



Full wwPDB EM Validation Report ⓘ

Sep 8, 2025 – 02:34 PM EDT

PDB ID : 9NGY / pdb_00009ngy
EMDB ID : EMD-49396
Title : In situ cryo-EM structure of protochannel (DotA-IcmX) of the Legionella Dot/Icm T4SS machine
Authors : Yue, J.; Liu, J.
Deposited on : 2025-02-22
Resolution : 3.63 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

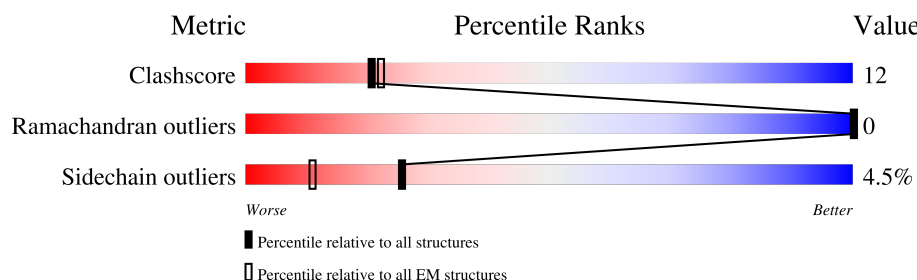
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.63 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	AP1	466	<div> <div>11%</div> <div>69%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>
1	BP1	466	<div> <div>10%</div> <div>67%</div> <div>22%</div> <div>•</div> <div>11%</div> </div>
1	CP1	466	<div> <div>10%</div> <div>70%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>
1	DP1	466	<div> <div>11%</div> <div>69%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
1	EP1	466	<div> <div>11%</div> <div>70%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>
2	FP1	1048	<div> <div>46%</div> <div>60%</div> <div>20%</div> <div>•</div> <div>18%</div> </div>
2	GP1	1048	<div> <div>47%</div> <div>57%</div> <div>23%</div> <div>•</div> <div>18%</div> </div>
2	HP1	1048	<div> <div>46%</div> <div>57%</div> <div>23%</div> <div>•</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
2	IP1	1048	<div><div><div>47%</div><div>58%</div><div>23%</div><div>18%</div></div></div>
2	JP1	1048	<div><div><div>46%</div><div>57%</div><div>23%</div><div>18%</div></div></div>
3	KP1	1048	<div><div><div></div><div>96%</div></div></div>
3	LP1	1048	<div><div><div></div><div>96%</div></div></div>
3	MP1	1048	<div><div><div></div><div>96%</div></div></div>
3	NP1	1048	<div><div><div></div><div>96%</div></div></div>
3	OP1	1048	<div><div><div></div><div>96%</div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 50535 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 IcmX (IcmY).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	BP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	CP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	DP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
1	EP1	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		

- Molecule 2 is a protein called DotA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	GP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	HP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	IP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
2	JP1	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		

- Molecule 3 is a protein called IcmE (DotG).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	KP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
3	LP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
3	MP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		

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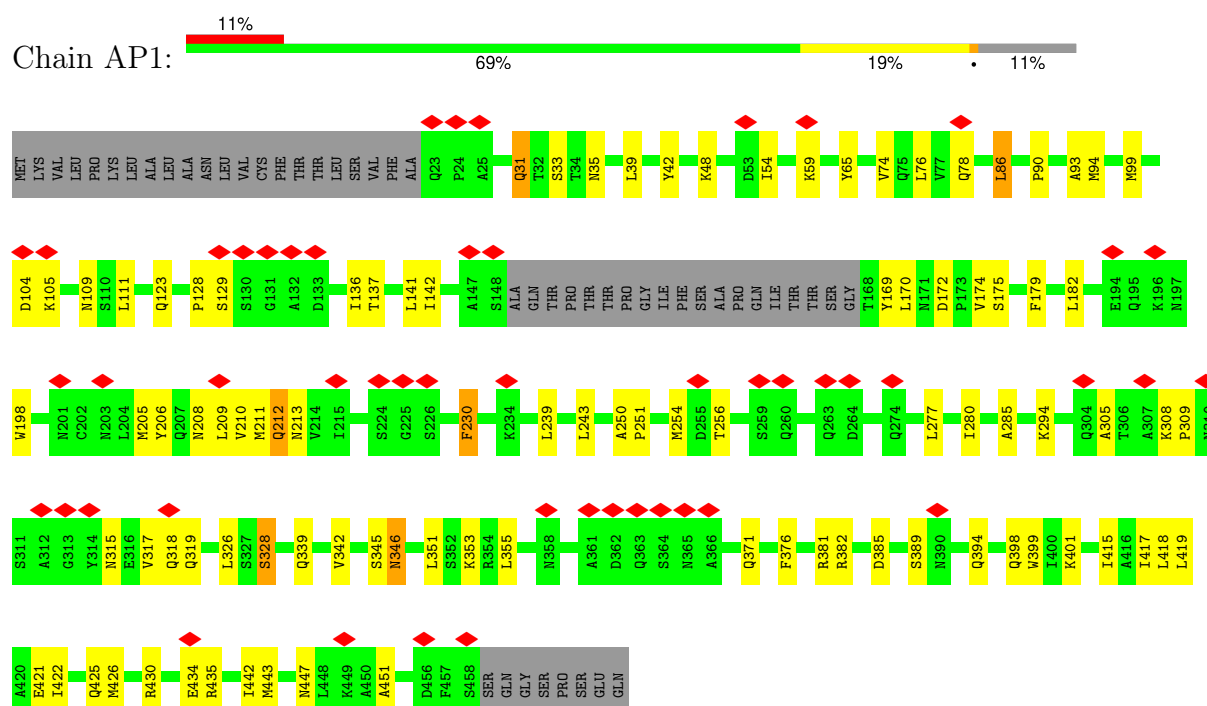
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	NP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
3	OP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		

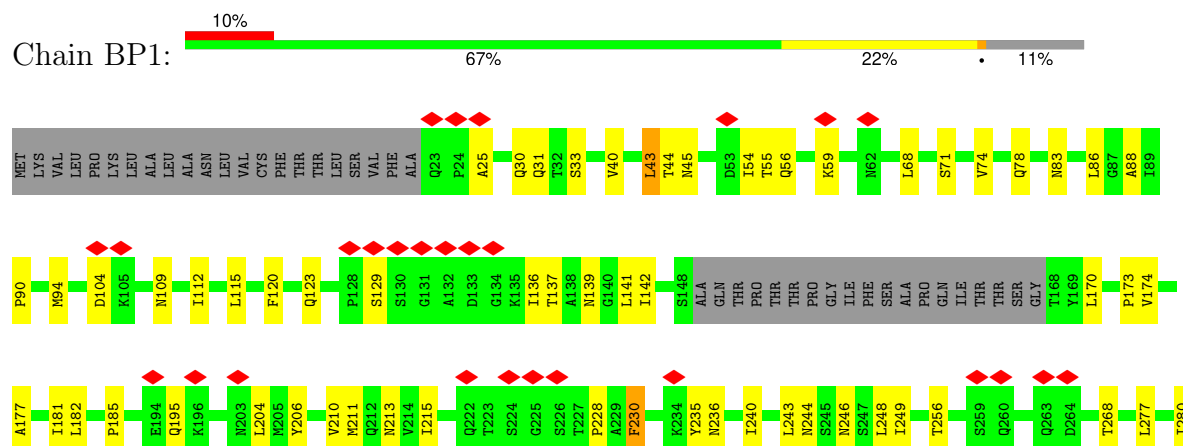
3 Residue-property plots

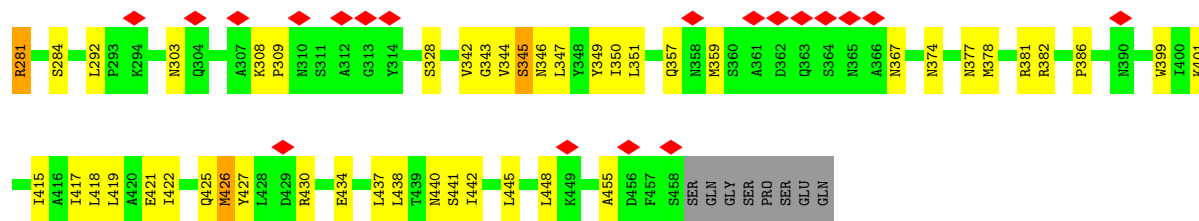
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

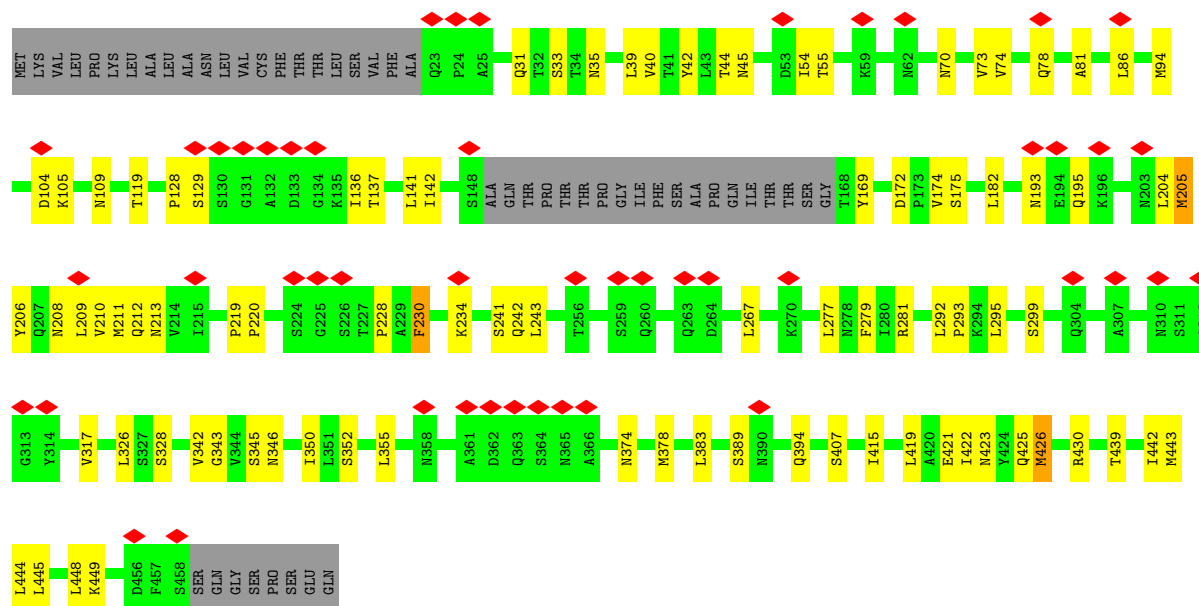
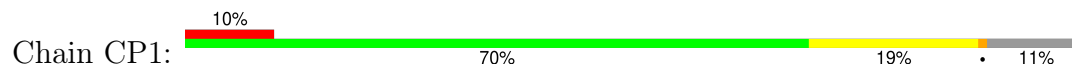


• Molecule 1: IcmX (IcmY)

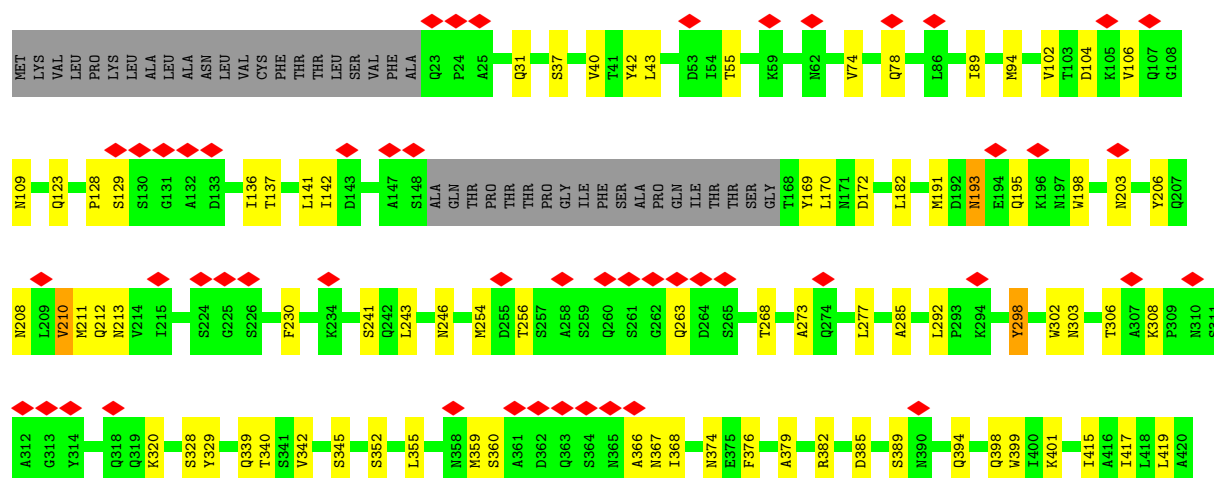
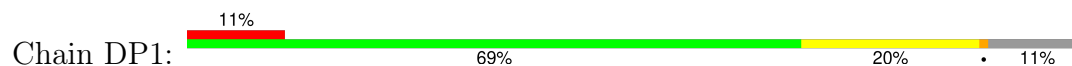


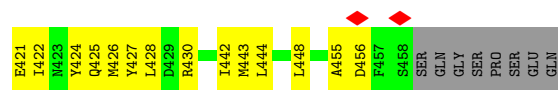


• Molecule 1: IcmX (IcmY)

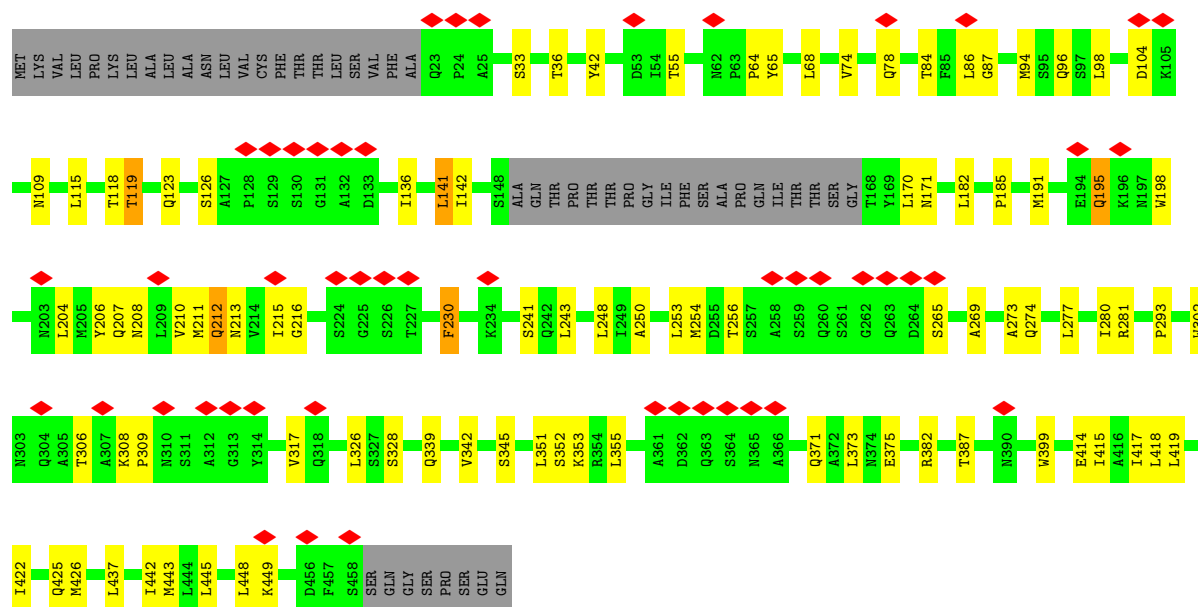
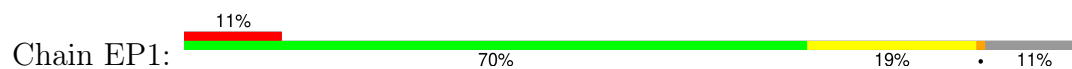


• Molecule 1: IcmX (IcmY)

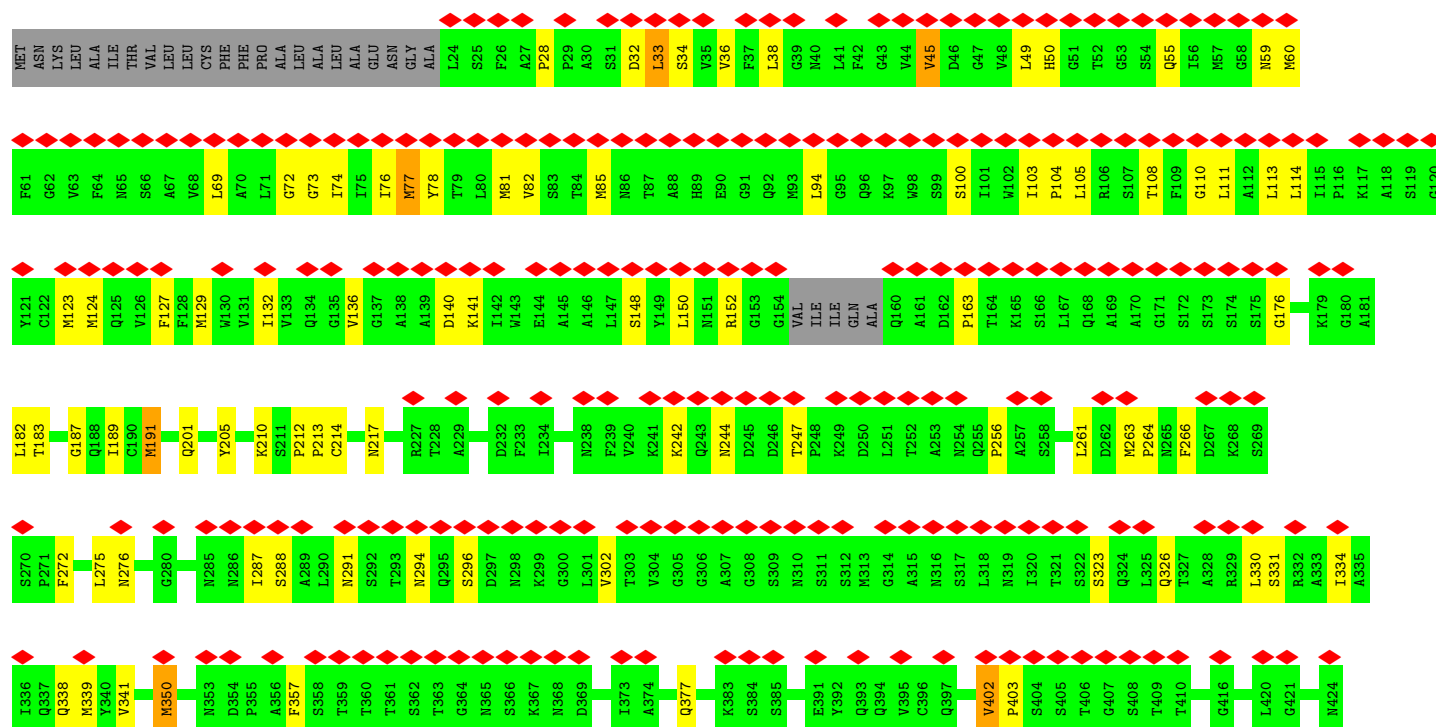


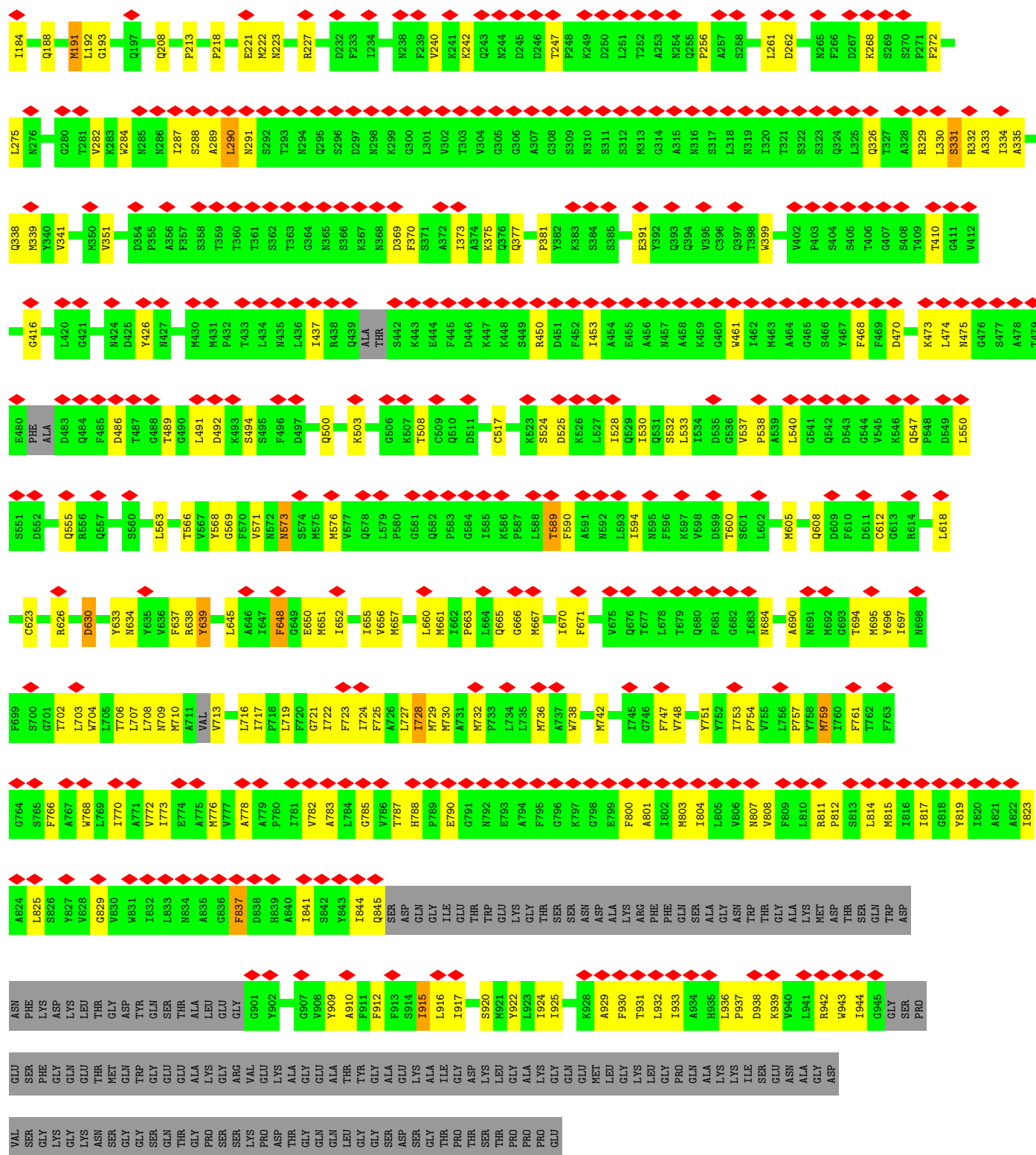


• Molecule 1: IcmX (IcmY)



