



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:11 AM UTC

PDB ID : 8W1I / pdb_00008w1i
EMDB ID : EMD-43726
Title : Cryo-EM structure of BTV subcore
Authors : Xia, X.; Sung, P.Y.; Martynowycz, M.W.; Gonen, T.; Roy, P.; Zhou, Z.H.
Deposited on : 2024-02-16
Resolution : 6.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

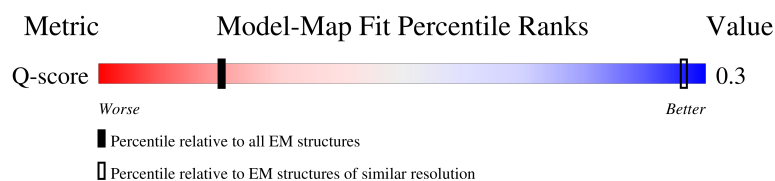
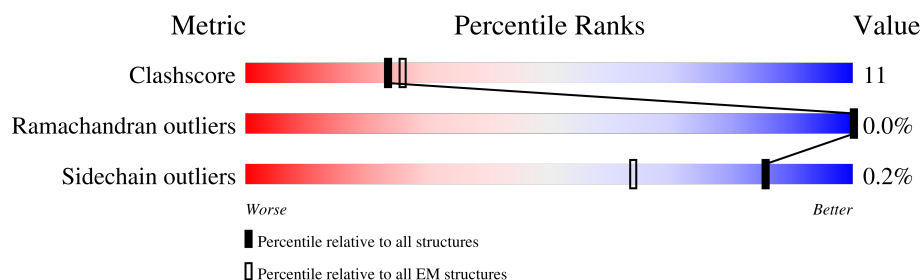
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	556 (6.00 - 7.00)

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

Mol	Chain	Length	Quality of chain
1	A	901	51% 68% 25% 6%
1	B	901	63% 71% 27% .
1	D	901	51% 70% 24% 6%
1	E	901	50% 70% 24% 6%

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Mol	Chain	Length	Quality of chain
1	F	901	
1	G	901	
1	H	901	
1	I	901	
1	J	901	
1	K	901	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 69810 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.

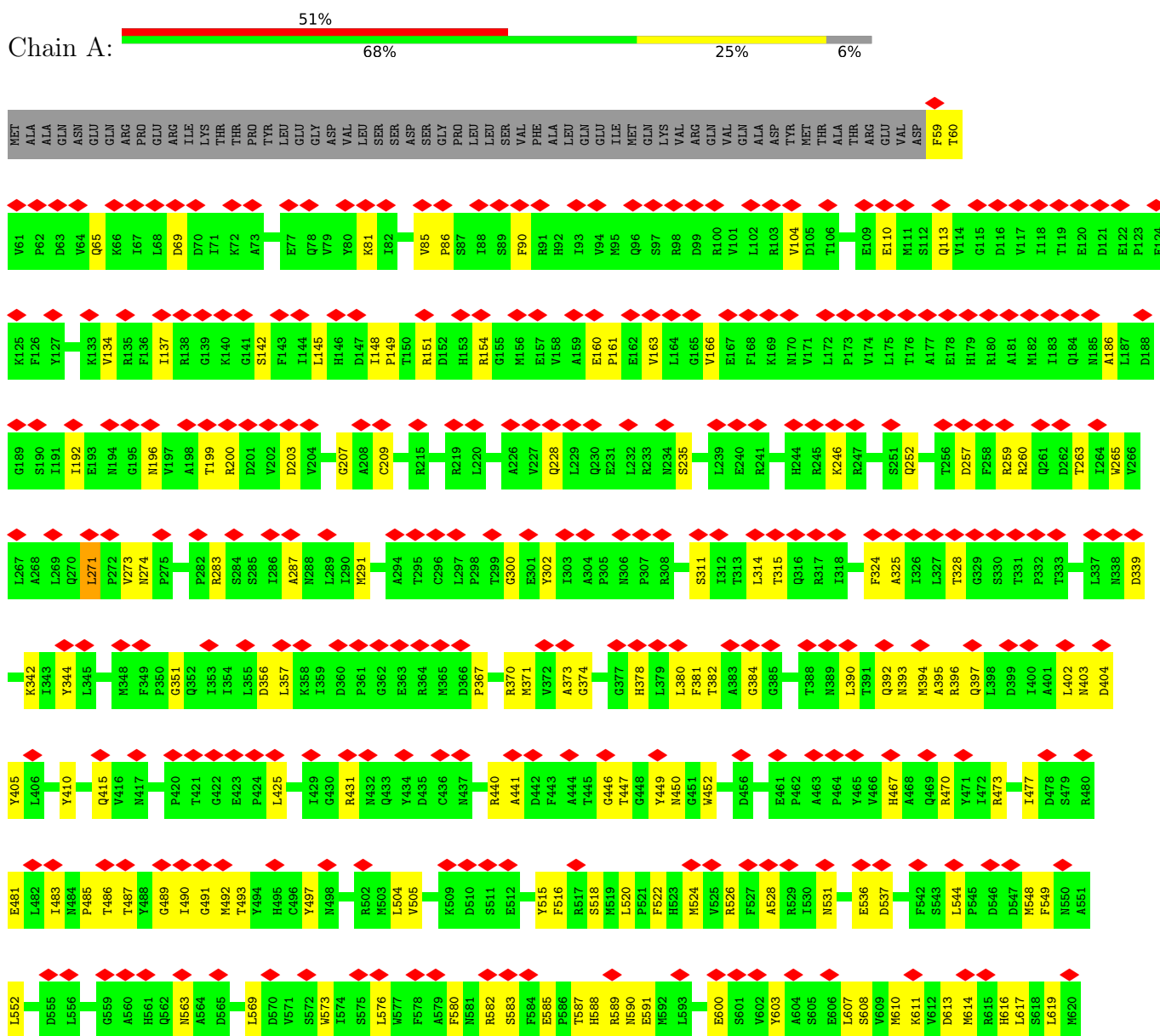
- Molecule 1 is a protein called Core protein VP3.

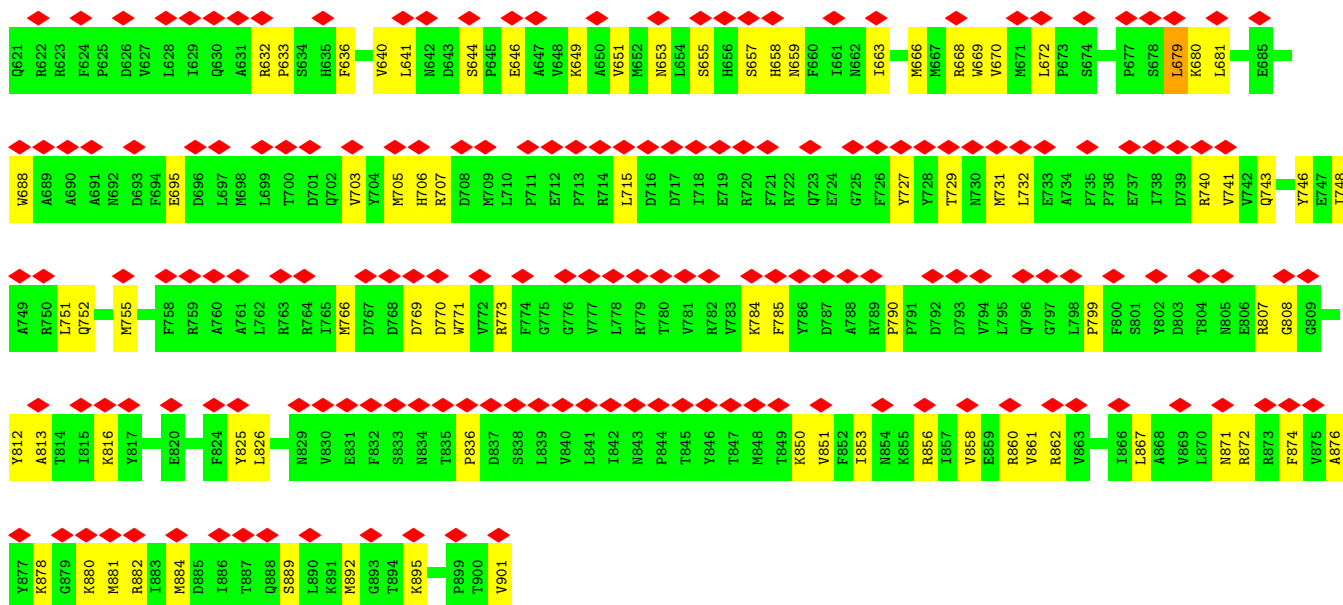
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	B	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	D	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	E	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	F	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	G	843	Total	C	N	O	S	0	0
			6811	4348	1182	1242	39		
1	H	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	I	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	J	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
1	K	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		

3 Residue-property plots

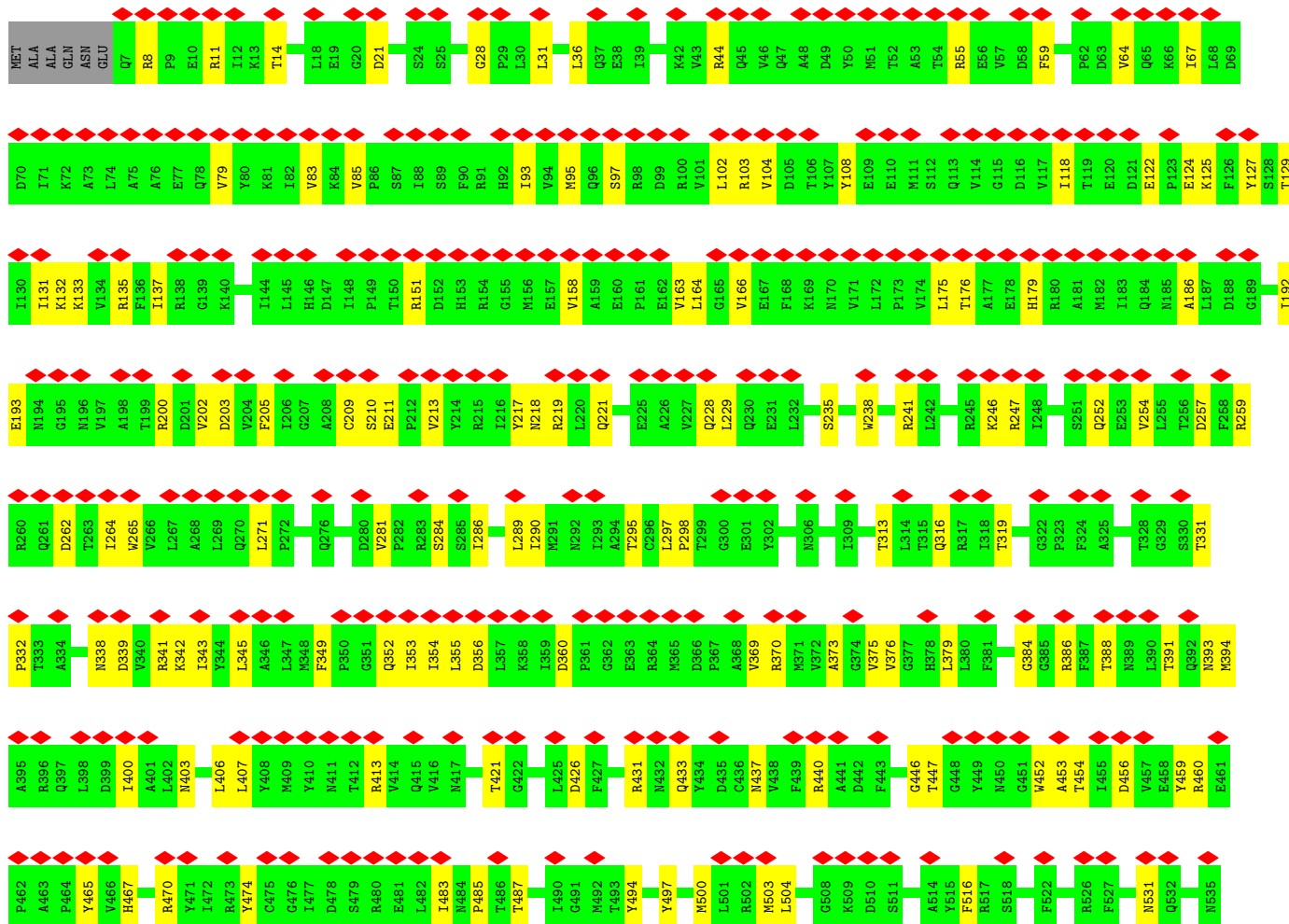
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

