



Full wwPDB EM Validation Report ⓘ

Oct 14, 2025 – 05:00 PM JST

PDB ID : 8Z5Y / pdb_00008z5y
EMDB ID : EMD-39788
Title : Cryo-EM structure of the L-hook of the polar flagellum
Authors : Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2024-04-18
Resolution : 3.22 Å(reported)
Based on initial model : .

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:

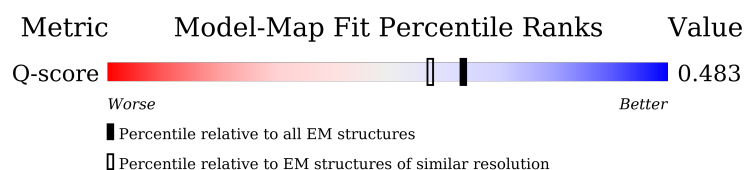
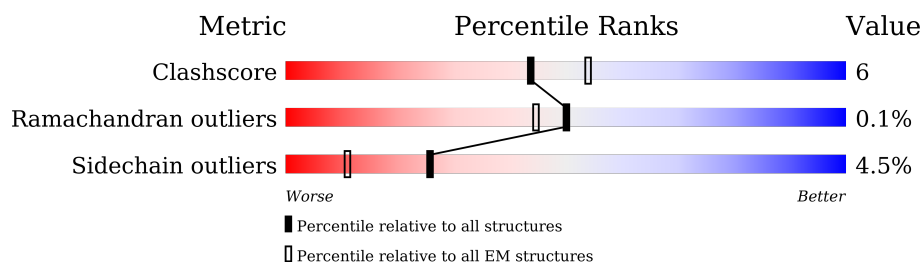
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance

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

The reported resolution of this entry is 3.22 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.









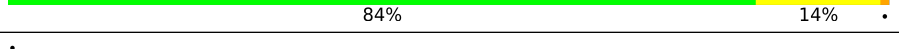
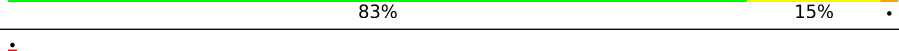
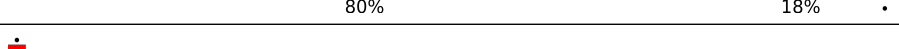
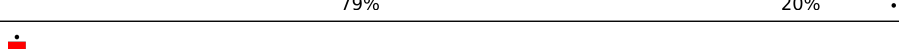
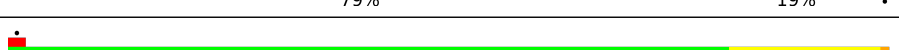

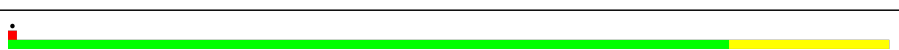

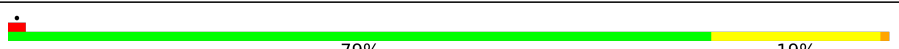





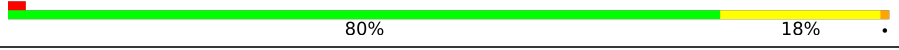
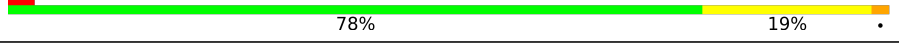



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14612 (2.72 - 3.72)

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	D	437	
1	E	437	
1	F	437	
1	G	437	







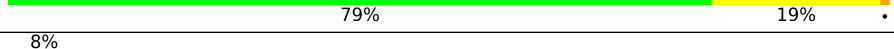
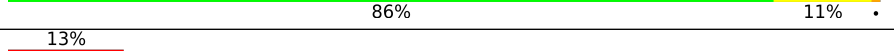
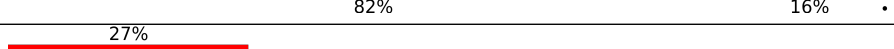
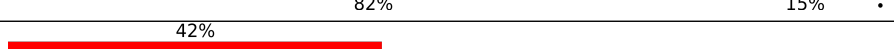
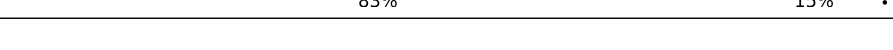
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Mol	Chain	Length	Quality of chain
1	H	437	
1	I	437	
1	J	437	
1	K	437	
1	L	437	
1	M	437	
1	N	437	
1	O	437	
1	P	437	
1	Q	437	
1	R	437	
1	S	437	
1	T	437	
1	U	437	
1	V	437	
1	W	437	
1	X	437	
1	Y	437	
1	Z	437	
1	a	437	
1	b	437	
1	c	437	
1	d	437	
1	e	437	
1	f	437	

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Mol	Chain	Length	Quality of chain
1	g	437	 83% 14%
1	h	437	 81% 17%
1	i	437	 83% 15%
1	j	437	 78% 19%
1	k	437	 82% 16%
1	l	437	 82% 16%
1	m	437	 79% 19%
1	n	437	 86% 11%
1	o	437	 82% 16%
1	p	437	 82% 15%
1	q	437	 83% 15%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 132760 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 Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	E	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	F	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	G	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	H	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	I	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	J	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	K	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	L	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	M	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	N	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	O	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	P	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	Q	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	R	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	S	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		
1	T	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	V	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	W	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	X	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	Y	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	Z	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	a	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	b	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	c	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	d	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	e	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	f	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	g	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	h	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	i	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	j	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	k	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	l	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	m	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	n	435	Total 3319	C 2052	N 563	O 696	S 8	0	0
1	o	435	Total 3319	C 2052	N 563	O 696	S 8	0	0

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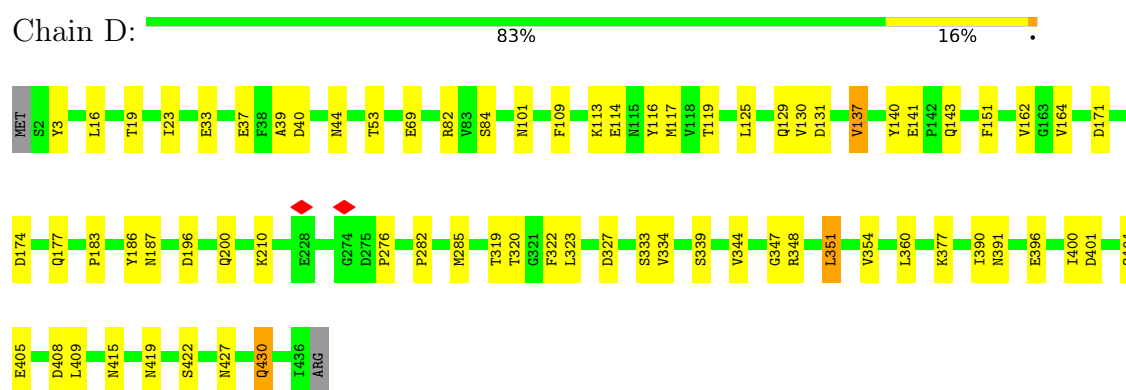
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	435	Total	C	N	O	S	0	0
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1	q	435	Total	C	N	O	S	0	0
			3319	2052	563	696	8		

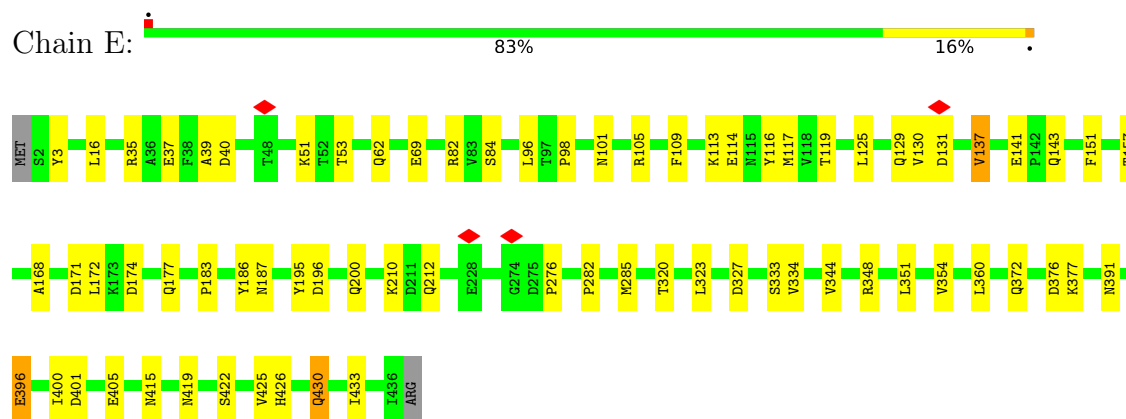
3 Residue-property plots

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.

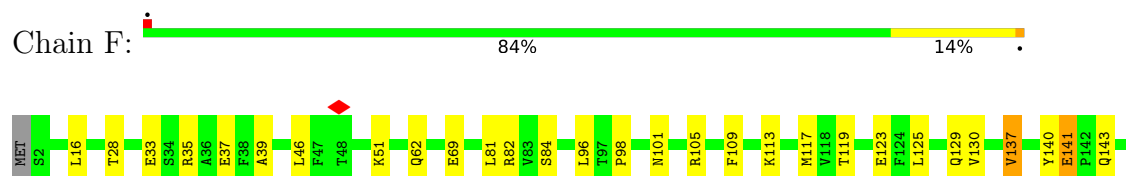
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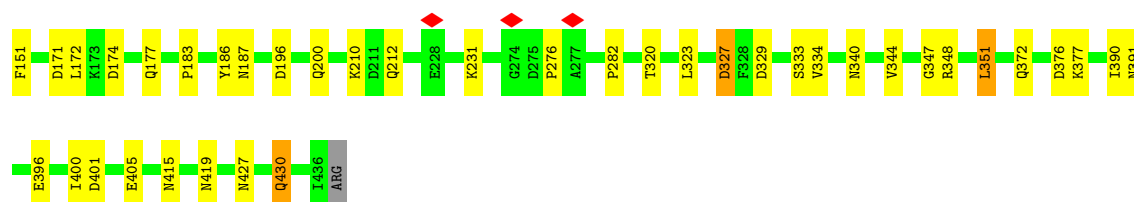


• Molecule 1: Flagellar hook protein FlgE



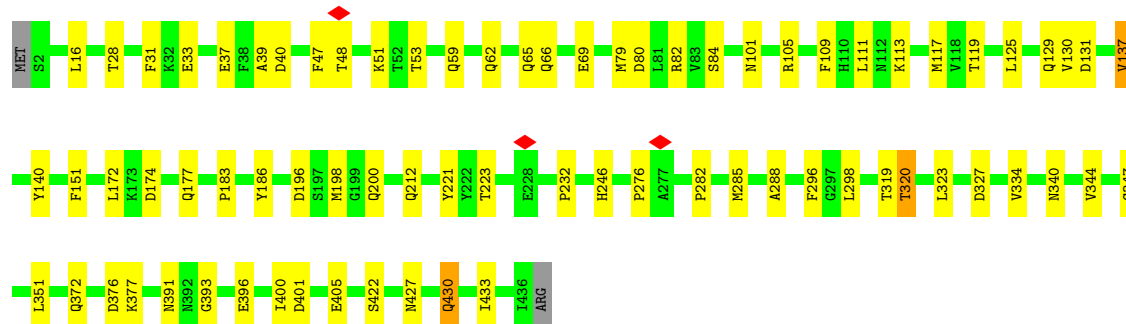
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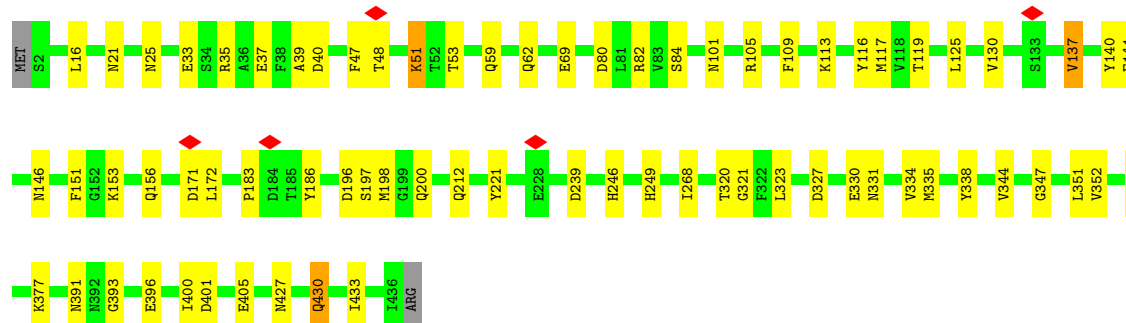
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Chain G: 82% 16%



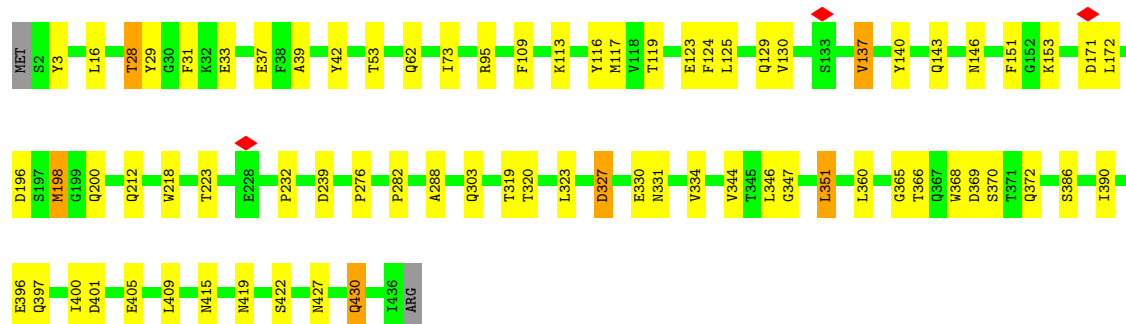
• Molecule 1: Flagellar hook protein FlgE

Chain H: 83% 16%

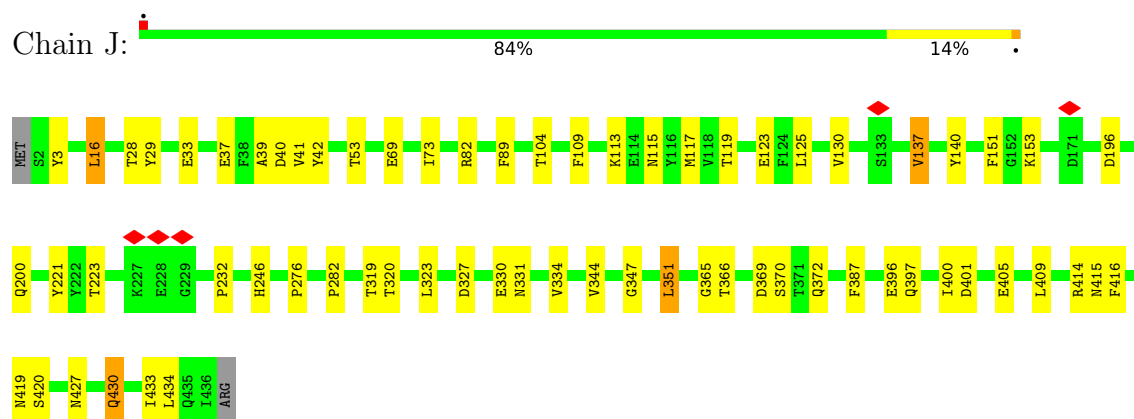


• Molecule 1: Flagellar hook protein FlgE

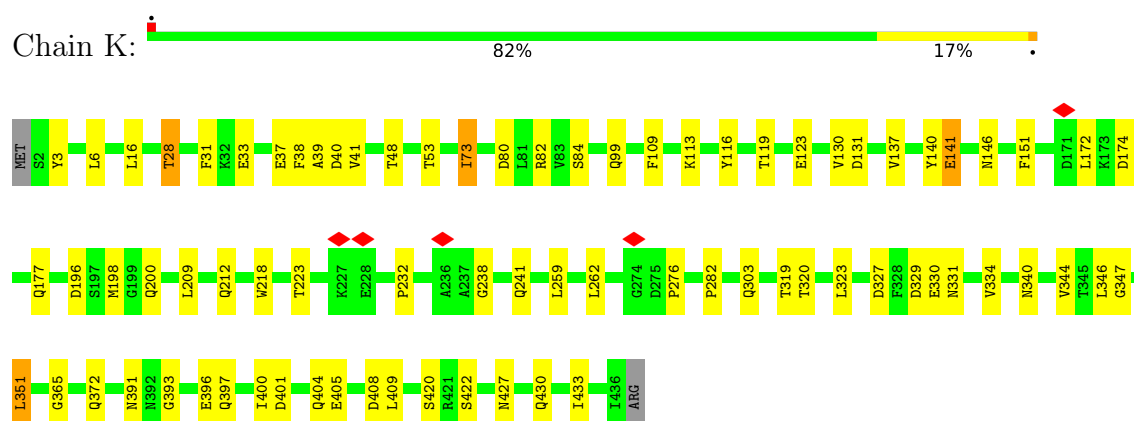
Chain I: 83% 16%



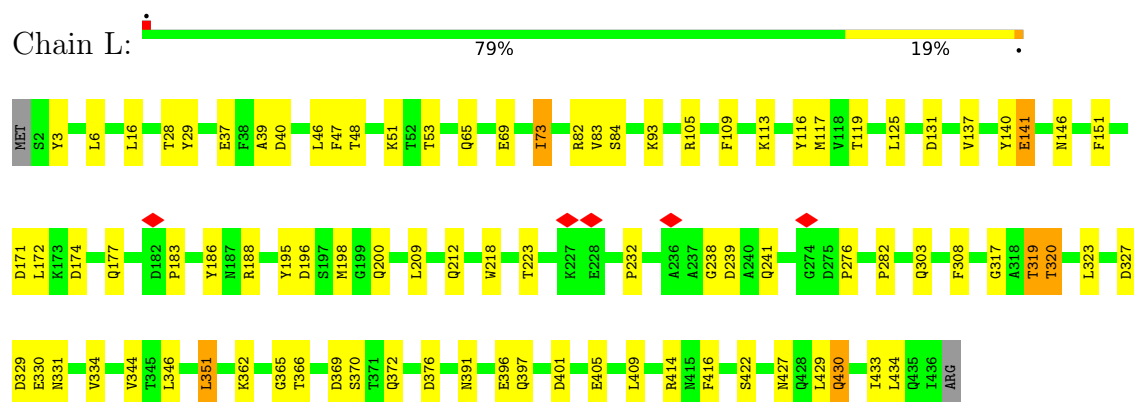
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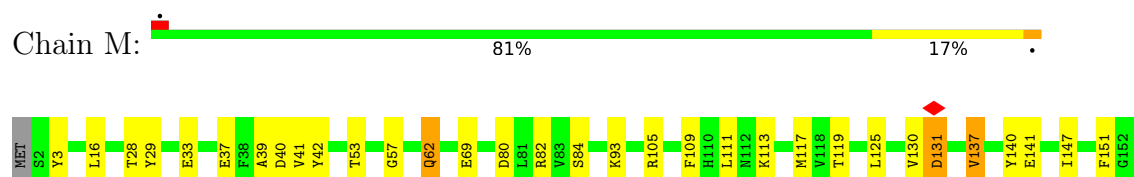
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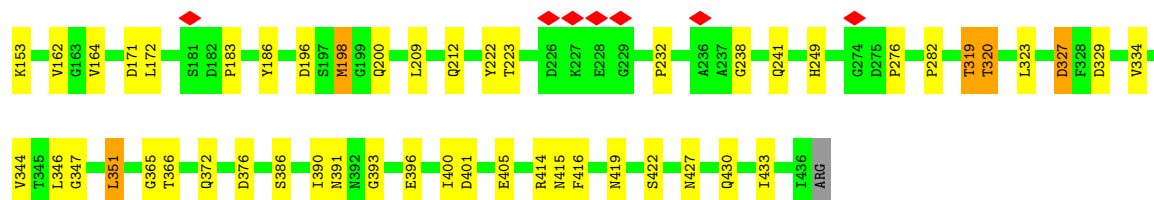


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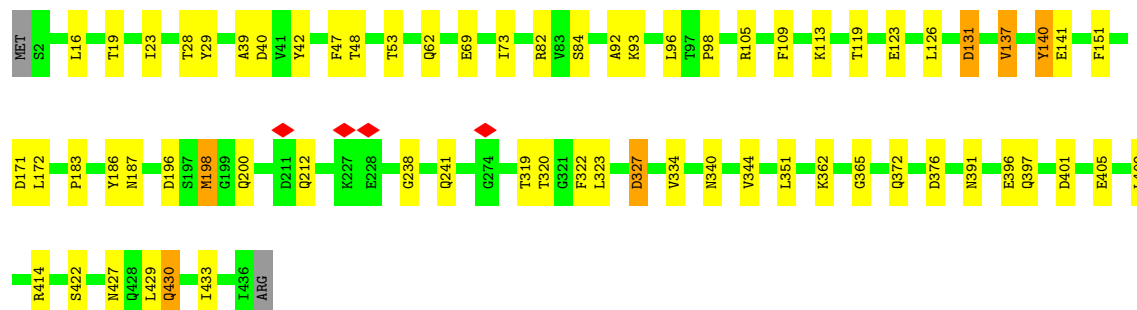
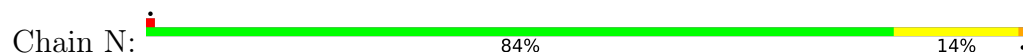


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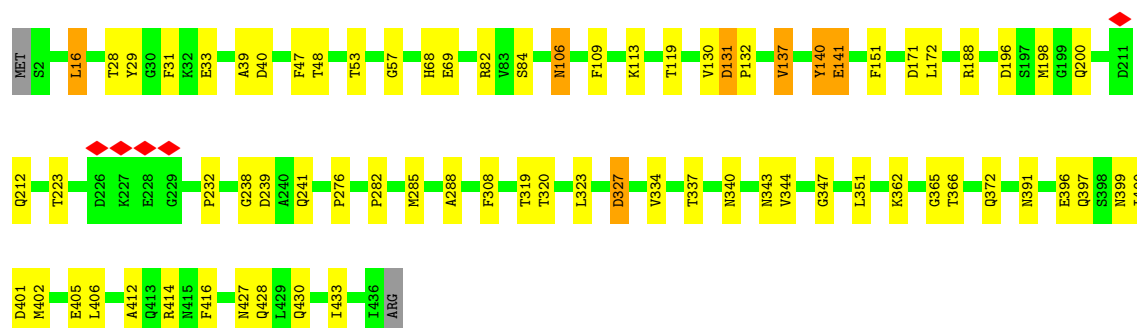
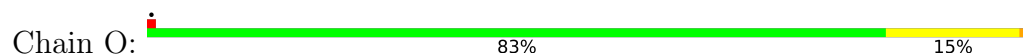




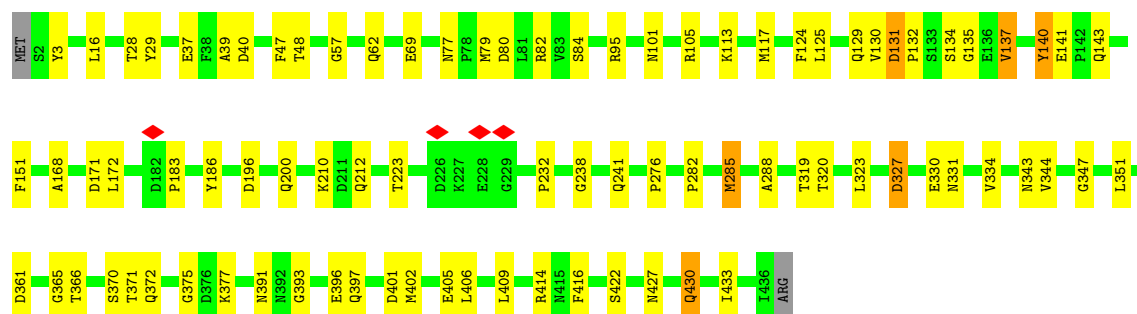
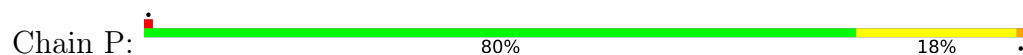
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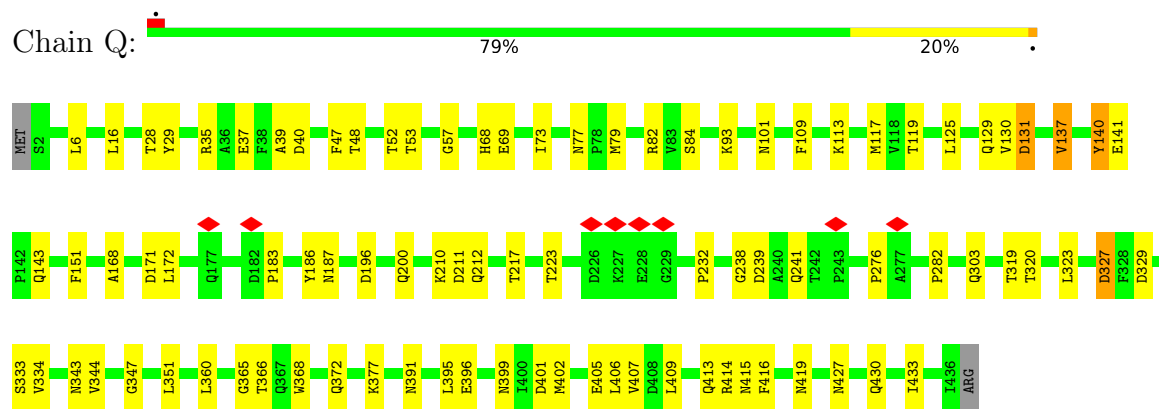
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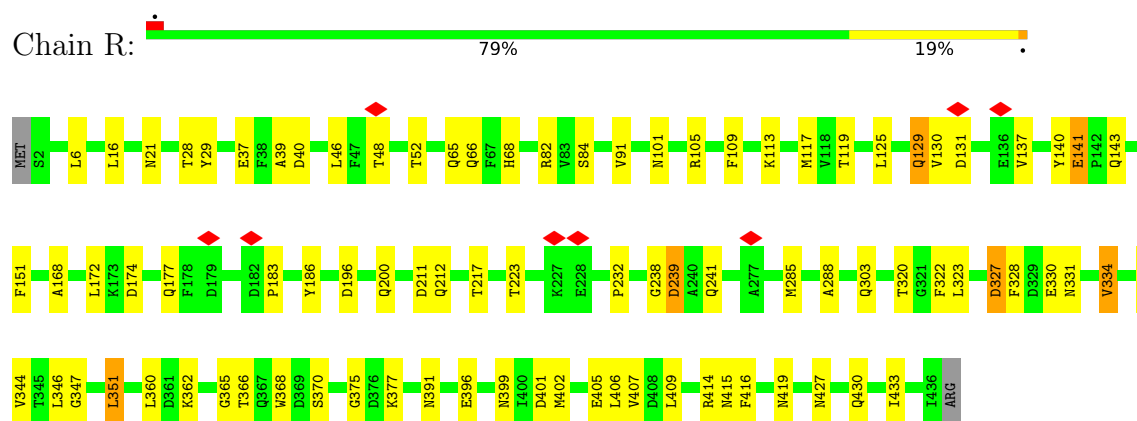
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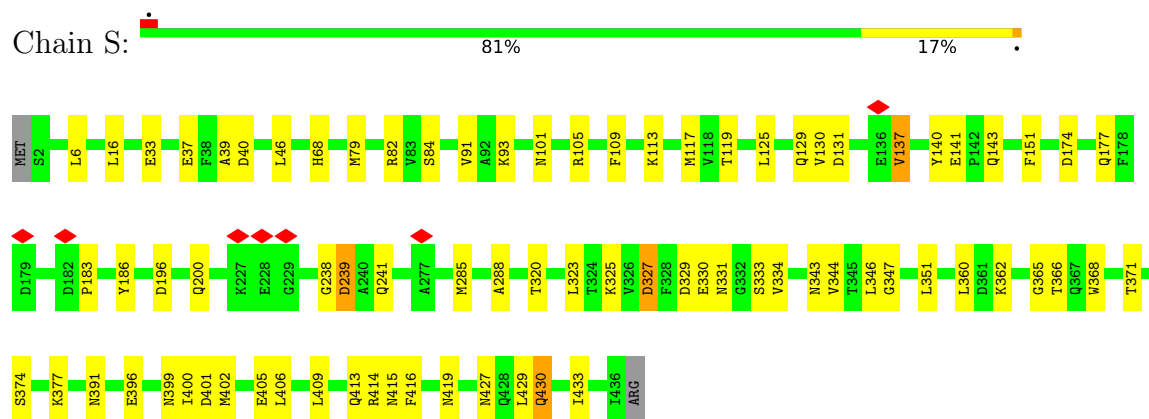
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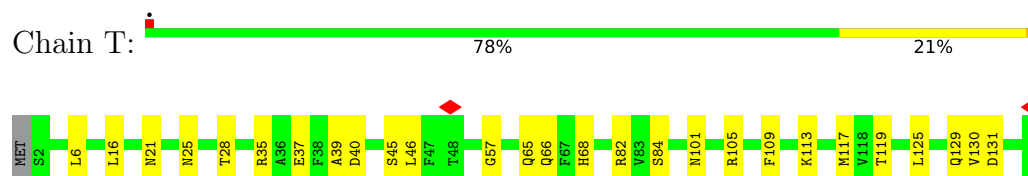
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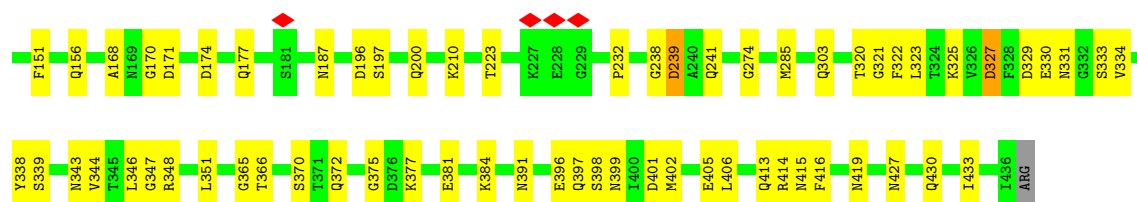


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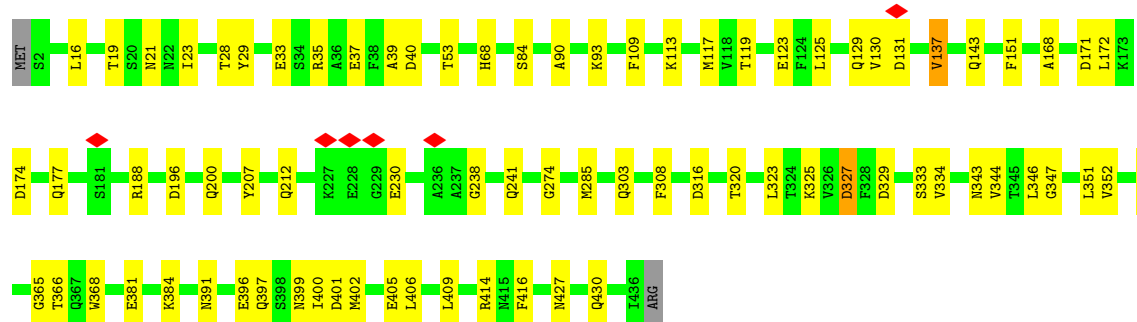
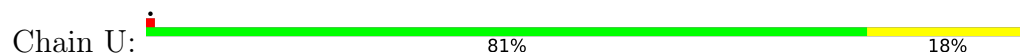


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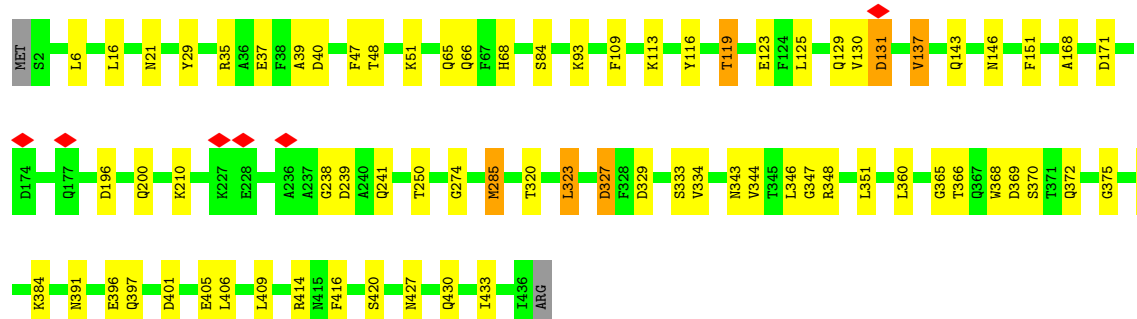
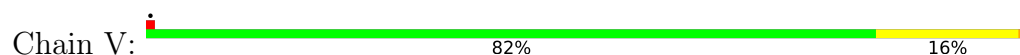




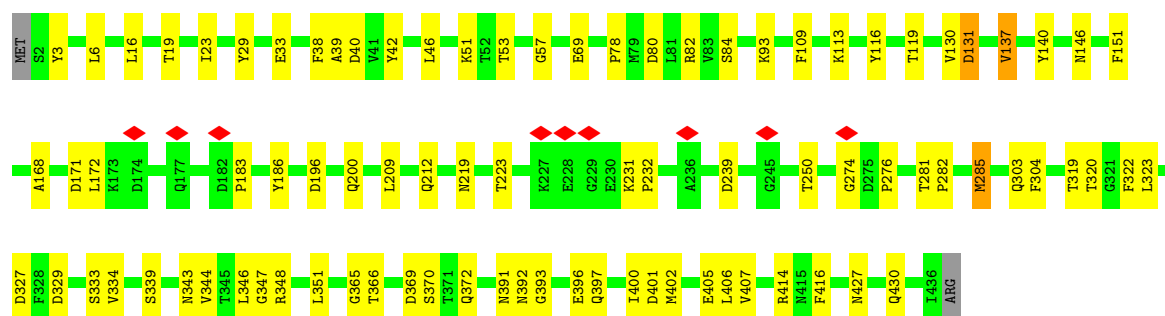
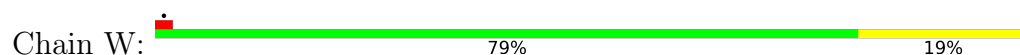
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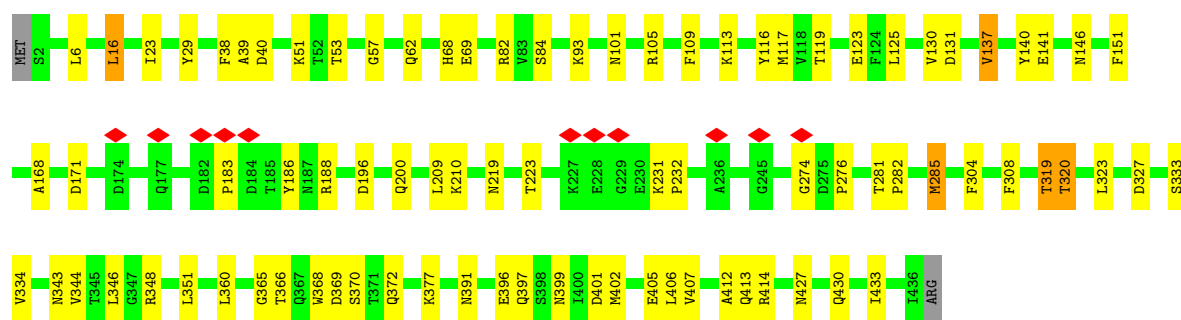