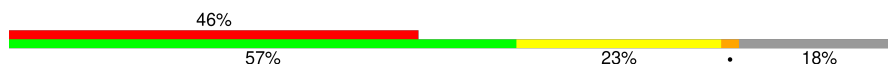
• Molecule 2: DotA





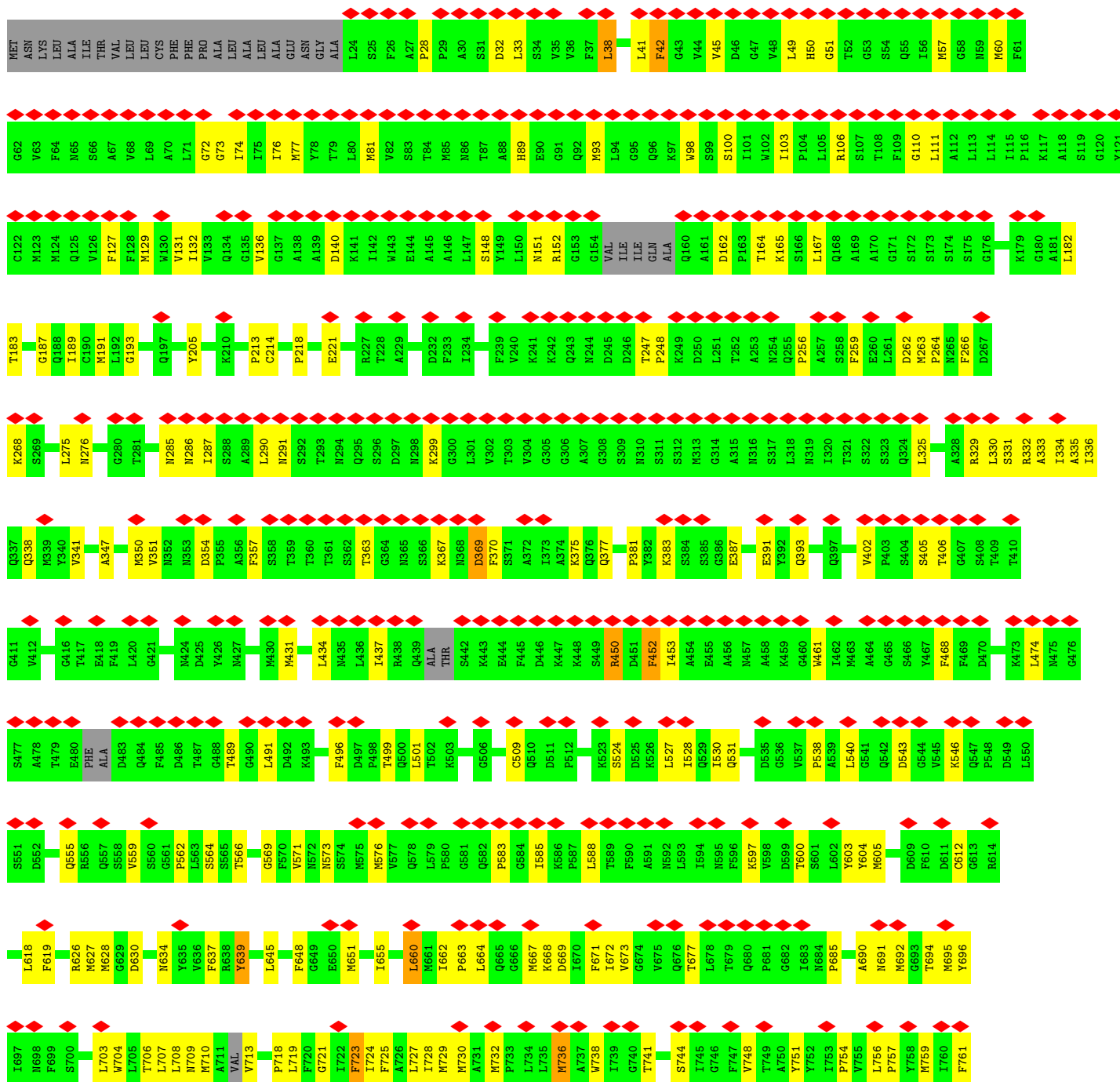
• Molecule 2: DotA

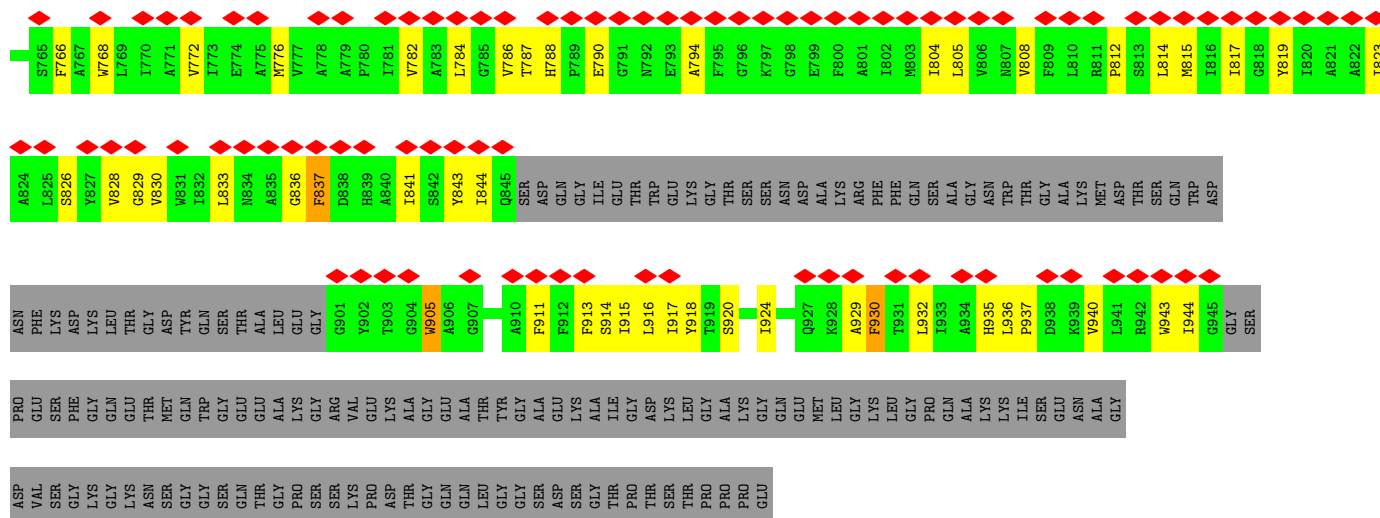
Chain HP1:



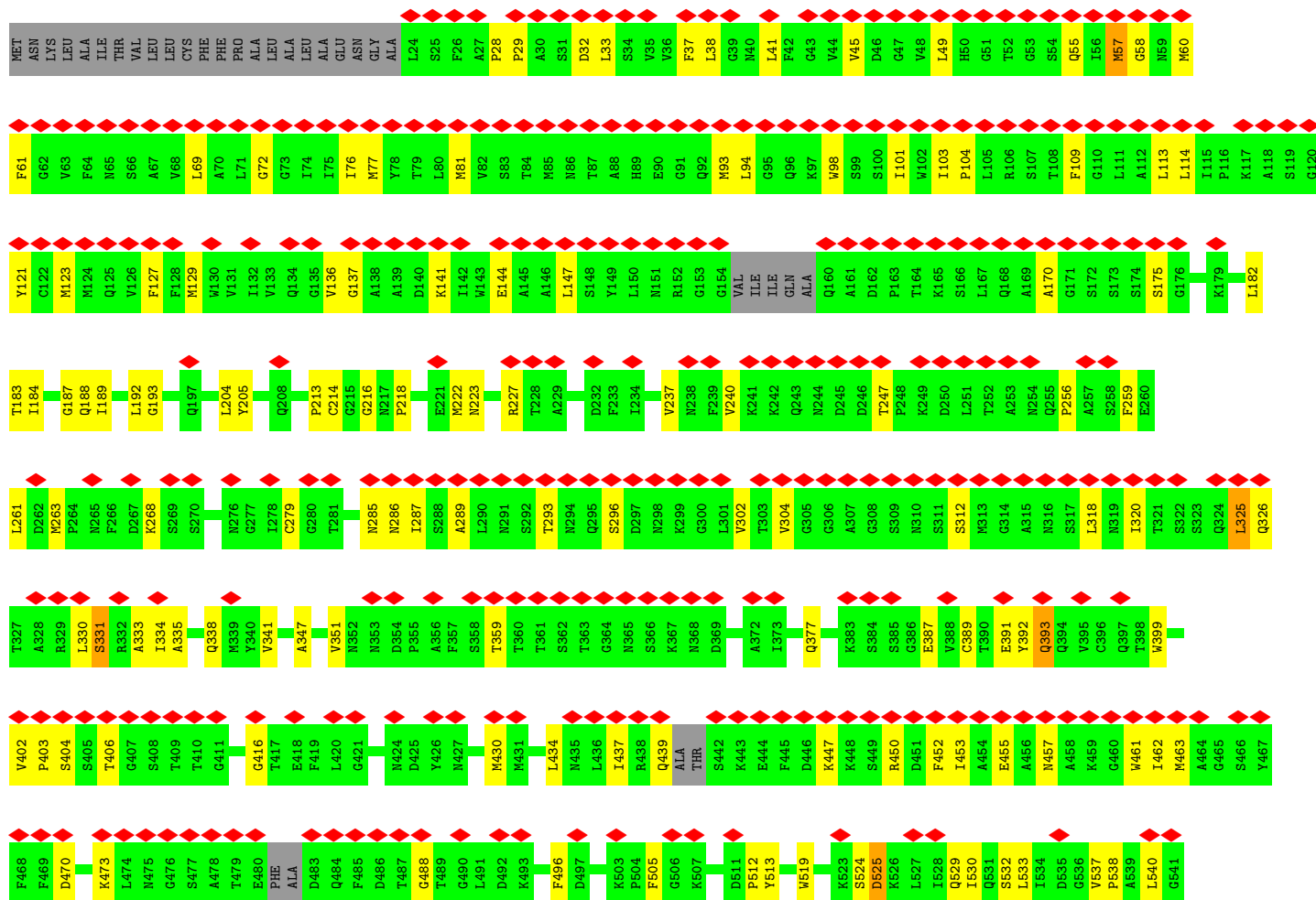
MET	ASN	LYS	LEU	ALA	ILE	THR	VAL	LEU	LEU	CYS	PHE	PHE	PRO	ALA	ALA	LEU	LEU	ALA	ALA	GLY	ASN	ALA	L24	S25	F26	A27	P28	P29	A30	S31	D32	L33	S34	V35	V36	F37	L38	G39	I40	L41	F42	G43	V44	V45	D46	G47	V48	L49	H50	G51	T52	G53	S54	Q55	I56	H57	G58	N59	H60
F61	G62	V63	F64	N65	S66	A67	V68	L69	A70	L71	G72	G73	I74	I75	I76	I77	I78	T79	L80	H81	H82	S83	T84	H85	H86	T87	A88	H89	E90	G91	D92	H93	L94	G95	D96	K97	K98	S99	S100	I101	I102	I103	P104	L105	S107	T108	F109	G110	L111	A112	L113	L114	I115	P116	K117	S118	S119	G120	
Y121	C122	M123	M124	Q125	V126	F127	F128	M129	W130	I131	I132	V133	Q134	G135	V136	G137	A138	A139	D140	K141	I142	W143	E144	A145	L147	S148	L150	N151	R152	G153	G154	VAL	ILE	ILE	GLN	ALA	Q160	A161	D162	P163	T164	K165	S166	L167	Q168	A169	G171	S172	S173	S174	S175	G176	K179	G180	A181				
L182	T183	I184	Q188	I189	C190	M191	L192	G193	K196	Q197	K210	S211	P212	G215	E221	M222	N223	R227	T228	A229	D232	F233	I234	V237	N238	F239	V240	K241	K242	Q243	N244	D245	D246	T247	P248	K249	D250	L251	T252	A253	N254	D255	P256	A257	S258	F259	E260	L261	D262	M263	P264								
N265	F266	D267	K268	A269	L275	N276	G277	L278	C279	T281	V282	N285	N286	L287	S288	A289	L290	N291	S292	T293	N294	Q295	S296	D297	N298	K299	G300	L301	V302	T303	V304	G305	G306	A307	G308	S309	N310	S311	S312	M313	G314	A315	N316	S317	L318	N319	I320	T321	S322	S323	Q324	Q326	A328	R329					
L330	S331	R332	A333	I334	A335	L336	Q337	Q338	M339	Y340	V341	Q348	N350	V351	N352	N353	D354	P355	A356	P357	T358	T359	T360	T361	S362	T363	G364	N365	S366	K367	N368	D369	S370	A372	I373	Q377	K383	S384	S385	E391	Y392	Q393	C396	Q397	V402	P403	S404	S405	T406	G407	S408								
T409	T410	G411	V412	G416	L420	G421	N424	D425	Y426	N427	G428	I429	M430	M431	L434	N435	L436	I437	R438	Q439	ALA	THR	S442	K443	E444	F445	D446	K447	K448	S449	R450	A451	F452	I453	A454	E455	A456	N457	A458	K459	G460	V461	I462	M463	A464	G465	S466	Y467	F468	D470	L471	K473	L474						
N475	G476	S477	T479	E480	PHE	ALA	D483	Q484	F485	D486	T487	G488	T489	L491	D492	K493	S494	D497	K503	G506	C509	Q510	D511	P512	Y513	S514	L515	L516	W519	D525	K526	L527	I528	Q529	I530	L533	I534	D535	P538	A539	L540	G541	Q542	D543	G544	V545	K546	Q547	P548										
D549	L550	S551	D552	Q557	S560	S564	S565	T566	G569	F570	V571	G578	L579	P580	G581	Q582	P583	G584	M585	K586	P587	L588	T589	F590	A591	N592	L593	I594	N595	F596	K597	V598	D599	L602	Y603	D609	F610	D611	C612	G613	R614	I617	L618	F619	G622	R626	M627												
M628	G629	D630	N634	Y635	Y639	V640	Y641	N642	F643	F644	L645	I647	G648	G649	M651	I652	I655	V656	M657	A658	F659	L660	M661	I662	P663	L664	Q665	G666	M667	K668	D669	I670	F671	I672	G674	V675	Q676	T677	L678	T679	Q680	P681	G682	I683	M692	M695	Y696	I697	N698	F699	S700								
G701	T702	L703	T706	L707	M710	A711	VAL	V713	L716	F723	I724	F725	A726	G727	I728	M729	M730	A731	F732	F733	L734	L735	M736	A737	W738	M742	V743	S744	I745	G746	F747	V748	T749	A750	Y751	I752	I753	P754	V755	L756	P757	Y758	M759	I760	F761	G762	F763	G764	S765	F766	A767	W768	L769	I770					
A771	V772	I773	E774	A775	A778	A779	V782	A783	L784	G785	T787	H788	P789	E790	G791	N792	E793	A794	F795	G796	N797	G798	E799	F800	A801	I802	N803	I804	L805	V806	N807	V808	F809	L810	R811	P812	L814	M815	I816	I817	G818	Y819	I820	A821	I823	A824	L825	S826	Y827	V828	G829	I832	L833						
N834	A835	G836	F837	D838	H839	A840	I841	S842	Y843	L844	Q845	SER	ASP	GLN	GLY	ILE	GLU	THR	TRP	GLU	LYS	THR	ARG	PHE	GLN	SER	ALA	GLY	ASN	TRP	THR	GLY	ALA	MET	ASP	THR	GLN	TRP	ASP	ASN	PHE	LYS	ASP	LYS	LEU	THR	GLY	ASP	PHE	GLY	GLN	GLU							
G901	Y902	T903	G904	Y905	A906	G907	Y908	Y909	A910	F911	F912	F913	L916	I917	T919	S920	N921	Y922	L923	I924	I925	V926	Q927	K928	A929	F930	T931	L932	I933	A934	H935	D938	K939	V940	L941	R942	V943	I944	G945	GLY	SER	PRO	GLU	SER	PHE	GLY	GLN	GLU											

- Molecule 2: DotA





• Molecule 2: DotA









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	73	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.818	Depositor
Minimum map value	-0.526	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	640.8192, 640.8192, 640.8192	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2516, 1.2516, 1.2516	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	AP1	0.17	0/3277	0.35	0/4473
1	BP1	0.17	0/3277	0.35	0/4473
1	CP1	0.16	0/3277	0.32	0/4473
1	DP1	0.16	0/3277	0.32	0/4473
1	EP1	0.17	0/3277	0.32	0/4473
2	FP1	0.16	0/6715	0.36	0/9115
2	GP1	0.16	0/6715	0.39	0/9115
2	HP1	0.16	0/6715	0.39	0/9115
2	IP1	0.16	0/6715	0.39	0/9115
2	JP1	0.16	0/6715	0.36	0/9115
3	KP1	0.16	0/337	0.52	0/451
3	LP1	0.09	0/337	0.27	0/451
3	MP1	0.12	0/337	0.38	0/451
3	NP1	0.14	0/337	0.41	0/451
3	OP1	0.18	0/337	0.54	0/451
All	All	0.16	0/51645	0.37	0/70195

There are no bond length outliers.

There are no bond angle outliers.

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	AP1	3213	0	3131	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BP1	3213	0	3131	91	0
1	CP1	3213	0	3131	74	0
1	DP1	3213	0	3131	75	0
1	EP1	3213	0	3131	78	0
2	FP1	6560	0	6545	165	0
2	GP1	6560	0	6545	208	0
2	HP1	6560	0	6545	198	0
2	IP1	6560	0	6545	185	0
2	JP1	6560	0	6545	174	0
3	KP1	334	0	378	15	0
3	LP1	334	0	378	14	0
3	MP1	334	0	378	12	0
3	NP1	334	0	378	11	0
3	OP1	334	0	378	13	0
All	All	50535	0	50270	1188	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 12.