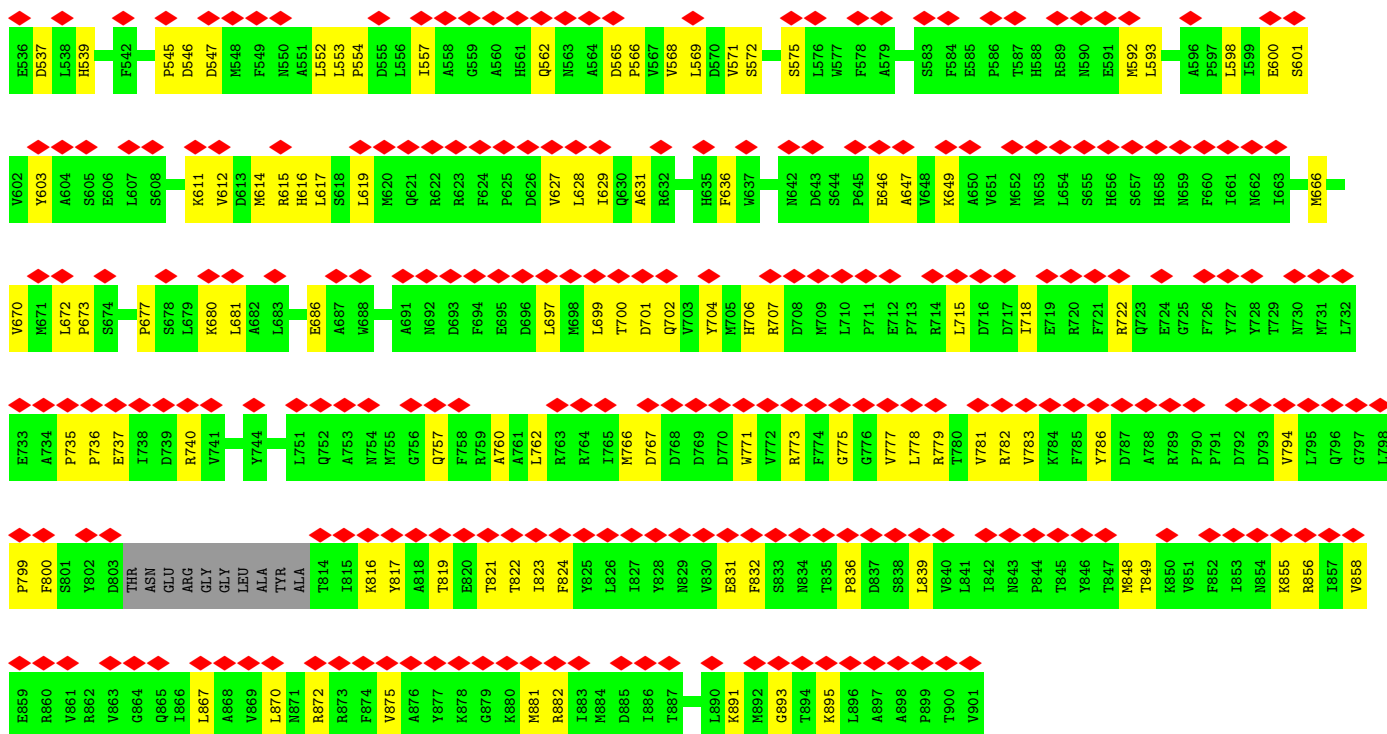
• Molecule 1: Core protein VP3



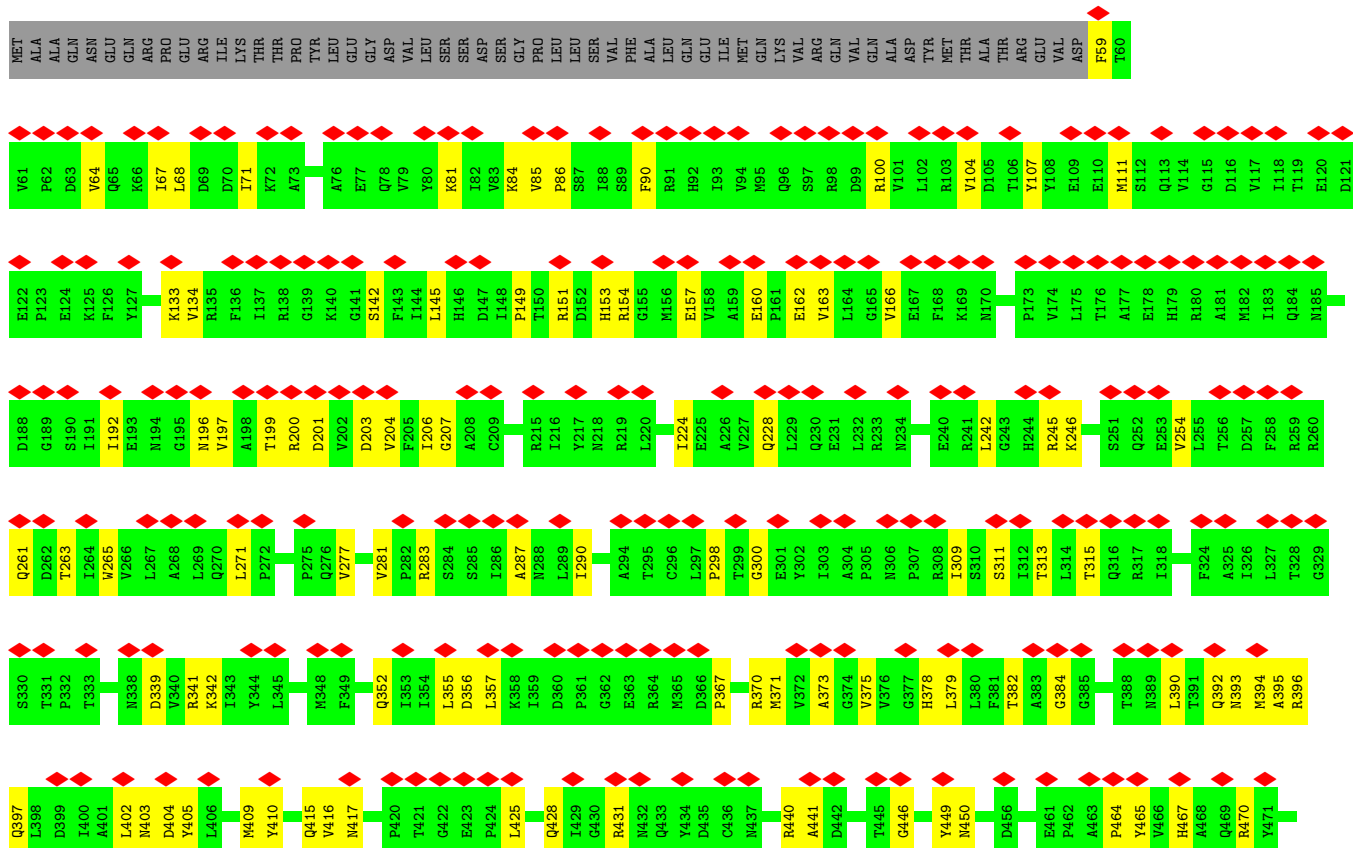


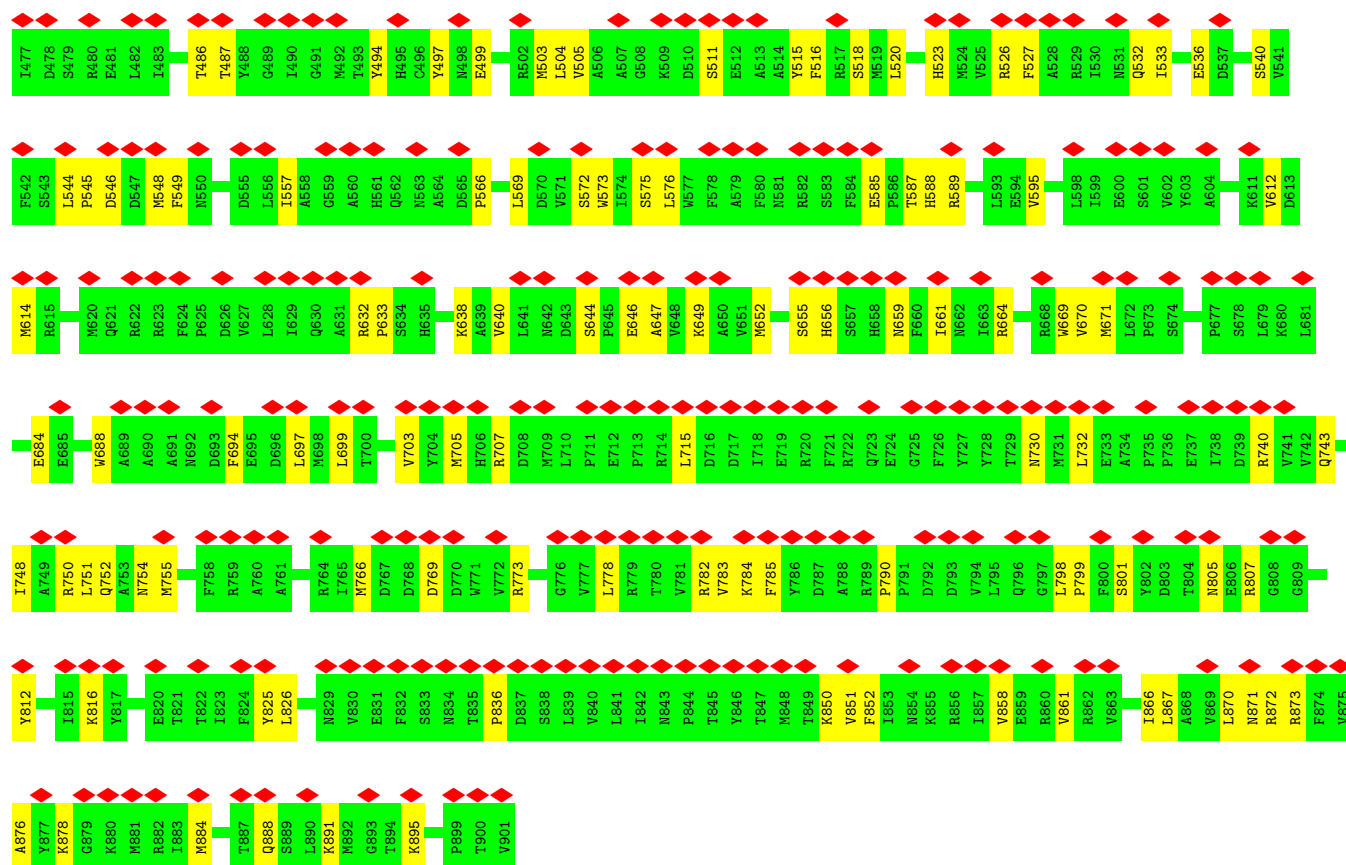
• Molecule 1: Core protein VP3



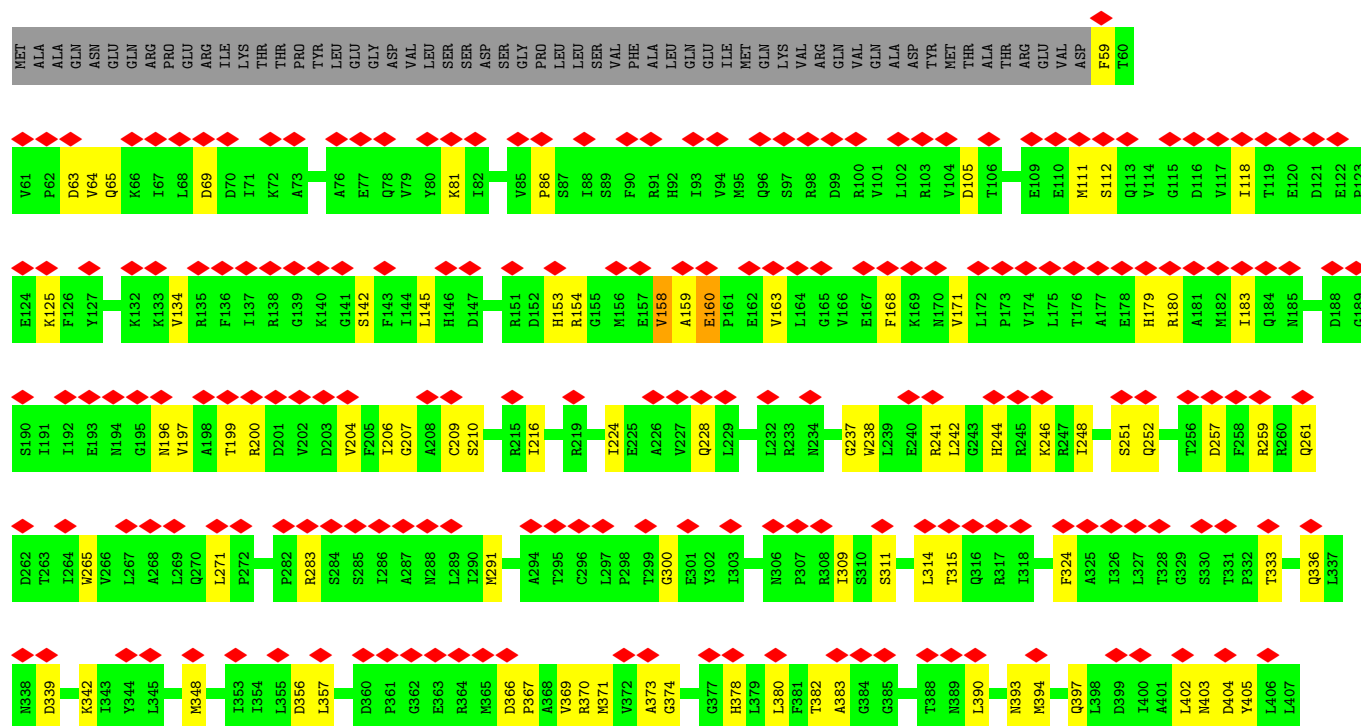


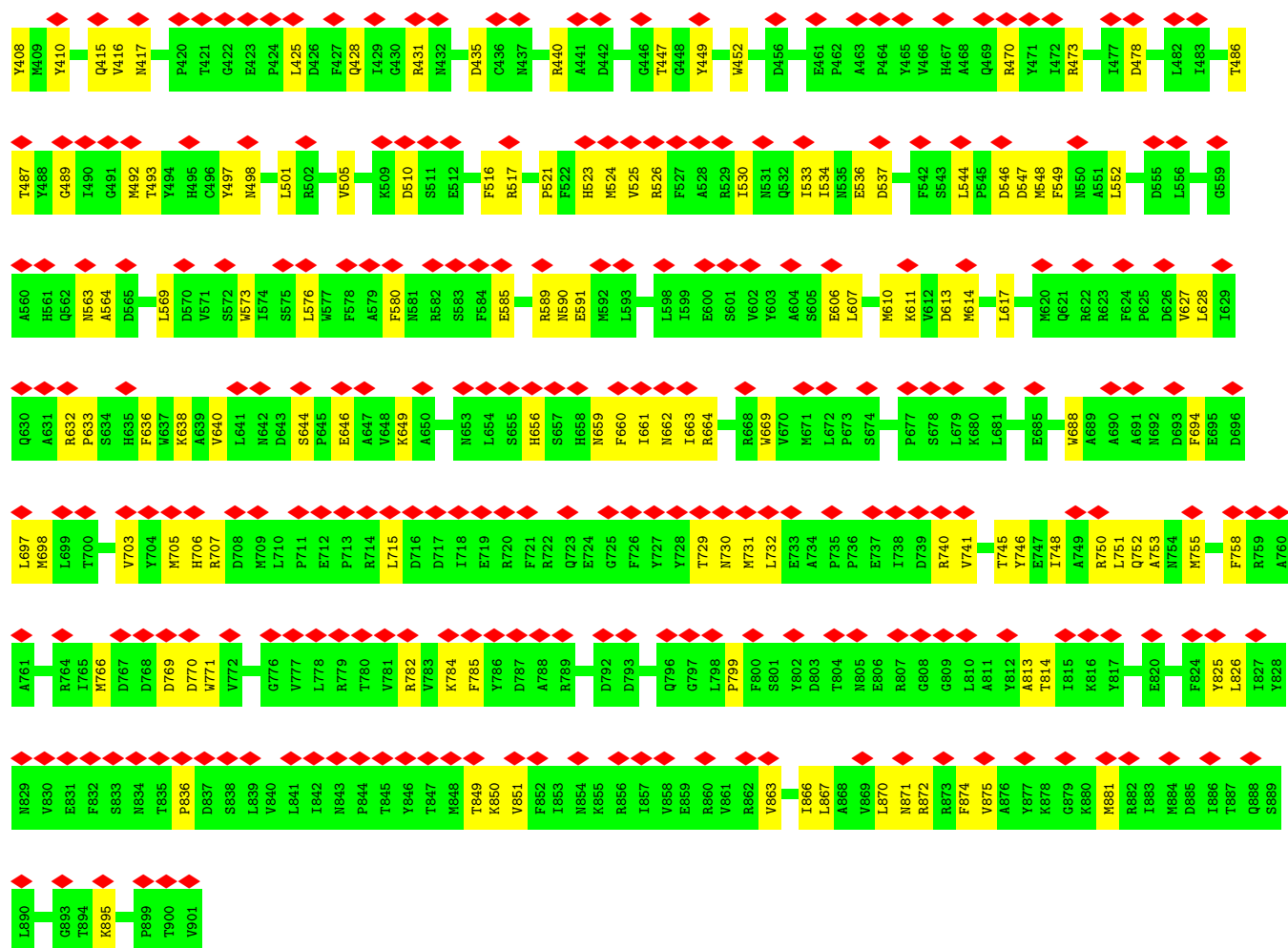
● Molecule 1: Core protein VP3



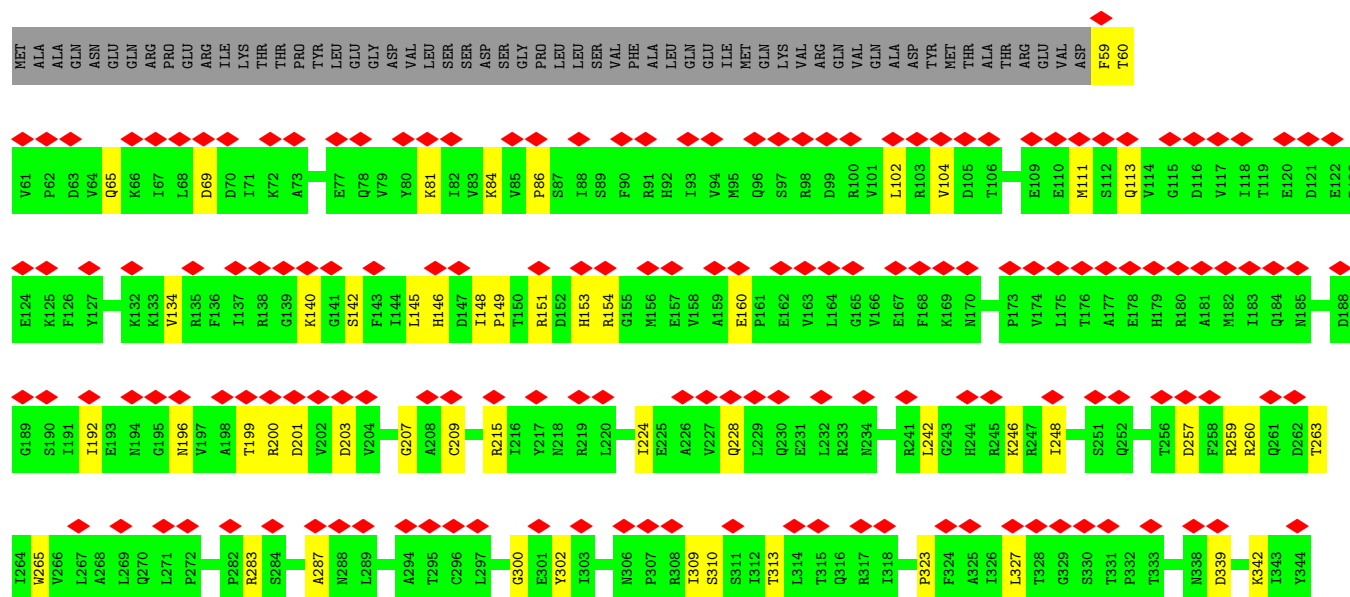


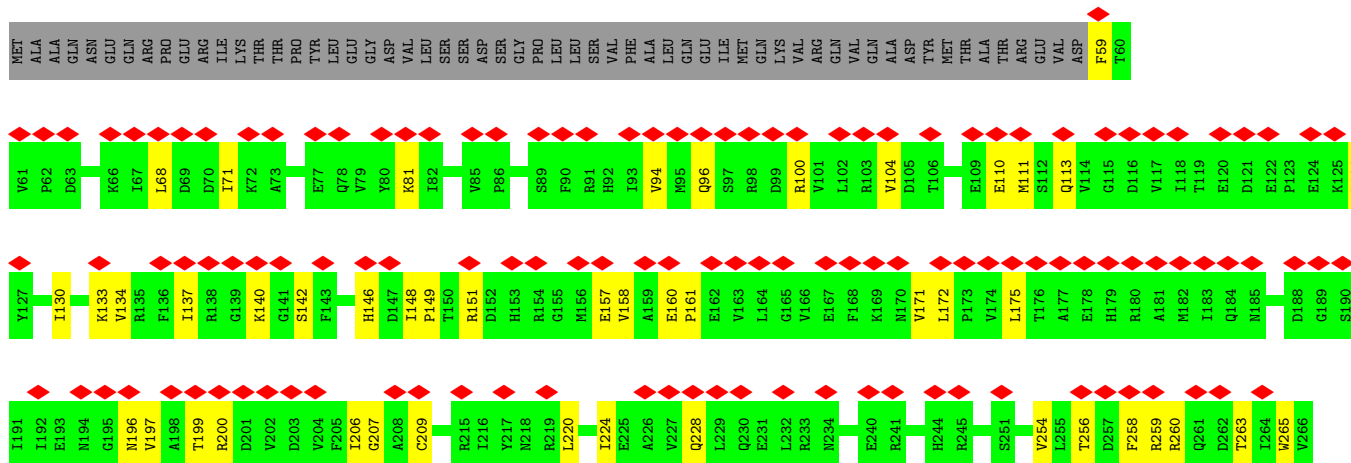
• Molecule 1: Core protein VP3

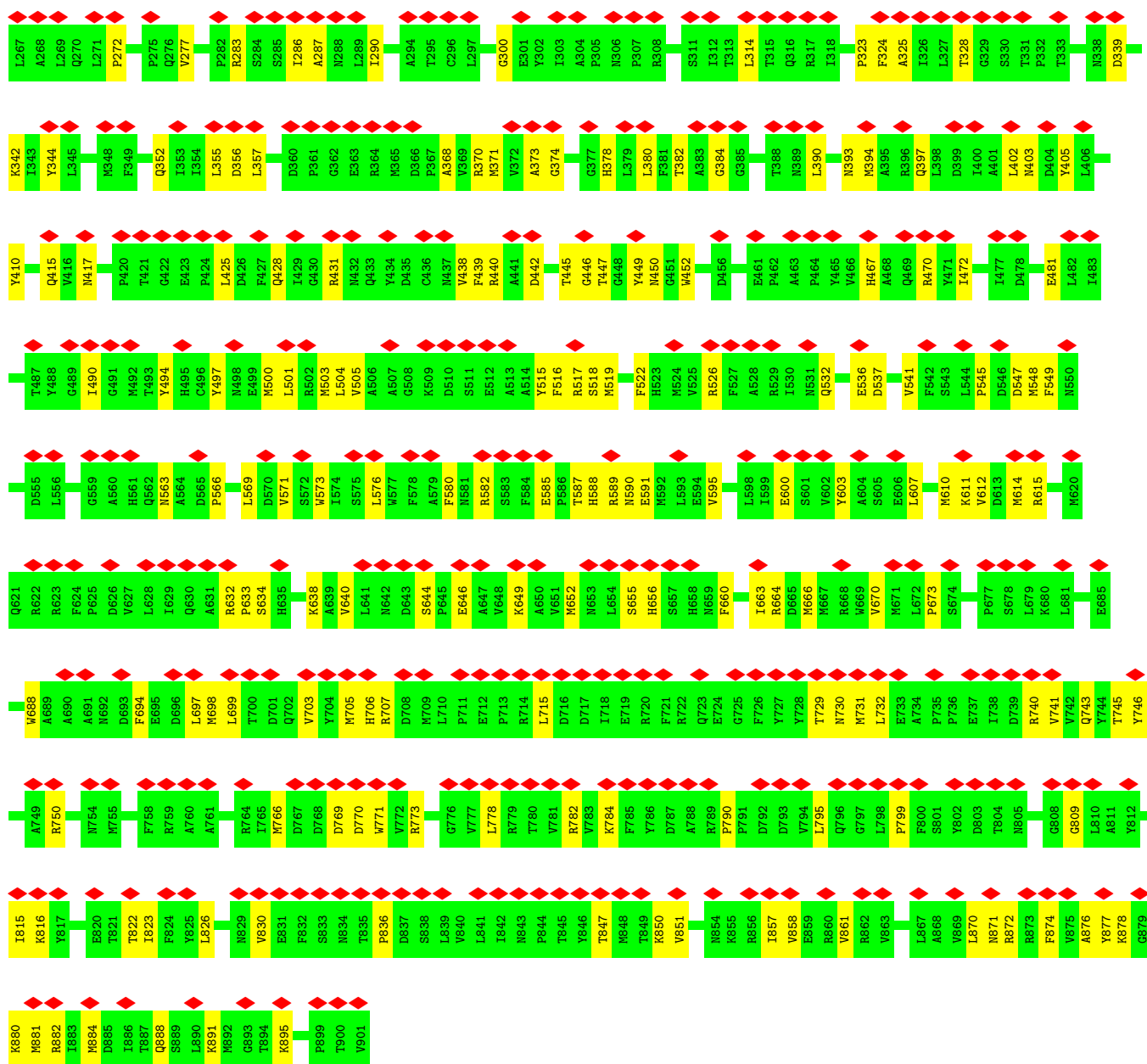




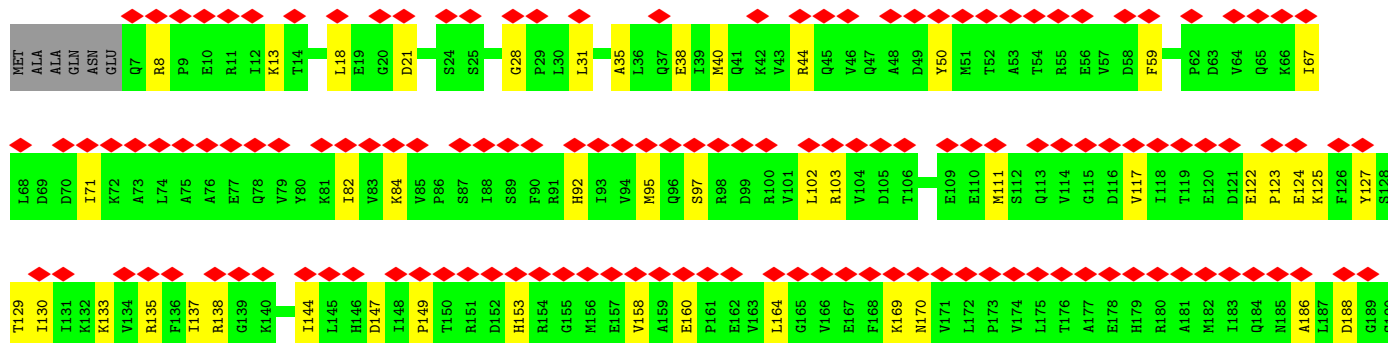
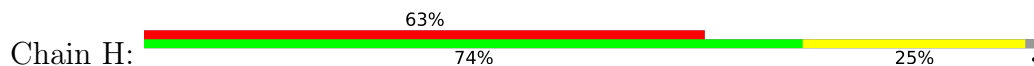
● Molecule 1: Core protein VP3

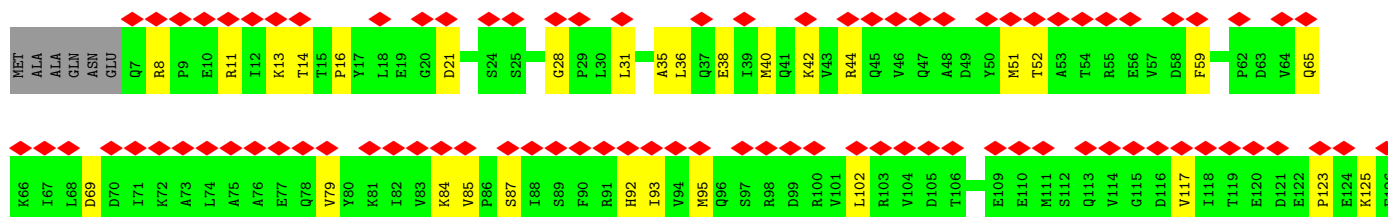
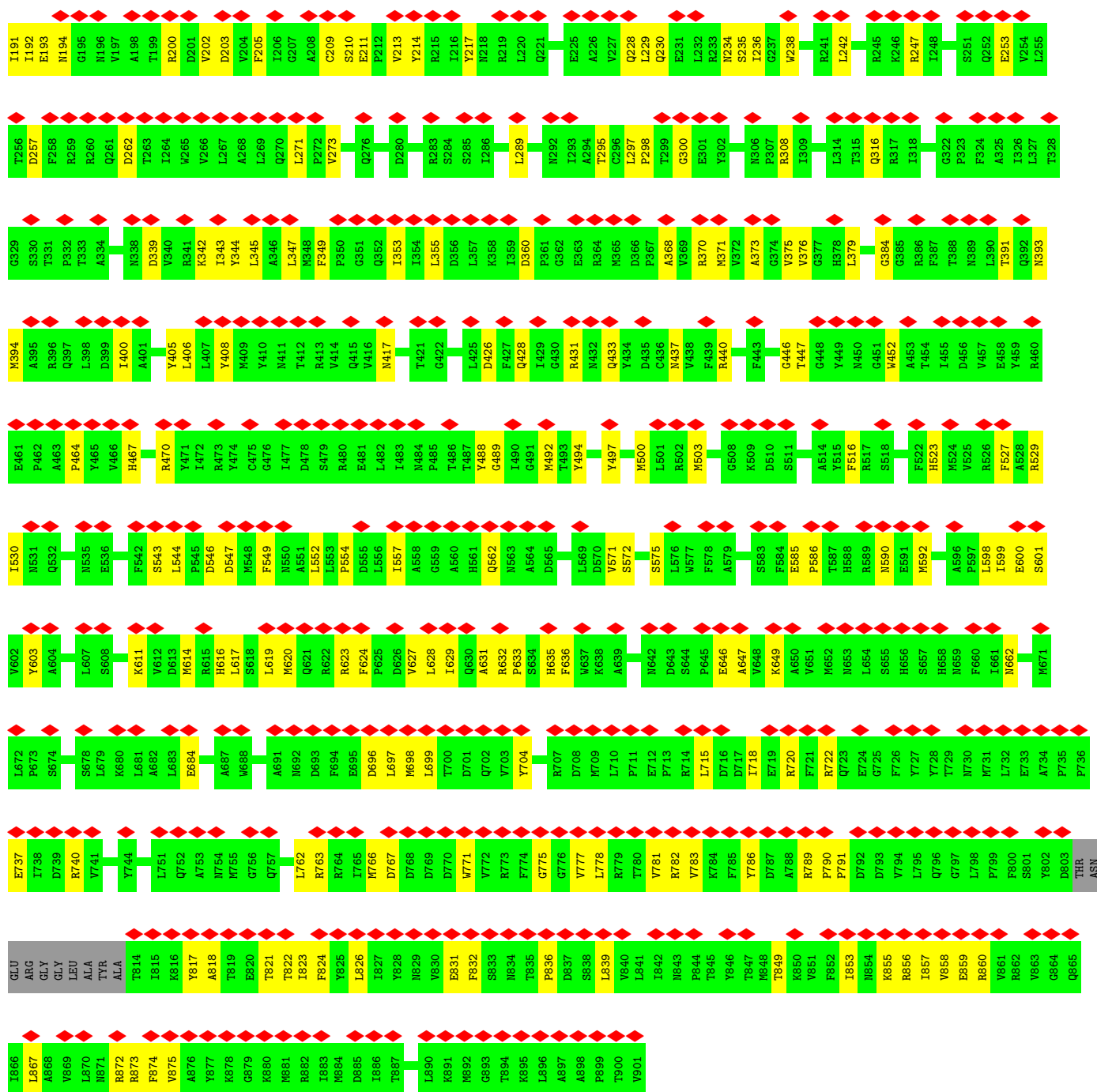


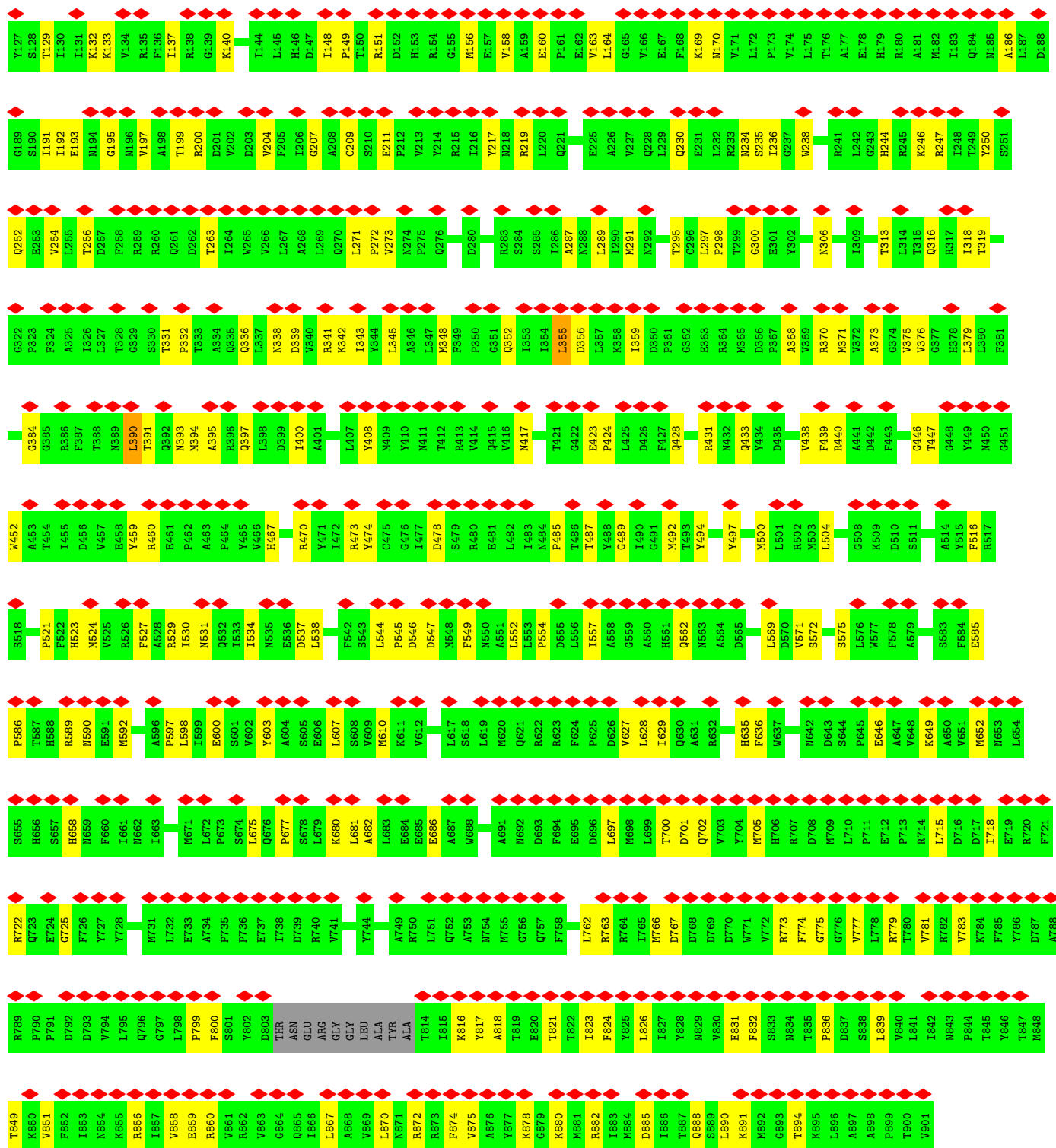




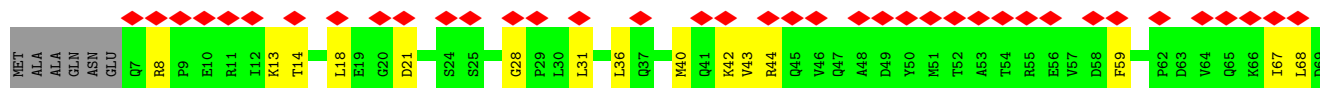
• Molecule 1: Core protein VP3

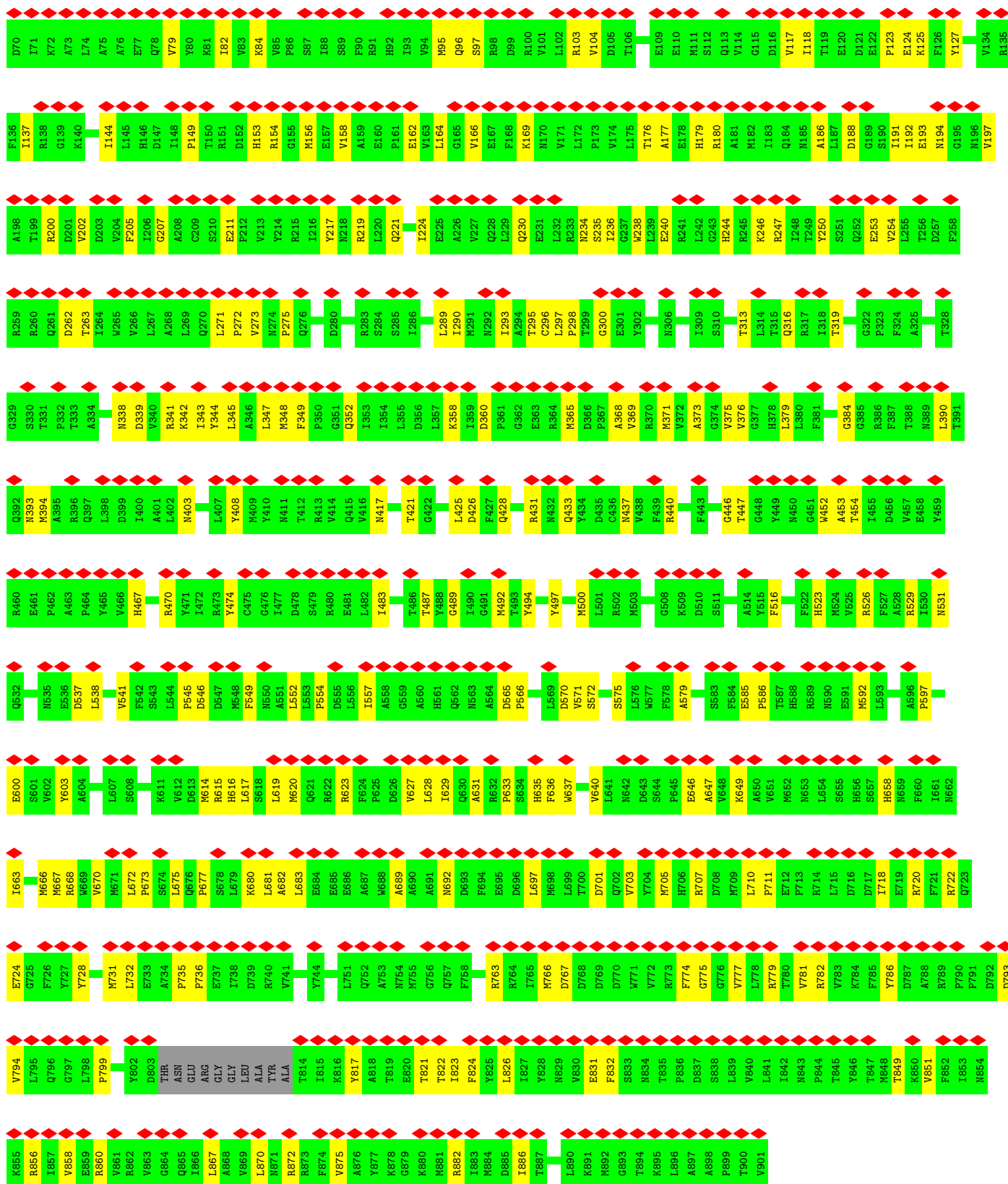






• Molecule 1: Core protein VP3





• Molecule 1: Core protein VP3



MET	ALA	ALA	GLN	ASN	GLU	Q7	R8	P9	E10	R11	I12	K13	T14	Y17	L18	E19	G20	D21	S24	S25	G28	P29	L30	L31	S32	A35	L36	Q37	E38	I39	M40	Q41	K42	V43	R44	Q45	V46	Q47	A48	D49	Y50	M51	T52	A53	T54	R55	E56	V57	D58	F59	T60	V61	P62	Q65			
K66	I67	L68	D69	D70	I71	K72	L74	A75	A76	E77	Q78	Y79	Y80	K81	I82	V83	K84	V85	P86	S87	I88	S89	F90	R91	H92	I93	V94	M95	Q96	S97	R98	D99	R100	V101	L102	R103	V104	D105	T106	E109	E110	M111	S112	Q113	V114	G115	D116	V117	I118	T119	Q184	E120	D121	E122	P123	K125	F126
Y127	I130	K133	V134	R135	P136	I137	R138	G139	K140	I144	L145	H146	D147	P149	T150	M156	E157	A159	E160	P161	V163	G165	V166	E167	F168	K169	N170	V171	L172	P173	V174	L175	T176	E178	H179	R180	A181	K246	R247	I248	S251	Q252	E253	L187	D188	G189	S190										
I191	I192	E193	N194	G195	N196	V197	A198	T199	R200	D201	V202	D203	V204	F205	I206	G207	A208	C209	S210	E211	P212	V213	Y214	R215	I216	Y217	M218	R219	I33	L220	Q221	G222	Y223	I224	E225	A226	Q228	L229	Q230	E231	L232	R233	N234	S235	W238	R241	L242	G243	H244	R245	K246	R247	I248	S251	Q252	E253	
V254	L255	T256	D257	F258	R259	Q261	D262	T263	L264	V265	L267	A268	L269	Q270	L271	P272	V273	M274	D280	V281	P282	R283	S284	S285	L286	L289	L290	M291	N292	L293	C296	L297	T299	G300	E301	Y302	N306	I309	T313	L314	T315	Q316	R317	I318	T319	G322	P323	F324									
A325	I326	L327	T328	G329	S330	T331	P332	T333	A334	N338	V340	K341	K342	I343	Y344	L345	A346	L347	M348	F349	P350	G351	Q352	L353	I354	L355	L357	K358	I359	D360	P361	G362	E363	R364	D366	P367	V369	R370	K371	V372	A373	V375	V376	G377	L378	Y379	L380	F381	G384	G385	R386	F387					
T388	N389	L390	T391	Q392	N393	K394	A395	R396	Q397	L398	D399	L400	A401	L402	N403	D404	Y405	L406	L407	Y408	N409	Y410	N411	T412	R413	V414	Q415	V416	N417	T421	G422	E423	P424	L425	D426	F427	Q428	R431	N432	Q433	Y434	D435	C436	F439	R440	F443	T447	Q448	Y449	N450	G451	W452	A453	T454			
I455	D456	V457	E458	Y459	R460	E461	P462	A463	P464	V465	Y466	H467	R470	R473	Y474	C475	C476	L477	D478	S479	N480	E481	L482	I483	N484	P485	T486	L487	L490	Q491	M492	Y494	Y497	M500	L501	R502	M503	G508	K509	D510	S511	A514	S518	M519	L520	P521	F522	H523	M524	V525							
R526	F527	A528	R529	N530	N531	Q532	N535	E536	V541	F542	P545	D546	D547	M548	F549	A551	L552	L553	P554	D555	R556	I557	A558	C559	A560	H561	Q562	N563	A564	D565	P566	V567	V568	L569	D570	S571	S572	S575	L576	W577	F578	A579	S583	F584	E585	P586	T587	H588	R589	N590	E591	M592	L593				
A596	P597	L598	T599	B600	S601	V602	Y603	A604	E605	E606	L607	S608	K611	V612	H616	L617	L619	M620	Q621	R622	R623	F624	P625	D626	V627	L628	L629	Q630	A631	R632	P633	T634	H635	F636	W637	N642	P645	E646	A647	K649	A650	V651	M652	N653	L654	S655	H656	S657	E658	N659	F660	L661					
M662	T663	B664	D665	M666	M667	R668	M671	L672	P673	S674	L675	Q676	P677	S678	L679	K680	L681	A682	L683	E684	E685	E686	A687	M688	A691	M692	D693	F694	E695	D696	L697	M698	L699	T700	D701	Q702	W703	Y704	M705	R707	D708	M709	L710	P711	E712	R713	R714	L715	D716	D717	I718	E719	R720	F721	R722	Q723	
E724	G725	F726	Y727	Y728	M731	L732	E733	A734	P735	L736	E737	T738	D739	R740	V741	Y744	L751	Q752	A753	N754	Y755	G756	Q757	A760	A761	L762	R763	R764	L765	M766	D767	D768	D769	W771	R772	R773	F774	G775	G776	V777	L778	R779	T780	V781	R782	V783	K784	F785	Y786	D787	W788	R789	P790	P791			
D792	D793	V794	L795	Q796	Q797	L798	P799	F800	S801	Y802	G803	THR	ASN	GLU	ARG	GLY	GLY	LEU	ALA	TYR	T814	I815	K816	Y817	A818	R819	E820	T821	T822	I823	F824	Y825	L826	I827	Y828	N829	V830	E831	F832	N833	N834	T835	A836	D837	S838	V840	L841	I842	N843	P844	T845	Y846	T847	W848	T849	F852	
I853	N854	K855	R856	I857	V858	E859	R860	V861	R862	V863	G864	Q865	I866	L867	A868	V869	L870	N871	R872	R873	F874	Y875	A876	Y877	K878	G879	K880	M881	R882	I883	M884	D885	I886	T887	L890	K891	M892	G893	T894	K895	L896	A897	A898	P899	T900	V901											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	2124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	A	0.28	0/6966	0.62	0/9462
1	B	0.19	0/7310	0.53	0/9927
1	D	0.25	0/6966	0.60	0/9462
1	E	0.24	0/6966	0.58	0/9462
1	F	0.24	0/6966	0.58	0/9462
1	G	0.24	0/6966	0.58	0/9462
1	H	0.19	0/7310	0.52	0/9927
1	I	0.24	0/7310	0.58	1/9927 (0.0%)
1	J	0.19	0/7310	0.53	0/9927
1	K	0.20	0/7310	0.55	0/9927
All	All	0.23	0/71380	0.57	1/96945 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	636	PHE	CA-CB-CG	5.43	119.23	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6811	0	6791	157	0
1	B	7151	0	7137	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6811	0	6791	155	0
1	E	6811	0	6791	148	0
1	F	6811	0	6791	150	0
1	G	6811	0	6791	160	0
1	H	7151	0	7137	158	0
1	I	7151	0	7137	181	0
1	J	7151	0	7137	164	0
1	K	7151	0	7137	178	0
All	All	69810	0	69640	1531	0