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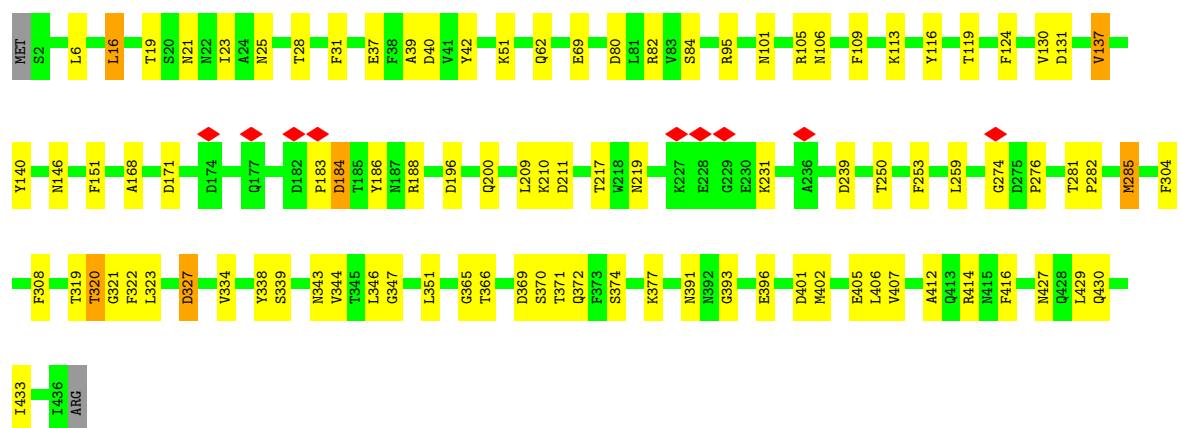
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Chain X: 




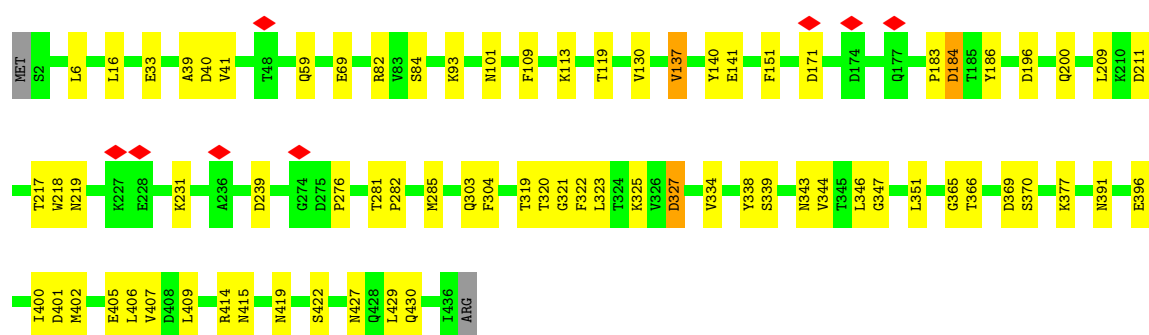
• Molecule 1: Flagellar hook protein FlgE

Chain Y: 




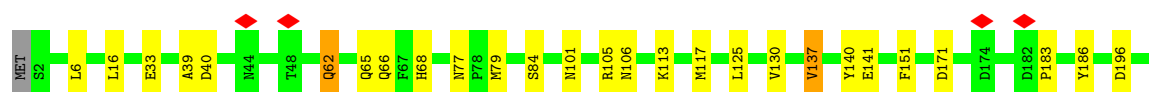
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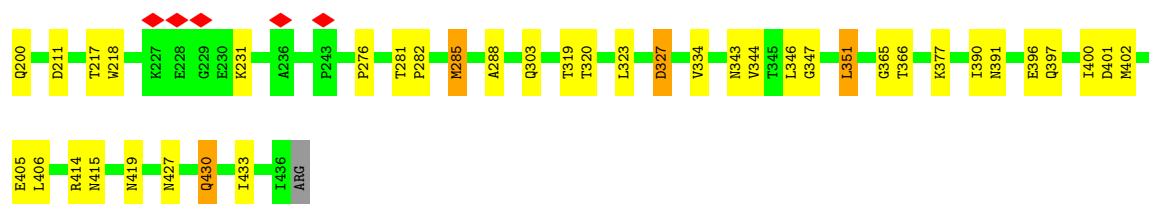
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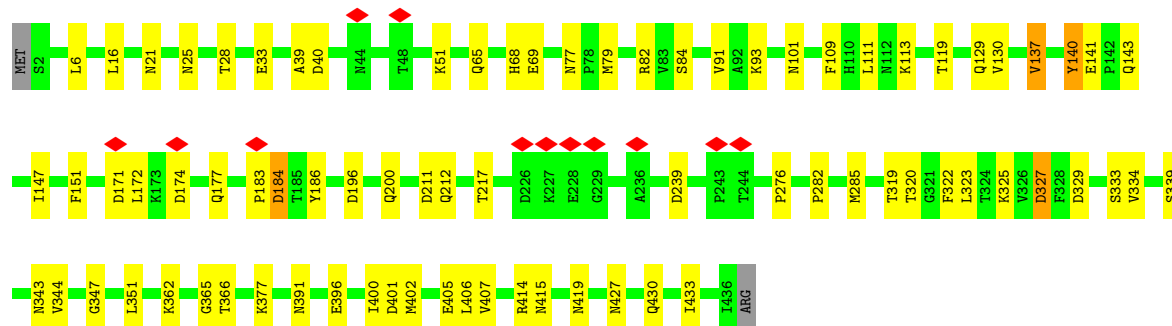
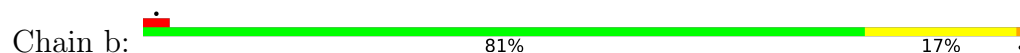
• Molecule 1: Flagellar hook protein FlgE

Chain a: 

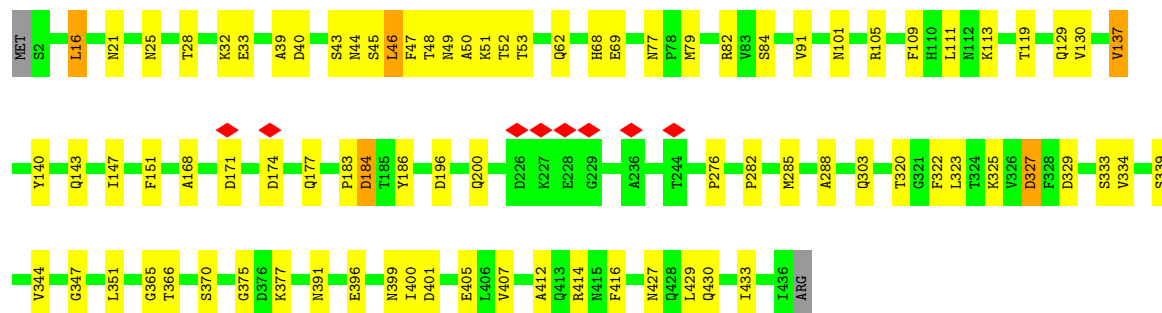
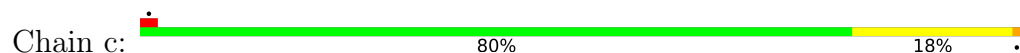




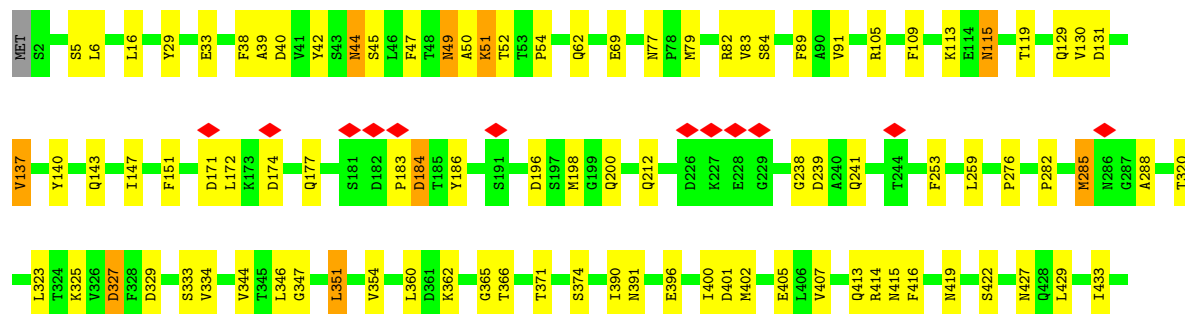
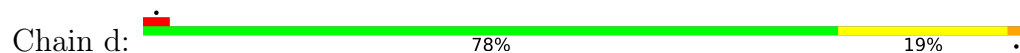
• Molecule 1: Flagellar hook protein FlgE



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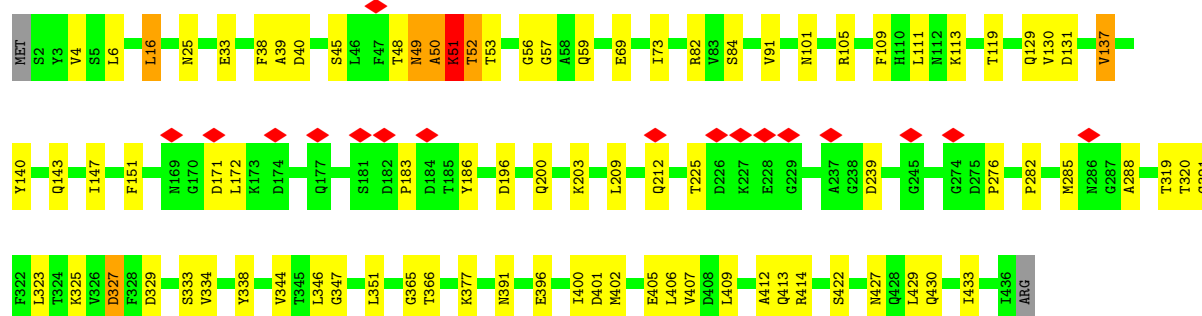
• Molecule 1: Flagellar hook protein FlgE





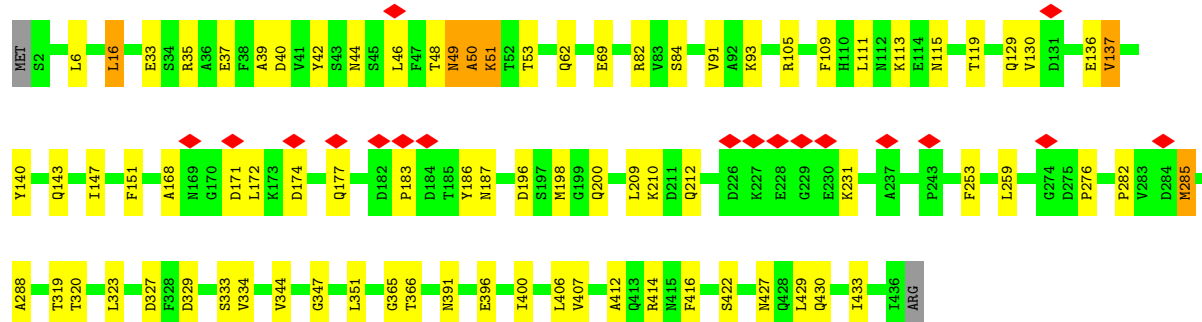
• Molecule 1: Flagellar hook protein FlgE

Chain e: 80% 18%



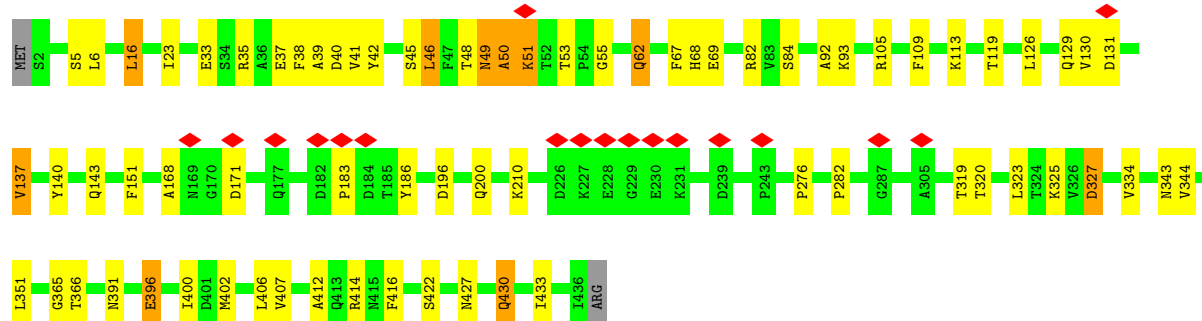
• Molecule 1: Flagellar hook protein FlgE

Chain f: 81% 17%



• Molecule 1: Flagellar hook protein FlgE

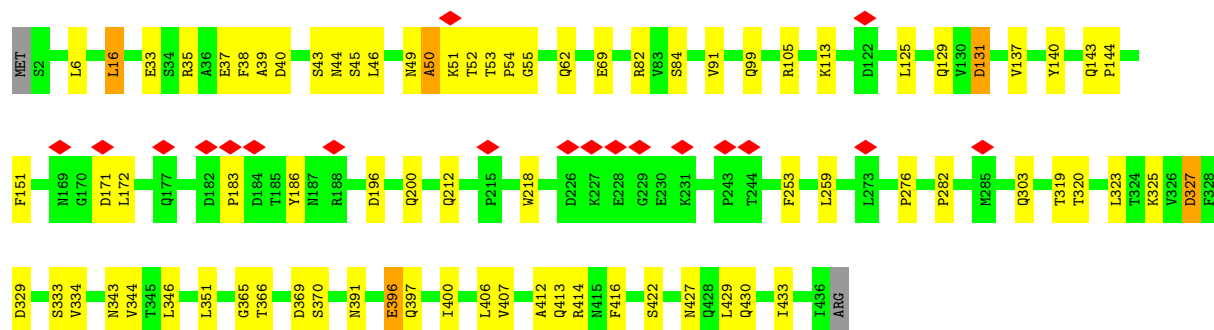
Chain g: 83% 14%



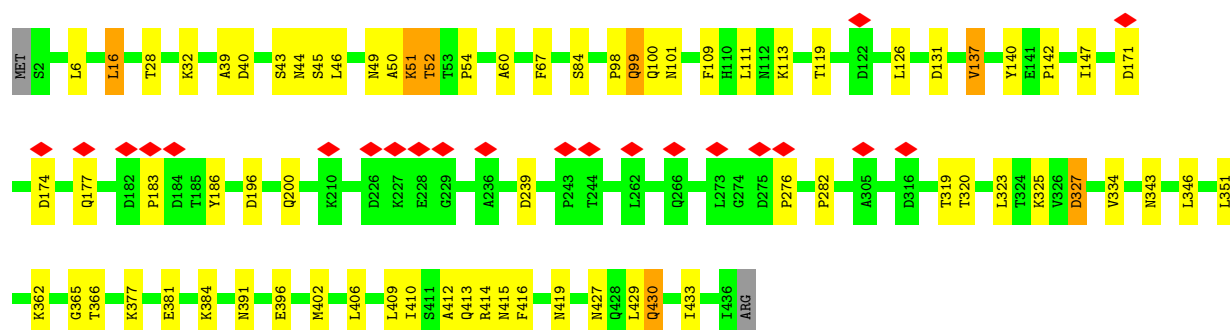
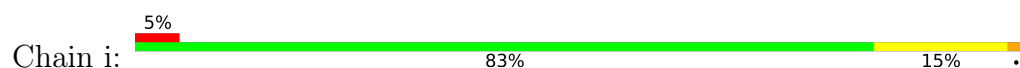
• Molecule 1: Flagellar hook protein FlgE

Chain h: 81% 17%

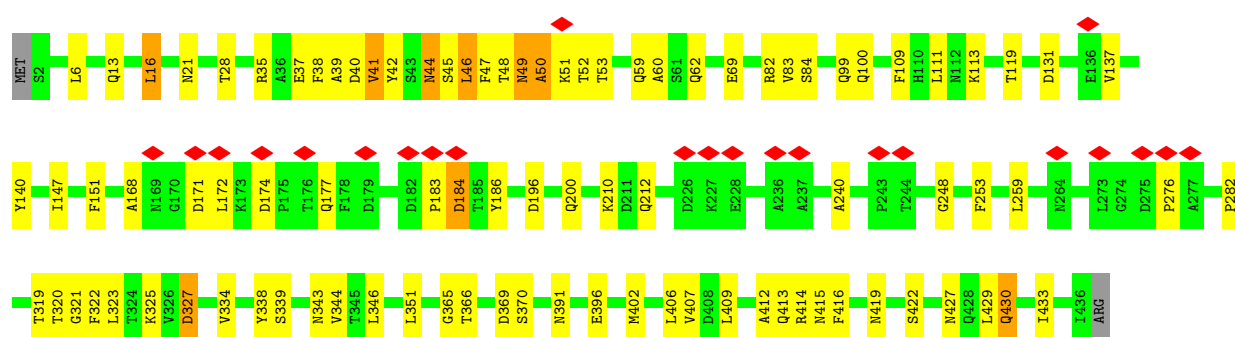
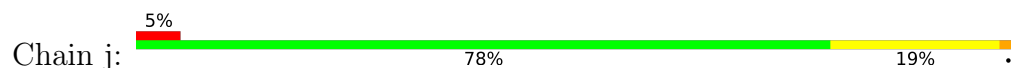




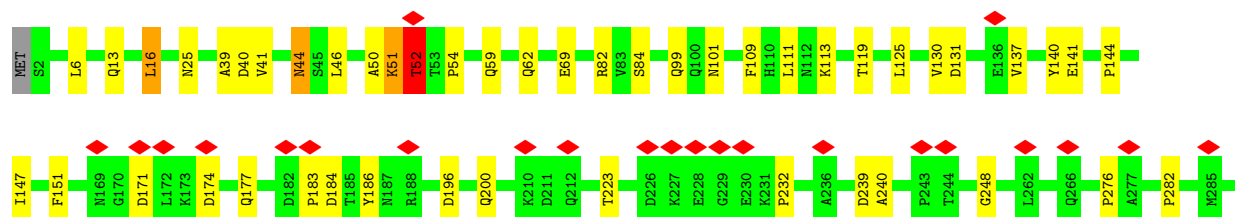
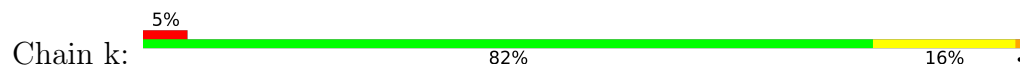
• Molecule 1: Flagellar hook protein FlgE



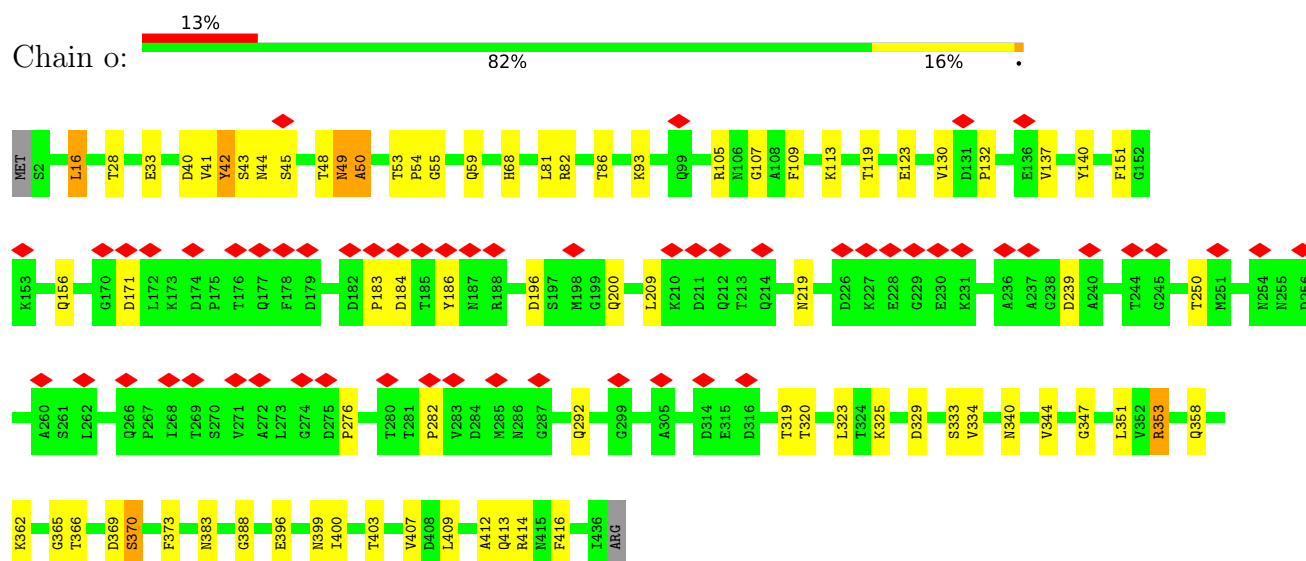
• Molecule 1: Flagellar hook protein FlgE



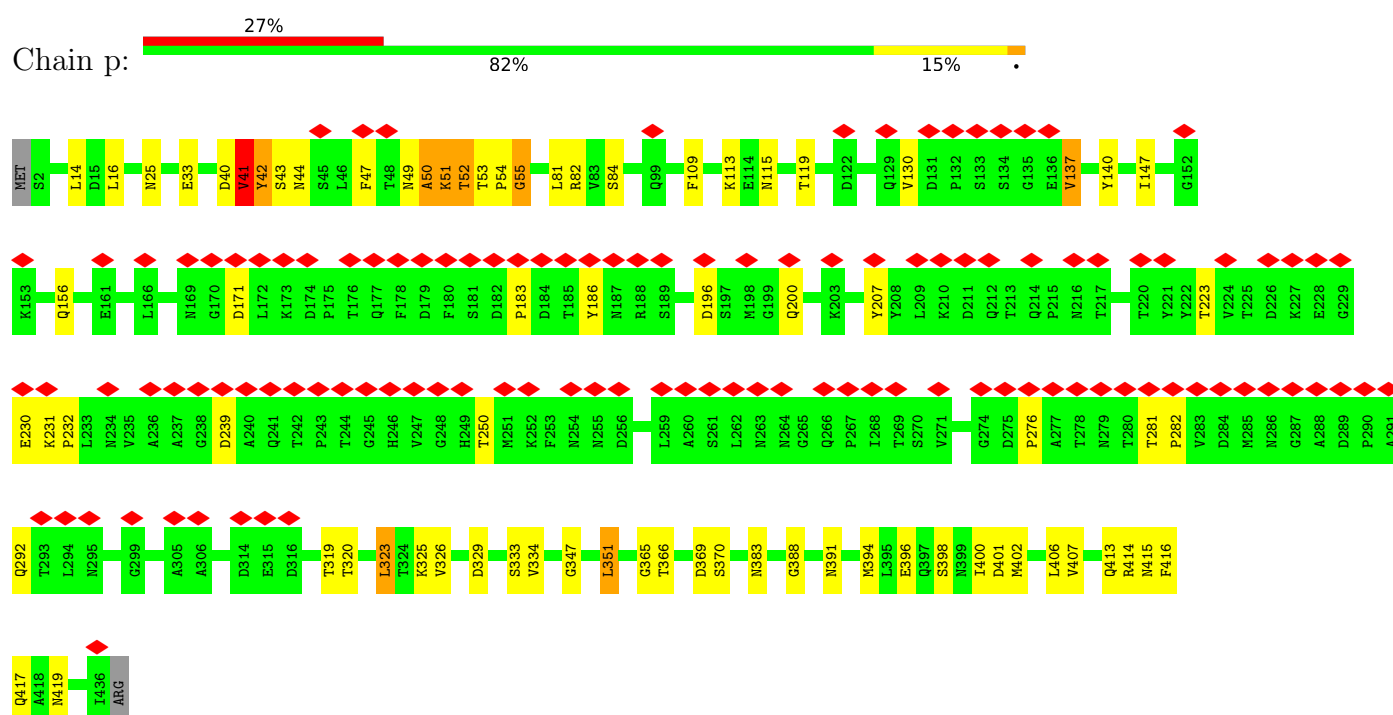
• Molecule 1: Flagellar hook protein FlgE



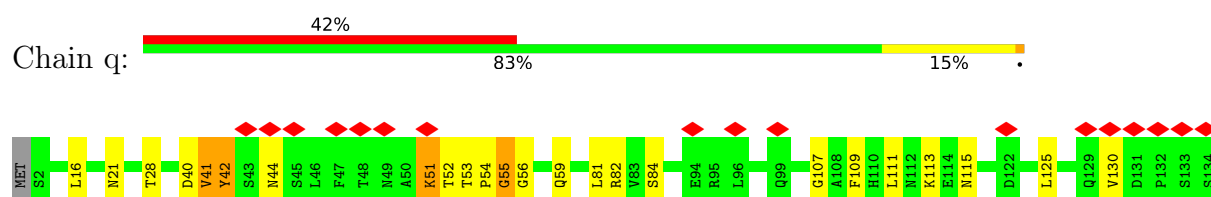
- Molecule 1: Flagellar hook protein FlgE



- Molecule 1: Flagellar hook protein FlgE



- Molecule 1: Flagellar hook protein FlgE



G135	E136	V137	S138	S139	Y140	E141	P144	I147	E150	F151	G152	K153	P154	K155	Q156	T157	A158	N159	I160	E161	V162	G163	V164	N165	L166	P167	A168	N169	G170	D171	L172	K173	D174	P175	T176	Q177	F178	D179	F180	S181	D182	P183	D184	T185	Y186	N187	R188	S189	T190	S191	S192	T193	I194	Y195	D196	S197																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
M198	G199	Q200	S201	Y202	K203	L204	T205	T206	Y207	Y208	L209	K210	D211	Q212	T213	Q214	P215	N216	T217	W218	N219	T220	Y221	Y222	T223	V224	T225	D226	K227	E228	G229	E230	K231	P232	L233	N234	V235	A236	A237	G238	D239	A240	Q241	T242	P243	T244	G245	H246	V247	G248	H249	T250	M251	K252	F253	N254	N255	D256	G257																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
T258	L259	A260	S261	L262	N263	N264	G265	Q266	P267	L268	T269	S270	V271	A272	L273	G274	D275	P276	A277	T278	N279	T280	T281	P282	V283	D284	M285	N286	G287	A288	D289	P290	A291	Q292	T293	L294	N295	F296	G297	L298	G299	S300	A301	T302	Q303	F304	A305	A306	P307	F308	E309	D314	E315	D316	G317	A318	T319	T320																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G321	F322	L323	V326	D329	V334	E342	G347	L351	L360	D361	K362	G365	T366	Q367	W368	D369	S370	T371	Q372	N383	K384	G385	G388	N391	E396	D401	V407	D408	L409	Q413	R414	N415	F416	Q417	A418	M419	L436	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32950	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.814	Depositor
Minimum map value	-1.223	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	456.00003, 456.00003, 456.00003	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	D	0.23	0/3385	0.34	0/4605
1	E	0.23	0/3385	0.34	0/4605
1	F	0.23	0/3385	0.33	0/4605
1	G	0.23	0/3385	0.33	0/4605
1	H	0.23	0/3385	0.33	0/4605
1	I	0.23	0/3385	0.33	0/4605
1	J	0.23	0/3385	0.33	0/4605
1	K	0.23	0/3385	0.33	0/4605
1	L	0.23	0/3385	0.33	0/4605
1	M	0.23	0/3385	0.33	0/4605
1	N	0.22	0/3385	0.33	0/4605
1	O	0.22	0/3385	0.33	0/4605
1	P	0.23	0/3385	0.33	0/4605
1	Q	0.22	0/3385	0.32	0/4605
1	R	0.22	0/3385	0.33	0/4605
1	S	0.22	0/3385	0.32	0/4605
1	T	0.21	0/3385	0.32	0/4605
1	U	0.22	0/3385	0.33	0/4605
1	V	0.22	0/3385	0.32	0/4605
1	W	0.21	0/3385	0.32	0/4605
1	X	0.21	0/3385	0.31	0/4605
1	Y	0.21	0/3385	0.31	0/4605
1	Z	0.20	0/3385	0.31	0/4605
1	a	0.21	0/3385	0.32	0/4605
1	b	0.20	0/3385	0.32	0/4605
1	c	0.27	0/3385	0.41	1/4605 (0.0%)
1	d	0.26	0/3385	0.40	1/4605 (0.0%)
1	e	0.26	0/3385	0.42	2/4605 (0.0%)
1	f	0.27	0/3385	0.41	0/4605
1	g	0.26	0/3385	0.42	3/4605 (0.1%)
1	h	0.28	1/3385 (0.0%)	0.44	2/4605 (0.0%)
1	i	0.29	0/3385	0.43	1/4605 (0.0%)
1	j	0.29	0/3385	0.45	3/4605 (0.1%)
1	k	0.27	0/3385	0.41	2/4605 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	l	0.25	0/3385	0.43	3/4605 (0.1%)
1	m	0.26	0/3385	0.41	1/4605 (0.0%)
1	n	0.27	0/3385	0.46	3/4605 (0.1%)
1	o	0.27	1/3385 (0.0%)	0.47	4/4605 (0.1%)
1	p	0.25	0/3385	0.45	4/4605 (0.1%)
1	q	0.23	0/3385	0.41	2/4605 (0.0%)
All	All	0.24	2/135400 (0.0%)	0.37	32/184200 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	m	0	1
1	n	0	1
1	o	0	1
1	p	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h	45	SER	CA-CB	-5.19	1.45	1.53
1	o	43	SER	CA-CB	-5.15	1.44	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	54	PRO	N-CA-C	-12.35	92.00	111.03
1	e	49	ASN	CB-CA-C	-10.21	104.79	116.63
1	o	54	PRO	N-CA-C	-10.19	95.20	111.19
1	p	54	PRO	N-CA-C	-9.42	96.40	111.19
1	h	46	LEU	N-CA-C	-8.75	102.60	113.28
1	l	51	LYS	N-CA-C	-8.73	102.41	113.23
1	q	54	PRO	N-CA-C	-8.63	96.97	110.95
1	m	54	PRO	N-CA-C	-7.49	99.43	111.19
1	n	51	LYS	N-CA-C	-7.40	103.29	111.36
1	q	42	TYR	CB-CA-C	-7.07	99.92	110.24
1	k	46	LEU	N-CA-C	-6.70	104.36	112.54
1	d	51	LYS	N-CA-C	-6.66	104.18	112.90
1	c	51	LYS	N-CA-C	-6.20	104.78	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	46	LEU	N-CA-C	-5.98	104.67	111.07
1	p	55	GLY	N-CA-C	5.96	121.35	112.41
1	g	46	LEU	N-CA-C	-5.88	106.10	113.28
1	p	41	VAL	O-C-N	-5.81	116.99	123.26
1	j	41	VAL	O-C-N	-5.69	117.17	123.20
1	o	42	TYR	CB-CA-C	-5.67	103.68	110.94
1	h	55	GLY	CA-C-O	-5.65	116.43	122.76
1	l	373	PHE	N-CA-C	-5.59	106.81	113.97
1	p	47	PHE	N-CA-C	-5.44	106.52	112.72
1	i	46	LEU	N-CA-C	-5.41	105.78	112.38
1	k	44	ASN	CB-CA-C	5.30	119.84	109.35
1	n	62	GLN	CB-CA-C	-5.27	100.38	109.86
1	g	41	VAL	O-C-N	-5.26	117.62	123.20
1	g	51	LYS	N-CA-C	-5.18	106.06	112.38
1	e	48	THR	N-CA-C	-5.17	106.52	114.16
1	o	373	PHE	N-CA-C	-5.16	106.25	112.54
1	l	54	PRO	N-CA-CB	-5.11	96.58	102.86
1	o	370	SER	O-C-N	5.03	128.64	122.96
1	j	44	ASN	CB-CA-C	5.01	119.56	109.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	m	353	ARG	Sidechain
1	n	353	ARG	Sidechain
1	o	353	ARG	Sidechain
1	p	41	VAL	Mainchain

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	D	3319	0	3124	36	0
1	E	3319	0	3124	43	0
1	F	3319	0	3124	44	0
1	G	3319	0	3124	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3319	0	3124	41	0
1	I	3319	0	3124	44	0
1	J	3319	0	3124	43	0
1	K	3319	0	3124	43	0
1	L	3319	0	3124	53	0
1	M	3319	0	3124	50	0
1	N	3319	0	3124	42	0
1	O	3319	0	3124	50	0
1	P	3319	0	3124	58	0
1	Q	3319	0	3124	59	0
1	R	3319	0	3124	52	0
1	S	3319	0	3124	50	0
1	T	3319	0	3124	58	0
1	U	3319	0	3124	47	0
1	V	3319	0	3124	48	0
1	W	3319	0	3124	53	0
1	X	3319	0	3124	54	0
1	Y	3319	0	3124	58	0
1	Z	3319	0	3124	44	0
1	a	3319	0	3124	40	0
1	b	3319	0	3124	54	0
1	c	3319	0	3124	55	0
1	d	3319	0	3124	64	0
1	e	3319	0	3124	59	0
1	f	3319	0	3124	53	0
1	g	3319	0	3124	51	0
1	h	3319	0	3124	50	0
1	i	3319	0	3124	47	0
1	j	3319	0	3124	58	0
1	k	3319	0	3124	48	0
1	l	3319	0	3124	48	0
1	m	3319	0	3124	56	0
1	n	3319	0	3124	38	0
1	o	3319	0	3124	46	0
1	p	3319	0	3124	44	0
1	q	3319	0	3124	43	0
All	All	132760	0	124960	1623	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 6.

