



Full wwPDB EM Validation Report ⓘ

Jul 9, 2024 – 11:01 pm BST

PDB ID : 7PTY
EMDB ID : EMD-13643
Title : Delta-latroinsectotoxin dimer
Authors : Chen, M.; Gatsogiannis, C.
Deposited on : 2021-09-27
Resolution : 4.63 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

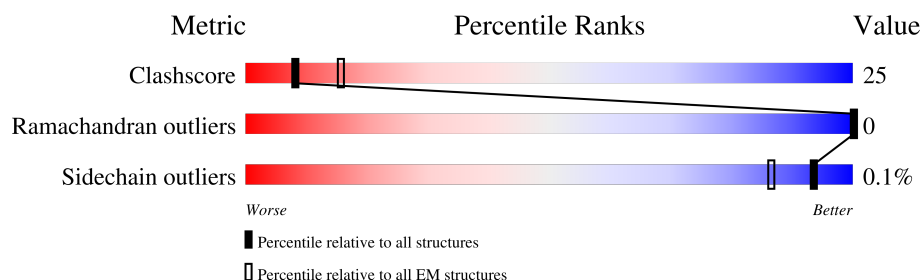
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1296	<div> <div>17%</div> <div>36%</div> <div>29%</div> <div>34%</div> </div>
1	B	1296	<div> <div>10%</div> <div>35%</div> <div>32%</div> <div>33%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13433 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 Delta-latroinsectotoxin-Lt1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	850	Total	C	N	O	S	0	0
			6663	4229	1125	1293	16		
1	B	865	Total	C	N	O	S	0	0
			6770	4293	1142	1318	17		

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-62	MET	-	initiating methionine	UNP Q25338
A	-61	LYS	-	expression tag	UNP Q25338
A	-60	PHE	-	expression tag	UNP Q25338
A	-59	LEU	-	expression tag	UNP Q25338
A	-58	VAL	-	expression tag	UNP Q25338
A	-57	ASN	-	expression tag	UNP Q25338
A	-56	VAL	-	expression tag	UNP Q25338
A	-55	ALA	-	expression tag	UNP Q25338
A	-54	LEU	-	expression tag	UNP Q25338
A	-53	VAL	-	expression tag	UNP Q25338
A	-52	PHE	-	expression tag	UNP Q25338
A	-51	MET	-	expression tag	UNP Q25338
A	-50	VAL	-	expression tag	UNP Q25338
A	-49	VAL	-	expression tag	UNP Q25338
A	-48	TYR	-	expression tag	UNP Q25338
A	-47	ILE	-	expression tag	UNP Q25338
A	-46	SER	-	expression tag	UNP Q25338
A	-45	TYR	-	expression tag	UNP Q25338
A	-44	ILE	-	expression tag	UNP Q25338
A	-43	TYR	-	expression tag	UNP Q25338
A	-42	ALA	-	expression tag	UNP Q25338
A	-41	MET	-	expression tag	UNP Q25338
A	-40	TRP	-	expression tag	UNP Q25338
A	-39	SER	-	expression tag	UNP Q25338
A	-38	HIS	-	expression tag	UNP Q25338
A	-37	PRO	-	expression tag	UNP Q25338

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	GLN	-	expression tag	UNP Q25338
A	-35	PHE	-	expression tag	UNP Q25338
A	-34	GLU	-	expression tag	UNP Q25338
A	-33	LYS	-	expression tag	UNP Q25338
A	-32	GLY	-	expression tag	UNP Q25338
A	-31	SER	-	expression tag	UNP Q25338
A	-30	ALA	-	expression tag	UNP Q25338
A	-29	GLY	-	expression tag	UNP Q25338
A	-28	SER	-	expression tag	UNP Q25338
A	-27	ALA	-	expression tag	UNP Q25338
A	-26	ALA	-	expression tag	UNP Q25338
A	-25	GLY	-	expression tag	UNP Q25338
A	-24	SER	-	expression tag	UNP Q25338
A	-23	GLY	-	expression tag	UNP Q25338
A	-22	ALA	-	expression tag	UNP Q25338
A	-21	GLY	-	expression tag	UNP Q25338
A	-20	TRP	-	expression tag	UNP Q25338
A	-19	SER	-	expression tag	UNP Q25338
A	-18	HIS	-	expression tag	UNP Q25338
A	-17	PRO	-	expression tag	UNP Q25338
A	-16	GLN	-	expression tag	UNP Q25338
A	-15	PHE	-	expression tag	UNP Q25338
A	-14	GLU	-	expression tag	UNP Q25338
A	-13	LYS	-	expression tag	UNP Q25338
A	-12	GLY	-	expression tag	UNP Q25338
A	-11	ALA	-	expression tag	UNP Q25338
A	-10	GLY	-	expression tag	UNP Q25338
A	-9	LEU	-	expression tag	UNP Q25338
A	-8	GLU	-	expression tag	UNP Q25338
A	-7	VAL	-	expression tag	UNP Q25338
A	-6	LEU	-	expression tag	UNP Q25338
A	-5	PHE	-	expression tag	UNP Q25338
A	-4	GLN	-	expression tag	UNP Q25338
A	-3	GLY	-	expression tag	UNP Q25338
A	-2	PRO	-	expression tag	UNP Q25338
A	-1	PRO	-	expression tag	UNP Q25338
A	0	TRP	-	expression tag	UNP Q25338
A	1215	LEU	-	expression tag	UNP Q25338
A	1216	GLU	-	expression tag	UNP Q25338
A	1217	SER	-	expression tag	UNP Q25338
A	1218	SER	-	expression tag	UNP Q25338
A	1219	GLY	-	expression tag	UNP Q25338

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	LEU	-	expression tag	UNP Q25338
A	1221	VAL	-	expression tag	UNP Q25338
A	1222	PRO	-	expression tag	UNP Q25338
A	1223	ARG	-	expression tag	UNP Q25338
A	1224	GLY	-	expression tag	UNP Q25338
A	1225	SER	-	expression tag	UNP Q25338
A	1226	HIS	-	expression tag	UNP Q25338
A	1227	HIS	-	expression tag	UNP Q25338
A	1228	HIS	-	expression tag	UNP Q25338
A	1229	HIS	-	expression tag	UNP Q25338
A	1230	HIS	-	expression tag	UNP Q25338
A	1231	HIS	-	expression tag	UNP Q25338
A	1232	HIS	-	expression tag	UNP Q25338
A	1233	HIS	-	expression tag	UNP Q25338
B	-62	MET	-	initiating methionine	UNP Q25338
B	-61	LYS	-	expression tag	UNP Q25338
B	-60	PHE	-	expression tag	UNP Q25338
B	-59	LEU	-	expression tag	UNP Q25338
B	-58	VAL	-	expression tag	UNP Q25338
B	-57	ASN	-	expression tag	UNP Q25338
B	-56	VAL	-	expression tag	UNP Q25338
B	-55	ALA	-	expression tag	UNP Q25338
B	-54	LEU	-	expression tag	UNP Q25338
B	-53	VAL	-	expression tag	UNP Q25338
B	-52	PHE	-	expression tag	UNP Q25338
B	-51	MET	-	expression tag	UNP Q25338
B	-50	VAL	-	expression tag	UNP Q25338
B	-49	VAL	-	expression tag	UNP Q25338
B	-48	TYR	-	expression tag	UNP Q25338
B	-47	ILE	-	expression tag	UNP Q25338
B	-46	SER	-	expression tag	UNP Q25338
B	-45	TYR	-	expression tag	UNP Q25338
B	-44	ILE	-	expression tag	UNP Q25338
B	-43	TYR	-	expression tag	UNP Q25338
B	-42	ALA	-	expression tag	UNP Q25338
B	-41	MET	-	expression tag	UNP Q25338
B	-40	TRP	-	expression tag	UNP Q25338
B	-39	SER	-	expression tag	UNP Q25338
B	-38	HIS	-	expression tag	UNP Q25338
B	-37	PRO	-	expression tag	UNP Q25338
B	-36	GLN	-	expression tag	UNP Q25338
B	-35	PHE	-	expression tag	UNP Q25338

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	GLU	-	expression tag	UNP Q25338
B	-33	LYS	-	expression tag	UNP Q25338
B	-32	GLY	-	expression tag	UNP Q25338
B	-31	SER	-	expression tag	UNP Q25338
B	-30	ALA	-	expression tag	UNP Q25338
B	-29	GLY	-	expression tag	UNP Q25338
B	-28	SER	-	expression tag	UNP Q25338
B	-27	ALA	-	expression tag	UNP Q25338
B	-26	ALA	-	expression tag	UNP Q25338
B	-25	GLY	-	expression tag	UNP Q25338
B	-24	SER	-	expression tag	UNP Q25338
B	-23	GLY	-	expression tag	UNP Q25338
B	-22	ALA	-	expression tag	UNP Q25338
B	-21	GLY	-	expression tag	UNP Q25338
B	-20	TRP	-	expression tag	UNP Q25338
B	-19	SER	-	expression tag	UNP Q25338
B	-18	HIS	-	expression tag	UNP Q25338
B	-17	PRO	-	expression tag	UNP Q25338
B	-16	GLN	-	expression tag	UNP Q25338
B	-15	PHE	-	expression tag	UNP Q25338
B	-14	GLU	-	expression tag	UNP Q25338
B	-13	LYS	-	expression tag	UNP Q25338
B	-12	GLY	-	expression tag	UNP Q25338
B	-11	ALA	-	expression tag	UNP Q25338
B	-10	GLY	-	expression tag	UNP Q25338
B	-9	LEU	-	expression tag	UNP Q25338
B	-8	GLU	-	expression tag	UNP Q25338
B	-7	VAL	-	expression tag	UNP Q25338
B	-6	LEU	-	expression tag	UNP Q25338
B	-5	PHE	-	expression tag	UNP Q25338
B	-4	GLN	-	expression tag	UNP Q25338
B	-3	GLY	-	expression tag	UNP Q25338
B	-2	PRO	-	expression tag	UNP Q25338
B	-1	PRO	-	expression tag	UNP Q25338
B	0	TRP	-	expression tag	UNP Q25338
B	1215	LEU	-	expression tag	UNP Q25338
B	1216	GLU	-	expression tag	UNP Q25338
B	1217	SER	-	expression tag	UNP Q25338
B	1218	SER	-	expression tag	UNP Q25338
B	1219	GLY	-	expression tag	UNP Q25338
B	1220	LEU	-	expression tag	UNP Q25338
B	1221	VAL	-	expression tag	UNP Q25338