All (1188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:671:PHE:HE1	2:FP1:915:ILE:HD13	1.29	0.97
2:HP1:193:GLY:HA3	2:HP1:530:ILE:HD11	1.51	0.92
1:DP1:443:MET:HE2	1:EP1:443:MET:HE1	1.53	0.91
2:GP1:929:ALA:O	2:GP1:932:LEU:HB3	1.73	0.88
2:GP1:193:GLY:HA3	2:GP1:530:ILE:HD11	1.55	0.87
3:MP1:16:ARG:HE	3:MP1:20:ILE:HD11	1.37	0.87
2:HP1:326:GLN:HA	2:HP1:329:ARG:HE	1.39	0.86
2:JP1:193:GLY:HA3	2:JP1:530:ILE:HD11	1.57	0.85
2:FP1:594:ILE:HG23	2:JP1:705:LEU:HD11	1.59	0.84
2:FP1:671:PHE:CE1	2:FP1:915:ILE:HD13	2.13	0.84
2:FP1:78:TYR:HA	2:FP1:81:MET:HE2	1.59	0.84
1:BP1:94:MET:HE1	1:BP1:170:LEU:HD23	1.56	0.83
2:GP1:768:TRP:HB2	2:GP1:815:MET:HE1	1.59	0.83
2:IP1:662:ILE:HG23	2:IP1:663:PRO:HD3	1.59	0.83
2:FP1:828:VAL:HG21	2:JP1:41:LEU:HB2	1.62	0.82
1:CP1:426:MET:HE1	1:DP1:422:ILE:HG23	1.64	0.80
2:FP1:766:PHE:HZ	2:GP1:829:GLY:HA2	1.46	0.79
2:FP1:60:MET:HE1	2:GP1:817:ILE:HG12	1.65	0.78
2:IP1:193:GLY:HA3	2:IP1:530:ILE:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:660:LEU:HD21	2:FP1:661:MET:HE2	1.64	0.78
2:FP1:73:GLY:HA2	2:FP1:76:ILE:HD12	1.64	0.78
2:HP1:909:TYR:O	2:HP1:912:PHE:HB2	1.85	0.76
2:HP1:41:LEU:HB2	2:IP1:828:VAL:HG11	1.66	0.76
2:HP1:917:ILE:HA	2:HP1:920:SER:HB3	1.67	0.75
2:HP1:60:MET:HE3	2:IP1:817:ILE:HD13	1.69	0.75
1:DP1:444:LEU:HD23	1:EP1:443:MET:HB2	1.69	0.74
1:AP1:422:ILE:HG23	1:EP1:426:MET:HE1	1.68	0.74
2:IP1:540:LEU:HD23	2:IP1:562:PRO:HB2	1.69	0.74
1:DP1:94:MET:HE1	1:DP1:170:LEU:HD23	1.67	0.74
2:JP1:302:VAL:HG11	2:JP1:325:LEU:HD13	1.70	0.73
2:IP1:612:CYS:HB2	2:IP1:626:ARG:HE	1.52	0.73
2:HP1:101:ILE:HD13	3:OP1:16:ARG:HH21	1.54	0.73
2:GP1:697:ILE:HD12	2:GP1:751:TYR:HE2	1.53	0.72
2:JP1:612:CYS:HB2	2:JP1:626:ARG:HE	1.53	0.72
2:FP1:72:GLY:HA3	2:FP1:784:LEU:HD21	1.71	0.72
2:IP1:41:LEU:HB2	2:JP1:828:VAL:HG11	1.72	0.72
1:DP1:123:GLN:HE22	1:DP1:256:THR:HG21	1.54	0.72
2:IP1:756:LEU:HA	2:IP1:759:MET:HG3	1.73	0.71
1:DP1:426:MET:HE1	1:EP1:422:ILE:HG23	1.72	0.71
2:IP1:266:PHE:H	2:IP1:276:ASN:HD21	1.36	0.71
2:GP1:759:MET:HE3	2:HP1:917:ILE:HG12	1.71	0.71
2:HP1:103:ILE:HG13	2:HP1:104:PRO:HD3	1.73	0.71
1:BP1:139:ASN:HB2	1:BP1:281:ARG:HH12	1.56	0.70
2:IP1:377:GLN:HE22	2:IP1:402:VAL:HG12	1.56	0.70
2:JP1:627:MET:HG2	2:JP1:628:MET:HE2	1.73	0.70
1:EP1:371:GLN:O	1:EP1:375:GLU:HB2	1.91	0.70
2:GP1:180:GLY:O	2:GP1:184:ILE:HD12	1.90	0.70
1:DP1:328:SER:HA	1:EP1:211:MET:HE2	1.74	0.70
2:FP1:732:MET:HA	2:FP1:732:MET:HE2	1.74	0.69
2:JP1:662:ILE:HG12	2:JP1:703:LEU:HD12	1.74	0.69
2:JP1:920:SER:O	2:JP1:924:ILE:HD12	1.92	0.69
2:GP1:648:PHE:O	2:GP1:652:ILE:HG13	1.93	0.69
1:BP1:94:MET:HG3	1:CP1:241:SER:HB2	1.73	0.69
1:DP1:426:MET:HE3	1:EP1:425:GLN:HB2	1.75	0.69
2:FP1:566:THR:HG23	2:FP1:569:GLY:H	1.56	0.69
2:HP1:377:GLN:HE22	2:HP1:402:VAL:H	1.40	0.69
2:GP1:788:HIS:HB3	2:GP1:790:GLU:HG3	1.75	0.68
2:HP1:320:ILE:HD11	2:HP1:325:LEU:HD12	1.75	0.68
2:IP1:932:LEU:HA	2:IP1:935:HIS:HB3	1.75	0.68
2:FP1:74:ILE:HA	2:FP1:77:MET:HE2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:104:ASP:HA	1:BP1:109:ASN:HD22	1.58	0.68
2:IP1:920:SER:O	2:IP1:924:ILE:HD12	1.94	0.68
2:GP1:716:LEU:HA	2:HP1:723:PHE:CD1	2.29	0.68
1:CP1:342:VAL:HG21	1:CP1:442:ILE:HG13	1.75	0.68
2:IP1:391:GLU:HG3	2:IP1:393:GLN:H	1.59	0.68
2:IP1:741:THR:HG23	2:IP1:916:LEU:HD21	1.75	0.68
1:BP1:342:VAL:HG21	1:BP1:442:ILE:HG13	1.75	0.68
2:IP1:566:THR:HG23	2:IP1:569:GLY:H	1.58	0.68
2:HP1:929:ALA:O	2:HP1:932:LEU:HD12	1.94	0.68
2:FP1:266:PHE:H	2:FP1:276:ASN:HD21	1.42	0.68
1:AP1:104:ASP:HA	1:AP1:109:ASN:HD22	1.59	0.67
2:HP1:757:PRO:HG3	2:HP1:930:PHE:HE1	1.60	0.67
1:EP1:185:PRO:HG3	1:EP1:204:LEU:HD12	1.76	0.67
1:BP1:123:GLN:HE22	1:BP1:256:THR:HG21	1.59	0.67
1:EP1:74:VAL:O	1:EP1:78:GLN:HG2	1.95	0.67
2:GP1:920:SER:O	2:GP1:924:ILE:HD12	1.95	0.67
2:GP1:656:VAL:HG12	2:GP1:660:LEU:HD23	1.76	0.67
2:JP1:723:PHE:CD2	2:JP1:724:ILE:HD13	2.29	0.67
1:AP1:342:VAL:HG21	1:AP1:442:ILE:HG13	1.75	0.67
1:BP1:248:LEU:HD22	1:BP1:249:ILE:HG22	1.75	0.67
2:HP1:192:LEU:HB2	2:HP1:351:VAL:HG21	1.75	0.67
2:HP1:594:ILE:HB	2:HP1:660:LEU:HD12	1.75	0.67
2:FP1:242:LYS:HG2	2:FP1:261:LEU:HD23	1.76	0.67
2:HP1:651:MET:O	2:HP1:655:ILE:HG13	1.95	0.67
3:MP1:25:ALA:O	3:MP1:29:ILE:HG12	1.95	0.67
2:FP1:78:TYR:O	2:FP1:82:VAL:HG23	1.95	0.66
1:BP1:54:ILE:HG22	1:CP1:42:TYR:HD2	1.60	0.66
2:FP1:745:ILE:HG23	2:FP1:919:THR:HG21	1.78	0.66
2:IP1:709:ASN:HD21	2:JP1:597:LYS:H	1.44	0.66
1:CP1:136:ILE:HG23	1:CP1:277:LEU:HD22	1.77	0.66
1:CP1:328:SER:HA	1:DP1:211:MET:HE2	1.78	0.66
2:IP1:72:GLY:O	2:IP1:76:ILE:HG13	1.95	0.66
1:BP1:40:VAL:O	1:BP1:44:THR:HG23	1.96	0.66
2:IP1:759:MET:HA	2:JP1:921:MET:HE1	1.76	0.66
2:GP1:450:ARG:O	2:GP1:453:ILE:HG13	1.96	0.65
2:GP1:651:MET:O	2:GP1:655:ILE:HG12	1.96	0.65
2:HP1:242:LYS:HG2	2:HP1:261:LEU:HD23	1.76	0.65
2:IP1:72:GLY:HA3	2:IP1:784:LEU:HD11	1.76	0.65
2:JP1:566:THR:HG23	2:JP1:569:GLY:H	1.60	0.65
1:BP1:430:ARG:HH21	1:CP1:425:GLN:HB3	1.59	0.65
1:DP1:74:VAL:O	1:DP1:78:GLN:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:627:MET:HG2	2:IP1:628:MET:HE2	1.78	0.65
3:LP1:24:THR:HA	3:LP1:27:LEU:HD12	1.77	0.65
1:AP1:33:SER:HB2	1:BP1:31:GLN:OE1	1.96	0.65
2:GP1:732:MET:HE2	2:GP1:732:MET:HA	1.79	0.65
2:IP1:757:PRO:HG3	2:IP1:930:PHE:CE1	2.32	0.64
2:IP1:841:ILE:HD12	2:IP1:844:ILE:HB	1.79	0.64
2:GP1:702:THR:HG23	2:HP1:905:TRP:HE1	1.61	0.64
2:HP1:180:GLY:O	2:HP1:184:ILE:HD12	1.96	0.64
1:CP1:74:VAL:O	1:CP1:78:GLN:HG2	1.96	0.64
2:GP1:706:THR:HG22	2:GP1:710:MET:HE2	1.80	0.64
2:HP1:662:ILE:HG12	2:HP1:703:LEU:HD11	1.80	0.64
2:JP1:72:GLY:HA3	2:JP1:784:LEU:HD11	1.79	0.64
3:MP1:16:ARG:O	3:MP1:20:ILE:HG13	1.97	0.64
1:AP1:74:VAL:O	1:AP1:78:GLN:HG2	1.98	0.64
2:HP1:738:TRP:CD1	2:HP1:912:PHE:HZ	2.15	0.64
2:HP1:648:PHE:O	2:HP1:652:ILE:HG22	1.98	0.64
2:IP1:639:TYR:HE2	2:JP1:605:MET:HE1	1.61	0.64
2:HP1:932:LEU:HA	2:HP1:935:HIS:CD2	2.33	0.64
2:GP1:132:ILE:HG13	2:GP1:772:VAL:HG13	1.80	0.63
2:GP1:759:MET:HG3	2:HP1:921:MET:HE2	1.78	0.63
2:FP1:667:MET:HE1	2:FP1:915:ILE:HG21	1.80	0.63
2:HP1:182:LEU:HD23	2:HP1:571:VAL:HG21	1.80	0.63
2:IP1:332:ARG:HH21	2:IP1:489:THR:HA	1.63	0.63
2:FP1:741:THR:O	2:FP1:745:ILE:HG13	1.99	0.63
2:GP1:766:PHE:HZ	2:HP1:829:GLY:HA3	1.63	0.63
2:JP1:807:ASN:HD22	2:JP1:941:LEU:HG	1.64	0.63
1:AP1:254:MET:HG3	1:AP1:355:LEU:HD12	1.81	0.63
1:EP1:136:ILE:HG23	1:EP1:277:LEU:HD22	1.81	0.63
2:HP1:728:ILE:HD11	2:IP1:729:MET:HE3	1.80	0.63
1:EP1:141:LEU:HB3	1:EP1:213:ASN:HB3	1.81	0.63
1:AP1:111:LEU:HD23	1:BP1:386:PRO:HB3	1.81	0.62
2:HP1:804:ILE:HD12	2:HP1:807:ASN:HD22	1.64	0.62
2:IP1:45:VAL:HG11	2:IP1:129:MET:HG2	1.81	0.62
1:DP1:129:SER:HB2	1:DP1:137:THR:HG21	1.81	0.62
2:HP1:932:LEU:HB3	2:HP1:936:LEU:HD12	1.82	0.62
2:IP1:100:SER:HA	2:IP1:103:ILE:HD12	1.81	0.62
1:BP1:83:ASN:HB2	1:BP1:359:MET:HE1	1.82	0.62
2:GP1:110:GLY:HA3	2:GP1:787:THR:HG23	1.82	0.62
2:JP1:905:TRP:HA	2:JP1:908:VAL:HB	1.80	0.62
3:MP1:16:ARG:NE	3:MP1:20:ILE:HD11	2.13	0.62
1:AP1:211:MET:HE2	1:EP1:328:SER:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:804:ILE:O	2:HP1:808:VAL:HG22	2.00	0.62
2:IP1:744:SER:O	2:IP1:748:VAL:HG23	2.00	0.62
1:DP1:427:TYR:HA	1:DP1:430:ARG:NH1	2.15	0.62
2:IP1:704:TRP:HA	2:IP1:707:LEU:HD12	1.81	0.62
1:CP1:104:ASP:HA	1:CP1:109:ASN:HD22	1.65	0.61
3:KP1:16:ARG:O	3:KP1:20:ILE:HG12	2.00	0.61
1:AP1:31:GLN:HE21	1:EP1:33:SER:HB2	1.63	0.61
2:JP1:402:VAL:HG12	2:JP1:404:SER:H	1.65	0.61
2:HP1:732:MET:HA	2:HP1:732:MET:HE2	1.80	0.61
2:JP1:616:LYS:HA	2:JP1:620:PHE:O	2.00	0.61
3:MP1:24:THR:HA	3:MP1:27:LEU:HD12	1.82	0.61
1:BP1:142:ILE:HA	1:BP1:210:VAL:HG23	1.83	0.61
2:IP1:131:VAL:HG21	2:IP1:805:LEU:HD11	1.82	0.61
2:JP1:101:ILE:HG12	3:MP1:16:ARG:HH22	1.65	0.61
1:DP1:427:TYR:HA	1:DP1:430:ARG:HH11	1.65	0.61
2:GP1:708:LEU:HD13	2:HP1:730:MET:HB3	1.81	0.61
2:GP1:768:TRP:O	2:GP1:772:VAL:HG23	2.00	0.61
2:IP1:528:ILE:HD11	2:IP1:538:PRO:HD3	1.81	0.61
2:JP1:590:PHE:CE2	2:JP1:664:LEU:HD13	2.35	0.61
2:JP1:630:ASP:HA	2:JP1:634:ASN:HB2	1.82	0.61
1:DP1:427:TYR:HD1	1:DP1:430:ARG:HH12	1.49	0.61
1:EP1:104:ASP:HA	1:EP1:109:ASN:HD22	1.65	0.61
2:FP1:330:LEU:O	2:FP1:334:ILE:HG13	2.00	0.61
2:GP1:721:GLY:HA3	2:HP1:723:PHE:HE1	1.66	0.61
2:IP1:183:THR:HG23	2:IP1:496:PHE:HB2	1.83	0.61
1:DP1:136:ILE:HG23	1:DP1:277:LEU:HD22	1.82	0.61
2:GP1:103:ILE:HG13	2:GP1:104:PRO:HD3	1.82	0.61
3:NP1:16:ARG:HE	3:NP1:17:THR:HG22	1.65	0.61
2:JP1:932:LEU:HA	2:JP1:935:HIS:HB3	1.82	0.61
2:FP1:804:ILE:O	2:FP1:808:VAL:HG22	2.00	0.60
2:GP1:747:PHE:HA	2:GP1:751:TYR:HD2	1.65	0.60
2:IP1:106:ARG:HE	2:IP1:794:ALA:HA	1.67	0.60
1:BP1:129:SER:HB2	1:BP1:137:THR:HG21	1.83	0.60
2:FP1:113:LEU:HD13	2:FP1:123:MET:HG3	1.82	0.60
2:FP1:593:LEU:H	2:FP1:593:LEU:HD23	1.67	0.60
2:GP1:804:ILE:O	2:GP1:808:VAL:HG22	2.00	0.60
2:HP1:816:ILE:O	2:HP1:820:ILE:HG13	2.02	0.60
1:BP1:55:THR:HA	1:CP1:42:TYR:HE2	1.67	0.60
2:HP1:928:LYS:O	2:HP1:931:THR:HG22	2.01	0.60
1:AP1:339:GLN:HB3	1:EP1:448:LEU:HD11	1.84	0.60
1:CP1:81:ALA:HB2	1:CP1:378:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:470:ASP:HA	2:GP1:473:LYS:HD2	1.84	0.59
1:CP1:40:VAL:O	1:CP1:44:THR:HG23	2.02	0.59
2:GP1:757:PRO:HG3	2:GP1:930:PHE:CE2	2.38	0.59
2:IP1:732:MET:HE2	2:IP1:732:MET:HA	1.84	0.59
1:AP1:174:VAL:HG13	1:BP1:244:ASN:HD21	1.67	0.59
1:CP1:141:LEU:HD22	1:CP1:213:ASN:HB3	1.83	0.59
2:HP1:907:GLY:O	2:HP1:910:ALA:HB3	2.02	0.59
1:DP1:182:LEU:HD11	1:EP1:243:LEU:HD12	1.84	0.59
2:GP1:612:CYS:HB3	2:GP1:626:ARG:HB2	1.85	0.59
2:HP1:391:GLU:HG3	2:HP1:393:GLN:H	1.67	0.59
1:DP1:352:SER:HA	1:DP1:355:LEU:HD23	1.84	0.59
2:FP1:504:PRO:HG3	2:FP1:513:TYR:HB2	1.85	0.59
2:GP1:785:GLY:HA2	2:GP1:788:HIS:CD2	2.37	0.59
1:CP1:352:SER:HA	1:CP1:355:LEU:HD12	1.85	0.59
2:JP1:188:GLN:O	2:JP1:192:LEU:HD13	2.03	0.59
2:FP1:287:ILE:HD12	2:FP1:287:ILE:H	1.68	0.59
2:JP1:287:ILE:HD12	2:JP1:287:ILE:H	1.67	0.59
2:FP1:675:VAL:O	2:FP1:679:THR:HG23	2.03	0.59
2:HP1:566:THR:HG23	2:HP1:569:GLY:H	1.67	0.59
2:JP1:289:ALA:HA	2:JP1:312:SER:HB2	1.84	0.59
2:HP1:150:LEU:HD12	2:HP1:474:LEU:HG	1.85	0.59
2:JP1:136:VAL:HG22	2:JP1:461:TRP:HE1	1.68	0.59
1:BP1:430:ARG:NH2	1:CP1:425:GLN:HB3	2.18	0.58
2:GP1:182:LEU:HD23	2:GP1:571:VAL:HG21	1.85	0.58
2:IP1:38:LEU:HD21	2:IP1:129:MET:HE1	1.85	0.58
2:IP1:77:MET:O	2:IP1:81:MET:HG3	2.02	0.58
2:FP1:722:ILE:O	2:FP1:725:PHE:HB3	2.04	0.58
2:JP1:556:ARG:HD2	2:JP1:576:MET:HG2	1.85	0.58
2:HP1:938:ASP:O	2:HP1:941:LEU:HB2	2.04	0.58
1:DP1:191:MET:HG2	1:DP1:198:TRP:HA	1.86	0.58
2:FP1:403:PRO:HB3	2:JP1:268:LYS:HB3	1.84	0.58
2:FP1:588:LEU:HD13	2:FP1:661:MET:HG3	1.86	0.58
2:FP1:627:MET:HG2	2:FP1:628:MET:HE2	1.84	0.58
2:GP1:147:LEU:HB2	2:GP1:453:ILE:HG23	1.84	0.58
2:JP1:296:SER:HA	2:JP1:302:VAL:HG13	1.86	0.58
3:KP1:38:LYS:HE2	3:KP1:38:LYS:HA	1.86	0.58
2:IP1:367:LYS:HD3	2:IP1:367:LYS:N	2.19	0.58
1:EP1:142:ILE:HA	1:EP1:210:VAL:HG23	1.86	0.58
2:JP1:824:ALA:O	2:JP1:827:TYR:HB2	2.03	0.58
2:GP1:814:LEU:HD23	2:GP1:937:PRO:HA	1.87	0.57
3:OP1:30:ILE:O	3:OP1:34:ILE:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:242:LYS:HG2	2:GP1:261:LEU:HD23	1.86	0.57
1:CP1:105:LYS:HZ3	1:DP1:367:ASN:HA	1.67	0.57
1:AP1:141:LEU:HD23	1:AP1:213:ASN:HB3	1.86	0.57
1:AP1:94:MET:HE3	1:BP1:240:ILE:HB	1.85	0.57
1:BP1:427:TYR:HD1	1:BP1:430:ARG:HH12	1.51	0.57
2:GP1:528:ILE:HD11	2:GP1:538:PRO:HD3	1.86	0.57
2:IP1:77:MET:HE1	3:NP1:32:VAL:HG11	1.86	0.57
1:BP1:136:ILE:HG23	1:BP1:277:LEU:HD22	1.87	0.57
2:GP1:489:THR:HG23	2:GP1:491:LEU:H	1.70	0.57
2:JP1:512:PRO:HG2	2:JP1:513:TYR:CE1	2.39	0.57
2:JP1:702:THR:O	2:JP1:706:THR:HG23	2.05	0.57
2:GP1:785:GLY:HA2	2:GP1:788:HIS:NE2	2.19	0.57
2:HP1:757:PRO:HG3	2:HP1:930:PHE:CE1	2.40	0.57
2:IP1:402:VAL:HG13	2:IP1:405:SER:HB3	1.86	0.57
1:AP1:353:LYS:HG2	1:AP1:371:GLN:HE21	1.69	0.57
2:FP1:247:THR:HG22	2:FP1:256:PRO:HD2	1.87	0.57
2:HP1:151:ASN:HB3	2:HP1:152:ARG:HH11	1.69	0.56
2:JP1:668:LYS:HA	2:JP1:911:PHE:HE2	1.70	0.56
2:JP1:793:GLU:HG3	2:JP1:795:PHE:H	1.68	0.56
2:GP1:122:CYS:H	2:GP1:125:GLN:HG3	1.71	0.56
2:IP1:766:PHE:CZ	2:JP1:829:GLY:HA2	2.40	0.56
1:DP1:385:ASP:H	1:DP1:398:GLN:HE22	1.52	0.56
2:GP1:770:ILE:HA	2:GP1:773:ILE:HD12	1.87	0.56
2:IP1:766:PHE:CD1	2:JP1:925:ILE:HD11	2.40	0.56
2:IP1:940:VAL:O	2:IP1:944:ILE:HD12	2.05	0.56
2:FP1:807:ASN:HB2	2:FP1:941:LEU:HD11	1.87	0.56
2:HP1:287:ILE:HG22	2:HP1:289:ALA:H	1.71	0.56
2:HP1:766:PHE:HZ	2:IP1:829:GLY:HA2	1.71	0.56
1:BP1:236:ASN:O	1:BP1:240:ILE:HG13	2.05	0.56
2:FP1:33:LEU:HA	2:FP1:36:VAL:HB	1.86	0.56
2:FP1:148:SER:O	2:FP1:152:ARG:HD3	2.05	0.56
2:FP1:660:LEU:HD23	2:FP1:661:MET:H	1.70	0.56
2:HP1:528:ILE:HD11	2:HP1:538:PRO:HD3	1.87	0.56
2:GP1:690:ALA:O	2:GP1:694:THR:HG23	2.06	0.56
2:IP1:837:PHE:O	2:IP1:841:ILE:HG22	2.06	0.56
1:EP1:94:MET:HB2	1:EP1:98:LEU:HD23	1.88	0.56
2:HP1:383:LYS:HA	2:HP1:396:CYS:HA	1.88	0.56
2:JP1:222:MET:HE1	2:JP1:519:TRP:HA	1.87	0.56
2:FP1:685:PRO:HB2	2:FP1:830:VAL:HG11	1.88	0.56
2:IP1:136:VAL:HG13	2:IP1:461:TRP:HE1	1.71	0.56
2:FP1:555:GLN:HE22	2:FP1:588:LEU:HD12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:684:ASN:HD22	2:FP1:687:VAL:HG23	1.71	0.56
2:GP1:600:THR:HB	2:GP1:645:LEU:HD22	1.87	0.56
1:AP1:426:MET:HE1	1:BP1:422:ILE:HG23	1.88	0.56
2:FP1:640:VAL:HG22	2:GP1:605:MET:HE1	1.88	0.56
2:IP1:434:LEU:HD13	2:IP1:437:ILE:HD12	1.88	0.56
1:AP1:123:GLN:HE22	1:AP1:256:THR:HG21	1.70	0.55
1:DP1:263:GLN:H	1:DP1:268:THR:HG21	1.71	0.55
1:EP1:208:ASN:O	1:EP1:212:GLN:HG2	2.06	0.55
2:HP1:593:LEU:HD21	2:HP1:905:TRP:HB3	1.87	0.55
2:IP1:690:ALA:O	2:IP1:694:THR:HG23	2.05	0.55
2:JP1:590:PHE:HE2	2:JP1:664:LEU:HD13	1.70	0.55
1:CP1:208:ASN:O	1:CP1:212:GLN:HG2	2.06	0.55
2:HP1:630:ASP:HA	2:HP1:634:ASN:HB2	1.87	0.55
3:NP1:14:ASN:HB3	3:NP1:17:THR:HG23	1.88	0.55
1:AP1:285:ALA:HB1	1:EP1:449:LYS:HE3	1.89	0.55
2:GP1:724:ILE:O	2:GP1:728:ILE:HG22	2.06	0.55
2:HP1:35:VAL:HA	2:HP1:38:LEU:HB2	1.87	0.55
2:HP1:331:SER:HA	2:HP1:334:ILE:HD12	1.87	0.55
2:FP1:548:PRO:HD3	2:FP1:568:TYR:CD1	2.41	0.55
2:JP1:844:ILE:HA	2:JP1:902:TYR:HE2	1.72	0.55
1:CP1:142:ILE:HD11	1:CP1:267:LEU:HD22	1.88	0.55
1:BP1:426:MET:HE1	1:CP1:422:ILE:HG23	1.88	0.55
1:EP1:342:VAL:HG21	1:EP1:442:ILE:HG13	1.89	0.55
2:JP1:667:MET:HE2	2:JP1:912:PHE:CD1	2.41	0.55
1:DP1:193:ASN:HD21	2:JP1:216:GLY:HA3	1.71	0.55
2:FP1:821:ALA:HA	2:JP1:57:MET:HE1	1.88	0.55
2:GP1:773:ILE:HD11	2:HP1:825:LEU:HD21	1.88	0.55
2:IP1:618:LEU:HD23	2:JP1:618:LEU:HB2	1.89	0.55
2:GP1:179:LYS:HA	2:GP1:550:LEU:HD23	1.89	0.55
2:JP1:807:ASN:ND2	2:JP1:941:LEU:HG	2.22	0.55
2:GP1:671:PHE:CG	2:GP1:915:ILE:HD11	2.42	0.55
2:IP1:788:HIS:HB3	2:IP1:790:GLU:HG3	1.89	0.54
2:IP1:911:PHE:O	2:IP1:915:ILE:HG22	2.07	0.54
2:JP1:392:TYR:HE2	2:JP1:585:ILE:HG21	1.71	0.54
1:BP1:139:ASN:HB2	1:BP1:281:ARG:NH1	2.22	0.54
2:HP1:180:GLY:HA3	2:HP1:491:LEU:HD23	1.88	0.54
2:HP1:931:THR:HG23	2:HP1:935:HIS:NE2	2.22	0.54
1:EP1:123:GLN:HE22	1:EP1:256:THR:HG21	1.71	0.54
2:IP1:768:TRP:HB2	2:IP1:815:MET:HE1	1.89	0.54
2:FP1:648:PHE:CZ	2:FP1:652:ILE:HD11	2.42	0.54
2:HP1:814:LEU:HD13	2:HP1:937:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:822:ALA:HB1	2:HP1:930:PHE:HD2	1.72	0.54
1:AP1:93:ALA:HB3	1:AP1:172:ASP:HB2	1.90	0.54
1:CP1:129:SER:H	1:CP1:137:THR:HG21	1.72	0.54
2:HP1:738:TRP:CD1	2:HP1:912:PHE:CZ	2.96	0.54
2:IP1:162:ASP:HB3	2:IP1:165:LYS:HB2	1.90	0.54
2:IP1:932:LEU:HB3	2:IP1:936:LEU:HD23	1.90	0.54
2:GP1:532:SER:HA	2:GP1:537:VAL:H	1.71	0.54
2:HP1:212:PRO:HA	2:HP1:215:GLY:H	1.73	0.54
3:KP1:23:PHE:O	3:KP1:27:LEU:HG	2.07	0.54
2:HP1:745:ILE:HG12	2:HP1:919:THR:HG21	1.89	0.54
2:IP1:287:ILE:HG13	2:IP1:332:ARG:HH12	1.73	0.54
1:AP1:206:TYR:O	1:AP1:210:VAL:HG12	2.08	0.54
1:BP1:185:PRO:HG3	1:BP1:204:LEU:HD22	1.88	0.54
2:IP1:837:PHE:HZ	2:IP1:917:ILE:HG23	1.72	0.54
2:JP1:147:LEU:HD22	2:JP1:453:ILE:HG23	1.90	0.54
2:FP1:60:MET:CE	2:GP1:817:ILE:HG12	2.36	0.54
2:FP1:182:LEU:HD23	2:FP1:571:VAL:HG21	1.89	0.54
2:FP1:556:ARG:HD2	2:FP1:576:MET:HG2	1.90	0.54
2:JP1:554:PRO:HB3	2:JP1:587:PRO:HA	1.89	0.54
1:BP1:280:ILE:HG23	1:BP1:347:LEU:HD23	1.90	0.53
2:GP1:594:ILE:HG21	2:GP1:660:LEU:HD22	1.89	0.53
2:IP1:73:GLY:C	2:IP1:77:MET:HE2	2.32	0.53
2:JP1:187:GLY:HA2	2:JP1:279:CYS:HB3	1.90	0.53
3:OP1:16:ARG:O	3:OP1:20:ILE:HG22	2.08	0.53
3:OP1:38:LYS:HE2	3:OP1:38:LYS:HA	1.89	0.53
2:HP1:822:ALA:HB1	2:HP1:930:PHE:CD2	2.43	0.53
2:JP1:450:ARG:HG2	2:JP1:453:ILE:HD11	1.90	0.53
1:BP1:177:ALA:O	1:BP1:181:ILE:HG12	2.08	0.53
1:DP1:298:TYR:HD1	1:DP1:298:TYR:O	1.91	0.53
2:GP1:648:PHE:HA	2:GP1:651:MET:HB2	1.90	0.53
2:IP1:669:ASP:HA	2:IP1:672:ILE:HG12	1.90	0.53
2:JP1:532:SER:HA	2:JP1:537:VAL:H	1.74	0.53
1:BP1:182:LEU:HD11	1:CP1:243:LEU:HD12	1.89	0.53
2:FP1:45:VAL:HG21	2:FP1:129:MET:HG2	1.90	0.53
2:FP1:548:PRO:HD3	2:FP1:568:TYR:HD1	1.74	0.53
2:GP1:667:MET:HE2	2:GP1:912:PHE:CD2	2.44	0.53
2:HP1:725:PHE:CD1	2:IP1:729:MET:HE1	2.43	0.53
2:HP1:725:PHE:CE1	2:IP1:729:MET:HE1	2.43	0.53
3:OP1:9:LYS:HD3	3:OP1:9:LYS:N	2.23	0.53
2:GP1:261:LEU:HB2	2:GP1:284:TRP:HZ3	1.71	0.53
2:GP1:841:ILE:HD12	2:GP1:844:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:721:GLY:O	2:IP1:724:ILE:HG22	2.09	0.53
2:FP1:617:ILE:HG22	2:FP1:618:LEU:H	1.73	0.53
2:HP1:725:PHE:CD1	2:HP1:725:PHE:C	2.87	0.53
3:KP1:16:ARG:NH1	3:KP1:20:ILE:HD13	2.24	0.53
1:BP1:141:LEU:HB3	1:BP1:213:ASN:HB3	1.91	0.53
2:HP1:732:MET:O	2:HP1:736:MET:HB2	2.09	0.53
2:IP1:151:ASN:HB2	2:IP1:453:ILE:HD13	1.89	0.53
2:IP1:668:LYS:O	2:IP1:672:ILE:HG23	2.09	0.53
2:FP1:618:LEU:HD23	2:GP1:618:LEU:HB2	1.91	0.53
2:FP1:756:LEU:HA	2:FP1:759:MET:HG3	1.91	0.53
2:IP1:929:ALA:O	2:IP1:932:LEU:HD12	2.09	0.53
1:AP1:90:PRO:HG2	1:BP1:246:ASN:HD21	1.73	0.53
1:CP1:421:GLU:O	1:CP1:425:GLN:HG3	2.09	0.53
2:FP1:630:ASP:HA	2:FP1:634:ASN:HB2	1.89	0.53
2:IP1:164:THR:HG21	2:IP1:583:PRO:HA	1.90	0.53
2:IP1:588:LEU:HD13	2:IP1:660:LEU:HD11	1.90	0.53
2:JP1:94:LEU:HD13	2:JP1:98:TRP:HD1	1.74	0.53
2:JP1:347:ALA:O	2:JP1:351:VAL:HG12	2.08	0.53
2:GP1:221:GLU:CD	2:GP1:221:GLU:H	2.17	0.52
2:GP1:652:ILE:O	2:GP1:656:VAL:HG23	2.09	0.52
2:HP1:920:SER:O	2:HP1:924:ILE:HD12	2.09	0.52
2:HP1:640:VAL:HG22	2:IP1:605:MET:HE1	1.91	0.52
2:IP1:148:SER:O	2:IP1:152:ARG:HD3	2.09	0.52
2:IP1:685:PRO:HB2	2:IP1:830:VAL:HG11	1.92	0.52
2:JP1:33:LEU:HD12	2:JP1:37:PHE:CZ	2.43	0.52
3:OP1:23:PHE:O	3:OP1:27:LEU:HD22	2.09	0.52
2:FP1:722:ILE:HG23	2:FP1:723:PHE:HD1	1.74	0.52
2:GP1:176:GLY:HA3	2:GP1:492:ASP:HB2	1.90	0.52
2:HP1:673:VAL:O	2:HP1:677:THR:HG22	2.10	0.52
2:IP1:213:PRO:O	2:IP1:218:PRO:HB3	2.09	0.52
2:IP1:804:ILE:O	2:IP1:808:VAL:HG22	2.09	0.52
2:JP1:757:PRO:HB3	2:JP1:930:PHE:HE2	1.74	0.52
3:NP1:18:ARG:O	3:NP1:22:ILE:HD13	2.10	0.52
2:FP1:663:PRO:HG3	2:FP1:703:LEU:HD11	1.91	0.52
2:IP1:706:THR:O	2:IP1:710:MET:HG2	2.09	0.52
2:IP1:713:VAL:HG13	2:JP1:723:PHE:CD1	2.44	0.52
1:AP1:305:ALA:HA	1:AP1:319:GLN:HG2	1.91	0.52
1:BP1:328:SER:HA	1:CP1:211:MET:HE2	1.92	0.52
1:CP1:42:TYR:HA	1:CP1:45:ASN:ND2	2.23	0.52
2:FP1:723:PHE:CZ	2:JP1:724:ILE:HG13	2.44	0.52
1:AP1:48:LYS:HG2	1:EP1:64:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:819:TYR:O	2:FP1:823:ILE:HG22	2.10	0.52
1:AP1:280:ILE:HD11	1:AP1:351:LEU:HB2	1.90	0.52
2:FP1:124:MET:HG3	2:FP1:779:ALA:HB1	1.91	0.52
2:FP1:732:MET:O	2:FP1:736:MET:HB2	2.10	0.52
2:GP1:757:PRO:HG3	2:GP1:930:PHE:CZ	2.45	0.52
2:FP1:725:PHE:CD2	2:GP1:729:MET:HE1	2.44	0.52
2:HP1:122:CYS:H	2:HP1:125:GLN:HG3	1.74	0.52
2:HP1:766:PHE:CZ	2:IP1:829:GLY:HA2	2.45	0.52
2:JP1:304:VAL:HB	2:JP1:318:LEU:H	1.74	0.52
2:JP1:237:VAL:HG13	2:JP1:261:LEU:HD21	1.90	0.52
3:KP1:15:THR:HG22	3:KP1:18:ARG:HH22	1.75	0.52
2:HP1:747:PHE:HA	2:HP1:751:TYR:HD2	1.74	0.52
1:DP1:254:MET:HB3	1:DP1:273:ALA:HB2	1.93	0.51
2:HP1:275:LEU:O	2:HP1:278:ILE:HG22	2.10	0.51
2:HP1:905:TRP:HA	2:HP1:908:VAL:HG13	1.92	0.51
2:JP1:175:SER:HB2	2:JP1:488:GLY:H	1.74	0.51
1:CP1:55:THR:HA	1:DP1:42:TYR:CE1	2.46	0.51
2:GP1:468:PHE:CD1	2:GP1:757:PRO:HG2	2.44	0.51