All (1623) 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:E:426:HIS:HE1	1:J:16:LEU:HD12	1.37	0.90
1:R:105:ARG:NH1	1:R:396:GLU:OE2	2.09	0.84
1:E:426:HIS:CE1	1:J:16:LEU:HD12	2.16	0.81
1:p:42:TYR:HE1	1:p:55:GLY:HA3	1.45	0.80
1:p:42:TYR:CE1	1:p:55:GLY:HA3	2.17	0.79
1:m:50:ALA:O	1:m:51:LYS:C	2.28	0.77
1:e:52:THR:HG21	1:j:60:ALA:HB1	1.67	0.75
1:g:6:LEU:HD13	1:m:407:VAL:HG11	1.71	0.73
1:h:6:LEU:HD13	1:n:407:VAL:HG11	1.71	0.72
1:G:105:ARG:NH1	1:G:396:GLU:OE2	2.21	0.70
1:i:6:LEU:HD13	1:o:407:VAL:HG11	1.72	0.70
1:E:39:ALA:HB1	1:J:365:GLY:HA2	1.73	0.70
1:H:109:PHE:HE1	1:H:119:THR:HG22	1.57	0.70
1:R:82:ARG:HH11	1:R:396:GLU:HG2	1.57	0.69
1:P:39:ALA:HB1	1:U:365:GLY:HA2	1.73	0.69
1:J:33:GLU:HB3	1:J:400:ILE:HG22	1.76	0.68
1:S:105:ARG:NH1	1:S:396:GLU:OE2	2.26	0.68
1:R:239:ASP:OD1	1:R:239:ASP:N	2.27	0.68
1:g:433:ILE:HD11	1:l:416:PHE:HZ	1.59	0.68
1:D:39:ALA:HB1	1:I:365:GLY:HA2	1.76	0.68
1:a:196:ASP:OD1	1:a:200:GLN:N	2.26	0.68
1:h:33:GLU:HB3	1:h:400:ILE:HG22	1.75	0.67
1:W:40:ASP:H	1:b:366:THR:HG23	1.59	0.67
1:Z:427:ASN:OD1	1:f:414:ARG:NH1	2.27	0.67
1:M:238:GLY:O	1:M:241:GLN:NE2	2.28	0.67
1:P:101:ASN:OD1	1:P:377:LYS:NZ	2.27	0.67
1:h:50:ALA:HA	1:h:53:THR:HG22	1.77	0.67
1:b:427:ASN:OD1	1:h:414:ARG:NH1	2.28	0.67
1:T:39:ALA:HB1	1:Y:365:GLY:HA2	1.76	0.66
1:N:131:ASP:OD1	1:N:131:ASP:N	2.27	0.66
1:L:40:ASP:H	1:Q:366:THR:HG23	1.60	0.66
1:M:105:ARG:NH1	1:M:396:GLU:OE2	2.28	0.66
1:g:50:ALA:HA	1:g:53:THR:HG22	1.76	0.66
1:b:33:GLU:HB3	1:b:400:ILE:HG22	1.78	0.66
1:Y:82:ARG:HH11	1:Y:396:GLU:HG2	1.60	0.66
1:b:40:ASP:H	1:g:366:THR:HG23	1.59	0.66
1:N:39:ALA:HB1	1:S:365:GLY:HA2	1.77	0.66
1:p:82:ARG:HH11	1:p:396:GLU:HG2	1.61	0.66
1:K:33:GLU:HB3	1:K:400:ILE:HG22	1.78	0.66
1:T:238:GLY:O	1:T:241:GLN:NE2	2.29	0.66
1:d:327:ASP:OD1	1:d:327:ASP:N	2.28	0.66
1:O:372:GLN:HB2	1:Z:343:ASN:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:372:GLN:HB2	1:Y:343:ASN:HD22	1.61	0.65
1:S:109:PHE:HE1	1:S:119:THR:HG22	1.62	0.65
1:Z:40:ASP:OD1	1:e:25:ASN:ND2	2.30	0.65
1:o:33:GLU:HB3	1:o:400:ILE:HG22	1.78	0.65
1:a:40:ASP:H	1:f:366:THR:HG23	1.62	0.65
1:T:427:ASN:OD1	1:Z:414:ARG:NH1	2.30	0.65
1:n:41:VAL:CG2	1:n:59:GLN:HB2	2.27	0.65
1:K:433:ILE:HD11	1:P:416:PHE:HZ	1.61	0.65
1:E:101:ASN:OD1	1:E:377:LYS:NZ	2.29	0.64
1:Y:196:ASP:OD1	1:Y:200:GLN:N	2.29	0.64
1:c:40:ASP:H	1:h:366:THR:HG23	1.63	0.64
1:I:427:ASN:OD1	1:O:414:ARG:NH1	2.30	0.64
1:P:327:ASP:OD1	1:P:327:ASP:N	2.30	0.64
1:T:327:ASP:N	1:T:327:ASP:OD1	2.31	0.64
1:H:427:ASN:OD1	1:N:414:ARG:NH1	2.30	0.64
1:Y:39:ALA:HB1	1:d:365:GLY:HA2	1.79	0.64
1:G:430:GLN:HG2	1:M:414:ARG:HD2	1.78	0.64
1:J:330:GLU:OE2	1:J:331:ASN:ND2	2.31	0.64
1:M:39:ALA:HB1	1:R:365:GLY:HA2	1.80	0.64
1:b:109:PHE:HE1	1:b:119:THR:HG22	1.61	0.64
1:M:327:ASP:OD1	1:M:327:ASP:N	2.31	0.64
1:R:327:ASP:OD1	1:R:327:ASP:N	2.31	0.64
1:Y:427:ASN:OD1	1:e:414:ARG:NH1	2.31	0.64
1:i:415:ASN:O	1:i:419:ASN:ND2	2.31	0.64
1:M:40:ASP:H	1:R:366:THR:HG23	1.63	0.63
1:S:174:ASP:HB3	1:S:177:GLN:HB2	1.81	0.63
1:c:50:ALA:HA	1:c:53:THR:HB	1.80	0.63
1:S:82:ARG:HH11	1:S:396:GLU:HG2	1.63	0.63
1:Z:196:ASP:OD1	1:Z:200:GLN:N	2.30	0.63
1:f:42:TYR:CE2	1:k:362:LYS:HD2	2.32	0.63
1:i:327:ASP:OD1	1:i:327:ASP:N	2.30	0.63
1:a:327:ASP:OD1	1:a:327:ASP:N	2.30	0.63
1:F:84:SER:OG	1:F:391:ASN:ND2	2.32	0.63
1:a:101:ASN:OD1	1:a:377:LYS:NZ	2.31	0.63
1:I:415:ASN:O	1:I:419:ASN:ND2	2.32	0.63
1:a:427:ASN:OD1	1:g:414:ARG:NH1	2.30	0.63
1:F:372:GLN:HB2	1:Q:343:ASN:HD22	1.63	0.63
1:G:33:GLU:HB3	1:G:400:ILE:HG22	1.79	0.63
1:g:109:PHE:HE1	1:g:119:THR:HG22	1.63	0.63
1:o:82:ARG:HH11	1:o:396:GLU:HG2	1.62	0.63
1:P:40:ASP:H	1:U:366:THR:HG23	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:101:ASN:OD1	1:Z:377:LYS:NZ	2.32	0.63
1:d:40:ASP:H	1:i:366:THR:HG23	1.64	0.63
1:d:427:ASN:OD1	1:j:414:ARG:NH1	2.32	0.63
1:P:77:ASN:HD21	1:P:79:MET:HB2	1.63	0.62
1:g:430:GLN:OE1	1:m:414:ARG:NH1	2.33	0.62
1:h:427:ASN:OD1	1:n:414:ARG:NH1	2.32	0.62
1:H:33:GLU:HB3	1:H:400:ILE:HG22	1.80	0.62
1:J:427:ASN:OD1	1:P:414:ARG:NH1	2.32	0.62
1:b:327:ASP:N	1:b:327:ASP:OD1	2.31	0.62
1:l:174:ASP:HB3	1:l:177:GLN:HB2	1.81	0.62
1:Q:84:SER:OG	1:Q:391:ASN:ND2	2.32	0.62
1:d:52:THR:HG21	1:i:60:ALA:HB1	1.80	0.62
1:O:131:ASP:OD1	1:O:131:ASP:N	2.29	0.62
1:W:427:ASN:OD1	1:c:414:ARG:NH1	2.33	0.62
1:c:47:PHE:CD2	1:n:67:PHE:HB2	2.34	0.62
1:K:40:ASP:H	1:P:366:THR:HG23	1.65	0.62
1:K:238:GLY:O	1:K:241:GLN:NE2	2.33	0.62
1:K:330:GLU:OE2	1:K:331:ASN:ND2	2.32	0.62
1:S:238:GLY:O	1:S:241:GLN:NE2	2.31	0.62
1:q:82:ARG:HH11	1:q:396:GLU:HG2	1.63	0.62
1:F:33:GLU:HB3	1:F:400:ILE:HG22	1.81	0.62
1:K:82:ARG:HH11	1:K:396:GLU:HG2	1.65	0.62
1:c:46:LEU:HD13	1:n:353:ARG:NH1	2.15	0.62
1:F:327:ASP:OD1	1:F:327:ASP:N	2.31	0.62
1:c:39:ALA:HB1	1:h:365:GLY:HA2	1.81	0.62
1:f:6:LEU:HD13	1:l:407:VAL:HG11	1.80	0.62
1:g:39:ALA:HB1	1:l:365:GLY:HA2	1.81	0.62
1:j:6:LEU:HD13	1:p:407:VAL:HG11	1.81	0.62
1:U:427:ASN:OD1	1:a:414:ARG:NH1	2.33	0.62
1:H:37:GLU:HG2	1:M:29:TYR:HE2	1.65	0.61
1:e:52:THR:HG21	1:j:60:ALA:CB	2.30	0.61
1:Z:327:ASP:OD1	1:Z:327:ASP:N	2.33	0.61
1:j:327:ASP:N	1:j:327:ASP:OD1	2.33	0.61
1:o:86:THR:HG21	1:o:353:ARG:HH11	1.64	0.61
1:p:33:GLU:HB3	1:p:400:ILE:HG22	1.81	0.61
1:Y:40:ASP:H	1:d:366:THR:HG23	1.66	0.61
1:l:433:ILE:HD11	1:q:416:PHE:HZ	1.65	0.61
1:N:40:ASP:H	1:S:366:THR:HG23	1.65	0.61
1:e:49:ASN:O	1:e:50:ALA:HB2	2.01	0.61
1:n:53:THR:O	1:n:54:PRO:C	2.42	0.61
1:G:39:ALA:HB1	1:L:365:GLY:HA2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:VAL:HG12	1:G:137:VAL:HA	1.82	0.61
1:X:38:PHE:HB2	1:c:28:THR:HG22	1.81	0.61
1:L:238:GLY:O	1:L:241:GLN:NE2	2.34	0.61
1:e:39:ALA:HB1	1:j:365:GLY:HA2	1.83	0.61
1:H:430:GLN:HE21	1:S:402:MET:HB2	1.66	0.60
1:Q:327:ASP:N	1:Q:327:ASP:OD1	2.34	0.60
1:V:327:ASP:N	1:V:327:ASP:OD1	2.33	0.60
1:S:327:ASP:OD1	1:S:327:ASP:N	2.31	0.60
1:X:105:ARG:NH1	1:X:396:GLU:OE2	2.31	0.60
1:I:109:PHE:HE1	1:I:119:THR:HG22	1.66	0.60
1:N:430:GLN:HE21	1:Y:402:MET:HB2	1.66	0.60
1:Q:101:ASN:OD1	1:Q:377:LYS:NZ	2.35	0.60
1:Q:427:ASN:OD1	1:W:414:ARG:NH1	2.34	0.60
1:U:327:ASP:OD1	1:U:327:ASP:N	2.33	0.60
1:X:196:ASP:OD1	1:X:200:GLN:N	2.34	0.60
1:c:327:ASP:OD1	1:c:327:ASP:N	2.32	0.60
1:D:130:VAL:HG12	1:D:137:VAL:HA	1.82	0.60
1:N:238:GLY:O	1:N:241:GLN:NE2	2.34	0.60
1:f:39:ALA:HB1	1:k:365:GLY:HA2	1.82	0.60
1:N:196:ASP:OD1	1:N:200:GLN:N	2.33	0.60
1:E:109:PHE:HE1	1:E:119:THR:HG22	1.66	0.60
1:I:39:ALA:HB1	1:N:365:GLY:HA2	1.84	0.60
1:U:40:ASP:H	1:Z:366:THR:HG23	1.66	0.60
1:k:40:ASP:H	1:p:366:THR:HG23	1.65	0.60
1:O:427:ASN:OD1	1:U:414:ARG:NH1	2.35	0.60
1:c:101:ASN:OD1	1:c:377:LYS:NZ	2.35	0.60
1:f:109:PHE:HE1	1:f:119:THR:HG22	1.66	0.60
1:Z:40:ASP:H	1:e:366:THR:HG23	1.67	0.60
1:O:39:ALA:HB1	1:T:365:GLY:HA2	1.84	0.60
1:S:84:SER:OG	1:S:391:ASN:ND2	2.34	0.60
1:Z:84:SER:OG	1:Z:391:ASN:ND2	2.35	0.60
1:f:129:GLN:HB2	1:f:143:GLN:HE21	1.67	0.60
1:j:39:ALA:HB1	1:o:365:GLY:HA2	1.84	0.59
1:l:45:SER:HB3	1:l:48:THR:HG23	1.84	0.59
1:G:427:ASN:OD1	1:M:414:ARG:NH1	2.35	0.59
1:W:196:ASP:OD1	1:W:200:GLN:N	2.35	0.59
1:g:42:TYR:CZ	1:l:362:LYS:HD2	2.36	0.59
1:M:33:GLU:HB3	1:M:400:ILE:HG22	1.84	0.59
1:X:39:ALA:HB1	1:c:365:GLY:HA2	1.83	0.59
1:g:33:GLU:HB3	1:g:400:ILE:HG22	1.83	0.59
1:V:109:PHE:HE1	1:V:119:THR:HG22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:196:ASP:OD1	1:J:200:GLN:N	2.36	0.59
1:d:171:ASP:OD1	1:d:171:ASP:N	2.35	0.59
1:L:433:ILE:HD11	1:Q:416:PHE:HZ	1.67	0.59
1:N:427:ASN:OD1	1:T:414:ARG:NH1	2.36	0.59
1:O:40:ASP:H	1:T:366:THR:HG23	1.67	0.59
1:W:84:SER:OG	1:W:391:ASN:ND2	2.36	0.59
1:O:238:GLY:O	1:O:241:GLN:NE2	2.35	0.59
1:V:381:GLU:OE1	1:V:384:LYS:NZ	2.29	0.59
1:Z:39:ALA:HB1	1:e:365:GLY:HA2	1.83	0.59
1:h:84:SER:OG	1:h:391:ASN:ND2	2.35	0.59
1:I:372:GLN:HB2	1:T:343:ASN:HD22	1.68	0.59
1:X:69:GLU:OE1	1:X:82:ARG:NH2	2.36	0.59
1:N:82:ARG:HH11	1:N:396:GLU:HG2	1.67	0.58
1:H:196:ASP:OD1	1:H:200:GLN:N	2.36	0.58
1:R:427:ASN:OD1	1:X:414:ARG:NH1	2.36	0.58
1:H:109:PHE:CE1	1:H:119:THR:HG22	2.38	0.58
1:h:52:THR:O	1:h:52:THR:HG22	2.03	0.58
1:k:174:ASP:HB3	1:k:177:GLN:HB2	1.86	0.58
1:N:327:ASP:OD1	1:N:327:ASP:N	2.36	0.58
1:i:39:ALA:HB1	1:n:365:GLY:HA2	1.85	0.58
1:T:82:ARG:HH11	1:T:396:GLU:HG2	1.68	0.58
1:Y:84:SER:OG	1:Y:391:ASN:ND2	2.36	0.58
1:T:171:ASP:OD1	1:T:187:ASN:ND2	2.37	0.58
1:e:109:PHE:HE1	1:e:119:THR:HG22	1.68	0.58
1:O:82:ARG:HH11	1:O:396:GLU:HG2	1.69	0.58
1:e:327:ASP:N	1:e:327:ASP:OD1	2.35	0.58
1:U:84:SER:OG	1:U:391:ASN:ND2	2.37	0.58
1:V:427:ASN:OD1	1:b:414:ARG:NH1	2.37	0.58
1:E:84:SER:OG	1:E:391:ASN:ND2	2.37	0.58
1:E:422:SER:HA	1:J:409:LEU:HD21	1.85	0.58
1:Y:101:ASN:OD1	1:Y:377:LYS:NZ	2.36	0.58
1:d:6:LEU:HD13	1:j:407:VAL:HG11	1.86	0.58
1:c:111:LEU:HD11	1:c:147:ILE:HD12	1.86	0.58
1:j:100:GLN:HE21	1:j:100:GLN:HA	1.69	0.58
1:n:82:ARG:HH11	1:n:396:GLU:HG2	1.68	0.58
1:M:427:ASN:OD1	1:S:414:ARG:NH1	2.37	0.57
1:R:101:ASN:OD1	1:R:377:LYS:NZ	2.37	0.57
1:T:129:GLN:HB2	1:T:143:GLN:HE21	1.67	0.57
1:V:84:SER:OG	1:V:391:ASN:ND2	2.37	0.57
1:h:327:ASP:OD1	1:h:327:ASP:N	2.36	0.57
1:h:433:ILE:HD11	1:m:416:PHE:HZ	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:218:TRP:NE1	1:L:303:GLN:OE1	2.32	0.57
1:S:239:ASP:OD1	1:S:239:ASP:N	2.28	0.57
1:U:39:ALA:HB1	1:Z:365:GLY:HA2	1.85	0.57
1:k:50:ALA:O	1:k:52:THR:N	2.35	0.57
1:a:39:ALA:HB1	1:f:365:GLY:HA2	1.86	0.57
1:n:42:TYR:CE2	1:n:55:GLY:HA2	2.39	0.57
1:Y:105:ARG:NH1	1:Y:396:GLU:OE2	2.35	0.57
1:c:196:ASP:OD1	1:c:200:GLN:N	2.34	0.57
1:f:82:ARG:HH11	1:f:396:GLU:HG2	1.68	0.57
1:h:52:THR:HG23	1:m:60:ALA:HB1	1.87	0.57
1:E:327:ASP:N	1:E:327:ASP:OD1	2.38	0.57
1:R:168:ALA:HA	1:R:303:GLN:HE21	1.69	0.57
1:S:427:ASN:OD1	1:Y:414:ARG:NH1	2.38	0.57
1:T:109:PHE:HE1	1:T:119:THR:HG22	1.70	0.57
1:F:231:LYS:NZ	1:F:282:PRO:O	2.27	0.57
1:c:171:ASP:N	1:c:171:ASP:OD1	2.35	0.57
1:d:39:ALA:HB1	1:i:365:GLY:HA2	1.86	0.57
1:k:433:ILE:HD11	1:p:416:PHE:HZ	1.69	0.57
1:D:84:SER:OG	1:D:391:ASN:ND2	2.37	0.57
1:G:84:SER:OG	1:G:391:ASN:ND2	2.38	0.57
1:U:196:ASP:OD1	1:U:200:GLN:N	2.38	0.57
1:l:40:ASP:H	1:q:366:THR:HG23	1.70	0.57
1:Y:231:LYS:HB3	1:Y:281:THR:HB	1.87	0.57
1:c:183:PRO:HA	1:c:186:TYR:CZ	2.40	0.57
1:g:171:ASP:OD1	1:g:171:ASP:N	2.37	0.57
1:D:33:GLU:HB3	1:D:400:ILE:HG22	1.86	0.57
1:M:372:GLN:HB2	1:X:343:ASN:HD22	1.70	0.57
1:d:183:PRO:HA	1:d:186:TYR:CZ	2.40	0.57
1:d:371:THR:H	1:d:374:SER:HG	1.52	0.57
1:e:101:ASN:OD1	1:e:377:LYS:NZ	2.37	0.57
1:K:427:ASN:OD1	1:Q:414:ARG:NH1	2.39	0.56
1:c:427:ASN:OD1	1:i:414:ARG:NH1	2.38	0.56
1:e:427:ASN:OD1	1:k:414:ARG:NH1	2.38	0.56
1:q:369:ASP:OD1	1:q:370:SER:N	2.37	0.56
1:O:327:ASP:N	1:O:327:ASP:OD1	2.35	0.56
1:d:44:ASN:OD1	1:d:44:ASN:N	2.38	0.56
1:Q:109:PHE:HE1	1:Q:119:THR:HG22	1.70	0.56
1:X:427:ASN:OD1	1:d:414:ARG:NH1	2.38	0.56
1:c:33:GLU:HB3	1:c:400:ILE:HG22	1.87	0.56
1:c:433:ILE:HD11	1:h:416:PHE:HZ	1.70	0.56
1:e:38:PHE:HB2	1:j:28:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:40:ASP:H	1:k:366:THR:HG23	1.71	0.56
1:i:40:ASP:H	1:n:366:THR:HG23	1.69	0.56
1:q:231:LYS:HB3	1:q:281:THR:HB	1.88	0.56
1:I:327:ASP:OD1	1:I:327:ASP:N	2.37	0.56
1:J:40:ASP:H	1:O:366:THR:HG23	1.70	0.56
1:e:433:ILE:HD11	1:j:416:PHE:HZ	1.70	0.56
1:G:82:ARG:HH11	1:G:396:GLU:HG2	1.70	0.56
1:I:196:ASP:OD1	1:I:200:GLN:N	2.38	0.56
1:L:330:GLU:OE2	1:L:331:ASN:ND2	2.39	0.56
1:T:105:ARG:NH1	1:T:396:GLU:OE2	2.33	0.56
1:e:40:ASP:H	1:j:366:THR:HG23	1.70	0.56
1:b:196:ASP:OD1	1:b:200:GLN:N	2.36	0.56
1:c:45:SER:OG	1:c:46:LEU:N	2.38	0.56
1:e:430:GLN:OE1	1:k:414:ARG:NH1	2.38	0.56
1:f:427:ASN:OD1	1:l:414:ARG:NH1	2.39	0.56
1:q:115:ASN:ND2	1:q:147:ILE:O	2.39	0.56
1:K:218:TRP:NE1	1:K:303:GLN:OE1	2.33	0.56
1:d:415:ASN:O	1:d:419:ASN:ND2	2.36	0.56
1:h:105:ARG:NH1	1:h:396:GLU:OE1	2.39	0.56
1:o:40:ASP:OD2	1:o:42:TYR:CE1	2.58	0.56
1:E:415:ASN:O	1:E:419:ASN:ND2	2.38	0.56
1:F:101:ASN:OD1	1:F:377:LYS:NZ	2.38	0.56
1:X:84:SER:OG	1:X:391:ASN:ND2	2.39	0.56
1:Y:327:ASP:N	1:Y:327:ASP:OD1	2.37	0.56
1:b:433:ILE:HD11	1:g:416:PHE:HZ	1.71	0.56
1:e:84:SER:OG	1:e:391:ASN:ND2	2.39	0.56
1:j:82:ARG:HH11	1:j:396:GLU:HG2	1.69	0.56
1:M:84:SER:OG	1:M:391:ASN:ND2	2.39	0.56
1:N:69:GLU:OE1	1:N:82:ARG:NH2	2.39	0.56
1:N:198:MET:HE1	1:Y:304:PHE:HA	1.88	0.56
1:f:49:ASN:O	1:f:50:ALA:HB2	2.06	0.56
1:i:109:PHE:HE1	1:i:119:THR:HG22	1.71	0.56
1:H:330:GLU:OE2	1:H:331:ASN:ND2	2.39	0.56
1:I:117:MET:HE3	1:I:125:LEU:HD23	1.86	0.56
1:c:84:SER:OG	1:c:391:ASN:ND2	2.38	0.56
1:q:111:LEU:HD11	1:q:147:ILE:HD12	1.88	0.56
1:e:183:PRO:HA	1:e:186:TYR:CZ	2.41	0.55
1:D:40:ASP:H	1:I:366:THR:HG23	1.70	0.55
1:H:84:SER:OG	1:H:391:ASN:ND2	2.39	0.55
1:q:42:TYR:CD1	1:q:55:GLY:HA2	2.41	0.55
1:R:129:GLN:HB2	1:R:143:GLN:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:73:ILE:HD13	1:I:397:GLN:HE21	1.71	0.55
1:Z:33:GLU:HB3	1:Z:400:ILE:HG22	1.89	0.55
1:h:39:ALA:HB1	1:m:365:GLY:HA2	1.89	0.55
1:m:42:TYR:CE2	1:m:55:GLY:HA3	2.41	0.55
1:M:415:ASN:O	1:M:419:ASN:ND2	2.40	0.55
1:O:130:VAL:HG22	1:O:347:GLY:HA2	1.88	0.55
1:d:84:SER:OG	1:d:391:ASN:ND2	2.39	0.55
1:b:174:ASP:HB3	1:b:177:GLN:HB2	1.88	0.55
1:i:84:SER:OG	1:i:391:ASN:ND2	2.40	0.55
1:k:39:ALA:HB1	1:p:365:GLY:HA2	1.88	0.55
1:F:427:ASN:OD1	1:L:414:ARG:NH1	2.40	0.55
1:H:372:GLN:HB2	1:S:343:ASN:HD22	1.72	0.55
1:g:38:PHE:HB2	1:l:28:THR:HG22	1.89	0.55
1:g:40:ASP:H	1:l:366:THR:HG23	1.72	0.55
1:g:276:PRO:HA	1:g:282:PRO:HG3	1.89	0.55
1:Q:39:ALA:HB1	1:V:365:GLY:HA2	1.88	0.55
1:P:131:ASP:N	1:P:131:ASP:OD1	2.40	0.55
1:p:239:ASP:OD2	1:p:250:THR:OG1	2.23	0.55
1:D:327:ASP:OD1	1:D:327:ASP:N	2.37	0.55
1:R:330:GLU:OE2	1:R:331:ASN:ND2	2.40	0.55
1:T:168:ALA:HA	1:T:303:GLN:HE21	1.71	0.55
1:b:77:ASN:HD21	1:b:79:MET:HB2	1.72	0.55
1:i:276:PRO:HA	1:i:282:PRO:HG3	1.89	0.55
1:k:327:ASP:OD1	1:k:327:ASP:N	2.40	0.55
1:f:111:LEU:HD11	1:f:147:ILE:HD12	1.89	0.54
1:i:101:ASN:OD1	1:i:377:LYS:NZ	2.41	0.54
1:O:84:SER:OG	1:O:391:ASN:ND2	2.40	0.54
1:Y:130:VAL:HG22	1:Y:347:GLY:HA2	1.90	0.54
1:g:327:ASP:N	1:g:327:ASP:OD1	2.37	0.54
1:j:84:SER:OG	1:j:391:ASN:ND2	2.40	0.54
1:n:40:ASP:OD2	1:n:42:TYR:CE1	2.61	0.54
1:Z:415:ASN:O	1:Z:419:ASN:ND2	2.36	0.54
1:e:171:ASP:OD1	1:e:171:ASP:N	2.36	0.54
1:h:276:PRO:HA	1:h:282:PRO:HG3	1.90	0.54
1:O:196:ASP:OD1	1:O:200:GLN:N	2.36	0.54
1:Q:82:ARG:HH11	1:Q:396:GLU:HG2	1.73	0.54
1:X:372:GLN:HB2	1:i:343:ASN:HD22	1.72	0.54
1:k:109:PHE:HE1	1:k:119:THR:HG22	1.73	0.54
1:e:57:GLY:H	1:j:21:ASN:HD22	1.54	0.54
1:f:16:LEU:HD22	1:f:412:ALA:HB1	1.89	0.54
1:j:40:ASP:H	1:o:366:THR:HG23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ASP:OD1	1:D:200:GLN:N	2.36	0.54
1:L:422:SER:HA	1:Q:409:LEU:HD21	1.90	0.54
1:a:415:ASN:O	1:a:419:ASN:ND2	2.41	0.54
1:b:183:PRO:HA	1:b:186:TYR:CZ	2.43	0.54
1:J:415:ASN:O	1:J:419:ASN:ND2	2.41	0.54
1:K:196:ASP:OD1	1:K:200:GLN:N	2.36	0.54
1:L:117:MET:HE3	1:L:125:LEU:HD23	1.90	0.54
1:M:111:LEU:HD11	1:M:147:ILE:HD12	1.89	0.54
1:S:39:ALA:HB1	1:X:365:GLY:HA2	1.87	0.54
1:S:129:GLN:HB2	1:S:143:GLN:NE2	2.23	0.54
1:T:129:GLN:HB2	1:T:143:GLN:NE2	2.23	0.54
1:V:238:GLY:O	1:V:241:GLN:NE2	2.41	0.54
1:f:430:GLN:OE1	1:l:414:ARG:NH1	2.41	0.54
1:j:174:ASP:HB3	1:j:177:GLN:HB2	1.89	0.54
1:E:372:GLN:HB2	1:P:343:ASN:HD22	1.73	0.54
1:G:196:ASP:OD1	1:G:200:GLN:N	2.40	0.54
1:n:171:ASP:OD1	1:n:171:ASP:N	2.40	0.54
1:P:196:ASP:OD1	1:P:200:GLN:N	2.39	0.54
1:P:430:GLN:HE21	1:a:402:MET:HB2	1.73	0.54
1:a:276:PRO:HA	1:a:282:PRO:HG3	1.89	0.54
1:d:47:PHE:HE2	1:o:358:GLN:HG2	1.73	0.54
1:d:115:ASN:ND2	1:d:147:ILE:O	2.41	0.54
1:e:69:GLU:OE1	1:e:82:ARG:NH2	2.40	0.54
1:e:129:GLN:HB2	1:e:143:GLN:HE21	1.73	0.54
1:p:50:ALA:O	1:p:52:THR:N	2.40	0.54
1:M:37:GLU:HG2	1:R:29:TYR:HE2	1.72	0.53
1:M:422:SER:HA	1:R:409:LEU:HD21	1.89	0.53
1:b:109:PHE:CE1	1:b:119:THR:HG22	2.42	0.53
1:G:372:GLN:HB2	1:R:343:ASN:HD22	1.71	0.53
1:I:218:TRP:NE1	1:I:303:GLN:OE1	2.39	0.53
1:k:196:ASP:OD1	1:k:200:GLN:N	2.38	0.53
1:q:239:ASP:OD2	1:q:250:THR:OG1	2.25	0.53
1:e:50:ALA:O	1:e:51:LYS:C	2.51	0.53
1:f:276:PRO:HA	1:f:282:PRO:HG3	1.91	0.53
1:f:327:ASP:OD1	1:f:327:ASP:N	2.41	0.53
1:T:174:ASP:HB3	1:T:177:GLN:HB2	1.88	0.53
1:Z:239:ASP:OD1	1:Z:239:ASP:N	2.39	0.53
1:f:168:ALA:O	1:f:210:LYS:NZ	2.41	0.53
1:D:422:SER:HA	1:I:409:LEU:HD21	1.90	0.53
1:T:196:ASP:OD1	1:T:200:GLN:N	2.41	0.53
1:d:433:ILE:HD11	1:i:416:PHE:HZ	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415:ASN:O	1:F:419:ASN:ND2	2.42	0.53
1:U:174:ASP:HB3	1:U:177:GLN:HB2	1.90	0.53
1:W:327:ASP:OD1	1:W:327:ASP:N	2.41	0.53
1:X:23:ILE:HG23	1:X:402:MET:HE1	1.91	0.53
1:X:231:LYS:HB3	1:X:281:THR:HB	1.91	0.53
1:g:23:ILE:HG23	1:g:402:MET:HE1	1.89	0.53
1:k:84:SER:OG	1:k:391:ASN:ND2	2.42	0.53
1:o:183:PRO:HA	1:o:186:TYR:CZ	2.44	0.53
1:K:422:SER:HA	1:P:409:LEU:HD21	1.90	0.53
1:L:82:ARG:HH11	1:L:396:GLU:HG2	1.73	0.53
1:L:427:ASN:OD1	1:R:414:ARG:NH1	2.42	0.53
1:d:433:ILE:HD11	1:i:416:PHE:CZ	2.43	0.53
1:k:427:ASN:OD1	1:q:414:ARG:NH1	2.42	0.53
1:l:183:PRO:HA	1:l:186:TYR:CZ	2.44	0.53
1:d:172:LEU:HB3	1:d:212:GLN:HB2	1.89	0.53
1:h:52:THR:HG23	1:m:60:ALA:CB	2.39	0.53
1:l:196:ASP:OD1	1:l:200:GLN:N	2.35	0.53
1:F:82:ARG:HH11	1:F:396:GLU:HG2	1.74	0.53
1:J:39:ALA:HB1	1:O:365:GLY:HA2	1.91	0.53
1:T:84:SER:OG	1:T:391:ASN:ND2	2.42	0.53
1:Y:372:GLN:HB2	1:j:343:ASN:HD22	1.73	0.53
1:L:327:ASP:OD1	1:L:327:ASP:N	2.40	0.52
1:T:130:VAL:HG12	1:T:137:VAL:HA	1.90	0.52
1:b:276:PRO:HA	1:b:282:PRO:HG3	1.91	0.52
1:f:69:GLU:OE1	1:f:82:ARG:NH2	2.38	0.52
1:h:44:ASN:OD1	1:h:44:ASN:N	2.42	0.52
1:k:6:LEU:HD13	1:q:407:VAL:HG11	1.91	0.52
1:o:41:VAL:HG22	1:o:59:GLN:HB2	1.91	0.52
1:S:196:ASP:OD1	1:S:200:GLN:N	2.41	0.52
1:W:82:ARG:HH11	1:W:396:GLU:HG2	1.74	0.52
1:g:168:ALA:O	1:g:210:LYS:NZ	2.43	0.52
1:D:427:ASN:OD1	1:J:414:ARG:NH1	2.42	0.52
1:L:37:GLU:HG2	1:Q:29:TYR:HE2	1.73	0.52
1:R:84:SER:OG	1:R:391:ASN:ND2	2.43	0.52
1:U:109:PHE:HE1	1:U:119:THR:HG22	1.74	0.52
1:X:82:ARG:HH11	1:X:396:GLU:HG2	1.74	0.52
1:i:137:VAL:HG11	1:i:140:TYR:CE2	2.45	0.52
1:l:386:SER:HB3	1:q:322:PHE:HB3	1.92	0.52
1:J:69:GLU:OE1	1:J:82:ARG:NH2	2.43	0.52
1:K:433:ILE:HD11	1:P:416:PHE:CZ	2.42	0.52
1:Q:196:ASP:OD1	1:Q:200:GLN:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:183:PRO:HA	1:a:186:TYR:CZ	2.45	0.52
1:d:196:ASP:OD1	1:d:200:GLN:N	2.35	0.52
1:n:183:PRO:HA	1:n:186:TYR:CZ	2.44	0.52
1:Q:35:ARG:NH2	1:Q:37:GLU:OE2	2.32	0.52
1:j:253:PHE:HD2	1:j:259:LEU:HA	1.74	0.52
1:m:69:GLU:OE1	1:m:82:ARG:NH2	2.43	0.52
1:p:415:ASN:O	1:p:419:ASN:ND2	2.41	0.52
1:q:84:SER:OG	1:q:391:ASN:ND2	2.43	0.52
1:J:327:ASP:N	1:J:327:ASP:OD1	2.42	0.52
1:L:196:ASP:OD1	1:L:200:GLN:N	2.36	0.52
1:L:430:GLN:HE21	1:W:402:MET:HB2	1.75	0.52
1:X:40:ASP:H	1:c:366:THR:HG23	1.75	0.52
1:Z:82:ARG:HH11	1:Z:396:GLU:HG2	1.74	0.52
1:j:16:LEU:HD22	1:j:412:ALA:HB1	1.91	0.52
1:M:69:GLU:OE1	1:M:82:ARG:NH2	2.43	0.52
1:Q:239:ASP:OD1	1:Q:239:ASP:N	2.35	0.52
1:b:130:VAL:HG12	1:b:137:VAL:HA	1.92	0.52
1:e:433:ILE:HD11	1:j:416:PHE:CZ	2.45	0.52
1:V:168:ALA:O	1:V:210:LYS:NZ	2.43	0.52
1:n:42:TYR:HE2	1:n:55:GLY:HA2	1.75	0.52
1:p:413:GLN:HE21	1:p:417:GLN:NE2	2.08	0.52
1:q:41:VAL:O	1:q:56:GLY:N	2.38	0.52
1:F:196:ASP:OD1	1:F:200:GLN:N	2.43	0.52
1:H:130:VAL:HG12	1:H:137:VAL:HA	1.91	0.52
1:M:131:ASP:OD1	1:M:131:ASP:N	2.41	0.52
1:U:129:GLN:HB2	1:U:143:GLN:NE2	2.25	0.52
1:d:82:ARG:HH11	1:d:396:GLU:HG2	1.74	0.52
1:f:115:ASN:ND2	1:f:147:ILE:O	2.35	0.52
1:j:184:ASP:N	1:j:184:ASP:OD1	2.42	0.52
1:S:151:PHE:CE2	1:S:344:VAL:HG21	2.45	0.51
1:l:105:ARG:NH1	1:l:396:GLU:OE1	2.43	0.51
1:E:35:ARG:NH2	1:E:37:GLU:OE2	2.38	0.51
1:F:174:ASP:HB3	1:F:177:GLN:HB2	1.91	0.51
1:N:92:ALA:HB2	1:N:126:LEU:HD11	1.93	0.51
1:R:68:HIS:CD2	1:R:399:ASN:HB2	2.46	0.51
1:S:37:GLU:HG2	1:X:29:TYR:HE2	1.74	0.51
1:X:130:VAL:HG12	1:X:137:VAL:HA	1.91	0.51
1:Y:239:ASP:OD2	1:Y:250:THR:OG1	2.24	0.51
1:c:174:ASP:HB3	1:c:177:GLN:HB2	1.90	0.51
1:e:6:LEU:HD13	1:k:407:VAL:HG11	1.92	0.51
1:e:203:LYS:HB3	1:e:225:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:109:PHE:CE1	1:g:119:THR:HG22	2.45	0.51
1:l:276:PRO:HA	1:l:282:PRO:HG3	1.92	0.51
1:Q:6:LEU:HD13	1:W:407:VAL:HG11	1.91	0.51
1:Q:183:PRO:HA	1:Q:186:TYR:CZ	2.46	0.51
1:U:35:ARG:NH2	1:U:37:GLU:OE2	2.37	0.51
1:X:168:ALA:O	1:X:210:LYS:NZ	2.43	0.51
1:c:130:VAL:HG12	1:c:137:VAL:HA	1.92	0.51
1:e:129:GLN:HB2	1:e:143:GLN:NE2	2.26	0.51
1:g:196:ASP:OD1	1:g:200:GLN:N	2.40	0.51
1:i:111:LEU:HD11	1:i:147:ILE:HD12	1.92	0.51
1:p:183:PRO:HA	1:p:186:TYR:CZ	2.46	0.51
1:G:327:ASP:OD1	1:G:327:ASP:N	2.43	0.51
1:Z:369:ASP:OD1	1:Z:370:SER:N	2.43	0.51
1:e:16:LEU:HD22	1:e:412:ALA:HB1	1.91	0.51
1:G:422:SER:HA	1:L:409:LEU:HD21	1.92	0.51
1:H:39:ALA:HB1	1:M:365:GLY:HA2	1.92	0.51
1:J:372:GLN:HB2	1:U:343:ASN:HD22	1.76	0.51
1:Q:57:GLY:H	1:V:21:ASN:HD22	1.59	0.51
1:e:82:ARG:HH11	1:e:396:GLU:HG2	1.76	0.51
1:G:430:GLN:HE21	1:R:402:MET:HB2	1.74	0.51
1:I:430:GLN:HE21	1:T:402:MET:HB2	1.75	0.51
1:V:196:ASP:OD1	1:V:200:GLN:N	2.44	0.51
1:b:172:LEU:HB3	1:b:212:GLN:HB2	1.92	0.51
1:i:427:ASN:OD1	1:o:414:ARG:NH1	2.44	0.51
1:l:327:ASP:N	1:l:327:ASP:OD1	2.43	0.51
1:q:413:GLN:HE21	1:q:417:GLN:NE2	2.09	0.51
1:c:429:LEU:HD21	1:h:413:GLN:HG3	1.93	0.51
1:j:42:TYR:CE2	1:o:362:LYS:HD2	2.45	0.51
1:G:69:GLU:OE1	1:G:82:ARG:NH2	2.43	0.51
1:P:372:GLN:HB2	1:a:343:ASN:HD22	1.76	0.51
1:Y:109:PHE:HE1	1:Y:119:THR:HG22	1.76	0.51
1:c:370:SER:OG	1:c:375:GLY:O	2.29	0.51
1:g:84:SER:OG	1:g:391:ASN:ND2	2.44	0.51
1:i:433:ILE:HD11	1:n:416:PHE:HZ	1.75	0.51
1:n:184:ASP:OD1	1:n:184:ASP:N	2.44	0.51
1:L:151:PHE:CE2	1:L:344:VAL:HG21	2.45	0.51
1:P:330:GLU:OE2	1:P:331:ASN:ND2	2.44	0.51
1:X:101:ASN:OD1	1:X:377:LYS:NZ	2.44	0.51
1:X:276:PRO:HA	1:X:282:PRO:HG3	1.92	0.51
1:a:84:SER:OG	1:a:391:ASN:ND2	2.44	0.51
1:n:35:ARG:HB3	1:n:66:GLN:HE21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:130:VAL:HG22	1:p:347:GLY:HA2	1.93	0.51
1:D:101:ASN:OD1	1:D:377:LYS:NZ	2.43	0.50
1:D:130:VAL:HG22	1:D:347:GLY:HA2	1.92	0.50
1:E:151:PHE:CE2	1:E:344:VAL:HG21	2.46	0.50
1:F:430:GLN:HE21	1:Q:402:MET:HB2	1.76	0.50
1:I:37:GLU:HG2	1:N:29:TYR:HE2	1.76	0.50
1:K:39:ALA:HB1	1:P:365:GLY:HA2	1.93	0.50
1:R:172:LEU:HD22	1:R:212:GLN:HA	1.93	0.50
1:R:370:SER:OG	1:R:375:GLY:O	2.29	0.50
1:E:105:ARG:NH1	1:E:396:GLU:OE1	2.44	0.50
1:R:183:PRO:HA	1:R:186:TYR:CZ	2.47	0.50
1:b:101:ASN:OD1	1:b:377:LYS:NZ	2.44	0.50
1:F:430:GLN:HG2	1:L:414:ARG:HD2	1.92	0.50
1:V:93:LYS:NZ	1:V:123:GLU:OE2	2.31	0.50
1:c:427:ASN:HD21	1:i:410:ILE:HG21	1.76	0.50
1:E:196:ASP:OD1	1:E:200:GLN:N	2.43	0.50
1:J:117:MET:HE3	1:J:125:LEU:HD23	1.94	0.50
1:N:151:PHE:CE2	1:N:344:VAL:HG21	2.46	0.50
1:P:57:GLY:H	1:U:21:ASN:HD22	1.59	0.50
1:W:39:ALA:HB1	1:b:365:GLY:HA2	1.92	0.50
1:d:77:ASN:HD21	1:d:79:MET:HB2	1.76	0.50
1:f:33:GLU:HB3	1:f:400:ILE:HG22	1.93	0.50
1:E:109:PHE:CE1	1:E:119:THR:HG22	2.45	0.50
1:E:187:ASN:OD1	1:E:210:LYS:N	2.44	0.50
1:I:151:PHE:CE2	1:I:344:VAL:HG21	2.47	0.50
1:M:151:PHE:CE2	1:M:344:VAL:HG21	2.46	0.50
1:O:16:LEU:HD22	1:O:412:ALA:HB1	1.91	0.50
1:f:171:ASP:N	1:f:171:ASP:OD1	2.40	0.50
1:h:69:GLU:OE1	1:h:82:ARG:NH2	2.45	0.50
1:D:117:MET:HE3	1:D:125:LEU:HD23	1.92	0.50
1:F:105:ARG:NH1	1:F:396:GLU:OE2	2.45	0.50
1:H:40:ASP:H	1:M:366:THR:HG23	1.77	0.50
1:J:119:THR:HG23	1:J:123:GLU:O	2.12	0.50
1:P:129:GLN:HB2	1:P:143:GLN:NE2	2.27	0.50
1:Y:171:ASP:N	1:Y:171:ASP:OD1	2.45	0.50
1:Z:276:PRO:HA	1:Z:282:PRO:HG3	1.92	0.50
1:d:69:GLU:OE1	1:d:82:ARG:NH2	2.45	0.50
1:k:101:ASN:OD1	1:k:377:LYS:NZ	2.43	0.50
1:m:50:ALA:O	1:m:52:THR:N	2.44	0.50
1:H:82:ARG:HH11	1:H:396:GLU:HG2	1.77	0.50
1:X:369:ASP:OD1	1:X:370:SER:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:321:GLY:HA3	1:Y:338:TYR:HB3	1.94	0.50
1:b:171:ASP:OD1	1:b:171:ASP:N	2.43	0.50
1:j:183:PRO:HA	1:j:186:TYR:CZ	2.46	0.50
1:D:82:ARG:HH11	1:D:396:GLU:HG2	1.76	0.50
1:T:117:MET:HE3	1:T:125:LEU:HD23	1.93	0.50
1:T:170:GLY:O	1:T:210:LYS:NZ	2.42	0.50
1:T:415:ASN:O	1:T:419:ASN:ND2	2.43	0.50
1:U:130:VAL:HG12	1:U:137:VAL:HA	1.94	0.50
1:U:381:GLU:OE1	1:U:384:LYS:NZ	2.31	0.50
1:a:33:GLU:HB3	1:a:400:ILE:HG22	1.94	0.50
1:e:196:ASP:OD1	1:e:200:GLN:N	2.40	0.50
1:f:183:PRO:HA	1:f:186:TYR:CZ	2.47	0.50
1:h:171:ASP:OD1	1:h:171:ASP:N	2.43	0.50
1:j:196:ASP:OD1	1:j:200:GLN:N	2.41	0.50
1:k:111:LEU:HD11	1:k:147:ILE:HD12	1.92	0.50
1:F:39:ALA:HB1	1:K:365:GLY:HA2	1.94	0.49
1:Q:130:VAL:HG22	1:Q:347:GLY:HA2	1.94	0.49
1:g:427:ASN:OD1	1:m:414:ARG:NH1	2.45	0.49
1:N:105:ARG:NH1	1:N:396:GLU:OE2	2.45	0.49
1:R:196:ASP:OD1	1:R:200:GLN:N	2.39	0.49
1:X:109:PHE:HE1	1:X:119:THR:HG22	1.76	0.49
1:g:69:GLU:OE1	1:g:82:ARG:NH2	2.45	0.49
1:h:40:ASP:H	1:m:366:THR:HG23	1.77	0.49
1:D:151:PHE:CE2	1:D:344:VAL:HG21	2.47	0.49
1:J:130:VAL:HG12	1:J:137:VAL:HA	1.93	0.49
1:L:433:ILE:HD11	1:Q:416:PHE:CZ	2.47	0.49
1:b:21:ASN:O	1:b:25:ASN:ND2	2.41	0.49
1:c:109:PHE:CE1	1:c:119:THR:HG22	2.47	0.49
1:f:174:ASP:HB3	1:f:177:GLN:HB2	1.95	0.49
1:j:276:PRO:HA	1:j:282:PRO:HG3	1.94	0.49
1:m:105:ARG:NH1	1:m:396:GLU:OE1	2.46	0.49
1:n:33:GLU:HB3	1:n:400:ILE:HG22	1.93	0.49
1:q:40:ASP:OD2	1:q:42:TYR:CE2	2.65	0.49
1:G:174:ASP:HB3	1:G:177:GLN:HB2	1.95	0.49
1:R:151:PHE:CE2	1:R:344:VAL:HG21	2.46	0.49
1:S:415:ASN:O	1:S:419:ASN:ND2	2.45	0.49
1:b:6:LEU:HD13	1:h:407:VAL:HG11	1.94	0.49
1:g:105:ARG:NH1	1:g:396:GLU:OE1	2.44	0.49
1:k:276:PRO:HA	1:k:282:PRO:HG3	1.93	0.49
1:o:369:ASP:OD1	1:o:370:SER:N	2.44	0.49
1:M:82:ARG:HH11	1:M:396:GLU:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:39:ALA:HB1	1:W:365:GLY:HA2	1.93	0.49
1:U:93:LYS:NZ	1:U:123:GLU:OE2	2.36	0.49
1:W:33:GLU:HB3	1:W:400:ILE:HG22	1.94	0.49
1:X:223:THR:HG22	1:X:232:PRO:HA	1.95	0.49
1:b:433:ILE:HD11	1:g:416:PHE:CZ	2.48	0.49
1:c:130:VAL:HG22	1:c:347:GLY:HA2	1.94	0.49
1:i:126:LEU:HD13	1:i:142:PRO:HB2	1.94	0.49
1:D:37:GLU:HG2	1:I:29:TYR:HE2	1.77	0.49
1:J:430:GLN:HE21	1:U:402:MET:HB2	1.77	0.49
1:P:132:PRO:HB3	1:P:344:VAL:HG13	1.93	0.49
1:I:386:SER:HB3	1:N:322:PHE:HB3	1.94	0.49
1:d:354:VAL:HG21	1:d:360:LEU:HD21	1.93	0.49
1:m:174:ASP:HB3	1:m:177:GLN:HB2	1.93	0.49
1:J:130:VAL:HG22	1:J:347:GLY:HA2	1.93	0.49
1:L:105:ARG:NH1	1:L:396:GLU:OE2	2.41	0.49
1:M:196:ASP:OD1	1:M:200:GLN:N	2.37	0.49
1:N:73:ILE:HD13	1:N:397:GLN:HE21	1.77	0.49
1:P:84:SER:OG	1:P:391:ASN:ND2	2.46	0.49
1:Y:130:VAL:HG12	1:Y:137:VAL:HA	1.95	0.49
1:d:429:LEU:HD21	1:i:413:GLN:HG3	1.94	0.49
1:f:422:SER:HA	1:k:409:LEU:HD21	1.93	0.49
1:i:196:ASP:OD1	1:i:200:GLN:N	2.42	0.49
1:m:183:PRO:HA	1:m:186:TYR:CZ	2.47	0.49
1:E:430:GLN:HE21	1:P:402:MET:HB2	1.78	0.49
1:H:35:ARG:NH2	1:H:37:GLU:OE2	2.40	0.49
1:H:327:ASP:N	1:H:327:ASP:OD1	2.45	0.49
1:T:101:ASN:OD1	1:T:377:LYS:NZ	2.46	0.49
1:T:151:PHE:CE2	1:T:344:VAL:HG21	2.48	0.49
1:X:360:LEU:HB3	1:X:368:TRP:HB3	1.94	0.49
1:Y:21:ASN:O	1:Y:25:ASN:ND2	2.42	0.49
1:d:151:PHE:CE2	1:d:344:VAL:HG21	2.48	0.49
1:d:172:LEU:HD22	1:d:212:GLN:HA	1.95	0.49
1:e:105:ARG:NH1	1:e:396:GLU:OE1	2.45	0.49
1:i:109:PHE:CE1	1:i:119:THR:HG22	2.48	0.49
1:D:401:ASP:O	1:D:405:GLU:HG2	2.13	0.49
1:Q:415:ASN:O	1:Q:419:ASN:ND2	2.43	0.49
1:j:422:SER:HA	1:o:409:LEU:HD21	1.95	0.49
1:D:430:GLN:HE21	1:O:402:MET:HB2	1.78	0.48
1:E:130:VAL:HG12	1:E:137:VAL:HA	1.93	0.48
1:F:172:LEU:HB3	1:F:212:GLN:HB2	1.94	0.48
1:G:40:ASP:H	1:L:366:THR:HG23	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:401:ASP:O	1:W:405:GLU:HG2	2.14	0.48
1:b:69:GLU:OE1	1:b:82:ARG:NH2	2.45	0.48
1:j:41:VAL:HG22	1:j:59:GLN:HB2	1.95	0.48
1:F:69:GLU:OE1	1:F:82:ARG:NH2	2.45	0.48
1:H:117:MET:HE3	1:H:125:LEU:HD23	1.94	0.48
1:L:429:LEU:HD21	1:Q:413:GLN:HG3	1.93	0.48
1:M:386:SER:HB3	1:R:322:PHE:HB3	1.95	0.48
1:O:151:PHE:CE2	1:O:344:VAL:HG21	2.48	0.48
1:R:37:GLU:HG2	1:W:29:TYR:HE2	1.78	0.48
1:S:33:GLU:HB3	1:S:400:ILE:HG22	1.94	0.48
1:S:130:VAL:HG12	1:S:137:VAL:HA	1.95	0.48
1:W:131:ASP:N	1:W:131:ASP:OD1	2.46	0.48
1:n:196:ASP:OD1	1:n:200:GLN:N	2.42	0.48
1:E:276:PRO:HA	1:E:282:PRO:HG3	1.95	0.48
1:H:130:VAL:HG22	1:H:347:GLY:HA2	1.94	0.48
1:K:372:GLN:HB2	1:V:343:ASN:HD22	1.78	0.48
1:P:223:THR:HG22	1:P:232:PRO:HA	1.95	0.48
1:V:151:PHE:CE2	1:V:344:VAL:HG21	2.49	0.48
1:V:372:GLN:HB2	1:g:343:ASN:HD22	1.79	0.48
1:W:239:ASP:OD2	1:W:250:THR:OG1	2.25	0.48
1:e:33:GLU:HB3	1:e:400:ILE:HG22	1.95	0.48
1:p:196:ASP:OD1	1:p:200:GLN:N	2.39	0.48
1:J:37:GLU:HG2	1:O:29:TYR:HE2	1.79	0.48
1:N:171:ASP:OD1	1:N:187:ASN:ND2	2.47	0.48
1:Y:69:GLU:OE1	1:Y:82:ARG:NH2	2.46	0.48
1:a:117:MET:HE3	1:a:125:LEU:HD23	1.94	0.48
1:a:130:VAL:HG22	1:a:347:GLY:HA2	1.95	0.48
1:f:196:ASP:OD1	1:f:200:GLN:N	2.43	0.48
1:n:109:PHE:HE1	1:n:119:THR:HG22	1.78	0.48
1:E:117:MET:HE3	1:E:125:LEU:HD23	1.96	0.48
1:P:57:GLY:H	1:U:21:ASN:ND2	2.11	0.48
1:R:415:ASN:O	1:R:419:ASN:ND2	2.46	0.48
1:W:231:LYS:HB3	1:W:281:THR:HB	1.95	0.48
1:d:49:ASN:O	1:d:50:ALA:HB3	2.14	0.48
1:e:130:VAL:HG22	1:e:347:GLY:HA2	1.96	0.48
1:k:223:THR:HG22	1:k:232:PRO:HA	1.95	0.48
1:E:174:ASP:HB3	1:E:177:GLN:HB2	1.95	0.48
1:K:327:ASP:OD1	1:K:327:ASP:N	2.44	0.48
1:M:3:TYR:CZ	1:X:397:GLN:HG3	2.48	0.48
1:P:117:MET:HE3	1:P:125:LEU:HD23	1.94	0.48
1:Q:276:PRO:HA	1:Q:282:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:109:PHE:HE1	1:W:119:THR:HG22	1.79	0.48
1:W:223:THR:HG22	1:W:232:PRO:HA	1.96	0.48
1:Z:6:LEU:HD13	1:f:407:VAL:HG11	1.94	0.48
1:e:151:PHE:CE2	1:e:344:VAL:HG21	2.48	0.48
1:i:171:ASP:OD1	1:i:171:ASP:N	2.41	0.48
1:i:174:ASP:HB3	1:i:177:GLN:HB2	1.95	0.48
1:m:276:PRO:HA	1:m:282:PRO:HG3	1.95	0.48
1:I:109:PHE:CE1	1:I:119:THR:HG22	2.47	0.48
1:M:117:MET:HE3	1:M:125:LEU:HD23	1.95	0.48
1:g:49:ASN:O	1:g:50:ALA:HB2	2.13	0.48
1:G:130:VAL:HG22	1:G:347:GLY:HA2	1.94	0.48
1:R:360:LEU:HB3	1:R:368:TRP:HB3	1.96	0.48
1:U:68:HIS:CD2	1:U:399:ASN:HB2	2.49	0.48
1:V:131:ASP:OD1	1:V:131:ASP:N	2.47	0.48
1:Z:151:PHE:CE2	1:Z:344:VAL:HG21	2.49	0.48
1:J:109:PHE:HE1	1:J:119:THR:HG22	1.78	0.48
1:L:6:LEU:HD13	1:R:407:VAL:HG11	1.96	0.48
1:X:171:ASP:OD1	1:X:171:ASP:N	2.46	0.48
1:a:430:GLN:CD	1:g:414:ARG:HD2	2.38	0.48
1:j:49:ASN:O	1:j:50:ALA:HB2	2.13	0.48
1:n:69:GLU:OE1	1:n:82:ARG:NH2	2.46	0.48
1:q:41:VAL:HG22	1:q:59:GLN:HB2	1.96	0.48
1:q:44:ASN:HD21	1:q:53:THR:HG23	1.78	0.48
1:O:106:ASN:HD22	1:O:106:ASN:H	1.60	0.48
1:R:40:ASP:H	1:W:366:THR:HG23	1.78	0.48
1:S:40:ASP:H	1:X:366:THR:HG23	1.79	0.48
1:U:238:GLY:O	1:U:241:GLN:NE2	2.46	0.48
1:d:129:GLN:HB2	1:d:143:GLN:NE2	2.28	0.48
1:e:422:SER:HA	1:j:409:LEU:HD21	1.95	0.48
1:h:50:ALA:HA	1:h:53:THR:CG2	2.44	0.48
1:o:109:PHE:HE1	1:o:119:THR:HG22	1.79	0.48
1:q:42:TYR:CE1	1:q:55:GLY:HA2	2.48	0.48
1:Q:109:PHE:CE1	1:Q:119:THR:HG22	2.49	0.47
1:S:109:PHE:CE1	1:S:119:THR:HG22	2.46	0.47
1:U:33:GLU:HB3	1:U:400:ILE:HG22	1.96	0.47
1:U:129:GLN:HB2	1:U:143:GLN:HE21	1.79	0.47
1:W:38:PHE:HB2	1:b:28:THR:HG22	1.95	0.47
1:a:433:ILE:HD11	1:f:416:PHE:HZ	1.79	0.47
1:b:111:LEU:HD11	1:b:147:ILE:HD12	1.96	0.47
1:f:84:SER:OG	1:f:391:ASN:ND2	2.47	0.47
1:f:433:ILE:HD11	1:k:416:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:130:VAL:HG22	1:o:347:GLY:HA2	1.96	0.47
1:I:33:GLU:HB3	1:I:400:ILE:HG22	1.96	0.47
1:I:130:VAL:HG12	1:I:137:VAL:HA	1.95	0.47
1:W:57:GLY:H	1:b:21:ASN:HD22	1.62	0.47
1:X:433:ILE:HD11	1:c:416:PHE:HZ	1.77	0.47
1:Z:171:ASP:OD1	1:Z:171:ASP:N	2.46	0.47
1:a:130:VAL:HG12	1:a:137:VAL:HA	1.96	0.47
1:k:171:ASP:OD1	1:k:171:ASP:N	2.44	0.47
1:p:115:ASN:ND2	1:p:147:ILE:O	2.45	0.47
1:F:130:VAL:HG12	1:F:137:VAL:HA	1.95	0.47
1:G:109:PHE:CE1	1:G:119:THR:HG22	2.49	0.47
1:H:401:ASP:O	1:H:405:GLU:HG2	2.14	0.47
1:J:73:ILE:HD13	1:J:397:GLN:HE21	1.77	0.47
1:N:433:ILE:HD11	1:S:416:PHE:HZ	1.79	0.47
1:P:130:VAL:HG12	1:P:137:VAL:HA	1.95	0.47
1:Q:211:ASP:HB3	1:Q:217:THR:HB	1.97	0.47
1:e:321:GLY:HA3	1:e:338:TYR:HB3	1.96	0.47
1:e:430:GLN:CD	1:k:414:ARG:HD2	2.39	0.47
1:q:239:ASP:OD1	1:q:239:ASP:N	2.39	0.47
1:G:172:LEU:HD13	1:G:212:GLN:HA	1.96	0.47
1:X:117:MET:HE3	1:X:125:LEU:HD23	1.97	0.47
1:l:184:ASP:OD1	1:l:184:ASP:N	2.48	0.47
1:K:37:GLU:HG2	1:P:29:TYR:HE2	1.80	0.47
1:L:372:GLN:HB2	1:W:343:ASN:HD22	1.79	0.47
1:M:433:ILE:HD11	1:R:416:PHE:HZ	1.78	0.47
1:P:427:ASN:OD1	1:V:414:ARG:NH1	2.48	0.47
1:R:174:ASP:HB3	1:R:177:GLN:HB2	1.95	0.47
1:S:330:GLU:OE2	1:S:331:ASN:ND2	2.48	0.47
1:X:401:ASP:O	1:X:405:GLU:HG2	2.14	0.47
1:f:433:ILE:HD11	1:k:416:PHE:HZ	1.79	0.47
1:i:16:LEU:HD22	1:i:412:ALA:HB1	1.97	0.47
1:k:13:GLN:NE2	1:q:401:ASP:OD2	2.47	0.47
1:I:422:SER:HA	1:N:409:LEU:HD21	1.96	0.47
1:V:274:GLY:HA3	1:V:285:MET:HG3	1.96	0.47
1:W:3:TYR:CZ	1:h:397:GLN:HG3	2.50	0.47
1:Z:429:LEU:HD21	1:e:413:GLN:HG3	1.96	0.47
1:f:105:ARG:NH1	1:f:396:GLU:OE1	2.48	0.47
1:g:430:GLN:CD	1:m:414:ARG:HD2	2.39	0.47
1:h:196:ASP:OD1	1:h:200:GLN:N	2.45	0.47
1:j:35:ARG:NH2	1:j:37:GLU:OE2	2.41	0.47
1:F:172:LEU:HD13	1:F:212:GLN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:ASP:O	1:F:405:GLU:HG2	2.15	0.47
1:K:84:SER:OG	1:K:391:ASN:ND2	2.48	0.47
1:K:151:PHE:CE2	1:K:344:VAL:HG21	2.49	0.47
1:L:39:ALA:HB1	1:Q:365:GLY:HA2	1.97	0.47
1:M:171:ASP:OD1	1:M:171:ASP:N	2.48	0.47
1:O:172:LEU:HD22	1:O:212:GLN:HA	1.96	0.47
1:Q:57:GLY:H	1:V:21:ASN:ND2	2.13	0.47
1:S:429:LEU:HD21	1:X:413:GLN:HG3	1.95	0.47
1:V:360:LEU:HB3	1:V:368:TRP:HB3	1.96	0.47
1:W:369:ASP:OD1	1:W:370:SER:N	2.47	0.47
1:X:327:ASP:OD1	1:X:327:ASP:N	2.47	0.47
1:Y:209:LEU:HD22	1:Y:219:ASN:HD22	1.80	0.47
1:c:168:ALA:HA	1:c:303:GLN:HE21	1.78	0.47
1:h:430:GLN:CD	1:n:414:ARG:HD2	2.39	0.47
1:l:16:LEU:HD22	1:l:412:ALA:HB1	1.95	0.47
1:m:223:THR:HG22	1:m:232:PRO:HA	1.97	0.47
1:n:327:ASP:OD1	1:n:327:ASP:N	2.48	0.47
1:o:42:TYR:CE2	1:o:55:GLY:HA2	2.50	0.47
1:o:171:ASP:OD1	1:o:171:ASP:N	2.47	0.47
1:o:196:ASP:OD1	1:o:200:GLN:N	2.40	0.47
1:q:51:LYS:HE3	1:q:51:LYS:HB2	1.51	0.47
1:G:117:MET:HE3	1:G:125:LEU:HD23	1.96	0.47
1:L:73:ILE:HD13	1:L:397:GLN:HG2	1.96	0.47
1:V:39:ALA:HB1	1:a:365:GLY:HA2	1.97	0.47
1:W:116:TYR:CE1	1:W:146:ASN:HB2	2.50	0.47
1:Y:80:ASP:O	1:Y:393:GLY:N	2.48	0.47
1:d:401:ASP:O	1:d:405:GLU:HG2	2.15	0.47
1:e:109:PHE:CE1	1:e:119:THR:HG22	2.48	0.47
1:p:239:ASP:OD1	1:p:239:ASP:N	2.36	0.47
1:I:223:THR:HG22	1:I:232:PRO:HA	1.97	0.47
1:K:276:PRO:HA	1:K:282:PRO:HG3	1.97	0.47
1:K:401:ASP:O	1:K:405:GLU:HG2	2.15	0.47
1:L:171:ASP:OD1	1:L:171:ASP:N	2.47	0.47
1:P:3:TYR:CZ	1:a:397:GLN:HG3	2.50	0.47
1:Q:372:GLN:HB2	1:b:343:ASN:HD22	1.80	0.47
1:Z:130:VAL:HG22	1:Z:347:GLY:HA2	1.96	0.47
1:b:151:PHE:CE2	1:b:344:VAL:HG21	2.50	0.47
1:e:130:VAL:HG12	1:e:137:VAL:HA	1.96	0.47
1:o:239:ASP:OD2	1:o:250:THR:OG1	2.33	0.47
1:G:183:PRO:HA	1:G:186:TYR:CZ	2.50	0.47
1:H:183:PRO:HA	1:H:186:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:401:ASP:O	1:U:405:GLU:HG2	2.14	0.47
1:W:130:VAL:HG22	1:W:347:GLY:HA2	1.96	0.47
1:c:69:GLU:OE1	1:c:82:ARG:NH2	2.46	0.47
1:f:329:ASP:OD2	1:f:333:SER:HB2	2.15	0.47
1:g:5:SER:OG	1:g:422:SER:OG	2.27	0.47
1:i:402:MET:O	1:i:406:LEU:HD23	2.15	0.47
1:p:130:VAL:HG12	1:p:137:VAL:HA	1.96	0.47
1:H:80:ASP:O	1:H:393:GLY:N	2.46	0.46
1:J:151:PHE:CE2	1:J:344:VAL:HG21	2.50	0.46
1:K:6:LEU:HD13	1:Q:407:VAL:HG11	1.96	0.46
1:M:276:PRO:HA	1:M:282:PRO:HG3	1.97	0.46
1:T:330:GLU:OE2	1:T:331:ASN:ND2	2.48	0.46
1:e:429:LEU:HD21	1:j:413:GLN:HG3	1.97	0.46
1:n:239:ASP:OD1	1:n:239:ASP:N	2.41	0.46
1:q:196:ASP:OD1	1:q:200:GLN:N	2.41	0.46
1:E:40:ASP:H	1:J:366:THR:HG23	1.81	0.46
1:I:116:TYR:CE1	1:I:146:ASN:HB2	2.50	0.46
1:I:119:THR:HG23	1:I:123:GLU:O	2.14	0.46
1:I:130:VAL:HG22	1:I:347:GLY:HA2	1.96	0.46
1:N:422:SER:HA	1:S:409:LEU:HD21	1.97	0.46
1:R:223:THR:HG22	1:R:232:PRO:HA	1.96	0.46
1:R:238:GLY:O	1:R:241:GLN:NE2	2.49	0.46
1:S:430:GLN:HE21	1:d:402:MET:HB2	1.80	0.46
1:o:49:ASN:O	1:o:50:ALA:CB	2.63	0.46
1:E:401:ASP:O	1:E:405:GLU:HG2	2.16	0.46
1:F:109:PHE:HE1	1:F:119:THR:HG22	1.80	0.46
1:F:171:ASP:N	1:F:171:ASP:OD1	2.47	0.46
1:K:141:GLU:H	1:K:141:GLU:HG3	1.60	0.46
1:P:238:GLY:O	1:P:241:GLN:NE2	2.49	0.46
1:R:6:LEU:HD13	1:X:407:VAL:HG11	1.95	0.46
1:T:40:ASP:H	1:Y:366:THR:HG23	1.80	0.46
1:V:119:THR:HG23	1:V:123:GLU:O	2.15	0.46
1:Z:69:GLU:OE1	1:Z:82:ARG:NH2	2.47	0.46
1:c:151:PHE:CE2	1:c:344:VAL:HG21	2.50	0.46
1:m:42:TYR:HE2	1:m:55:GLY:HA3	1.77	0.46
1:F:109:PHE:CE1	1:F:119:THR:HG22	2.50	0.46
1:I:330:GLU:OE2	1:I:331:ASN:ND2	2.48	0.46
1:Y:402:MET:O	1:Y:406:LEU:HD23	2.14	0.46
1:b:65:GLN:HE21	1:b:362:LYS:HE2	1.81	0.46
1:h:183:PRO:HA	1:h:186:TYR:CZ	2.50	0.46
1:l:422:SER:HA	1:q:409:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:45:SER:HB3	1:o:48:THR:HG23	1.96	0.46
1:p:41:VAL:O	1:p:42:TYR:CD1	2.69	0.46
1:O:47:PHE:O	1:O:48:THR:OG1	2.33	0.46
1:P:183:PRO:HA	1:P:186:TYR:CZ	2.50	0.46
1:Q:47:PHE:O	1:Q:48:THR:OG1	2.33	0.46
1:Q:69:GLU:OE1	1:Q:82:ARG:NH2	2.48	0.46
1:U:168:ALA:HA	1:U:303:GLN:HE21	1.79	0.46
1:V:370:SER:OG	1:V:375:GLY:O	2.34	0.46
1:X:274:GLY:HA3	1:X:285:MET:HG3	1.98	0.46
1:Y:276:PRO:HA	1:Y:282:PRO:HG3	1.97	0.46
1:b:39:ALA:HB1	1:g:365:GLY:HA2	1.97	0.46
1:b:415:ASN:O	1:b:419:ASN:ND2	2.48	0.46
1:e:4:VAL:HG12	1:e:56:GLY:C	2.41	0.46
1:g:38:PHE:CB	1:l:28:THR:HG22	2.44	0.46
1:L:183:PRO:HA	1:L:186:TYR:CZ	2.51	0.46