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

All (1531) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:GLY:HA3	1:F:585:GLU:O	1.56	1.03
1:E:300:GLY:HA3	1:E:585:GLU:O	1.59	1.02
1:A:300:GLY:HA3	1:A:585:GLU:O	1.60	1.00
1:D:300:GLY:HA3	1:D:585:GLU:O	1.66	0.95
1:G:300:GLY:HA3	1:G:585:GLU:O	1.67	0.94
1:I:355:LEU:HD21	1:I:571:VAL:HG13	1.50	0.93
1:D:207:GLY:O	1:D:872:ARG:HB2	1.72	0.88
1:J:84:LYS:HE3	1:J:149:PRO:HD2	1.57	0.87
1:G:207:GLY:O	1:G:872:ARG:HB2	1.76	0.86
1:E:207:GLY:O	1:E:872:ARG:HB2	1.75	0.85
1:B:707:ARG:HG2	1:B:766:MET:HE3	1.59	0.85
1:F:207:GLY:O	1:F:872:ARG:HB2	1.76	0.84
1:G:707:ARG:H	1:G:766:MET:HE2	1.45	0.82
1:B:891:LYS:HD2	1:B:893:GLY:H	1.44	0.80
1:H:617:LEU:HD13	1:H:636:PHE:HB2	1.64	0.78
1:J:617:LEU:HA	1:J:620:MET:HE3	1.64	0.78
1:G:882:ARG:NH1	1:K:47:GLN:OE1	2.15	0.78
1:A:707:ARG:H	1:A:766:MET:HE2	1.49	0.78
1:A:492:MET:HB3	1:A:524:MET:HE1	1.66	0.77
1:I:523:HIS:HE1	1:I:527:PHE:CE2	2.02	0.77
1:E:373:ALA:HA	1:E:576:LEU:HD11	1.67	0.76
1:K:520:LEU:HG	1:K:524:MET:HE2	1.68	0.76
1:D:261:GLN:OE1	1:H:562:GLN:NE2	2.20	0.75
1:A:207:GLY:O	1:A:872:ARG:HB2	1.86	0.74
1:B:132:LYS:HE2	1:B:135:ARG:HH11	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:GLU:HA	1:J:872:ARG:HH12	1.51	0.74
1:J:263:THR:HG22	1:J:882:ARG:HE	1.52	0.74
1:H:617:LEU:HA	1:H:620:MET:HE3	1.70	0.74
1:K:523:HIS:HE1	1:K:527:PHE:CE2	2.06	0.74
1:F:649:LYS:HA	1:F:652:MET:HE2	1.69	0.73
1:G:110:GLU:OE2	1:G:140:LYS:NZ	2.22	0.73
1:G:344:TYR:OH	1:G:526:ARG:NH2	2.22	0.73
1:A:314:LEU:HD13	1:A:324:PHE:HB3	1.71	0.72
1:H:523:HIS:HE1	1:H:527:PHE:CE2	2.08	0.72
1:J:137:ILE:HD11	1:J:697:LEU:HD21	1.72	0.72
1:J:494:TYR:OH	1:J:523:HIS:HD2	1.72	0.72
1:H:529:ARG:HH12	1:H:585:GLU:HG3	1.53	0.72
1:K:211:GLU:HA	1:K:872:ARG:HH12	1.52	0.71
1:B:137:ILE:HD11	1:B:697:LEU:HD21	1.72	0.71
1:F:707:ARG:H	1:F:766:MET:HE2	1.55	0.71
1:F:287:ALA:HB2	1:F:655:SER:HB2	1.73	0.71
1:K:668:ARG:HA	1:K:671:MET:HE3	1.71	0.71
1:K:84:LYS:HE3	1:K:149:PRO:HD2	1.73	0.71
1:A:339:ASP:HA	1:A:342:LYS:HD2	1.71	0.71
1:B:391:THR:H	1:B:394:MET:HE2	1.56	0.70
1:A:373:ALA:HA	1:A:576:LEU:HD11	1.71	0.70
1:E:283:ARG:NH1	1:E:660:PHE:O	2.24	0.70
1:H:620:MET:HA	1:H:623:ARG:HB2	1.74	0.70
1:I:521:PRO:HA	1:I:524:MET:HE2	1.74	0.70
1:F:259:ARG:NH1	1:F:880:LYS:O	2.24	0.70
1:J:786:TYR:HB2	1:J:824:PHE:HE1	1.55	0.70
1:I:263:THR:HG22	1:I:882:ARG:HE	1.56	0.70
1:I:529:ARG:HH12	1:I:585:GLU:HG3	1.56	0.70
1:D:339:ASP:HA	1:D:342:LYS:HD2	1.74	0.69
1:E:339:ASP:HA	1:E:342:LYS:HD2	1.74	0.69
1:F:410:TYR:HD2	1:G:505:VAL:HG21	1.57	0.69
1:I:137:ILE:HD11	1:I:697:LEU:HD21	1.73	0.69
1:B:615:ARG:HH12	1:B:673:PRO:HA	1.57	0.69
1:G:373:ALA:HA	1:G:576:LEU:HD11	1.72	0.69
1:B:219:ARG:HD2	1:B:686:GLU:HG3	1.75	0.69
1:F:339:ASP:HA	1:F:342:LYS:HD2	1.75	0.69
1:G:374:GLY:O	1:G:378:HIS:ND1	2.26	0.69
1:D:263:THR:HG21	1:D:884:MET:HE3	1.74	0.69
1:F:113:GLN:HA	1:F:782:ARG:HH22	1.58	0.69
1:E:283:ARG:NH1	1:E:659:ASN:OD1	2.26	0.69
1:F:382:THR:HA	1:F:449:TYR:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:ARG:NH1	1:F:686:GLU:O	2.27	0.68
1:I:117:VAL:O	1:I:125:LYS:NZ	2.27	0.68
1:B:715:LEU:HD11	1:B:839:LEU:HD13	1.76	0.67
1:I:207:GLY:HA2	1:I:870:LEU:HD22	1.76	0.67
1:F:646:GLU:HA	1:F:649:LYS:HE2	1.77	0.67
1:E:440:ARG:O	1:E:447:THR:OG1	2.12	0.67
1:G:339:ASP:HA	1:G:342:LYS:HD2	1.76	0.67
1:H:699:LEU:HD23	1:H:778:LEU:HD13	1.76	0.67
1:J:217:TYR:OH	1:J:875:VAL:O	2.12	0.67
1:B:821:THR:HG21	1:B:849:THR:HG21	1.77	0.67
1:F:417:ASN:HB3	1:F:428:GLN:HB2	1.77	0.67
1:G:263:THR:HG21	1:G:884:MET:HE3	1.75	0.67
1:G:740:ARG:NH1	1:G:769:ASP:O	2.28	0.67
1:K:529:ARG:HH11	1:K:586:PRO:HD2	1.60	0.67
1:G:795:LEU:HD11	1:G:847:THR:HG22	1.77	0.67
1:K:379:LEU:HD21	1:K:500:MET:HG3	1.75	0.67
1:F:390:LEU:HD13	1:F:394:MET:HB3	1.76	0.66
1:G:393:ASN:O	1:G:397:GLN:NE2	2.27	0.66
1:J:84:LYS:NZ	1:J:162:GLU:OE2	2.28	0.66
1:A:440:ARG:O	1:A:447:THR:OG1	2.13	0.66
1:B:193:GLU:O	1:B:200:ARG:NH1	2.28	0.66
1:D:67:ILE:HD11	1:D:647:ALA:HA	1.77	0.66
1:F:260:ARG:NH1	1:J:566:PRO:O	2.29	0.66
1:H:211:GLU:HG3	1:H:872:ARG:HH12	1.61	0.66
1:B:264:ILE:HG12	1:B:881:MET:HE2	1.76	0.66
1:G:149:PRO:HG2	1:G:160:GLU:HG3	1.77	0.66
1:B:704:TYR:HB3	1:B:771:TRP:HD1	1.60	0.66
1:A:374:GLY:O	1:A:378:HIS:ND1	2.24	0.66
1:B:881:MET:HE3	1:B:882:ARG:H	1.59	0.66
1:I:492:MET:SD	1:I:524:MET:HE1	2.36	0.66
1:J:371:MET:HE1	1:J:408:TYR:HB3	1.77	0.66
1:E:536:GLU:OE2	1:E:589:ARG:NH1	2.29	0.66
1:H:40:MET:HE2	1:H:59:PHE:HB3	1.78	0.66
1:D:245:ARG:HH21	1:D:464:PRO:HD2	1.61	0.66
1:G:481:GLU:HA	1:K:407:LEU:HD21	1.78	0.66
1:I:8:ARG:HB3	1:I:11:ARG:HE	1.60	0.66
1:D:393:ASN:O	1:D:397:GLN:NE2	2.28	0.65
1:H:230:GLN:NE2	1:H:234:ASN:OD1	2.30	0.65
1:J:823:ILE:HG12	1:J:851:VAL:HG11	1.77	0.65
1:G:259:ARG:NH1	1:G:880:LYS:O	2.29	0.65
1:A:490:ILE:HD12	1:G:370:ARG:HH12	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:HIS:HE1	1:F:402:LEU:HB2	1.62	0.65
1:F:470:ARG:NH1	1:F:544:LEU:O	2.30	0.65
1:I:523:HIS:HE1	1:I:527:PHE:HE2	1.45	0.65
1:J:781:VAL:HG13	1:J:823:ILE:HD13	1.78	0.65
1:A:536:GLU:OE2	1:A:589:ARG:NH1	2.30	0.65
1:K:246:LYS:HE3	1:K:593:LEU:HD21	1.78	0.65
1:B:483:ILE:O	1:G:632:ARG:NH2	2.30	0.65
1:D:154:ARG:HH22	1:H:629:ILE:HG23	1.61	0.65
1:F:740:ARG:NH1	1:F:769:ASP:O	2.30	0.65
1:H:489:GLY:HA2	1:H:492:MET:HE2	1.78	0.65
1:K:459:TYR:O	1:K:460:ARG:NE	2.28	0.65
1:H:391:THR:H	1:H:394:MET:HE2	1.62	0.65
1:J:720:ARG:HE	1:J:724:GLU:HG2	1.62	0.65
1:B:781:VAL:HG13	1:B:823:ILE:HD13	1.77	0.65
1:F:260:ARG:HH11	1:J:565:ASP:HB2	1.62	0.65
1:F:379:LEU:HD21	1:F:500:MET:HE3	1.79	0.65
1:A:110:GLU:O	1:A:113:GLN:NE2	2.29	0.65
1:A:740:ARG:NH1	1:A:769:ASP:O	2.30	0.65
1:A:644:SER:O	1:A:649:LYS:NZ	2.30	0.65
1:G:260:ARG:NH1	1:K:566:PRO:O	2.30	0.65
1:H:193:GLU:O	1:H:200:ARG:NH1	2.30	0.65
1:K:521:PRO:HA	1:K:524:MET:HE3	1.79	0.65
1:K:617:LEU:HA	1:K:620:MET:HE3	1.78	0.65
1:D:133:LYS:HZ1	1:D:697:LEU:HA	1.62	0.64
1:E:393:ASN:O	1:E:397:GLN:NE2	2.31	0.64
1:B:600:GLU:O	1:B:603:TYR:HB3	1.97	0.64
1:D:715:LEU:HB2	1:D:836:PRO:HA	1.79	0.64
1:H:8:ARG:HH22	1:H:247:ARG:HG2	1.62	0.64
1:I:230:GLN:NE2	1:I:234:ASN:OD1	2.30	0.64
1:G:548:MET:SD	1:G:563:ASN:ND2	2.70	0.64
1:K:8:ARG:HB3	1:K:11:ARG:HE	1.62	0.64
1:D:638:LYS:HE3	1:I:14:THR:HG22	1.77	0.64
1:J:117:VAL:O	1:J:125:LYS:NZ	2.30	0.64
1:J:494:TYR:OH	1:J:523:HIS:CD2	2.50	0.64
1:D:740:ARG:NH1	1:D:769:ASP:O	2.30	0.64
1:J:338:ASN:HA	1:J:341:ARG:HD3	1.80	0.64
1:A:871:ASN:OD1	1:A:872:ARG:NH2	2.31	0.64
1:D:382:THR:HA	1:D:449:TYR:HB3	1.79	0.64
1:E:366:ASP:HB3	1:E:369:VAL:HB	1.80	0.64
1:F:373:ALA:HA	1:F:576:LEU:HD11	1.80	0.64
1:G:694:PHE:HA	1:G:697:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:GLY:HA2	1:I:297:LEU:HD23	1.78	0.64
1:I:821:THR:HG21	1:I:849:THR:HG21	1.80	0.64
1:J:230:GLN:NE2	1:J:234:ASN:OD1	2.30	0.64
1:B:67:ILE:HD11	1:B:647:ALA:HA	1.80	0.63
1:B:617:LEU:HD13	1:B:636:PHE:HB2	1.80	0.63
1:E:644:SER:O	1:E:649:LYS:NZ	2.31	0.63
1:H:628:LEU:HB3	1:H:631:ALA:HB2	1.80	0.63
1:I:379:LEU:HD21	1:I:500:MET:HG2	1.79	0.63
1:F:393:ASN:O	1:F:397:GLN:NE2	2.31	0.63
1:F:638:LYS:NZ	1:K:13:LYS:O	2.31	0.63
1:G:283:ARG:NH2	1:G:660:PHE:O	2.30	0.63
1:I:600:GLU:O	1:I:603:TYR:HB3	1.99	0.63
1:K:230:GLN:NE2	1:K:234:ASN:OD1	2.30	0.63
1:B:211:GLU:HA	1:B:872:ARG:HH12	1.64	0.63
1:B:246:LYS:HE2	1:B:537:ASP:HA	1.80	0.63
1:E:707:ARG:H	1:E:766:MET:HE2	1.63	0.63
1:I:352:GLN:HE21	1:I:544:LEU:HD22	1.63	0.63
1:A:390:LEU:HD13	1:A:394:MET:HB3	1.81	0.63
1:D:470:ARG:NH1	1:D:544:LEU:O	2.31	0.63
1:G:151:ARG:HH12	1:G:161:PRO:HD3	1.64	0.63
1:K:426:ASP:OD1	1:K:440:ARG:NH1	2.31	0.63
1:D:644:SER:O	1:D:649:LYS:NZ	2.31	0.63
1:G:382:THR:HA	1:G:449:TYR:HB3	1.81	0.63
1:I:390:LEU:HG	1:I:391:THR:N	2.13	0.63
1:I:856:ARG:NH1	1:I:858:VAL:O	2.31	0.63
1:B:8:ARG:HB3	1:B:11:ARG:HE	1.64	0.63
1:D:283:ARG:HD3	1:D:659:ASN:HB3	1.81	0.63
1:E:740:ARG:NH1	1:E:769:ASP:O	2.32	0.63
1:E:814:THR:OG1	1:J:253:GLU:OE1	2.15	0.63
1:K:193:GLU:O	1:K:200:ARG:NH1	2.32	0.63
1:E:729:THR:HG22	1:E:731:MET:H	1.63	0.62
1:F:283:ARG:O	1:F:655:SER:OG	2.17	0.62
1:G:871:ASN:OD1	1:G:872:ARG:NH2	2.31	0.62
1:H:28:GLY:HA2	1:H:297:LEU:HD23	1.81	0.62
1:E:871:ASN:OD1	1:E:872:ARG:NH2	2.32	0.62
1:B:217:TYR:OH	1:B:875:VAL:O	2.17	0.62
1:K:616:HIS:HA	1:K:619:LEU:HD12	1.79	0.62
1:A:260:ARG:NH1	1:B:566:PRO:O	2.33	0.62
1:B:375:VAL:HG13	1:B:500:MET:HE2	1.81	0.62
1:E:314:LEU:HD13	1:E:324:PHE:HB3	1.82	0.62
1:D:203:ASP:HB2	1:D:876:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:LEU:HA	1:G:175:LEU:HD12	1.81	0.62
1:D:370:ARG:NH1	1:D:404:ASP:OD2	2.33	0.62
1:G:287:ALA:HB2	1:G:655:SER:HB2	1.82	0.62
1:I:235:SER:HB3	1:I:271:LEU:HD13	1.80	0.62
1:I:534:ILE:HA	1:I:538:LEU:HD12	1.79	0.62
1:J:235:SER:HB3	1:J:271:LEU:HD13	1.81	0.62
1:D:151:ARG:HH22	1:D:160:GLU:HA	1.64	0.62
1:F:548:MET:SD	1:F:563:ASN:ND2	2.70	0.62
1:F:743:GLN:NE2	1:F:773:ARG:O	2.33	0.62
1:A:257:ASP:OD2	1:A:882:ARG:NH1	2.32	0.62
1:A:273:VAL:O	1:A:274:ASN:C	2.43	0.62
1:D:356:ASP:N	1:D:569:LEU:O	2.31	0.62
1:I:217:TYR:OH	1:I:875:VAL:O	2.17	0.62
1:I:431:ARG:O	1:I:433:GLN:NE2	2.33	0.62
1:K:217:TYR:OH	1:K:875:VAL:O	2.17	0.62
1:A:382:THR:HA	1:A:449:TYR:HB3	1.81	0.62
1:F:440:ARG:O	1:F:447:THR:OG1	2.18	0.62
1:H:856:ARG:NH1	1:H:858:VAL:O	2.33	0.61
1:J:193:GLU:O	1:J:200:ARG:NH1	2.33	0.61
1:K:523:HIS:HE1	1:K:527:PHE:HE2	1.46	0.61
1:A:646:GLU:HA	1:A:649:LYS:HE2	1.82	0.61
1:B:125:LYS:NZ	1:B:129:THR:OG1	2.27	0.61
1:H:821:THR:HG21	1:H:849:THR:HG21	1.82	0.61
1:K:235:SER:HB3	1:K:271:LEU:HD13	1.82	0.61
1:A:149:PRO:HG2	1:A:160:GLU:HG3	1.82	0.61
1:A:283:ARG:HD3	1:A:659:ASN:HB3	1.81	0.61
1:F:65:GLN:NE2	1:F:69:ASP:OD2	2.34	0.61
1:H:117:VAL:O	1:H:125:LYS:NZ	2.32	0.61
1:J:67:ILE:HD11	1:J:647:ALA:HA	1.82	0.61
1:D:878:LYS:NZ	1:H:662:ASN:OD1	2.31	0.61
1:E:370:ARG:NH1	1:E:404:ASP:OD2	2.34	0.61
1:A:415:GLN:OE1	1:A:431:ARG:NH2	2.33	0.61
1:A:486:THR:HG23	1:A:487:THR:HG23	1.83	0.61
1:F:731:MET:HE3	1:F:732:LEU:H	1.66	0.61
1:B:459:TYR:O	1:B:460:ARG:NE	2.29	0.61
1:K:628:LEU:HB3	1:K:631:ALA:HB2	1.83	0.61
1:F:644:SER:O	1:F:649:LYS:NZ	2.34	0.61
1:E:374:GLY:O	1:E:378:HIS:ND1	2.27	0.61
1:E:417:ASN:HB3	1:E:428:GLN:HB2	1.81	0.61
1:J:28:GLY:HA2	1:J:297:LEU:HD23	1.83	0.61
1:E:548:MET:SD	1:E:563:ASN:ND2	2.70	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:GLU:HG3	1:I:872:ARG:HH12	1.66	0.61
1:J:620:MET:HA	1:J:623:ARG:HB2	1.83	0.61
1:G:325:ALA:O	1:G:328:THR:OG1	2.15	0.60
1:J:774:PHE:O	1:J:779:ARG:NH1	2.33	0.60
1:B:379:LEU:HD21	1:B:500:MET:HG2	1.83	0.60
1:A:548:MET:SD	1:A:563:ASN:ND2	2.74	0.60
1:B:552:LEU:HD11	1:B:566:PRO:HG3	1.82	0.60
1:H:600:GLU:O	1:H:603:TYR:HB3	2.01	0.60
1:I:391:THR:HG22	1:I:394:MET:HG2	1.83	0.60
1:F:590:ASN:O	1:F:895:LYS:NZ	2.35	0.60
1:B:235:SER:HB3	1:B:271:LEU:HD13	1.83	0.60
1:B:431:ARG:O	1:B:433:GLN:NE2	2.35	0.60
1:H:431:ARG:O	1:H:433:GLN:NE2	2.33	0.60
1:H:235:SER:HB3	1:H:271:LEU:HD13	1.83	0.60
1:I:489:GLY:HA2	1:I:492:MET:HE2	1.83	0.60
1:F:263:THR:HG21	1:F:884:MET:HE2	1.82	0.60
1:H:343:ILE:HG13	1:H:571:VAL:HG11	1.83	0.60
1:A:743:GLN:NE2	1:A:773:ARG:O	2.35	0.60
1:D:373:ALA:HA	1:D:576:LEU:HD11	1.84	0.60
1:E:200:ARG:HH22	1:E:228:GLN:HB3	1.67	0.60
1:H:67:ILE:HD11	1:H:647:ALA:HA	1.83	0.60
1:H:781:VAL:HG13	1:H:823:ILE:HD13	1.83	0.60
1:K:821:THR:HG21	1:K:849:THR:HG21	1.83	0.60
1:D:149:PRO:HG2	1:D:160:GLU:HG3	1.84	0.60
1:I:715:LEU:HD11	1:I:839:LEU:HD13	1.82	0.60
1:I:779:ARG:HD2	1:I:818:ALA:HB1	1.84	0.60
1:J:103:ARG:O	1:J:858:VAL:HA	2.01	0.60
1:J:646:GLU:HA	1:J:649:LYS:HE3	1.84	0.60
1:J:600:GLU:O	1:J:603:TYR:HB3	2.02	0.59
1:D:871:ASN:OD1	1:D:872:ARG:NH2	2.35	0.59
1:E:632:ARG:NH2	1:J:483:ILE:O	2.35	0.59
1:F:871:ASN:OD1	1:F:872:ARG:NH2	2.34	0.59
1:J:8:ARG:NH1	1:J:247:ARG:O	2.36	0.59
1:D:200:ARG:HH12	1:D:228:GLN:HB3	1.67	0.59
1:H:763:ARG:NH2	1:H:767:ASP:OD1	2.36	0.59
1:F:531:ASN:OD1	1:F:535:ASN:ND2	2.35	0.59
1:K:523:HIS:CE1	1:K:527:PHE:CE2	2.89	0.59
1:A:263:THR:HG21	1:A:884:MET:HE3	1.85	0.59
1:B:93:ILE:HB	1:B:102:LEU:HB2	1.83	0.59
1:G:355:LEU:HD11	1:G:571:VAL:HG22	1.84	0.59
1:H:696:ASP:OD1	1:H:855:LYS:NZ	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:627:VAL:HG22	1:I:777:VAL:HG13	1.83	0.59
1:K:762:LEU:O	1:K:766:MET:HB2	2.03	0.59
1:F:526:ARG:NH2	1:F:583:SER:OG	2.36	0.59
1:I:95:MET:HE3	1:I:725:GLY:HA3	1.85	0.59
1:D:371:MET:HB2	1:D:405:TYR:HD2	1.68	0.59
1:D:544:LEU:HD23	1:D:549:PHE:HD1	1.67	0.59
1:E:367:PRO:HA	1:E:370:ARG:HG2	1.84	0.59
1:G:815:ILE:O	1:G:816:LYS:NZ	2.36	0.59
1:I:775:GLY:HA2	1:I:779:ARG:HH12	1.66	0.59
1:J:856:ARG:NH1	1:J:858:VAL:O	2.36	0.59
1:A:481:GLU:HA	1:B:407:LEU:HD21	1.85	0.59
1:B:339:ASP:HA	1:B:342:LYS:HD2	1.85	0.59
1:G:536:GLU:OE2	1:G:589:ARG:NH1	2.35	0.59
1:H:339:ASP:HA	1:H:342:LYS:HE2	1.84	0.59
1:I:823:ILE:HG12	1:I:851:VAL:HG11	1.83	0.59
1:J:431:ARG:O	1:J:433:GLN:NE2	2.36	0.59
1:K:84:LYS:CE	1:K:149:PRO:HD2	2.32	0.59
1:H:704:TYR:HB3	1:H:771:TRP:HD1	1.68	0.59
1:D:357:LEU:HD13	1:D:573:TRP:HE1	1.68	0.59
1:E:410:TYR:HD2	1:F:505:VAL:HG21	1.67	0.59
1:H:44:ARG:HH21	1:H:59:PHE:HB2	1.67	0.59
1:K:431:ARG:O	1:K:433:GLN:NE2	2.36	0.59
1:A:65:GLN:NE2	1:A:69:ASP:OD2	2.35	0.58
1:F:149:PRO:HG2	1:F:160:GLU:HG3	1.85	0.58
1:G:415:GLN:OE1	1:G:431:ARG:NH2	2.35	0.58
1:G:595:VAL:HG12	1:G:891:LYS:HB2	1.85	0.58
1:I:79:VAL:HG11	1:I:680:LYS:HD3	1.84	0.58
1:G:537:ASP:OD1	1:G:589:ARG:NH1	2.29	0.58
1:H:137:ILE:HD11	1:H:697:LEU:HD21	1.85	0.58
1:D:752:GLN:HA	1:D:755:MET:HE3	1.85	0.58
1:G:111:MET:HE1	1:G:698:MET:HB2	1.85	0.58
1:B:437:ASN:HA	1:B:440:ARG:HH11	1.68	0.58
1:I:338:ASN:OD1	1:I:341:ARG:NH1	2.32	0.58
1:J:705:MET:HE1	1:J:799:PRO:HD3	1.85	0.58
1:K:424:PRO:O	1:K:440:ARG:NH1	2.32	0.58
1:F:715:LEU:HB2	1:F:836:PRO:HA	1.86	0.58
1:F:729:THR:HG22	1:F:731:MET:H	1.67	0.58
1:G:356:ASP:N	1:G:569:LEU:O	2.34	0.58
1:J:675:LEU:HD11	1:J:681:LEU:HD21	1.86	0.58
1:K:856:ARG:NH1	1:K:859:GLU:OE1	2.35	0.58
1:A:715:LEU:HB2	1:A:836:PRO:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:LYS:NZ	1:E:537:ASP:O	2.36	0.58
1:G:134:VAL:HG21	1:G:688:TRP:CZ2	2.38	0.58
1:B:338:ASN:HA	1:B:341:ARG:HD3	1.85	0.58
1:F:104:VAL:HG23	1:F:858:VAL:HG22	1.85	0.58
1:F:228:GLN:NE2	1:F:265:TRP:O	2.35	0.58
1:K:295:THR:HG22	1:K:592:MET:HE1	1.84	0.58
1:A:483:ILE:HG13	1:A:528:ALA:HB1	1.84	0.58
1:D:228:GLN:NE2	1:D:265:TRP:O	2.36	0.58
1:E:154:ARG:HH22	1:I:629:ILE:HG23	1.68	0.58
1:G:649:LYS:HA	1:G:652:MET:HE2	1.84	0.58
1:J:426:ASP:OD1	1:J:440:ARG:NH1	2.37	0.58
1:B:297:LEU:HD12	1:B:298:PRO:HD2	1.85	0.58
1:I:355:LEU:HD23	1:I:356:ASP:H	1.68	0.58
1:K:297:LEU:HD12	1:K:298:PRO:HD2	1.86	0.58
1:D:68:LEU:HA	1:D:71:ILE:HD12	1.86	0.58
1:D:313:THR:O	1:D:511:SER:OG	2.19	0.58
1:F:703:VAL:HG12	1:F:851:VAL:HG22	1.86	0.58
1:I:246:LYS:NZ	1:I:537:ASP:O	2.37	0.58
1:J:615:ARG:HH22	1:J:673:PRO:HB3	1.69	0.58
1:J:628:LEU:HB3	1:J:631:ALA:HB2	1.85	0.58
1:K:28:GLY:HA2	1:K:297:LEU:HD23	1.86	0.58
1:K:667:MET:SD	1:K:671:MET:HE2	2.44	0.58
1:B:487:THR:O	1:G:664:ARG:NH1	2.36	0.57
1:I:523:HIS:CE1	1:I:527:PHE:CE2	2.88	0.57
1:K:696:ASP:OD1	1:K:855:LYS:NZ	2.34	0.57
1:E:382:THR:HA	1:E:449:TYR:HB3	1.86	0.57
1:A:381:PHE:HD2	1:A:390:LEU:HD23	1.70	0.57
1:G:888:GLN:HE21	1:G:891:LYS:HD3	1.70	0.57
1:J:44:ARG:HD2	1:J:59:PHE:HB2	1.85	0.57
1:K:391:THR:H	1:K:394:MET:HE2	1.69	0.57
1:H:102:LEU:HG	1:H:860:ARG:HE	1.69	0.57
1:J:297:LEU:HD12	1:J:298:PRO:HD2	1.85	0.57
1:A:393:ASN:O	1:A:397:GLN:NE2	2.38	0.57
1:A:505:VAL:HG21	1:G:410:TYR:HD2	1.67	0.57
1:A:703:VAL:HG12	1:A:851:VAL:HG22	1.86	0.57
1:B:722:ARG:HH11	1:B:831:GLU:HA	1.68	0.57
1:J:219:ARG:HH22	1:J:682:ALA:HB1	1.68	0.57
1:J:295:THR:HG22	1:J:592:MET:HE1	1.86	0.57
1:B:252:GLN:OE1	1:G:750:ARG:NH1	2.37	0.57
1:J:365:MET:HE2	1:J:369:VAL:HB	1.86	0.57
1:K:339:ASP:HA	1:K:342:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:MET:HB2	1:A:405:TYR:HD2	1.70	0.57
1:B:848:MET:SD	1:B:848:MET:N	2.78	0.57
1:E:390:LEU:HD13	1:E:394:MET:HB3	1.86	0.57
1:H:297:LEU:HD12	1:H:298:PRO:HD2	1.86	0.57
1:J:31:LEU:HD12	1:J:345:LEU:HD11	1.86	0.57
1:D:536:GLU:OE1	1:D:589:ARG:NH1	2.37	0.57
1:I:890:LEU:O	1:I:891:LYS:HG3	2.04	0.57
1:A:878:LYS:HB3	1:A:881:MET:HG2	1.86	0.57
1:H:13:LYS:NZ	1:H:18:LEU:O	2.37	0.57
1:H:300:GLY:HA2	1:H:586:PRO:HA	1.86	0.57
1:J:775:GLY:N	1:J:817:TYR:OH	2.38	0.57
1:K:627:VAL:HG22	1:K:777:VAL:HG13	1.87	0.57
1:E:380:LEU:HD11	1:E:580:PHE:HB2	1.87	0.56
1:E:415:GLN:OE1	1:E:431:ARG:NH2	2.38	0.56
1:E:715:LEU:HB2	1:E:836:PRO:HA	1.87	0.56
1:G:371:MET:HB2	1:G:405:TYR:HD2	1.69	0.56
1:A:370:ARG:NH1	1:A:404:ASP:OD2	2.38	0.56
1:F:323:PRO:HB3	1:F:368:ALA:HB1	1.87	0.56
1:G:644:SER:O	1:G:649:LYS:NZ	2.38	0.56
1:H:135:ARG:HE	1:H:138:ARG:HE	1.53	0.56
1:K:371:MET:HB3	1:K:405:TYR:HD2	1.70	0.56
1:B:28:GLY:HA2	1:B:297:LEU:HD23	1.87	0.56
1:B:393:ASN:OD1	1:B:394:MET:N	2.37	0.56
1:F:302:TYR:HA	1:F:583:SER:O	2.06	0.56
1:I:8:ARG:NH1	1:I:247:ARG:O	2.37	0.56
1:J:440:ARG:O	1:J:447:THR:OG1	2.22	0.56
1:D:801:SER:HB3	1:D:816:LYS:HB2	1.86	0.56
1:E:356:ASP:N	1:E:569:LEU:O	2.37	0.56
1:G:497:TYR:OH	1:G:516:PHE:O	2.23	0.56
1:I:297:LEU:HD12	1:I:298:PRO:HD2	1.87	0.56
1:K:620:MET:HA	1:K:623:ARG:HB2	1.87	0.56
1:D:670:VAL:HG13	1:D:671:MET:HE2	1.87	0.56
1:D:743:GLN:NE2	1:D:773:ARG:O	2.39	0.56
1:F:356:ASP:N	1:F:569:LEU:O	2.37	0.56
1:F:752:GLN:HA	1:F:755:MET:HE3	1.87	0.56
1:J:728:TYR:HB3	1:J:826:LEU:HB3	1.86	0.56
1:B:254:VAL:HG12	1:B:895:LYS:HD2	1.87	0.56
1:B:627:VAL:HG22	1:B:777:VAL:HG13	1.87	0.56