2:GP1:605:MET:HE2	2:GP1:637:PHE:HE2	1.74	0.51
2:HP1:841:ILE:HD12	2:HP1:844:ILE:HB	1.92	0.51
2:IP1:73:GLY:O	2:IP1:77:MET:HE2	2.11	0.51
2:JP1:183:THR:HG23	2:JP1:496:PHE:HB2	1.92	0.51
2:FP1:77:MET:HG2	3:LP1:28:LEU:HD11	1.91	0.51
2:HP1:33:LEU:HD23	2:HP1:462:ILE:HD11	1.91	0.51
1:AP1:346:ASN:OD1	1:EP1:437:LEU:HD11	2.09	0.51
2:GP1:41:LEU:HD22	2:GP1:42:PHE:CD2	2.45	0.51
2:IP1:182:LEU:HD23	2:IP1:571:VAL:HG21	1.91	0.51
2:IP1:468:PHE:CE1	2:IP1:930:PHE:HZ	2.28	0.51
2:IP1:74:ILE:HA	2:IP1:77:MET:HG2	1.91	0.51
2:JP1:318:LEU:HD11	2:JP1:439:GLN:HB2	1.91	0.51
1:CP1:430:ARG:HH21	1:DP1:425:GLN:HB3	1.76	0.51
2:FP1:718:PRO:HB3	2:GP1:719:LEU:HD11	1.92	0.51
2:GP1:107:SER:HA	2:GP1:787:THR:HG22	1.91	0.51
2:GP1:290:LEU:HB2	2:GP1:329:ARG:NH1	2.26	0.51
2:IP1:673:VAL:O	2:IP1:677:THR:HG22	2.11	0.51
1:AP1:182:LEU:HD11	1:BP1:243:LEU:HD12	1.92	0.51
2:FP1:745:ILE:HD13	2:FP1:915:ILE:HG13	1.93	0.51
2:GP1:656:VAL:HG12	2:GP1:660:LEU:CD2	2.41	0.51
2:GP1:909:TYR:O	2:GP1:912:PHE:HB2	2.11	0.51
2:IP1:944:ILE:HD12	2:IP1:944:ILE:H	1.76	0.51
1:AP1:451:ALA:HB1	2:HP1:619:PHE:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:78:TYR:HA	2:GP1:81:MET:SD	2.51	0.51
2:GP1:179:LYS:HE2	2:GP1:547:GLN:HE22	1.75	0.51
2:GP1:192:LEU:HB2	2:GP1:351:VAL:HG21	1.93	0.51
2:GP1:373:ILE:HG13	2:GP1:533:LEU:HD23	1.92	0.51
2:HP1:713:VAL:O	2:HP1:716:LEU:HD23	2.11	0.51
2:IP1:728:ILE:HD11	2:JP1:730:MET:SD	2.51	0.51
3:OP1:15:THR:HG22	3:OP1:18:ARG:HH22	1.76	0.51
1:AP1:136:ILE:HG23	1:AP1:277:LEU:HD22	1.93	0.51
2:GP1:566:THR:HG23	2:GP1:569:GLY:H	1.76	0.51
2:GP1:670:ILE:HD13	2:GP1:695:MET:HB3	1.93	0.51
2:HP1:222:MET:HE1	2:HP1:519:TRP:HA	1.91	0.51
2:HP1:669:ASP:O	2:HP1:673:VAL:HG13	2.10	0.51
2:IP1:501:LEU:HB3	2:IP1:527:LEU:HD23	1.93	0.51
1:BP1:230:PHE:CD1	1:BP1:230:PHE:C	2.89	0.50
1:DP1:142:ILE:HG22	1:DP1:210:VAL:HG23	1.94	0.50
2:FP1:69:LEU:HD21	3:LP1:31:ALA:HB1	1.94	0.50
2:FP1:150:LEU:HD12	2:FP1:474:LEU:HD23	1.93	0.50
2:FP1:648:PHE:HB2	2:FP1:717:ILE:HD12	1.92	0.50
2:IP1:60:MET:SD	2:JP1:817:ILE:HD13	2.51	0.50
2:IP1:338:GLN:HA	2:IP1:341:VAL:HG22	1.91	0.50
2:JP1:182:LEU:HD23	2:JP1:571:VAL:HG21	1.92	0.50
3:OP1:15:THR:HA	3:OP1:18:ARG:CZ	2.41	0.50
2:FP1:132:ILE:HG12	2:FP1:772:VAL:HG23	1.93	0.50
2:FP1:450:ARG:O	2:FP1:453:ILE:HD12	2.11	0.50
2:JP1:470:ASP:O	2:JP1:473:LYS:HG2	2.11	0.50
1:BP1:206:TYR:O	1:BP1:210:VAL:HG12	2.11	0.50
2:GP1:634:ASN:O	2:GP1:638:ARG:HB3	2.12	0.50
2:HP1:706:THR:O	2:HP1:710:MET:HG2	2.11	0.50
2:HP1:922:TYR:O	2:HP1:925:ILE:HB	2.12	0.50
1:AP1:208:ASN:O	1:AP1:212:GLN:HG2	2.11	0.50
1:CP1:182:LEU:HD11	1:DP1:243:LEU:HD12	1.92	0.50
2:FP1:643:PHE:O	2:FP1:647:ILE:HG22	2.12	0.50
2:IP1:330:LEU:HB3	2:IP1:333:ALA:HB3	1.93	0.50
2:IP1:814:LEU:HD13	2:IP1:937:PRO:HA	1.93	0.50
1:AP1:54:ILE:HG23	1:BP1:45:ASN:OD1	2.12	0.50
1:BP1:174:VAL:HG11	1:BP1:345:SER:HB2	1.94	0.50
2:GP1:630:ASP:HA	2:GP1:634:ASN:HB2	1.93	0.50
2:IP1:468:PHE:HE1	2:IP1:930:PHE:HZ	1.59	0.50
2:GP1:722:ILE:O	2:GP1:725:PHE:HB3	2.11	0.50
2:IP1:370:PHE:CD1	2:IP1:377:GLN:HB3	2.46	0.50
2:IP1:662:ILE:HD13	2:IP1:703:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JP1:113:LEU:HA	2:JP1:123:MET:HB2	1.93	0.50
2:JP1:392:TYR:CE2	2:JP1:585:ILE:HG21	2.46	0.50
2:JP1:661:MET:O	2:JP1:665:GLN:HB2	2.12	0.50
1:AP1:42:TYR:CE1	1:EP1:55:THR:HA	2.47	0.50
2:FP1:841:ILE:HD12	2:FP1:844:ILE:HB	1.93	0.50
2:GP1:77:MET:HG3	2:GP1:81:MET:HE3	1.93	0.50
2:IP1:167:LEU:HD12	2:IP1:585:ILE:HD11	1.94	0.50
2:IP1:347:ALA:O	2:IP1:351:VAL:HG22	2.11	0.50
2:IP1:655:ILE:HD11	2:IP1:710:MET:HB2	1.92	0.50
3:LP1:7:ASN:O	3:LP1:11:LEU:HG	2.12	0.50
1:AP1:142:ILE:HA	1:AP1:210:VAL:HG23	1.93	0.50
1:BP1:55:THR:HA	1:CP1:42:TYR:CE2	2.47	0.50
1:BP1:347:LEU:HA	1:BP1:350:ILE:HG22	1.91	0.50
2:GP1:370:PHE:HB2	2:GP1:410:THR:HG21	1.93	0.50
1:AP1:179:PHE:HB2	1:BP1:240:ILE:HD13	1.93	0.49
1:DP1:104:ASP:HA	1:DP1:109:ASN:HD22	1.75	0.49
2:HP1:49:LEU:HG	2:HP1:51:GLY:H	1.77	0.49
2:HP1:468:PHE:CD1	2:HP1:757:PRO:HG2	2.47	0.49
2:HP1:939:LYS:HE3	2:HP1:939:LYS:HA	1.94	0.49
1:EP1:280:ILE:HD11	1:EP1:351:LEU:HB2	1.94	0.49
2:GP1:103:ILE:HG22	2:GP1:106:ARG:HH21	1.76	0.49
2:HP1:147:LEU:HB2	2:HP1:453:ILE:HG23	1.94	0.49
1:AP1:35:ASN:O	1:AP1:39:LEU:HD23	2.12	0.49
2:FP1:594:ILE:HB	2:FP1:660:LEU:HD12	1.95	0.49
2:HP1:738:TRP:HD1	2:HP1:912:PHE:CZ	2.29	0.49
2:IP1:268:LYS:HB3	2:JP1:403:PRO:HB3	1.95	0.49
2:JP1:338:GLN:HA	2:JP1:341:VAL:HG12	1.94	0.49
1:AP1:434:GLU:OE2	1:BP1:350:ILE:HD11	2.12	0.49
1:CP1:94:MET:HG3	1:DP1:241:SER:HB3	1.94	0.49
1:DP1:206:TYR:O	1:DP1:210:VAL:HG12	2.12	0.49
2:FP1:183:THR:HG23	2:FP1:496:PHE:HB2	1.94	0.49
2:GP1:381:PRO:HD2	2:GP1:573:ASN:ND2	2.27	0.49
2:HP1:593:LEU:HD11	2:HP1:905:TRP:HB3	1.93	0.49
2:IP1:692:MET:HA	2:IP1:695:MET:HE3	1.94	0.49
2:IP1:718:PRO:O	2:IP1:719:LEU:HB2	2.11	0.49
3:KP1:18:ARG:O	3:KP1:22:ILE:HD13	2.12	0.49
1:CP1:172:ASP:HB3	1:CP1:175:SER:OG	2.12	0.49
1:DP1:342:VAL:HG21	1:DP1:442:ILE:HG13	1.94	0.49
1:EP1:269:ALA:HB1	1:EP1:274:GLN:HB3	1.93	0.49
2:FP1:124:MET:HG2	2:FP1:783:ALA:HB2	1.94	0.49
2:GP1:666:GLY:O	2:GP1:670:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:110:GLY:HA3	2:IP1:787:THR:HG22	1.94	0.49
3:MP1:36:PHE:HA	3:MP1:39:ILE:HD11	1.95	0.49
2:GP1:713:VAL:HG22	2:HP1:727:LEU:HB2	1.94	0.49
2:JP1:103:ILE:HG22	2:JP1:104:PRO:HD3	1.93	0.49
3:KP1:28:LEU:O	3:KP1:32:VAL:HG13	2.11	0.49
2:GP1:223:ASN:O	2:GP1:227:ARG:HG2	2.13	0.49
2:GP1:766:PHE:CZ	2:HP1:925:ILE:HG23	2.48	0.49
2:HP1:84:THR:HA	2:HP1:87:THR:HG22	1.94	0.49
2:IP1:663:PRO:HG3	2:IP1:738:TRP:CH2	2.48	0.49
1:BP1:280:ILE:HD11	1:BP1:351:LEU:HB2	1.93	0.49
1:CP1:444:LEU:HD13	1:DP1:443:MET:HB2	1.95	0.49
2:GP1:136:VAL:HG22	2:GP1:461:TRP:HE1	1.78	0.49
2:JP1:259:PHE:HE2	2:JP1:286:ASN:HB2	1.77	0.49
1:AP1:230:PHE:C	1:AP1:230:PHE:CD1	2.91	0.49
2:FP1:605:MET:HE1	2:JP1:640:VAL:HG22	1.95	0.49
2:HP1:664:LEU:O	2:HP1:668:LYS:HB2	2.13	0.49
1:CP1:86:LEU:HD21	1:DP1:376:PHE:CZ	2.48	0.48
1:DP1:455:ALA:HB1	1:EP1:293:PRO:HA	1.95	0.48
1:EP1:382:ARG:HB3	1:EP1:399:TRP:CD2	2.48	0.48
2:GP1:61:PHE:CE1	2:GP1:776:MET:HG3	2.48	0.48
2:JP1:247:THR:HG22	2:JP1:256:PRO:HD2	1.94	0.48
2:JP1:540:LEU:HD23	2:JP1:562:PRO:HB2	1.94	0.48
1:AP1:415:ILE:HG23	1:EP1:419:LEU:HD12	1.96	0.48
2:FP1:78:TYR:HA	2:FP1:81:MET:CE	2.36	0.48
2:FP1:111:LEU:HD13	3:LP1:31:ALA:HB2	1.96	0.48
2:GP1:57:MET:HE1	2:HP1:821:ALA:HA	1.93	0.48
2:IP1:662:ILE:HB	2:IP1:703:LEU:HD11	1.93	0.48
2:FP1:920:SER:O	2:FP1:924:ILE:HD12	2.13	0.48
2:HP1:111:LEU:HD13	3:OP1:31:ALA:HB2	1.95	0.48
2:HP1:176:GLY:HA3	2:HP1:492:ASP:HB2	1.95	0.48
1:CP1:119:THR:HG21	1:CP1:352:SER:HB2	1.96	0.48
2:JP1:184:ILE:HG13	2:JP1:263:MET:HE1	1.96	0.48
1:DP1:141:LEU:HD23	1:DP1:213:ASN:HB3	1.94	0.48
1:EP1:68:LEU:HD11	1:EP1:417:ILE:HD11	1.96	0.48
2:FP1:113:LEU:HD12	2:FP1:124:MET:HE2	1.96	0.48
2:FP1:769:LEU:HA	2:FP1:772:VAL:HG12	1.95	0.48
2:GP1:837:PHE:O	2:GP1:841:ILE:HG22	2.13	0.48
2:JP1:391:GLU:HG3	2:JP1:393:GLN:H	1.79	0.48
1:AP1:308:LYS:HG2	1:AP1:309:PRO:HD2	1.95	0.48
1:AP1:419:LEU:HD12	1:BP1:415:ILE:HG23	1.96	0.48
1:BP1:86:LEU:HD21	1:BP1:112:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:292:LEU:HD13	1:CP1:230:PHE:HE2	1.78	0.48
1:BP1:382:ARG:HB3	1:BP1:399:TRP:CE3	2.49	0.48
2:GP1:147:LEU:HB2	2:GP1:453:ILE:CG2	2.43	0.48
2:HP1:132:ILE:HG13	2:HP1:772:VAL:HG23	1.95	0.48
1:AP1:205:MET:HG3	1:AP1:209:LEU:HG	1.94	0.48
2:HP1:589:THR:HG22	2:HP1:664:LEU:HD21	1.96	0.48
2:JP1:461:TRP:CZ2	2:JP1:812:PRO:HB3	2.48	0.48
2:JP1:647:ILE:HG22	2:JP1:717:ILE:HG12	1.95	0.48
1:BP1:419:LEU:HD12	1:CP1:415:ILE:HG23	1.96	0.48
1:CP1:142:ILE:HD12	1:CP1:281:ARG:HD2	1.96	0.48
2:FP1:766:PHE:CE2	2:GP1:925:ILE:HD12	2.49	0.48
2:GP1:468:PHE:CG	2:GP1:757:PRO:HG2	2.49	0.48
2:GP1:612:CYS:HB2	2:GP1:623:CYS:HB2	1.61	0.48
2:HP1:936:LEU:O	2:HP1:940:VAL:HG23	2.14	0.48
2:IP1:450:ARG:HD3	2:IP1:474:LEU:HD11	1.95	0.48
2:FP1:723:PHE:HZ	2:JP1:724:ILE:HG13	1.79	0.48
2:GP1:663:PRO:HG3	2:GP1:703:LEU:HD11	1.96	0.48
2:HP1:338:GLN:HA	2:HP1:341:VAL:HG12	1.95	0.48
2:IP1:129:MET:O	2:IP1:132:ILE:HG13	2.13	0.48
2:JP1:799:GLU:HA	2:JP1:802:ILE:HD12	1.96	0.48
1:AP1:376:PHE:CZ	1:EP1:86:LEU:HD21	2.49	0.48
1:EP1:207:GLN:O	1:EP1:211:MET:HB2	2.13	0.48
2:FP1:434:LEU:HA	2:FP1:437:ILE:HG22	1.95	0.48
2:FP1:707:LEU:HD13	2:FP1:735:LEU:HD21	1.95	0.48
2:GP1:738:TRP:O	2:GP1:742:MET:HG3	2.14	0.48
2:HP1:165:LYS:HB3	2:HP1:485:PHE:HE2	1.78	0.48
2:IP1:136:VAL:HG13	2:IP1:461:TRP:NE1	2.28	0.48
2:IP1:354:ASP:HB3	2:IP1:357:PHE:HD1	1.78	0.48
2:IP1:732:MET:O	2:IP1:736:MET:HB2	2.13	0.48
1:BP1:90:PRO:HG3	1:BP1:349:TYR:HB2	1.95	0.47
1:BP1:421:GLU:O	1:BP1:425:GLN:HG3	2.14	0.47
1:EP1:206:TYR:O	1:EP1:210:VAL:HG12	2.14	0.47
2:GP1:114:LEU:HD21	2:GP1:783:ALA:HB3	1.96	0.47
2:GP1:179:LYS:HG2	2:GP1:492:ASP:HA	1.95	0.47
2:GP1:288:SER:HA	2:GP1:291:ASN:HB3	1.95	0.47
2:HP1:223:ASN:O	2:HP1:227:ARG:HG2	2.14	0.47
1:AP1:418:LEU:HD12	1:AP1:418:LEU:HA	1.77	0.47
1:EP1:126:SER:HB2	1:EP1:171:ASN:HA	1.96	0.47
2:HP1:526:LYS:HA	2:HP1:529:GLN:HE21	1.79	0.47
1:BP1:25:ALA:HB1	1:BP1:30:GLN:HE22	1.80	0.47
2:HP1:60:MET:HE3	2:IP1:817:ILE:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:732:MET:O	2:HP1:736:MET:CB	2.62	0.47
2:JP1:768:TRP:HB2	2:JP1:815:MET:HE1	1.96	0.47
2:FP1:829:GLY:HA2	2:JP1:766:PHE:CZ	2.50	0.47
2:FP1:940:VAL:O	2:FP1:944:ILE:HG13	2.14	0.47
2:HP1:188:GLN:O	2:HP1:191:MET:HB2	2.14	0.47
2:IP1:406:THR:O	2:IP1:406:THR:HG22	2.14	0.47
1:EP1:191:MET:HE3	1:EP1:195:GLN:HA	1.96	0.47
2:IP1:41:LEU:HD12	2:JP1:825:LEU:HA	1.96	0.47
3:LP1:5:LYS:O	3:LP1:9:LYS:HG3	2.15	0.47
1:CP1:443:MET:SD	1:DP1:443:MET:HE1	2.55	0.47
1:DP1:389:SER:HB3	1:DP1:394:GLN:OE1	2.15	0.47
2:IP1:189:ILE:HD11	2:IP1:350:MET:HB3	1.95	0.47
2:IP1:524:SER:O	2:IP1:528:ILE:HG22	2.14	0.47
2:JP1:58:GLY:HA2	2:JP1:121:TYR:CE1	2.50	0.47
2:JP1:77:MET:HE3	2:JP1:77:MET:HB2	1.77	0.47
2:JP1:103:ILE:HD11	2:JP1:789:PRO:HA	1.97	0.47
2:JP1:558:SER:HB3	2:JP1:576:MET:HE1	1.97	0.47
2:JP1:732:MET:HE2	2:JP1:732:MET:HA	1.95	0.47
1:BP1:437:LEU:HD11	1:CP1:346:ASN:HB3	1.96	0.47
2:FP1:94:LEU:HD21	3:LP1:21:ILE:HD11	1.96	0.47
2:GP1:608:GLN:HG2	2:GP1:633:TYR:CE2	2.50	0.47
2:HP1:79:THR:HA	2:HP1:82:VAL:HG22	1.97	0.47
2:HP1:713:VAL:HG22	2:IP1:727:LEU:HB2	1.96	0.47
2:JP1:462:ILE:HG13	2:JP1:463:MET:SD	2.55	0.47
2:JP1:833:LEU:HD21	2:JP1:921:MET:HB3	1.97	0.47
3:KP1:35:GLY:O	3:KP1:39:ILE:HG12	2.15	0.47
3:OP1:24:THR:HA	3:OP1:27:LEU:HD23	1.95	0.47
1:BP1:88:ALA:HB2	1:BP1:357:GLN:HE22	1.80	0.47
2:GP1:338:GLN:HA	2:GP1:341:VAL:HG12	1.97	0.47
2:HP1:82:VAL:HA	2:HP1:85:MET:HG3	1.96	0.47
2:HP1:106:ARG:HH11	2:HP1:789:PRO:HA	1.80	0.47
1:BP1:68:LEU:HD11	1:BP1:417:ILE:HD11	1.96	0.47
2:FP1:716:LEU:HD13	2:GP1:648:PHE:HE2	1.80	0.47
2:FP1:826:SER:O	2:FP1:830:VAL:HG23	2.15	0.47
2:GP1:213:PRO:HB2	2:GP1:222:MET:HE2	1.96	0.47
2:HP1:759:MET:HE3	2:IP1:917:ILE:HD11	1.96	0.47
1:AP1:243:LEU:HD12	1:EP1:182:LEU:HD11	1.97	0.46
2:GP1:117:LYS:HA	2:GP1:117:LYS:HD3	1.66	0.46
2:IP1:111:LEU:HD13	3:NP1:31:ALA:HB2	1.96	0.46
2:IP1:287:ILE:HG13	2:IP1:332:ARG:NH1	2.29	0.46
2:IP1:559:VAL:HG22	2:IP1:573:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JP1:72:GLY:O	2:JP1:76:ILE:HG12	2.14	0.46
2:JP1:189:ILE:HD11	2:JP1:533:LEU:HD21	1.96	0.46
2:JP1:747:PHE:HA	2:JP1:751:TYR:HD2	1.81	0.46
1:AP1:35:ASN:HB3	1:EP1:36:THR:HB	1.96	0.46
2:HP1:189:ILE:HD11	2:HP1:533:LEU:HD21	1.96	0.46
1:BP1:228:PRO:HB2	1:BP1:235:TYR:HB2	1.97	0.46
2:FP1:829:GLY:HA2	2:JP1:766:PHE:HZ	1.79	0.46
2:GP1:55:GLN:HB3	2:HP1:149:TYR:OH	2.15	0.46
2:HP1:778:ALA:HB2	2:IP1:943:TRP:CH2	2.50	0.46
2:IP1:336:ILE:HD11	2:IP1:491:LEU:HD21	1.97	0.46
2:IP1:826:SER:O	2:IP1:830:VAL:HG23	2.14	0.46
3:LP1:28:LEU:O	3:LP1:32:VAL:HG13	2.15	0.46
1:CP1:445:LEU:HD11	1:DP1:340:THR:HG23	1.97	0.46
2:JP1:69:LEU:HD21	2:JP1:114:LEU:HB3	1.97	0.46
1:AP1:430:ARG:NH2	1:BP1:425:GLN:HE21	2.14	0.46
2:FP1:338:GLN:HA	2:FP1:341:VAL:HG12	1.97	0.46
2:GP1:150:LEU:HD12	2:GP1:474:LEU:HG	1.97	0.46
2:HP1:196:LYS:NZ	2:HP1:357:PHE:HB3	2.31	0.46
3:LP1:4:LYS:H	3:LP1:4:LYS:HD3	1.79	0.46
1:BP1:30:GLN:CD	1:BP1:30:GLN:H	2.24	0.46
1:EP1:254:MET:HG3	1:EP1:355:LEU:HD23	1.97	0.46
2:FP1:55:GLN:HB3	2:GP1:149:TYR:OH	2.16	0.46
2:FP1:925:ILE:HG12	2:JP1:766:PHE:CE2	2.51	0.46
2:GP1:41:LEU:HB2	2:HP1:828:VAL:HG21	1.97	0.46
2:GP1:111:LEU:HD13	3:KP1:31:ALA:HB2	1.98	0.46
2:GP1:475:ASN:HB3	2:GP1:684:ASN:HD21	1.80	0.46
2:HP1:698:ASN:HA	2:IP1:905:TRP:CZ3	2.50	0.46
2:HP1:751:TYR:HB3	2:IP1:913:PHE:CD2	2.50	0.46
2:JP1:757:PRO:HB3	2:JP1:930:PHE:CE2	2.51	0.46
2:JP1:811:ARG:O	2:JP1:815:MET:HE3	2.14	0.46
1:BP1:94:MET:HE2	1:BP1:94:MET:HA	1.97	0.46
1:BP1:438:LEU:HD12	1:CP1:350:ILE:HD13	1.98	0.46
2:FP1:464:ALA:HB3	2:FP1:761:PHE:HE2	1.80	0.46
2:IP1:663:PRO:HB3	2:IP1:738:TRP:CD2	2.50	0.46
2:JP1:434:LEU:HA	2:JP1:437:ILE:HG22	1.97	0.46
2:JP1:608:GLN:HG3	2:JP1:633:TYR:HE2	1.80	0.46
2:JP1:659:PHE:CZ	2:JP1:707:LEU:HD11	2.51	0.46
3:KP1:23:PHE:CZ	3:KP1:27:LEU:HD21	2.51	0.46
1:CP1:419:LEU:HD12	1:DP1:415:ILE:HG23	1.98	0.46
1:DP1:419:LEU:HD12	1:EP1:415:ILE:HG23	1.98	0.46
2:FP1:189:ILE:HD11	2:FP1:350:MET:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:659:PHE:HA	2:HP1:662:ILE:HD11	1.97	0.46
2:IP1:667:MET:HE2	2:IP1:915:ILE:HD13	1.98	0.46
1:DP1:89:ILE:HD11	1:EP1:250:ALA:HA	1.98	0.46
2:FP1:357:PHE:HZ	2:FP1:530:ILE:HD13	1.80	0.46
2:IP1:77:MET:SD	3:NP1:28:LEU:HD21	2.56	0.46
1:DP1:421:GLU:O	1:DP1:425:GLN:HG3	2.16	0.46
2:FP1:741:THR:HG23	2:FP1:916:LEU:HD21	1.97	0.46
2:FP1:757:PRO:HG3	2:FP1:930:PHE:CE2	2.51	0.46
2:GP1:589:THR:H	2:GP1:665:GLN:HE22	1.64	0.46
2:GP1:944:ILE:HD12	2:GP1:944:ILE:H	1.81	0.46
2:HP1:212:PRO:HB3	2:HP1:215:GLY:O	2.16	0.46
2:IP1:708:LEU:HA	2:JP1:730:MET:HG2	1.97	0.46
2:IP1:713:VAL:HG13	2:JP1:723:PHE:HD1	1.81	0.46
2:IP1:819:TYR:CZ	2:IP1:823:ILE:HD11	2.51	0.46
2:JP1:28:PRO:HB2	2:JP1:32:ASP:OD2	2.16	0.46
2:JP1:184:ILE:O	2:JP1:188:GLN:HG3	2.16	0.46
1:CP1:242:GLN:O	1:CP1:279:PHE:HB2	2.16	0.45
1:DP1:382:ARG:HD3	1:DP1:399:TRP:CE2	2.51	0.45
1:DP1:401:LYS:HA	1:DP1:401:LYS:HD2	1.79	0.45
2:GP1:330:LEU:O	2:GP1:334:ILE:HG13	2.16	0.45
2:GP1:399:TRP:CE3	2:GP1:416:GLY:HA3	2.51	0.45
2:IP1:132:ILE:HG22	2:IP1:808:VAL:HB	1.98	0.45
2:JP1:49:LEU:HD23	2:JP1:129:MET:HE3	1.98	0.45
2:JP1:822:ALA:HB1	2:JP1:930:PHE:CD1	2.51	0.45
1:BP1:78:GLN:HB3	1:CP1:383:LEU:HD13	1.98	0.45
1:BP1:377:ASN:O	1:BP1:381:ARG:HB2	2.15	0.45
2:FP1:94:LEU:HD23	2:FP1:94:LEU:HA	1.81	0.45
2:IP1:132:ILE:HG21	2:IP1:772:VAL:HG23	1.97	0.45
2:JP1:377:GLN:OE1	2:JP1:402:VAL:HB	2.16	0.45
2:JP1:643:PHE:O	2:JP1:647:ILE:HG13	2.16	0.45
1:CP1:326:LEU:HD23	1:CP1:326:LEU:HA	1.82	0.45
2:FP1:201:GLN:O	2:FP1:205:TYR:HD1	1.99	0.45
2:FP1:697:ILE:HG13	2:FP1:751:TYR:HE2	1.81	0.45
2:FP1:708:LEU:HA	2:GP1:730:MET:HG2	1.97	0.45
2:GP1:55:GLN:NE2	2:GP1:58:GLY:HA3	2.32	0.45
2:GP1:247:THR:HG22	2:GP1:256:PRO:HD2	1.98	0.45
2:HP1:143:TRP:O	2:HP1:147:LEU:HG	2.16	0.45
2:IP1:247:THR:HG22	2:IP1:256:PRO:HD2	1.97	0.45
2:IP1:618:LEU:HD11	2:IP1:619:PHE:CE2	2.51	0.45
2:JP1:740:GLY:HA2	2:JP1:743:VAL:HG12	1.98	0.45
3:OP1:16:ARG:NH1	3:OP1:20:ILE:HG21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CP1:277:LEU:HD21	1:CP1:281:ARG:HH21	1.81	0.45
1:CP1:292:LEU:HD13	1:DP1:230:PHE:HE1	1.81	0.45
1:DP1:170:LEU:HD12	1:DP1:170:LEU:H	1.81	0.45
2:FP1:28:PRO:HB2	2:FP1:32:ASP:OD2	2.16	0.45
2:FP1:602:LEU:HD23	2:JP1:647:ILE:HD13	1.99	0.45
2:HP1:468:PHE:CE2	2:HP1:930:PHE:HZ	2.34	0.45
2:JP1:103:ILE:HD12	2:JP1:103:ILE:HA	1.88	0.45
1:EP1:353:LYS:HE3	1:EP1:353:LYS:HB3	1.68	0.45
2:HP1:473:LYS:HE3	2:IP1:843:TYR:CZ	2.52	0.45
2:HP1:659:PHE:CE1	2:HP1:707:LEU:HD22	2.51	0.45
1:AP1:105:LYS:HZ3	1:BP1:367:ASN:HA	1.82	0.45
1:BP1:74:VAL:O	1:BP1:78:GLN:HG2	2.16	0.45
1:CP1:81:ALA:CB	1:CP1:378:MET:HE1	2.45	0.45
1:DP1:55:THR:HA	1:EP1:42:TYR:CE1	2.52	0.45
1:DP1:208:ASN:O	1:DP1:212:GLN:HG2	2.17	0.45
2:FP1:103:ILE:N	2:FP1:104:PRO:HD2	2.32	0.45
2:FP1:435:ASN:HA	2:FP1:438:ARG:HD2	1.98	0.45
2:FP1:908:VAL:HG23	2:FP1:909:TYR:HD1	1.82	0.45
2:GP1:290:LEU:HB2	2:GP1:329:ARG:HH12	1.82	0.45
2:JP1:223:ASN:O	2:JP1:227:ARG:HG2	2.16	0.45
1:AP1:328:SER:HA	1:BP1:211:MET:CE	2.46	0.45
1:AP1:417:ILE:O	1:AP1:421:GLU:HG2	2.16	0.45
1:CP1:378:MET:HE3	1:CP1:378:MET:HB2	1.69	0.45
1:DP1:94:MET:HG3	1:EP1:241:SER:HB3	1.98	0.45
1:EP1:248:LEU:HD13	1:EP1:280:ILE:HD11	1.98	0.45
2:FP1:612:CYS:HB2	2:FP1:626:ARG:HE	1.82	0.45
2:GP1:819:TYR:CZ	2:GP1:823:ILE:HD11	2.52	0.45
2:IP1:461:TRP:CZ2	2:IP1:812:PRO:HB3	2.52	0.45
2:JP1:334:ILE:HD12	2:JP1:335:ALA:N	2.32	0.45
1:BP1:343:GLY:HA2	1:BP1:346:ASN:HD22	1.82	0.45
2:GP1:105:LEU:HD12	2:GP1:106:ARG:N	2.32	0.45
2:GP1:326:GLN:O	2:GP1:329:ARG:HB2	2.17	0.45
2:GP1:667:MET:CE	2:GP1:915:ILE:HD12	2.47	0.45
2:HP1:511:ASP:HB3	2:HP1:512:PRO:HA	1.98	0.45
2:HP1:905:TRP:O	2:HP1:908:VAL:HG22	2.16	0.45
2:JP1:330:LEU:O	2:JP1:334:ILE:HG13	2.17	0.45
2:JP1:741:THR:HG23	2:JP1:916:LEU:HG	1.99	0.45
1:AP1:389:SER:HB3	1:AP1:394:GLN:OE1	2.17	0.45
1:DP1:142:ILE:C	1:DP1:142:ILE:HD12	2.42	0.45
1:EP1:104:ASP:HA	1:EP1:109:ASN:ND2	2.32	0.45
2:FP1:288:SER:HA	2:FP1:291:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:820:ILE:HA	2:HP1:823:ILE:HG22	1.98	0.45
2:IP1:290:LEU:HB3	2:IP1:329:ARG:NH1	2.31	0.45
2:IP1:648:PHE:HE1	2:IP1:723:PHE:CD2	2.35	0.45
2:JP1:809:PHE:CD1	2:JP1:809:PHE:C	2.95	0.45
1:AP1:385:ASP:H	1:AP1:398:GLN:HE22	1.65	0.45
2:GP1:284:TRP:CD1	2:GP1:332:ARG:HG2	2.52	0.45
2:HP1:628:MET:HA	2:HP1:628:MET:HE2	1.99	0.45
1:BP1:378:MET:HE3	1:BP1:378:MET:HB2	1.65	0.44
1:CP1:389:SER:HB3	1:CP1:394:GLN:OE1	2.17	0.44
1:EP1:141:LEU:H	1:EP1:141:LEU:HD12	1.82	0.44
1:EP1:399:TRP:HE1	1:EP1:414:GLU:CD	2.25	0.44
2:FP1:100:SER:C	3:LP1:16:ARG:HH12	2.25	0.44
2:FP1:713:VAL:HG21	2:GP1:727:LEU:HD12	1.99	0.44
2:GP1:287:ILE:HG13	2:GP1:332:ARG:NH2	2.33	0.44
2:GP1:778:ALA:HB2	2:HP1:943:TRP:CH2	2.52	0.44
2:HP1:191:MET:CE	2:HP1:263:MET:HB3	2.47	0.44
2:HP1:932:LEU:HA	2:HP1:935:HIS:HD2	1.81	0.44
2:IP1:725:PHE:CZ	2:JP1:722:ILE:HG23	2.53	0.44
3:KP1:16:ARG:HA	3:KP1:19:VAL:HG22	1.98	0.44
1:EP1:302:TRP:NE1	1:EP1:306:THR:HG21	2.32	0.44
2:GP1:667:MET:HE2	2:GP1:912:PHE:HD2	1.82	0.44
2:GP1:930:PHE:O	2:GP1:933:ILE:HB	2.17	0.44
1:AP1:421:GLU:O	1:AP1:425:GLN:HG3	2.18	0.44
2:FP1:176:GLY:HA3	2:FP1:492:ASP:HB2	1.99	0.44
2:FP1:472:VAL:HG13	2:FP1:827:TYR:HE1	1.83	0.44
2:JP1:452:PHE:O	2:JP1:455:GLU:HG3	2.17	0.44
2:JP1:689:LEU:HD23	2:JP1:922:TYR:CE2	2.52	0.44
2:FP1:605:MET:HE3	2:FP1:605:MET:HB3	1.81	0.44
2:GP1:563:LEU:HD23	2:GP1:563:LEU:HA	1.82	0.44
2:GP1:639:TYR:CD1	2:GP1:639:TYR:C	2.94	0.44
2:HP1:247:THR:HG22	2:HP1:256:PRO:HD2	2.00	0.44
2:HP1:282:VAL:HA	2:HP1:494:SER:HB3	2.00	0.44
2:IP1:450:ARG:HD2	2:IP1:453:ILE:HD11	1.99	0.44
1:AP1:315:ASN:OD1	1:AP1:318:GLN:HB3	2.17	0.44
1:BP1:43:LEU:HD12	1:CP1:39:LEU:HD13	2.00	0.44
1:EP1:418:LEU:HD12	1:EP1:418:LEU:HA	1.80	0.44
2:FP1:34:SER:HA	2:FP1:462:ILE:HD13	1.99	0.44
2:GP1:213:PRO:O	2:GP1:218:PRO:HB3	2.17	0.44
2:GP1:369:ASP:OD1	2:GP1:369:ASP:N	2.51	0.44
2:GP1:525:ASP:HA	2:GP1:528:ILE:HG22	2.00	0.44
2:HP1:639:TYR:CD1	2:HP1:639:TYR:C	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:833:LEU:O	2:IP1:837:PHE:HB2	2.17	0.44
2:FP1:49:LEU:HD22	2:FP1:50:HIS:H	1.83	0.44
2:FP1:77:MET:O	2:FP1:81:MET:HG3	2.17	0.44
2:FP1:331:SER:HA	2:FP1:334:ILE:HD12	1.99	0.44
2:GP1:370:PHE:CD1	2:GP1:377:GLN:HB3	2.52	0.44
2:GP1:651:MET:HE1	2:GP1:655:ILE:HD11	2.00	0.44
2:HP1:753:ILE:HG13	2:HP1:922:TYR:CE2	2.52	0.44
2:IP1:555:GLN:NE2	2:IP1:588:LEU:HD12	2.32	0.44
2:IP1:664:LEU:O	2:IP1:668:LYS:HB2	2.18	0.44
2:JP1:537:VAL:HA	2:JP1:538:PRO:HA	1.86	0.44
3:KP1:40:ARG:HD2	3:KP1:40:ARG:HA	1.78	0.44
1:BP1:359:MET:HB2	1:BP1:367:ASN:OD1	2.18	0.44
1:DP1:104:ASP:HA	1:DP1:109:ASN:ND2	2.33	0.44
1:DP1:424:TYR:CZ	1:DP1:428:LEU:HD11	2.52	0.44
1:DP1:448:LEU:HD11	1:EP1:339:GLN:HB3	1.99	0.44
