



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:14 PM UTC

PDB ID : 9X0F / pdb_00009x0f
EMDB ID : EMD-66433
Title : Cryo-EM structure of EvSS
Authors : Bai, L.; Lyu, R.Q.
Deposited on : 2025-09-30
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

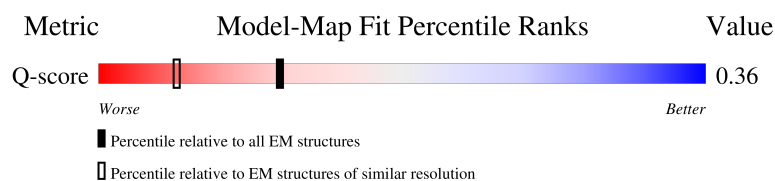
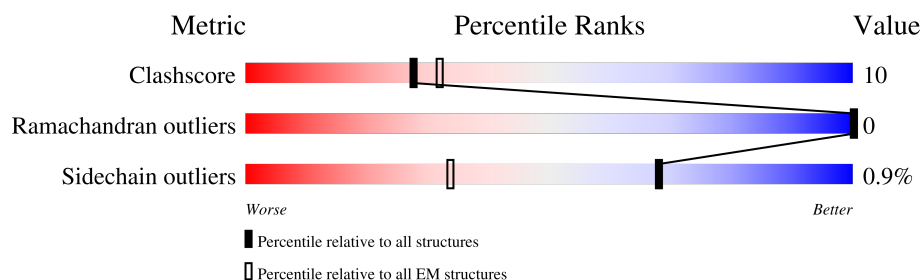
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

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

Mol	Chain	Length	Quality of chain
1	A	714	22% 31%10%59%
1	B	714	32% 32%8%59%
1	C	714	33% 30%11%59%
1	D	714	32% 33%8%59%

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Mol	Chain	Length	Quality of chain
1	E	714	
1	F	714	
1	G	714	
1	H	714	
1	I	714	
1	J	714	
1	K	714	
1	L	714	
1	M	714	
1	N	714	
1	O	714	
1	P	714	
1	Q	714	
1	R	714	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 42552 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.

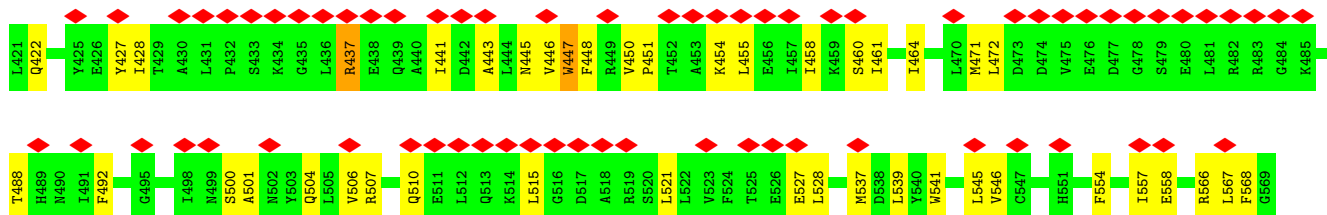
- Molecule 1 is a protein called Stelatatriene synthase.

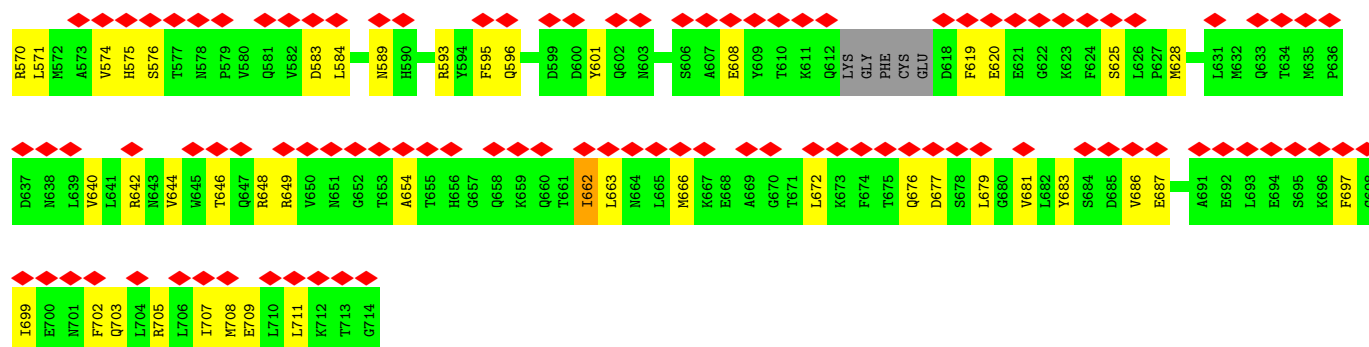
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	B	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	C	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	D	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	E	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	F	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	G	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	H	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	I	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	J	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	K	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	L	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	M	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	N	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	O	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	P	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		
1	Q	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		

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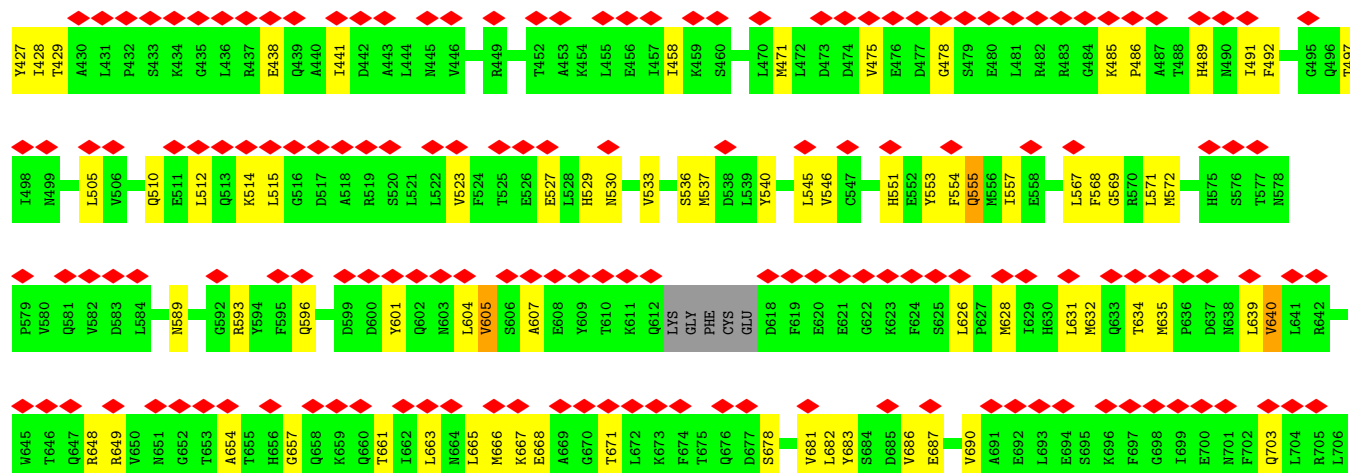
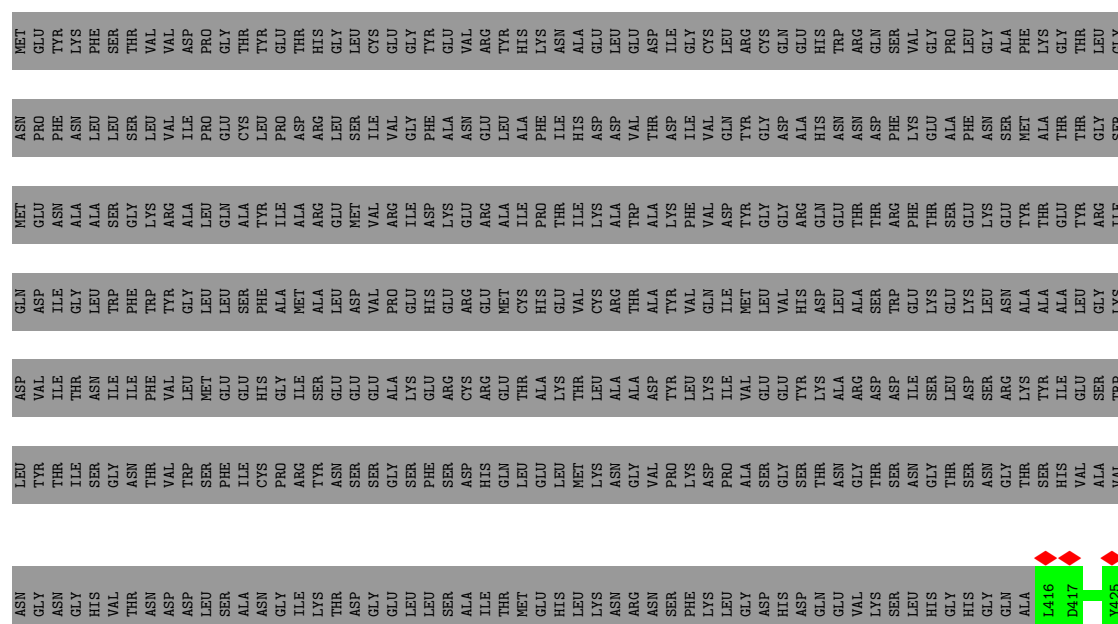
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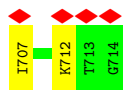
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	294	Total	C	N	O	S	0	0
			2364	1502	407	444	11		



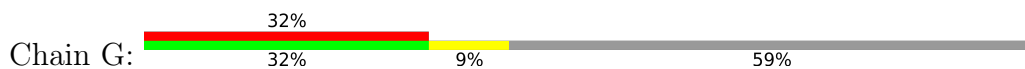


• Molecule 1: Stellatatriene synthase





- Molecule 1: Stellatatriene synthase

[illegible]

ASN	GLY	ASN	GLY	HIS	VAL	THR	ASN	ASP	ASP	LEU	SER	ALA	ASN	GLY	ILE	LYS	THR	ASP	GLY	GLU	LEU	LEU	SER	ALA	ILE	THR	MET	GLU	HIS	HIS	LEU	LYS	ASN	ASN	ARG	ASN	ASN	SER	SER	PHE	LYS	LEU	LEU	GLY	ASP	HIS	ASP	GLN	GLU	VAL	VAL	LYS	SER	SER	LEU	LEU	HIS	GLY	HIS	HIS	GLY	GLN	ALA	L416	D417	P418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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Q422	A423	P424	Y425	E426	Y427	I428	T429	A430	L431	P432	S433	S434	S435	G436	L437	R438	E439	Q439	A440	I441	D442	A443	L444	M445	V446	W447	F448	R449	V450	P451	T452	A453	K454	L455	E456	I457	L458	K459	S460	T461	T462	T463	L464	S465	L470	M471	L472	D473	D474	V475	D476	G477	G478	S479	E480	L481	R482	R483	A484
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K485	P486	A487	T488	H489	M490	T491	G495	R507	A508	L509	Q510	E511	L512	Q513	K514	L515	G516	D517	A518	R519	S520	L521	L522	V523	F524	T525	E526	E527	L528	H529	M530	G534	Q535	S536	M537	D538	L539	V540	H541	T542	S543	M544	L545	P548	S549	M550	H551	E552	V553	F554	Q555	M556	L557	E558
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G562	G563	L564	F565	R566	L567	F568	G569	R570	L571	M572	A573	V574	H575	S576	T577	M578	F579	V580	Q581	V582	D583	L584	T585	D586	F587	T588	M589	H590	L591	G592	R593	V594	F595	Q596	T597	D598	D599	D600	Y601	Q602	M603	L604	V605	S606	A607	E608	V609	T610	K611	Q612	LYS	GLY	PHE	CYS	GLU	D618	F619	E620	F621
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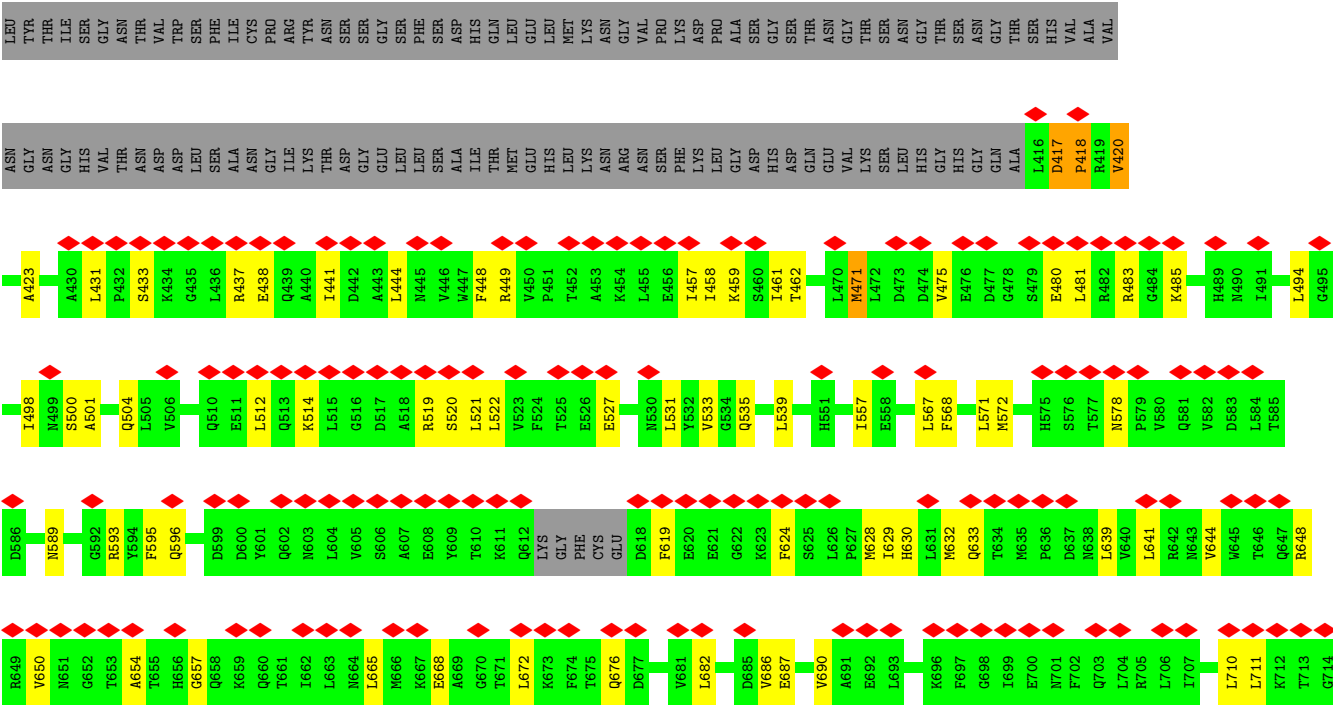
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L682	Y683	S684	S685	Y686	S687	K688	S689	Y690	A691	S692	L693	S694	S695	K696	F697	G698	L699	E700	N701	F702	Q703	L704	R705	L706	L707	N708	E709	L710	L711	K712	T713	G714
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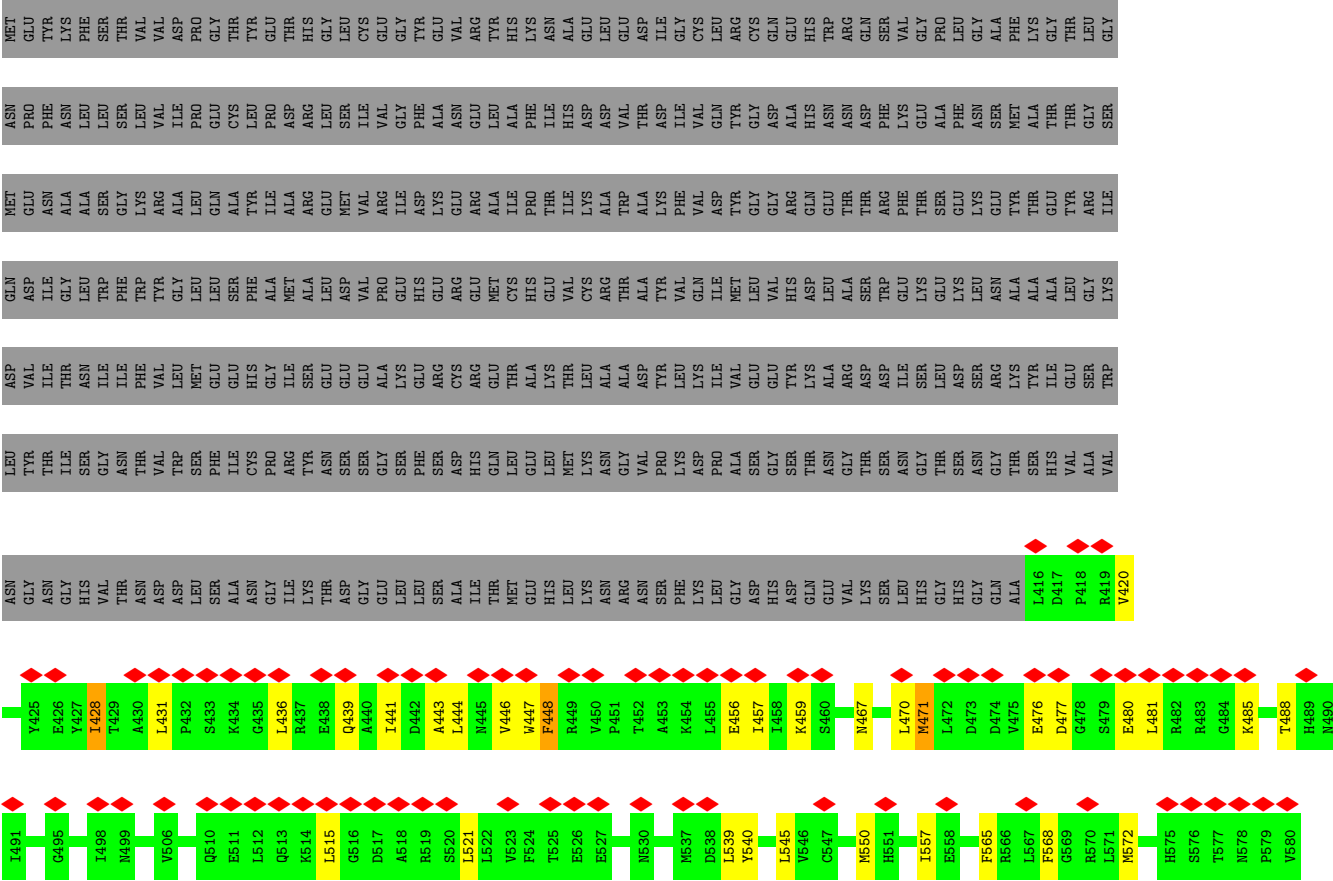
- Molecule 1: Stellatatriene synthase

