:333:ASP:N	2.53	0.42
1:4:209:ARG:HD2	1:4:230:THR:HG23	2.02	0.42
1:6:7:ALA:HB1	1:E:40:TYR:CE1	2.52	0.42
1:B:54:VAL:HG23	1:F:79:LYS:HG2	2.02	0.42
1:C:34:PHE:HZ	1:C:75:PRO:HG3	1.84	0.42
1:C:128:GLU:OE2	1:C:132:VAL:HG23	2.20	0.42
1:I:116:MET:HA	1:I:119:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:TYR:OH	1:J:183:ASP:OD2	2.32	0.42
1:K:197:ILE:N	1:K:248:VAL:HG13	2.35	0.42
1:R:141:THR:HG22	1:R:151:GLU:OE1	2.20	0.42
2:X:211:TYR:CD1	2:X:212:PRO:HD3	2.55	0.42
2:Z:34:GLN:NE2	2:a:256:GLU:OE2	2.40	0.42
2:Z:474:THR:HG22	2:a:493:GLN:HG3	2.01	0.42
2:c:348:ASP:OD2	2:c:352:SER:OG	2.31	0.42
2:d:251:PHE:CD1	2:d:258:MET:HE1	2.55	0.42
1:h:162:ILE:O	1:h:338:VAL:HA	2.20	0.42
1:2:83:GLU:HB2	1:2:318:PHE:CD1	2.54	0.42
1:4:100:ASN:HA	2:W:55:ARG:NH1	2.35	0.42
1:5:113:MET:O	1:5:117:ARG:HG3	2.19	0.42
1:6:148:ASP:N	1:6:148:ASP:OD1	2.53	0.42
1:P:90:LEU:HD12	1:P:90:LEU:HA	1.91	0.42
1:P:234:ASP:C	1:P:235:LEU:HD12	2.44	0.42
1:P:290:ASP:O	1:P:294:GLN:HG2	2.20	0.42
1:Q:81:LYS:HG3	1:Q:320:MET:HE2	2.02	0.42
2:V:403:VAL:HG23	2:V:404:ALA:N	2.35	0.42
2:Z:345:GLN:HG3	2:Z:346:ASP:O	2.20	0.42
2:a:127:ASP:OD2	2:a:130:ARG:N	2.52	0.42
2:a:249:ASN:OD1	2:a:251:PHE:HB2	2.19	0.42
2:e:368:VAL:HG12	2:e:396:PHE:HZ	1.85	0.42
1:h:259:GLU:O	1:h:264:LYS:NZ	2.52	0.42
1:h:283:ARG:HG3	1:h:327:MET:SD	2.59	0.42
1:0:51:ALA:HB3	1:4:126:VAL:HG21	2.02	0.41
1:A:175:LYS:HD3	1:A:175:LYS:HA	1.84	0.41
1:C:81:LYS:HB3	1:C:320:MET:HB2	2.01	0.41
1:D:73:PHE:CE2	1:D:328:LEU:HD21	2.55	0.41
1:D:269:ASP:OD1	1:D:269:ASP:N	2.53	0.41
1:O:119:GLU:H	1:O:119:GLU:HG2	1.59	0.41
2:V:133:THR:HG23	2:V:136:MET:HE1	2.02	0.41
2:V:166:ARG:HE	2:V:422:ARG:NH2	2.05	0.41
2:X:85:PHE:CD2	2:X:87:ARG:HG3	2.53	0.41
2:Y:42:SER:HB2	2:Z:58:ALA:HB2	2.02	0.41
2:Z:199:GLY:HA3	2:a:129:GLU:HG2	2.02	0.41
2:b:180:PRO:O	2:b:183:THR:HG23	2.20	0.41
2:b:420:ILE:HD12	2:b:427:LEU:HD21	2.02	0.41
1:g:130:GLN:HE21	1:g:142:MET:HG2	1.85	0.41
1:g:205:TRP:CZ3	1:g:250:ILE:HG21	2.55	0.41
1:h:329:LEU:HD12	1:h:329:LEU:HA	1.88	0.41
1:0:77:TYR:HE1	1:0:324:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:ILE:HD11	1:P:95:ASP:OD1	2.19	0.41
1:J:90:LEU:HD23	1:J:90:LEU:HA	1.93	0.41
1:M:83:GLU:HB2	1:M:318:PHE:CD1	2.55	0.41
1:Q:86:PRO:O	1:Q:89:THR:N	2.53	0.41
2:W:101:GLU:O	2:W:105:ARG:HG3	2.20	0.41
2:c:358:LEU:HD23	2:c:358:LEU:HA	1.89	0.41
2:d:49:LEU:HD11	2:d:53:PHE:HD1	1.85	0.41
2:d:144:MET:HE1	2:d:173:SER:HA	2.02	0.41
2:e:386:ARG:HE	2:e:452:ARG:NH2	2.19	0.41
1:0:219:ASP:OD1	1:Q:220:THR:HG23	2.20	0.41
1:3:185:GLU:HG3	1:C:235:LEU:HD21	2.01	0.41
1:4:201:ASP:O	1:4:202:PRO:C	2.62	0.41
1:4:316:ARG:HH21	1:4:318:PHE:HZ	1.68	0.41
1:6:34:PHE:HZ	1:6:75:PRO:HG3	1.85	0.41
1:C:270:ASN:O	1:C:339:GLN:HG2	2.20	0.41
1:E:213:ALA:O	1:E:216:GLU:HG2	2.20	0.41
1:I:178:TYR:O	1:I:213:ALA:HB2	2.21	0.41
1:I:328:LEU:HD23	1:I:328:LEU:HA	1.69	0.41
1:T:283:ARG:HG2	1:T:327:MET:SD	2.61	0.41
2:W:327:GLY:H	2:e:31:PHE:HE2	1.67	0.41
2:b:96:TYR:HE2	2:b:433:PHE:HE2	1.68	0.41
2:b:397:MET:HE2	2:b:397:MET:HA	2.03	0.41
1:0:174:ASP:OD2	1:0:177:THR:OG1	2.38	0.41
1:2:201:ASP:HB2	1:2:202:PRO:HD2	2.01	0.41
1:5:130:GLN:O	1:5:130:GLN:NE2	2.48	0.41
1:6:320:MET:HE1	1:6:322:GLN:CD	2.45	0.41
1:I:109:ARG:O	1:I:112:ILE:HG22	2.21	0.41
1:J:130:GLN:NE2	1:J:326:LEU:HA	2.36	0.41
1:N:295:ARG:HE	1:N:295:ARG:HB2	1.73	0.41
1:N:296:GLU:H	1:N:296:GLU:HG2	1.53	0.41
1:P:309:VAL:HG22	1:P:317:GLU:HB3	2.02	0.41
1:Q:328:LEU:HD23	1:Q:328:LEU:HA	1.91	0.41
1:S:76:GLY:HA3	1:S:142:MET:HE2	2.03	0.41
1:S:164:GLN:HB3	1:S:168:THR:O	2.21	0.41
1:T:180:PRO:HD3	1:T:211:PHE:HD2	1.84	0.41
2:e:406:ARG:HH22	2:f:136:MET:HE1	1.86	0.41
2:f:166:ARG:HD3	2:f:422:ARG:HH12	1.84	0.41
1:g:75:PRO:HA	1:g:326:LEU:HD12	2.02	0.41
1:g:310:THR:HG22	1:g:311:THR:N	2.33	0.41
1:2:156:ARG:HD3	1:2:161:ASN:OD1	2.20	0.41
1:5:195:VAL:HG22	1:B:235:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:HD2	1:A:327:MET:SD	2.61	0.41
1:C:214:VAL:O	1:C:218:LEU:HG	2.21	0.41
1:D:282:LEU:HB2	1:D:328:LEU:HB2	2.03	0.41
1:Q:54:VAL:HG22	1:Q:58:VAL:HG23	2.01	0.41
1:R:81:LYS:HA	1:R:320:MET:HB2	2.02	0.41
2:U:61:ASP:OD1	2:U:65:ARG:NE	2.54	0.41
2:W:474:THR:HG21	2:X:492:GLN:HG2	2.00	0.41
2:Y:63:LEU:HD23	2:Y:63:LEU:HA	1.81	0.41
2:Z:144:MET:SD	2:Z:174:PRO:HD3	2.60	0.41
2:Z:163:ARG:NH1	2:Z:165:PHE:O	2.53	0.41
2:b:283:GLU:HB3	2:b:338:SER:HB2	2.01	0.41
2:e:370:TYR:OH	2:e:376:ASN:ND2	2.51	0.41
2:f:381:SER:OG	2:f:382:TYR:N	2.54	0.41
1:1:201:ASP:OD2	1:1:201:ASP:N	2.52	0.41
1:2:51:ALA:HB2	1:3:122:ALA:HB1	2.02	0.41
1:3:75:PRO:HB3	1:3:326:LEU:HB2	2.03	0.41
1:6:36:THR:HG22	1:6:37:GLU:N	2.35	0.41
1:A:201:ASP:OD1	1:A:202:PRO:HD2	2.20	0.41
1:E:109:ARG:O	1:E:113:MET:HG2	2.21	0.41
1:G:283:ARG:HG3	1:G:327:MET:HE1	2.01	0.41
1:I:36:THR:OG1	1:I:37:GLU:N	2.53	0.41
1:J:43:GLN:O	1:J:68:GLY:HA3	2.21	0.41
1:K:24:LEU:HD21	1:K:283:ARG:NH2	2.34	0.41
1:P:66:ARG:H	1:P:66:ARG:HG2	1.71	0.41
2:U:334:MET:HG3	2:U:335:PRO:CD	2.49	0.41
2:W:288:THR:O	2:W:292:MET:HG3	2.19	0.41
2:Z:105:ARG:NH2	2:a:495:ARG:HH21	2.19	0.41
2:Z:356:GLN:HG2	2:Z:370:TYR:OH	2.21	0.41
2:b:193:VAL:HG13	2:b:204:TYR:CE2	2.55	0.41
2:c:364:ALA:HA	2:d:375:ARG:HE	1.85	0.41
1:4:7:ALA:HB3	1:4:98:PRO:HG2	2.02	0.41
1:6:256:GLN:HA	1:6:265:ASN:HA	2.01	0.41
1:B:63:ILE:HB	1:F:82:HIS:CE1	2.56	0.41
1:D:115:ASN:O	1:D:119:GLU:OE1	2.38	0.41
1:D:274:LEU:HB2	1:D:336:VAL:HB	2.03	0.41
1:E:226:SER:HB3	1:E:246:GLY:H	1.85	0.41
1:F:108:ARG:NH1	1:F:317:GLU:OE1	2.53	0.41
1:J:36:THR:HG21	1:K:7:ALA:C	2.46	0.41
1:L:73:PHE:CD1	1:L:152:VAL:HG23	2.54	0.41
1:L:78:VAL:O	1:L:79:LYS:HG3	2.21	0.41
1:M:61:GLU:HG2	1:M:62:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:47:LEU:HD12	1:N:47:LEU:HA	1.88	0.41
1:P:162:ILE:HB	1:P:338:VAL:HG12	2.01	0.41
2:W:453:MET:HE2	2:W:453:MET:HB3	1.89	0.41
2:Z:386:ARG:HG2	2:a:455:ILE:O	2.21	0.41
2:a:29:SER:OG	2:a:33:GLY:HA2	2.21	0.41
1:3:201:ASP:CG	1:3:202:PRO:HD2	2.45	0.41
1:4:201:ASP:OD2	1:4:270:ASN:N	2.40	0.41
1:5:21:PRO:HA	1:5:128:GLU:OE2	2.21	0.41
1:6:38:LYS:HD3	1:6:72:GLU:HB2	2.02	0.41
1:7:13:ASN:HD22	1:F:331:ASP:HB3	1.86	0.41
1:7:55:SER:OG	1:R:147:PHE:HA	2.21	0.41
1:7:131:ALA:HB2	1:7:327:MET:HE2	2.02	0.41
1:7:196:ASN:C	1:7:248:VAL:HG23	2.45	0.41
1:A:41:LEU:HD12	1:A:73:PHE:HE2	1.86	0.41
1:C:77:TYR:OH	1:C:322:GLN:OE1	2.36	0.41
1:F:234:ASP:N	1:F:234:ASP:OD1	2.53	0.41
1:F:303:ARG:O	1:F:305:PRO:HD3	2.20	0.41
1:G:247:ASP:HB3	1:O:233:LYS:O	2.20	0.41
1:I:40:TYR:CE1	1:I:72:GLU:HB3	2.55	0.41
1:J:21:PRO:HB2	1:J:24:LEU:HB3	2.03	0.41
1:K:84:VAL:HG11	1:K:112:ILE:HD11	2.03	0.41
1:L:85:ASN:H	1:L:88:MET:HE2	1.85	0.41
1:N:23:PHE:HE2	1:N:135:VAL:HG11	1.86	0.41
1:N:35:THR:HA	1:N:287:CYS:SG	2.60	0.41
1:O:170:TRP:HB3	1:O:207:LEU:HD21	2.03	0.41
1:P:178:TYR:HB3	1:P:211:PHE:HE2	1.86	0.41
2:W:27:GLY:O	2:X:52:ASN:ND2	2.53	0.41
2:W:211:TYR:HB3	2:W:212:PRO:HD3	2.03	0.41
2:e:124:CYS:O	2:e:130:ARG:HA	2.20	0.41
2:f:61:ASP:HA	2:f:64:VAL:HG12	2.02	0.41
2:f:81:ILE:HG23	2:f:400:ARG:HB2	2.02	0.41
1:0:130:GLN:NE2	1:0:142:MET:SD	2.94	0.41
1:1:192:SER:HB3	1:1:333:ASP:O	2.20	0.41
1:1:245:TYR:HB3	1:1:250:ILE:HD11	2.02	0.41
1:2:36:THR:HG22	1:2:37:GLU:N	2.34	0.41
1:2:118:ASP:OD2	1:S:66:ARG:NE	2.49	0.41
1:A:36:THR:OG1	1:A:37:GLU:N	2.54	0.41
1:A:184:ILE:HD11	1:A:208:PHE:HE1	1.86	0.41
1:A:272:MET:HE2	1:A:272:MET:HB3	1.87	0.41
1:B:293:ALA:HB2	1:B:304:TYR:CE2	2.56	0.41
