



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 08:30 pm GMT

PDB ID : 6Z6O
EMDB ID : EMD-11101
Title : HDAC-TC
Authors : Lee, J.-H.; Bollschweiler, D.; Schaefer, T.; Huber, R.
Deposited on : 2020-05-28
Resolution : 3.80 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

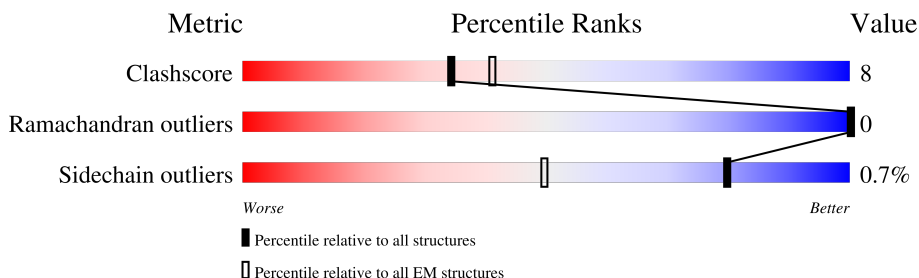
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	661	79% 20% .
1	E	661	78% 21% .
1	I	661	78% 21% .
1	M	661	79% 20% .
2	B	672	78% 20% .
2	F	672	79% 20% .
2	J	672	79% 19% .
2	N	672	80% 19% .

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Mol	Chain	Length	Quality of chain
3	C	629	<div><div>5%</div><div><div></div><div>65%</div><div>22%</div><div>13%</div></div></div>
3	G	629	<div><div>5%</div><div><div></div><div>65%</div><div>22%</div><div>13%</div></div></div>
3	K	629	<div><div>5%</div><div><div></div><div>65%</div><div>22%</div><div>13%</div></div></div>
3	O	629	<div><div>5%</div><div><div></div><div>65%</div><div>22%</div><div>13%</div></div></div>
4	D	542	<div><div>18%</div><div><div></div><div>77%</div><div>22%</div><div></div></div></div>
4	H	542	<div><div>18%</div><div><div></div><div>78%</div><div>22%</div><div></div></div></div>
4	L	542	<div><div>18%</div><div><div></div><div>79%</div><div>21%</div><div></div></div></div>
4	P	542	<div><div>18%</div><div><div></div><div>77%</div><div>23%</div><div></div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 77516 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 Histone deacetylase HDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	656	Total	C	N	O	S	0	0
			5220	3328	883	981	28		
1	E	656	Total	C	N	O	S	0	0
			5220	3328	883	981	28		
1	I	656	Total	C	N	O	S	0	0
			5220	3328	883	981	28		
1	M	656	Total	C	N	O	S	0	0
			5220	3328	883	981	28		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	LEU	ILE	conflict	UNP P53973
E	446	LEU	ILE	conflict	UNP P53973
I	446	LEU	ILE	conflict	UNP P53973
M	446	LEU	ILE	conflict	UNP P53973

- Molecule 2 is a protein called Histone deacetylase HDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	661	Total	C	N	O	S	0	0
			5245	3339	883	995	28		
2	F	661	Total	C	N	O	S	0	0
			5245	3339	883	995	28		
2	J	661	Total	C	N	O	S	0	0
			5245	3339	883	995	28		
2	N	661	Total	C	N	O	S	0	0
			5245	3339	883	995	28		

- Molecule 3 is a protein called HDA1 complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	548	Total	C	N	O	S	0	0
			4472	2835	768	856	13		
3	G	548	Total	C	N	O	S	0	0
			4472	2835	768	856	13		
3	K	548	Total	C	N	O	S	0	0
			4472	2835	768	856	13		
3	O	548	Total	C	N	O	S	0	0
			4472	2835	768	856	13		

- Molecule 4 is a protein called HDA1 complex subunit 3,HDA1 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	542	Total	C	N	O	S	0	0
			4440	2803	750	867	20		
4	H	542	Total	C	N	O	S	0	0
			4440	2803	750	867	20		
4	L	542	Total	C	N	O	S	0	0
			4440	2803	750	867	20		
4	P	542	Total	C	N	O	S	0	0
			4440	2803	750	867	20		

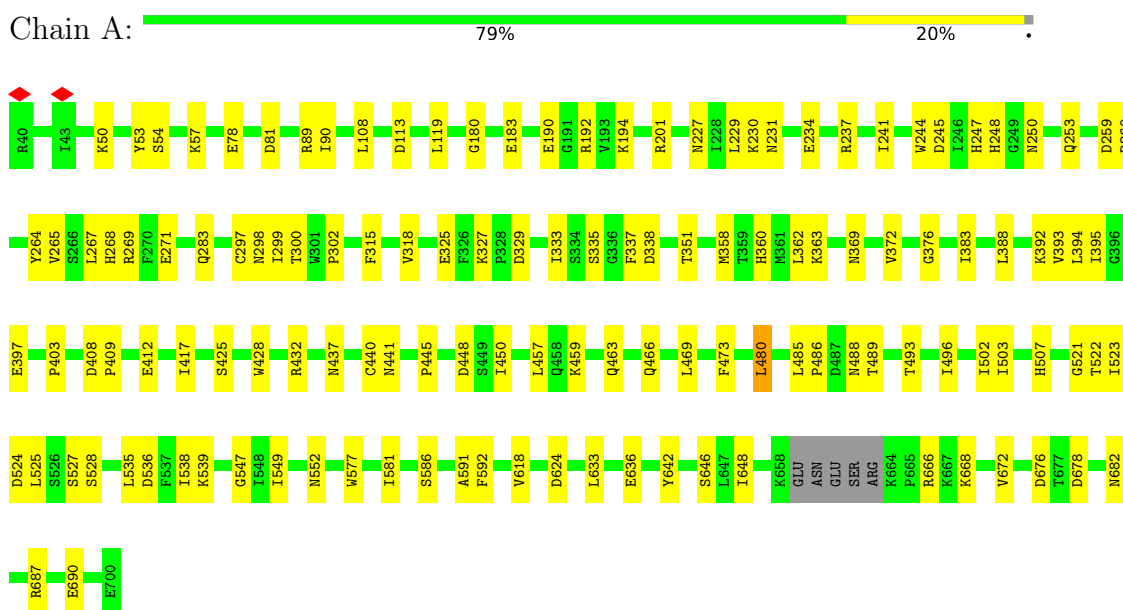
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	J	1	Total	Zn	0
			1	1	
5	M	1	Total	Zn	0
			1	1	
5	N	1	Total	Zn	0
			1	1	

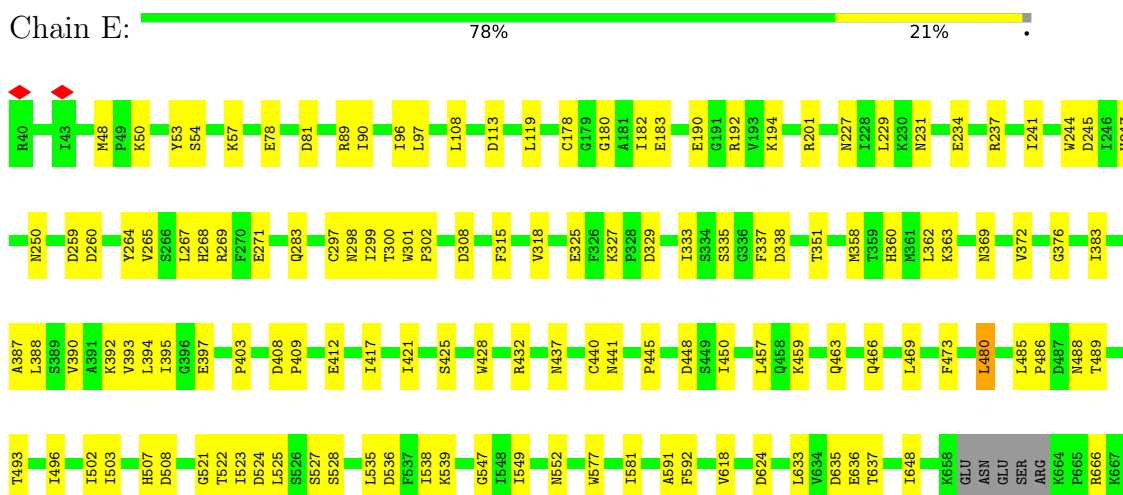
3 Residue-property plots

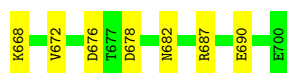
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Histone deacetylase HDA1