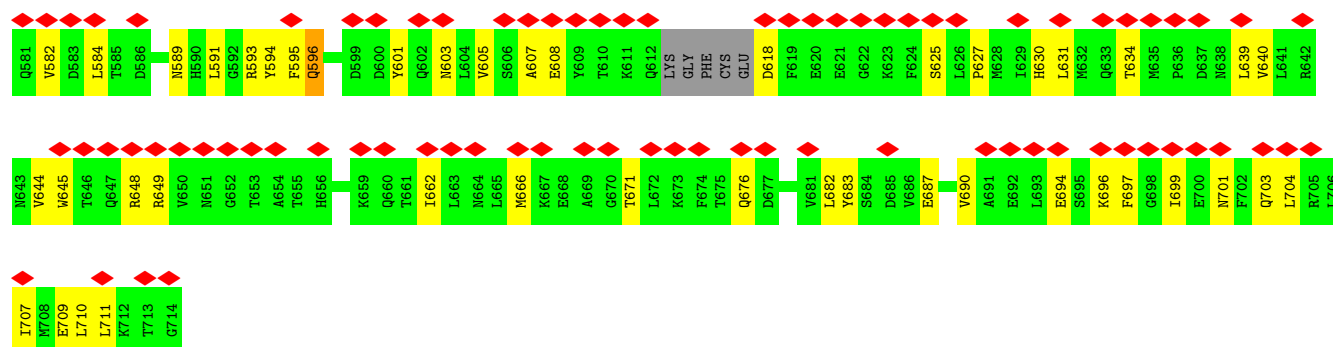


MET	GLU	TYR	LYS	PHE	THR	VAL	ASP	PRO	GLY	THR	TYR	GLU	GLU	GLY	TYR	GLU	VAL	ASN	ALA	GLU	LEU	GLU	GLY	ASP	ILE	GLY	CYS	LEU	ARG	CYS	GLN	GLU	HIS	TRP	ARG	GLN	SER	VAL	GLY	PRO	PRO	LEU	GLY	ALA	PHE	LYS	THR	LEU	TYR
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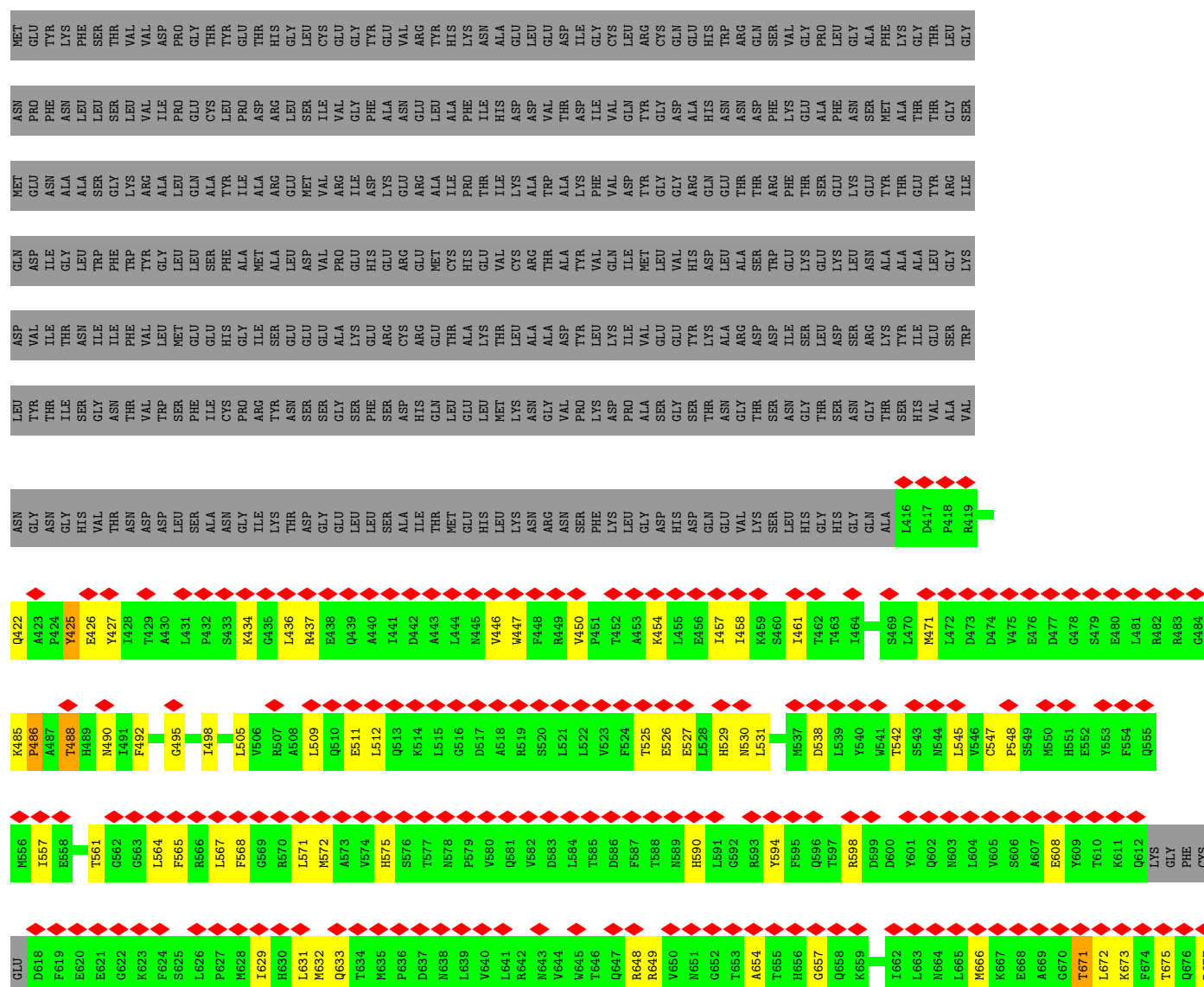


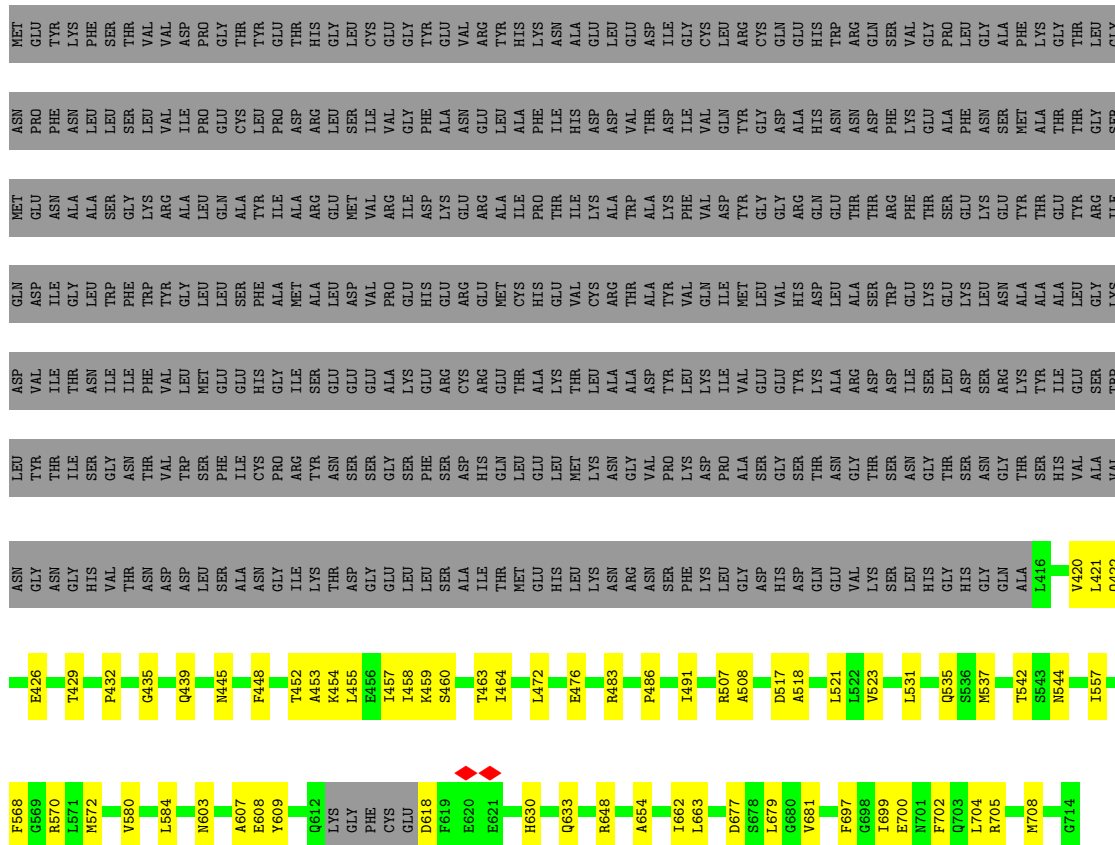
● Molecule 1: Steltatriene synthase



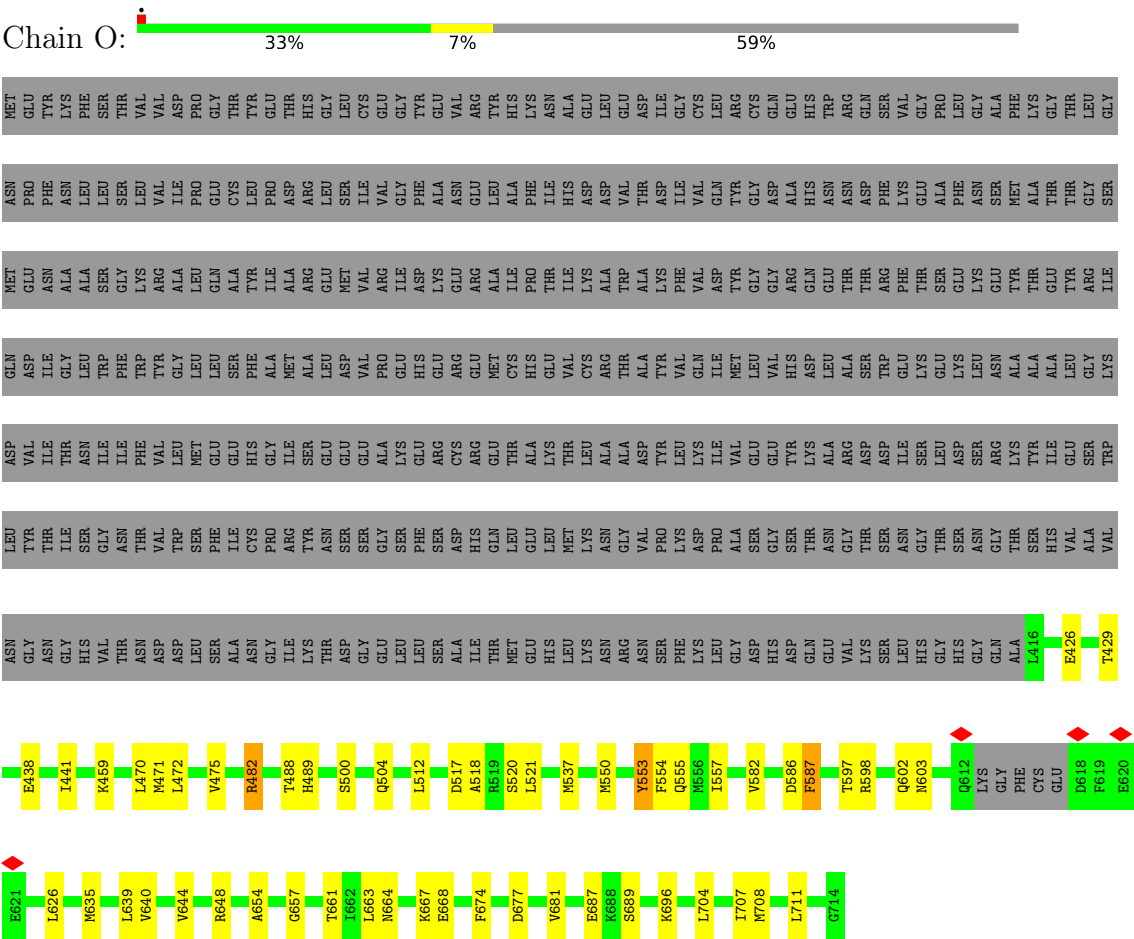


• Molecule 1: Steltatriene synthase

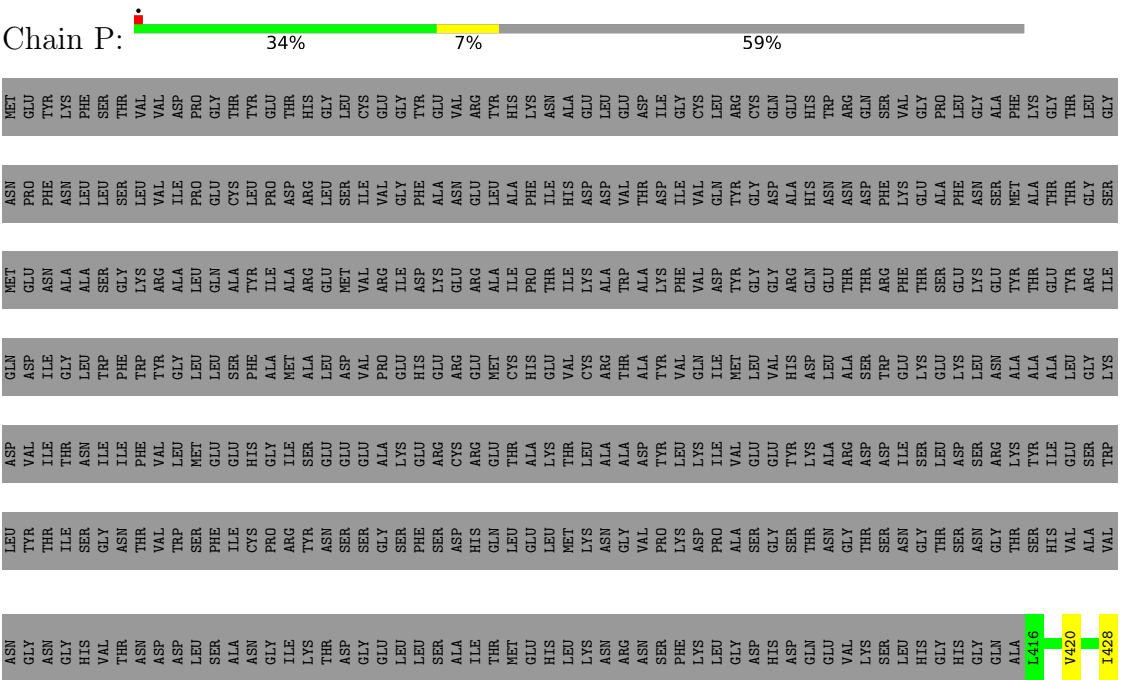




● Molecule 1: Stellatatriene synthase

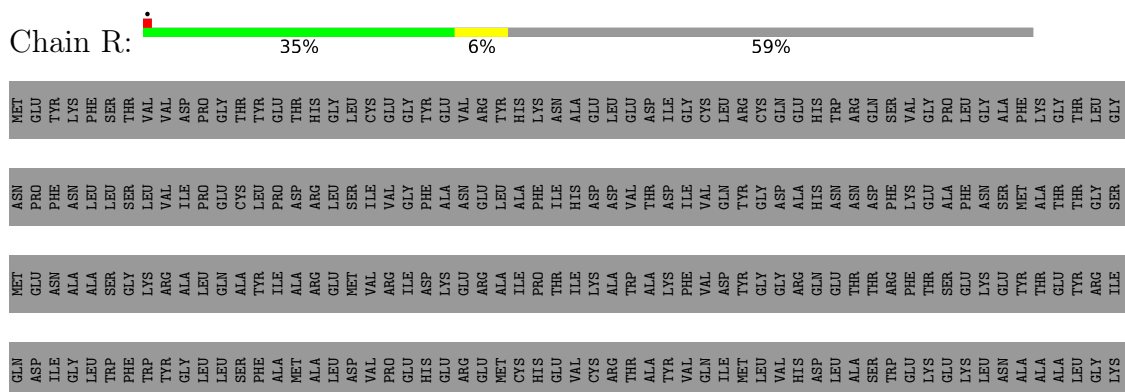


● Molecule 1: Stellatatriene synthase



- Molecule 1: Stellatatriene synthase

- Molecule 1: Stellatatriene synthase



Q633	E426	ASN	LEU	ASP
T634	Y427	GLY	THR	ILE
M635	T428	ASN	THR	VAL
	T429	GLY	ILE	ASN
W645		HIS	SER	ILE
	P432	VAL	GLY	ILE
R648	S433	THR	ASN	ILE
R649		ASN	THR	VAL
	K454	ASP	VAL	ASP
G657		ASP	THR	LEU
	T458	LEU	SER	MET
T661		SER	PHE	GLU
I662	A468	ALA	ILE	GLU
L663	S469	ASN	CYS	GLY
N664	L470	GLY	PRO	HIS
L665	M471	ILE	ARG	ILE
W666	L472	LYS	THR	SER
K667		THR	ASN	GLU
E668	V475	ASP	SER	GLU
		GLY	SER	GLU
K696	R483	LEU	GLY	ALA
		LEU	SER	LYS
Q703	A487	LEU	PHE	ARG
	T488	SER	SER	GLY
I707	H489	ALA	ASP	CYS
	N490	ILE	HIS	ARG
G714		THR	GLN	GLU
	L505	MET	LEU	THR
		GLY	GLU	ALA
	Q513	HIS	LEU	LYS
		LEU	MET	THR
	T542	LYS	LYS	LEU
	S543	ARG	ASN	ALA
	N544	ASN	GLY	ALA
		ASN	VAL	ASP
	V582	SER	PRO	TYR
		PHE	LYS	LEU
	T597	LYS	ASP	LYS
		LEU	PRO	ILE
	V605	GLY	ALA	VAL
	S606	ASP	SER	GLU
	A607	HIS	GLY	GLU
	E608	ASP	SER	TYR
		GLN	THR	LYS
		GLU	ASN	ALA
	Q612	VAL	GLY	ARG
		LYS	THR	ASP
	GLY	GLY	SER	ASP
	PHE	LEU	ASN	ILE
	CYS	HIS	GLY	SER
	GLU	GLY	THR	LEU
	D618	HIS	SER	ASP
	F619	GLY	ASN	SER
	E620	GLN	GLY	ARG
	E621	ALA	THR	LYS
	Q622	L416	SER	TYR
		L416	HIS	ILE
		Q422	VAL	GLU
		A423	ALA	SER
			VAL	TRP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108639	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.482	Depositor
Minimum map value	-0.295	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	296.0, 296.0, 296.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	1/2409 (0.0%)	0.51	7/3257 (0.2%)
1	B	0.18	0/2409	0.66	12/3257 (0.4%)
1	C	0.17	0/2409	0.54	5/3257 (0.2%)
1	D	0.15	0/2409	0.42	2/3257 (0.1%)
1	E	0.20	0/2409	0.56	6/3257 (0.2%)
1	F	0.22	0/2409	0.64	11/3257 (0.3%)
1	G	0.15	0/2409	0.51	6/3257 (0.2%)
1	H	0.27	2/2409 (0.1%)	0.59	12/3257 (0.4%)
1	I	0.23	1/2409 (0.0%)	0.38	3/3257 (0.1%)
1	J	0.21	1/2409 (0.0%)	0.63	9/3257 (0.3%)
1	K	0.24	1/2409 (0.0%)	0.68	11/3257 (0.3%)
1	L	0.19	1/2409 (0.0%)	0.46	2/3257 (0.1%)
1	M	0.15	0/2409	0.46	8/3257 (0.2%)
1	N	0.20	1/2409 (0.0%)	0.51	6/3257 (0.2%)
1	O	0.15	0/2409	0.48	6/3257 (0.2%)
1	P	0.16	0/2409	0.49	6/3257 (0.2%)
1	Q	0.20	1/2409 (0.0%)	0.53	4/3257 (0.1%)
1	R	0.17	0/2409	0.52	9/3257 (0.3%)
All	All	0.19	9/43362 (0.0%)	0.54	125/58626 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	418	PRO	N-CD	9.71	1.61	1.47
1	I	418	PRO	N-CD	9.19	1.60	1.47
1	L	636	PRO	N-CD	-6.14	1.39	1.47
1	N	608	GLU	CA-C	6.03	1.60	1.52
1	Q	451	PRO	N-CD	-6.02	1.39	1.47
1	J	477	ASP	CA-C	5.98	1.60	1.52
1	K	486	PRO	N-CD	-5.63	1.39	1.47
1	H	637	ASP	CA-C	5.55	1.60	1.52
1	A	477	ASP	CA-C	5.10	1.60	1.52