1:C:327:MET:HA	1:C:327:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:PRO:HG3	1:H:211:PHE:CD2	2.55	0.41
1:I:31:SER:HA	1:I:283:ARG:HB2	2.03	0.41
1:J:41:LEU:HD11	1:J:328:LEU:HD13	2.02	0.41
1:L:181:THR:HG21	1:L:217:LYS:NZ	2.36	0.41
1:P:287:CYS:HA	1:P:300:ALA:H	1.85	0.41
2:V:172:VAL:HG13	2:V:176:ARG:NH1	2.36	0.41
2:W:388:SER:HA	2:X:377:TYR:HE1	1.86	0.41
2:W:391:GLU:HG3	2:X:377:TYR:OH	2.20	0.41
2:X:65:ARG:O	2:X:66:ASN:ND2	2.52	0.41
2:Z:63:LEU:HD23	2:Z:63:LEU:HA	1.89	0.41
2:Z:428:PRO:HD2	2:Z:442:TRP:HH2	1.86	0.41
2:c:467:LEU:HD23	2:c:467:LEU:HA	1.88	0.41
2:c:475:TYR:HB2	2:d:496:GLU:CD	2.46	0.41
1:g:36:THR:OG1	1:g:37:GLU:N	2.54	0.41
1:1:6:THR:HG1	1:R:37:GLU:CD	2.29	0.41
1:5:121:LEU:HD12	1:5:121:LEU:HA	1.86	0.41
1:7:303:ARG:O	1:7:305:PRO:HD3	2.21	0.41
1:B:109:ARG:O	1:B:112:ILE:HG22	2.20	0.41
1:C:66:ARG:HH21	1:G:118:ASP:CG	2.29	0.41
1:D:143:THR:OG1	1:D:144:GLY:N	2.54	0.41
1:J:326:LEU:HD23	1:J:327:MET:N	2.36	0.41
1:L:178:TYR:OH	1:L:183:ASP:OD2	2.31	0.41
1:L:316:ARG:H	1:L:316:ARG:HG2	1.47	0.41
1:M:82:HIS:CD2	1:T:63:ILE:HB	2.56	0.41
1:T:42:SER:HA	1:T:70:THR:HA	2.03	0.41
1:T:232:VAL:HG13	1:T:235:LEU:HD21	2.03	0.41
2:U:324:ARG:HA	2:U:324:ARG:HD3	1.73	0.41
2:V:359:LEU:HA	2:V:359:LEU:HD23	1.85	0.41
2:V:490:PHE:O	2:V:494:VAL:HG13	2.20	0.41
2:W:386:ARG:HG2	2:X:455:ILE:O	2.21	0.41
2:X:295:ILE:O	2:X:331:PRO:HB3	2.20	0.41
2:c:393:TRP:CG	2:c:452:ARG:HH21	2.38	0.41
1:h:41:LEU:HA	1:h:41:LEU:HD23	1.78	0.41
1:h:77:TYR:CD1	1:h:324:ALA:HB2	2.55	0.41
1:0:218:LEU:HD13	1:Q:223:GLY:HA2	2.03	0.40
1:0:338:VAL:HG23	1:0:340:LEU:HD22	2.03	0.40
1:4:101:LEU:HD23	1:4:101:LEU:HA	1.88	0.40
1:5:191:ALA:HB2	1:5:336:VAL:HG23	2.02	0.40
1:B:201:ASP:CG	1:B:202:PRO:HD2	2.45	0.40
1:C:57:ILE:HG13	1:C:58:VAL:HG13	2.02	0.40
1:C:79:LYS:HB3	1:C:322:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ARG:HD2	1:C:327:MET:HE1	2.03	0.40
1:D:268:PRO:HG2	1:D:271:THR:OG1	2.21	0.40
1:F:77:TYR:CE2	1:F:79:LYS:HD2	2.51	0.40
2:W:44:SER:OG	2:W:45:VAL:N	2.54	0.40
2:X:455:ILE:H	2:X:455:ILE:HD12	1.86	0.40
2:Y:180:PRO:O	2:Y:183:THR:HG23	2.22	0.40
2:Y:435:PHE:HD1	2:Y:442:TRP:CD1	2.39	0.40
2:a:69:TYR:CE2	2:a:359:LEU:HD21	2.56	0.40
2:a:169:PHE:CD1	2:a:411:MET:HG2	2.56	0.40
1:2:86:PRO:HD3	1:N:291:ALA:HB2	2.03	0.40
1:3:80:PRO:HG2	1:3:119:GLU:HB2	2.03	0.40
1:6:45:PRO:HD3	1:6:68:GLY:HA2	2.03	0.40
1:6:82:HIS:O	1:6:318:PHE:HB2	2.21	0.40
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.97	0.40
1:D:113:MET:O	1:D:117:ARG:HG2	2.22	0.40
1:D:129:MET:HE3	1:D:133:SER:HB2	2.02	0.40
1:J:234:ASP:N	1:J:234:ASP:OD1	2.55	0.40
1:K:49:ASN:HA	1:L:258:VAL:HG23	2.03	0.40
1:N:180:PRO:O	1:N:184:ILE:HG13	2.21	0.40
1:N:239:VAL:HG12	1:N:253:TYR:HD1	1.85	0.40
1:O:30:GLU:OE2	1:O:280:ARG:NH2	2.53	0.40
1:O:91:ARG:HD2	1:O:92:ARG:H	1.86	0.40
1:R:274:LEU:HD23	1:R:274:LEU:H	1.87	0.40
2:V:358:LEU:HD23	2:V:358:LEU:HA	1.85	0.40
2:V:386:ARG:HG2	2:W:455:ILE:O	2.21	0.40
2:W:475:TYR:HB2	2:X:496:GLU:OE1	2.22	0.40
2:X:101:GLU:HB3	2:X:105:ARG:HH12	1.86	0.40
2:Z:358:LEU:HD23	2:Z:358:LEU:HA	1.92	0.40
2:Z:359:LEU:HD23	2:Z:359:LEU:HA	1.94	0.40
2:a:132:ARG:HA	2:a:136:MET:HE3	2.03	0.40
2:a:137:MET:HE3	2:a:137:MET:HB2	1.76	0.40
2:b:254:VAL:HG12	2:b:361:TYR:CE2	2.56	0.40
2:d:47:ALA:HA	2:e:211:TYR:CD1	2.57	0.40
1:1:77:TYR:HE2	1:1:289:GLN:HG2	1.87	0.40
1:4:134:ALA:HB2	1:4:140:TYR:CE2	2.56	0.40
1:4:237:LYS:HE3	1:4:237:LYS:HB2	1.94	0.40
1:6:19:PHE:CZ	1:6:128:GLU:HG3	2.57	0.40
1:6:201:ASP:HB3	1:6:267:LEU:HD22	2.04	0.40
1:C:180:PRO:HG3	1:C:211:PHE:CD2	2.50	0.40
1:O:36:THR:HG22	1:O:37:GLU:N	2.35	0.40
1:R:92:ARG:H	1:R:107:ARG:NH1	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:491:ALA:HA	2:V:494:VAL:HG22	2.03	0.40
2:X:94:TRP:CD1	2:X:94:TRP:H	2.38	0.40
2:Z:370:TYR:OH	2:Z:376:ASN:ND2	2.54	0.40
1:6:305:PRO:HB3	1:6:321:ILE:HG12	2.04	0.40
1:7:41:LEU:HD12	1:7:73:PHE:HE2	1.87	0.40
1:7:257:TYR:HB3	1:7:266:PHE:CE1	2.57	0.40
1:7:329:LEU:HD23	1:7:332:PRO:HA	2.03	0.40
1:H:108:ARG:NH1	1:H:317:GLU:OE1	2.54	0.40
1:K:42:SER:HB3	1:K:70:THR:HG23	2.02	0.40
1:M:112:ILE:HD13	1:M:112:ILE:HA	1.96	0.40
1:O:26:LEU:HD23	1:O:26:LEU:HA	1.94	0.40
1:R:40:TYR:HE1	1:R:72:GLU:HG2	1.86	0.40
2:U:206:VAL:HG21	2:U:222:ILE:HD12	2.03	0.40
2:X:204:TYR:CD1	2:X:233:PHE:HD2	2.39	0.40
2:X:378:ALA:O	2:X:380:MET:HG2	2.22	0.40
2:Y:356:GLN:HE21	2:Y:376:ASN:HD21	1.70	0.40
2:c:63:LEU:HD13	2:c:258:MET:HE3	2.03	0.40
2:f:195:ILE:HD11	2:f:245:THR:HG22	2.03	0.40
1:2:154:MET:HB3	1:2:332:PRO:HG3	2.03	0.40
1:5:165:SER:OG	1:5:166:GLY:N	2.53	0.40
1:A:51:ALA:HB3	1:E:126:VAL:HG21	2.04	0.40
1:D:218:LEU:HD13	1:N:223:GLY:HA2	2.04	0.40
1:K:74:THR:HA	1:K:75:PRO:HD3	1.86	0.40
1:P:80:PRO:HD2	1:P:321:ILE:O	2.21	0.40
1:P:198:ILE:HG12	1:P:274:LEU:HD13	2.04	0.40
1:R:22:LEU:HD13	1:R:239:VAL:HG21	2.04	0.40
1:T:200:PHE:CD2	1:T:205:TRP:HE3	2.39	0.40
2:W:158:ASP:OD1	2:W:158:ASP:N	2.55	0.40
2:a:386:ARG:HG2	2:b:455:ILE:O	2.22	0.40
2:b:277:MET:CE	2:c:325:LEU:HD12	2.51	0.40
2:e:125:CYS:SG	2:e:163:ARG:NH2	2.94	0.40
2:e:324:ARG:HD3	2:e:324:ARG:HA	1.93	0.40
2:f:397:MET:HE1	2:f:400:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	338/341 (99%)	315 (93%)	22 (6%)	1 (0%)	36	70
1	1	338/341 (99%)	318 (94%)	18 (5%)	2 (1%)	21	57
1	2	338/341 (99%)	312 (92%)	23 (7%)	3 (1%)	14	48
1	3	335/341 (98%)	302 (90%)	31 (9%)	2 (1%)	21	57
1	4	335/341 (98%)	303 (90%)	31 (9%)	1 (0%)	36	70
1	5	335/341 (98%)	305 (91%)	28 (8%)	2 (1%)	21	57
1	6	338/341 (99%)	311 (92%)	25 (7%)	2 (1%)	21	57
1	7	338/341 (99%)	313 (93%)	23 (7%)	2 (1%)	21	57
1	A	338/341 (99%)	320 (95%)	17 (5%)	1 (0%)	36	70
1	B	338/341 (99%)	321 (95%)	17 (5%)	0	100	100
1	C	338/341 (99%)	317 (94%)	20 (6%)	1 (0%)	36	70
1	D	338/341 (99%)	318 (94%)	19 (6%)	1 (0%)	36	70
1	E	338/341 (99%)	320 (95%)	18 (5%)	0	100	100
1	F	338/341 (99%)	318 (94%)	20 (6%)	0	100	100
1	G	338/341 (99%)	318 (94%)	20 (6%)	0	100	100
1	H	338/341 (99%)	318 (94%)	20 (6%)	0	100	100
1	I	322/341 (94%)	302 (94%)	19 (6%)	1 (0%)	36	70
1	J	338/341 (99%)	320 (95%)	18 (5%)	0	100	100
1	K	338/341 (99%)	313 (93%)	23 (7%)	2 (1%)	21	57
1	L	338/341 (99%)	313 (93%)	24 (7%)	1 (0%)	36	70
1	M	338/341 (99%)	311 (92%)	26 (8%)	1 (0%)	36	70
1	N	335/341 (98%)	306 (91%)	27 (8%)	2 (1%)	21	57
1	O	338/341 (99%)	315 (93%)	20 (6%)	3 (1%)	14	48
1	P	338/341 (99%)	308 (91%)	28 (8%)	2 (1%)	21	57
1	Q	338/341 (99%)	316 (94%)	21 (6%)	1 (0%)	36	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	338/341 (99%)	314 (93%)	22 (6%)	2 (1%)	21	57
1	S	338/341 (99%)	308 (91%)	28 (8%)	2 (1%)	21	57
1	T	338/341 (99%)	313 (93%)	23 (7%)	2 (1%)	21	57
1	g	338/341 (99%)	315 (93%)	22 (6%)	1 (0%)	36	70
1	h	335/341 (98%)	304 (91%)	28 (8%)	3 (1%)	14	48
2	U	453/533 (85%)	438 (97%)	15 (3%)	0	100	100
2	V	468/533 (88%)	449 (96%)	19 (4%)	0	100	100
2	W	468/533 (88%)	449 (96%)	19 (4%)	0	100	100
2	X	468/533 (88%)	444 (95%)	24 (5%)	0	100	100
2	Y	468/533 (88%)	448 (96%)	20 (4%)	0	100	100
2	Z	468/533 (88%)	453 (97%)	14 (3%)	1 (0%)	43	75
2	a	472/533 (89%)	455 (96%)	16 (3%)	1 (0%)	43	75
2	b	468/533 (88%)	451 (96%)	17 (4%)	0	100	100
2	c	468/533 (88%)	449 (96%)	17 (4%)	2 (0%)	30	65
2	d	468/533 (88%)	452 (97%)	16 (3%)	0	100	100
2	e	468/533 (88%)	450 (96%)	18 (4%)	0	100	100
2	f	468/533 (88%)	450 (96%)	18 (4%)	0	100	100
All	All	15714/16626 (94%)	14775 (94%)	894 (6%)	45 (0%)	37	70