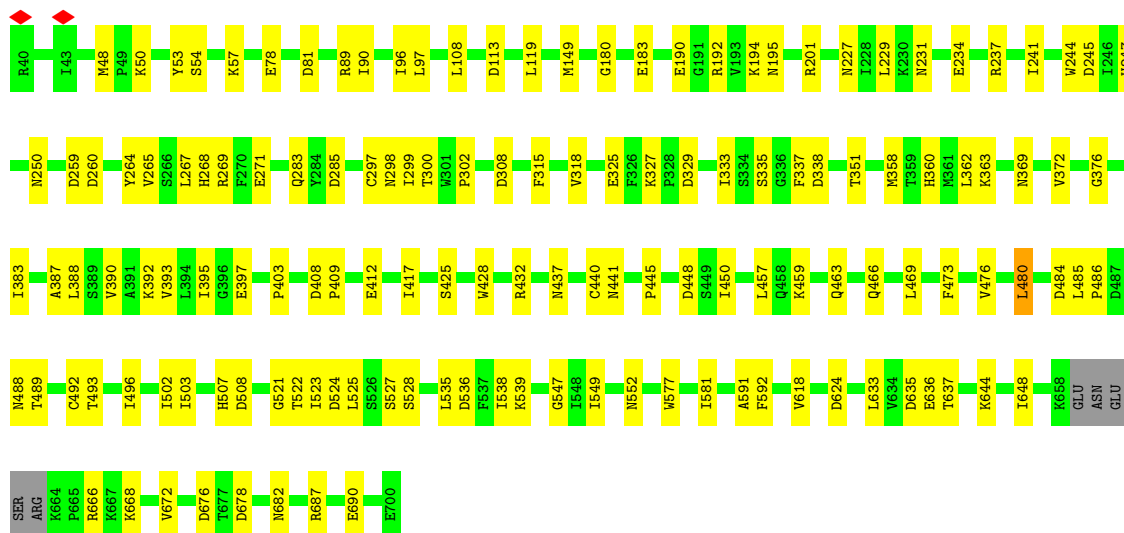
• Molecule 1: Histone deacetylase HDA1





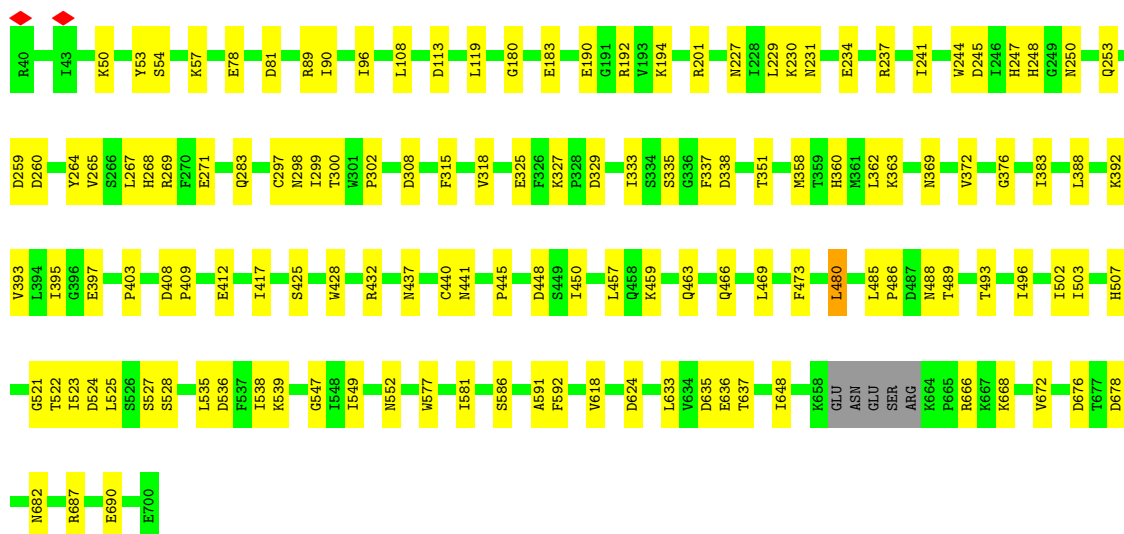
• Molecule 1: Histone deacetylase HDA1

Chain I: 78% 21%



• Molecule 1: Histone deacetylase HDA1

Chain M: 79% 20%

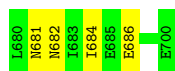


• Molecule 2: Histone deacetylase HDA1

Chain B: 78% 20%

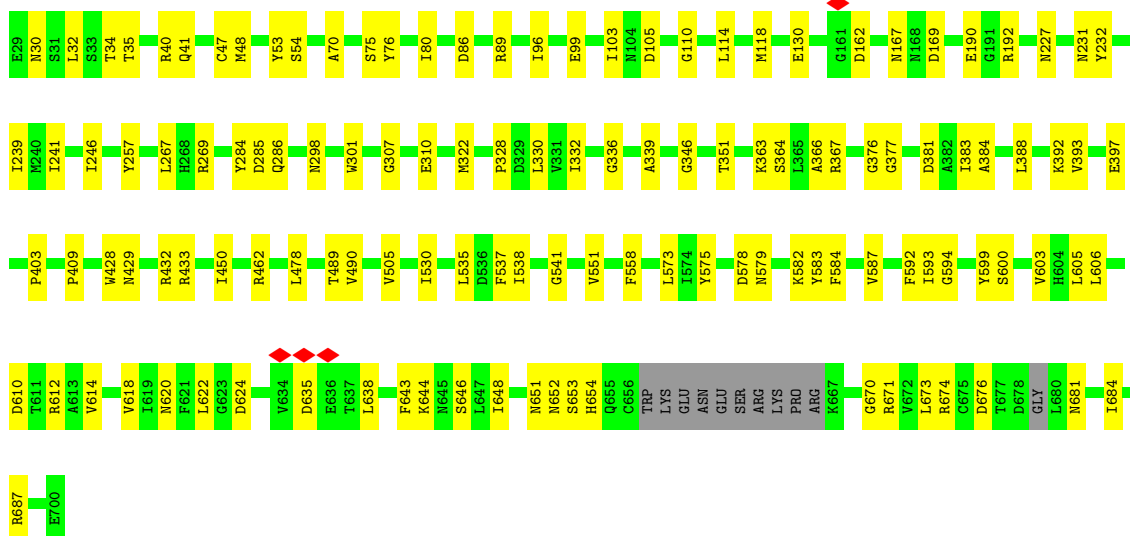






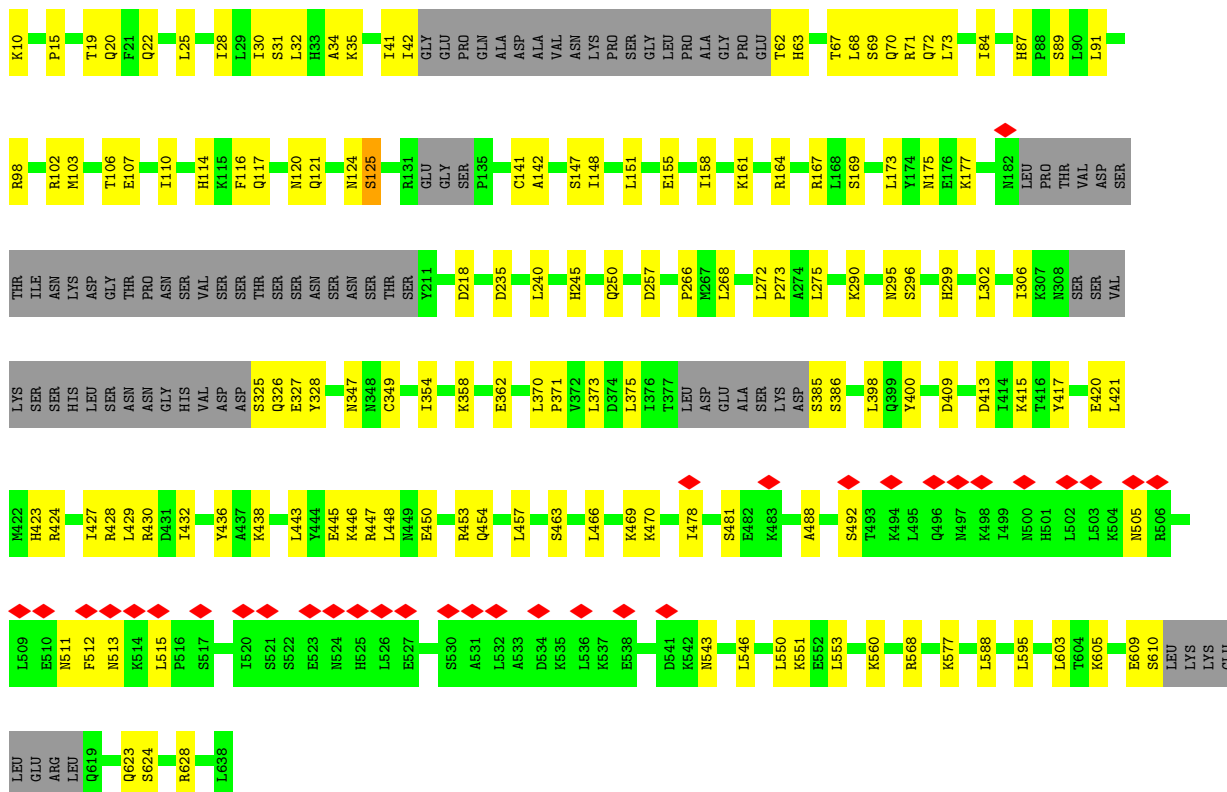
• Molecule 2: Histone deacetylase HDA1

Chain N: 80% 19%



• Molecule 3: HDA1 complex subunit 2

Chain C: 5% 65% 22% 13%



Chain G:

65% 22% 13%

Residue	Category
L638	Green
I520	Red
S521	Red
S522	Green
E523	Red
N524	Red
H525	Red
L526	Red
E527	Red
S530	Red
A531	Red
D534	Red
K535	Red
L536	Red
K537	Red
E538	Red
D541	Red
K542	Red
N543	Red
L546	Yellow
L550	Yellow
K551	Yellow
E552	Green
L553	Yellow
K560	Yellow
R568	Yellow
K577	Yellow
L588	Yellow
L595	Yellow
L603	Yellow
T604	Green
K605	Yellow
E609	Yellow
S610	Yellow
L610	Grey
L611	Grey
L612	Grey
L613	Grey
L614	Grey
L615	Grey
L616	Grey
L617	Grey
