



Full wwPDB EM Validation Report ⓘ

Mar 1, 2026 – 07:10 AM UTC

PDB ID : 7NTX / pdb_00007ntx
EMDB ID : EMD-10889
Title : Vip3Bc1 tetramer in processed, activated state
Authors : Thompson, R.F.; Byrne, M.J.; Iadanza, M.I.
Deposited on : 2021-03-11
Resolution : 4.75 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

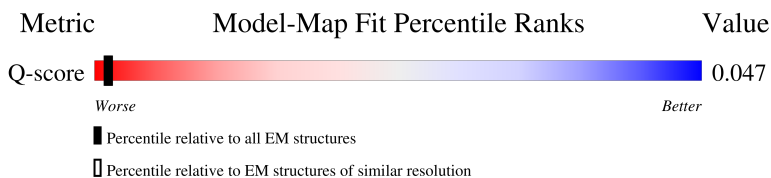
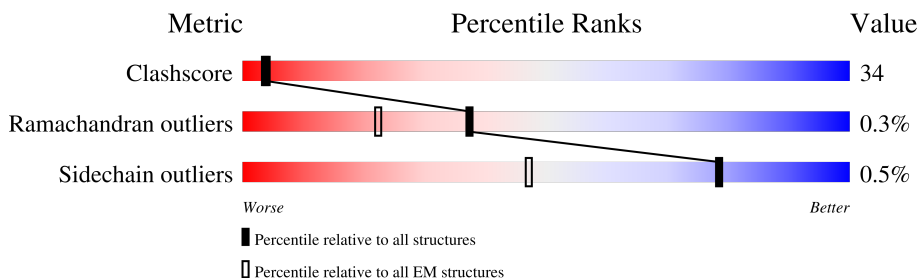
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.75 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	1575 (4.30 - 5.30)

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	803	25% 40% 40% 19%
1	B	803	26% 39% 41% 19%
1	C	803	25% 39% 41% 19%
1	D	803	26% 38% 42% 19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20848 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.

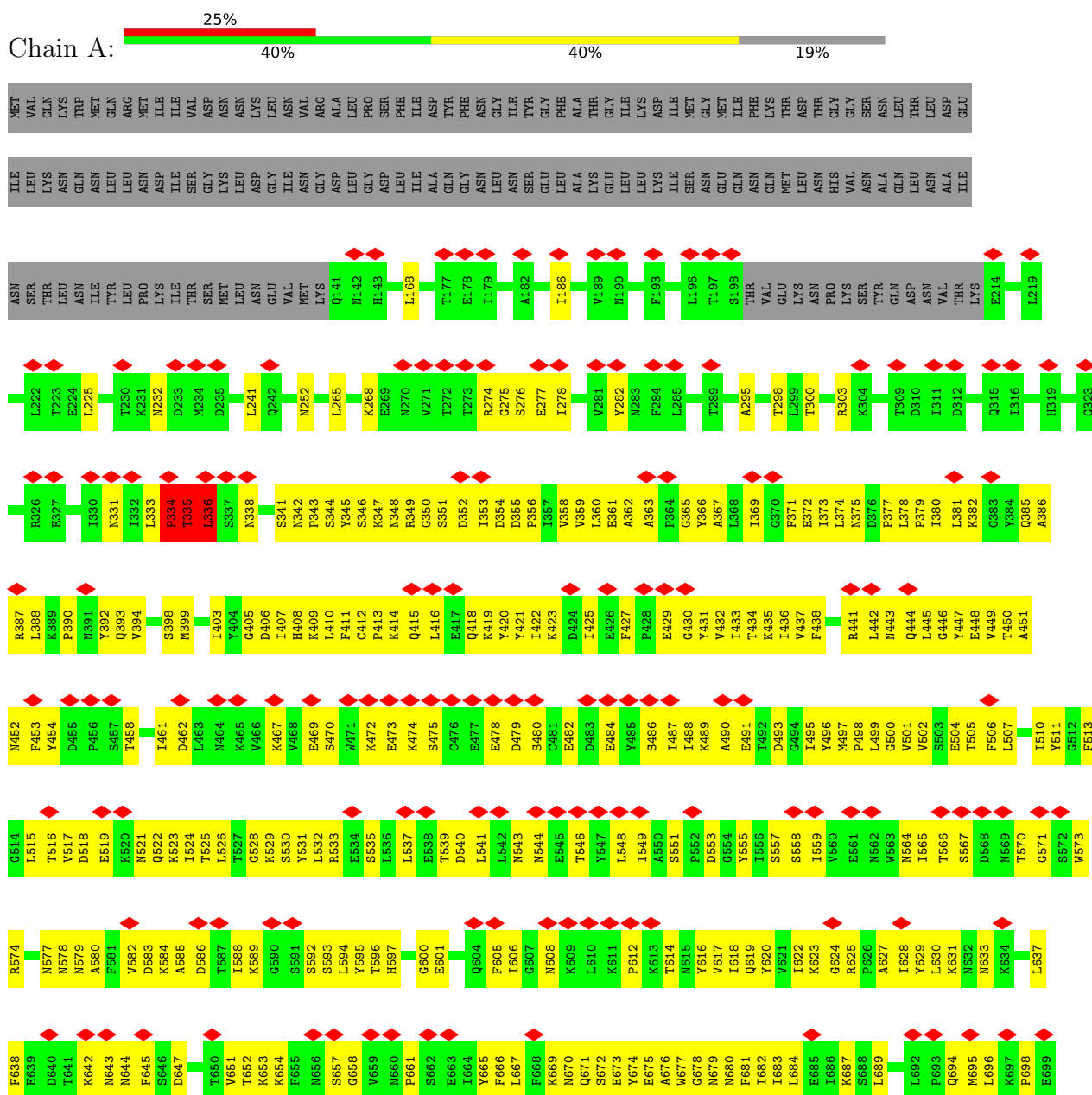
- Molecule 1 is a protein called Vegetative insecticidal protein.

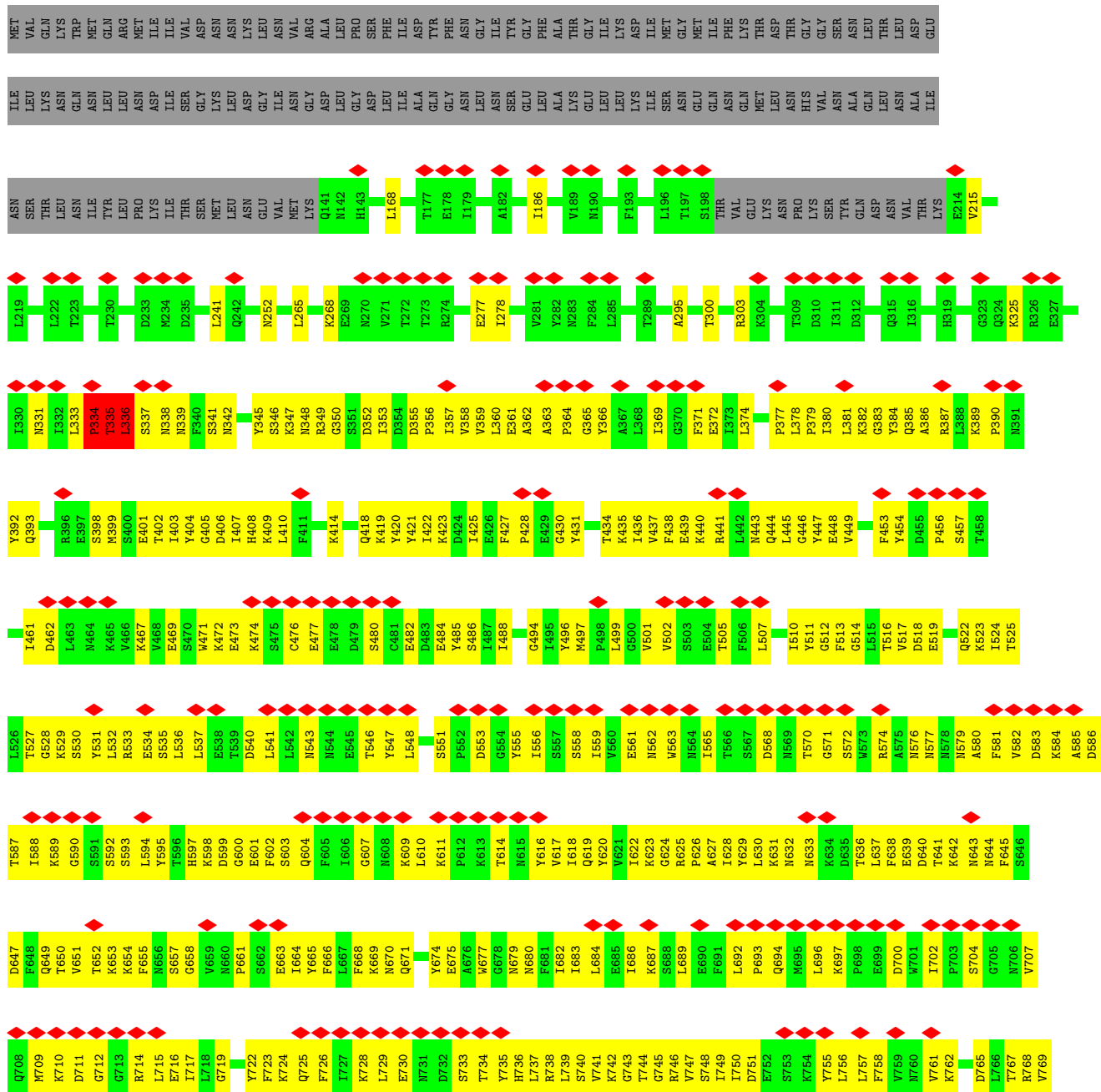
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	648	Total	C	N	O	S	0	0
			5212	3328	843	1029	12		
1	B	648	Total	C	N	O	S	0	0
			5212	3328	843	1029	12		
1	C	648	Total	C	N	O	S	0	0
			5212	3328	843	1029	12		
1	D	648	Total	C	N	O	S	0	0
			5212	3328	843	1029	12		

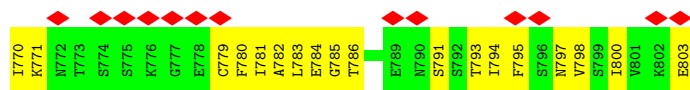
3 Residue-property plots

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.

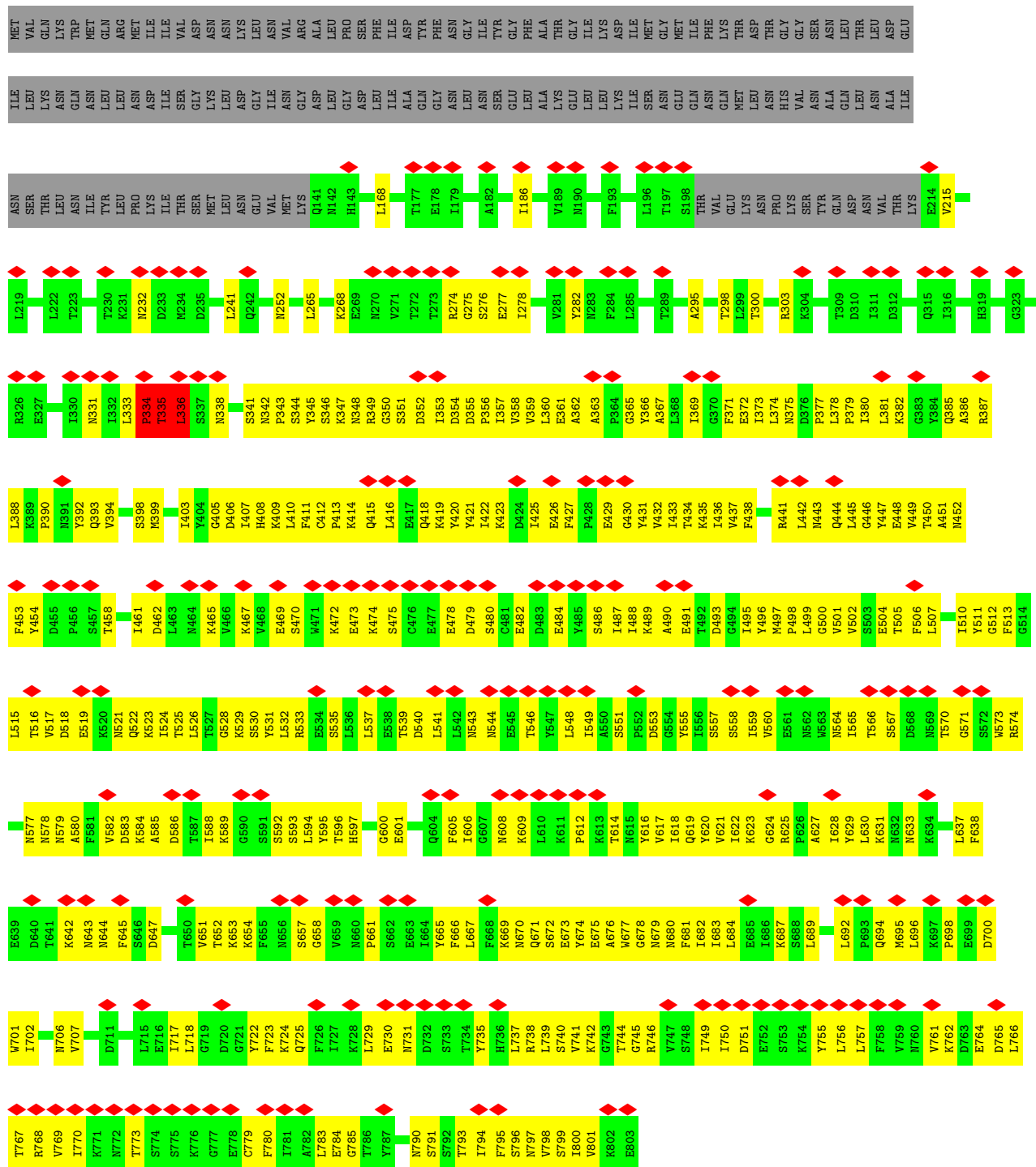
• Molecule 1: Vegetative insecticidal protein







• Molecule 1: Vegetative insecticidal protein



• Molecule 1: Vegetative insecticidal protein

Chain D: 26% 38% 42% 19%

R768	V707	S646	D586	T525	T458	N391	I330	L222	ASN	ILE
V769	Q708	D647	T587	L526	I461	Y392	I332	T223	SER	LEU
K771	M709	F648	I588	G528	D462	Q393	I333	E224	THR	LYS
N772	D711	V651	G590	K529	L463	R396	L333	L225	ASN	GLN
S774	G712	T652	S591	Y531	M464	E397	P334	T230	ILE	ASN
S775	R713	K654	S593	L532	K465	S398	T335	K231	TYR	GLN
K776	G714	F655	L594	R533	V466	N400	L336	ASN	LEU	LEU
G777	L715	N656	L595	E534	K467	E401	S337	LYS	LEU	ASN
E778	E716	S657	T596	L536	V468	T402	D233	ILE	THR	ASP
C779	L717	G658	H597	L537	S470	I403	M234	THR	SER	GLY
F780	L718	V659	K598	L537	K471	G405	D235	MET	LYS	LEU
I781	N660	N660	D599	E538	K472	D406	L241	ASN	LEU	ASN
A782	P661	S662	G600	T539	E473	H408	Q242	GLY	LEU	GLY
L783	F723	E663	E601	D540	K474	K409	N252	VAL	ASN	ILE
E784	K724	I664	F602	L541	S475	L410	L265	GLU	LEU	ILE
G785	Q725	Y665	Q604	L542	C476	F411	N142	VAL	ASP	GLY
T786	F726	F666	F605	N543	E477	K414	H143	MET	ALA	ASN
E789	I727	L667	T606	N544	E478	D424	Q141	LYS	LEU	LEU
N790	K728	F668	G607	E545	D479	K419	K268	ASN	GLY	PRO
S791	L729	K669	N608	T546	S480	K418	E269	SER	ASP	PHE
S792	N670	Y547	K609	Y547	S480	Y420	N270	LEU	LEU	ILE
T793	E730	Q671	L610	L548	C481	Y421	V271	ALA	ALA	ASP
I794	N731	Y674	K611	S551	D483	I422	T272	TYR	GLN	GLY
F795	D732	E675	P612	P552	E484	K423	T273	ASN	ASN	ASN
S796	S733	A676	K613	D553	Y485	I425	R274	GLY	GLY	GLY
N797	T734	W677	T614	G554	S486	E426	E277	ASN	ASN	ASN
V798	H735	G678	G554	I487	I488	F427	I278	ILE	ILE	ILE
S799	H736	N679	N615	Y555	I488	P428	L278	GLY	GLY	GLY
I800	L737	N680	N615	I556	G494	E429	V281	LEU	LEU	LEU
V801	R738	F681	V616	S557	L495	G430	Y282	LYS	LYS	LYS
K802	L739	I682	V617	E557	Y495	A363	N283	GLY	GLY	GLY
E803	S740	T683	Q619	S558	M497	Y431	F284	LEU	LEU	LEU
	V741	L684	V559	I559	P498	T434	L285	LYS	LYS	LYS
	K742	E685	V620	V560	L499	K435	L289	ASP	ASP	ASP
	G743	I686	V621	E561	G500	I436	L196	ILE	ILE	ILE
	T744	K687	K623	N562	V501	V437	T197	SER	SER	SER
	G745	S686	G624	V563	V502	F438	S198	ASN	ASN	ASN
	R746	L689	R625	N664	S603	E439	A295	GLY	GLY	GLY
	V747	E690	P626	I565	S604	K440	M295	MET	MET	MET
	S748	F691	A627	T566	E504	R441	T300	ILE	ILE	ILE
	I749	L692	T628	T566	T505	K440	F371	GLN	GLN	GLN
	T750	P693	V629	S567	F506	L442	THR	LYS	LYS	LYS
	D751	L693	D568	D568	L507	N443	GLY	LEU	LEU	LEU
	E752	Q694	K631	N669	L507	Q444	ASN	ASN	ASN	ASN
	S753	N632	K631	N669	L507	Q444	THR	THR	THR	THR
	K754	N695	N633	T570	I510	L445	ASN	ASN	ASN	ASN
	Y755	L696	K634	G571	Y511	G446	HIS	HIS	HIS	HIS
	L756	D635	D635	S571	G512	P379	VAL	VAL	VAL	VAL
	L757	P698	T636	S572	F513	Y447	SER	SER	SER	SER
	F758	E699	L637	N573	G514	E448	TYR	TYR	TYR	TYR
	N759	D700	F638	R574	L515	F453	GLM	GLM	GLM	GLM
	V760	W701	E639	A575	T516	G383	ASP	ASP	ASP	ASP
	V761	I702	T641	N576	V517	Y384	ASN	ASN	ASN	ASN
	K762	L702	K642	N577	D518	Q385	LEU	LEU	LEU	LEU
	D763	S704	N643	N578	E519	A386	THR	THR	THR	THR
	E764	G705	N644	N578	E519	R387	VAL	VAL	VAL	VAL
	T766	N706	F645	N579	Q522	L388	LYS	LYS	LYS	LYS
				A580	K523	K389	E214	E214	E214	E214
				F581	I524	P390	L219	L219	L219	L219
				V582		G323	G323	G323	G323	G323
				D583		K325	K325	K325	K325	K325
				K584		E327	E327	E327	E327	E327
				A585						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158763	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 ($e^-/\text{\AA}^2$)	70.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.779	Depositor
Minimum map value	-0.787	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	319.50003, 319.50003, 319.50003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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	0.53	4/5311 (0.1%)	0.96	10/7183 (0.1%)
1	B	0.53	3/5311 (0.1%)	0.97	13/7183 (0.2%)
1	C	0.53	4/5311 (0.1%)	0.96	12/7183 (0.2%)
1	D	0.52	3/5311 (0.1%)	0.97	13/7183 (0.2%)
All	All	0.53	14/21244 (0.1%)	0.97	48/28732 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	3
All	All	0	10

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	LEU	N-CA	8.70	1.57	1.46
1	C	336	LEU	N-CA	8.61	1.57	1.46
1	B	336	LEU	C-N	7.69	1.43	1.33
1	D	336	LEU	C-N	7.58	1.42	1.33
1	C	335	THR	N-CA	7.26	1.54	1.45
1	A	335	THR	N-CA	7.23	1.54	1.45
1	D	336	LEU	N-CA	6.78	1.54	1.46
1	B	336	LEU	N-CA	6.67	1.54	1.46
1	A	335	THR	C-N	6.12	1.42	1.33
1	C	335	THR	C-N	6.08	1.42	1.33
1	A	336	LEU	C-N	5.57	1.41	1.33
1	C	336	LEU	C-N	5.54	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	335	THR	CA-C	5.30	1.59	1.52
1	B	335	THR	CA-C	5.24	1.59	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	PRO	O-C-N	-12.61	105.61	122.64
1	C	334	PRO	O-C-N	-12.51	105.75	122.64
1	B	335	THR	CB-CA-C	12.27	134.84	110.42
1	D	335	THR	CB-CA-C	11.65	133.61	110.42
1	A	335	THR	CA-C-O	-10.40	109.36	121.11
1	C	335	THR	CA-C-O	-10.35	109.42	121.11
1	D	335	THR	N-CA-CB	-8.78	95.65	110.49
1	B	335	THR	N-CA-CB	-8.61	95.94	110.49
1	B	336	LEU	CB-CA-C	-7.91	94.69	110.42
1	D	336	LEU	CB-CA-C	-7.80	94.91	110.42
1	B	334	PRO	O-C-N	-7.69	112.25	122.64
1	D	334	PRO	O-C-N	-7.67	112.29	122.64
1	D	334	PRO	CA-C-N	7.48	135.83	121.54
1	D	334	PRO	C-N-CA	7.48	135.83	121.54
1	B	336	LEU	N-CA-C	7.36	126.47	110.80
1	D	336	LEU	N-CA-C	7.31	126.37	110.80
1	A	335	THR	CA-C-N	6.94	134.79	121.54
1	A	335	THR	C-N-CA	6.94	134.79	121.54
1	C	335	THR	CA-C-N	6.89	134.70	121.54
1	C	335	THR	C-N-CA	6.89	134.70	121.54
1	B	336	LEU	N-CA-CB	-6.87	98.88	110.49
1	B	334	PRO	CA-C-N	6.74	134.42	121.54
1	B	334	PRO	C-N-CA	6.74	134.42	121.54
1	D	336	LEU	N-CA-CB	-6.60	99.34	110.49
1	D	232	ASN	CA-CB-CG	-6.44	106.16	112.60
1	C	232	ASN	CA-CB-CG	-6.42	106.18	112.60
1	D	300	THR	N-CA-CB	5.87	118.75	110.12
1	B	300	THR	N-CA-CB	5.85	118.71	110.12
1	A	300	THR	N-CA-CB	5.72	118.53	110.12
1	B	335	THR	CA-C-O	-5.61	112.49	120.51
1	C	300	THR	N-CA-CB	5.50	118.20	110.12
1	D	335	THR	CA-C-O	-5.48	112.67	120.51
1	B	252	ASN	CA-CB-CG	-5.47	107.13	112.60
1	D	252	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	252	ASN	CA-CB-CG	-5.39	107.21	112.60
1	C	252	ASN	CA-CB-CG	-5.39	107.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	VAL	CB-CA-C	-5.30	105.19	111.97
1	B	215	VAL	CB-CA-C	-5.28	105.21	111.97
1	B	331	ASN	CA-CB-CG	-5.16	107.44	112.60
1	C	215	VAL	N-CA-C	5.14	115.35	110.42
1	D	331	ASN	CA-CB-CG	-5.13	107.47	112.60
1	C	331	ASN	CA-CB-CG	-5.12	107.48	112.60
1	A	336	LEU	N-CA-C	5.11	121.68	110.80
1	A	336	LEU	CB-CA-C	-5.10	100.28	110.42
1	C	336	LEU	CB-CA-C	-5.10	100.28	110.42
1	A	331	ASN	CA-CB-CG	-5.09	107.51	112.60
1	C	336	LEU	N-CA-C	5.05	121.55	110.80
1	A	232	ASN	CA-CB-CG	-5.02	107.58	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	ARG	Sidechain
1	A	334	PRO	Mainchain
1	B	303	ARG	Sidechain
1	B	334	PRO	Mainchain
1	B	335	THR	Peptide
1	C	303	ARG	Sidechain
1	C	334	PRO	Mainchain
1	D	303	ARG	Sidechain
1	D	334	PRO	Mainchain
1	D	335	THR	Peptide

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	5212	0	5169	327	0
1	B	5212	0	5169	362	0
1	C	5212	0	5169	343	0
1	D	5212	0	5168	362	0
All	All	20848	0	20675	1394	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 34.