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	334	GLU
1	4	316	ARG
1	5	316	ARG
1	C	316	ARG
1	L	262	VAL
1	N	316	ARG
1	O	177	THR
1	Q	262	VAL
1	R	262	VAL
1	R	313	ASP
1	S	262	VAL
1	S	313	ASP
1	T	262	VAL
1	h	316	ARG

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Mol	Chain	Res	Type
1	1	157	SER
1	3	316	ARG
1	7	325	PRO
1	P	325	PRO
1	T	92	ARG
2	c	164	LEU
1	0	262	VAL
1	5	100	ASN
1	6	325	PRO
1	K	325	PRO
1	N	100	ASN
2	c	217	GLN
1	A	314	PRO
1	I	314	PRO
1	g	157	SER
1	h	100	ASN
1	1	262	VAL
1	2	262	VAL
1	M	262	VAL
1	O	325	PRO
2	a	301	GLN
1	h	315	ALA
1	2	157	SER
1	3	100	ASN
1	7	201	ASP
1	K	201	ASP
1	6	201	ASP
1	O	201	ASP
1	P	201	ASP
2	Z	215	MET
1	D	314	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	1	289/290 (100%)	289 (100%)	0	100	100
1	2	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	3	286/290 (99%)	286 (100%)	0	100	100
1	4	286/290 (99%)	286 (100%)	0	100	100
1	5	286/290 (99%)	286 (100%)	0	100	100
1	6	289/290 (100%)	289 (100%)	0	100	100
1	7	289/290 (100%)	287 (99%)	2 (1%)	76	79
1	A	289/290 (100%)	289 (100%)	0	100	100
1	B	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	C	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	D	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	E	289/290 (100%)	289 (100%)	0	100	100
1	F	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	G	289/290 (100%)	289 (100%)	0	100	100
1	H	289/290 (100%)	289 (100%)	0	100	100
1	I	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	J	289/290 (100%)	289 (100%)	0	100	100
1	K	289/290 (100%)	289 (100%)	0	100	100
1	L	289/290 (100%)	287 (99%)	2 (1%)	76	79
1	M	289/290 (100%)	287 (99%)	2 (1%)	76	79
1	N	286/290 (99%)	284 (99%)	2 (1%)	76	79
1	O	289/290 (100%)	287 (99%)	2 (1%)	76	79
1	P	289/290 (100%)	289 (100%)	0	100	100
1	Q	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	R	289/290 (100%)	289 (100%)	0	100	100
1	S	289/290 (100%)	288 (100%)	1 (0%)	86	85
1	T	289/290 (100%)	286 (99%)	3 (1%)	68	76
1	g	289/290 (100%)	286 (99%)	3 (1%)	68	76
1	h	286/290 (99%)	286 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	377/428 (88%)	377 (100%)	0	100	100
2	V	380/428 (89%)	377 (99%)	3 (1%)	73	77
2	W	380/428 (89%)	380 (100%)	0	100	100
2	X	380/428 (89%)	379 (100%)	1 (0%)	86	85
2	Y	380/428 (89%)	380 (100%)	0	100	100
2	Z	380/428 (89%)	380 (100%)	0	100	100
2	a	383/428 (90%)	383 (100%)	0	100	100
2	b	380/428 (89%)	378 (100%)	2 (0%)	81	82
2	c	380/428 (89%)	380 (100%)	0	100	100
2	d	380/428 (89%)	379 (100%)	1 (0%)	86	85
2	e	380/428 (89%)	380 (100%)	0	100	100
2	f	380/428 (89%)	380 (100%)	0	100	100
All	All	13215/13836 (96%)	13183 (100%)	32 (0%)	85	87