L618	Grey
L619	Grey
L620	Grey
L621	Grey
L622	Grey
L623	Grey
L624	Grey
L625	Grey
L626	Grey
L627	Grey
L628	Grey
L629	Grey
L630	Grey
L631	Grey
L632	Grey
L633	Grey
L634	Grey
L635	Grey
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L777	Grey
L778	Grey
L779	Grey
L780	Grey
L781	Grey
L782	Grey
L783	Grey
L784	Grey
L785	Grey
L786	Grey
L787	Grey
L788	Grey
L789	Grey
L790	Grey
L791	Grey
L792	Grey
L793	Grey
L794	Grey
L795	Grey
L796	Grey
L797	Grey
L798	Grey

Chain K:

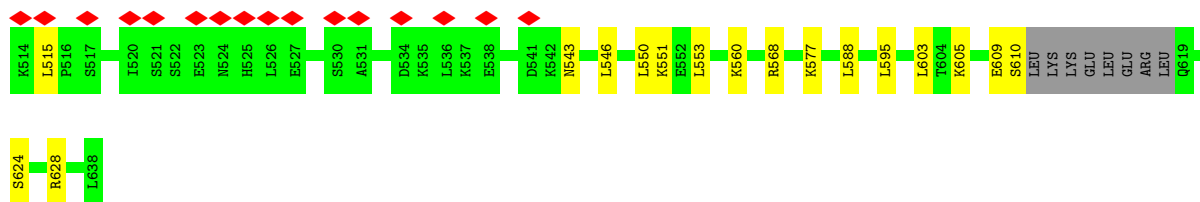
5% 65% 22% 13%

R428 R429 R430 R431 R432 R436 R437 R438 R443 R444 R445 R446 R447 R448 R449 R450 R453 R454 R457 R463 R466 R469 R470 R478 R481 R482 R483 R488 R492 R493 R494 R495 R496 R497 R499 R500 R501 R502 R504 R505 R506 R509 R510 R511 R512 R513

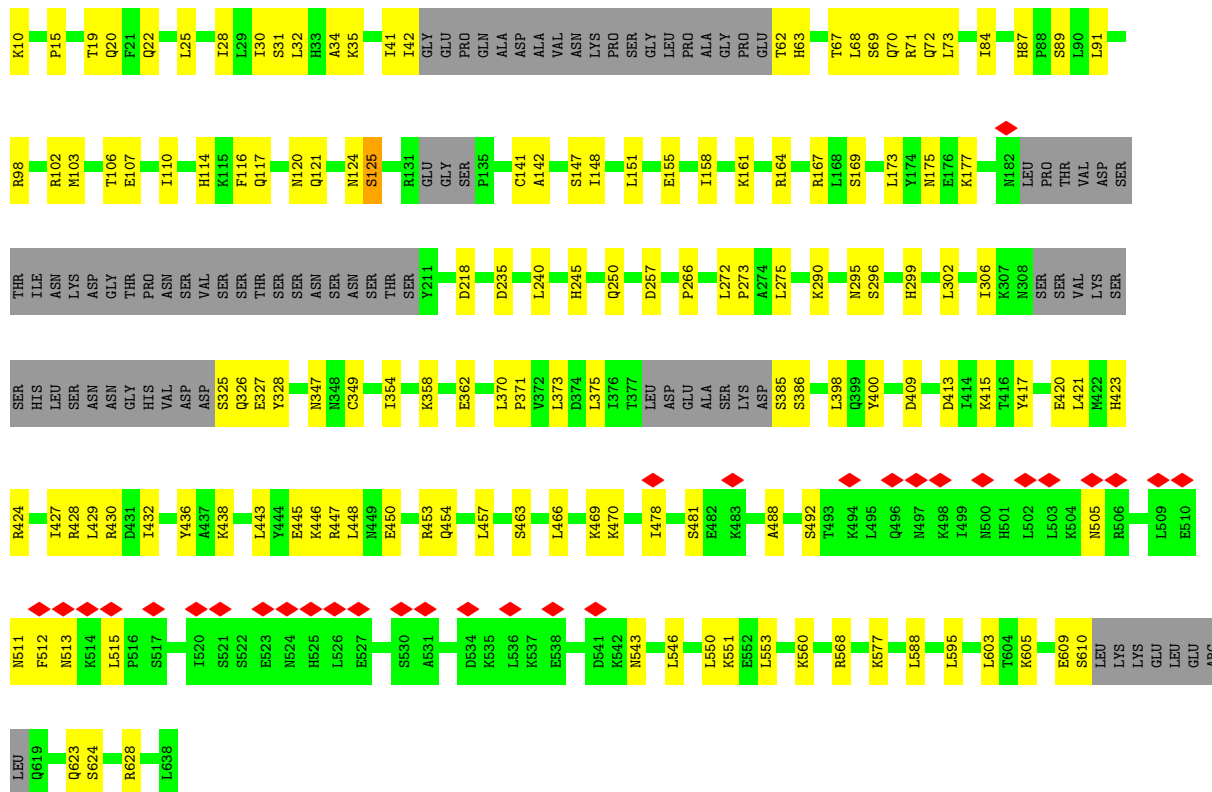
SER HIS LEU SER ASN ASN GLY HIS VAL ASP S325 Q326 K327 Y328 N347 N348 C349 K358 E362 L370 P371 P372 L373 L374 L375 L376 L377 LEU ASP GLU ALA SER LYS ASP S385 S386 L398 Q399 Y400 L405 P406 D413 Y417 E420 L421 Q422 H423 R424 I427