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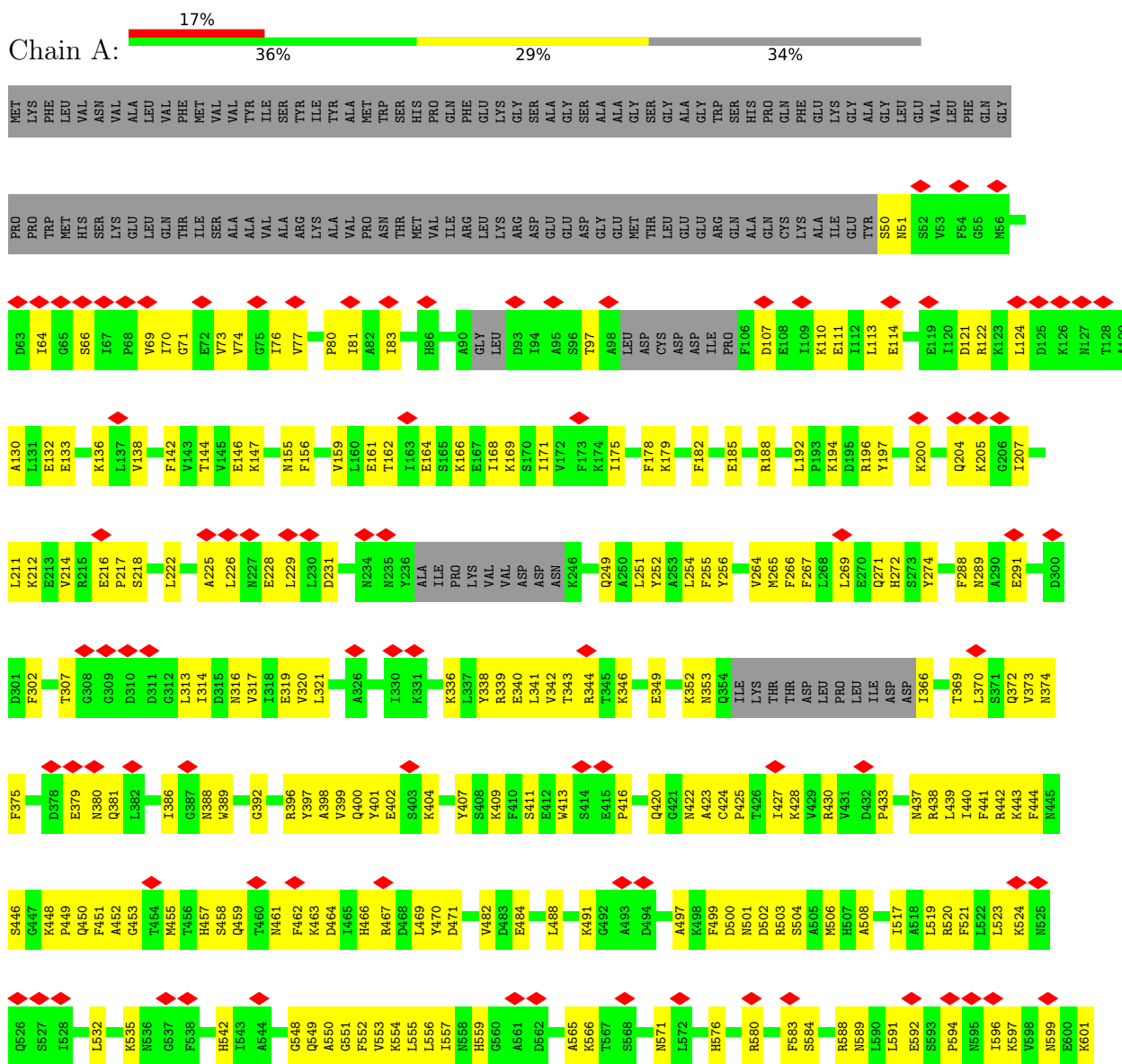
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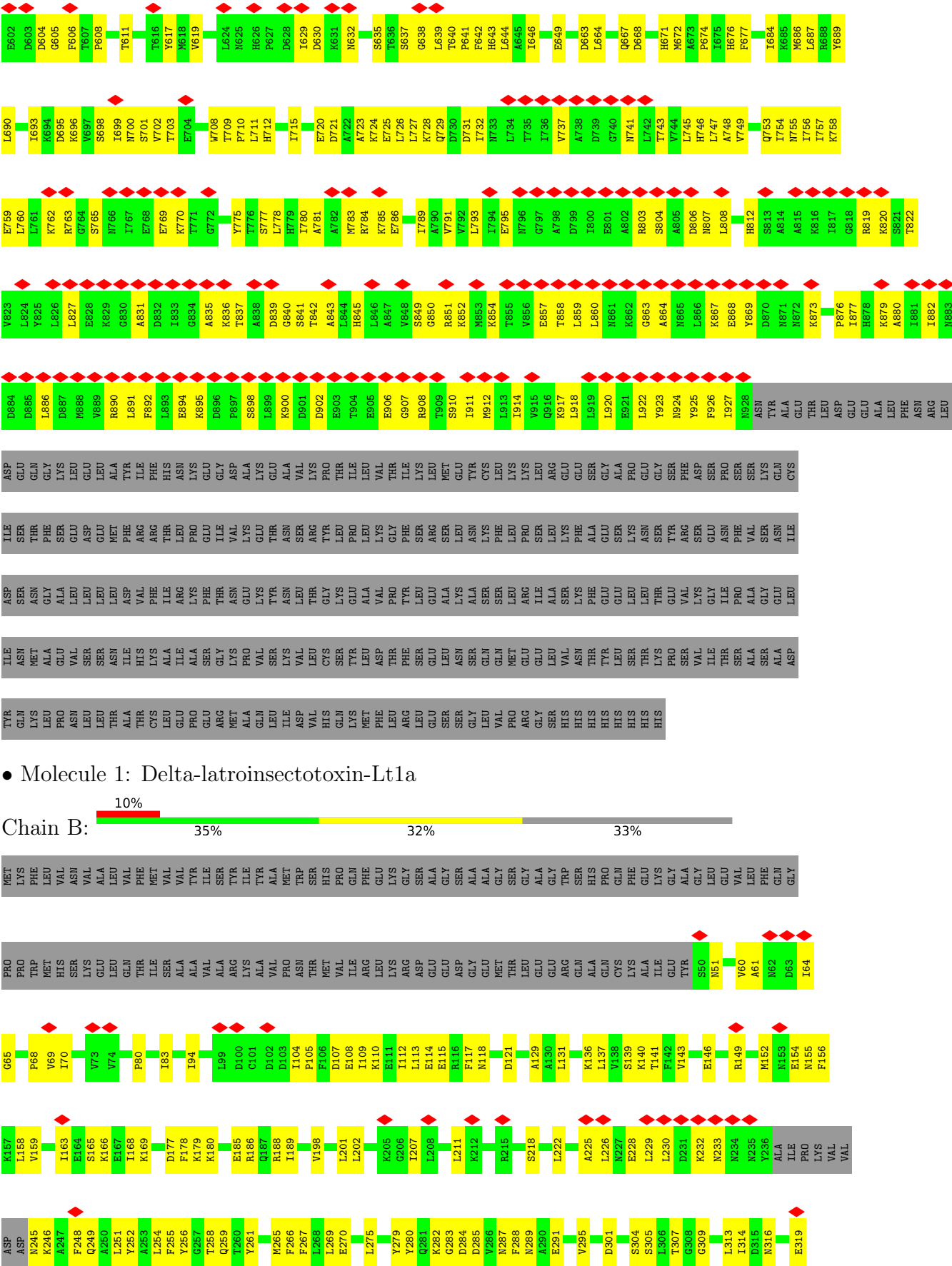
Chain	Residue	Modelled	Actual	Comment	Reference
B	1222	PRO	-	expression tag	UNP Q25338
B	1223	ARG	-	expression tag	UNP Q25338
B	1224	GLY	-	expression tag	UNP Q25338
B	1225	SER	-	expression tag	UNP Q25338
B	1226	HIS	-	expression tag	UNP Q25338
B	1227	HIS	-	expression tag	UNP Q25338
B	1228	HIS	-	expression tag	UNP Q25338
B	1229	HIS	-	expression tag	UNP Q25338
B	1230	HIS	-	expression tag	UNP Q25338
B	1231	HIS	-	expression tag	UNP Q25338
B	1232	HIS	-	expression tag	UNP Q25338
B	1233	HIS	-	expression tag	UNP Q25338

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: Delta-latroinsectotoxin-Lt1a





MET	LYS	ASN	VAL	ASP	D901	T837	G764	1684	V598	K524	Q459	V390	N322
ALA	PRO	GLU	LYS	ALA	D902	A838	S765	K885	R999	N525	Q461	D391	T323
LEU	VAL	TYR	THR	GLU	E903	D839	N766	M886	E600	Q526	N461	G392	V324
ILE	ASN	TYR	ASN	VAL	E904			L687	K601	S27	F462	V393	K325
VAL	LEU	THR	ASN	VAL	E905	L844	K770	R688	E602	I528	K463	V395	A326
GLY	LEU	GLY	ARG	THR	E906	H845	T771	Y689	D604	D529	D464	L327	L327
THR	CYS	THR	THR	PRO	E907	L846	G772	L690		I530	I465	R396	P328
PRO	THR	THR	THR	THR	E908	A847	E773	I691	P008	E531	H466	V397	F329
TYR	TYR	ILE	PRO	ILE	E909	V848	G774	I693	L609	L532	D468	I330	I330
LEU	ALA	LEU	LEU	LEU	S910	S849	T775	S692	H610	K533	Q400	K331	K331
ALA	VAL	ALA	LEU	VAL	S911	G850	T776	K696	V613	K534	L469	Y401	N332
THR	PRO	THR	GLY	THR	N912	R851	S777	S701	M614	D534	Y470	E402	A332
ILE	THR	THR	PHE	ILE	N913	K852	T778	T703		K535		S403	
LYS	LYS	LYS	ARG	LYS	N914	N853	H779	W702	Y617	F538	L474	K404	K336
LEU	LEU	LEU	SER	MET	N915	T854	I780	T703	M618	G537	M475	S404	K337
ALA	ALA	ALA	SER	ALA	N916	V855			V619	T539	M476	K405	L337
ASN	LYS	GLY	ASN	GLY	K917	V856			V620	H542	M477	G406	K338
ASN	TYR	TYR	ASN	TYR	L918		M783	N706	V619	I543	K478	M406	Y338
GLN	CYS	CYS	LYS	CYS	L919	L859	R784	N707	V620		K480	Y407	R339
SER	LYS	LYS	PHE	LYS	L920	L860	T785	W708	D621		K481	F410	
PRO	LEU	LEU	PRO	LYS	L921	N861	E786	P710	A622	A547	F411	S411	V342
ARG	ARG	ARG	PRO	LYS	E921	K862	P787	L711	L624	Q548	E481	E412	T343
GLY	GLY	ILE	SER	LEU	L922	G863		H712	L624	G549	S411	E413	R344
LEU	LEU	ALA	LEU	ARG	L923	A864	A790	F713	M626	A550	E414	S414	L348
VAL	VAL	SER	LYS	GLY	N924	N865	V791	A714	P627	G551	T486	S415	L351
ASN	PHE	LYS	PHE	GLY	Y925	L866	I794	D721	D628	F552	T487		
THR	THR	GLY	ALA	SER	F926	R867	A798	A722	L629	L488	L488	Q420	Q354
PRO	GLY	ALA	GLY	ALA	N927	E868	D798	A723	D630	K554	K491	M422	I355
ASN	LYS	ASN	LYS	PRO	N928	Y869		K724		L555	Q492	A423	LYS
THR	THR	THR	ASN	GLY		D870		E725	Q634	L556	G493	A424	THR
LYS	LYS	GLY	TYR	GLY	ASN	N871	A798	L726	S635	I557	D494	C424	THR
PRO	PRO	VAL	TYR	SER	ALA	K872	F801	L727	S636		I495	P425	ASP
VAL	VAL	VAL	VAL	ASP	THR	R873	A802	K728	S637	A561	T495	T426	LEU
GLY	GLY	GLY	GLY	SER	LEU	Y874	R803	Q729	G638	K566	E496	I427	PRO
ILE	ILE	ILE	ASN	PRO	ASP	L875	S804	D730	L639	K569	F499	K428	L362
THR	THR	THR	ASN	PRO	ASP	P876	A805	D731		T570	D500	I363	I363
SER	SER	SER	VAL	SER	GLY	H877	D806	T735	P641	N571	N501	D364	D365
ALA	ALA	ALA	VAL	SER	ALA	H878	L808	I736	F642		R503	I366	I366
ALA	ALA	ALA	ASN	GLN	LEU	K879		I737	H643		S504	P367	P367
ASP	ASP	ASP	ILE	CYS	PHE	A880	H812	A738			M506	E368	T369
TYR	TYR	ILE	ASP	ILE	ASN	I881		D739			A508	L370	L370
GLN	GLN	ASN	SER	SER	ARG	T882	T817	G740	Q667	R580	A510	S371	S371
LEU	LEU	ASN	THR	THR	LEU	N883	G818	N741	D668	S881	A511	Q372	Q372
PRO	PRO	ALA	PHE	PHE	ASP	N884	R819	G742	V669	F583	R512	F441	F441
VAL	VAL	ALA	GLY	GLY	GLN	D885	K820	L742	N670		G513	V373	V373
LEU	LEU	VAL	GLY	ASP	GLY	L886	T822	H746	H671		N514	N374	N374
SER	SER	VAL	LEU	ASP	LYS	D887	V823	L747	M672	V587	N515	F375	F375
ASN	ASN	ASN	LEU	MET	LEU	N888	L624	A748	A673	R588	K516	P376	P376
THR	THR	ILE	VAL	PHE	GLU	V889	Y825	V749	P674	N589	I517	N377	N377
ALA	ALA	VAL	VAL	ARG	LEU	N890	L826	S750	I675	L590	A518	D378	D378
LYS	CYS	LYS	PHE	THR	ALA	L891	L827	T751	H676	L591	L519	Q381	Q381
LEU	LEU	ALA	ILE	ARG	LEU	F892	K829	G752	F677	E592	R520	L382	L382
GLU	GLU	ILE	ARG	LEU	PRO	N893		K758	A679	P594	F521	P383	P383
PRO	PRO	ALA	LYS	THR	PHE	E894	D832	K762	A679	N595	L522	G387	G387
GLY	GLY	SER	PHE	GLU	ILE	K895	T833	R763			L523	N388	N388
ARG	ARG	GLY	THR	ILE	THR	P897	A835					K389	K389
						S898	R836						
						L899							
						K900							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81192	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	78.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.003	Depositor
Map size (\AA)	324.0, 324.0, 324.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.9, 0.9, 0.9	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/6769	0.49	0/9147
1	B	0.27	0/6878	0.49	0/9300
All	All	0.27	0/13647	0.49	0/18447

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	A	6663	0	6706	329	0
1	B	6770	0	6807	337	0
All	All	13433	0	13513	663	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 25.