1:H:853:ILE:HG23	1:H:855:LYS:H	1.69	0.56
1:J:238:TRP:CZ3	1:J:272:PRO:HA	2.41	0.56
1:B:349:PHE:HB2	1:B:353:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:720:ARG:O	1:H:720:ARG:NH2	2.38	0.56
1:K:391:THR:HG22	1:K:394:MET:HE2	1.87	0.56
1:D:415:GLN:OE1	1:D:431:ARG:NH2	2.39	0.56
1:E:523:HIS:HA	1:E:526:ARG:CZ	2.36	0.56
1:K:572:SER:O	1:K:575:SER:OG	2.20	0.56
1:A:81:LYS:NZ	1:A:142:SER:OG	2.39	0.56
1:G:314:LEU:HD13	1:G:324:PHE:HB3	1.88	0.56
1:H:523:HIS:CE1	1:H:527:PHE:CE2	2.93	0.56
1:E:741:VAL:HG22	1:E:771:TRP:HB2	1.87	0.56
1:F:415:GLN:OE1	1:F:431:ARG:NH2	2.38	0.56
1:A:658:HIS:CE1	1:H:308:ARG:HB3	2.40	0.55
1:B:122:GLU:HB3	1:B:125:LYS:HB3	1.87	0.55
1:D:707:ARG:H	1:D:766:MET:HE2	1.70	0.55
1:F:694:PHE:HA	1:F:697:LEU:HD23	1.87	0.55
1:H:238:TRP:HE3	1:H:271:LEU:HD23	1.72	0.55
1:H:295:THR:HG22	1:H:592:MET:HE1	1.88	0.55
1:J:489:GLY:HA2	1:J:492:MET:HE2	1.87	0.55
1:J:523:HIS:ND1	1:J:526:ARG:NH1	2.46	0.55
1:A:196:ASN:OD1	1:A:200:ARG:N	2.39	0.55
1:K:470:ARG:NH2	1:K:546:ASP:OD1	2.34	0.55
1:A:356:ASP:N	1:A:569:LEU:O	2.39	0.55
1:B:164:LEU:HD12	1:B:205:PHE:HZ	1.71	0.55
1:B:700:THR:OG1	1:B:702:GLN:OE1	2.22	0.55
1:E:646:GLU:HA	1:E:649:LYS:HE2	1.87	0.55
1:F:611:LYS:HZ1	1:F:669:TRP:C	2.14	0.55
1:G:196:ASN:OD1	1:G:200:ARG:N	2.39	0.55
1:I:417:ASN:HB2	1:I:428:GLN:HG2	1.87	0.55
1:K:856:ARG:NH1	1:K:858:VAL:O	2.39	0.55
1:F:425:LEU:O	1:F:440:ARG:NH2	2.38	0.55
1:G:790:PRO:HG3	1:G:826:LEU:HD21	1.88	0.55
1:H:82:ILE:HG22	1:H:144:ILE:HB	1.88	0.55
1:A:410:TYR:HD2	1:D:505:VAL:HG21	1.71	0.55
1:D:417:ASN:HB3	1:D:428:GLN:HG2	1.87	0.55
1:K:84:LYS:HE3	1:K:149:PRO:CD	2.37	0.55
1:K:440:ARG:O	1:K:447:THR:OG1	2.24	0.55
1:F:257:ASP:OD2	1:F:882:ARG:NH1	2.39	0.55
1:G:715:LEU:HB2	1:G:836:PRO:HA	1.87	0.55
1:I:373:ALA:HA	1:I:376:VAL:HG12	1.88	0.55
1:F:283:ARG:NH2	1:F:660:PHE:O	2.37	0.55
1:E:750:ARG:HE	1:J:254:VAL:HG11	1.71	0.55
1:G:263:THR:HG23	1:G:882:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:GLU:HA	1:B:649:LYS:HE3	1.88	0.55
1:I:148:ILE:HB	1:I:163:VAL:HG21	1.89	0.55
1:D:707:ARG:H	1:D:766:MET:CE	2.20	0.55
1:G:545:PRO:O	1:G:549:PHE:N	2.40	0.55
1:I:44:ARG:HH21	1:I:59:PHE:HB2	1.71	0.55
1:I:781:VAL:HG13	1:I:823:ILE:HD13	1.89	0.55
1:E:447:THR:HG22	1:E:452:TRP:NE1	2.21	0.54
1:A:200:ARG:HH12	1:A:228:GLN:HB3	1.72	0.54
1:B:403:ASN:O	1:B:407:LEU:HB2	2.06	0.54
1:F:242:LEU:O	1:F:246:LYS:HB2	2.07	0.54
1:G:382:THR:HB	1:G:450:ASN:HB2	1.88	0.54
1:G:743:GLN:NE2	1:G:773:ARG:O	2.40	0.54
1:H:92:HIS:NE2	1:H:170:ASN:OD1	2.38	0.54
1:B:175:LEU:HD22	1:B:179:HIS:HB3	1.90	0.54
1:H:149:PRO:HG2	1:H:160:GLU:HG3	1.88	0.54
1:H:217:TYR:OH	1:H:875:VAL:O	2.25	0.54
1:J:97:SER:HB3	1:J:860:ARG:HH12	1.72	0.54
1:K:707:ARG:HG2	1:K:766:MET:HE3	1.88	0.54
1:A:302:TYR:HA	1:A:583:SER:O	2.07	0.54
1:B:238:TRP:HE3	1:B:271:LEU:HD23	1.71	0.54
1:E:81:LYS:NZ	1:E:142:SER:OG	2.41	0.54
1:F:633:PRO:HB2	1:F:663:ILE:HD13	1.89	0.54
1:J:176:THR:OG1	1:J:179:HIS:ND1	2.40	0.54
1:K:417:ASN:HB2	1:K:428:GLN:HG2	1.89	0.54
1:D:732:LEU:HB2	1:D:852:PHE:HB2	1.90	0.54
1:F:357:LEU:HD13	1:F:573:TRP:HE1	1.72	0.54
1:J:192:ILE:HD12	1:J:200:ARG:HH22	1.73	0.54
1:E:633:PRO:HB2	1:E:663:ILE:HD13	1.90	0.54
1:E:752:GLN:HA	1:E:755:MET:HE2	1.90	0.54
1:I:572:SER:O	1:I:575:SER:OG	2.24	0.54
1:I:598:LEU:HD21	1:I:890:LEU:HB2	1.89	0.54
1:J:529:ARG:NH2	1:J:585:GLU:OE1	2.40	0.54
1:K:371:MET:HE1	1:K:408:TYR:HD2	1.71	0.54
1:K:492:MET:HE3	1:K:524:MET:HE1	1.89	0.54
1:A:252:GLN:HE21	1:B:393:ASN:HD22	1.53	0.54
1:B:615:ARG:NH1	1:B:672:LEU:O	2.41	0.54
1:B:775:GLY:N	1:B:817:TYR:OH	2.40	0.54
1:D:378:HIS:NE2	1:D:402:LEU:HB2	2.22	0.54
1:E:371:MET:HB2	1:E:405:TYR:HD2	1.72	0.54
1:E:544:LEU:HD23	1:E:549:PHE:HD1	1.72	0.54
1:F:148:ILE:HD12	1:F:876:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:373:ALA:HA	1:J:376:VAL:HG12	1.90	0.54
1:A:526:ARG:HH12	1:A:582:ARG:N	2.06	0.54
1:D:403:ASN:HB2	1:D:425:LEU:HG	1.89	0.54
1:E:730:ASN:HB2	1:E:850:LYS:HD3	1.89	0.54
1:I:297:LEU:O	1:I:590:ASN:ND2	2.41	0.54
1:D:888:GLN:HE21	1:H:50:TYR:HE1	1.55	0.54
1:G:589:ARG:HD3	1:G:895:LYS:HD3	1.90	0.54
1:H:135:ARG:NH1	1:H:684:GLU:OE1	2.41	0.54
1:H:572:SER:O	1:H:575:SER:OG	2.21	0.54
1:K:373:ALA:HA	1:K:376:VAL:HG12	1.90	0.54
1:D:638:LYS:NZ	1:I:13:LYS:O	2.41	0.54
1:E:86:PRO:HD3	1:E:145:LEU:HD11	1.89	0.54
1:E:813:ALA:N	1:J:253:GLU:OE2	2.41	0.54
1:F:200:ARG:HH12	1:F:228:GLN:HB3	1.73	0.54
1:A:367:PRO:HG2	1:D:309:ILE:HG12	1.90	0.53
1:B:44:ARG:HH21	1:B:59:PHE:HB2	1.73	0.53
1:J:344:TYR:OH	1:J:579:ALA:O	2.22	0.53
1:A:90:PHE:HB2	1:A:166:VAL:HG23	1.90	0.53
1:A:752:GLN:HA	1:A:755:MET:HE3	1.91	0.53
1:G:390:LEU:HD13	1:G:394:MET:HB3	1.90	0.53
1:B:124:GLU:HA	1:B:127:TYR:HD2	1.73	0.53
1:J:614:MET:SD	1:J:640:VAL:HG21	2.49	0.53
1:J:627:VAL:HG22	1:J:777:VAL:HG13	1.89	0.53
1:J:821:THR:HG21	1:J:849:THR:HG21	1.90	0.53
1:K:87:SER:OG	1:K:140:LYS:NZ	2.41	0.53
1:A:489:GLY:HA2	1:A:524:MET:SD	2.49	0.53
1:K:116:ASP:HB2	1:K:125:LYS:HE2	1.90	0.53
1:A:228:GLN:NE2	1:A:265:TRP:O	2.41	0.53
1:D:390:LEU:HD13	1:D:394:MET:HB2	1.90	0.53
1:F:741:VAL:HG22	1:F:771:TRP:HB2	1.90	0.53
1:G:501:LEU:HD13	1:G:517:ARG:HH12	1.73	0.53
1:G:646:GLU:HA	1:G:649:LYS:HE2	1.91	0.53
1:K:549:PHE:HA	1:K:552:LEU:HD23	1.90	0.53
1:F:327:LEU:HD11	1:F:369:VAL:HG22	1.89	0.53
1:F:664:ARG:NH1	1:K:487:THR:O	2.42	0.53
1:I:93:ILE:HB	1:I:102:LEU:HB2	1.90	0.53
1:I:209:CYS:HB2	1:I:874:PHE:HZ	1.73	0.53
1:I:775:GLY:N	1:I:817:TYR:OH	2.41	0.53
1:J:617:LEU:HD13	1:J:636:PHE:HB2	1.90	0.53
1:A:705:MET:HB2	1:A:799:PRO:HG2	1.91	0.53
1:E:486:THR:HG23	1:E:487:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:748:ILE:HD12	1:F:751:LEU:HD11	1.91	0.53
1:K:200:ARG:NE	1:K:202:VAL:O	2.41	0.53
1:A:790:PRO:HG3	1:A:826:LEU:HD21	1.91	0.53
1:D:86:PRO:HD3	1:D:145:LEU:HD11	1.91	0.53
1:D:703:VAL:HG12	1:D:851:VAL:HG22	1.90	0.53
1:F:750:ARG:NH1	1:K:252:GLN:OE1	2.42	0.53
1:I:65:GLN:NE2	1:I:69:ASP:OD1	2.40	0.53
1:B:151:ARG:HB3	1:B:158:VAL:HG23	1.91	0.53
1:B:373:ALA:HA	1:B:376:VAL:HG12	1.90	0.53
1:D:196:ASN:OD1	1:D:200:ARG:N	2.42	0.53
1:H:379:LEU:HD21	1:H:500:MET:HG2	1.91	0.53
1:K:598:LEU:O	1:K:601:SER:HB3	2.09	0.53
1:B:440:ARG:O	1:B:447:THR:OG1	2.26	0.53
1:B:453:ALA:C	1:B:454:THR:HG23	2.35	0.53
1:D:499:GLU:O	1:D:503:MET:HG2	2.08	0.53
1:F:445:THR:HG23	1:F:447:THR:HG23	1.91	0.53
1:J:393:ASN:OD1	1:J:394:MET:N	2.42	0.53
1:K:36:LEU:HD21	1:K:62:PRO:HD2	1.90	0.53
1:E:300:GLY:CA	1:E:585:GLU:O	2.47	0.52
1:A:380:LEU:HD21	1:A:580:PHE:HB2	1.89	0.52
1:B:406:LEU:HD21	1:B:503:MET:HE3	1.89	0.52
1:E:428:GLN:NE2	1:E:435:ASP:OD1	2.41	0.52
1:G:300:GLY:CA	1:G:585:GLU:O	2.51	0.52
1:A:246:LYS:NZ	1:A:537:ASP:O	2.41	0.52
1:F:151:ARG:HH22	1:F:160:GLU:HA	1.74	0.52
1:J:707:ARG:HH11	1:J:766:MET:HG3	1.73	0.52
1:E:664:ARG:NH1	1:J:487:THR:O	2.42	0.52
1:G:706:HIS:ND1	1:G:770:ASP:O	2.35	0.52
1:H:262:ASP:OD1	1:H:262:ASP:N	2.42	0.52
1:A:235:SER:HB3	1:A:271:LEU:HD23	1.92	0.52
1:E:248:ILE:HD12	1:E:895:LYS:HG3	1.91	0.52
1:F:532:GLN:O	1:F:536:GLU:HB3	2.09	0.52
1:F:732:LEU:HD11	1:F:850:LYS:HB3	1.91	0.52
1:I:193:GLU:O	1:I:200:ARG:NH1	2.42	0.52
1:I:722:ARG:HH11	1:I:831:GLU:HA	1.75	0.52
1:B:14:THR:HG22	1:G:638:LYS:HD3	1.91	0.52
1:B:209:CYS:O	1:B:872:ARG:NH2	2.41	0.52
1:F:403:ASN:HB2	1:F:425:LEU:HG	1.91	0.52
1:H:375:VAL:HG13	1:H:500:MET:HE2	1.92	0.52
1:H:762:LEU:O	1:H:766:MET:HB2	2.09	0.52
1:H:777:VAL:HG21	1:H:818:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:500:MET:O	1:I:504:LEU:HD12	2.09	0.52
1:I:700:THR:OG1	1:I:702:GLN:OE1	2.26	0.52
1:A:812:TYR:HB3	1:H:253:GLU:OE2	2.09	0.52
1:E:196:ASN:HD21	1:E:199:THR:HA	1.75	0.52
1:G:342:LYS:HB3	1:G:569:LEU:HD21	1.91	0.52
1:H:373:ALA:HA	1:H:376:VAL:HG12	1.90	0.52
1:J:470:ARG:NH2	1:J:546:ASP:OD1	2.35	0.52
1:A:729:THR:HG22	1:A:731:MET:H	1.73	0.52
1:B:259:ARG:NH2	1:G:809:GLY:O	2.43	0.52
1:E:403:ASN:HB2	1:E:425:LEU:HG	1.91	0.52
1:G:157:GLU:OE1	1:K:632:ARG:NH1	2.42	0.52
1:E:204:VAL:HG22	1:E:875:VAL:HG22	1.92	0.52
1:G:81:LYS:NZ	1:G:142:SER:OG	2.43	0.52
1:B:176:THR:OG1	1:B:179:HIS:ND1	2.43	0.52
1:E:607:LEU:O	1:E:611:LYS:HG2	2.09	0.52
1:D:497:TYR:OH	1:D:516:PHE:O	2.28	0.51
1:D:750:ARG:NH1	1:I:252:GLN:OE1	2.43	0.51
1:G:666:MET:O	1:G:670:VAL:HG23	2.10	0.51
1:I:209:CYS:O	1:I:872:ARG:NH2	2.43	0.51
1:I:339:ASP:HA	1:I:342:LYS:HE2	1.92	0.51
1:J:339:ASP:HA	1:J:342:LYS:HD2	1.91	0.51
1:J:379:LEU:HD21	1:J:500:MET:HG2	1.92	0.51
1:J:710:LEU:HD12	1:J:711:PRO:HD2	1.92	0.51
1:F:442:ASP:HB3	1:F:445:THR:HG22	1.91	0.51
1:G:68:LEU:HA	1:G:71:ILE:HD12	1.92	0.51
1:H:95:MET:HE3	1:H:97:SER:HB3	1.92	0.51
1:K:740:ARG:HB3	1:K:771:TRP:H	1.75	0.51
1:A:196:ASN:HD21	1:A:199:THR:HA	1.74	0.51
1:A:741:VAL:HG22	1:A:771:TRP:HB2	1.92	0.51
1:D:384:GLY:HA3	1:D:446:GLY:HA2	1.92	0.51
1:E:638:LYS:HD3	1:J:14:THR:HG22	1.92	0.51
1:G:323:PRO:HB3	1:G:368:ALA:HB1	1.93	0.51
1:J:13:LYS:NZ	1:J:18:LEU:O	2.39	0.51
1:G:615:ARG:HG2	1:G:670:VAL:HG13	1.93	0.51
1:K:646:GLU:HA	1:K:649:LYS:HE3	1.91	0.51
1:D:367:PRO:HA	1:D:370:ARG:HG2	1.93	0.51
1:H:824:PHE:CZ	1:H:826:LEU:HB2	2.46	0.51
1:I:197:VAL:HG12	1:I:199:THR:H	1.75	0.51
1:I:375:VAL:HG13	1:I:500:MET:HE2	1.92	0.51
1:K:92:HIS:NE2	1:K:170:ASN:OD1	2.32	0.51
1:K:421:THR:OG1	1:K:426:ASP:OD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LYS:NZ	1:D:142:SER:O	2.37	0.51
1:E:63:ASP:OD1	1:E:64:VAL:N	2.43	0.51
1:E:342:LYS:HB3	1:E:569:LEU:HD21	1.92	0.51
1:H:447:THR:HA	1:H:452:TRP:CG	2.45	0.51
1:J:262:ASP:N	1:J:262:ASP:OD1	2.44	0.51
1:D:367:PRO:HG2	1:E:309:ILE:HG12	1.93	0.51
1:F:342:LYS:HB3	1:F:569:LEU:HD21	1.90	0.51
1:F:497:TYR:CE2	1:F:520:LEU:HD12	2.45	0.51
1:G:110:GLU:O	1:G:113:GLN:NE2	2.33	0.51
1:A:611:LYS:HZ1	1:A:669:TRP:CG	2.29	0.51
1:A:632:ARG:HG3	1:A:633:PRO:HD2	1.93	0.51
1:E:238:TRP:HD1	1:E:241:ARG:HH12	1.57	0.51
1:G:148:ILE:HD12	1:G:876:ALA:HB2	1.92	0.51
1:H:355:LEU:HD21	1:H:571:VAL:HG22	1.93	0.51
1:I:394:MET:HA	1:I:397:GLN:HG2	1.92	0.51
1:K:58:ASP:OD1	1:K:59:PHE:N	2.43	0.51
1:A:209:CYS:HB2	1:A:874:PHE:HZ	1.76	0.51
1:D:154:ARG:HH12	1:H:629:ILE:HG12	1.76	0.51
1:D:357:LEU:HG	1:D:394:MET:SD	2.51	0.51
1:D:783:VAL:C	1:D:784:LYS:HZ2	2.19	0.51
1:E:607:LEU:HA	1:E:610:MET:HE2	1.92	0.51
1:H:549:PHE:HA	1:H:552:LEU:HD23	1.92	0.51
1:I:186:ALA:HB1	1:I:867:LEU:HD12	1.92	0.51
1:J:616:HIS:O	1:J:619:LEU:HB2	2.11	0.51
1:K:83:VAL:HG12	1:K:85:VAL:H	1.74	0.51
1:A:378:HIS:CE1	1:A:402:LEU:HB2	2.46	0.51
1:A:470:ARG:HH22	1:A:549:PHE:HB3	1.75	0.51
1:D:85:VAL:HG13	1:D:163:VAL:HA	1.92	0.51
1:F:447:THR:HG22	1:F:452:TRP:NE1	2.24	0.51
1:H:782:ARG:O	1:H:823:ILE:N	2.36	0.51
1:I:774:PHE:O	1:I:779:ARG:NH1	2.44	0.51
1:B:572:SER:O	1:B:575:SER:OG	2.23	0.50
1:E:470:ARG:NH1	1:E:546:ASP:OD1	2.34	0.50
1:E:732:LEU:HD11	1:E:850:LYS:HB3	1.93	0.50
1:H:494:TYR:CZ	1:H:497:TYR:HB2	2.46	0.50
1:I:497:TYR:OH	1:I:516:PHE:O	2.28	0.50
1:J:246:LYS:NZ	1:J:537:ASP:O	2.43	0.50
1:J:572:SER:O	1:J:575:SER:OG	2.22	0.50
1:K:164:LEU:HG	1:K:166:VAL:HG22	1.91	0.50
1:F:669:TRP:HA	1:F:672:LEU:HD12	1.93	0.50
1:G:94:VAL:HB	1:G:171:VAL:HG12	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:ASN:HD21	1:G:199:THR:HA	1.74	0.50
1:H:523:HIS:CE1	1:H:527:PHE:CD2	2.99	0.50
1:J:732:LEU:N	1:J:851:VAL:O	2.38	0.50
1:B:497:TYR:OH	1:B:516:PHE:O	2.29	0.50
1:E:348:MET:HA	1:E:534:ILE:HD11	1.93	0.50
1:F:616:HIS:CD2	1:F:688:TRP:HB3	2.47	0.50
1:G:151:ARG:HG3	1:G:158:VAL:HG13	1.92	0.50
1:J:221:GLN:HA	1:J:224:ILE:HD12	1.93	0.50
1:A:425:LEU:O	1:A:440:ARG:NH2	2.45	0.50
1:I:447:THR:HA	1:I:452:TRP:CG	2.47	0.50
1:B:200:ARG:NE	1:B:202:VAL:O	2.44	0.50
1:B:453:ALA:O	1:B:454:THR:HG23	2.11	0.50
1:D:81:LYS:NZ	1:D:142:SER:OG	2.44	0.50
1:E:705:MET:HB2	1:E:799:PRO:HG2	1.94	0.50
1:F:81:LYS:NZ	1:F:142:SER:OG	2.45	0.50
1:G:403:ASN:HB2	1:G:425:LEU:HG	1.92	0.50
1:G:607:LEU:HD13	1:G:610:MET:HE2	1.93	0.50
1:I:31:LEU:HD12	1:I:345:LEU:HD11	1.93	0.50
1:I:368:ALA:HA	1:I:371:MET:HB2	1.93	0.50
1:J:200:ARG:NE	1:J:202:VAL:O	2.44	0.50
1:J:701:ASP:OD1	1:J:701:ASP:N	2.44	0.50
1:A:614:MET:HE3	1:A:640:VAL:HG21	1.93	0.50
1:D:705:MET:HB2	1:D:799:PRO:HG2	1.93	0.50
1:E:526:ARG:O	1:E:530:ILE:HG12	2.12	0.50
1:E:656:HIS:CE1	1:E:661:ILE:HG12	2.47	0.50
1:E:694:PHE:HA	1:E:697:LEU:HD23	1.94	0.50
1:E:706:HIS:ND1	1:E:770:ASP:O	2.42	0.50
1:G:220:LEU:O	1:G:224:ILE:HG12	2.11	0.50
1:I:777:VAL:O	1:I:779:ARG:NH2	2.44	0.50
1:J:176:THR:O	1:J:180:ARG:HG3	2.11	0.50
1:K:192:ILE:HD12	1:K:200:ARG:HH22	1.75	0.50
1:E:111:MET:HE2	1:E:697:LEU:HA	1.94	0.50
1:F:192:ILE:HD11	1:F:203:ASP:HB3	1.94	0.50
1:F:705:MET:HB2	1:F:799:PRO:HG2	1.93	0.50
1:G:228:GLN:NE2	1:G:265:TRP:O	2.44	0.50
1:H:200:ARG:NE	1:H:202:VAL:O	2.45	0.50
1:H:470:ARG:NH2	1:H:546:ASP:OD1	2.35	0.50
1:I:197:VAL:HB	1:I:200:ARG:HG2	1.94	0.50
1:J:177:ALA:HA	1:J:180:ARG:NE	2.27	0.50
1:A:85:VAL:HG13	1:A:163:VAL:HA	1.93	0.50
1:D:393:ASN:CG	1:D:397:GLN:HE22	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:790:PRO:HG3	1:D:826:LEU:HD21	1.94	0.50
1:F:393:ASN:CG	1:F:397:GLN:HE22	2.20	0.50
1:H:497:TYR:OH	1:H:516:PHE:O	2.30	0.50
1:I:300:GLY:HA2	1:I:586:PRO:HA	1.94	0.50
1:K:358:LYS:HB2	1:K:570:ASP:OD2	2.12	0.50
1:A:311:SER:O	1:A:315:THR:OG1	2.29	0.50
1:A:695:GLU:OE2	1:A:853:ILE:HG13	2.12	0.50
1:E:154:ARG:HH12	1:I:629:ILE:HG12	1.77	0.50
1:F:790:PRO:HG3	1:F:826:LEU:HD21	1.94	0.50
1:H:722:ARG:HH11	1:H:831:GLU:HA	1.76	0.50
1:K:453:ALA:C	1:K:454:THR:HG23	2.37	0.50
1:F:547:ASP:OD1	1:F:547:ASP:N	2.44	0.49
1:I:129:THR:O	1:I:133:LYS:HG2	2.11	0.49
1:I:295:THR:HA	1:I:592:MET:HE1	1.93	0.49
1:I:885:ASP:N	1:I:885:ASP:OD1	2.45	0.49
1:K:700:THR:OG1	1:K:702:GLN:OE1	2.30	0.49
1:B:453:ALA:O	1:B:454:THR:CG2	2.60	0.49
1:H:437:ASN:HA	1:H:440:ARG:HH11	1.77	0.49
1:I:164:LEU:HD21	1:I:870:LEU:HD21	1.94	0.49
1:J:453:ALA:C	1:J:454:THR:HG23	2.36	0.49
1:A:727:TYR:HE1	1:A:860:ARG:HE	1.59	0.49
1:D:732:LEU:HD11	1:D:850:LYS:HB3	1.94	0.49
1:F:352:GLN:HA	1:F:566:PRO:HB3	1.95	0.49
1:H:789:ARG:NH2	1:H:790:PRO:O	2.45	0.49
1:K:79:VAL:HG11	1:K:680:LYS:HD3	1.94	0.49
1:A:613:ASP:O	1:A:617:LEU:HB2	2.12	0.49
1:B:500:MET:HE3	1:B:504:LEU:HD21	1.94	0.49
1:F:544:LEU:HD11	1:F:549:PHE:HD1	1.77	0.49
1:G:732:LEU:HD11	1:G:850:LYS:HB3	1.93	0.49
1:I:343:ILE:HG13	1:I:571:VAL:HG11	1.94	0.49
1:J:104:VAL:HG22	1:J:858:VAL:HG22	1.94	0.49
1:A:813:ALA:N	1:H:253:GLU:OE2	2.45	0.49
1:F:666:MET:O	1:F:670:VAL:HG23	2.13	0.49
1:G:417:ASN:HB3	1:G:428:GLN:HB3	1.94	0.49
1:H:95:MET:SD	1:H:860:ARG:NH2	2.85	0.49
1:H:297:LEU:O	1:H:590:ASN:ND2	2.42	0.49
1:J:421:THR:OG1	1:J:426:ASP:OD2	2.31	0.49
1:F:248:ILE:HD11	1:F:589:ARG:HH22	1.76	0.49
1:F:489:GLY:HA2	1:F:524:MET:SD	2.52	0.49
1:G:547:ASP:OD1	1:G:547:ASP:N	2.46	0.49
1:K:194:ASN:OD1	1:K:200:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:262:ASP:OD1	1:K:262:ASP:N	2.45	0.49
1:I:92:HIS:NE2	1:I:170:ASN:OD1	2.42	0.49
1:I:597:PRO:O	1:I:600:GLU:HG2	2.13	0.49
1:K:238:TRP:HE3	1:K:271:LEU:HD23	1.78	0.49
1:K:343:ILE:HG13	1:K:571:VAL:HG11	1.93	0.49
1:K:732:LEU:HD21	1:K:771:TRP:CH2	2.48	0.49
1:B:8:ARG:HH22	1:B:247:ARG:HG2	1.77	0.49
1:D:730:ASN:HB2	1:D:850:LYS:HD3	1.94	0.49
1:F:86:PRO:HD3	1:F:145:LEU:HD11	1.94	0.49
1:K:853:ILE:HG12	1:K:857:ILE:HD11	1.93	0.49
1:A:607:LEU:HD13	1:A:610:MET:HE3	1.94	0.49
1:E:206:ILE:HG22	1:E:870:LEU:HD12	1.95	0.49
1:H:393:ASN:OD1	1:H:394:MET:N	2.45	0.49
1:I:219:ARG:HH22	1:I:682:ALA:C	2.21	0.49
1:J:158:VAL:HG12	1:J:191:ILE:HG22	1.94	0.49
1:D:807:ARG:HH12	1:I:888:GLN:HE22	1.60	0.49
1:E:501:LEU:HD13	1:E:517:ARG:HH12	1.78	0.49
1:E:730:ASN:ND2	1:E:849:THR:OG1	2.45	0.49
1:H:35:ALA:O	1:H:38:GLU:HG2	2.13	0.49
1:H:417:ASN:HB2	1:H:428:GLN:HG2	1.95	0.49
1:H:853:ILE:HG12	1:H:857:ILE:HD11	1.94	0.49
1:K:40:MET:SD	1:K:59:PHE:HB3	2.53	0.49
1:B:470:ARG:NH2	1:B:546:ASP:OD1	2.36	0.48
1:D:515:TYR:O	1:D:518:SER:OG	2.26	0.48
1:D:523:HIS:NE2	1:D:527:PHE:HE2	2.11	0.48
1:F:532:GLN:O	1:F:536:GLU:CB	2.61	0.48
1:H:84:LYS:HE2	1:H:147:ASP:O	2.13	0.48
1:H:214:TYR:OH	1:H:873:ARG:N	2.44	0.48
1:H:737:GLU:HG3	1:H:740:ARG:HH11	1.77	0.48
1:I:158:VAL:HG12	1:I:191:ILE:HG22	1.95	0.48
1:J:494:TYR:HH	1:J:523:HIS:HD2	1.60	0.48
1:K:853:ILE:HG23	1:K:855:LYS:H	1.77	0.48
1:B:262:ASP:N	1:B:262:ASP:OD1	2.44	0.48
1:D:395:ALA:HB1	1:D:441:ALA:HB3	1.95	0.48
1:H:84:LYS:HZ1	1:H:149:PRO:HD3	1.78	0.48
1:H:646:GLU:HA	1:H:649:LYS:HE3	1.95	0.48
1:J:293:ILE:HD13	1:J:349:PHE:HE2	1.77	0.48
1:J:375:VAL:HG13	1:J:500:MET:HE2	1.93	0.48
1:K:494:TYR:CZ	1:K:497:TYR:HB2	2.47	0.48
1:B:131:ILE:HD12	1:B:135:ARG:HH22	1.79	0.48
1:B:762:LEU:O	1:B:766:MET:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:PHE:O	1:K:316:GLN:N	2.46	0.48
1:F:410:TYR:HE1	1:F:416:VAL:HB	1.77	0.48
1:H:633:PRO:HA	1:H:636:PHE:CE2	2.49	0.48
1:I:460:ARG:HA	1:I:460:ARG:NH2	2.28	0.48
1:J:124:GLU:HA	1:J:127:TYR:HD2	1.78	0.48
1:J:186:ALA:HB1	1:J:867:LEU:HD12	1.94	0.48
1:K:554:PRO:HA	1:K:557:ILE:HG22	1.96	0.48
1:B:494:TYR:CE1	1:B:497:TYR:HB2	2.48	0.48
1:D:100:ARG:HA	1:D:861:VAL:O	2.13	0.48
1:F:370:ARG:HH12	1:G:490:ILE:HG13	1.77	0.48
1:G:200:ARG:HH12	1:G:228:GLN:HB3	1.78	0.48
1:G:880:LYS:HG3	1:K:55:ARG:HH21	1.78	0.48
1:K:355:LEU:HD21	1:K:571:VAL:HG22	1.93	0.48
1:B:79:VAL:HG11	1:B:680:LYS:HD3	1.94	0.48
1:D:486:THR:HG23	1:D:487:THR:HG23	1.96	0.48
1:F:367:PRO:O	1:F:371:MET:HE3	2.14	0.48
1:G:425:LEU:O	1:G:440:ARG:NH2	2.47	0.48
1:G:442:ASP:HB3	1:G:445:THR:HG22	1.95	0.48
1:G:526:ARG:NH1	1:G:580:PHE:O	2.46	0.48
1:H:21:ASP:N	1:H:21:ASP:OD1	2.46	0.48
