



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:19 PM UTC

PDB ID : 8EB7 / pdb_00008eb7
EMDB ID : EMD-27793
Title : Cryo-EM structure of the in-situ gp4-gp10-gp9N from bacteriophage P22
Authors : Wang, C.; Liu, J.; Molineux, I.J.
Deposited on : 2022-08-30
Resolution : 3.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

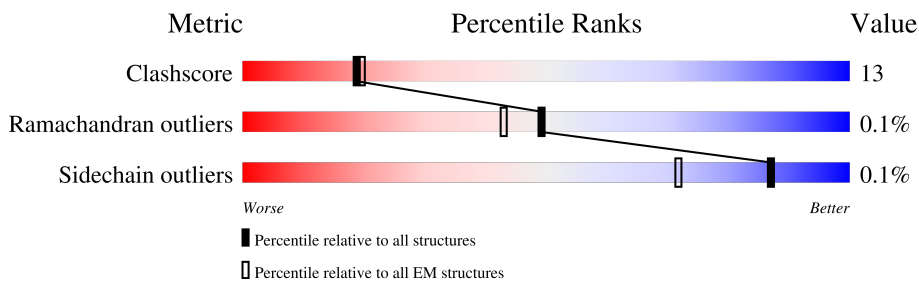
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	0	111	
1	A	111	
1	B	111	
1	C	111	
1	D	111	
1	F	111	
1	X	111	
1	Y	111	

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Mol	Chain	Length	Quality of chain	
1	Z	111	89%	33%
1	a	111	95%	32%
1	b	111	95%	29%
1	c	111	95%	32%
1	d	111	95%	32%
1	e	111	92%	36%
1	f	111	91%	36%
1	g	111	90%	35%
1	h	111	92%	35%
1	i	111	90%	31%
2	E	150	93%	33%
2	G	150	93%	29%
2	H	150	92%	31%
2	I	150	93%	30%
2	J	150	94%	28%
2	K	150	94%	29%
2	L	150	92%	27%
2	M	150	93%	31%
2	N	150	93%	30%
2	O	150	94%	37%
2	P	150	93%	31%
2	Q	150	93%	30%
3	R	471	96%	29%
3	S	471	96%	28%
3	T	471	96%	29%

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Mol	Chain	Length	Quality of chain
3	U	471	<p>97% 71% 29%</p>
3	V	471	<p>96% 72% 28%</p>
3	W	471	<p>97% 70% 30%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 51240 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 Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	111	855	543	144	167	1	0	0
1	A	111	855	543	144	167	1	0	0
1	B	111	855	543	144	167	1	0	0
1	C	111	855	543	144	167	1	0	0
1	D	111	855	543	144	167	1	0	0
1	F	111	855	543	144	167	1	0	0
1	X	111	855	543	144	167	1	0	0
1	Y	111	855	543	144	167	1	0	0
1	Z	111	855	543	144	167	1	0	0
1	a	111	855	543	144	167	1	0	0
1	b	111	855	543	144	167	1	0	0
1	c	111	855	543	144	167	1	0	0
1	d	111	855	543	144	167	1	0	0
1	e	111	855	543	144	167	1	0	0
1	f	111	855	543	144	167	1	0	0
1	g	111	855	543	144	167	1	0	0
1	h	111	855	543	144	167	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	111	Total	C	N	O	S	0	0
			855	543	144	167	1		

- Molecule 2 is a protein called Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	G	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	H	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	I	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	J	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	K	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	L	150	Total	C	N	O	S	0	0
			1149	721	198	225	5		
2	M	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	N	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	O	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	P	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
2	Q	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		

- Molecule 3 is a protein called Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
3	S	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
3	T	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		
3	U	471	Total	C	N	O	S	0	0
			3686	2326	631	711	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	V	471	3686	2326	631	711	18	0	0
3	W	471	3686	2326	631	711	18	0	0

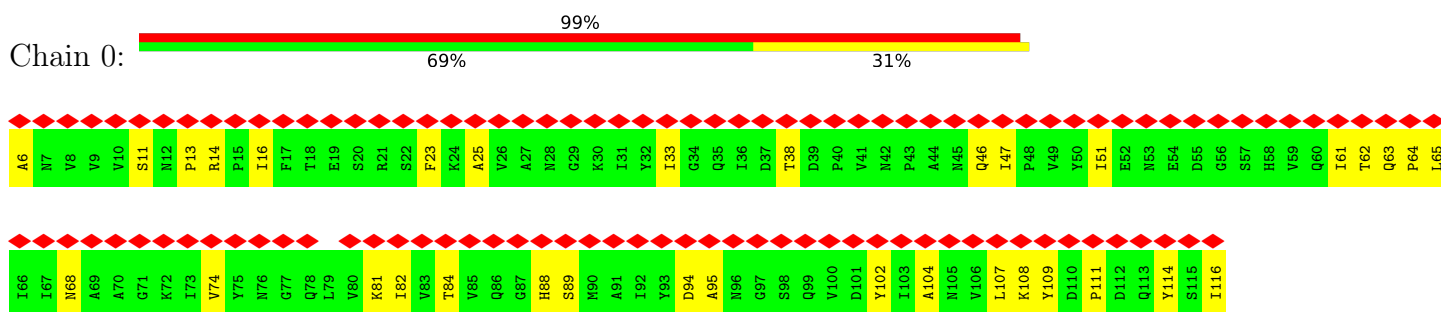
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	233	SER	GLY	conflict	UNP P26749
S	233	SER	GLY	conflict	UNP P26749
T	233	SER	GLY	conflict	UNP P26749
U	233	SER	GLY	conflict	UNP P26749
V	233	SER	GLY	conflict	UNP P26749
W	233	SER	GLY	conflict	UNP P26749

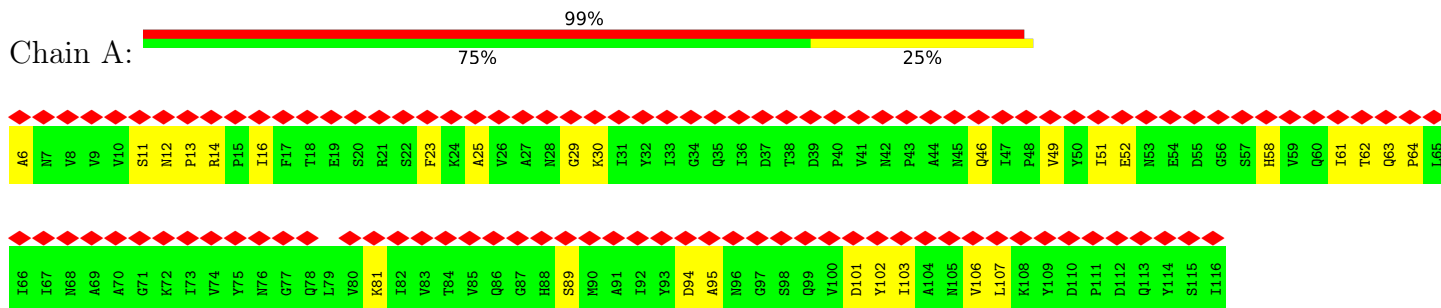
3 Residue-property plots

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

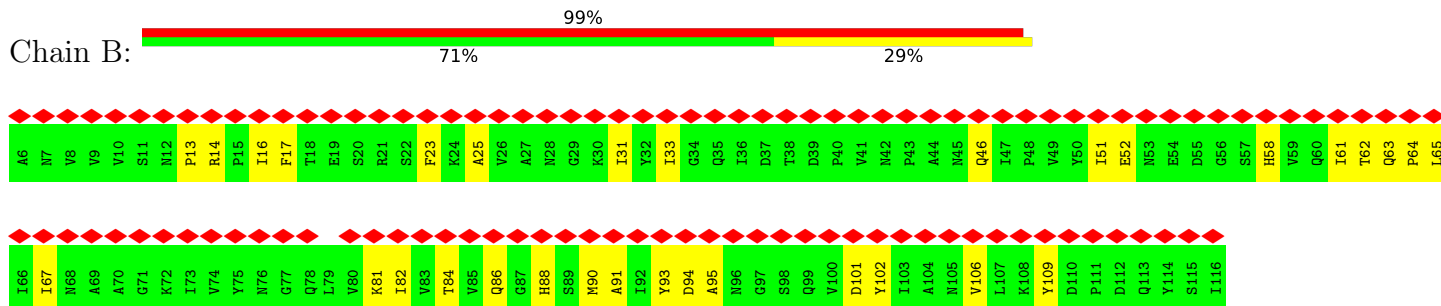
- Molecule 1: Tail spike protein



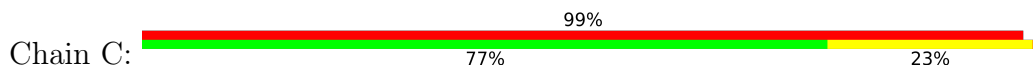
- Molecule 1: Tail spike protein

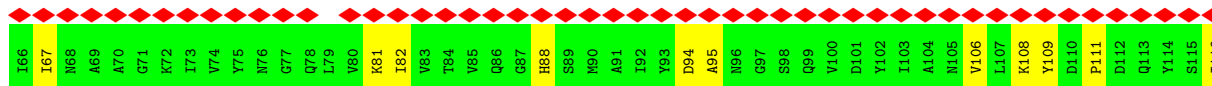


- Molecule 1: Tail spike protein

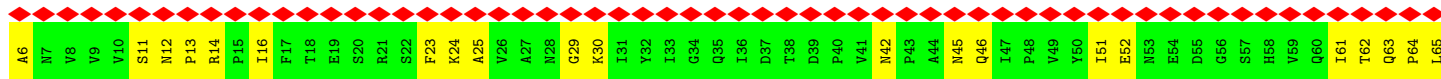


- Molecule 1: Tail spike protein

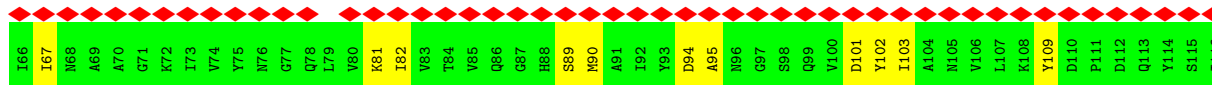
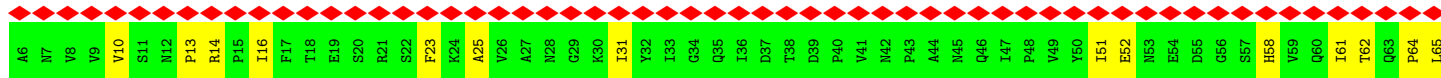
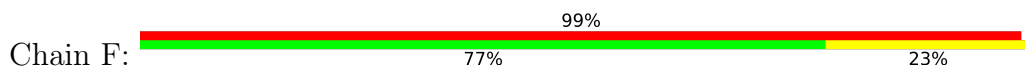




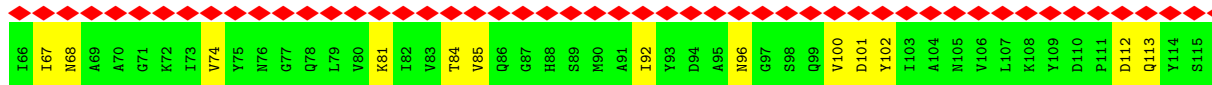
• Molecule 1: Tail spike protein



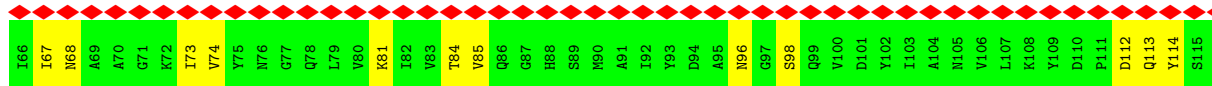
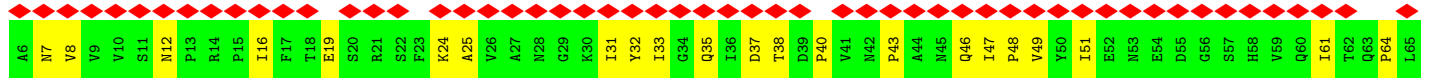
• Molecule 1: Tail spike protein



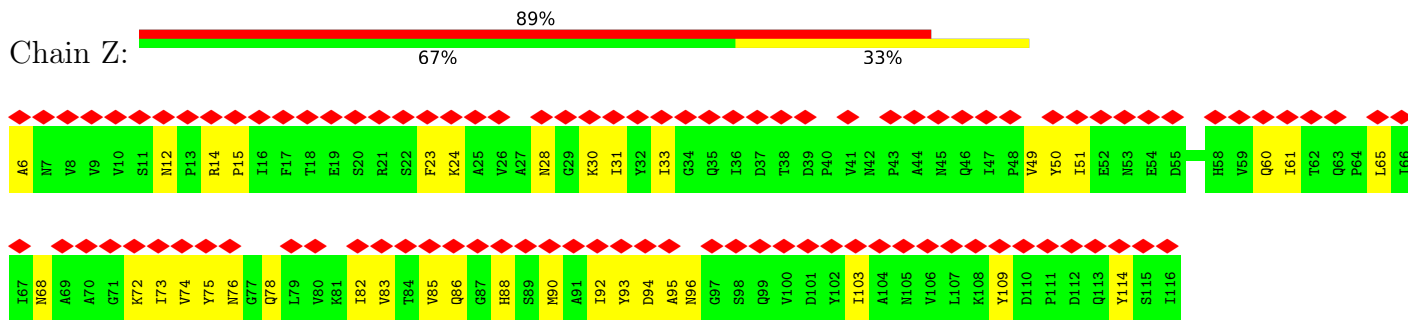
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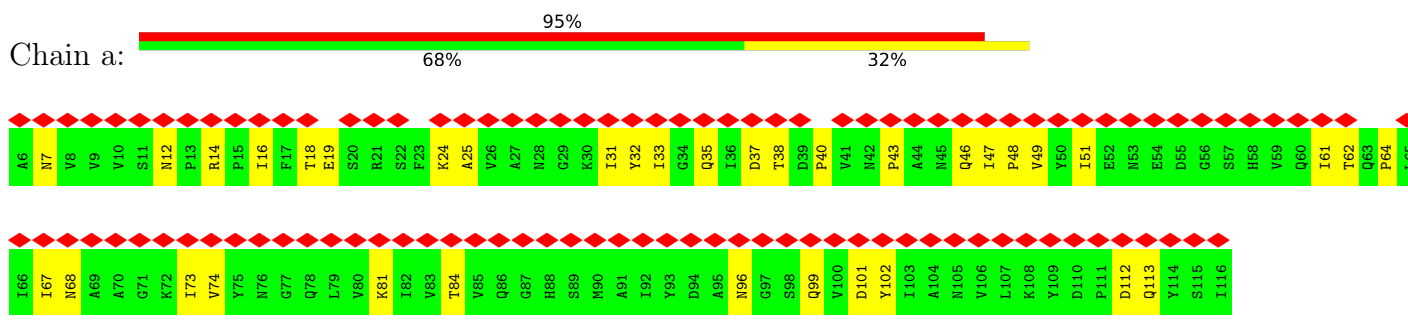
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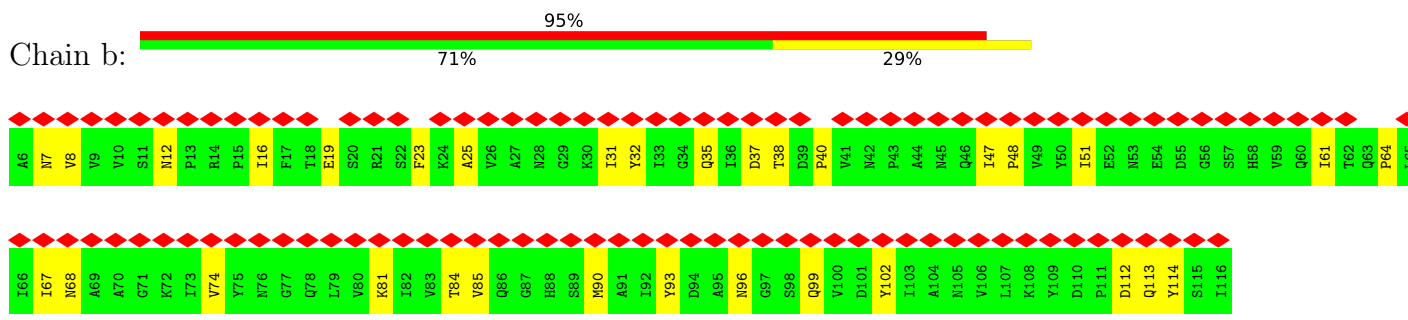
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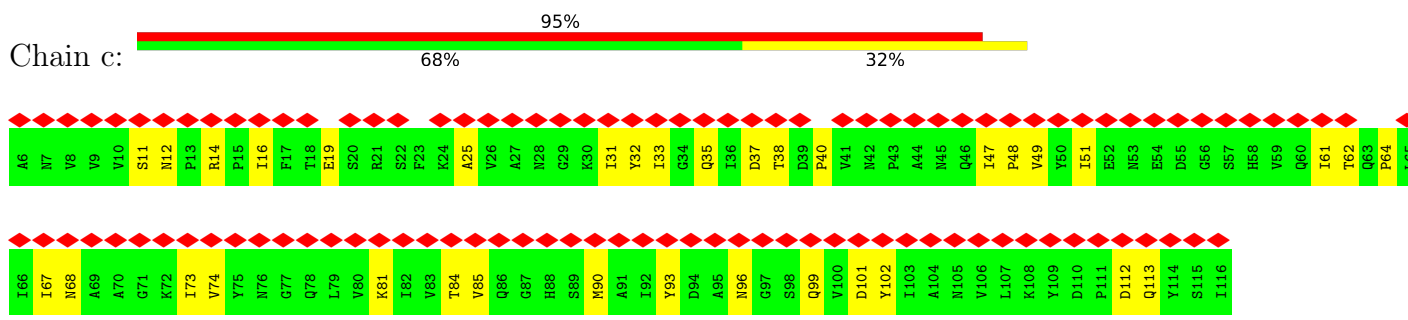
• Molecule 1: Tail spike protein



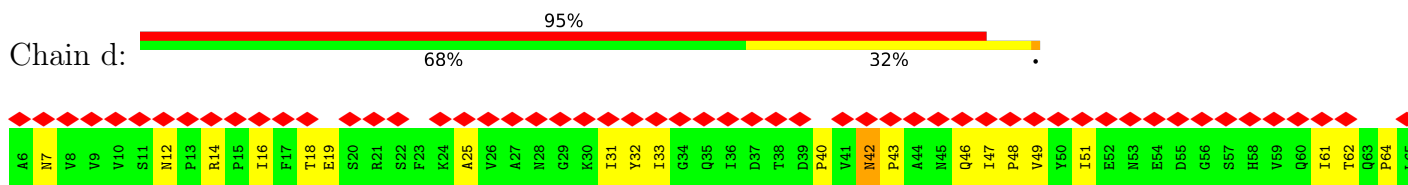
• Molecule 1: Tail spike protein

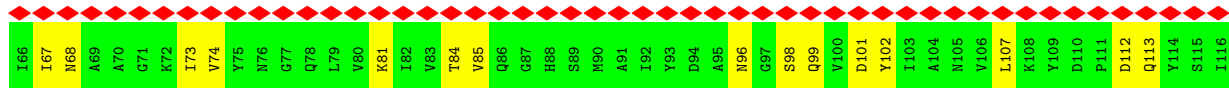


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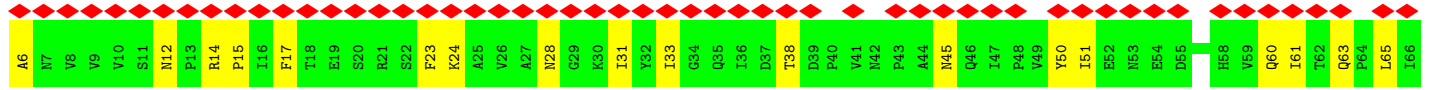
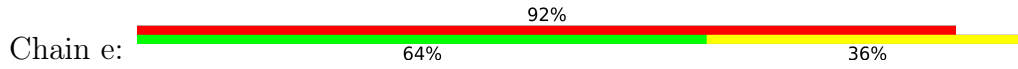


• Molecule 1: Tail spike protein

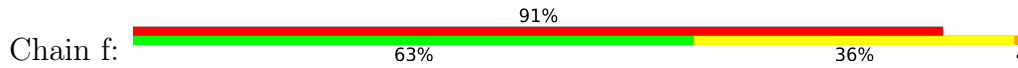




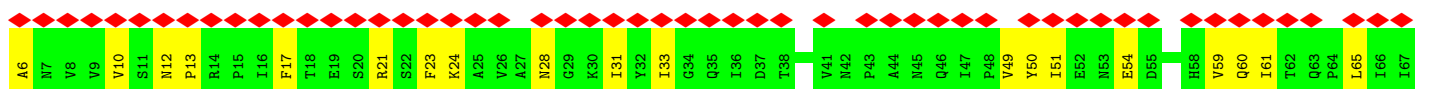
• Molecule 1: Tail spike protein



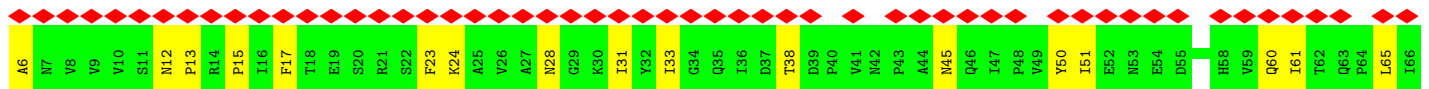
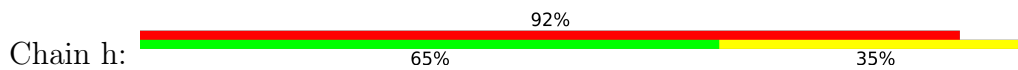
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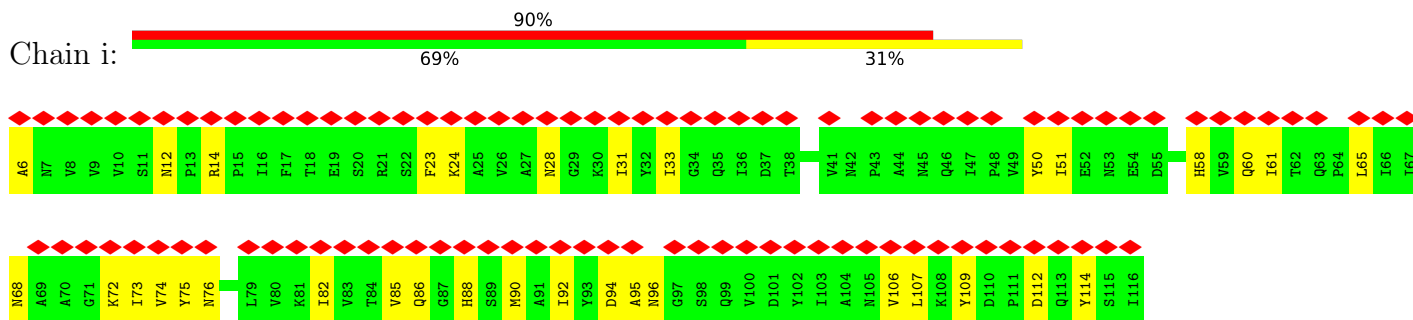


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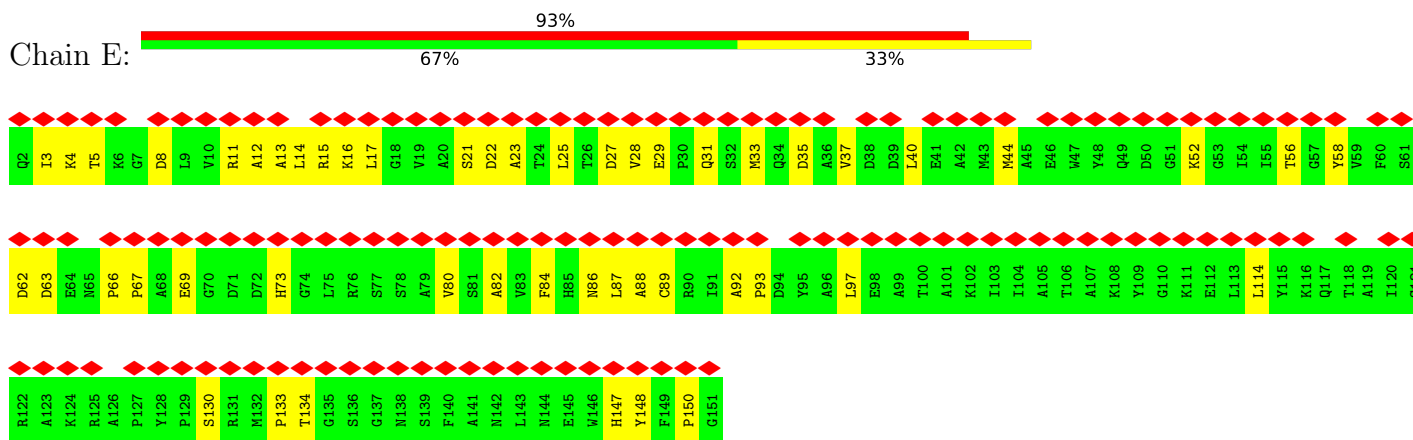


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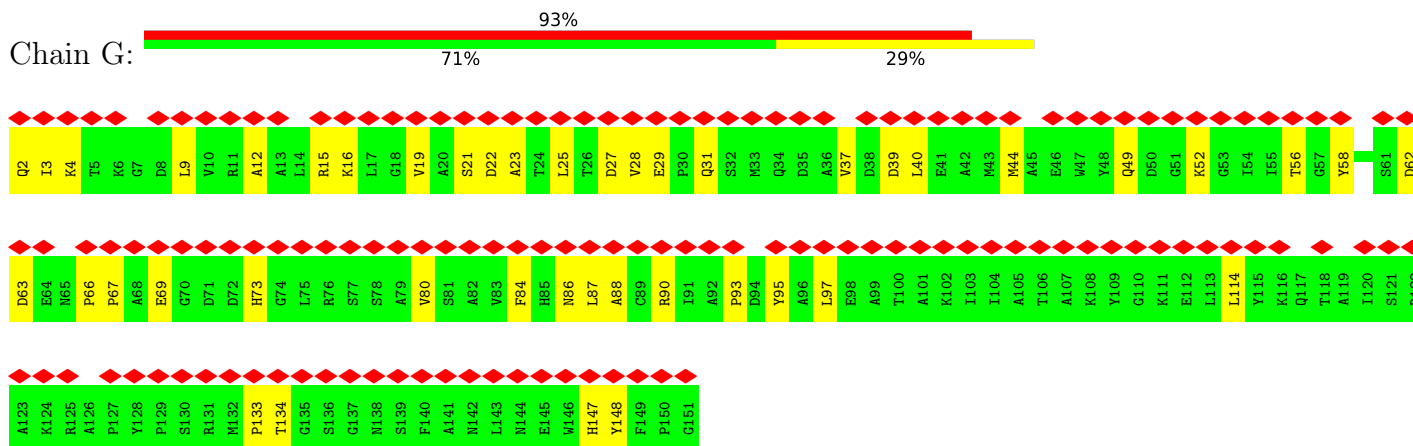