THR ILE ASN LYS ASP GLY THR PRO ASN SER VAL SER SER SER THR SER ASN SER Y211 D218 D235 L240 L245 Q250 D257 ALA P266 L272 P273 A274 L275 K290 N295 S296 H299 L302 I306 K307 N308 SER SER THR VAL LYS SER

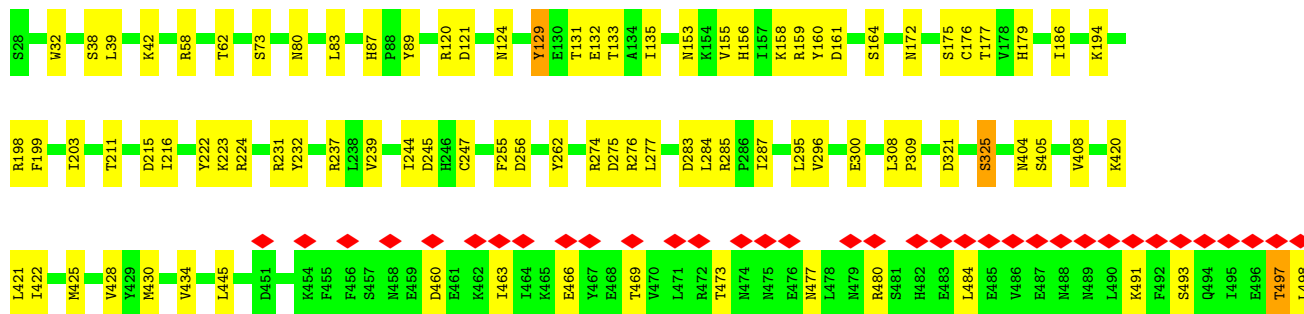
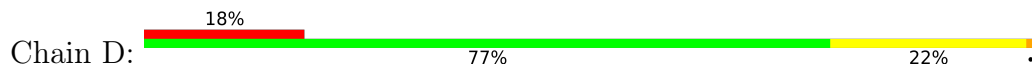
R98 R102 M103 T106 E107 I110 H114 K115 F116 Q117 N120 Q121 N124 S125 R131 GLU GLY SER P135 C141 A142 S147 I148 L151 E155 I158 K161 R164 R167 L168 S169 T173 Y174 L175 N175 K177 N182 LEU PRO THR VAL ASP SER

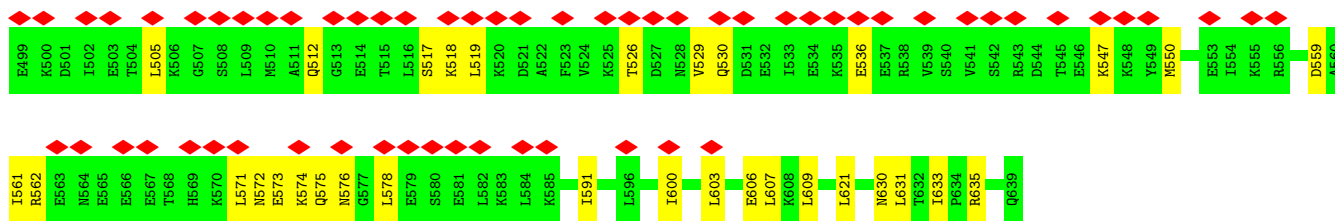


• Molecule 3: HDA1 complex subunit 2

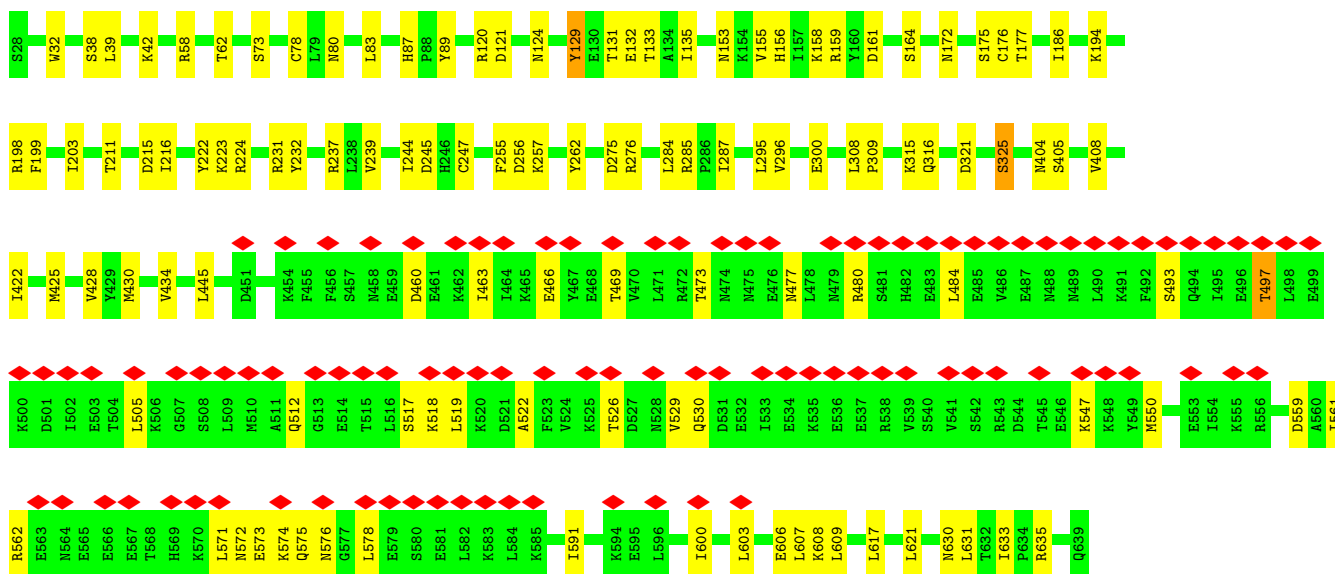
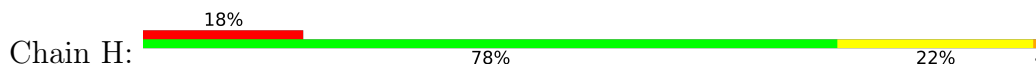


• Molecule 4: HDA1 complex subunit 3, HDA1 complex subunit 3

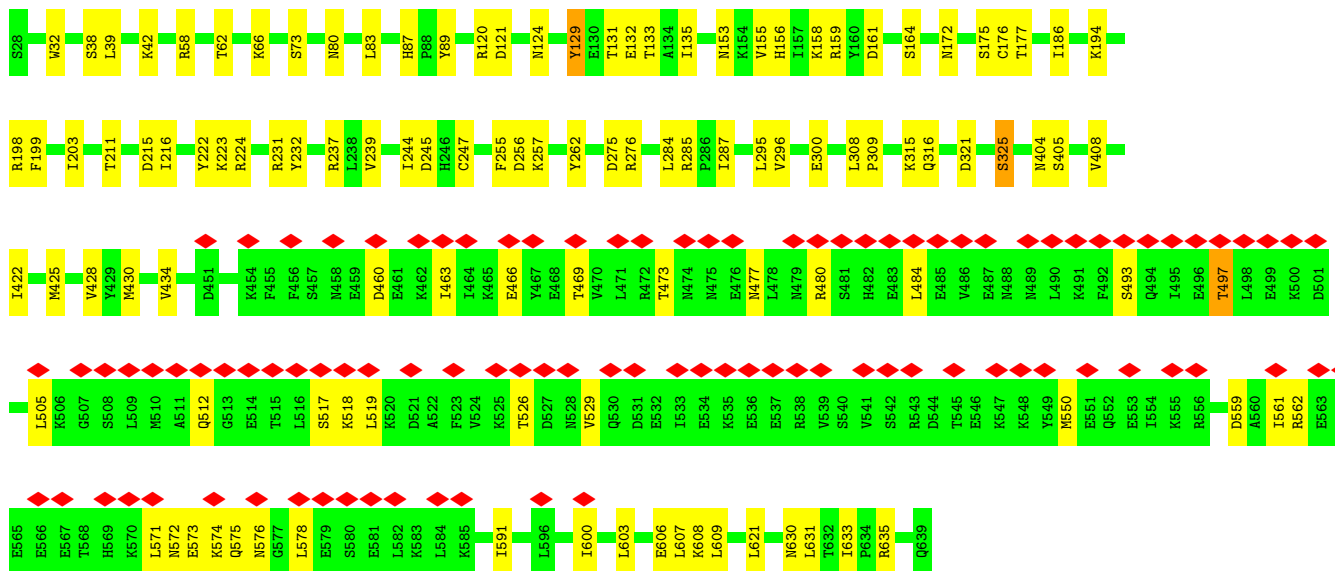
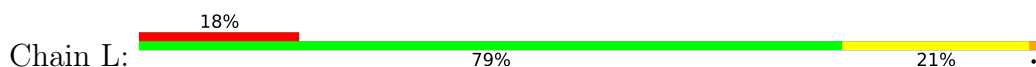