All (663) 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:288:PHE:CE1	1:A:409:LYS:HD2	1.37	1.58
1:A:288:PHE:CE1	1:A:409:LYS:CD	2.25	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PHE:CD1	1:A:409:LYS:HD2	1.89	1.07
1:A:407:TYR:CE2	1:A:409:LYS:HE3	1.91	1.04
1:A:130:ALA:HB3	1:A:409:LYS:HZ1	1.27	0.98
1:A:130:ALA:HB3	1:A:409:LYS:NZ	1.86	0.91
1:A:640:THR:HG21	1:A:664:LEU:HB3	1.57	0.86
1:B:452:ALA:HA	1:B:467:ARG:HD2	1.56	0.85
1:A:430:ARG:HD3	1:A:458:SER:HB2	1.58	0.85
1:A:288:PHE:HE1	1:A:409:LYS:HD2	1.36	0.83
1:A:400:GLN:HG2	1:A:409:LYS:HA	1.62	0.82
1:A:407:TYR:HE2	1:A:409:LYS:HE3	1.41	0.82
1:A:444:PHE:H	1:A:448:LYS:HG3	1.46	0.80
1:B:94:ILE:HG12	1:B:783:MET:HE3	1.64	0.79
1:A:549:GLN:HB3	1:A:552:PHE:HD2	1.46	0.79
1:A:80:PRO:HA	1:A:83:ILE:HG12	1.64	0.79
1:A:372:GLN:HB2	1:B:512:ARG:HA	1.65	0.79
1:B:245:ASN:HB3	1:B:248:PHE:HB2	1.63	0.78
1:A:255:PHE:HB2	1:A:338:TYR:HE1	1.50	0.77
1:A:288:PHE:CD1	1:A:409:LYS:CD	2.62	0.76
1:A:748:ALA:HB1	1:A:757:ILE:HG12	1.67	0.76
1:B:587:VAL:HG11	1:B:619:VAL:HG23	1.66	0.76
1:B:441:PHE:HA	1:B:452:ALA:HB3	1.67	0.76
1:A:860:LEU:HA	1:A:864:ALA:HA	1.67	0.76
1:A:226:LEU:HD13	1:A:254:LEU:HD22	1.68	0.76
1:A:820:LYS:HD2	1:A:854:LYS:HB3	1.68	0.76
1:A:130:ALA:CB	1:A:409:LYS:HZ1	2.00	0.75
1:A:288:PHE:CZ	1:A:409:LYS:CE	2.70	0.75
1:B:474:LEU:HA	1:B:512:ARG:HG3	1.67	0.75
1:A:164:GLU:H	1:A:169:LYS:HD2	1.51	0.74
1:A:467:ARG:HA	1:A:470:TYR:CE1	2.21	0.74
1:A:715:ILE:HG21	1:A:747:LEU:HB3	1.70	0.74
1:B:511:TYR:O	1:B:549:GLN:NE2	2.20	0.74
1:B:741:ASN:HB3	1:B:772:GLY:H	1.54	0.72
1:A:891:LEU:HA	1:A:895:LYS:HB3	1.72	0.72
1:B:634:GLN:HG3	1:B:638:GLY:HA2	1.70	0.72
1:A:321:LEU:HD22	1:A:342:VAL:HG11	1.72	0.71
1:B:462:PHE:O	1:B:466:HIS:ND1	2.21	0.71
1:A:521:PHE:O	1:A:524:LYS:NZ	2.23	0.71
1:B:401:TYR:HB3	1:B:408:SER:HB3	1.72	0.70
1:A:640:THR:HG22	1:A:642:PHE:H	1.54	0.70
1:A:711:LEU:HD13	1:A:726:LEU:HD11	1.73	0.70
1:A:381:GLN:O	1:A:491:LYS:NZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ASP:OD1	1:A:503:ARG:N	2.25	0.70
1:A:920:LEU:HB3	1:A:923:TYR:HB2	1.75	0.69
1:B:812:HIS:HB3	1:B:846:LEU:HD12	1.74	0.69
1:B:900:LYS:HD2	1:B:928:ASN:HB2	1.74	0.69
1:A:375:PHE:HB2	1:A:424:CYS:HB3	1.76	0.68
1:B:279:TYR:HA	1:B:283:GLY:HA3	1.74	0.68
1:B:598:VAL:HG11	1:B:629:ILE:HA	1.75	0.68
1:A:667:GLN:HE22	1:A:703:THR:HA	1.58	0.68
1:A:469:LEU:HD13	1:A:488:LEU:HD11	1.73	0.68
1:A:121:ASP:O	1:A:194:LYS:NZ	2.24	0.68
1:A:556:LEU:O	1:A:559:HIS:ND1	2.27	0.68
1:A:185:GLU:OE1	1:A:188:ARG:NH2	2.27	0.68
1:A:188:ARG:O	1:A:200:LYS:NZ	2.27	0.67
1:B:679:ALA:HB1	1:B:714:ALA:HB2	1.75	0.67
1:B:365:ASP:HA	1:B:438:ARG:HH12	1.59	0.67
1:A:638:GLY:HA3	1:A:668:ASP:HB2	1.77	0.66
1:A:693:ILE:HG22	1:A:695:ASP:H	1.59	0.66
1:A:803:ARG:NH1	1:A:804:SER:O	2.28	0.66
1:B:448:LYS:HG3	1:B:450:GLN:H	1.61	0.66
1:A:542:HIS:NE2	1:A:565:ALA:O	2.27	0.66
1:B:322:ASN:OD1	1:B:325:LYS:NZ	2.28	0.66
1:A:695:ASP:OD1	1:A:696:LYS:NZ	2.28	0.66
1:B:910:SER:O	1:B:914:ILE:HD12	1.96	0.65
1:A:83:ILE:HG21	1:A:677:PHE:HE1	1.62	0.65
1:B:726:LEU:HA	1:B:729:GLN:HG2	1.78	0.65
1:B:601:LYS:NZ	1:B:634:GLN:O	2.30	0.65
1:B:370:LEU:HD22	1:B:442:ARG:HH12	1.61	0.65
1:A:849:SER:O	1:A:851:ARG:NH2	2.29	0.65
1:B:156:PHE:HA	1:B:159:VAL:HB	1.77	0.65
1:B:784:ARG:HG3	1:B:786:GLU:H	1.61	0.65
1:A:430:ARG:HE	1:B:583:PHE:HE1	1.45	0.65
1:A:159:VAL:HG13	1:A:249:GLN:HB3	1.78	0.64
1:A:482:VAL:HA	1:A:517:ILE:HD11	1.79	0.64
1:A:803:ARG:NH1	1:A:807:ASN:OD1	2.29	0.64
1:B:787:PRO:HB2	1:B:825:TYR:HE2	1.63	0.64
1:A:640:THR:HG23	1:A:641:PRO:HD2	1.80	0.64
1:B:725:GLU:O	1:B:729:GLN:NE2	2.20	0.64
1:B:908:ARG:O	1:B:912:MET:N	2.27	0.64
1:B:503:ARG:NE	1:B:533:LYS:O	2.31	0.64
1:B:702:VAL:HB	1:B:707:ASN:HA	1.79	0.64
1:B:289:ASN:OD1	1:B:411:SER:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PHE:HA	1:B:269:LEU:HD12	1.79	0.63
1:B:551:GLY:HA2	1:B:554:LYS:HE2	1.79	0.63
1:A:122:ARG:HA	1:A:194:LYS:HG2	1.80	0.63
1:A:396:ARG:HB3	1:A:413:TRP:CD1	2.34	0.63
1:B:776:THR:OG1	1:B:779:HIS:ND1	2.29	0.63
1:B:916:GLN:HE21	1:B:919:LEU:HD21	1.62	0.63
1:B:402:GLU:HB2	1:B:407:TYR:HD1	1.63	0.63
1:A:130:ALA:CB	1:A:409:LYS:NZ	2.61	0.63
1:A:107:ASP:OD1	1:A:110:LYS:NZ	2.31	0.62
1:B:163:ILE:HD12	1:B:169:LYS:HG2	1.81	0.62
1:B:478:LYS:HA	1:B:514:ASN:HD21	1.64	0.62
1:A:727:LEU:O	1:A:763:ARG:NH2	2.31	0.62
1:B:779:HIS:NE2	1:B:808:LEU:O	2.22	0.62
1:A:205:LYS:NZ	1:A:291:GLU:OE2	2.32	0.62
1:B:622:ALA:O	1:B:626:HIS:ND1	2.32	0.62
1:A:908:ARG:O	1:A:912:MET:N	2.30	0.62
1:B:576:HIS:O	1:B:580:ARG:NH1	2.32	0.62
1:A:902:ASP:HA	1:A:907:GLY:HA3	1.80	0.62
1:A:910:SER:O	1:A:914:ILE:HG12	2.00	0.62
1:A:920:LEU:HG	1:A:922:LEU:H	1.63	0.62
1:A:729:GLN:O	1:A:763:ARG:NH2	2.32	0.61
1:A:265:MET:SD	1:A:302:PHE:HB2	2.40	0.61
1:A:869:TYR:HB2	1:A:873:LYS:HA	1.82	0.61
1:B:737:VAL:HG13	1:B:741:ASN:HA	1.82	0.61
1:B:779:HIS:HE1	1:B:803:ARG:HA	1.65	0.61
1:B:887:ASP:OD1	1:B:888:MET:N	2.33	0.61
1:B:910:SER:HA	1:B:913:LEU:HD12	1.83	0.61
1:A:640:THR:CG2	1:A:641:PRO:HD2	2.30	0.61
1:B:143:VAL:O	1:B:146:GLU:HG2	1.99	0.61
1:A:396:ARG:HD3	1:A:416:PRO:HB2	1.82	0.60
1:A:155:ASN:HB2	1:A:252:TYR:OH	2.00	0.60
1:A:427:ILE:HD11	1:A:459:GLN:HB3	1.83	0.60
1:A:138:VAL:HG13	1:A:266:PHE:HD1	1.66	0.60
1:A:288:PHE:CE1	1:A:409:LYS:CE	2.82	0.60
1:A:288:PHE:CZ	1:A:409:LYS:HE2	2.36	0.60
1:B:186:ARG:HA	1:B:189:ILE:HD12	1.83	0.60
1:A:372:GLN:OE1	1:A:372:GLN:N	2.34	0.60
1:A:785:LYS:HG2	1:A:819:ARG:HH21	1.66	0.60
1:B:178:PHE:HE1	1:B:211:LEU:HD22	1.66	0.60
1:A:852:LYS:HE3	1:A:854:LYS:HG3	1.82	0.60
1:A:381:GLN:O	1:A:422:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:THR:HG23	1:A:664:LEU:HD23	1.84	0.60
1:B:685:LYS:HG3	1:B:686:MET:SD	2.42	0.60
1:A:255:PHE:CZ	1:A:341:LEU:HB3	2.37	0.60
1:A:924:ASN:OD1	1:A:925:TYR:N	2.34	0.60
1:A:601:LYS:NZ	1:A:605:GLY:O	2.29	0.60
1:B:874:TYR:O	1:B:879:LYS:NZ	2.35	0.60
1:A:50:SER:OG	1:A:51:ASN:N	2.32	0.59
1:A:806:ASP:HB3	1:A:808:LEU:HG	1.84	0.59
1:B:285:ASP:O	1:B:409:LYS:NZ	2.35	0.59
1:B:364:ASP:O	1:B:438:ARG:NH1	2.35	0.59
1:A:519:LEU:HD11	1:A:555:LEU:HB3	1.83	0.59
1:A:455:MET:SD	1:A:457:HIS:N	2.70	0.59
1:A:721:ASP:HA	1:A:724:LYS:HE3	1.85	0.59
1:B:267:PHE:HA	1:B:270:GLU:OE2	2.03	0.59
1:B:501:ASN:HB3	1:B:535:LYS:HD3	1.84	0.59
1:A:837:THR:HG22	1:A:841:SER:H	1.68	0.59
1:B:185:GLU:OE1	1:B:188:ARG:NH2	2.36	0.59
1:B:528:ILE:HG23	1:B:532:LEU:HD22	1.83	0.59
1:B:784:ARG:NE	1:B:786:GLU:OE1	2.35	0.59
1:A:440:ILE:HG23	1:A:452:ALA:HB3	1.85	0.58
1:B:571:ASN:N	1:B:603:ASP:OD2	2.36	0.58
1:A:302:PHE:HZ	1:A:352:LYS:HB2	1.67	0.58
1:A:375:PHE:N	1:A:424:CYS:O	2.28	0.58
1:A:778:LEU:HD13	1:A:793:LEU:HD22	1.86	0.58
1:B:533:LYS:HB3	1:B:537:GLY:HA2	1.85	0.58
1:B:684:ILE:HG22	1:B:688:ARG:HH21	1.67	0.58
1:B:228:GLU:HB3	1:B:232:LYS:HE3	1.85	0.58
1:A:341:LEU:HA	1:A:344:ARG:HE	1.68	0.58
1:A:906:GLU:HG3	1:A:908:ARG:HG2	1.86	0.58
1:A:64:ILE:HG22	1:A:66:SER:H	1.68	0.58
1:A:877:ILE:HD12	1:A:880:ALA:HB3	1.85	0.58
1:A:396:ARG:HA	1:A:416:PRO:HB3	1.86	0.58
1:A:617:TYR:HB3	1:A:619:VAL:HG12	1.86	0.58
1:B:407:TYR:CZ	1:B:409:LYS:HB2	2.39	0.57
1:A:288:PHE:CZ	1:A:409:LYS:NZ	2.71	0.57
1:A:501:ASN:HB3	1:A:535:LYS:HD3	1.86	0.57
1:A:130:ALA:HB2	1:A:407:TYR:HD2	1.70	0.57
1:A:741:ASN:ND2	1:A:770:LYS:O	2.38	0.57
1:B:477:ASN:HB3	1:B:480:LYS:HB2	1.85	0.57
1:A:388:ASN:ND2	1:A:471:ASP:OD2	2.37	0.57
1:B:849:SER:O	1:B:851:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ASN:HB2	1:B:708:TRP:NE1	2.20	0.57
1:A:254:LEU:HD21	1:A:317:VAL:HG12	1.86	0.57
1:A:462:PHE:HB3	1:A:466:HIS:CE1	2.40	0.57
1:A:422:ASN:OD1	1:A:423:ALA:N	2.37	0.57
1:A:725:GLU:HA	1:A:728:LYS:HD2	1.86	0.57
1:B:904:THR:H	1:B:907:GLY:HA2	1.69	0.57
1:A:451:PHE:HB3	1:A:499:PHE:CE1	2.39	0.56
1:B:539:THR:OG1	1:B:542:HIS:ND1	2.27	0.56
1:A:836:LYS:HD3	1:A:840:GLY:HA2	1.88	0.56
1:B:114:GLU:O	1:B:118:ASN:ND2	2.38	0.56
1:B:469:LEU:HG	1:B:488:LEU:HD22	1.87	0.56
1:B:233:ASN:HD22	1:B:323:THR:HG21	1.70	0.56
1:A:923:TYR:HA	1:A:926:PHE:HD2	1.70	0.56
1:B:750:SER:O	1:B:784:ARG:NH1	2.37	0.56
1:A:138:VAL:HG21	1:A:269:LEU:HD22	1.88	0.56
1:A:594:PRO:HB2	1:A:596:ILE:HG22	1.87	0.56
1:A:316:ASN:O	1:A:319:GLU:HG3	2.05	0.56
1:B:839:ASP:O	1:B:871:ASN:ND2	2.38	0.56
1:B:875:LEU:HD12	1:B:877:ILE:HD11	1.88	0.56
1:A:255:PHE:HB2	1:A:338:TYR:CE1	2.36	0.55
1:A:754:ILE:HA	1:A:757:ILE:HD12	1.89	0.55
1:A:827:LEU:HD23	1:A:831:ALA:HB3	1.87	0.55
1:B:427:ILE:HD11	1:B:442:ARG:HH21	1.70	0.55
1:B:533:LYS:NZ	1:B:566:LYS:O	2.31	0.55
1:A:144:THR:HA	1:A:147:LYS:HD3	1.89	0.55
1:A:554:LYS:HA	1:A:557:ILE:HG22	1.88	0.55
1:B:114:GLU:HA	1:B:117:PHE:CD2	2.42	0.55
1:B:338:TYR:O	1:B:342:VAL:HG23	2.07	0.55
1:B:156:PHE:CZ	1:B:256:TYR:HB2	2.42	0.55
1:A:444:PHE:N	1:A:448:LYS:HG3	2.21	0.54
1:B:107:ASP:OD1	1:B:108:GLU:N	2.40	0.54
1:A:424:CYS:N	1:A:425:PRO:HD3	2.22	0.54
1:A:700:ASN:ND2	1:A:731:ASP:O	2.31	0.54
1:B:149:ARG:HH22	1:B:179:LYS:HD3	1.72	0.54
1:A:668:ASP:OD1	1:A:671:HIS:N	2.40	0.54
1:A:759:GLU:HA	1:A:762:LYS:HE3	1.89	0.54
1:A:401:TYR:OH	1:A:404:LYS:HB2	2.07	0.54
1:A:484:GLU:HG2	1:A:488:LEU:HD23	1.90	0.54
1:B:502:ASP:HB2	1:B:535:LYS:HZ3	1.73	0.54
1:B:859:LEU:O	1:B:863:GLY:N	2.40	0.54
1:B:255:PHE:O	1:B:258:THR:OG1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:GLU:OE1	1:B:786:GLU:N	2.41	0.54
1:A:349:GLU:OE2	1:A:353:ASN:ND2	2.41	0.54
1:B:668:ASP:OD1	1:B:672:MET:N	2.29	0.53
1:B:547:ALA:HB1	1:B:549:GLN:HE22	1.74	0.53
1:B:577:LEU:HD12	1:B:580:ARG:HH22	1.73	0.53
1:A:162:THR:O	1:A:169:LYS:NZ	2.27	0.53
1:A:407:TYR:CD2	1:A:409:LYS:NZ	2.77	0.53
1:B:552:PHE:HA	1:B:555:LEU:HB2	1.89	0.53
1:B:875:LEU:HG	1:B:878:HIS:CE1	2.43	0.53
1:B:482:VAL:HG22	1:B:517:ILE:HG21	1.89	0.53
1:A:640:THR:CG2	1:A:664:LEU:HB3	2.32	0.53
1:A:886:LEU:HD12	1:A:890:ARG:HH11	1.74	0.53
1:B:670:ASN:HB2	1:B:672:MET:HE2	1.91	0.53
1:B:397:TYR:OH	1:B:414:SER:OG	2.26	0.53
1:B:721:ASP:OD1	1:B:722:ALA:N	2.40	0.53
1:B:226:LEU:O	1:B:230:LEU:HG	2.09	0.53
1:B:517:ILE:HA	1:B:520:ARG:HG2	1.90	0.53