All (1394) 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:275:GLY:HA2	1:A:505:THR:CG2	1.16	1.64
1:A:278:ILE:HG13	1:A:336:LEU:CD1	1.27	1.60
1:A:278:ILE:CG1	1:A:336:LEU:HD13	1.32	1.58
1:C:275:GLY:CA	1:C:505:THR:CG2	1.84	1.53
1:C:275:GLY:HA2	1:C:505:THR:CG2	1.17	1.53
1:C:278:ILE:HG13	1:C:336:LEU:CD1	1.29	1.53
1:A:275:GLY:CA	1:A:505:THR:CG2	1.84	1.52
1:C:278:ILE:CG1	1:C:336:LEU:HD13	1.35	1.50
1:D:325:LYS:HZ1	1:D:543:ASN:ND2	1.06	1.41
1:B:325:LYS:HZ1	1:B:543:ASN:ND2	1.15	1.39
1:C:275:GLY:CA	1:C:505:THR:HG22	1.43	1.38
1:B:325:LYS:NZ	1:B:543:ASN:HD21	1.18	1.36
1:A:275:GLY:CA	1:A:505:THR:HG22	1.43	1.31
1:D:325:LYS:NZ	1:D:543:ASN:HD21	1.25	1.30
1:A:333:LEU:CD2	1:A:541:LEU:HD21	1.70	1.19
1:C:333:LEU:CD2	1:C:541:LEU:HD21	1.71	1.19
1:C:276:SER:N	1:C:505:THR:HG21	1.58	1.19
1:A:276:SER:N	1:A:505:THR:HG21	1.59	1.17
1:B:325:LYS:NZ	1:B:543:ASN:ND2	1.78	1.17
1:D:325:LYS:NZ	1:D:543:ASN:ND2	1.84	1.14
1:C:275:GLY:CA	1:C:505:THR:HG21	1.71	1.10
1:B:333:LEU:O	1:B:335:THR:OG1	1.66	1.10
1:A:275:GLY:CA	1:A:505:THR:HG21	1.69	1.09
1:B:325:LYS:NZ	1:B:543:ASN:CG	2.13	1.04
1:D:325:LYS:NZ	1:D:543:ASN:CG	2.16	1.03
1:C:275:GLY:C	1:C:505:THR:HG21	1.84	1.02
1:A:275:GLY:C	1:A:505:THR:HG21	1.83	1.01
1:A:333:LEU:HD21	1:A:541:LEU:CD2	1.91	1.01
1:A:278:ILE:N	1:A:336:LEU:HD11	1.77	1.00
1:C:278:ILE:N	1:C:336:LEU:HD11	1.79	0.98
1:C:333:LEU:HD21	1:C:541:LEU:CD2	1.92	0.98
1:A:282:TYR:OH	1:A:540:ASP:OD1	1.80	0.98
1:D:333:LEU:C	1:D:335:THR:H	1.64	0.97
1:C:282:TYR:OH	1:C:540:ASP:OD1	1.81	0.97
1:B:533:ARG:O	1:B:537:LEU:HB2	1.65	0.97
1:D:325:LYS:NZ	1:D:543:ASN:OD1	1.98	0.96
1:C:333:LEU:HD21	1:C:541:LEU:HD21	0.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:ARG:O	1:D:537:LEU:HB2	1.65	0.96
1:A:276:SER:H	1:A:505:THR:HG21	1.23	0.95
1:B:325:LYS:NZ	1:B:543:ASN:OD1	1.99	0.95
1:A:333:LEU:HD21	1:A:541:LEU:HD21	0.96	0.94
1:C:275:GLY:C	1:C:505:THR:CG2	2.42	0.92
1:C:276:SER:H	1:C:505:THR:HG21	1.20	0.91
1:B:333:LEU:C	1:B:335:THR:H	1.66	0.91
1:D:333:LEU:C	1:D:335:THR:HG23	1.97	0.89
1:B:325:LYS:HZ1	1:B:543:ASN:CG	1.75	0.89
1:A:333:LEU:CD2	1:A:541:LEU:CD2	2.50	0.88
1:A:275:GLY:HA3	1:A:505:THR:CG2	2.02	0.88
1:A:275:GLY:C	1:A:505:THR:CG2	2.43	0.88
1:A:275:GLY:HA2	1:A:505:THR:CB	2.04	0.87
1:C:745:GLY:HA2	1:C:785:GLY:HA2	1.57	0.87
1:B:601:GLU:HA	1:B:669:LYS:HA	1.56	0.87
1:A:745:GLY:HA2	1:A:785:GLY:HA2	1.57	0.86
1:D:601:GLU:HA	1:D:669:LYS:HA	1.56	0.85
1:C:275:GLY:HA2	1:C:505:THR:CB	2.04	0.85
1:B:325:LYS:HZ2	1:B:543:ASN:HD21	1.23	0.84
1:C:333:LEU:CD2	1:C:541:LEU:CD2	2.52	0.84
1:C:275:GLY:HA3	1:C:505:THR:CG2	2.03	0.84
1:D:751:ASP:HB2	1:D:756:LEU:HD11	1.61	0.83
1:A:381:LEU:HB2	1:A:407:ILE:HG13	1.61	0.83
1:B:277:GLU:HB2	1:B:336:LEU:HD21	1.59	0.82
1:A:276:SER:OG	1:A:336:LEU:CD2	2.27	0.82
1:C:381:LEU:HB2	1:C:407:ILE:HG13	1.61	0.82
1:B:751:ASP:HB2	1:B:756:LEU:HD11	1.61	0.82
1:A:275:GLY:CA	1:A:505:THR:CB	2.58	0.82
1:D:670:ASN:HD21	1:D:674:TYR:H	1.28	0.81
1:B:670:ASN:HD21	1:B:674:TYR:H	1.28	0.81
1:C:746:ARG:HB2	1:C:784:GLU:HG3	1.63	0.80
1:A:435:LYS:HD3	1:A:437:VAL:HG23	1.62	0.80
1:C:276:SER:N	1:C:505:THR:CG2	2.42	0.80
1:B:336:LEU:HD23	1:B:337:SER:H	1.45	0.80
1:C:435:LYS:HD3	1:C:437:VAL:HG23	1.62	0.80
1:D:333:LEU:O	1:D:335:THR:N	2.15	0.80
1:A:746:ARG:HB2	1:A:784:GLU:HG3	1.63	0.80
1:C:276:SER:OG	1:C:336:LEU:CD2	2.29	0.80
1:D:624:GLY:N	1:D:645:PHE:O	2.16	0.79
1:D:671:GLN:HG2	1:D:674:TYR:HD2	1.47	0.79
1:A:623:LYS:HG3	1:A:647:ASP:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:GLY:CA	1:C:505:THR:CB	2.58	0.78
1:C:749:ILE:HD12	1:C:757:LEU:HD12	1.65	0.78
1:A:521:ASN:HB2	1:A:523:LYS:HG2	1.65	0.78
1:B:333:LEU:O	1:B:335:THR:N	2.16	0.78
1:D:277:GLU:HB2	1:D:336:LEU:HD21	1.64	0.78
1:B:371:PHE:HB2	1:B:502:VAL:HB	1.66	0.78
1:C:623:LYS:HG3	1:C:647:ASP:HA	1.65	0.78
1:A:360:LEU:N	1:A:436:ILE:O	2.15	0.77
1:B:624:GLY:N	1:B:645:PHE:O	2.15	0.77
1:B:671:GLN:HG2	1:B:674:TYR:HD2	1.47	0.77
1:C:351:SER:HB3	1:C:409:LYS:HD3	1.65	0.77
1:C:521:ASN:HB2	1:C:523:LYS:HG2	1.65	0.77
1:A:351:SER:HB3	1:A:409:LYS:HD3	1.65	0.77
1:A:722:TYR:HB3	1:A:784:GLU:HB3	1.67	0.77
1:D:371:PHE:HB2	1:D:502:VAL:HB	1.66	0.77
1:D:372:GLU:HB2	1:D:384:TYR:HE2	1.49	0.77
1:B:372:GLU:HB2	1:B:384:TYR:HE2	1.49	0.77
1:B:333:LEU:C	1:B:335:THR:HG1	1.92	0.77
1:B:514:GLY:N	1:B:527:THR:O	2.16	0.77
1:A:418:GLN:HA	1:A:443:ASN:HB3	1.67	0.77
1:A:749:ILE:HD12	1:A:757:LEU:HD12	1.65	0.77
1:D:757:LEU:HD12	1:D:770:ILE:HD11	1.68	0.76
1:D:579:ASN:ND2	1:D:599:ASP:OD1	2.19	0.76
1:D:336:LEU:HD23	1:D:337:SER:H	1.49	0.76
1:D:746:ARG:NH2	1:D:785:GLY:O	2.18	0.76
1:C:418:GLN:HA	1:C:443:ASN:HB3	1.67	0.76
1:C:722:TYR:HB3	1:C:784:GLU:HB3	1.67	0.76
1:D:742:LYS:HB2	1:D:794:ILE:HB	1.68	0.76
1:B:710:LYS:HB2	1:B:714:ARG:HB2	1.68	0.76
1:B:579:ASN:ND2	1:B:599:ASP:OD1	2.19	0.76
1:B:742:LYS:HB2	1:B:794:ILE:HB	1.68	0.76
1:B:746:ARG:NH2	1:B:785:GLY:O	2.18	0.76
1:D:514:GLY:N	1:D:527:THR:O	2.16	0.76
1:C:631:LYS:HG3	1:C:633:ASN:H	1.52	0.75
1:C:360:LEU:N	1:C:436:ILE:O	2.15	0.75
1:A:502:VAL:HG21	1:A:526:LEU:HB2	1.68	0.75
1:C:502:VAL:HG21	1:C:526:LEU:HB2	1.68	0.75
1:A:419:LYS:HB3	1:A:444:GLN:HA	1.68	0.75
1:B:757:LEU:HD12	1:B:770:ILE:HD11	1.68	0.75
1:A:278:ILE:H	1:A:336:LEU:HD11	1.52	0.75
1:A:276:SER:N	1:A:505:THR:CG2	2.44	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:LYS:HB3	1:D:444:GLN:HA	1.69	0.74
1:D:737:LEU:HA	1:D:800:ILE:HA	1.70	0.74
1:B:737:LEU:HA	1:B:800:ILE:HA	1.70	0.74
1:C:596:THR:HB	1:C:600:GLY:HA3	1.70	0.74
1:C:419:LYS:HB3	1:C:444:GLN:HA	1.68	0.73
1:D:710:LYS:HB2	1:D:714:ARG:HB2	1.68	0.73
1:B:333:LEU:C	1:B:335:THR:HG23	2.13	0.73
1:B:419:LYS:HB3	1:B:444:GLN:HA	1.69	0.73
1:B:355:ASP:HB3	1:B:692:LEU:HB2	1.71	0.73
1:B:350:GLY:O	1:B:414:LYS:NZ	2.21	0.73
1:D:355:ASP:HB3	1:D:692:LEU:HB2	1.71	0.73
1:C:495:ILE:HG23	1:C:522:GLN:HB3	1.71	0.73
1:A:411:PHE:O	1:A:420:TYR:OH	2.07	0.72
1:A:584:LYS:HE3	1:A:592:SER:HA	1.71	0.72
1:D:350:GLY:O	1:D:414:LYS:NZ	2.21	0.72
1:A:596:THR:HB	1:A:600:GLY:HA3	1.70	0.72
1:A:631:LYS:HG3	1:A:633:ASN:H	1.52	0.72
1:B:747:VAL:HB	1:B:781:ILE:HD11	1.72	0.72
1:C:411:PHE:O	1:C:420:TYR:OH	2.07	0.71
1:A:495:ILE:HG23	1:A:522:GLN:HB3	1.71	0.71
1:A:707:VAL:HG12	1:A:717:ILE:HA	1.72	0.71
1:A:698:PRO:HA	1:A:701:TRP:HD1	1.55	0.71
1:A:361:GLU:HA	1:A:435:LYS:HA	1.73	0.71
1:C:278:ILE:H	1:C:336:LEU:HD11	1.55	0.71
1:D:747:VAL:HB	1:D:781:ILE:HD11	1.72	0.71
1:C:361:GLU:HA	1:C:435:LYS:HA	1.73	0.71
1:B:333:LEU:C	1:B:335:THR:OG1	2.34	0.71
1:A:518:ASP:HB3	1:A:523:LYS:HB2	1.73	0.70
1:B:586:ASP:OD2	1:B:593:SER:N	2.22	0.70
1:C:717:ILE:HB	1:C:793:THR:HB	1.73	0.70
1:D:586:ASP:OD2	1:D:593:SER:N	2.22	0.70
1:B:372:GLU:HB3	1:B:382:LYS:HB3	1.71	0.70
1:D:496:TYR:HB2	1:D:523:LYS:HA	1.73	0.70
1:D:510:ILE:HA	1:D:530:SER:HA	1.73	0.70
1:C:510:ILE:HA	1:C:530:SER:HA	1.73	0.70
1:C:584:LYS:HE3	1:C:592:SER:HA	1.71	0.70
1:D:620:TYR:OH	1:D:653:LYS:NZ	2.20	0.70
1:C:707:VAL:HG12	1:C:717:ILE:HA	1.72	0.70
1:D:372:GLU:HB3	1:D:382:LYS:HB3	1.71	0.70
1:B:734:THR:HB	1:B:803:GLU:HB3	1.73	0.70
1:D:611:LYS:O	1:D:614:THR:OG1	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:734:THR:HB	1:D:803:GLU:HB3	1.73	0.70
1:A:596:THR:O	1:A:670:ASN:ND2	2.25	0.70
1:B:611:LYS:O	1:B:614:THR:OG1	2.10	0.70
1:D:349:ARG:O	1:D:408:HIS:ND1	2.24	0.70
1:C:698:PRO:HA	1:C:701:TRP:HD1	1.55	0.70
1:B:349:ARG:O	1:B:408:HIS:ND1	2.24	0.69
1:C:738:ARG:O	1:C:799:SER:OG	2.11	0.69
1:C:518:ASP:HB3	1:C:523:LYS:HB2	1.73	0.69
1:A:510:ILE:HA	1:A:530:SER:HA	1.73	0.69
1:A:278:ILE:CD1	1:A:336:LEU:HD13	2.20	0.69
1:B:510:ILE:HA	1:B:530:SER:HA	1.73	0.69
1:A:546:THR:HG22	1:A:548:LEU:HD22	1.75	0.69
1:A:738:ARG:O	1:A:799:SER:OG	2.11	0.69
1:B:496:TYR:HB2	1:B:523:LYS:HA	1.74	0.69
1:B:513:PHE:HA	1:B:528:GLY:HA2	1.74	0.69
1:D:421:TYR:HA	1:D:485:TYR:HA	1.75	0.69
1:D:558:SER:HB2	1:D:682:ILE:HA	1.75	0.69
1:A:360:LEU:HB2	1:A:436:ILE:HB	1.75	0.68
1:A:717:ILE:HB	1:A:793:THR:HB	1.73	0.68
1:C:546:THR:HG22	1:C:548:LEU:HD22	1.75	0.68
1:B:278:ILE:HG13	1:B:336:LEU:HD22	1.75	0.68
1:D:361:GLU:HA	1:D:435:LYS:HA	1.75	0.68
1:A:670:ASN:ND2	1:A:674:TYR:O	2.27	0.68
1:B:719:GLY:HA2	1:B:791:SER:HB3	1.76	0.68
1:A:278:ILE:HG13	1:A:336:LEU:HD11	1.63	0.68
1:B:558:SER:HB2	1:B:682:ILE:HA	1.75	0.68
1:C:360:LEU:HB2	1:C:436:ILE:HB	1.75	0.68
1:C:670:ASN:ND2	1:C:674:TYR:O	2.27	0.68
1:A:558:SER:HB2	1:A:682:ILE:HD13	1.76	0.68
1:C:558:SER:HB2	1:C:682:ILE:HD13	1.76	0.68
1:B:325:LYS:HZ2	1:B:543:ASN:ND2	1.79	0.68
1:D:513:PHE:HA	1:D:528:GLY:HA2	1.74	0.68
1:B:559:ILE:HG13	1:B:684:LEU:HD23	1.76	0.67
1:C:596:THR:O	1:C:670:ASN:ND2	2.25	0.67
1:D:333:LEU:C	1:D:335:THR:CG2	2.66	0.67
1:D:719:GLY:HA2	1:D:791:SER:HB3	1.76	0.67
1:B:349:ARG:HH11	1:B:494:GLY:HA2	1.60	0.67
1:B:746:ARG:H	1:B:785:GLY:HA2	1.59	0.67
1:B:437:VAL:HB	1:B:448:GLU:HB3	1.75	0.67
1:D:559:ILE:HG13	1:D:684:LEU:HD23	1.76	0.67
1:D:746:ARG:H	1:D:785:GLY:HA2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:TYR:HA	1:B:485:TYR:HA	1.75	0.67
1:D:593:SER:HA	1:D:679:ASN:HB3	1.76	0.67
1:D:437:VAL:HB	1:D:448:GLU:HB3	1.75	0.67
1:D:356:PRO:HG2	1:D:440:LYS:HB3	1.77	0.67
1:D:737:LEU:HD23	1:D:757:LEU:HD13	1.77	0.67
1:A:346:SER:HB2	1:A:499:LEU:HD22	1.76	0.67
1:C:564:ASN:HA	1:C:680:ASN:H	1.59	0.67
1:B:737:LEU:HD23	1:B:757:LEU:HD13	1.77	0.67
1:C:342:ASN:ND2	1:C:344:SER:O	2.28	0.66
1:A:352:ASP:H	1:A:414:LYS:HZ3	1.44	0.66
1:C:507:LEU:HD22	1:C:549:ILE:HB	1.77	0.66
1:A:507:LEU:HD22	1:A:549:ILE:HB	1.77	0.66
1:C:278:ILE:CG1	1:C:336:LEU:CD1	2.23	0.66
1:C:352:ASP:H	1:C:414:LYS:HZ3	1.42	0.66
1:B:361:GLU:HA	1:B:435:LYS:HA	1.75	0.66
1:B:427:PHE:HD2	1:B:467:LYS:HE3	1.60	0.66
1:D:700:ASP:HB3	1:D:725:GLN:HG3	1.77	0.66
1:B:593:SER:HA	1:B:679:ASN:HB3	1.76	0.66
1:D:278:ILE:HG13	1:D:336:LEU:HD22	1.76	0.66
1:B:339:ASN:HB3	1:B:527:THR:HG23	1.77	0.66
1:D:278:ILE:HG13	1:D:336:LEU:HD13	1.76	0.66
1:C:593:SER:HA	1:C:679:ASN:HB3	1.78	0.66
1:D:339:ASN:HB3	1:D:527:THR:HG23	1.77	0.66
1:D:372:GLU:HG2	1:D:501:VAL:HG22	1.77	0.66
1:D:349:ARG:HH11	1:D:494:GLY:HA2	1.60	0.66
1:B:700:ASP:HB3	1:B:725:GLN:HG3	1.77	0.66
1:C:168:LEU:HD21	1:C:265:LEU:HA	1.78	0.65
1:D:427:PHE:HD2	1:D:467:LYS:HE3	1.60	0.65
1:D:597:HIS:HB2	1:D:675:GLU:HG2	1.78	0.65
1:B:356:PRO:HG2	1:B:440:LYS:HB3	1.77	0.65
1:C:278:ILE:HG13	1:C:336:LEU:HD11	1.65	0.65
1:D:641:THR:O	1:D:671:GLN:NE2	2.30	0.65
1:C:346:SER:HB2	1:C:499:LEU:HD22	1.76	0.65
1:D:168:LEU:HD21	1:D:265:LEU:HA	1.78	0.65
1:B:620:TYR:OH	1:B:653:LYS:NZ	2.20	0.65
1:A:564:ASN:HA	1:A:680:ASN:H	1.59	0.65
1:B:333:LEU:C	1:B:335:THR:N	2.49	0.65
1:B:735:TYR:O	1:B:770:ILE:N	2.30	0.65
1:D:517:VAL:HG23	1:D:524:ILE:HA	1.79	0.65
1:A:342:ASN:ND2	1:A:344:SER:O	2.28	0.65
1:B:278:ILE:HG13	1:B:336:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLY:HA3	1:A:505:THR:HB	1.79	0.65
1:C:392:TYR:OH	1:C:429:GLU:OE2	2.13	0.65
1:C:275:GLY:HA3	1:C:505:THR:HB	1.78	0.65
1:C:619:GLN:HB3	1:C:682:ILE:HB	1.79	0.65
1:D:386:ALA:HB2	1:D:399:MET:HA	1.78	0.65
1:A:392:TYR:OH	1:A:429:GLU:OE2	2.13	0.64
1:A:593:SER:HA	1:A:679:ASN:HB3	1.78	0.64
1:B:168:LEU:HD21	1:B:265:LEU:HA	1.78	0.64
1:B:597:HIS:HB2	1:B:675:GLU:HG2	1.78	0.64
1:D:359:VAL:HA	1:D:437:VAL:HA	1.79	0.64
1:B:386:ALA:HB2	1:B:399:MET:HA	1.78	0.64
1:A:168:LEU:HD21	1:A:265:LEU:HA	1.78	0.64
1:B:372:GLU:HG2	1:B:501:VAL:HG22	1.77	0.64
1:C:519:GLU:O	1:C:522:GLN:NE2	2.30	0.64
1:A:519:GLU:O	1:A:522:GLN:NE2	2.30	0.64
1:A:619:GLN:HB3	1:A:682:ILE:HB	1.79	0.64
1:B:641:THR:O	1:B:671:GLN:NE2	2.30	0.64
1:C:517:VAL:HG12	1:C:524:ILE:HA	1.79	0.64
1:C:352:ASP:OD1	1:C:443:ASN:ND2	2.28	0.64
1:C:413:PRO:HB3	1:C:418:GLN:HB2	1.80	0.64
1:A:413:PRO:HB3	1:A:418:GLN:HB2	1.80	0.64
1:B:277:GLU:HB2	1:B:336:LEU:CD2	2.27	0.64
1:B:358:VAL:O	1:B:438:PHE:N	2.30	0.64
1:B:359:VAL:HA	1:B:437:VAL:HA	1.79	0.64
1:B:453:PHE:O	1:B:462:ASP:N	2.29	0.64
1:C:390:PRO:O	1:C:393:GLN:HG2	1.98	0.64
1:D:392:TYR:HB2	1:D:535:SER:HB2	1.80	0.64
1:A:275:GLY:HA3	1:A:505:THR:CB	2.26	0.63
1:B:517:VAL:HG23	1:B:524:ILE:HA	1.79	0.63
1:D:358:VAL:O	1:D:438:PHE:N	2.30	0.63
1:B:392:TYR:HB2	1:B:535:SER:HB2	1.80	0.63
1:A:517:VAL:HG12	1:A:524:ILE:HA	1.79	0.63
1:C:622:ILE:HA	1:C:678:GLY:HA2	1.80	0.63
1:B:730:GLU:N	1:B:735:TYR:OH	2.23	0.63
1:D:611:LYS:O	1:D:657:SER:OG	2.16	0.63
1:D:734:THR:HG23	1:D:771:LYS:HA	1.80	0.63
1:B:631:LYS:HG2	1:B:633:ASN:H	1.63	0.63
1:C:532:LEU:HD12	1:C:535:SER:HB2	1.81	0.63
1:D:474:LYS:HE3	1:D:484:GLU:HG2	1.81	0.63