1:A:81:LYS:NZ	1:A:142:SER:O	2.39	0.48
1:D:283:ARG:HH21	1:D:661:ILE:HG22	1.79	0.48
1:D:425:LEU:O	1:D:440:ARG:NH2	2.46	0.48
1:E:614:MET:HE3	1:E:640:VAL:HG21	1.96	0.48
1:F:313:THR:O	1:F:511:SER:OG	2.29	0.48
1:I:85:VAL:HG12	1:I:163:VAL:HG23	1.95	0.48
1:I:219:ARG:HH12	1:I:682:ALA:HB1	1.78	0.48
1:J:343:ILE:HG13	1:J:571:VAL:HG11	1.94	0.48
1:K:523:HIS:CE1	1:K:527:PHE:HE2	2.28	0.48
1:A:325:ALA:O	1:A:328:THR:HG22	2.14	0.48
1:A:528:ALA:HA	1:A:531:ASN:ND2	2.28	0.48
1:D:153:HIS:ND1	1:D:154:ARG:HG2	2.29	0.48
1:I:856:ARG:NH1	1:I:859:GLU:OE1	2.41	0.48
1:K:403:ASN:O	1:K:407:LEU:HB2	2.13	0.48
1:A:154:ARG:HD2	1:B:629:ILE:HG23	1.95	0.48
1:A:732:LEU:HD11	1:A:850:LYS:HB3	1.96	0.48
1:D:782:ARG:HB3	1:D:784:LYS:NZ	2.29	0.48
1:E:393:ASN:CG	1:E:397:GLN:HE22	2.22	0.48
1:G:380:LEU:HD21	1:G:580:PHE:CG	2.49	0.48
1:G:515:TYR:O	1:G:518:SER:OG	2.26	0.48
1:J:763:ARG:NH2	1:J:767:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:745:THR:OG1	1:G:746:TYR:N	2.47	0.48
1:H:437:ASN:OD1	1:H:440:ARG:NH1	2.46	0.48
1:J:731:MET:HG2	1:J:851:VAL:HG13	1.95	0.48
1:B:677:PRO:HA	1:B:681:LEU:HD23	1.96	0.48
1:E:547:ASP:N	1:E:547:ASP:OD1	2.42	0.48
1:G:151:ARG:HH22	1:G:160:GLU:HA	1.79	0.48
1:G:378:HIS:CE1	1:G:402:LEU:HB2	2.49	0.48
1:H:856:ARG:NH1	1:H:859:GLU:OE1	2.46	0.48
1:J:36:LEU:HD11	1:J:290:ILE:HG12	1.95	0.48
1:K:281:VAL:O	1:K:284:SER:OG	2.29	0.48
1:K:370:ARG:NH1	1:K:404:ASP:OD2	2.44	0.48
1:K:786:TYR:HE2	1:K:791:PRO:HD2	1.78	0.48
1:A:342:LYS:HB3	1:A:569:LEU:HD21	1.96	0.47
1:A:497:TYR:OH	1:A:516:PHE:O	2.31	0.47
1:B:21:ASP:OD1	1:B:21:ASP:N	2.47	0.47
1:B:554:PRO:HA	1:B:557:ILE:HG22	1.96	0.47
1:D:59:PHE:O	1:I:316:GLN:N	2.46	0.47
1:D:732:LEU:HD21	1:D:850:LYS:HB3	1.96	0.47
1:E:425:LEU:O	1:E:440:ARG:NH2	2.47	0.47
1:F:632:ARG:NH2	1:K:483:ILE:O	2.46	0.47
1:G:133:LYS:HE2	1:G:697:LEU:HA	1.96	0.47
1:H:158:VAL:HG12	1:H:191:ILE:HG22	1.96	0.47
1:I:16:PRO:O	1:I:306:ASN:ND2	2.47	0.47
1:I:554:PRO:HA	1:I:557:ILE:HG22	1.96	0.47
1:K:35:ALA:O	1:K:38:GLU:HG2	2.13	0.47
1:B:355:LEU:HD21	1:B:571:VAL:HG22	1.95	0.47
1:B:628:LEU:HB3	1:B:631:ALA:HB2	1.96	0.47
1:D:342:LYS:HB3	1:D:569:LEU:HD21	1.96	0.47
1:D:785:PHE:HD1	1:D:825:TYR:HB2	1.79	0.47
1:H:130:ILE:HD11	1:H:699:LEU:HD21	1.96	0.47
1:I:35:ALA:O	1:I:38:GLU:HG2	2.13	0.47
1:K:722:ARG:HH11	1:K:831:GLU:HA	1.78	0.47
1:B:467:HIS:HB2	1:B:545:PRO:HB3	1.96	0.47
1:E:428:GLN:HE22	1:E:435:ASP:HA	1.79	0.47
1:F:310:SER:HA	1:F:313:THR:HG22	1.95	0.47
1:A:148:ILE:HD12	1:A:876:ALA:HB2	1.97	0.47
1:A:151:ARG:HH12	1:A:161:PRO:HD3	1.78	0.47
1:E:81:LYS:NZ	1:E:142:SER:O	2.38	0.47
1:E:228:GLN:NE2	1:E:265:TRP:O	2.48	0.47
1:E:367:PRO:HG2	1:F:309:ILE:HG12	1.96	0.47
1:F:196:ASN:HD21	1:F:199:THR:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:729:THR:HG22	1:G:731:MET:H	1.80	0.47
1:G:857:ILE:HG12	1:G:858:VAL:HG23	1.96	0.47
1:I:87:SER:OG	1:I:140:LYS:NZ	2.47	0.47
1:J:95:MET:HG2	1:J:96:GLN:H	1.78	0.47
1:K:349:PHE:HB2	1:K:353:ILE:HD12	1.96	0.47
1:A:104:VAL:HG22	1:A:858:VAL:HG22	1.96	0.47
1:D:352:GLN:HA	1:D:566:PRO:HB3	1.96	0.47
1:E:160:GLU:O	1:E:163:VAL:HG12	2.14	0.47
1:G:100:ARG:HA	1:G:861:VAL:O	2.15	0.47
1:G:614:MET:HE3	1:G:640:VAL:HG21	1.96	0.47
1:J:82:ILE:HG22	1:J:144:ILE:HB	1.96	0.47
1:J:718:ILE:HG21	1:J:832:PHE:HA	1.96	0.47
1:A:748:ILE:HD12	1:A:751:LEU:HD11	1.96	0.47
1:B:316:GLN:N	1:G:59:PHE:O	2.47	0.47
1:B:616:HIS:O	1:B:619:LEU:HB2	2.14	0.47
1:D:298:PRO:HG2	1:D:533:ILE:HD11	1.97	0.47
1:E:378:HIS:CE1	1:E:402:LEU:HB2	2.50	0.47
1:I:677:PRO:HA	1:I:681:LEU:HD23	1.97	0.47
1:K:633:PRO:HA	1:K:636:PHE:CE2	2.50	0.47
1:A:403:ASN:HB2	1:A:425:LEU:HG	1.96	0.47
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.79	0.47
1:A:658:HIS:HE1	1:H:308:ARG:HB3	1.77	0.47
1:B:246:LYS:HE3	1:B:593:LEU:HD21	1.96	0.47
1:B:816:LYS:HE3	1:B:816:LYS:HA	1.96	0.47
1:D:84:LYS:HE3	1:D:149:PRO:HG3	1.97	0.47
1:D:134:VAL:HG21	1:D:688:TRP:CZ3	2.49	0.47
1:E:65:GLN:NE2	1:E:69:ASP:OD2	2.47	0.47
1:G:133:LYS:HE2	1:G:697:LEU:HD13	1.95	0.47
1:H:129:THR:O	1:H:133:LYS:HG2	2.14	0.47
1:H:554:PRO:HA	1:H:557:ILE:HG22	1.97	0.47
1:I:470:ARG:NH2	1:I:546:ASP:OD1	2.35	0.47
1:J:244:HIS:ND1	1:J:250:TYR:OH	2.39	0.47
1:J:417:ASN:HB2	1:J:428:GLN:HG2	1.96	0.47
1:J:447:THR:HA	1:J:452:TRP:CD1	2.50	0.47
1:J:554:PRO:HA	1:J:557:ILE:HG22	1.97	0.47
1:J:663:ILE:HA	1:J:666:MET:HG3	1.97	0.47
1:K:10:GLU:HG2	1:K:11:ARG:HD3	1.97	0.47
1:A:522:PHE:HE2	1:A:526:ARG:HH11	1.63	0.47
1:A:731:MET:SD	1:A:853:ILE:HG22	2.55	0.47
1:B:447:THR:HA	1:B:452:TRP:CD1	2.50	0.47
1:D:410:TYR:HE2	1:D:416:VAL:HB	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:LYS:HG2	1:F:149:PRO:HD3	1.97	0.47
1:F:632:ARG:HG2	1:F:633:PRO:HD2	1.97	0.47
1:H:391:THR:HG22	1:H:394:MET:HE2	1.97	0.47
1:I:718:ILE:HG21	1:I:832:PHE:HA	1.97	0.47
1:A:192:ILE:HD11	1:A:203:ASP:HB3	1.97	0.47
1:D:157:GLU:OE1	1:H:632:ARG:NH1	2.47	0.47
1:F:608:SER:HB3	1:F:681:LEU:HD12	1.97	0.47
1:K:757:GLN:HG2	1:K:760:ALA:HB3	1.97	0.47
1:B:36:LEU:HD11	1:B:290:ILE:HG12	1.97	0.47
1:H:164:LEU:HD12	1:H:205:PHE:HZ	1.80	0.47
1:J:707:ARG:HE	1:J:766:MET:HE3	1.80	0.47
1:K:21:ASP:OD1	1:K:21:ASP:N	2.47	0.47
1:B:31:LEU:HD12	1:B:345:LEU:HD11	1.97	0.46
1:B:437:ASN:OD1	1:B:440:ARG:NH1	2.48	0.46
1:D:694:PHE:HA	1:D:697:LEU:HD23	1.97	0.46
1:F:470:ARG:NE	1:F:546:ASP:OD1	2.39	0.46
1:G:447:THR:HG22	1:G:452:TRP:NE1	2.30	0.46
1:H:349:PHE:HB2	1:H:353:ILE:HD12	1.96	0.46
1:I:149:PRO:HB2	1:I:160:GLU:HG3	1.97	0.46
1:I:209:CYS:HB2	1:I:874:PHE:CZ	2.50	0.46
1:I:858:VAL:HG12	1:I:860:ARG:HH12	1.80	0.46
1:J:289:LEU:HD21	1:J:352:GLN:HG2	1.97	0.46
1:J:467:HIS:HB2	1:J:545:PRO:HB3	1.96	0.46
1:D:409:MET:HE3	1:E:510:ASP:HB3	1.96	0.46
1:F:357:LEU:HD21	1:F:394:MET:HE1	1.98	0.46
1:G:652:MET:HB2	1:G:656:HIS:NE2	2.29	0.46
1:H:529:ARG:NH1	1:H:586:PRO:HD2	2.30	0.46
1:J:447:THR:HG22	1:J:452:TRP:NE1	2.30	0.46
1:J:453:ALA:O	1:J:454:THR:HG23	2.15	0.46
1:K:158:VAL:HG12	1:K:191:ILE:HG22	1.97	0.46
1:K:297:LEU:O	1:K:590:ASN:ND2	2.45	0.46
1:K:681:LEU:O	1:K:685:GLU:HG3	2.16	0.46
1:A:344:TYR:OH	1:A:526:ARG:NH2	2.48	0.46
1:A:526:ARG:NH2	1:A:582:ARG:O	2.32	0.46
1:D:652:MET:HB2	1:D:656:HIS:NE2	2.31	0.46
1:E:59:PHE:O	1:J:316:GLN:N	2.47	0.46
1:E:105:ASP:OD2	1:E:210:SER:OG	2.34	0.46
1:E:261:GLN:NE2	1:I:562:GLN:O	2.35	0.46
1:E:866:ILE:HG22	1:E:867:LEU:HD22	1.96	0.46
1:F:371:MET:HB2	1:F:405:TYR:HD2	1.81	0.46
1:F:499:GLU:O	1:F:503:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:730:ASN:HB2	1:F:850:LYS:HD3	1.97	0.46
1:G:782:ARG:H	1:G:822:THR:HA	1.79	0.46
1:H:547:ASP:OD1	1:H:547:ASP:N	2.47	0.46
1:K:254:VAL:HG12	1:K:895:LYS:NZ	2.30	0.46
1:B:598:LEU:O	1:B:601:SER:HB3	2.15	0.46
1:E:785:PHE:HD1	1:E:825:TYR:HB2	1.80	0.46
1:F:384:GLY:HA3	1:F:446:GLY:HA2	1.97	0.46
1:F:416:VAL:HA	1:F:428:GLN:O	2.16	0.46
1:G:500:MET:O	1:G:503:MET:HG2	2.14	0.46
1:H:111:MET:HE3	1:H:111:MET:HA	1.97	0.46
1:H:368:ALA:HA	1:H:371:MET:HG3	1.97	0.46
1:I:238:TRP:HH2	1:I:273:VAL:HG12	1.81	0.46
1:B:131:ILE:HG13	1:B:135:ARG:NH1	2.29	0.46
1:B:706:HIS:HB3	1:B:771:TRP:HA	1.96	0.46
1:D:670:VAL:HG13	1:D:671:MET:CE	2.46	0.46
1:E:159:ALA:HB1	1:E:163:VAL:HG11	1.96	0.46
1:H:718:ILE:HG21	1:H:832:PHE:HA	1.97	0.46
1:I:244:HIS:ND1	1:I:250:TYR:OH	2.47	0.46
1:I:356:ASP:N	1:I:569:LEU:O	2.48	0.46
1:J:453:ALA:O	1:J:454:THR:CG2	2.63	0.46
1:K:436:CYS:HA	1:K:503:MET:HE1	1.98	0.46
1:B:218:ASN:HA	1:B:221:GLN:HE21	1.81	0.46
1:B:718:ILE:HG21	1:B:832:PHE:HA	1.96	0.46
1:D:104:VAL:HG22	1:D:858:VAL:HG22	1.97	0.46
1:F:113:GLN:HA	1:F:782:ARG:NH2	2.29	0.46
1:G:519:MET:HB3	1:G:522:PHE:HB3	1.97	0.46
1:G:632:ARG:HG2	1:G:634:SER:H	1.80	0.46
1:I:701:ASP:OD1	1:I:701:ASP:N	2.47	0.46
1:J:153:HIS:NE2	1:J:188:ASP:OD2	2.49	0.46
1:A:287:ALA:HB2	1:A:655:SER:HB2	1.98	0.46
1:A:633:PRO:HB2	1:A:663:ILE:HD13	1.98	0.46
1:B:295:THR:HA	1:B:592:MET:HE1	1.96	0.46
1:B:794:VAL:HG13	1:B:822:THR:HB	1.97	0.46
1:F:209:CYS:HB2	1:F:874:PHE:HZ	1.80	0.46
1:G:206:ILE:HG22	1:G:870:LEU:HD12	1.98	0.46
1:I:40:MET:SD	1:I:59:PHE:HB3	2.55	0.46
1:J:549:PHE:HA	1:J:552:LEU:HD23	1.98	0.46
1:B:701:ASP:OD1	1:B:701:ASP:N	2.48	0.46
1:D:287:ALA:HB2	1:D:655:SER:HB2	1.97	0.46
1:E:228:GLN:HE22	1:E:265:TRP:HB2	1.80	0.46
1:F:81:LYS:NZ	1:F:142:SER:O	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:PRO:HG2	1:H:635:HIS:CD2	2.51	0.46
1:J:403:ASN:ND2	1:J:425:LEU:H	2.13	0.46
1:K:423:GLU:HG2	1:K:424:PRO:HD2	1.97	0.46
1:A:653:ASN:OD1	1:A:657:SER:OG	2.33	0.46
1:B:384:GLY:HA3	1:B:446:GLY:HA3	1.98	0.46
1:F:196:ASN:OD1	1:F:200:ARG:N	2.49	0.46
1:H:371:MET:HE1	1:H:408:TYR:HB3	1.98	0.46
1:I:390:LEU:HD21	1:I:395:ALA:HB2	1.98	0.46
1:J:21:ASP:N	1:J:21:ASP:OD1	2.47	0.46
1:K:111:MET:HE3	1:K:111:MET:HA	1.97	0.46
1:A:746:TYR:HE2	1:A:816:LYS:HZ3	1.63	0.46
1:B:228:GLN:OE1	1:B:229:LEU:N	2.49	0.46
1:B:281:VAL:O	1:B:284:SER:OG	2.31	0.46
1:E:134:VAL:HG21	1:E:688:TRP:CZ3	2.51	0.46
1:G:283:ARG:O	1:G:655:SER:OG	2.32	0.46
1:H:523:HIS:HE1	1:H:527:PHE:CD2	2.34	0.46
1:J:497:TYR:OH	1:J:516:PHE:O	2.34	0.46
1:K:57:VAL:HG13	1:K:59:PHE:CE1	2.51	0.46
1:B:369:VAL:O	1:B:373:ALA:HB2	2.16	0.45
1:D:632:ARG:HG2	1:D:633:PRO:HD2	1.97	0.45
1:G:260:ARG:HH11	1:K:565:ASP:HB2	1.80	0.45
1:G:438:VAL:HG13	1:G:439:PHE:CD1	2.50	0.45
1:K:130:ILE:HD11	1:K:699:LEU:HD21	1.98	0.45
1:K:243:GLY:O	1:K:247:ARG:N	2.45	0.45
1:K:447:THR:HG22	1:K:452:TRP:NE1	2.30	0.45
1:K:547:ASP:OD1	1:K:547:ASP:N	2.47	0.45
1:K:708:ASP:HB3	1:K:847:THR:HG23	1.98	0.45
1:B:85:VAL:HG23	1:B:163:VAL:HA	1.97	0.45
1:B:186:ALA:HB1	1:B:867:LEU:HD12	1.98	0.45
1:B:782:ARG:O	1:B:823:ILE:N	2.33	0.45
1:B:783:VAL:HG22	1:B:823:ILE:HB	1.98	0.45
1:D:64:VAL:HA	1:D:67:ILE:HG22	1.98	0.45
1:E:209:CYS:HB2	1:E:874:PHE:HZ	1.82	0.45
1:F:520:LEU:HB3	1:F:521:PRO:HD3	1.99	0.45
1:H:242:LEU:HD22	1:H:464:PRO:HB3	1.97	0.45
1:I:763:ARG:NH2	1:I:767:ASP:OD1	2.50	0.45
1:J:156:MET:HE3	1:J:156:MET:HA	1.99	0.45
1:K:186:ALA:HB1	1:K:867:LEU:HD12	1.98	0.45
1:K:789:ARG:NH2	1:K:790:PRO:O	2.48	0.45
1:A:300:GLY:CA	1:A:585:GLU:O	2.48	0.45
1:D:379:LEU:O	1:D:450:ASN:ND2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:ASP:OD1	1:F:201:ASP:N	2.49	0.45
1:G:126:PHE:O	1:G:130:ILE:HG12	2.17	0.45
1:H:370:ARG:HH22	1:H:400:ILE:HG22	1.80	0.45
1:H:611:LYS:O	1:H:614:MET:HB2	2.17	0.45
1:I:289:LEU:HD21	1:I:352:GLN:HG2	1.98	0.45
1:I:549:PHE:HA	1:I:552:LEU:HD23	1.98	0.45
1:K:453:ALA:O	1:K:454:THR:HG23	2.17	0.45
1:B:104:VAL:HG22	1:B:858:VAL:HG22	1.99	0.45
1:E:408:TYR:HA	1:F:517:ARG:HD2	1.99	0.45
1:E:497:TYR:OH	1:E:516:PHE:O	2.33	0.45
1:F:378:HIS:CE1	1:F:402:LEU:HB2	2.47	0.45
1:I:348:MET:SD	1:I:538:LEU:HD11	2.56	0.45
1:A:669:TRP:HA	1:A:672:LEU:HD12	1.99	0.45
1:D:589:ARG:HB2	1:D:895:LYS:HD2	1.99	0.45
1:D:866:ILE:HG22	1:D:867:LEU:HD22	1.98	0.45
1:E:489:GLY:HA2	1:E:524:MET:SD	2.56	0.45
1:H:71:ILE:HG21	1:H:599:ILE:HG23	1.99	0.45
1:I:195:GLY:HA2	1:I:200:ARG:HD2	1.99	0.45
1:I:824:PHE:CE2	1:I:826:LEU:HB2	2.52	0.45
1:J:360:ASP:N	1:J:360:ASP:OD1	2.48	0.45
1:J:474:TYR:H	1:J:531:ASN:HD21	1.63	0.45
1:J:637:TRP:HZ2	1:J:658:HIS:HE1	1.64	0.45
1:A:587:THR:HG23	1:A:588:HIS:ND1	2.32	0.45
1:E:473:ARG:HD2	1:E:478:ASP:HA	1.99	0.45
1:G:254:VAL:HG11	1:K:50:TYR:HE2	1.81	0.45
1:G:703:VAL:HG12	1:G:851:VAL:HG22	1.98	0.45
1:H:200:ARG:NH1	1:H:203:ASP:HA	2.32	0.45
1:I:21:ASP:OD1	1:I:21:ASP:N	2.47	0.45
1:I:371:MET:HE1	1:I:408:TYR:HB3	1.98	0.45
1:I:702:GLN:HA	1:I:773:ARG:HH22	1.82	0.45
1:J:368:ALA:HA	1:J:371:MET:HB2	1.99	0.45
1:J:677:PRO:HA	1:J:681:LEU:HD23	1.99	0.45
1:A:134:VAL:HG21	1:A:688:TRP:CH2	2.51	0.45
1:D:339:ASP:HB3	1:D:575:SER:HB2	1.99	0.45
1:D:750:ARG:HE	1:I:254:VAL:HG11	1.81	0.45
1:E:244:HIS:NE2	1:I:424:PRO:HG3	2.31	0.45
1:E:333:THR:N	1:E:336:GLN:OE1	2.48	0.45
1:H:194:ASN:OD1	1:H:200:ARG:NE	2.50	0.45
1:H:447:THR:HG22	1:H:452:TRP:NE1	2.32	0.45
1:K:701:ASP:N	1:K:701:ASP:OD1	2.49	0.45
1:D:196:ASN:HD21	1:D:199:THR:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:VAL:HG22	1:D:873:ARG:HH22	1.81	0.45
1:D:300:GLY:CA	1:D:585:GLU:O	2.51	0.45
1:E:748:ILE:HD12	1:E:751:LEU:HD11	1.99	0.45
1:H:783:VAL:HG22	1:H:823:ILE:HB	1.99	0.45
1:I:523:HIS:CE1	1:I:527:PHE:HE2	2.28	0.45
1:A:611:LYS:HA	1:A:611:LYS:HD3	1.56	0.45
1:B:83:VAL:HG12	1:B:85:VAL:H	1.82	0.45
1:D:196:ASN:OD1	1:D:197:VAL:N	2.50	0.45
1:E:492:MET:HE3	1:E:524:MET:HE2	1.98	0.45
1:F:339:ASP:HB3	1:F:575:SER:HB2	1.98	0.45
1:H:122:GLU:HB3	1:H:125:LYS:HB3	1.98	0.45
1:I:646:GLU:HA	1:I:649:LYS:HE3	1.98	0.45
1:J:123:PRO:HG2	1:J:635:HIS:CD2	2.51	0.45
1:J:793:ASP:OD1	1:J:793:ASP:N	2.50	0.45
1:J:794:VAL:HG13	1:J:822:THR:HB	1.98	0.45
1:K:388:THR:HB	1:K:553:LEU:HD13	1.98	0.45
1:K:453:ALA:O	1:K:454:THR:CG2	2.64	0.45
1:B:129:THR:O	1:B:133:LYS:HG2	2.16	0.44
1:E:118:ILE:HD13	1:E:125:LYS:HZ1	1.82	0.44
1:F:153:HIS:O	1:F:154:ARG:HG2	2.18	0.44
1:F:370:ARG:HH22	1:G:490:ILE:HD12	1.82	0.44
1:G:140:LYS:HA	1:G:140:LYS:HD3	1.73	0.44
1:G:541:VAL:HG21	1:G:600:GLU:CD	2.41	0.44
1:H:289:LEU:HD21	1:H:544:LEU:HD11	1.99	0.44
1:H:371:MET:HE2	1:H:405:TYR:HA	1.99	0.44
1:I:164:LEU:HD11	1:I:870:LEU:HD11	1.99	0.44
1:I:438:VAL:HG13	1:I:439:PHE:HD1	1.81	0.44
1:K:123:PRO:HG2	1:K:635:HIS:CD2	2.52	0.44
1:K:300:GLY:HA2	1:K:586:PRO:HA	1.99	0.44
1:K:732:LEU:HD21	1:K:771:TRP:HH2	1.80	0.44
1:A:235:SER:CB	1:A:271:LEU:HB2	2.47	0.44
1:A:679:LEU:HD12	1:A:680:LYS:H	1.83	0.44
1:A:785:PHE:HD1	1:A:825:TYR:HB2	1.83	0.44
1:D:392:GLN:O	1:D:396:ARG:HG2	2.18	0.44
1:G:352:GLN:HA	1:G:566:PRO:HB3	1.99	0.44
1:H:103:ARG:O	1:H:858:VAL:HA	2.18	0.44
1:H:124:GLU:HA	1:H:127:TYR:HD2	1.81	0.44
1:I:467:HIS:HB2	1:I:545:PRO:HB3	2.00	0.44
1:K:289:LEU:HD21	1:K:352:GLN:HG3	1.98	0.44
1:K:447:THR:HA	1:K:452:TRP:CD1	2.52	0.44
1:B:545:PRO:HB2	1:B:547:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ARG:HH12	1:I:487:THR:N	2.14	0.44
1:D:754:ASN:HA	1:I:256:THR:HB	1.99	0.44
1:H:209:CYS:HB2	1:H:874:PHE:CZ	2.52	0.44
1:K:282:PRO:HB3	1:K:665:ASP:HB3	2.00	0.44
1:A:632:ARG:HE	1:A:663:ILE:HD12	1.82	0.44
1:A:633:PRO:HA	1:A:636:PHE:CE2	2.53	0.44
1:E:563:ASN:OD1	1:E:564:ALA:N	2.51	0.44
1:F:200:ARG:HH22	1:F:228:GLN:HB3	1.83	0.44
1:G:415:GLN:HE22	1:G:431:ARG:HH12	1.65	0.44
1:H:84:LYS:HZ1	1:H:149:PRO:CD	2.29	0.44
1:H:360:ASP:N	1:H:360:ASP:OD1	2.50	0.44
1:J:79:VAL:HG11	1:J:680:LYS:HD3	2.00	0.44
1:K:611:LYS:HZ1	1:K:673:PRO:HA	1.82	0.44
1:B:370:ARG:HH22	1:B:400:ILE:HG22	1.83	0.44
1:D:587:THR:HG23	1:D:588:HIS:ND1	2.33	0.44
1:D:798:LEU:HD23	1:D:798:LEU:H	1.83	0.44
1:E:257:ASP:HA	1:I:42:LYS:NZ	2.32	0.44
1:F:111:MET:HE2	1:F:697:LEU:HA	1.99	0.44
1:F:632:ARG:HH22	1:K:483:ILE:C	2.25	0.44
1:H:209:CYS:HB2	1:H:874:PHE:HZ	1.81	0.44
1:K:718:ILE:HG23	1:K:830:VAL:HG13	1.98	0.44
1:D:375:VAL:HA	1:D:378:HIS:CD2	2.52	0.44
1:F:443:PHE:HB3	1:F:553:LEU:HD11	2.00	0.44
1:G:96:GLN:HE22	1:G:830:VAL:H	1.65	0.44
1:G:256:THR:HB	1:K:568:VAL:HG11	2.00	0.44
1:G:445:THR:HG23	1:G:447:THR:HG23	2.00	0.44
1:G:730:ASN:HD21	1:G:823:ILE:HA	1.81	0.44
1:G:741:VAL:HG22	1:G:771:TRP:HB2	1.99	0.44
1:H:192:ILE:HD12	1:H:200:ARG:HH22	1.82	0.44
1:I:132:LYS:HD2	1:I:132:LYS:HA	1.86	0.44
1:J:154:ARG:HD3	1:J:154:ARG:HA	1.84	0.44
1:K:207:GLY:HA2	1:K:870:LEU:HB3	1.98	0.44
1:K:705:MET:HE1	1:K:799:PRO:HD3	1.99	0.44
1:B:699:LEU:HB3	1:B:778:LEU:HD13	2.00	0.44
1:E:153:HIS:CD2	1:E:158:VAL:HG11	2.52	0.44
1:E:179:HIS:CD2	1:E:863:VAL:HG21	2.52	0.44
1:F:370:ARG:HH12	1:G:490:ILE:HG21	1.83	0.44
1:F:861:VAL:HG12	1:F:862:ARG:O	2.18	0.44
1:G:209:CYS:HB2	1:G:874:PHE:HZ	1.83	0.44
1:G:526:ARG:HH12	1:G:582:ARG:C	2.26	0.44
1:H:467:HIS:CE1	1:H:543:SER:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:598:LEU:O	1:H:601:SER:HB3	2.18	0.44
1:J:194:ASN:OD1	1:J:200:ARG:NE	2.51	0.44
1:J:219:ARG:HH11	1:J:683:LEU:HD23	1.81	0.44
1:K:17:TYR:OH	1:K:521:PRO:HG2	2.18	0.44
1:A:395:ALA:HB1	1:A:441:ALA:HB3	2.00	0.44
1:B:735:PRO:HA	1:B:736:PRO:HD3	1.91	0.44
1:D:201:ASP:OD1	1:D:201:ASP:N	2.51	0.44
1:D:545:PRO:O	1:D:549:PHE:N	2.48	0.44
1:E:662:ASN:ND2	1:E:664:ARG:HH11	2.15	0.44
1:F:515:TYR:O	1:F:518:SER:OG	2.31	0.44
1:G:494:TYR:CZ	1:G:497:TYR:HB2	2.53	0.44
1:I:151:ARG:HB3	1:I:158:VAL:HG23	2.00	0.44
1:I:529:ARG:NH1	1:I:586:PRO:HD2	2.33	0.44
1:J:597:PRO:O	1:J:600:GLU:HB2	2.17	0.44
1:A:447:THR:HG22	1:A:452:TRP:NE1	2.33	0.44
1:F:153:HIS:CE1	1:F:154:ARG:HD3	2.53	0.44
1:F:633:PRO:HA	1:F:636:PHE:CE2	2.53	0.44
1:G:504:LEU:HD23	1:G:504:LEU:HA	1.79	0.44
1:G:699:LEU:HB3	1:G:778:LEU:HB3	1.99	0.44
1:H:186:ALA:HB1	1:H:867:LEU:HD12	2.00	0.44
1:H:624:PHE:HB3	1:H:627:VAL:HG22	1.99	0.44
1:I:423:GLU:OE1	1:I:440:ARG:NE	2.50	0.44
1:A:59:PHE:HB2	1:A:60:THR:H	1.66	0.43
1:B:262:ASP:C	1:B:881:MET:HE1	2.43	0.43
1:B:474:TYR:H	1:B:531:ASN:HD21	1.66	0.43
1:B:786:TYR:HB2	1:B:824:PHE:CE1	2.52	0.43
1:F:798:LEU:HD23	1:F:798:LEU:HA	1.90	0.43
1:H:775:GLY:N	1:H:817:TYR:OH	2.51	0.43
1:I:219:ARG:NH1	1:I:682:ALA:HB1	2.33	0.43
1:I:295:THR:HG22	1:I:592:MET:HE1	2.00	0.43
1:K:223:TYR:CZ	1:K:679:LEU:HB2	2.53	0.43
1:K:313:THR:HA	1:K:319:THR:HG23	1.99	0.43
1:B:447:THR:HA	1:B:452:TRP:CG	2.53	0.43
1:F:300:GLY:CA	1:F:585:GLU:O	2.45	0.43
1:F:572:SER:O	1:F:575:SER:OG	2.31	0.43
1:G:286:ILE:O	1:G:290:ILE:HG12	2.18	0.43
1:H:614:MET:HE2	1:H:617:LEU:HD12	2.01	0.43
1:I:652:MET:HE3	1:I:658:HIS:CD2	2.53	0.43
1:J:782:ARG:O	1:J:823:ILE:N	2.35	0.43
1:K:370:ARG:HH22	1:K:400:ILE:HG22	1.83	0.43
1:A:861:VAL:HG12	1:A:862:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ASP:OD1	1:B:440:ARG:NH1	2.42	0.43
1:G:587:THR:HG23	1:G:588:HIS:ND1	2.33	0.43