1:B:806:ASP:O	1:B:837:THR:OG1	2.24	0.53
1:B:401:TYR:CE1	1:B:403:SER:HB3	2.44	0.52
1:B:549:GLN:HB3	1:B:552:PHE:HD2	1.74	0.52
1:B:233:ASN:OD1	1:B:245:ASN:ND2	2.43	0.52
1:A:441:PHE:HB2	1:A:450:GLN:C	2.29	0.52
1:B:787:PRO:HB2	1:B:825:TYR:CE2	2.45	0.52
1:B:879:LYS:O	1:B:883:ASN:ND2	2.36	0.52
1:A:396:ARG:HB3	1:A:413:TRP:HD1	1.74	0.52
1:B:399:VAL:HA	1:B:440:ILE:HA	1.92	0.52
1:A:444:PHE:H	1:A:448:LYS:CG	2.19	0.52
1:B:847:ALA:O	1:B:851:ARG:N	2.35	0.52
1:A:576:HIS:HE2	1:A:608:PRO:HG3	1.74	0.52
1:B:578:ALA:O	1:B:581:SER:OG	2.24	0.52
1:B:706:ASN:HB2	1:B:708:TRP:HE1	1.75	0.52
1:A:218:SER:O	1:A:222:LEU:HB2	2.10	0.52
1:A:401:TYR:O	1:A:407:TYR:HD1	1.93	0.51
1:A:402:GLU:HG3	1:A:407:TYR:HB2	1.92	0.51
1:B:80:PRO:HA	1:B:83:ILE:HG12	1.92	0.51
1:B:309:GLY:O	1:B:313:LEU:HG	2.10	0.51
1:A:746:HIS:NE2	1:A:769:GLU:O	2.42	0.51
1:A:911:ILE:HA	1:A:914:ILE:HG12	1.92	0.51
1:B:159:VAL:HG13	1:B:249:GLN:HE21	1.74	0.51
1:B:448:LYS:O	1:B:450:GLN:HG3	2.10	0.51
1:B:903:GLU:HG2	1:B:904:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:HE2	1:A:256:TYR:HE2	1.76	0.51
1:A:413:TRP:NE1	1:A:443:LYS:HE3	2.25	0.51
1:B:366:ILE:N	1:B:367:PRO:HD3	2.26	0.51
1:B:600:GLU:O	1:B:608:PRO:HD3	2.10	0.51
1:B:701:SER:OG	1:B:702:VAL:N	2.40	0.51
1:A:556:LEU:HD12	1:A:557:ILE:N	2.25	0.51
1:A:702:VAL:HG12	1:A:709:THR:HG22	1.92	0.51
1:A:860:LEU:HD21	1:A:892:PHE:HE1	1.76	0.51
1:A:225:ALA:O	1:A:229:LEU:HD13	2.10	0.51
1:A:321:LEU:HD11	1:A:339:ARG:HD2	1.93	0.51
1:A:566:LYS:HD3	1:A:571:ASN:HB3	1.92	0.51
1:A:708:TRP:HE3	1:A:712:HIS:HB3	1.76	0.51
1:A:854:LYS:O	1:A:857:GLU:HG3	2.10	0.51
1:B:149:ARG:HA	1:B:152:MET:HE2	1.93	0.51
1:A:466:HIS:CD2	1:A:497:ALA:HB3	2.46	0.51
1:B:375:PHE:H	1:B:425:PRO:HG3	1.76	0.51
1:B:819:ARG:HH21	1:B:821:SER:H	1.58	0.50
1:A:786:GLU:HG2	1:A:789:ILE:HG12	1.94	0.50
1:A:588:ARG:O	1:A:592:GLU:HG3	2.11	0.50
1:B:207:ILE:O	1:B:211:LEU:HG	2.11	0.50
1:B:291:GLU:O	1:B:295:VAL:HG13	2.11	0.50
1:B:819:ARG:HE	1:B:821:SER:H	1.58	0.50
1:A:69:VAL:HG12	1:A:71:GLY:H	1.76	0.50
1:A:302:PHE:CZ	1:A:352:LYS:HB2	2.46	0.50
1:A:366:ILE:HG12	1:A:438:ARG:HH21	1.77	0.50
1:B:424:CYS:HA	1:B:461:ASN:HB2	1.93	0.50
1:B:534:ASP:H	1:B:538:PHE:H	1.56	0.50
1:A:554:LYS:NZ	1:A:589:ASN:OD1	2.27	0.50
1:A:370:LEU:HG	1:A:373:VAL:HG23	1.93	0.50
1:A:467:ARG:HA	1:A:470:TYR:HE1	1.71	0.50
1:B:365:ASP:HB3	1:B:400:GLN:HA	1.93	0.50
1:A:81:ILE:HG13	1:A:113:LEU:HG	1.93	0.50
1:B:818:GLY:HA2	1:B:855:THR:HG21	1.92	0.50
1:B:576:HIS:CE1	1:B:608:PRO:HG3	2.47	0.50
1:B:609:LEU:HD23	1:B:641:PRO:HG2	1.94	0.50
1:A:197:TYR:OH	1:A:271:GLN:NE2	2.35	0.49
1:A:251:LEU:O	1:A:254:LEU:HB3	2.12	0.49
1:A:179:LYS:HE2	1:A:256:TYR:CE2	2.47	0.49
1:A:552:PHE:HA	1:A:555:LEU:HB2	1.94	0.49
1:A:386:ILE:HG22	1:A:389:TRP:H	1.78	0.49
1:A:604:ASP:HB2	1:A:606:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:PHE:O	1:A:898:SER:N	2.45	0.49
1:B:201:LEU:HD21	1:B:275:LEU:HD22	1.94	0.49
1:B:370:LEU:HB2	1:B:442:ARG:HH22	1.78	0.49
1:A:754:ILE:HG22	1:A:758:LYS:HZ3	1.77	0.49
1:B:426:THR:HG21	1:B:430:ARG:NH2	2.27	0.49
1:B:866:LEU:HB2	1:B:868:GLU:HG2	1.93	0.49
1:A:407:TYR:CD2	1:A:409:LYS:HE3	2.44	0.49
1:B:502:ASP:OD1	1:B:503:ARG:N	2.45	0.49
1:B:913:LEU:HB2	1:B:923:TYR:OH	2.13	0.49
1:B:109:ILE:O	1:B:113:LEU:HG	2.13	0.49
1:B:261:TYR:O	1:B:265:MET:HG3	2.13	0.49
1:A:424:CYS:HA	1:A:461:ASN:ND2	2.27	0.49
1:B:588:ARG:HA	1:B:591:LEU:HD12	1.95	0.49
1:B:486:THR:O	1:B:490:GLU:HG3	2.13	0.49
1:B:779:HIS:CE1	1:B:803:ARG:HA	2.45	0.49
1:B:507:HIS:HB3	1:B:543:ILE:HG13	1.94	0.49
1:A:178:PHE:HE1	1:A:211:LEU:HD11	1.78	0.48
1:A:379:GLU:OE2	1:A:380:ASN:ND2	2.46	0.48
1:A:606:PHE:CD1	1:A:635:SER:OG	2.53	0.48
1:A:166:LYS:HE3	1:A:168:ILE:H	1.77	0.48
1:A:462:PHE:HB3	1:A:466:HIS:HE1	1.76	0.48
1:A:850:GLY:O	1:A:851:ARG:HG2	2.13	0.48
1:B:370:LEU:HD23	1:B:397:TYR:HB3	1.95	0.48
1:B:794:ILE:HG13	1:B:829:LYS:HE2	1.94	0.48
1:A:430:ARG:HH11	1:A:458:SER:HA	1.77	0.48
1:A:637:SER:HB2	1:A:639:LEU:HD13	1.94	0.48
1:B:365:ASP:HA	1:B:438:ARG:HH22	1.79	0.48
1:B:154:GLU:O	1:B:158:LEU:HG	2.14	0.48
1:B:229:LEU:HA	1:B:232:LYS:HB2	1.95	0.48
1:B:676:HIS:HA	1:B:710:PRO:HB3	1.95	0.48
1:B:218:SER:O	1:B:222:LEU:HG	2.13	0.48
1:B:609:LEU:O	1:B:613:VAL:HG23	2.12	0.48
1:A:430:ARG:O	1:A:433:PRO:HD3	2.13	0.48
1:A:503:ARG:HB3	1:A:506:MET:HE2	1.95	0.48
1:A:890:ARG:O	1:A:895:LYS:N	2.40	0.48
1:B:885:ASP:HB3	1:B:888:MET:HB2	1.95	0.48
1:A:428:LYS:HA	1:A:430:ARG:NH2	2.28	0.48
1:B:490:GLU:OE1	1:B:491:LYS:NZ	2.46	0.48
1:B:503:ARG:HB2	1:B:507:HIS:CE1	2.48	0.48
1:B:620:VAL:O	1:B:624:LEU:HG	2.13	0.48
1:B:869:TYR:HB2	1:B:873:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:878:HIS:HA	1:B:881:ILE:HD12	1.95	0.48
1:A:517:ILE:HA	1:A:520:ARG:HB3	1.95	0.48
1:A:819:ARG:O	1:A:822:THR:OG1	2.31	0.48
1:B:667:GLN:HB3	1:B:671:HIS:HA	1.96	0.48
1:A:374:ASN:HB2	1:B:476:ILE:HD12	1.96	0.48
1:A:519:LEU:O	1:A:523:LEU:HB2	2.13	0.48
1:B:177:ASP:O	1:B:180:LYS:HG2	2.13	0.48
1:A:877:ILE:HA	1:A:880:ALA:HB3	1.96	0.47
1:A:443:LYS:HG2	1:A:448:LYS:HG2	1.97	0.47
1:A:548:GLY:HA3	1:A:583:PHE:CG	2.49	0.47
1:A:920:LEU:HG	1:A:922:LEU:N	2.29	0.47
1:B:443:LYS:HA	1:B:448:LYS:HD3	1.95	0.47
1:A:142:PHE:HE1	1:A:267:PHE:HB2	1.78	0.47
1:B:791:VAL:O	1:B:794:ILE:HB	2.15	0.47
1:A:97:THR:O	1:A:784:ARG:NH1	2.46	0.47
1:A:640:THR:HG22	1:A:641:PRO:N	2.30	0.47
1:A:689:TYR:CZ	1:A:693:ILE:HD11	2.50	0.47
1:A:698:SER:HB2	1:A:701:SER:HB2	1.96	0.47
1:B:376:PRO:O	1:B:422:ASN:ND2	2.45	0.47
1:B:397:TYR:OH	1:B:412:GLU:OE2	2.26	0.47
1:B:136:LYS:O	1:B:140:LYS:HG2	2.15	0.47
1:B:198:VAL:O	1:B:202:LEU:HG	2.15	0.47
1:B:706:ASN:HB2	1:B:708:TRP:CD1	2.50	0.47
1:A:550:ALA:HB1	1:A:589:ASN:OD1	2.14	0.47
1:A:684:ILE:HA	1:A:687:LEU:HB3	1.97	0.47
1:B:362:LEU:N	1:B:408:SER:HG	2.12	0.47
1:B:397:TYR:HA	1:B:442:ARG:HG2	1.96	0.47
1:B:519:LEU:HD22	1:B:523:LEU:HD13	1.96	0.47
1:B:588:ARG:HA	1:B:591:LEU:HB2	1.97	0.47
1:B:912:MET:HA	1:B:915:VAL:HG12	1.96	0.47
1:B:362:LEU:HD22	1:B:410:PHE:HD1	1.78	0.47
1:B:383:PRO:HG3	1:B:421:GLY:HA2	1.97	0.47
1:A:338:TYR:HA	1:A:341:LEU:HD12	1.97	0.47
1:A:453:GLY:HA3	1:A:463:LYS:NZ	2.29	0.47
1:B:251:LEU:O	1:B:254:LEU:HG	2.15	0.47
1:A:77:VAL:O	1:A:81:ILE:HG12	2.14	0.47
1:A:211:LEU:HA	1:A:214:VAL:HB	1.97	0.47
1:A:307:THR:HG22	1:A:352:LYS:HE3	1.97	0.47
1:A:632:ASN:HB3	1:A:664:LEU:HD13	1.97	0.47
1:B:370:LEU:HD21	1:B:415:GLU:O	2.15	0.47
1:B:426:THR:HG22	1:B:428:LYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:GLN:HB3	1:B:552:PHE:HB2	1.96	0.47
1:B:602:GLU:HG2	1:B:604:ASP:H	1.80	0.47
1:B:853:MET:SD	1:B:853:MET:N	2.88	0.47
1:A:640:THR:CG2	1:A:641:PRO:CD	2.93	0.46
1:B:186:ARG:HG3	1:B:267:PHE:CZ	2.49	0.46
1:B:475:ASN:OD1	1:B:476:ILE:N	2.48	0.46
1:B:502:ASP:HA	1:B:534:ASP:HB2	1.97	0.46
1:A:914:ILE:HD12	1:A:927:ILE:HG12	1.97	0.46
1:A:182:PHE:CE1	1:A:264:VAL:HG22	2.50	0.46
1:B:504:SER:O	1:B:508:ALA:HB3	2.15	0.46
1:B:824:LEU:O	1:B:828:GLU:OE1	2.34	0.46
1:A:369:THR:HG23	1:A:397:TYR:CE1	2.50	0.46
1:A:917:LYS:HG3	1:A:918:LEU:H	1.80	0.46
1:B:104:ILE:HB	1:B:105:PRO:HD3	1.96	0.46
1:B:482:VAL:HG22	1:B:517:ILE:HD13	1.96	0.46
1:A:430:ARG:HD3	1:A:458:SER:CB	2.37	0.46
1:B:258:THR:OG1	1:B:259:GLN:NE2	2.48	0.46
1:B:284:ASP:HB3	1:B:287:ASN:HB2	1.98	0.46
1:A:720:GLU:HA	1:A:756:ILE:HD11	1.97	0.46
1:B:65:GLY:O	1:B:68:PRO:HD2	2.16	0.46
1:B:519:LEU:HD12	1:B:555:LEU:HD12	1.97	0.46
1:B:691:ILE:HG21	1:B:729:GLN:OE1	2.15	0.46
1:B:790:ALA:O	1:B:794:ILE:HG12	2.15	0.46
1:B:905:GLU:O	1:B:906:GLU:HG2	2.15	0.46
1:A:448:LYS:HB3	1:A:449:PRO:HD2	1.97	0.46
1:A:503:ARG:HG2	1:A:532:LEU:HD11	1.97	0.46
1:B:107:ASP:HB2	1:B:110:LYS:NZ	2.31	0.46
1:B:506:MET:HA	1:B:509:VAL:HG12	1.98	0.46
1:A:342:VAL:O	1:A:346:LYS:HG2	2.16	0.46
1:B:504:SER:O	1:B:508:ALA:CB	2.64	0.46
1:B:280:TYR:HE1	1:B:407:TYR:HH	1.63	0.46
1:B:289:ASN:ND2	1:B:409:LYS:O	2.49	0.46
1:B:534:ASP:OD1	1:B:537:GLY:N	2.49	0.46
1:B:825:TYR:O	1:B:829:LYS:HD2	2.16	0.46
1:A:461:ASN:ND2	1:A:464:ASP:OD2	2.43	0.45
1:B:304:SER:O	1:B:307:THR:OG1	2.25	0.45
1:B:874:TYR:HB3	1:B:878:HIS:HB2	1.98	0.45
1:A:743:THR:HG21	1:A:769:GLU:HG2	1.97	0.45
1:B:201:LEU:HD11	1:B:275:LEU:HB2	1.97	0.45
1:A:708:TRP:CE3	1:A:712:HIS:HB3	2.52	0.45
1:B:374:ASN:HA	1:B:425:PRO:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:ARG:HB2	1:A:911:ILE:HB	1.99	0.45
1:B:288:PHE:CE1	1:B:409:LYS:HB3	2.51	0.45
1:B:391:ASP:HB3	1:B:420:GLN:HG3	1.97	0.45
1:B:636:THR:HG23	1:B:637:SER:N	2.32	0.45
1:A:249:GLN:OE1	1:A:249:GLN:N	2.37	0.45
1:A:879:LYS:HE2	1:A:882:ILE:HD12	1.97	0.45
1:B:115:GLU:HA	1:B:118:ASN:HD21	1.81	0.45
1:B:395:VAL:O	1:B:395:VAL:HG13	2.16	0.45
1:B:635:SER:H	1:B:639:LEU:H	1.64	0.45
1:B:451:PHE:CE2	1:B:499:PHE:HA	2.52	0.45
1:A:520:ARG:O	1:A:520:ARG:NH1	2.37	0.45
1:A:923:TYR:O	1:A:927:ILE:HG13	2.16	0.45
1:B:617:TYR:O	1:B:620:VAL:HG22	2.16	0.45
1:B:673:ALA:H	1:B:676:HIS:CE1	2.34	0.45
1:B:687:LEU:HD21	1:B:726:LEU:HG	1.98	0.45
1:A:313:LEU:O	1:A:317:VAL:HG13	2.16	0.45
1:A:709:THR:HG23	1:A:712:HIS:CE1	2.52	0.45
1:A:721:ASP:OD1	1:A:721:ASP:N	2.50	0.45
1:A:749:VAL:HG21	1:A:777:SER:HB3	1.99	0.45
1:B:643:HIS:CD2	1:B:674:PRO:HG3	2.51	0.45
1:B:780:ILE:O	1:B:784:ARG:N	2.48	0.45
1:A:668:ASP:OD1	1:A:672:MET:HG3	2.17	0.45
1:A:869:TYR:CD2	1:A:873:LYS:HD2	2.52	0.45
1:B:443:LYS:HD2	1:B:447:GLY:HA2	1.99	0.45
1:B:535:LYS:O	1:B:569:LYS:NZ	2.40	0.45
1:B:602:GLU:HG2	1:B:603:ASP:N	2.31	0.45
1:A:503:ARG:N	1:A:503:ARG:HD2	2.32	0.45
1:A:591:LEU:O	1:A:594:PRO:HD3	2.17	0.45
1:B:549:GLN:O	1:B:553:VAL:N	2.47	0.45
1:B:856:VAL:HA	1:B:859:LEU:HB2	1.99	0.45
1:A:226:LEU:HD11	1:A:320:VAL:HG21	1.99	0.44
1:A:343:THR:HA	1:A:346:LYS:HE2	1.99	0.44
1:A:837:THR:HG23	1:A:839:ASP:H	1.81	0.44
1:B:448:LYS:HZ1	1:B:452:ALA:N	2.15	0.44
1:B:823:VAL:O	1:B:827:LEU:HD23	2.17	0.44
1:A:407:TYR:CE2	1:A:409:LYS:CE	2.81	0.44
1:A:724:LYS:HG3	1:A:728:LYS:HZ2	1.82	0.44
1:B:424:CYS:N	1:B:425:PRO:HD2	2.31	0.44
1:B:549:GLN:O	1:B:553:VAL:HG23	2.17	0.44