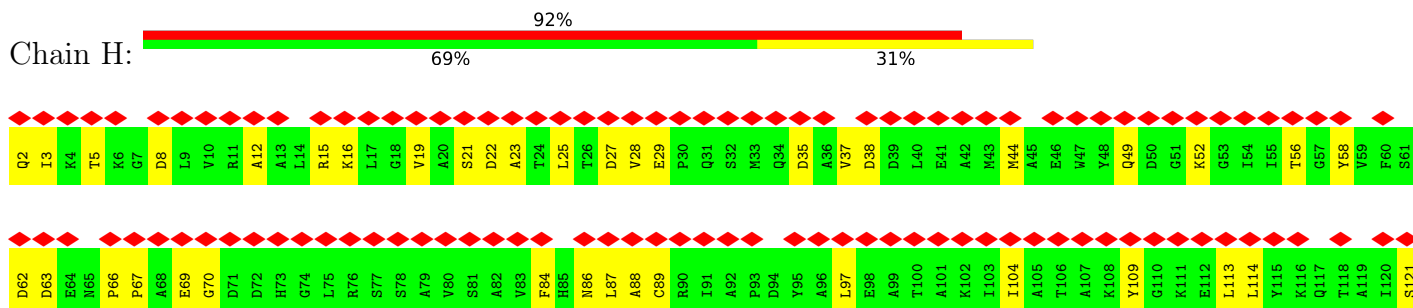
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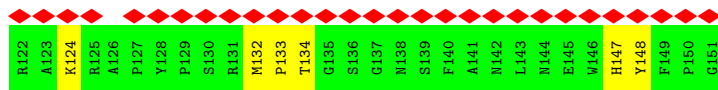


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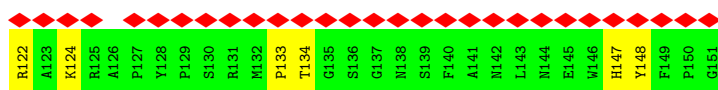
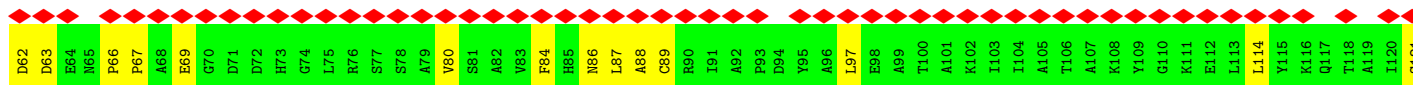
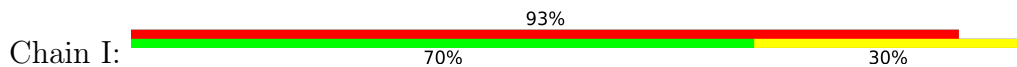


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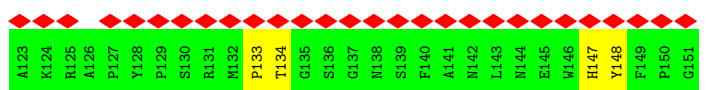
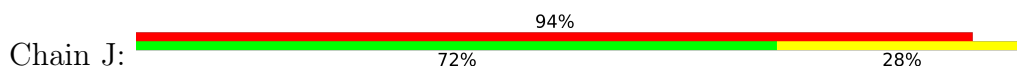




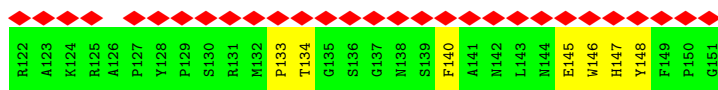
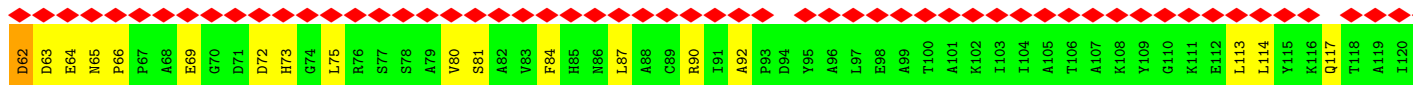
• Molecule 2: Peptidoglycan hydrolase gp4



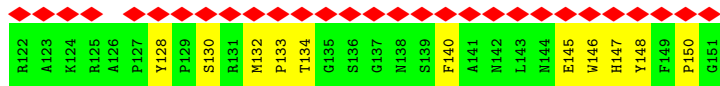
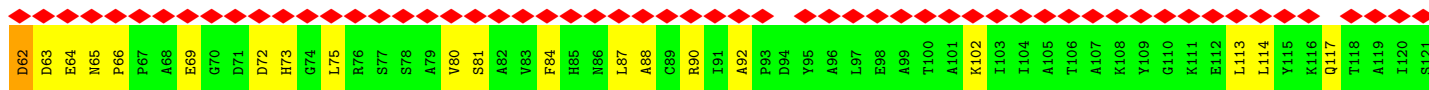
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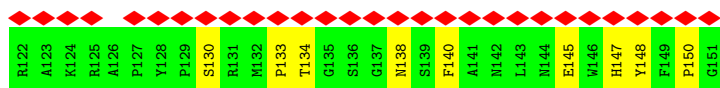
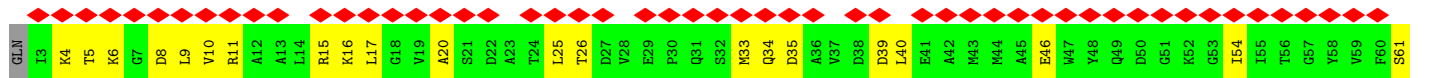
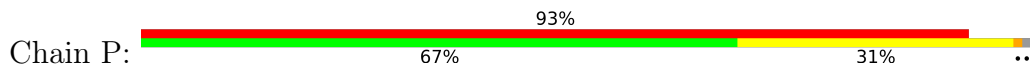
• Molecule 2: Peptidoglycan hydrolase gp4



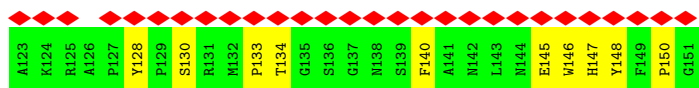
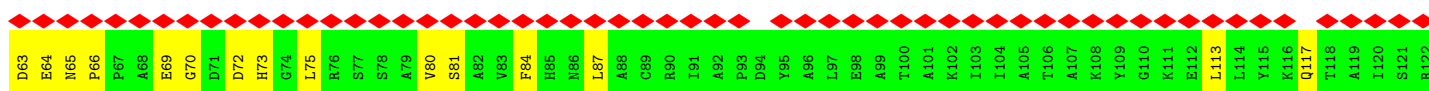
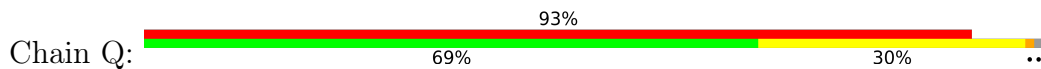
• Molecule 2: Peptidoglycan hydrolase gp4



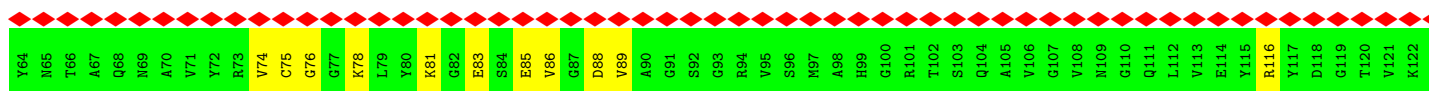
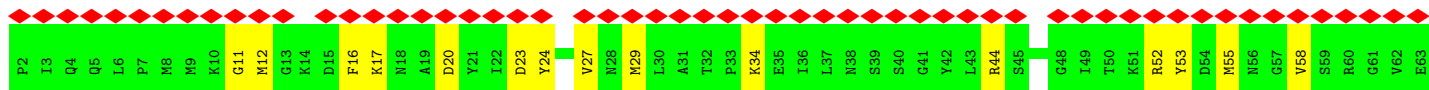
• Molecule 2: Peptidoglycan hydrolase gp4



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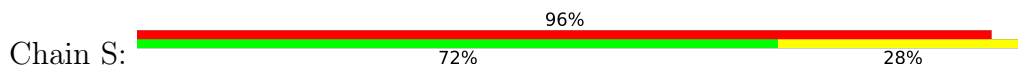


• Molecule 3: Packaged DNA stabilization protein gp10

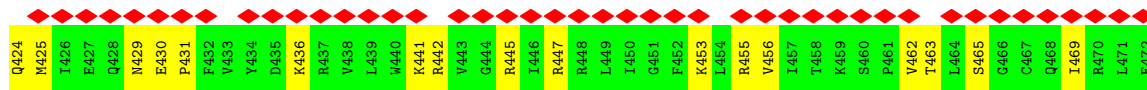


V124	P184	A244	L304	Q364	M425
S125	P185	D245	I305	F365	I426
N126	D186	S246	I306	D366	E427
W127	G187	Y247	H307	I367	Q428
P128	I188	A248	L308	S368	M429
A129	I189	F249	R310	S369	E430
D130	G190	I250	H311	Q370	P431
S131	I191	S251	V312	Y371	F432
S132	G192	H252	L313	D372	W433
F133	T193	P253	V314	S373	Y434
T134	W194	A254	Y315	Q374	D435
Q135	R195	T255	G316	Q375	K436
Y136	D196	G256	D316	E376	K437
E137	F197	G257	A317	H377	W438
L138	I198	P258	S318	L378	L439
G139	V199	S259	S319	L379	W440
V141	C200	V260	S320	F380	K441
R142	F201	Y261	N321	T381	R442
D143	G202	I262	G323	P382	W443
L144	S203	I263	P324	L383	G444
T145	T205	G264	Q325	F384	R445
R146	T206	S265	W326	K385	I446
L147	I207	G266	C327	A386	R447
R148	E207	Q267	V328	D387	R448
G149	F208	A268	L329	N388	L449
R150	Y209	S269	K330	A389	I450
Y151	S210	P270	T331	R390	G451
A152	L211	I271	G332	C391	F452
W153	T212	A272	L333	F392	K453
S154	G213	T273	Y334	D393	L454
K155	A214	A274	D335	L394	R455
D156	T215	S275	D336	E395	W456
G157	T216	I276	Y337	E396	I457
T158	A217	E277	V338	E397	T458
D159	G218	K278	R339	S398	K459
S160	A219	I279	G340	S399	S460
W161	A220	I280	V341	T400	P461
F162	Y222	R281	D342	W401	W462
I163	V223	S282	F343	Y402	L464
T164	V224	Y283	M344	A403	S465
D165	A224	T284	Y345	Q404	G466
L166	Q225	A285	E346	Y405	C467
E167	P226	E286	G347	A406	Q468
D168	S227	E287	N348	D407	I469
E169	L228	M288	Q349	R408	R470
S170	M229	A289	I350	L409	L471
H171	V230	T290	T351	F410	E472
P172	Q231	G291	C352	L411	
D173	K232	V292	G353	S412	
R174	S233	M293	D354	A413	
Y175	I234	E294	K355	T414	
S176	A235	T295	S356	T415	
A177	G236	L296	E357	D416	
Q178	T237	R297	A358	G417	
Y179	Y238	F298	V359	I418	
R180	C239	D299	V360	W419	
A181	K240	S300	G361	Y420	
E182	P242	H301	Q362	G421	
S183	F243	L303	L363	R422	

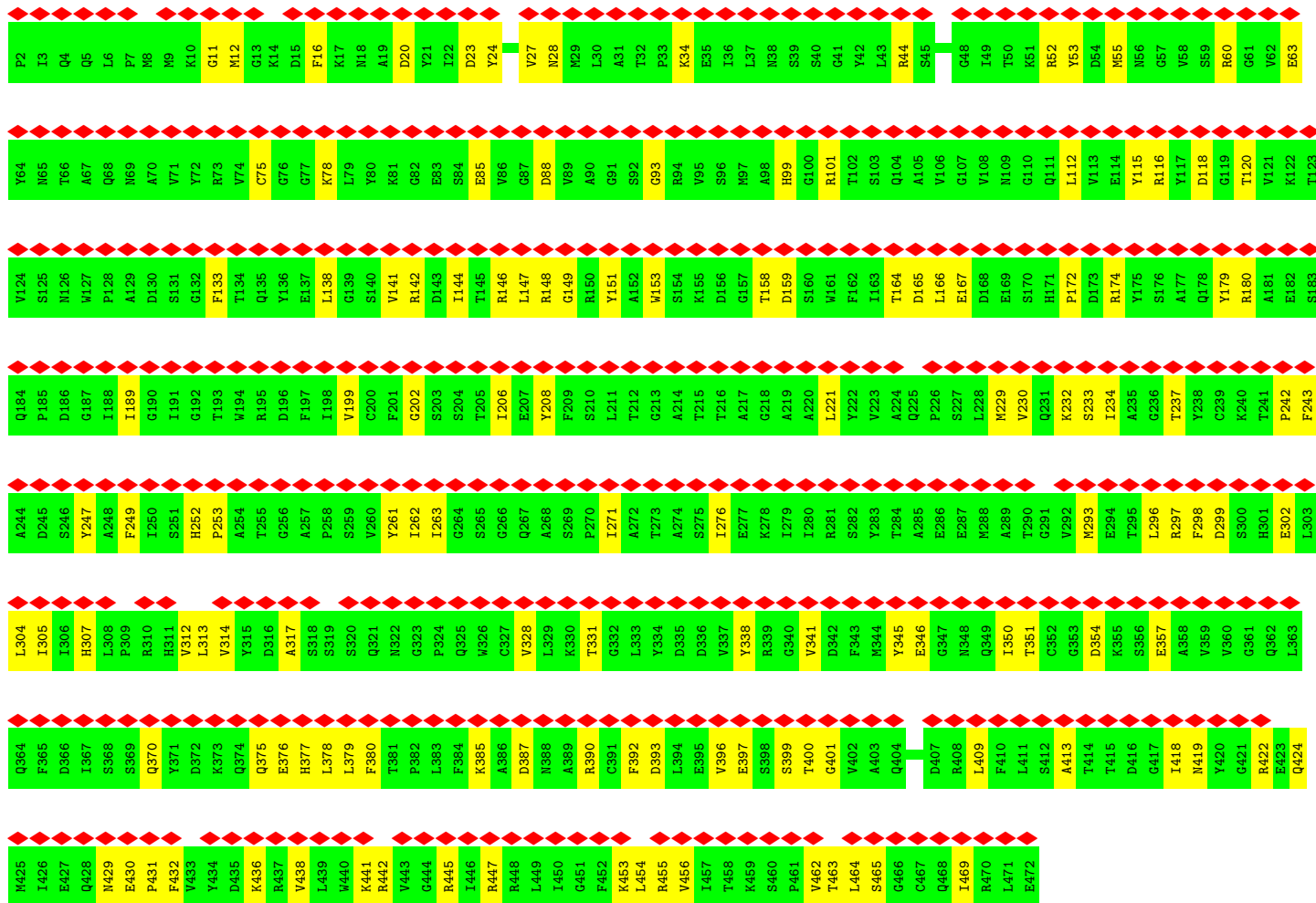
• Molecule 3: Packaged DNA stabilization protein gp10



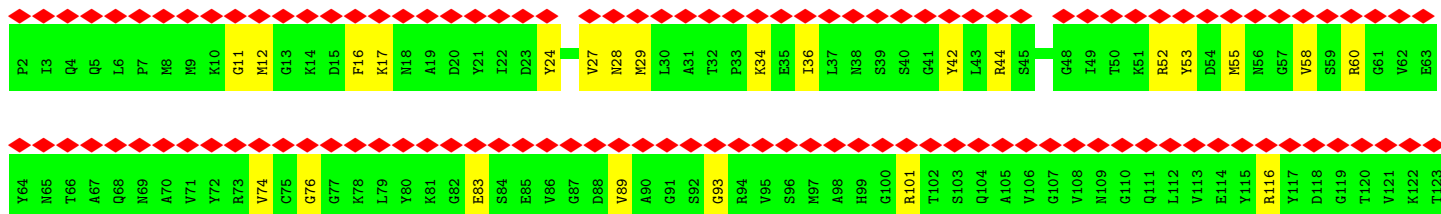
P2	E63	T123	S183	F243	L303	L363	L363
I3	Y64	V124	Q184	A244	L304	Q364	Q364
Q4	M65	S125	P185	D245	L305	F365	F365
Q5	T66	N126	D186	S246	L306	D366	D366
L6	A67	W127	G187	Y247	H307	I367	I367
P7	Q68	P128	I188	A248	L308	S368	S368
M8	M69	A129	I189	F249	P309	S369	S369
M9	A70	D130	G190	I250	R310	Q370	Q370
K10	V71	S131	I191	S251	H311	Y371	Y371
G11	Y72	G132	G192	H252	V312	D372	D372
M12	R73	F133	T193	P253	L313	S373	S373
G13	V74	T134	W194	A254	V314	Y374	Y374
K14	C75	Q135	R195	T255	Y315	Q375	Q375
D15	G76	Y136	D196	G256	D316	E376	E376
F16	G77	E137	F197	G257	A317	H377	H377
K17	K78	L138	I198	P258	S318	L378	L378
N18	L79	G139	V199	S259	S319	L379	L379
A19	Y80	S140	C200	V260	S320	F380	F380
D20	K81	V141	F201	Y261	N321	T381	T381
Y21	G82	R142	G202	I262	G323	P382	P382
I22	E83	D143	S203	I263	P324	L383	L383
D23	S84	I144	S204	G264	Q325	F384	F384
Y24	E85	T145	T205	S265	W326	K385	K385
V27	V86	R146	I206	G266	C327	A386	A386
M28	G87	L147	E207	Q267	V328	D387	D387
N29	D88	R148	Y208	A268	L329	N388	N388
L30	V89	G149	F209	S269	K330	A389	A389
A31	A90	R150	S210	P270	T331	R390	R390
T32	G91	Y151	G332	I271	G332	C391	C391
P33	S92	A152	L212	A272	L333	F392	F392
K34	G93	W153	G213	T273	Y334	D393	D393
E35	R94	S154	A214	A274	D335	L394	L394
I36	V95	K155	T215	S275	D336	E395	E395
L37	S96	D156	T216	I276	Y337	V396	V396
N38	M97	G157	A217	E277	V338	E397	E397
R39	A98	T158	G218	K278	R339	S398	S398
S40	H99	D159	A219	I279	G340	S399	S399
G41	G100	S160	A220	I280	V341	T400	T400
Y42	R101	W161	L221	R281	D342	W401	W401
L43	T102	F162	Y222	Y222	F343	Y402	Y402
R44	S103	I163	V223	V223	M344	A403	A403
S45	Q104	T164	A224	A224	Y345	Q404	Q404
F46	A105	D165	Q225	Q225	E346	Y405	Y405
P47	V106	E166	P226	P226	G347	A406	A406
G48	G107	L167	S227	S227	N348	D407	D407
I49	F108	D168	L228	M288	Q349	R408	R408
T50	N109	E169	M229	A289	I350	L409	L409
K51	G110	S170	V230	T290	T351	F410	F410
R52	Q111	H171	Q231	G291	C352	L411	L411
Y53	L112	P172	K232	V292	R232	S412	S412
D54	V113	D173	S233	M293	D293	A413	A413
M55	E114	R174	I234	E294	E294	T414	T414
G56	Y115	Y175	A235	T295	T295	T415	T415
N57	R116	S176	G236	L296	L296	D416	D416
V58	Y117	A177	T237	R297	R297	G417	G417
S59	D118	Q178	Y238	F298	F298	I418	I418
R60	G119	Y179	C239	D299	D299	W419	W419
G61	T120	R180	K240	S300	S300	Y420	Y420
V62	V121	A181	T241	H301	H301	G421	G421
K122	K122	E182	P242	L303	L303	R422	R422

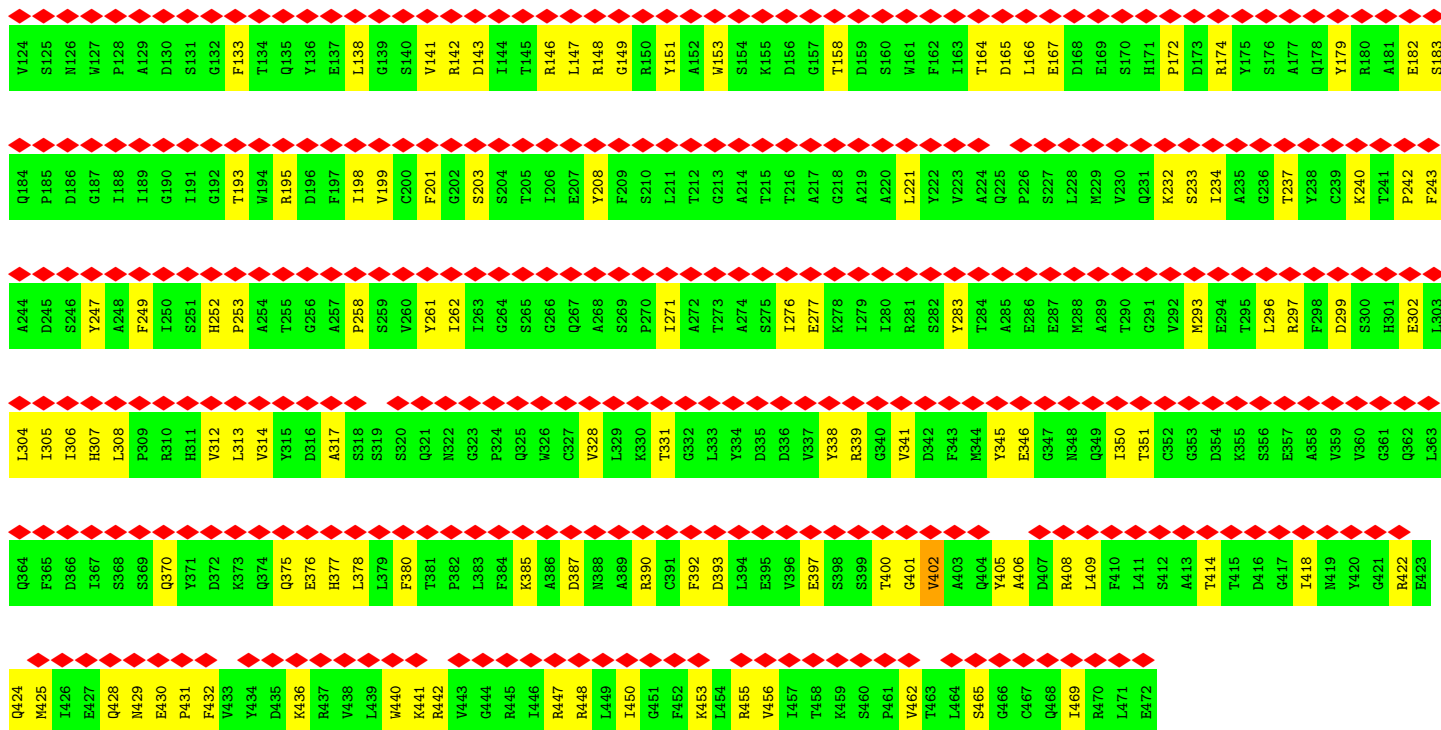


• Molecule 3: Packaged DNA stabilization protein gp10

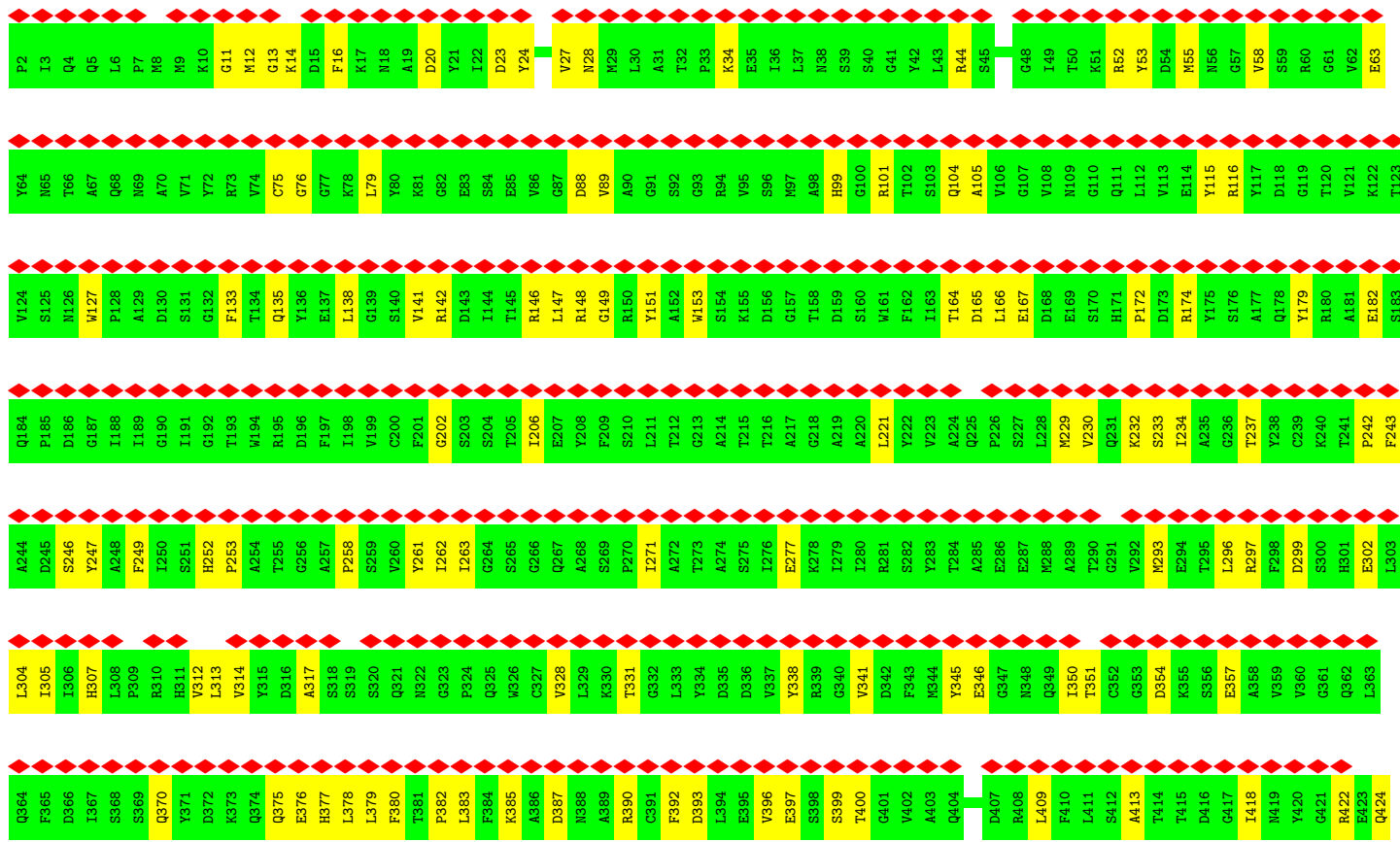
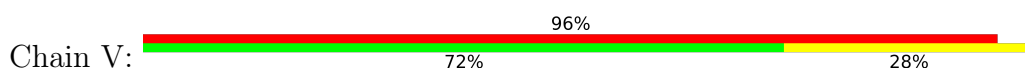


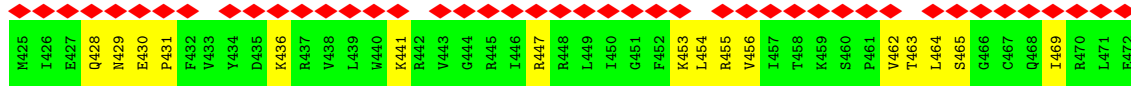
• Molecule 3: Packaged DNA stabilization protein gp10