1:A:390:PRO:O	1:A:393:GLN:HG2	1.98	0.62
1:A:742:LYS:N	1:A:794:ILE:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ARG:O	1:B:537:LEU:CB	2.45	0.62
1:D:631:LYS:HG2	1:D:633:ASN:H	1.63	0.62
1:D:735:TYR:O	1:D:770:ILE:N	2.30	0.62
1:A:352:ASP:OD1	1:A:443:ASN:ND2	2.27	0.62
1:A:717:ILE:N	1:A:793:THR:O	2.32	0.62
1:C:717:ILE:N	1:C:793:THR:O	2.32	0.62
1:D:333:LEU:CA	1:D:335:THR:CG2	2.76	0.62
1:D:453:PHE:O	1:D:462:ASP:N	2.30	0.62
1:B:611:LYS:O	1:B:657:SER:OG	2.16	0.62
1:A:532:LEU:HD12	1:A:535:SER:HB2	1.81	0.62
1:C:537:LEU:HA	1:C:541:LEU:HD13	1.81	0.62
1:B:707:VAL:HG12	1:B:717:ILE:HA	1.82	0.62
1:A:532:LEU:HA	1:A:535:SER:HB2	1.82	0.62
1:D:421:TYR:HB3	1:D:473:GLU:HB3	1.81	0.62
1:B:734:THR:HG23	1:B:771:LYS:HA	1.80	0.62
1:A:622:ILE:HA	1:A:678:GLY:HA2	1.80	0.61
1:A:741:VAL:HA	1:A:795:PHE:HA	1.82	0.61
1:B:607:GLY:N	1:B:664:ILE:O	2.33	0.61
1:C:282:TYR:HH	1:C:540:ASP:CG	1.99	0.61
1:C:349:ARG:HH22	1:C:415:GLN:HB3	1.65	0.61
1:C:761:VAL:HB	1:C:766:LEU:HD21	1.82	0.61
1:D:742:LYS:O	1:D:794:ILE:N	2.28	0.61
1:B:746:ARG:HH12	1:B:786:THR:HA	1.65	0.61
1:D:707:VAL:HG12	1:D:717:ILE:HA	1.82	0.61
1:B:421:TYR:HB3	1:B:473:GLU:HB3	1.81	0.61
1:D:586:ASP:HB3	1:D:677:TRP:HD1	1.66	0.61
1:A:537:LEU:HA	1:A:541:LEU:HD13	1.81	0.61
1:B:430:GLY:O	1:B:454:TYR:N	2.34	0.61
1:B:742:LYS:O	1:B:794:ILE:N	2.28	0.61
1:C:742:LYS:N	1:C:794:ILE:O	2.31	0.61
1:D:746:ARG:HH12	1:D:786:THR:HA	1.65	0.61
1:A:761:VAL:HB	1:A:766:LEU:HD21	1.82	0.61
1:B:559:ILE:HG23	1:B:609:LYS:HD2	1.82	0.61
1:D:325:LYS:HZ3	1:D:543:ASN:CG	1.99	0.61
1:B:352:ASP:OD1	1:B:443:ASN:ND2	2.33	0.61
1:D:430:GLY:O	1:D:454:TYR:N	2.34	0.61
1:D:559:ILE:HG23	1:D:609:LYS:HD2	1.82	0.61
1:B:440:LYS:HA	1:B:445:LEU:HA	1.83	0.60
1:D:352:ASP:OD1	1:D:443:ASN:ND2	2.33	0.60
1:D:421:TYR:HB2	1:D:472:LYS:HB2	1.82	0.60
1:A:349:ARG:HH22	1:A:415:GLN:HB3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LYS:HE3	1:B:484:GLU:HG2	1.81	0.60
1:B:421:TYR:HB2	1:B:472:LYS:HB2	1.82	0.60
1:B:586:ASP:HB3	1:B:677:TRP:HD1	1.66	0.60
1:D:352:ASP:HA	1:D:443:ASN:HD21	1.67	0.60
1:D:440:LYS:HB2	1:D:445:LEU:HD13	1.84	0.60
1:B:726:PHE:HD1	1:B:780:PHE:HB3	1.66	0.60
1:C:532:LEU:HA	1:C:535:SER:HB2	1.82	0.60
1:C:741:VAL:HA	1:C:795:PHE:HA	1.82	0.60
1:D:637:LEU:HD13	1:D:655:PHE:HE2	1.67	0.60
1:D:277:GLU:HB2	1:D:336:LEU:CD2	2.31	0.60
1:B:537:LEU:HA	1:B:541:LEU:HD12	1.83	0.60
1:D:670:ASN:ND2	1:D:674:TYR:O	2.35	0.60
1:A:751:ASP:HB2	1:A:756:LEU:HD21	1.84	0.60
1:C:505:THR:O	1:C:551:SER:N	2.35	0.60
1:C:631:LYS:HG2	1:C:667:LEU:HD13	1.84	0.60
1:A:744:THR:HB	1:A:762:LYS:HD2	1.84	0.60
1:B:403:ILE:HG21	1:B:686:ILE:HA	1.84	0.60
1:C:275:GLY:HA3	1:C:505:THR:CB	2.26	0.60
1:C:447:TYR:CE1	1:C:515:LEU:HB2	2.37	0.60
1:D:607:GLY:N	1:D:664:ILE:O	2.34	0.60
1:C:513:PHE:HA	1:C:528:GLY:HA2	1.83	0.59
1:C:744:THR:HB	1:C:762:LYS:HD2	1.84	0.59
1:B:440:LYS:HB2	1:B:445:LEU:HD13	1.84	0.59
1:B:670:ASN:ND2	1:B:674:TYR:O	2.35	0.59
1:D:726:PHE:HD1	1:D:780:PHE:HB3	1.66	0.59
1:B:783:LEU:HB3	1:B:795:PHE:HE2	1.67	0.59
1:D:365:GLY:HA3	1:D:387:ARG:HH21	1.67	0.59
1:D:736:HIS:NE2	1:D:803:GLU:OE2	2.35	0.59
1:D:744:THR:HA	1:D:762:LYS:HA	1.84	0.59
1:A:276:SER:OG	1:A:336:LEU:HD21	2.02	0.59
1:A:419:LYS:N	1:A:443:ASN:O	2.36	0.59
1:B:637:LEU:HD13	1:B:655:PHE:HE2	1.67	0.59
1:D:537:LEU:HA	1:D:541:LEU:HD12	1.84	0.59
1:A:513:PHE:HA	1:A:528:GLY:HA2	1.83	0.59
1:A:631:LYS:HG2	1:A:667:LEU:HD13	1.84	0.59
1:B:365:GLY:HA3	1:B:387:ARG:HH21	1.67	0.59
1:B:510:ILE:HG22	1:B:530:SER:HB2	1.84	0.59
1:C:278:ILE:CD1	1:C:336:LEU:HD13	2.23	0.59
1:A:447:TYR:CE1	1:A:515:LEU:HB2	2.37	0.59
1:A:505:THR:O	1:A:551:SER:N	2.35	0.59
1:B:511:TYR:HB3	1:B:531:TYR:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:THR:HA	1:B:762:LYS:HA	1.84	0.59
1:C:745:GLY:N	1:C:761:VAL:O	2.24	0.59
1:C:751:ASP:HB2	1:C:756:LEU:HD21	1.84	0.59
1:D:404:TYR:HA	1:D:687:LYS:HD2	1.85	0.59
1:D:510:ILE:HG22	1:D:530:SER:HB2	1.84	0.59
1:A:488:ILE:HG12	1:A:519:GLU:HB3	1.85	0.59
1:C:423:LYS:HE2	1:C:473:GLU:H	1.67	0.59
1:D:440:LYS:HA	1:D:445:LEU:HA	1.83	0.59
1:A:423:LYS:HE2	1:A:473:GLU:H	1.67	0.59
1:C:698:PRO:HA	1:C:701:TRP:CD1	2.38	0.59
1:A:513:PHE:HZ	1:A:526:LEU:HD22	1.67	0.58
1:D:572:SER:O	1:D:574:ARG:NH1	2.36	0.58
1:A:701:TRP:HA	1:A:725:GLN:HB2	1.85	0.58
1:B:710:LYS:NZ	1:B:716:GLU:OE1	2.34	0.58
1:C:441:ARG:HG2	1:C:442:LEU:HD12	1.84	0.58
1:D:511:TYR:HB3	1:D:531:TYR:CZ	2.37	0.58
1:B:627:ALA:HB1	1:B:629:TYR:HE2	1.68	0.58
1:D:783:LEU:HB3	1:D:795:PHE:HE2	1.67	0.58
1:A:278:ILE:CG1	1:A:336:LEU:CD1	2.21	0.58
1:C:701:TRP:HA	1:C:725:GLN:HB2	1.86	0.58
1:D:598:LYS:H	1:D:670:ASN:ND2	2.01	0.58
1:A:584:LYS:HG3	1:A:585:ALA:N	2.18	0.58
1:A:441:ARG:HG2	1:A:442:LEU:HD12	1.84	0.58
1:B:404:TYR:HA	1:B:687:LYS:HD2	1.85	0.58
1:B:598:LYS:H	1:B:670:ASN:ND2	2.01	0.58
1:C:421:TYR:HB2	1:C:446:GLY:HA2	1.86	0.58
1:C:513:PHE:HZ	1:C:526:LEU:HD22	1.67	0.58
1:D:488:ILE:HG12	1:D:519:GLU:HB3	1.84	0.58
1:A:277:GLU:HB2	1:A:336:LEU:HG	1.86	0.58
1:B:742:LYS:N	1:B:794:ILE:O	2.33	0.58
1:C:595:TYR:HE2	1:C:675:GLU:HB3	1.69	0.58
1:D:403:ILE:HG21	1:D:686:ILE:HA	1.84	0.58
1:A:275:GLY:CA	1:A:505:THR:HB	2.34	0.58
1:A:275:GLY:HA3	1:A:505:THR:HG21	1.72	0.58
1:B:352:ASP:HA	1:B:443:ASN:HD21	1.67	0.58
1:B:488:ILE:HG12	1:B:519:GLU:HB3	1.84	0.58
1:D:625:ARG:NE	1:D:642:LYS:O	2.32	0.58
1:D:627:ALA:HB1	1:D:629:TYR:HE2	1.68	0.58
1:D:730:GLU:N	1:D:735:TYR:OH	2.23	0.58
1:A:497:MET:HA	1:A:524:ILE:HB	1.85	0.58
1:B:335:THR:HB	1:B:336:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:ILE:HG12	1:C:519:GLU:HB3	1.85	0.58
1:D:627:ALA:HA	1:D:641:THR:HG22	1.86	0.58
1:B:625:ARG:NE	1:B:642:LYS:O	2.32	0.57
1:B:423:LYS:HB2	1:B:473:GLU:C	2.30	0.57
1:B:767:THR:OG1	1:B:768:ARG:NH2	2.37	0.57
1:C:346:SER:OG	1:C:375:ASN:ND2	2.37	0.57
1:C:497:MET:HA	1:C:524:ILE:HB	1.85	0.57
1:D:423:LYS:HB2	1:D:473:GLU:C	2.30	0.57
1:D:767:THR:OG1	1:D:768:ARG:NH2	2.37	0.57
1:A:421:TYR:HB2	1:A:446:GLY:HA2	1.86	0.57
1:A:749:ILE:HG22	1:A:756:LEU:HB2	1.86	0.57
1:B:439:GLU:O	1:B:446:GLY:N	2.35	0.57
1:B:572:SER:O	1:B:574:ARG:NH1	2.36	0.57
1:B:736:HIS:NE2	1:B:803:GLU:OE2	2.35	0.57
1:A:346:SER:OG	1:A:375:ASN:ND2	2.37	0.57
1:A:453:PHE:HB3	1:A:462:ASP:OD1	2.05	0.57
1:A:630:LEU:O	1:A:637:LEU:N	2.33	0.57
1:C:453:PHE:HB3	1:C:462:ASP:OD1	2.05	0.57
1:D:533:ARG:O	1:D:537:LEU:CB	2.45	0.57
1:C:345:TYR:HH	1:C:525:THR:HG1	1.51	0.57
1:A:338:ASN:ND2	1:A:530:SER:O	2.38	0.57
1:A:595:TYR:HE2	1:A:675:GLU:HB3	1.69	0.57
1:B:438:PHE:HA	1:B:447:TYR:HA	1.87	0.57
1:B:604:GLN:O	1:B:666:PHE:N	2.31	0.57
1:D:333:LEU:CA	1:D:335:THR:HG23	2.32	0.57
1:A:412:CYS:SG	1:A:497:MET:HB3	2.44	0.57
1:B:748:SER:O	1:B:782:ALA:N	2.37	0.57
1:C:338:ASN:ND2	1:C:530:SER:O	2.38	0.57
1:C:412:CYS:SG	1:C:497:MET:HB3	2.43	0.57
1:D:631:LYS:HB2	1:D:636:THR:HG23	1.87	0.57
1:D:632:ASN:HB2	1:D:663:GLU:HB2	1.86	0.57
1:D:742:LYS:N	1:D:794:ILE:O	2.33	0.57
1:C:345:TYR:OH	1:C:525:THR:OG1	2.22	0.57
1:C:419:LYS:N	1:C:443:ASN:O	2.36	0.57
1:A:511:TYR:N	1:A:529:LYS:O	2.37	0.57
1:B:632:ASN:HB2	1:B:663:GLU:HB2	1.86	0.57
1:D:748:SER:O	1:D:782:ALA:N	2.37	0.57
1:C:420:TYR:CE1	1:C:488:ILE:HD12	2.40	0.57
1:D:418:GLN:NE2	1:D:420:TYR:OH	2.35	0.57
1:A:377:PRO:HG2	1:A:380:ILE:HD12	1.86	0.56
1:A:422:ILE:O	1:A:484:GLU:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:GLY:N	1:A:761:VAL:O	2.24	0.56
1:B:389:LYS:N	1:B:393:GLN:O	2.37	0.56
1:B:623:LYS:HB3	1:B:677:TRP:HB2	1.86	0.56
1:A:696:LEU:HD13	1:A:798:VAL:HB	1.86	0.56
1:D:346:SER:HB2	1:D:499:LEU:HD22	1.86	0.56
1:D:623:LYS:HB3	1:D:677:TRP:HB2	1.86	0.56
1:A:557:SER:HB2	1:A:684:LEU:HD11	1.88	0.56
1:A:558:SER:HB2	1:A:682:ILE:HA	1.88	0.56
1:B:602:PHE:HB2	1:B:668:PHE:HD1	1.71	0.56
1:C:277:GLU:HB2	1:C:336:LEU:CG	2.36	0.56
1:C:422:ILE:O	1:C:484:GLU:HG3	2.04	0.56
1:C:448:GLU:HA	1:C:470:SER:HA	1.87	0.56
1:C:735:TYR:HB2	1:C:770:ILE:HD11	1.87	0.56
1:D:335:THR:HB	1:D:336:LEU:HD12	1.88	0.56
1:D:438:PHE:HA	1:D:447:TYR:HA	1.87	0.56
1:D:710:LYS:NZ	1:D:716:GLU:OE1	2.34	0.56
1:A:420:TYR:CE1	1:A:488:ILE:HD12	2.40	0.56
1:A:448:GLU:HA	1:A:470:SER:HA	1.86	0.56
1:A:735:TYR:HB2	1:A:770:ILE:HD11	1.86	0.56
1:B:361:GLU:HB2	1:B:435:LYS:HD3	1.87	0.56
1:B:730:GLU:OE1	1:B:735:TYR:OH	2.20	0.56
1:D:657:SER:HB2	1:D:661:PRO:HG3	1.87	0.56
1:B:627:ALA:HA	1:B:641:THR:HG22	1.86	0.56
1:B:631:LYS:HB2	1:B:636:THR:HG23	1.87	0.56
1:C:511:TYR:N	1:C:529:LYS:O	2.37	0.56
1:C:584:LYS:HG3	1:C:585:ALA:N	2.18	0.56
1:C:696:LEU:HD13	1:C:798:VAL:HB	1.86	0.56
1:B:631:LYS:O	1:B:665:TYR:N	2.39	0.56
1:C:346:SER:OG	1:C:348:ASN:ND2	2.38	0.56
1:C:377:PRO:HG2	1:C:380:ILE:HD12	1.86	0.56
1:C:434:THR:OG1	1:C:452:ASN:OD1	2.24	0.56
1:C:558:SER:HB2	1:C:682:ILE:HA	1.88	0.56
1:C:744:THR:HA	1:C:762:LYS:HA	1.87	0.56
1:D:369:ILE:HD12	1:D:507:LEU:HD22	1.88	0.56
1:B:369:ILE:HD12	1:B:507:LEU:HD22	1.88	0.56
1:B:733:SER:OG	1:B:735:TYR:OH	2.19	0.56
1:D:709:MET:HA	1:D:715:LEU:HA	1.87	0.56
1:A:577:ASN:HB2	1:A:580:ALA:HB3	1.88	0.56
1:B:600:GLY:O	1:B:670:ASN:N	2.36	0.56
1:D:355:ASP:O	1:D:692:LEU:N	2.33	0.56
1:D:383:GLY:O	1:D:402:THR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:THR:OG1	1:A:452:ASN:OD1	2.24	0.56
1:A:698:PRO:HA	1:A:701:TRP:CD1	2.38	0.56
1:B:447:TYR:O	1:B:472:LYS:HD2	2.06	0.56
1:B:657:SER:HB2	1:B:661:PRO:HG3	1.87	0.56
1:D:602:PHE:HB2	1:D:668:PHE:HD1	1.71	0.56
1:B:696:LEU:HG	1:B:800:ILE:HG22	1.88	0.55
1:B:709:MET:HA	1:B:715:LEU:HA	1.87	0.55
1:C:277:GLU:HB2	1:C:336:LEU:HG	1.87	0.55
1:C:630:LEU:O	1:C:637:LEU:N	2.33	0.55
1:D:447:TYR:O	1:D:472:LYS:HD2	2.06	0.55
1:C:557:SER:HB2	1:C:684:LEU:HD11	1.87	0.55
1:D:696:LEU:HG	1:D:800:ILE:HG22	1.88	0.55
1:A:277:GLU:HB2	1:A:336:LEU:CG	2.36	0.55
1:A:744:THR:HA	1:A:762:LYS:HA	1.87	0.55
1:C:749:ILE:HG22	1:C:756:LEU:HB2	1.87	0.55
1:D:716:GLU:HG3	1:D:794:ILE:HG13	1.88	0.55
1:B:694:GLN:NE2	1:B:798:VAL:O	2.40	0.55
1:C:540:ASP:O	1:C:543:ASN:ND2	2.39	0.55
1:C:584:LYS:HG3	1:C:585:ALA:H	1.71	0.55
1:B:346:SER:HB2	1:B:499:LEU:HD22	1.86	0.55
1:C:577:ASN:HB2	1:C:580:ALA:HB3	1.88	0.55
1:D:631:LYS:O	1:D:665:TYR:N	2.39	0.55
1:C:750:ILE:HG22	1:C:755:TYR:HA	1.89	0.55
1:A:346:SER:OG	1:A:348:ASN:ND2	2.39	0.55
1:B:532:LEU:HD12	1:B:533:ARG:HG3	1.89	0.55
1:D:694:GLN:NE2	1:D:798:VAL:O	2.40	0.55
1:A:790:ASN:OD1	1:A:791:SER:N	2.40	0.55
1:C:496:TYR:HD2	1:C:522:GLN:HB2	1.72	0.55
1:A:559:ILE:HB	1:A:683:ILE:HB	1.89	0.55
1:B:383:GLY:O	1:B:402:THR:N	2.39	0.55
1:B:594:LEU:HB2	1:B:668:PHE:CE1	2.42	0.55
1:B:632:ASN:N	1:B:664:ILE:HD13	2.22	0.55
1:C:276:SER:OG	1:C:336:LEU:HD21	2.05	0.55
1:D:738:ARG:HG2	1:D:767:THR:HA	1.89	0.55
1:B:362:ALA:N	1:B:434:THR:O	2.31	0.55
1:B:716:GLU:HG3	1:B:794:ILE:HG13	1.88	0.55
1:C:559:ILE:HB	1:C:683:ILE:HB	1.89	0.55
1:D:361:GLU:HB2	1:D:435:LYS:HD3	1.87	0.55
1:D:439:GLU:O	1:D:446:GLY:N	2.35	0.55
1:D:702:ILE:HD12	1:D:724:LYS:HG3	1.88	0.55
1:B:418:GLN:NE2	1:B:420:TYR:OH	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LEU:O	1:A:436:ILE:N	2.35	0.54
1:A:584:LYS:HG3	1:A:585:ALA:H	1.72	0.54
1:A:730:GLU:O	1:A:773:THR:OG1	2.25	0.54
1:B:347:LYS:HE3	1:B:496:TYR:CZ	2.42	0.54
1:B:355:ASP:O	1:B:692:LEU:N	2.33	0.54
1:B:738:ARG:HG2	1:B:767:THR:HA	1.89	0.54
1:C:504:GLU:HG3	1:C:532:LEU:HD22	1.89	0.54
1:C:790:ASN:OD1	1:C:791:SER:N	2.40	0.54
1:A:540:ASP:O	1:A:543:ASN:ND2	2.39	0.54
1:D:347:LYS:HE3	1:D:496:TYR:CZ	2.42	0.54
1:D:616:TYR:HA	1:D:686:ILE:H	1.73	0.54
1:D:636:THR:HG21	1:D:639:GLU:HB2	1.90	0.54
1:A:750:ILE:HG22	1:A:755:TYR:HA	1.89	0.54
1:B:431:TYR:HA	1:B:453:PHE:HA	1.89	0.54
1:C:406:ASP:OD1	1:C:406:ASP:N	2.40	0.54
1:C:573:TRP:O	1:C:574:ARG:NH1	2.36	0.54
1:B:702:ILE:HD12	1:B:724:LYS:HG3	1.88	0.54
1:A:365:GLY:HA3	1:A:387:ARG:HE	1.73	0.54
1:B:616:TYR:HA	1:B:686:ILE:H	1.73	0.54
1:D:431:TYR:HA	1:D:453:PHE:HA	1.89	0.54
1:A:504:GLU:HG3	1:A:532:LEU:HD22	1.90	0.54
1:B:636:THR:HG21	1:B:639:GLU:HB2	1.90	0.54
1:D:735:TYR:HB2	1:D:770:ILE:HB	1.89	0.54
1:D:378:LEU:HD12	1:D:654:LYS:HE2	1.89	0.54
1:D:532:LEU:HD12	1:D:533:ARG:HG3	1.89	0.54
1:D:594:LEU:HB2	1:D:668:PHE:CE1	2.42	0.54
1:D:632:ASN:N	1:D:664:ILE:HD13	2.22	0.54
1:A:496:TYR:HD2	1:A:522:GLN:HB2	1.72	0.53
1:B:745:GLY:N	1:B:761:VAL:O	2.36	0.53
1:C:365:GLY:HA3	1:C:387:ARG:HE	1.73	0.53
1:C:539:THR:HA	1:C:544:ASN:HD21	1.73	0.53
1:B:378:LEU:HD12	1:B:654:LYS:HE2	1.89	0.53
1:B:420:TYR:O	1:B:486:SER:N	2.38	0.53
1:D:454:TYR:HA	1:D:461:ILE:HA	1.89	0.53
1:D:471:TRP:HB2	1:D:476:CYS:SG	2.48	0.53
1:D:730:GLU:OE1	1:D:735:TYR:OH	2.20	0.53
1:A:539:THR:HA	1:A:544:ASN:HD21	1.73	0.53