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	588	THR	N-CA-C	11.31	123.61	111.28
1	B	618	ASP	N-CA-CB	11.12	129.41	110.50
1	K	633	GLN	N-CA-C	10.90	123.24	111.36
1	B	476	GLU	N-CA-C	10.43	122.73	111.36
1	B	618	ASP	N-CA-C	-10.29	82.20	111.00
1	J	640	VAL	N-CA-C	10.18	120.19	110.42
1	N	608	GLU	N-CA-C	10.12	124.13	111.69
1	P	453	ALA	N-CA-C	9.64	121.79	111.28
1	B	573	ALA	N-CA-C	9.58	122.73	111.71
1	G	475	VAL	N-CA-C	-9.53	101.57	110.53
1	B	611	LYS	N-CA-C	9.41	124.71	113.23
1	K	427	TYR	N-CA-C	9.33	121.45	111.28
1	A	601	TYR	N-CA-C	9.15	120.86	111.07
1	K	531	LEU	N-CA-C	8.97	121.88	111.11
1	N	609	TYR	N-CA-C	8.95	124.89	112.45
1	K	673	LYS	N-CA-C	-8.92	101.50	111.14
1	E	437	ARG	N-CA-C	8.74	120.81	111.28
1	F	569	GLY	N-CA-C	-8.74	101.91	112.49
1	F	555	GLN	N-CA-C	-8.74	101.72	111.07
1	R	605	VAL	N-CA-C	8.62	119.41	110.62
1	Q	475	VAL	N-CA-C	-8.61	102.44	110.53
1	J	476	GLU	N-CA-C	8.59	121.79	111.82
1	P	512	LEU	N-CA-C	-8.48	102.12	111.36
1	G	473	ASP	N-CA-C	8.24	119.89	111.07
1	F	553	TYR	N-CA-C	8.21	119.85	111.07
1	K	671	THR	N-CA-C	8.04	122.34	112.54
1	R	470	LEU	N-CA-C	7.92	119.54	111.07
1	G	475	VAL	N-CA-CB	7.80	120.56	110.57
1	M	542	THR	N-CA-C	7.80	119.42	111.07
1	A	476	GLU	N-CA-C	7.79	119.40	111.07
1	F	426	GLU	N-CA-C	7.67	121.73	112.38
1	P	510	GLN	N-CA-C	7.64	119.61	111.28
1	A	446	VAL	N-CA-C	7.60	118.37	110.62
1	G	663	LEU	N-CA-C	7.58	119.55	111.28
1	F	640	VAL	N-CA-C	7.57	118.34	110.62
1	B	542	THR	N-CA-C	7.51	119.11	111.07
1	J	594	TYR	N-CA-C	7.50	119.10	111.07
1	N	542	THR	N-CA-C	7.50	119.09	111.07
1	R	472	LEU	N-CA-C	-7.43	103.26	111.36
1	F	555	GLN	N-CA-CB	7.37	120.69	110.01
1	E	447	TRP	N-CA-C	7.36	122.44	113.17
1	A	448	PHE	N-CA-CB	7.13	121.02	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	557	ILE	N-CA-C	-7.12	103.83	110.53
1	D	696	LYS	N-CA-C	7.09	119.00	111.28
1	K	673	LYS	N-CA-CB	7.02	120.25	110.07
1	M	544	ASN	N-CA-CB	6.98	120.82	110.49
1	N	609	TYR	N-CA-CB	-6.98	99.86	110.26
1	R	472	LEU	N-CA-CB	6.97	120.48	110.16
1	J	596	GLN	N-CA-C	-6.95	103.64	111.14
1	M	594	TYR	N-CA-C	6.91	118.82	111.28
1	R	542	THR	N-CA-C	6.91	118.46	111.07
1	H	636	PRO	N-CA-C	6.90	123.13	114.92
1	N	544	ASN	N-CA-CB	6.89	120.69	110.49
1	F	607	ALA	N-CA-CB	6.89	121.14	110.46
1	G	665	LEU	N-CA-C	-6.88	103.86	111.36
1	K	631	LEU	N-CA-C	-6.85	103.89	111.36
1	J	596	GLN	N-CA-CB	6.79	119.92	110.07
1	Q	475	VAL	N-CA-CB	6.79	119.26	110.57
1	P	451	PRO	N-CA-C	6.76	120.99	111.33
1	O	555	GLN	N-CA-C	-6.73	103.87	111.14
1	C	554	PHE	N-CA-C	6.69	118.57	111.28
1	O	587	PHE	N-CA-C	6.66	118.54	111.28
1	I	418	PRO	N-CA-CB	6.57	109.06	102.17
1	M	596	GLN	N-CA-C	-6.54	104.08	111.07
1	K	488	THR	N-CA-C	6.52	119.21	111.71
1	L	542	THR	N-CA-C	6.51	118.04	111.07
1	R	544	ASN	N-CA-CB	6.51	120.12	110.49
1	F	428	ILE	N-CA-C	-6.48	103.94	111.00
1	H	588	THR	N-CA-C	6.46	118.32	111.28
1	F	605	VAL	N-CA-C	6.45	121.38	113.00
1	Q	473	ASP	N-CA-C	6.44	117.96	111.07
1	P	512	LEU	N-CA-CB	6.41	119.65	110.16
1	B	544	ASN	N-CA-CB	6.37	119.91	110.49
1	F	428	ILE	N-CA-CB	6.35	121.17	110.56
1	K	490	ASN	N-CA-C	-6.33	104.81	112.54
1	B	571	LEU	N-CA-C	-6.33	104.46	111.36
1	G	665	LEU	N-CA-CB	6.30	119.48	110.16
1	M	596	GLN	N-CA-CB	6.25	119.07	110.01
1	N	607	ALA	N-CA-C	-6.22	105.45	113.16
1	B	477	ASP	CB-CA-C	-6.19	99.35	110.37
1	K	425	TYR	N-CA-C	-6.19	104.61	111.36
1	J	446	VAL	N-CA-C	6.12	117.60	110.62
1	J	448	PHE	N-CA-CB	6.07	119.69	110.28
1	H	417	ASP	N-CA-C	6.04	119.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	529	HIS	N-CA-C	-6.03	104.79	111.36
1	R	607	ALA	N-CA-CB	5.98	120.03	110.46
1	C	585	THR	N-CA-C	5.95	117.46	110.97
1	I	417	ASP	N-CA-C	5.89	119.18	109.58
1	C	556	MET	N-CA-C	-5.88	104.95	111.36
1	H	418	PRO	N-CA-C	-5.86	108.59	114.68
1	E	574	VAL	N-CA-C	5.83	119.78	113.43
1	E	601	TYR	N-CA-C	5.80	117.60	111.28
1	J	477	ASP	CA-C-O	5.78	126.41	119.59
1	B	477	ASP	N-CA-CB	5.70	118.74	110.47
1	O	482	ARG	N-CA-C	5.66	117.74	108.52
1	L	544	ASN	N-CA-CB	5.64	119.07	110.44
1	E	448	PHE	N-CA-C	5.62	120.15	113.12
1	H	508	ALA	N-CA-C	-5.59	105.27	111.36
1	J	477	ASP	CB-CA-C	-5.57	101.30	110.72
1	H	607	ALA	N-CA-CB	5.56	118.72	110.49
1	M	550	MET	N-CA-C	-5.54	104.87	111.69
1	H	638	ASN	N-CA-C	-5.51	98.29	107.99
1	H	418	PRO	CA-N-CD	-5.49	104.31	112.00
1	C	588	THR	N-CA-CB	-5.49	102.06	110.12
1	H	637	ASP	CA-C-O	5.48	126.99	120.53
1	P	453	ALA	N-CA-CB	-5.46	102.09	110.12
1	A	599	ASP	N-CA-C	-5.39	105.31	111.14
1	R	607	ALA	N-CA-C	-5.39	102.54	110.52
1	Q	438	GLU	N-CA-C	-5.36	105.51	111.36
1	B	475	VAL	N-CA-C	5.36	115.57	110.42
1	I	418	PRO	N-CA-C	-5.31	108.60	114.92
1	A	477	ASP	CA-C-O	5.29	125.83	119.43
1	E	576	SER	N-CA-C	-5.28	102.24	110.42
1	R	471	MET	N-CA-C	5.25	117.91	111.82
1	B	477	ASP	CA-C-O	5.23	125.76	119.43
1	A	477	ASP	CB-CA-C	-5.22	101.08	110.37
1	F	607	ALA	N-CA-C	-5.21	102.74	110.46
1	H	605	VAL	N-CA-C	5.21	119.33	112.04
1	O	687	GLU	N-CA-C	5.20	116.64	111.07
1	H	607	ALA	N-CA-C	-5.18	106.64	113.17
1	M	543	SER	CA-C-O	5.06	125.21	119.18
1	H	418	PRO	N-CA-CB	5.05	108.50	102.60
1	O	553	TYR	N-CA-C	5.03	116.45	111.07
1	M	595	PHE	N-CA-C	5.02	116.83	111.36
1	O	689	SER	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2364	0	2359	48	0
1	B	2364	0	2360	49	0
1	C	2364	0	2360	66	0
1	D	2364	0	2360	60	0
1	E	2364	0	2360	60	0
1	F	2364	0	2360	63	0
1	G	2364	0	2360	40	0
1	H	2364	0	2360	49	0
1	I	2364	0	2360	57	0
1	J	2364	0	2360	65	0
1	K	2364	0	2360	46	0
1	L	2364	0	2360	59	0
1	M	2364	0	2360	37	0
1	N	2364	0	2360	40	0
1	O	2364	0	2360	39	0
1	P	2364	0	2360	29	0
1	Q	2364	0	2359	44	0
1	R	2364	0	2360	22	0
All	All	42552	0	42478	823	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 10.