1:M:223:THR:HA	1:M:232:PRO:HA	1.97	0.46
1:U:207:TYR:OH	1:U:230:GLU:OE2	2.33	0.46
1:Z:321:GLY:HA3	1:Z:338:TYR:HB3	1.97	0.46
1:h:49:ASN:O	1:h:50:ALA:HB3	2.16	0.46
1:E:172:LEU:HB3	1:E:212:GLN:HB2	1.98	0.46
1:L:3:TYR:CZ	1:W:397:GLN:HG3	2.51	0.46
1:M:130:VAL:HG12	1:M:137:VAL:HA	1.97	0.46
1:Q:433:ILE:HD11	1:V:416:PHE:CZ	2.50	0.46
1:X:38:PHE:CB	1:c:28:THR:HG22	2.44	0.46
1:b:402:MET:O	1:b:406:LEU:HD23	2.15	0.46
1:D:171:ASP:OD1	1:D:171:ASP:N	2.49	0.46
1:E:69:GLU:OE1	1:E:82:ARG:NH2	2.48	0.46
1:E:171:ASP:OD1	1:E:171:ASP:N	2.49	0.46
1:M:183:PRO:HA	1:M:186:TYR:CZ	2.51	0.46
1:O:401:ASP:O	1:O:405:GLU:HG2	2.16	0.46
1:R:433:ILE:HD11	1:W:416:PHE:HZ	1.81	0.46
1:S:46:LEU:HD12	1:i:325:LYS:HA	1.98	0.46
1:U:151:PHE:CE2	1:U:344:VAL:HG21	2.50	0.46
1:V:130:VAL:HG22	1:V:347:GLY:HA2	1.98	0.46
1:b:172:LEU:HD22	1:b:212:GLN:HA	1.98	0.46
1:j:430:GLN:CD	1:p:414:ARG:HD2	2.41	0.46
1:k:16:LEU:HD22	1:k:412:ALA:HB1	1.98	0.46
1:q:223:THR:HG22	1:q:232:PRO:HA	1.97	0.46
1:D:187:ASN:OD1	1:D:210:LYS:N	2.49	0.46
1:F:187:ASN:OD1	1:F:210:LYS:N	2.48	0.46
1:P:402:MET:O	1:P:406:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:37:GLU:HG2	1:V:29:TYR:HE2	1.80	0.46
1:Q:40:ASP:H	1:V:366:THR:HG23	1.80	0.46
1:R:117:MET:HE3	1:R:125:LEU:HD23	1.96	0.46
1:W:78:PRO:HA	1:W:392:ASN:HD22	1.80	0.46
1:b:84:SER:OG	1:b:391:ASN:ND2	2.48	0.46
1:c:47:PHE:CE2	1:n:67:PHE:HB2	2.50	0.46
1:c:49:ASN:O	1:c:50:ALA:HB3	2.16	0.46
1:l:171:ASP:OD1	1:l:171:ASP:N	2.49	0.46
1:m:239:ASP:OD2	1:m:250:THR:OG1	2.34	0.46
1:G:172:LEU:HB3	1:G:212:GLN:HB2	1.98	0.46
1:G:340:ASN:OD1	1:G:340:ASN:N	2.49	0.46
1:O:340:ASN:OD1	1:O:340:ASN:N	2.49	0.46
1:P:422:SER:HA	1:U:409:LEU:HD21	1.97	0.46
1:R:130:VAL:HG22	1:R:347:GLY:HA2	1.97	0.46
1:V:6:LEU:HD13	1:b:407:VAL:HG11	1.97	0.46
1:X:188:ARG:HG3	1:X:308:PHE:CG	2.52	0.46
1:d:239:ASP:OD1	1:d:239:ASP:N	2.40	0.46
1:l:38:PHE:HB2	1:q:28:THR:HG22	1.98	0.46
1:F:276:PRO:HA	1:F:282:PRO:HG3	1.97	0.45
1:J:89:PHE:HB2	1:J:104:THR:HG22	1.97	0.45
1:J:369:ASP:OD1	1:J:370:SER:N	2.50	0.45
1:K:116:TYR:CE1	1:K:146:ASN:HB2	2.51	0.45
1:O:28:THR:OG1	1:O:31:PHE:HB2	2.16	0.45
1:P:69:GLU:OE1	1:P:82:ARG:NH2	2.49	0.45
1:R:46:LEU:HD12	1:h:325:LYS:HA	1.98	0.45
1:R:285:MET:HB3	1:R:288:ALA:HB3	1.97	0.45
1:T:401:ASP:O	1:T:405:GLU:HG2	2.16	0.45
1:Z:401:ASP:O	1:Z:405:GLU:HG2	2.17	0.45
1:a:6:LEU:HD13	1:g:407:VAL:HG11	1.98	0.45
1:b:130:VAL:HG22	1:b:347:GLY:HA2	1.98	0.45
1:f:172:LEU:HB3	1:f:212:GLN:HB2	1.97	0.45
1:j:369:ASP:OD1	1:j:370:SER:N	2.46	0.45
1:m:40:ASP:OD2	1:m:42:TYR:CE1	2.69	0.45
1:D:174:ASP:HB3	1:D:177:GLN:HB2	1.97	0.45
1:I:276:PRO:HA	1:I:282:PRO:HG3	1.98	0.45
1:U:360:LEU:HB3	1:U:368:TRP:HB3	1.97	0.45
1:V:130:VAL:HG12	1:V:137:VAL:HA	1.98	0.45
1:W:151:PHE:CE2	1:W:344:VAL:HG21	2.52	0.45
1:X:57:GLY:H	1:c:21:ASN:HD22	1.65	0.45
1:c:325:LYS:HE3	1:c:325:LYS:HB2	1.79	0.45
1:d:422:SER:HA	1:i:409:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:111:LEU:HD11	1:e:147:ILE:HD12	1.98	0.45
1:e:329:ASP:OD2	1:e:333:SER:HB2	2.16	0.45
1:i:429:LEU:HD21	1:n:413:GLN:HG3	1.98	0.45
1:l:402:MET:O	1:l:406:LEU:HD23	2.15	0.45
1:p:40:ASP:OD2	1:p:42:TYR:CE2	2.69	0.45
1:q:183:PRO:HA	1:q:186:TYR:CZ	2.52	0.45
1:D:109:PHE:CE1	1:D:119:THR:HG22	2.51	0.45
1:H:171:ASP:OD1	1:H:171:ASP:N	2.49	0.45
1:L:65:GLN:HE21	1:L:362:LYS:HE2	1.82	0.45
1:O:132:PRO:HB3	1:O:344:VAL:HG13	1.97	0.45
1:Z:109:PHE:HE1	1:Z:119:THR:HG22	1.81	0.45
1:f:151:PHE:CE2	1:f:344:VAL:HG21	2.51	0.45
1:f:198:MET:HG3	1:f:288:ALA:HA	1.99	0.45
1:g:35:ARG:NH2	1:g:37:GLU:OE2	2.45	0.45
1:M:109:PHE:HE1	1:M:119:THR:HG22	1.81	0.45
1:M:198:MET:HE1	1:X:304:PHE:HA	1.98	0.45
1:N:172:LEU:HD22	1:N:212:GLN:HA	1.97	0.45
1:P:47:PHE:O	1:P:48:THR:OG1	2.32	0.45
1:P:401:ASP:O	1:P:405:GLU:HG2	2.16	0.45
1:V:129:GLN:HB2	1:V:143:GLN:NE2	2.32	0.45
1:Y:37:GLU:HG2	1:d:29:TYR:HE2	1.82	0.45
1:b:329:ASP:OD2	1:b:333:SER:HB2	2.16	0.45
1:c:430:GLN:OE1	1:i:414:ARG:NH1	2.50	0.45
1:e:239:ASP:OD1	1:e:239:ASP:N	2.42	0.45
1:h:429:LEU:HD21	1:m:413:GLN:HG3	1.97	0.45
1:i:183:PRO:HA	1:i:186:TYR:CZ	2.51	0.45
1:i:239:ASP:OD1	1:i:239:ASP:N	2.43	0.45
1:m:16:LEU:HD13	1:m:16:LEU:HA	1.80	0.45
1:q:156:GLN:HB2	1:q:292:GLN:NE2	2.31	0.45
1:E:37:GLU:HG2	1:J:29:TYR:HE2	1.81	0.45
1:F:35:ARG:NH2	1:F:37:GLU:OE2	2.38	0.45
1:I:360:LEU:HB3	1:I:368:TRP:HB3	1.99	0.45
1:Q:187:ASN:OD1	1:Q:210:LYS:N	2.49	0.45
1:Q:238:GLY:O	1:Q:241:GLN:NE2	2.49	0.45
1:a:285:MET:HB3	1:a:288:ALA:HB3	1.97	0.45
1:c:433:ILE:HD11	1:h:416:PHE:CZ	2.49	0.45
1:f:231:LYS:NZ	1:f:282:PRO:O	2.38	0.45
1:h:172:LEU:HB3	1:h:212:GLN:HB2	1.98	0.45
1:j:13:GLN:NE2	1:p:401:ASP:OD2	2.49	0.45
1:j:402:MET:O	1:j:406:LEU:HD23	2.17	0.45
1:n:151:PHE:CE2	1:n:344:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:223:THR:HG22	1:n:232:PRO:HA	1.98	0.45
1:p:369:ASP:OD1	1:p:370:SER:N	2.49	0.45
1:J:3:TYR:CE1	1:U:397:GLN:HG3	2.52	0.45
1:J:82:ARG:HG3	1:J:396:GLU:HG2	1.99	0.45
1:J:223:THR:HA	1:J:232:PRO:HA	1.98	0.45
1:O:285:MET:HB3	1:O:288:ALA:HB3	1.98	0.45
1:P:370:SER:OG	1:P:375:GLY:O	2.34	0.45
1:S:130:VAL:HG22	1:S:347:GLY:HA2	1.98	0.45
1:V:401:ASP:O	1:V:405:GLU:HG2	2.17	0.45
1:a:433:ILE:HD11	1:f:416:PHE:CZ	2.52	0.45
1:b:82:ARG:HH11	1:b:396:GLU:HG2	1.82	0.45
1:k:402:MET:O	1:k:406:LEU:HD23	2.16	0.45
1:m:92:ALA:HB2	1:m:126:LEU:HD21	1.98	0.45
1:n:276:PRO:HA	1:n:282:PRO:HG3	1.99	0.45
1:D:114:GLU:HB2	1:D:116:TYR:HD2	1.81	0.45
1:E:129:GLN:HB2	1:E:143:GLN:NE2	2.31	0.45
1:F:183:PRO:HA	1:F:186:TYR:CZ	2.52	0.45
1:I:401:ASP:O	1:I:405:GLU:HG2	2.16	0.45
1:O:16:LEU:HD13	1:O:16:LEU:HA	1.82	0.45
1:R:401:ASP:O	1:R:405:GLU:HG2	2.17	0.45
1:T:68:HIS:CD2	1:T:399:ASN:HB2	2.52	0.45
1:f:109:PHE:CE1	1:f:119:THR:HG22	2.48	0.45
1:h:16:LEU:HD22	1:h:412:ALA:HB1	1.99	0.45
1:o:49:ASN:O	1:o:50:ALA:HB3	2.16	0.45
1:L:116:TYR:CE1	1:L:146:ASN:HB2	2.52	0.45
1:S:401:ASP:O	1:S:405:GLU:HG2	2.17	0.45
1:W:329:ASP:OD2	1:W:333:SER:HB2	2.17	0.45
1:a:211:ASP:HB3	1:a:217:THR:HB	1.99	0.45
1:a:401:ASP:O	1:a:405:GLU:HG2	2.17	0.45
1:d:198:MET:HG3	1:d:288:ALA:HA	1.99	0.45
1:o:132:PRO:HB3	1:o:344:VAL:HG13	1.98	0.45
1:q:130:VAL:HG22	1:q:347:GLY:HA2	1.99	0.45
1:J:276:PRO:HA	1:J:282:PRO:HG3	1.97	0.45
1:S:430:GLN:HA	1:S:433:ILE:HD12	1.99	0.45
1:T:321:GLY:HA3	1:T:338:TYR:HB3	1.98	0.45
1:Y:6:LEU:HD13	1:e:407:VAL:HG11	1.98	0.45
1:g:422:SER:HA	1:l:409:LEU:HD21	1.98	0.45
1:k:183:PRO:HA	1:k:186:TYR:CZ	2.51	0.45
1:n:16:LEU:HD22	1:n:412:ALA:HB1	1.98	0.45
1:q:259:LEU:HD21	1:q:262:LEU:HG	1.99	0.45
1:L:109:PHE:HE1	1:L:119:THR:HG22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:151:PHE:CE2	1:P:344:VAL:HG21	2.52	0.45
1:P:433:ILE:HD11	1:U:416:PHE:HZ	1.82	0.45
1:c:21:ASN:O	1:c:25:ASN:ND2	2.49	0.45
1:d:83:VAL:HG23	1:d:89:PHE:CE2	2.52	0.45
1:d:276:PRO:HA	1:d:282:PRO:HG3	1.99	0.45
1:e:105:ARG:HD2	1:e:396:GLU:OE2	2.17	0.45
1:l:16:LEU:HD13	1:l:16:LEU:HA	1.81	0.45
1:E:129:GLN:HB2	1:E:143:GLN:HE21	1.83	0.44
1:G:79:MET:HE3	1:G:111:LEU:HD21	1.98	0.44
1:G:276:PRO:HA	1:G:282:PRO:HG3	1.98	0.44
1:G:401:ASP:O	1:G:405:GLU:HG2	2.16	0.44
1:N:183:PRO:HA	1:N:186:TYR:CZ	2.52	0.44
1:T:25:ASN:O	1:T:398:SER:OG	2.34	0.44
1:U:316:ASP:OD1	1:U:316:ASP:N	2.49	0.44
1:Y:109:PHE:CE1	1:Y:119:THR:HG22	2.52	0.44
1:Z:231:LYS:HB3	1:Z:281:THR:HB	1.97	0.44
1:c:43:SER:OG	1:c:44:ASN:N	2.47	0.44
1:d:130:VAL:HG12	1:d:137:VAL:HA	1.99	0.44
1:m:50:ALA:C	1:m:52:THR:N	2.74	0.44
1:o:93:LYS:NZ	1:o:123:GLU:OE2	2.33	0.44
1:p:109:PHE:HE1	1:p:119:THR:HG22	1.82	0.44
1:F:129:GLN:HB2	1:F:143:GLN:NE2	2.32	0.44
1:K:223:THR:HA	1:K:232:PRO:HA	1.98	0.44
1:M:172:LEU:HD22	1:M:212:GLN:HA	1.98	0.44
1:O:109:PHE:HE1	1:O:119:THR:HG22	1.82	0.44
1:O:188:ARG:HG3	1:O:308:PHE:CG	2.53	0.44
1:O:239:ASP:OD1	1:O:239:ASP:N	2.49	0.44
1:P:276:PRO:HA	1:P:282:PRO:HG3	1.98	0.44
1:Q:68:HIS:CD2	1:Q:399:ASN:HB2	2.52	0.44
1:S:6:LEU:HD13	1:Y:407:VAL:HG11	1.99	0.44
1:V:329:ASP:OD2	1:V:333:SER:HB2	2.18	0.44
1:W:171:ASP:N	1:W:171:ASP:OD1	2.49	0.44
1:Y:184:ASP:N	1:Y:184:ASP:OD1	2.50	0.44
1:a:151:PHE:CE2	1:a:344:VAL:HG21	2.52	0.44
1:g:45:SER:OG	1:g:46:LEU:N	2.50	0.44
1:j:111:LEU:HD11	1:j:147:ILE:HD12	1.97	0.44
1:k:151:PHE:CE2	1:k:344:VAL:HG21	2.53	0.44
1:m:415:ASN:O	1:m:419:ASN:ND2	2.48	0.44
1:I:153:LYS:HA	1:I:153:LYS:HD3	1.78	0.44
1:J:433:ILE:HD11	1:O:416:PHE:HZ	1.82	0.44
1:N:433:ILE:HD11	1:S:416:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:130:VAL:HG22	1:P:347:GLY:HA2	1.98	0.44
1:T:274:GLY:HA3	1:T:285:MET:HG3	1.99	0.44
1:e:285:MET:HB3	1:e:288:ALA:HB3	1.99	0.44
1:m:125:LEU:O	1:m:144:PRO:HA	2.18	0.44
1:m:130:VAL:HG12	1:m:137:VAL:HA	1.99	0.44
1:m:172:LEU:HD22	1:m:212:GLN:HA	1.99	0.44
1:p:42:TYR:CE1	1:p:55:GLY:CA	2.96	0.44
1:D:3:TYR:CZ	1:O:397:GLN:HG3	2.53	0.44
1:L:276:PRO:HA	1:L:282:PRO:HG3	1.99	0.44
1:M:130:VAL:HG22	1:M:347:GLY:HA2	1.99	0.44
1:Q:73:ILE:HD11	1:Q:395:LEU:HD12	2.00	0.44
1:j:168:ALA:O	1:j:210:LYS:NZ	2.50	0.44
1:l:223:THR:HG22	1:l:232:PRO:HA	1.99	0.44
1:m:151:PHE:CE2	1:m:344:VAL:HG21	2.52	0.44
1:G:51:LYS:HB2	1:G:51:LYS:HE3	1.76	0.44
1:I:239:ASP:OD1	1:I:239:ASP:N	2.42	0.44
1:O:33:GLU:HB3	1:O:400:ILE:HG22	1.98	0.44
1:Q:401:ASP:O	1:Q:405:GLU:HG2	2.18	0.44
1:Q:433:ILE:HD11	1:V:416:PHE:HZ	1.82	0.44
1:T:223:THR:HG22	1:T:232:PRO:HA	2.00	0.44
1:V:40:ASP:H	1:a:366:THR:HG23	1.82	0.44
1:a:351:LEU:HD13	1:a:390:ILE:HD11	1.99	0.44
1:b:93:LYS:HE2	1:b:93:LYS:HB2	1.82	0.44
1:m:109:PHE:HE1	1:m:119:THR:HG22	1.82	0.44
1:q:415:ASN:O	1:q:419:ASN:ND2	2.44	0.44
1:D:19:THR:O	1:D:23:ILE:HG13	2.17	0.44
1:G:101:ASN:OD1	1:G:377:LYS:NZ	2.49	0.44
1:H:47:PHE:O	1:H:48:THR:OG1	2.35	0.44
1:K:38:PHE:CB	1:P:28:THR:HG22	2.47	0.44
1:N:109:PHE:HE1	1:N:119:THR:HG22	1.83	0.44
1:O:109:PHE:CE1	1:O:119:THR:HG22	2.52	0.44
1:O:276:PRO:HA	1:O:282:PRO:HG3	1.99	0.44
1:Q:360:LEU:HB3	1:Q:368:TRP:HB3	2.00	0.44
1:U:109:PHE:CE1	1:U:119:THR:HG22	2.53	0.44
1:Z:209:LEU:HD22	1:Z:219:ASN:HD22	1.82	0.44
1:d:130:VAL:HG22	1:d:347:GLY:HA2	2.00	0.44
1:i:98:PRO:HD2	1:i:99:GLN:OE1	2.17	0.44
1:j:171:ASP:OD1	1:j:171:ASP:N	2.44	0.44
1:D:109:PHE:HE1	1:D:119:THR:HG22	1.82	0.44
1:I:172:LEU:HB3	1:I:212:GLN:HB2	1.99	0.44
1:I:198:MET:HG3	1:I:288:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:174:ASP:HB3	1:L:177:GLN:HB2	1.98	0.44
1:N:119:THR:HG23	1:N:123:GLU:O	2.17	0.44
1:T:45:SER:HB3	1:e:69:GLU:HG3	2.00	0.44
1:a:141:GLU:H	1:a:141:GLU:HG3	1.65	0.44
1:a:171:ASP:N	1:a:171:ASP:OD1	2.49	0.44
1:f:130:VAL:HG22	1:f:347:GLY:HA2	2.00	0.44
1:i:430:GLN:CD	1:o:414:ARG:HD2	2.43	0.44
1:j:46:LEU:HD12	1:j:46:LEU:H	1.82	0.44
1:k:369:ASP:OD1	1:k:370:SER:N	2.51	0.44
1:l:132:PRO:HB3	1:l:344:VAL:HG13	1.99	0.44
1:o:340:ASN:OD1	1:o:340:ASN:N	2.51	0.44
1:F:333:SER:OG	1:F:348:ARG:NH2	2.51	0.44
1:K:3:TYR:CZ	1:V:397:GLN:HG3	2.53	0.44
1:P:137:VAL:HG11	1:P:140:TYR:CE2	2.53	0.44
1:T:35:ARG:NH2	1:T:37:GLU:OE2	2.37	0.44
1:U:329:ASP:OD2	1:U:333:SER:HB2	2.18	0.44
1:X:116:TYR:CE1	1:X:146:ASN:HB2	2.53	0.44
1:Y:116:TYR:CE1	1:Y:146:ASN:HB2	2.52	0.44
1:Z:211:ASP:HB3	1:Z:217:THR:HB	1.99	0.44
1:c:184:ASP:N	1:c:184:ASP:OD1	2.50	0.44
1:e:276:PRO:HA	1:e:282:PRO:HG3	1.99	0.44
1:h:125:LEU:O	1:h:144:PRO:HA	2.18	0.44
1:i:32:LYS:HG3	1:i:67:PHE:CE1	2.53	0.44
1:m:16:LEU:HD22	1:m:412:ALA:HB1	1.99	0.44
1:m:285:MET:SD	1:m:290:PRO:HA	2.57	0.44
1:q:360:LEU:HB3	1:q:368:TRP:HB3	1.99	0.44
1:K:119:THR:HG23	1:K:123:GLU:O	2.18	0.44
1:Q:131:ASP:OD1	1:Q:131:ASP:N	2.51	0.44
1:T:57:GLY:H	1:Y:21:ASN:HD22	1.66	0.44
1:T:370:SER:OG	1:T:375:GLY:O	2.36	0.44
1:W:276:PRO:HA	1:W:282:PRO:HG3	1.98	0.44
1:Z:183:PRO:HA	1:Z:186:TYR:CZ	2.52	0.44
1:c:129:GLN:HB2	1:c:143:GLN:NE2	2.33	0.44
1:d:52:THR:HG21	1:i:60:ALA:CB	2.47	0.44
1:f:93:LYS:HE2	1:f:93:LYS:HB2	1.86	0.44
1:i:52:THR:HG22	1:i:52:THR:O	2.18	0.44
1:j:429:LEU:HD21	1:o:413:GLN:HG3	2.00	0.44
1:l:42:TYR:CE1	1:q:362:LYS:HD3	2.53	0.44
1:m:171:ASP:OD1	1:m:187:ASN:ND2	2.51	0.44
1:o:276:PRO:HA	1:o:282:PRO:HG3	2.00	0.44
1:p:25:ASN:O	1:p:398:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:PRO:HA	1:E:186:TYR:CZ	2.53	0.43
1:F:105:ARG:HH11	1:F:396:GLU:CD	2.25	0.43
1:H:151:PHE:CE2	1:H:344:VAL:HG21	2.53	0.43
1:P:285:MET:HB3	1:P:288:ALA:HB3	1.99	0.43
1:T:6:LEU:HD13	1:Z:407:VAL:HG11	1.99	0.43
1:T:46:LEU:HD12	1:j:325:LYS:HA	1.99	0.43
1:Z:402:MET:O	1:Z:406:LEU:HD23	2.18	0.43
1:f:49:ASN:O	1:f:50:ALA:CB	2.66	0.43
1:f:253:PHE:HD2	1:f:259:LEU:HA	1.83	0.43
1:k:25:ASN:O	1:k:398:SER:OG	2.35	0.43
1:l:39:ALA:HB1	1:q:365:GLY:HA2	2.00	0.43
1:l:351:LEU:HD12	1:l:351:LEU:HA	1.90	0.43
1:n:402:MET:O	1:n:406:LEU:HD23	2.17	0.43
1:p:51:LYS:HB3	1:p:51:LYS:HE2	1.68	0.43
1:F:151:PHE:CE2	1:F:344:VAL:HG21	2.52	0.43
1:G:433:ILE:HD11	1:L:416:PHE:HZ	1.83	0.43
1:J:221:TYR:HB3	1:J:246:HIS:CE1	2.53	0.43
1:K:174:ASP:HB3	1:K:177:GLN:HB2	1.99	0.43
1:T:109:PHE:CE1	1:T:119:THR:HG22	2.49	0.43
1:c:82:ARG:HH11	1:c:396:GLU:HG2	1.82	0.43
1:f:129:GLN:HB2	1:f:143:GLN:NE2	2.33	0.43
1:l:69:GLU:OE1	1:l:82:ARG:NH2	2.50	0.43
1:p:323:LEU:HD11	1:p:326:VAL:HG23	1.99	0.43
1:O:428:GLN:NE2	1:T:413:GLN:HE22	2.15	0.43
1:Q:48:THR:CG2	1:b:68:HIS:HB2	2.48	0.43
1:W:69:GLU:OE1	1:W:82:ARG:NH2	2.48	0.43
1:Y:19:THR:O	1:Y:23:ILE:HG13	2.19	0.43
1:i:49:ASN:O	1:i:50:ALA:HB3	2.18	0.43
1:F:130:VAL:HG22	1:F:347:GLY:HA2	1.99	0.43
1:G:151:PHE:CE2	1:G:344:VAL:HG21	2.54	0.43
1:K:38:PHE:HB2	1:P:28:THR:HG22	1.99	0.43
1:R:211:ASP:HB3	1:R:217:THR:HB	2.01	0.43
1:X:402:MET:O	1:X:406:LEU:HD23	2.19	0.43
1:e:325:LYS:HE3	1:e:325:LYS:HB2	1.63	0.43
1:g:325:LYS:HB2	1:g:325:LYS:HE3	1.74	0.43
1:o:209:LEU:HD22	1:o:219:ASN:HD22	1.83	0.43
1:H:221:TYR:HB3	1:H:246:HIS:CE1	2.54	0.43
1:W:6:LEU:HD13	1:c:407:VAL:HG11	1.99	0.43
1:Z:93:LYS:HE2	1:Z:93:LYS:HB2	1.88	0.43
1:b:137:VAL:HG11	1:b:140:TYR:CE2	2.54	0.43
1:c:401:ASP:O	1:c:405:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:92:ALA:HB2	1:g:126:LEU:HD21	1.99	0.43
1:g:151:PHE:CE2	1:g:344:VAL:HG21	2.52	0.43
1:h:38:PHE:HB2	1:m:28:THR:HG22	2.00	0.43
1:m:109:PHE:CE1	1:m:119:THR:HG22	2.54	0.43
1:H:239:ASP:OD1	1:H:239:ASP:N	2.45	0.43
1:N:47:PHE:C	1:N:48:THR:HG1	2.26	0.43
1:O:68:HIS:NE2	1:O:399:ASN:O	2.50	0.43
1:Q:117:MET:HE3	1:Q:125:LEU:HD23	1.99	0.43
1:Q:151:PHE:CE2	1:Q:344:VAL:HG21	2.54	0.43
1:U:274:GLY:HA3	1:U:285:MET:HG3	1.99	0.43
1:X:183:PRO:HA	1:X:186:TYR:CZ	2.54	0.43
1:c:46:LEU:HD13	1:n:353:ARG:HH11	1.84	0.43
1:c:276:PRO:HA	1:c:282:PRO:HG3	2.00	0.43
1:i:16:LEU:HA	1:i:16:LEU:HD13	1.82	0.43
1:l:33:GLU:HG2	1:l:68:HIS:HE1	1.83	0.43
1:m:327:ASP:OD1	1:m:327:ASP:N	2.52	0.43
1:G:80:ASP:O	1:G:393:GLY:N	2.51	0.43
1:H:51:LYS:HB2	1:H:51:LYS:HE3	1.79	0.43
1:O:141:GLU:H	1:O:141:GLU:HG3	1.64	0.43
1:W:42:TYR:CE2	1:b:362:LYS:HD2	2.54	0.43
1:b:322:PHE:H	1:b:339:SER:H	1.67	0.43
1:j:433:ILE:HD11	1:o:416:PHE:HZ	1.82	0.43
1:m:171:ASP:OD1	1:m:171:ASP:N	2.50	0.43
1:J:223:THR:HG22	1:J:232:PRO:HA	2.00	0.43
1:K:259:LEU:HD21	1:K:262:LEU:HD11	2.00	0.43
1:L:47:PHE:O	1:L:48:THR:OG1	2.35	0.43
1:L:93:LYS:HE2	1:L:93:LYS:HB2	1.87	0.43
1:L:239:ASP:OD1	1:L:239:ASP:N	2.43	0.43
1:M:57:GLY:H	1:R:21:ASN:HD22	1.67	0.43
1:T:130:VAL:HG22	1:T:347:GLY:HA2	2.01	0.43
1:W:322:PHE:H	1:W:339:SER:H	1.66	0.43
1:X:51:LYS:HE3	1:X:51:LYS:HB2	1.81	0.43
1:Y:16:LEU:HD22	1:Y:412:ALA:HB1	2.00	0.43
1:Y:151:PHE:CE2	1:Y:344:VAL:HG21	2.54	0.43
1:d:325:LYS:HB2	1:d:325:LYS:HE3	1.75	0.43
1:e:59:GLN:NE2	1:p:394:MET:HE1	2.34	0.43
1:f:51:LYS:HZ2	1:k:62:GLN:HB3	1.83	0.43
1:h:35:ARG:NH2	1:h:37:GLU:OE2	2.38	0.43
1:i:351:LEU:HD12	1:i:351:LEU:HA	1.90	0.43
1:k:125:LEU:O	1:k:144:PRO:HA	2.19	0.43
1:l:141:GLU:H	1:l:141:GLU:HG3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:151:PHE:CE2	1:o:344:VAL:HG21	2.54	0.43
1:E:82:ARG:NH1	1:E:396:GLU:HB3	2.34	0.43
1:N:137:VAL:HG11	1:N:140:TYR:CE2	2.54	0.43
1:P:48:THR:CG2	1:a:68:HIS:HB2	2.49	0.43
1:Q:129:GLN:HB2	1:Q:143:GLN:NE2	2.34	0.43
1:S:371:THR:H	1:S:374:SER:HG	1.63	0.43
1:c:105:ARG:HD2	1:c:396:GLU:OE2	2.19	0.43
1:e:16:LEU:HD13	1:e:16:LEU:HA	1.85	0.43
1:h:151:PHE:CE2	1:h:344:VAL:HG21	2.54	0.43
1:h:369:ASP:OD1	1:h:370:SER:N	2.51	0.43
1:j:109:PHE:CE1	1:j:119:THR:HG22	2.53	0.43
1:E:433:ILE:HD11	1:J:416:PHE:HZ	1.82	0.43
1:O:69:GLU:OE1	1:O:82:ARG:NH2	2.52	0.43
1:T:322:PHE:H	1:T:339:SER:H	1.67	0.43
1:T:329:ASP:OD2	1:T:333:SER:HB2	2.18	0.43
1:g:183:PRO:HA	1:g:186:TYR:CZ	2.54	0.43
1:k:51:LYS:O	1:k:52:THR:OG1	2.28	0.43
1:m:82:ARG:HH11	1:m:396:GLU:HG2	1.84	0.43
1:o:16:LEU:HD13	1:o:16:LEU:HA	1.91	0.43
1:H:335:MET:HE3	1:H:335:MET:HB2	1.93	0.42
1:K:340:ASN:OD1	1:K:340:ASN:N	2.51	0.42
1:M:80:ASP:O	1:M:393:GLY:N	2.50	0.42
1:M:351:LEU:HD13	1:M:390:ILE:HD11	2.00	0.42
1:R:48:THR:CG2	1:c:68:HIS:HB2	2.48	0.42
1:U:325:LYS:HE3	1:U:325:LYS:HB2	1.83	0.42
1:V:35:ARG:NH2	1:V:37:GLU:OE2	2.41	0.42
1:Y:274:GLY:HA3	1:Y:285:MET:HG3	2.01	0.42
1:e:401:ASP:O	1:e:405:GLU:HG2	2.19	0.42
1:g:16:LEU:HD22	1:g:412:ALA:HB1	2.01	0.42
1:g:105:ARG:HD2	1:g:396:GLU:OE2	2.19	0.42
1:h:129:GLN:HB2	1:h:143:GLN:NE2	2.34	0.42
1:k:184:ASP:OD1	1:k:184:ASP:N	2.51	0.42
1:m:184:ASP:N	1:m:184:ASP:OD1	2.48	0.42
1:p:351:LEU:HD12	1:p:351:LEU:HA	1.89	0.42
1:D:351:LEU:HD13	1:D:390:ILE:HD11	2.01	0.42
1:G:37:GLU:HG2	1:L:29:TYR:HE2	1.84	0.42
1:G:223:THR:HA	1:G:232:PRO:HA	2.02	0.42
1:I:95:ARG:HB2	1:I:124:PHE:CZ	2.54	0.42
1:J:433:ILE:HD11	1:O:416:PHE:CZ	2.54	0.42
1:K:28:THR:OG1	1:K:31:PHE:HB2	2.20	0.42
1:L:69:GLU:OE1	1:L:82:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:183:PRO:HA	1:S:186:TYR:CE2	2.55	0.42
1:b:211:ASP:HB3	1:b:217:THR:HB	2.01	0.42
1:d:238:GLY:O	1:d:241:GLN:NE2	2.51	0.42
1:g:42:TYR:CD2	1:g:55:GLY:HA2	2.55	0.42
1:j:151:PHE:CE2	1:j:344:VAL:HG21	2.54	0.42
1:j:172:LEU:HB3	1:j:212:GLN:HB2	2.02	0.42
1:j:321:GLY:HA3	1:j:338:TYR:HB3	2.00	0.42
1:p:276:PRO:HA	1:p:282:PRO:HG3	2.02	0.42
1:D:322:PHE:H	1:D:339:SER:H	1.67	0.42
1:D:333:SER:OG	1:D:348:ARG:NH2	2.52	0.42
1:F:372:GLN:HE21	1:F:372:GLN:HB3	1.66	0.42
1:M:401:ASP:O	1:M:405:GLU:HG2	2.19	0.42
1:S:325:LYS:HE3	1:S:325:LYS:HB2	1.89	0.42
1:U:171:ASP:OD1	1:U:171:ASP:N	2.52	0.42
1:X:200:GLN:HE21	1:X:200:GLN:HB3	1.66	0.42
1:e:57:GLY:H	1:j:21:ASN:ND2	2.17	0.42
1:m:369:ASP:OD1	1:m:370:SER:N	2.51	0.42
1:n:101:ASN:OD1	1:n:377:LYS:NZ	2.52	0.42
1:o:16:LEU:HD22	1:o:412:ALA:HB1	2.01	0.42
1:F:51:LYS:HB2	1:F:51:LYS:HE3	1.67	0.42
1:F:348:ARG:HE	1:F:348:ARG:HB3	1.62	0.42
1:H:105:ARG:NH1	1:H:396:GLU:OE2	2.44	0.42
1:K:80:ASP:O	1:K:393:GLY:N	2.50	0.42
1:L:198:MET:HE1	1:W:304:PHE:HA	2.01	0.42
1:O:137:VAL:HG11	1:O:140:TYR:CE2	2.55	0.42
1:P:171:ASP:N	1:P:171:ASP:OD1	2.51	0.42
1:P:433:ILE:HD11	1:U:416:PHE:CZ	2.53	0.42
1:Q:223:THR:HG22	1:Q:232:PRO:HA	2.00	0.42
1:T:333:SER:OG	1:T:348:ARG:NH2	2.50	0.42
1:V:171:ASP:OD1	1:V:171:ASP:N	2.51	0.42
1:W:274:GLY:HA3	1:W:285:MET:HG3	2.00	0.42
1:b:401:ASP:O	1:b:405:GLU:HG2	2.19	0.42
1:d:33:GLU:HB3	1:d:400:ILE:HG22	2.00	0.42
1:d:184:ASP:OD1	1:d:184:ASP:N	2.52	0.42
1:e:172:LEU:HB3	1:e:212:GLN:HB2	2.00	0.42
1:h:131:ASP:OD1	1:h:131:ASP:N	2.52	0.42
1:k:82:ARG:HH11	1:k:396:GLU:HG2	1.84	0.42
1:k:239:ASP:OD1	1:k:239:ASP:N	2.44	0.42
1:l:329:ASP:OD2	1:l:333:SER:HB2	2.20	0.42
1:m:164:VAL:HG12	1:m:310:LEU:HA	2.01	0.42
1:m:207:TYR:OH	1:m:230:GLU:OE2	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:351:LEU:HD12	1:m:351:LEU:HA	1.88	0.42
1:p:402:MET:O	1:p:406:LEU:HD23	2.20	0.42
1:q:81:LEU:HD13	1:q:109:PHE:HD2	1.85	0.42
1:D:354:VAL:HG21	1:D:360:LEU:HD21	2.01	0.42
1:E:105:ARG:HH11	1:E:396:GLU:CD	2.27	0.42
1:H:172:LEU:HB3	1:H:212:GLN:HB2	2.00	0.42
1:N:84:SER:OG	1:N:391:ASN:ND2	2.52	0.42
1:Q:130:VAL:HG12	1:Q:137:VAL:HA	2.01	0.42
1:S:101:ASN:OD1	1:S:377:LYS:NZ	2.53	0.42
1:U:130:VAL:HG22	1:U:347:GLY:HA2	2.01	0.42
1:V:51:LYS:HE3	1:V:51:LYS:HB2	1.79	0.42
1:Y:429:LEU:HD21	1:d:413:GLN:HG3	2.01	0.42
1:Z:322:PHE:H	1:Z:339:SER:H	1.67	0.42
1:b:239:ASP:OD1	1:b:239:ASP:N	2.42	0.42
1:b:430:GLN:CD	1:h:414:ARG:HD2	2.44	0.42
1:d:47:PHE:HE2	1:o:358:GLN:HE21	1.67	0.42
1:d:105:ARG:HD2	1:d:396:GLU:OE2	2.20	0.42
1:i:381:GLU:OE1	1:i:384:LYS:HG3	2.19	0.42
1:k:54:PRO:HD3	1:p:14:LEU:CD1	2.50	0.42
1:n:40:ASP:OD2	1:n:42:TYR:CZ	2.73	0.42
1:D:276:PRO:HA	1:D:282:PRO:HG3	2.02	0.42
1:F:117:MET:HE3	1:F:125:LEU:HD23	2.01	0.42
1:J:401:ASP:O	1:J:405:GLU:HG2	2.19	0.42
1:Q:329:ASP:OD2	1:Q:333:SER:HB2	2.20	0.42
1:S:129:GLN:HB2	1:S:143:GLN:HE21	1.84	0.42
1:Z:184:ASP:OD1	1:Z:184:ASP:N	2.51	0.42
1:d:5:SER:OG	1:d:422:SER:OG	2.30	0.42
1:h:54:PRO:HD3	1:m:14:LEU:CD1	2.50	0.42
1:K:351:LEU:HD12	1:K:351:LEU:HA	1.89	0.42
1:L:223:THR:HG22	1:L:232:PRO:HA	2.02	0.42
1:N:171:ASP:OD1	1:N:171:ASP:N	2.52	0.42
1:N:401:ASP:O	1:N:405:GLU:HG2	2.18	0.42
1:W:172:LEU:HB3	1:W:212:GLN:HB2	2.02	0.42
1:Y:95:ARG:HB2	1:Y:124:PHE:CZ	2.54	0.42
1:Z:422:SER:HA	1:e:409:LEU:HD21	2.02	0.42
1:d:109:PHE:CE1	1:d:119:THR:HG22	2.54	0.42
1:g:129:GLN:HB2	1:g:143:GLN:NE2	2.34	0.42
1:k:130:VAL:HG22	1:k:347:GLY:HA2	2.02	0.42
1:k:430:GLN:OE1	1:q:414:ARG:NH1	2.53	0.42
1:n:351:LEU:HD12	1:n:351:LEU:HA	1.85	0.42
1:o:329:ASP:OD2	1:o:333:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:81:LEU:HD13	1:p:109:PHE:HD2	1.85	0.42
1:p:231:LYS:HB3	1:p:281:THR:HB	2.02	0.42
1:D:162:VAL:HG12	1:D:164:VAL:HG13	2.02	0.42
1:E:3:TYR:CZ	1:P:397:GLN:HG3	2.55	0.42
1:F:81:LEU:HD23	1:F:390:ILE:HG21	2.02	0.42
1:G:28:THR:OG1	1:G:31:PHE:HB2	2.20	0.42
1:L:172:LEU:HD22	1:L:212:GLN:HA	2.01	0.42
1:N:109:PHE:CE1	1:N:119:THR:HG22	2.55	0.42
1:P:37:GLU:HG2	1:U:29:TYR:HE2	1.83	0.42
1:T:156:GLN:HB3	1:T:197:SER:HA	2.01	0.42
1:W:93:LYS:HB2	1:W:93:LYS:HE2	1.84	0.42
1:X:141:GLU:H	1:X:141:GLU:HG3	1.66	0.42
1:Y:51:LYS:HB2	1:Y:51:LYS:HE3	1.80	0.42
1:a:231:LYS:HB3	1:a:281:THR:HB	2.01	0.42
1:b:51:LYS:HB2	1:b:51:LYS:HE3	1.79	0.42
1:b:184:ASP:OD1	1:b:184:ASP:N	2.52	0.42
1:i:49:ASN:O	1:i:51:LYS:N	2.47	0.42
1:j:69:GLU:OE1	1:j:82:ARG:NH2	2.52	0.42
1:m:35:ARG:HB3	1:m:66:GLN:HE21	1.85	0.42
1:m:84:SER:OG	1:m:391:ASN:ND2	2.52	0.42
1:o:156:GLN:HB2	1:o:292:GLN:NE2	2.35	0.42
1:G:285:MET:HB3	1:G:288:ALA:HB3	2.02	0.42
1:O:337:THR:HG22	1:O:343:ASN:OD1	2.19	0.42
1:S:117:MET:HE3	1:S:125:LEU:HD23	2.01	0.42
1:S:285:MET:HB3	1:S:288:ALA:HB3	2.02	0.42
1:T:171:ASP:OD1	1:T:171:ASP:N	2.52	0.42
1:V:116:TYR:CE1	1:V:146:ASN:HB2	2.55	0.42
1:W:183:PRO:HA	1:W:186:TYR:CZ	2.55	0.42
1:d:329:ASP:OD2	1:d:333:SER:HB2	2.20	0.42
1:e:38:PHE:CB	1:j:28:THR:HG22	2.49	0.42
1:f:130:VAL:HG12	1:f:137:VAL:HA	2.01	0.42
1:g:49:ASN:HB3	1:g:50:ALA:H	1.66	0.42
1:h:129:GLN:HB2	1:h:143:GLN:HE21	1.85	0.42
1:o:383:ASN:N	1:o:388:GLY:O	2.47	0.42
1:p:84:SER:OG	1:p:391:ASN:ND2	2.52	0.42
1:p:207:TYR:OH	1:p:230:GLU:OE2	2.30	0.42
1:q:125:LEU:O	1:q:144:PRO:HA	2.20	0.42
1:D:69:GLU:OE1	1:D:82:ARG:NH2	2.53	0.42
1:E:96:LEU:O	1:E:98:PRO:HD3	2.20	0.42
1:E:354:VAL:HG21	1:E:360:LEU:HD21	2.01	0.42
1:F:46:LEU:HD11	1:V:323:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:129:GLN:HB2	1:I:143:GLN:NE2	2.35	0.42
1:I:351:LEU:HD13	1:I:390:ILE:HD11	2.01	0.42
1:Q:172:LEU:HD22	1:Q:212:GLN:HA	2.02	0.42
1:S:93:LYS:HE2	1:S:93:LYS:HB2	1.83	0.42
1:a:105:ARG:NH1	1:a:396:GLU:OE1	2.53	0.42
1:d:42:TYR:CE2	1:i:362:LYS:HD2	2.55	0.42
1:f:187:ASN:OD1	1:f:210:LYS:N	2.53	0.42
1:h:422:SER:HA	1:m:409:LEU:HD21	2.02	0.42
1:j:49:ASN:O	1:j:50:ALA:CB	2.68	0.42
1:j:109:PHE:HE1	1:j:119:THR:HG22	1.85	0.42
1:k:240:ALA:HB3	1:k:248:GLY:C	2.45	0.42
1:n:132:PRO:HB3	1:n:344:VAL:HG13	2.02	0.42
1:q:207:TYR:OH	1:q:230:GLU:OE2	2.30	0.42
1:H:116:TYR:CE1	1:H:146:ASN:HB2	2.55	0.41
1:H:352:VAL:HG13	1:H:377:LYS:HB3	2.02	0.41
1:K:172:LEU:HD22	1:K:212:GLN:HA	2.02	0.41
1:M:109:PHE:CE1	1:M:119:THR:HG22	2.55	0.41
1:O:433:ILE:HD11	1:T:416:PHE:HZ	1.84	0.41
1:P:105:ARG:HD2	1:P:396:GLU:OE2	2.20	0.41
1:Q:93:LYS:HE2	1:Q:93:LYS:HB2	1.90	0.41
1:W:168:ALA:HA	1:W:303:GLN:HE21	1.84	0.41
1:a:433:ILE:HD13	1:l:403:THR:HG23	2.02	0.41
1:j:240:ALA:HB3	1:j:248:GLY:C	2.45	0.41
1:k:430:GLN:CD	1:q:414:ARG:HD2	2.45	0.41
1:E:157:THR:HG1	1:E:195:TYR:H	1.67	0.41
1:G:221:TYR:HB3	1:G:246:HIS:CE1	2.55	0.41
1:O:198:MET:HE1	1:Z:304:PHE:HA	2.01	0.41
1:T:381:GLU:OE1	1:T:384:LYS:HG3	2.20	0.41
1:V:47:PHE:HE2	1:g:67:PHE:HB2	1.85	0.41
1:X:151:PHE:CE2	1:X:344:VAL:HG21	2.55	0.41
1:b:325:LYS:HB2	1:b:325:LYS:HE3	1.85	0.41
1:d:253:PHE:HD2	1:d:259:LEU:HA	1.84	0.41
1:g:93:LYS:HB2	1:g:93:LYS:HE2	1.84	0.41
1:k:69:GLU:OE1	1:k:82:ARG:NH2	2.53	0.41
1:l:330:GLU:H	1:l:330:GLU:CD	2.28	0.41
1:m:325:LYS:HB2	1:m:325:LYS:HE3	1.80	0.41
1:m:402:MET:O	1:m:406:LEU:HD23	2.20	0.41
1:n:188:ARG:HG3	1:n:308:PHE:CG	2.55	0.41
1:o:81:LEU:O	1:o:107:GLY:HA3	2.20	0.41
1:E:141:GLU:H	1:E:141:GLU:HG3	1.62	0.41
1:E:433:ILE:HD11	1:J:416:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:LEU:O	1:F:98:PRO:HD3	2.21	0.41
1:F:340:ASN:OD1	1:F:340:ASN:N	2.53	0.41
1:H:433:ILE:HD11	1:M:416:PHE:HZ	1.85	0.41
1:I:3:TYR:CE1	1:T:397:GLN:HG3	2.55	0.41
1:I:369:ASP:OD1	1:I:370:SER:N	2.53	0.41
1:J:153:LYS:HD3	1:J:153:LYS:HA	1.80	0.41
1:K:109:PHE:CE1	1:K:119:THR:HG22	2.55	0.41
1:N:42:TYR:CE2	1:S:362:LYS:HD2	2.55	0.41
1:T:433:ILE:HD11	1:Y:416:PHE:CZ	2.56	0.41
1:V:239:ASP:OD2	1:V:250:THR:OG1	2.28	0.41
1:d:82:ARG:HD2	1:d:396:GLU:HG2	2.02	0.41
1:j:322:PHE:H	1:j:339:SER:H	1.68	0.41
1:l:125:LEU:O	1:l:144:PRO:HA	2.20	0.41
1:l:415:ASN:O	1:l:419:ASN:ND2	2.54	0.41
1:o:109:PHE:CE1	1:o:119:THR:HG22	2.55	0.41
1:q:81:LEU:O	1:q:107:GLY:HA3	2.20	0.41
1:D:404:GLN:NE2	1:D:408:ASP:OD1	2.53	0.41
1:E:168:ALA:O	1:E:210:LYS:NZ	2.52	0.41
1:J:351:LEU:HD12	1:J:351:LEU:HA	1.85	0.41
1:O:172:LEU:HB3	1:O:212:GLN:HB2	2.02	0.41
1:P:80:ASP:O	1:P:393:GLY:N	2.54	0.41
1:P:172:LEU:HB3	1:P:212:GLN:HB2	2.03	0.41
1:V:200:GLN:HE21	1:V:200:GLN:HB3	1.66	0.41
1:Y:433:ILE:HD11	1:d:416:PHE:HZ	1.85	0.41
1:b:433:ILE:HD13	1:m:403:THR:HG23	2.01	0.41
1:c:32:LYS:HD2	1:c:399:ASN:ND2	2.35	0.41
1:d:109:PHE:HE1	1:d:119:THR:HG22	1.85	0.41
1:D:129:GLN:HB2	1:D:143:GLN:NE2	2.35	0.41
1:K:130:VAL:HG22	1:K:347:GLY:HA2	2.02	0.41
1:M:222:TYR:OH	1:M:249:HIS:NE2	2.48	0.41
1:O:57:GLY:H	1:T:21:ASN:HD22	1.69	0.41
1:Q:168:ALA:HA	1:Q:303:GLN:HE21	1.84	0.41
1:W:19:THR:O	1:W:23:ILE:HG13	2.20	0.41
1:X:209:LEU:HD22	1:X:219:ASN:HD22	1.85	0.41
1:X:319:THR:O	1:X:320:THR:HG23	2.21	0.41
1:Y:319:THR:O	1:Y:320:THR:HG23	2.20	0.41
1:Y:401:ASP:O	1:Y:405:GLU:HG2	2.20	0.41
1:a:65:GLN:O	1:a:66:GLN:C	2.63	0.41
1:l:134:SER:OG	1:l:135:GLY:N	2.54	0.41
1:m:329:ASP:OD2	1:m:333:SER:HB2	2.19	0.41
1:o:68:HIS:NE2	1:o:399:ASN:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:325:LYS:HE3	1:o:325:LYS:HB2	1.77	0.41
1:G:47:PHE:O	1:G:48:THR:OG1	2.35	0.41
1:H:101:ASN:OD1	1:H:377:LYS:NZ	2.54	0.41
1:H:141:GLU:H	1:H:141:GLU:HG3	1.63	0.41
1:H:156:GLN:HB3	1:H:197:SER:HA	2.02	0.41
1:K:109:PHE:HE1	1:K:119:THR:HG22	1.85	0.41
1:K:404:GLN:NE2	1:K:408:ASP:OD1	2.53	0.41
1:L:51:LYS:HE3	1:L:51:LYS:HB2	1.86	0.41
1:M:62:GLN:HE21	1:M:62:GLN:HB2	1.62	0.41
1:M:162:VAL:HG12	1:M:164:VAL:HG13	2.03	0.41
1:O:171:ASP:OD1	1:O:171:ASP:N	2.52	0.41
1:Q:151:PHE:CZ	1:Q:344:VAL:HG11	2.55	0.41
1:R:129:GLN:HB2	1:R:129:GLN:HE21	1.65	0.41
1:T:381:GLU:OE1	1:T:384:LYS:NZ	2.36	0.41
1:W:209:LEU:HD22	1:W:219:ASN:HD22	1.85	0.41
1:X:16:LEU:HD22	1:X:412:ALA:HB1	2.02	0.41
1:X:68:HIS:NE2	1:X:399:ASN:O	2.53	0.41
1:d:433:ILE:HD13	1:o:403:THR:HG23	2.01	0.41
1:j:427:ASN:OD1	1:p:414:ARG:NH1	2.53	0.41
1:k:16:LEU:HD13	1:k:16:LEU:HA	1.83	0.41
1:l:40:ASP:OD2	1:l:42:TYR:HD1	2.03	0.41
1:o:184:ASP:N	1:o:184:ASP:OD1	2.53	0.41
1:F:329:ASP:OD2	1:F:333:SER:HB2	2.21	0.41
1:I:172:LEU:HD22	1:I:212:GLN:HA	2.02	0.41
1:K:48:THR:CG2	1:V:68:HIS:HB2	2.50	0.41
1:P:361:ASP:HB3	1:P:371:THR:HG21	2.03	0.41
1:R:141:GLU:H	1:R:141:GLU:HG3	1.61	0.41
1:S:183:PRO:HA	1:S:186:TYR:CZ	2.54	0.41
1:S:329:ASP:OD2	1:S:333:SER:HB2	2.21	0.41
1:S:360:LEU:HB3	1:S:368:TRP:HB3	2.01	0.41
1:T:239:ASP:OD1	1:T:239:ASP:N	2.31	0.41
1:W:46:LEU:HD12	1:m:325:LYS:HA	2.02	0.41
1:W:130:VAL:HG12	1:W:137:VAL:HA	2.01	0.41
1:Y:188:ARG:HG3	1:Y:308:PHE:CG	2.55	0.41
1:Y:253:PHE:HD2	1:Y:259:LEU:HA	1.86	0.41
1:h:99:GLN:H	1:h:99:GLN:HG2	1.72	0.41
1:p:156:GLN:HB2	1:p:292:GLN:NE2	2.35	0.41
1:p:325:LYS:HE3	1:p:325:LYS:HB2	1.87	0.41
1:M:319:THR:O	1:M:320:THR:HG23	2.21	0.41
1:Q:172:LEU:HB3	1:Q:212:GLN:HB2	2.03	0.41
1:R:328:PHE:CE2	1:R:334:VAL:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:117:MET:HE3	1:U:125:LEU:HD23	2.02	0.41
1:V:369:ASP:OD1	1:V:370:SER:N	2.53	0.41
1:W:51:LYS:HE3	1:W:51:LYS:HB2	1.81	0.41
1:W:200:GLN:HE21	1:W:200:GLN:HB3	1.65	0.41
1:Y:183:PRO:HA	1:Y:186:TYR:CZ	2.55	0.41
1:Y:211:ASP:HB3	1:Y:217:THR:HB	2.02	0.41
1:Z:41:VAL:HG22	1:Z:59:GLN:HB2	2.02	0.41
1:a:218:TRP:NE1	1:a:303:GLN:OE1	2.46	0.41
1:h:218:TRP:NE1	1:h:303:GLN:OE1	2.44	0.41
1:h:329:ASP:OD2	1:h:333:SER:HB2	2.21	0.41
1:l:57:GLY:H	1:q:21:ASN:HD22	1.69	0.41
1:l:151:PHE:CE2	1:l:344:VAL:HG21	2.56	0.41
1:n:325:LYS:HE3	1:n:325:LYS:HB2	1.91	0.41
1:E:333:SER:OG	1:E:348:ARG:NH2	2.53	0.41
1:H:21:ASN:O	1:H:25:ASN:ND2	2.47	0.41
1:H:153:LYS:HD3	1:H:153:LYS:HA	1.87	0.41
1:H:321:GLY:HA3	1:H:338:TYR:HB3	2.03	0.41
1:I:42:TYR:CE2	1:N:362:LYS:HD2	2.56	0.41
1:J:351:LEU:HB3	1:J:387:PHE:CD1	2.56	0.41
1:N:429:LEU:HD21	1:S:413:GLN:HG3	2.03	0.41
1:P:105:ARG:HH11	1:P:396:GLU:CD	2.28	0.41
1:S:79:MET:O	1:S:109:PHE:HB2	2.21	0.41
1:T:433:ILE:HD11	1:Y:416:PHE:HZ	1.85	0.41
1:U:188:ARG:HG3	1:U:308:PHE:CG	2.56	0.41
1:V:65:GLN:O	1:V:66:GLN:C	2.64	0.41
1:X:109:PHE:CE1	1:X:119:THR:HG22	2.55	0.41
1:X:119:THR:HG23	1:X:123:GLU:O	2.20	0.41
1:Y:168:ALA:O	1:Y:210:LYS:NZ	2.49	0.41
1:b:129:GLN:HB2	1:b:143:GLN:NE2	2.36	0.41
1:c:77:ASN:HD21	1:c:79:MET:HB2	1.85	0.41
1:d:105:ARG:NH1	1:d:396:GLU:OE1	2.54	0.41
1:d:174:ASP:HB3	1:d:177:GLN:HB2	2.02	0.41
1:d:285:MET:HB3	1:d:288:ALA:HB3	2.03	0.41
1:g:62:GLN:HE21	1:g:62:GLN:HB2	1.66	0.41
1:g:130:VAL:HG12	1:g:137:VAL:HA	2.02	0.41
1:h:253:PHE:HD2	1:h:259:LEU:HA	1.85	0.41
1:l:111:LEU:HD11	1:l:147:ILE:HD12	2.03	0.41
1:p:329:ASP:OD2	1:p:333:SER:HB2	2.20	0.41
1:I:28:THR:OG1	1:I:31:PHE:HB2	2.21	0.41
1:M:42:TYR:CE2	1:R:362:LYS:HD2	2.56	0.41
1:O:402:MET:O	1:O:406:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:65:GLN:O	1:T:66:GLN:C	2.64	0.41
1:U:19:THR:O	1:U:23:ILE:HG13	2.20	0.41
1:U:90:ALA:HB2	1:U:352:VAL:HG21	2.03	0.41
1:W:333:SER:OG	1:W:348:ARG:NH2	2.54	0.41
1:W:372:GLN:HB2	1:h:343:ASN:HD22	1.86	0.41
1:Z:109:PHE:CE1	1:Z:119:THR:HG22	2.56	0.41
1:f:429:LEU:HD21	1:k:413:GLN:HG3	2.03	0.41
1:E:114:GLU:HB2	1:E:116:TYR:HD2	1.86	0.40
1:G:372:GLN:HE21	1:G:372:GLN:HB3	1.65	0.40
1:L:84:SER:OG	1:L:391:ASN:ND2	2.53	0.40
1:L:141:GLU:H	1:L:141:GLU:HG3	1.62	0.40
1:L:195:TYR:HD2	1:L:317:GLY:HA3	1.86	0.40
1:L:369:ASP:OD1	1:L:370:SER:N	2.54	0.40
1:M:153:LYS:HA	1:M:153:LYS:HD3	1.86	0.40
1:N:19:THR:O	1:N:23:ILE:HG13	2.20	0.40
1:R:65:GLN:O	1:R:66:GLN:C	2.64	0.40
1:S:68:HIS:CD2	1:S:399:ASN:HB2	2.56	0.40
1:T:325:LYS:HB2	1:T:325:LYS:HE3	1.81	0.40
1:U:172:LEU:HB3	1:U:212:GLN:HB2	2.02	0.40
1:V:109:PHE:CE2	1:V:125:LEU:HD22	2.55	0.40
1:e:402:MET:O	1:e:406:LEU:HD23	2.21	0.40
1:f:35:ARG:NH2	1:f:37:GLU:OE2	2.37	0.40
1:j:415:ASN:O	1:j:419:ASN:ND2	2.54	0.40
1:l:221:TYR:HB3	1:l:246:HIS:CE1	2.55	0.40
1:E:51:LYS:HE3	1:E:51:LYS:HB2	1.77	0.40
1:I:372:GLN:HE21	1:I:372:GLN:HB3	1.67	0.40
1:K:223:THR:HG22	1:K:232:PRO:HA	2.03	0.40
1:L:319:THR:O	1:L:320:THR:HG23	2.22	0.40
1:L:351:LEU:HD12	1:L:351:LEU:HA	1.92	0.40
1:L:401:ASP:O	1:L:405:GLU:HG2	2.21	0.40
1:M:93:LYS:HE2	1:M:93:LYS:HB2	1.82	0.40
1:M:433:ILE:HD11	1:R:416:PHE:CZ	2.56	0.40
1:N:340:ASN:N	1:N:340:ASN:OD1	2.51	0.40
1:P:95:ARG:HB2	1:P:124:PHE:CZ	2.56	0.40
1:P:168:ALA:O	1:P:210:LYS:NZ	2.54	0.40
1:T:372:GLN:HE21	1:T:372:GLN:HB3	1.65	0.40
1:V:48:THR:CG2	1:g:68:HIS:HB2	2.51	0.40
1:X:6:LEU:HD13	1:d:407:VAL:HG11	2.03	0.40
1:X:333:SER:OG	1:X:348:ARG:NH2	2.54	0.40
1:Y:28:THR:OG1	1:Y:31:PHE:HB2	2.22	0.40
1:Y:322:PHE:H	1:Y:339:SER:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:369:ASP:OD1	1:Y:370:SER:N	2.54	0.40
1:Z:325:LYS:HE3	1:Z:325:LYS:HB2	1.95	0.40
1:a:105:ARG:HH11	1:a:396:GLU:CD	2.29	0.40
1:c:322:PHE:H	1:c:339:SER:H	1.70	0.40
1:c:329:ASP:OD2	1:c:333:SER:HB2	2.21	0.40
1:f:136:GLU:H	1:f:136:GLU:HG2	1.69	0.40
1:f:285:MET:HB3	1:f:288:ALA:HB3	2.02	0.40
1:g:42:TYR:CE2	1:l:362:LYS:HD2	2.57	0.40
1:j:38:PHE:HB2	1:o:28:THR:HG22	2.02	0.40
1:j:50:ALA:O	1:j:53:THR:HG22	2.21	0.40
1:m:73:ILE:HD11	1:m:395:LEU:HD12	2.02	0.40
1:p:171:ASP:OD1	1:p:171:ASP:N	2.53	0.40
1:p:383:ASN:N	1:p:388:GLY:O	2.47	0.40
1:D:183:PRO:HA	1:D:186:TYR:CZ	2.56	0.40
1:H:69:GLU:OE1	1:H:82:ARG:NH2	2.53	0.40
1:H:249:HIS:CG	1:H:268:ILE:HD13	2.56	0.40
1:J:42:TYR:CE2	1:O:362:LYS:HD2	2.57	0.40
1:N:93:LYS:HE2	1:N:93:LYS:HB2	1.87	0.40
1:O:223:THR:HG22	1:O:232:PRO:HA	2.03	0.40
1:P:134:SER:OG	1:P:135:GLY:N	2.55	0.40
1:Q:137:VAL:HG11	1:Q:140:TYR:CE2	2.56	0.40
1:Y:371:THR:H	1:Y:374:SER:HG	1.65	0.40
1:a:62:GLN:HE21	1:a:62:GLN:HB2	1.62	0.40
1:a:77:ASN:HD21	1:a:79:MET:HB2	1.87	0.40
1:d:38:PHE:HB2	1:i:28:THR:HG22	2.03	0.40
1:l:40:ASP:OD2	1:l:42:TYR:CD1	2.75	0.40
1:m:196:ASP:OD1	1:m:200:GLN:N	2.42	0.40
1:p:223:THR:HG22	1:p:232:PRO:HA	2.03	0.40
1:q:383:ASN:N	1:q:388:GLY:O	2.44	0.40
1:D:415:ASN:O	1:D:419:ASN:ND2	2.54	0.40
1:F:141:GLU:H	1:F:141:GLU:HG3	1.60	0.40
1:G:296:PHE:HB3	1:G:298:LEU:HD11	2.03	0.40
1:L:188:ARG:HG3	1:L:308:PHE:CG	2.56	0.40
1:N:96:LEU:O	1:N:98:PRO:HD3	2.21	0.40
1:R:351:LEU:HD12	1:R:351:LEU:HA	1.91	0.40
1:W:80:ASP:O	1:W:393:GLY:N	2.50	0.40
1:Y:42:TYR:CE2	1:d:362:LYS:HD2	2.56	0.40
1:Z:141:GLU:H	1:Z:141:GLU:HG3	1.66	0.40
1:Z:218:TRP:NE1	1:Z:303:GLN:OE1	2.47	0.40
1:b:141:GLU:H	1:b:141:GLU:HG3	1.64	0.40
1:c:16:LEU:HD22	1:c:412:ALA:HB1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:351:LEU:HD13	1:d:390:ILE:HD11	2.04	0.40
1:f:16:LEU:HA	1:f:16:LEU:HD13	1.80	0.40
1:k:141:GLU:H	1:k:141:GLU:HG3	1.67	0.40
1:F:119:THR:HG23	1:F:123:GLU:O	2.22	0.40
1:F:351:LEU:HD13	1:F:390:ILE:HD11	2.04	0.40
1:G:65:GLN:O	1:G:66:GLN:C	2.65	0.40
1:G:319:THR:O	1:G:320:THR:HG23	2.21	0.40
1:I:171:ASP:N	1:I:171:ASP:OD1	2.54	0.40
1:K:40:ASP:OD1	1:K:41:VAL:N	2.55	0.40
1:K:73:ILE:HD13	1:K:397:GLN:HE21	1.87	0.40
1:L:46:LEU:HD12	1:b:325:LYS:HA	2.04	0.40
1:Q:77:ASN:HD21	1:Q:79:MET:HB2	1.86	0.40
1:Q:171:ASP:N	1:Q:171:ASP:OD1	2.53	0.40
1:R:109:PHE:HE1	1:R:119:THR:HG22	1.87	0.40
1:U:381:GLU:OE1	1:U:384:LYS:HG3	2.21	0.40
1:V:333:SER:OG	1:V:348:ARG:NH2	2.54	0.40
1:X:93:LYS:HE2	1:X:93:LYS:HB2	1.92	0.40
1:Z:130:VAL:HG12	1:Z:137:VAL:HA	2.03	0.40
1:c:285:MET:HB3	1:c:288:ALA:HB3	2.04	0.40
1:f:105:ARG:HD2	1:f:396:GLU:OE2	2.22	0.40
1:m:2:SER:HB3	1:m:426:HIS:CE1	2.56	0.40
1:o:105:ARG:HD2	1:o:396:GLU:OE2	2.21	0.40
1:q:323:LEU:HD11	1:q:326:VAL:HG23	2.04	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	D	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	E	433/437 (99%)	416 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	G	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	H	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	I	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	J	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	K	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	L	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	M	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	N	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	O	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	P	433/437 (99%)	416 (96%)	17 (4%)	0	100	100
1	Q	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	R	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	S	433/437 (99%)	422 (98%)	11 (2%)	0	100	100
1	T	433/437 (99%)	417 (96%)	16 (4%)	0	100	100
1	U	433/437 (99%)	417 (96%)	16 (4%)	0	100	100
1	V	433/437 (99%)	417 (96%)	16 (4%)	0	100	100
1	W	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	X	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	Y	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	Z	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	a	433/437 (99%)	418 (96%)	15 (4%)	0	100	100
1	b	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	c	433/437 (99%)	422 (98%)	11 (2%)	0	100	100
1	d	433/437 (99%)	416 (96%)	16 (4%)	1 (0%)	44	74
1	e	433/437 (99%)	418 (96%)	13 (3%)	2 (0%)	25	59
1	f	433/437 (99%)	417 (96%)	14 (3%)	2 (0%)	25	59
1	g	433/437 (99%)	417 (96%)	14 (3%)	2 (0%)	25	59
1	h	433/437 (99%)	420 (97%)	12 (3%)	1 (0%)	44	74
1	i	433/437 (99%)	417 (96%)	14 (3%)	2 (0%)	25	59
1	j	433/437 (99%)	422 (98%)	8 (2%)	3 (1%)	19	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	433/437 (99%)	416 (96%)	15 (4%)	2 (0%)	25	59
1	l	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	m	433/437 (99%)	420 (97%)	12 (3%)	1 (0%)	44	74
1	n	433/437 (99%)	417 (96%)	15 (4%)	1 (0%)	44	74
1	o	433/437 (99%)	419 (97%)	12 (3%)	2 (0%)	25	59
1	p	433/437 (99%)	418 (96%)	13 (3%)	2 (0%)	25	59
1	q	433/437 (99%)	419 (97%)	13 (3%)	1 (0%)	44	74
All	All	17320/17480 (99%)	16740 (97%)	558 (3%)	22 (0%)	50	79