1:I:370:ARG:HA	1:I:373:ALA:HB3	2.00	0.43
1:I:370:ARG:HH22	1:I:400:ILE:HG22	1.82	0.43
1:J:300:GLY:HA2	1:J:586:PRO:HA	2.00	0.43
1:K:541:VAL:HG11	1:K:600:GLU:HG3	2.00	0.43
1:K:763:ARG:NH2	1:K:767:ASP:OD1	2.51	0.43
1:A:382:THR:HB	1:A:450:ASN:HB2	1.99	0.43
1:A:889:SER:HB2	1:A:892:MET:HE3	2.00	0.43
1:E:627:VAL:HG23	1:E:628:LEU:HG	2.00	0.43
1:G:784:LYS:HA	1:G:784:LYS:HD3	1.75	0.43
1:I:705:MET:HE1	1:I:799:PRO:HD3	2.00	0.43
1:K:44:ARG:HH21	1:K:59:PHE:HD2	1.67	0.43
1:K:447:THR:HA	1:K:452:TRP:CG	2.53	0.43
1:B:386:ARG:NH1	1:B:456:ASP:OD1	2.50	0.43
1:B:701:ASP:O	1:B:773:ARG:NH1	2.40	0.43
1:H:782:ARG:HB2	1:H:822:THR:HA	1.99	0.43
1:I:169:LYS:HA	1:I:169:LYS:HD3	1.83	0.43
1:K:390:LEU:HD22	1:K:394:MET:HE3	1.99	0.43
1:K:522:PHE:CZ	1:K:583:SER:HB3	2.53	0.43
1:A:134:VAL:HA	1:A:137:ILE:HG22	2.01	0.43
1:A:367:PRO:HA	1:A:370:ARG:HG2	2.00	0.43
1:B:118:ILE:HG21	1:B:779:ARG:HA	2.00	0.43
1:B:229:LEU:HD11	1:B:257:ASP:HB2	2.00	0.43
1:B:485:PRO:HG2	1:G:664:ARG:NE	2.33	0.43
1:D:206:ILE:HG22	1:D:870:LEU:HD12	2.00	0.43
1:D:523:HIS:CE1	1:D:527:PHE:HE2	2.37	0.43
1:E:238:TRP:CD1	1:E:241:ARG:HH12	2.36	0.43
1:G:607:LEU:O	1:G:611:LYS:HG2	2.18	0.43
1:H:715:LEU:HB2	1:H:836:PRO:HA	1.99	0.43
1:J:437:ASN:OD1	1:J:440:ARG:NH1	2.42	0.43
1:K:786:TYR:HB2	1:K:824:PHE:HE1	1.84	0.43
1:D:224:ILE:O	1:D:228:GLN:HG2	2.19	0.43
1:D:572:SER:O	1:D:575:SER:OG	2.32	0.43
1:D:805:ASN:OD1	1:D:812:TYR:HB2	2.18	0.43
1:E:196:ASN:OD1	1:E:197:VAL:N	2.52	0.43
1:E:606:GLU:O	1:E:610:MET:HG3	2.19	0.43
1:E:633:PRO:HA	1:E:636:PHE:CE2	2.53	0.43
1:F:503:MET:N	1:F:503:MET:SD	2.91	0.43
1:H:228:GLN:OE1	1:H:229:LEU:N	2.51	0.43
1:I:474:TYR:H	1:I:531:ASN:HD21	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:715:LEU:HB2	1:I:836:PRO:HA	2.01	0.43
1:J:637:TRP:HZ2	1:J:658:HIS:CE1	2.37	0.43
1:A:260:ARG:NH1	1:B:565:ASP:HB2	2.34	0.43
1:A:641:LEU:HD23	1:A:641:LEU:HA	1.89	0.43
1:A:878:LYS:HG2	1:A:880:LYS:H	1.83	0.43
1:B:611:LYS:O	1:B:614:MET:HB2	2.19	0.43
1:D:254:VAL:HG11	1:H:50:TYR:OH	2.19	0.43
1:E:196:ASN:OD1	1:E:200:ARG:N	2.52	0.43
1:F:563:ASN:OD1	1:F:564:ALA:N	2.52	0.43
1:G:603:TYR:O	1:G:607:LEU:HD23	2.18	0.43
1:I:523:HIS:CE1	1:I:527:PHE:CD2	3.07	0.43
1:I:527:PHE:O	1:I:530:ILE:HG22	2.19	0.43
1:J:384:GLY:HA3	1:J:446:GLY:HA3	2.01	0.43
1:A:616:HIS:O	1:A:619:LEU:HG	2.18	0.43
1:B:286:ILE:HA	1:B:289:LEU:HD12	2.01	0.43
1:B:388:THR:HB	1:B:553:LEU:HD13	2.01	0.43
1:D:85:VAL:HG11	1:D:162:GLU:HG2	2.01	0.43
1:D:90:PHE:HD2	1:D:166:VAL:HG22	1.84	0.43
1:E:611:LYS:HZ2	1:E:669:TRP:CG	2.37	0.43
1:G:224:ILE:O	1:G:228:GLN:HG2	2.19	0.43
1:G:782:ARG:O	1:G:823:ILE:N	2.41	0.43
1:G:878:LYS:HB3	1:G:881:MET:HG2	2.01	0.43
1:H:447:THR:HA	1:H:452:TRP:CD1	2.54	0.43
1:I:8:ARG:HH22	1:I:247:ARG:HG2	1.82	0.43
1:B:349:PHE:HB3	1:B:352:GLN:NE2	2.33	0.43
1:B:707:ARG:NH2	1:B:767:ASP:HA	2.34	0.43
1:D:532:GLN:O	1:D:536:GLU:HG3	2.19	0.43
1:E:311:SER:O	1:E:315:THR:OG1	2.31	0.43
1:E:492:MET:HB3	1:E:524:MET:HE1	1.99	0.43
1:F:154:ARG:H	1:J:629:ILE:HG23	1.83	0.43
1:F:224:ILE:O	1:F:228:GLN:HG2	2.18	0.43
1:H:153:HIS:NE2	1:H:188:ASP:OD2	2.51	0.43
1:I:156:MET:HA	1:I:156:MET:HE3	1.99	0.43
1:I:447:THR:HG22	1:I:452:TRP:NE1	2.34	0.43
1:J:447:THR:HA	1:J:452:TRP:CG	2.54	0.43
1:A:86:PRO:HD3	1:A:145:LEU:HD11	2.01	0.42
1:A:384:GLY:HA3	1:A:446:GLY:HA2	2.01	0.42
1:A:668:ARG:NH2	1:H:488:TYR:OH	2.52	0.42
1:B:103:ARG:O	1:B:858:VAL:HA	2.18	0.42
1:B:200:ARG:NH1	1:B:203:ASP:HA	2.33	0.42
1:B:360:ASP:OD1	1:B:360:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:THR:OG1	1:B:426:ASP:OD2	2.37	0.42
1:B:447:THR:HG22	1:B:452:TRP:NE1	2.33	0.42
1:B:465:TYR:HB2	1:B:539:HIS:CE1	2.54	0.42
1:D:192:ILE:HA	1:D:204:VAL:O	2.19	0.42
1:E:112:SER:O	1:E:782:ARG:NH2	2.52	0.42
1:E:168:PHE:O	1:E:171:VAL:HG22	2.19	0.42
1:E:590:ASN:OD1	1:E:591:GLU:N	2.52	0.42
1:F:866:ILE:HG22	1:F:867:LEU:HD22	2.01	0.42
1:I:355:LEU:CD2	1:I:571:VAL:HG13	2.35	0.42
1:K:737:GLU:HG3	1:K:740:ARG:HH11	1.84	0.42
1:A:357:LEU:HD22	1:A:573:TRP:CD1	2.54	0.42
1:A:392:GLN:O	1:A:396:ARG:HG2	2.19	0.42
1:D:523:HIS:HA	1:D:526:ARG:CZ	2.49	0.42
1:G:705:MET:HB2	1:G:799:PRO:HG2	2.02	0.42
1:I:459:TYR:O	1:I:460:ARG:HD2	2.19	0.42
1:J:40:MET:HA	1:J:43:VAL:HG12	2.00	0.42
1:A:492:MET:SD	1:A:493:THR:N	2.92	0.42
1:A:867:LEU:HD23	1:A:867:LEU:H	1.85	0.42
1:A:880:LYS:HG3	1:B:55:ARG:HH21	1.84	0.42
1:D:497:TYR:CE2	1:D:520:LEU:HD12	2.54	0.42
1:E:242:LEU:HD21	1:E:246:LYS:HD3	2.01	0.42
1:E:544:LEU:HD21	1:E:552:LEU:HD11	2.01	0.42
1:F:746:TYR:HB3	1:F:750:ARG:NH2	2.34	0.42
1:G:384:GLY:HA3	1:G:446:GLY:HA2	2.01	0.42
1:J:667:MET:HA	1:J:670:VAL:HG12	2.01	0.42
1:K:124:GLU:HB3	1:K:635:HIS:HD2	1.84	0.42
1:K:600:GLU:O	1:K:603:TYR:HB3	2.19	0.42
1:A:895:LYS:HB2	1:A:895:LYS:HE2	1.90	0.42
1:B:95:MET:HE3	1:B:97:SER:HB3	2.02	0.42
1:B:614:MET:HE2	1:B:614:MET:HA	2.01	0.42
1:E:237:GLY:O	1:E:241:ARG:HG3	2.19	0.42
1:E:611:LYS:NZ	1:E:669:TRP:O	2.43	0.42
1:G:324:PHE:O	1:G:328:THR:HG23	2.19	0.42
1:I:192:ILE:HG13	1:I:200:ARG:HH12	1.84	0.42
1:I:800:PHE:HA	1:I:816:LYS:O	2.19	0.42
1:K:677:PRO:HA	1:K:681:LEU:HD23	2.01	0.42
1:B:192:ILE:HD12	1:B:200:ARG:HH22	1.85	0.42
1:D:410:TYR:CE1	1:E:505:VAL:HG11	2.55	0.42
1:D:646:GLU:HA	1:D:649:LYS:HE2	2.01	0.42
1:E:291:MET:HE2	1:E:291:MET:HB2	1.87	0.42
1:E:826:LEU:HD23	1:E:826:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:VAL:HG22	1:G:858:VAL:HG22	2.01	0.42
1:I:211:GLU:HA	1:I:872:ARG:HH12	1.83	0.42
1:I:332:PRO:HB3	1:I:336:GLN:HB3	2.01	0.42
1:J:238:TRP:HH2	1:J:273:VAL:HG12	1.84	0.42
1:J:390:LEU:HD22	1:J:394:MET:HE3	2.00	0.42
1:K:197:VAL:HB	1:K:200:ARG:HB2	2.01	0.42
1:B:354:ILE:O	1:B:569:LEU:N	2.39	0.42
1:G:196:ASN:OD1	1:G:197:VAL:N	2.52	0.42
1:I:51:MET:HE3	1:I:52:THR:N	2.35	0.42
1:I:238:TRP:CZ3	1:I:272:PRO:HA	2.54	0.42
1:J:348:MET:HE1	1:J:538:LEU:HD11	2.02	0.42
1:K:124:GLU:HA	1:K:127:TYR:HD2	1.84	0.42
1:K:710:LEU:HD12	1:K:711:PRO:HD2	2.01	0.42
1:A:706:HIS:ND1	1:A:770:ASP:O	2.41	0.42
1:B:210:SER:HB3	1:B:213:VAL:HB	2.02	0.42
1:B:370:ARG:HA	1:B:373:ALA:HB3	2.01	0.42
1:D:311:SER:O	1:D:315:THR:OG1	2.25	0.42
1:E:410:TYR:HE1	1:E:416:VAL:HB	1.85	0.42
1:F:731:MET:HE3	1:F:732:LEU:N	2.33	0.42
1:G:470:ARG:HD3	1:G:472:ILE:HD11	2.02	0.42
1:I:219:ARG:HD3	1:I:686:GLU:HG3	2.01	0.42
1:I:675:LEU:HD11	1:I:681:LEU:HD21	2.02	0.42
1:J:68:LEU:HD13	1:J:592:MET:HE2	2.01	0.42
1:J:275:PRO:HB3	1:J:541:VAL:HG23	2.02	0.42
1:J:633:PRO:HA	1:J:636:PHE:CZ	2.55	0.42
1:A:807:ARG:NH1	1:A:808:GLY:HA3	2.35	0.42
1:B:354:ILE:HB	1:B:568:VAL:HG22	2.02	0.42
1:B:737:GLU:HG3	1:B:740:ARG:HH11	1.84	0.42
1:D:228:GLN:HE22	1:D:265:TRP:HB2	1.85	0.42
1:D:612:VAL:HG11	1:D:684:GLU:CD	2.45	0.42
1:F:638:LYS:HG3	1:K:12:ILE:HD11	2.02	0.42
1:G:151:ARG:NH2	1:G:160:GLU:OE1	2.52	0.42
1:H:406:LEU:HD21	1:H:503:MET:HE3	2.02	0.42
1:H:529:ARG:HH11	1:H:586:PRO:HD2	1.83	0.42
1:H:616:HIS:HA	1:H:619:LEU:HD12	2.01	0.42
1:I:204:VAL:HA	1:I:874:PHE:O	2.20	0.42
1:A:473:ARG:HB3	1:A:477:ILE:O	2.20	0.42
1:A:603:TYR:CE1	1:A:651:VAL:HG11	2.55	0.42
1:A:608:SER:HB3	1:A:681:LEU:HD12	2.02	0.42
1:A:784:LYS:HA	1:A:784:LYS:HD3	1.86	0.42
1:D:357:LEU:HD22	1:D:573:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:TYR:CE2	1:D:540:SER:HA	2.54	0.42
1:D:614:MET:HE3	1:D:640:VAL:HG21	2.00	0.42
1:F:410:TYR:CD2	1:G:505:VAL:HG21	2.46	0.42
1:G:633:PRO:HB2	1:G:663:ILE:HD13	2.02	0.42
1:J:735:PRO:HA	1:J:736:PRO:HD3	1.89	0.42
1:K:32:SER:O	1:K:290:ILE:HD11	2.20	0.42
1:K:219:ARG:CZ	1:K:686:GLU:HG3	2.50	0.42
1:A:856:ARG:H	1:A:856:ARG:HG2	1.70	0.42
1:B:715:LEU:HB2	1:B:836:PRO:HA	2.01	0.42
1:B:757:GLN:HG2	1:B:760:ALA:HB3	2.01	0.42
1:D:573:TRP:O	1:D:576:LEU:HG	2.20	0.42
1:F:392:GLN:O	1:F:396:ARG:HG2	2.20	0.42
1:J:180:ARG:HE	1:J:180:ARG:HB2	1.66	0.42
1:J:207:GLY:HA2	1:J:870:LEU:HB3	2.01	0.42
1:K:95:MET:HG3	1:K:97:SER:H	1.85	0.42
1:K:242:LEU:HD22	1:K:464:PRO:HB3	2.01	0.42
1:A:497:TYR:CE1	1:A:520:LEU:HD12	2.55	0.41
1:F:667:MET:HE2	1:F:667:MET:HA	2.02	0.41
1:J:344:TYR:HD1	1:J:347:LEU:HD12	1.85	0.41
1:K:719:GLU:HG2	1:K:832:PHE:HE1	1.85	0.41
1:K:800:PHE:HA	1:K:816:LYS:O	2.20	0.41
1:E:134:VAL:HG11	1:E:688:TRP:CE2	2.55	0.41
1:E:530:ILE:HA	1:E:533:ILE:HG22	2.02	0.41
1:E:703:VAL:HG12	1:E:851:VAL:HG22	2.02	0.41
1:G:258:PHE:HE1	1:K:43:VAL:HG11	1.84	0.41
1:H:698:MET:HB3	1:H:781:VAL:HB	2.02	0.41
1:I:473:ARG:NE	1:I:478:ASP:OD1	2.53	0.41
1:J:95:MET:HG2	1:J:96:GLN:N	2.35	0.41
1:K:125:LYS:HD2	1:K:125:LYS:O	2.20	0.41
1:K:221:GLN:HA	1:K:224:ILE:HD12	2.01	0.41
1:A:410:TYR:CE2	1:D:505:VAL:HG11	2.55	0.41
1:A:666:MET:O	1:A:670:VAL:HG23	2.20	0.41
1:A:826:LEU:HA	1:A:826:LEU:HD23	1.85	0.41
1:B:799:PRO:O	1:B:819:THR:OG1	2.27	0.41
1:D:355:LEU:HG	1:D:394:MET:HE2	2.02	0.41
1:D:494:TYR:CZ	1:D:497:TYR:HB2	2.55	0.41
1:D:638:LYS:HA	1:D:638:LYS:HD3	1.89	0.41
1:D:748:ILE:HD12	1:D:751:LEU:HD11	2.02	0.41
1:E:224:ILE:O	1:E:228:GLN:HG2	2.20	0.41
1:F:434:TYR:CE1	1:F:503:MET:HE3	2.55	0.41
1:G:590:ASN:OD1	1:G:591:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:SER:HB3	1:H:213:VAL:HB	2.01	0.41
1:I:890:LEU:O	1:I:891:LYS:CG	2.67	0.41
1:K:545:PRO:HB2	1:K:547:ASP:OD1	2.20	0.41
1:B:313:THR:HA	1:B:319:THR:HG23	2.02	0.41
1:E:112:SER:HA	1:E:698:MET:HG3	2.02	0.41
1:E:180:ARG:HA	1:E:183:ILE:HG22	2.03	0.41
1:E:357:LEU:HD22	1:E:573:TRP:CD1	2.55	0.41
1:F:146:HIS:HE1	1:F:878:LYS:O	2.03	0.41
1:G:134:VAL:HA	1:G:137:ILE:HG22	2.02	0.41
1:H:229:LEU:HD11	1:H:257:ASP:HB2	2.02	0.41
1:H:384:GLY:HA3	1:H:446:GLY:HA3	2.01	0.41
1:I:355:LEU:HD22	1:I:571:VAL:HG22	2.02	0.41
1:I:878:LYS:HB3	1:I:880:LYS:HG2	2.01	0.41
1:A:491:GLY:H	1:B:413:ARG:HH12	1.69	0.41
1:B:487:THR:N	1:G:664:ARG:HH12	2.18	0.41
1:F:798:LEU:HA	1:F:799:PRO:HD3	1.94	0.41
1:H:467:HIS:HE1	1:H:543:SER:O	2.02	0.41
1:I:384:GLY:HA3	1:I:446:GLY:HA3	2.03	0.41
1:I:470:ARG:NH1	1:I:544:LEU:O	2.49	0.41
1:A:590:ASN:OD1	1:A:591:GLU:N	2.53	0.41
1:D:134:VAL:HG11	1:D:688:TRP:CE2	2.55	0.41
1:D:287:ALA:HA	1:D:290:ILE:HG12	2.02	0.41
1:F:102:LEU:HD23	1:F:102:LEU:HA	1.90	0.41
1:H:169:LYS:HA	1:H:169:LYS:HD3	1.90	0.41
1:I:547:ASP:OD1	1:I:547:ASP:N	2.51	0.41
1:J:164:LEU:HD12	1:J:205:PHE:HZ	1.86	0.41
1:J:617:LEU:HA	1:J:617:LEU:HD23	1.88	0.41
1:A:373:ALA:HB1	1:A:576:LEU:HD21	2.03	0.41
1:D:470:ARG:HH11	1:D:546:ASP:HA	1.86	0.41
1:E:745:THR:OG1	1:E:746:TYR:N	2.54	0.41
1:I:236:ILE:HD11	1:I:894:THR:HB	2.01	0.41
1:I:494:TYR:CE1	1:I:497:TYR:HB2	2.55	0.41
1:K:95:MET:HE3	1:K:97:SER:HB3	2.01	0.41
1:K:153:HIS:NE2	1:K:188:ASP:OD2	2.54	0.41
1:A:259:ARG:NH1	1:A:880:LYS:O	2.54	0.41
1:A:732:LEU:HD21	1:A:850:LYS:HB3	2.03	0.41
1:B:355:LEU:HD23	1:B:356:ASP:N	2.36	0.41
1:D:504:LEU:HD23	1:D:504:LEU:HA	1.80	0.41
1:D:595:VAL:HG12	1:D:891:LYS:HB2	2.02	0.41
1:D:664:ARG:NE	1:I:485:PRO:HG2	2.35	0.41
1:D:699:LEU:HB3	1:D:778:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:816:LYS:NZ	1:I:252:GLN:HG2	2.36	0.41
1:E:259:ARG:HH12	1:E:881:MET:HA	1.85	0.41
1:E:753:ALA:HA	1:E:758:PHE:HB2	2.03	0.41
1:E:782:ARG:HB3	1:E:784:LYS:CE	2.51	0.41
1:F:140:LYS:HB3	1:F:140:LYS:HE3	1.83	0.41
1:H:715:LEU:HD21	1:H:839:LEU:HD12	2.02	0.41
1:J:358:LYS:HB2	1:J:570:ASP:OD2	2.21	0.41
1:K:646:GLU:OE2	1:K:649:LYS:NZ	2.47	0.41
1:A:186:ALA:HB1	1:A:867:LEU:HD11	2.02	0.41
1:A:544:LEU:HD11	1:A:549:PHE:HD1	1.86	0.41
1:B:108:TYR:CE2	1:B:855:LYS:HD2	2.56	0.41
1:B:228:GLN:HA	1:B:265:TRP:HE1	1.86	0.41
1:B:238:TRP:HD1	1:B:241:ARG:HE	1.69	0.41
1:B:343:ILE:HG13	1:B:571:VAL:HG11	2.02	0.41
1:B:612:VAL:HG21	1:B:681:LEU:HD11	2.03	0.41
1:D:548:MET:HE2	1:D:548:MET:HA	2.03	0.41
1:D:826:LEU:HD23	1:D:826:LEU:HA	1.89	0.41
1:E:613:ASP:O	1:E:617:LEU:HB2	2.20	0.41
1:F:59:PHE:HB2	1:F:60:THR:H	1.69	0.41
1:G:357:LEU:HD22	1:G:573:TRP:CD1	2.56	0.41
1:G:393:ASN:CG	1:G:397:GLN:HE22	2.28	0.41
1:H:95:MET:HG3	1:H:97:SER:H	1.86	0.41
1:H:786:TYR:CE2	1:H:791:PRO:HD2	2.55	0.41
1:I:607:LEU:HD13	1:I:610:MET:CE	2.51	0.41
1:J:169:LYS:HA	1:J:169:LYS:HD3	1.92	0.41
1:J:296:CYS:HB2	1:J:538:LEU:HD13	2.03	0.41
1:J:703:VAL:HB	1:J:774:PHE:O	2.21	0.41
1:K:238:TRP:CZ3	1:K:272:PRO:HA	2.55	0.41
1:K:676:GLN:HA	1:K:677:PRO:HD3	1.97	0.41
1:A:59:PHE:O	1:H:316:GLN:N	2.50	0.41
1:A:273:VAL:HG11	1:A:600:GLU:HB2	2.02	0.41
1:A:291:MET:HE2	1:A:291:MET:HB3	1.82	0.41
1:D:341:ARG:HB3	1:I:318:ILE:HD11	2.02	0.41
1:G:371:MET:HB2	1:G:405:TYR:CD2	2.53	0.41
1:G:532:GLN:O	1:G:536:GLU:CB	2.69	0.41
1:H:344:TYR:HD1	1:H:347:LEU:HD12	1.86	0.41
1:I:123:PRO:HG2	1:I:635:HIS:CD2	2.56	0.41
1:I:313:THR:HA	1:I:319:THR:HG23	2.02	0.41
1:K:735:PRO:HA	1:K:736:PRO:HD3	1.86	0.41
1:K:775:GLY:N	1:K:817:TYR:OH	2.54	0.41
1:B:211:GLU:HA	1:B:872:ARG:HH22	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ASP:OD1	1:B:547:ASP:N	2.53	0.40
1:B:800:PHE:HA	1:B:816:LYS:O	2.21	0.40
1:B:867:LEU:HD22	1:B:870:LEU:HD11	2.03	0.40
1:E:216:ILE:HD13	1:E:216:ILE:HA	1.94	0.40
1:E:252:GLN:HG3	1:I:393:ASN:ND2	2.36	0.40
1:F:257:ASP:HA	1:J:42:LYS:NZ	2.36	0.40
1:H:236:ILE:HD12	1:H:236:ILE:HA	1.94	0.40
1:H:238:TRP:HH2	1:H:273:VAL:HG12	1.87	0.40
1:H:527:PHE:O	1:H:530:ILE:HG22	2.22	0.40
1:I:246:LYS:HD2	1:I:589:ARG:HH22	1.85	0.40
1:I:287:ALA:O	1:I:291:MET:HG3	2.20	0.40
1:I:339:ASP:HB3	1:I:571:VAL:HB	2.04	0.40
1:J:96:GLN:HB3	1:J:722:ARG:HD3	2.03	0.40
1:J:197:VAL:HB	1:J:200:ARG:HB2	2.03	0.40
1:J:313:THR:HA	1:J:319:THR:HG23	2.02	0.40
1:K:751:LEU:O	1:K:755:MET:HG2	2.21	0.40
1:A:485:PRO:HG2	1:A:901:VAL:HG22	2.02	0.40
1:A:515:TYR:O	1:A:518:SER:OG	2.29	0.40
1:B:64:VAL:O	1:B:67:ILE:HG22	2.22	0.40
1:B:331:THR:HA	1:B:332:PRO:HD3	1.95	0.40
1:B:855:LYS:HD3	1:B:856:ARG:N	2.36	0.40
1:D:107:TYR:O	1:D:111:MET:HE2	2.21	0.40
1:E:521:PRO:O	1:E:525:VAL:HG22	2.22	0.40
1:I:36:LEU:HD23	1:I:36:LEU:HA	1.91	0.40
1:I:84:LYS:HB2	1:I:84:LYS:HE3	1.82	0.40
1:I:783:VAL:HG22	1:I:823:ILE:HB	2.03	0.40
1:K:230:GLN:HA	1:K:233:ARG:HD3	2.03	0.40
1:K:338:ASN:HA	1:K:341:ARG:HD3	2.03	0.40
1:A:351:GLY:HA3	1:A:552:LEU:HD13	2.04	0.40
1:B:666:MET:O	1:B:670:VAL:HG23	2.21	0.40
1:D:242:LEU:HD12	1:D:246:LYS:HD2	2.03	0.40
1:D:557:ILE:HD12	1:D:557:ILE:HA	1.94	0.40
1:E:251:SER:OG	1:I:359:ILE:HG12	2.20	0.40
1:F:431:ARG:HD3	1:F:431:ARG:HA	1.95	0.40
1:F:544:LEU:HA	1:F:545:PRO:HD3	1.92	0.40
1:G:612:VAL:HA	1:G:615:ARG:HB2	2.04	0.40
1:G:615:ARG:HH12	1:G:673:PRO:HA	1.86	0.40
1:G:816:LYS:HD3	1:G:816:LYS:HA	1.85	0.40
1:H:557:ILE:HD12	1:H:557:ILE:HA	1.91	0.40
1:H:737:GLU:HG3	1:H:740:ARG:NH1	2.36	0.40
1:I:762:LEU:O	1:I:766:MET:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:164:LEU:HD22	1:J:166:VAL:HG22	2.03	0.40
1:J:668:ARG:O	1:J:672:LEU:HD23	2.22	0.40
1:J:689:ALA:HA	1:J:692:ASN:ND2	2.37	0.40
1:J:722:ARG:HH11	1:J:831:GLU:HA	1.86	0.40
1:K:93:ILE:HB	1:K:102:LEU:HD12	2.03	0.40
1:K:386:ARG:NH1	1:K:456:ASP:OD1	2.46	0.40
1:K:456:ASP:OD1	1:K:456:ASP:N	2.47	0.40
1:A:403:ASN:ND2	1:A:425:LEU:H	2.19	0.40
1:A:431:ARG:HA	1:A:431:ARG:HD3	1.90	0.40
1:B:465:TYR:HB3	1:B:467:HIS:CE1	2.57	0.40
1:E:238:TRP:HA	1:E:241:ARG:CZ	2.52	0.40
1:E:383:ALA:HB3	1:E:449:TYR:CE1	2.57	0.40
1:E:493:THR:OG1	1:E:498:ASN:OD1	2.34	0.40
1:F:611:LYS:HA	1:F:611:LYS:HD2	1.76	0.40
1:H:426:ASP:OD1	1:H:440:ARG:NH1	2.43	0.40
1:J:118:ILE:HG21	1:J:779:ARG:HA	2.03	0.40
1:J:236:ILE:O	1:J:240:GLU:HG2	2.22	0.40
1:A:544:LEU:HD11	1:A:552:LEU:HD11	2.03	0.40
1:B:164:LEU:HD22	1:B:166:VAL:HG22	2.03	0.40
1:B:485:PRO:HB2	1:G:664:ARG:NH1	2.36	0.40
1:D:281:VAL:HG22	1:D:669:TRP:HZ2	1.86	0.40
1:F:134:VAL:HG21	1:F:688:TRP:CZ3	2.57	0.40
1:G:146:HIS:CD2	1:G:877:TYR:HB2	2.57	0.40
1:G:880:LYS:HG2	1:K:660:PHE:HA	2.03	0.40
1:H:31:LEU:HD12	1:H:345:LEU:HD11	2.04	0.40
1:I:331:THR:HA	1:I:332:PRO:HD3	1.92	0.40
1:I:447:THR:HA	1:I:452:TRP:CD1	2.56	0.40
1:K:103:ARG:O	1:K:858:VAL:HA	2.21	0.40
1:K:133:LYS:HB3	1:K:697:LEU:HD23	2.03	0.40
1:K:238:TRP:HH2	1:K:273:VAL:HG12	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	841/901 (93%)	813 (97%)	28 (3%)	0	100	100
1	B	881/901 (98%)	845 (96%)	36 (4%)	0	100	100
1	D	841/901 (93%)	811 (96%)	30 (4%)	0	100	100
1	E	841/901 (93%)	819 (97%)	22 (3%)	0	100	100
1	F	841/901 (93%)	822 (98%)	19 (2%)	0	100	100
1	G	841/901 (93%)	816 (97%)	24 (3%)	1 (0%)	48	83
1	H	881/901 (98%)	849 (96%)	32 (4%)	0	100	100
1	I	881/901 (98%)	842 (96%)	39 (4%)	0	100	100
1	J	881/901 (98%)	844 (96%)	37 (4%)	0	100	100
1	K	881/901 (98%)	845 (96%)	36 (4%)	0	100	100
All	All	8610/9010 (96%)	8306 (96%)	303 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	272	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	741/792 (94%)	738 (100%)	3 (0%)	84	84
1	B	782/792 (99%)	781 (100%)	1 (0%)	88	89
1	D	741/792 (94%)	738 (100%)	3 (0%)	84	84
1	E	741/792 (94%)	738 (100%)	3 (0%)	84	84
1	F	741/792 (94%)	740 (100%)	1 (0%)	88	89
1	G	741/792 (94%)	739 (100%)	2 (0%)	86	86
1	H	782/792 (99%)	782 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	782/792 (99%)	779 (100%)	3 (0%)	84	84
1	J	782/792 (99%)	781 (100%)	1 (0%)	88	89
1	K	782/792 (99%)	782 (100%)	0	100	100
All	All	7615/7920 (96%)	7598 (100%)	17 (0%)	85	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	271	LEU
1	A	467	HIS
1	A	679	LEU
1	B	562	GLN
1	D	271	LEU
1	D	277	VAL
1	D	467	HIS
1	E	158	VAL
1	E	160	GLU
1	E	271	LEU
1	F	467	HIS
1	G	277	VAL
1	G	467	HIS
1	I	355	LEU
1	I	390	LEU
1	I	628	LEU
1	J	886	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	234	ASN
1	A	252	GLN
1	A	532	GLN
1	A	656	HIS
1	A	658	HIS
1	A	754	ASN
1	A	843	ASN
1	B	45	GLN
1	B	185	ASN
1	B	221	GLN