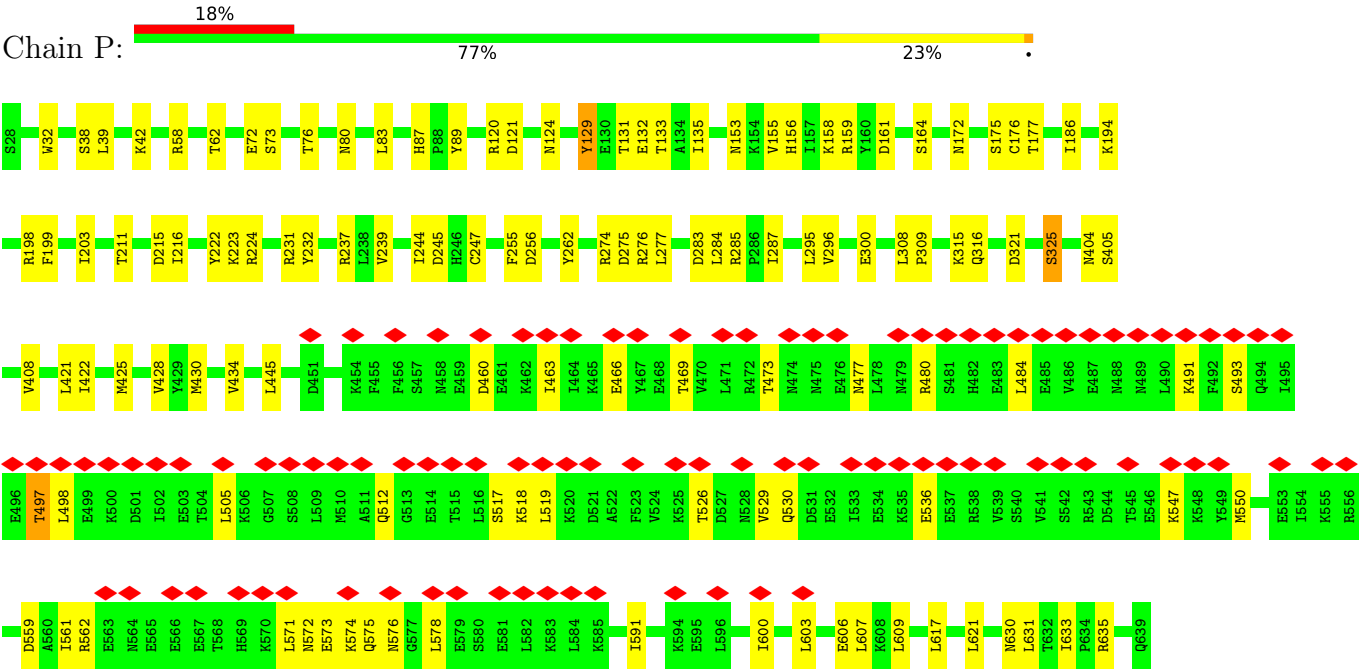
• Molecule 4: HDA1 complex subunit 3,HDA1 complex subunit 3



• Molecule 4: HDA1 complex subunit 3,HDA1 complex subunit 3



• Molecule 4: HDA1 complex subunit 3,HDA1 complex subunit 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	53757	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	86	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.650	Depositor
Minimum map value	-2.931	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.361	Depositor
Recommended contour level	1.3	Depositor
Map size (\AA)	510.72, 510.72, 510.72	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8512, 0.8512, 0.8512	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.37	0/5345	0.54	2/7251 (0.0%)
1	E	0.37	0/5345	0.55	2/7251 (0.0%)
1	I	0.37	0/5345	0.54	2/7251 (0.0%)
1	M	0.37	0/5345	0.54	2/7251 (0.0%)
2	B	0.37	0/5366	0.53	0/7277
2	F	0.37	0/5366	0.53	0/7277
2	J	0.37	0/5366	0.53	0/7277
2	N	0.37	0/5366	0.53	0/7277
3	C	0.31	0/4545	0.54	0/6120
3	G	0.31	0/4545	0.54	0/6120
3	K	0.31	0/4545	0.54	0/6120
3	O	0.31	0/4545	0.54	0/6120
4	D	0.31	0/4515	0.54	1/6087 (0.0%)
4	H	0.31	0/4515	0.54	1/6087 (0.0%)
4	L	0.31	0/4515	0.54	1/6087 (0.0%)
4	P	0.31	0/4515	0.54	1/6087 (0.0%)
All	All	0.34	0/79084	0.54	12/106940 (0.0%)

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	3
1	E	0	3
1	I	0	3
1	M	0	3
2	B	0	1
2	F	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1
3	C	0	2
3	G	0	2
3	K	0	2
3	O	0	2
4	D	0	2
4	H	0	2
4	L	0	2
4	P	0	2
All	All	0	32

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ILE	CG1-CB-CG2	-6.93	96.16	111.40
1	E	450	ILE	CG1-CB-CG2	-6.93	96.15	111.40
1	M	450	ILE	CG1-CB-CG2	-6.92	96.18	111.40
1	I	450	ILE	CG1-CB-CG2	-6.91	96.19	111.40
4	D	607	LEU	CA-CB-CG	5.75	128.53	115.30
4	H	607	LEU	CA-CB-CG	5.75	128.53	115.30
4	P	607	LEU	CA-CB-CG	5.74	128.50	115.30
4	L	607	LEU	CA-CB-CG	5.74	128.49	115.30
1	E	480	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	480	LEU	CA-CB-CG	5.36	127.62	115.30
1	M	480	LEU	CA-CB-CG	5.36	127.62	115.30
1	I	480	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	445	PRO	Peptide
1	A	521	GLY	Peptide
1	A	54	SER	Peptide
2	B	54	SER	Peptide
3	C	512	PHE	Peptide
3	C	605	LYS	Peptide
4	D	231	ARG	Peptide
4	D	256	ASP	Peptide
1	E	445	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	E	521	GLY	Peptide
1	E	54	SER	Peptide
2	F	54	SER	Peptide
3	G	512	PHE	Peptide
3	G	605	LYS	Peptide
4	H	231	ARG	Peptide
4	H	256	ASP	Peptide
1	I	445	PRO	Peptide
1	I	521	GLY	Peptide
1	I	54	SER	Peptide
2	J	54	SER	Peptide
3	K	512	PHE	Peptide
3	K	605	LYS	Peptide
4	L	231	ARG	Peptide
4	L	256	ASP	Peptide
1	M	445	PRO	Peptide
1	M	521	GLY	Peptide
1	M	54	SER	Peptide
2	N	54	SER	Peptide
3	O	512	PHE	Peptide
3	O	605	LYS	Peptide
4	P	231	ARG	Peptide
4	P	256	ASP	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	5220	0	5136	85	0
1	E	5220	0	5136	91	0
1	I	5220	0	5136	93	0
1	M	5220	0	5136	87	0
2	B	5245	0	5155	91	0
2	F	5245	0	5155	90	0
2	J	5245	0	5155	86	0
2	N	5245	0	5155	86	0
3	C	4472	0	4536	86	0
3	G	4472	0	4536	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	4472	0	4536	85	0
3	O	4472	0	4536	85	0
4	D	4440	0	4447	70	0
4	H	4440	0	4447	68	0
4	L	4440	0	4447	63	0
4	P	4440	0	4447	71	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
All	All	77516	0	77096	1226	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 8.