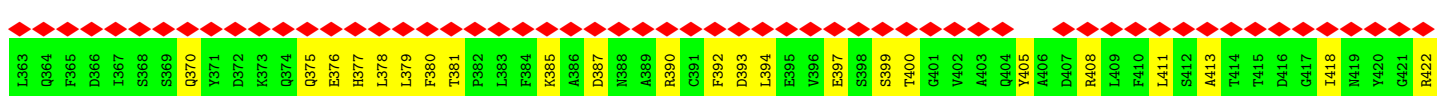
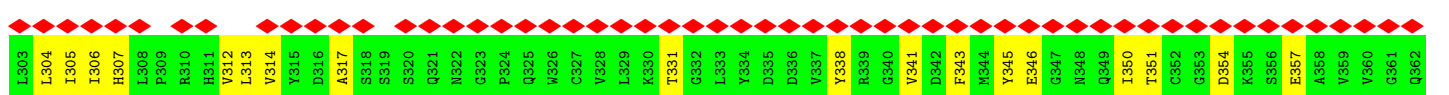
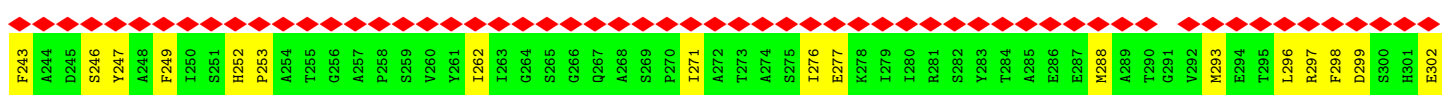
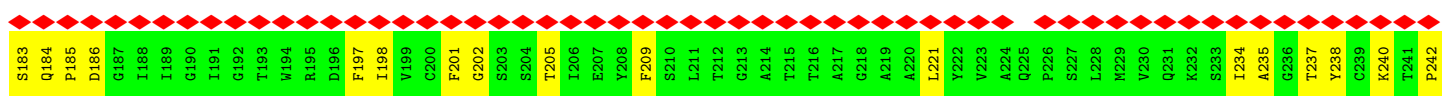
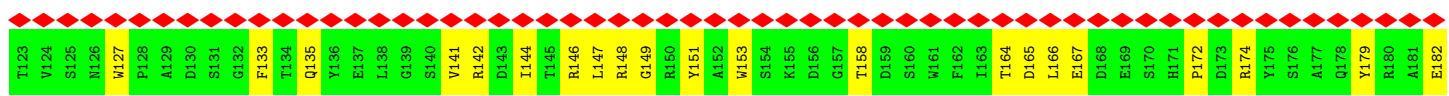
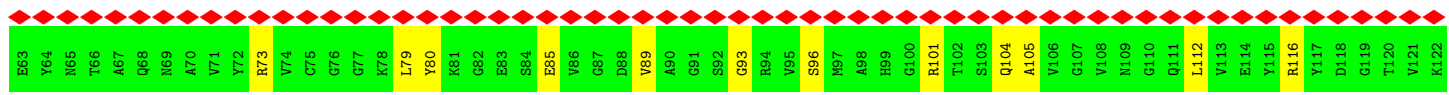
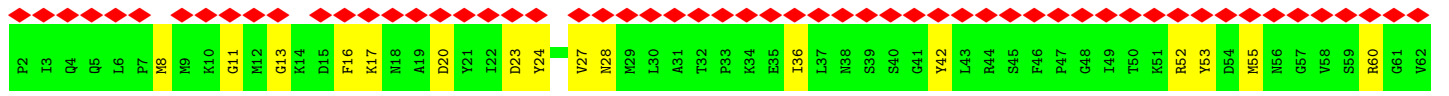
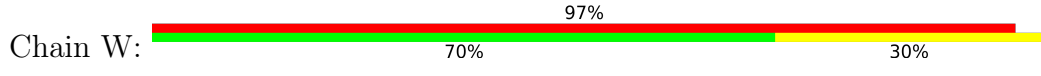


• Molecule 3: Packaged DNA stabilization protein gp10





• Molecule 3: Packaged DNA stabilization protein gp10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32650	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.35	0/872	0.49	0/1192
1	A	0.16	0/872	0.37	0/1192
1	B	0.27	0/872	0.41	0/1192
1	C	0.44	0/872	0.56	0/1192
1	D	0.16	0/872	0.37	0/1192
1	F	0.14	0/872	0.31	0/1192
1	X	0.16	0/872	0.35	0/1192
1	Y	0.17	0/872	0.36	0/1192
1	Z	0.17	0/872	0.39	0/1192
1	a	0.17	0/872	0.35	0/1192
1	b	0.17	0/872	0.37	0/1192
1	c	0.17	0/872	0.35	0/1192
1	d	0.17	0/872	0.35	0/1192
1	e	0.18	0/872	0.39	0/1192
1	f	0.18	0/872	0.40	0/1192
1	g	0.18	0/872	0.40	0/1192
1	h	0.18	0/872	0.40	0/1192
1	i	0.18	0/872	0.40	0/1192
2	E	0.29	0/1174	0.49	0/1592
2	G	0.25	0/1174	0.44	0/1592
2	H	0.18	0/1174	0.36	0/1592
2	I	0.17	0/1174	0.36	0/1592
2	J	0.30	0/1174	0.49	0/1592
2	K	0.27	0/1165	0.56	0/1580
2	L	0.17	0/1174	0.36	0/1592
2	M	0.18	0/1165	0.48	0/1580
2	N	0.19	0/1165	0.48	0/1580
2	O	0.30	0/1165	0.58	0/1580
2	P	0.18	0/1165	0.45	0/1580
2	Q	0.19	0/1165	0.48	0/1580
3	R	0.16	0/3767	0.31	0/5100
3	S	0.16	0/3767	0.33	0/5100
3	T	0.19	0/3767	0.34	0/5100
3	U	0.25	0/3767	0.41	1/5100 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	V	0.22	0/3767	0.37	1/5100 (0.0%)
3	W	0.25	0/3767	0.39	1/5100 (0.0%)
All	All	0.22	0/52332	0.40	3/71088 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	299	ASP	CB-CA-C	-5.17	110.59	116.54
3	U	299	ASP	CB-CA-C	-5.16	110.61	116.54
3	V	299	ASP	CB-CA-C	-5.07	110.71	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	855	0	846	23	0
1	A	855	0	846	23	0
1	B	855	0	846	22	0
1	C	855	0	846	22	0
1	D	855	0	846	25	0
1	F	855	0	846	17	0
1	X	855	0	846	26	0
1	Y	855	0	846	27	0
1	Z	855	0	846	33	0
1	a	855	0	846	29	0
1	b	855	0	846	26	0
1	c	855	0	846	27	0
1	d	855	0	846	28	0
1	e	855	0	846	38	0
1	f	855	0	846	37	0
1	g	855	0	846	38	0
1	h	855	0	846	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	i	855	0	846	30	0
2	E	1149	0	1115	42	0
2	G	1149	0	1115	41	0
2	H	1149	0	1115	40	0
2	I	1149	0	1115	38	0
2	J	1149	0	1115	40	0
2	K	1140	0	1107	33	0
2	L	1149	0	1115	34	0
2	M	1140	0	1107	36	0
2	N	1140	0	1107	37	0
2	O	1140	0	1107	43	0
2	P	1140	0	1107	35	0
2	Q	1140	0	1107	37	0
3	R	3686	0	3592	105	0
3	S	3686	0	3592	105	0
3	T	3686	0	3592	102	0
3	U	3686	0	3592	107	0
3	V	3686	0	3592	92	0
3	W	3686	0	3592	105	0
All	All	51240	0	50112	1307	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 13.