All (823) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:TRP:CZ2	1:A:701:ASN:ND2	1.71	1.55
1:F:427:TYR:OH	1:F:485:LYS:HG2	1.20	1.31
1:C:582:VAL:HG11	1:C:697:PHE:CZ	1.67	1.29
1:O:470:LEU:HD22	1:O:482:ARG:HH22	1.06	1.18
1:B:582:VAL:HG11	1:B:697:PHE:HE1	1.05	1.18
1:A:447:TRP:CE2	1:A:701:ASN:ND2	2.13	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:VAL:HG11	1:B:697:PHE:CE1	1.83	1.14
1:O:470:LEU:HD22	1:O:482:ARG:NH2	1.62	1.13
1:D:582:VAL:HG21	1:D:697:PHE:CZ	1.85	1.12
1:D:555:GLN:HE21	1:D:556:MET:HE3	0.95	1.12
1:D:555:GLN:HE21	1:D:556:MET:CE	1.62	1.11
1:J:447:TRP:NE1	1:J:701:ASN:HD22	1.49	1.09
1:M:591:LEU:HD11	1:M:595:PHE:CZ	1.88	1.08
1:A:447:TRP:CZ2	1:A:701:ASN:CG	2.32	1.07
1:D:582:VAL:CG2	1:D:697:PHE:HZ	1.65	1.07
1:C:582:VAL:HG11	1:C:697:PHE:CE1	1.93	1.04
1:I:431:LEU:HD21	1:I:485:LYS:HG3	1.41	1.01
1:F:568:PHE:HA	1:F:571:LEU:HB2	1.43	1.01
1:F:427:TYR:OH	1:F:485:LYS:CG	2.13	0.97
1:F:491:ILE:HG23	1:F:492:PHE:CD2	1.99	0.97
1:L:491:ILE:HG23	1:L:492:PHE:CD2	2.00	0.97
1:L:450:VAL:HG21	1:L:572:MET:HG3	1.44	0.97
1:D:555:GLN:NE2	1:D:556:MET:HE3	1.79	0.95
1:D:582:VAL:HG21	1:D:697:PHE:HZ	1.17	0.95
1:D:582:VAL:CG2	1:D:697:PHE:CZ	2.45	0.95
1:A:447:TRP:HZ2	1:A:701:ASN:CG	1.74	0.93
1:B:582:VAL:CG1	1:B:697:PHE:HE1	1.81	0.92
1:C:693:LEU:O	1:C:697:PHE:HD2	1.54	0.90
1:O:586:ASP:OD1	1:O:587:PHE:N	2.05	0.90
1:I:417:ASP:OD1	1:I:418:PRO:HD2	1.74	0.87
1:H:503:TYR:CE2	1:H:507:ARG:HD2	2.10	0.87
1:C:587:PHE:HE1	1:C:690:VAL:HG22	1.39	0.86
1:C:582:VAL:CG1	1:C:697:PHE:CZ	2.56	0.85
1:C:693:LEU:O	1:C:697:PHE:CD2	2.29	0.85
1:E:557:ILE:HD12	1:E:596:GLN:HG3	1.58	0.85
1:A:645:TRP:HA	1:A:648:ARG:HE	1.43	0.84
1:O:470:LEU:CD2	1:O:482:ARG:HH22	1.90	0.84
1:E:447:TRP:HE3	1:E:697:PHE:CE2	1.94	0.83
1:I:539:LEU:CD1	1:L:499:ASN:ND2	2.42	0.83
1:Q:648:ARG:HG3	1:Q:654:ALA:HB2	1.60	0.83
1:F:554:PHE:CZ	1:F:626:LEU:CD1	2.63	0.82
1:B:608:GLU:CD	1:B:608:GLU:O	2.23	0.81
1:C:582:VAL:CG1	1:C:697:PHE:CE1	2.63	0.81
1:F:427:TYR:CZ	1:F:485:LYS:HG2	2.16	0.81
1:J:595:PHE:HE1	1:J:711:LEU:CD2	1.94	0.80
1:M:595:PHE:CE1	1:M:711:LEU:CD2	2.65	0.80
1:J:595:PHE:CE1	1:J:711:LEU:CD2	2.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:487:ALA:HB3	1:R:490:ASN:HD22	1.46	0.79
1:C:582:VAL:HG21	1:C:697:PHE:HZ	1.48	0.78
1:J:447:TRP:CZ2	1:J:701:ASN:HB2	2.18	0.78
1:A:475:VAL:HG11	1:A:498:ILE:HD11	1.66	0.78
1:A:447:TRP:CH2	1:A:701:ASN:ND2	2.51	0.78
1:C:582:VAL:HG21	1:C:697:PHE:CZ	2.18	0.78
1:B:477:ASP:HB2	1:B:621:GLU:HG3	1.67	0.77
1:B:565:PHE:HA	1:B:568:PHE:CE1	2.21	0.76
1:R:468:ALA:HA	1:R:471:MET:HE3	1.68	0.75
1:I:539:LEU:CD1	1:L:499:ASN:HD21	1.99	0.75
1:J:595:PHE:CE1	1:J:711:LEU:HD21	2.21	0.75
1:H:620:GLU:HA	1:H:648:ARG:HH21	1.51	0.75
1:F:554:PHE:CZ	1:F:626:LEU:HD13	2.21	0.75
1:B:513:GLN:HG3	1:E:521:LEU:HD13	1.69	0.75
1:A:416:LEU:N	1:D:556:MET:HE1	2.02	0.75
1:P:517:ASP:OD1	1:P:518:ALA:N	2.19	0.75
1:F:554:PHE:CZ	1:F:626:LEU:HD11	2.21	0.74
1:J:710:LEU:HD12	1:J:711:LEU:N	2.03	0.74
1:K:657:GLY:HA3	1:L:486:PRO:HG2	1.68	0.73
1:M:595:PHE:HE1	1:M:711:LEU:HD23	1.53	0.73
1:G:664:ASN:OD1	1:G:665:LEU:N	2.21	0.73
1:C:436:LEU:HD22	1:C:711:LEU:HD21	1.70	0.73
1:G:632:MET:HG3	1:G:641:LEU:HD21	1.71	0.73
1:I:431:LEU:CD2	1:I:485:LYS:HG3	2.16	0.73
1:L:438:GLU:HA	1:L:441:ILE:HD12	1.71	0.73
1:D:555:GLN:NE2	1:D:556:MET:CE	2.45	0.72
1:D:563:GLY:HA2	1:D:566:ARG:HH11	1.54	0.72
1:M:591:LEU:CD1	1:M:595:PHE:CZ	2.69	0.72
1:A:447:TRP:HE1	1:A:701:ASN:HB3	1.55	0.72
1:N:517:ASP:OD1	1:N:518:ALA:N	2.19	0.72
1:B:568:PHE:HD2	1:B:572:MET:HE3	1.54	0.71
1:I:438:GLU:HG2	1:I:459:LYS:HE2	1.73	0.71
1:L:537:MET:HB3	1:L:556:MET:SD	2.29	0.71
1:M:475:VAL:HG22	1:M:489:HIS:HB3	1.70	0.71
1:I:417:ASP:OD1	1:I:418:PRO:CD	2.39	0.71
1:C:587:PHE:CE1	1:C:690:VAL:HG22	2.23	0.70
1:C:587:PHE:HZ	1:C:704:LEU:HD21	1.56	0.70
1:I:521:LEU:HD13	1:L:513:GLN:HG3	1.74	0.70
1:D:582:VAL:HG22	1:D:697:PHE:HZ	1.53	0.70
1:E:447:TRP:CE3	1:E:697:PHE:CE2	2.78	0.69
1:A:521:LEU:HD13	1:D:513:GLN:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:441:ILE:HG23	1:F:572:MET:HE1	1.73	0.69
1:O:517:ASP:OD1	1:O:518:ALA:N	2.21	0.69
1:F:557:ILE:HD12	1:F:596:GLN:HG3	1.74	0.69
1:J:447:TRP:CD1	1:J:701:ASN:HD22	2.09	0.69
1:B:445:ASN:HD21	1:B:455:LEU:HD22	1.58	0.69
1:L:450:VAL:CG2	1:L:572:MET:HG3	2.21	0.69
1:Q:474:ASP:CG	1:Q:482:ARG:HH21	2.00	0.69
1:J:709:GLU:HG3	1:M:706:LEU:HD11	1.74	0.69
1:L:631:LEU:HD12	1:L:635:MET:HE3	1.75	0.69
1:F:568:PHE:O	1:F:572:MET:HG3	1.93	0.68
1:M:595:PHE:CE1	1:M:711:LEU:HD21	2.26	0.68
1:L:538:ASP:N	1:L:556:MET:SD	2.67	0.68
1:R:635:MET:HE1	1:R:665:LEU:HD11	1.74	0.68
1:L:457:ILE:O	1:L:461:ILE:HG13	1.94	0.68
1:Q:437:ARG:O	1:Q:441:ILE:HG22	1.93	0.68
1:G:474:ASP:OD2	1:G:482:ARG:HD2	1.93	0.67
1:H:417:ASP:OD1	1:H:418:PRO:HD2	1.94	0.67
1:B:582:VAL:HG21	1:B:697:PHE:CZ	2.30	0.67
1:K:545:LEU:HD21	1:K:649:ARG:HG2	1.77	0.67
1:J:428:ILE:HD12	1:J:471:MET:HG3	1.75	0.67
1:K:527:GLU:HA	1:K:530:ASN:HD22	1.60	0.67
1:J:443:ALA:HB1	1:J:704:LEU:HD12	1.77	0.66
1:H:417:ASP:OD1	1:H:418:PRO:CD	2.44	0.66
1:C:582:VAL:HG11	1:C:697:PHE:CE2	2.28	0.66
1:K:648:ARG:HH21	1:K:649:ARG:HB2	1.61	0.65
1:E:683:TYR:O	1:E:687:GLU:HG2	1.96	0.65
1:I:539:LEU:HD11	1:L:499:ASN:HD21	1.61	0.65
1:Q:447:TRP:CD1	1:Q:697:PHE:CE2	2.84	0.65
1:C:535:GLN:HA	1:C:560:LYS:HZ1	1.62	0.64
1:G:470:LEU:HD22	1:G:482:ARG:NH2	2.12	0.64
1:C:558:GLU:HG3	1:C:589:ASN:HB3	1.77	0.64
1:F:491:ILE:HG23	1:F:492:PHE:CE2	2.31	0.64
1:I:423:ALA:HB2	1:J:639:LEU:HD22	1.79	0.64
1:M:595:PHE:HE1	1:M:711:LEU:CD2	2.10	0.64
1:L:437:ARG:HH11	1:L:564:LEU:HD22	1.63	0.64
1:O:704:LEU:HG	1:O:708:MET:HE1	1.80	0.64
1:K:485:LYS:HB3	1:K:486:PRO:HD2	1.80	0.64
1:A:536:SER:HB2	1:D:421:LEU:HD13	1.79	0.63
1:H:574:VAL:HG23	1:H:575:HIS:ND1	2.14	0.63
1:I:568:PHE:O	1:I:572:MET:HG2	1.99	0.63
1:D:557:ILE:HD12	1:D:596:GLN:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:450:VAL:HG21	1:K:572:MET:HE1	1.79	0.63
1:N:704:LEU:O	1:N:708:MET:HG2	1.99	0.62
1:K:561:THR:HG22	1:K:565:PHE:HE2	1.65	0.62
1:L:513:GLN:HE22	1:L:521:LEU:HD21	1.63	0.62
1:B:554:PHE:CD2	1:B:593:ARG:HD3	2.34	0.62
1:N:445:ASN:ND2	1:N:455:LEU:HD22	2.14	0.62
1:Q:447:TRP:CD1	1:Q:697:PHE:CD2	2.88	0.62
1:P:545:LEU:HD21	1:P:649:ARG:HG2	1.81	0.62
1:D:582:VAL:HG21	1:D:697:PHE:CE2	2.33	0.62
1:H:503:TYR:HE2	1:H:507:ARG:HD2	1.65	0.62
1:A:683:TYR:O	1:A:687:GLU:HG2	1.99	0.61
1:A:557:ILE:HD11	1:A:596:GLN:HE21	1.64	0.61
1:H:634:THR:HG22	1:H:635:MET:SD	2.39	0.61
1:Q:677:ASP:O	1:Q:681:VAL:HG23	2.00	0.61
1:I:628:MET:O	1:I:632:MET:HG3	2.00	0.61
1:P:704:LEU:O	1:P:708:MET:HG2	2.00	0.61
1:G:470:LEU:HD13	1:G:482:ARG:HH21	1.64	0.61
1:I:521:LEU:HD22	1:L:513:GLN:HE21	1.66	0.61
1:D:537:MET:HG2	1:D:556:MET:SD	2.41	0.60
1:K:672:LEU:HA	1:K:675:THR:HB	1.84	0.60
1:J:710:LEU:HD12	1:J:710:LEU:C	2.26	0.60
1:N:432:PRO:HG2	1:N:483:ARG:HH11	1.66	0.60
1:B:445:ASN:ND2	1:B:455:LEU:HD22	2.16	0.60
1:J:447:TRP:HZ2	1:J:701:ASN:HB2	1.66	0.60
1:I:539:LEU:HD12	1:L:499:ASN:ND2	2.15	0.60
1:J:645:TRP:CD1	1:J:648:ARG:HH21	2.20	0.60
1:E:447:TRP:CE3	1:E:697:PHE:CZ	2.90	0.60
1:A:512:LEU:HD11	1:A:520:SER:HB3	1.84	0.59
1:B:447:TRP:CE3	1:B:697:PHE:HE2	2.20	0.59
1:J:545:LEU:HD11	1:J:649:ARG:HG2	1.84	0.59
1:P:677:ASP:O	1:P:681:VAL:HG23	2.02	0.59
1:H:537:MET:HE2	1:H:537:MET:HA	1.84	0.59
1:O:704:LEU:HA	1:O:707:ILE:HD12	1.83	0.59
1:C:639:LEU:HD23	1:C:639:LEU:H	1.68	0.59
1:H:663:LEU:O	1:H:667:LYS:HG3	2.02	0.59
1:I:437:ARG:O	1:I:441:ILE:HD12	2.02	0.59
1:A:475:VAL:HG22	1:A:489:HIS:HB3	1.84	0.59
1:G:422:GLN:HE22	1:G:507:ARG:NH1	2.00	0.59
1:L:631:LEU:CD1	1:L:635:MET:HE3	2.32	0.59
1:O:639:LEU:H	1:O:639:LEU:HD23	1.68	0.59
1:B:565:PHE:HA	1:B:568:PHE:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:438:GLU:HG2	1:L:459:LYS:HE2	1.83	0.59
1:A:423:ALA:HB2	1:F:639:LEU:HD12	1.83	0.59
1:F:471:MET:O	1:F:475:VAL:HG23	2.02	0.58
1:H:628:MET:O	1:H:632:MET:HG3	2.03	0.58
1:N:453:ALA:O	1:N:457:ILE:HG13	2.03	0.58
1:H:557:ILE:HD12	1:H:596:GLN:HG2	1.83	0.58
1:L:708:MET:HG3	1:L:712:LYS:NZ	2.16	0.58
1:G:568:PHE:HA	1:G:571:LEU:HD12	1.84	0.58
1:I:650:VAL:HG21	1:K:649:ARG:HH22	1.68	0.58
1:R:597:THR:HG23	1:R:626:LEU:HD22	1.84	0.58
1:B:582:VAL:HG21	1:B:697:PHE:CE1	2.38	0.58
1:I:639:LEU:HD23	1:I:639:LEU:H	1.69	0.58
1:J:550:MET:HE2	1:J:550:MET:HA	1.85	0.58
1:O:470:LEU:CD2	1:O:482:ARG:NH2	2.52	0.58
1:O:521:LEU:HD23	1:R:513:GLN:HG3	1.84	0.58
1:F:478:GLY:HA2	1:F:489:HIS:CE1	2.39	0.58
1:I:420:VAL:HA	1:J:639:LEU:CD2	2.33	0.57
1:H:507:ARG:O	1:H:511:GLU:HG2	2.03	0.57
1:K:666:MET:HE3	1:K:671:THR:HG21	1.86	0.57
1:F:485:LYS:HD2	1:F:486:PRO:HD2	1.86	0.57
1:H:687:GLU:HA	1:H:690:VAL:HG12	1.87	0.57
1:L:509:LEU:O	1:L:513:GLN:HG2	2.04	0.57
1:Q:447:TRP:HD1	1:Q:697:PHE:CZ	2.22	0.57
1:F:648:ARG:HH21	1:F:654:ALA:HB3	1.69	0.57
1:B:434:LYS:HG2	1:B:436:LEU:HD13	1.87	0.57
1:N:448:PHE:HZ	1:N:584:LEU:HD11	1.68	0.57
1:C:628:MET:O	1:C:632:MET:HG3	2.05	0.57
1:J:644:VAL:O	1:J:648:ARG:HG3	2.04	0.57
1:O:664:ASN:O	1:O:668:GLU:HG2	2.05	0.57
1:A:505:LEU:HD13	1:D:505:LEU:HD23	1.87	0.56
1:G:542:THR:HA	1:G:624:PHE:HE1	1.70	0.56
1:I:519:ARG:HA	1:I:522:LEU:HD23	1.87	0.56
1:L:437:ARG:NH1	1:L:564:LEU:HD22	2.20	0.56
1:P:447:TRP:HZ2	1:P:694:GLU:HG3	1.70	0.56
1:B:529:HIS:O	1:B:533:VAL:HG12	2.06	0.56
1:J:447:TRP:NE1	1:J:701:ASN:ND2	2.35	0.56
1:R:657:GLY:O	1:R:661:THR:HG23	2.06	0.56
1:G:664:ASN:OD1	1:G:665:LEU:HD12	2.05	0.56
1:J:625:SER:HB2	1:J:627:PRO:HD2	1.87	0.56
1:K:434:LYS:HG2	1:K:436:LEU:HD21	1.86	0.56
1:L:568:PHE:HA	1:L:571:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:607:ALA:O	1:J:608:GLU:HG2	2.06	0.56
1:E:537:MET:HE3	1:E:537:MET:HA	1.87	0.56
1:C:485:LYS:HG3	1:C:486:PRO:HD2	1.87	0.56
1:B:418:PRO:HB3	1:B:421:LEU:HD12	1.87	0.56
1:L:541:TRP:CZ3	1:L:556:MET:HE2	2.41	0.56
1:L:564:LEU:HD23	1:L:564:LEU:O	2.06	0.56
1:M:595:PHE:CE1	1:M:711:LEU:HD23	2.33	0.56
1:K:701:ASN:HD21	1:K:704:LEU:HD13	1.69	0.56
1:M:591:LEU:HD11	1:M:595:PHE:CE2	2.39	0.56
1:B:476:GLU:C	1:B:476:GLU:CD	2.74	0.55
1:F:663:LEU:O	1:F:667:LYS:HG3	2.06	0.55
1:H:471:MET:HB2	1:H:488:THR:HG21	1.89	0.55
1:K:565:PHE:HA	1:K:568:PHE:CZ	2.40	0.55
1:L:657:GLY:O	1:L:661:THR:HG23	2.05	0.55
1:H:445:ASN:ND2	1:H:455:LEU:HD22	2.21	0.55
1:C:703:GLN:O	1:C:707:ILE:HG13	2.06	0.55
1:O:553:TYR:CD2	1:O:554:PHE:CD1	2.95	0.55
1:M:512:LEU:HD11	1:M:520:SER:HB3	1.89	0.55
1:B:431:LEU:HD21	1:B:485:LYS:HB2	1.88	0.55
1:E:640:VAL:O	1:E:644:VAL:HG23	2.07	0.55
1:I:420:VAL:HA	1:J:639:LEU:HD21	1.88	0.55
1:B:703:GLN:O	1:B:707:ILE:HG13	2.07	0.54
1:Q:557:ILE:HD12	1:Q:596:GLN:HG2	1.90	0.54
1:F:527:GLU:HG3	1:F:567:LEU:HA	1.90	0.54
1:B:538:ASP:O	1:B:542:THR:HG23	2.07	0.54
1:N:697:PHE:HB3	1:N:699:ILE:HG22	1.89	0.54
1:E:575:HIS:CG	1:E:575:HIS:O	2.59	0.54
1:F:657:GLY:O	1:F:661:THR:HG23	2.08	0.54
1:J:631:LEU:HD22	1:J:666:MET:SD	2.48	0.54
1:K:677:ASP:O	1:K:681:VAL:HG13	2.08	0.54
1:F:491:ILE:HG13	1:F:491:ILE:O	2.06	0.54
1:C:598:ARG:NH1	1:C:598:ARG:HA	2.22	0.54
1:H:464:ILE:HD11	1:H:508:ALA:HA	1.90	0.54
1:M:663:LEU:O	1:M:667:LYS:HG3	2.06	0.54
1:G:470:LEU:HD22	1:G:482:ARG:HH22	1.71	0.54
1:Q:447:TRP:HD1	1:Q:697:PHE:CE1	2.26	0.54
1:R:475:VAL:HG22	1:R:489:HIS:HB3	1.88	0.54
1:R:630:HIS:HA	1:R:633:GLN:HG2	1.90	0.54
1:D:512:LEU:HD11	1:D:520:SER:HB3	1.90	0.54
1:F:478:GLY:HA2	1:F:489:HIS:HE1	1.71	0.53
1:I:444:LEU:HD12	1:I:448:PHE:HE2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:690:VAL:O	1:J:694:GLU:HG3	2.08	0.53
1:D:657:GLY:O	1:D:661:THR:HG23	2.08	0.53
1:I:512:LEU:HD11	1:I:520:SER:HB3	1.89	0.53
1:R:582:VAL:HG23	1:R:696:LYS:HD2	1.90	0.53
1:A:457:ILE:HG21	1:A:515:LEU:HG	1.91	0.53
1:I:500:SER:O	1:I:504:GLN:HG2	2.08	0.53
1:P:431:LEU:HD22	1:P:485:LYS:HG3	1.90	0.53
1:Q:450:VAL:CG2	1:Q:451:PRO:HD2	2.38	0.53
1:L:635:MET:O	1:L:635:MET:HG3	2.09	0.53
1:C:444:LEU:HD23	1:C:448:PHE:HE2	1.74	0.53
1:E:454:LYS:HD3	1:E:515:LEU:HG	1.91	0.53
1:I:557:ILE:HD11	1:I:596:GLN:HE21	1.73	0.53
1:B:554:PHE:HD2	1:B:593:ARG:HD3	1.73	0.53
1:F:634:THR:HG22	1:F:635:MET:SD	2.49	0.53
1:H:417:ASP:OD1	1:H:418:PRO:N	2.42	0.53
1:H:632:MET:HG2	1:H:641:LEU:HD21	1.90	0.53
1:E:437:ARG:O	1:E:441:ILE:HG22	2.08	0.53
1:F:426:GLU:HA	1:F:429:THR:HG22	1.90	0.53
1:H:683:TYR:O	1:H:687:GLU:HG2	2.09	0.53
1:K:471:MET:SD	1:K:488:THR:HG21	2.48	0.53
1:O:640:VAL:O	1:O:644:VAL:HG23	2.08	0.53
1:P:448:PHE:HZ	1:P:584:LEU:HD11	1.74	0.53
1:A:631:LEU:HD22	1:A:666:MET:SD	2.48	0.53
1:H:511:GLU:HA	1:H:514:LYS:NZ	2.24	0.53
1:K:538:ASP:O	1:K:542:THR:HG23	2.09	0.53
1:K:446:VAL:HG23	1:K:447:TRP:CD1	2.44	0.53
1:A:438:GLU:HG3	1:A:459:LYS:HD2	1.91	0.52
1:H:505:LEU:HD23	1:K:505:LEU:HD23	1.91	0.52
1:D:450:VAL:HG11	1:D:572:MET:HB2	1.91	0.52
1:K:458:ILE:HD12	1:K:572:MET:HE2	1.90	0.52
1:K:705:ARG:O	1:K:709:GLU:HG2	2.08	0.52
1:E:527:GLU:HB2	1:E:567:LEU:HD13	1.91	0.52
1:E:583:ASP:OD1	1:E:584:LEU:N	2.42	0.52
1:F:554:PHE:CE2	1:F:626:LEU:HD11	2.43	0.52
1:I:619:PHE:HB3	1:I:648:ARG:HH12	1.74	0.52
1:E:662:ILE:O	1:E:666:MET:HG3	2.09	0.52
1:F:545:LEU:HD11	1:F:649:ARG:HG2	1.90	0.52
1:H:648:ARG:NH1	1:H:654:ALA:HB3	2.24	0.52
1:M:422:GLN:HE22	1:M:507:ARG:NH1	2.08	0.52
1:Q:705:ARG:O	1:Q:709:GLU:HG2	2.09	0.52
1:C:439:GLN:HB3	1:C:707:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:PHE:HA	1:D:571:LEU:HD12	1.91	0.52
1:N:426:GLU:HA	1:N:429:THR:HG22	1.91	0.52
1:R:664:ASN:O	1:R:668:GLU:HG2	2.09	0.52
1:I:672:LEU:O	1:I:676:GLN:HG2	2.10	0.52
1:M:677:ASP:O	1:M:681:VAL:HG23	2.09	0.52
1:E:450:VAL:CG2	1:E:451:PRO:HD2	2.40	0.52
1:F:628:MET:O	1:F:632:MET:HG3	2.10	0.52
1:H:443:ALA:HB1	1:H:704:LEU:HD23	1.91	0.52
1:H:509:LEU:HD22	1:K:525:THR:HG21	1.92	0.52
1:L:491:ILE:HG23	1:L:492:PHE:CE2	2.44	0.52
1:C:594:TYR:O	1:C:598:ARG:HG2	2.10	0.52
1:C:601:TYR:O	1:C:605:VAL:HG12	2.10	0.52
1:M:448:PHE:HZ	1:M:584:LEU:HD11	1.75	0.52
1:Q:450:VAL:HG22	1:Q:451:PRO:HD2	1.92	0.52
1:A:664:ASN:HA	1:A:667:LYS:HE2	1.91	0.51
1:F:527:GLU:HB2	1:F:567:LEU:HD13	1.92	0.51
1:I:475:VAL:HG11	1:I:498:ILE:HD11	1.93	0.51
1:B:646:THR:O	1:B:650:VAL:HG12	2.10	0.51
1:H:630:HIS:HA	1:H:633:GLN:HG2	1.91	0.51
1:Q:528:LEU:HD23	1:Q:531:LEU:HD12	1.92	0.51
1:B:435:GLY:HA2	1:B:438:GLU:HG2	1.91	0.51
1:G:565:PHE:HA	1:G:568:PHE:CE2	2.44	0.51
1:J:601:TYR:HE2	1:J:676:GLN:HG3	1.75	0.51
1:A:639:LEU:HD12	1:A:639:LEU:H	1.75	0.51
1:I:417:ASP:OD1	1:I:418:PRO:N	2.44	0.51
1:E:445:ASN:HD22	1:E:455:LEU:HD22	1.74	0.51
1:E:642:ARG:O	1:E:646:THR:HG23	2.10	0.51
1:E:648:ARG:HH21	1:E:654:ALA:HB3	1.75	0.51
1:P:517:ASP:CG	1:P:518:ALA:H	2.17	0.51
1:Q:447:TRP:CD1	1:Q:697:PHE:CZ	2.99	0.51
1:A:677:ASP:O	1:A:681:VAL:HG23	2.11	0.51
1:D:489:HIS:HA	1:D:497:THR:HG21	1.93	0.51
1:G:475:VAL:HG22	1:G:489:HIS:HB3	1.93	0.51
1:E:460:SER:O	1:E:464:ILE:HG13	2.11	0.51
1:G:557:ILE:HD12	1:G:596:GLN:HG3	1.93	0.51
1:H:642:ARG:O	1:H:646:THR:HG23	2.11	0.51
1:L:426:GLU:HA	1:L:429:THR:HG22	1.91	0.51
1:Q:666:MET:HE3	1:Q:666:MET:HA	1.93	0.51
1:J:521:LEU:HD12	1:J:521:LEU:H	1.76	0.51
1:L:475:VAL:HG22	1:L:489:HIS:HB3	1.93	0.51
1:R:703:GLN:O	1:R:707:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:SER:HB3	1:C:483:ARG:HH12	1.75	0.51
1:C:505:LEU:HD23	1:F:505:LEU:HD22	1.93	0.50
1:E:663:LEU:HD13	1:E:666:MET:SD	2.52	0.50
1:H:445:ASN:HD21	1:H:455:LEU:HD22	1.76	0.50
1:H:509:LEU:HD12	1:K:509:LEU:HD21	1.93	0.50
1:J:589:ASN:O	1:J:593:ARG:HG3	2.10	0.50
1:B:420:VAL:HG21	1:E:537:MET:HE1	1.93	0.50
1:B:657:GLY:O	1:B:661:THR:HG23	2.10	0.50
1:D:570:ARG:O	1:D:574:VAL:HG23	2.11	0.50
1:P:570:ARG:O	1:P:574:VAL:HG23	2.11	0.50
1:R:426:GLU:HA	1:R:429:THR:HG22	1.94	0.50
1:B:589:ASN:HB3	1:B:593:ARG:HH21	1.76	0.50
1:H:639:LEU:HD12	1:H:639:LEU:H	1.76	0.50
1:E:450:VAL:HG22	1:E:451:PRO:HD2	1.93	0.50
1:E:705:ARG:HA	1:E:708:MET:HB3	1.94	0.50
1:L:541:TRP:CE3	1:L:556:MET:CE	2.95	0.50
1:H:424:PRO:O	1:H:428:ILE:HG22	2.11	0.50
1:H:624:PHE:HE1	1:H:645:TRP:HE1	1.58	0.50
1:I:444:LEU:HD12	1:I:448:PHE:CE2	2.47	0.50
1:L:648:ARG:HG3	1:L:654:ALA:HB2	1.94	0.50
1:G:598:ARG:O	1:G:602:GLN:HG2	2.11	0.50
1:J:441:ILE:HG21	1:J:459:LYS:HG3	1.92	0.50
1:O:441:ILE:HG21	1:O:459:LYS:HG3	1.94	0.50
1:C:558:GLU:HB2	1:C:593:ARG:HH12	1.76	0.50
1:E:619:PHE:CE1	1:E:666:MET:HE1	2.47	0.50
1:J:630:HIS:O	1:J:634:THR:HG23	2.12	0.50
1:L:688:LYS:O	1:L:692:GLU:HG2	2.11	0.50
1:N:460:SER:O	1:N:464:ILE:HG23	2.12	0.50
1:B:557:ILE:HG12	1:B:596:GLN:HG2	1.94	0.50
1:C:598:ARG:HH11	1:C:679:LEU:HD11	1.76	0.50
1:D:582:VAL:HG22	1:D:697:PHE:CZ	2.33	0.50
1:E:443:ALA:HB2	1:E:707:ILE:HD12	1.92	0.50
1:F:683:TYR:CZ	1:F:712:LYS:HE3	2.46	0.50
1:J:557:ILE:HD12	1:J:596:GLN:HG3	1.93	0.50
1:N:603:ASN:HD21	1:N:618:ASP:HB2	1.76	0.50
1:P:686:VAL:HG11	1:P:708:MET:HE2	1.94	0.50
1:Q:454:LYS:O	1:Q:458:ILE:HG13	2.12	0.50
1:A:687:GLU:HA	1:A:690:VAL:HG12	1.94	0.50
1:C:545:LEU:HD11	1:C:649:ARG:HG2	1.94	0.50
1:C:568:PHE:HA	1:C:571:LEU:HD12	1.93	0.50
1:Q:445:ASN:HD22	1:Q:455:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:582:VAL:HG11	1:D:697:PHE:CZ	2.47	0.49
1:J:683:TYR:O	1:J:687:GLU:HG2	2.12	0.49
1:M:452:THR:O	1:M:456:GLU:HG2	2.12	0.49
1:O:553:TYR:HD2	1:O:554:PHE:CD1	2.30	0.49
1:B:608:GLU:CD	1:B:608:GLU:C	2.80	0.49
1:J:595:PHE:CD1	1:J:711:LEU:HD21	2.47	0.49
1:A:603:ASN:HD21	1:A:618:ASP:HB2	1.77	0.49
1:E:672:LEU:O	1:E:676:GLN:HG3	2.12	0.49
1:I:433:SER:HB3	1:I:483:ARG:HH12	1.77	0.49
1:I:632:MET:HG2	1:I:641:LEU:HD21	1.93	0.49
1:J:591:LEU:HD11	1:J:595:PHE:CZ	2.47	0.49
1:D:630:HIS:O	1:D:634:THR:HG23	2.12	0.49
1:D:646:THR:O	1:D:650:VAL:HG12	2.13	0.49
1:J:447:TRP:HH2	1:J:694:GLU:HG2	1.77	0.49
1:P:656:HIS:O	1:P:660:GLN:HG2	2.12	0.49
1:A:447:TRP:NE1	1:A:701:ASN:HB3	2.23	0.49
1:F:665:LEU:O	1:F:668:GLU:HG3	2.12	0.49
1:F:683:TYR:O	1:F:687:GLU:HG2	2.13	0.49
1:M:603:ASN:HD21	1:M:618:ASP:HB2	1.77	0.49
1:A:500:SER:O	1:A:504:GLN:HG2	2.13	0.49
1:C:421:LEU:HD11	1:F:533:VAL:HA	1.94	0.49
1:C:451:PRO:HD2	1:C:454:LYS:HZ1	1.77	0.49
1:C:598:ARG:HH22	1:C:601:TYR:HD2	1.61	0.49
1:D:631:LEU:HD11	1:D:665:LEU:HG	1.95	0.49
1:I:624:PHE:HB3	1:I:629:ILE:HD11	1.95	0.49
1:Q:665:LEU:HD23	1:Q:668:GLU:HB3	1.94	0.49
1:R:630:HIS:O	1:R:634:THR:HG22	2.13	0.49
1:J:545:LEU:HD21	1:J:649:ARG:HD3	1.94	0.49
1:O:707:ILE:HG22	1:O:711:LEU:HD23	1.95	0.49
1:D:602:GLN:HA	1:D:605:VAL:HG22	1.95	0.49
1:E:428:ILE:HD13	1:E:471:MET:HB2	1.95	0.49
1:I:441:ILE:HG23	1:I:572:MET:HE1	1.94	0.49
1:J:444:LEU:HD12	1:J:448:PHE:HE2	1.77	0.49
1:J:447:TRP:CE2	1:J:701:ASN:HB2	2.48	0.49
1:M:591:LEU:HD11	1:M:595:PHE:HZ	1.68	0.49
1:D:509:LEU:O	1:D:513:GLN:HG2	2.13	0.49
1:D:582:VAL:CG1	1:D:697:PHE:CZ	2.95	0.49
1:H:460:SER:O	1:H:464:ILE:HG23	2.13	0.49
1:J:447:TRP:CH2	1:J:694:GLU:HG2	2.48	0.49
1:J:595:PHE:CE1	1:J:711:LEU:HD22	2.47	0.49
1:K:568:PHE:HA	1:K:571:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:SER:O	1:B:464:ILE:HG23	2.13	0.48
1:E:702:PHE:HB3	1:N:702:PHE:CG	2.48	0.48
1:L:527:GLU:HB2	1:L:567:LEU:HD13	1.94	0.48
1:L:541:TRP:HZ3	1:L:556:MET:HE2	1.78	0.48
1:Q:422:GLN:HE22	1:Q:507:ARG:NH1	2.11	0.48
1:G:482:ARG:HG2	1:G:483:ARG:HG2	1.94	0.48
1:G:540:TYR:HB2	1:J:420:VAL:HG21	1.95	0.48
1:D:542:THR:HA	1:D:624:PHE:CE1	2.48	0.48
1:I:533:VAL:HG22	1:L:421:LEU:HD11	1.95	0.48
1:J:601:TYR:O	1:J:605:VAL:HG13	2.13	0.48
1:J:703:GLN:O	1:J:707:ILE:HG13	2.14	0.48
1:L:538:ASP:HA	1:L:556:MET:HE1	1.95	0.48
1:R:645:TRP:HZ3	1:R:648:ARG:HH21	1.62	0.48