1:C:559:ILE:HD12	1:C:683:ILE:HG22	1.91	0.53
1:D:709:MET:HB3	1:D:715:LEU:HD23	1.91	0.53
1:A:436:ILE:HG12	1:A:449:VAL:HG22	1.90	0.53
1:B:735:TYR:HB2	1:B:770:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:TRP:HB3	1:A:723:PHE:HD1	1.74	0.53
1:C:366:TYR:CE1	1:C:387:ARG:HG2	2.44	0.53
1:C:518:ASP:O	1:C:523:LYS:N	2.39	0.53
1:C:701:TRP:HB3	1:C:723:PHE:HD1	1.74	0.53
1:D:511:TYR:N	1:D:529:LYS:O	2.42	0.53
1:D:647:ASP:O	1:D:649:GLN:NE2	2.42	0.53
1:D:733:SER:OG	1:D:735:TYR:OH	2.19	0.53
1:A:625:ARG:HE	1:A:674:TYR:HB3	1.74	0.53
1:C:730:GLU:O	1:C:773:THR:OG1	2.25	0.53
1:D:570:THR:HG23	1:D:582:VAL:HG22	1.91	0.53
1:B:454:TYR:HA	1:B:461:ILE:HA	1.89	0.53
1:C:333:LEU:C	1:C:335:THR:H	2.17	0.53
1:C:625:ARG:HE	1:C:674:TYR:HB3	1.74	0.53
1:D:697:LYS:N	1:D:725:GLN:HE22	2.07	0.53
1:A:341:SER:HA	1:A:502:VAL:HG13	1.91	0.53
1:B:471:TRP:HB2	1:B:476:CYS:SG	2.49	0.53
1:C:275:GLY:HA3	1:C:505:THR:HG21	1.74	0.53
1:A:366:TYR:CE1	1:A:387:ARG:HG2	2.43	0.53
1:B:563:TRP:HE3	1:B:680:ASN:HA	1.74	0.53
1:B:697:LYS:N	1:B:725:GLN:HE22	2.07	0.53
1:D:339:ASN:HD21	1:D:529:LYS:HG2	1.74	0.53
1:A:371:PHE:HB2	1:A:502:VAL:HB	1.91	0.52
1:A:386:ALA:HB2	1:A:399:MET:HA	1.91	0.52
1:A:518:ASP:O	1:A:523:LYS:N	2.39	0.52
1:B:647:ASP:O	1:B:649:GLN:NE2	2.42	0.52
1:C:423:LYS:HG3	1:C:425:ILE:HG13	1.91	0.52
1:D:333:LEU:HA	1:D:335:THR:CG2	2.39	0.52
1:B:555:TYR:CG	1:B:682:ILE:HG21	2.44	0.52
1:B:570:THR:HG23	1:B:582:VAL:HG22	1.91	0.52
1:C:430:GLY:O	1:C:454:TYR:N	2.42	0.52
1:C:386:ALA:HB2	1:C:399:MET:HA	1.90	0.52
1:B:363:ALA:HB3	1:B:366:TYR:CG	2.45	0.52
1:B:423:LYS:HD2	1:B:477:GLU:HB2	1.91	0.52
1:A:333:LEU:C	1:A:335:THR:H	2.16	0.52
1:A:423:LYS:HG3	1:A:425:ILE:HG13	1.91	0.52
1:A:430:GLY:O	1:A:454:TYR:N	2.42	0.52
1:D:532:LEU:O	1:D:536:LEU:HG	2.09	0.52
1:D:555:TYR:CG	1:D:682:ILE:HG21	2.44	0.52
1:A:406:ASP:HB2	1:A:408:HIS:CD2	2.45	0.52
1:A:559:ILE:HD12	1:A:683:ILE:HG22	1.91	0.52
1:C:436:ILE:HG12	1:C:449:VAL:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:VAL:HB	1:C:507:LEU:HG	1.92	0.52
1:B:377:PRO:HD3	1:B:652:THR:OG1	2.09	0.52
1:B:622:ILE:HB	1:B:626:PRO:HG3	1.92	0.52
1:B:739:LEU:HD12	1:B:798:VAL:HA	1.92	0.52
1:C:360:LEU:O	1:C:436:ILE:N	2.35	0.52
1:B:511:TYR:N	1:B:529:LYS:O	2.42	0.52
1:B:709:MET:HB3	1:B:715:LEU:HD23	1.91	0.52
1:D:423:LYS:O	1:D:514:GLY:HA2	2.10	0.52
1:D:604:GLN:O	1:D:666:PHE:N	2.31	0.52
1:D:745:GLY:N	1:D:761:VAL:O	2.36	0.52
1:C:341:SER:HA	1:C:502:VAL:HG13	1.91	0.52
1:C:488:ILE:HD11	1:C:517:VAL:HB	1.92	0.52
1:C:740:SER:HA	1:C:765:ASP:HA	1.92	0.52
1:D:389:LYS:N	1:D:393:GLN:O	2.37	0.52
1:C:729:LEU:HD13	1:C:779:CYS:HB3	1.92	0.51
1:D:600:GLY:O	1:D:670:ASN:N	2.36	0.51
1:D:751:ASP:HA	1:D:779:CYS:HA	1.92	0.51
1:A:740:SER:HA	1:A:765:ASP:HA	1.92	0.51
1:B:588:ILE:HG12	1:B:590:GLY:H	1.74	0.51
1:B:769:VAL:O	1:B:771:LYS:NZ	2.29	0.51
1:D:277:GLU:HB2	1:D:336:LEU:HD11	1.92	0.51
1:D:338:ASN:HB3	1:D:533:ARG:NH2	2.25	0.51
1:D:711:ASP:OD1	1:D:714:ARG:NH2	2.44	0.51
1:A:333:LEU:O	1:A:335:THR:N	2.44	0.51
1:B:338:ASN:HB3	1:B:533:ARG:NH2	2.25	0.51
1:B:532:LEU:O	1:B:536:LEU:HG	2.09	0.51
1:C:584:LYS:HB2	1:C:588:ILE:HG12	1.92	0.51
1:D:363:ALA:HB3	1:D:366:TYR:CG	2.45	0.51
1:D:377:PRO:HD3	1:D:652:THR:OG1	2.09	0.51
1:D:588:ILE:HG12	1:D:590:GLY:H	1.74	0.51
1:C:275:GLY:CA	1:C:505:THR:HB	2.34	0.51
1:D:739:LEU:HD12	1:D:798:VAL:HA	1.92	0.51
1:A:488:ILE:HD11	1:A:517:VAL:HB	1.92	0.51
1:B:423:LYS:O	1:B:514:GLY:HA2	2.10	0.51
1:A:394:VAL:HB	1:A:507:LEU:HG	1.92	0.51
1:A:586:ASP:N	1:A:586:ASP:OD1	2.44	0.51
1:B:711:ASP:OD1	1:B:714:ARG:NH2	2.44	0.51
1:C:586:ASP:N	1:C:586:ASP:OD1	2.44	0.51
1:B:339:ASN:HD21	1:B:529:LYS:HG2	1.74	0.51
1:C:447:TYR:OH	1:C:515:LEU:N	2.44	0.51
1:C:620:TYR:HA	1:C:680:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LYS:HZ3	1:A:473:GLU:HB3	1.76	0.51
1:A:589:LYS:HE2	1:A:677:TRP:CD1	2.46	0.51
1:A:620:TYR:HA	1:A:680:ASN:O	2.11	0.51
1:C:371:PHE:HB2	1:C:502:VAL:HB	1.91	0.51
1:D:341:SER:OG	1:D:342:ASN:N	2.44	0.51
1:D:599:ASP:OD1	1:D:599:ASP:N	2.44	0.51
1:D:622:ILE:HB	1:D:626:PRO:HG3	1.92	0.51
1:A:564:ASN:OD1	1:A:679:ASN:HB2	2.11	0.51
1:B:346:SER:OG	1:B:348:ASN:ND2	2.44	0.51
1:C:564:ASN:OD1	1:C:679:ASN:HB2	2.11	0.51
1:A:278:ILE:H	1:A:336:LEU:CD1	2.22	0.51
1:B:346:SER:O	1:B:497:MET:N	2.44	0.51
1:D:333:LEU:HA	1:D:335:THR:HG21	1.93	0.51
1:D:423:LYS:HD2	1:D:477:GLU:HB2	1.91	0.51
1:D:586:ASP:OD1	1:D:595:TYR:N	2.44	0.51
1:B:586:ASP:OD1	1:B:595:TYR:N	2.44	0.50
1:C:333:LEU:O	1:C:335:THR:N	2.44	0.50
1:D:563:TRP:HE3	1:D:680:ASN:HA	1.74	0.50
1:B:333:LEU:C	1:B:335:THR:CG2	2.83	0.50
1:B:736:HIS:HD2	1:B:803:GLU:HB2	1.75	0.50
1:C:406:ASP:HB2	1:C:408:HIS:CD2	2.45	0.50
1:C:488:ILE:HG21	1:C:495:ILE:HG21	1.92	0.50
1:C:605:PHE:HA	1:C:665:TYR:HB3	1.94	0.50
1:D:345:TYR:CE2	1:D:523:LYS:HD3	2.47	0.50
1:A:488:ILE:HG21	1:A:495:ILE:HG21	1.92	0.50
1:B:341:SER:OG	1:B:342:ASN:N	2.44	0.50
1:B:751:ASP:HA	1:B:779:CYS:HA	1.92	0.50
1:C:275:GLY:HA2	1:C:505:THR:HG22	0.51	0.50
1:C:372:GLU:HA	1:C:501:VAL:HA	1.94	0.50
1:A:352:ASP:H	1:A:414:LYS:NZ	2.09	0.50
1:A:374:LEU:HB2	1:A:380:ILE:HB	1.94	0.50
1:A:431:TYR:HA	1:A:453:PHE:HA	1.93	0.50
1:A:605:PHE:HA	1:A:665:TYR:HB3	1.94	0.50
1:C:282:TYR:CZ	1:C:540:ASP:OD1	2.65	0.50
1:C:589:LYS:HE2	1:C:677:TRP:CD1	2.46	0.50
1:D:372:GLU:HB2	1:D:384:TYR:CE2	2.39	0.50
1:D:736:HIS:HD2	1:D:803:GLU:HB2	1.75	0.50
1:C:606:ILE:HD11	1:C:630:LEU:HD11	1.94	0.50
1:A:447:TYR:OH	1:A:515:LEU:N	2.44	0.50
1:B:427:PHE:CD2	1:B:467:LYS:HE3	2.45	0.50
1:D:346:SER:OG	1:D:348:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:LEU:HD11	1:D:658:GLY:H	1.77	0.50
1:A:729:LEU:HD13	1:A:779:CYS:HB3	1.92	0.50
1:C:374:LEU:HB2	1:C:380:ILE:HB	1.94	0.50
1:C:566:THR:OG1	1:C:567:SER:N	2.44	0.50
1:C:596:THR:OG1	1:C:676:ALA:HB3	2.12	0.50
1:D:346:SER:O	1:D:497:MET:N	2.44	0.50
1:D:594:LEU:HB2	1:D:668:PHE:HE1	1.77	0.50
1:A:358:VAL:HG21	1:A:410:LEU:HD22	1.94	0.50
1:B:277:GLU:HB2	1:B:336:LEU:CG	2.42	0.50
1:B:345:TYR:CE2	1:B:523:LYS:HD3	2.47	0.50
1:B:599:ASP:OD1	1:B:599:ASP:N	2.43	0.50
1:C:413:PRO:HG2	1:C:490:ALA:HB2	1.94	0.50
1:D:519:GLU:O	1:D:522:GLN:NE2	2.36	0.50
1:A:582:VAL:HG13	1:A:585:ALA:HB2	1.94	0.50
1:B:707:VAL:HB	1:B:723:PHE:CZ	2.47	0.50
1:C:423:LYS:HZ3	1:C:473:GLU:HB3	1.77	0.50
1:D:420:TYR:O	1:D:486:SER:N	2.38	0.50
1:B:380:ILE:HG21	1:B:403:ILE:HG23	1.93	0.49
1:B:454:TYR:CE2	1:B:456:PRO:HA	2.47	0.49
1:B:625:ARG:HA	1:B:643:ASN:O	2.12	0.49
1:B:640:ASP:HA	1:B:642:LYS:HE2	1.94	0.49
1:C:533:ARG:HG2	1:C:537:LEU:HD23	1.94	0.49
1:A:584:LYS:HB2	1:A:588:ILE:HG12	1.92	0.49
1:B:381:LEU:HB2	1:B:407:ILE:HG12	1.94	0.49
1:D:277:GLU:HB2	1:D:336:LEU:CG	2.42	0.49
1:D:353:ILE:HG13	1:D:797:ASN:HD22	1.78	0.49
1:D:380:ILE:HG21	1:D:403:ILE:HG23	1.93	0.49
1:D:381:LEU:HB2	1:D:407:ILE:HG12	1.94	0.49
1:A:606:ILE:HD11	1:A:630:LEU:HD11	1.94	0.49
1:C:356:PRO:HB3	1:C:689:LEU:HD21	1.94	0.49
1:D:357:ILE:HG13	1:D:438:PHE:O	2.13	0.49
1:D:516:THR:HG23	1:D:525:THR:HB	1.94	0.49
1:D:702:ILE:N	1:D:724:LYS:O	2.45	0.49
1:A:573:TRP:O	1:A:574:ARG:NH1	2.36	0.49
1:B:594:LEU:HB3	1:B:602:PHE:CE2	2.48	0.49
1:A:282:TYR:CZ	1:A:540:ASP:OD1	2.64	0.49
1:A:425:ILE:HG23	1:A:469:GLU:HB2	1.95	0.49
1:A:533:ARG:HG2	1:A:537:LEU:HD23	1.94	0.49
1:B:357:ILE:HG13	1:B:438:PHE:O	2.13	0.49
1:A:359:VAL:HA	1:A:437:VAL:HA	1.94	0.49
1:A:422:ILE:HA	1:A:515:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:VAL:HG13	1:C:585:ALA:HB2	1.95	0.49
1:D:562:ASN:OD1	1:D:571:GLY:HA3	2.13	0.49
1:A:372:GLU:HA	1:A:501:VAL:HA	1.93	0.49
1:A:382:LYS:HD2	1:A:555:TYR:CE1	2.48	0.49
1:B:471:TRP:C	1:B:472:LYS:HD3	2.38	0.49
1:B:511:TYR:HB3	1:B:531:TYR:CE2	2.48	0.49
1:B:630:LEU:HD12	1:B:638:PHE:HB3	1.94	0.49
1:B:637:LEU:HD11	1:B:658:GLY:H	1.77	0.49
1:B:670:ASN:ND2	1:B:674:TYR:H	2.04	0.49
1:C:362:ALA:HA	1:C:385:GLN:OE1	2.13	0.49
1:C:427:PHE:CE2	1:C:467:LYS:HB2	2.48	0.49
1:C:783:LEU:HB3	1:C:795:PHE:CE2	2.48	0.49
1:D:359:VAL:HG23	1:D:437:VAL:HG22	1.95	0.49
1:D:594:LEU:HB3	1:D:602:PHE:CE2	2.48	0.49
1:D:745:GLY:HA3	1:D:793:THR:HG21	1.94	0.49
1:A:594:LEU:HD13	1:A:681:PHE:HE2	1.77	0.49
1:B:345:TYR:HB3	1:B:496:TYR:HB3	1.94	0.49
1:B:359:VAL:HG23	1:B:437:VAL:HG22	1.95	0.49
1:C:359:VAL:HA	1:C:437:VAL:HA	1.94	0.49
1:C:382:LYS:HD2	1:C:555:TYR:CE1	2.48	0.49
1:C:408:HIS:O	1:C:412:CYS:N	2.46	0.49
1:C:478:GLU:HG3	1:C:480:SER:N	2.28	0.49
1:D:345:TYR:HB3	1:D:496:TYR:HB3	1.94	0.49
1:D:471:TRP:C	1:D:472:LYS:HD3	2.38	0.49
1:A:356:PRO:HB3	1:A:689:LEU:HD21	1.94	0.49
1:A:362:ALA:HA	1:A:385:GLN:OE1	2.13	0.49
1:A:427:PHE:CE2	1:A:467:LYS:HB2	2.48	0.49
1:A:548:LEU:O	1:A:549:ILE:HD13	2.13	0.49
1:A:749:ILE:HB	1:A:757:LEU:HB2	1.95	0.49
1:C:373:ILE:HG12	1:C:498:PRO:HG2	1.95	0.49
1:C:431:TYR:HA	1:C:453:PHE:HA	1.93	0.49
1:D:602:PHE:O	1:D:668:PHE:N	2.46	0.49
1:A:373:ILE:HG12	1:A:498:PRO:HG2	1.95	0.49
1:D:454:TYR:CE2	1:D:456:PRO:HA	2.47	0.49
1:A:579:ASN:HB2	1:A:597:HIS:CE1	2.48	0.48
1:A:783:LEU:HB3	1:A:795:PHE:CE2	2.48	0.48
1:B:562:ASN:OD1	1:B:571:GLY:HA3	2.13	0.48
1:B:602:PHE:O	1:B:668:PHE:N	2.46	0.48
1:C:358:VAL:HG21	1:C:410:LEU:HD22	1.94	0.48
1:A:345:TYR:CG	1:A:523:LYS:HD2	2.48	0.48
1:A:408:HIS:O	1:A:412:CYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ILE:HG23	1:C:469:GLU:HB2	1.95	0.48
1:A:275:GLY:HA2	1:A:505:THR:HG22	0.50	0.48
1:A:348:ASN:ND2	1:A:379:PRO:HG3	2.28	0.48
1:B:333:LEU:HA	1:B:335:THR:OG1	2.13	0.48
1:B:574:ARG:O	1:B:602:PHE:HA	2.13	0.48
1:B:744:THR:HG23	1:B:762:LYS:HG3	1.96	0.48
1:C:345:TYR:CG	1:C:523:LYS:HD2	2.48	0.48
1:C:348:ASN:ND2	1:C:379:PRO:HG3	2.28	0.48
1:C:548:LEU:O	1:C:549:ILE:HD13	2.13	0.48
1:C:594:LEU:HD13	1:C:681:PHE:HE2	1.77	0.48
1:D:630:LEU:HD12	1:D:638:PHE:HB3	1.94	0.48
1:D:707:VAL:HB	1:D:723:PHE:CZ	2.47	0.48
1:A:427:PHE:HD2	1:A:467:LYS:HD3	1.78	0.48
1:A:489:LYS:NZ	1:A:490:ALA:O	2.47	0.48
1:B:277:GLU:CB	1:B:336:LEU:HD11	2.44	0.48
1:B:580:ALA:HB2	1:B:601:GLU:N	2.29	0.48
1:B:745:GLY:HA3	1:B:793:THR:HG21	1.94	0.48
1:D:625:ARG:HA	1:D:643:ASN:O	2.12	0.48
1:B:353:ILE:HG13	1:B:797:ASN:HD22	1.78	0.48
1:B:401:GLU:OE2	1:B:555:TYR:HA	2.14	0.48
1:B:702:ILE:N	1:B:724:LYS:O	2.45	0.48
1:C:584:LYS:HB3	1:C:589:LYS:HB3	1.95	0.48
1:C:749:ILE:HB	1:C:757:LEU:HB2	1.95	0.48
1:A:413:PRO:HG2	1:A:490:ALA:HB2	1.94	0.48
1:D:277:GLU:CB	1:D:336:LEU:HD11	2.43	0.48
1:D:278:ILE:H	1:D:336:LEU:HD22	1.79	0.48
1:A:407:ILE:HG23	1:A:410:LEU:HD23	1.96	0.48
1:A:687:LYS:HA	1:A:687:LYS:HD3	1.74	0.48
1:B:519:GLU:C	1:B:522:GLN:H	2.22	0.48
1:C:422:ILE:HA	1:C:515:LEU:HB3	1.94	0.48
1:D:333:LEU:C	1:D:335:THR:N	2.48	0.48
1:A:418:GLN:HB3	1:A:420:TYR:CE1	2.49	0.48
1:A:596:THR:OG1	1:A:676:ALA:HB3	2.12	0.48
1:B:516:THR:HG23	1:B:525:THR:HB	1.94	0.48
1:C:407:ILE:HG23	1:C:410:LEU:HD23	1.96	0.48
1:C:418:GLN:HB3	1:C:420:TYR:CE1	2.49	0.48
1:C:629:TYR:HB2	1:C:667:LEU:O	2.14	0.48
1:D:697:LYS:H	1:D:725:GLN:HE22	1.62	0.48
1:A:373:ILE:HG21	1:A:498:PRO:O	2.14	0.48
1:A:478:GLU:HG3	1:A:480:SER:N	2.28	0.48
1:A:629:TYR:HB2	1:A:667:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLU:HB2	1:B:336:LEU:HD11	1.95	0.48
1:C:427:PHE:HD2	1:C:467:LYS:HD3	1.78	0.48
1:D:422:ILE:O	1:D:474:LYS:N	2.47	0.48
1:D:744:THR:HG23	1:D:762:LYS:HG3	1.96	0.48
1:B:505:THR:O	1:B:551:SER:N	2.47	0.48
1:C:373:ILE:HG21	1:C:498:PRO:O	2.14	0.48
1:C:387:ARG:N	1:C:398:SER:OG	2.46	0.48
1:C:579:ASN:HB2	1:C:597:HIS:CE1	2.48	0.48
1:D:511:TYR:HB3	1:D:531:TYR:CE2	2.48	0.48
1:D:640:ASP:HA	1:D:642:LYS:HE2	1.94	0.48
1:A:584:LYS:HB3	1:A:589:LYS:HB3	1.96	0.47
1:B:697:LYS:H	1:B:725:GLN:HE22	1.62	0.47
1:D:363:ALA:N	1:D:366:TYR:HB2	2.29	0.47
1:D:505:THR:O	1:D:551:SER:N	2.47	0.47
1:A:511:TYR:HB3	1:A:531:TYR:CE2	2.49	0.47
1:A:739:LEU:HD21	1:A:795:PHE:HB3	1.95	0.47
1:B:783:LEU:HD13	1:B:795:PHE:HD2	1.78	0.47
1:C:479:ASP:OD1	1:C:480:SER:N	2.47	0.47
1:C:489:LYS:NZ	1:C:490:ALA:O	2.47	0.47
1:C:740:SER:O	1:C:796:SER:N	2.47	0.47
1:D:783:LEU:HB3	1:D:795:PHE:CE2	2.49	0.47
1:A:372:GLU:HB3	1:A:382:LYS:HB2	1.97	0.47
1:A:740:SER:O	1:A:796:SER:N	2.47	0.47
1:D:519:GLU:C	1:D:522:GLN:H	2.22	0.47
1:A:355:ASP:OD1	1:A:738:ARG:NH1	2.46	0.47
1:A:722:TYR:HB3	1:A:784:GLU:CB	2.42	0.47
1:B:631:LYS:HA	1:B:636:THR:HA	1.95	0.47
1:C:372:GLU:HB3	1:C:382:LYS:HB2	1.97	0.47
1:C:436:ILE:HG23	1:C:449:VAL:HG22	1.96	0.47
1:C:511:TYR:HB3	1:C:531:TYR:CE2	2.49	0.47
1:D:401:GLU:OE2	1:D:555:TYR:HA	2.14	0.47
1:D:419:LYS:HE3	1:D:419:LYS:HB2	1.70	0.47
1:D:574:ARG:O	1:D:602:PHE:HA	2.13	0.47