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	335	GLN
1	B	389	ASN
1	B	532	GLN
1	B	642	ASN
1	B	706	HIS
1	B	871	ASN
1	D	252	GLN
1	D	276	GLN
1	D	397	GLN
1	D	428	GLN
1	D	484	ASN
1	D	531	ASN
1	D	829	ASN
1	D	843	ASN
1	E	234	ASN
1	E	397	GLN
1	E	428	GLN
1	E	532	GLN
1	E	561	HIS
1	E	581	ASN
1	E	723	GLN
1	E	730	ASN
1	E	829	ASN
1	E	843	ASN
1	F	96	GLN
1	F	397	GLN
1	F	532	GLN
1	F	561	HIS
1	F	616	HIS
1	F	702	GLN
1	F	752	GLN
1	F	796	GLN
1	F	829	ASN
1	F	843	ASN
1	G	276	GLN
1	G	397	GLN
1	G	498	ASN
1	G	532	GLN
1	G	561	HIS
1	G	616	HIS
1	G	843	ASN

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Mol	Chain	Res	Type
1	H	45	GLN
1	H	335	GLN
1	H	389	ASN
1	H	411	ASN
1	H	467	HIS
1	H	523	HIS
1	H	561	HIS
1	H	562	GLN
1	I	45	GLN
1	I	185	ASN
1	I	335	GLN
1	I	352	GLN
1	I	393	ASN
1	I	450	ASN
1	I	495	HIS
1	I	523	HIS
1	I	561	HIS
1	I	621	GLN
1	I	642	ASN
1	I	676	GLN
1	I	888	GLN
1	J	45	GLN
1	J	185	ASN
1	J	221	GLN
1	J	335	GLN
1	J	352	GLN
1	J	389	ASN
1	J	403	ASN
1	J	411	ASN
1	J	450	ASN
1	J	523	HIS
1	J	630	GLN
1	J	692	ASN
1	K	185	ASN
1	K	335	GLN
1	K	389	ASN
1	K	411	ASN
1	K	523	HIS
1	K	532	GLN
1	K	561	HIS
1	K	630	GLN
1	K	658	HIS

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Mol	Chain	Res	Type
1	K	676	GLN
1	K	706	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

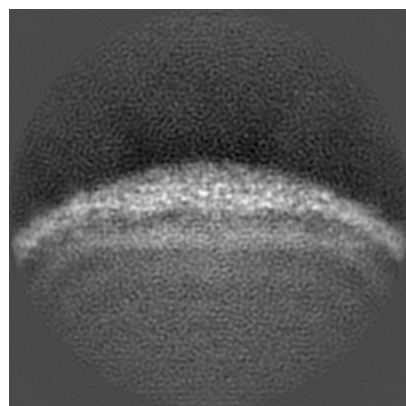
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43726. These allow visual inspection of the internal detail of the map and identification of artifacts.

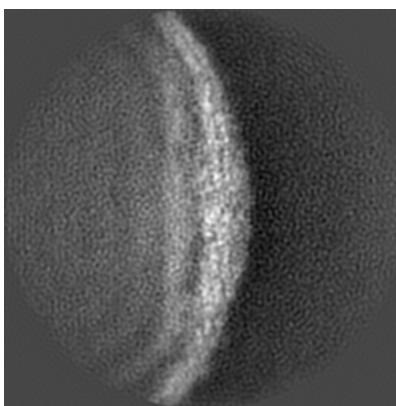
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

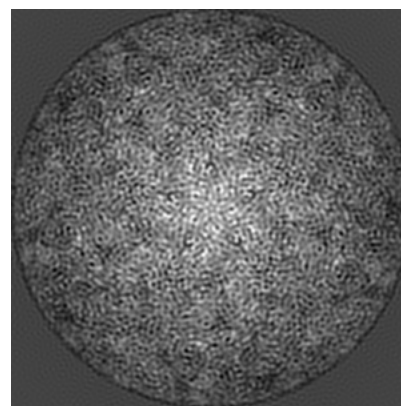
6.1.1 Primary map



X

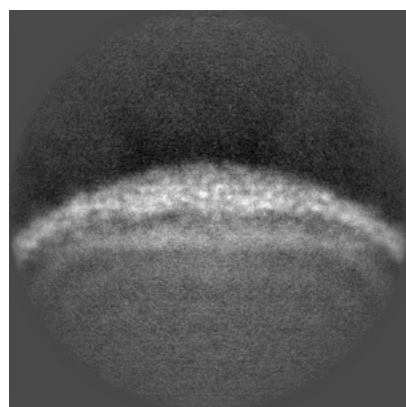


Y

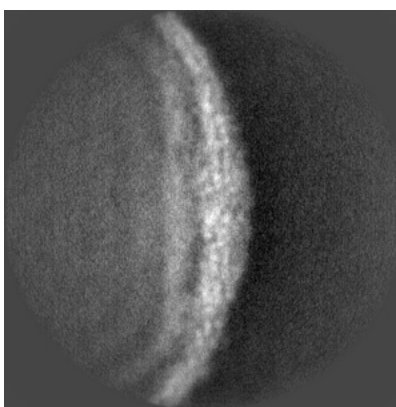


Z

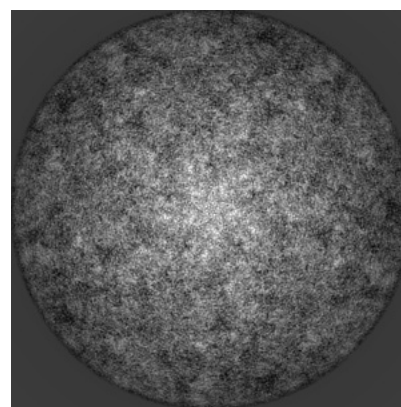
6.1.2 Raw map



X



Y

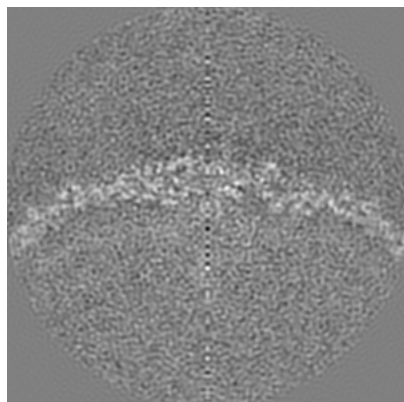


Z

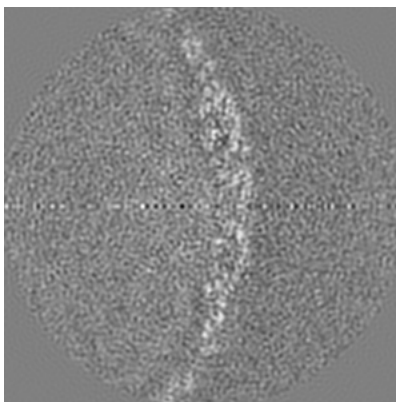
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

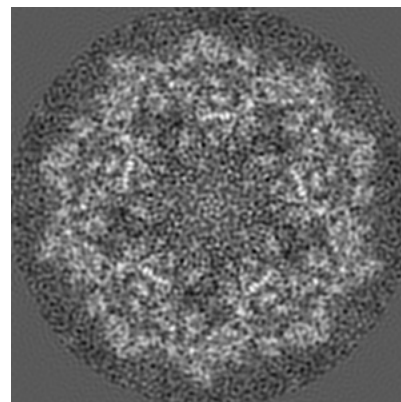
6.2.1 Primary map



X Index: 160

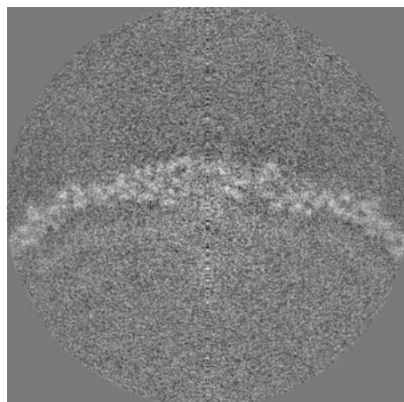


Y Index: 160

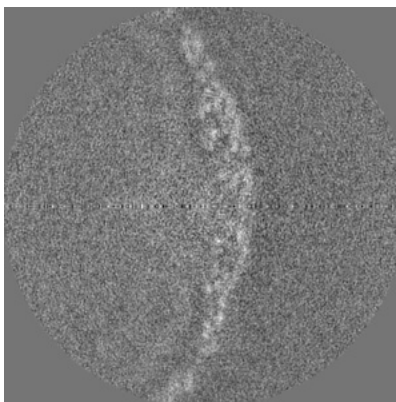


Z Index: 160

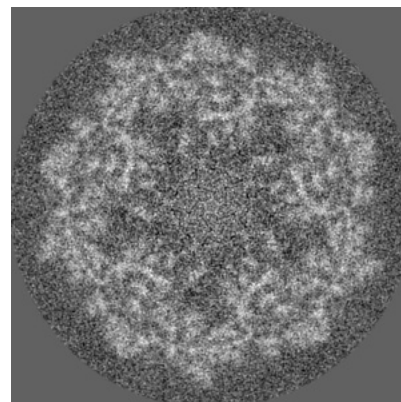
6.2.2 Raw map



X Index: 160



Y Index: 160

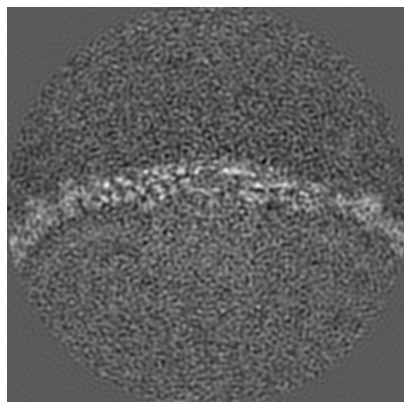


Z Index: 160

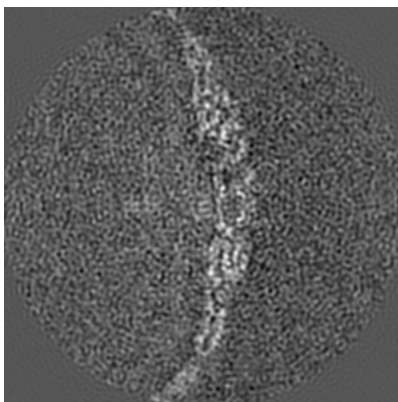
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

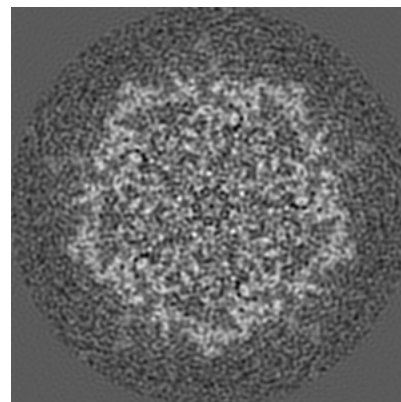
6.3.1 Primary map



X Index: 153

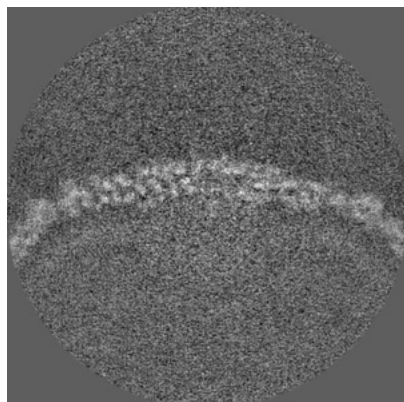


Y Index: 164

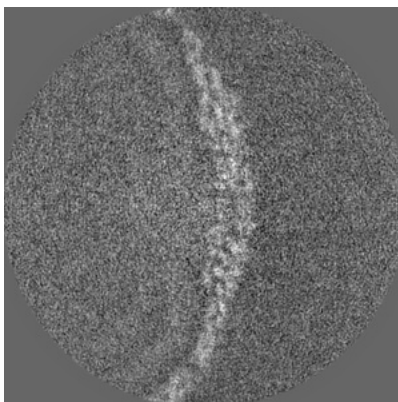


Z Index: 170

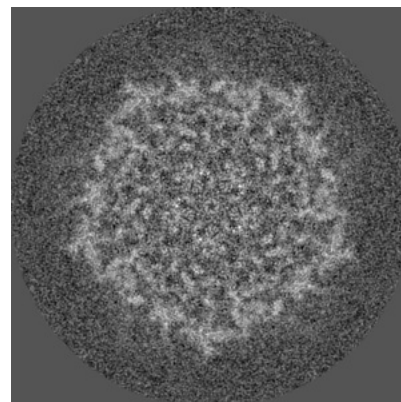
6.3.2 Raw map



X Index: 152



Y Index: 156

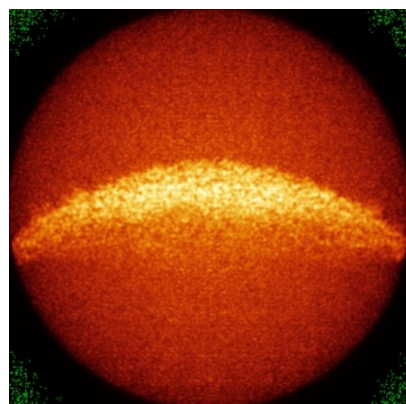


Z Index: 171

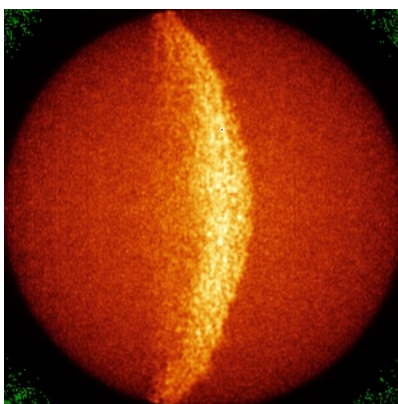
The images above show the largest variance slices of the map in three orthogonal directions.