1:A:470:LEU:HD22	1:A:482:ARG:NH2	2.28	0.48
1:A:684:SER:O	1:A:688:LYS:HE2	2.13	0.48
1:C:705:ARG:O	1:C:709:GLU:HG2	2.12	0.48
1:L:664:ASN:O	1:L:668:GLU:HG2	2.14	0.48
1:B:582:VAL:HG21	1:B:697:PHE:HZ	1.78	0.48
1:C:658:GLN:O	1:C:662:ILE:HG12	2.14	0.48
1:J:431:LEU:HD22	1:J:485:LYS:HG3	1.95	0.48
1:L:466:HIS:O	1:L:470:LEU:HG	2.14	0.48
1:N:700:GLU:OE1	1:N:702:PHE:HE2	1.97	0.48
1:P:703:GLN:O	1:P:707:ILE:HG22	2.14	0.48
1:A:570:ARG:O	1:A:574:VAL:HG23	2.14	0.48
1:D:683:TYR:CE2	1:D:708:MET:HE1	2.48	0.48
1:F:686:VAL:O	1:F:690:VAL:HG12	2.13	0.48
1:G:582:VAL:HG21	1:G:696:LYS:HG2	1.96	0.48
1:J:568:PHE:O	1:J:572:MET:HG3	2.14	0.48
1:N:677:ASP:O	1:N:681:VAL:HG12	2.14	0.48
1:E:554:PHE:O	1:E:558:GLU:HG2	2.13	0.48
1:I:441:ILE:HD11	1:I:462:THR:HG21	1.96	0.48
1:J:697:PHE:HB3	1:J:699:ILE:HD12	1.95	0.48
1:L:448:PHE:HD2	1:L:572:MET:SD	2.37	0.48
1:A:444:LEU:HD12	1:A:448:PHE:CE2	2.49	0.47
1:E:418:PRO:O	1:E:422:GLN:HG3	2.14	0.47
1:A:527:GLU:HG3	1:A:567:LEU:HA	1.96	0.47
1:C:683:TYR:CE2	1:C:708:MET:HE1	2.48	0.47
1:M:481:LEU:HD12	1:M:482:ARG:H	1.79	0.47
1:B:486:PRO:HG3	1:C:657:GLY:HA3	1.96	0.47
1:E:471:MET:SD	1:E:488:THR:HG21	2.54	0.47
1:F:678:SER:O	1:F:682:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:554:PHE:CG	1:G:593:ARG:HD3	2.49	0.47
1:I:531:LEU:O	1:I:535:GLN:HG3	2.14	0.47
1:C:454:LYS:HE2	1:C:454:LYS:HB3	1.70	0.47
1:C:656:HIS:O	1:C:660:GLN:HG3	2.14	0.47
1:E:447:TRP:HH2	1:E:584:LEU:HD12	1.79	0.47
1:K:547:CYS:SG	1:K:632:MET:HE2	2.54	0.47
1:Q:597:THR:HG23	1:Q:626:LEU:HD23	1.95	0.47
1:C:438:GLU:HG2	1:C:459:LYS:NZ	2.30	0.47
1:C:582:VAL:CG2	1:C:697:PHE:CZ	2.92	0.47
1:F:554:PHE:HZ	1:F:626:LEU:HD11	1.76	0.47
1:G:562:GLY:O	1:G:566:ARG:HG3	2.14	0.47
1:I:457:ILE:HD13	1:I:514:LYS:HG3	1.96	0.47
1:Q:702:PHE:CD1	1:Q:705:ARG:HG3	2.49	0.47
1:C:505:LEU:O	1:C:509:LEU:HG	2.15	0.47
1:J:467:ASN:HA	1:J:470:LEU:HD12	1.96	0.47
1:M:472:LEU:HD23	1:M:472:LEU:HA	1.73	0.47
1:Q:422:GLN:HE22	1:Q:507:ARG:HH11	1.61	0.47
1:E:608:GLU:O	1:E:608:GLU:HG3	2.15	0.47
1:F:554:PHE:HZ	1:F:626:LEU:CD1	2.24	0.47
1:G:620:GLU:HG3	1:G:654:ALA:HB3	1.97	0.47
1:J:582:VAL:HG21	1:J:697:PHE:HE1	1.80	0.47
1:Q:434:LYS:HB2	1:Q:434:LYS:HE2	1.69	0.47
1:A:545:LEU:HD11	1:A:649:ARG:HG2	1.96	0.47
1:F:551:HIS:O	1:F:555:GLN:HG3	2.15	0.47
1:N:472:LEU:HD23	1:N:472:LEU:HA	1.68	0.47
1:O:426:GLU:HA	1:O:429:THR:HG22	1.97	0.47
1:G:543:SER:HA	1:G:649:ARG:NH2	2.29	0.47
1:H:598:ARG:HH11	1:H:598:ARG:HG2	1.79	0.47
1:K:598:ARG:HG2	1:K:679:LEU:HD11	1.97	0.47
1:P:528:LEU:HD12	1:P:532:TYR:HE2	1.78	0.47
1:F:512:LEU:HA	1:F:515:LEU:HD12	1.96	0.47
1:L:635:MET:O	1:L:635:MET:CG	2.63	0.47
1:G:535:GLN:O	1:G:539:LEU:HD23	2.14	0.46
1:H:447:TRP:HB3	1:H:697:PHE:CE2	2.51	0.46
1:I:458:ILE:HD11	1:I:571:LEU:HB3	1.97	0.46
1:I:589:ASN:O	1:I:593:ARG:HG3	2.15	0.46
1:K:608:GLU:HG3	1:K:608:GLU:O	2.15	0.46
1:Q:582:VAL:HG12	1:Q:696:LYS:HE3	1.97	0.46
1:A:531:LEU:O	1:A:535:GLN:HG3	2.15	0.46
1:B:447:TRP:CE3	1:B:697:PHE:CE2	3.02	0.46
1:C:426:GLU:HA	1:C:429:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:677:ASP:O	1:G:681:VAL:HG23	2.14	0.46
1:Q:447:TRP:NE1	1:Q:697:PHE:CE2	2.83	0.46
1:A:657:GLY:O	1:A:661:THR:HG22	2.15	0.46
1:D:568:PHE:HA	1:D:571:LEU:HB2	1.98	0.46
1:N:432:PRO:HG2	1:N:483:ARG:NH1	2.30	0.46
1:O:582:VAL:HG12	1:O:696:LYS:HG2	1.97	0.46
1:D:598:ARG:O	1:D:602:GLN:HG2	2.15	0.46
1:H:637:ASP:C	1:H:637:ASP:OD1	2.58	0.46
1:L:708:MET:HG3	1:L:712:LYS:HZ1	1.80	0.46
1:M:598:ARG:O	1:M:602:GLN:HG2	2.16	0.46
1:O:553:TYR:CD2	1:O:554:PHE:CE1	3.03	0.46
1:O:554:PHE:HA	1:O:557:ILE:HB	1.98	0.46
1:A:471:MET:HE3	1:A:501:ALA:HB2	1.97	0.46
1:L:545:LEU:HD11	1:L:649:ARG:HG2	1.98	0.46
1:P:562:GLY:HA2	1:P:565:PHE:HD2	1.81	0.46
1:R:663:LEU:O	1:R:667:LYS:HG3	2.15	0.46
1:B:438:GLU:HB3	1:B:459:LYS:NZ	2.31	0.46
1:M:630:HIS:ND1	1:M:671:THR:HG22	2.30	0.46
1:M:712:LYS:HB3	1:M:712:LYS:HE2	1.81	0.46
1:F:601:TYR:O	1:F:605:VAL:HG13	2.16	0.46
1:C:678:SER:O	1:C:682:LEU:HG	2.15	0.46
1:G:664:ASN:OD1	1:G:664:ASN:C	2.59	0.46
1:B:507:ARG:O	1:B:511:GLU:HG2	2.16	0.46
1:C:535:GLN:HA	1:C:560:LYS:NZ	2.28	0.46
1:K:461:ILE:HD11	1:K:512:LEU:HA	1.97	0.46
1:P:441:ILE:HD13	1:P:572:MET:HE2	1.98	0.46
1:C:594:TYR:OH	1:C:712:LYS:HD3	2.16	0.46
1:F:589:ASN:O	1:F:593:ARG:HG3	2.16	0.46
1:K:422:GLN:O	1:K:426:GLU:HG2	2.15	0.46
1:K:678:SER:HA	1:K:681:VAL:HG22	1.98	0.46
1:C:449:ARG:HG3	1:C:449:ARG:O	2.16	0.45
1:D:582:VAL:HG11	1:D:697:PHE:CE2	2.51	0.45
1:E:500:SER:O	1:E:504:GLN:HG2	2.16	0.45
1:G:594:TYR:HE2	1:G:711:LEU:HD23	1.81	0.45
1:K:567:LEU:O	1:K:571:LEU:HG	2.15	0.45
1:C:503:TYR:OH	1:F:529:HIS:HE1	1.99	0.45
1:C:660:GLN:O	1:C:664:ASN:ND2	2.40	0.45
1:G:521:LEU:O	1:G:525:THR:HG23	2.16	0.45
1:O:500:SER:O	1:O:504:GLN:HG2	2.16	0.45
1:Q:506:VAL:O	1:Q:510:GLN:HG3	2.16	0.45
1:G:452:THR:O	1:G:456:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:521:LEU:HG	1:I:522:LEU:HD22	1.97	0.45
1:N:420:VAL:HG11	1:Q:540:TYR:HB2	1.98	0.45
1:N:531:LEU:HG	1:N:535:GLN:OE1	2.17	0.45
1:I:641:LEU:O	1:I:644:VAL:HG12	2.17	0.45
1:J:436:LEU:HA	1:J:439:GLN:CD	2.41	0.45
1:Q:582:VAL:HG12	1:Q:696:LYS:CE	2.46	0.45
1:B:690:VAL:HG11	1:B:705:ARG:HH12	1.82	0.45
1:E:427:TYR:HB2	1:E:492:PHE:HE2	1.81	0.45
1:I:710:LEU:HA	1:I:710:LEU:HD23	1.80	0.45
1:K:557:ILE:HA	1:K:557:ILE:HD12	1.75	0.45
1:N:464:ILE:HD11	1:N:508:ALA:HA	1.99	0.45
1:E:447:TRP:HH2	1:E:584:LEU:CD1	2.30	0.45
1:H:472:LEU:HD23	1:H:472:LEU:HA	1.83	0.45
1:H:555:GLN:O	1:H:558:GLU:HG2	2.16	0.45
1:J:601:TYR:CE2	1:J:676:GLN:HG3	2.52	0.45
1:O:553:TYR:CE2	1:O:554:PHE:CE1	3.04	0.45
1:R:471:MET:O	1:R:475:VAL:HG23	2.16	0.45
1:D:565:PHE:HA	1:D:568:PHE:CZ	2.52	0.45
1:L:538:ASP:CA	1:L:556:MET:SD	3.05	0.45
1:M:472:LEU:HD11	1:P:502:ASN:HD21	1.82	0.45
1:D:708:MET:HE3	1:D:708:MET:C	2.42	0.45
1:E:677:ASP:O	1:E:681:VAL:HG22	2.16	0.45
1:F:681:VAL:HG13	1:F:682:LEU:HD23	1.99	0.45
1:L:470:LEU:HD22	1:L:482:ARG:HH22	1.82	0.45
1:N:568:PHE:O	1:N:572:MET:HG3	2.17	0.45
1:A:548:PRO:HD2	1:A:624:PHE:CE2	2.52	0.45
1:E:705:ARG:O	1:E:709:GLU:HG2	2.16	0.45
1:G:458:ILE:HD12	1:G:572:MET:HB3	1.98	0.45
1:J:666:MET:HE3	1:J:671:THR:OG1	2.17	0.45
1:C:562:GLY:O	1:C:566:ARG:HD3	2.17	0.44
1:D:444:LEU:HD23	1:D:444:LEU:HA	1.79	0.44
1:D:514:LYS:HE2	1:D:514:LYS:HB3	1.76	0.44
1:E:506:VAL:O	1:E:510:GLN:HG3	2.17	0.44
1:O:677:ASP:O	1:O:681:VAL:HG23	2.17	0.44
1:Q:422:GLN:NE2	1:Q:507:ARG:HD3	2.32	0.44
1:B:495:GLY:HA3	1:E:539:LEU:HD12	1.98	0.44
1:C:587:PHE:CZ	1:C:704:LEU:HD21	2.44	0.44
1:D:449:ARG:HG2	1:D:449:ARG:O	2.17	0.44
1:F:485:LYS:HD2	1:F:486:PRO:CD	2.47	0.44
1:J:687:GLU:HA	1:J:690:VAL:HG12	2.00	0.44
1:C:640:VAL:O	1:C:644:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:620:GLU:HA	1:E:648:ARG:NH1	2.33	0.44
1:N:537:MET:HE1	1:Q:420:VAL:HG21	1.98	0.44
1:O:471:MET:HG3	1:O:488:THR:HG21	1.98	0.44
1:H:551:HIS:O	1:H:555:GLN:HG3	2.18	0.44
1:J:582:VAL:HG23	1:J:584:LEU:CD1	2.48	0.44
1:K:682:LEU:O	1:K:686:VAL:HG13	2.18	0.44
1:O:597:THR:HG23	1:O:626:LEU:HD23	1.99	0.44
1:Q:608:GLU:O	1:Q:608:GLU:HG3	2.18	0.44
1:F:666:MET:HE3	1:F:671:THR:OG1	2.17	0.44
1:N:452:THR:O	1:N:455:LEU:HG	2.17	0.44
1:O:512:LEU:HD11	1:O:520:SER:HB3	2.00	0.44
1:Q:445:ASN:ND2	1:Q:455:LEU:HD22	2.33	0.44
1:R:607:ALA:HB1	1:R:663:LEU:HD11	1.99	0.44
1:C:587:PHE:CD1	1:C:693:LEU:HD12	2.52	0.44
1:D:562:GLY:HA2	1:D:565:PHE:HD2	1.81	0.44
1:D:703:GLN:O	1:D:707:ILE:HG22	2.17	0.44
1:J:565:PHE:HA	1:J:568:PHE:CE2	2.53	0.44
1:O:635:MET:HE2	1:O:635:MET:HB3	1.92	0.44
1:P:630:HIS:O	1:P:634:THR:HG23	2.17	0.44
1:A:619:PHE:HB2	1:A:659:LYS:HE3	1.98	0.44
1:H:672:LEU:O	1:H:676:GLN:HG2	2.18	0.44
1:K:548:PRO:HG2	1:K:629:ILE:HD11	1.99	0.44
1:O:663:LEU:O	1:O:667:LYS:HG3	2.17	0.44
1:Q:422:GLN:HE22	1:Q:507:ARG:HD3	1.82	0.44
1:C:598:ARG:HD2	1:C:679:LEU:HD11	2.00	0.44
1:Q:458:ILE:HD13	1:Q:571:LEU:HB3	1.99	0.44
1:G:542:THR:HA	1:G:624:PHE:CE1	2.52	0.44
1:H:452:THR:O	1:H:455:LEU:HG	2.18	0.44
1:N:422:GLN:OE1	1:N:422:GLN:HA	2.18	0.44
1:P:517:ASP:CG	1:P:518:ALA:N	2.76	0.44
1:B:648:ARG:HE	1:B:654:ALA:HB2	1.83	0.43
1:F:631:LEU:HD22	1:F:666:MET:SD	2.57	0.43
1:J:696:LYS:HD3	1:J:696:LYS:HA	1.82	0.43
1:K:526:GLU:O	1:K:530:ASN:ND2	2.51	0.43
1:N:435:GLY:O	1:N:439:GLN:HG3	2.18	0.43
1:Q:447:TRP:CD1	1:Q:697:PHE:CG	3.06	0.43
1:A:710:LEU:HD23	1:A:710:LEU:HA	1.87	0.43
1:B:485:LYS:HG3	1:B:486:PRO:HD2	2.00	0.43
1:J:457:ILE:HG21	1:J:515:LEU:HG	2.00	0.43
1:C:648:ARG:HG3	1:C:654:ALA:HB2	1.99	0.43
1:E:584:LEU:O	1:E:584:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:540:TYR:HE1	1:F:546:VAL:HG21	1.84	0.43
1:I:630:HIS:HA	1:I:633:GLN:HG2	1.99	0.43
1:L:513:GLN:HE22	1:L:521:LEU:HD11	1.84	0.43
1:Q:639:LEU:HD12	1:R:423:ALA:HB2	1.99	0.43
1:D:538:ASP:O	1:D:542:THR:HG23	2.18	0.43
1:E:568:PHE:HA	1:E:571:LEU:HB2	2.01	0.43
1:N:421:LEU:HD13	1:Q:536:SER:HB3	2.00	0.43
1:B:435:GLY:O	1:B:439:GLN:HG3	2.19	0.43
1:B:552:GLU:HA	1:B:555:GLN:HG2	2.00	0.43
1:E:545:LEU:HD11	1:E:649:ARG:HG2	2.00	0.43
1:G:662:ILE:HD13	1:G:662:ILE:HA	1.89	0.43
1:J:645:TRP:HA	1:J:648:ARG:HH21	1.84	0.43
1:O:553:TYR:HE2	1:O:554:PHE:HE1	1.67	0.43
1:E:566:ARG:O	1:E:570:ARG:HG3	2.19	0.43
1:F:554:PHE:HA	1:F:557:ILE:HB	2.00	0.43
1:G:476:GLU:CD	1:G:539:LEU:HD11	2.43	0.43
1:I:480:GLU:O	1:I:481:LEU:HD23	2.18	0.43
1:K:437:ARG:NH1	1:K:564:LEU:HD23	2.32	0.43
1:B:459:LYS:HB2	1:B:459:LYS:HE2	1.88	0.43
1:P:472:LEU:HD23	1:P:472:LEU:HA	1.86	0.43
1:R:432:PRO:HD2	1:R:483:ARG:HH21	1.84	0.43
1:L:625:SER:O	1:L:629:ILE:HG12	2.18	0.43
1:C:517:ASP:CG	1:C:519:ARG:H	2.27	0.43
1:I:471:MET:HE3	1:I:501:ALA:HB2	2.00	0.43
1:J:471:MET:HG2	1:J:488:THR:HG21	2.00	0.43
1:K:447:TRP:HE1	1:K:701:ASN:ND2	2.17	0.43
1:K:648:ARG:HG2	1:K:654:ALA:HB2	2.00	0.43
1:L:472:LEU:HD23	1:L:472:LEU:HA	1.85	0.43
1:L:607:ALA:HB1	1:L:663:LEU:HD11	2.00	0.43
1:O:475:VAL:HG22	1:O:489:HIS:HB3	1.99	0.43
1:B:489:HIS:HA	1:B:497:THR:HG21	2.01	0.43
1:H:711:LEU:HD12	1:H:711:LEU:HA	1.89	0.43
1:K:495:GLY:O	1:K:498:ILE:HG22	2.19	0.43
1:A:472:LEU:HD11	1:D:502:ASN:ND2	2.33	0.42
1:C:594:TYR:O	1:C:597:THR:HG22	2.19	0.42
1:E:447:TRP:CZ3	1:E:697:PHE:CZ	3.07	0.42
1:E:541:TRP:HA	1:E:546:VAL:HG22	2.01	0.42
1:E:702:PHE:CD1	1:E:705:ARG:HD3	2.54	0.42
1:I:533:VAL:HA	1:L:421:LEU:HD21	2.00	0.42
1:J:447:TRP:CD1	1:J:701:ASN:ND2	2.83	0.42
1:C:420:VAL:HG13	1:F:536:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:630:HIS:HA	1:N:633:GLN:HG2	1.99	0.42
1:A:637:ASP:OD1	1:A:637:ASP:C	2.62	0.42
1:A:711:LEU:HD12	1:A:711:LEU:HA	1.87	0.42
1:C:503:TYR:OH	1:F:529:HIS:CE1	2.72	0.42
1:F:491:ILE:CG2	1:F:492:PHE:CE2	3.02	0.42
1:F:554:PHE:CE2	1:F:626:LEU:CD1	3.00	0.42
1:N:472:LEU:O	1:N:476:GLU:HG3	2.18	0.42
1:O:472:LEU:HA	1:O:472:LEU:HD23	1.73	0.42
1:G:431:LEU:HD22	1:G:485:LYS:HG3	2.01	0.42
1:M:438:GLU:HG3	1:M:459:LYS:HD3	2.01	0.42
1:M:666:MET:HG2	1:M:671:THR:OG1	2.19	0.42
1:R:454:LYS:O	1:R:458:ILE:HG13	2.19	0.42
1:E:697:PHE:HB3	1:E:699:ILE:HD12	2.02	0.42
1:K:454:LYS:HD2	1:K:575:HIS:CE1	2.55	0.42
1:K:708:MET:HE3	1:K:712:LYS:HB2	2.02	0.42
1:L:708:MET:HE2	1:L:708:MET:HB2	1.92	0.42
1:O:550:MET:HE3	1:O:550:MET:HA	2.01	0.42
1:O:657:GLY:O	1:O:661:THR:HG23	2.19	0.42
1:P:708:MET:HE3	1:P:708:MET:HB3	1.86	0.42
1:D:679:LEU:HD23	1:D:679:LEU:HA	1.88	0.42
1:H:574:VAL:HG23	1:H:575:HIS:CE1	2.55	0.42
1:P:565:PHE:HA	1:P:568:PHE:CE2	2.54	0.42
1:R:422:GLN:OE1	1:R:422:GLN:HA	2.19	0.42
1:C:521:LEU:O	1:C:525:THR:HG23	2.20	0.42
1:D:677:ASP:O	1:D:681:VAL:HG13	2.20	0.42
1:H:437:ARG:O	1:H:441:ILE:HG13	2.20	0.42
1:N:459:LYS:O	1:N:463:THR:HG22	2.19	0.42
1:A:421:LEU:HD21	1:A:503:TYR:CG	2.55	0.42
1:B:557:ILE:HD12	1:B:557:ILE:HA	1.81	0.42
1:D:472:LEU:HD23	1:D:472:LEU:HA	1.92	0.42
1:E:445:ASN:ND2	1:E:455:LEU:HD22	2.35	0.42
1:F:703:GLN:O	1:F:707:ILE:HG13	2.19	0.42
1:G:570:ARG:O	1:G:574:VAL:HG23	2.20	0.42
1:I:648:ARG:HH21	1:I:654:ALA:HB3	1.84	0.42
1:J:480:GLU:HG2	1:J:481:LEU:HG	2.01	0.42
1:J:662:ILE:HD13	1:J:662:ILE:HA	1.89	0.42
1:M:570:ARG:O	1:M:574:VAL:HG23	2.19	0.42
1:N:705:ARG:NH1	1:N:705:ARG:HG3	2.35	0.42
1:O:648:ARG:HD3	1:O:654:ALA:HB2	2.01	0.42
1:C:448:PHE:HZ	1:C:584:LEU:HD11	1.84	0.42
1:E:528:LEU:HD23	1:E:528:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:640:VAL:HA	1:K:492:PHE:HE1	1.85	0.42
1:I:682:LEU:O	1:I:686:VAL:HG12	2.19	0.42
1:L:527:GLU:HG3	1:L:567:LEU:HA	2.01	0.42
1:P:635:MET:HE2	1:P:638:ASN:HD22	1.84	0.42
1:P:704:LEU:HD23	1:P:704:LEU:HA	1.87	0.42
1:D:537:MET:CB	1:D:556:MET:SD	3.08	0.42
1:F:458:ILE:HG21	1:F:572:MET:HE2	2.02	0.42
1:K:425:TYR:HA	1:K:471:MET:HE1	2.01	0.42
1:A:645:TRP:HA	1:A:648:ARG:NE	2.24	0.41
1:A:646:THR:O	1:A:650:VAL:HG23	2.20	0.41
1:F:529:HIS:O	1:F:533:VAL:HG12	2.20	0.41
1:I:431:LEU:HD23	1:I:431:LEU:HA	1.92	0.41
1:L:561:THR:HG22	1:L:565:PHE:HE2	1.85	0.41
1:L:708:MET:O	1:L:712:LYS:HG2	2.20	0.41
1:M:448:PHE:CZ	1:M:584:LEU:HD11	2.55	0.41
1:M:557:ILE:HD13	1:M:557:ILE:HA	1.84	0.41
1:N:454:LYS:O	1:N:458:ILE:HG13	2.19	0.41
1:N:523:VAL:HG12	1:N:570:ARG:NH2	2.35	0.41
1:G:486:PRO:HG3	1:L:657:GLY:HA3	2.02	0.41
1:I:461:ILE:HD12	1:I:512:LEU:HB2	2.02	0.41
1:N:662:ILE:HD13	1:N:662:ILE:HA	1.95	0.41
1:F:438:GLU:HA	1:F:441:ILE:HD12	2.01	0.41
1:J:540:TYR:OH	1:L:642:ARG:HD2	2.20	0.41
1:O:598:ARG:O	1:O:602:GLN:HG2	2.20	0.41
1:Q:450:VAL:CG2	1:Q:451:PRO:CD	2.98	0.41
1:B:417:ASP:HA	1:B:418:PRO:HD3	1.89	0.41
1:G:509:LEU:O	1:G:512:LEU:HG	2.21	0.41
1:I:687:GLU:HA	1:I:690:VAL:HG12	2.01	0.41
1:J:603:ASN:HD21	1:J:618:ASP:N	2.18	0.41
1:K:594:TYR:CZ	1:K:598:ARG:HD2	2.55	0.41
1:L:541:TRP:CZ3	1:L:556:MET:CE	3.02	0.41
1:I:665:LEU:HA	1:I:668:GLU:HG2	2.02	0.41
1:M:548:PRO:HG2	1:M:629:ILE:HD11	2.02	0.41
1:M:632:MET:HG2	1:M:641:LEU:HD21	2.02	0.41
1:A:444:LEU:HD12	1:A:448:PHE:HE2	1.83	0.41
1:B:452:THR:O	1:B:455:LEU:HG	2.21	0.41
1:B:608:GLU:O	1:B:608:GLU:CG	2.68	0.41
1:C:598:ARG:NH1	1:C:679:LEU:HD11	2.35	0.41
1:D:505:LEU:O	1:D:509:LEU:HG	2.20	0.41
1:E:589:ASN:O	1:E:593:ARG:HG3	2.21	0.41
1:F:537:MET:HE2	1:F:537:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:500:SER:O	1:H:504:GLN:HG2	2.20	0.41
1:I:527:GLU:HG3	1:I:567:LEU:HA	2.02	0.41
1:L:564:LEU:HD23	1:L:564:LEU:C	2.46	0.41
1:M:521:LEU:HD12	1:M:521:LEU:HA	1.90	0.41
1:N:491:ILE:HG23	1:O:644:VAL:HG22	2.02	0.41
1:C:663:LEU:O	1:C:667:LYS:HG2	2.20	0.41
1:E:644:VAL:HG22	1:F:491:ILE:HD11	2.03	0.41
1:E:683:TYR:O	1:E:686:VAL:HG12	2.21	0.41
1:F:648:ARG:NH2	1:F:654:ALA:HB3	2.34	0.41
1:K:561:THR:HG22	1:K:565:PHE:CE2	2.51	0.41
1:N:486:PRO:HG3	1:O:657:GLY:HA3	2.02	0.41
1:P:454:LYS:O	1:P:458:ILE:HG13	2.20	0.41
1:P:650:VAL:HG21	1:R:649:ARG:NH2	2.35	0.41
1:A:712:LYS:HE2	1:A:712:LYS:HB3	1.86	0.41
1:E:472:LEU:HD13	1:E:501:ALA:HB1	2.02	0.41
1:E:507:ARG:HH11	1:E:507:ARG:HG2	1.86	0.41
1:M:565:PHE:HA	1:M:568:PHE:CE2	2.56	0.41
1:N:422:GLN:HE22	1:N:507:ARG:HH11	1.69	0.41
1:O:553:TYR:CE2	1:O:554:PHE:HE1	2.39	0.41
1:Q:557:ILE:CD1	1:Q:596:GLN:HG2	2.50	0.41
1:A:420:VAL:HG21	1:D:540:TYR:HB2	2.01	0.41
1:D:557:ILE:HD13	1:D:557:ILE:HA	1.95	0.41
1:E:458:ILE:O	1:E:461:ILE:HG22	2.21	0.41
1:E:595:PHE:HE1	1:E:711:LEU:HD22	1.86	0.41
1:F:510:GLN:C	1:F:514:LYS:HZ3	2.29	0.41
1:G:597:THR:HG23	1:G:679:LEU:HD12	2.02	0.41
1:G:620:GLU:HA	1:G:648:ARG:HH12	1.85	0.41
1:H:441:ILE:HG23	1:H:572:MET:CE	2.51	0.41
1:H:459:LYS:O	1:H:463:THR:HG22	2.20	0.41
1:H:461:ILE:O	1:H:464:ILE:HG12	2.20	0.41
1:H:706:LEU:HD13	1:Q:709:GLU:HG3	2.03	0.41
1:I:441:ILE:HG23	1:I:572:MET:CE	2.51	0.41
1:N:452:THR:HA	1:N:455:LEU:CD2	2.51	0.41
1:N:648:ARG:HE	1:N:654:ALA:HB2	1.84	0.41
1:Q:475:VAL:HG22	1:Q:489:HIS:HB3	2.03	0.41
1:Q:693:LEU:HD23	1:Q:693:LEU:HA	1.97	0.41
1:F:682:LEU:O	1:F:686:VAL:HG12	2.20	0.41
1:G:425:TYR:HA	1:G:428:ILE:HG22	2.03	0.41
1:I:449:ARG:HH21	1:I:578:ASN:ND2	2.19	0.41
1:M:500:SER:O	1:M:504:GLN:HG2	2.22	0.41
1:N:557:ILE:HD13	1:N:557:ILE:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:626:LEU:HD11	1:O:674:PHE:HE2	1.86	0.41
1:C:451:PRO:HD2	1:C:454:LYS:NZ	2.35	0.40
1:D:568:PHE:HB2	1:D:572:MET:CE	2.51	0.40
1:E:625:SER:HB3	1:E:628:MET:HG2	2.04	0.40
1:F:530:ASN:HA	1:F:533:VAL:HG12	2.03	0.40
1:I:494:LEU:HD12	1:I:494:LEU:HA	1.89	0.40
1:J:456:GLU:OE1	1:J:456:GLU:HA	2.20	0.40
1:J:539:LEU:HD23	1:J:539:LEU:HA	1.82	0.40
1:K:457:ILE:HG23	1:K:511:GLU:OE2	2.21	0.40
1:K:590:HIS:HB3	1:K:686:VAL:HG12	2.02	0.40
1:P:630:HIS:ND1	1:P:671:THR:HG22	2.36	0.40
1:Q:436:LEU:C	1:Q:436:LEU:HD12	2.46	0.40
1:B:548:PRO:HG2	1:B:629:ILE:HD11	2.03	0.40
1:C:417:ASP:OD1	1:C:418:PRO:HD2	2.21	0.40
1:G:447:TRP:CZ3	1:G:693:LEU:HB3	2.57	0.40
1:D:444:LEU:HD22	1:D:448:PHE:CE2	2.57	0.40
1:M:663:LEU:HD13	1:M:663:LEU:HA	1.89	0.40
1:N:521:LEU:HD23	1:N:521:LEU:HA	1.94	0.40
1:N:679:LEU:HD23	1:N:679:LEU:HA	1.83	0.40
1:P:662:ILE:HD13	1:P:662:ILE:HA	1.90	0.40
1:Q:426:GLU:HA	1:Q:429:THR:HG22	2.01	0.40
1:C:683:TYR:HE2	1:C:712:LYS:HG2	1.85	0.40
1:D:448:PHE:HD2	1:D:572:MET:HG3	1.87	0.40
1:D:448:PHE:CD2	1:D:572:MET:HG3	2.56	0.40
1:D:482:ARG:HG2	1:D:483:ARG:HG2	2.03	0.40
1:D:580:VAL:HG21	1:D:697:PHE:HD1	1.85	0.40
1:D:593:ARG:NH1	1:D:593:ARG:HB2	2.36	0.40
1:E:446:VAL:HG21	1:E:703:GLN:HE21	1.85	0.40
1:F:632:MET:HE2	1:F:632:MET:HB3	1.93	0.40
1:J:447:TRP:HB3	1:J:697:PHE:CE2	2.57	0.40
1:L:448:PHE:CD2	1:L:572:MET:HG2	2.57	0.40
1:M:431:LEU:HD22	1:M:485:LYS:HD3	2.02	0.40
1:N:705:ARG:HG3	1:N:705:ARG:HH11	1.85	0.40
1:P:632:MET:HE1	1:P:645:TRP:CE3	2.55	0.40
1:D:704:LEU:HD23	1:D:704:LEU:HA	1.93	0.40
1:H:486:PRO:HG3	1:I:657:GLY:HA3	2.02	0.40
1:M:432:PRO:O	1:M:483:ARG:HD3	2.22	0.40
1:P:626:LEU:HD12	1:P:626:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/714 (41%)	287 (99%)	3 (1%)	0	100	100
1	B	290/714 (41%)	286 (99%)	4 (1%)	0	100	100
1	C	290/714 (41%)	283 (98%)	7 (2%)	0	100	100
1	D	290/714 (41%)	284 (98%)	6 (2%)	0	100	100
1	E	290/714 (41%)	284 (98%)	6 (2%)	0	100	100
1	F	290/714 (41%)	280 (97%)	10 (3%)	0	100	100
1	G	290/714 (41%)	287 (99%)	3 (1%)	0	100	100
1	H	290/714 (41%)	286 (99%)	4 (1%)	0	100	100
1	I	290/714 (41%)	286 (99%)	4 (1%)	0	100	100
1	J	290/714 (41%)	286 (99%)	4 (1%)	0	100	100
1	K	290/714 (41%)	281 (97%)	9 (3%)	0	100	100
1	L	290/714 (41%)	281 (97%)	9 (3%)	0	100	100
1	M	290/714 (41%)	288 (99%)	2 (1%)	0	100	100
1	N	290/714 (41%)	287 (99%)	3 (1%)	0	100	100
1	O	290/714 (41%)	286 (99%)	4 (1%)	0	100	100
1	P	290/714 (41%)	283 (98%)	7 (2%)	0	100	100
1	Q	290/714 (41%)	284 (98%)	6 (2%)	0	100	100
1	R	290/714 (41%)	285 (98%)	5 (2%)	0	100	100
All	All	5220/12852 (41%)	5124 (98%)	96 (2%)	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	A	261/616 (42%)	259 (99%)	2 (1%)	73	78
1	B	261/616 (42%)	261 (100%)	0	100	100
1	C	261/616 (42%)	260 (100%)	1 (0%)	84	84
1	D	261/616 (42%)	260 (100%)	1 (0%)	84	84
1	E	261/616 (42%)	258 (99%)	3 (1%)	65	75
1	F	261/616 (42%)	257 (98%)	4 (2%)	57	71
1	G	261/616 (42%)	257 (98%)	4 (2%)	57	71
1	H	261/616 (42%)	260 (100%)	1 (0%)	84	84
1	I	261/616 (42%)	257 (98%)	4 (2%)	57	71
1	J	261/616 (42%)	258 (99%)	3 (1%)	65	75
1	K	261/616 (42%)	261 (100%)	0	100	100
1	L	261/616 (42%)	259 (99%)	2 (1%)	73	78
1	M	261/616 (42%)	259 (99%)	2 (1%)	73	78
1	N	261/616 (42%)	259 (99%)	2 (1%)	73	78
1	O	261/616 (42%)	258 (99%)	3 (1%)	65	75
1	P	261/616 (42%)	258 (99%)	3 (1%)	65	75
1	Q	261/616 (42%)	259 (99%)	2 (1%)	73	78
1	R	261/616 (42%)	258 (99%)	3 (1%)	65	75
All	All	4698/11088 (42%)	4658 (99%)	40 (1%)	68	76