1:B:406:ASP:HB3	1:B:408:HIS:NE2	2.30	0.47
1:B:594:LEU:HB2	1:B:668:PHE:HE1	1.77	0.47
1:B:628:ILE:HB	1:B:640:ASP:HB3	1.96	0.47
1:C:352:ASP:H	1:C:414:LYS:NZ	2.09	0.47
1:D:631:LYS:HA	1:D:636:THR:HA	1.95	0.47
1:A:479:ASP:OD1	1:A:480:SER:N	2.47	0.47
1:B:278:ILE:H	1:B:336:LEU:HD22	1.78	0.47
1:B:333:LEU:O	1:B:335:THR:CB	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:SER:N	1:B:497:MET:O	2.48	0.47
1:B:627:ALA:N	1:B:670:ASN:O	2.48	0.47
1:C:652:THR:O	1:C:653:LYS:HD2	2.15	0.47
1:D:627:ALA:N	1:D:670:ASN:O	2.48	0.47
1:B:349:ARG:HB3	1:B:414:LYS:HZ2	1.80	0.47
1:B:350:GLY:HA2	1:B:408:HIS:HD1	1.79	0.47
1:B:372:GLU:HB2	1:B:384:TYR:CE2	2.39	0.47
1:C:278:ILE:H	1:C:336:LEU:CD1	2.24	0.47
1:C:355:ASP:OD1	1:C:738:ARG:NH1	2.46	0.47
1:C:739:LEU:HD21	1:C:795:PHE:HB3	1.96	0.47
1:D:346:SER:N	1:D:497:MET:O	2.48	0.47
1:D:406:ASP:HB3	1:D:408:HIS:NE2	2.30	0.47
1:D:645:PHE:CD2	1:D:649:GLN:HB2	2.50	0.47
1:D:651:VAL:HG23	1:D:653:LYS:NZ	2.30	0.47
1:D:783:LEU:HD13	1:D:795:PHE:HD2	1.78	0.47
1:A:652:THR:O	1:A:653:LYS:HD2	2.15	0.47
1:A:701:TRP:CE3	1:A:723:PHE:HB3	2.50	0.47
1:B:325:LYS:CE	1:B:543:ASN:HD21	2.17	0.47
1:B:339:ASN:ND2	1:B:528:GLY:O	2.47	0.47
1:B:518:ASP:OD2	1:B:523:LYS:HB2	2.14	0.47
1:D:339:ASN:ND2	1:D:528:GLY:O	2.47	0.47
1:D:518:ASP:OD2	1:D:523:LYS:HB2	2.14	0.47
1:D:625:ARG:HE	1:D:642:LYS:C	2.21	0.47
1:D:697:LYS:HB2	1:D:725:GLN:HE22	1.80	0.47
1:A:373:ILE:N	1:A:500:GLY:O	2.32	0.47
1:B:437:VAL:O	1:B:447:TYR:HB2	2.15	0.47
1:B:783:LEU:HB3	1:B:795:PHE:CE2	2.49	0.47
1:C:595:TYR:HH	1:C:597:HIS:CE1	2.30	0.47
1:C:701:TRP:CE3	1:C:723:PHE:HB3	2.50	0.47
1:D:580:ALA:HB2	1:D:601:GLU:N	2.29	0.47
1:D:628:ILE:HB	1:D:640:ASP:HB3	1.96	0.47
1:A:282:TYR:OH	1:A:540:ASP:CG	2.54	0.47
1:A:366:TYR:HE1	1:A:387:ARG:HG2	1.80	0.47
1:A:578:ASN:OD1	1:A:579:ASN:N	2.45	0.47
1:B:363:ALA:N	1:B:366:TYR:HB2	2.29	0.47
1:B:625:ARG:HE	1:B:642:LYS:C	2.21	0.47
1:B:697:LYS:HB2	1:B:725:GLN:HE22	1.80	0.47
1:C:274:ARG:NH2	1:C:553:ASP:OD2	2.47	0.47
1:D:427:PHE:CD2	1:D:467:LYS:HE3	2.45	0.47
1:A:434:THR:HG1	1:A:452:ASN:CG	2.23	0.46
1:A:516:THR:O	1:A:525:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ILE:O	1:B:474:LYS:N	2.47	0.46
1:B:724:LYS:HB2	1:B:780:PHE:HB2	1.97	0.46
1:B:737:LEU:HD22	1:B:749:ILE:HD11	1.97	0.46
1:C:347:LYS:HD2	1:C:496:TYR:CZ	2.51	0.46
1:A:595:TYR:HH	1:A:597:HIS:CE1	2.30	0.46
1:B:512:GLY:O	1:B:529:LYS:N	2.40	0.46
1:B:558:SER:HB3	1:B:563:TRP:CG	2.50	0.46
1:B:737:LEU:HB2	1:B:800:ILE:HG13	1.97	0.46
1:D:362:ALA:N	1:D:434:THR:O	2.31	0.46
1:D:441:ARG:NH1	1:D:693:PRO:O	2.37	0.46
1:D:670:ASN:ND2	1:D:674:TYR:H	2.04	0.46
1:A:353:ILE:HD11	1:A:739:LEU:HA	1.98	0.46
1:A:416:LEU:HD21	1:A:767:THR:HG21	1.98	0.46
1:A:436:ILE:HG23	1:A:449:VAL:HG22	1.96	0.46
1:A:627:ALA:HB3	1:A:669:LYS:HB2	1.98	0.46
1:A:737:LEU:HD22	1:A:749:ILE:HD11	1.97	0.46
1:B:533:ARG:NH1	1:B:534:GLU:OE2	2.48	0.46
1:B:645:PHE:CD2	1:B:649:GLN:HB2	2.50	0.46
1:B:651:VAL:HG23	1:B:653:LYS:NZ	2.30	0.46
1:C:432:VAL:N	1:C:452:ASN:O	2.34	0.46
1:C:517:VAL:HG12	1:C:524:ILE:HG23	1.98	0.46
1:D:533:ARG:NH1	1:D:534:GLU:OE2	2.48	0.46
1:D:574:ARG:NH1	1:D:604:GLN:HA	2.30	0.46
1:D:619:GLN:HB2	1:D:652:THR:HG22	1.97	0.46
1:D:740:SER:HB2	1:D:765:ASP:OD1	2.15	0.46
1:A:623:LYS:CG	1:A:647:ASP:HA	2.42	0.46
1:B:619:GLN:N	1:B:682:ILE:O	2.37	0.46
1:C:434:THR:HG1	1:C:452:ASN:CG	2.23	0.46
1:C:601:GLU:OE2	1:C:667:LEU:HD23	2.15	0.46
1:C:694:GLN:HB3	1:C:801:VAL:HG12	1.98	0.46
1:D:350:GLY:HA2	1:D:408:HIS:HD1	1.79	0.46
1:D:769:VAL:O	1:D:771:LYS:NZ	2.29	0.46
1:A:372:GLU:HB3	1:A:382:LYS:CB	2.45	0.46
1:C:366:TYR:HE1	1:C:387:ARG:HG2	1.80	0.46
1:C:372:GLU:HB3	1:C:382:LYS:CB	2.46	0.46
1:C:578:ASN:OD1	1:C:579:ASN:N	2.45	0.46
1:D:558:SER:HB3	1:D:563:TRP:CG	2.50	0.46
1:A:387:ARG:N	1:A:398:SER:OG	2.46	0.46
1:B:349:ARG:NH2	1:B:414:LYS:HA	2.31	0.46
1:C:621:VAL:O	1:C:679:ASN:N	2.38	0.46
1:D:423:LYS:HB2	1:D:474:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:GLU:N	1:D:604:GLN:HE22	2.14	0.46
1:D:737:LEU:HB2	1:D:800:ILE:HG13	1.97	0.46
1:A:586:ASP:O	1:A:588:ILE:HG23	2.16	0.46
1:A:601:GLU:OE2	1:A:667:LEU:HD23	2.14	0.46
1:B:696:LEU:HG	1:B:800:ILE:CG2	2.45	0.46
1:C:623:LYS:HB3	1:C:677:TRP:HB2	1.98	0.46
1:C:737:LEU:HG	1:C:800:ILE:HG13	1.98	0.46
1:C:737:LEU:HD22	1:C:749:ILE:HD11	1.97	0.46
1:D:390:PRO:HB3	1:D:457:SER:O	2.15	0.46
1:A:624:GLY:O	1:A:644:ASN:HA	2.16	0.46
1:B:186:ILE:HG23	1:B:295:ALA:HB2	1.97	0.46
1:B:390:PRO:HB3	1:B:457:SER:O	2.15	0.46
1:C:186:ILE:HG23	1:C:295:ALA:HB2	1.97	0.46
1:C:423:LYS:HG3	1:C:425:ILE:CG1	2.46	0.46
1:C:583:ASP:HB2	1:C:595:TYR:HB2	1.97	0.46
1:D:558:SER:HB3	1:D:563:TRP:CD1	2.51	0.46
1:A:413:PRO:HB2	1:A:416:LEU:O	2.16	0.46
1:A:623:LYS:HB3	1:A:677:TRP:HB2	1.98	0.46
1:A:695:MET:HE3	1:A:695:MET:HB2	1.81	0.46
1:C:416:LEU:HD21	1:C:767:THR:HG21	1.98	0.46
1:C:516:THR:O	1:C:525:THR:HB	2.15	0.46
1:C:738:ARG:HA	1:C:766:LEU:O	2.16	0.46
1:C:739:LEU:HD21	1:C:795:PHE:HD1	1.80	0.46
1:A:406:ASP:N	1:A:406:ASP:OD1	2.40	0.46
1:A:511:TYR:CZ	1:A:529:LYS:HB3	2.51	0.46
1:A:517:VAL:HG12	1:A:524:ILE:HG23	1.98	0.46
1:B:467:LYS:HE3	1:B:467:LYS:HB3	1.86	0.46
1:B:580:ALA:HB2	1:B:601:GLU:H	1.81	0.46
1:B:610:LEU:HA	1:B:616:TYR:CZ	2.51	0.46
1:B:740:SER:HB2	1:B:765:ASP:OD1	2.15	0.46
1:D:349:ARG:HD2	1:D:349:ARG:HA	1.60	0.46
1:D:437:VAL:O	1:D:447:TYR:HB2	2.15	0.46
1:A:347:LYS:HD2	1:A:496:TYR:CZ	2.50	0.45
1:B:353:ILE:HB	1:B:738:ARG:HB3	1.98	0.45
1:B:574:ARG:NH1	1:B:604:GLN:HA	2.30	0.45
1:B:619:GLN:HB2	1:B:652:THR:HG22	1.97	0.45
1:D:186:ILE:HG23	1:D:295:ALA:HB2	1.96	0.45
1:D:349:ARG:HB3	1:D:414:LYS:HZ2	1.80	0.45
1:D:724:LYS:HB2	1:D:780:PHE:HB2	1.97	0.45
1:D:734:THR:O	1:D:803:GLU:N	2.49	0.45
1:A:438:PHE:HD1	1:A:445:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LYS:HD2	1:A:633:ASN:HA	1.99	0.45
1:A:738:ARG:HA	1:A:766:LEU:O	2.16	0.45
1:C:374:LEU:O	1:C:379:PRO:HA	2.16	0.45
1:C:413:PRO:HB2	1:C:416:LEU:O	2.15	0.45
1:C:586:ASP:O	1:C:588:ILE:HG23	2.16	0.45
1:D:372:GLU:HB3	1:D:382:LYS:CB	2.44	0.45
1:D:576:ASN:HD21	1:D:603:SER:HB3	1.81	0.45
1:D:580:ALA:HB2	1:D:601:GLU:H	1.81	0.45
1:A:423:LYS:HG3	1:A:425:ILE:CG1	2.46	0.45
1:A:746:ARG:N	1:A:784:GLU:O	2.24	0.45
1:B:619:GLN:HG2	1:B:650:THR:OG1	2.16	0.45
1:B:647:ASP:OD1	1:B:647:ASP:N	2.49	0.45
1:C:438:PHE:HD1	1:C:445:LEU:HD11	1.81	0.45
1:C:627:ALA:HB3	1:C:669:LYS:HB2	1.98	0.45
1:D:349:ARG:NH2	1:D:414:LYS:HA	2.31	0.45
1:D:393:GLN:HE22	1:D:547:TYR:HD1	1.64	0.45
1:D:610:LEU:HD12	1:D:664:ILE:HB	1.98	0.45
1:A:374:LEU:O	1:A:379:PRO:HA	2.16	0.45
1:B:369:ILE:HG13	1:B:384:TYR:HB3	1.98	0.45
1:B:558:SER:HB3	1:B:563:TRP:CD1	2.51	0.45
1:B:561:GLU:N	1:B:604:GLN:HE22	2.14	0.45
1:B:610:LEU:HD12	1:B:664:ILE:HB	1.98	0.45
1:C:353:ILE:HD11	1:C:739:LEU:HA	1.98	0.45
1:C:511:TYR:CZ	1:C:529:LYS:HB3	2.51	0.45
1:A:612:PRO:HA	1:A:658:GLY:O	2.17	0.45
1:B:423:LYS:HB2	1:B:474:LYS:N	2.31	0.45
1:B:748:SER:HB3	1:B:758:PHE:HD1	1.81	0.45
1:D:338:ASN:HD22	1:D:533:ARG:CZ	2.29	0.45
1:C:738:ARG:HH21	1:C:799:SER:HB2	1.82	0.45
1:D:353:ILE:HB	1:D:738:ARG:HB3	1.98	0.45
1:A:186:ILE:HG23	1:A:295:ALA:HB2	1.97	0.45
1:A:583:ASP:HB2	1:A:595:TYR:HB2	1.97	0.45
1:A:672:SER:OG	1:A:673:GLU:OE1	2.31	0.45
1:A:739:LEU:HD21	1:A:795:PHE:HD1	1.80	0.45
1:B:734:THR:O	1:B:803:GLU:N	2.49	0.45
1:C:454:TYR:CD1	1:C:461:ILE:HG22	2.52	0.45
1:C:624:GLY:O	1:C:644:ASN:HA	2.16	0.45
1:C:687:LYS:HD3	1:C:687:LYS:HA	1.74	0.45
1:A:694:GLN:HB3	1:A:801:VAL:HG12	1.98	0.45
1:D:737:LEU:HD22	1:D:749:ILE:HD11	1.98	0.45
1:B:372:GLU:HB3	1:B:382:LYS:CB	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:610:LEU:HA	1:D:616:TYR:CZ	2.51	0.45
1:D:619:GLN:HG2	1:D:650:THR:OG1	2.16	0.45
1:D:619:GLN:N	1:D:682:ILE:O	2.37	0.45
1:A:625:ARG:HB3	1:A:671:GLN:HB3	1.99	0.45
1:B:576:ASN:HD21	1:B:603:SER:HB3	1.81	0.45
1:C:392:TYR:O	1:C:535:SER:OG	2.22	0.45
1:C:631:LYS:HD2	1:C:633:ASN:HA	1.99	0.45
1:D:405:GLY:HA2	1:D:687:LYS:O	2.17	0.45
1:D:565:ILE:HG22	1:D:592:SER:HB2	1.99	0.45
1:D:756:LEU:HD12	1:D:756:LEU:H	1.82	0.45
1:B:338:ASN:HD22	1:B:533:ARG:CZ	2.29	0.44
1:B:372:GLU:O	1:B:381:LEU:HD12	2.18	0.44
1:B:393:GLN:HE22	1:B:547:TYR:HD1	1.64	0.44
1:B:405:GLY:HA2	1:B:687:LYS:O	2.16	0.44
1:B:546:THR:HB	1:B:548:LEU:HG	1.99	0.44
1:D:540:ASP:HB2	1:D:548:LEU:HD11	2.00	0.44
1:D:580:ALA:HA	1:D:595:TYR:O	2.17	0.44
1:D:587:THR:HB	1:D:677:TRP:NE1	2.32	0.44
1:D:711:ASP:OD1	1:D:712:GLY:N	2.50	0.44
1:A:343:PRO:HD3	1:A:501:VAL:O	2.18	0.44
1:A:480:SER:OG	1:A:482:GLU:OE1	2.32	0.44
1:A:628:ILE:HD12	1:A:681:PHE:HE1	1.82	0.44
1:B:587:THR:HB	1:B:677:TRP:NE1	2.32	0.44
1:B:625:ARG:CZ	1:B:644:ASN:HB2	2.47	0.44
1:C:623:LYS:CG	1:C:647:ASP:HA	2.42	0.44
1:C:625:ARG:HB3	1:C:671:GLN:HB3	1.99	0.44
1:C:651:VAL:HG13	1:C:653:LYS:HG2	1.99	0.44
1:D:476:CYS:SG	1:D:480:SER:HA	2.58	0.44
1:A:423:LYS:O	1:A:447:TYR:OH	2.24	0.44
1:A:651:VAL:HG13	1:A:653:LYS:HG2	1.99	0.44
1:A:737:LEU:HG	1:A:800:ILE:HG13	1.98	0.44
1:C:694:GLN:CD	1:C:799:SER:HA	2.43	0.44
1:D:372:GLU:O	1:D:381:LEU:HD12	2.18	0.44
1:D:696:LEU:HG	1:D:800:ILE:CG2	2.45	0.44
1:A:454:TYR:CD1	1:A:461:ILE:HG22	2.52	0.44
1:B:756:LEU:H	1:B:756:LEU:HD12	1.82	0.44
1:C:378:LEU:HB3	1:C:654:LYS:HD3	1.99	0.44
1:C:378:LEU:HD22	1:C:654:LYS:HE3	2.00	0.44
1:D:647:ASP:OD1	1:D:647:ASP:N	2.49	0.44
1:D:750:ILE:HG12	1:D:755:TYR:HE1	1.82	0.44
1:B:339:ASN:ND2	1:B:529:LYS:HG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:GLY:HA3	1:B:664:ILE:N	2.33	0.44
1:C:390:PRO:HG3	1:C:458:THR:HA	2.00	0.44
1:D:726:PHE:CD1	1:D:780:PHE:HB3	2.50	0.44
1:A:378:LEU:HD22	1:A:654:LYS:HE3	2.00	0.44
1:B:241:LEU:HD21	1:B:295:ALA:HB1	2.00	0.44
1:C:282:TYR:OH	1:C:540:ASP:CG	2.54	0.44
1:C:343:PRO:HD3	1:C:501:VAL:O	2.17	0.44
1:C:414:LYS:O	1:C:415:GLN:HG2	2.18	0.44
1:C:480:SER:OG	1:C:482:GLU:OE1	2.32	0.44
1:D:431:TYR:N	1:D:531:TYR:OH	2.50	0.44
1:D:553:ASP:OD1	1:D:553:ASP:N	2.51	0.44
1:D:625:ARG:CZ	1:D:644:ASN:HB2	2.47	0.44
1:D:748:SER:HB3	1:D:758:PHE:HD1	1.81	0.44
1:A:346:SER:O	1:A:497:MET:HG2	2.18	0.44
1:B:611:LYS:N	1:B:616:TYR:OH	2.47	0.44
1:D:369:ILE:HG13	1:D:384:TYR:HB3	1.98	0.44
1:A:414:LYS:O	1:A:415:GLN:HG2	2.18	0.44
1:A:418:GLN:HB3	1:A:420:TYR:HE1	1.83	0.44
1:A:738:ARG:HH21	1:A:799:SER:HB2	1.82	0.44
1:B:350:GLY:CA	1:B:409:LYS:HA	2.48	0.44
1:B:561:GLU:H	1:B:604:GLN:HE22	1.66	0.44
1:D:581:PHE:CD2	1:D:583:ASP:HB2	2.53	0.44
1:D:726:PHE:O	1:D:728:LYS:NZ	2.51	0.44
1:A:241:LEU:HD21	1:A:295:ALA:HB1	2.00	0.44
1:A:378:LEU:HB3	1:A:654:LYS:HD3	1.99	0.44
1:B:540:ASP:HB2	1:B:548:LEU:HD11	1.99	0.44
1:B:568:ASP:C	1:B:582:VAL:HG11	2.43	0.44
1:B:584:LYS:HE3	1:B:589:LYS:O	2.18	0.44
1:B:722:TYR:HB3	1:B:784:GLU:HA	2.00	0.44
1:C:372:GLU:OE1	1:C:382:LYS:HB2	2.18	0.44
1:D:618:ILE:HG23	1:D:683:ILE:HG12	2.00	0.44
1:B:427:PHE:CE2	1:B:469:GLU:HG2	2.53	0.43
1:B:565:ILE:HG22	1:B:592:SER:HB2	1.99	0.43
1:B:711:ASP:OD1	1:B:712:GLY:N	2.51	0.43
1:B:750:ILE:HG12	1:B:755:TYR:HE1	1.82	0.43
1:D:410:LEU:HA	1:D:440:LYS:HD3	2.00	0.43
1:D:607:GLY:HA3	1:D:664:ILE:N	2.33	0.43
1:A:168:LEU:HD22	1:A:268:LYS:HG3	1.99	0.43
1:B:476:CYS:SG	1:B:480:SER:HA	2.58	0.43
1:B:697:LYS:HA	1:B:697:LYS:HD3	1.87	0.43
1:C:628:ILE:HD12	1:C:681:PHE:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:GLY:CA	1:D:409:LYS:HA	2.48	0.43
1:D:364:PRO:O	1:D:461:ILE:HD11	2.18	0.43
1:D:561:GLU:H	1:D:604:GLN:HE22	1.66	0.43
1:A:274:ARG:NH2	1:A:553:ASP:OD2	2.51	0.43
1:A:423:LYS:HE2	1:A:473:GLU:N	2.33	0.43
1:A:566:THR:OG1	1:A:567:SER:N	2.44	0.43
1:A:742:LYS:HB3	1:A:794:ILE:HB	2.00	0.43
1:B:401:GLU:CD	1:B:556:ILE:H	2.26	0.43
1:B:428:PRO:HG2	1:B:431:TYR:CE2	2.54	0.43
1:B:441:ARG:NH1	1:B:693:PRO:O	2.37	0.43
1:C:381:LEU:HD13	1:C:407:ILE:HG21	1.99	0.43
1:C:612:PRO:HA	1:C:658:GLY:O	2.17	0.43
1:C:618:ILE:HG21	1:C:638:PHE:CE1	2.53	0.43
1:A:349:ARG:NH2	1:A:414:LYS:HB2	2.33	0.43
1:A:390:PRO:HG3	1:A:458:THR:HA	2.00	0.43
1:A:392:TYR:O	1:A:535:SER:OG	2.22	0.43
1:A:702:ILE:HD12	1:A:724:LYS:HG3	2.00	0.43
1:B:692:LEU:HB3	1:B:693:PRO:HD2	2.00	0.43
1:C:241:LEU:HD21	1:C:295:ALA:HB1	2.00	0.43
1:C:346:SER:O	1:C:497:MET:HG2	2.18	0.43
1:C:349:ARG:NH2	1:C:414:LYS:HB2	2.33	0.43
1:C:405:GLY:O	1:C:407:ILE:HG12	2.19	0.43
1:C:605:PHE:O	1:C:609:LYS:NZ	2.46	0.43
1:C:742:LYS:HB3	1:C:794:ILE:HB	2.01	0.43
1:D:168:LEU:HD22	1:D:268:LYS:HG3	1.99	0.43
1:D:568:ASP:C	1:D:582:VAL:HG11	2.43	0.43
1:D:616:TYR:HB2	1:D:655:PHE:CE1	2.53	0.43
1:D:722:TYR:HB3	1:D:784:GLU:HA	2.00	0.43
1:D:783:LEU:HD22	1:D:795:PHE:CE2	2.54	0.43