All (1226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:575:TYR:O	2:J:579:ASN:HB2	1.77	0.84
2:F:575:TYR:O	2:F:579:ASN:HB2	1.79	0.83
2:B:575:TYR:O	2:B:579:ASN:HB2	1.80	0.81
2:N:575:TYR:O	2:N:579:ASN:HB2	1.80	0.81
3:C:358:LYS:O	3:C:362:GLU:HB2	1.83	0.77
3:G:358:LYS:O	3:G:362:GLU:HB2	1.83	0.77
3:O:358:LYS:O	3:O:362:GLU:HB2	1.83	0.76
3:K:358:LYS:O	3:K:362:GLU:HB2	1.83	0.76
1:A:459:LYS:O	1:A:463:GLN:HB2	1.89	0.73
1:M:459:LYS:O	1:M:463:GLN:HB2	1.89	0.73
1:E:459:LYS:O	1:E:463:GLN:HB2	1.88	0.73
1:I:459:LYS:O	1:I:463:GLN:HB2	1.89	0.72
2:F:96:ILE:HG13	2:F:384:ALA:HB1	1.77	0.66
2:J:96:ILE:HG13	2:J:384:ALA:HB1	1.78	0.66
2:J:32:LEU:HA	4:L:58:ARG:HH12	1.60	0.65
2:N:96:ILE:HG13	2:N:384:ALA:HB1	1.77	0.65
2:B:96:ILE:HG13	2:B:384:ALA:HB1	1.78	0.65
1:E:592:PHE:HB2	1:E:618:VAL:HG23	1.81	0.63
2:B:47:CYS:SG	2:B:48:MET:N	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:47:CYS:SG	2:N:48:MET:N	2.72	0.63
1:A:592:PHE:HB2	1:A:618:VAL:HG23	1.81	0.63
2:J:47:CYS:SG	2:J:48:MET:N	2.72	0.63
1:M:592:PHE:HB2	1:M:618:VAL:HG23	1.81	0.63
2:F:47:CYS:SG	2:F:48:MET:N	2.72	0.63
1:I:592:PHE:HB2	1:I:618:VAL:HG23	1.81	0.63
4:H:133:THR:HA	4:H:199:PHE:HB3	1.80	0.62
4:D:133:THR:HA	4:D:199:PHE:HB3	1.80	0.62
4:P:133:THR:HA	4:P:199:PHE:HB3	1.80	0.62
4:L:133:THR:HA	4:L:199:PHE:HB3	1.80	0.62
2:B:239:ILE:HG12	2:B:330:LEU:HB3	1.82	0.61
2:N:239:ILE:HG12	2:N:330:LEU:HB3	1.82	0.61
2:B:535:LEU:HD12	2:B:538:ILE:HD12	1.83	0.61
2:B:32:LEU:HA	4:D:58:ARG:HH12	1.65	0.61
2:N:535:LEU:HD12	2:N:538:ILE:HD12	1.83	0.61
3:G:15:PRO:HG3	3:G:370:LEU:HD12	1.83	0.61
3:C:15:PRO:HG3	3:C:370:LEU:HD12	1.83	0.61
3:K:15:PRO:HG3	3:K:370:LEU:HD12	1.83	0.61
2:F:535:LEU:HD12	2:F:538:ILE:HD12	1.83	0.60
2:J:535:LEU:HD12	2:J:538:ILE:HD12	1.83	0.60
2:N:328:PRO:HG2	2:N:366:ALA:HB2	1.83	0.60
2:F:32:LEU:HA	4:H:58:ARG:HH12	1.66	0.60
3:O:15:PRO:HG3	3:O:370:LEU:HD12	1.83	0.60
2:B:328:PRO:HG2	2:B:366:ALA:HB2	1.83	0.60
2:J:620:ASN:HD21	2:J:622:LEU:HD13	1.66	0.60
2:F:620:ASN:HD21	2:F:622:LEU:HD13	1.67	0.60
3:K:347:ASN:ND2	3:K:349:CYS:SG	2.75	0.60
1:E:244:TRP:HE1	1:E:335:SER:HG	1.47	0.60
1:I:244:TRP:HE1	1:I:335:SER:HG	1.47	0.60
3:G:347:ASN:ND2	3:G:349:CYS:SG	2.75	0.60
2:N:32:LEU:HA	4:P:58:ARG:HH12	1.66	0.60
2:F:328:PRO:HG2	2:F:366:ALA:HB2	1.83	0.60
2:B:600:SER:O	2:B:603:VAL:HB	2.02	0.59
1:E:522:THR:OG1	1:E:523:ILE:N	2.35	0.59
1:I:522:THR:OG1	1:I:523:ILE:N	2.35	0.59
2:J:328:PRO:HG2	2:J:366:ALA:HB2	1.83	0.59
2:F:239:ILE:HG12	2:F:330:LEU:HB3	1.82	0.59
1:I:265:VAL:HG22	1:I:297:CYS:HB3	1.84	0.59
2:N:310:GLU:HG3	2:N:409:PRO:HB3	1.84	0.59
2:B:620:ASN:HD21	2:B:622:LEU:HD13	1.66	0.59
1:E:265:VAL:HG22	1:E:297:CYS:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:ASP:OD1	1:E:536:ASP:N	2.36	0.59
2:N:620:ASN:HD21	2:N:622:LEU:HD13	1.66	0.59
3:O:347:ASN:ND2	3:O:349:CYS:SG	2.75	0.59
3:C:347:ASN:ND2	3:C:349:CYS:SG	2.75	0.59
2:J:239:ILE:HG12	2:J:330:LEU:HB3	1.82	0.59
1:M:536:ASP:N	1:M:536:ASP:OD1	2.36	0.59
2:N:600:SER:O	2:N:603:VAL:HB	2.03	0.59
1:A:265:VAL:HG22	1:A:297:CYS:HB3	1.84	0.59
1:A:536:ASP:N	1:A:536:ASP:OD1	2.36	0.59
1:A:525:LEU:O	1:A:528:SER:OG	2.21	0.59
2:F:592:PHE:HB2	2:F:618:VAL:HG12	1.85	0.59
4:H:512:GLN:NE2	4:H:526:THR:OG1	2.36	0.59
1:M:265:VAL:HG22	1:M:297:CYS:HB3	1.84	0.59
1:M:525:LEU:O	1:M:528:SER:OG	2.21	0.59
1:A:244:TRP:HE1	1:A:335:SER:HG	1.50	0.59
4:L:512:GLN:NE2	4:L:526:THR:OG1	2.36	0.59
2:J:592:PHE:HB2	2:J:618:VAL:HG12	1.85	0.59
1:E:194:LYS:NZ	1:E:395:ILE:O	2.36	0.59
1:I:194:LYS:NZ	1:I:395:ILE:O	2.36	0.58
2:J:600:SER:O	2:J:603:VAL:HB	2.03	0.58
1:M:397:GLU:HG3	2:N:53:TYR:HB3	1.85	0.58
1:A:397:GLU:HG3	2:B:53:TYR:HB3	1.85	0.58
4:H:159:ARG:HH21	4:H:161:ASP:HB3	1.68	0.58
2:F:600:SER:O	2:F:603:VAL:HB	2.03	0.58
2:N:285:ASP:OD1	2:N:285:ASP:N	2.36	0.58
2:B:644:LYS:HD3	2:B:671:ARG:HH22	1.68	0.58
4:D:198:ARG:HG2	4:D:223:LYS:HB2	1.85	0.58
4:P:198:ARG:HG2	4:P:223:LYS:HB2	1.85	0.58
4:P:512:GLN:NE2	4:P:526:THR:OG1	2.36	0.58
2:B:404:ASP:OD1	2:B:404:ASP:N	2.37	0.58
4:D:512:GLN:NE2	4:D:526:THR:OG1	2.36	0.58
4:L:159:ARG:HH21	4:L:161:ASP:HB3	1.69	0.58
2:N:644:LYS:HD3	2:N:671:ARG:HH22	1.69	0.58
4:P:159:ARG:HH21	4:P:161:ASP:HB3	1.69	0.58
2:B:310:GLU:HG3	2:B:409:PRO:HB3	1.86	0.58
2:J:310:GLU:HG3	2:J:409:PRO:HB3	1.84	0.58