2:FP1:323:SER:O	2:FP1:326:GLN:HG3	2.18	0.44
2:GP1:766:PHE:CZ	2:HP1:829:GLY:HA3	2.49	0.44
2:IP1:461:TRP:CH2	2:IP1:812:PRO:HB3	2.52	0.44
2:JP1:600:THR:HG22	2:JP1:648:PHE:HE2	1.82	0.44
2:JP1:608:GLN:HG3	2:JP1:633:TYR:CE2	2.52	0.44
1:CP1:174:VAL:HG21	1:DP1:246:ASN:HD21	1.82	0.44
1:DP1:417:ILE:O	1:DP1:421:GLU:HG2	2.17	0.44
2:FP1:272:PHE:HD2	2:FP1:275:LEU:HD12	1.83	0.44
2:GP1:272:PHE:HD2	2:GP1:275:LEU:HD12	1.82	0.44
2:GP1:290:LEU:HD11	2:GP1:437:ILE:HD11	2.00	0.44
2:GP1:939:LYS:HA	2:GP1:939:LYS:HD2	1.86	0.44
2:JP1:240:VAL:HA	2:JP1:333:ALA:HB1	1.99	0.44
1:AP1:128:PRO:HB3	1:AP1:169:TYR:CE2	2.53	0.44
1:AP1:443:MET:HE1	1:EP1:443:MET:CE	2.48	0.44
2:FP1:377:GLN:HE22	2:FP1:402:VAL:HB	1.83	0.44
2:FP1:751:TYR:C	2:FP1:754:PRO:HD2	2.43	0.44
2:HP1:110:GLY:HA3	2:HP1:787:THR:HG22	2.00	0.44
2:HP1:516:LEU:HD23	2:HP1:516:LEU:HA	1.78	0.44
2:HP1:617:ILE:O	2:HP1:618:LEU:C	2.61	0.44
2:IP1:49:LEU:HD13	2:IP1:51:GLY:N	2.33	0.44
1:AP1:435:ARG:NH1	1:BP1:249:ILE:HD11	2.32	0.43
1:DP1:102:VAL:HG21	1:DP1:106:VAL:HG12	2.00	0.43
1:EP1:87:GLY:HA3	1:EP1:118:THR:HG22	2.00	0.43
2:FP1:33:LEU:HD12	2:FP1:459:LYS:O	2.19	0.43
2:FP1:921:MET:HA	2:FP1:924:ILE:HD12	2.00	0.43
2:GP1:188:GLN:O	2:GP1:191:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:335:ALA:HB1	2:GP1:426:TYR:CD1	2.53	0.43
2:GP1:612:CYS:HB3	2:GP1:626:ARG:H	1.83	0.43
2:GP1:704:TRP:CZ2	2:HP1:730:MET:HE3	2.52	0.43
2:GP1:753:ILE:HG13	2:GP1:922:TYR:CE2	2.53	0.43
2:GP1:811:ARG:HE	2:GP1:815:MET:HE2	1.82	0.43
2:IP1:89:HIS:HA	3:NP1:1:MET:HG2	1.99	0.43
2:IP1:452:PHE:CE1	2:IP1:453:ILE:HG13	2.53	0.43
1:CP1:448:LEU:HD11	1:DP1:339:GLN:HB3	2.00	0.43
2:FP1:38:LEU:HD12	2:FP1:38:LEU:HA	1.79	0.43
2:GP1:113:LEU:O	2:GP1:122:CYS:HB3	2.19	0.43
2:HP1:175:SER:HB2	2:HP1:488:GLY:H	1.82	0.43
2:HP1:643:PHE:CZ	2:HP1:647:ILE:HD11	2.53	0.43
1:AP1:419:LEU:HA	1:AP1:419:LEU:HD23	1.80	0.43
1:BP1:401:LYS:HD2	1:BP1:401:LYS:HA	1.75	0.43
1:CP1:33:SER:HB2	1:DP1:31:GLN:OE1	2.17	0.43
1:CP1:206:TYR:CZ	1:CP1:209:LEU:HB2	2.53	0.43
1:DP1:37:SER:O	1:DP1:40:VAL:HG12	2.18	0.43
2:HP1:818:GLY:HA2	2:HP1:936:LEU:HD13	2.01	0.43
2:IP1:667:MET:HE3	2:IP1:696:TYR:OH	2.18	0.43
2:IP1:917:ILE:HD12	2:IP1:917:ILE:HA	1.82	0.43
1:BP1:455:ALA:HB1	1:CP1:293:PRO:HA	2.01	0.43
1:EP1:119:THR:HG21	1:EP1:352:SER:OG	2.19	0.43
2:FP1:73:GLY:O	2:FP1:77:MET:HG3	2.18	0.43
2:FP1:205:TYR:HE2	2:FP1:213:PRO:HG2	1.83	0.43
2:FP1:720:PHE:HD1	2:JP1:716:LEU:HD12	1.83	0.43
2:FP1:766:PHE:CZ	2:GP1:829:GLY:HA2	2.36	0.43
2:GP1:261:LEU:HB2	2:GP1:284:TRP:CZ3	2.52	0.43
2:GP1:725:PHE:O	2:GP1:728:ILE:HG23	2.18	0.43
2:HP1:188:GLN:O	2:HP1:192:LEU:HG	2.18	0.43
2:IP1:334:ILE:HD12	2:IP1:335:ALA:N	2.33	0.43
2:IP1:381:PRO:HD3	2:IP1:573:ASN:HB3	1.99	0.43
2:IP1:756:LEU:O	2:IP1:759:MET:HB2	2.17	0.43
3:OP1:14:ASN:HB3	3:OP1:17:THR:HB	1.99	0.43
1:EP1:115:LEU:HD23	1:EP1:115:LEU:HA	1.79	0.43
1:EP1:123:GLN:NE2	1:EP1:256:THR:HG21	2.33	0.43
2:FP1:645:LEU:HD12	2:FP1:645:LEU:HA	1.84	0.43
2:FP1:716:LEU:HA	2:GP1:723:PHE:CG	2.54	0.43
2:FP1:778:ALA:HB2	2:GP1:943:TRP:CH2	2.53	0.43
2:GP1:79:THR:HA	2:GP1:82:VAL:HG12	2.01	0.43
2:GP1:125:GLN:H	2:GP1:125:GLN:HG2	1.66	0.43
2:HP1:139:ALA:HB2	2:HP1:812:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:152:ARG:N	2:HP1:152:ARG:HD3	2.33	0.43
2:HP1:264:PRO:O	2:HP1:276:ASN:ND2	2.51	0.43
2:HP1:434:LEU:O	2:HP1:437:ILE:HG22	2.18	0.43
2:HP1:769:LEU:HD23	2:HP1:769:LEU:HA	1.82	0.43
2:HP1:807:ASN:O	2:HP1:811:ARG:HG2	2.18	0.43
2:JP1:259:PHE:CE2	2:JP1:286:ASN:HB2	2.54	0.43
2:JP1:548:PRO:HD3	2:JP1:568:TYR:HD2	1.82	0.43
2:JP1:586:LYS:HB3	2:JP1:586:LYS:HE3	1.90	0.43
1:BP1:308:LYS:HG2	1:BP1:309:PRO:HD2	2.01	0.43
1:CP1:328:SER:HA	1:DP1:211:MET:CE	2.48	0.43
1:EP1:170:LEU:H	1:EP1:170:LEU:HD12	1.83	0.43
1:EP1:445:LEU:HD13	1:EP1:445:LEU:HA	1.84	0.43
2:GP1:105:LEU:HA	2:GP1:108:THR:HG22	2.00	0.43
2:JP1:45:VAL:HG12	2:JP1:49:LEU:HB2	2.01	0.43
1:CP1:423:ASN:HD21	1:DP1:379:ALA:HA	1.83	0.43
1:EP1:419:LEU:HD23	1:EP1:419:LEU:HA	1.81	0.43
2:GP1:717:ILE:HD12	2:GP1:717:ILE:O	2.19	0.43
2:HP1:377:GLN:HE22	2:HP1:402:VAL:HB	1.83	0.43
2:IP1:383:LYS:HG3	2:IP1:387:GLU:O	2.18	0.43
2:JP1:38:LEU:HD23	2:JP1:38:LEU:HA	1.80	0.43
1:AP1:86:LEU:HA	1:AP1:86:LEU:HD12	1.81	0.43
1:AP1:123:GLN:NE2	1:AP1:256:THR:HG21	2.33	0.43
1:CP1:206:TYR:O	1:CP1:210:VAL:HG12	2.18	0.43
1:EP1:355:LEU:HD23	1:EP1:355:LEU:HA	1.85	0.43
2:FP1:163:PRO:HG2	2:FP1:581:GLY:HA3	1.99	0.43
2:HP1:136:VAL:HG13	2:HP1:461:TRP:HE1	1.84	0.43
2:JP1:399:TRP:CE3	2:JP1:416:GLY:HA3	2.54	0.43
2:JP1:447:LYS:HE2	2:JP1:447:LYS:HB2	1.87	0.43
3:LP1:26:ALA:HA	3:LP1:29:ILE:HG12	2.01	0.43
3:NP1:16:ARG:HA	3:NP1:19:VAL:HG22	2.01	0.43
1:AP1:211:MET:CE	1:EP1:328:SER:HA	2.48	0.43
1:CP1:205:MET:HA	1:CP1:209:LEU:HD23	2.00	0.43
1:CP1:449:LYS:HE2	1:DP1:285:ALA:HB1	1.99	0.43
1:EP1:84:THR:HB	1:EP1:371:GLN:HA	2.01	0.43
2:HP1:103:ILE:HA	2:HP1:106:ARG:HG2	2.01	0.43
2:HP1:922:TYR:HA	2:HP1:925:ILE:HD12	2.00	0.43
2:IP1:766:PHE:HZ	2:JP1:829:GLY:HA2	1.81	0.43
1:AP1:31:GLN:HE22	1:AP1:35:ASN:ND2	2.16	0.43
1:AP1:99:MET:HE2	1:AP1:99:MET:HB2	1.86	0.43
1:EP1:142:ILE:HD13	1:EP1:281:ARG:HD3	2.01	0.43
2:FP1:716:LEU:HA	2:GP1:723:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:739:ILE:O	2:FP1:743:VAL:HG22	2.19	0.43
2:GP1:725:PHE:HE1	2:HP1:729:MET:SD	2.42	0.43
2:HP1:503:LYS:HE2	2:HP1:503:LYS:HB2	1.73	0.43
2:IP1:330:LEU:O	2:IP1:334:ILE:HG13	2.19	0.43
2:IP1:612:CYS:HB2	2:IP1:626:ARG:NE	2.27	0.43
2:JP1:573:ASN:HA	2:JP1:576:MET:HE2	2.01	0.43
1:AP1:175:SER:HB3	1:BP1:244:ASN:HD22	1.84	0.42
1:BP1:351:LEU:C	1:BP1:351:LEU:HD23	2.44	0.42
1:DP1:359:MET:HB2	1:DP1:367:ASN:OD1	2.19	0.42
2:FP1:205:TYR:HB3	2:FP1:214:CYS:SG	2.59	0.42
2:GP1:67:ALA:O	2:GP1:71:LEU:HD12	2.18	0.42
2:GP1:125:GLN:HB3	2:GP1:776:MET:SD	2.59	0.42
2:GP1:547:GLN:HA	2:GP1:568:TYR:CD2	2.54	0.42
2:HP1:45:VAL:HG11	2:HP1:129:MET:HG2	2.00	0.42
2:HP1:692:MET:HE3	2:HP1:696:TYR:HE2	1.83	0.42
2:IP1:766:PHE:CG	2:JP1:925:ILE:HD11	2.54	0.42
2:JP1:331:SER:HA	2:JP1:334:ILE:HD11	2.01	0.42
2:JP1:725:PHE:HA	2:JP1:728:ILE:HG22	2.01	0.42
2:HP1:143:TRP:HB2	2:HP1:816:ILE:HG12	2.00	0.42
2:IP1:370:PHE:CE2	2:IP1:562:PRO:HA	2.53	0.42
2:JP1:213:PRO:O	2:JP1:218:PRO:HB3	2.19	0.42
2:JP1:612:CYS:HB2	2:JP1:626:ARG:NE	2.27	0.42
2:JP1:922:TYR:O	2:JP1:925:ILE:HG22	2.19	0.42
1:AP1:172:ASP:HB3	1:AP1:175:SER:OG	2.18	0.42
2:FP1:664:LEU:HD23	2:FP1:664:LEU:HA	1.89	0.42
2:FP1:769:LEU:HA	2:FP1:769:LEU:HD23	1.87	0.42
2:IP1:41:LEU:HD23	2:IP1:42:PHE:CD1	2.54	0.42
2:IP1:708:LEU:HD13	2:JP1:730:MET:HB3	2.01	0.42
2:JP1:525:ASP:OD2	2:JP1:525:ASP:N	2.52	0.42
1:BP1:56:GLN:HB3	1:BP1:59:LYS:HG3	2.01	0.42
1:BP1:445:LEU:HD21	1:CP1:343:GLY:HA3	2.01	0.42
1:CP1:317:VAL:HA	1:DP1:198:TRP:HE1	1.84	0.42
1:DP1:320:LYS:HD2	1:EP1:198:TRP:CE2	2.55	0.42
2:FP1:588:LEU:HD22	2:FP1:665:GLN:HE22	1.83	0.42
2:FP1:817:ILE:HD13	2:JP1:60:MET:HE3	2.00	0.42
2:HP1:33:LEU:HA	2:HP1:36:VAL:HB	2.01	0.42
1:BP1:328:SER:HA	1:CP1:211:MET:CE	2.50	0.42
2:FP1:724:ILE:O	2:FP1:728:ILE:HG22	2.19	0.42
2:GP1:268:LYS:HB3	2:HP1:403:PRO:HB3	2.01	0.42
2:GP1:375:LYS:HE3	2:GP1:375:LYS:HB2	1.91	0.42
2:GP1:391:GLU:OE1	2:GP1:391:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:461:TRP:CH2	2:GP1:812:PRO:HB3	2.55	0.42
2:GP1:751:TYR:HB3	2:HP1:913:PHE:CD2	2.55	0.42
2:HP1:162:ASP:HB3	2:HP1:165:LYS:HB3	2.02	0.42
2:HP1:299:LYS:H	2:HP1:299:LYS:HG2	1.67	0.42
2:HP1:768:TRP:O	2:HP1:772:VAL:HG12	2.20	0.42
2:HP1:837:PHE:O	2:HP1:841:ILE:HG22	2.18	0.42
1:BP1:33:SER:HB2	1:CP1:31:GLN:OE1	2.20	0.42
1:CP1:54:ILE:HD13	1:CP1:54:ILE:HA	1.87	0.42
1:EP1:216:GLY:HA3	1:EP1:265:SER:O	2.20	0.42
2:FP1:103:ILE:HD11	3:LP1:20:ILE:HD12	2.00	0.42
2:HP1:162:ASP:H	2:HP1:485:PHE:HZ	1.67	0.42
2:HP1:617:ILE:HG22	2:HP1:618:LEU:H	1.85	0.42
2:JP1:101:ILE:O	2:JP1:104:PRO:HD2	2.19	0.42
2:JP1:204:LEU:HD23	2:JP1:204:LEU:HA	1.75	0.42
2:JP1:589:THR:HG23	2:JP1:590:PHE:CD1	2.55	0.42
2:JP1:755:VAL:O	2:JP1:759:MET:HG3	2.19	0.42
2:JP1:936:LEU:N	2:JP1:937:PRO:HD2	2.34	0.42
1:AP1:382:ARG:HB3	1:AP1:399:TRP:CE3	2.55	0.42
1:BP1:204:LEU:HD23	1:BP1:204:LEU:HA	1.82	0.42
1:DP1:308:LYS:HA	1:DP1:308:LYS:HD2	1.75	0.42
2:GP1:35:VAL:HA	2:GP1:38:LEU:HB2	2.02	0.42
2:GP1:524:SER:O	2:GP1:528:ILE:HG22	2.19	0.42
2:GP1:657:MET:O	2:GP1:661:MET:HG2	2.19	0.42
2:GP1:667:MET:HE3	2:GP1:915:ILE:HD12	2.01	0.42
2:HP1:237:VAL:HG13	2:HP1:261:LEU:HD11	2.01	0.42
2:IP1:725:PHE:CE2	2:JP1:722:ILE:HG23	2.55	0.42
3:KP1:24:THR:HA	3:KP1:27:LEU:HD12	2.02	0.42
1:BP1:292:LEU:HD13	1:CP1:230:PHE:CE2	2.55	0.42
2:FP1:187:GLY:HA3	2:FP1:263:MET:HE3	2.02	0.42
2:GP1:334:ILE:HD12	2:GP1:335:ALA:N	2.34	0.42
2:HP1:728:ILE:HD12	2:IP1:730:MET:SD	2.60	0.42
2:IP1:751:TYR:C	2:IP1:754:PRO:HD2	2.45	0.42
2:JP1:804:ILE:O	2:JP1:808:VAL:HG22	2.20	0.42
3:LP1:38:LYS:HA	3:LP1:38:LYS:HD2	1.77	0.42
3:MP1:35:GLY:O	3:MP1:39:ILE:HG13	2.20	0.42
1:AP1:430:ARG:NH2	1:BP1:425:GLN:NE2	2.68	0.42
2:FP1:617:ILE:O	2:FP1:618:LEU:C	2.63	0.42
2:FP1:730:MET:O	2:FP1:733:PRO:HD2	2.20	0.42
2:FP1:759:MET:HE1	2:GP1:917:ILE:HD12	2.01	0.42
2:GP1:240:VAL:HA	2:GP1:333:ALA:HB1	2.01	0.42
2:GP1:573:ASN:O	2:GP1:576:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EP1:96:GLN:OE1	1:EP1:96:GLN:N	2.52	0.42
1:EP1:230:PHE:C	1:EP1:230:PHE:CD2	2.97	0.42
2:FP1:191:MET:HE1	2:FP1:264:PRO:HA	2.02	0.42
2:GP1:41:LEU:HD22	2:GP1:42:PHE:CE2	2.55	0.42
2:GP1:143:TRP:CE2	2:GP1:147:LEU:HD23	2.55	0.42
2:GP1:782:VAL:HG11	2:GP1:801:ALA:HB2	2.02	0.42
2:HP1:667:MET:HE3	2:HP1:911:PHE:HD2	1.84	0.42
2:HP1:799:GLU:HG2	2:HP1:800:PHE:H	1.85	0.42
3:LP1:4:LYS:HB2	3:LP1:4:LYS:HE2	1.83	0.42
1:BP1:303:ASN:HD22	2:GP1:208:GLN:CD	2.28	0.41
1:CP1:219:PRO:HA	1:CP1:220:PRO:HD3	1.91	0.41
1:DP1:298:TYR:HE2	1:EP1:230:PHE:CD1	2.38	0.41
2:FP1:105:LEU:HA	2:FP1:108:THR:HG22	2.02	0.41
2:GP1:703:LEU:O	2:GP1:707:LEU:HG	2.20	0.41
2:HP1:179:LYS:HE3	2:HP1:547:GLN:HE22	1.84	0.41
2:HP1:336:ILE:HD11	2:HP1:491:LEU:HD11	2.01	0.41
2:FP1:59:ASN:HD22	2:GP1:149:TYR:HB2	1.84	0.41
2:GP1:330:LEU:HB3	2:GP1:333:ALA:HB3	2.01	0.41
2:HP1:335:ALA:HB1	2:HP1:426:TYR:CD1	2.55	0.41
2:HP1:448:LYS:HE2	2:HP1:448:LYS:HB2	1.66	0.41
2:HP1:588:LEU:HD22	2:HP1:665:GLN:CD	2.45	0.41
2:IP1:259:PHE:HE1	2:IP1:286:ASN:HB2	1.85	0.41
2:IP1:331:SER:O	2:IP1:334:ILE:HD12	2.19	0.41
2:IP1:837:PHE:CE2	2:IP1:918:TYR:HB2	2.55	0.41
2:JP1:57:MET:SD	2:JP1:61:PHE:HE1	2.43	0.41
2:JP1:137:GLY:O	2:JP1:141:LYS:HG3	2.21	0.41
2:JP1:141:LYS:HA	2:JP1:144:GLU:HG2	2.02	0.41
1:DP1:128:PRO:HB3	1:DP1:169:TYR:CE2	2.55	0.41
1:EP1:215:ILE:HD13	1:EP1:215:ILE:HA	1.75	0.41
1:EP1:253:LEU:HD22	1:EP1:373:LEU:HD22	2.02	0.41
2:HP1:753:ILE:HD13	2:HP1:753:ILE:HA	1.94	0.41
2:HP1:758:TYR:OH	2:IP1:836:GLY:HA3	2.21	0.41
2:JP1:547:GLN:HA	2:JP1:568:TYR:CE2	2.55	0.41
1:AP1:250:ALA:HB3	1:AP1:251:PRO:HD3	2.02	0.41
1:AP1:419:LEU:HD23	1:AP1:422:ILE:HD12	2.02	0.41
2:FP1:136:VAL:HG13	2:FP1:461:TRP:HE1	1.85	0.41
2:GP1:144:GLU:HA	2:GP1:147:LEU:HG	2.01	0.41
2:GP1:329:ARG:HA	2:GP1:329:ARG:HD3	1.81	0.41
2:HP1:105:LEU:HA	2:HP1:108:THR:HG22	2.02	0.41
2:HP1:603:TYR:O	2:HP1:641:TYR:HE2	2.04	0.41
2:HP1:645:LEU:HD23	2:HP1:645:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:701:GLY:HA3	2:IP1:905:TRP:CH2	2.55	0.41
2:IP1:131:VAL:HG11	2:IP1:805:LEU:HG	2.01	0.41
2:IP1:600:THR:HB	2:IP1:645:LEU:HD22	2.01	0.41
2:JP1:939:LYS:HE3	2:JP1:939:LYS:HB3	1.86	0.41
3:NP1:21:ILE:HD13	3:NP1:21:ILE:HA	1.84	0.41
1:AP1:104:ASP:OD1	1:AP1:104:ASP:C	2.64	0.41
1:BP1:115:LEU:HD23	1:BP1:115:LEU:HA	1.88	0.41
1:DP1:102:VAL:HG23	1:EP1:253:LEU:HD23	2.01	0.41
1:DP1:302:TRP:O	1:DP1:306:THR:HG22	2.21	0.41
1:DP1:368:ILE:HD13	1:DP1:368:ILE:HA	1.88	0.41
2:FP1:468:PHE:CE1	2:FP1:757:PRO:HG2	2.56	0.41
2:FP1:705:LEU:HD12	2:GP1:594:ILE:HG23	2.03	0.41
2:GP1:147:LEU:HD12	2:GP1:148:SER:N	2.34	0.41
2:GP1:290:LEU:HD12	2:GP1:290:LEU:H	1.85	0.41
2:GP1:671:PHE:CD1	2:GP1:915:ILE:HD11	2.55	0.41
2:GP1:841:ILE:HG13	2:GP1:845:GLN:HG2	2.01	0.41
2:HP1:612:CYS:HB2	2:HP1:626:ARG:HE	1.85	0.41
2:HP1:833:LEU:O	2:HP1:837:PHE:HB2	2.20	0.41
2:IP1:187:GLY:O	2:IP1:191:MET:HG2	2.20	0.41
2:IP1:499:THR:HA	2:IP1:531:GLN:NE2	2.35	0.41
2:IP1:630:ASP:HA	2:IP1:634:ASN:HB2	2.01	0.41
2:JP1:505:PHE:CG	2:JP1:524:SER:HB3	2.56	0.41
3:MP1:36:PHE:O	3:MP1:39:ILE:HD12	2.19	0.41
1:CP1:228:PRO:HG3	1:CP1:234:LYS:HD2	2.01	0.41
2:GP1:184:ILE:HD12	2:GP1:184:ILE:H	1.85	0.41
2:GP1:282:VAL:HA	2:GP1:494:SER:HB3	2.03	0.41
2:GP1:589:THR:HG23	2:GP1:590:PHE:CD1	2.55	0.41
2:GP1:751:TYR:C	2:GP1:754:PRO:HD2	2.46	0.41
2:HP1:210:LYS:HE2	2:HP1:210:LYS:HB2	1.81	0.41
2:IP1:205:TYR:HB3	2:IP1:214:CYS:SG	2.60	0.41
2:IP1:369:ASP:HB3	2:IP1:375:LYS:HA	2.02	0.41
2:IP1:782:VAL:O	2:IP1:786:VAL:HG23	2.20	0.41
2:JP1:685:PRO:HB2	2:JP1:830:VAL:HG11	2.02	0.41
2:JP1:816:ILE:HD13	2:JP1:816:ILE:HA	1.83	0.41
3:MP1:15:THR:HG22	3:MP1:18:ARG:HH22	1.85	0.41
1:AP1:206:TYR:CZ	1:AP1:209:LEU:HB2	2.56	0.41
1:AP1:294:LYS:H	1:AP1:294:LYS:HG2	1.61	0.41
2:GP1:100:SER:HB3	3:KP1:16:ARG:HH12	1.85	0.41
2:GP1:748:VAL:O	2:GP1:753:ILE:HG12	2.20	0.41
2:GP1:803:MET:HE3	2:GP1:804:ILE:N	2.36	0.41
2:HP1:469:PHE:O	2:HP1:473:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:691:ASN:HA	2:IP1:694:THR:HG23	2.02	0.41
2:IP1:841:ILE:HG12	2:IP1:914:SER:HB3	2.03	0.41
2:JP1:302:VAL:HB	2:JP1:320:ILE:HG13	2.02	0.41
3:MP1:4:LYS:O	3:MP1:8:LEU:HG	2.20	0.41
3:NP1:16:ARG:O	3:NP1:20:ILE:HG23	2.21	0.41
1:AP1:239:LEU:O	1:AP1:243:LEU:HG	2.21	0.41
1:AP1:339:GLN:HG2	1:AP1:442:ILE:HG23	2.02	0.41
1:AP1:443:MET:HE1	1:EP1:443:MET:HE2	2.01	0.41
1:CP1:70:ASN:HB3	1:CP1:73:VAL:HG22	2.02	0.41
2:FP1:334:ILE:HG13	2:FP1:334:ILE:H	1.69	0.41
2:IP1:98:TRP:CD1	2:IP1:103:ILE:HD11	2.56	0.41
2:JP1:170:ALA:HA	2:JP1:175:SER:H	1.84	0.41
2:JP1:205:TYR:HB3	2:JP1:214:CYS:SG	2.61	0.41
1:AP1:170:LEU:HD12	1:AP1:170:LEU:H	1.86	0.41
1:AP1:326:LEU:HD23	1:AP1:326:LEU:HA	1.81	0.41
1:BP1:104:ASP:OD2	1:BP1:104:ASP:C	2.64	0.41
1:BP1:418:LEU:HD12	1:BP1:418:LEU:HA	1.84	0.41
1:BP1:440:ASN:HB3	1:CP1:439:THR:HG21	2.03	0.41
1:BP1:441:SER:O	1:BP1:445:LEU:HD23	2.19	0.41
1:CP1:448:LEU:HD23	1:CP1:448:LEU:HA	1.77	0.41
1:DP1:292:LEU:HD13	1:DP1:329:TYR:OH	2.21	0.41
1:DP1:360:SER:HB2	1:DP1:366:ALA:HA	2.02	0.41
1:EP1:254:MET:HB3	1:EP1:273:ALA:HB2	2.03	0.41
1:EP1:426:MET:HB2	1:EP1:426:MET:HE3	1.71	0.41
2:FP1:725:PHE:CD2	2:FP1:725:PHE:C	2.98	0.41
2:FP1:725:PHE:CE2	2:GP1:729:MET:HE1	2.55	0.41
2:FP1:937:PRO:HA	2:FP1:940:VAL:HG22	2.03	0.41
2:GP1:56:ILE:O	2:GP1:60:MET:HB2	2.21	0.41
2:GP1:184:ILE:O	2:GP1:188:GLN:HG3	2.20	0.41
2:GP1:287:ILE:HD12	2:GP1:287:ILE:H	1.86	0.41
2:GP1:331:SER:HA	2:GP1:334:ILE:HD11	2.03	0.41
2:GP1:766:PHE:CE2	2:HP1:925:ILE:HG23	2.55	0.41
2:HP1:103:ILE:HG13	2:HP1:104:PRO:CD	2.47	0.41
2:HP1:114:LEU:HD21	2:HP1:783:ALA:HB3	2.03	0.41
2:HP1:301:LEU:HD21	2:HP1:319:ASN:HD21	1.86	0.41
2:HP1:696:TYR:CD1	2:HP1:742:MET:HG2	2.55	0.41
2:HP1:751:TYR:C	2:HP1:754:PRO:HD2	2.46	0.41
2:IP1:28:PRO:HB2	2:IP1:32:ASP:OD2	2.21	0.41
2:IP1:191:MET:HE1	2:IP1:264:PRO:N	2.36	0.41
2:IP1:651:MET:HB2	2:IP1:651:MET:HE2	1.79	0.41
2:IP1:713:VAL:HG11	2:JP1:596:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JP1:752:TYR:HE1	2:JP1:756:LEU:HD22	1.86	0.41
1:BP1:284:SER:HB2	1:BP1:344:VAL:HG22	2.03	0.41
1:BP1:419:LEU:HD23	1:BP1:419:LEU:HA	1.84	0.41
1:DP1:43:LEU:HD12	1:DP1:43:LEU:HA	1.92	0.41
2:FP1:210:LYS:HB2	2:FP1:210:LYS:HE2	1.76	0.41
2:IP1:660:LEU:O	2:IP1:663:PRO:HD2	2.21	0.41
2:JP1:704:TRP:CD1	2:JP1:704:TRP:C	3.00	0.41
3:MP1:12:PHE:CZ	3:MP1:22:ILE:HD11	2.56	0.41
1:BP1:120:PHE:CZ	1:BP1:173:PRO:HG3	2.56	0.40
1:BP1:215:ILE:HD12	1:BP1:215:ILE:HA	1.80	0.40
1:EP1:142:ILE:HG22	1:EP1:210:VAL:HG23	2.03	0.40
2:FP1:751:TYR:CE1	2:GP1:910:ALA:HA	2.56	0.40
2:HP1:447:LYS:HD2	2:HP1:447:LYS:H	1.86	0.40
2:IP1:191:MET:CE	2:IP1:263:MET:HB3	2.51	0.40
2:JP1:525:ASP:O	2:JP1:529:GLN:HG3	2.21	0.40
2:JP1:814:LEU:O	2:JP1:817:ILE:HB	2.21	0.40
1:AP1:129:SER:HB3	1:AP1:137:THR:HG21	2.04	0.40
2:FP1:110:GLY:O	2:FP1:114:LEU:HD23	2.21	0.40
2:FP1:296:SER:HA	2:FP1:302:VAL:HG13	2.03	0.40
2:FP1:588:LEU:HD22	2:FP1:665:GLN:NE2	2.35	0.40
2:FP1:708:LEU:O	2:FP1:713:VAL:HG23	2.21	0.40
2:GP1:149:TYR:C	2:GP1:149:TYR:CD2	2.99	0.40
2:GP1:650:GLU:CD	2:GP1:650:GLU:H	2.30	0.40
2:HP1:816:ILE:HD12	2:HP1:816:ILE:HA	1.94	0.40
2:IP1:248:PRO:HD2	2:IP1:256:PRO:HD3	2.03	0.40
2:IP1:597:LYS:HA	2:IP1:597:LYS:HD2	1.79	0.40
2:IP1:725:PHE:O	2:IP1:728:ILE:HG22	2.21	0.40
2:IP1:844:ILE:N	2:IP1:844:ILE:HD13	2.36	0.40
2:JP1:331:SER:O	2:JP1:334:ILE:HD12	2.21	0.40
2:JP1:547:GLN:HA	2:JP1:568:TYR:HE2	1.86	0.40
1:BP1:448:LEU:HD23	1:BP1:448:LEU:HA	1.95	0.40
2:FP1:462:ILE:HG13	2:FP1:463:MET:SD	2.61	0.40
2:FP1:752:TYR:CE1	2:FP1:756:LEU:HB2	2.56	0.40
2:GP1:732:MET:O	2:GP1:736:MET:HB2	2.21	0.40
2:HP1:377:GLN:NE2	2:HP1:402:VAL:H	2.13	0.40
2:IP1:528:ILE:CD1	2:IP1:538:PRO:HD3	2.50	0.40
2:JP1:664:LEU:HD23	2:JP1:664:LEU:HA	1.67	0.40
2:JP1:769:LEU:HD23	2:JP1:769:LEU:HA	1.84	0.40
3:OP1:30:ILE:HD13	3:OP1:30:ILE:HA	1.94	0.40
2:FP1:844:ILE:HD13	2:FP1:844:ILE:N	2.37	0.40
2:HP1:58:GLY:HA2	2:HP1:121:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:370:PHE:HE2	2:HP1:565:SER:HB3	1.87	0.40
2:IP1:290:LEU:HD11	2:IP1:437:ILE:HG12	2.02	0.40
2:JP1:935:HIS:HE1	2:JP1:939:LYS:HD2	1.86	0.40
1:AP1:198:TRP:CD1	1:EP1:317:VAL:HG22	2.56	0.40
1:AP1:401:LYS:HD2	1:AP1:401:LYS:HA	1.70	0.40
1:CP1:35:ASN:O	1:CP1:39:LEU:HD23	2.22	0.40
1:CP1:128:PRO:HG3	1:CP1:169:TYR:CE2	2.56	0.40
1:CP1:295:LEU:HD11	2:FP1:212:PRO:HG3	2.03	0.40
1:EP1:308:LYS:HG2	1:EP1:309:PRO:HD2	2.03	0.40
1:EP1:326:LEU:HD23	1:EP1:326:LEU:HA	1.81	0.40
2:FP1:448:LYS:HA	2:FP1:451:ASP:OD2	2.21	0.40
2:FP1:915:ILE:HD12	2:FP1:915:ILE:HA	1.93	0.40
2:GP1:289:ALA:HB3	2:GP1:437:ILE:HD13	2.04	0.40
2:GP1:500:GLN:HA	2:GP1:503:LYS:HB2	2.02	0.40
2:GP1:800:PHE:HZ	2:HP1:943:TRP:CE2	2.39	0.40
2:GP1:939:LYS:HA	2:GP1:942:ARG:HG3	2.02	0.40
2:HP1:617:ILE:HG22	2:HP1:618:LEU:N	2.37	0.40
2:HP1:619:PHE:HD1	2:HP1:619:PHE:HA	1.76	0.40
2:IP1:93:MET:HE1	3:NP1:17:THR:HG22	2.03	0.40
2:JP1:596:PHE:CD2	2:JP1:656:VAL:HG21	2.56	0.40
3:KP1:5:LYS:HG3	3:KP1:6:GLU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AP1	413/466 (89%)	401 (97%)	12 (3%)	0	100	100
1	BP1	413/466 (89%)	405 (98%)	8 (2%)	0	100	100
1	CP1	413/466 (89%)	406 (98%)	7 (2%)	0	100	100
1	DP1	413/466 (89%)	402 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EP1	413/466 (89%)	406 (98%)	7 (2%)	0	100	100
2	FP1	847/1048 (81%)	816 (96%)	31 (4%)	0	100	100
2	GP1	847/1048 (81%)	813 (96%)	34 (4%)	0	100	100
2	HP1	847/1048 (81%)	807 (95%)	40 (5%)	0	100	100
2	IP1	847/1048 (81%)	813 (96%)	34 (4%)	0	100	100
2	JP1	847/1048 (81%)	811 (96%)	36 (4%)	0	100	100
3	KP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	LP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	MP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	NP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	OP1	41/1048 (4%)	41 (100%)	0	0	100	100
All	All	6505/12810 (51%)	6285 (97%)	220 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AP1	360/401 (90%)	347 (96%)	13 (4%)	30	55
1	BP1	360/401 (90%)	350 (97%)	10 (3%)	38	60
1	CP1	360/401 (90%)	350 (97%)	10 (3%)	38	60
1	DP1	360/401 (90%)	350 (97%)	10 (3%)	38	60
1	EP1	360/401 (90%)	352 (98%)	8 (2%)	47	66
2	FP1	715/858 (83%)	683 (96%)	32 (4%)	23	49
2	GP1	715/858 (83%)	683 (96%)	32 (4%)	23	49
2	HP1	715/858 (83%)	674 (94%)	41 (6%)	17	43
2	IP1	715/858 (83%)	678 (95%)	37 (5%)	19	45
2	JP1	715/858 (83%)	677 (95%)	38 (5%)	19	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	KP1	36/765 (5%)	32 (89%)	4 (11%)	5	22
3	LP1	36/765 (5%)	35 (97%)	1 (3%)	38	60
3	MP1	36/765 (5%)	32 (89%)	4 (11%)	5	22
3	NP1	36/765 (5%)	31 (86%)	5 (14%)	3	15
3	OP1	36/765 (5%)	31 (86%)	5 (14%)	3	15
All	All	5555/10120 (55%)	5305 (96%)	250 (4%)	26	49