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	e	50	ALA
1	f	49	ASN
1	f	50	ALA
1	g	49	ASN
1	i	52	THR
1	k	52	THR
1	n	53	THR
1	o	50	ALA
1	p	50	ALA
1	e	51	LYS
1	g	50	ALA
1	j	49	ASN
1	j	50	ALA
1	k	51	LYS
1	o	49	ASN
1	j	48	THR
1	p	51	LYS
1	m	49	ASN
1	h	50	ALA
1	i	54	PRO
1	q	55	GLY
1	d	54	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	D	364/366 (100%)	348 (96%)	16 (4%)	24	55	
1	E	364/366 (100%)	348 (96%)	16 (4%)	24	55	
1	F	364/366 (100%)	350 (96%)	14 (4%)	28	59	
1	G	364/366 (100%)	348 (96%)	16 (4%)	24	55	
1	H	364/366 (100%)	350 (96%)	14 (4%)	28	59	
1	I	364/366 (100%)	347 (95%)	17 (5%)	22	53	
1	J	364/366 (100%)	348 (96%)	16 (4%)	24	55	
1	K	364/366 (100%)	342 (94%)	22 (6%)	16	46	
1	L	364/366 (100%)	343 (94%)	21 (6%)	17	47	
1	M	364/366 (100%)	342 (94%)	22 (6%)	16	46	
1	N	364/366 (100%)	346 (95%)	18 (5%)	21	53	
1	O	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	P	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	Q	364/366 (100%)	347 (95%)	17 (5%)	22	53	
1	R	364/366 (100%)	345 (95%)	19 (5%)	19	50	
1	S	364/366 (100%)	348 (96%)	16 (4%)	24	55	
1	T	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	U	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	V	364/366 (100%)	346 (95%)	18 (5%)	21	53	
1	W	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	X	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	Y	364/366 (100%)	348 (96%)	16 (4%)	24	55	
1	Z	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	a	364/366 (100%)	348 (96%)	16 (4%)	24	55	
1	b	364/366 (100%)	351 (96%)	13 (4%)	30	60	
1	c	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	d	364/366 (100%)	344 (94%)	20 (6%)	18	49	
1	e	364/366 (100%)	345 (95%)	19 (5%)	19	50	
1	f	364/366 (100%)	345 (95%)	19 (5%)	19	50	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	g	364/366 (100%)	347 (95%)	17 (5%)	22	53	
1	h	364/366 (100%)	346 (95%)	18 (5%)	21	53	
1	i	364/366 (100%)	346 (95%)	18 (5%)	21	53	
1	j	364/366 (100%)	342 (94%)	22 (6%)	16	46	
1	k	364/366 (100%)	346 (95%)	18 (5%)	21	53	
1	l	364/366 (100%)	347 (95%)	17 (5%)	22	53	
1	m	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	n	364/366 (100%)	353 (97%)	11 (3%)	36	64	
1	o	364/366 (100%)	353 (97%)	11 (3%)	36	64	
1	p	364/366 (100%)	349 (96%)	15 (4%)	26	57	
1	q	364/366 (100%)	352 (97%)	12 (3%)	33	62	
All	All	14560/14640 (100%)	13901 (96%)	659 (4%)	26	54	