1:A:222:LEU:HD11	1:A:254:LEU:HA	1.99	0.44
1:A:366:ILE:HD13	1:A:438:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:VAL:HG13	1:A:517:ILE:HD13	1.97	0.44
1:A:859:LEU:O	1:A:863:GLY:N	2.49	0.44
1:A:868:GLU:O	1:A:876:PRO:HD3	2.17	0.44
1:B:69:VAL:HG13	1:B:69:VAL:O	2.18	0.44
1:B:139:SER:O	1:B:143:VAL:HG23	2.17	0.44
1:B:152:MET:HA	1:B:155:ASN:HB3	1.98	0.44
1:B:333:ALA:HA	1:B:336:LYS:HD3	2.00	0.44
1:B:439:LEU:HG	1:B:454:THR:HA	1.99	0.44
1:A:551:GLY:O	1:A:555:LEU:HD23	2.17	0.44
1:A:745:LEU:HD13	1:A:760:LEU:HD22	1.99	0.44
1:B:600:GLU:OE1	1:B:601:LYS:N	2.51	0.44
1:A:166:LYS:HG3	1:A:168:ILE:HG22	1.99	0.44
1:A:446:SER:O	1:A:448:LYS:HG2	2.18	0.44
1:B:159:VAL:HG13	1:B:249:GLN:NE2	2.33	0.44
1:B:177:ASP:HA	1:B:180:LYS:HG2	1.99	0.44
1:B:683:SER:OG	1:B:686:MET:HB2	2.17	0.44
1:A:73:VAL:HG12	1:A:74:VAL:H	1.83	0.44
1:A:255:PHE:CE2	1:A:341:LEU:HB3	2.53	0.44
1:A:396:ARG:HA	1:A:416:PRO:CB	2.48	0.44
1:A:500:ASP:C	1:A:502:ASP:H	2.21	0.44
1:A:608:PRO:O	1:A:611:THR:OG1	2.29	0.44
1:B:222:LEU:O	1:B:226:LEU:HG	2.17	0.44
1:B:514:ASN:HB3	1:B:517:ILE:HG12	2.00	0.44
1:A:204:GLN:HA	1:A:207:ILE:HD13	2.00	0.44
1:A:373:VAL:HG21	1:A:428:LYS:HD3	2.00	0.44
1:B:365:ASP:O	1:B:438:ARG:NH2	2.48	0.44
1:B:461:ASN:O	1:B:465:ILE:HG12	2.17	0.44
1:B:819:ARG:NH2	1:B:821:SER:OG	2.51	0.44
1:A:166:LYS:HG3	1:A:168:ILE:H	1.83	0.44
1:A:389:TRP:CE2	1:A:423:ALA:HB2	2.53	0.44
1:A:820:LYS:HE3	1:A:858:THR:OG1	2.18	0.44
1:B:710:PRO:HA	1:B:713:PHE:HD2	1.82	0.44
1:A:132:GLU:OE2	1:A:133:GLU:HG2	2.18	0.44
1:A:192:LEU:HB3	1:A:196:ARG:HB2	2.00	0.44
1:A:399:VAL:HG23	1:A:439:LEU:C	2.38	0.43
1:B:400:GLN:HB2	1:B:408:SER:O	2.18	0.43
1:B:466:HIS:NE2	1:B:494:ASP:HB3	2.32	0.43
1:B:889:VAL:O	1:B:893:LEU:HG	2.17	0.43
1:A:908:ARG:HA	1:A:911:ILE:HD13	2.00	0.43
1:B:577:LEU:HD12	1:B:580:ARG:NH2	2.33	0.43
1:A:289:ASN:OD1	1:A:411:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LYS:HD3	1:A:448:LYS:HA	1.73	0.43
1:B:400:GLN:HB2	1:B:409:LYS:HA	2.00	0.43
1:B:593:SER:HB3	1:B:594:PRO:HD3	2.00	0.43
1:B:803:ARG:NE	1:B:807:ASN:OD1	2.35	0.43
1:B:892:PHE:O	1:B:896:ASP:HB3	2.18	0.43
1:B:908:ARG:HA	1:B:911:ILE:HD12	2.01	0.43
1:A:597:LYS:HD2	1:A:597:LYS:O	2.19	0.43
1:A:737:VAL:HG13	1:A:741:ASN:HA	1.99	0.43
1:A:812:HIS:HE2	1:A:835:ALA:HB3	1.84	0.43
1:B:327:LEU:HD12	1:B:328:PRO:HD2	2.00	0.43
1:B:396:ARG:HA	1:B:413:TRP:HB3	2.01	0.43
1:A:630:ASP:OD1	1:A:630:ASP:N	2.49	0.43
1:B:110:LYS:O	1:B:114:GLU:OE1	2.36	0.43
1:B:396:ARG:HB3	1:B:413:TRP:CD1	2.54	0.43
1:B:876:PRO:HA	1:B:879:LYS:HD3	2.00	0.43
1:B:894:GLU:HG2	1:B:895:LYS:N	2.33	0.43
1:A:443:LYS:HB2	1:A:450:GLN:HG2	2.01	0.43
1:A:699:ILE:HD11	1:A:731:ASP:HB3	2.01	0.43
1:A:900:LYS:HD2	1:A:900:LYS:HA	1.86	0.43
1:B:348:LEU:O	1:B:351:LEU:HB3	2.18	0.43
1:B:770:LYS:NZ	1:B:774:GLY:HA2	2.34	0.43
1:A:171:ILE:O	1:A:175:ILE:HG23	2.19	0.43
1:A:549:GLN:O	1:A:553:VAL:HG23	2.19	0.43
1:A:686:MET:O	1:A:690:LEU:HG	2.17	0.43
1:A:786:GLU:N	1:A:786:GLU:OE1	2.52	0.43
1:B:61:ALA:O	1:B:64:ILE:HB	2.18	0.43
1:B:903:GLU:HG2	1:B:904:THR:N	2.33	0.43
1:A:288:PHE:CD1	1:A:409:LYS:HD3	2.52	0.43
1:A:642:PHE:CE2	1:A:663:ASP:HA	2.53	0.43
1:A:676:HIS:HD2	1:A:710:PRO:HB3	1.84	0.43
1:B:316:ASN:O	1:B:319:GLU:HG3	2.18	0.43
1:B:427:ILE:HD11	1:B:442:ARG:NH2	2.32	0.43
1:B:534:ASP:OD1	1:B:538:PHE:N	2.52	0.43
1:B:556:LEU:HD12	1:B:557:ILE:N	2.34	0.43
1:B:137:LEU:O	1:B:141:THR:HG23	2.18	0.43
1:B:401:TYR:HE2	1:B:406:MET:HG3	1.83	0.43
1:B:667:GLN:HE22	1:B:703:THR:HA	1.83	0.43
1:A:124:LEU:HG	1:A:274:TYR:HE1	1.84	0.42
1:A:349:GLU:O	1:A:352:LYS:HG2	2.19	0.42
1:A:398:ALA:O	1:A:440:ILE:HG13	2.19	0.42
1:A:584:SER:OG	1:A:619:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:HG12	1:B:225:ALA:HB2	2.01	0.42
1:B:400:GLN:HG3	1:B:409:LYS:HA	2.00	0.42
1:A:891:LEU:HD13	1:A:895:LYS:HD2	2.01	0.42
1:B:118:ASN:HA	1:B:121:ASP:OD2	2.18	0.42
1:B:703:THR:OG1	1:B:708:TRP:N	2.50	0.42
1:B:886:LEU:HD12	1:B:887:ASP:N	2.35	0.42
1:A:441:PHE:HB2	1:A:450:GLN:O	2.19	0.42
1:A:808:LEU:HA	1:A:812:HIS:ND1	2.34	0.42
1:A:837:THR:HG23	1:A:839:ASP:N	2.35	0.42
1:A:341:LEU:N	1:A:344:ARG:HH21	2.17	0.42
1:A:401:TYR:HE1	1:A:437:ASN:H	1.68	0.42
1:B:255:PHE:O	1:B:259:GLN:HG2	2.19	0.42
1:B:669:VAL:HG23	1:B:670:ASN:ND2	2.35	0.42
1:B:727:LEU:HD21	1:B:763:ARG:HG3	2.01	0.42
1:B:783:MET:HA	1:B:817:ILE:HD13	2.01	0.42
1:A:443:LYS:HG2	1:A:448:LYS:CG	2.50	0.42
1:A:504:SER:O	1:A:508:ALA:HB3	2.19	0.42
1:A:890:ARG:O	1:A:894:GLU:N	2.46	0.42
1:B:282:LYS:NZ	1:B:447:GLY:O	2.51	0.42
1:B:478:LYS:O	1:B:482:VAL:HG23	2.20	0.42
1:A:111:GLU:O	1:A:114:GLU:HG3	2.19	0.42
1:A:599:ASN:OD1	1:A:629:ILE:HA	2.19	0.42
1:B:441:PHE:HB2	1:B:448:LYS:NZ	2.35	0.42
1:B:516:LYS:HB2	1:B:520:ARG:HH22	1.84	0.42
1:A:200:LYS:O	1:A:204:GLN:HG2	2.19	0.42
1:A:639:LEU:HD23	1:A:644:LEU:HD21	2.02	0.42
1:A:723:ALA:O	1:A:726:LEU:HG	2.19	0.42
1:A:753:GLN:OE1	1:A:755:ASN:ND2	2.53	0.42
1:B:252:TYR:HA	1:B:338:TYR:CE1	2.55	0.42
1:B:377:ASN:OD1	1:B:378:ASP:N	2.53	0.42
1:B:441:PHE:HB2	1:B:448:LYS:HZ1	1.85	0.42
1:B:478:LYS:HG3	1:B:514:ASN:OD1	2.19	0.42
1:B:566:LYS:HB3	1:B:571:ASN:HB3	2.01	0.42
1:B:890:ARG:HA	1:B:893:LEU:HD12	2.01	0.42
1:A:142:PHE:O	1:A:146:GLU:HG2	2.19	0.42
1:A:754:ILE:HG22	1:A:758:LYS:NZ	2.35	0.42
1:A:760:LEU:HD21	1:A:765:SER:HB3	2.02	0.42
1:B:396:ARG:HB2	1:B:443:LYS:HB2	2.01	0.42
1:A:216:GLU:OE1	1:A:217:PRO:HD3	2.19	0.42
1:A:336:LYS:O	1:A:340:GLU:OE1	2.38	0.42
1:B:776:THR:O	1:B:780:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:LYS:HB2	1:B:855:THR:OG1	2.20	0.42
1:A:73:VAL:H	1:A:76:ILE:HB	1.85	0.42
1:A:212:LYS:HE3	1:A:212:LYS:HB3	1.86	0.42
1:A:775:TYR:HD2	1:A:780:ILE:HD11	1.84	0.42
1:B:179:LYS:HE2	1:B:256:TYR:CE2	2.54	0.42
1:B:525:ASN:OD1	1:B:527:SER:OG	2.23	0.42
1:B:587:VAL:O	1:B:590:LEU:HG	2.19	0.42
1:B:624:LEU:O	1:B:629:ILE:HG21	2.20	0.42
1:A:147:LYS:HB2	1:A:147:LYS:HE2	1.84	0.41
1:A:392:GLY:C	1:A:420:GLN:HE21	2.23	0.41
1:B:70:ILE:HD11	1:B:580:ARG:NE	2.35	0.41
1:B:149:ARG:NH2	1:B:179:LYS:HD3	2.34	0.41
1:B:165:SER:OG	1:B:246:LYS:HE2	2.20	0.41
1:B:370:LEU:HD23	1:B:397:TYR:CD1	2.55	0.41
1:B:470:TYR:O	1:B:474:LEU:HG	2.20	0.41
1:B:516:LYS:HB2	1:B:520:ARG:NH2	2.34	0.41
1:B:581:SER:HB2	1:B:583:PHE:CE2	2.55	0.41
1:A:155:ASN:O	1:A:159:VAL:HG23	2.19	0.41
1:A:349:GLU:HA	1:A:352:LYS:HG2	2.01	0.41
1:A:407:TYR:HD2	1:A:409:LYS:NZ	2.16	0.41
1:A:780:ILE:HA	1:A:783:MET:HG3	2.01	0.41
1:B:689:TYR:CD2	1:B:690:LEU:HD22	2.55	0.41
1:B:845:HIS:HA	1:B:848:VAL:HG22	2.02	0.41
1:A:845:HIS:O	1:A:849:SER:OG	2.30	0.41
1:B:689:TYR:CZ	1:B:693:ILE:HD11	2.55	0.41
1:A:255:PHE:CE1	1:A:341:LEU:HD22	2.56	0.41
1:A:442:ARG:HH12	1:A:444:PHE:HD1	1.67	0.41
1:A:778:LEU:HA	1:A:781:ALA:HB3	2.01	0.41
1:B:819:ARG:O	1:B:823:VAL:HG23	2.21	0.41
1:A:205:LYS:HE3	1:A:272:HIS:NE2	2.36	0.41
1:A:407:TYR:CD2	1:A:409:LYS:CE	3.03	0.41
1:B:179:LYS:HE2	1:B:256:TYR:HE2	1.85	0.41
1:B:314:ILE:HD13	1:B:314:ILE:HA	1.89	0.41
1:B:742:LEU:HD21	1:B:773:GLU:HG3	2.01	0.41
1:B:894:GLU:N	1:B:894:GLU:OE1	2.54	0.41
1:B:515:ASN:HB3	1:B:552:PHE:CD1	2.56	0.41
1:B:581:SER:HB2	1:B:583:PHE:CD2	2.55	0.41
1:B:610:HIS:NE2	1:B:639:LEU:O	2.53	0.41
1:B:708:TRP:HE3	1:B:712:HIS:CG	2.38	0.41
1:B:855:THR:O	1:B:859:LEU:HD13	2.21	0.41
1:A:448:LYS:HB2	1:A:450:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ILE:O	1:A:649:GLU:HG3	2.21	0.41
1:B:486:THR:HA	1:B:489:ILE:HG22	2.02	0.41
1:B:683:SER:O	1:B:687:LEU:HB2	2.21	0.41
1:A:413:TRP:HA	1:A:416:PRO:HD2	2.02	0.41
1:B:643:HIS:HD2	1:B:677:PHE:HE2	1.68	0.41
1:B:844:LEU:O	1:B:848:VAL:HG13	2.20	0.41
1:A:194:LYS:H	1:A:194:LYS:HG3	1.66	0.41
1:A:314:ILE:HA	1:A:317:VAL:HG22	2.02	0.41
1:A:676:HIS:CD2	1:A:676:HIS:N	2.89	0.41
1:A:842:THR:HG22	1:A:843:ALA:N	2.36	0.41
1:B:129:ALA:HB3	1:B:131:LEU:HD22	2.01	0.41
1:B:684:ILE:HG23	1:B:725:GLU:OE1	2.21	0.41
1:B:703:THR:HG21	1:B:713:PHE:HZ	1.85	0.41
1:A:136:LYS:HB3	1:A:136:LYS:HE2	1.80	0.41
1:A:727:LEU:HD23	1:A:732:ILE:HG21	2.03	0.41
1:B:60:VAL:O	1:B:64:ILE:HG12	2.21	0.41
1:B:166:LYS:HD2	1:B:166:LYS:HA	1.95	0.41
1:B:443:LYS:HG2	1:B:448:LYS:H	1.86	0.41
1:B:500:ASP:O	1:B:535:LYS:NZ	2.39	0.41
1:B:746:HIS:CD2	1:B:777:SER:HB3	2.56	0.41
1:B:112:ILE:HD12	1:B:112:ILE:H	1.86	0.40
1:B:324:VAL:HG22	1:B:339:ARG:HH21	1.86	0.40
1:B:375:PHE:H	1:B:425:PRO:CG	2.33	0.40
1:B:470:TYR:CZ	1:B:504:SER:HB2	2.56	0.40
1:B:724:LYS:HB3	1:B:728:LYS:NZ	2.36	0.40
1:A:70:ILE:HD12	1:A:70:ILE:HA	1.95	0.40
1:B:448:LYS:HE2	1:B:452:ALA:HB2	2.04	0.40
1:B:837:THR:OG1	1:B:838:ALA:N	2.54	0.40
1:A:867:LYS:HE2	1:A:876:PRO:HG2	2.03	0.40
1:B:51:ASN:N	1:B:51:ASN:OD1	2.53	0.40
1:B:301:ASP:O	1:B:305:SER:OG	2.32	0.40
1:B:575:LEU:CD2	1:B:608:PRO:HB3	2.51	0.40
1:B:676:HIS:CD2	1:B:710:PRO:HG3	2.57	0.40
1:B:758:LYS:O	1:B:762:LYS:HG2	2.21	0.40
1:A:156:PHE:N	1:A:252:TYR:HE2	2.20	0.40
1:A:228:GLU:O	1:A:231:ASP:HB2	2.22	0.40
1:A:640:THR:HB	1:A:643:HIS:ND1	2.37	0.40
1:A:712:HIS:O	1:A:715:ILE:HB	2.22	0.40
1:A:791:VAL:HG12	1:A:795:GLU:OE2	2.21	0.40
1:B:630:ASP:N	1:B:630:ASP:OD1	2.53	0.40
1:A:161:GLU:OE1	1:A:161:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:HIS:NE2	1:A:608:PRO:HG3	2.35	0.40
1:A:643:HIS:CE1	1:A:674:PRO:HG3	2.57	0.40
1:B:403:SER:OG	1:B:404:LYS:HG3	2.21	0.40
1:B:580:ARG:HG2	1:B:614:MET:HB2	2.02	0.40
1:B:861:ASN:O	1:B:862:LYS:HE2	2.22	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	A	840/1296 (65%)	761 (91%)	79 (9%)	0	100	100
1	B	859/1296 (66%)	753 (88%)	106 (12%)	0	100	100
All	All	1699/2592 (66%)	1514 (89%)	185 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	732/1127 (65%)	731 (100%)	1 (0%)	93	96
1	B	745/1127 (66%)	745 (100%)	0	100	100
All	All	1477/2254 (66%)	1476 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	580	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	B	249	GLN
1	B	916	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 monosaccharides 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.