All (1307) 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)
2:P:63:ASP:HB3	2:P:69:GLU:HB3	1.46	0.97
2:Q:63:ASP:HB3	2:Q:69:GLU:HB3	1.45	0.97
2:M:63:ASP:HB3	2:M:69:GLU:HB3	1.45	0.97
2:O:63:ASP:HB3	2:O:69:GLU:HB3	1.45	0.96
2:N:63:ASP:HB3	2:N:69:GLU:HB3	1.46	0.96
2:K:63:ASP:HB3	2:K:69:GLU:HB3	1.46	0.95
2:P:9:LEU:HD21	2:P:80:VAL:HG13	1.52	0.92
2:M:25:LEU:HD13	3:V:447:ARG:HD2	1.51	0.91
1:0:62:THR:HG22	1:0:64:PRO:HD2	1.55	0.89
1:B:62:THR:HG22	1:B:64:PRO:HD2	1.55	0.89
1:C:62:THR:HG22	1:C:64:PRO:HD2	1.55	0.89
2:M:9:LEU:HD21	2:M:80:VAL:HG13	1.53	0.88
1:F:62:THR:HG22	1:F:64:PRO:HD2	1.54	0.88
1:A:62:THR:HG22	1:A:64:PRO:HD2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3:ILE:HG22	2:G:9:LEU:HD12	1.57	0.87
1:D:62:THR:HG22	1:D:64:PRO:HD2	1.56	0.86
3:R:12:MET:HE3	3:S:34:LYS:HE3	1.57	0.84
2:Q:40:LEU:HD12	2:Q:87:LEU:HD22	1.61	0.82
2:M:40:LEU:HD12	2:M:87:LEU:HD22	1.62	0.81
2:N:40:LEU:HD12	2:N:87:LEU:HD22	1.62	0.81
2:K:40:LEU:HD12	2:K:87:LEU:HD22	1.60	0.80
2:P:40:LEU:HD12	2:P:87:LEU:HD22	1.61	0.79
2:N:9:LEU:CD2	2:N:80:VAL:HG13	2.12	0.79
2:O:40:LEU:HD12	2:O:87:LEU:HD22	1.63	0.79
3:V:397:GLU:HB2	3:V:465:SER:HB3	1.66	0.78
1:Z:94:ASP:OD1	1:Z:95:ALA:N	2.18	0.77
1:h:94:ASP:OD1	1:h:95:ALA:N	2.18	0.77
2:P:9:LEU:CD2	2:P:80:VAL:HG13	2.14	0.76
1:g:94:ASP:OD1	1:g:95:ALA:N	2.18	0.76
1:i:85:VAL:HG23	1:i:86:GLN:H	1.51	0.76
1:f:94:ASP:OD1	1:f:95:ALA:N	2.18	0.76
1:h:85:VAL:HG23	1:h:86:GLN:H	1.50	0.76
2:N:140:PHE:HB3	2:N:145:GLU:HB3	1.67	0.76
1:Z:85:VAL:HG23	1:Z:86:GLN:H	1.51	0.76
1:i:94:ASP:OD1	1:i:95:ALA:N	2.18	0.76
3:S:397:GLU:HB2	3:S:465:SER:HB3	1.67	0.75
2:K:140:PHE:HB3	2:K:145:GLU:HB3	1.68	0.75
2:O:140:PHE:HB3	2:O:145:GLU:HB3	1.69	0.75
3:R:385:LYS:NZ	3:R:387:ASP:OD2	2.20	0.75
1:e:94:ASP:OD1	1:e:95:ALA:N	2.19	0.75
1:f:85:VAL:HG23	1:f:86:GLN:H	1.51	0.75
1:g:85:VAL:HG23	1:g:86:GLN:H	1.51	0.75
2:Q:9:LEU:CD2	2:Q:80:VAL:HG13	2.16	0.74
3:U:397:GLU:HB2	3:U:465:SER:HB3	1.69	0.74
1:e:85:VAL:HG23	1:e:86:GLN:H	1.50	0.74
2:M:9:LEU:CD2	2:M:80:VAL:HG13	2.17	0.74
2:P:140:PHE:HB3	2:P:145:GLU:HB3	1.70	0.74
3:R:229:MET:O	3:S:195:ARG:NH2	2.21	0.74
2:I:16:LYS:NZ	2:O:39:ASP:OD2	2.21	0.74
2:K:17:LEU:HD21	2:K:92:ALA:HA	1.69	0.74
1:b:90:MET:HE2	1:g:10:VAL:HG23	1.70	0.73
3:V:385:LYS:NZ	3:V:387:ASP:OD2	2.22	0.73
3:S:385:LYS:NZ	3:S:387:ASP:OD2	2.22	0.73
3:R:23:ASP:OD1	3:S:34:LYS:NZ	2.21	0.72
2:G:16:LYS:NZ	2:M:39:ASP:OD2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:385:LYS:NZ	3:T:387:ASP:OD2	2.22	0.72
1:C:16:ILE:O	1:b:12:ASN:ND2	2.23	0.72
2:M:140:PHE:HB3	2:M:145:GLU:HB3	1.70	0.72
2:J:12:ALA:HB1	2:J:84:PHE:CE1	2.24	0.72
2:Q:140:PHE:HB3	2:Q:145:GLU:HB3	1.72	0.72
3:V:44:ARG:NH1	3:W:20:ASP:OD1	2.23	0.71
2:I:21:SER:O	3:T:442:ARG:NH2	2.23	0.71
2:H:21:SER:HB2	3:S:442:ARG:HH21	1.55	0.71
2:N:9:LEU:HD21	2:N:80:VAL:HG13	1.70	0.71
2:J:16:LYS:NZ	2:P:39:ASP:OD2	2.23	0.71
2:N:25:LEU:HD13	3:R:447:ARG:HD2	1.72	0.71
3:U:385:LYS:NZ	3:U:387:ASP:OD2	2.22	0.71
3:U:167:GLU:OE1	3:U:174:ARG:NH2	2.24	0.70
1:a:81:LYS:NZ	1:a:112:ASP:OD2	2.24	0.70
1:g:31:ILE:HD11	1:g:90:MET:HB3	1.73	0.70
2:E:16:LYS:NZ	2:K:39:ASP:OD2	2.24	0.70
2:J:12:ALA:HB1	2:J:84:PHE:HE1	1.56	0.70
2:G:21:SER:O	3:R:442:ARG:NH2	2.24	0.70
2:L:21:SER:HB2	3:W:442:ARG:HH21	1.55	0.70
3:S:20:ASP:OD1	3:T:44:ARG:NH1	2.24	0.70
3:R:167:GLU:OE1	3:R:174:ARG:NH2	2.24	0.70
3:W:385:LYS:NZ	3:W:387:ASP:OD2	2.23	0.70
1:Z:31:ILE:HD11	1:Z:90:MET:HB3	1.74	0.70
1:b:19:GLU:O	1:g:72:LYS:NZ	2.24	0.70
1:B:14:ARG:NH2	1:f:109:TYR:OH	2.25	0.70
2:N:43:MET:HE3	2:N:44:MET:HE2	1.73	0.70
3:U:370:GLN:HB2	3:U:375:GLN:HE21	1.58	0.69
3:W:201:PHE:HZ	3:W:247:TYR:HD2	1.40	0.69
1:d:81:LYS:NZ	1:d:112:ASP:OD2	2.25	0.69
2:Q:43:MET:HE3	2:Q:44:MET:HE2	1.73	0.69
1:X:81:LYS:NZ	1:X:112:ASP:OD2	2.26	0.69
2:O:25:LEU:HD13	3:S:447:ARG:HD3	1.75	0.69
1:f:31:ILE:HD13	1:f:92:ILE:HD13	1.73	0.69
1:c:81:LYS:NZ	1:c:112:ASP:OD2	2.26	0.69
2:J:21:SER:O	3:U:442:ARG:NH2	2.26	0.69
2:L:21:SER:O	3:W:442:ARG:NH2	2.26	0.69
3:W:397:GLU:HB2	3:W:465:SER:HB3	1.75	0.69
1:Y:19:GLU:O	1:Z:72:LYS:NZ	2.26	0.68
1:c:90:MET:HE2	1:h:13:PRO:HG3	1.75	0.68
2:P:25:LEU:HD13	3:T:447:ARG:HD3	1.75	0.68
3:R:370:GLN:HB2	3:R:375:GLN:HE21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:SER:O	3:S:442:ARG:NH2	2.26	0.68
2:H:37:VAL:HG21	2:H:69:GLU:HG2	1.76	0.68
1:d:19:GLU:O	1:i:72:LYS:NZ	2.27	0.68
2:K:9:LEU:CD2	2:K:80:VAL:HG13	2.24	0.67
3:S:370:GLN:HB2	3:S:375:GLN:HE21	1.59	0.67
2:G:31:GLN:OE1	1:e:28:ASN:ND2	2.28	0.67
2:J:21:SER:HB2	3:U:442:ARG:HH21	1.60	0.67
2:J:37:VAL:HG21	2:J:69:GLU:HG2	1.77	0.67
3:R:20:ASP:OD1	3:S:44:ARG:NH1	2.28	0.67
3:T:370:GLN:HB2	3:T:375:GLN:HE21	1.60	0.66
3:W:164:THR:HA	3:W:172:PRO:HA	1.78	0.66
1:Y:81:LYS:NZ	1:Y:112:ASP:OD2	2.25	0.66
2:P:46:GLU:OE1	2:P:90:ARG:NH2	2.28	0.66
2:I:80:VAL:O	2:I:84:PHE:HB2	1.96	0.66
3:W:370:GLN:HB2	3:W:375:GLN:HE21	1.59	0.66
1:a:19:GLU:O	1:f:72:LYS:NZ	2.27	0.66
2:I:21:SER:HB2	3:T:442:ARG:HH21	1.60	0.66
3:W:235:ALA:HB1	3:W:288:MET:HE3	1.78	0.66
3:U:302:GLU:HB2	3:U:317:ALA:HB3	1.78	0.66
3:U:147:LEU:HD23	3:U:148:ARG:HG3	1.78	0.66
2:G:40:LEU:HD12	2:G:87:LEU:HD22	1.76	0.65
2:M:46:GLU:OE1	2:M:90:ARG:NH2	2.29	0.65
2:Q:25:LEU:HD13	3:U:447:ARG:HD2	1.78	0.65
3:R:397:GLU:HB2	3:R:465:SER:HB3	1.77	0.65
3:S:302:GLU:HB2	3:S:317:ALA:HB3	1.77	0.65
1:d:51:ILE:HD11	1:d:61:ILE:HD12	1.78	0.65
3:W:147:LEU:HD23	3:W:148:ARG:HG3	1.79	0.65
1:b:81:LYS:NZ	1:b:112:ASP:OD2	2.26	0.65
3:S:147:LEU:HD23	3:S:148:ARG:HG3	1.78	0.65
3:T:23:ASP:OD1	3:U:34:LYS:NZ	2.30	0.65
3:V:302:GLU:HB2	3:V:317:ALA:HB3	1.78	0.65
3:U:164:THR:HA	3:U:172:PRO:HA	1.79	0.65
2:G:21:SER:HB2	3:R:442:ARG:HH21	1.60	0.65
2:H:27:ASP:OD1	2:H:28:VAL:N	2.30	0.65
3:U:29:MET:HE2	3:U:377:HIS:HB3	1.79	0.64
3:R:34:LYS:NZ	3:V:23:ASP:OD1	2.29	0.64
3:T:147:LEU:HD23	3:T:148:ARG:HG3	1.79	0.64
3:V:370:GLN:HB2	3:V:375:GLN:HE21	1.62	0.64
1:Y:51:ILE:HD11	1:Y:61:ILE:HD12	1.79	0.64
3:V:34:LYS:NZ	3:W:23:ASP:OD1	2.26	0.64
3:V:164:THR:HA	3:V:172:PRO:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:GLN:OE1	1:i:28:ASN:ND2	2.30	0.64
3:S:296:LEU:HD11	3:S:350:ILE:HD13	1.80	0.64
2:I:121:SER:O	2:I:124:LYS:NZ	2.31	0.64
2:O:54:ILE:HD11	2:O:114:LEU:HB3	1.79	0.64
3:R:235:ALA:HB1	3:R:288:MET:HE3	1.78	0.64
3:U:277:GLU:OE2	3:W:297:ARG:NH1	2.21	0.64
2:I:37:VAL:HG21	2:I:69:GLU:HG2	1.80	0.64
3:W:302:GLU:HB2	3:W:317:ALA:HB3	1.79	0.64
3:T:397:GLU:HB2	3:T:465:SER:HB3	1.80	0.64
2:G:15:ARG:NH1	2:M:35:ASP:OD1	2.31	0.63
2:G:39:ASP:OD2	2:N:15:ARG:NH2	2.31	0.63
2:L:27:ASP:OD1	2:L:28:VAL:N	2.31	0.63
2:L:40:LEU:HD12	2:L:87:LEU:HD22	1.79	0.63
3:V:147:LEU:HD23	3:V:148:ARG:HG3	1.79	0.63
3:U:296:LEU:HD11	3:U:350:ILE:HD13	1.79	0.63
2:J:40:LEU:HD12	2:J:87:LEU:HD22	1.78	0.63
2:K:54:ILE:HD11	2:K:114:LEU:HB3	1.79	0.63
3:S:23:ASP:OD1	3:T:34:LYS:NZ	2.26	0.63
3:S:167:GLU:OE2	3:S:174:ARG:NH2	2.31	0.63
3:R:296:LEU:HD11	3:R:350:ILE:HD13	1.81	0.63
2:E:31:GLN:OE1	1:Z:28:ASN:ND2	2.32	0.63
1:a:51:ILE:HD11	1:a:61:ILE:HD12	1.80	0.63
2:P:130:SER:HB2	2:P:150:PRO:HB3	1.81	0.63
2:Q:9:LEU:HD21	2:Q:80:VAL:HG13	1.80	0.63
3:S:164:THR:HA	3:S:172:PRO:HA	1.80	0.63
2:I:25:LEU:O	1:g:78:GLN:NE2	2.32	0.63
3:T:138:LEU:HD22	3:T:153:TRP:HZ2	1.64	0.63
1:F:16:ILE:O	1:d:12:ASN:ND2	2.32	0.62
2:G:37:VAL:HG21	2:G:69:GLU:HG2	1.81	0.62
3:W:167:GLU:OE2	3:W:174:ARG:NH2	2.32	0.62
2:L:37:VAL:HG21	2:L:69:GLU:HG2	1.81	0.62
3:V:400:THR:HG21	3:V:436:LYS:HB3	1.81	0.62
2:E:27:ASP:OD1	2:E:28:VAL:N	2.33	0.62
2:J:31:GLN:OE1	1:h:28:ASN:ND2	2.33	0.62
3:R:138:LEU:HD22	3:R:153:TRP:HZ2	1.64	0.62
3:R:147:LEU:HD23	3:R:148:ARG:HG3	1.81	0.62
3:R:164:THR:HA	3:R:172:PRO:HA	1.79	0.62
1:B:52:GLU:OE1	1:B:81:LYS:NZ	2.32	0.62
2:E:37:VAL:HG21	2:E:69:GLU:HG2	1.80	0.62
2:G:15:ARG:HG3	2:G:21:SER:HB2	1.79	0.62
1:c:19:GLU:O	1:h:72:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:201:PHE:CZ	3:W:247:TYR:HD2	2.18	0.62
3:U:138:LEU:HD22	3:U:153:TRP:HZ2	1.65	0.62
3:R:195:ARG:NH2	3:V:229:MET:O	2.31	0.62
2:Q:72:ASP:OD1	2:Q:73:HIS:N	2.33	0.61
1:A:14:ARG:NH2	1:e:109:TYR:OH	2.33	0.61
2:P:54:ILE:HD11	2:P:114:LEU:HB3	1.82	0.61
3:T:229:MET:O	3:U:195:ARG:NH2	2.33	0.61
1:F:52:GLU:OE1	1:F:81:LYS:NZ	2.33	0.61
2:O:17:LEU:HD21	2:O:92:ALA:HA	1.82	0.61
3:T:164:THR:HA	3:T:172:PRO:HA	1.80	0.61
3:W:296:LEU:HD11	3:W:350:ILE:HD13	1.83	0.61
2:M:54:ILE:HD11	2:M:114:LEU:HB3	1.82	0.61
3:T:302:GLU:HB2	3:T:317:ALA:HB3	1.82	0.61
2:L:16:LYS:NZ	2:Q:39:ASP:OD2	2.32	0.61
3:V:138:LEU:HD22	3:V:153:TRP:HZ2	1.64	0.61
1:B:33:ILE:HG23	1:B:88:HIS:HB2	1.82	0.61
3:V:296:LEU:HD11	3:V:350:ILE:HD13	1.83	0.61
2:I:31:GLN:OE1	1:g:28:ASN:ND2	2.33	0.61
3:V:293:MET:HE2	3:V:304:LEU:HD11	1.82	0.61
3:W:447:ARG:NH2	1:i:76:ASN:OD1	2.27	0.61
2:G:27:ASP:OD1	2:G:28:VAL:N	2.34	0.60
2:J:27:ASP:OD1	2:J:28:VAL:N	2.34	0.60
2:K:133:PRO:HA	2:K:147:HIS:HA	1.83	0.60
2:N:134:THR:HG22	2:N:148:TYR:HE1	1.64	0.60
1:b:51:ILE:HD11	1:b:61:ILE:HD12	1.83	0.60
2:G:56:THR:HG22	2:G:114:LEU:HD22	1.83	0.60
2:N:72:ASP:OD1	2:N:73:HIS:N	2.34	0.60
1:C:94:ASP:OD1	1:C:95:ALA:N	2.35	0.60
1:F:14:ARG:NH2	1:i:109:TYR:OH	2.33	0.60
3:R:447:ARG:NH2	1:e:76:ASN:OD1	2.35	0.60
3:R:58:VAL:O	3:R:76:GLY:N	2.30	0.60
3:R:201:PHE:HZ	3:R:247:TYR:HD2	1.50	0.60
1:X:84:THR:O	1:e:6:ALA:N	2.34	0.60
1:0:94:ASP:OD1	1:0:95:ALA:N	2.35	0.60
3:U:179:TYR:OH	3:U:221:LEU:N	2.35	0.60
3:V:165:ASP:OD1	3:V:166:LEU:N	2.35	0.60
3:W:400:THR:HG21	3:W:436:LYS:HB3	1.83	0.60
2:O:56:THR:HG22	2:O:114:LEU:HD22	1.84	0.60
3:T:296:LEU:HD11	3:T:350:ILE:HD13	1.83	0.60
1:c:84:THR:O	1:h:6:ALA:N	2.35	0.60
1:B:16:ILE:O	1:a:12:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ARG:NH2	1:g:109:TYR:OH	2.35	0.59
3:R:165:ASP:OD1	3:R:166:LEU:N	2.35	0.59
3:S:179:TYR:OH	3:S:221:LEU:N	2.35	0.59
2:I:27:ASP:OD1	2:I:28:VAL:N	2.35	0.59
3:S:293:MET:HE2	3:S:304:LEU:HD11	1.84	0.59
3:V:127:TRP:O	3:V:135:GLN:NE2	2.35	0.59
3:W:165:ASP:OD1	3:W:166:LEU:N	2.35	0.59
3:R:179:TYR:OH	3:R:221:LEU:N	2.34	0.59
2:G:80:VAL:O	2:G:84:PHE:HB2	2.02	0.59
2:O:5:THR:HG23	2:O:8:ASP:H	1.66	0.59
3:U:165:ASP:OD1	3:U:166:LEU:N	2.35	0.59
3:V:179:TYR:OH	3:V:221:LEU:N	2.36	0.59
1:X:51:ILE:HD11	1:X:61:ILE:HD12	1.83	0.59
1:Y:84:THR:O	1:Z:6:ALA:N	2.35	0.59
1:b:84:THR:O	1:g:6:ALA:N	2.35	0.59
2:Q:134:THR:HG22	2:Q:148:TYR:HE1	1.66	0.59
2:K:56:THR:HG22	2:K:114:LEU:HD22	1.85	0.59
3:S:165:ASP:OD1	3:S:166:LEU:N	2.35	0.59
3:T:456:VAL:HG11	3:T:462:VAL:HG11	1.84	0.59
3:S:142:ARG:NH1	3:S:237:THR:OG1	2.36	0.59
3:W:293:MET:HE2	3:W:304:LEU:HD11	1.85	0.59
1:X:19:GLU:O	1:e:72:LYS:NZ	2.35	0.59
2:H:15:ARG:HG3	2:H:21:SER:HB2	1.84	0.58
2:J:29:GLU:HG3	3:U:447:ARG:HH12	1.68	0.58
2:N:54:ILE:HD11	2:N:114:LEU:HB3	1.84	0.58
3:T:179:TYR:OH	3:T:221:LEU:N	2.36	0.58
2:E:80:VAL:O	2:E:84:PHE:HB2	2.02	0.58
3:S:400:THR:HG21	3:S:436:LYS:HB3	1.84	0.58
3:T:165:ASP:OD1	3:T:166:LEU:N	2.35	0.58
2:H:121:SER:O	2:H:124:LYS:NZ	2.36	0.58
2:N:5:THR:HG23	2:N:8:ASP:H	1.67	0.58
3:V:63:GLU:OE2	3:V:99:HIS:ND1	2.36	0.58
1:a:84:THR:O	1:f:6:ALA:N	2.36	0.58
1:C:111:PRO:HG2	1:b:8:VAL:CG2	2.33	0.58
2:E:35:ASP:OD2	2:M:15:ARG:NH1	2.37	0.58
2:L:15:ARG:HG3	2:L:21:SER:HB2	1.83	0.58
3:V:456:VAL:HG11	3:V:462:VAL:HG11	1.85	0.58
2:E:15:ARG:NH1	2:K:35:ASP:OD1	2.37	0.58
2:H:89:CYS:HB3	2:O:102:LYS:HE2	1.85	0.58
1:d:84:THR:O	1:i:6:ALA:N	2.35	0.58
3:W:142:ARG:NH1	3:W:237:THR:OG1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:179:TYR:OH	3:W:221:LEU:N	2.35	0.58
1:i:31:ILE:HD13	1:i:92:ILE:HD13	1.85	0.58
2:Q:5:THR:HG23	2:Q:8:ASP:H	1.67	0.58
3:S:127:TRP:O	3:S:135:GLN:NE2	2.36	0.58
1:C:25:ALA:HB2	1:g:23:PHE:CD2	2.39	0.58
2:I:35:ASP:OD2	2:P:15:ARG:NH1	2.37	0.58
3:T:63:GLU:OE2	3:T:99:HIS:ND1	2.36	0.58
1:D:16:ILE:O	1:c:12:ASN:ND2	2.37	0.58
1:F:89:SER:OG	1:F:103:ILE:O	2.21	0.58
2:L:121:SER:O	2:L:124:LYS:NZ	2.36	0.58
1:0:111:PRO:HG2	1:Y:8:VAL:CG2	2.34	0.58
2:O:130:SER:HB2	2:O:150:PRO:HB3	1.85	0.58
3:R:11:GLY:HA3	3:R:380:PHE:HB2	1.86	0.58
3:V:16:PHE:HB3	3:V:418:ILE:HG21	1.84	0.58
1:C:33:ILE:HG23	1:C:88:HIS:HB2	1.85	0.57
2:K:134:THR:HG22	2:K:148:TYR:HE1	1.69	0.57
3:T:293:MET:HE2	3:T:304:LEU:HD11	1.85	0.57
3:W:127:TRP:O	3:W:135:GLN:NE2	2.37	0.57
1:A:52:GLU:OE1	1:A:81:LYS:NZ	2.37	0.57
3:S:394:LEU:HD22	3:S:411:LEU:HD11	1.85	0.57
1:D:14:ARG:NH2	1:h:109:TYR:OH	2.37	0.57
2:E:13:ALA:O	2:E:16:LYS:N	2.36	0.57
3:S:194:TRP:CG	3:S:195:ARG:H	2.23	0.57
2:H:62:ASP:OD1	2:H:63:ASP:N	2.37	0.57
2:J:80:VAL:O	2:J:84:PHE:HB2	2.03	0.57
2:O:133:PRO:HA	2:O:147:HIS:HA	1.87	0.57
3:S:408:ARG:HE	3:S:425:MET:HE3	1.68	0.57
1:0:114:TYR:O	1:0:116:ILE:HG12	2.05	0.57
2:K:9:LEU:HD21	2:K:80:VAL:HG13	1.85	0.57
2:L:56:THR:HG22	2:L:114:LEU:HD22	1.85	0.57
2:M:17:LEU:HD21	2:M:92:ALA:HA	1.86	0.57
2:Q:31:GLN:HG3	1:d:98:SER:HB2	1.87	0.57
3:R:293:MET:HE2	3:R:304:LEU:HD11	1.86	0.57
3:U:201:PHE:CE2	3:U:247:TYR:HD2	2.23	0.57
3:W:394:LEU:HD22	3:W:411:LEU:HD11	1.86	0.57
3:S:27:VAL:HB	3:S:378:LEU:HB2	1.86	0.56
3:T:11:GLY:O	3:T:24:TYR:N	2.38	0.56
3:U:447:ARG:NH2	1:h:76:ASN:OD1	2.38	0.56
3:R:11:GLY:O	3:R:24:TYR:N	2.39	0.56
3:T:27:VAL:HB	3:T:378:LEU:HB2	1.87	0.56
3:U:201:PHE:CZ	3:U:247:TYR:HD2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:203:SER:HA	3:U:233:SER:OG	2.05	0.56
3:W:11:GLY:O	3:W:24:TYR:N	2.38	0.56
1:C:45:ASN:HD22	1:C:45:ASN:H	1.53	0.56
2:N:6:LYS:HD2	2:N:70:GLY:HA2	1.87	0.56
3:V:14:LYS:HB2	3:V:418:ILE:HG12	1.87	0.56
3:V:409:LEU:HD23	3:V:428:GLN:HB2	1.86	0.56
3:W:27:VAL:HB	3:W:378:LEU:HB2	1.86	0.56
1:D:52:GLU:OE1	1:D:81:LYS:NZ	2.38	0.56
1:O:25:ALA:HB2	1:Z:23:PHE:CD2	2.40	0.56
2:H:44:MET:HG2	2:H:58:TYR:CD2	2.41	0.56
1:d:16:ILE:O	1:i:12:ASN:ND2	2.39	0.56
2:M:44:MET:HE3	2:M:44:MET:HA	1.88	0.56
2:O:134:THR:HG22	2:O:148:TYR:HE1	1.71	0.56
2:P:17:LEU:HD21	2:P:92:ALA:HA	1.88	0.56
3:R:331:THR:HG23	3:R:375:GLN:HE22	1.70	0.56
3:U:455:ARG:NH1	1:c:37:ASP:OD1	2.39	0.56
2:P:20:ALA:HA	2:P:26:THR:HB	1.88	0.56
3:U:11:GLY:O	3:U:24:TYR:N	2.39	0.56
1:e:91:ALA:HB1	1:e:93:TYR:HE1	1.70	0.56
2:I:40:LEU:HD12	2:I:87:LEU:HD22	1.88	0.56
2:Q:34:GLN:NE2	2:Q:69:GLU:OE2	2.34	0.56
3:U:409:LEU:HD23	3:U:428:GLN:HB2	1.87	0.56
3:U:27:VAL:HB	3:U:378:LEU:HB2	1.87	0.55
1:c:51:ILE:HD11	1:c:61:ILE:HD12	1.88	0.55
3:R:27:VAL:HB	3:R:378:LEU:HB2	1.87	0.55
3:V:146:ARG:HD2	3:V:151:TYR:HE1	1.71	0.55
2:G:49:GLN:HE22	2:N:113:LEU:HB3	1.70	0.55
2:I:29:GLU:HG3	3:T:447:ARG:HH22	1.70	0.55
2:M:20:ALA:HA	2:M:26:THR:HB	1.89	0.55
2:G:2:GLN:HG3	2:M:63:ASP:OD2	2.05	0.55
2:H:113:LEU:HB3	2:N:49:GLN:HE21	1.72	0.55
2:N:133:PRO:HA	2:N:147:HIS:HA	1.89	0.55
3:S:146:ARG:HD2	3:S:151:TYR:HE1	1.71	0.55
3:T:432:PHE:HD2	1:f:60:GLN:HE21	1.54	0.55
2:M:6:LYS:HD2	2:M:70:GLY:HA2	1.87	0.55
3:U:448:ARG:NH1	3:W:397:GLU:OE1	2.39	0.55
1:B:23:PHE:CD2	1:a:25:ALA:HB2	2.41	0.55
2:E:62:ASP:OD1	2:E:63:ASP:N	2.39	0.55
3:S:331:THR:HG23	3:S:375:GLN:HE22	1.72	0.55
3:R:78:LYS:HD2	3:R:85:GLU:HG3	1.89	0.55
3:S:11:GLY:O	3:S:24:TYR:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:142:ARG:NH1	3:T:237:THR:OG1	2.40	0.55
1:F:23:PHE:CD2	1:d:25:ALA:HB2	2.41	0.55
3:R:142:ARG:NH1	3:R:237:THR:OG1	2.40	0.55
3:T:78:LYS:HD3	3:T:85:GLU:CD	2.32	0.55
3:U:293:MET:HE2	3:U:304:LEU:HD11	1.88	0.55
1:D:25:ALA:HB2	1:h:23:PHE:CD2	2.42	0.55
3:R:116:ARG:NH1	3:R:116:ARG:HB2	2.22	0.55
3:T:20:ASP:OD1	3:U:44:ARG:NH1	2.40	0.55
3:W:331:THR:HG23	3:W:375:GLN:HE22	1.72	0.55
2:K:81:SER:HA	2:K:84:PHE:CE2	2.42	0.55
3:V:116:ARG:HB2	3:V:116:ARG:NH1	2.22	0.55
1:X:32:TYR:HE1	1:X:64:PRO:HB3	1.71	0.55
1:d:112:ASP:OD1	1:d:113:GLN:NE2	2.40	0.55
2:M:81:SER:HA	2:M:84:PHE:CE2	2.42	0.54
3:S:201:PHE:HZ	3:S:247:TYR:HD2	1.55	0.54
3:U:331:THR:HG23	3:U:375:GLN:HE22	1.71	0.54
2:P:65:ASN:OD1	2:P:66:PRO:HD3	2.07	0.54
3:T:146:ARG:HD2	3:T:151:TYR:HE1	1.72	0.54
3:U:312:VAL:HG21	3:U:338:TYR:HB3	1.89	0.54
3:U:456:VAL:HG11	3:U:462:VAL:HG11	1.89	0.54
1:a:16:ILE:O	1:f:12:ASN:ND2	2.40	0.54
1:d:99:GLN:HE21	1:d:102:TYR:HB2	1.72	0.54
2:O:9:LEU:CD2	2:O:80:VAL:HG13	2.38	0.54
3:U:116:ARG:NH1	3:U:116:ARG:HB2	2.22	0.54
3:V:141:VAL:HG22	3:V:153:TRP:CD1	2.42	0.54
1:A:16:ILE:O	1:X:12:ASN:ND2	2.41	0.54
3:R:147:LEU:HD13	3:R:198:ILE:HG12	1.88	0.54
3:U:141:VAL:HG22	3:U:153:TRP:CD1	2.42	0.54
3:V:27:VAL:HB	3:V:378:LEU:HB2	1.88	0.54
2:M:134:THR:HG22	2:M:148:TYR:CZ	2.42	0.54
2:P:81:SER:HA	2:P:84:PHE:CE2	2.42	0.54
3:R:158:THR:HA	3:S:101:ARG:HH21	1.73	0.54
3:R:456:VAL:HG11	3:R:462:VAL:HG11	1.88	0.54
2:G:3:ILE:CG2	2:G:9:LEU:HD12	2.33	0.54
2:J:15:ARG:NE	2:P:35:ASP:OD1	2.41	0.54
2:N:81:SER:HA	2:N:84:PHE:CE2	2.43	0.54
3:U:142:ARG:NH1	3:U:237:THR:OG1	2.41	0.54
2:M:5:THR:HG23	2:M:8:ASP:H	1.73	0.54
2:O:46:GLU:OE1	2:O:90:ARG:NH2	2.40	0.54
3:R:141:VAL:HG22	3:R:153:TRP:CD1	2.42	0.54
3:R:312:VAL:HG21	3:R:338:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:116:ARG:HB2	3:S:116:ARG:NH1	2.23	0.54
1:A:25:ALA:HB2	1:e:23:PHE:CD2	2.42	0.54
2:L:133:PRO:HA	2:L:147:HIS:HA	1.88	0.54
2:Q:6:LYS:HD2	2:Q:70:GLY:HA2	1.90	0.54
2:E:3:ILE:HG23	2:E:8:ASP:HB3	1.87	0.54
1:F:101:ASP:OD1	1:F:102:TYR:N	2.41	0.54
3:T:52:ARG:HG2	3:T:53:TYR:CD2	2.43	0.54
3:W:141:VAL:HG22	3:W:153:TRP:CD1	2.43	0.54
1:b:16:ILE:O	1:g:12:ASN:ND2	2.41	0.54
1:b:47:ILE:HG13	1:b:48:PRO:HD2	1.90	0.54
3:T:88:ASP:O	3:T:115:TYR:OH	2.21	0.54
3:V:142:ARG:NH1	3:V:237:THR:OG1	2.41	0.54
1:i:33:ILE:HG23	1:i:88:HIS:HB2	1.89	0.54
2:E:89:CYS:HB2	2:M:102:LYS:HE2	1.90	0.53
2:P:9:LEU:CD2	2:P:80:VAL:CG1	2.84	0.53
1:Y:47:ILE:HG13	1:Y:48:PRO:HD2	1.89	0.53
2:L:62:ASP:OD1	2:L:63:ASP:N	2.38	0.53
2:P:5:THR:HG23	2:P:8:ASP:H	1.72	0.53
3:S:305:ILE:HG12	3:S:314:VAL:HG22	1.90	0.53
3:S:456:VAL:HG11	3:S:462:VAL:HG11	1.90	0.53
2:I:133:PRO:HA	2:I:147:HIS:HA	1.90	0.53
2:L:113:LEU:HB3	2:Q:49:GLN:HE21	1.72	0.53
2:M:65:ASN:OD1	2:M:66:PRO:HD3	2.08	0.53
3:R:146:ARG:HD2	3:R:151:TYR:HE1	1.73	0.53
3:V:88:ASP:O	3:V:115:TYR:OH	2.20	0.53
1:Y:16:ILE:O	1:Z:12:ASN:ND2	2.42	0.53
1:g:49:VAL:O	1:g:60:GLN:HG3	2.08	0.53
2:H:15:ARG:NH1	2:N:35:ASP:OD1	2.41	0.53
2:N:65:ASN:OD1	2:N:66:PRO:HD3	2.09	0.53
3:R:184:GLN:HG3	3:R:205:THR:HG21	1.90	0.53
3:S:141:VAL:HG22	3:S:153:TRP:CD1	2.43	0.53
3:T:116:ARG:NH1	3:T:116:ARG:HB2	2.23	0.53
1:Z:75:TYR:CG	1:Z:76:ASN:N	2.76	0.53
1:c:32:TYR:HE1	1:c:64:PRO:HB3	1.73	0.53
3:T:331:THR:HG23	3:T:375:GLN:HE22	1.73	0.53
3:U:146:ARG:HD2	3:U:151:TYR:HE1	1.74	0.53
3:W:116:ARG:NH1	3:W:116:ARG:HB2	2.23	0.53
2:H:16:LYS:NZ	2:N:39:ASP:OD2	2.34	0.53
2:O:81:SER:HA	2:O:84:PHE:CE2	2.43	0.53
3:U:16:PHE:HB3	3:U:418:ILE:HG21	1.90	0.53
3:W:399:SER:HB3	3:W:463:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASP:OD1	1:B:102:TYR:N	2.41	0.53
2:P:134:THR:HG22	2:P:148:TYR:CZ	2.44	0.53
3:S:399:SER:HB3	3:S:463:THR:HB	1.91	0.53
1:A:103:ILE:HG21	1:A:106:VAL:HA	1.91	0.53
2:O:9:LEU:HD21	2:O:80:VAL:HG13	1.89	0.53
2:O:65:ASN:OD1	2:O:66:PRO:HD3	2.09	0.53
3:S:354:ASP:OD1	3:S:357:GLU:N	2.41	0.53
1:O:16:ILE:O	1:Y:12:ASN:ND2	2.42	0.53
2:K:65:ASN:OD1	2:K:66:PRO:HD3	2.09	0.53
2:M:9:LEU:CD2	2:M:80:VAL:CG1	2.87	0.53
3:T:141:VAL:HG22	3:T:153:TRP:CD1	2.43	0.53
3:W:312:VAL:HG21	3:W:338:TYR:HB3	1.90	0.53
1:d:101:ASP:OD2	1:i:14:ARG:NH1	2.42	0.53
2:E:15:ARG:HG3	2:E:21:SER:HB2	1.91	0.53
1:g:51:ILE:HD11	1:g:61:ILE:HD13	1.90	0.53
2:E:29:GLU:HG3	3:V:447:ARG:HH12	1.74	0.52
2:K:34:GLN:NE2	2:K:69:GLU:OE2	2.39	0.52
1:O:38:THR:O	1:O:102:TYR:OH	2.24	0.52
1:A:46:GLN:HB3	1:A:63:GLN:HG2	1.91	0.52
3:V:399:SER:HB3	3:V:463:THR:HB	1.91	0.52
1:X:16:ILE:O	1:e:12:ASN:ND2	2.42	0.52
1:Y:32:TYR:HE1	1:Y:64:PRO:HB3	1.74	0.52
1:F:31:ILE:HG13	1:F:67:ILE:HD11	1.90	0.52
2:G:49:GLN:NE2	2:N:113:LEU:HB3	2.24	0.52
2:J:49:GLN:HE22	2:Q:113:LEU:HB3	1.73	0.52
2:Q:81:SER:HA	2:Q:84:PHE:CE2	2.44	0.52
3:R:116:ARG:HB2	3:R:116:ARG:HH11	1.74	0.52