1:B:168:LEU:HD22	1:B:268:LYS:HG3	1.99	0.43
1:B:553:ASP:OD1	1:B:553:ASP:N	2.51	0.43
1:B:580:ALA:HA	1:B:595:TYR:O	2.17	0.43
1:B:726:PHE:O	1:B:728:LYS:NZ	2.51	0.43
1:C:373:ILE:N	1:C:500:GLY:O	2.32	0.43
1:C:570:THR:HB	1:C:573:TRP:HB2	1.99	0.43
1:D:428:PRO:HG2	1:D:431:TYR:CE2	2.54	0.43
1:B:476:CYS:HA	1:B:480:SER:H	1.83	0.43
1:C:168:LEU:HD22	1:C:268:LYS:HG3	1.99	0.43
1:C:363:ALA:HB3	1:C:366:TYR:CD2	2.54	0.43
1:C:433:ILE:HA	1:C:451:ALA:HA	2.01	0.43
1:C:625:ARG:O	1:C:676:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ASN:ND2	1:D:529:LYS:HG2	2.33	0.43
1:D:476:CYS:HA	1:D:480:SER:H	1.83	0.43
1:A:277:GLU:N	1:A:336:LEU:HD21	2.33	0.43
1:A:378:LEU:HD12	1:A:379:PRO:HD2	2.01	0.43
1:A:381:LEU:HD13	1:A:407:ILE:HG21	1.99	0.43
1:A:614:THR:HB	1:A:616:TYR:HE2	1.84	0.43
1:B:431:TYR:N	1:B:531:TYR:OH	2.50	0.43
1:B:519:GLU:O	1:B:522:GLN:NE2	2.36	0.43
1:B:581:PHE:CD2	1:B:583:ASP:HB2	2.53	0.43
1:B:726:PHE:CD1	1:B:780:PHE:HB3	2.50	0.43
1:C:276:SER:H	1:C:505:THR:CG2	2.09	0.43
1:C:702:ILE:HD12	1:C:724:LYS:HG3	2.00	0.43
1:D:379:PRO:C	1:D:407:ILE:HG22	2.44	0.43
1:D:425:ILE:HG21	1:D:449:VAL:HB	2.01	0.43
1:D:512:GLY:O	1:D:529:LYS:N	2.40	0.43
1:D:584:LYS:HE3	1:D:589:LYS:O	2.18	0.43
1:D:617:VAL:N	1:D:684:LEU:O	2.48	0.43
1:D:743:GLY:O	1:D:793:THR:HG23	2.19	0.43
1:A:413:PRO:HB2	1:A:490:ALA:HB2	2.01	0.43
1:A:570:THR:HB	1:A:573:TRP:HB2	1.99	0.43
1:A:625:ARG:O	1:A:676:ALA:HB2	2.18	0.43
1:B:616:TYR:HB2	1:B:655:PHE:CE1	2.54	0.43
1:B:618:ILE:HG23	1:B:683:ILE:HG12	2.00	0.43
1:B:743:GLY:O	1:B:793:THR:HG23	2.19	0.43
1:C:378:LEU:HD12	1:C:379:PRO:HD2	2.01	0.43
1:C:418:GLN:HB3	1:C:420:TYR:HE1	1.83	0.43
1:D:692:LEU:HB3	1:D:693:PRO:HD2	2.00	0.43
1:A:333:LEU:HD23	1:A:541:LEU:CD2	2.47	0.43
1:A:608:ASN:OD1	1:A:608:ASN:N	2.51	0.43
1:B:360:LEU:HD22	1:B:371:PHE:CE1	2.54	0.43
1:B:364:PRO:O	1:B:461:ILE:HD11	2.18	0.43
1:B:410:LEU:HA	1:B:440:LYS:HD3	2.00	0.43
1:C:403:ILE:HD13	1:C:617:VAL:HG11	2.00	0.43
1:D:427:PHE:CE2	1:D:469:GLU:HG2	2.54	0.43
1:D:707:VAL:HB	1:D:723:PHE:CE1	2.54	0.43
1:A:363:ALA:HB3	1:A:366:TYR:CD2	2.54	0.43
1:A:371:PHE:HE2	1:A:513:PHE:CE2	2.37	0.43
1:A:372:GLU:OE1	1:A:382:LYS:HB2	2.18	0.43
1:B:736:HIS:CD2	1:B:803:GLU:HB2	2.52	0.43
1:C:371:PHE:HE2	1:C:513:PHE:CE2	2.37	0.43
1:C:672:SER:OG	1:C:673:GLU:OE1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:LEU:HD21	1:D:295:ALA:HB1	2.00	0.43
1:D:546:THR:HB	1:D:548:LEU:HG	1.99	0.43
1:A:403:ILE:HD13	1:A:617:VAL:HG11	2.00	0.42
1:A:618:ILE:HG21	1:A:638:PHE:CE1	2.53	0.42
1:A:694:GLN:CD	1:A:799:SER:HA	2.43	0.42
1:B:345:TYR:HE2	1:B:523:LYS:HD3	1.83	0.42
1:B:617:VAL:N	1:B:684:LEU:O	2.48	0.42
1:B:707:VAL:HB	1:B:723:PHE:CE1	2.54	0.42
1:B:729:LEU:HD13	1:B:779:CYS:SG	2.59	0.42
1:C:472:LYS:HB3	1:C:475:SER:OG	2.19	0.42
1:C:764:GLU:OE2	1:C:764:GLU:N	2.52	0.42
1:D:577:ASN:HB3	1:D:600:GLY:HA2	2.01	0.42
1:A:433:ILE:HA	1:A:451:ALA:HA	2.01	0.42
1:C:435:LYS:NZ	1:C:448:GLU:HG2	2.34	0.42
1:C:701:TRP:HB3	1:C:723:PHE:CD1	2.54	0.42
1:D:611:LYS:N	1:D:616:TYR:OH	2.47	0.42
1:A:739:LEU:HD21	1:A:795:PHE:CD1	2.54	0.42
1:A:769:VAL:O	1:A:769:VAL:HG13	2.19	0.42
1:B:436:ILE:HA	1:B:448:GLU:O	2.20	0.42
1:C:277:GLU:N	1:C:336:LEU:HD21	2.34	0.42
1:B:576:ASN:HD22	1:B:601:GLU:HG2	1.84	0.42
1:B:577:ASN:HB3	1:B:600:GLY:HA2	2.01	0.42
1:C:344:SER:O	1:C:499:LEU:N	2.51	0.42
1:C:608:ASN:OD1	1:C:608:ASN:N	2.51	0.42
1:C:630:LEU:HD13	1:C:666:PHE:CD1	2.55	0.42
1:D:360:LEU:HD22	1:D:371:PHE:CE1	2.54	0.42
1:A:731:ASN:HA	1:A:773:THR:O	2.19	0.42
1:B:423:LYS:HD3	1:B:473:GLU:O	2.20	0.42
1:B:425:ILE:HG21	1:B:449:VAL:HB	2.01	0.42
1:B:704:SER:N	1:B:722:TYR:O	2.52	0.42
1:C:489:LYS:HA	1:C:489:LYS:HD2	1.85	0.42
1:D:423:LYS:HD3	1:D:473:GLU:O	2.20	0.42
1:D:658:GLY:O	1:D:661:PRO:HD3	2.20	0.42
1:D:736:HIS:CD2	1:D:803:GLU:HB2	2.52	0.42
1:B:379:PRO:C	1:B:407:ILE:HG22	2.44	0.42
1:D:434:THR:HG21	1:D:461:ILE:HD12	2.02	0.42
1:D:562:ASN:O	1:D:565:ILE:HG13	2.19	0.42
1:D:746:ARG:NE	1:D:784:GLU:OE2	2.45	0.42
1:A:405:GLY:O	1:A:407:ILE:HG12	2.19	0.42
1:A:472:LYS:HB3	1:A:475:SER:OG	2.19	0.42
1:B:427:PHE:CD2	1:B:467:LYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ALA:HB2	1:B:589:LYS:HB3	2.02	0.42
1:B:652:THR:C	1:B:653:LYS:HD3	2.45	0.42
1:B:658:GLY:O	1:B:661:PRO:HD3	2.20	0.42
1:C:423:LYS:HE2	1:C:473:GLU:N	2.33	0.42
1:D:471:TRP:HA	1:D:472:LYS:HD3	2.01	0.42
1:D:473:GLU:OE2	1:D:482:GLU:HA	2.20	0.42
1:D:623:LYS:C	1:D:677:TRP:HE3	2.28	0.42
1:B:562:ASN:O	1:B:565:ILE:HG13	2.19	0.42
1:B:623:LYS:C	1:B:677:TRP:HE3	2.28	0.42
1:B:744:THR:O	1:B:793:THR:OG1	2.35	0.42
1:B:783:LEU:HD22	1:B:795:PHE:CE2	2.54	0.42
1:C:435:LYS:HE3	1:C:450:THR:HB	2.01	0.42
1:C:571:GLY:O	1:C:574:ARG:NH1	2.53	0.42
1:D:399:MET:HE3	1:D:507:LEU:HD22	2.01	0.42
1:D:436:ILE:HA	1:D:448:GLU:O	2.20	0.42
1:A:420:TYR:HB3	1:A:515:LEU:HD21	2.02	0.42
1:A:435:LYS:HE3	1:A:450:THR:HB	2.01	0.42
1:B:399:MET:HE3	1:B:507:LEU:HD22	2.01	0.42
1:C:625:ARG:HE	1:C:674:TYR:CB	2.33	0.42
1:C:642:LYS:HG3	1:C:643:ASN:OD1	2.20	0.42
1:C:739:LEU:HD21	1:C:795:PHE:CD1	2.54	0.42
1:C:746:ARG:N	1:C:784:GLU:O	2.24	0.42
1:D:401:GLU:CD	1:D:556:ILE:H	2.26	0.42
1:D:704:SER:N	1:D:722:TYR:O	2.52	0.42
1:A:378:LEU:CB	1:A:654:LYS:HD3	2.50	0.42
1:A:555:TYR:CG	1:A:682:ILE:HG21	2.55	0.42
1:A:571:GLY:O	1:A:574:ARG:NH1	2.53	0.42
1:A:706:ASN:O	1:A:718:LEU:HB2	2.20	0.42
1:B:349:ARG:HD2	1:B:349:ARG:HA	1.60	0.42
1:B:446:GLY:CA	1:B:472:LYS:HE3	2.50	0.42
1:B:680:ASN:O	1:B:682:ILE:HD12	2.20	0.42
1:C:744:THR:O	1:C:793:THR:OG1	2.38	0.42
1:D:585:ALA:HB2	1:D:589:LYS:HB3	2.02	0.42
1:A:282:TYR:CZ	1:A:540:ASP:CG	2.98	0.41
1:A:435:LYS:NZ	1:A:448:GLU:HG2	2.34	0.41
1:B:333:LEU:CA	1:B:335:THR:CG2	2.97	0.41
1:B:423:LYS:HE3	1:B:425:ILE:HG12	2.02	0.41
1:D:427:PHE:CD2	1:D:467:LYS:HB3	2.54	0.41
1:D:744:THR:O	1:D:793:THR:OG1	2.35	0.41
1:D:783:LEU:HD13	1:D:795:PHE:CD2	2.55	0.41
1:A:333:LEU:C	1:A:335:THR:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:LEU:HD13	1:A:666:PHE:CD1	2.55	0.41
1:A:642:LYS:HG3	1:A:643:ASN:OD1	2.20	0.41
1:C:413:PRO:HB2	1:C:490:ALA:HB2	2.01	0.41
1:C:425:ILE:N	1:C:513:PHE:O	2.53	0.41
1:C:490:ALA:HA	1:C:495:ILE:HD11	2.02	0.41
1:C:555:TYR:CG	1:C:682:ILE:HG21	2.55	0.41
1:C:757:LEU:HD23	1:C:757:LEU:HA	1.89	0.41
1:C:769:VAL:HG13	1:C:769:VAL:O	2.19	0.41
1:D:325:LYS:HZ1	1:D:543:ASN:HD21	0.44	0.41
1:D:356:PRO:HB3	1:D:689:LEU:HD21	2.02	0.41
1:D:369:ILE:HG12	1:D:385:GLN:CA	2.50	0.41
1:D:729:LEU:HD13	1:D:779:CYS:SG	2.60	0.41
1:D:761:VAL:HA	1:D:764:GLU:OE2	2.21	0.41
1:B:715:LEU:HD12	1:B:798:VAL:HG11	2.02	0.41
1:C:731:ASN:HA	1:C:773:THR:O	2.19	0.41
1:D:366:TYR:CZ	1:D:398:SER:HB2	2.56	0.41
1:D:425:ILE:N	1:D:513:PHE:O	2.53	0.41
1:D:563:TRP:CE3	1:D:680:ASN:HA	2.55	0.41
1:D:628:ILE:HG23	1:D:666:PHE:CZ	2.55	0.41
1:D:680:ASN:O	1:D:682:ILE:HD12	2.20	0.41
1:A:701:TRP:HB3	1:A:723:PHE:CD1	2.54	0.41
1:B:356:PRO:HB3	1:B:689:LEU:HD21	2.02	0.41
1:B:425:ILE:N	1:B:513:PHE:O	2.53	0.41
1:B:628:ILE:HG23	1:B:666:PHE:CZ	2.55	0.41
1:B:783:LEU:HD13	1:B:795:PHE:CD2	2.55	0.41
1:C:465:LYS:HA	1:C:465:LYS:HD2	1.84	0.41
1:C:614:THR:HB	1:C:616:TYR:HE2	1.84	0.41
1:D:576:ASN:HD22	1:D:601:GLU:HG2	1.84	0.41
1:D:613:LYS:HD3	1:D:613:LYS:HA	1.82	0.41
1:A:505:THR:OG1	1:A:506:PHE:N	2.53	0.41
1:A:625:ARG:HE	1:A:674:TYR:CB	2.33	0.41
1:B:333:LEU:CA	1:B:335:THR:HG23	2.50	0.41
1:B:372:GLU:OE2	1:B:374:LEU:HG	2.21	0.41
1:B:471:TRP:HA	1:B:472:LYS:HD3	2.01	0.41
1:C:768:ARG:HA	1:C:768:ARG:HD3	1.88	0.41
1:D:423:LYS:CD	1:D:477:GLU:HB2	2.51	0.41
1:D:472:LYS:HD3	1:D:472:LYS:N	2.36	0.41
1:D:587:THR:HG21	1:D:623:LYS:HD2	2.03	0.41
1:A:432:VAL:N	1:A:452:ASN:O	2.34	0.41
1:B:366:TYR:CZ	1:B:398:SER:HB2	2.56	0.41
1:B:472:LYS:HD3	1:B:472:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:LYS:HE2	1:B:675:GLU:HG3	2.03	0.41
1:C:378:LEU:CB	1:C:654:LYS:HD3	2.50	0.41
1:C:486:SER:OG	1:C:487:ILE:N	2.54	0.41
1:C:491:GLU:HG3	1:C:493:ASP:OD1	2.21	0.41
1:D:710:LYS:HA	1:D:710:LYS:HD3	1.92	0.41
1:D:715:LEU:HD12	1:D:798:VAL:HG11	2.02	0.41
1:A:757:LEU:HD23	1:A:757:LEU:HA	1.89	0.41
1:B:369:ILE:HG12	1:B:385:GLN:CA	2.50	0.41
1:B:434:THR:HG21	1:B:461:ILE:HD12	2.02	0.41
1:B:607:GLY:HA3	1:B:664:ILE:H	1.86	0.41
1:C:282:TYR:CZ	1:C:540:ASP:CG	2.99	0.41
1:C:512:GLY:C	1:C:529:LYS:HE2	2.46	0.41
1:C:532:LEU:HD12	1:C:532:LEU:HA	1.74	0.41
1:C:783:LEU:HD23	1:C:783:LEU:HA	1.92	0.41
1:D:736:HIS:HA	1:D:769:VAL:HA	2.02	0.41
1:D:748:SER:HB3	1:D:758:PHE:CD1	2.55	0.41
1:A:350:GLY:HA3	1:A:412:CYS:O	2.21	0.41
1:A:354:ASP:OD1	1:A:797:ASN:ND2	2.53	0.41
1:A:716:GLU:HA	1:A:794:ILE:HG12	2.03	0.41
1:B:654:LYS:HE3	1:B:654:LYS:HB3	1.90	0.41
1:C:367:ALA:HB3	1:C:388:LEU:HD11	2.03	0.41
1:A:344:SER:O	1:A:499:LEU:N	2.52	0.41
1:A:367:ALA:O	1:A:369:ILE:HG23	2.21	0.41
1:A:657:SER:OG	1:A:661:PRO:HG3	2.21	0.41
1:B:278:ILE:HG13	1:B:336:LEU:CD2	2.49	0.41
1:B:473:GLU:OE2	1:B:482:GLU:HA	2.20	0.41
1:B:587:THR:HG21	1:B:623:LYS:HD2	2.03	0.41
1:B:798:VAL:O	1:B:798:VAL:HG23	2.21	0.41
1:C:420:TYR:CD2	1:C:517:VAL:HG11	2.56	0.41
1:C:722:TYR:HB3	1:C:784:GLU:CB	2.42	0.41
1:D:376:ASP:OD2	1:D:652:THR:OG1	2.28	0.41
1:D:446:GLY:CA	1:D:472:LYS:HE3	2.50	0.41
1:D:619:GLN:O	1:D:682:ILE:N	2.54	0.41
1:D:798:VAL:O	1:D:798:VAL:HG23	2.21	0.41
1:A:425:ILE:N	1:A:513:PHE:O	2.53	0.41
1:A:474:LYS:HG2	1:A:478:GLU:HB3	2.02	0.41
1:A:491:GLU:HG3	1:A:493:ASP:OD1	2.21	0.41
1:A:619:GLN:HA	1:A:651:VAL:O	2.21	0.41
1:B:748:SER:HB3	1:B:758:PHE:CD1	2.55	0.41
1:C:354:ASP:OD1	1:C:797:ASN:ND2	2.53	0.41
1:C:367:ALA:O	1:C:369:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:THR:OG1	1:C:506:PHE:N	2.53	0.41
1:C:605:PHE:HA	1:C:665:TYR:CB	2.51	0.41
1:C:695:MET:HE1	1:C:735:TYR:CD2	2.56	0.41
1:D:739:LEU:HD21	1:D:795:PHE:CG	2.56	0.41
1:B:563:TRP:CE3	1:B:680:ASN:HA	2.55	0.40
1:C:350:GLY:HA3	1:C:412:CYS:O	2.21	0.40
1:C:426:GLU:HG2	1:C:512:GLY:HA3	2.03	0.40
1:C:631:LYS:O	1:C:665:TYR:N	2.51	0.40
1:C:657:SER:OG	1:C:661:PRO:HG3	2.21	0.40
1:C:700:ASP:HB2	1:C:725:GLN:NE2	2.36	0.40
1:A:367:ALA:HB3	1:A:388:LEU:HD11	2.03	0.40
1:A:594:LEU:HD12	1:A:594:LEU:H	1.87	0.40
1:C:594:LEU:H	1:C:594:LEU:HD12	1.87	0.40
1:C:706:ASN:O	1:C:718:LEU:HB2	2.20	0.40
1:D:343:PRO:HG2	1:D:500:GLY:HA3	2.04	0.40
1:D:596:THR:HB	1:D:670:ASN:HB2	2.03	0.40
1:D:652:THR:C	1:D:653:LYS:HD3	2.45	0.40
1:A:490:ALA:HA	1:A:495:ILE:HD11	2.02	0.40
1:B:561:GLU:H	1:B:604:GLN:NE2	2.19	0.40
1:C:295:ALA:HA	1:C:298:THR:HG22	2.04	0.40
1:C:427:PHE:CD2	1:C:467:LYS:HB2	2.57	0.40
1:C:474:LYS:HG2	1:C:478:GLU:HB3	2.02	0.40
1:C:695:MET:HE1	1:C:735:TYR:CE2	2.56	0.40
1:C:725:GLN:O	1:C:780:PHE:HB2	2.21	0.40
1:D:607:GLY:HA3	1:D:664:ILE:H	1.86	0.40
1:A:700:ASP:HB2	1:A:725:GLN:NE2	2.36	0.40
1:B:423:LYS:CD	1:B:477:GLU:HB2	2.51	0.40
1:B:619:GLN:O	1:B:682:ILE:N	2.54	0.40
1:C:333:LEU:HD23	1:C:541:LEU:CD2	2.48	0.40
1:C:643:ASN:HB3	1:C:645:PHE:CE2	2.56	0.40
1:D:708:GLN:O	1:D:716:GLU:N	2.55	0.40
1:D:735:TYR:HA	1:D:802:LYS:HA	2.03	0.40
1:A:276:SER:H	1:A:505:THR:CG2	2.11	0.40
1:A:295:ALA:HA	1:A:298:THR:HG22	2.04	0.40
1:A:486:SER:OG	1:A:487:ILE:N	2.54	0.40
1:A:643:ASN:HB3	1:A:645:PHE:CE2	2.56	0.40
1:A:672:SER:HB3	1:A:674:TYR:HD2	1.87	0.40
1:A:695:MET:HE1	1:A:735:TYR:CE2	2.56	0.40
1:A:725:GLN:O	1:A:780:PHE:HB2	2.21	0.40
1:C:275:GLY:C	1:C:505:THR:HG22	2.23	0.40
1:C:357:ILE:HD12	1:C:692:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:TYR:HB3	1:C:515:LEU:HD21	2.02	0.40
1:C:560:VAL:HG11	1:C:681:PHE:HB2	2.03	0.40
1:D:423:LYS:HE3	1:D:425:ILE:HG12	2.02	0.40
1:D:594:LEU:HD13	1:D:602:PHE:CG	2.57	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	644/803 (80%)	576 (89%)	66 (10%)	2 (0%)	36	71
1	B	644/803 (80%)	580 (90%)	62 (10%)	2 (0%)	36	71
1	C	644/803 (80%)	578 (90%)	64 (10%)	2 (0%)	36	71
1	D	644/803 (80%)	579 (90%)	63 (10%)	2 (0%)	36	71
All	All	2576/3212 (80%)	2313 (90%)	255 (10%)	8 (0%)	37	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	LEU
1	B	335	THR
1	C	336	LEU
1	D	335	THR
1	A	334	PRO
1	C	334	PRO
1	B	334	PRO
1	D	334	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/730 (81%)	588 (99%)	4 (1%)	76	79
1	B	592/730 (81%)	590 (100%)	2 (0%)	86	84
1	C	592/730 (81%)	589 (100%)	3 (0%)	81	82
1	D	592/730 (81%)	589 (100%)	3 (0%)	81	82
All	All	2368/2920 (81%)	2356 (100%)	12 (0%)	78	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	LEU
1	A	335	THR
1	A	336	LEU
1	A	565	ILE
1	B	336	LEU
1	B	741	VAL
1	C	335	THR
1	C	336	LEU
1	C	565	ILE
1	D	225	LEU
1	D	336	LEU
1	D	741	VAL