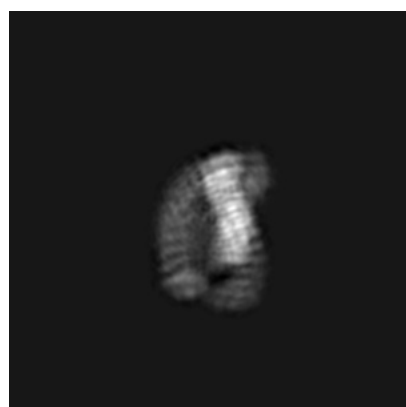
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13643. These allow visual inspection of the internal detail of the map and identification of artifacts.

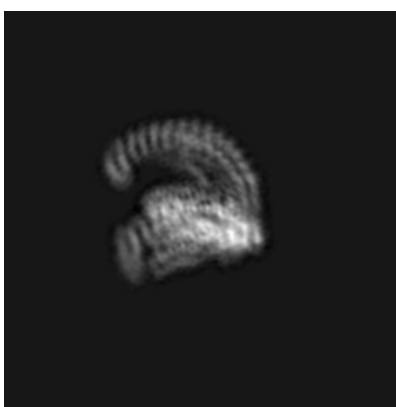
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

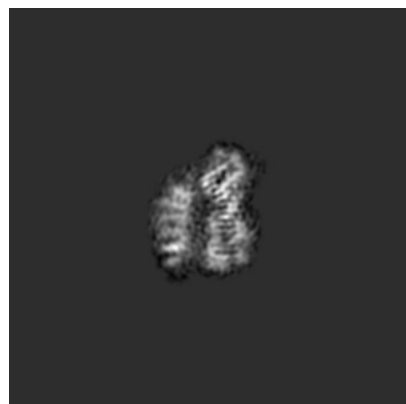


Z

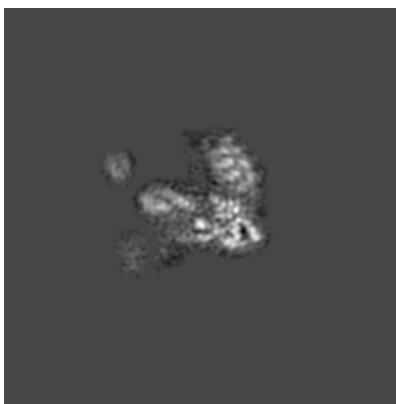
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