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	36	THR
1	2	333	ASP
1	7	199	VAL
1	7	201	ASP
1	B	13	ASN
1	C	310	THR
1	D	310	THR
1	F	201	ASP
1	I	148	ASP
1	L	93	LEU
1	L	201	ASP
1	M	333	ASP
1	M	334	GLU
1	N	103	ASP
1	N	296	GLU
1	O	119	GLU
1	O	328	LEU
1	Q	90	LEU
1	S	309	VAL
1	T	91	ARG
1	T	96	GLU

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Mol	Chain	Res	Type
1	T	311	THR
2	V	178	SER
2	V	179	ASN
2	V	183	THR
2	X	72	ASN
2	b	156	THR
2	b	161	SER
2	d	167	THR
1	g	128	GLU
1	g	258	VAL
1	g	262	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	125	GLN
1	0	164	GLN
1	0	196	ASN
1	0	294	GLN
1	1	256	GLN
1	1	270	ASN
1	1	289	GLN
1	2	43	GLN
1	2	256	GLN
1	2	270	ASN
1	3	190	ASN
1	3	289	GLN
1	3	339	GLN
1	4	289	GLN
1	4	294	GLN
1	4	339	GLN
1	5	8	GLN
1	5	13	ASN
1	5	289	GLN
1	5	294	GLN
1	5	299	ASN
1	6	164	GLN
1	7	130	GLN
1	A	130	GLN
1	A	289	GLN
1	B	87	GLN
1	B	115	ASN

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Mol	Chain	Res	Type
1	C	100	ASN
1	D	161	ASN
1	E	278	GLN
1	F	164	GLN
1	F	265	ASN
1	F	299	ASN
1	G	82	HIS
1	H	43	GLN
1	H	125	GLN
1	I	160	ASN
1	I	289	GLN
1	J	115	ASN
1	J	130	GLN
1	K	8	GLN
1	K	130	GLN
1	K	190	ASN
1	L	115	ASN
1	L	130	GLN
1	M	8	GLN
1	M	190	ASN
1	M	307	ASN
1	N	82	HIS
1	N	115	ASN
1	N	339	GLN
1	O	8	GLN
1	O	82	HIS
1	O	87	GLN
1	O	130	GLN
1	Q	125	GLN
1	Q	161	ASN
1	Q	256	GLN
1	R	99	GLN
1	R	270	ASN
1	R	289	GLN
1	R	339	GLN
1	S	299	ASN
1	T	161	ASN
1	T	190	ASN
2	U	77	HIS
2	U	356	GLN
2	V	217	GLN
2	V	235	HIS

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Mol	Chain	Res	Type
2	W	39	ASN
2	W	194	GLN
2	W	345	GLN
2	W	376	ASN
2	X	77	HIS
2	X	196	ASN
2	Y	332	HIS
2	Y	345	GLN
2	Y	376	ASN
2	Z	179	ASN
2	Z	182	ASN
2	a	436	GLN
2	a	487	GLN
2	b	66	ASN
2	b	145	HIS
2	b	196	ASN
2	b	235	HIS
2	c	145	HIS
2	c	244	GLN
2	d	356	GLN
2	e	39	ASN
2	e	244	GLN
2	e	270	GLN
2	e	289	GLN
2	e	299	ASN
2	e	376	ASN
2	e	407	GLN
2	f	181	ASN
2	f	244	GLN
1	g	130	GLN
1	g	160	ASN
1	g	164	GLN
1	g	307	ASN
1	h	87	GLN
1	h	99	GLN
1	h	190	ASN
1	h	299	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

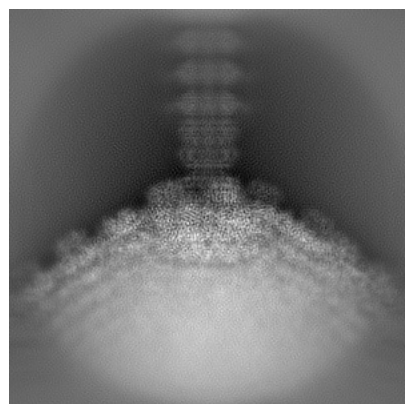
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36848. These allow visual inspection of the internal detail of the map and identification of artifacts.

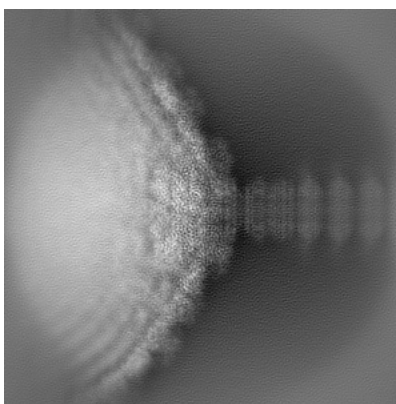
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