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

Mol	Chain	Res	Type
1	A	148	GLN
1	A	155	GLN
1	A	292	GLN
1	A	324	GLN
1	A	331	ASN
1	A	348	ASN
1	A	375	ASN

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Mol	Chain	Res	Type
1	A	543	ASN
1	A	615	ASN
1	A	708	GLN
1	B	148	GLN
1	B	155	GLN
1	B	292	GLN
1	B	324	GLN
1	B	331	ASN
1	B	339	ASN
1	B	348	ASN
1	B	393	GLN
1	B	418	GLN
1	B	443	ASN
1	B	452	ASN
1	B	543	ASN
1	B	576	ASN
1	B	604	GLN
1	B	670	ASN
1	B	671	GLN
1	B	725	GLN
1	B	797	ASN
1	C	148	GLN
1	C	155	GLN
1	C	292	GLN
1	C	324	GLN
1	C	348	ASN
1	C	375	ASN
1	C	543	ASN
1	C	708	GLN
1	D	148	GLN
1	D	155	GLN
1	D	292	GLN
1	D	324	GLN
1	D	331	ASN
1	D	338	ASN
1	D	339	ASN
1	D	348	ASN
1	D	393	GLN
1	D	418	GLN
1	D	443	ASN
1	D	452	ASN
1	D	543	ASN

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Mol	Chain	Res	Type
1	D	576	ASN
1	D	670	ASN
1	D	671	GLN
1	D	725	GLN
1	D	797	ASN

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.

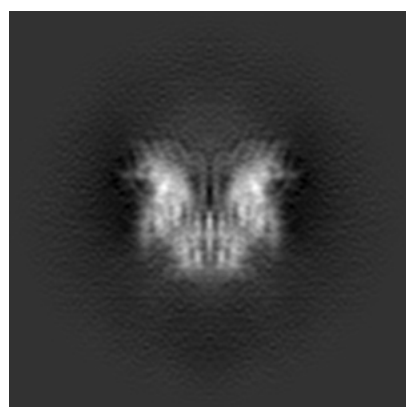
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10889. These allow visual inspection of the internal detail of the map and identification of artifacts.

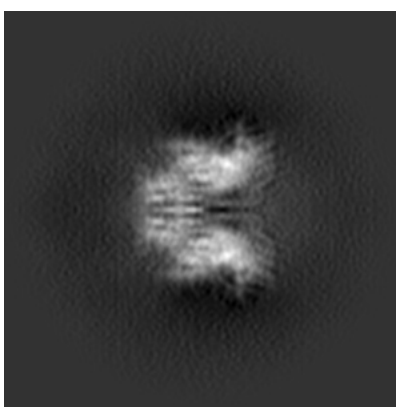
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

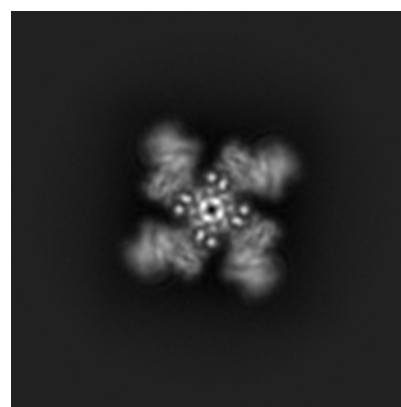
6.1.1 Primary map



X



Y

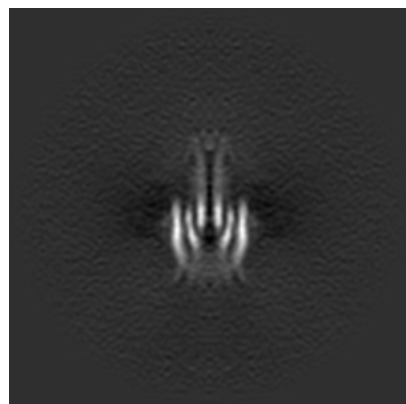


Z

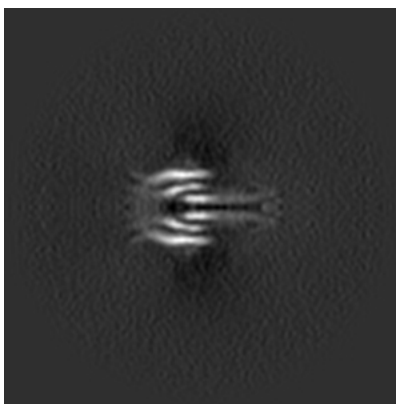
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

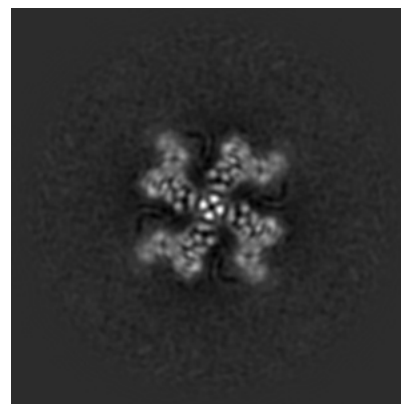
6.2.1 Primary map



X Index: 150



Y Index: 150

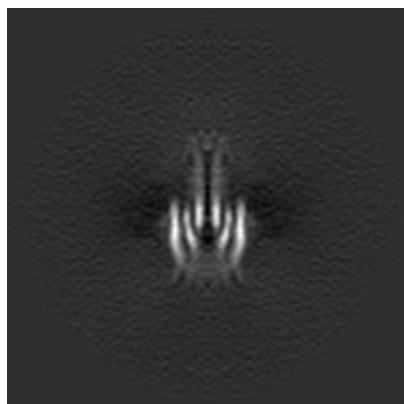


Z Index: 150

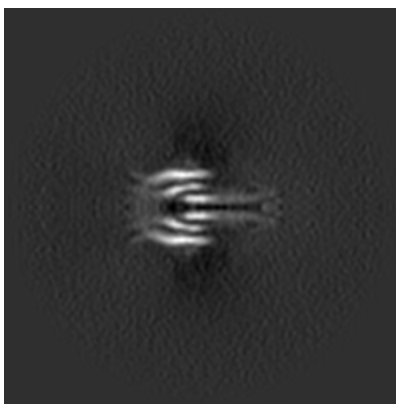
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

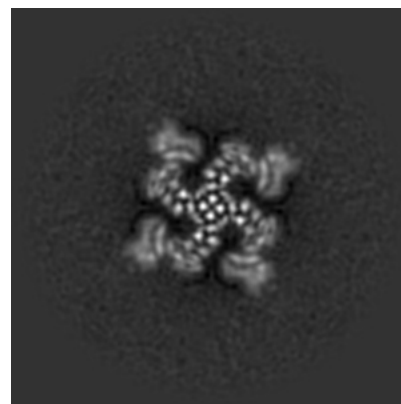
6.3.1 Primary map



X Index: 150



Y Index: 150

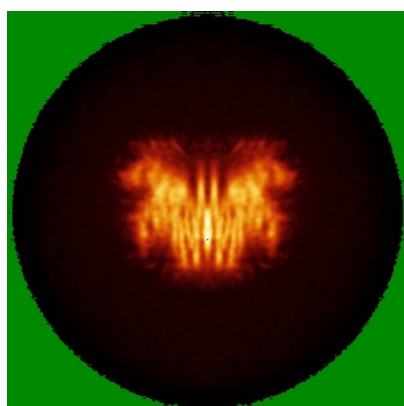


Z Index: 143

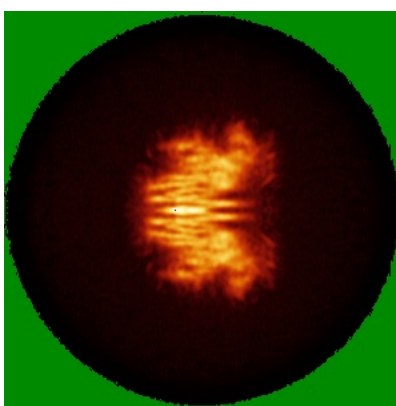
The images above show the largest variance slices of the map in three orthogonal directions.

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

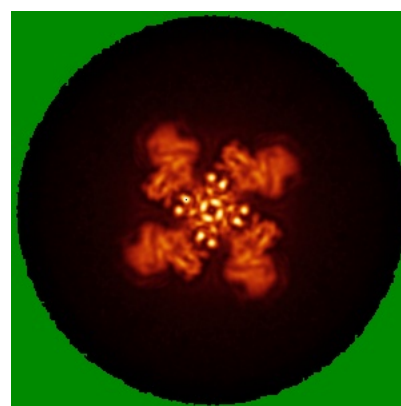
6.4.1 Primary map



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

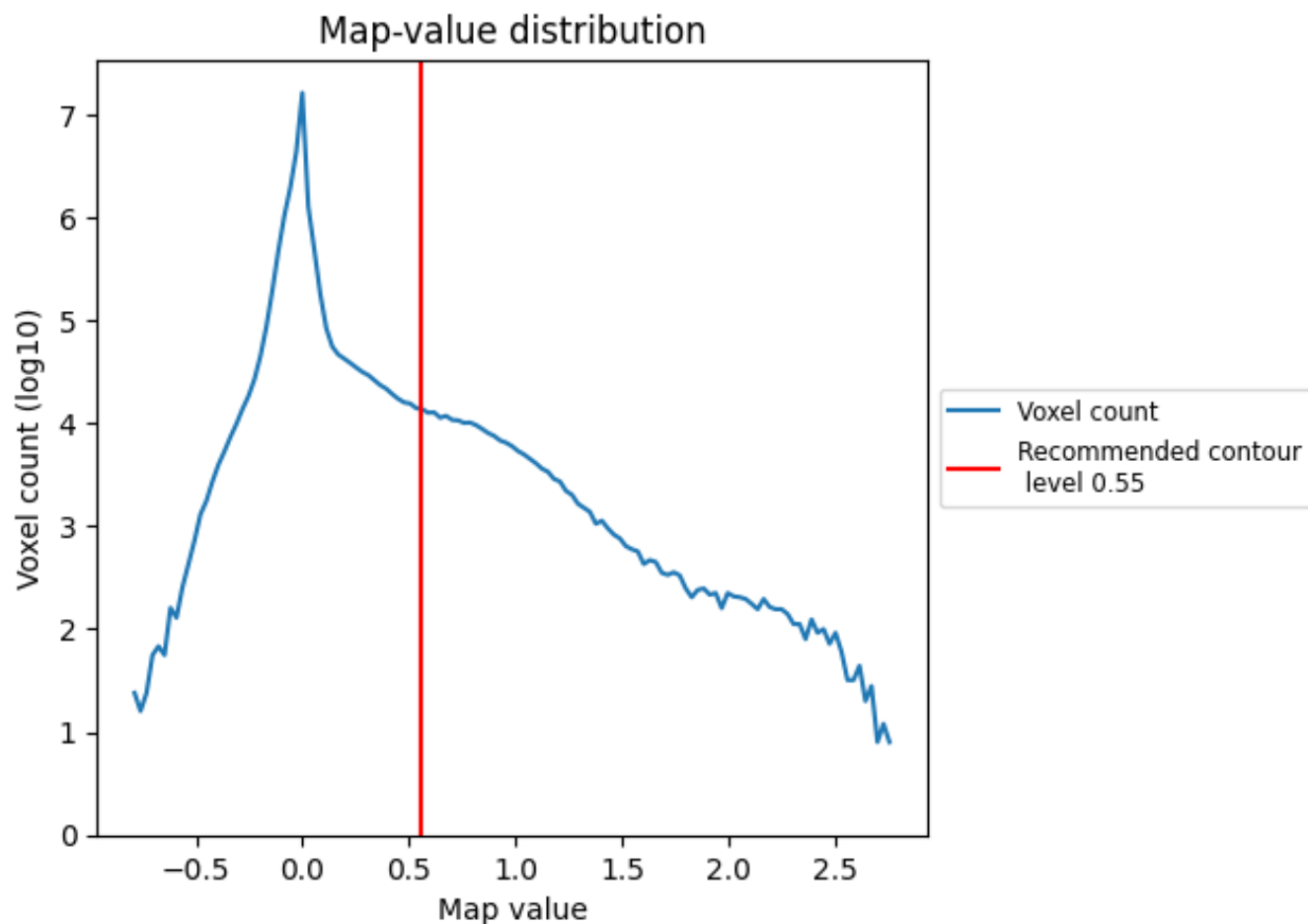
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