3:S:455:ARG:NH1	1:a:37:ASP:OD1	2.42	0.52
3:V:116:ARG:HB2	3:V:116:ARG:HH11	1.75	0.52
1:c:16:ILE:O	1:h:12:ASN:ND2	2.43	0.52
1:i:14:ARG:HB3	1:i:72:LYS:HD2	1.92	0.52
2:H:133:PRO:HA	2:H:147:HIS:HA	1.92	0.52
2:P:6:LYS:HD2	2:P:70:GLY:HA2	1.90	0.52
3:S:184:GLN:HG3	3:S:205:THR:HG21	1.92	0.52
3:W:307:HIS:CD2	3:W:341:VAL:HG23	2.45	0.52
1:d:43:PRO:HA	1:d:46:GLN:HG3	1.91	0.52
2:H:132:MET:HA	2:H:132:MET:HE2	1.92	0.52
2:J:44:MET:HG2	2:J:58:TYR:CD2	2.45	0.52
2:M:34:GLN:HB2	1:X:96:ASN:HD22	1.75	0.52
2:Q:65:ASN:OD1	2:Q:66:PRO:HD3	2.09	0.52
1:a:112:ASP:OD1	1:a:113:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:32:TYR:HE1	1:d:64:PRO:HB3	1.73	0.52
2:E:3:ILE:HG23	2:E:8:ASP:CB	2.40	0.52
3:R:52:ARG:HG2	3:R:53:TYR:CD2	2.44	0.52
3:S:423:GLU:O	1:a:99:GLN:NE2	2.42	0.52
3:V:52:ARG:HG2	3:V:53:TYR:CD2	2.45	0.52
1:d:99:GLN:NE2	1:d:102:TYR:HB2	2.25	0.52
1:g:75:TYR:CG	1:g:76:ASN:N	2.77	0.52
1:B:88:HIS:CD2	1:B:90:MET:HG3	2.44	0.52
1:C:46:GLN:HB3	1:C:63:GLN:HG2	1.92	0.52
3:U:116:ARG:HB2	3:U:116:ARG:HH11	1.74	0.52
1:b:32:TYR:HE1	1:b:64:PRO:HB3	1.73	0.52
2:L:15:ARG:NH1	2:Q:35:ASP:OD1	2.42	0.52
3:S:312:VAL:HG21	3:S:338:TYR:HB3	1.90	0.52
3:T:202:GLY:O	3:T:233:SER:OG	2.27	0.52
3:U:52:ARG:HG2	3:U:53:TYR:CD2	2.44	0.52
1:C:65:LEU:HD11	1:C:82:ILE:HG21	1.92	0.52
2:H:22:ASP:OD1	2:H:23:ALA:N	2.42	0.52
2:K:34:GLN:OE1	1:Y:96:ASN:ND2	2.37	0.52
2:Q:133:PRO:HA	2:Q:147:HIS:HA	1.92	0.52
3:V:312:VAL:HG21	3:V:338:TYR:HB3	1.91	0.52
2:L:22:ASP:OD1	2:L:23:ALA:N	2.42	0.52
2:N:128:TYR:HB2	2:N:148:TYR:HD2	1.74	0.52
1:a:32:TYR:HE1	1:a:64:PRO:HB3	1.74	0.52
1:i:75:TYR:CG	1:i:76:ASN:N	2.77	0.52
3:T:298:PHE:HB3	3:T:350:ILE:HD11	1.92	0.51
3:T:312:VAL:HG21	3:T:338:TYR:HB3	1.91	0.51
3:T:455:ARG:NH2	1:g:54:GLU:OE2	2.44	0.51
3:V:331:THR:HG23	3:V:375:GLN:HE22	1.75	0.51
1:c:47:ILE:HG13	1:c:48:PRO:HD2	1.92	0.51
3:R:307:HIS:CD2	3:R:341:VAL:HG23	2.45	0.51
3:T:252:HIS:CG	3:T:253:PRO:HD2	2.46	0.51
3:W:116:ARG:HB2	3:W:116:ARG:HH11	1.76	0.51
3:W:430:GLU:HG3	3:W:431:PRO:HD2	1.93	0.51
1:a:101:ASP:OD2	1:f:14:ARG:NH1	2.43	0.51
2:E:97:LEU:HD22	3:V:390:ARG:NH1	2.26	0.51
2:I:62:ASP:OD1	2:I:63:ASP:N	2.39	0.51
3:S:158:THR:HA	3:T:101:ARG:HH21	1.75	0.51
3:S:307:HIS:CD2	3:S:341:VAL:HG23	2.45	0.51
3:W:432:PHE:CE2	1:h:60:GLN:NE2	2.79	0.51
1:Z:33:ILE:HG23	1:Z:88:HIS:HB2	1.92	0.51
2:H:56:THR:HG22	2:H:114:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:101:ARG:HH21	3:W:158:THR:HA	1.76	0.51
3:V:297:ARG:NH1	3:W:277:GLU:OE2	2.30	0.51
1:e:14:ARG:HH11	1:e:14:ARG:HG2	1.74	0.51
1:f:14:ARG:HB3	1:f:72:LYS:HD2	1.92	0.51
2:G:133:PRO:HA	2:G:147:HIS:HA	1.93	0.51
2:J:9:LEU:HD12	2:J:9:LEU:H	1.75	0.51
2:K:20:ALA:HA	2:K:26:THR:HB	1.93	0.51
2:O:6:LYS:O	2:O:10:VAL:HG12	2.10	0.51
3:W:52:ARG:HG2	3:W:53:TYR:CD2	2.46	0.51
1:h:91:ALA:HB1	1:h:93:TYR:HE1	1.76	0.51
2:H:86:ASN:C	2:H:88:ALA:H	2.19	0.51
1:b:112:ASP:OD1	1:b:113:GLN:NE2	2.44	0.51
1:0:23:PHE:CD1	1:Y:25:ALA:HB2	2.46	0.51
2:E:12:ALA:HB1	2:E:84:PHE:CE1	2.46	0.51
2:I:97:LEU:HD22	3:T:390:ARG:NH1	2.26	0.51
1:Z:50:TYR:CE1	1:Z:60:GLN:HB2	2.46	0.51
1:h:31:ILE:HD13	1:h:92:ILE:HD13	1.93	0.51
1:0:109:TYR:O	1:0:111:PRO:HD3	2.10	0.51
2:O:10:VAL:HG23	2:O:36:ALA:HB3	1.93	0.51
3:R:53:TYR:HE1	3:R:55:MET:HE1	1.76	0.51
3:V:53:TYR:HE1	3:V:55:MET:HE1	1.76	0.51
3:V:243:PHE:HZ	3:V:317:ALA:HB2	1.76	0.51
1:0:14:ARG:NE	1:Z:109:TYR:OH	2.43	0.50
1:0:65:LEU:HD11	1:0:82:ILE:HG21	1.92	0.50
2:J:56:THR:HG22	2:J:114:LEU:HD22	1.93	0.50
2:K:134:THR:HG23	2:K:146:TRP:O	2.11	0.50
2:O:134:THR:HG23	2:O:146:TRP:O	2.10	0.50
3:S:116:ARG:HB2	3:S:116:ARG:HH11	1.75	0.50
3:W:305:ILE:HG12	3:W:314:VAL:HG22	1.93	0.50
2:J:66:PRO:HB3	1:h:96:ASN:ND2	2.26	0.50
2:L:19:VAL:HG13	3:W:445:ARG:HD3	1.94	0.50
2:N:33:MET:HA	2:N:33:MET:HE2	1.93	0.50
3:T:199:VAL:HG12	3:T:208:TYR:CE1	2.46	0.50
3:T:305:ILE:HG12	3:T:314:VAL:HG22	1.93	0.50
3:V:305:ILE:HG12	3:V:314:VAL:HG22	1.92	0.50
1:C:23:PHE:CD1	1:b:25:ALA:HB2	2.47	0.50
2:J:15:ARG:HG2	2:J:21:SER:HB2	1.92	0.50
2:Q:33:MET:HE2	2:Q:33:MET:HA	1.93	0.50
3:U:158:THR:HA	3:W:101:ARG:HH21	1.75	0.50
3:U:262:ILE:HD12	3:U:271:ILE:HG21	1.94	0.50
1:e:33:ILE:HG23	1:e:88:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:33:ILE:HG23	1:h:88:HIS:HB2	1.93	0.50
2:J:9:LEU:HD11	2:J:73:HIS:CD2	2.47	0.50
2:J:133:PRO:HA	2:J:147:HIS:HA	1.93	0.50
3:R:29:MET:HE2	3:R:377:HIS:HB3	1.93	0.50
3:R:252:HIS:CG	3:R:253:PRO:HD2	2.46	0.50
3:S:52:ARG:HG2	3:S:53:TYR:CD2	2.45	0.50
3:V:252:HIS:CG	3:V:253:PRO:HD2	2.46	0.50
1:f:75:TYR:CG	1:f:76:ASN:N	2.79	0.50
1:D:90:MET:HE1	1:c:11:SER:H	1.76	0.50
2:K:117:GLN:NE2	2:L:52:LYS:HG3	2.26	0.50
2:Q:73:HIS:ND1	2:Q:75:LEU:HB3	2.27	0.50
3:V:297:ARG:HH11	3:V:297:ARG:HG2	1.77	0.50
1:a:47:ILE:HG13	1:a:48:PRO:HD2	1.94	0.50
1:g:33:ILE:HG23	1:g:88:HIS:HB2	1.92	0.50
2:E:8:ASP:HA	2:E:11:ARG:HG2	1.94	0.50
2:E:56:THR:HG22	2:E:114:LEU:HD22	1.93	0.50
2:H:19:VAL:HG13	3:S:445:ARG:HD3	1.93	0.50
2:J:49:GLN:NE2	2:Q:113:LEU:HB3	2.27	0.50
2:M:33:MET:HE2	2:M:33:MET:HA	1.94	0.50
3:T:307:HIS:CD2	3:T:341:VAL:HG23	2.47	0.50
1:X:68:ASN:HB3	1:X:74:VAL:HG11	1.94	0.50
1:f:50:TYR:O	1:f:83:VAL:N	2.42	0.50
1:g:31:ILE:HD13	1:g:92:ILE:HD13	1.94	0.50
2:H:29:GLU:HG3	3:S:447:ARG:HH22	1.77	0.50
3:T:116:ARG:HB2	3:T:116:ARG:HH11	1.75	0.50
3:W:262:ILE:HD12	3:W:271:ILE:HG21	1.93	0.50
3:W:297:ARG:HG2	3:W:297:ARG:HH11	1.74	0.50
1:e:38:THR:HB	1:e:45:ASN:HD22	1.77	0.50
1:D:23:PHE:CD1	1:c:25:ALA:HB2	2.46	0.50
2:L:97:LEU:HD22	3:W:390:ARG:NH1	2.26	0.50
3:R:262:ILE:HD12	3:R:271:ILE:HG21	1.93	0.50
2:G:62:ASP:OD1	2:G:63:ASP:N	2.38	0.50
2:G:97:LEU:HD22	3:R:390:ARG:NH1	2.27	0.50
2:N:134:THR:HG23	2:N:146:TRP:O	2.12	0.50
3:V:202:GLY:O	3:V:233:SER:OG	2.26	0.50
3:V:307:HIS:CD2	3:V:341:VAL:HG23	2.47	0.50
3:W:184:GLN:HG3	3:W:205:THR:HG21	1.94	0.50
3:T:396:VAL:HG11	3:T:454:LEU:HD21	1.94	0.49
3:U:307:HIS:CD2	3:U:341:VAL:HG23	2.47	0.49
3:U:418:ILE:HD12	3:W:434:TYR:CD1	2.47	0.49
1:X:47:ILE:HG13	1:X:48:PRO:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:31:ILE:HD13	1:Z:92:ILE:HD13	1.94	0.49
1:A:29:GLY:O	1:A:30:LYS:HD3	2.13	0.49
2:I:86:ASN:C	2:I:88:ALA:H	2.20	0.49
3:R:86:VAL:HG12	3:R:86:VAL:O	2.11	0.49
3:U:58:VAL:O	3:U:76:GLY:N	2.37	0.49
1:Z:14:ARG:HG2	1:Z:14:ARG:HH11	1.77	0.49
1:a:38:THR:O	1:a:102:TYR:OH	2.26	0.49
1:h:65:LEU:HD23	1:h:73:ILE:HG21	1.94	0.49
3:R:293:MET:HE3	3:R:306:ILE:HG12	1.95	0.49
3:U:252:HIS:CG	3:U:253:PRO:HD2	2.47	0.49
3:W:354:ASP:OD1	3:W:357:GLU:N	2.42	0.49
2:P:33:MET:HE2	2:P:33:MET:HA	1.93	0.49
3:U:430:GLU:HG3	3:U:431:PRO:HD2	1.93	0.49
2:E:22:ASP:OD1	2:E:23:ALA:N	2.45	0.49
2:O:11:ARG:HE	2:O:33:MET:HE1	1.77	0.49
1:D:29:GLY:O	1:D:30:LYS:HD3	2.13	0.49
2:I:22:ASP:OD1	2:I:23:ALA:N	2.44	0.49
2:J:97:LEU:HD22	3:U:390:ARG:NH1	2.27	0.49
3:T:422:ARG:NH2	3:T:424:GLN:OE1	2.45	0.49
3:U:400:THR:HA	3:U:429:ASN:ND2	2.28	0.49
3:V:11:GLY:O	3:V:24:TYR:N	2.44	0.49
1:f:28:ASN:HB3	1:f:95:ALA:HB2	1.95	0.49
1:C:109:TYR:O	1:C:111:PRO:HD3	2.12	0.49
3:U:305:ILE:HG12	3:U:314:VAL:HG22	1.95	0.49
3:W:60:ARG:HD2	3:W:93:GLY:O	2.13	0.49
3:W:252:HIS:CG	3:W:253:PRO:HD2	2.47	0.49
3:R:74:VAL:HG13	3:R:89:VAL:HG11	1.94	0.49
3:V:146:ARG:NH2	3:V:149:GLY:HA2	2.28	0.49
1:Y:43:PRO:HA	1:Y:46:GLN:HG3	1.95	0.49
1:i:51:ILE:HD11	1:i:61:ILE:HD13	1.94	0.49
1:B:94:ASP:OD1	1:B:95:ALA:N	2.46	0.49
3:R:193:THR:O	3:R:247:TYR:OH	2.21	0.49
3:T:53:TYR:HE1	3:T:55:MET:HE1	1.77	0.49
3:T:243:PHE:HZ	3:T:317:ALA:HB2	1.76	0.49
3:T:430:GLU:HG3	3:T:431:PRO:HD2	1.94	0.49
3:U:400:THR:HG21	3:U:436:LYS:HB3	1.93	0.49
3:V:354:ASP:OD1	3:V:357:GLU:N	2.43	0.49
3:W:197:PHE:HA	3:W:209:PHE:O	2.13	0.49
1:X:112:ASP:OD1	1:X:113:GLN:NE2	2.46	0.49
1:b:90:MET:SD	1:g:13:PRO:HG3	2.52	0.49
1:D:91:ALA:HB1	1:D:93:TYR:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ASP:OD1	1:F:95:ALA:N	2.46	0.48
2:G:52:LYS:HG3	2:N:117:GLN:NE2	2.28	0.48
2:P:61:SER:O	2:P:62:ASP:HB3	2.13	0.48
3:T:146:ARG:NH2	3:T:149:GLY:HA2	2.28	0.48
1:d:47:ILE:HG13	1:d:48:PRO:HD2	1.95	0.48
1:A:103:ILE:HD12	1:A:106:VAL:HG22	1.96	0.48
2:L:86:ASN:C	2:L:88:ALA:H	2.20	0.48
2:N:79:ALA:HB1	2:N:114:LEU:HD21	1.93	0.48
3:R:243:PHE:HZ	3:R:317:ALA:HB2	1.78	0.48
3:S:296:LEU:HD12	3:S:297:ARG:H	1.78	0.48
3:S:297:ARG:HG2	3:S:297:ARG:HH11	1.77	0.48
3:U:401:GLY:O	3:U:402:VAL:HB	2.13	0.48
3:V:400:THR:HA	3:V:429:ASN:HD22	1.77	0.48
1:X:43:PRO:HA	1:X:46:GLN:HG3	1.94	0.48
1:Y:33:ILE:HG13	1:Y:49:VAL:HG11	1.96	0.48
1:Y:112:ASP:OD1	1:Y:113:GLN:NE2	2.47	0.48
1:h:38:THR:HB	1:h:45:ASN:HD22	1.78	0.48
2:G:29:GLU:HG3	3:R:447:ARG:HH12	1.78	0.48
2:H:97:LEU:HD22	3:S:390:ARG:NH1	2.27	0.48
3:U:232:LYS:HE2	3:U:261:TYR:HE2	1.78	0.48
1:g:50:TYR:O	1:g:83:VAL:N	2.41	0.48
1:A:13:PRO:HG3	1:e:106:VAL:HG22	1.95	0.48
1:B:65:LEU:HD11	1:B:82:ILE:HG21	1.95	0.48
2:K:46:GLU:OE1	2:K:90:ARG:NH2	2.47	0.48
3:T:346:GLU:OE2	3:T:351:THR:OG1	2.29	0.48
3:U:146:ARG:NH2	3:U:149:GLY:HA2	2.29	0.48
1:C:109:TYR:CE1	1:b:114:TYR:HB3	2.49	0.48
2:K:34:GLN:HB2	1:Y:96:ASN:ND2	2.29	0.48
2:Q:6:LYS:NZ	2:Q:72:ASP:O	2.44	0.48
1:D:94:ASP:OD1	1:D:95:ALA:N	2.47	0.48
2:H:52:LYS:HG3	2:O:117:GLN:NE2	2.28	0.48
2:I:44:MET:HG2	2:I:58:TYR:CG	2.48	0.48
2:I:56:THR:HG22	2:I:114:LEU:HD22	1.94	0.48
2:K:61:SER:O	2:K:62:ASP:HB3	2.14	0.48
3:U:293:MET:HE3	3:U:306:ILE:HG12	1.95	0.48
1:B:46:GLN:HB3	1:B:63:GLN:HG2	1.96	0.48
2:J:52:LYS:HG3	2:Q:117:GLN:NE2	2.29	0.48
2:K:11:ARG:HE	2:K:33:MET:HE1	1.79	0.48
2:M:61:SER:O	2:M:62:ASP:HB3	2.13	0.48
2:P:10:VAL:HG13	2:P:33:MET:HE1	1.96	0.48
3:W:146:ARG:HD2	3:W:151:TYR:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:OD1	1:A:102:TYR:N	2.46	0.48
1:F:65:LEU:HD11	1:F:82:ILE:HG21	1.95	0.48
2:L:12:ALA:HB1	2:L:84:PHE:CE1	2.49	0.48
2:L:29:GLU:HG3	3:W:447:ARG:HH12	1.79	0.48
2:O:72:ASP:OD1	2:O:73:HIS:N	2.47	0.48
3:T:354:ASP:OD1	3:T:357:GLU:N	2.42	0.48
3:V:400:THR:HA	3:V:429:ASN:ND2	2.28	0.48
1:h:75:TYR:CG	1:h:76:ASN:N	2.81	0.48
1:i:65:LEU:HD23	1:i:73:ILE:HG21	1.96	0.48
1:F:90:MET:HB3	1:F:103:ILE:HD12	1.96	0.48
2:N:8:ASP:OD1	2:N:11:ARG:NH1	2.35	0.48
3:R:430:GLU:HG3	3:R:431:PRO:HD2	1.95	0.48
3:U:147:LEU:HD12	3:U:193:THR:OG1	2.14	0.48
1:D:103:ILE:HG21	1:D:106:VAL:HA	1.94	0.48
2:H:12:ALA:HB1	2:H:84:PHE:CE1	2.48	0.48
2:O:34:GLN:HB2	1:b:96:ASN:ND2	2.29	0.48
1:f:31:ILE:HD11	1:f:90:MET:HG3	1.96	0.48
1:i:68:ASN:HB3	1:i:74:VAL:HG21	1.96	0.48
2:E:44:MET:HG2	2:E:58:TYR:CG	2.49	0.47
2:O:61:SER:O	2:O:62:ASP:HB3	2.14	0.47
3:S:293:MET:HE3	3:S:306:ILE:HG12	1.96	0.47
1:d:68:ASN:HB3	1:d:74:VAL:HG11	1.95	0.47
1:e:31:ILE:HD13	1:e:92:ILE:HD13	1.96	0.47
2:G:12:ALA:HB1	2:G:84:PHE:HE1	1.79	0.47
2:N:34:GLN:NE2	1:a:96:ASN:OD1	2.29	0.47
2:N:61:SER:O	2:N:62:ASP:HB3	2.14	0.47
2:O:4:LYS:H	2:O:4:LYS:HD2	1.78	0.47
3:V:206:ILE:HB	3:V:230:VAL:HB	1.96	0.47
3:W:146:ARG:NH2	3:W:149:GLY:HA2	2.29	0.47
1:X:33:ILE:HG13	1:X:49:VAL:HG11	1.96	0.47
1:Z:68:ASN:HB3	1:Z:74:VAL:HG21	1.95	0.47
1:a:43:PRO:HA	1:a:46:GLN:HG3	1.96	0.47
1:A:94:ASP:OD1	1:A:95:ALA:N	2.47	0.47
2:E:86:ASN:C	2:E:88:ALA:H	2.21	0.47
2:Q:61:SER:O	2:Q:62:ASP:HB3	2.14	0.47
1:d:33:ILE:HG13	1:d:49:VAL:HG11	1.96	0.47
1:A:23:PHE:CD1	1:X:25:ALA:HB2	2.48	0.47
2:M:11:ARG:HG2	2:M:28:VAL:HG11	1.95	0.47
3:S:146:ARG:NH2	3:S:149:GLY:HA2	2.29	0.47
3:V:12:MET:HB3	3:V:383:LEU:H	1.79	0.47
1:i:50:TYR:CE1	1:i:60:GLN:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:TYR:CZ	2:H:113:LEU:HD11	2.50	0.47
2:O:20:ALA:HA	2:O:26:THR:HB	1.96	0.47
3:U:60:ARG:HD2	3:U:93:GLY:O	2.14	0.47
3:U:297:ARG:HG2	3:U:297:ARG:NH1	2.29	0.47
1:b:68:ASN:HB3	1:b:74:VAL:HG11	1.95	0.47
1:D:81:LYS:HD3	1:h:109:TYR:CZ	2.49	0.47
2:J:12:ALA:CB	2:J:84:PHE:HE1	2.25	0.47
3:U:392:PHE:O	3:U:441:LYS:HA	2.14	0.47
3:U:408:ARG:NH2	1:c:93:TYR:OH	2.47	0.47
1:X:38:THR:O	1:X:102:TYR:OH	2.24	0.47
1:Y:68:ASN:HB3	1:Y:74:VAL:HG11	1.96	0.47
1:A:13:PRO:HG2	1:e:103:ILE:HD13	1.97	0.47
1:D:11:SER:HA	1:h:15:PRO:HB3	1.96	0.47
2:I:5:THR:OG1	2:I:8:ASP:OD2	2.26	0.47
2:J:86:ASN:C	2:J:88:ALA:H	2.22	0.47
2:K:72:ASP:OD1	2:K:73:HIS:N	2.47	0.47
3:R:146:ARG:NH2	3:R:149:GLY:HA2	2.29	0.47
3:R:446:ILE:HG23	3:R:450:ILE:HB	1.96	0.47
3:R:455:ARG:NH1	1:X:37:ASP:OD1	2.47	0.47
3:S:392:PHE:O	3:S:441:LYS:HA	2.14	0.47
3:W:293:MET:HE3	3:W:306:ILE:HG12	1.95	0.47
3:W:392:PHE:O	3:W:441:LYS:HA	2.15	0.47
1:Z:30:LYS:N	1:Z:93:TYR:O	2.43	0.47
1:Z:85:VAL:HG23	1:Z:86:GLN:N	2.26	0.47
1:e:38:THR:HB	1:e:45:ASN:ND2	2.30	0.47
1:e:75:TYR:CG	1:e:76:ASN:N	2.82	0.47
1:f:33:ILE:HG23	1:f:88:HIS:HB2	1.97	0.47
1:g:91:ALA:HB1	1:g:93:TYR:HE1	1.80	0.47
1:h:38:THR:HB	1:h:45:ASN:ND2	2.30	0.47
2:G:86:ASN:C	2:G:88:ALA:H	2.22	0.47
2:Q:134:THR:HG23	2:Q:146:TRP:O	2.15	0.47
3:S:193:THR:O	3:S:247:TYR:OH	2.22	0.47
3:V:262:ILE:HD12	3:V:271:ILE:HG21	1.96	0.47
1:a:62:THR:HG22	1:a:64:PRO:HD2	1.97	0.47
1:g:65:LEU:HD23	1:g:73:ILE:HG21	1.97	0.47
3:R:409:LEU:HD23	3:R:428:GLN:HB2	1.95	0.47
3:T:78:LYS:HD3	3:T:85:GLU:OE1	2.15	0.47
3:T:392:PHE:O	3:T:441:LYS:HA	2.14	0.47
1:f:90:MET:HB3	1:f:103:ILE:HB	1.96	0.47
3:W:79:LEU:HB2	3:W:89:VAL:HG23	1.96	0.47
3:W:276:ILE:HG23	3:W:313:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:31:ILE:HG13	1:a:67:ILE:HD11	1.97	0.47
1:e:50:TYR:CE1	1:e:60:GLN:HB2	2.50	0.47
1:f:30:LYS:N	1:f:93:TYR:O	2.40	0.47
2:J:13:ALA:O	2:J:14:LEU:C	2.58	0.46
2:P:34:GLN:HB2	1:c:96:ASN:OD1	2.16	0.46
3:T:262:ILE:HD12	3:T:271:ILE:HG21	1.96	0.46
3:U:201:PHE:CE2	3:U:247:TYR:CD2	3.03	0.46
2:I:33:MET:HE3	2:I:33:MET:HB2	1.86	0.46
2:L:67:PRO:HG2	1:i:24:LYS:HE2	1.96	0.46
2:N:73:HIS:ND1	2:N:75:LEU:HB3	2.30	0.46
2:Q:130:SER:HB2	2:Q:150:PRO:HB3	1.97	0.46
1:a:14:ARG:HG3	1:a:14:ARG:HH11	1.80	0.46
1:a:33:ILE:HG13	1:a:49:VAL:HG11	1.97	0.46
1:B:13:PRO:HG2	1:f:103:ILE:HD13	1.97	0.46
1:C:88:HIS:NE2	1:C:106:VAL:HG21	2.30	0.46
3:S:243:PHE:HZ	3:S:317:ALA:HB2	1.80	0.46
3:T:297:ARG:HG2	3:T:297:ARG:HH11	1.81	0.46
3:V:392:PHE:O	3:V:441:LYS:HA	2.15	0.46
1:g:50:TYR:CD1	1:g:60:GLN:HB2	2.50	0.46
1:B:25:ALA:HB2	1:f:23:PHE:CD1	2.50	0.46
1:F:25:ALA:HB2	1:i:23:PHE:CD1	2.51	0.46
2:N:130:SER:HB2	2:N:150:PRO:HB3	1.98	0.46
2:P:133:PRO:HA	2:P:147:HIS:HA	1.97	0.46
3:U:234:ILE:HG22	3:U:249:PHE:HB2	1.98	0.46
3:V:447:ARG:NH2	1:Z:76:ASN:OD1	2.48	0.46
1:C:12:ASN:HB2	1:g:17:PHE:CD1	2.51	0.46
3:S:430:GLU:HG3	3:S:431:PRO:HD2	1.96	0.46
3:U:414:THR:O	3:U:450:ILE:HA	2.14	0.46
1:D:13:PRO:HG2	1:h:103:ILE:HD13	1.98	0.46
1:D:46:GLN:HB3	1:D:63:GLN:HG2	1.97	0.46
2:J:8:ASP:HA	2:J:11:ARG:HG2	1.98	0.46
3:V:380:PHE:CE2	3:V:453:LYS:HG3	2.50	0.46
3:W:243:PHE:HZ	3:W:317:ALA:HB2	1.81	0.46
1:O:89:SER:HB2	1:O:104:ALA:O	2.15	0.46
2:K:113:LEU:HB3	2:L:49:GLN:NE2	2.30	0.46
3:S:262:ILE:HD12	3:S:271:ILE:HG21	1.97	0.46
1:X:35:GLN:HB2	1:X:38:THR:HG21	1.97	0.46
1:Y:31:ILE:HG13	1:Y:67:ILE:HD11	1.97	0.46
1:c:32:TYR:HB3	1:c:40:PRO:O	2.15	0.46
1:c:68:ASN:HB3	1:c:74:VAL:HG11	1.98	0.46
2:L:109:TYR:CZ	2:L:113:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:34:GLN:HB2	1:X:96:ASN:ND2	2.30	0.46
2:P:8:ASP:OD1	2:P:11:ARG:NH1	2.36	0.46
3:S:13:GLY:HA3	3:S:24:TYR:CE2	2.51	0.46
3:S:345:TYR:HD1	3:S:350:ILE:HG12	1.81	0.46
3:T:399:SER:HB3	3:T:463:THR:HB	1.98	0.46
1:X:92:ILE:O	1:X:100:VAL:N	2.46	0.46
1:a:68:ASN:HB3	1:a:74:VAL:HG11	1.98	0.46
1:d:14:ARG:HG3	1:d:14:ARG:HH11	1.80	0.46
1:d:31:ILE:HG13	1:d:67:ILE:HD11	1.97	0.46
1:e:51:ILE:HD11	1:e:61:ILE:HD13	1.96	0.46
1:A:89:SER:O	1:A:89:SER:OG	2.33	0.46
2:P:64:GLU:N	2:P:66:PRO:HD2	2.31	0.46
2:Q:8:ASP:OD1	2:Q:11:ARG:NH1	2.36	0.46
3:R:392:PHE:O	3:R:441:LYS:HA	2.16	0.46
3:S:183:SER:HA	3:T:148:ARG:HG2	1.98	0.46
3:U:193:THR:O	3:U:247:TYR:OH	2.23	0.46
3:W:242:PRO:HA	3:W:247:TYR:HD1	1.81	0.46
1:a:7:ASN:OD1	1:f:114:TYR:HB2	2.15	0.46
1:c:62:THR:HG22	1:c:64:PRO:HD2	1.98	0.46
1:f:51:ILE:HD11	1:f:61:ILE:HD13	1.96	0.46
1:h:50:TYR:O	1:h:83:VAL:N	2.41	0.46
1:i:85:VAL:HG23	1:i:86:GLN:N	2.27	0.46
1:B:109:TYR:OH	1:f:112:ASP:OD2	2.33	0.46
2:N:6:LYS:NZ	2:N:72:ASP:O	2.45	0.46
3:R:147:LEU:HD12	3:R:193:THR:OG1	2.16	0.46
3:S:400:THR:HA	3:S:429:ASN:HD22	1.80	0.46
3:U:36:ILE:HG21	3:U:42:TYR:HB3	1.97	0.46
3:V:258:PRO:O	3:V:277:GLU:HG3	2.16	0.46
1:C:45:ASN:N	1:C:45:ASN:ND2	2.64	0.45
2:E:133:PRO:HA	2:E:147:HIS:HA	1.97	0.45
2:O:10:VAL:CG2	2:O:36:ALA:HB3	2.47	0.45
3:V:455:ARG:NH1	1:Y:37:ASP:OD1	2.49	0.45
1:f:68:ASN:HB3	1:f:74:VAL:HG21	1.98	0.45
1:i:31:ILE:HD11	1:i:90:MET:HG2	1.98	0.45
1:D:51:ILE:HD11	1:D:61:ILE:HD13	1.98	0.45
2:E:52:LYS:HG3	2:M:117:GLN:NE2	2.31	0.45
2:I:15:ARG:HG3	2:I:21:SER:HB2	1.98	0.45
2:L:66:PRO:HB3	1:i:96:ASN:ND2	2.31	0.45
2:M:64:GLU:N	2:M:66:PRO:HD2	2.31	0.45
3:T:447:ARG:NH1	1:g:76:ASN:OD1	2.34	0.45
3:U:183:SER:HA	3:W:148:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:148:ARG:HG2	3:W:183:SER:HA	1.98	0.45
1:h:74:VAL:HG22	1:h:79:LEU:HD23	1.97	0.45
1:i:31:ILE:HD13	1:i:92:ILE:CD1	2.46	0.45
2:G:25:LEU:HB3	3:R:413:ALA:HB3	1.97	0.45
2:H:49:GLN:NE2	2:O:113:LEU:HB3	2.31	0.45
2:K:25:LEU:HD11	3:W:447:ARG:CZ	2.47	0.45
2:M:9:LEU:HD21	2:M:80:VAL:CG1	2.36	0.45
3:T:380:PHE:CE2	3:T:453:LYS:HG3	2.51	0.45
3:U:393:ASP:O	3:U:469:ILE:HA	2.17	0.45
1:0:109:TYR:CE1	1:Y:114:TYR:HB3	2.51	0.45
2:G:67:PRO:HG2	1:e:24:LYS:HE2	1.98	0.45
3:R:232:LYS:HE2	3:R:261:TYR:HE2	1.80	0.45
3:R:305:ILE:HG12	3:R:314:VAL:HG22	1.98	0.45
3:T:234:ILE:HG22	3:T:249:PHE:HB2	1.99	0.45
3:V:422:ARG:NH2	3:V:424:GLN:OE1	2.49	0.45
3:W:405:TYR:CE1	1:d:42:ASN:ND2	2.79	0.45
3:W:422:ARG:NH2	3:W:424:GLN:OE1	2.50	0.45
1:0:107:LEU:O	1:0:108:LYS:HB2	2.16	0.45
1:D:107:LEU:HD11	1:h:112:ASP:HB2	1.99	0.45
2:I:19:VAL:HG13	3:T:445:ARG:HD3	1.98	0.45
3:S:133:PHE:CE1	3:S:174:ARG:HD3	2.52	0.45
2:N:34:GLN:HB2	1:a:96:ASN:OD1	2.15	0.45
2:P:134:THR:HB	2:P:138:ASN:HD22	1.82	0.45
2:Q:20:ALA:HA	2:Q:26:THR:HB	1.97	0.45
3:S:422:ARG:NH2	3:S:424:GLN:OE1	2.48	0.45
3:T:133:PHE:CE1	3:T:174:ARG:HD3	2.51	0.45
3:V:234:ILE:HG22	3:V:249:PHE:HB2	1.98	0.45
3:W:380:PHE:CE2	3:W:453:LYS:HG3	2.51	0.45
1:X:62:THR:HG22	1:X:64:PRO:HD2	1.97	0.45
2:I:52:LYS:HG3	2:P:117:GLN:NE2	2.32	0.45
2:J:13:ALA:O	2:J:16:LYS:N	2.50	0.45
2:K:64:GLU:N	2:K:66:PRO:HD2	2.32	0.45
2:K:113:LEU:HB3	2:L:49:GLN:HE22	1.82	0.45
3:S:296:LEU:HD12	3:S:297:ARG:N	2.31	0.45
3:V:346:GLU:OE2	3:V:351:THR:OG1	2.29	0.45
3:W:376:GLU:OE2	3:W:455:ARG:HD2	2.16	0.45
1:f:49:VAL:O	1:f:60:GLN:HG3	2.16	0.45
1:g:50:TYR:CE1	1:g:60:GLN:HB2	2.52	0.45
3:S:376:GLU:OE2	3:S:455:ARG:HD2	2.17	0.45
3:V:13:GLY:HA3	3:V:24:TYR:CE2	2.52	0.45
3:W:400:THR:HA	3:W:429:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:39:ASP:OD2	2:P:16:LYS:NZ	2.46	0.45
2:N:64:GLU:N	2:N:66:PRO:HD2	2.32	0.45
3:R:258:PRO:O	3:R:277:GLU:HG3	2.15	0.45
3:R:376:GLU:OE2	3:R:455:ARG:HD2	2.17	0.45
3:U:242:PRO:HA	3:U:247:TYR:HD1	1.82	0.45
3:W:36:ILE:HG21	3:W:42:TYR:HB3	1.99	0.45
1:h:50:TYR:CE1	1:h:60:GLN:HB2	2.51	0.45
1:A:107:LEU:HD11	1:e:112:ASP:HB2	1.98	0.45
1:F:10:VAL:HG13	1:i:90:MET:HE2	1.99	0.45
2:I:89:CYS:HB2	2:P:102:LYS:HE2	1.99	0.45
3:R:133:PHE:CE1	3:R:174:ARG:HD3	2.52	0.45
3:U:74:VAL:HG13	3:U:89:VAL:HG11	1.99	0.45
2:E:4:LYS:HA	2:E:73:HIS:HE2	1.81	0.44
2:H:38:ASP:OD2	2:O:3:ILE:HG12	2.18	0.44
2:J:25:LEU:O	1:h:78:GLN:NE2	2.50	0.44
2:O:64:GLU:N	2:O:66:PRO:HD2	2.32	0.44
3:R:78:LYS:HE2	3:R:88:ASP:OD1	2.17	0.44
3:R:380:PHE:CE2	3:R:453:LYS:HG3	2.52	0.44
3:R:393:ASP:O	3:R:469:ILE:HA	2.17	0.44
3:V:230:VAL:HG21	3:V:263:ILE:HG23	1.99	0.44
1:Z:50:TYR:O	1:Z:83:VAL:N	2.44	0.44
1:C:25:ALA:HB2	1:g:23:PHE:HD2	1.81	0.44
1:D:52:GLU:CD	1:D:81:LYS:HZ1	2.25	0.44
2:G:19:VAL:HG21	2:G:95:TYR:CD2	2.53	0.44
3:S:17:LYS:HE2	3:S:17:LYS:HB2	1.82	0.44
3:S:55:MET:HE3	3:S:73:ARG:HD2	1.99	0.44
3:S:201:PHE:CZ	3:S:247:TYR:HD2	2.34	0.44
3:U:12:MET:SD	3:W:36:ILE:HD12	2.58	0.44
3:V:167:GLU:OE2	3:V:174:ARG:NH2	2.50	0.44