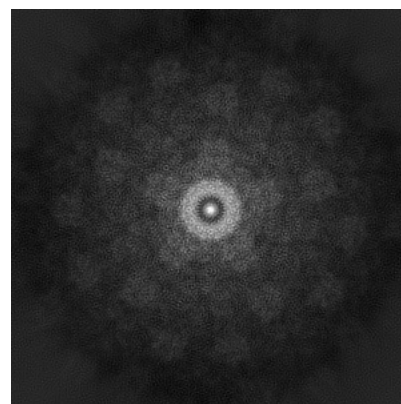
6.1.1 Primary map



X

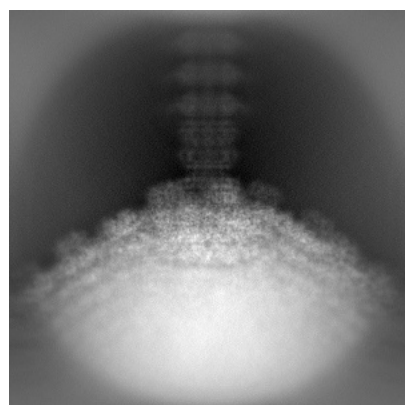


Y

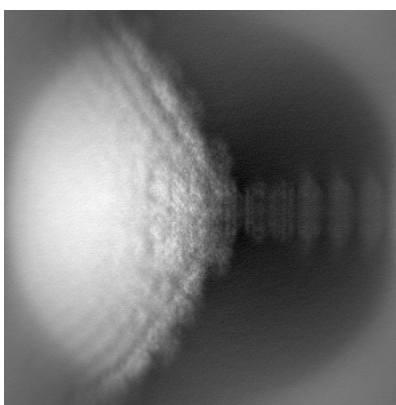


Z

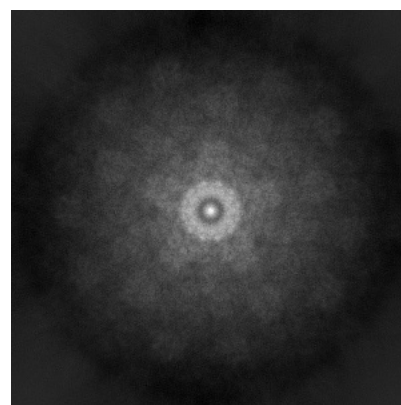
6.1.2 Raw map



X



Y

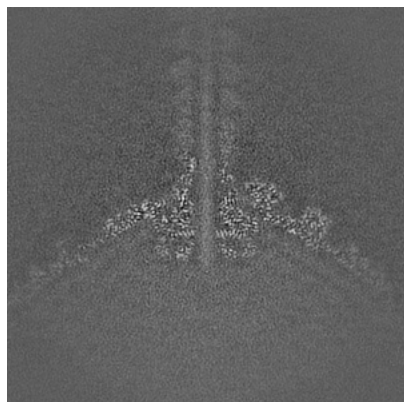


Z

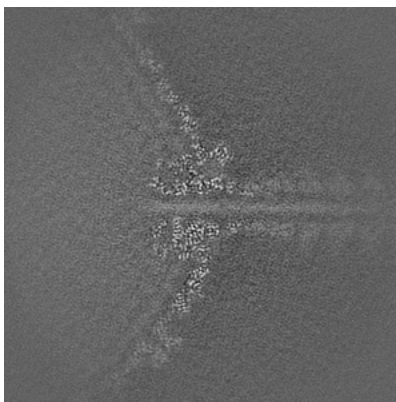
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

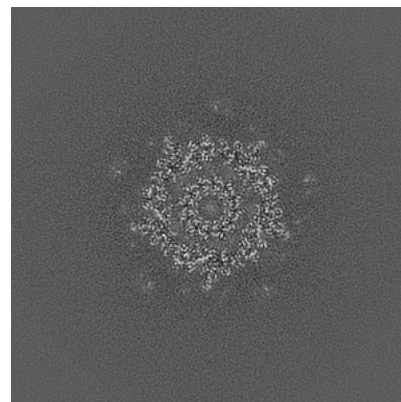
6.2.1 Primary map



X Index: 200

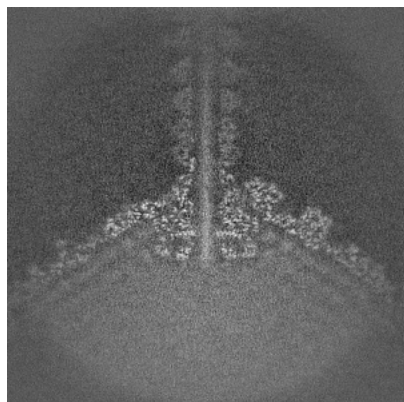


Y Index: 200

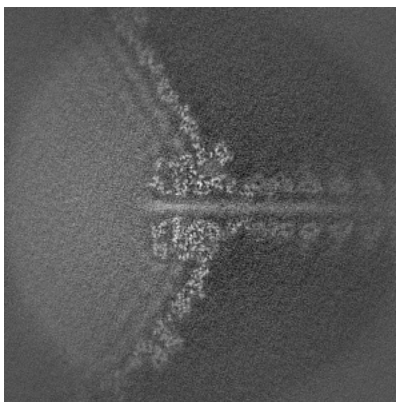


Z Index: 200

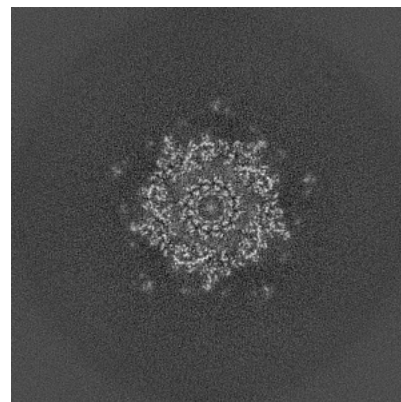
6.2.2 Raw map



X Index: 200



Y Index: 200

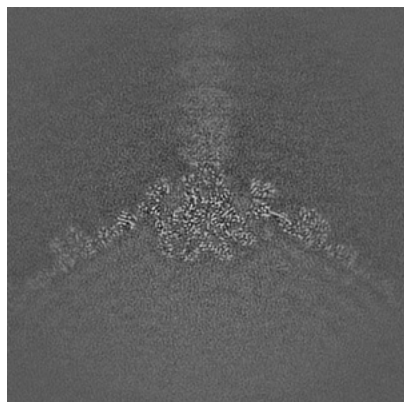


Z Index: 200

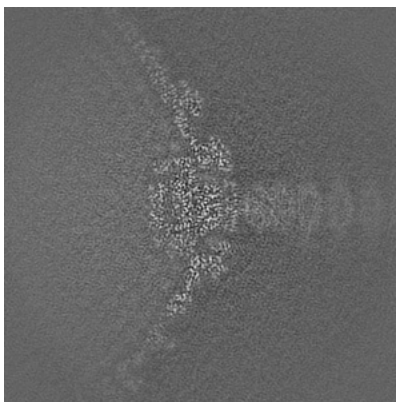
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