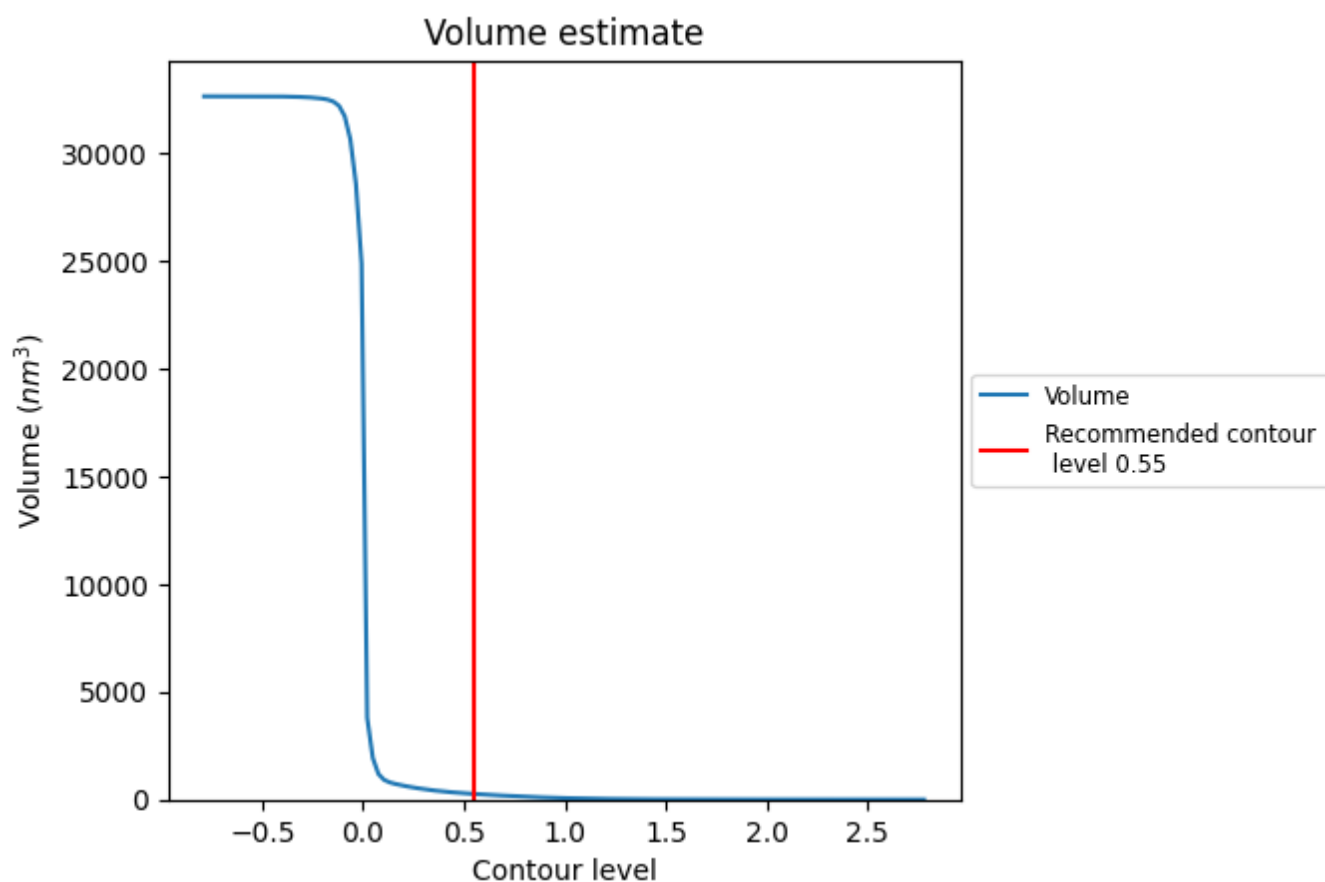
This section contains the results of statistical analysis of the map.

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.

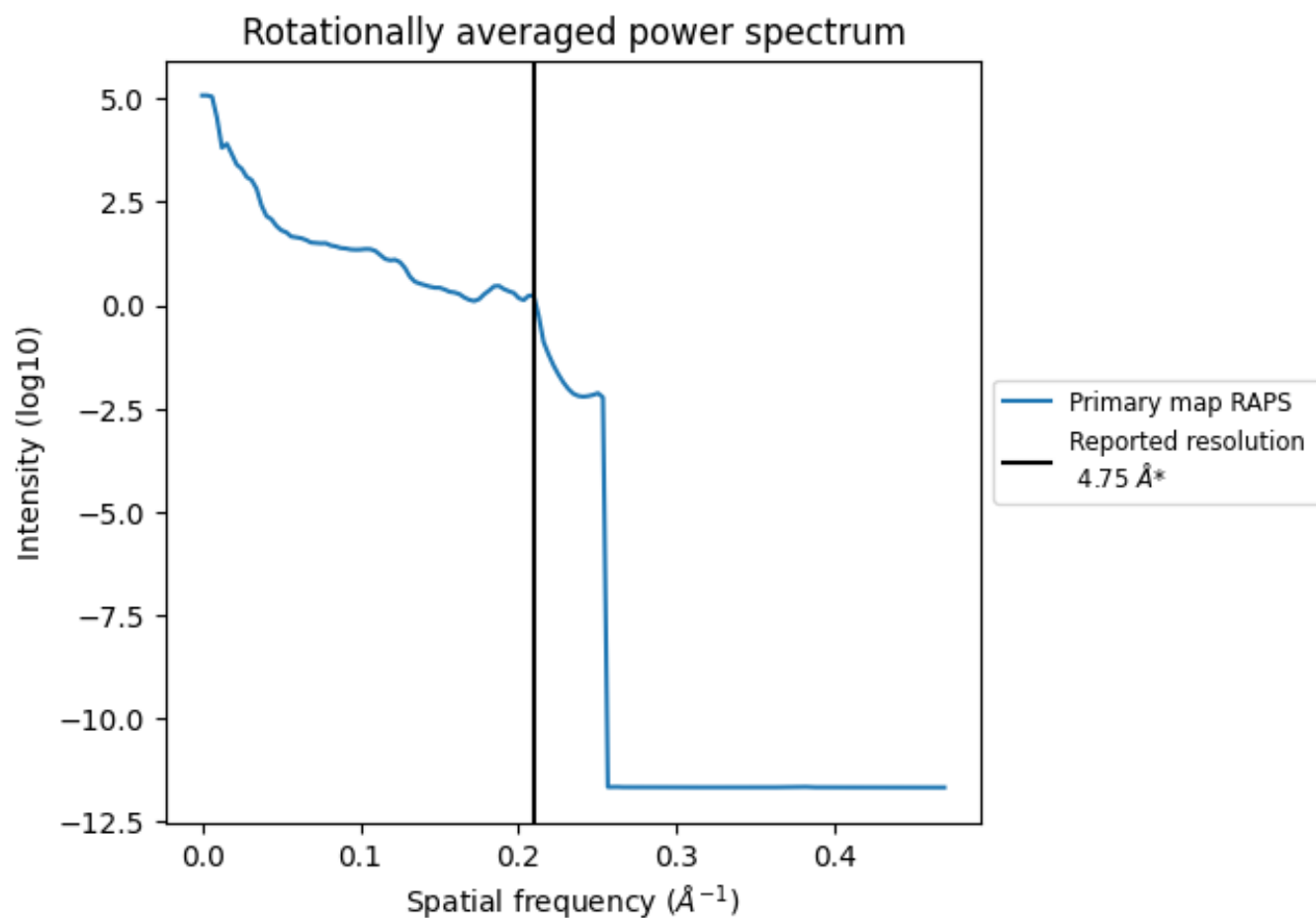
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm³; this corresponds to an approximate mass of 236 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 ⓘ

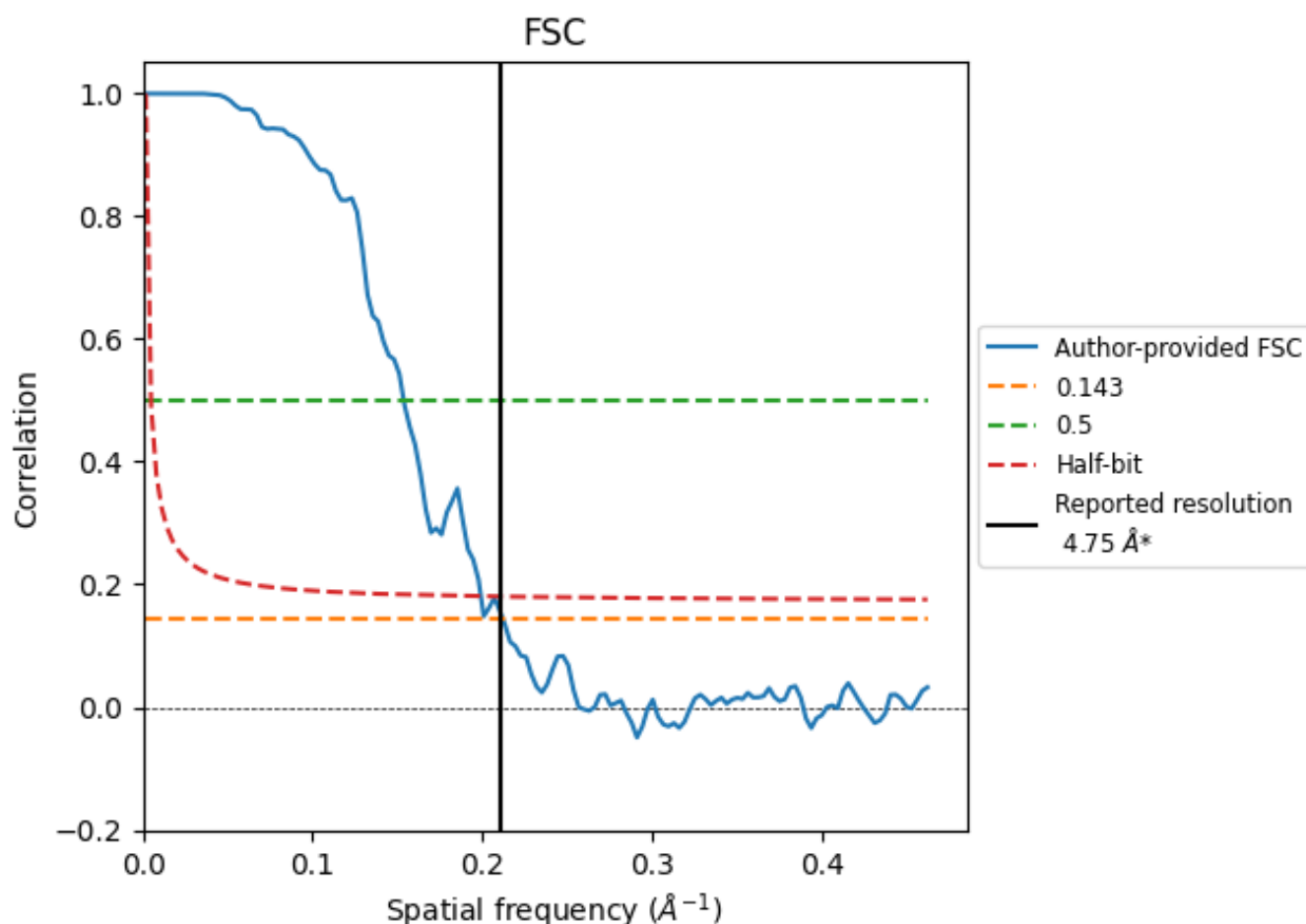


*Reported resolution corresponds to spatial frequency of 0.211 Å⁻¹

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 0.211 Å⁻¹

8.2 Resolution estimates [i](#)

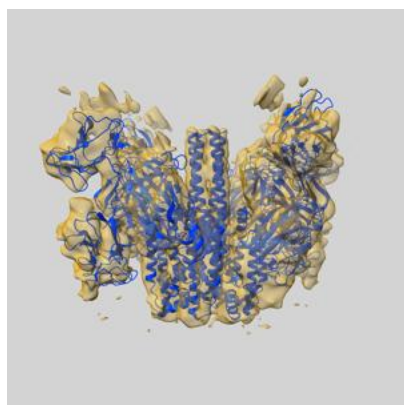
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.75	-	-
Author-provided FSC curve	4.71	6.51	5.02
Unmasked-calculated*	-	-	-

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

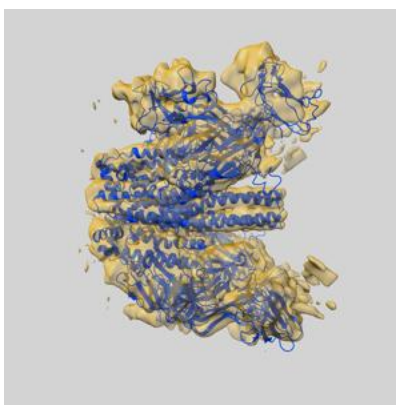
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10889 and PDB model 7NTX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

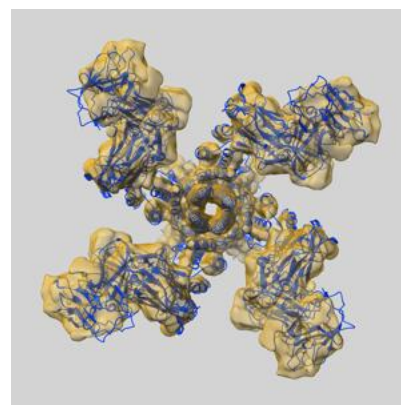
9.1 Map-model overlay [i](#)



X



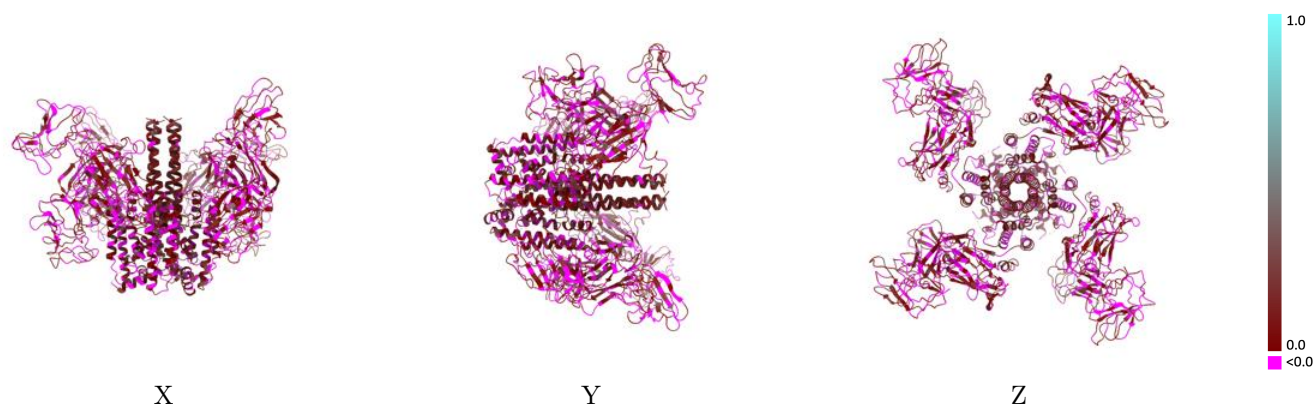
Y



Z

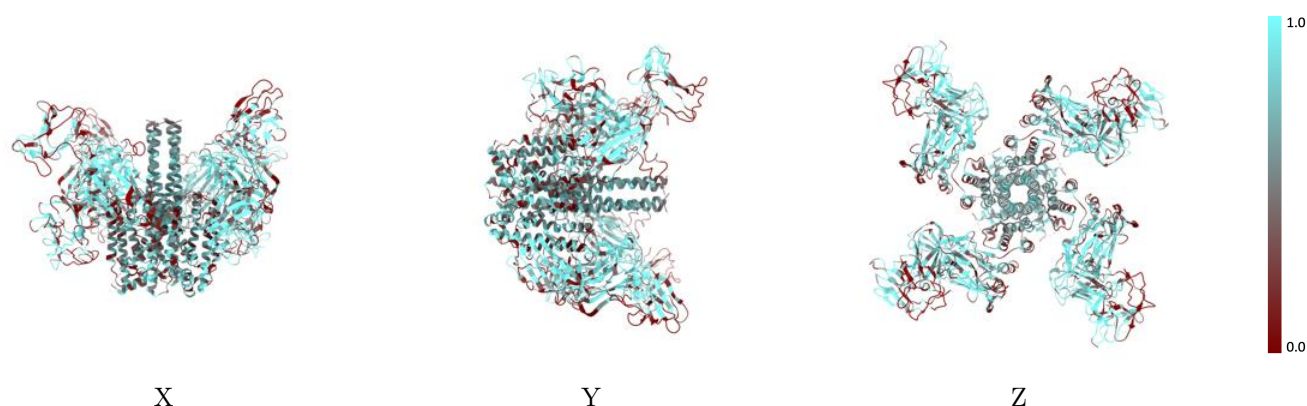
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



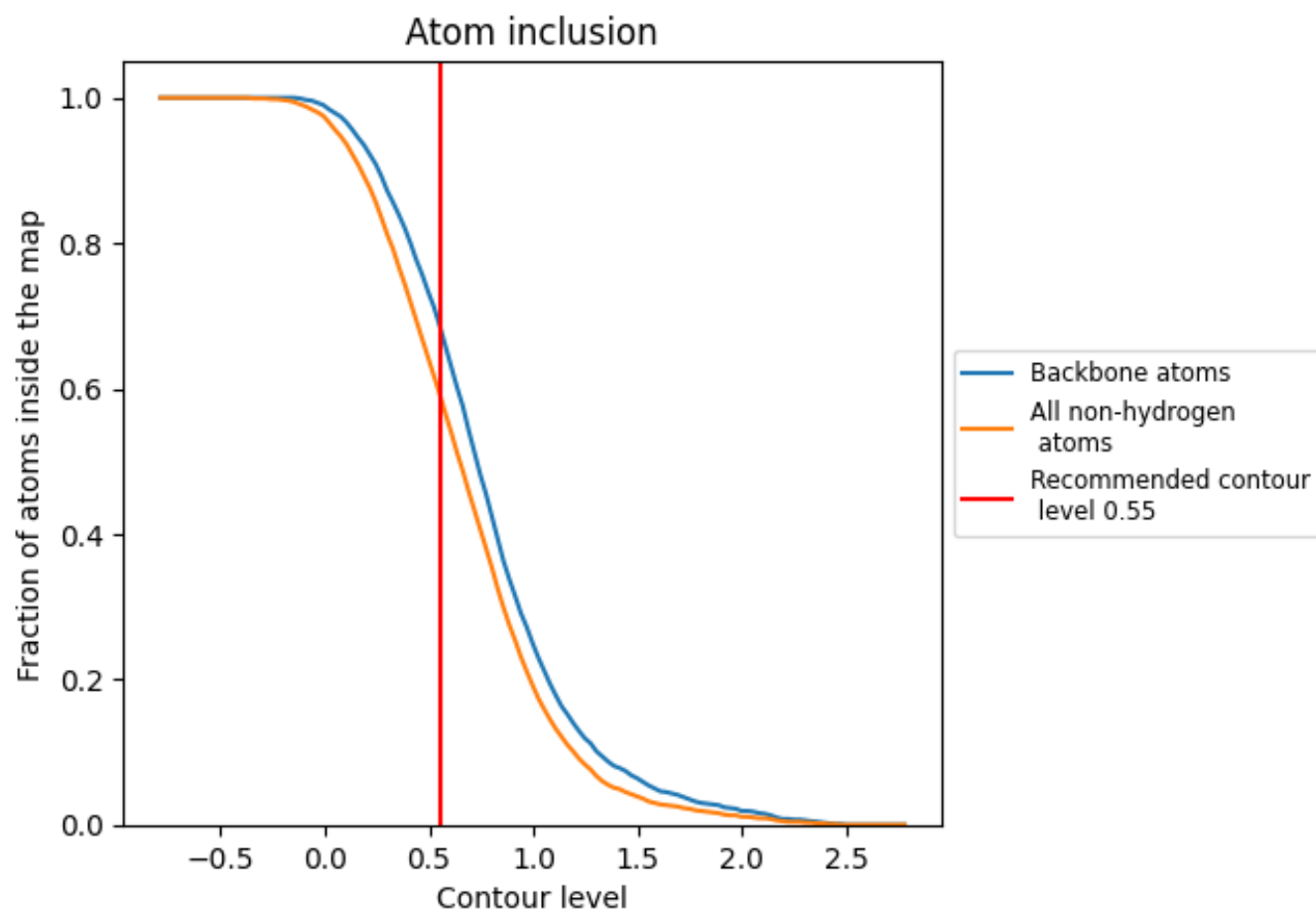
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 59% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5930	0.0470
A	0.5930	0.0510
B	0.5920	0.0460
C	0.5940	0.0500
D	0.5920	0.0410