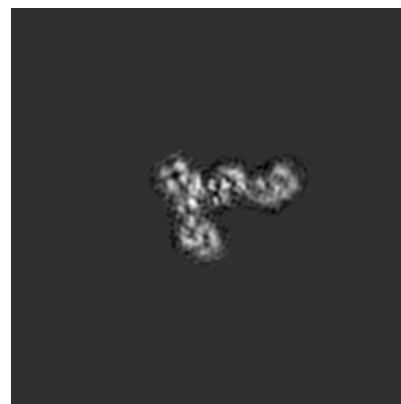
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

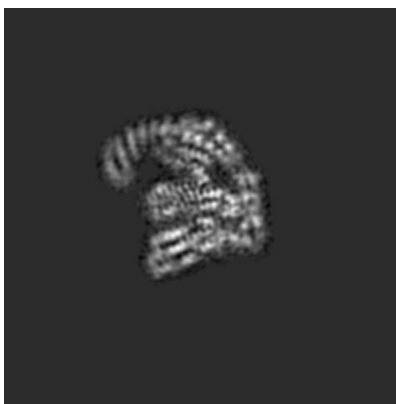
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

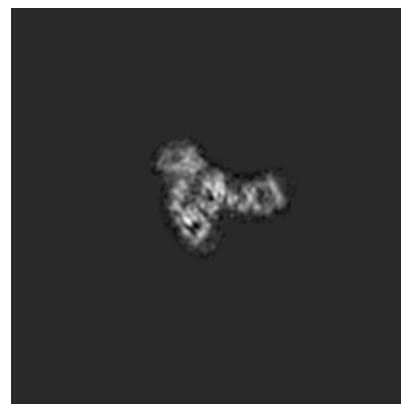
6.3.1 Primary map



X Index: 157



Y Index: 202

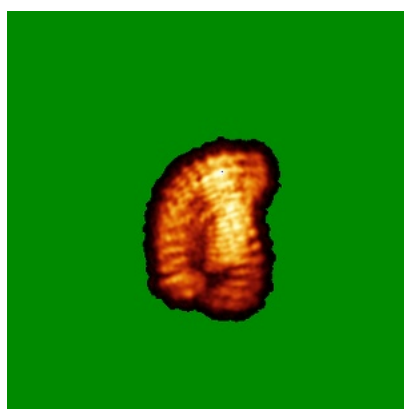


Z Index: 204

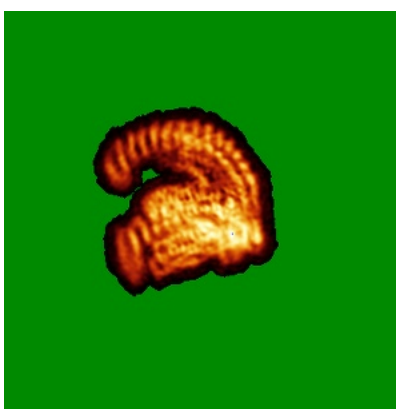
The images above show the largest variance slices of the map in three orthogonal directions.

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

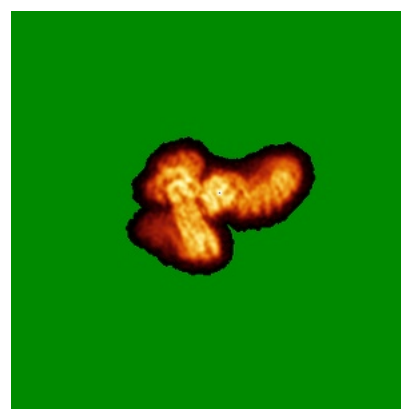
6.4.1 Primary map



X



Y

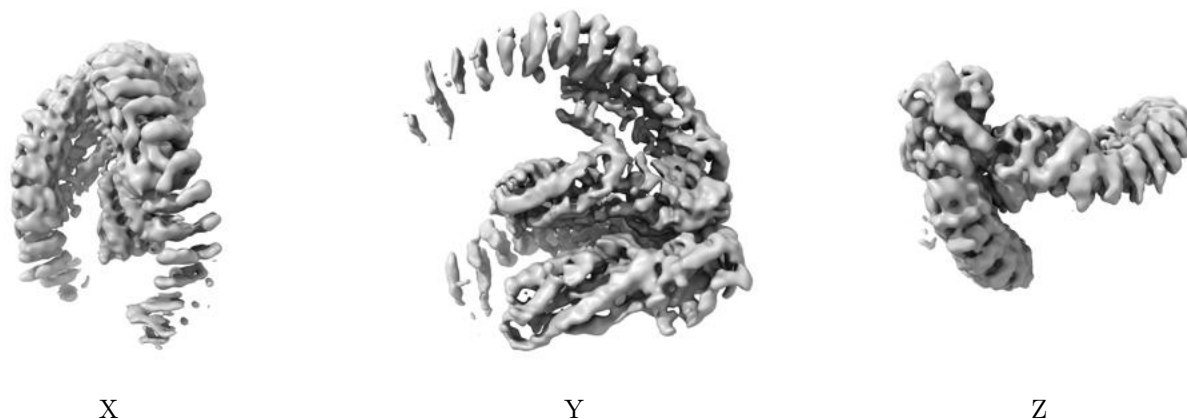


Z

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 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

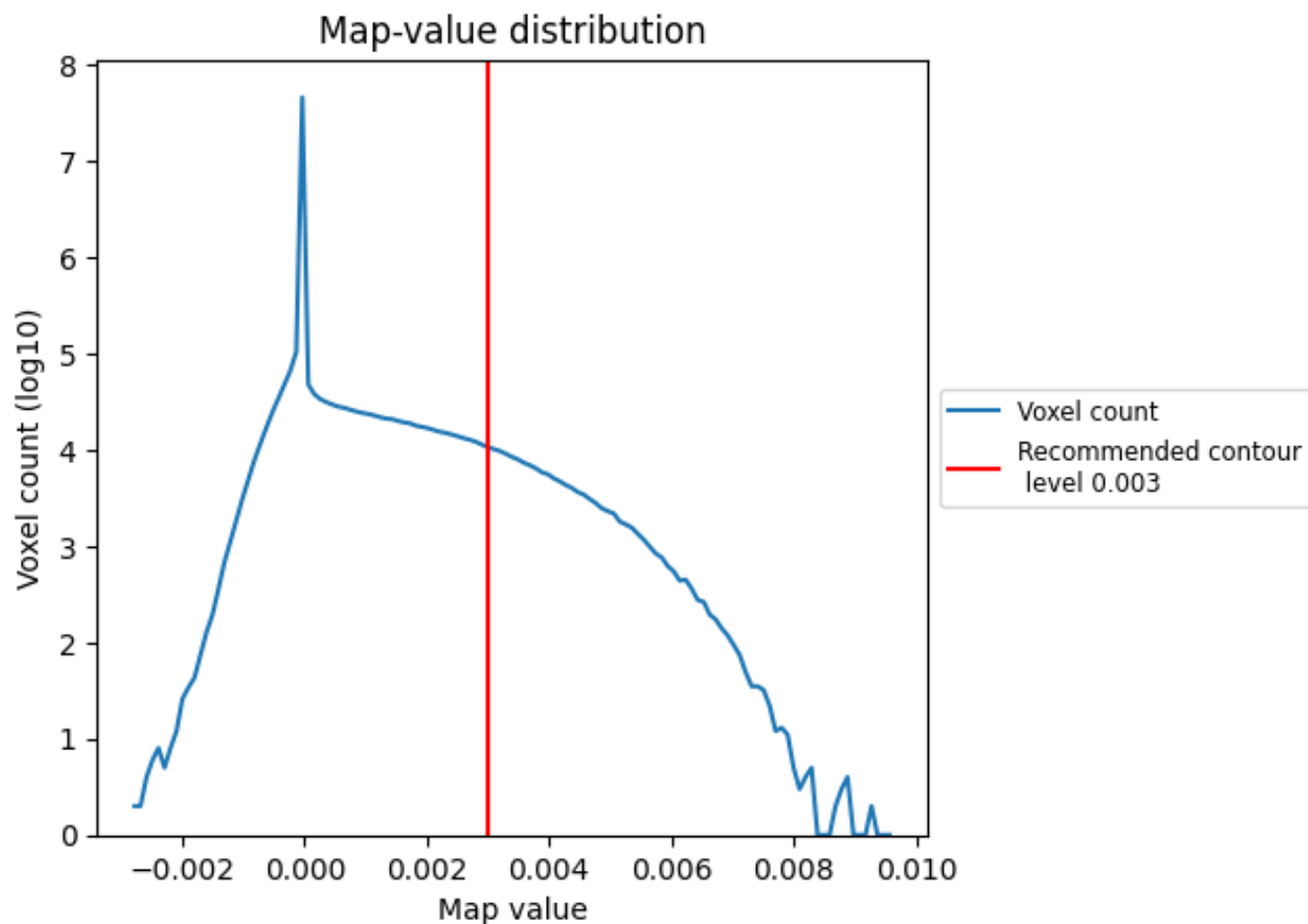
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

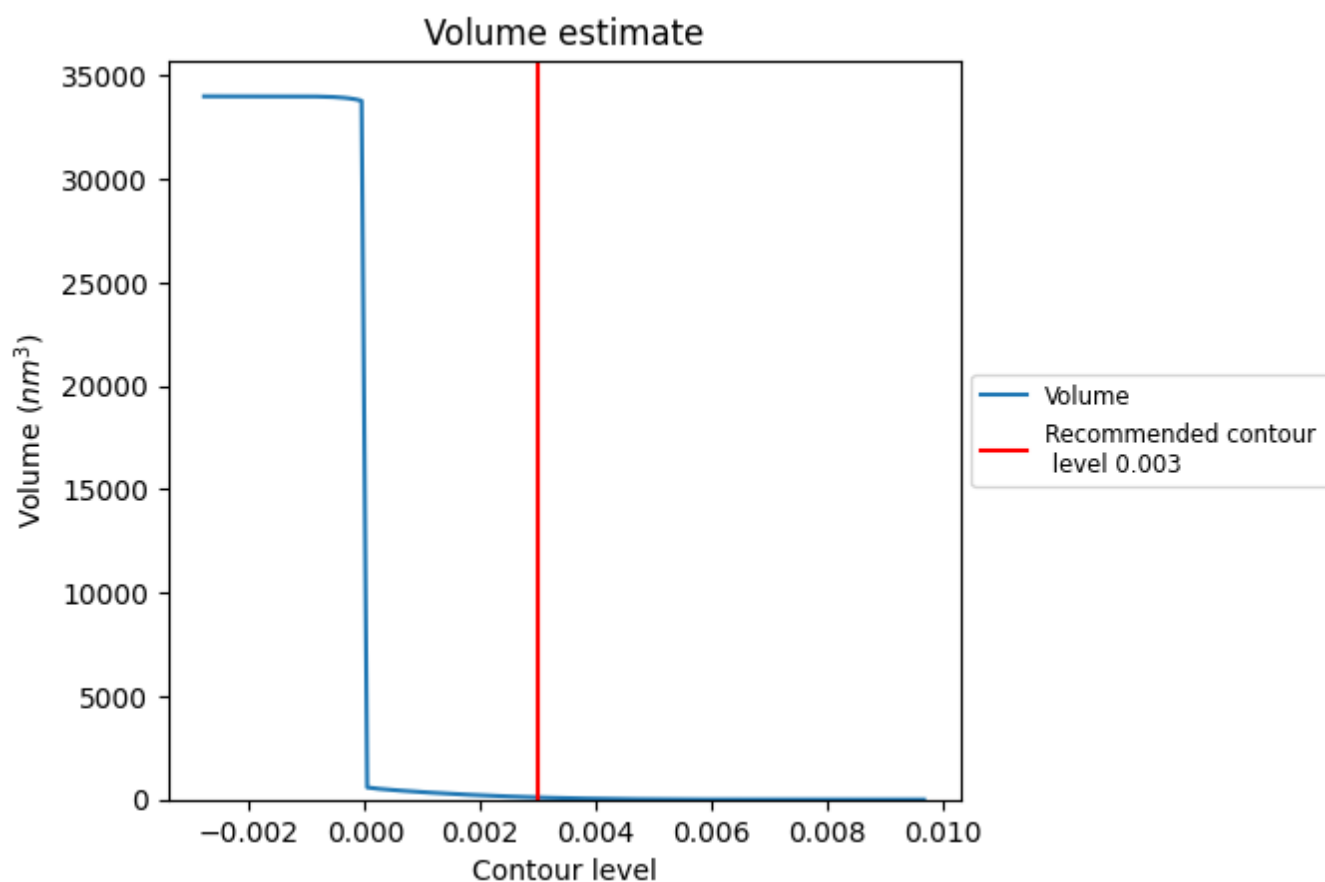
This section contains the results of statistical analysis of the map.