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	420	VAL
1	A	533	VAL
1	C	684	SER
1	D	465	LEU
1	E	420	VAL
1	E	662	ILE
1	E	679	LEU
1	F	497	THR
1	F	523	VAL
1	F	604	LEU
1	F	640	VAL

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Mol	Chain	Res	Type
1	G	549	SER
1	G	635	MET
1	G	672	LEU
1	G	684	SER
1	H	444	LEU
1	I	420	VAL
1	I	471	MET
1	I	595	PHE
1	I	711	LEU
1	J	428	ILE
1	J	471	MET
1	J	682	LEU
1	L	465	LEU
1	L	498	ILE
1	M	505	LEU
1	M	663	LEU
1	N	580	VAL
1	N	663	LEU
1	O	438	GLU
1	O	537	MET
1	O	603	ASN
1	P	420	VAL
1	P	428	ILE
1	P	580	VAL
1	Q	704	LEU
1	Q	711	LEU
1	R	428	ILE
1	R	505	LEU
1	R	635	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	GLN
1	A	502	ASN
1	A	555	GLN
1	A	596	GLN
1	A	612	GLN
1	B	445	ASN
1	B	555	GLN
1	B	602	GLN
1	C	496	GLN

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Mol	Chain	Res	Type
1	C	660	GLN
1	D	499	ASN
1	D	502	ASN
1	D	535	GLN
1	D	555	GLN
1	D	602	GLN
1	D	638	ASN
1	D	643	ASN
1	D	647	GLN
1	E	466	HIS
1	E	535	GLN
1	E	544	ASN
1	E	633	GLN
1	F	489	HIS
1	F	529	HIS
1	F	660	GLN
1	H	502	ASN
1	H	596	GLN
1	H	656	HIS
1	H	658	GLN
1	I	466	HIS
1	I	502	ASN
1	I	544	ASN
1	I	596	GLN
1	J	445	ASN
1	J	499	ASN
1	J	502	ASN
1	J	660	GLN
1	J	701	ASN
1	K	466	HIS
1	K	530	ASN
1	K	555	GLN
1	K	643	ASN
1	K	656	HIS
1	K	701	ASN
1	L	466	HIS
1	L	499	ASN
1	L	513	GLN
1	M	660	GLN
1	M	676	GLN
1	N	490	ASN
1	N	510	GLN

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Mol	Chain	Res	Type
1	N	603	ASN
1	O	499	ASN
1	O	544	ASN
1	O	596	GLN
1	P	499	ASN
1	P	638	ASN
1	P	660	GLN
1	Q	490	ASN
1	R	489	HIS
1	R	490	ASN
1	R	535	GLN
1	R	647	GLN
1	R	651	ASN
1	R	658	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

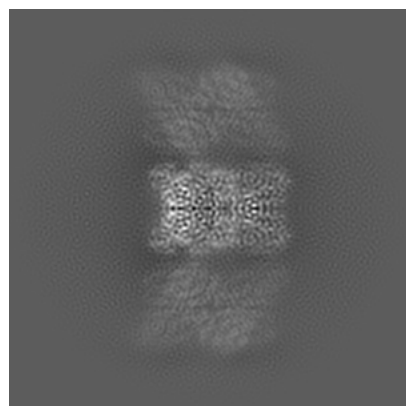
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66433. These allow visual inspection of the internal detail of the map and identification of artifacts.