2:H:12:ALA:HB1	2:H:84:PHE:HE1	1.82	0.44
2:H:35:ASP:OD1	2:O:15:ARG:NE	2.50	0.44
2:I:31:GLN:HA	1:g:28:ASN:HD21	1.81	0.44
3:R:379:LEU:HD23	3:R:379:LEU:HA	1.82	0.44
3:S:380:PHE:CE2	3:S:453:LYS:HG3	2.52	0.44
3:U:147:LEU:CD2	3:U:148:ARG:HG3	2.46	0.44
3:U:297:ARG:HG2	3:U:297:ARG:HH11	1.81	0.44
2:E:31:GLN:HA	1:Z:28:ASN:HD21	1.82	0.44
2:G:66:PRO:HB3	1:e:96:ASN:HD22	1.81	0.44
2:H:66:PRO:HB3	1:f:96:ASN:ND2	2.32	0.44
3:R:242:PRO:HA	3:R:247:TYR:HD1	1.82	0.44
3:S:346:GLU:OE2	3:S:351:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:53:TYR:HE1	3:U:55:MET:HE1	1.82	0.44
3:U:380:PHE:CE2	3:U:453:LYS:HG3	2.52	0.44
1:0:81:LYS:HD3	1:Z:109:TYR:CZ	2.52	0.44
1:B:51:ILE:HD11	1:B:61:ILE:HD13	2.00	0.44
1:B:88:HIS:NE2	1:B:106:VAL:HG21	2.33	0.44
2:G:66:PRO:HB3	1:e:96:ASN:ND2	2.33	0.44
2:H:2:GLN:HG3	2:H:3:ILE:H	1.82	0.44
2:I:15:ARG:NH2	2:I:84:PHE:HZ	2.15	0.44
2:K:73:HIS:ND1	2:K:75:LEU:HB3	2.32	0.44
2:Q:64:GLU:N	2:Q:66:PRO:HD2	2.32	0.44
3:R:408:ARG:HD3	1:X:39:ASP:OD2	2.18	0.44
3:S:422:ARG:HG2	1:f:78:GLN:OE1	2.18	0.44
3:T:206:ILE:HB	3:T:230:VAL:HB	1.98	0.44
3:T:232:LYS:HE2	3:T:261:TYR:HE2	1.82	0.44
3:V:28:ASN:HB3	3:V:377:HIS:HD2	1.82	0.44
3:R:44:ARG:NH1	3:V:20:ASP:OD1	2.51	0.44
3:T:242:PRO:HA	3:T:247:TYR:HD1	1.82	0.44
3:U:345:TYR:HD1	3:U:350:ILE:HG12	1.83	0.44
3:U:400:THR:HA	3:U:429:ASN:HD22	1.82	0.44
3:V:133:PHE:CE1	3:V:174:ARG:HD3	2.51	0.44
1:X:32:TYR:HB3	1:X:40:PRO:O	2.18	0.44
1:b:38:THR:O	1:b:102:TYR:OH	2.26	0.44
2:E:25:LEU:HB3	3:V:413:ALA:HB3	2.00	0.44
2:E:25:LEU:O	1:Z:78:GLN:NE2	2.51	0.44
2:I:134:THR:HG22	2:I:148:TYR:CZ	2.52	0.44
3:S:8:MET:HG2	3:S:381:THR:HG22	1.98	0.44
3:S:242:PRO:HA	3:S:247:TYR:HD1	1.83	0.44
3:T:158:THR:HA	3:U:101:ARG:NH2	2.33	0.44
3:W:133:PHE:CE1	3:W:174:ARG:HD3	2.52	0.44
3:W:345:TYR:HD1	3:W:350:ILE:HG12	1.83	0.44
1:e:85:VAL:HG23	1:e:86:GLN:N	2.26	0.44
1:f:31:ILE:HD11	1:f:90:MET:CG	2.48	0.44
1:f:50:TYR:CE1	1:f:60:GLN:HB2	2.52	0.44
2:G:87:LEU:HA	2:G:90:ARG:HB2	1.99	0.44
2:H:113:LEU:HB3	2:N:49:GLN:NE2	2.33	0.44
2:I:25:LEU:HB3	3:T:413:ALA:HB3	2.00	0.44
2:L:12:ALA:HB1	2:L:84:PHE:HE1	1.82	0.44
3:U:376:GLU:OE2	3:U:455:ARG:HD2	2.17	0.44
3:U:405:TYR:CG	3:U:406:ALA:N	2.85	0.44
3:W:8:MET:HG2	3:W:381:THR:HG22	2.00	0.44
1:Z:51:ILE:HD11	1:Z:61:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:35:GLN:HB2	1:a:38:THR:HG21	2.00	0.44
1:h:51:ILE:HD11	1:h:61:ILE:HD13	2.00	0.44
1:A:51:ILE:HD11	1:A:61:ILE:HD13	2.00	0.44
2:G:44:MET:HG2	2:G:58:TYR:CG	2.53	0.44
2:P:4:LYS:HB3	2:P:4:LYS:HE3	1.89	0.44
2:P:9:LEU:HD21	2:P:80:VAL:CG1	2.34	0.44
3:R:183:SER:HA	3:S:148:ARG:HG2	2.00	0.44
3:U:243:PHE:HZ	3:U:317:ALA:HB2	1.83	0.44
3:W:13:GLY:HA3	3:W:24:TYR:CE2	2.53	0.44
1:0:68:ASN:HB3	1:0:74:VAL:HG21	1.98	0.43
1:D:24:LYS:HB2	1:D:24:LYS:HE2	1.87	0.43
2:I:2:GLN:HG3	2:I:3:ILE:H	1.83	0.43
3:T:262:ILE:HD11	3:T:271:ILE:HD13	2.00	0.43
3:W:243:PHE:N	3:W:246:SER:O	2.38	0.43
1:c:14:ARG:HG3	1:c:14:ARG:HH11	1.82	0.43
2:H:5:THR:OG1	2:H:8:ASP:OD2	2.28	0.43
2:J:19:VAL:HG21	2:J:95:TYR:CD2	2.53	0.43
2:J:87:LEU:HA	2:J:90:ARG:HB2	2.01	0.43
2:L:113:LEU:HB3	2:Q:49:GLN:NE2	2.33	0.43
3:R:243:PHE:N	3:R:246:SER:O	2.40	0.43
3:U:133:PHE:CE1	3:U:174:ARG:HD3	2.52	0.43
1:f:63:GLN:O	1:f:65:LEU:N	2.50	0.43
1:i:107:LEU:HD12	1:i:107:LEU:HA	1.88	0.43
1:D:12:ASN:HB2	1:h:17:PHE:CD1	2.54	0.43
2:E:66:PRO:HB3	1:Z:96:ASN:ND2	2.34	0.43
2:G:19:VAL:HG13	3:R:445:ARG:HD3	1.99	0.43
2:I:86:ASN:O	2:I:87:LEU:HB3	2.18	0.43
2:J:21:SER:CB	3:U:442:ARG:HH21	2.30	0.43
3:R:158:THR:HA	3:S:101:ARG:NH2	2.33	0.43
3:S:202:GLY:O	3:S:233:SER:OG	2.23	0.43
3:T:455:ARG:NH1	1:b:37:ASP:OD1	2.51	0.43
3:V:58:VAL:O	3:V:76:GLY:N	2.38	0.43
3:V:242:PRO:HA	3:V:247:TYR:HD1	1.82	0.43
3:V:262:ILE:HD11	3:V:271:ILE:HD13	2.01	0.43
1:b:35:GLN:HB2	1:b:38:THR:HG21	1.99	0.43
1:h:31:ILE:HD11	1:h:90:MET:HB3	2.00	0.43
1:D:65:LEU:HD11	1:D:82:ILE:HG21	2.00	0.43
2:E:17:LEU:HD21	2:E:92:ALA:HA	2.00	0.43
1:F:51:ILE:O	1:F:58:HIS:HA	2.19	0.43
2:L:86:ASN:O	2:L:87:LEU:HB3	2.19	0.43
3:S:72:TYR:CE2	3:S:81:LYS:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:259:SER:OG	3:S:277:GLU:OE2	2.27	0.43
3:T:400:THR:HG21	3:T:436:LYS:HB3	1.99	0.43
3:U:158:THR:HA	3:W:101:ARG:NH2	2.33	0.43
3:V:379:LEU:HD23	3:V:379:LEU:HA	1.82	0.43
3:W:379:LEU:HD23	3:W:379:LEU:HA	1.83	0.43
3:W:456:VAL:HG11	3:W:462:VAL:HG11	1.99	0.43
2:K:5:THR:HG23	2:K:8:ASP:H	1.83	0.43
2:K:31:GLN:HG3	1:Y:98:SER:HB2	2.01	0.43
3:S:281:ARG:NH1	3:T:299:ASP:OD1	2.52	0.43
3:T:379:LEU:HD23	3:T:379:LEU:HA	1.82	0.43
3:T:409:LEU:HD21	3:T:438:VAL:HG11	2.01	0.43
3:W:201:PHE:CE2	3:W:240:LYS:HD2	2.53	0.43
1:c:112:ASP:OD1	1:c:113:GLN:NE2	2.51	0.43
1:e:65:LEU:HD23	1:e:73:ILE:HG21	2.00	0.43
1:h:85:VAL:HG23	1:h:86:GLN:N	2.26	0.43
3:R:345:TYR:HD1	3:R:350:ILE:HG12	1.83	0.43
3:S:186:ASP:OD2	3:S:202:GLY:HA3	2.18	0.43
3:V:243:PHE:N	3:V:246:SER:O	2.41	0.43
1:X:14:ARG:HH11	1:X:14:ARG:HG3	1.82	0.43
1:e:14:ARG:HG2	1:e:14:ARG:NH1	2.32	0.43
1:f:73:ILE:HG21	1:f:82:ILE:HG13	1.98	0.43
2:E:86:ASN:O	2:E:87:LEU:HB3	2.18	0.43
2:G:15:ARG:HD2	2:M:35:ASP:OD2	2.18	0.43
3:S:147:LEU:HD12	3:S:193:THR:OG1	2.19	0.43
3:T:400:THR:HA	3:T:429:ASN:ND2	2.33	0.43
3:U:143:ASP:OD2	3:U:240:LYS:NZ	2.42	0.43
3:V:376:GLU:OE2	3:V:455:ARG:HD2	2.18	0.43
3:W:400:THR:HA	3:W:429:ASN:ND2	2.33	0.43
1:d:107:LEU:HD23	1:d:107:LEU:HA	1.87	0.43
1:e:73:ILE:HG21	1:e:82:ILE:HG13	2.00	0.43
1:h:68:ASN:HB3	1:h:74:VAL:HG21	2.00	0.43
1:C:81:LYS:HD3	1:g:109:TYR:CZ	2.53	0.43
2:H:70:GLY:HA3	1:f:24:LYS:HD2	2.01	0.43
2:I:52:LYS:O	2:I:122:ARG:NH2	2.52	0.43
2:M:133:PRO:HA	2:M:147:HIS:HA	2.00	0.43
3:R:422:ARG:HG2	1:e:78:GLN:OE1	2.19	0.43
3:V:345:TYR:HD1	3:V:350:ILE:HG12	1.83	0.43
3:V:396:VAL:HG11	3:V:454:LEU:HD21	2.01	0.43
1:a:18:THR:HA	1:a:25:ALA:HA	2.01	0.43
1:e:31:ILE:HD13	1:e:92:ILE:CD1	2.49	0.43
1:i:51:ILE:O	1:i:58:HIS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HG13	1:A:63:GLN:HE22	1.84	0.43
2:G:134:THR:HG22	2:G:148:TYR:CZ	2.53	0.43
2:H:89:CYS:SG	2:H:104:ILE:HD13	2.59	0.43
2:I:66:PRO:HB3	1:g:96:ASN:HD22	1.83	0.43
2:L:2:GLN:HG3	2:L:3:ILE:H	1.83	0.43
3:S:234:ILE:HG22	3:S:249:PHE:HB2	2.01	0.43
3:S:400:THR:HA	3:S:429:ASN:ND2	2.34	0.43
3:T:28:ASN:HB3	3:T:377:HIS:HD2	1.84	0.43
3:T:230:VAL:HG21	3:T:263:ILE:HG23	2.01	0.43
1:b:84:THR:HG22	1:b:85:VAL:N	2.34	0.43
1:c:33:ILE:HG13	1:c:49:VAL:HG11	2.01	0.43
1:0:11:SER:HA	1:Z:15:PRO:HB3	1.99	0.43
2:E:67:PRO:HG2	1:Z:24:LYS:HE2	2.00	0.43
2:H:67:PRO:HG2	1:f:24:LYS:HE2	2.01	0.43
2:O:13:ALA:O	2:O:14:LEU:C	2.61	0.43
2:O:73:HIS:ND1	2:O:75:LEU:HB3	2.34	0.43
3:R:81:LYS:HB3	3:R:86:VAL:HG21	2.01	0.43
3:T:167:GLU:OE1	3:T:174:ARG:NH2	2.52	0.43
3:U:182:GLU:O	3:W:148:ARG:HA	2.19	0.43
3:U:431:PRO:O	3:U:432:PHE:HB2	2.18	0.43
3:W:234:ILE:HG22	3:W:249:PHE:HB2	1.99	0.43
3:W:296:LEU:HD12	3:W:297:ARG:N	2.33	0.43
1:Y:32:TYR:HB3	1:Y:40:PRO:O	2.19	0.43
1:b:93:TYR:HE1	1:b:99:GLN:HG2	1.83	0.43
1:e:74:VAL:HG22	1:e:79:LEU:HD23	2.01	0.43
2:E:13:ALA:O	2:E:14:LEU:C	2.62	0.42
2:J:15:ARG:HD3	2:P:35:ASP:OD2	2.19	0.42
2:J:67:PRO:HG2	1:h:24:LYS:HE2	2.01	0.42
2:M:8:ASP:OD1	2:M:11:ARG:NH1	2.40	0.42
3:R:182:GLU:O	3:S:148:ARG:HA	2.19	0.42
3:T:400:THR:HA	3:T:429:ASN:HD22	1.84	0.42
3:W:346:GLU:OE2	3:W:351:THR:OG1	2.28	0.42
1:f:33:ILE:CG2	1:f:88:HIS:HB2	2.49	0.42
1:h:31:ILE:HD13	1:h:92:ILE:CD1	2.48	0.42
1:D:87:GLY:N	1:D:111:PRO:HD2	2.34	0.42
2:E:5:THR:O	2:E:8:ASP:N	2.52	0.42
2:H:86:ASN:O	2:H:87:LEU:HB3	2.19	0.42
2:I:3:ILE:HG23	2:I:8:ASP:HB3	2.01	0.42
3:W:298:PHE:HB3	3:W:350:ILE:HD11	2.01	0.42
1:a:32:TYR:HB3	1:a:40:PRO:O	2.19	0.42
1:c:35:GLN:HB2	1:c:38:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:84:THR:HG22	1:c:85:VAL:N	2.35	0.42
2:G:86:ASN:O	2:G:87:LEU:HB3	2.20	0.42
2:K:25:LEU:HD11	3:W:447:ARG:NE	2.33	0.42
3:R:16:PHE:HB3	3:R:418:ILE:HG21	2.01	0.42
3:R:346:GLU:OE2	3:R:351:THR:OG1	2.26	0.42
3:R:448:ARG:NH1	3:S:397:GLU:OE1	2.52	0.42
3:S:28:ASN:HB3	3:S:377:HIS:HD2	1.84	0.42
3:T:16:PHE:HB3	3:T:418:ILE:HG21	2.01	0.42
3:U:276:ILE:HG23	3:U:313:LEU:HD13	2.00	0.42
3:V:148:ARG:HA	3:W:182:GLU:O	2.20	0.42
1:b:7:ASN:OD1	1:g:114:TYR:HB2	2.20	0.42
2:J:134:THR:HG22	2:J:148:TYR:CZ	2.54	0.42
2:O:3:ILE:HG13	2:O:8:ASP:HB3	2.01	0.42
3:T:20:ASP:OD1	3:U:44:ARG:HD3	2.20	0.42
3:U:331:THR:HG21	3:U:339:ARG:HD2	2.02	0.42
1:f:47:ILE:HB	1:f:48:PRO:HD2	2.02	0.42
1:A:51:ILE:O	1:A:58:HIS:HA	2.20	0.42
1:F:13:PRO:HG3	1:i:106:VAL:HG22	2.01	0.42
3:S:182:GLU:O	3:T:148:ARG:HA	2.19	0.42
3:T:296:LEU:HD12	3:T:297:ARG:N	2.35	0.42
3:U:346:GLU:OE2	3:U:351:THR:OG1	2.28	0.42
3:W:112:LEU:HD12	3:W:144:ILE:HG21	2.01	0.42
3:W:186:ASP:OD2	3:W:202:GLY:HA3	2.19	0.42
1:d:62:THR:HG22	1:d:64:PRO:HD2	2.02	0.42
1:A:11:SER:HA	1:e:15:PRO:HB3	2.00	0.42
1:B:51:ILE:O	1:B:58:HIS:HA	2.19	0.42
2:E:12:ALA:C	2:E:84:PHE:HE1	2.26	0.42
2:I:3:ILE:HG22	2:I:9:LEU:HD12	2.02	0.42
3:R:53:TYR:CE2	3:R:83:GLU:HG2	2.54	0.42
1:b:32:TYR:HB3	1:b:40:PRO:O	2.20	0.42
1:d:7:ASN:OD1	1:i:114:TYR:HB2	2.19	0.42
1:A:6:ALA:N	1:e:85:VAL:HG12	2.35	0.42
1:F:51:ILE:HD11	1:F:61:ILE:HD13	2.02	0.42
2:O:43:MET:SD	2:O:90:ARG:HD2	2.59	0.42
2:P:75:LEU:HD21	2:P:83:VAL:HG21	2.01	0.42
3:S:252:HIS:CG	3:S:253:PRO:HD2	2.54	0.42
3:T:396:VAL:HG23	3:T:396:VAL:O	2.20	0.42
3:U:53:TYR:CE2	3:U:83:GLU:HG2	2.55	0.42
3:U:296:LEU:HD12	3:U:297:ARG:N	2.34	0.42
3:W:147:LEU:CD2	3:W:148:ARG:HG3	2.47	0.42
1:Y:35:GLN:HB2	1:Y:38:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:38:THR:O	1:c:102:TYR:OH	2.30	0.42
1:e:68:ASN:HB3	1:e:74:VAL:HG21	2.01	0.42
1:C:108:LYS:HD2	1:b:113:GLN:HG3	2.00	0.42
2:E:134:THR:HG22	2:E:148:TYR:CZ	2.54	0.42
3:V:232:LYS:HE2	3:V:261:TYR:HE2	1.84	0.42
1:Z:31:ILE:HD13	1:Z:92:ILE:CD1	2.50	0.42
2:G:90:ARG:O	2:G:93:PRO:HD2	2.20	0.42
2:O:11:ARG:HG2	2:O:28:VAL:HG11	2.01	0.42
3:T:159:ASP:OD2	3:T:180:ARG:NH2	2.53	0.42
3:T:379:LEU:HD12	3:T:464:LEU:HD12	2.01	0.42
1:Z:49:VAL:O	1:Z:60:GLN:HG3	2.19	0.42
1:f:31:ILE:HD13	1:f:92:ILE:CD1	2.45	0.42
2:I:67:PRO:HG2	1:g:24:LYS:HE2	2.02	0.42
2:J:23:ALA:HB1	3:U:440:TRP:CZ2	2.55	0.42
2:J:90:ARG:O	2:J:93:PRO:HD2	2.20	0.42
2:Q:34:GLN:HB2	1:d:96:ASN:OD1	2.20	0.42
3:T:11:GLY:HA3	3:T:380:PHE:HB2	2.01	0.42
3:W:297:ARG:NH1	3:W:297:ARG:HG2	2.35	0.42
1:X:84:THR:HG22	1:X:85:VAL:N	2.35	0.42
1:Z:65:LEU:HD23	1:Z:73:ILE:HG21	2.01	0.42
2:E:8:ASP:OD2	1:Y:24:LYS:NZ	2.53	0.41
2:G:21:SER:CB	3:R:442:ARG:HH21	2.30	0.41
2:L:3:ILE:HG23	2:L:8:ASP:HB3	2.02	0.41
2:O:13:ALA:O	2:O:16:LYS:N	2.52	0.41
3:T:55:MET:HG2	3:T:75:CYS:SG	2.60	0.41
3:T:345:TYR:HD1	3:T:350:ILE:HG12	1.85	0.41
2:E:15:ARG:NH2	2:E:84:PHE:HZ	2.19	0.41
2:E:40:LEU:HD12	2:E:87:LEU:CD2	2.50	0.41
2:G:4:LYS:HA	2:G:73:HIS:HE2	1.83	0.41
2:H:8:ASP:OD1	1:a:24:LYS:NZ	2.35	0.41
2:H:25:LEU:HB3	3:S:413:ALA:HB3	2.01	0.41
2:J:33:MET:HE3	2:J:33:MET:HB2	1.85	0.41
3:R:12:MET:HE2	3:S:36:ILE:HD12	2.01	0.41
3:T:313:LEU:HD23	3:T:328:VAL:HG22	2.01	0.41
3:W:393:ASP:O	3:W:469:ILE:HA	2.20	0.41
1:d:73:ILE:HD12	1:d:73:ILE:H	1.86	0.41
2:G:12:ALA:HB1	2:G:84:PHE:CE1	2.55	0.41
2:Q:128:TYR:HD2	2:Q:148:TYR:CE2	2.38	0.41
3:R:262:ILE:HD11	3:R:271:ILE:HD13	2.02	0.41
3:U:17:LYS:HB2	3:U:17:LYS:HE2	1.84	0.41
3:V:104:GLN:OE1	3:V:105:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:7:ASN:OD1	1:Z:114:TYR:HB2	2.21	0.41
1:Y:84:THR:HG22	1:Y:85:VAL:N	2.35	0.41
1:b:31:ILE:HG13	1:b:67:ILE:HD11	2.00	0.41
1:g:31:ILE:HD13	1:g:92:ILE:CD1	2.49	0.41
1:g:68:ASN:HB3	1:g:74:VAL:HG21	2.02	0.41
1:C:33:ILE:HD12	1:C:88:HIS:CD2	2.56	0.41
2:H:134:THR:HG22	2:H:148:TYR:CZ	2.56	0.41
2:O:41:GLU:OE1	2:O:41:GLU:HA	2.19	0.41
2:Q:128:TYR:HB2	2:Q:148:TYR:HD2	1.85	0.41
3:T:12:MET:SD	3:U:36:ILE:HD12	2.60	0.41
3:T:276:ILE:HG23	3:T:313:LEU:HD13	2.02	0.41
3:U:199:VAL:HG12	3:U:208:TYR:CE2	2.55	0.41
3:U:422:ARG:NH2	3:U:424:GLN:OE1	2.50	0.41
3:V:55:MET:HG2	3:V:75:CYS:SG	2.60	0.41
3:V:379:LEU:HD12	3:V:464:LEU:HD12	2.03	0.41
3:W:96:SER:HB3	3:W:238:TYR:CE2	2.55	0.41
1:c:31:ILE:HG13	1:c:67:ILE:HD11	2.02	0.41
1:0:46:GLN:HB3	1:0:63:GLN:HG2	2.02	0.41
2:M:75:LEU:HD21	2:M:83:VAL:HG21	2.01	0.41
3:R:331:THR:HG21	3:R:339:ARG:HD2	2.01	0.41
3:R:391:CYS:SG	3:R:446:ILE:HD11	2.61	0.41
3:T:393:ASP:O	3:T:469:ILE:HA	2.20	0.41
3:U:283:TYR:HE2	3:U:308:LEU:HD13	1.85	0.41
3:W:55:MET:HE3	3:W:73:ARG:HD2	2.03	0.41
3:W:147:LEU:HB3	3:W:198:ILE:HD11	2.02	0.41
1:c:101:ASP:OD1	1:c:101:ASP:C	2.64	0.41
1:d:84:THR:HG22	1:d:85:VAL:N	2.36	0.41
1:e:74:VAL:HG12	1:e:75:TYR:O	2.20	0.41
1:0:6:ALA:N	1:Z:85:VAL:HG12	2.36	0.41
1:D:42:ASN:HB3	1:D:45:ASN:HD22	1.86	0.41
2:N:128:TYR:HD2	2:N:132:MET:HG2	1.85	0.41
3:R:408:ARG:HE	3:R:425:MET:HE2	1.85	0.41
3:V:79:LEU:HB2	3:V:89:VAL:HG23	2.03	0.41
3:W:80:TYR:CE1	3:W:85:GLU:HB3	2.56	0.41
1:g:85:VAL:HG23	1:g:86:GLN:N	2.26	0.41
1:0:47:ILE:HD11	1:0:88:HIS:HB3	2.01	0.41
2:E:33:MET:HE3	2:E:33:MET:HB2	1.87	0.41
2:H:49:GLN:HE22	2:O:113:LEU:HB3	1.86	0.41
2:L:8:ASP:HA	2:L:11:ARG:HG2	2.02	0.41
2:L:25:LEU:HB3	3:W:413:ALA:HB3	2.01	0.41
2:N:128:TYR:CD2	2:N:132:MET:HG2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:186:ASP:OD2	3:R:202:GLY:HA3	2.19	0.41
3:R:398:SER:HA	3:R:463:THR:O	2.20	0.41
3:R:400:THR:HA	3:R:429:ASN:ND2	2.35	0.41
3:S:147:LEU:CD2	3:S:148:ARG:HG3	2.49	0.41
3:T:419:ASN:HB3	1:g:59:VAL:HG21	2.02	0.41
3:W:262:ILE:HD11	3:W:271:ILE:HD13	2.02	0.41
1:0:51:ILE:HD11	1:0:61:ILE:HD13	2.03	0.41
1:D:90:MET:HE3	1:D:106:VAL:HG21	2.03	0.41
2:G:23:ALA:HB1	3:R:440:TRP:CZ2	2.55	0.41
2:O:128:TYR:HD2	2:O:132:MET:HG2	1.84	0.41
3:R:302:GLU:HB3	3:R:317:ALA:HB3	2.01	0.41
3:S:74:VAL:O	3:S:74:VAL:HG13	2.20	0.41
3:S:96:SER:HB3	3:S:238:TYR:CE2	2.55	0.41
3:S:112:LEU:HD12	3:S:144:ILE:HG21	2.03	0.41
3:U:370:GLN:CB	3:U:375:GLN:HE21	2.32	0.41
3:U:425:MET:HB2	1:c:99:GLN:NE2	2.36	0.41
3:V:296:LEU:HD12	3:V:297:ARG:N	2.34	0.41
3:W:17:LYS:HE2	3:W:17:LYS:HB2	1.84	0.41
1:Y:67:ILE:HG22	1:Y:68:ASN:O	2.21	0.41
1:d:32:TYR:HB3	1:d:40:PRO:O	2.20	0.41
1:e:63:GLN:O	1:e:65:LEU:N	2.52	0.41
1:f:85:VAL:HG23	1:f:86:GLN:N	2.26	0.41
1:B:91:ALA:HB1	1:B:93:TYR:HE1	1.85	0.41
1:D:6:ALA:N	1:h:85:VAL:HG12	2.36	0.41
2:G:22:ASP:OD1	2:G:23:ALA:N	2.54	0.41
2:O:13:ALA:HB1	2:O:88:ALA:HB2	2.03	0.41
3:R:55:MET:HG2	3:R:75:CYS:SG	2.60	0.41
3:R:375:GLN:HA	3:R:375:GLN:OE1	2.21	0.41
3:R:379:LEU:HD12	3:R:464:LEU:HD12	2.02	0.41
3:R:405:TYR:CG	3:R:406:ALA:N	2.88	0.41
3:S:185:PRO:HG2	3:T:99:HIS:NE2	2.36	0.41
3:S:338:TYR:HE2	3:S:343:PHE:HZ	1.67	0.41
3:T:376:GLU:OE2	3:T:455:ARG:HD2	2.20	0.41
3:U:16:PHE:HB3	3:U:418:ILE:CG2	2.50	0.41
3:U:147:LEU:HD13	3:U:198:ILE:HG12	2.03	0.41
3:V:12:MET:H	3:V:382:PRO:HA	1.86	0.41
3:V:99:HIS:CD2	3:W:185:PRO:HG2	2.55	0.41
3:W:408:ARG:HE	3:W:425:MET:HE3	1.85	0.41
1:d:18:THR:HA	1:d:25:ALA:HA	2.02	0.41
1:0:33:ILE:HG21	1:0:84:THR:HG21	2.03	0.41
2:J:14:LEU:O	2:J:15:ARG:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:15:ARG:HG3	2:K:21:SER:CB	2.51	0.41
3:R:148:ARG:HA	3:V:182:GLU:O	2.21	0.41
3:S:194:TRP:CE2	3:S:195:ARG:HG3	2.56	0.41
3:T:112:LEU:HD12	3:T:144:ILE:HG21	2.03	0.41
3:U:147:LEU:CB	3:U:198:ILE:HD11	2.51	0.41
3:U:258:PRO:O	3:U:277:GLU:HG3	2.21	0.41
3:V:313:LEU:HD23	3:V:328:VAL:HG22	2.02	0.41
3:V:393:ASP:O	3:V:469:ILE:HA	2.22	0.41
1:Z:73:ILE:HG21	1:Z:82:ILE:HG13	2.02	0.41
1:B:88:HIS:HD2	1:B:90:MET:HG3	1.86	0.40
1:C:31:ILE:HG13	1:C:67:ILE:HD11	2.03	0.40
1:C:51:ILE:O	1:C:58:HIS:HA	2.22	0.40
1:F:109:TYR:OH	1:i:112:ASP:OD2	2.36	0.40
2:M:4:LYS:HB3	2:M:4:LYS:HE3	1.89	0.40
2:M:130:SER:HB2	2:M:150:PRO:HB3	2.03	0.40
2:Q:11:ARG:HG2	2:Q:28:VAL:HG11	2.02	0.40
2:Q:41:GLU:HA	2:Q:41:GLU:OE1	2.22	0.40
3:S:297:ARG:HG2	3:S:297:ARG:NH1	2.36	0.40
3:S:313:LEU:HD23	3:S:328:VAL:HG22	2.02	0.40
3:T:142:ARG:HD3	3:T:189:ILE:O	2.21	0.40
3:W:338:TYR:HE2	3:W:343:PHE:HZ	1.69	0.40
1:X:101:ASP:OD1	1:X:101:ASP:C	2.64	0.40
1:B:33:ILE:HG21	1:B:84:THR:HG21	2.04	0.40
2:E:82:ALA:O	2:E:86:ASN:HB2	2.21	0.40
2:E:130:SER:HA	2:E:150:PRO:HD3	2.03	0.40
2:H:67:PRO:HD3	1:f:19:GLU:OE1	2.21	0.40
3:S:243:PHE:N	3:S:246:SER:O	2.42	0.40
3:S:375:GLN:OE1	3:S:375:GLN:HA	2.21	0.40
3:S:393:ASP:O	3:S:469:ILE:HA	2.21	0.40
3:T:118:ASP:OD1	3:T:120:THR:HG22	2.21	0.40
3:U:313:LEU:HD23	3:U:328:VAL:HG22	2.02	0.40
3:V:430:GLU:HG3	3:V:431:PRO:HD2	2.03	0.40
3:W:104:GLN:OE1	3:W:105:ALA:N	2.54	0.40
1:c:73:ILE:HD12	1:c:73:ILE:H	1.86	0.40
1:B:31:ILE:HG13	1:B:67:ILE:HD11	2.03	0.40
2:E:89:CYS:O	2:E:93:PRO:HD3	2.22	0.40
2:I:66:PRO:HB3	1:g:96:ASN:ND2	2.37	0.40
2:J:86:ASN:O	2:J:87:LEU:HB3	2.20	0.40
2:L:134:THR:HG22	2:L:148:TYR:CZ	2.56	0.40
3:R:17:LYS:HB2	3:R:17:LYS:HE2	1.84	0.40
3:R:44:ARG:HD3	3:V:20:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:283:TYR:HE2	3:R:308:LEU:HD13	1.86	0.40
3:T:60:ARG:HD2	3:T:93:GLY:O	2.21	0.40
3:T:401:GLY:O	3:T:432:PHE:HD1	2.05	0.40
3:V:147:LEU:CD2	3:V:148:ARG:HG3	2.50	0.40
3:W:28:ASN:HB3	3:W:377:HIS:HD2	1.86	0.40
1:Y:73:ILE:HD12	1:Y:73:ILE:H	1.86	0.40
1:a:73:ILE:HD12	1:a:73:ILE:H	1.85	0.40
1:B:17:PHE:CE1	1:a:12:ASN:HB3	2.57	0.40
3:S:104:GLN:OE1	3:S:105:ALA:N	2.54	0.40
3:U:28:ASN:HB3	3:U:377:HIS:HD2	1.86	0.40
3:U:201:PHE:HE2	3:U:247:TYR:CD2	2.39	0.40
3:W:16:PHE:HB3	3:W:418:ILE:HG21	2.03	0.40
1:g:21:ARG:HD3	1:g:21:ARG:HA	1.95	0.40
1:0:13:PRO:CG	1:Z:103:ILE:HD13	2.51	0.40
1:A:12:ASN:HB2	1:e:17:PHE:CE1	2.56	0.40
1:A:81:LYS:HD3	1:e:109:TYR:CZ	2.56	0.40
3:R:201:PHE:CZ	3:R:247:TYR:HD2	2.33	0.40
3:R:313:LEU:HD23	3:R:328:VAL:HG22	2.03	0.40
3:S:185:PRO:HG2	3:T:99:HIS:CD2	2.56	0.40
1:X:31:ILE:HG13	1:X:67:ILE:HD11	2.03	0.40
1:b:23:PHE:HE2	1:g:23:PHE:CE1	2.39	0.40
1:i:73:ILE:HG21	1:i:82:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
1	A	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
1	B	109/111 (98%)	108 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	109/111 (98%)	107 (98%)	2 (2%)	0	100	100
1	D	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
1	F	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
1	X	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
1	Y	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
1	Z	109/111 (98%)	97 (89%)	12 (11%)	0	100	100
1	a	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
1	b	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
1	c	109/111 (98%)	101 (93%)	8 (7%)	0	100	100
1	d	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
1	e	109/111 (98%)	99 (91%)	10 (9%)	0	100	100
1	f	109/111 (98%)	100 (92%)	9 (8%)	0	100	100
1	g	109/111 (98%)	98 (90%)	11 (10%)	0	100	100
1	h	109/111 (98%)	100 (92%)	9 (8%)	0	100	100
1	i	109/111 (98%)	98 (90%)	11 (10%)	0	100	100
2	E	148/150 (99%)	135 (91%)	13 (9%)	0	100	100
2	G	148/150 (99%)	137 (93%)	11 (7%)	0	100	100
2	H	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
2	I	148/150 (99%)	137 (93%)	11 (7%)	0	100	100
2	J	148/150 (99%)	137 (93%)	11 (7%)	0	100	100
2	K	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	51
2	L	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
2	M	147/150 (98%)	135 (92%)	11 (8%)	1 (1%)	18	51
2	N	147/150 (98%)	135 (92%)	11 (8%)	1 (1%)	18	51
2	O	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	18	51
2	P	147/150 (98%)	135 (92%)	11 (8%)	1 (1%)	18	51
2	Q	147/150 (98%)	135 (92%)	11 (8%)	1 (1%)	18	51
3	R	469/471 (100%)	444 (95%)	25 (5%)	0	100	100
3	S	469/471 (100%)	440 (94%)	29 (6%)	0	100	100
3	T	469/471 (100%)	436 (93%)	33 (7%)	0	100	100
3	U	469/471 (100%)	439 (94%)	29 (6%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	469/471 (100%)	439 (94%)	30 (6%)	0	100	100
3	W	469/471 (100%)	444 (95%)	25 (5%)	0	100	100
All	All	6546/6624 (99%)	6118 (94%)	421 (6%)	7 (0%)	49	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	U	402	VAL
2	K	62	ASP
2	M	62	ASP
2	N	62	ASP
2	O	62	ASP
2	P	62	ASP
2	Q	62	ASP