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AP1	31	GLN
1	AP1	59	LYS
1	AP1	65	TYR
1	AP1	76	LEU
1	AP1	86	LEU
1	AP1	212	GLN
1	AP1	230	PHE
1	AP1	317	VAL
1	AP1	328	SER
1	AP1	345	SER
1	AP1	346	ASN
1	AP1	381	ARG
1	AP1	447	ASN
1	BP1	43	LEU
1	BP1	71	SER
1	BP1	195	GLN
1	BP1	230	PHE
1	BP1	268	THR
1	BP1	281	ARG
1	BP1	345	SER
1	BP1	374	ASN
1	BP1	426	MET
1	BP1	434	GLU
1	CP1	193	ASN
1	CP1	195	GLN
1	CP1	204	LEU
1	CP1	205	MET
1	CP1	230	PHE
1	CP1	299	SER
1	CP1	345	SER

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Mol	Chain	Res	Type
1	CP1	374	ASN
1	CP1	407	SER
1	CP1	426	MET
1	DP1	172	ASP
1	DP1	193	ASN
1	DP1	195	GLN
1	DP1	203	ASN
1	DP1	210	VAL
1	DP1	298	TYR
1	DP1	303	ASN
1	DP1	345	SER
1	DP1	374	ASN
1	DP1	456	ASP
1	EP1	65	TYR
1	EP1	119	THR
1	EP1	141	LEU
1	EP1	195	GLN
1	EP1	212	GLN
1	EP1	230	PHE
1	EP1	345	SER
1	EP1	387	THR
2	FP1	33	LEU
2	FP1	45	VAL
2	FP1	77	MET
2	FP1	85	MET
2	FP1	127	PHE
2	FP1	140	ASP
2	FP1	141	LYS
2	FP1	191	MET
2	FP1	217	ASN
2	FP1	244	ASN
2	FP1	294	ASN
2	FP1	339	MET
2	FP1	350	MET
2	FP1	402	VAL
2	FP1	427	ASN
2	FP1	508	THR
2	FP1	509	CYS
2	FP1	517	CYS
2	FP1	596	PHE
2	FP1	603	TYR
2	FP1	637	PHE