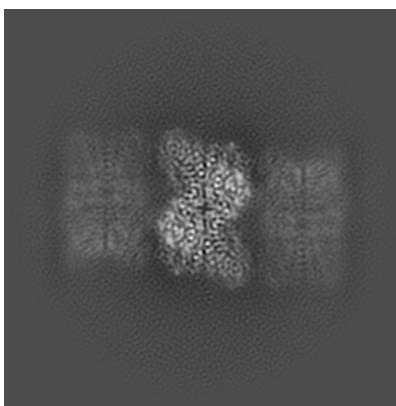
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

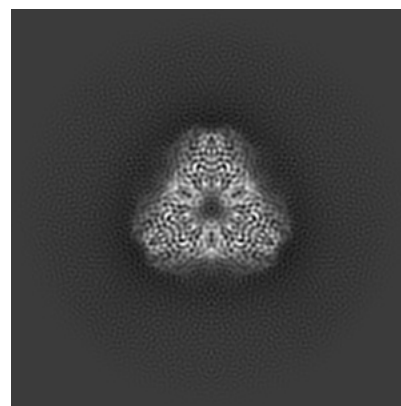
6.1.1 Primary map



X

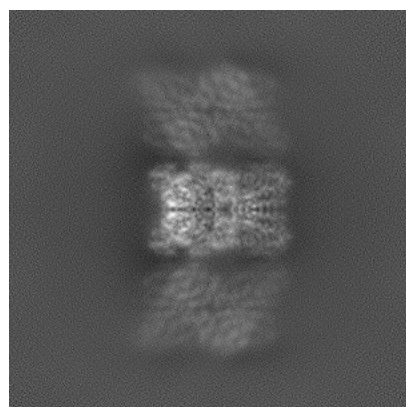


Y

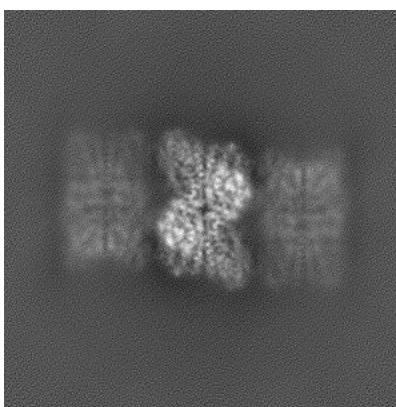


Z

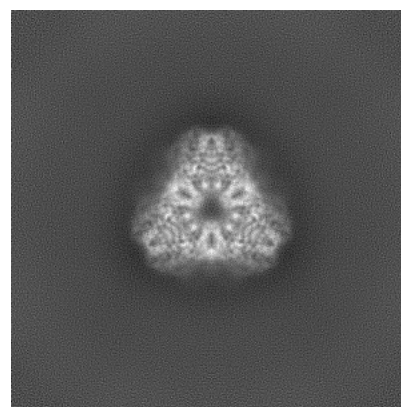
6.1.2 Raw map



X



Y

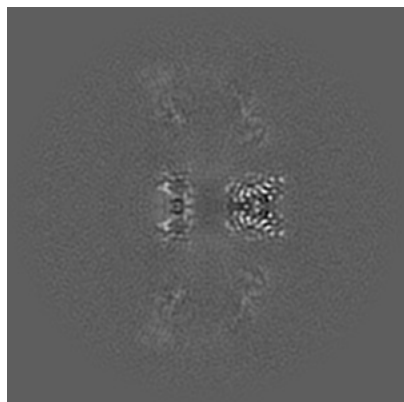


Z

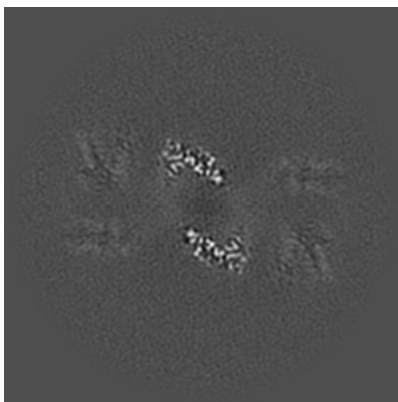
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

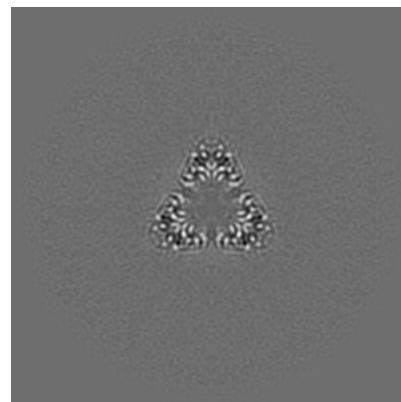
6.2.1 Primary map



X Index: 200

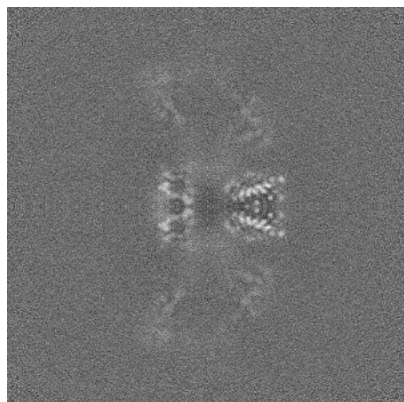


Y Index: 200

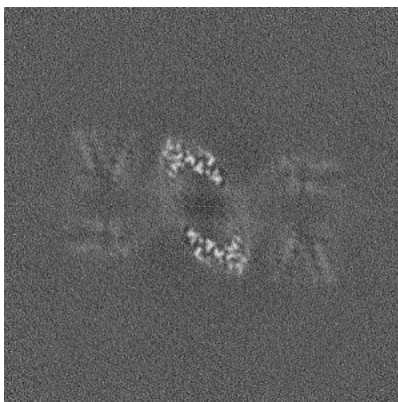


Z Index: 200

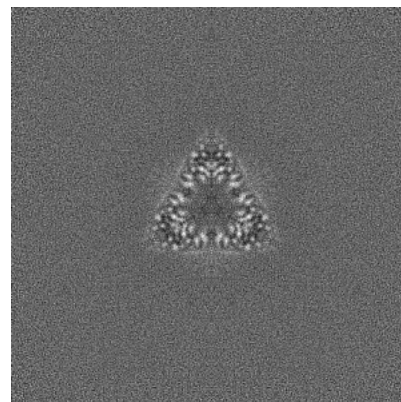
6.2.2 Raw map



X Index: 200



Y Index: 200

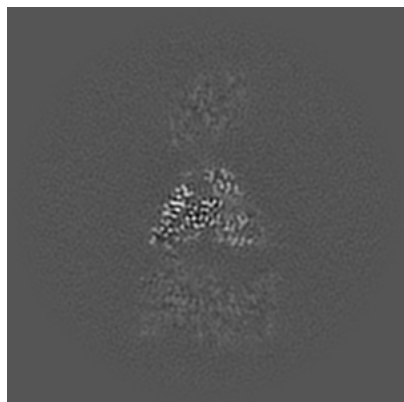


Z Index: 200

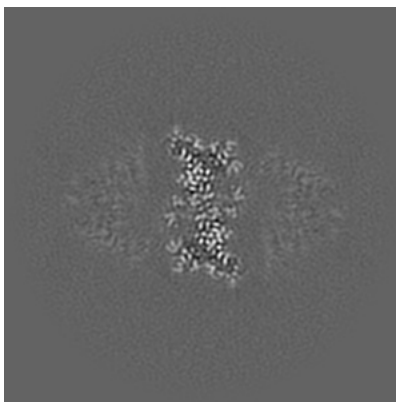
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

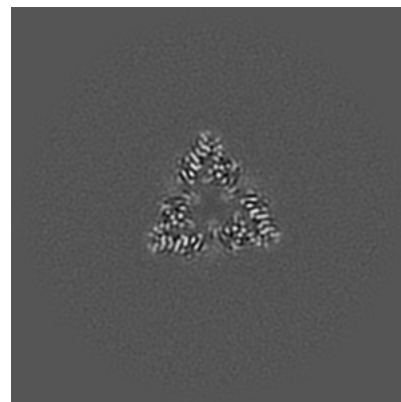
6.3.1 Primary map



X Index: 165

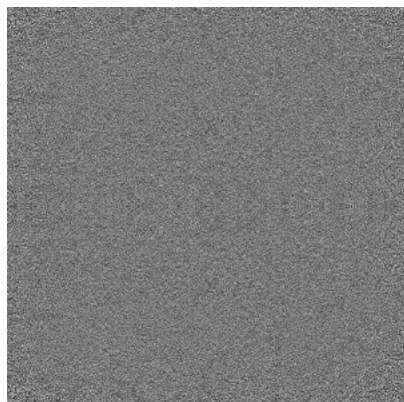


Y Index: 171

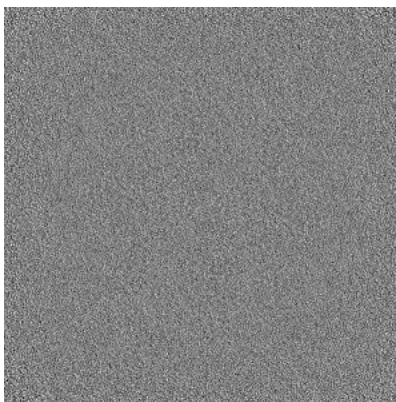


Z Index: 193

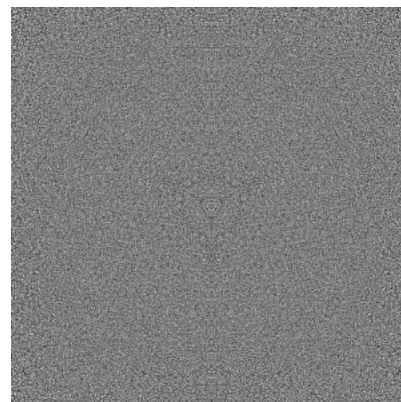
6.3.2 Raw map



X Index: 0



Y Index: 0

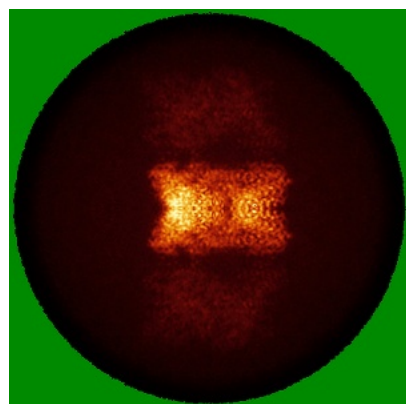


Z Index: 0

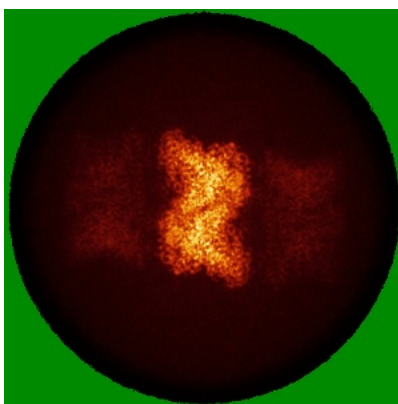
The images above show the largest variance slices of the map in three orthogonal directions.

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

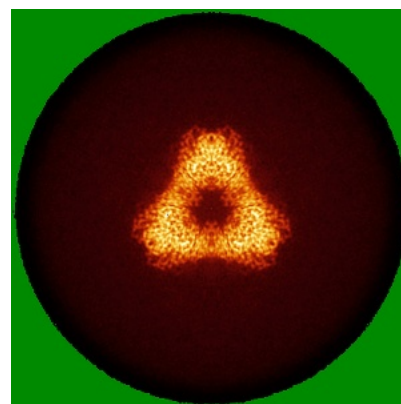
6.4.1 Primary map



X

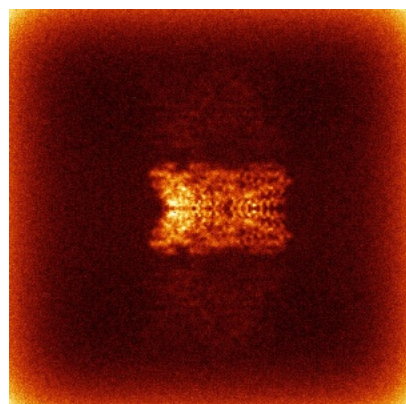


Y

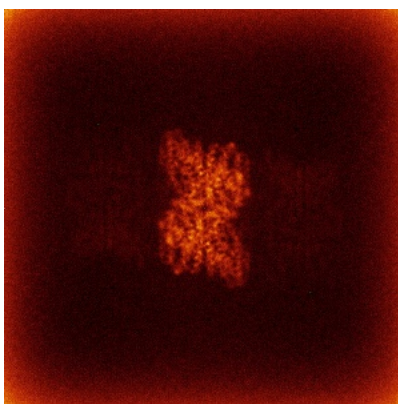


Z

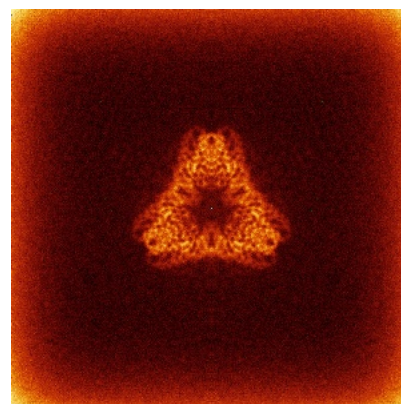
6.4.2 Raw map



X



Y

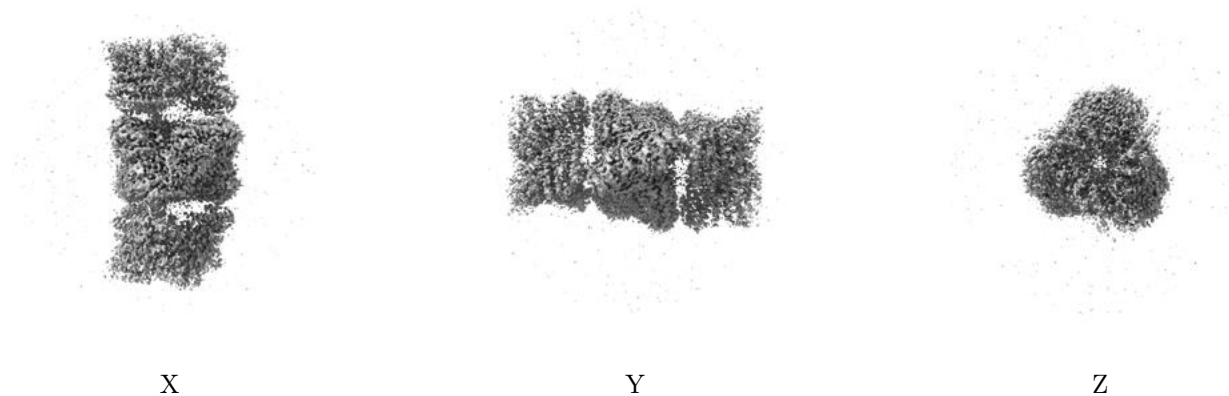


Z

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.

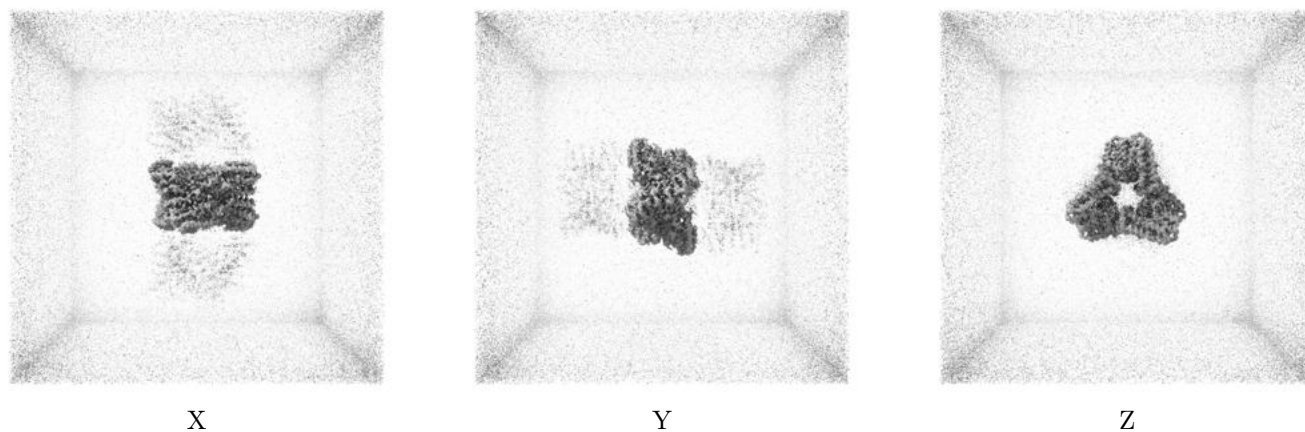
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

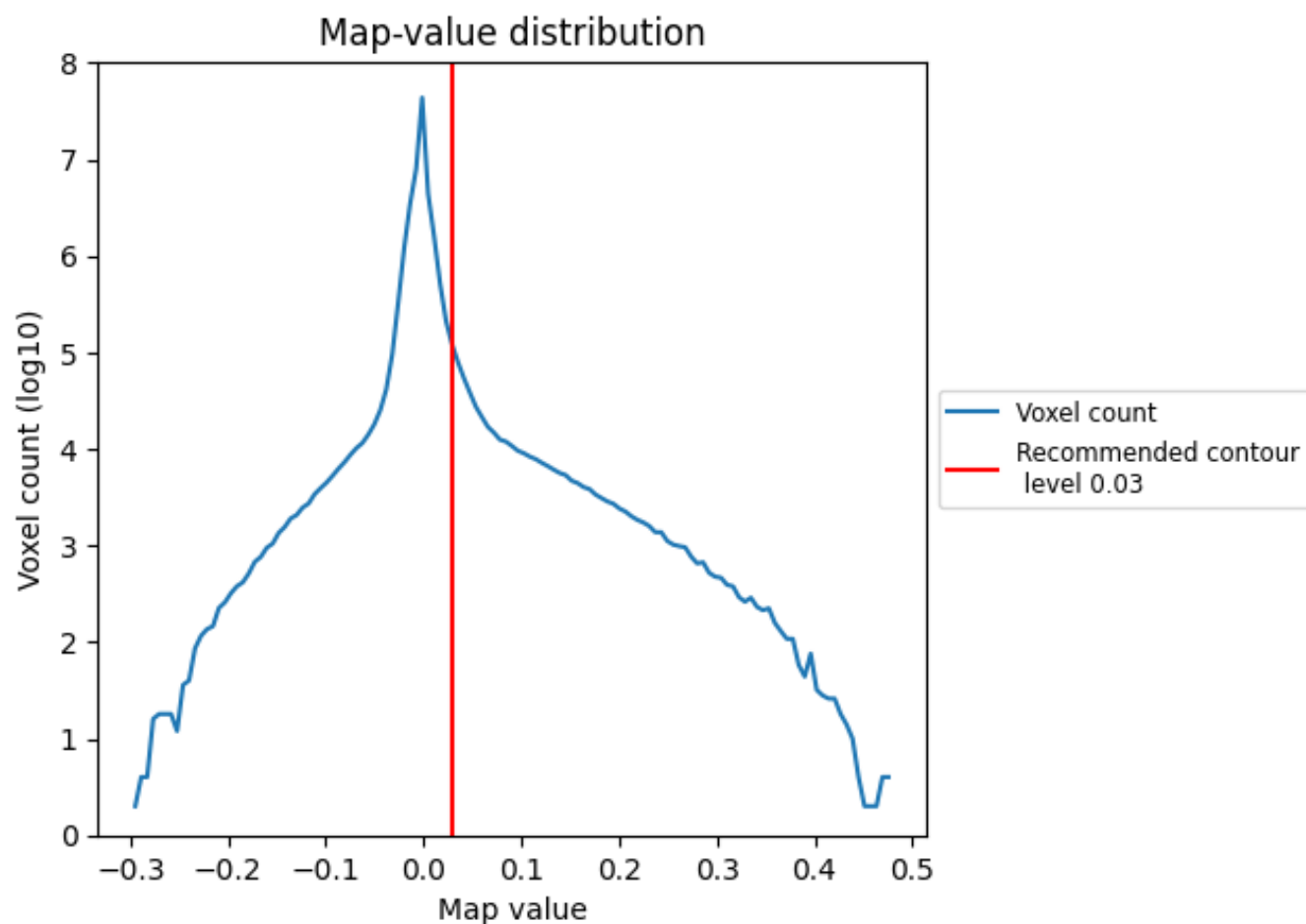
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