5.3.2 Protein sidechains [i](#)

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	0	95/95 (100%)	95 (100%)	0	100	100
1	A	95/95 (100%)	95 (100%)	0	100	100
1	B	95/95 (100%)	94 (99%)	1 (1%)	65	73
1	C	95/95 (100%)	93 (98%)	2 (2%)	47	64
1	D	95/95 (100%)	95 (100%)	0	100	100
1	F	95/95 (100%)	95 (100%)	0	100	100
1	X	95/95 (100%)	95 (100%)	0	100	100
1	Y	95/95 (100%)	95 (100%)	0	100	100
1	Z	95/95 (100%)	95 (100%)	0	100	100
1	a	95/95 (100%)	95 (100%)	0	100	100
1	b	95/95 (100%)	95 (100%)	0	100	100
1	c	95/95 (100%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	95/95 (100%)	94 (99%)	1 (1%)	65	73
1	e	95/95 (100%)	95 (100%)	0	100	100
1	f	95/95 (100%)	94 (99%)	1 (1%)	65	73
1	g	95/95 (100%)	95 (100%)	0	100	100
1	h	95/95 (100%)	95 (100%)	0	100	100
1	i	95/95 (100%)	95 (100%)	0	100	100
2	E	118/118 (100%)	118 (100%)	0	100	100
2	G	118/118 (100%)	118 (100%)	0	100	100
2	H	118/118 (100%)	118 (100%)	0	100	100
2	I	118/118 (100%)	118 (100%)	0	100	100
2	J	118/118 (100%)	118 (100%)	0	100	100
2	K	117/118 (99%)	117 (100%)	0	100	100
2	L	118/118 (100%)	118 (100%)	0	100	100
2	M	117/118 (99%)	117 (100%)	0	100	100
2	N	117/118 (99%)	117 (100%)	0	100	100
2	O	117/118 (99%)	114 (97%)	3 (3%)	40	60
2	P	117/118 (99%)	117 (100%)	0	100	100
2	Q	117/118 (99%)	117 (100%)	0	100	100
3	R	395/395 (100%)	395 (100%)	0	100	100
3	S	395/395 (100%)	395 (100%)	0	100	100
3	T	395/395 (100%)	395 (100%)	0	100	100
3	U	395/395 (100%)	395 (100%)	0	100	100
3	V	395/395 (100%)	395 (100%)	0	100	100
3	W	395/395 (100%)	395 (100%)	0	100	100
All	All	5490/5496 (100%)	5482 (100%)	8 (0%)	87	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	GLN
1	C	45	ASN
1	C	116	ILE
2	O	3	ILE
2	O	4	LYS

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Mol	Chain	Res	Type
2	O	10	VAL
1	d	42	ASN
1	f	28	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
2	E	85	HIS
2	G	2	GLN
2	G	85	HIS
2	G	138	ASN
2	H	34	GLN
2	H	138	ASN
2	H	142	ASN
2	I	85	HIS
2	J	85	HIS
2	J	138	ASN
2	K	144	ASN
2	L	138	ASN
2	O	144	ASN
2	P	117	GLN
2	Q	117	GLN
3	R	374	GLN
3	R	429	ASN
3	S	429	ASN
3	T	231	GLN
3	T	429	ASN
3	U	231	GLN
3	U	374	GLN
3	U	429	ASN
3	V	231	GLN
3	V	374	GLN
3	V	429	ASN
3	W	322	ASN
3	W	429	ASN
1	X	53	ASN
1	X	113	GLN
1	Y	12	ASN
1	Y	28	ASN
1	Y	45	ASN
1	Y	113	GLN

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Mol	Chain	Res	Type
1	Z	113	GLN
1	a	53	ASN
1	b	12	ASN
1	b	28	ASN
1	c	28	ASN
1	c	53	ASN
1	c	99	GLN
1	c	113	GLN
1	d	53	ASN
1	d	63	GLN
1	e	113	GLN
1	f	105	ASN
1	f	113	GLN
1	g	113	GLN
1	h	58	HIS
1	h	113	GLN
1	i	58	HIS
1	i	105	ASN
1	i	113	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

There are no chain breaks in this entry.

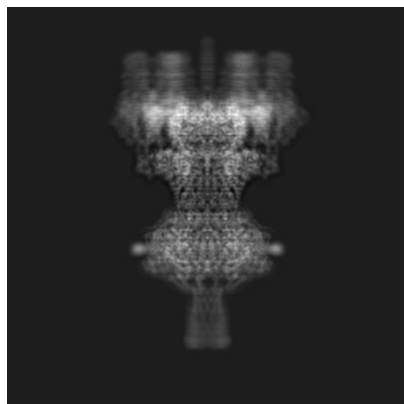
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27793. These allow visual inspection of the internal detail of the map and identification of artifacts.

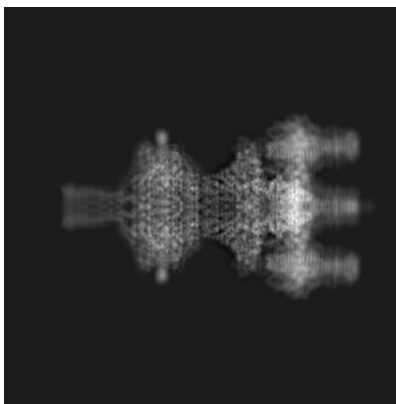
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

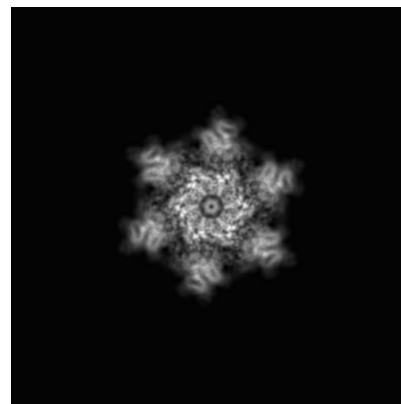
6.1.1 Primary map



X

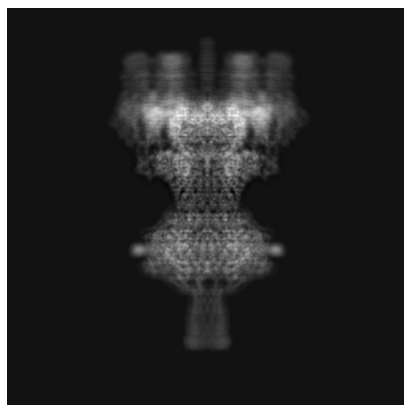


Y

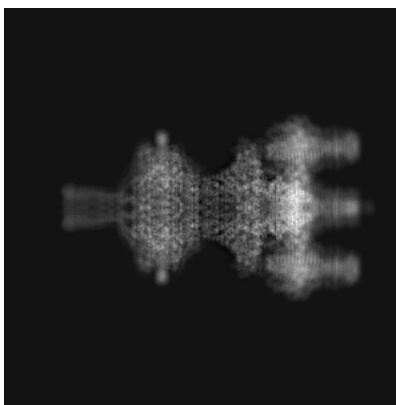


Z

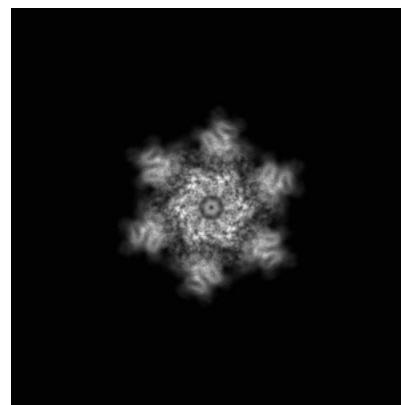
6.1.2 Raw map



X



Y

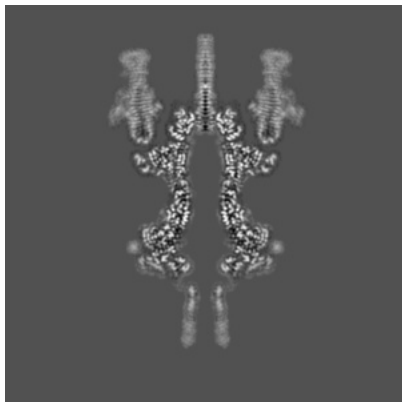


Z

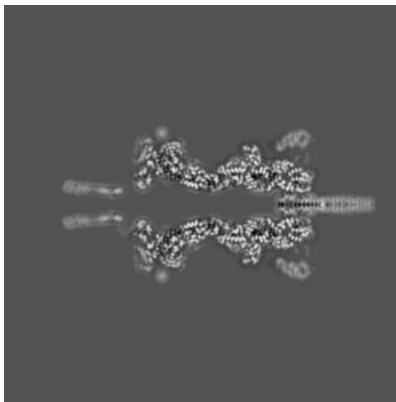
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

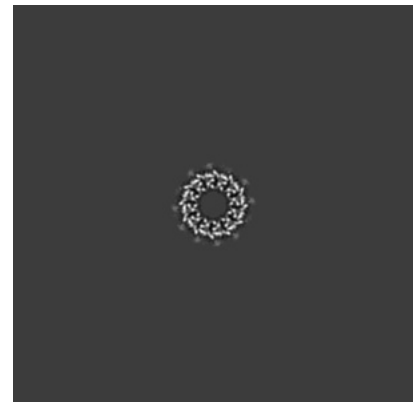
6.2.1 Primary map



X Index: 240

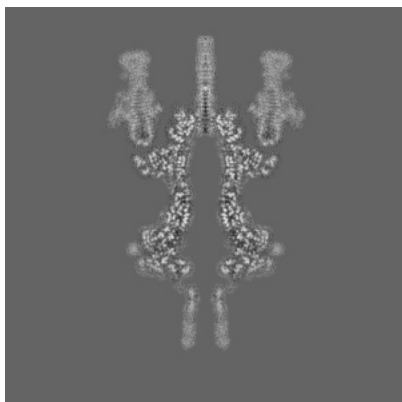


Y Index: 240

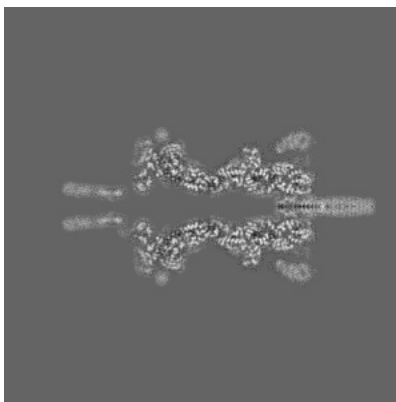


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

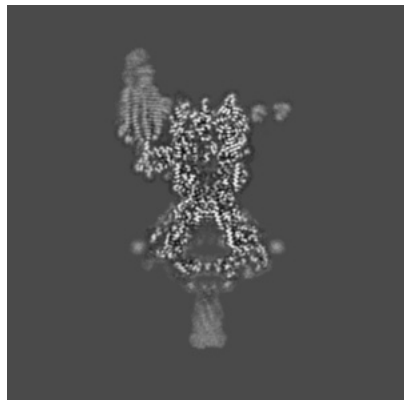


Z Index: 240

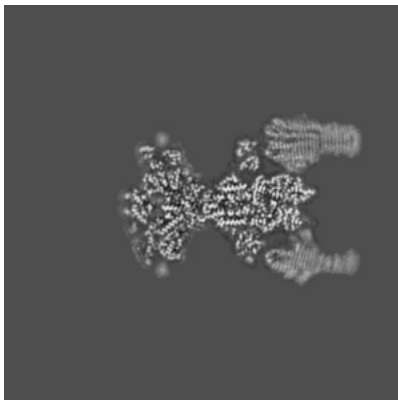
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

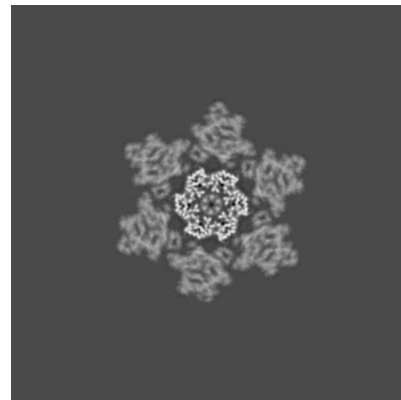
6.3.1 Primary map



X Index: 219

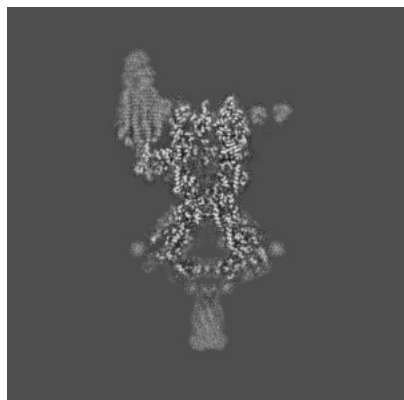


Y Index: 275

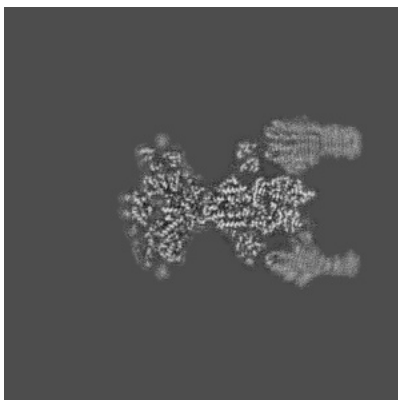


Z Index: 350

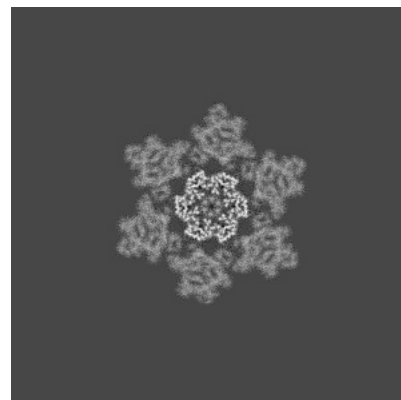
6.3.2 Raw map



X Index: 220



Y Index: 275

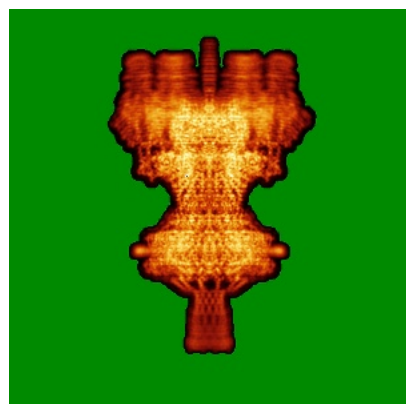


Z Index: 350

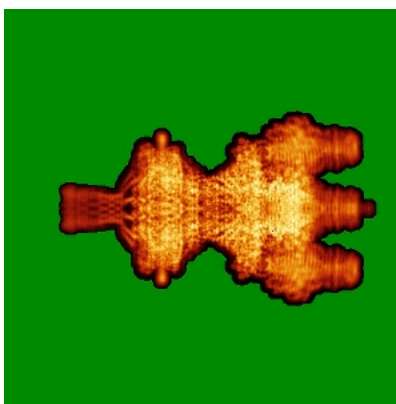
The images above show the largest variance slices of the map in three orthogonal directions.