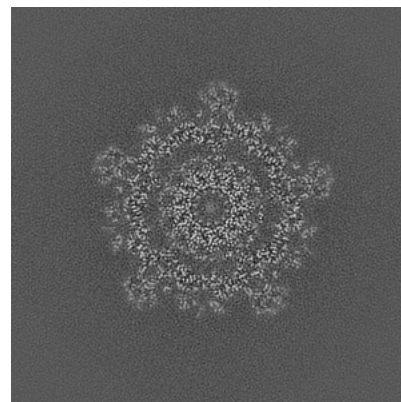
6.3.1 Primary map



X Index: 216

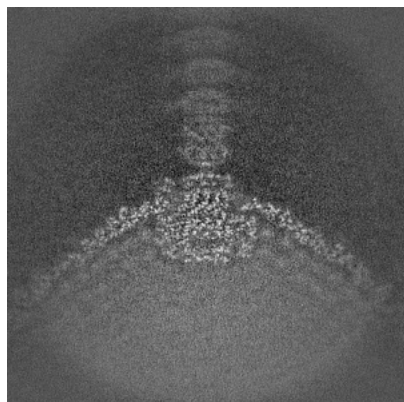


Y Index: 219

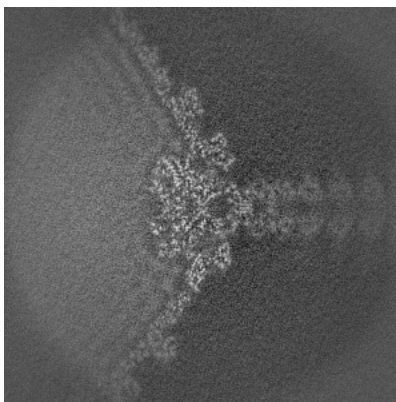


Z Index: 186

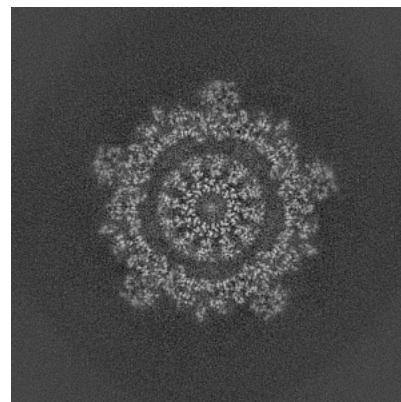
6.3.2 Raw map



X Index: 179



Y Index: 212

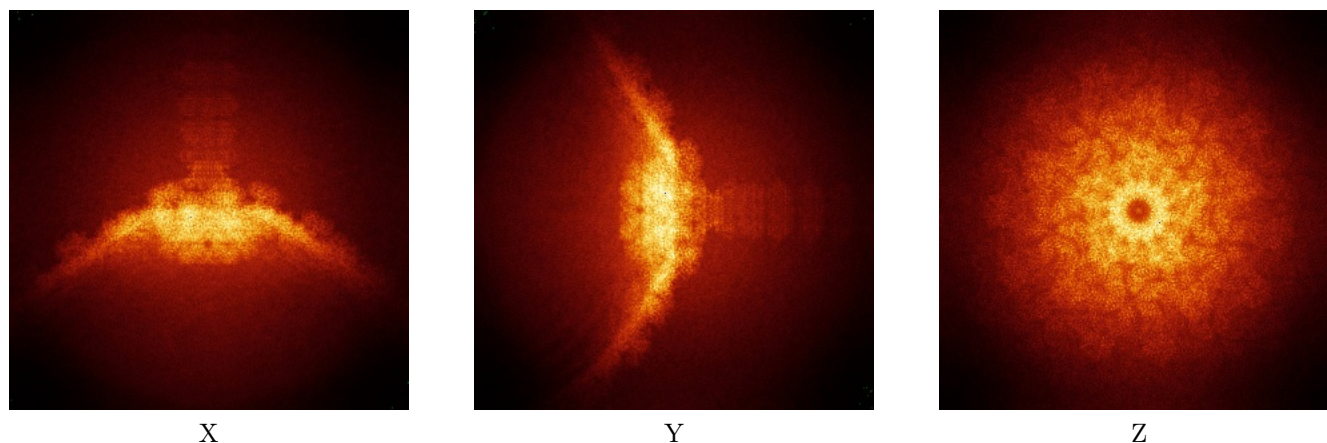


Z Index: 182

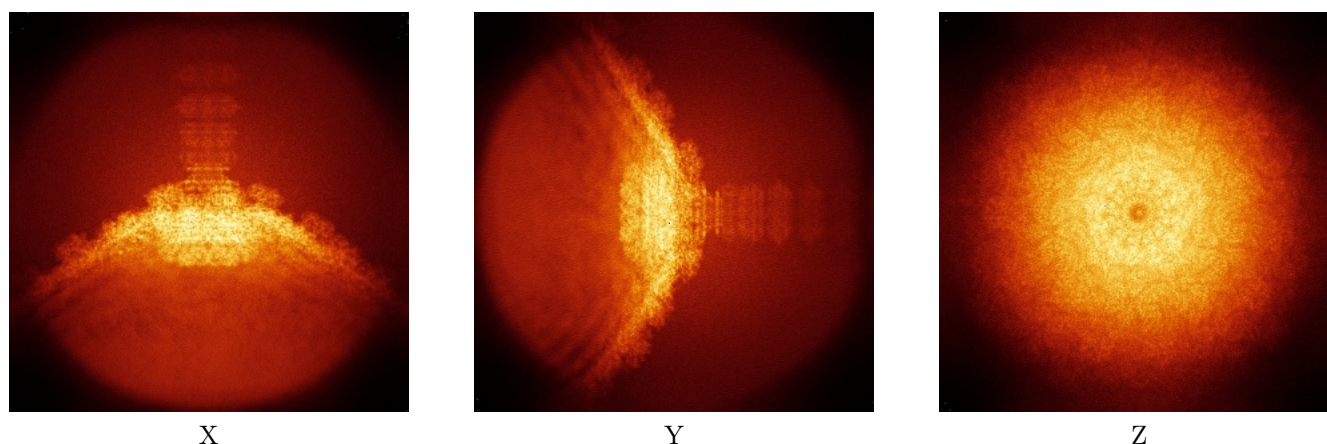
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

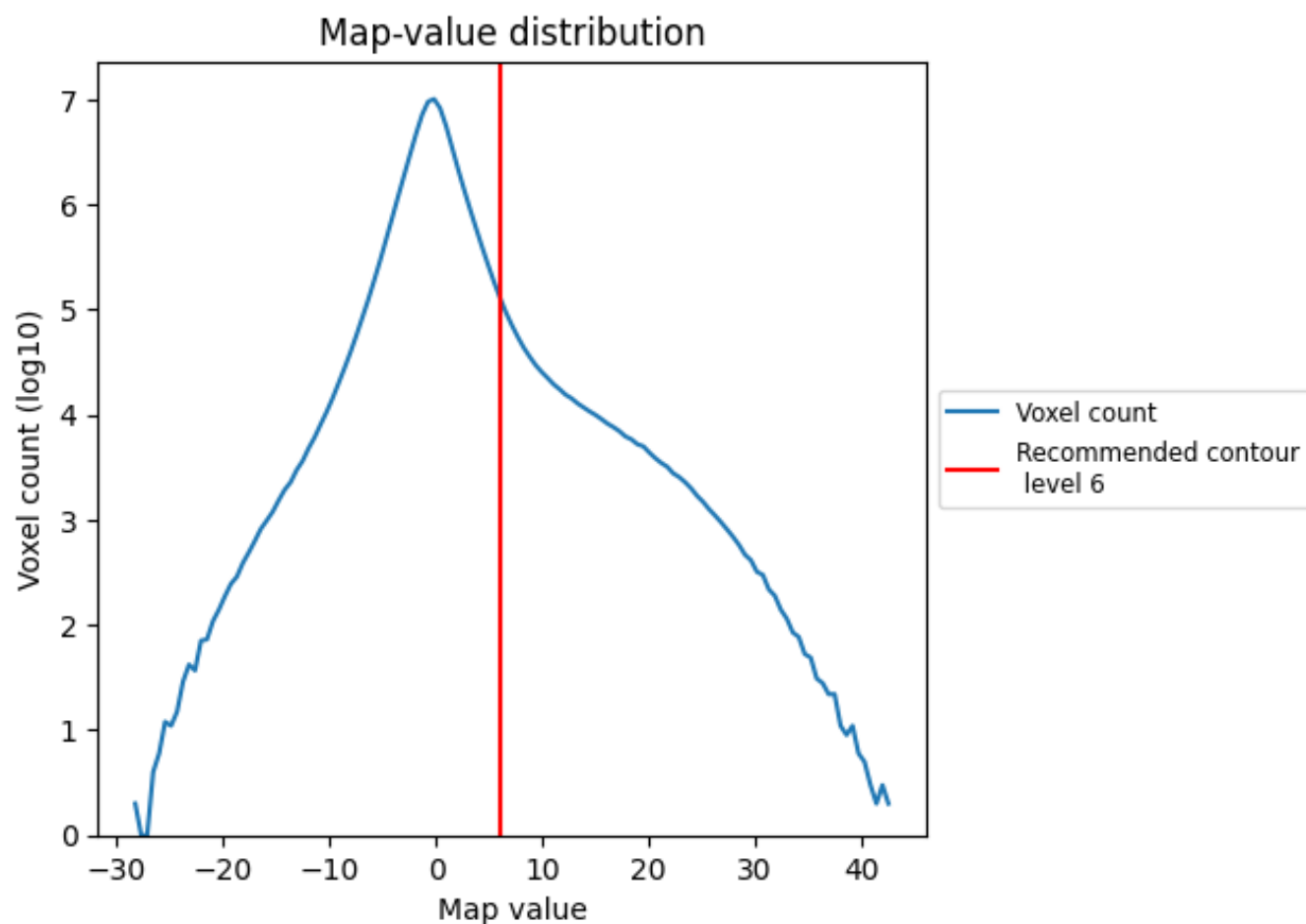
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

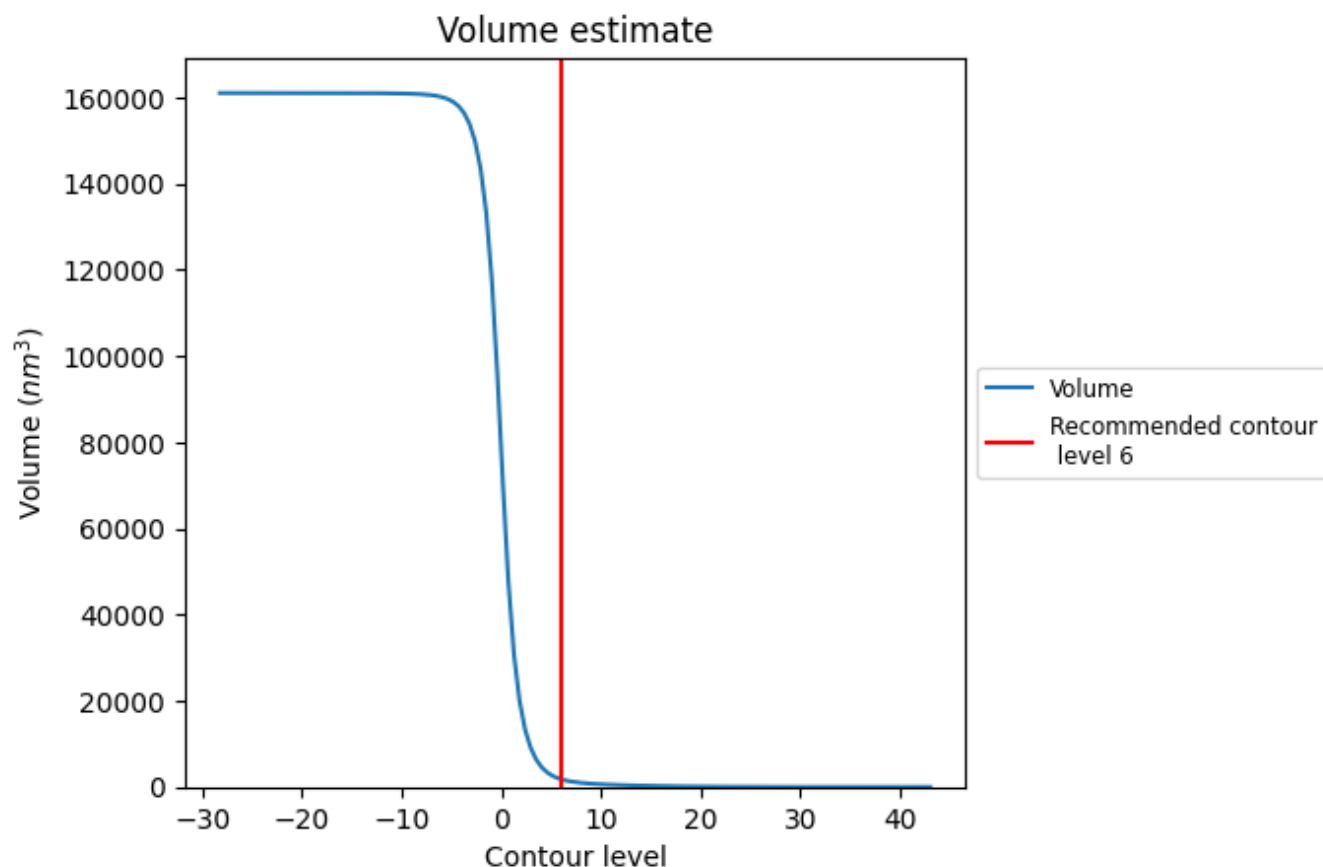
This section contains the results of statistical analysis of the map.