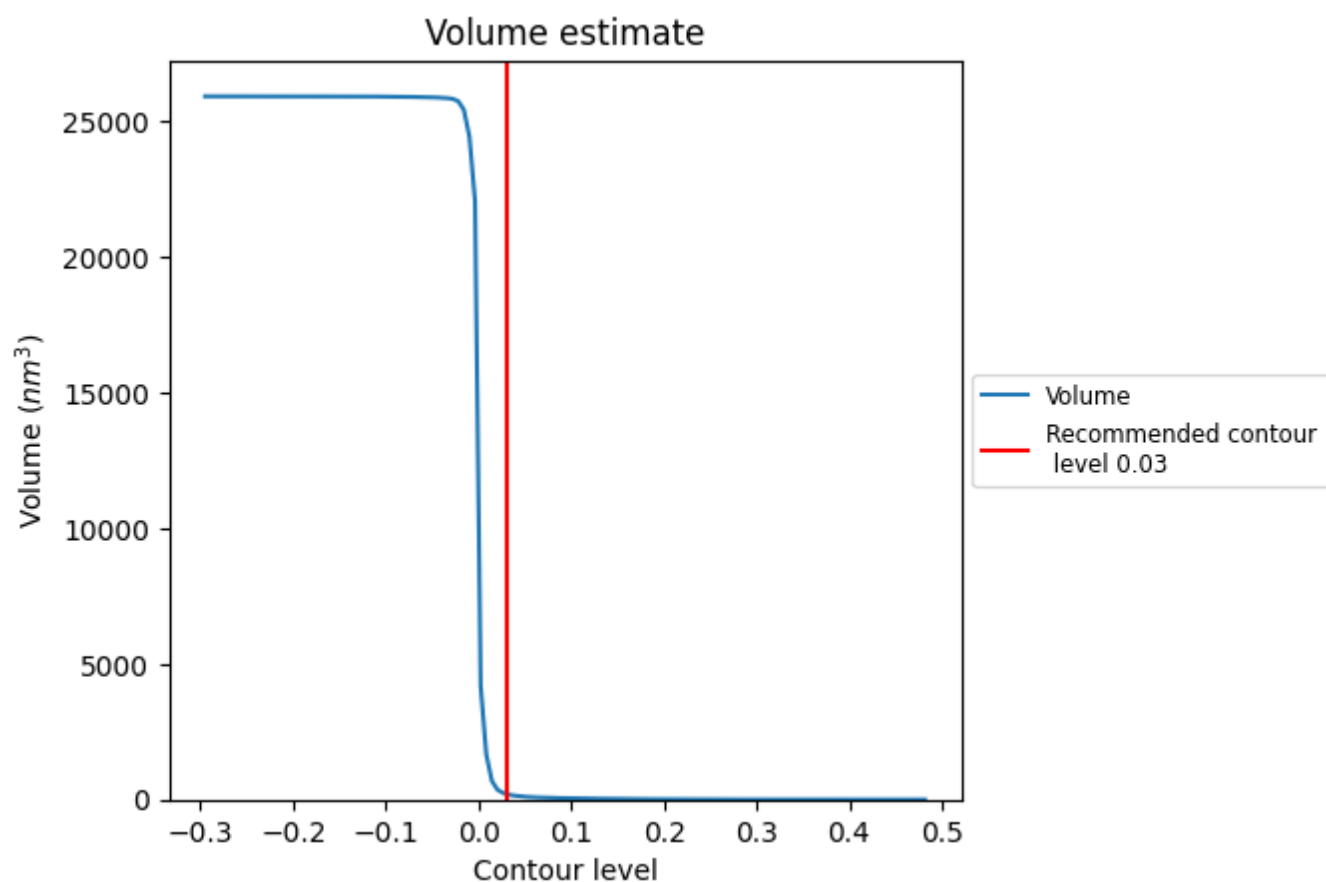
This section contains the results of statistical analysis of the map.

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.

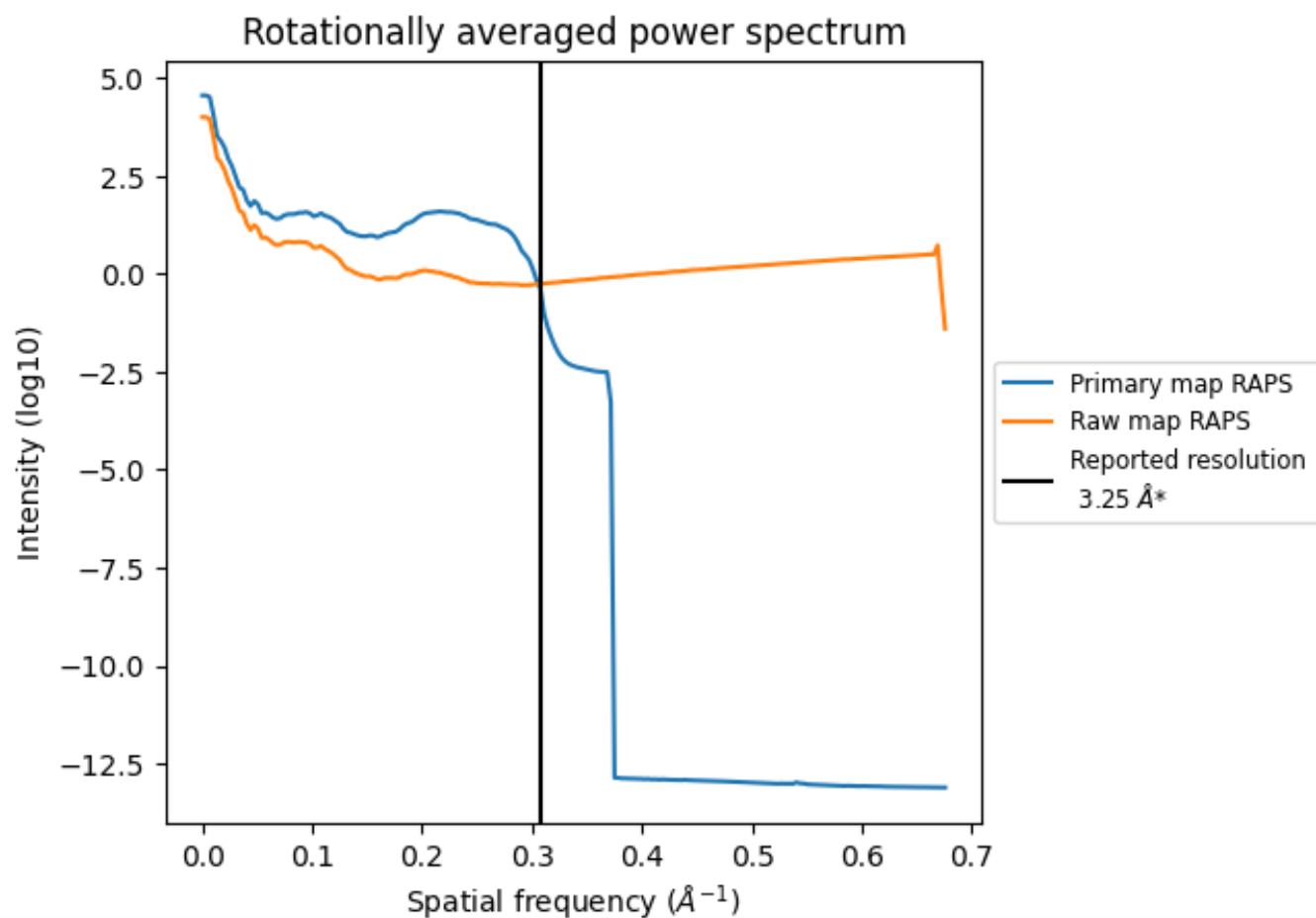
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209 nm³; this corresponds to an approximate mass of 189 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 ⓘ

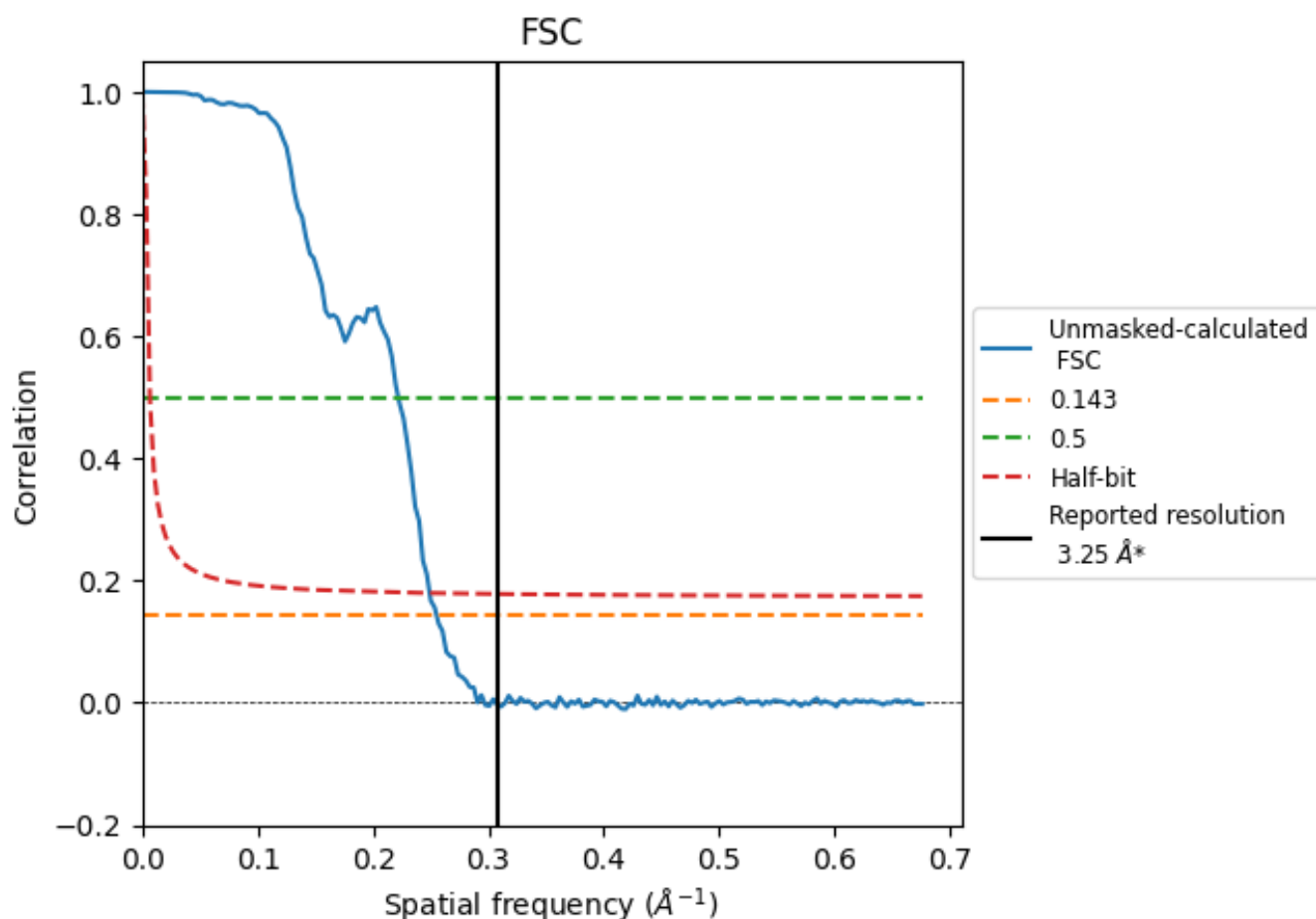


*Reported resolution corresponds to spatial frequency of 0.308 Å⁻¹

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 0.308 Å⁻¹

8.2 Resolution estimates [i](#)

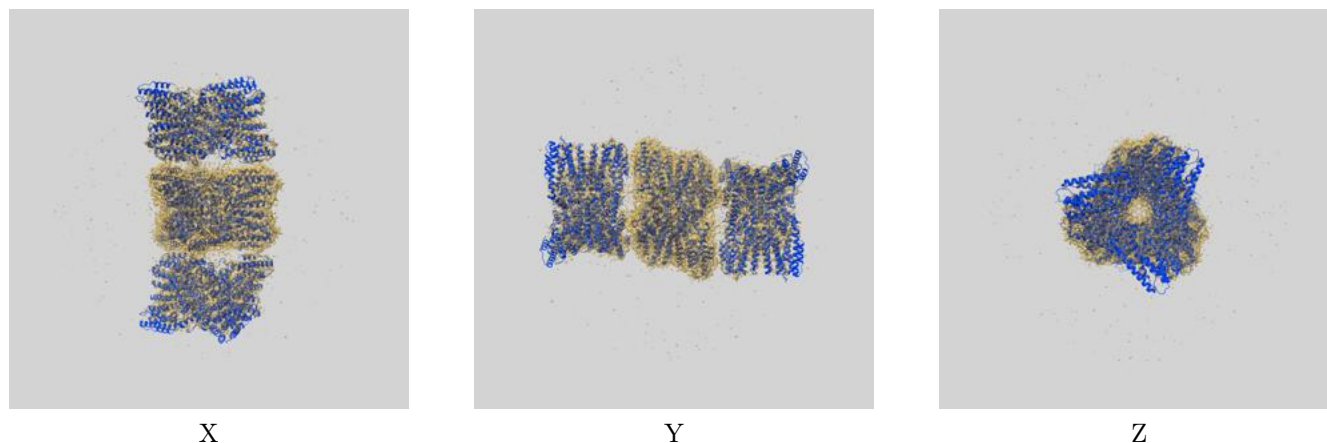
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	4.51	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

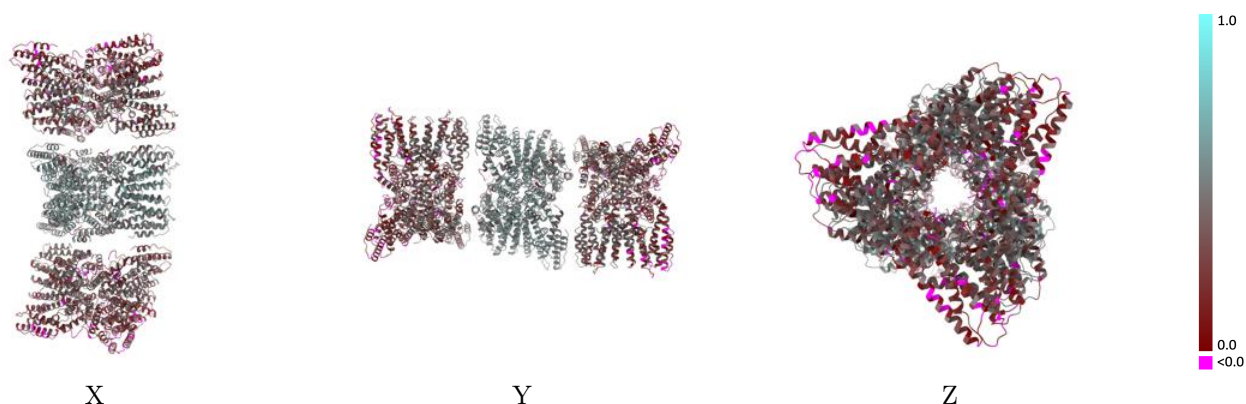
This section contains information regarding the fit between EMDB map EMD-66433 and PDB model 9X0F. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



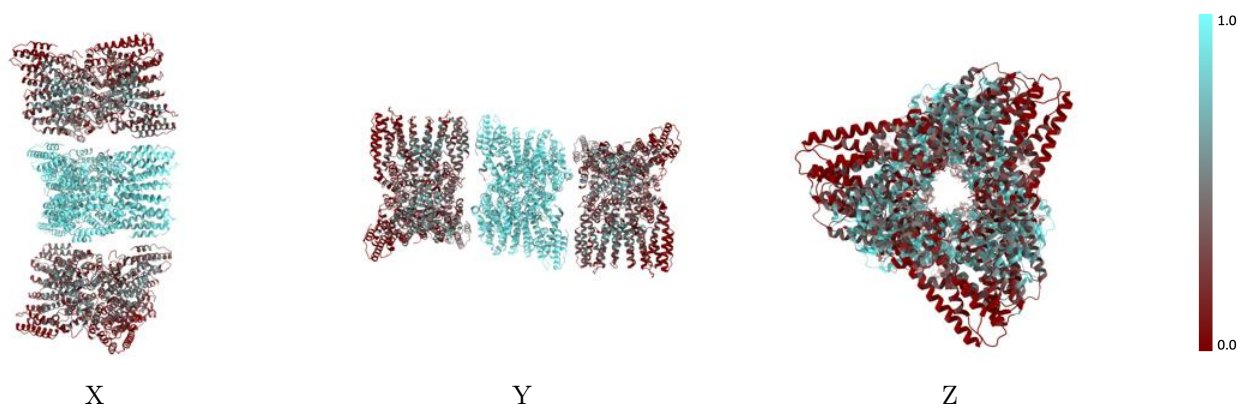
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



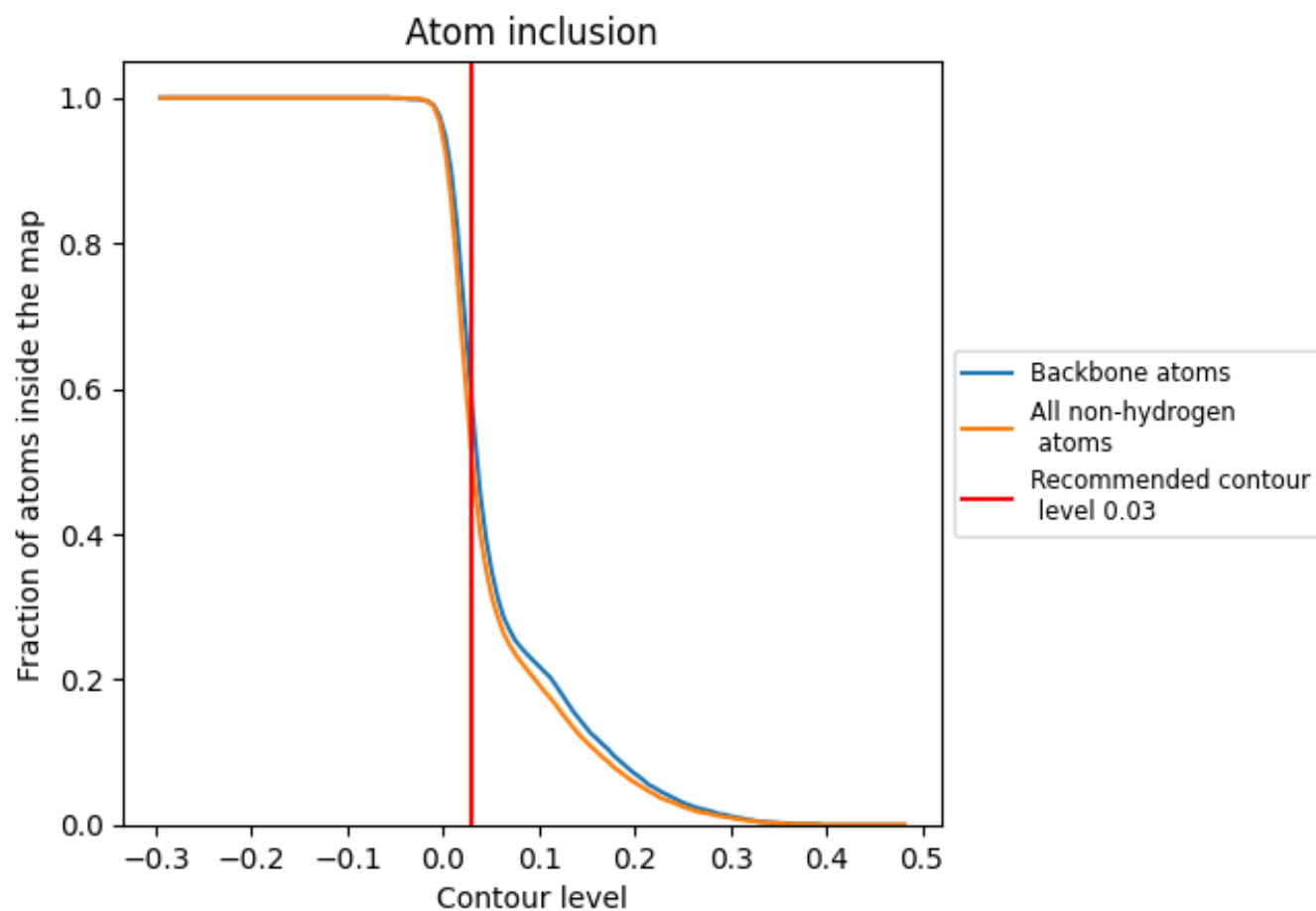
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 50% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.3600
A	 0.3860	 0.3470
B	 0.2310	 0.2390
C	 0.2260	 0.2370
D	 0.2310	 0.2380
E	 0.3700	 0.3220
F	 0.3790	 0.3400
G	 0.2310	 0.2370
H	 0.3880	 0.3480
I	 0.3870	 0.3380
J	 0.3860	 0.3450
K	 0.2190	 0.2400
L	 0.2260	 0.2330
M	 0.9060	 0.5060
N	 0.9110	 0.5070
O	 0.9040	 0.5060
P	 0.9040	 0.5040
Q	 0.8970	 0.4900
R	 0.9020	 0.5040