2:F:652:ASN:ND2	2:F:676:ASP:O	2.36	0.58
4:D:159:ARG:HH21	4:D:161:ASP:HB3	1.69	0.58
2:F:285:ASP:OD1	2:F:285:ASP:N	2.36	0.58
1:E:397:GLU:HG3	2:F:53:TYR:HB3	1.85	0.58
1:I:397:GLU:HG3	2:J:53:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:285:ASP:N	2:J:285:ASP:OD1	2.36	0.58
1:A:522:THR:OG1	1:A:523:ILE:N	2.36	0.57
3:C:450:GLU:OE2	3:C:453:ARG:NH2	2.37	0.57
2:F:310:GLU:HG3	2:F:409:PRO:HB3	1.85	0.57
4:H:198:ARG:HG2	4:H:223:LYS:HB2	1.85	0.57
4:L:198:ARG:HG2	4:L:223:LYS:HB2	1.85	0.57
1:M:522:THR:OG1	1:M:523:ILE:N	2.36	0.57
2:F:490:VAL:HG12	2:F:551:VAL:HA	1.86	0.57
2:F:644:LYS:HD3	2:F:671:ARG:HH22	1.68	0.57
2:N:592:PHE:HB2	2:N:618:VAL:HG12	1.85	0.57
3:O:450:GLU:OE2	3:O:453:ARG:NH2	2.37	0.57
1:E:325:GLU:O	1:E:327:LYS:NZ	2.38	0.57
1:I:325:GLU:O	1:I:327:LYS:NZ	2.38	0.57
2:J:490:VAL:HG12	2:J:551:VAL:HA	1.86	0.57
2:B:592:PHE:HB2	2:B:618:VAL:HG12	1.85	0.57
2:J:644:LYS:HD3	2:J:671:ARG:HH22	1.68	0.57
3:C:250:GLN:HG2	3:C:273:PRO:HB2	1.86	0.57
2:N:652:ASN:ND2	2:N:676:ASP:O	2.36	0.57
1:E:525:LEU:O	1:E:528:SER:OG	2.21	0.57
1:I:525:LEU:O	1:I:528:SER:OG	2.21	0.57
1:M:283:GLN:O	1:M:298:ASN:ND2	2.38	0.57
1:A:194:LYS:NZ	1:A:395:ILE:O	2.36	0.57
1:A:283:GLN:O	1:A:298:ASN:ND2	2.38	0.57
2:B:652:ASN:ND2	2:B:676:ASP:O	2.36	0.57
3:G:450:GLU:OE2	3:G:453:ARG:NH2	2.37	0.57
4:L:505:LEU:HD12	4:L:529:VAL:HG22	1.87	0.57
3:O:250:GLN:HG2	3:O:273:PRO:HB2	1.86	0.57
3:G:41:ILE:HG22	3:G:42:ILE:HG13	1.86	0.57
3:K:450:GLU:OE2	3:K:453:ARG:NH2	2.37	0.57
1:M:194:LYS:NZ	1:M:395:ILE:O	2.36	0.57
2:N:351:THR:HG21	2:N:403:PRO:HG2	1.87	0.57
3:O:84:ILE:HG13	3:O:91:LEU:HD21	1.85	0.57
1:A:337:PHE:HB2	1:A:383:ILE:HG22	1.87	0.57
3:C:41:ILE:HG22	3:C:42:ILE:HG13	1.86	0.57
3:C:84:ILE:HG13	3:C:91:LEU:HD21	1.85	0.57
1:E:283:GLN:O	1:E:298:ASN:ND2	2.38	0.57
4:H:505:LEU:HD12	4:H:529:VAL:HG22	1.87	0.57
1:M:337:PHE:HB2	1:M:383:ILE:HG22	1.87	0.57
3:O:41:ILE:HG22	3:O:42:ILE:HG13	1.86	0.57
3:G:250:GLN:HG2	3:G:273:PRO:HB2	1.86	0.56
2:J:284:TYR:HA	2:J:298:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:41:ILE:HG22	3:K:42:ILE:HG13	1.86	0.56
3:K:84:ILE:HG13	3:K:91:LEU:HD21	1.85	0.56
4:P:460:ASP:HA	4:P:463:ILE:HD12	1.87	0.56
1:A:50:LYS:NZ	2:B:99:GLU:O	2.38	0.56
3:G:84:ILE:HG13	3:G:91:LEU:HD21	1.85	0.56
2:B:490:VAL:HG12	2:B:551:VAL:HA	1.86	0.56
3:C:151:LEU:HD11	3:C:240:LEU:HB3	1.87	0.56
4:D:460:ASP:HA	4:D:463:ILE:HD12	1.87	0.56
3:K:250:GLN:HG2	3:K:273:PRO:HB2	1.86	0.56
1:M:50:LYS:NZ	2:N:99:GLU:O	2.38	0.56
1:M:463:GLN:NE2	1:M:466:GLN:OE1	2.39	0.56
2:N:490:VAL:HG12	2:N:551:VAL:HA	1.86	0.56
2:F:284:TYR:HA	2:F:298:ASN:HB2	1.88	0.56
4:H:460:ASP:HA	4:H:463:ILE:HD12	1.87	0.56
2:F:606:LEU:HD11	2:F:618:VAL:HG11	1.88	0.56
1:A:463:GLN:NE2	1:A:466:GLN:OE1	2.39	0.56
2:F:404:ASP:N	2:F:404:ASP:OD1	2.37	0.56
1:M:325:GLU:O	1:M:327:LYS:NZ	2.38	0.56
3:O:151:LEU:HD11	3:O:240:LEU:HB3	1.87	0.56
2:B:351:THR:HG21	2:B:403:PRO:HG2	1.88	0.56
2:J:606:LEU:HD11	2:J:618:VAL:HG11	1.88	0.56
4:L:460:ASP:HA	4:L:463:ILE:HD12	1.87	0.56
2:N:606:LEU:HD11	2:N:618:VAL:HG11	1.88	0.56
1:A:325:GLU:O	1:A:327:LYS:NZ	2.38	0.56
2:J:404:ASP:OD1	2:J:404:ASP:N	2.37	0.56
2:B:643:PHE:HA	2:B:670:GLY:HA2	1.88	0.56
1:M:244:TRP:HE1	1:M:335:SER:HG	1.54	0.56
2:N:643:PHE:HA	2:N:670:GLY:HA2	1.88	0.56
2:B:284:TYR:HA	2:B:298:ASN:HB2	1.87	0.56
2:B:606:LEU:HD11	2:B:618:VAL:HG11	1.88	0.56
1:E:50:LYS:NZ	2:F:99:GLU:O	2.38	0.56
2:J:643:PHE:HA	2:J:670:GLY:HA2	1.88	0.56
2:F:246:ILE:HB	2:F:339:ALA:HB2	1.88	0.55
3:G:151:LEU:HD11	3:G:240:LEU:HB3	1.87	0.55
1:I:50:LYS:NZ	2:J:99:GLU:O	2.38	0.55
1:I:466:GLN:OE1	1:I:488:ASN:ND2	2.39	0.55
2:J:351:THR:HG21	2:J:403:PRO:HG2	1.88	0.55
3:K:151:LEU:HD11	3:K:240:LEU:HB3	1.87	0.55
4:D:493:SER:O	4:D:497:THR:OG1	2.25	0.55
1:E:535:LEU:HG	1:E:539:LYS:HE2	1.89	0.55
3:O:436:TYR:HA	3:O:588:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:505:LEU:HD12	4:P:529:VAL:HG22	1.87	0.55
4:D:505:LEU:HD12	4:D:529:VAL:HG22	1.87	0.55
2:F:351:THR:HG21	2:F:403:PRO:HG2	1.88	0.55
3:G:436:TYR:HA	3:G:588:LEU:HD21	1.88	0.55
1:I:337:PHE:HB2	1:I:383:ILE:HG22	1.87	0.55
1:I:535:LEU:HG	1:I:539:LYS:HE2	1.89	0.55
2:J:246:ILE:HB	2:J:339:ALA:HB2	1.89	0.55
4:P:493:SER:O	4:P:497:THR:OG1	2.25	0.55
3:C:155:GLU:OE2	3:C:167:ARG:NH1	2.39	0.55
3:C:436:TYR:HA	3:C:588:LEU:HD21	1.88	0.55