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.

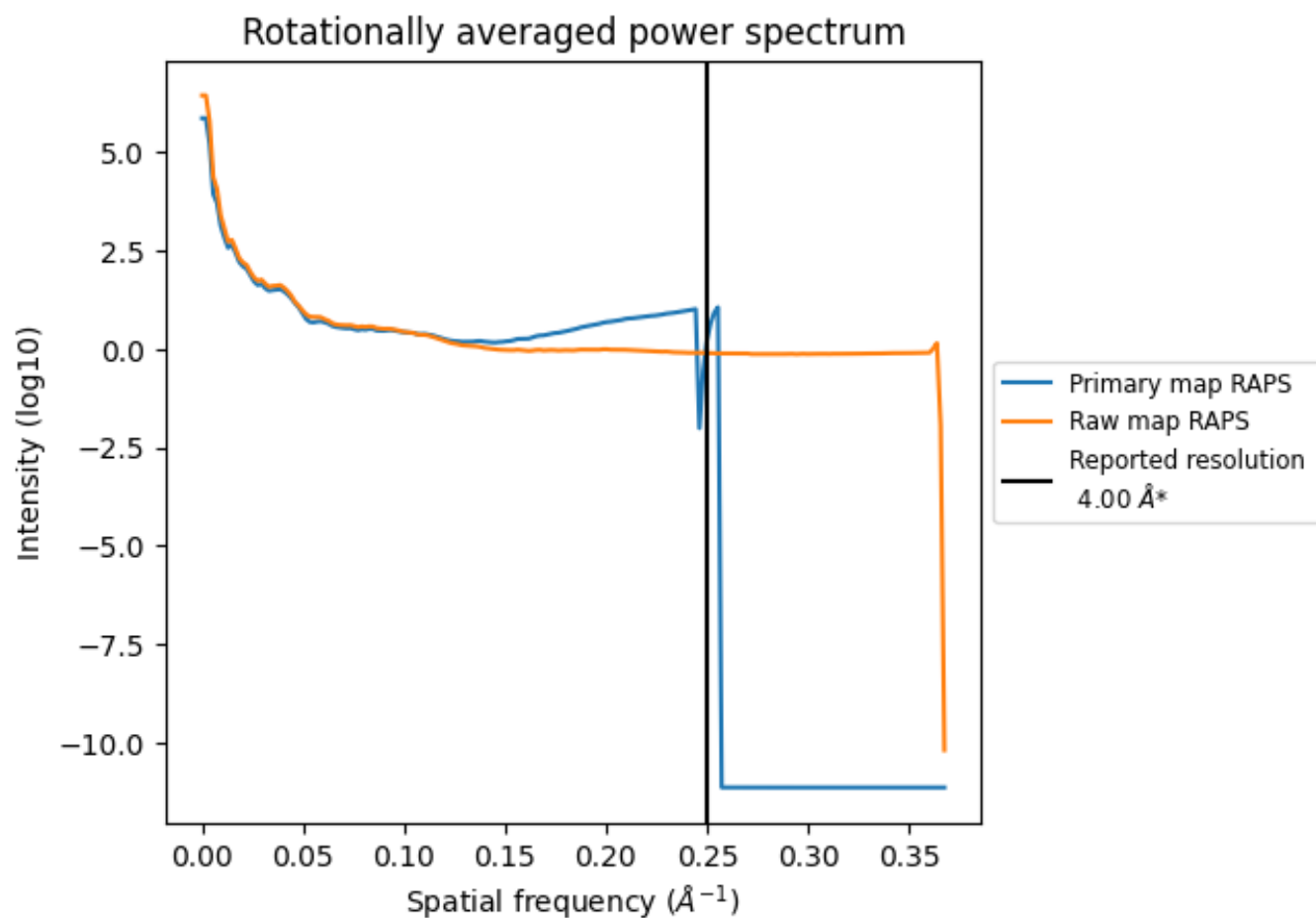
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1805 nm³; this corresponds to an approximate mass of 1631 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 ⓘ

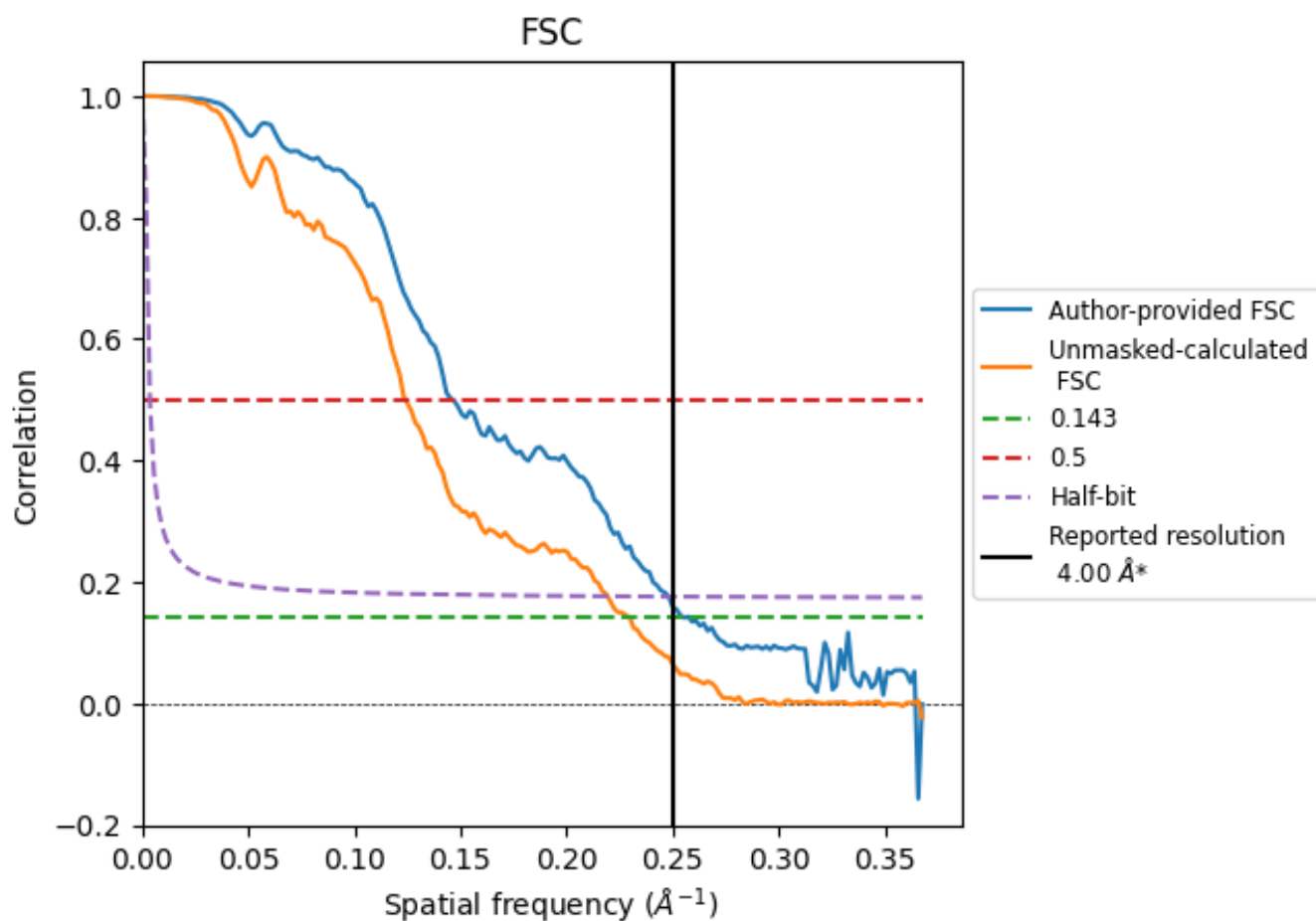


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

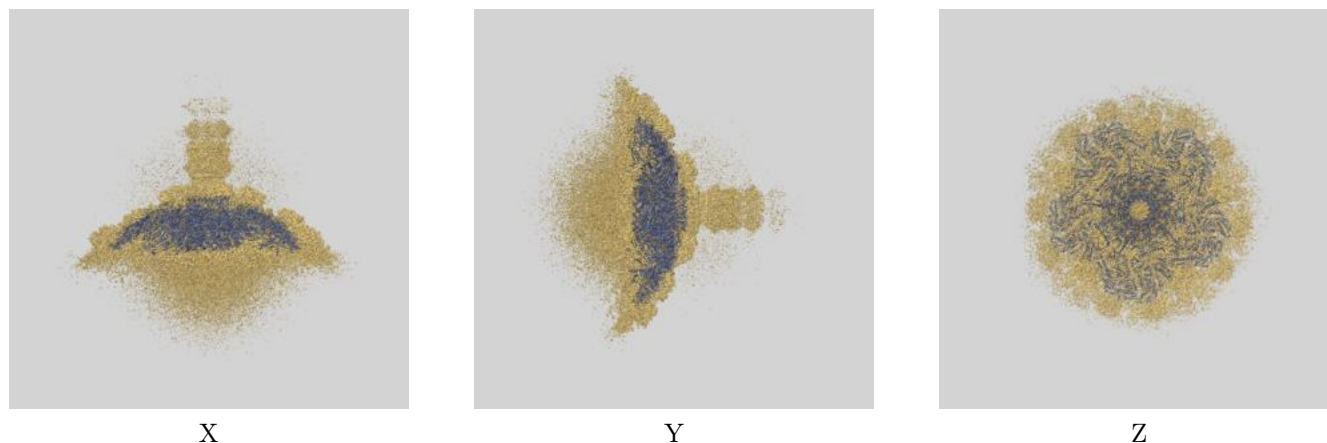
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.93	6.84	4.03
Unmasked-calculated*	4.37	8.06	4.56