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

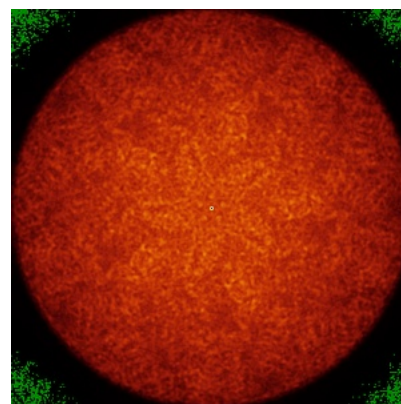
6.4.1 Primary map



X

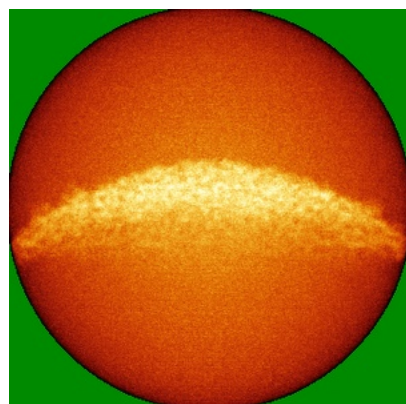


Y

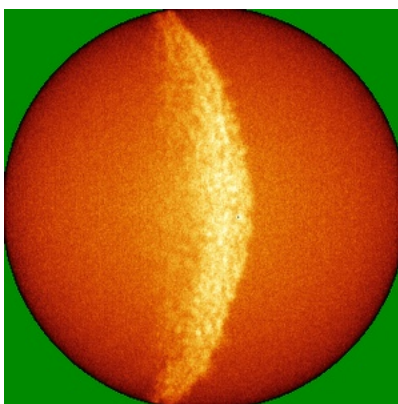


Z

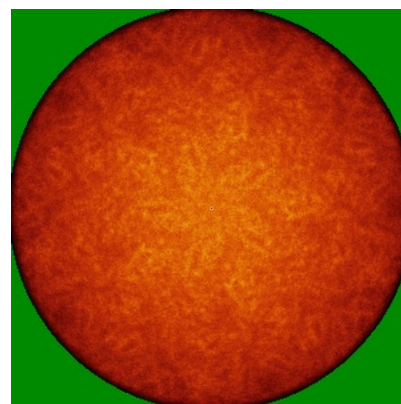
6.4.2 Raw map



X



Y

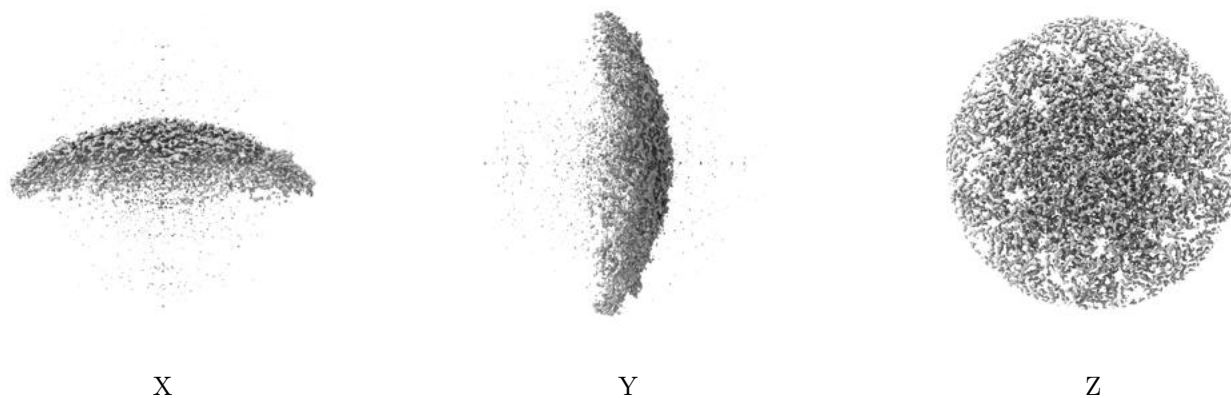


Z

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.

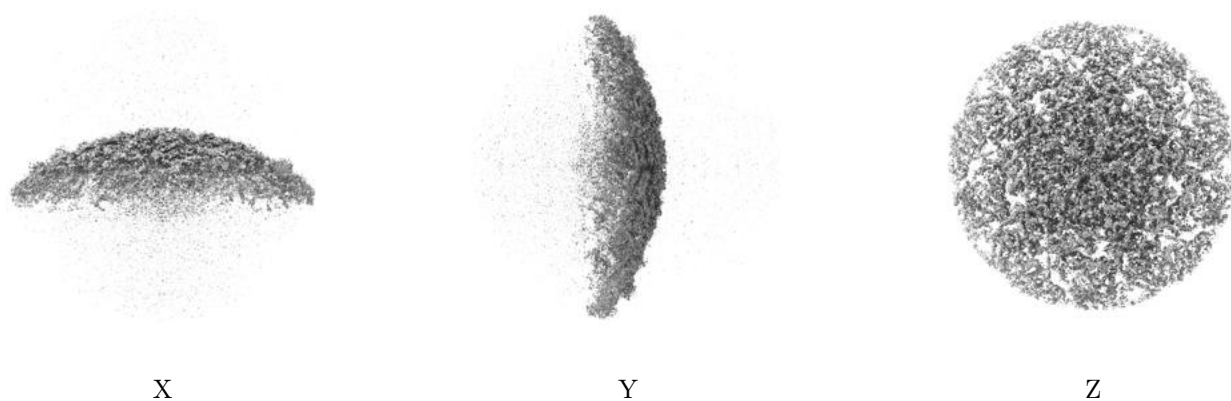
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

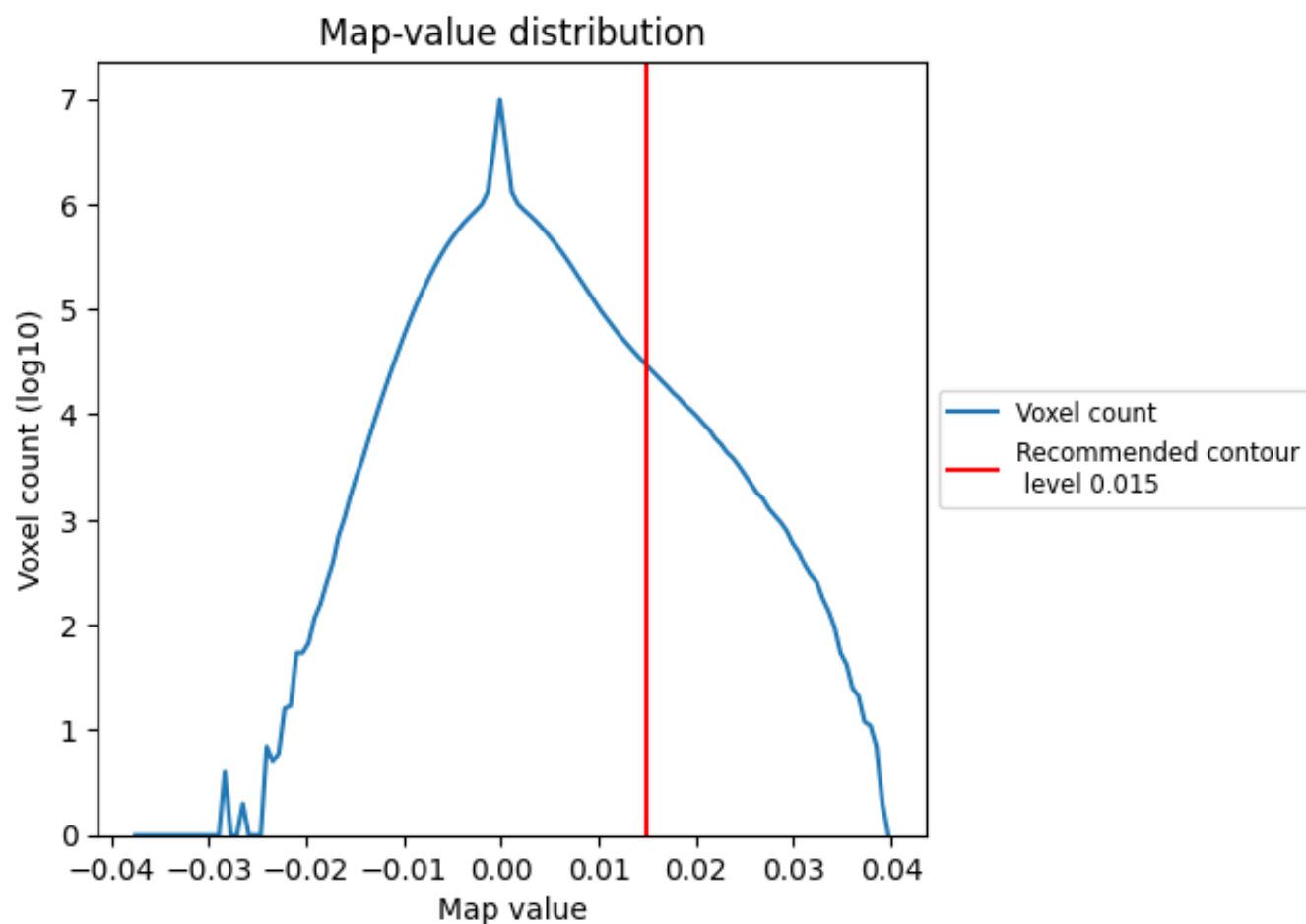
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

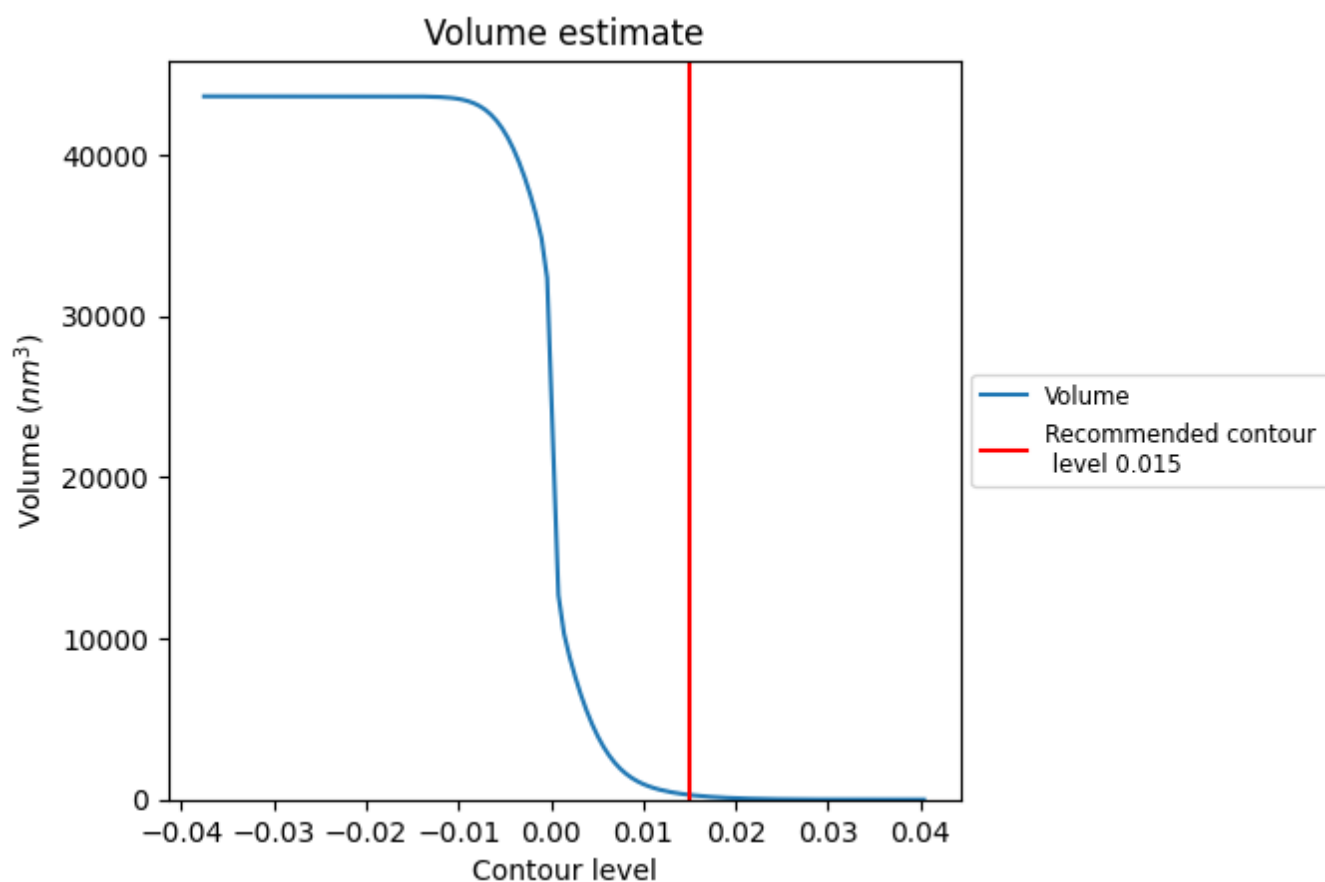
This section contains the results of statistical analysis of the map.

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.

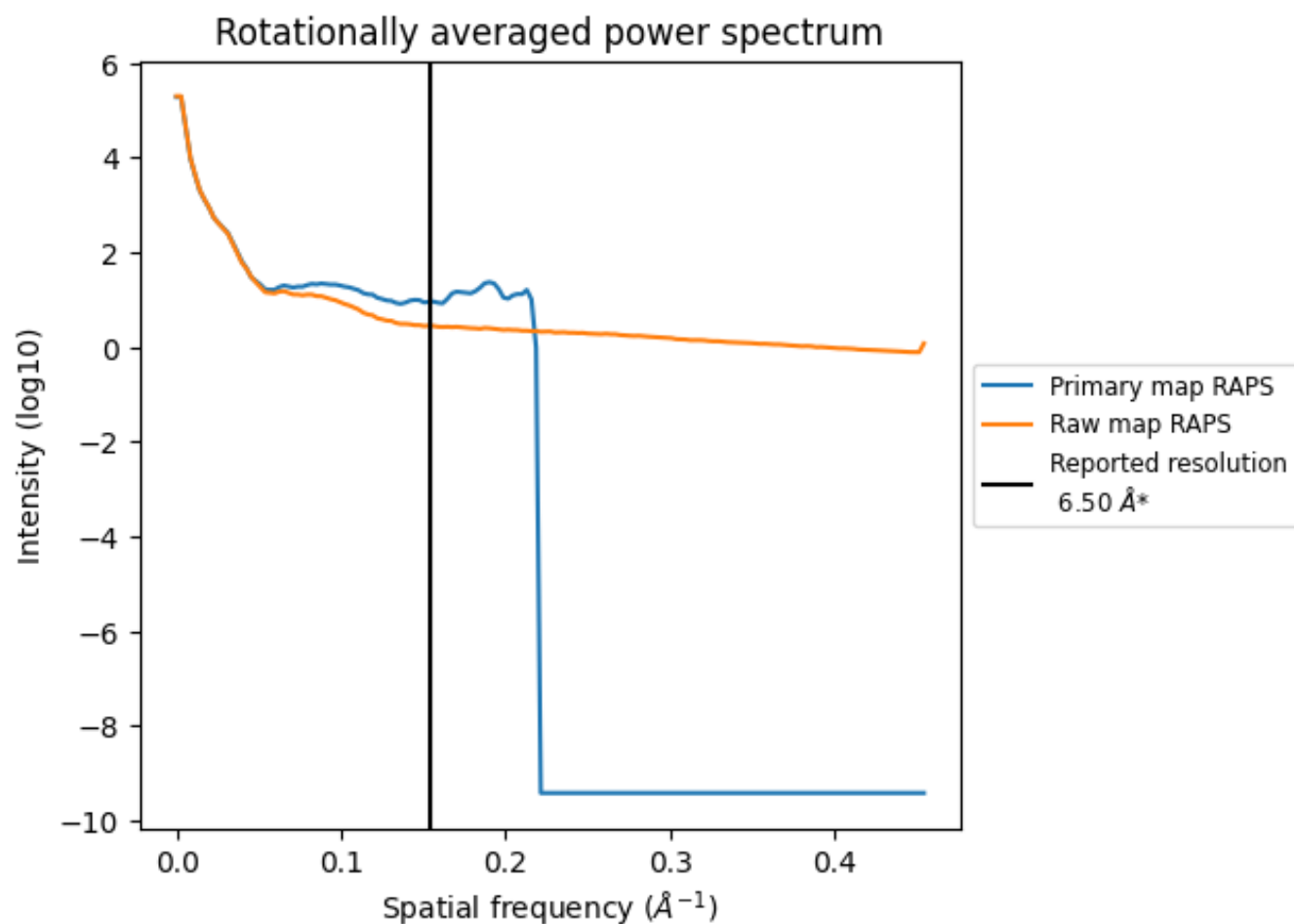
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm³; this corresponds to an approximate mass of 262 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

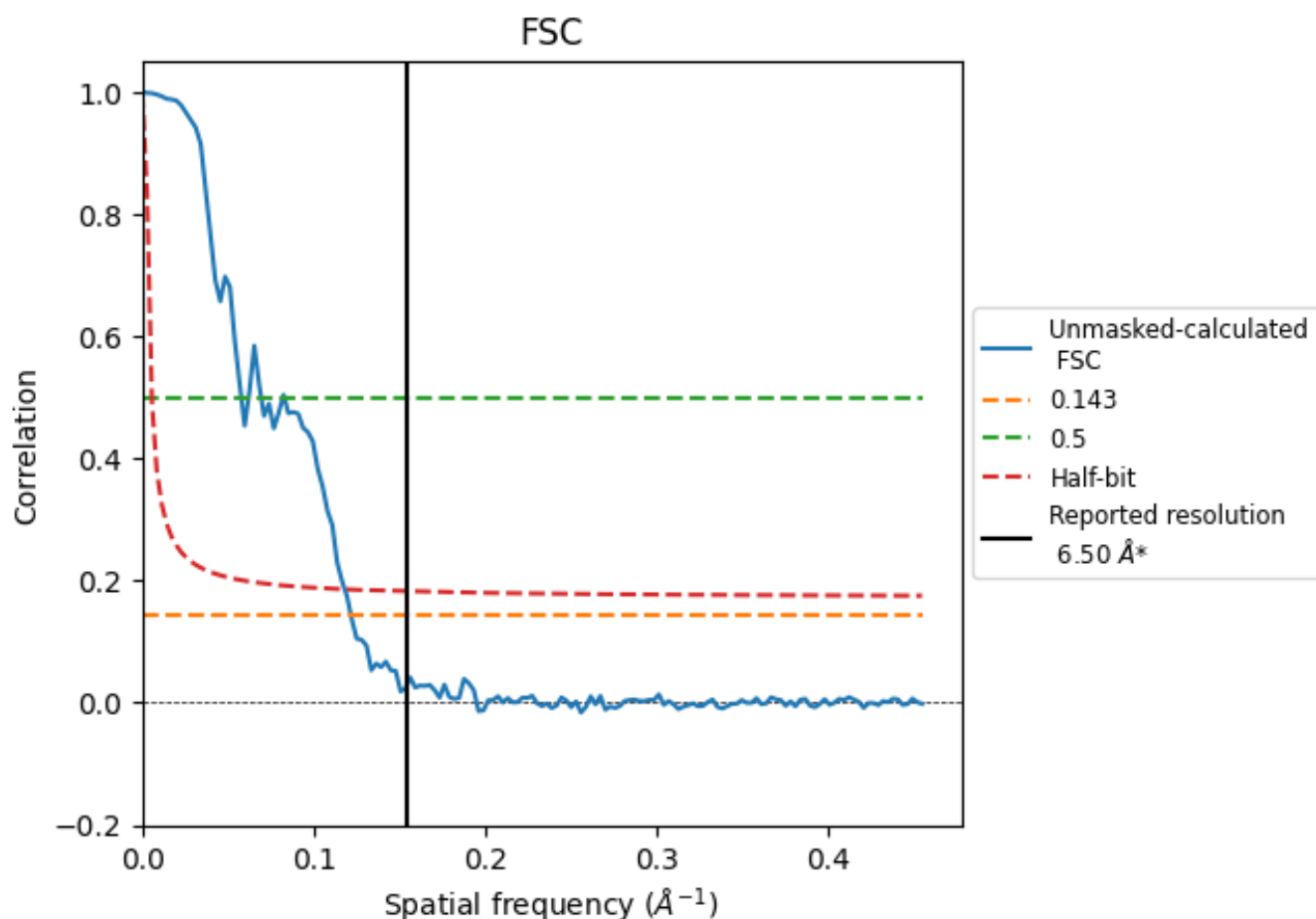


*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

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 0.154 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

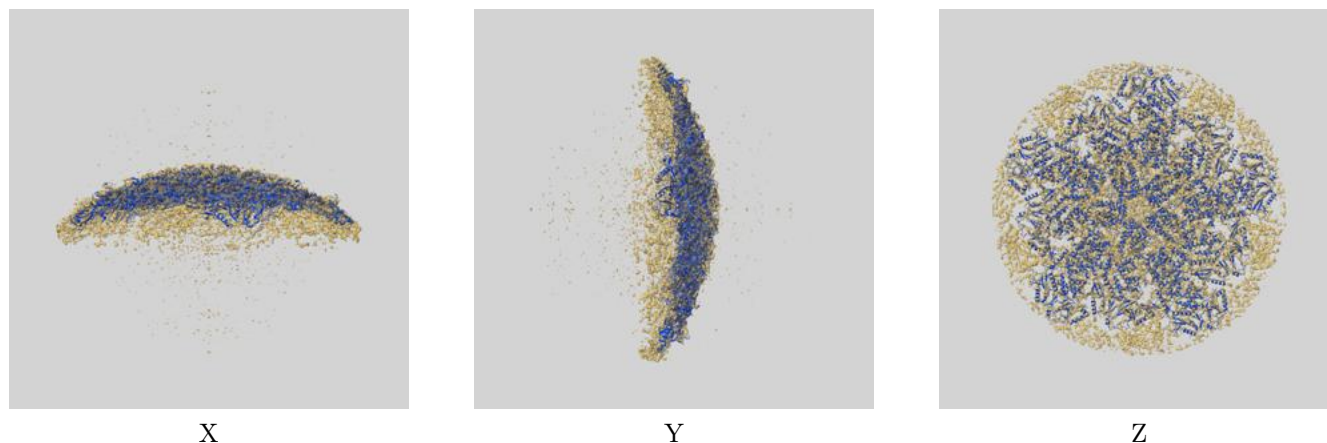
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.22	17.33	8.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.22 differs from the reported value 6.5 by more than 10 %

9 Map-model fit [i](#)

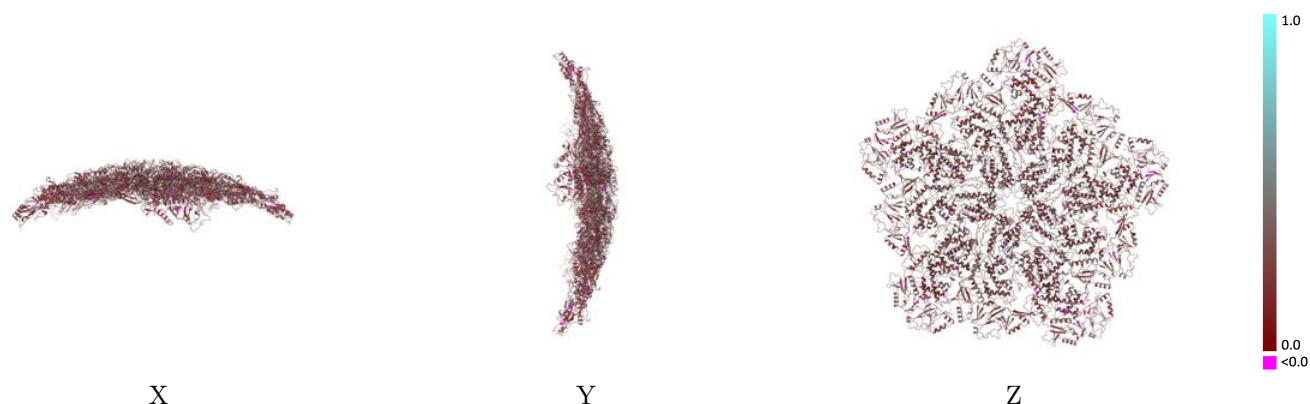
This section contains information regarding the fit between EMDB map EMD-43726 and PDB model 8W1I. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



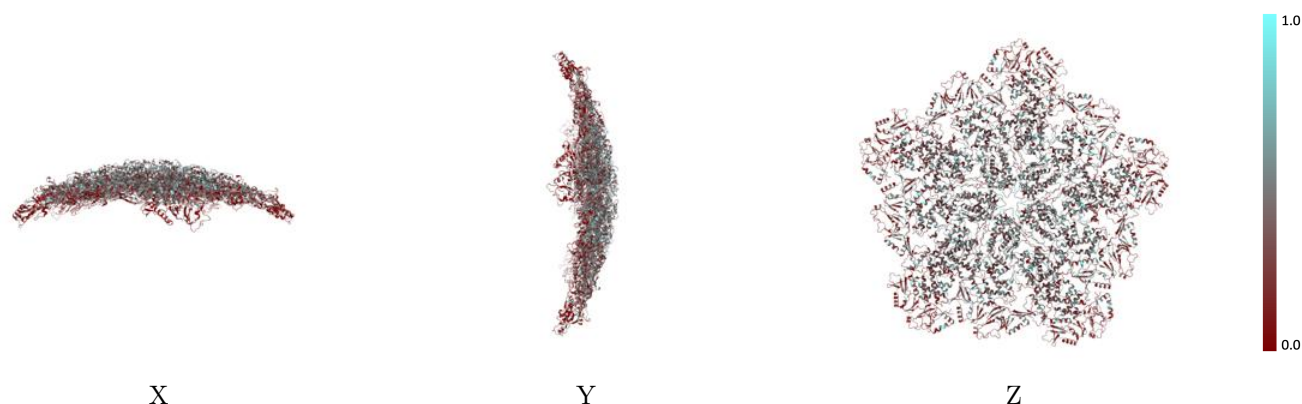
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



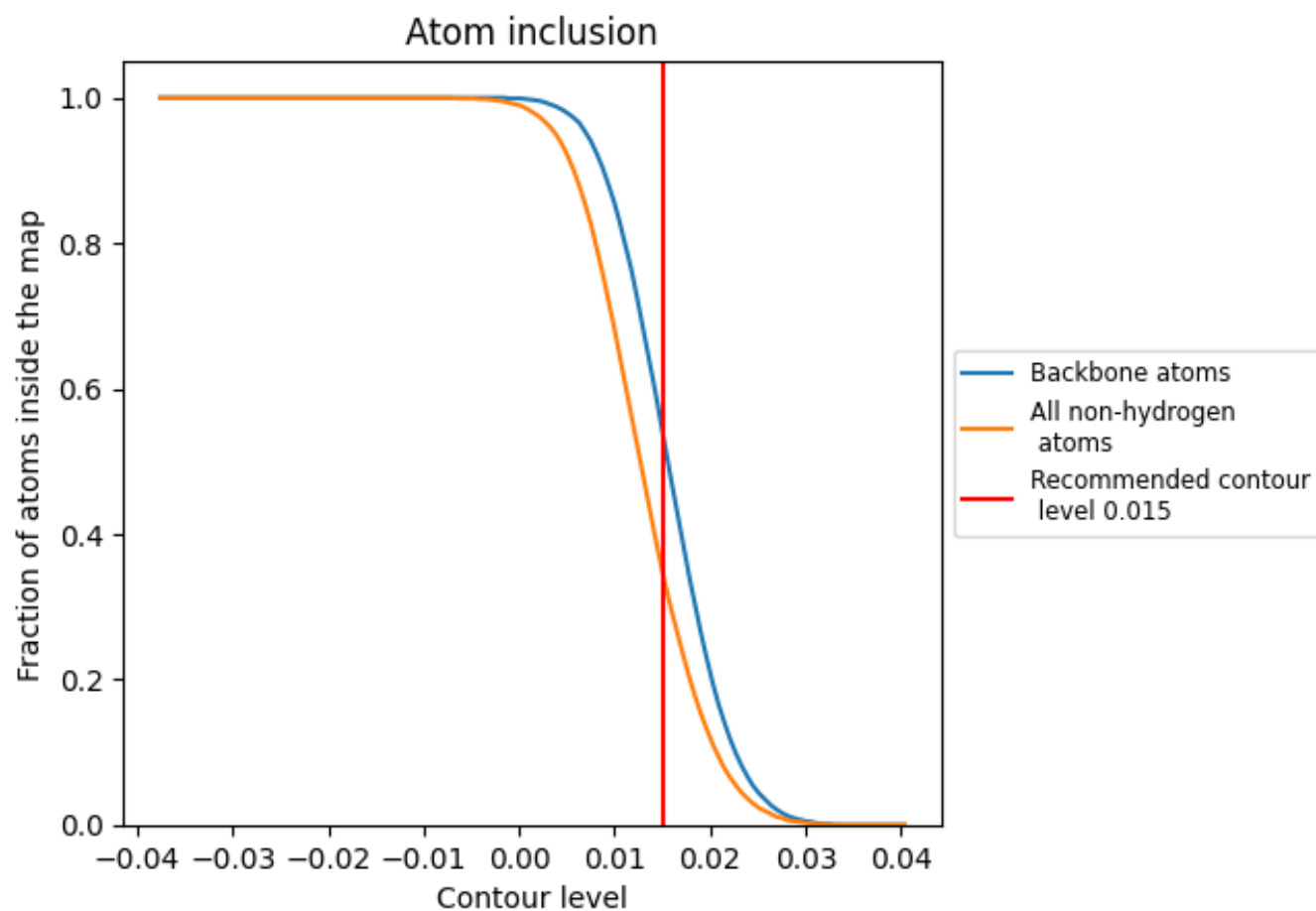
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 35% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3490	0.3000
A	0.3760	0.3080
B	0.3220	0.2950
D	0.3770	0.3090
E	0.3780	0.3070
F	0.3800	0.3070
G	0.3780	0.3080
H	0.3220	0.2930
I	0.3210	0.2910
J	0.3210	0.2920
K	0.3210	0.2940

1.0

0.0

<0.0