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Mol	Chain	Res	Type
2	FP1	660	LEU
2	FP1	716	LEU
2	FP1	725	PHE
2	FP1	728	ILE
2	FP1	732	MET
2	FP1	761	PHE
2	FP1	800	PHE
2	FP1	825	LEU
2	FP1	837	PHE
2	FP1	911	PHE
2	FP1	930	PHE
2	GP1	57	MET
2	GP1	127	PHE
2	GP1	140	ASP
2	GP1	149	TYR
2	GP1	191	MET
2	GP1	262	ASP
2	GP1	290	LEU
2	GP1	331	SER
2	GP1	339	MET
2	GP1	486	ASP
2	GP1	508	THR
2	GP1	517	CYS
2	GP1	540	LEU
2	GP1	555	GLN
2	GP1	573	ASN
2	GP1	589	THR
2	GP1	630	ASP
2	GP1	639	TYR
2	GP1	648	PHE
2	GP1	696	TYR
2	GP1	709	ASN
2	GP1	728	ILE
2	GP1	759	MET
2	GP1	761	PHE
2	GP1	807	ASN
2	GP1	825	LEU
2	GP1	837	PHE
2	GP1	915	ILE
2	GP1	916	LEU
2	GP1	931	THR
2	GP1	936	LEU

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Mol	Chain	Res	Type
2	GP1	938	ASP
2	HP1	33	LEU
2	HP1	85	MET
2	HP1	93	MET
2	HP1	125	GLN
2	HP1	127	PHE
2	HP1	140	ASP
2	HP1	147	LEU
2	HP1	149	TYR
2	HP1	196	LYS
2	HP1	262	ASP
2	HP1	285	ASN
2	HP1	295	GLN
2	HP1	299	LYS
2	HP1	325	LEU
2	HP1	326	GLN
2	HP1	348	GLN
2	HP1	368	ASN
2	HP1	369	ASP
2	HP1	393	GLN
2	HP1	430	MET
2	HP1	431	MET
2	HP1	509	CYS
2	HP1	514	SER
2	HP1	515	LEU
2	HP1	530	ILE
2	HP1	540	LEU
2	HP1	557	GLN
2	HP1	564	SER
2	HP1	603	TYR
2	HP1	612	CYS
2	HP1	639	TYR
2	HP1	661	MET
2	HP1	696	TYR
2	HP1	723	PHE
2	HP1	725	PHE
2	HP1	728	ILE
2	HP1	758	TYR
2	HP1	759	MET
2	HP1	837	PHE
2	HP1	911	PHE
2	HP1	936	LEU

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Mol	Chain	Res	Type
2	IP1	33	LEU
2	IP1	38	LEU
2	IP1	42	PHE
2	IP1	50	HIS
2	IP1	57	MET
2	IP1	127	PHE
2	IP1	140	ASP
2	IP1	221	GLU
2	IP1	262	ASP
2	IP1	275	LEU
2	IP1	285	ASN
2	IP1	291	ASN
2	IP1	299	LYS
2	IP1	325	LEU
2	IP1	363	THR
2	IP1	369	ASP
2	IP1	431	MET
2	IP1	450	ARG
2	IP1	452	PHE
2	IP1	509	CYS
2	IP1	543	ASP
2	IP1	546	LYS
2	IP1	564	SER
2	IP1	576	MET
2	IP1	603	TYR
2	IP1	604	TYR
2	IP1	637	PHE
2	IP1	639	TYR
2	IP1	660	LEU
2	IP1	671	PHE
2	IP1	723	PHE
2	IP1	736	MET
2	IP1	761	PHE
2	IP1	776	MET
2	IP1	837	PHE
2	IP1	905	TRP
2	IP1	930	PHE
2	JP1	29	PRO
2	JP1	55	GLN
2	JP1	57	MET
2	JP1	81	MET
2	JP1	93	MET

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Mol	Chain	Res	Type
2	JP1	109	PHE
2	JP1	127	PHE
2	JP1	285	ASN
2	JP1	293	THR
2	JP1	325	LEU
2	JP1	326	GLN
2	JP1	331	SER
2	JP1	359	THR
2	JP1	387	GLU
2	JP1	389	CYS
2	JP1	393	GLN
2	JP1	406	THR
2	JP1	430	MET
2	JP1	457	ASN
2	JP1	525	ASP
2	JP1	547	GLN
2	JP1	564	SER
2	JP1	568	TYR
2	JP1	596	PHE
2	JP1	603	TYR
2	JP1	611	ASP
2	JP1	624	LEU
2	JP1	661	MET
2	JP1	696	TYR
2	JP1	704	TRP
2	JP1	717	ILE
2	JP1	723	PHE
2	JP1	724	ILE
2	JP1	800	PHE
2	JP1	827	TYR
2	JP1	845	GLN
2	JP1	903	THR
2	JP1	941	LEU
3	KP1	12	PHE
3	KP1	16	ARG
3	KP1	36	PHE
3	KP1	38	LYS
3	LP1	12	PHE
3	MP1	7	ASN
3	MP1	12	PHE
3	MP1	37	PHE
3	MP1	40	ARG

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Mol	Chain	Res	Type
3	NP1	11	LEU
3	NP1	12	PHE
3	NP1	16	ARG
3	NP1	36	PHE
3	NP1	37	PHE
3	OP1	1	MET
3	OP1	12	PHE
3	OP1	16	ARG
3	OP1	18	ARG
3	OP1	37	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

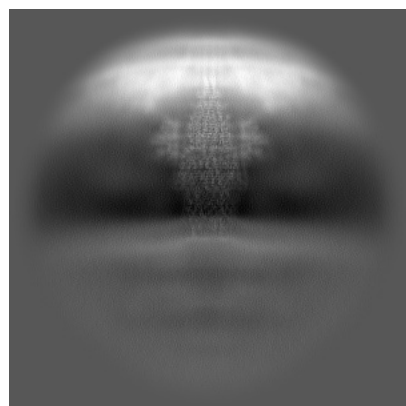
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49396. These allow visual inspection of the internal detail of the map and identification of artifacts.

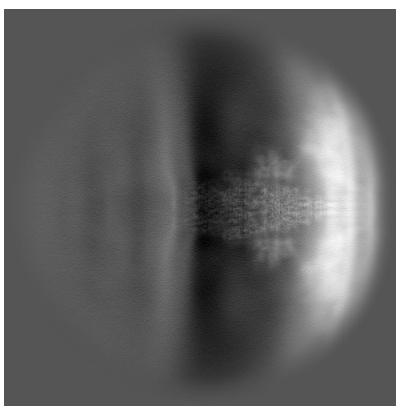
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

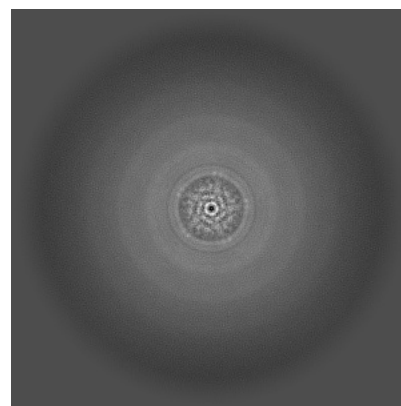
6.1.1 Primary map



X

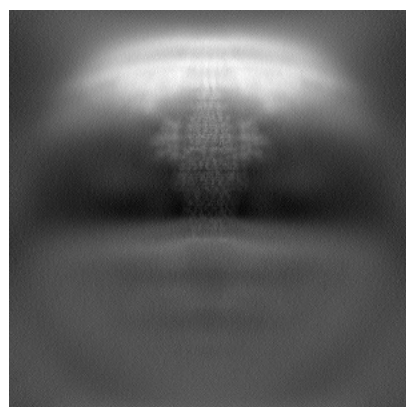


Y

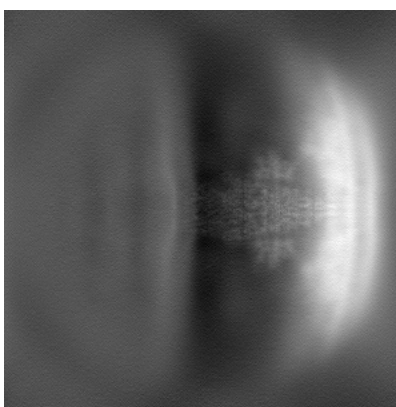


Z

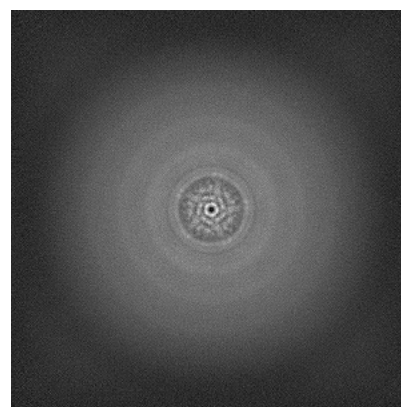
6.1.2 Raw map



X



Y

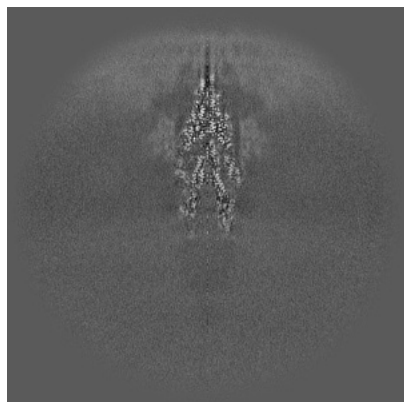


Z

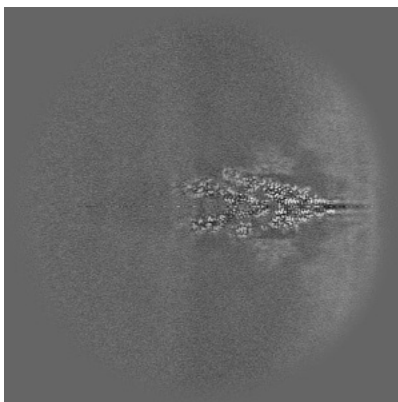
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

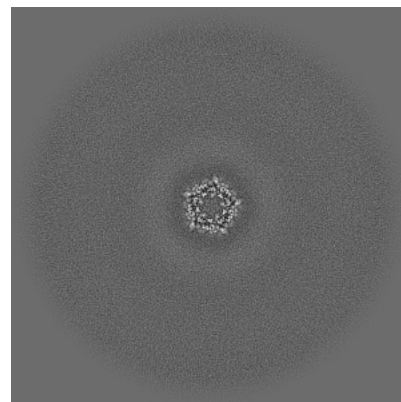
6.2.1 Primary map



X Index: 256

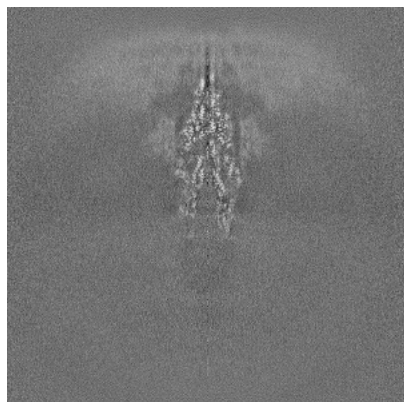


Y Index: 256

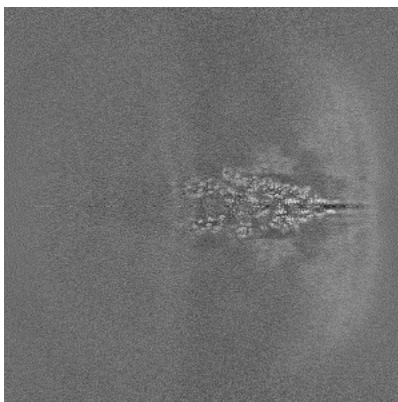


Z Index: 256

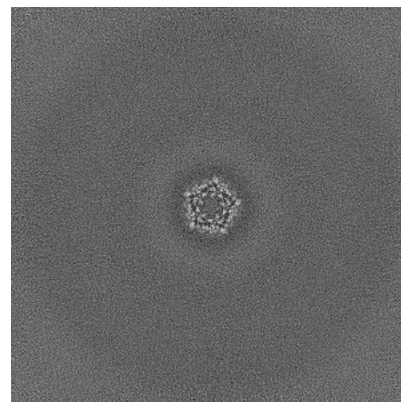
6.2.2 Raw map



X Index: 256



Y Index: 256

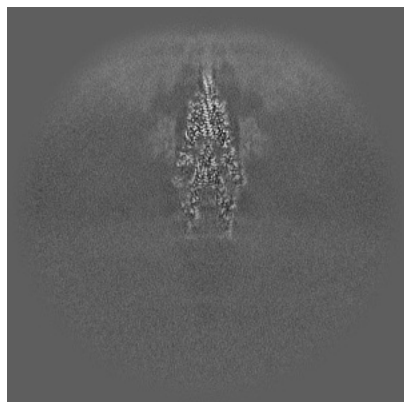


Z Index: 256

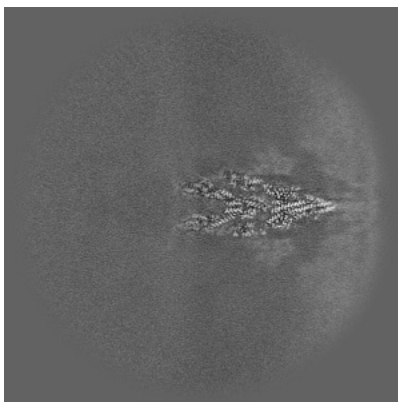
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

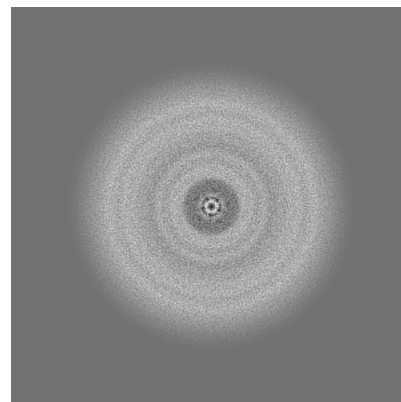
6.3.1 Primary map



X Index: 262

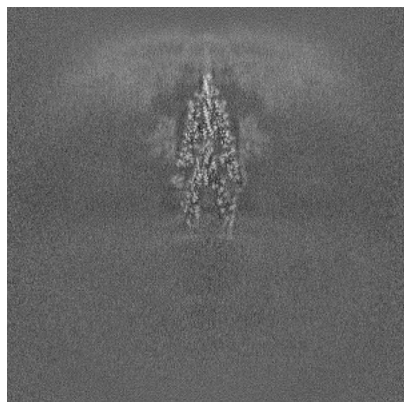


Y Index: 262

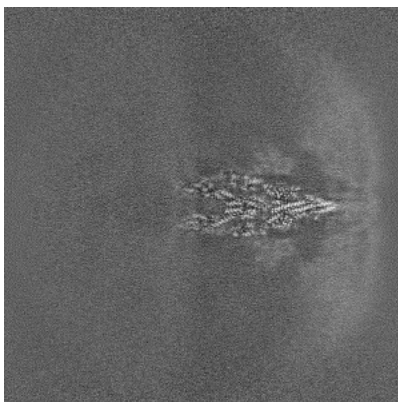


Z Index: 428

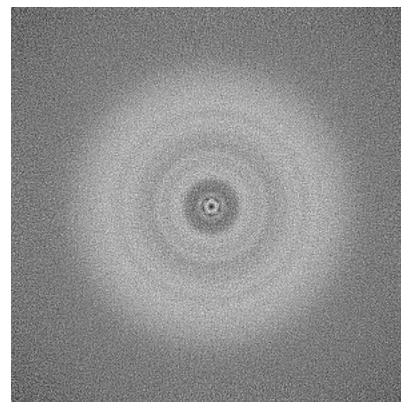
6.3.2 Raw map



X Index: 263



Y Index: 262

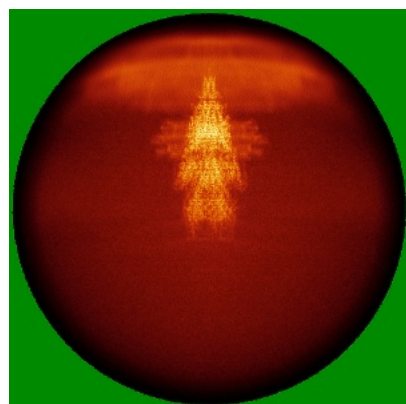


Z Index: 429

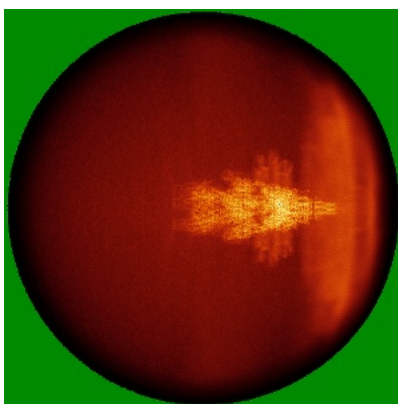
The images above show the largest variance slices of the map in three orthogonal directions.

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

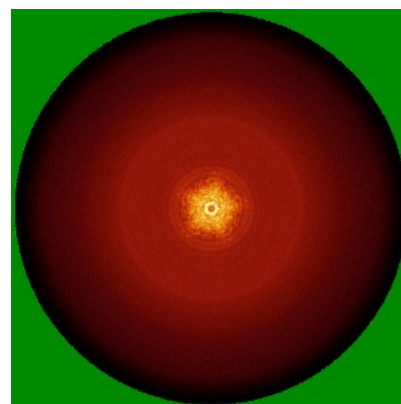
6.4.1 Primary map



X

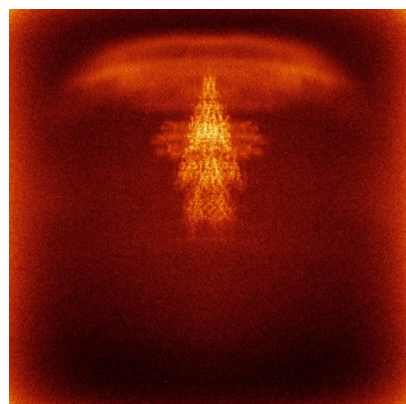


Y

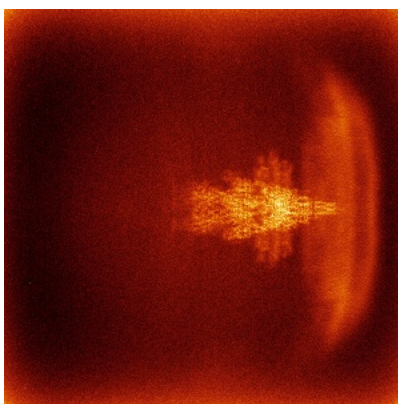


Z

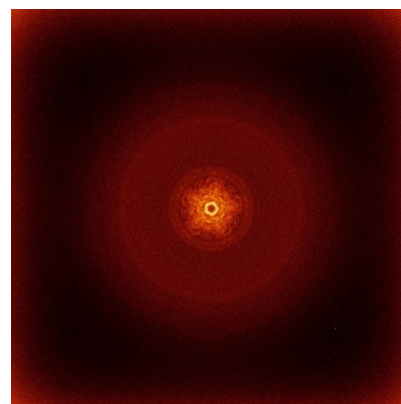
6.4.2 Raw map



X



Y

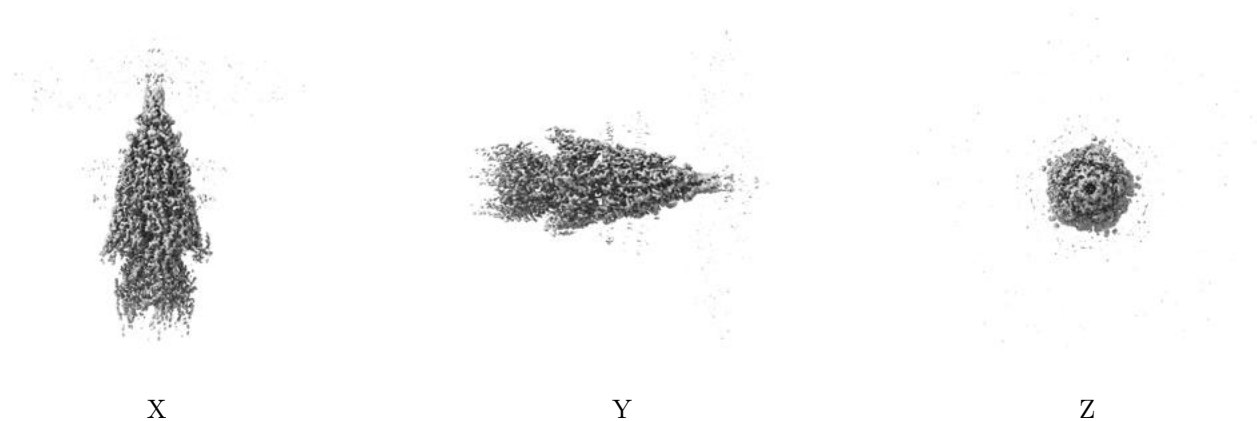


Z

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.