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

9 Map-model fit [i](#)

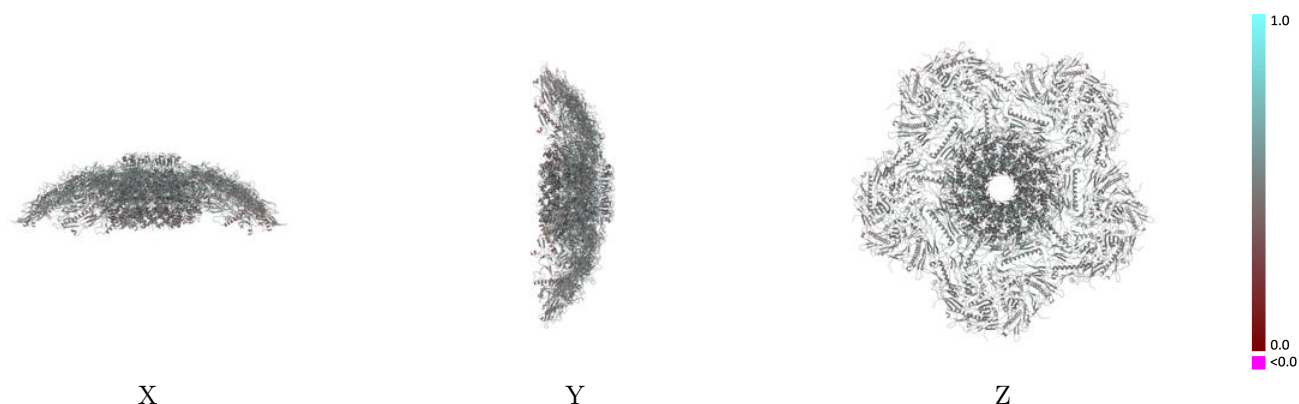
This section contains information regarding the fit between EMDB map EMD-36848 and PDB model 8K39. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



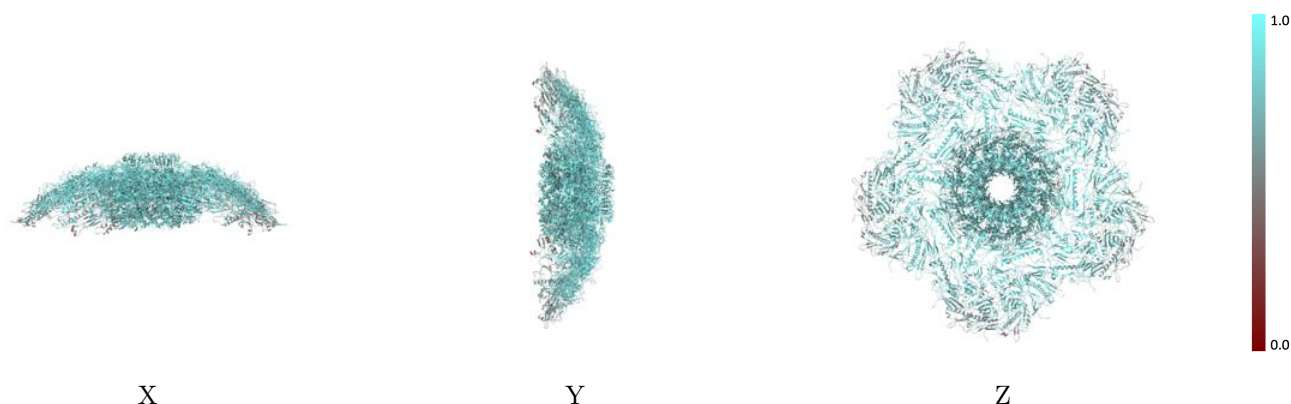
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



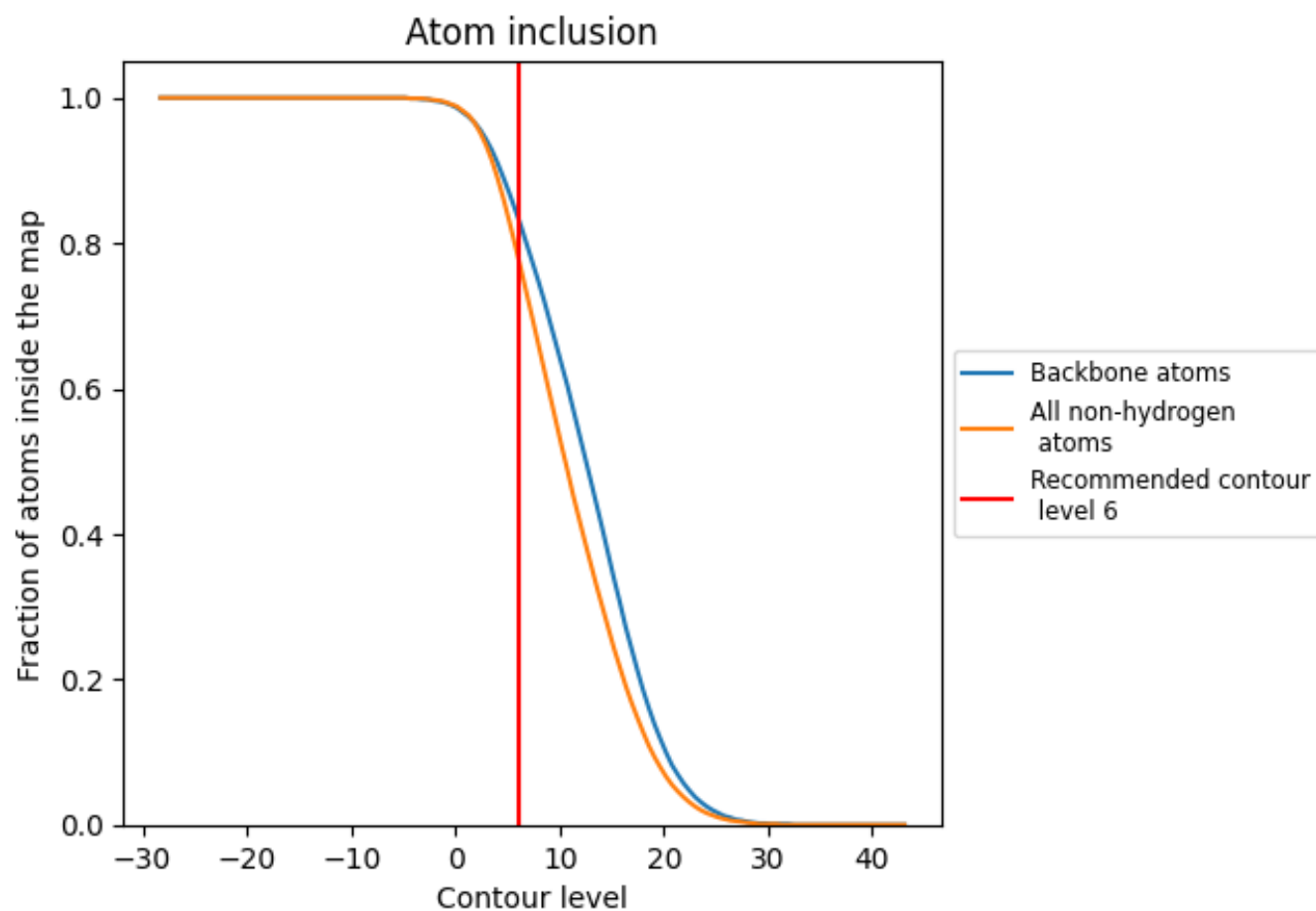
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.4900
0	 0.8470	 0.5080
1	 0.8330	 0.5030
2	 0.8360	 0.5030
3	 0.8340	 0.5030
4	 0.8320	 0.5040
5	 0.8220	 0.4970
6	 0.6990	 0.4810
7	 0.6870	 0.4720
A	 0.7760	 0.4930
B	 0.7730	 0.4950
C	 0.7670	 0.4930
D	 0.7660	 0.4920
E	 0.6500	 0.4740
F	 0.6440	 0.4690
G	 0.6410	 0.4690
H	 0.6370	 0.4690
I	 0.7740	 0.4900
J	 0.6500	 0.4680
K	 0.6920	 0.4780
L	 0.8020	 0.4930
M	 0.8390	 0.5080
N	 0.8270	 0.5010
O	 0.6940	 0.4750
P	 0.6870	 0.4780
Q	 0.8060	 0.4910
R	 0.8050	 0.4900
S	 0.8100	 0.4940
T	 0.8020	 0.4930
U	 0.8140	 0.4930
V	 0.8100	 0.4870
W	 0.8120	 0.4880
X	 0.8180	 0.4960
Y	 0.8220	 0.4940
Z	 0.8220	 0.4940



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Chain	Atom inclusion	Q-score
a	 0.8190	 0.4870
b	 0.8190	 0.4890
c	 0.8120	 0.4860
d	 0.8140	 0.4880
e	 0.8090	 0.4860
f	 0.8110	 0.4880
g	 0.8330	 0.5030
h	 0.8410	 0.5050