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.

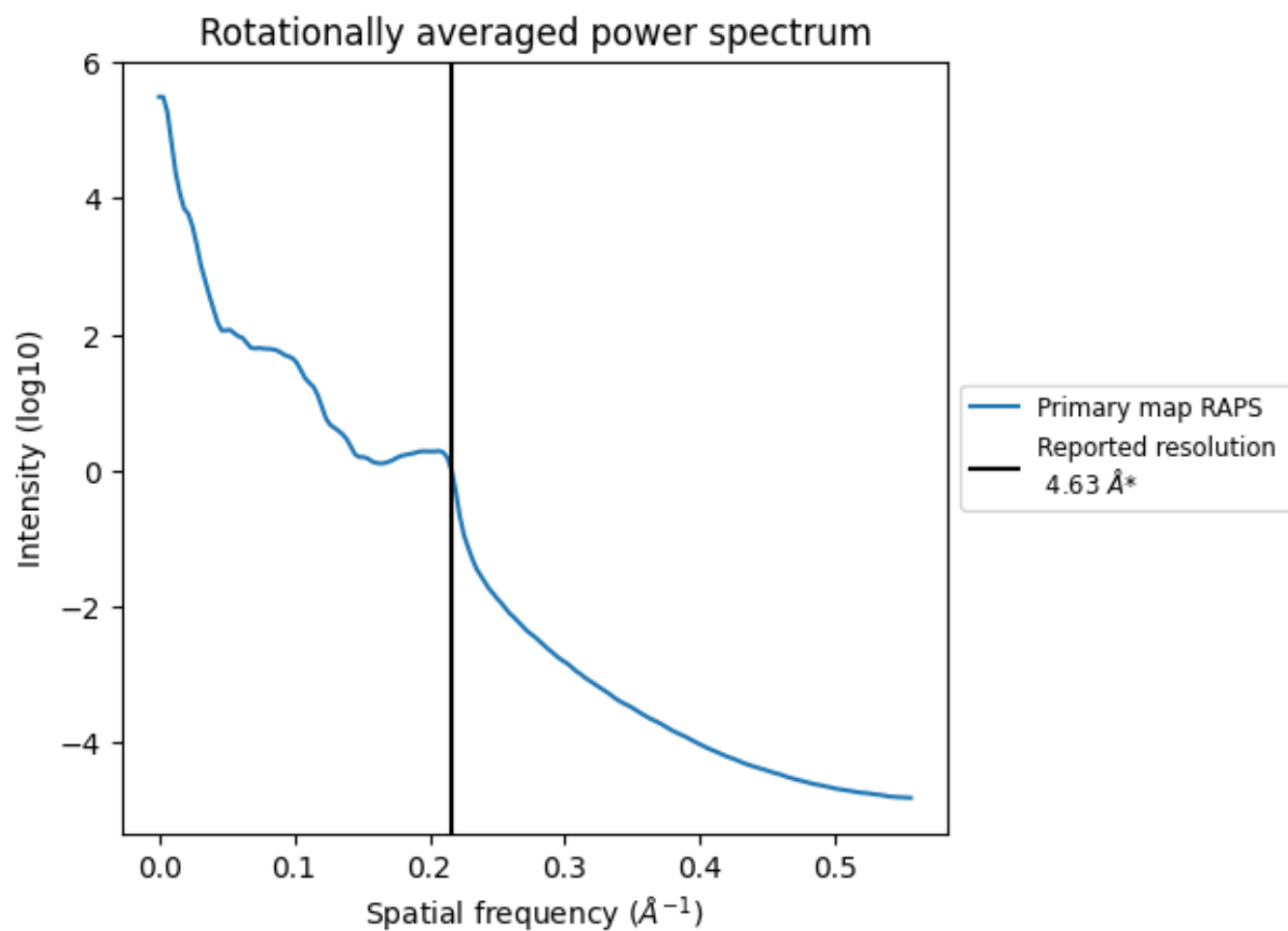
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm^3 ; this corresponds to an approximate mass of 92 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 0.216 Å⁻¹

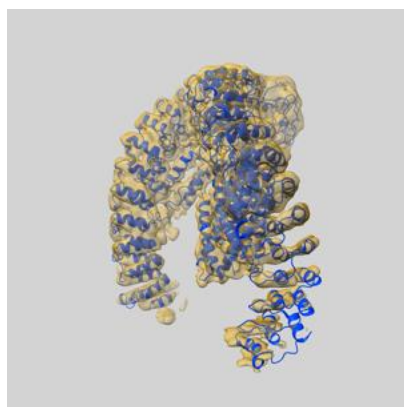
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

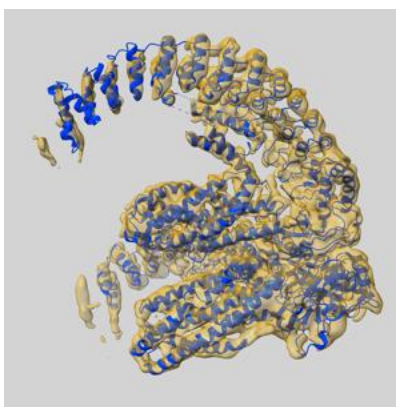
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13643 and PDB model 7PTY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

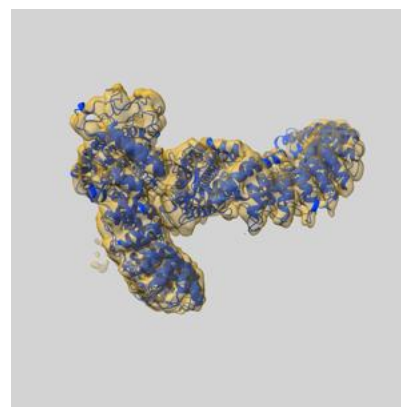
9.1 Map-model overlay [i](#)



X



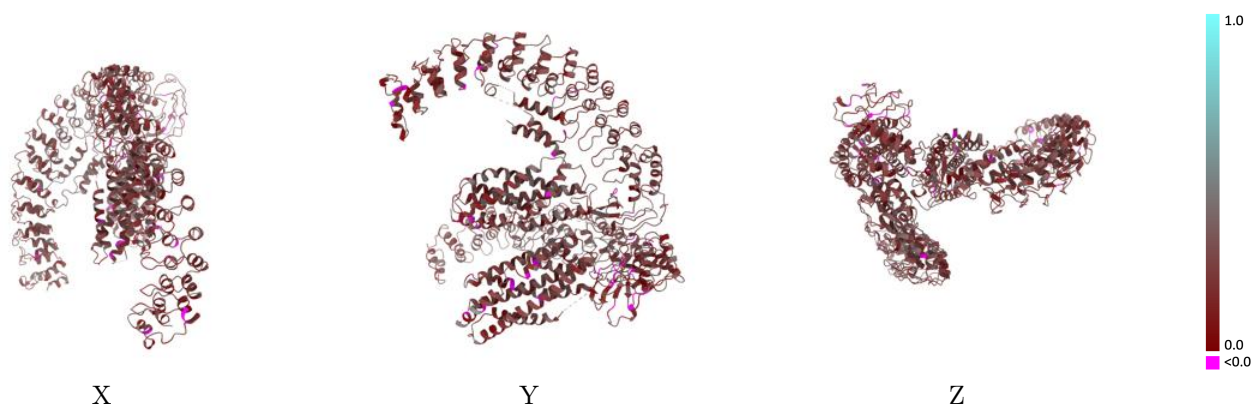
Y



Z

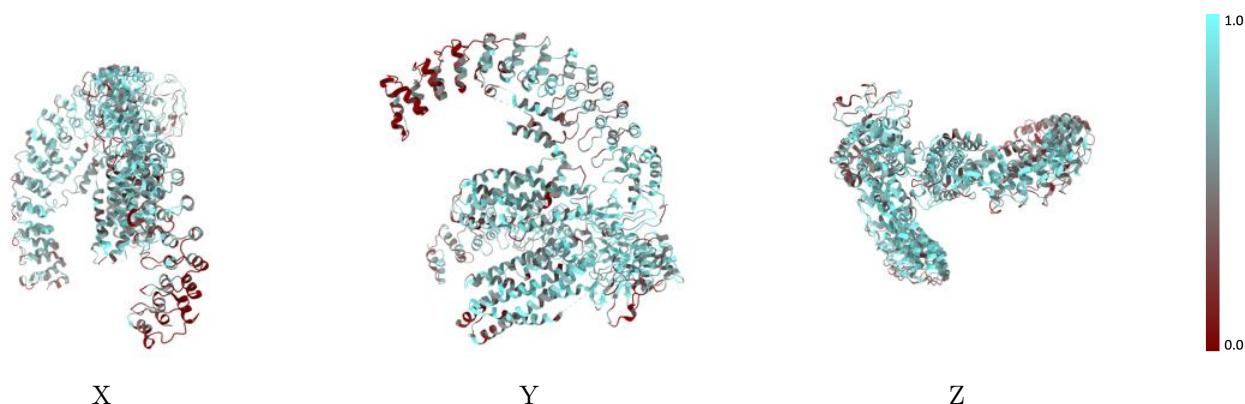
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



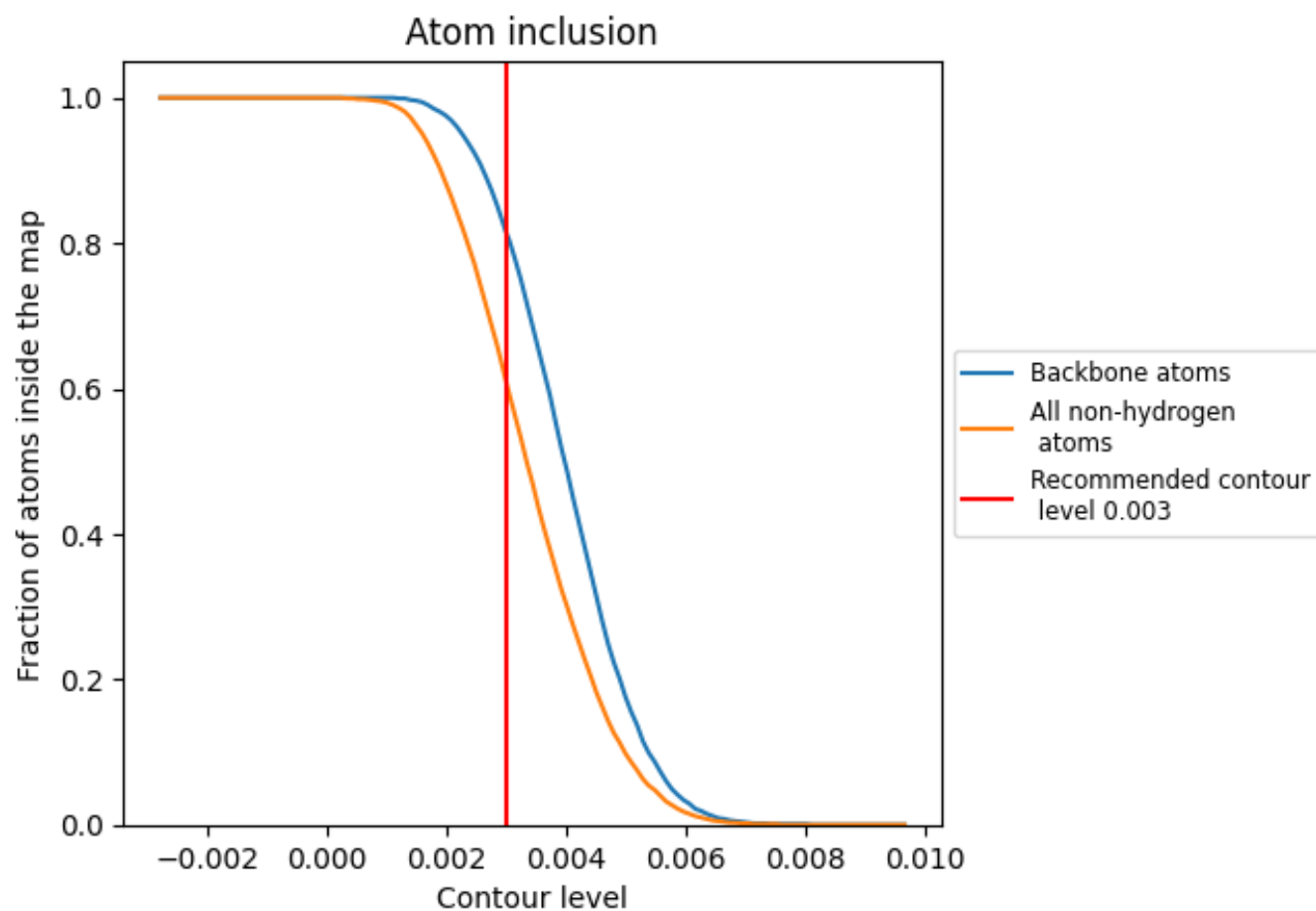
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 61% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6100	<div></div> 0.2530
A	<div></div> 0.5670	<div></div> 0.2540
B	<div></div> 0.6530	<div></div> 0.2520