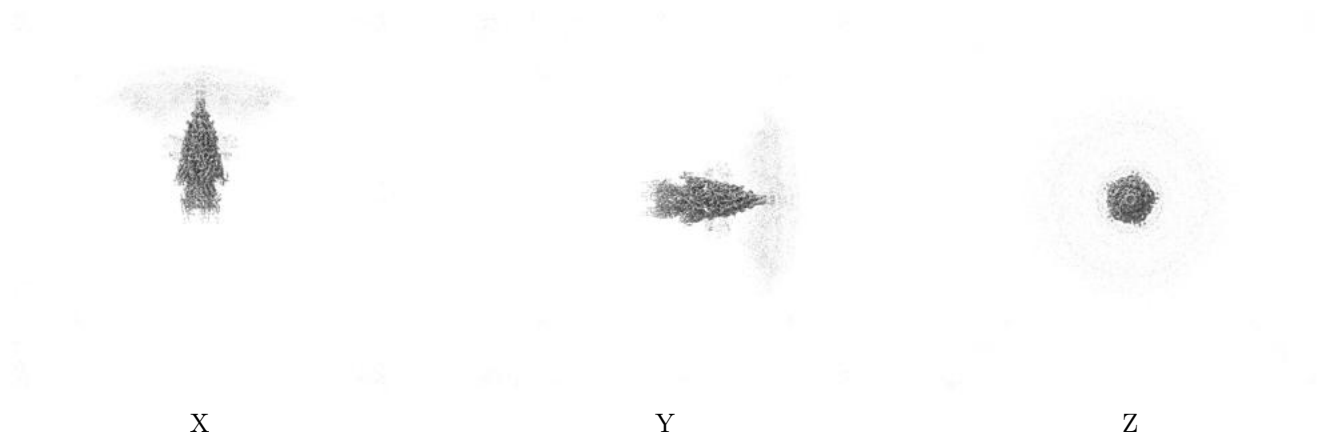
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

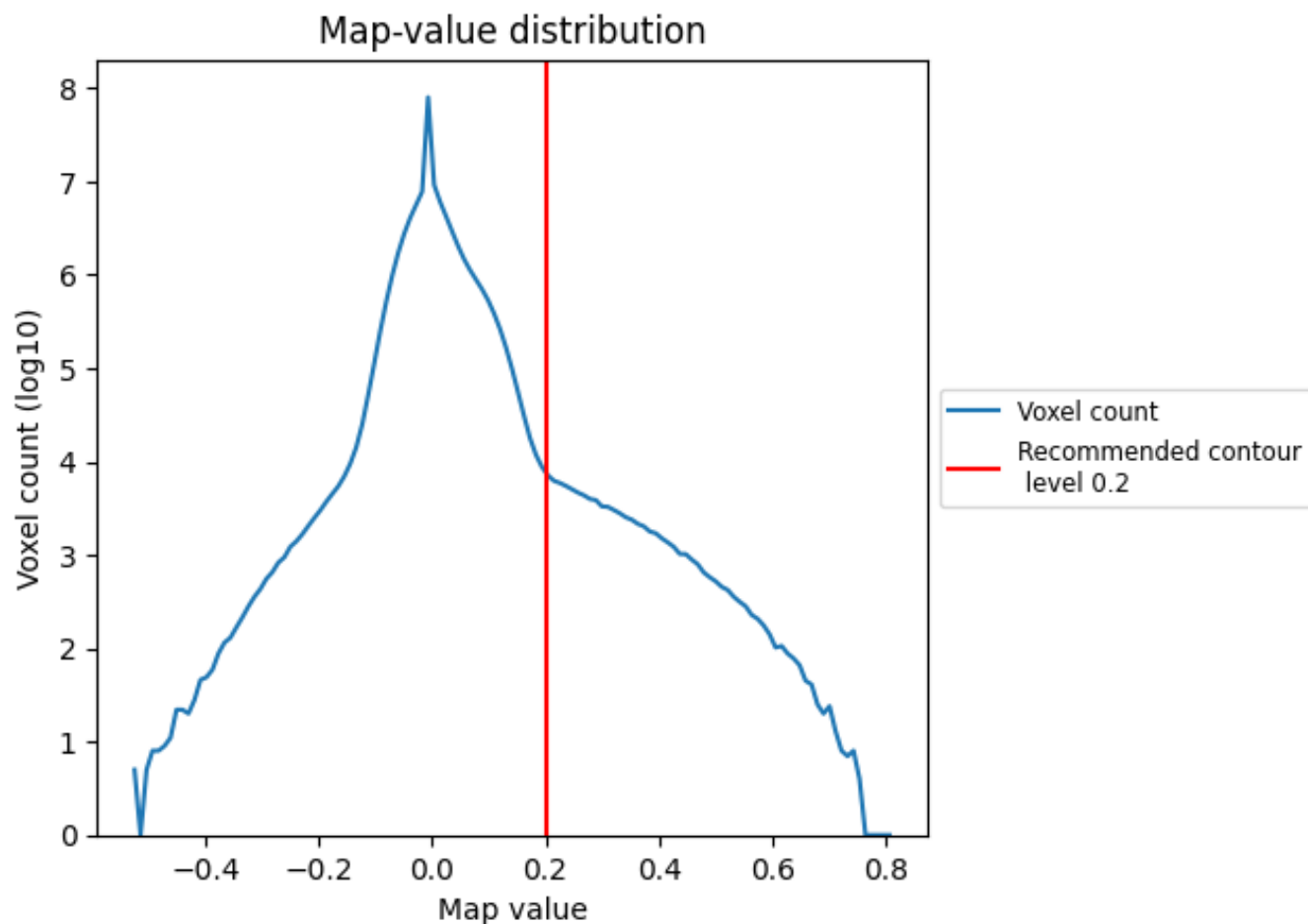
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

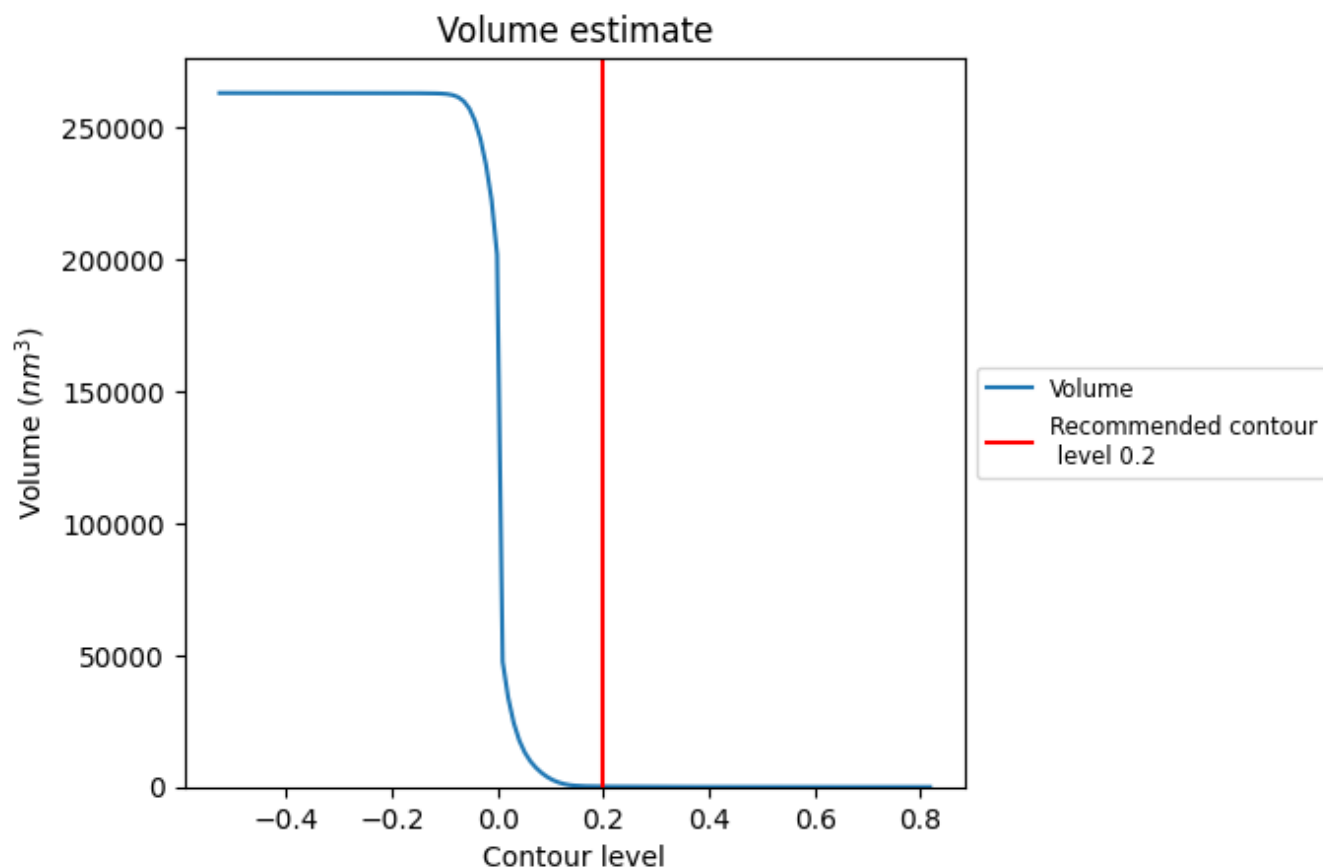
This section contains the results of statistical analysis of the map.

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.

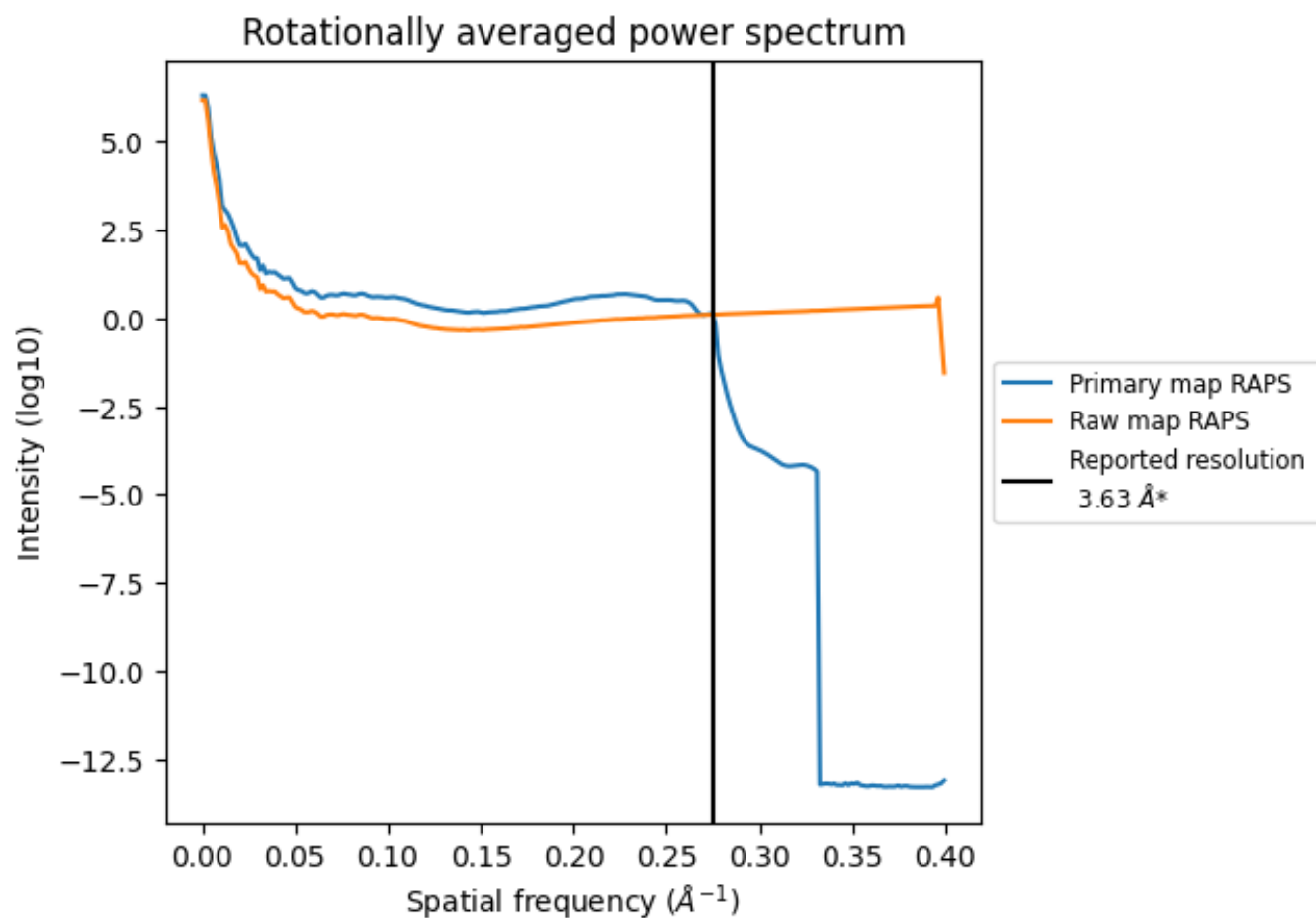
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm^3 ; this corresponds to an approximate mass of 156 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 ⓘ

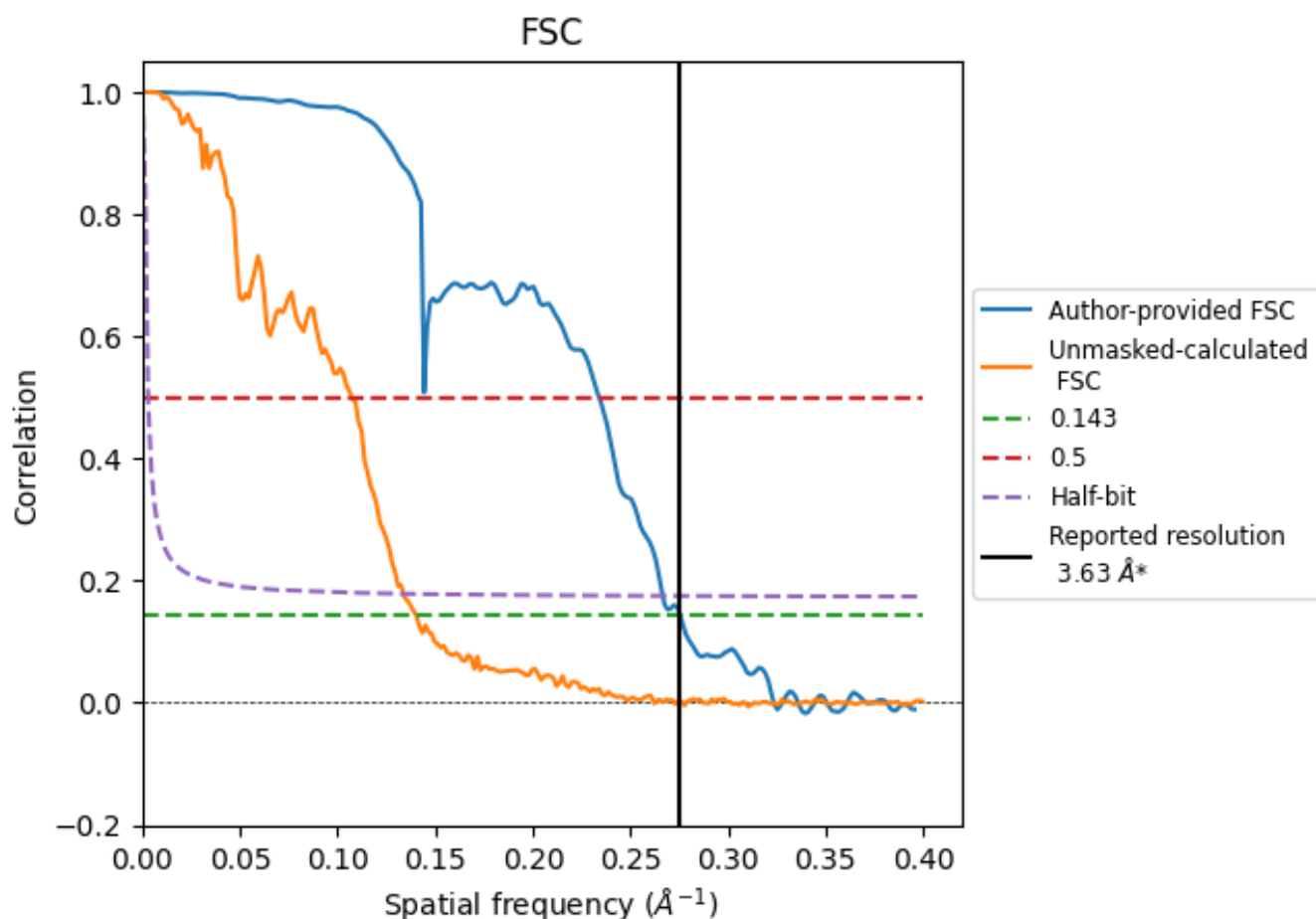


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

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 0.275 \AA^{-1}

8.2 Resolution estimates [i](#)

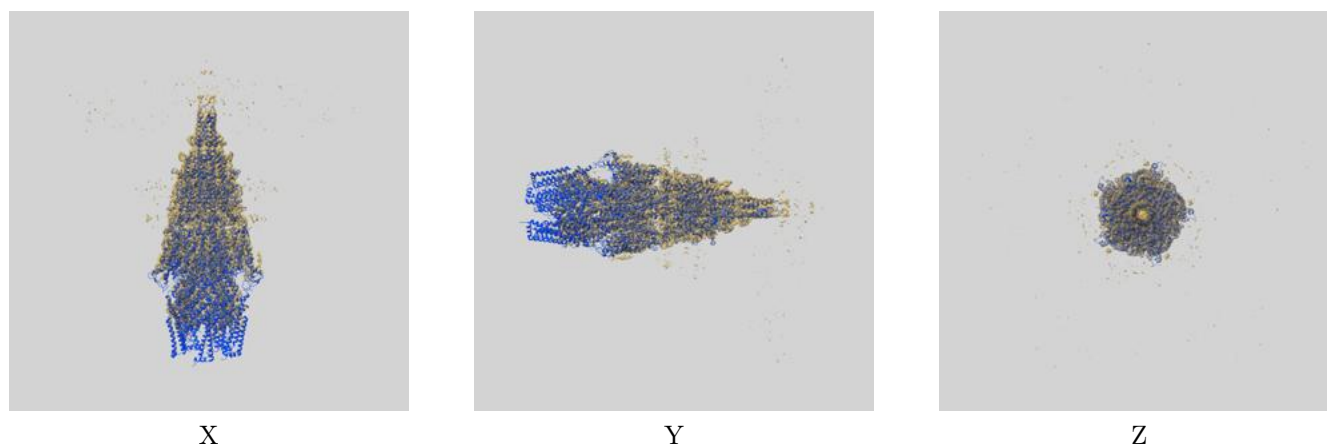
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	3.63	4.27	3.75
Unmasked-calculated*	7.12	9.32	7.47

*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 7.12 differs from the reported value 3.63 by more than 10 %

9 Map-model fit [i](#)

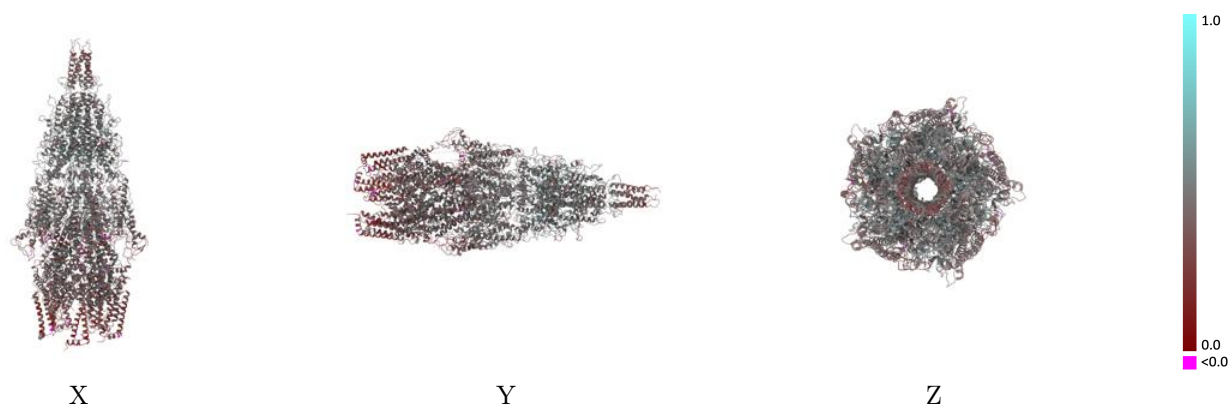
This section contains information regarding the fit between EMDB map EMD-49396 and PDB model 9NGY. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



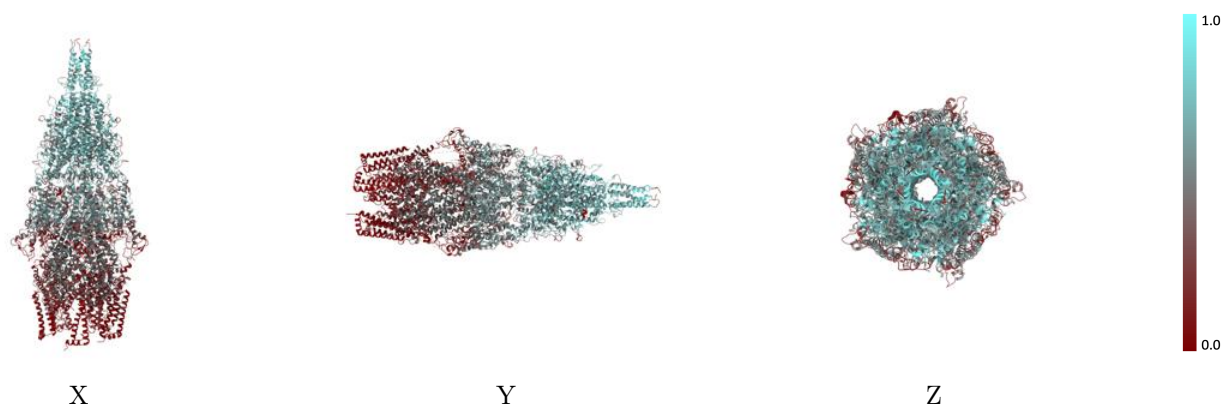
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



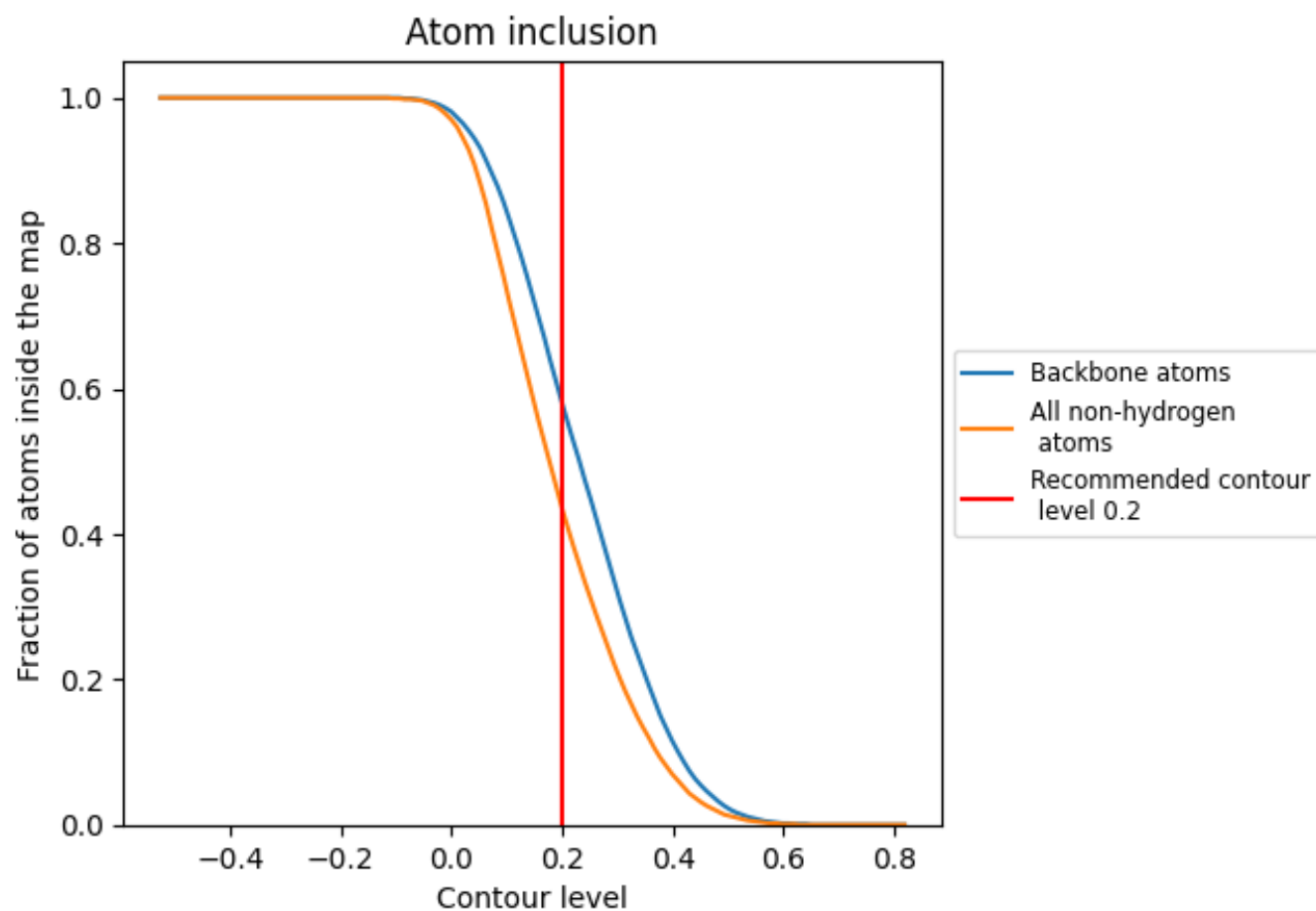
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 43% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4340	 0.4130
AP1	 0.6400	 0.4630
BP1	 0.6390	 0.4630
CP1	 0.6390	 0.4630
DP1	 0.6380	 0.4640
EP1	 0.6410	 0.4630
FP1	 0.3560	 0.3990
GP1	 0.3560	 0.3970
HP1	 0.3540	 0.3970
IP1	 0.3510	 0.3960
JP1	 0.3510	 0.3960
KP1	 0.0400	 0.2680
LP1	 0.0490	 0.2740
MP1	 0.0400	 0.2680
NP1	 0.0520	 0.2460
OP1	 0.0370	 0.2420