All (659) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	16	LEU
1	D	44	ASN
1	D	53	THR
1	D	113	LYS
1	D	131	ASP
1	D	137	VAL
1	D	140	TYR
1	D	141	GLU
1	D	285	MET
1	D	319	THR
1	D	320	THR
1	D	323	LEU
1	D	334	VAL
1	D	351	LEU
1	D	409	LEU
1	D	430	GLN
1	E	16	LEU
1	E	53	THR
1	E	62	GLN
1	E	113	LYS
1	E	131	ASP
1	E	137	VAL

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Mol	Chain	Res	Type
1	E	285	MET
1	E	320	THR
1	E	323	LEU
1	E	334	VAL
1	E	351	LEU
1	E	376	ASP
1	E	396	GLU
1	E	400	ILE
1	E	425	VAL
1	E	430	GLN
1	F	16	LEU
1	F	28	THR
1	F	62	GLN
1	F	113	LYS
1	F	137	VAL
1	F	140	TYR
1	F	141	GLU
1	F	320	THR
1	F	323	LEU
1	F	327	ASP
1	F	334	VAL
1	F	351	LEU
1	F	376	ASP
1	F	430	GLN
1	G	16	LEU
1	G	53	THR
1	G	59	GLN
1	G	62	GLN
1	G	113	LYS
1	G	129	GLN
1	G	131	ASP
1	G	137	VAL
1	G	140	TYR
1	G	198	MET
1	G	320	THR
1	G	323	LEU
1	G	334	VAL
1	G	351	LEU
1	G	376	ASP
1	G	430	GLN
1	H	16	LEU
1	H	51	LYS

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Mol	Chain	Res	Type
1	H	53	THR
1	H	59	GLN
1	H	62	GLN
1	H	113	LYS
1	H	137	VAL
1	H	140	TYR
1	H	198	MET
1	H	320	THR
1	H	323	LEU
1	H	334	VAL
1	H	351	LEU
1	H	430	GLN
1	I	16	LEU
1	I	28	THR
1	I	53	THR
1	I	62	GLN
1	I	113	LYS
1	I	137	VAL
1	I	140	TYR
1	I	198	MET
1	I	319	THR
1	I	320	THR
1	I	323	LEU
1	I	327	ASP
1	I	334	VAL
1	I	346	LEU
1	I	351	LEU
1	I	396	GLU
1	I	430	GLN
1	J	16	LEU
1	J	28	THR
1	J	41	VAL
1	J	53	THR
1	J	113	LYS
1	J	115	ASN
1	J	137	VAL
1	J	140	TYR
1	J	319	THR
1	J	320	THR
1	J	323	LEU
1	J	334	VAL
1	J	351	LEU