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

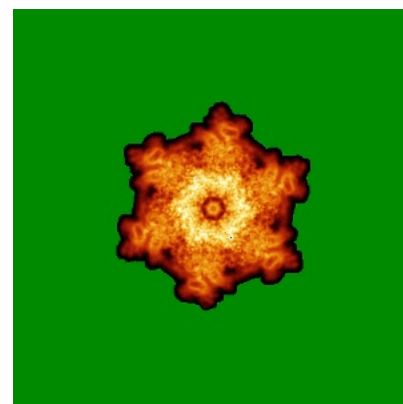
6.4.1 Primary map



X

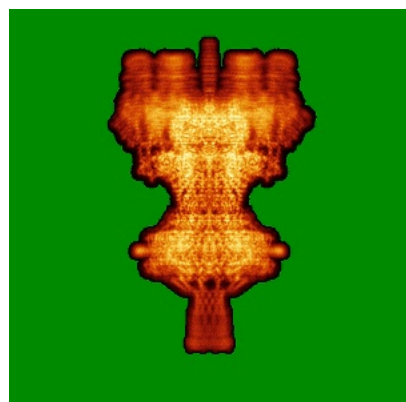


Y

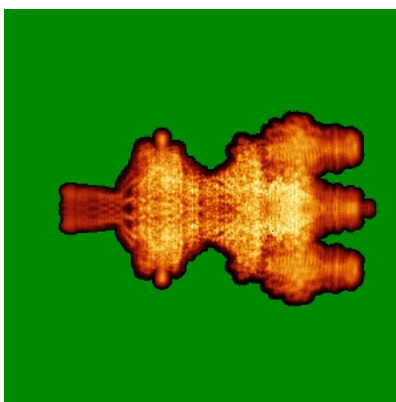


Z

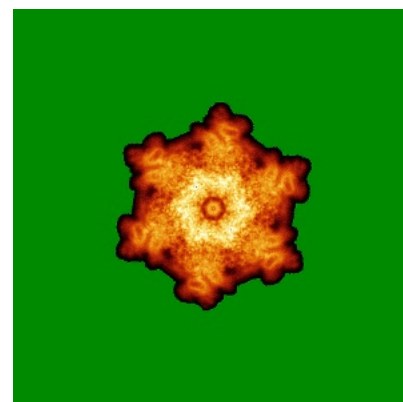
6.4.2 Raw map



X



Y

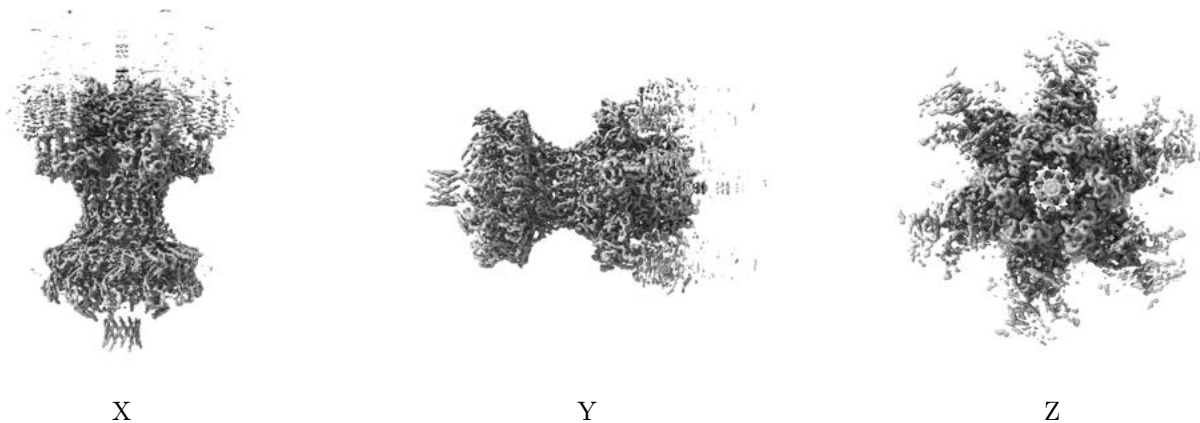


Z

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

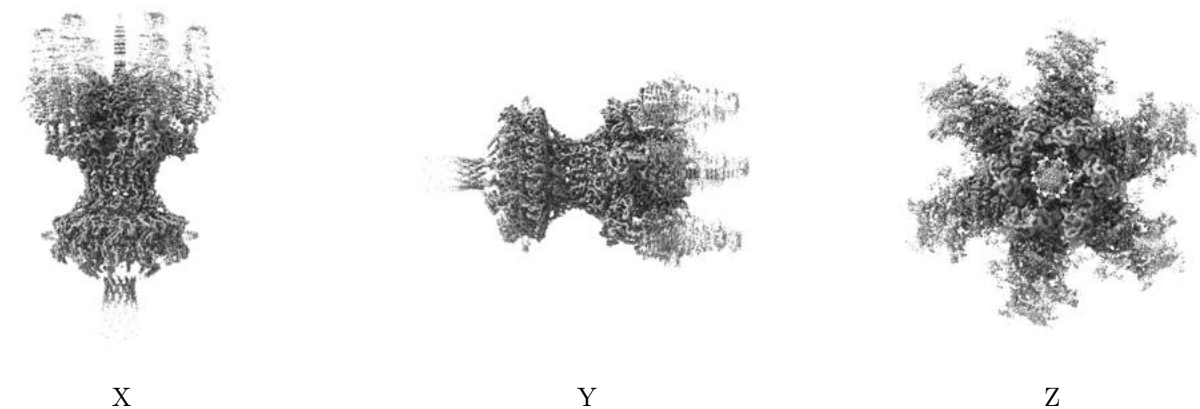
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

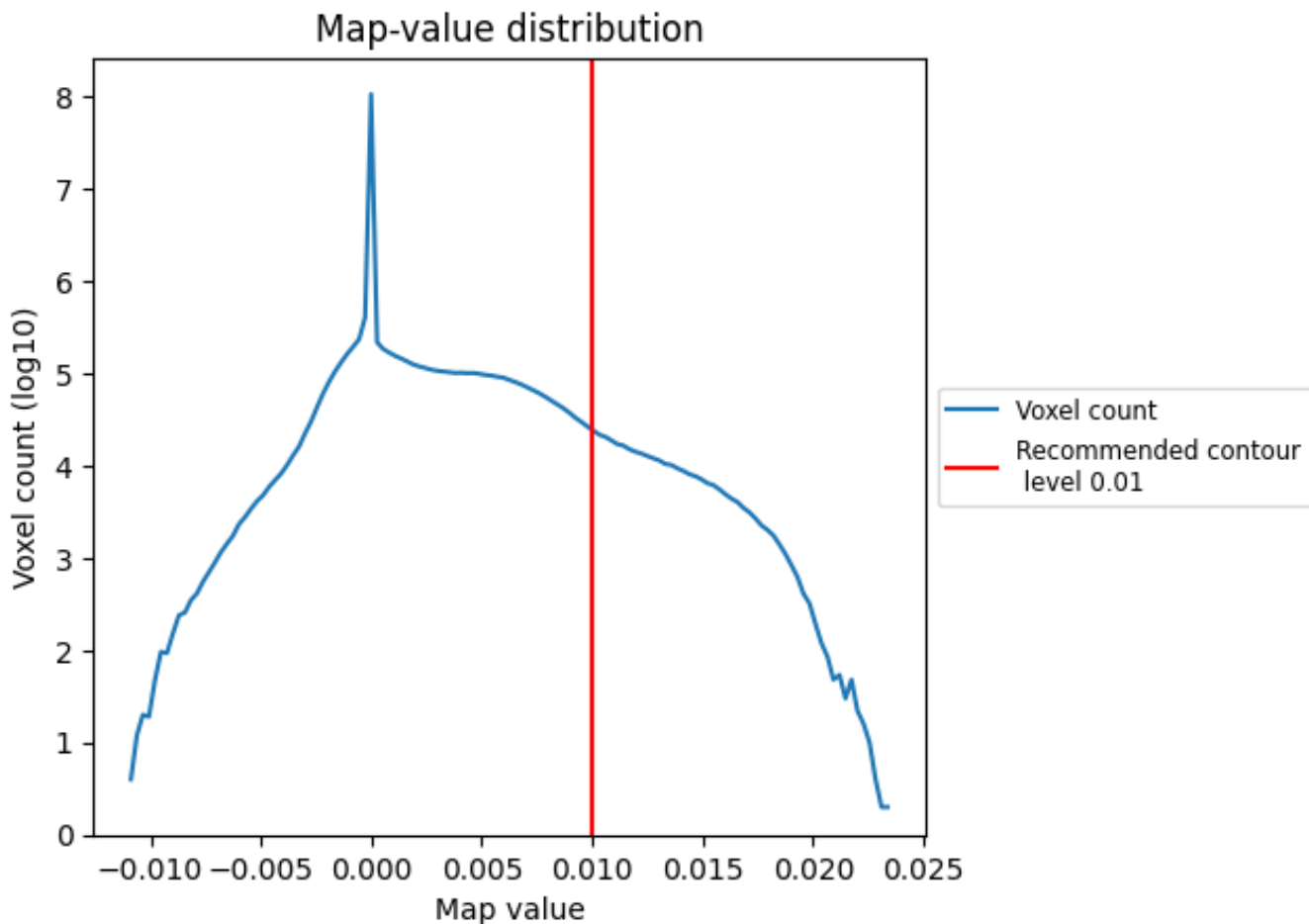
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

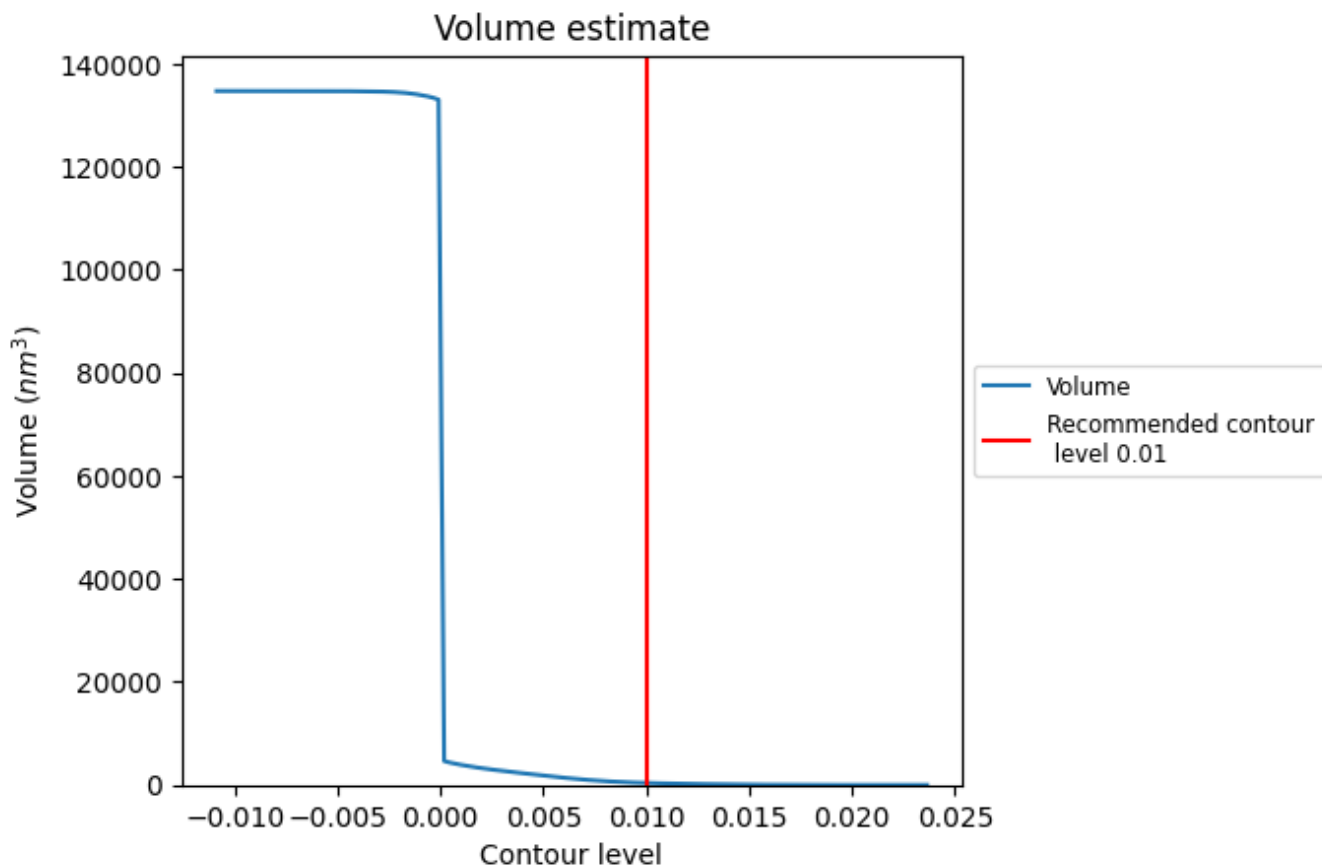
This section contains the results of statistical analysis of the map.

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.

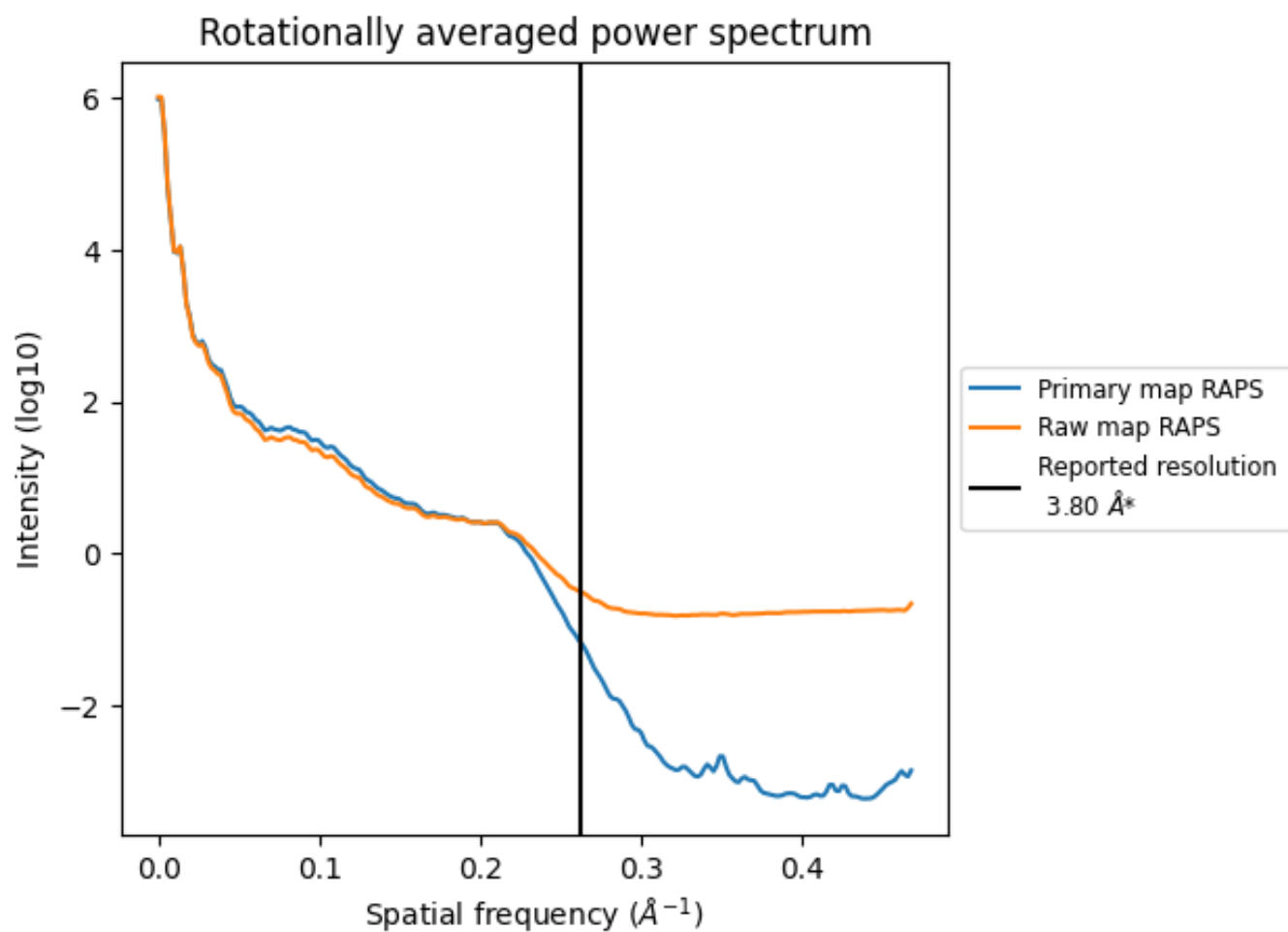
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 385 nm³; this corresponds to an approximate mass of 347 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 i

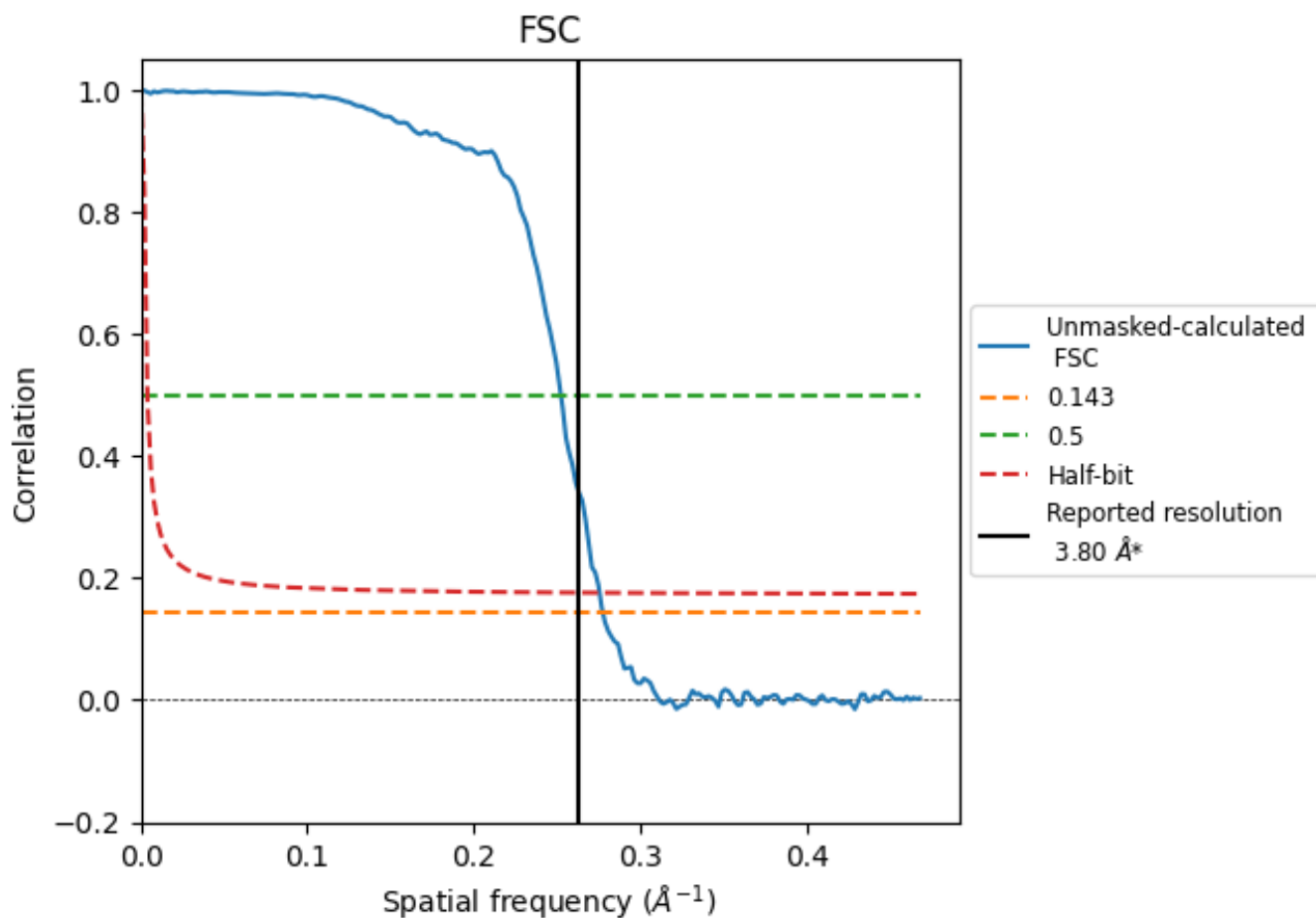


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

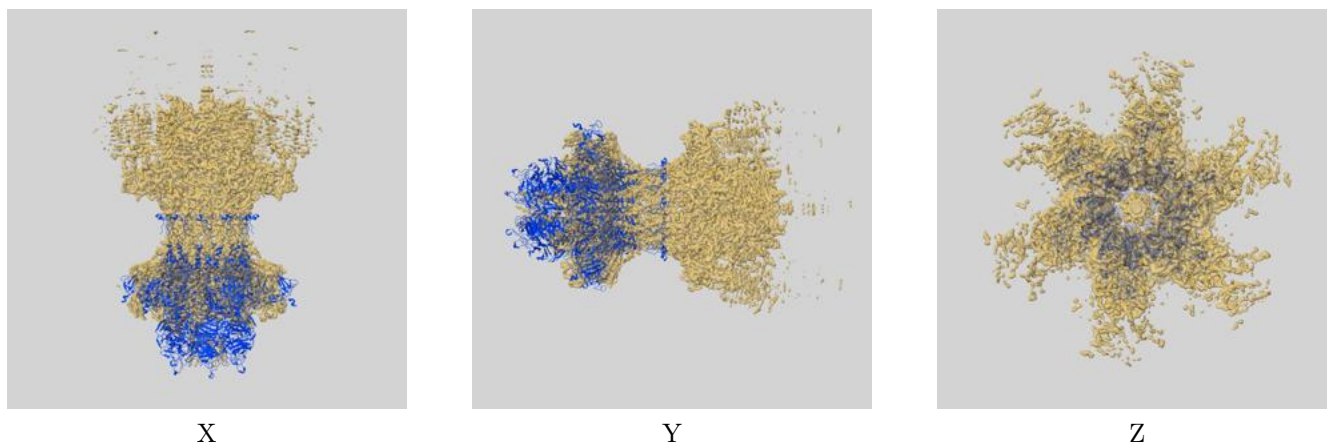
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	3.96	3.63

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

9 Map-model fit [i](#)

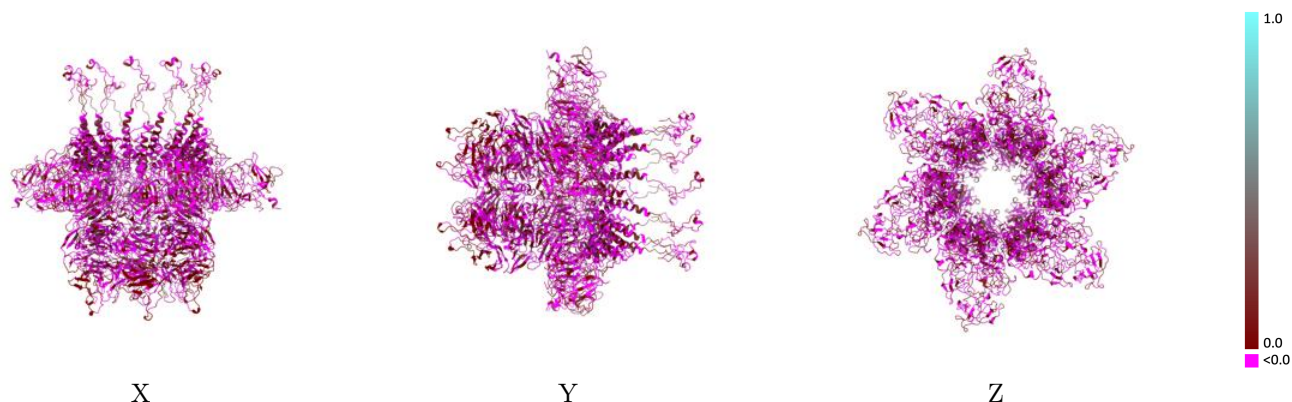
This section contains information regarding the fit between EMDB map EMD-27793 and PDB model 8EB7. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



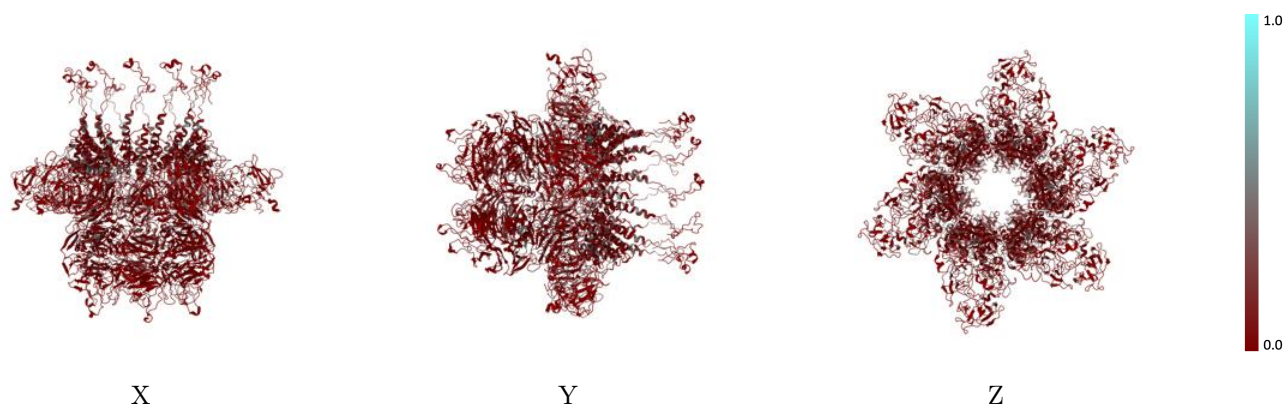
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



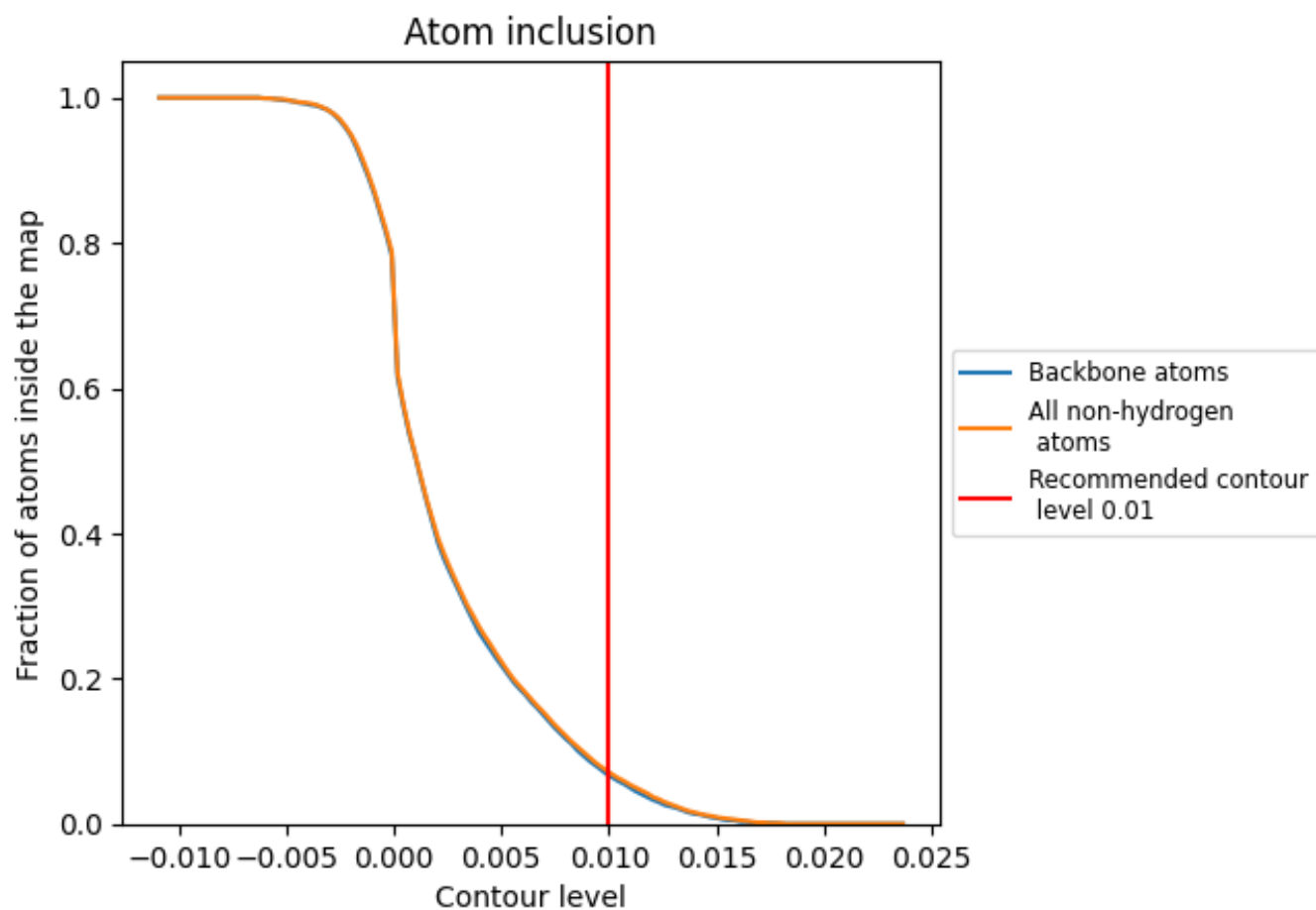
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 7% of all backbone atoms, 7% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0710	 -0.0240
0	 0.0340	 -0.0200
A	 0.0310	 -0.0170
B	 0.0340	 -0.0130
C	 0.0310	 -0.0190
D	 0.0300	 -0.0130
E	 0.0990	 -0.0350
F	 0.0340	 -0.0100
G	 0.1010	 -0.0390
H	 0.1050	 -0.0290
I	 0.0960	 -0.0340
J	 0.0910	 -0.0390
K	 0.0990	 -0.0350
L	 0.1000	 -0.0330
M	 0.1000	 -0.0350
N	 0.1030	 -0.0380
O	 0.0990	 -0.0360
P	 0.1000	 -0.0360
Q	 0.1030	 -0.0410
R	 0.0460	 -0.0240
S	 0.0450	 -0.0240
T	 0.0460	 -0.0240
U	 0.0350	 -0.0240
V	 0.0480	 -0.0220
W	 0.0330	 -0.0180
X	 0.0900	 -0.0270
Y	 0.0890	 -0.0280
Z	 0.1340	 -0.0070
a	 0.0890	 -0.0270
b	 0.0900	 -0.0260
c	 0.0900	 -0.0280
d	 0.0880	 -0.0290
e	 0.1360	 -0.0040
f	 0.1340	 -0.0070
g	 0.1350	 -0.0080



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Chain	Atom inclusion	Q-score
h	 0.1340	 -0.0060
i	 0.1340	 -0.0080