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Mol	Chain	Res	Type
1	J	420	SER
1	J	430	GLN
1	J	434	LEU
1	K	16	LEU
1	K	28	THR
1	K	53	THR
1	K	73	ILE
1	K	99	GLN
1	K	113	LYS
1	K	131	ASP
1	K	137	VAL
1	K	140	TYR
1	K	141	GLU
1	K	198	MET
1	K	209	LEU
1	K	319	THR
1	K	320	THR
1	K	323	LEU
1	K	329	ASP
1	K	334	VAL
1	K	346	LEU
1	K	351	LEU
1	K	409	LEU
1	K	420	SER
1	K	430	GLN
1	L	16	LEU
1	L	28	THR
1	L	53	THR
1	L	73	ILE
1	L	83	VAL
1	L	113	LYS
1	L	131	ASP
1	L	137	VAL
1	L	140	TYR
1	L	141	GLU
1	L	209	LEU
1	L	319	THR
1	L	320	THR
1	L	323	LEU
1	L	329	ASP
1	L	334	VAL
1	L	346	LEU

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Mol	Chain	Res	Type
1	L	351	LEU
1	L	376	ASP
1	L	430	GLN
1	L	434	LEU
1	M	16	LEU
1	M	28	THR
1	M	41	VAL
1	M	53	THR
1	M	62	GLN
1	M	113	LYS
1	M	131	ASP
1	M	137	VAL
1	M	140	TYR
1	M	141	GLU
1	M	198	MET
1	M	209	LEU
1	M	319	THR
1	M	320	THR
1	M	323	LEU
1	M	327	ASP
1	M	329	ASP
1	M	334	VAL
1	M	346	LEU
1	M	351	LEU
1	M	376	ASP
1	M	430	GLN
1	N	16	LEU
1	N	28	THR
1	N	53	THR
1	N	62	GLN
1	N	113	LYS
1	N	131	ASP
1	N	137	VAL
1	N	140	TYR
1	N	141	GLU
1	N	198	MET
1	N	319	THR
1	N	320	THR
1	N	323	LEU
1	N	327	ASP
1	N	334	VAL
1	N	351	LEU

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Mol	Chain	Res	Type
1	N	376	ASP
1	N	430	GLN
1	O	16	LEU
1	O	53	THR
1	O	106	ASN
1	O	113	LYS
1	O	131	ASP
1	O	137	VAL
1	O	140	TYR
1	O	141	GLU
1	O	319	THR
1	O	320	THR
1	O	323	LEU
1	O	327	ASP
1	O	334	VAL
1	O	351	LEU
1	O	430	GLN
1	P	16	LEU
1	P	62	GLN
1	P	113	LYS
1	P	131	ASP
1	P	137	VAL
1	P	140	TYR
1	P	141	GLU
1	P	285	MET
1	P	319	THR
1	P	320	THR
1	P	323	LEU
1	P	327	ASP
1	P	334	VAL
1	P	351	LEU
1	P	430	GLN
1	Q	16	LEU
1	Q	28	THR
1	Q	52	THR
1	Q	53	THR
1	Q	113	LYS
1	Q	131	ASP
1	Q	137	VAL
1	Q	140	TYR
1	Q	141	GLU
1	Q	319	THR

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Mol	Chain	Res	Type
1	Q	320	THR
1	Q	323	LEU
1	Q	327	ASP
1	Q	334	VAL
1	Q	351	LEU
1	Q	406	LEU
1	Q	430	GLN
1	R	16	LEU
1	R	28	THR
1	R	52	THR
1	R	91	VAL
1	R	113	LYS
1	R	129	GLN
1	R	131	ASP
1	R	137	VAL
1	R	140	TYR
1	R	141	GLU
1	R	239	ASP
1	R	320	THR
1	R	323	LEU
1	R	327	ASP
1	R	334	VAL
1	R	346	LEU
1	R	351	LEU
1	R	406	LEU
1	R	430	GLN
1	S	16	LEU
1	S	91	VAL
1	S	113	LYS
1	S	131	ASP
1	S	137	VAL
1	S	140	TYR
1	S	141	GLU
1	S	239	ASP
1	S	320	THR
1	S	323	LEU
1	S	327	ASP
1	S	334	VAL
1	S	346	LEU
1	S	351	LEU
1	S	406	LEU
1	S	430	GLN

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Mol	Chain	Res	Type
1	T	16	LEU
1	T	28	THR
1	T	113	LYS
1	T	131	ASP
1	T	137	VAL
1	T	140	TYR
1	T	239	ASP
1	T	320	THR
1	T	323	LEU
1	T	327	ASP
1	T	334	VAL
1	T	346	LEU
1	T	351	LEU
1	T	406	LEU
1	T	430	GLN
1	U	16	LEU
1	U	28	THR
1	U	53	THR
1	U	113	LYS
1	U	131	ASP
1	U	137	VAL
1	U	320	THR
1	U	323	LEU
1	U	327	ASP
1	U	334	VAL
1	U	346	LEU
1	U	351	LEU
1	U	396	GLU
1	U	406	LEU
1	U	430	GLN
1	V	16	LEU
1	V	113	LYS
1	V	119	THR
1	V	131	ASP
1	V	137	VAL
1	V	285	MET
1	V	320	THR
1	V	323	LEU
1	V	327	ASP
1	V	334	VAL
1	V	346	LEU
1	V	351	LEU

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Mol	Chain	Res	Type
1	V	396	GLU
1	V	406	LEU
1	V	409	LEU
1	V	420	SER
1	V	430	GLN
1	V	433	ILE
1	W	16	LEU
1	W	53	THR
1	W	113	LYS
1	W	131	ASP
1	W	137	VAL
1	W	140	TYR
1	W	285	MET
1	W	319	THR
1	W	320	THR
1	W	323	LEU
1	W	334	VAL
1	W	346	LEU
1	W	351	LEU
1	W	406	LEU
1	W	430	GLN
1	X	16	LEU
1	X	53	THR
1	X	62	GLN
1	X	113	LYS
1	X	131	ASP
1	X	137	VAL
1	X	140	TYR
1	X	285	MET
1	X	319	THR
1	X	320	THR
1	X	323	LEU
1	X	334	VAL
1	X	346	LEU
1	X	351	LEU
1	X	430	GLN
1	Y	16	LEU
1	Y	62	GLN
1	Y	106	ASN
1	Y	113	LYS
1	Y	131	ASP
1	Y	137	VAL

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Mol	Chain	Res	Type
1	Y	140	TYR
1	Y	184	ASP
1	Y	285	MET
1	Y	320	THR
1	Y	323	LEU
1	Y	327	ASP
1	Y	334	VAL
1	Y	346	LEU
1	Y	351	LEU
1	Y	430	GLN
1	Z	16	LEU
1	Z	113	LYS
1	Z	137	VAL
1	Z	140	TYR
1	Z	184	ASP
1	Z	285	MET
1	Z	319	THR
1	Z	320	THR
1	Z	323	LEU
1	Z	327	ASP
1	Z	334	VAL
1	Z	346	LEU
1	Z	351	LEU
1	Z	409	LEU
1	Z	430	GLN
1	a	16	LEU
1	a	62	GLN
1	a	106	ASN
1	a	113	LYS
1	a	137	VAL
1	a	140	TYR
1	a	285	MET
1	a	319	THR
1	a	320	THR
1	a	323	LEU
1	a	327	ASP
1	a	334	VAL
1	a	346	LEU
1	a	351	LEU
1	a	406	LEU
1	a	430	GLN
1	b	16	LEU

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Mol	Chain	Res	Type
1	b	91	VAL
1	b	113	LYS
1	b	137	VAL
1	b	140	TYR
1	b	184	ASP
1	b	285	MET
1	b	319	THR
1	b	320	THR
1	b	323	LEU
1	b	327	ASP
1	b	334	VAL
1	b	351	LEU
1	c	16	LEU
1	c	46	LEU
1	c	48	THR
1	c	52	THR
1	c	62	GLN
1	c	91	VAL
1	c	113	LYS
1	c	137	VAL
1	c	140	TYR
1	c	184	ASP
1	c	320	THR
1	c	323	LEU
1	c	327	ASP
1	c	334	VAL
1	c	351	LEU
1	d	16	LEU
1	d	44	ASN
1	d	45	SER
1	d	49	ASN
1	d	51	LYS
1	d	62	GLN
1	d	91	VAL
1	d	113	LYS
1	d	115	ASN
1	d	131	ASP
1	d	137	VAL
1	d	140	TYR
1	d	184	ASP
1	d	285	MET
1	d	320	THR

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Mol	Chain	Res	Type
1	d	323	LEU
1	d	327	ASP
1	d	334	VAL
1	d	346	LEU
1	d	351	LEU
1	e	16	LEU
1	e	45	SER
1	e	51	LYS
1	e	52	THR
1	e	53	THR
1	e	73	ILE
1	e	91	VAL
1	e	113	LYS
1	e	131	ASP
1	e	137	VAL
1	e	140	TYR
1	e	209	LEU
1	e	319	THR
1	e	320	THR
1	e	323	LEU
1	e	327	ASP
1	e	334	VAL
1	e	346	LEU
1	e	351	LEU
1	f	16	LEU
1	f	44	ASN
1	f	46	LEU
1	f	48	THR
1	f	51	LYS
1	f	53	THR
1	f	62	GLN
1	f	91	VAL
1	f	113	LYS
1	f	137	VAL
1	f	140	TYR
1	f	209	LEU
1	f	285	MET
1	f	319	THR
1	f	320	THR
1	f	323	LEU
1	f	334	VAL
1	f	351	LEU

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Mol	Chain	Res	Type
1	f	406	LEU
1	g	16	LEU
1	g	48	THR
1	g	51	LYS
1	g	62	GLN
1	g	113	LYS
1	g	131	ASP
1	g	137	VAL
1	g	140	TYR
1	g	319	THR
1	g	320	THR
1	g	323	LEU
1	g	327	ASP
1	g	334	VAL
1	g	351	LEU
1	g	396	GLU
1	g	406	LEU
1	g	430	GLN
1	h	16	LEU
1	h	43	SER
1	h	51	LYS
1	h	62	GLN
1	h	91	VAL
1	h	113	LYS
1	h	131	ASP
1	h	137	VAL
1	h	140	TYR
1	h	319	THR
1	h	320	THR
1	h	323	LEU
1	h	327	ASP
1	h	334	VAL
1	h	346	LEU
1	h	351	LEU
1	h	396	GLU
1	h	406	LEU
1	i	16	LEU
1	i	43	SER
1	i	44	ASN
1	i	45	SER
1	i	51	LYS
1	i	99	GLN

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Mol	Chain	Res	Type
1	i	100	GLN
1	i	113	LYS
1	i	131	ASP
1	i	137	VAL
1	i	319	THR
1	i	320	THR
1	i	323	LEU
1	i	327	ASP
1	i	334	VAL
1	i	346	LEU
1	i	396	GLU
1	i	430	GLN
1	j	16	LEU
1	j	44	ASN
1	j	45	SER
1	j	47	PHE
1	j	51	LYS
1	j	52	THR
1	j	62	GLN
1	j	83	VAL
1	j	99	GLN
1	j	113	LYS
1	j	131	ASP
1	j	137	VAL
1	j	140	TYR
1	j	184	ASP
1	j	319	THR
1	j	320	THR
1	j	323	LEU
1	j	327	ASP
1	j	334	VAL
1	j	346	LEU
1	j	351	LEU
1	j	430	GLN
1	k	16	LEU
1	k	41	VAL
1	k	44	ASN
1	k	52	THR
1	k	59	GLN
1	k	99	GLN
1	k	113	LYS
1	k	131	ASP

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Mol	Chain	Res	Type
1	k	137	VAL
1	k	140	TYR
1	k	319	THR
1	k	320	THR
1	k	323	LEU
1	k	327	ASP
1	k	334	VAL
1	k	346	LEU
1	k	351	LEU
1	k	430	GLN
1	l	16	LEU
1	l	42	TYR
1	l	44	ASN
1	l	49	ASN
1	l	53	THR
1	l	62	GLN
1	l	113	LYS
1	l	137	VAL
1	l	140	TYR
1	l	184	ASP
1	l	319	THR
1	l	320	THR
1	l	323	LEU
1	l	334	VAL
1	l	351	LEU
1	l	372	GLN
1	l	396	GLU
1	m	16	LEU
1	m	43	SER
1	m	44	ASN
1	m	53	THR
1	m	62	GLN
1	m	113	LYS
1	m	137	VAL
1	m	140	TYR
1	m	184	ASP
1	m	319	THR
1	m	320	THR
1	m	323	LEU
1	m	334	VAL
1	m	351	LEU
1	m	396	GLU

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Mol	Chain	Res	Type
1	n	16	LEU
1	n	51	LYS
1	n	113	LYS
1	n	137	VAL
1	n	140	TYR
1	n	184	ASP
1	n	319	THR
1	n	320	THR
1	n	334	VAL
1	n	351	LEU
1	n	353	ARG
1	o	16	LEU
1	o	44	ASN
1	o	53	THR
1	o	113	LYS
1	o	137	VAL
1	o	140	TYR
1	o	319	THR
1	o	320	THR
1	o	323	LEU
1	o	334	VAL
1	o	351	LEU
1	p	16	LEU
1	p	42	TYR
1	p	43	SER
1	p	44	ASN
1	p	49	ASN
1	p	52	THR
1	p	53	THR
1	p	113	LYS
1	p	137	VAL
1	p	140	TYR
1	p	319	THR
1	p	320	THR
1	p	323	LEU
1	p	334	VAL
1	p	351	LEU
1	q	16	LEU
1	q	41	VAL
1	q	51	LYS
1	q	52	THR
1	q	113	LYS

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Mol	Chain	Res	Type
1	q	137	VAL
1	q	140	TYR
1	q	319	THR
1	q	320	THR
1	q	323	LEU
1	q	334	VAL
1	q	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (589) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	44	ASN
1	D	62	GLN
1	D	99	GLN
1	D	129	GLN
1	D	200	GLN
1	D	234	ASN
1	D	246	HIS
1	D	356	ASN
1	D	372	GLN
1	D	391	ASN
1	D	404	GLN
1	D	428	GLN
1	D	435	GLN
1	E	44	ASN
1	E	62	GLN
1	E	110	HIS
1	E	129	GLN
1	E	143	GLN
1	E	200	GLN
1	E	234	ASN
1	E	372	GLN
1	E	391	ASN
1	E	397	GLN
1	E	426	HIS
1	E	428	GLN
1	E	435	GLN
1	F	21	ASN
1	F	62	GLN
1	F	99	GLN
1	F	106	ASN
1	F	110	HIS

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Mol	Chain	Res	Type
1	F	129	GLN
1	F	143	GLN
1	F	200	GLN
1	F	234	ASN
1	F	356	ASN
1	F	372	GLN
1	F	391	ASN
1	F	428	GLN
1	F	435	GLN
1	G	62	GLN
1	G	65	GLN
1	G	129	GLN
1	G	143	GLN
1	G	200	GLN
1	G	234	ASN
1	G	246	HIS
1	G	372	GLN
1	G	391	ASN
1	G	397	GLN
1	G	428	GLN
1	G	430	GLN
1	G	435	GLN
1	H	62	GLN
1	H	76	ASN
1	H	129	GLN
1	H	200	GLN
1	H	356	ASN
1	H	372	GLN
1	H	391	ASN
1	H	397	GLN
1	H	428	GLN
1	H	430	GLN
1	H	435	GLN
1	I	21	ASN
1	I	22	ASN
1	I	62	GLN
1	I	99	GLN
1	I	110	HIS
1	I	129	GLN
1	I	143	GLN
1	I	200	GLN
1	I	234	ASN

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Mol	Chain	Res	Type
1	I	246	HIS
1	I	263	ASN
1	I	356	ASN
1	I	372	GLN
1	I	391	ASN
1	I	397	GLN
1	I	417	GLN
1	I	428	GLN
1	I	430	GLN
1	I	435	GLN
1	J	21	ASN
1	J	62	GLN
1	J	99	GLN
1	J	129	GLN
1	J	143	GLN
1	J	200	GLN
1	J	234	ASN
1	J	246	HIS
1	J	263	ASN
1	J	266	GLN
1	J	331	ASN
1	J	372	GLN
1	J	391	ASN
1	J	397	GLN
1	J	417	GLN
1	J	428	GLN
1	J	430	GLN
1	J	435	GLN
1	K	21	ASN
1	K	62	GLN
1	K	99	GLN
1	K	106	ASN
1	K	110	HIS
1	K	129	GLN
1	K	143	GLN
1	K	200	GLN
1	K	246	HIS
1	K	356	ASN
1	K	372	GLN
1	K	391	ASN
1	K	397	GLN
1	K	428	GLN

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Mol	Chain	Res	Type
1	K	435	GLN
1	L	21	ASN
1	L	27	ASN
1	L	62	GLN
1	L	76	ASN
1	L	99	GLN
1	L	110	HIS
1	L	129	GLN
1	L	200	GLN
1	L	234	ASN
1	L	263	ASN
1	L	372	GLN
1	L	391	ASN
1	L	417	GLN
1	L	428	GLN
1	L	430	GLN
1	L	435	GLN
1	M	21	ASN
1	M	62	GLN
1	M	99	GLN
1	M	110	HIS
1	M	129	GLN
1	M	200	GLN
1	M	356	ASN
1	M	372	GLN
1	M	391	ASN
1	M	397	GLN
1	M	417	GLN
1	M	428	GLN
1	M	435	GLN
1	N	21	ASN
1	N	62	GLN
1	N	99	GLN
1	N	129	GLN
1	N	143	GLN
1	N	200	GLN
1	N	246	HIS
1	N	372	GLN
1	N	391	ASN
1	N	397	GLN
1	N	417	GLN
1	N	428	GLN

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Mol	Chain	Res	Type
1	N	430	GLN
1	N	435	GLN
1	O	21	ASN
1	O	62	GLN
1	O	99	GLN
1	O	106	ASN
1	O	110	HIS
1	O	129	GLN
1	O	143	GLN
1	O	156	GLN
1	O	200	GLN
1	O	234	ASN
1	O	246	HIS
1	O	372	GLN
1	O	391	ASN
1	O	417	GLN
1	O	428	GLN
1	O	435	GLN
1	P	21	ASN
1	P	62	GLN
1	P	77	ASN
1	P	99	GLN
1	P	129	GLN
1	P	143	GLN
1	P	200	GLN
1	P	234	ASN
1	P	246	HIS
1	P	343	ASN
1	P	372	GLN
1	P	391	ASN
1	P	417	GLN
1	P	428	GLN
1	P	435	GLN
1	Q	21	ASN
1	Q	62	GLN
1	Q	76	ASN
1	Q	77	ASN
1	Q	99	GLN
1	Q	129	GLN
1	Q	143	GLN
1	Q	200	GLN
1	Q	234	ASN

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Mol	Chain	Res	Type
1	Q	246	HIS
1	Q	343	ASN
1	Q	372	GLN
1	Q	391	ASN
1	Q	428	GLN
1	Q	435	GLN
1	R	21	ASN
1	R	27	ASN
1	R	62	GLN
1	R	99	GLN
1	R	129	GLN
1	R	143	GLN
1	R	200	GLN
1	R	234	ASN
1	R	246	HIS
1	R	303	GLN
1	R	343	ASN
1	R	372	GLN
1	R	391	ASN
1	R	397	GLN
1	R	417	GLN
1	R	428	GLN
1	R	430	GLN
1	R	435	GLN
1	S	21	ASN
1	S	27	ASN
1	S	62	GLN
1	S	99	GLN
1	S	129	GLN
1	S	143	GLN
1	S	200	GLN
1	S	246	HIS
1	S	343	ASN
1	S	356	ASN
1	S	372	GLN
1	S	391	ASN
1	S	417	GLN
1	S	428	GLN
1	S	430	GLN
1	S	435	GLN
1	T	21	ASN
1	T	44	ASN

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Mol	Chain	Res	Type
1	T	62	GLN
1	T	129	GLN
1	T	143	GLN
1	T	200	GLN
1	T	255	ASN
1	T	303	GLN
1	T	343	ASN
1	T	372	GLN
1	T	391	ASN
1	T	428	GLN
1	T	435	GLN
1	U	21	ASN
1	U	62	GLN
1	U	99	GLN
1	U	129	GLN
1	U	143	GLN
1	U	200	GLN
1	U	234	ASN
1	U	303	GLN
1	U	343	ASN
1	U	372	GLN
1	U	391	ASN
1	U	404	GLN
1	U	428	GLN
1	U	430	GLN
1	U	435	GLN
1	V	21	ASN
1	V	44	ASN
1	V	62	GLN
1	V	99	GLN
1	V	129	GLN
1	V	143	GLN
1	V	200	GLN
1	V	234	ASN
1	V	343	ASN
1	V	372	GLN
1	V	391	ASN
1	V	428	GLN
1	V	435	GLN
1	W	21	ASN
1	W	44	ASN
1	W	62	GLN

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Mol	Chain	Res	Type
1	W	76	ASN
1	W	129	GLN
1	W	200	GLN
1	W	219	ASN
1	W	234	ASN
1	W	303	GLN
1	W	343	ASN
1	W	372	GLN
1	W	391	ASN
1	W	428	GLN
1	W	432	ASN
1	W	435	GLN
1	X	21	ASN
1	X	44	ASN
1	X	62	GLN
1	X	129	GLN
1	X	200	GLN
1	X	234	ASN
1	X	343	ASN
1	X	356	ASN
1	X	372	GLN
1	X	391	ASN
1	X	417	GLN
1	X	428	GLN
1	X	435	GLN
1	Y	13	GLN
1	Y	21	ASN
1	Y	62	GLN
1	Y	99	GLN
1	Y	129	GLN
1	Y	156	GLN
1	Y	200	GLN
1	Y	219	ASN
1	Y	343	ASN
1	Y	372	GLN
1	Y	391	ASN
1	Y	417	GLN
1	Y	428	GLN
1	Y	432	ASN
1	Y	435	GLN
1	Z	21	ASN
1	Z	62	GLN

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Mol	Chain	Res	Type
1	Z	99	GLN
1	Z	110	HIS
1	Z	129	GLN
1	Z	156	GLN
1	Z	200	GLN
1	Z	219	ASN
1	Z	246	HIS
1	Z	343	ASN
1	Z	356	ASN
1	Z	372	GLN
1	Z	391	ASN
1	Z	417	GLN
1	Z	430	GLN
1	Z	435	GLN
1	a	21	ASN
1	a	62	GLN
1	a	77	ASN
1	a	106	ASN
1	a	129	GLN
1	a	200	GLN
1	a	343	ASN
1	a	372	GLN
1	a	391	ASN
1	a	417	GLN
1	a	428	GLN
1	a	430	GLN
1	a	432	ASN
1	a	435	GLN
1	b	21	ASN
1	b	62	GLN
1	b	77	ASN
1	b	99	GLN
1	b	110	HIS
1	b	129	GLN
1	b	143	GLN
1	b	200	GLN
1	b	246	HIS
1	b	343	ASN
1	b	372	GLN
1	b	391	ASN
1	b	417	GLN
1	b	428	GLN

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Mol	Chain	Res	Type
1	b	435	GLN
1	c	21	ASN
1	c	27	ASN
1	c	49	ASN
1	c	62	GLN
1	c	77	ASN
1	c	110	HIS
1	c	129	GLN
1	c	143	GLN
1	c	200	GLN
1	c	234	ASN
1	c	303	GLN
1	c	343	ASN
1	c	372	GLN
1	c	391	ASN
1	c	417	GLN
1	c	428	GLN
1	c	435	GLN
1	d	21	ASN
1	d	27	ASN
1	d	62	GLN
1	d	77	ASN
1	d	99	GLN
1	d	129	GLN
1	d	143	GLN
1	d	200	GLN
1	d	343	ASN
1	d	372	GLN
1	d	391	ASN
1	d	417	GLN
1	d	428	GLN
1	d	432	ASN
1	d	435	GLN
1	e	21	ASN
1	e	62	GLN
1	e	129	GLN
1	e	143	GLN
1	e	200	GLN
1	e	343	ASN
1	e	372	GLN
1	e	391	ASN
1	e	428	GLN

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Mol	Chain	Res	Type
1	e	435	GLN
1	f	21	ASN
1	f	44	ASN
1	f	62	GLN
1	f	99	GLN
1	f	129	GLN
1	f	143	GLN
1	f	200	GLN
1	f	343	ASN
1	f	372	GLN
1	f	391	ASN
1	f	417	GLN
1	f	428	GLN
1	f	435	GLN
1	g	22	ASN
1	g	49	ASN
1	g	62	GLN
1	g	77	ASN
1	g	99	GLN
1	g	129	GLN
1	g	143	GLN
1	g	146	ASN
1	g	200	GLN
1	g	343	ASN
1	g	372	GLN
1	g	391	ASN
1	g	417	GLN
1	g	428	GLN
1	g	435	GLN
1	h	21	ASN
1	h	49	ASN
1	h	62	GLN
1	h	99	GLN
1	h	129	GLN
1	h	143	GLN
1	h	146	ASN
1	h	200	GLN
1	h	286	ASN
1	h	343	ASN
1	h	372	GLN
1	h	391	ASN
1	h	428	GLN

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Mol	Chain	Res	Type
1	h	435	GLN
1	i	21	ASN
1	i	59	GLN
1	i	62	GLN
1	i	129	GLN
1	i	146	ASN
1	i	200	GLN
1	i	214	GLN
1	i	234	ASN
1	i	372	GLN
1	i	391	ASN
1	i	428	GLN
1	i	435	GLN
1	j	13	GLN
1	j	21	ASN
1	j	49	ASN
1	j	62	GLN
1	j	100	GLN
1	j	129	GLN
1	j	200	GLN
1	j	214	GLN
1	j	234	ASN
1	j	343	ASN
1	j	372	GLN
1	j	391	ASN
1	j	428	GLN
1	j	435	GLN
1	k	21	ASN
1	k	44	ASN
1	k	49	ASN
1	k	62	GLN
1	k	77	ASN
1	k	99	GLN
1	k	129	GLN
1	k	156	GLN
1	k	200	GLN
1	k	343	ASN
1	k	372	GLN
1	k	391	ASN
1	k	435	GLN
1	l	21	ASN
1	l	44	ASN

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Mol	Chain	Res	Type
1	l	62	GLN
1	l	99	GLN
1	l	129	GLN
1	l	156	GLN
1	l	200	GLN
1	l	214	GLN
1	l	234	ASN
1	l	246	HIS
1	l	343	ASN
1	l	391	ASN
1	l	426	HIS
1	l	428	GLN
1	l	432	ASN
1	l	435	GLN
1	m	21	ASN
1	m	49	ASN
1	m	62	GLN
1	m	99	GLN
1	m	129	GLN
1	m	143	GLN
1	m	156	GLN
1	m	187	ASN
1	m	200	GLN
1	m	234	ASN
1	m	246	HIS
1	m	343	ASN
1	m	372	GLN
1	m	391	ASN
1	m	426	HIS
1	m	428	GLN
1	m	435	GLN
1	n	21	ASN
1	n	49	ASN
1	n	99	GLN
1	n	129	GLN
1	n	143	GLN
1	n	187	ASN
1	n	200	GLN
1	n	234	ASN
1	n	246	HIS
1	n	372	GLN
1	n	391	ASN

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Mol	Chain	Res	Type
1	n	417	GLN
1	n	428	GLN
1	n	435	GLN
1	o	21	ASN
1	o	27	ASN
1	o	62	GLN
1	o	77	ASN
1	o	99	GLN
1	o	129	GLN
1	o	143	GLN
1	o	146	ASN
1	o	156	GLN
1	o	187	ASN
1	o	200	GLN
1	o	234	ASN
1	o	246	HIS
1	o	372	GLN
1	o	391	ASN
1	o	413	GLN
1	o	428	GLN
1	o	430	GLN
1	o	435	GLN
1	p	21	ASN
1	p	22	ASN
1	p	44	ASN
1	p	62	GLN
1	p	99	GLN
1	p	129	GLN
1	p	143	GLN
1	p	146	ASN
1	p	200	GLN
1	p	246	HIS
1	p	254	ASN
1	p	286	ASN
1	p	372	GLN
1	p	391	ASN
1	p	413	GLN
1	p	428	GLN
1	p	435	GLN
1	q	21	ASN
1	q	44	ASN
1	q	62	GLN

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Mol	Chain	Res	Type
1	q	99	GLN
1	q	110	HIS
1	q	129	GLN
1	q	200	GLN
1	q	219	ASN
1	q	234	ASN
1	q	286	ASN
1	q	372	GLN
1	q	391	ASN
1	q	413	GLN
1	q	428	GLN
1	q	435	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

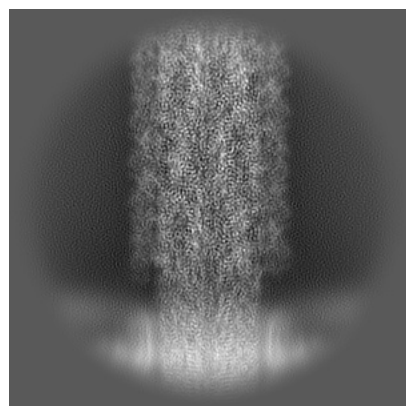
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39788. These allow visual inspection of the internal detail of the map and identification of artifacts.

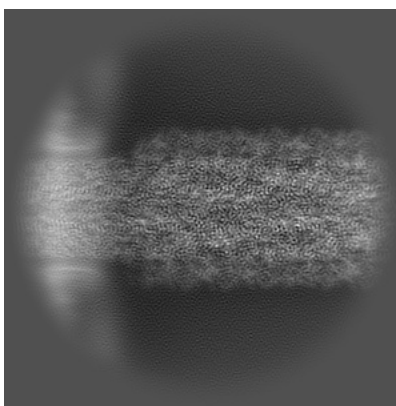
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

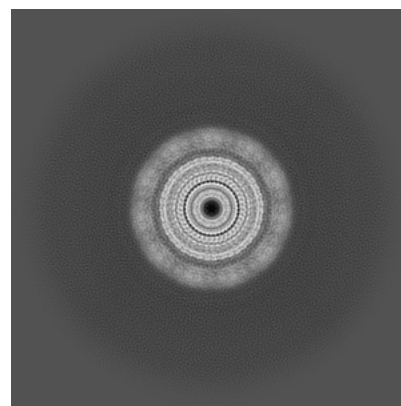
6.1.1 Primary map



X

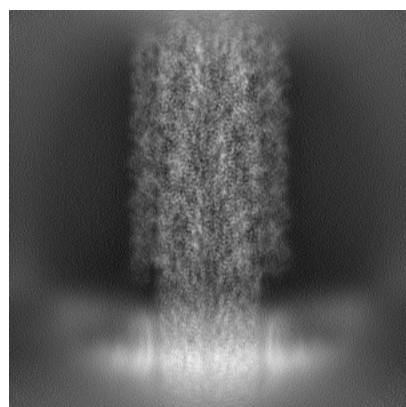


Y

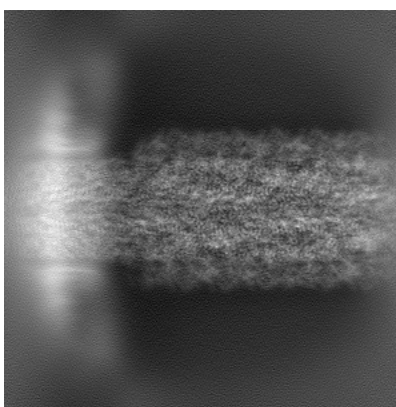


Z

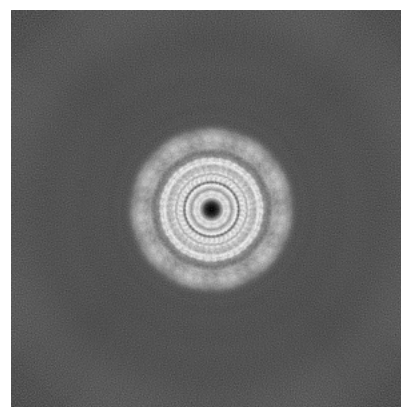
6.1.2 Raw map



X



Y

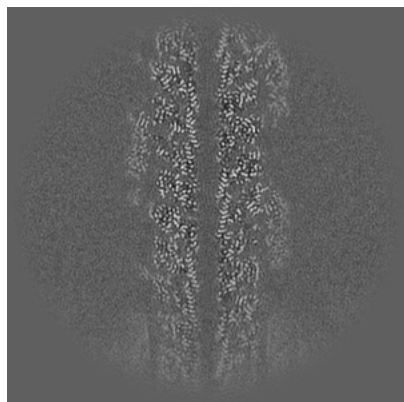


Z

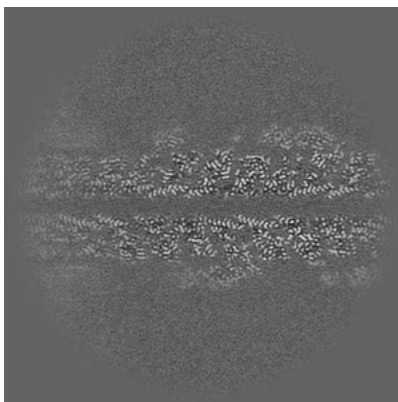
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

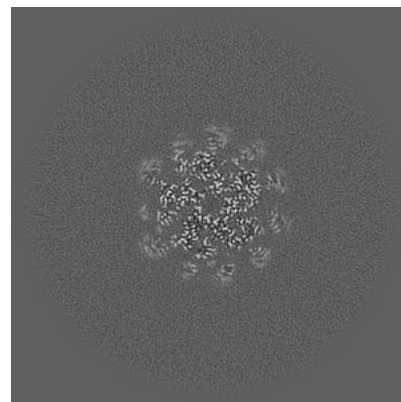
6.2.1 Primary map



X Index: 190

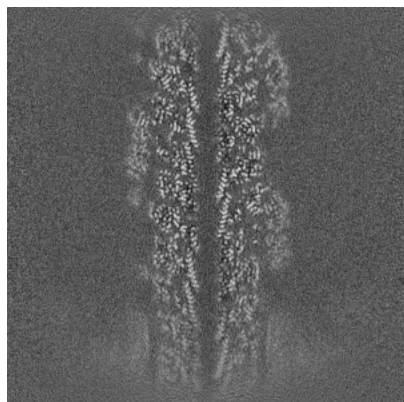


Y Index: 190

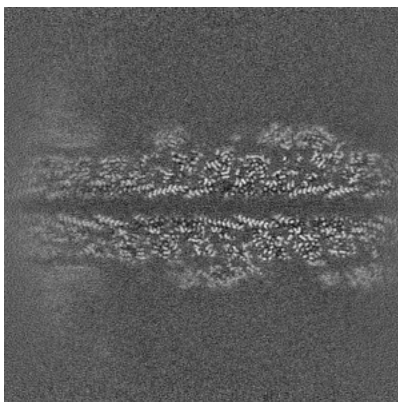


Z Index: 190

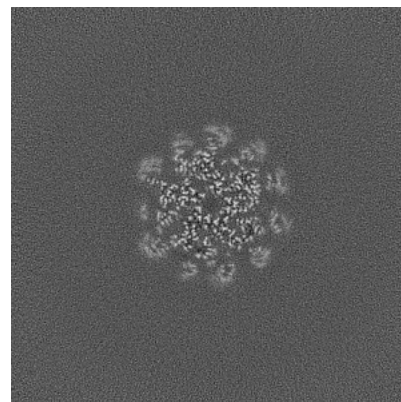
6.2.2 Raw map



X Index: 190



Y Index: 190

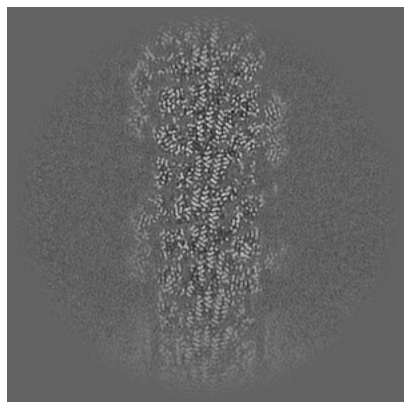


Z Index: 190

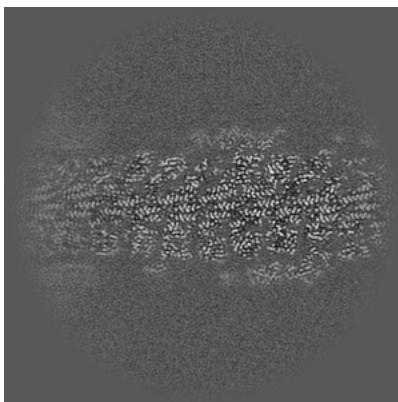
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

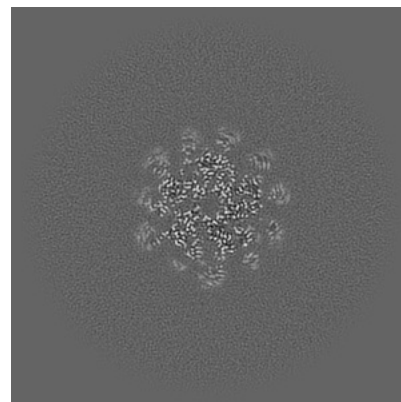
6.3.1 Primary map



X Index: 176

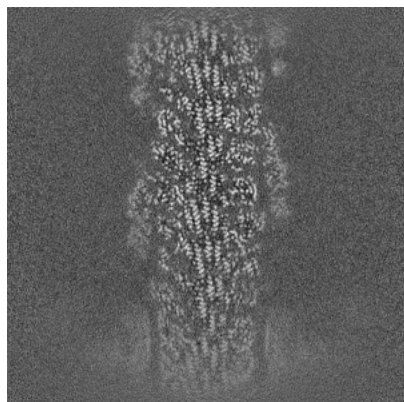


Y Index: 204

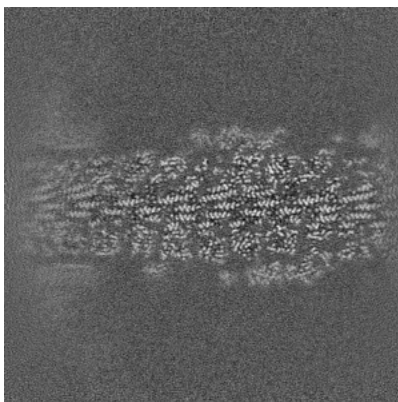


Z Index: 231

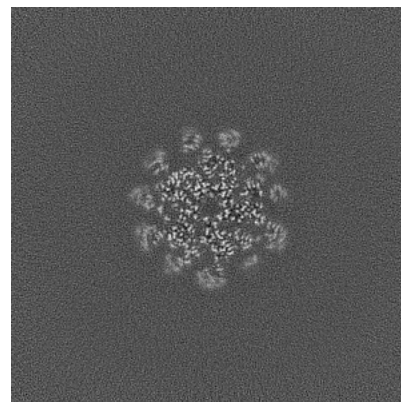
6.3.2 Raw map



X Index: 204



Y Index: 204

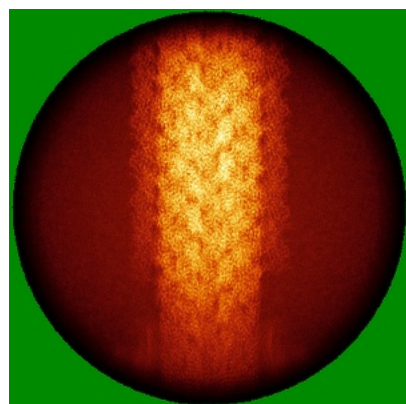


Z Index: 235

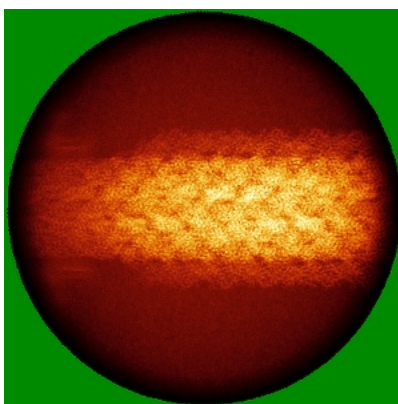
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

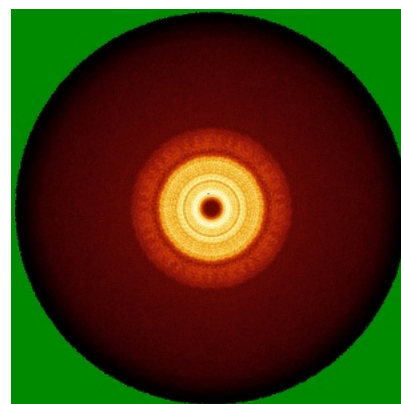
6.4.1 Primary map



X

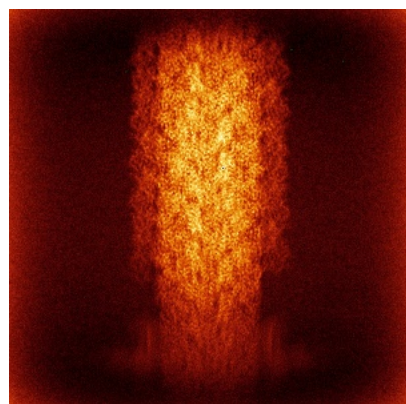


Y

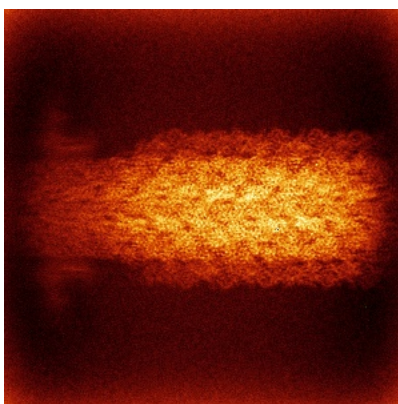


Z

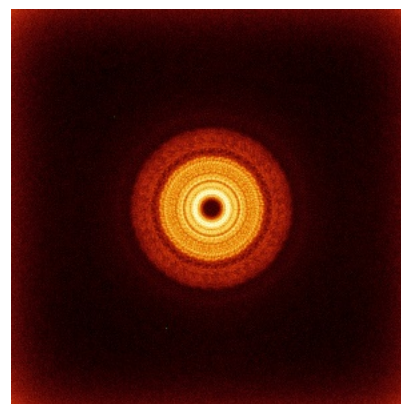
6.4.2 Raw map



X



Y

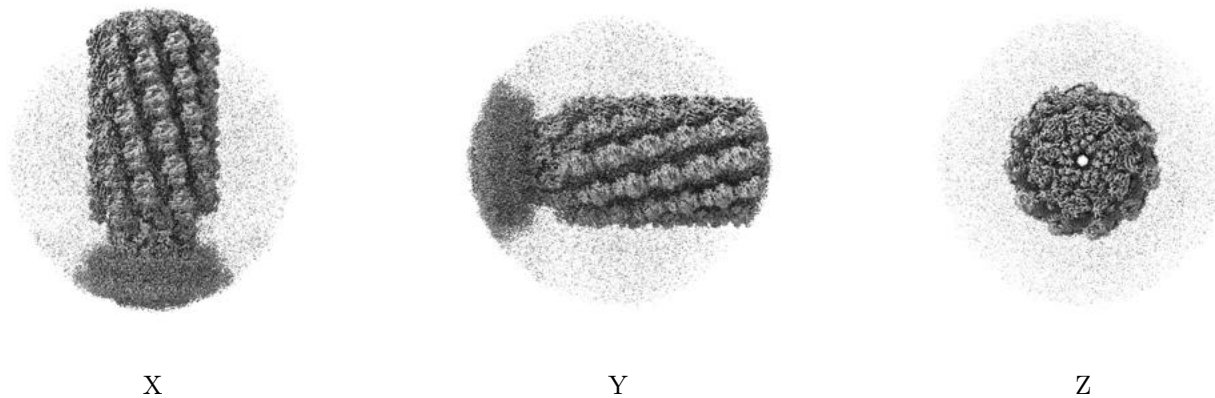


Z

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

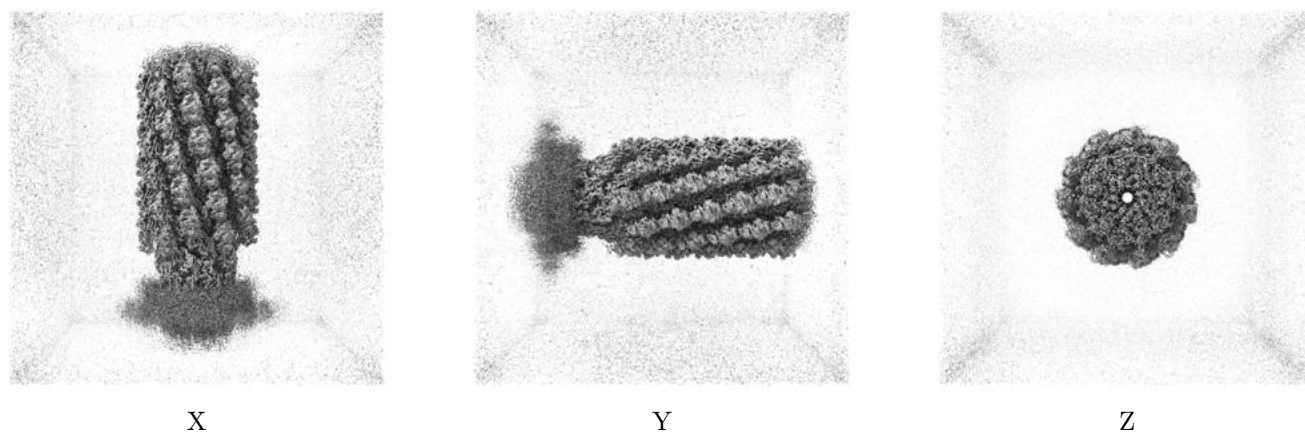
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

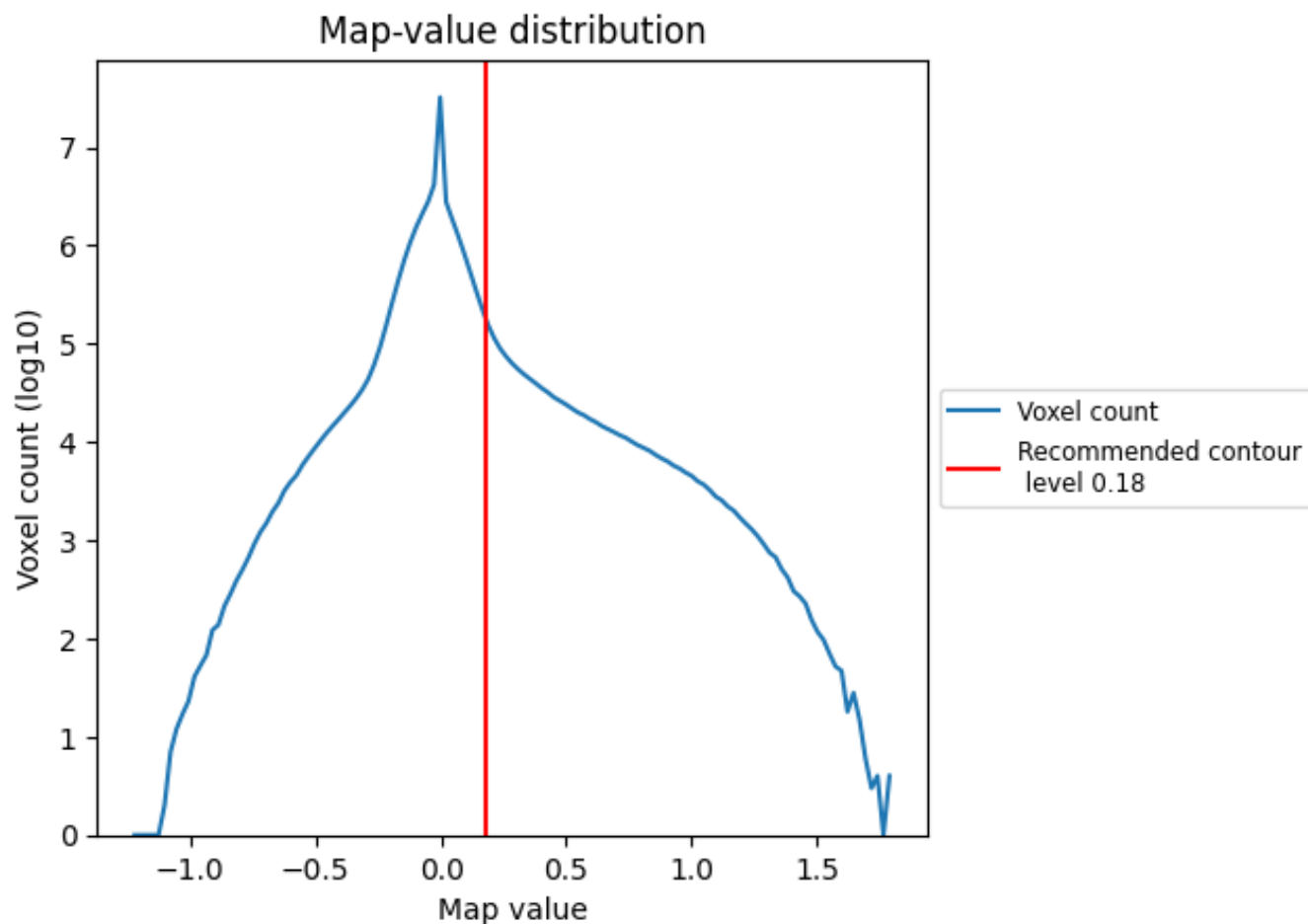
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

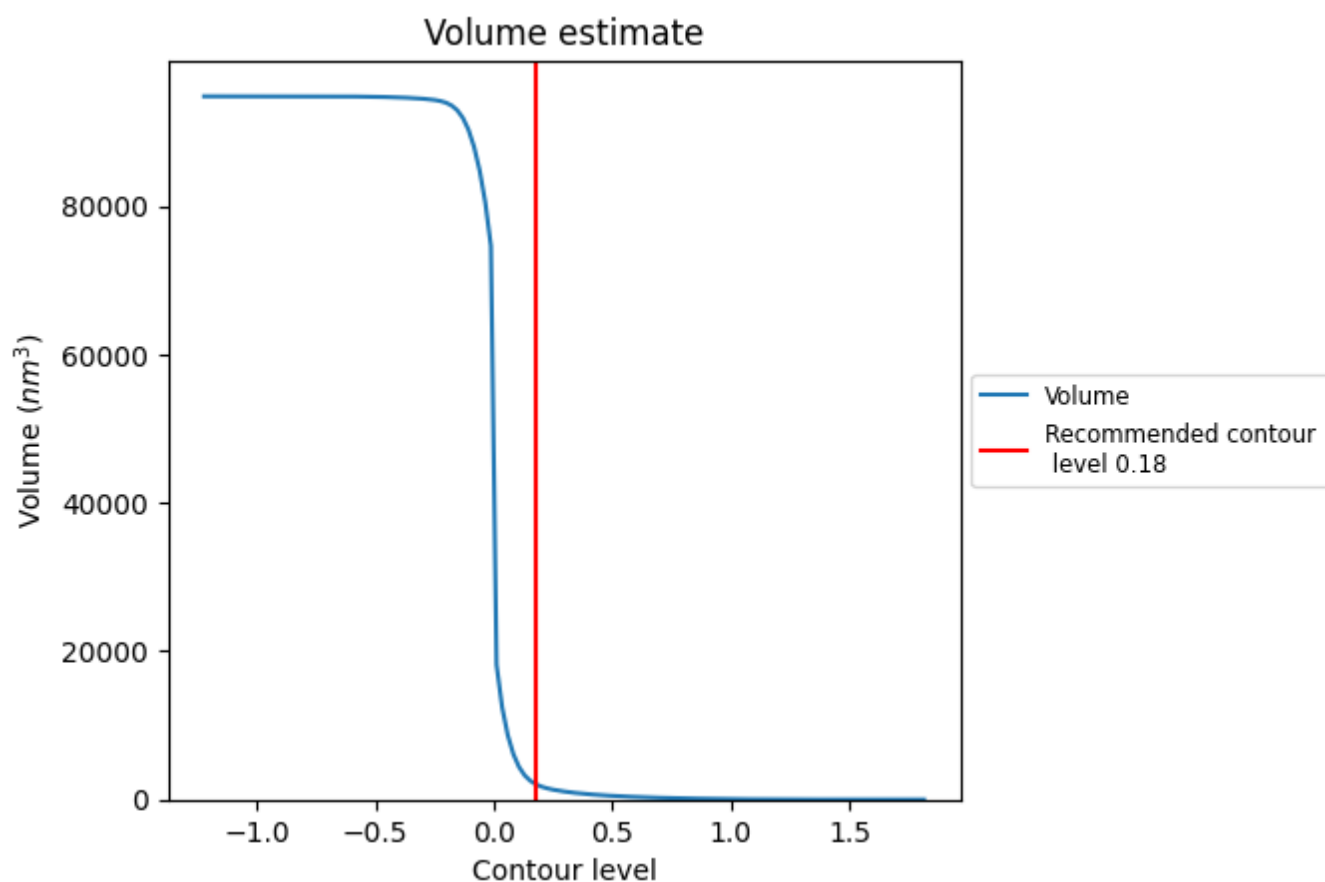
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

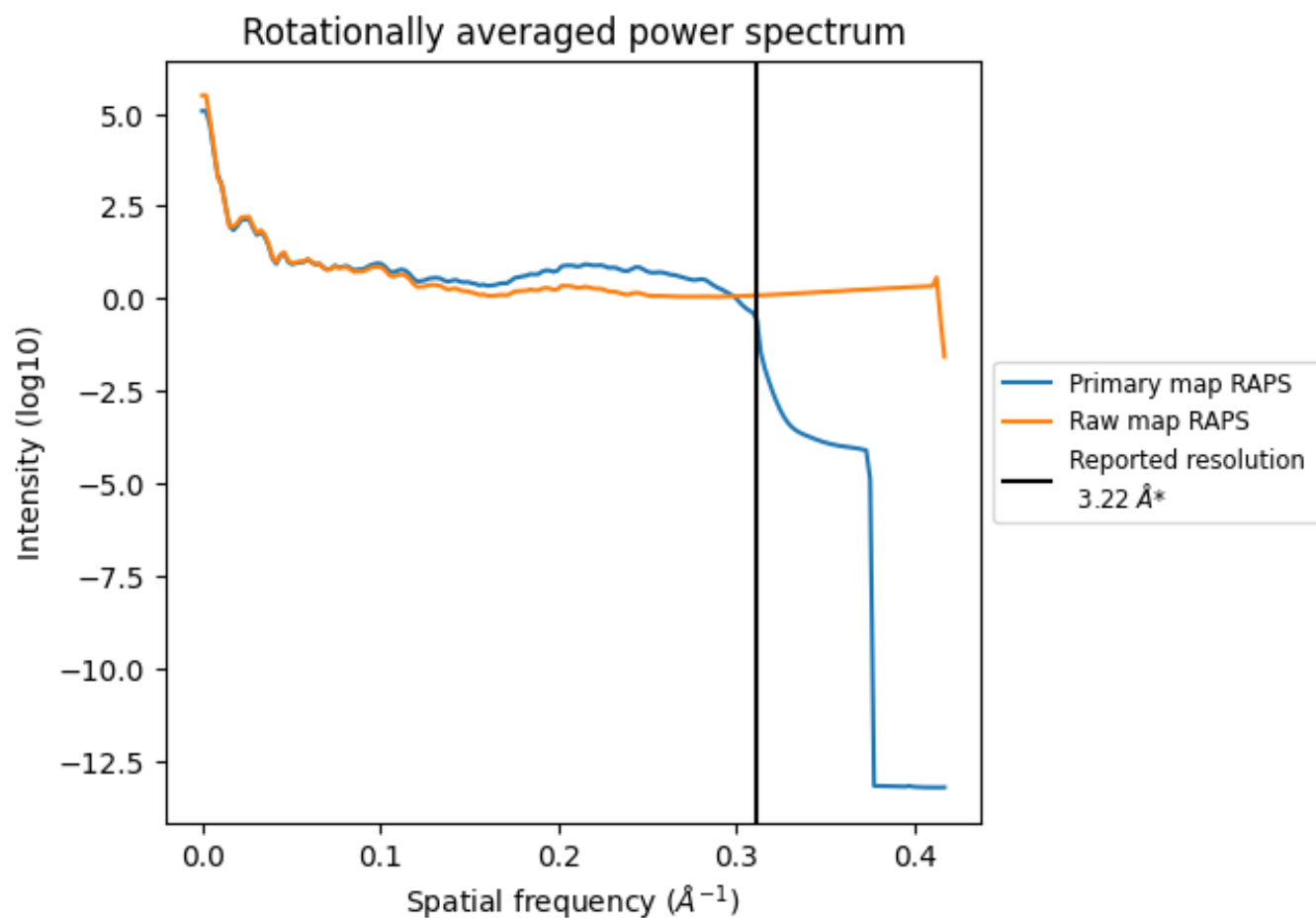
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2018 nm³; this corresponds to an approximate mass of 1823 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 ⓘ

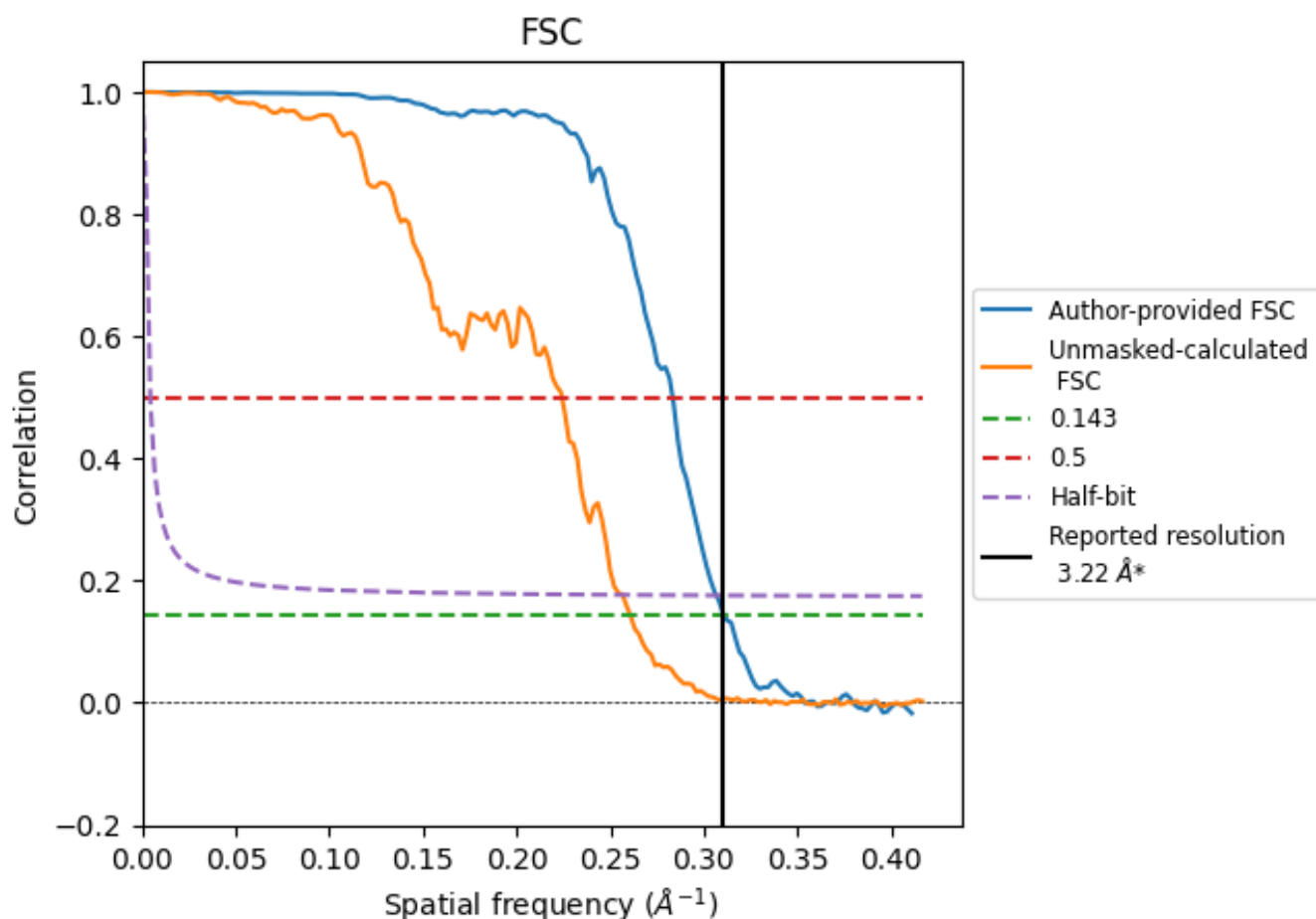


*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

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 0.311 \AA^{-1}

8.2 Resolution estimates [i](#)

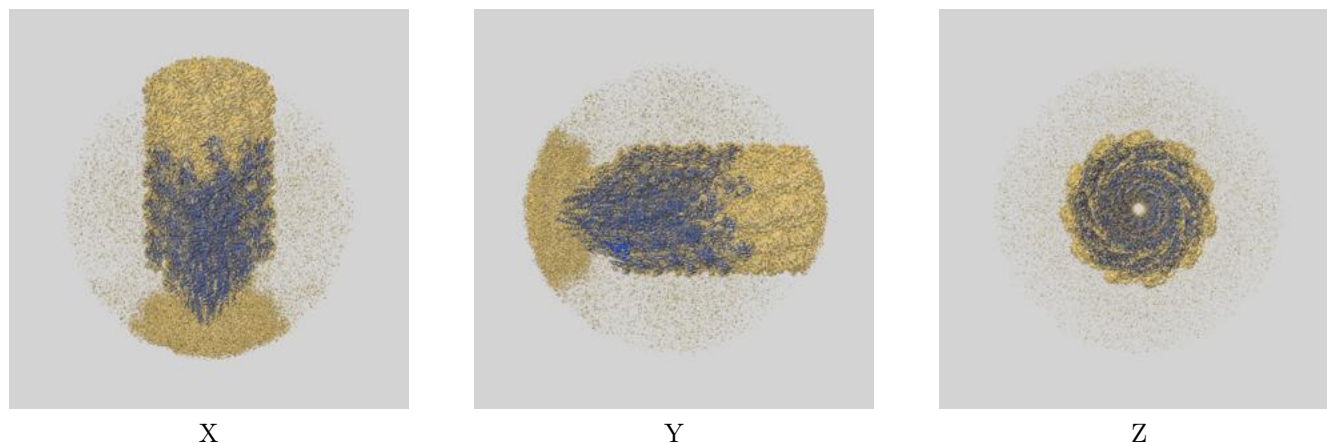
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.22	3.53	3.26
Unmasked-calculated*	3.83	4.46	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.22 by more than 10 %

9 Map-model fit [i](#)

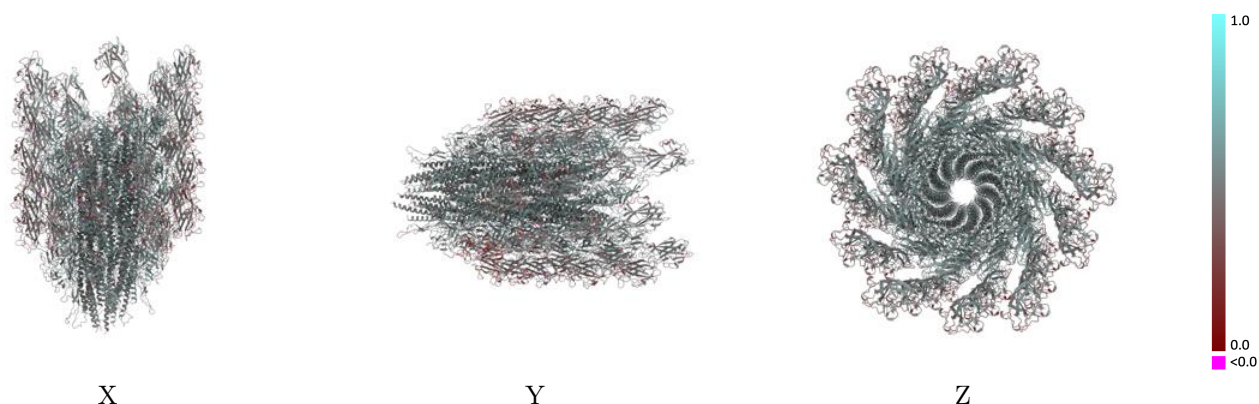
This section contains information regarding the fit between EMDB map EMD-39788 and PDB model 8Z5Y. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



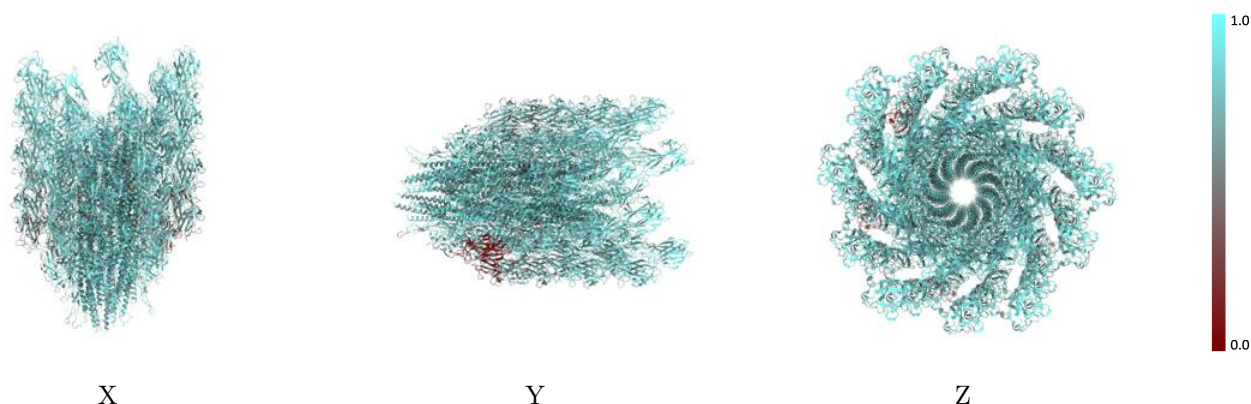
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



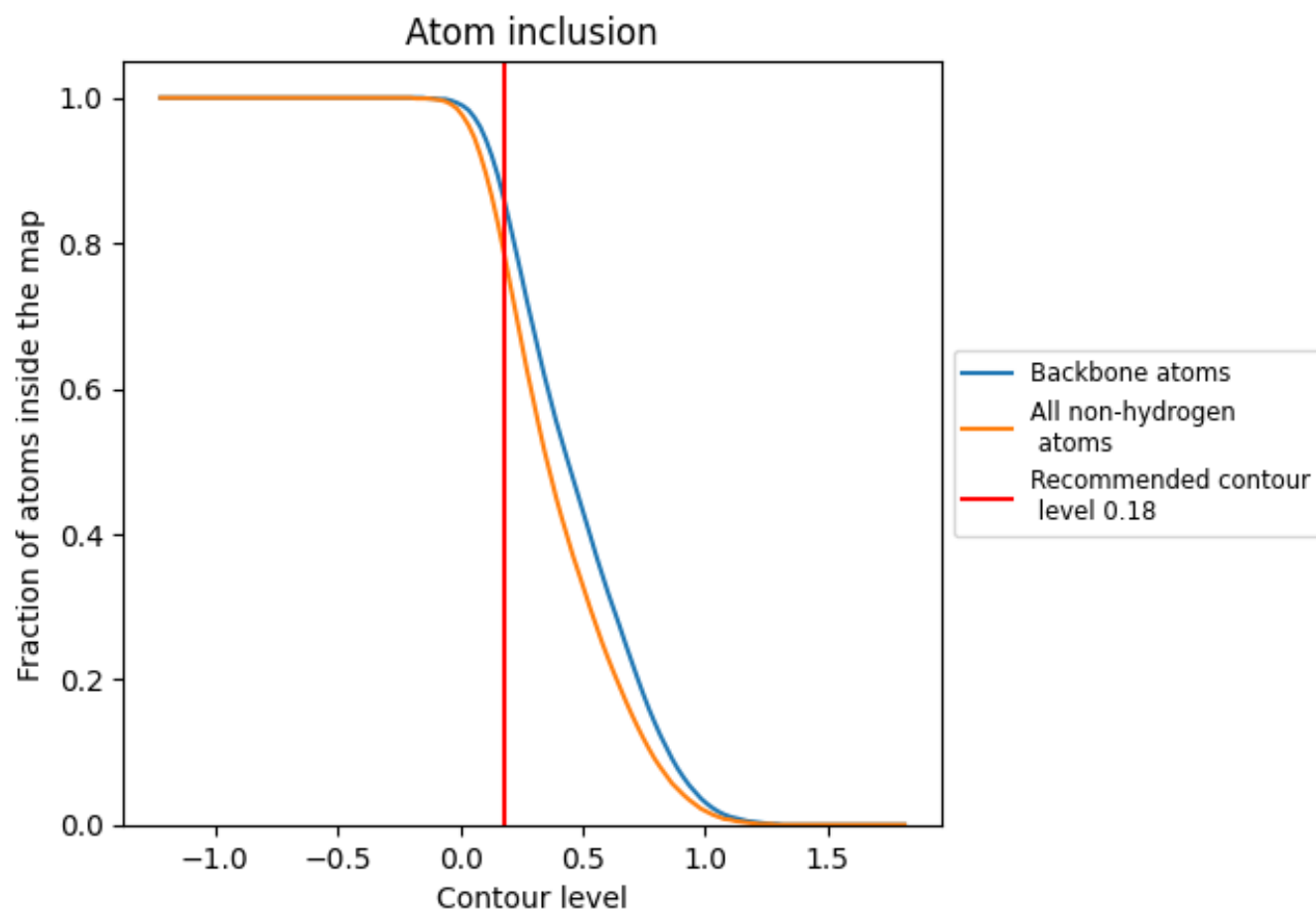
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.4830
D	 0.8410	 0.5030
E	 0.8330	 0.5010
F	 0.8320	 0.5010
G	 0.8330	 0.5050
H	 0.8370	 0.5040
I	 0.8320	 0.5030
J	 0.8380	 0.5070
K	 0.8350	 0.5040
L	 0.8350	 0.5010
M	 0.8340	 0.5010
N	 0.8350	 0.5000
O	 0.8270	 0.4970
P	 0.8280	 0.5000
Q	 0.8200	 0.4970
R	 0.8300	 0.5000
S	 0.8260	 0.4970
T	 0.8250	 0.4950
U	 0.8220	 0.4940
V	 0.8150	 0.4910
W	 0.8060	 0.4880
X	 0.8070	 0.4880
Y	 0.8120	 0.4880
Z	 0.8050	 0.4870
a	 0.8060	 0.4890
b	 0.7910	 0.4850
c	 0.7930	 0.4860
d	 0.7910	 0.4820
e	 0.7800	 0.4800
f	 0.7680	 0.4720
g	 0.7600	 0.4670
h	 0.7540	 0.4610
i	 0.7500	 0.4630
j	 0.7500	 0.4610
k	 0.7410	 0.4620



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Chain	Atom inclusion	Q-score
l	 0.7390	 0.4630
m	 0.7350	 0.4610
n	 0.7180	 0.4600
o	 0.6650	 0.4470
p	 0.5750	 0.4270
q	 0.4720	 0.3990