3:K:436:TYR:HA	3:K:588:LEU:HD21	1.88	0.55
2:F:643:PHE:HA	2:F:670:GLY:HA2	1.88	0.55
2:N:284:TYR:HA	2:N:298:ASN:HB2	1.87	0.55
1:E:337:PHE:HB2	1:E:383:ILE:HG22	1.87	0.55
2:F:587:VAL:HG22	2:F:614:VAL:HG11	1.89	0.55
1:I:536:ASP:OD1	1:I:536:ASP:N	2.36	0.55
2:N:587:VAL:HG22	2:N:614:VAL:HG11	1.89	0.55
3:O:155:GLU:OE2	3:O:167:ARG:NH1	2.39	0.55
2:B:587:VAL:HG22	2:B:614:VAL:HG11	1.89	0.55
2:F:363:LYS:NZ	2:F:393:VAL:O	2.40	0.55
2:J:363:LYS:NZ	2:J:393:VAL:O	2.40	0.55
3:K:302:LEU:O	3:K:306:ILE:HB	2.07	0.55
3:G:302:LEU:O	3:G:306:ILE:HB	2.07	0.55
1:I:190:GLU:OE1	1:I:192:ARG:NH1	2.37	0.55
3:K:218:ASP:OD1	3:K:218:ASP:N	2.40	0.55
1:A:89:ARG:NH2	1:A:376:GLY:O	2.40	0.55
3:G:218:ASP:OD1	3:G:218:ASP:N	2.40	0.55
1:M:89:ARG:NH2	1:M:376:GLY:O	2.40	0.55
1:M:535:LEU:HG	1:M:539:LYS:HE2	1.89	0.55
1:A:535:LEU:HG	1:A:539:LYS:HE2	1.89	0.54
4:H:477:ASN:HD22	4:H:561:ILE:HB	1.72	0.54
1:I:363:LYS:NZ	1:I:393:VAL:O	2.39	0.54
1:I:463:GLN:NE2	1:I:466:GLN:OE1	2.39	0.54
3:K:103:MET:O	3:K:624:SER:OG	2.25	0.54
4:D:32:TRP:NE1	4:D:309:PRO:O	2.31	0.54
1:E:190:GLU:OE1	1:E:192:ARG:NH1	2.37	0.54
3:G:103:MET:O	3:G:624:SER:OG	2.25	0.54
3:G:164:ARG:HG3	3:G:235:ASP:HB2	1.89	0.54
4:L:477:ASN:HD22	4:L:561:ILE:HB	1.72	0.54
4:P:58:ARG:O	4:P:62:THR:OG1	2.26	0.54
1:A:329:ASP:O	1:A:369:ASN:ND2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:ARG:O	4:D:62:THR:OG1	2.26	0.54
1:E:363:LYS:NZ	1:E:393:VAL:O	2.39	0.54
3:K:164:ARG:HG3	3:K:235:ASP:HB2	1.89	0.54
2:N:246:ILE:HB	2:N:339:ALA:HB2	1.88	0.54
2:B:246:ILE:HB	2:B:339:ALA:HB2	1.89	0.54
2:B:322:MET:SD	2:B:428:TRP:NE1	2.80	0.54
2:F:241:ILE:HG12	2:F:332:ILE:HB	1.89	0.54
2:J:587:VAL:HG22	2:J:614:VAL:HG11	1.90	0.54
4:P:477:ASN:HD22	4:P:561:ILE:HB	1.72	0.54
3:C:164:ARG:HG3	3:C:235:ASP:HB2	1.89	0.54
4:D:477:ASN:HD22	4:D:561:ILE:HB	1.72	0.54
1:I:268:HIS:O	1:I:300:THR:HA	2.08	0.54
1:I:480:LEU:HD11	1:I:485:LEU:HD12	1.88	0.54
2:J:241:ILE:HG12	2:J:332:ILE:HB	1.89	0.54
1:M:190:GLU:OE1	1:M:192:ARG:NH1	2.37	0.54
2:N:322:MET:SD	2:N:428:TRP:NE1	2.81	0.54
3:O:164:ARG:HG3	3:O:235:ASP:HB2	1.89	0.54
2:B:363:LYS:NZ	2:B:393:VAL:O	2.40	0.54
1:E:113:ASP:OD1	1:E:113:ASP:N	2.41	0.54
2:J:322:MET:SD	2:J:428:TRP:NE1	2.81	0.54
1:M:329:ASP:O	1:M:369:ASN:ND2	2.35	0.54
2:N:162:ASP:OD1	2:N:162:ASP:N	2.39	0.54
1:A:190:GLU:OE1	1:A:192:ARG:NH1	2.37	0.54
2:B:162:ASP:OD1	2:B:162:ASP:N	2.39	0.54
1:E:268:HIS:O	1:E:300:THR:HA	2.08	0.54
1:E:463:GLN:NE2	1:E:466:GLN:OE1	2.40	0.54
2:F:322:MET:SD	2:F:428:TRP:NE1	2.80	0.54
1:M:648:ILE:HB	1:M:672:VAL:HA	1.90	0.54
2:N:363:LYS:NZ	2:N:393:VAL:O	2.40	0.54
3:O:302:LEU:O	3:O:306:ILE:HB	2.07	0.54
4:P:32:TRP:NE1	4:P:309:PRO:O	2.31	0.54
1:A:648:ILE:HB	1:A:672:VAL:HA	1.90	0.54
3:C:302:LEU:O	3:C:306:ILE:HB	2.07	0.54
2:F:651:ASN:HB3	2:F:654:HIS:HB2	1.90	0.54
2:F:681:ASN:HA	2:F:684:ILE:HD12	1.90	0.54
3:G:147:SER:OG	3:G:148:ILE:N	2.40	0.54
3:K:147:SER:OG	3:K:148:ILE:N	2.40	0.54
4:L:493:SER:O	4:L:497:THR:OG1	2.25	0.54
2:N:241:ILE:HG12	2:N:332:ILE:HB	1.89	0.54
4:H:493:SER:O	4:H:497:THR:OG1	2.25	0.54
1:I:89:ARG:NH2	1:I:376:GLY:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:ASP:OD1	1:I:113:ASP:N	2.41	0.54
1:A:666:ARG:HH11	1:I:636:GLU:HG3	1.73	0.54
2:B:241:ILE:HG12	2:B:332:ILE:HB	1.90	0.54
2:B:681:ASN:HA	2:B:684:ILE:HD12	1.90	0.54
3:C:31:SER:OG	3:C:424:ARG:NH1	2.41	0.54
1:E:89:ARG:NH2	1:E:376:GLY:O	2.41	0.54
1:E:466:GLN:OE1	1:E:488:ASN:ND2	2.40	0.54
2:F:377:GLY:HA3	2:F:383:ILE:HD12	1.90	0.54
2:J:377:GLY:HA3	2:J:383:ILE:HD12	1.90	0.54
2:N:41:GLN:NE2	4:P:321:ASP:OD1	2.41	0.54
3:C:141:CYS:SG	3:C:142:ALA:N	2.82	0.53
1:E:636:GLU:HG3	1:M:666:ARG:HH11	1.73	0.53
2:F:70:ALA:O	2:F:167:ASN:ND2	2.41	0.53
1:I:283:GLN:O	1:I:298:ASN:ND2	2.38	0.53
2:J:70:ALA:O	2:J:167:ASN:ND2	2.41	0.53
2:J:681:ASN:HA	2:J:684:ILE:HD12	1.91	0.53
3:K:155:GLU:OE2	3:K:167:ARG:NH1	2.39	0.53
3:O:141:CYS:SG	3:O:142:ALA:N	2.82	0.53
1:A:480:LEU:HD11	1:A:485:LEU:HD12	1.90	0.53
2:B:285:ASP:OD1	2:B:285:ASP:N	2.36	0.53
4:D:135:ILE:HG12	4:D:203:ILE:HB	1.91	0.53
2:N:377:GLY:HA3	2:N:383:ILE:HD12	1.90	0.53
3:O:31:SER:OG	3:O:424:ARG:NH1	2.41	0.53
1:A:440:CYS:SG	1:A:441:ASN:N	2.81	0.53
2:B:377:GLY:HA3	2:B:383:ILE:HD12	1.91	0.53
3:G:141:CYS:SG	3:G:142:ALA:N	2.81	0.53
3:G:155:GLU:OE2	3:G:167:ARG:NH1	2.39	0.53
1:I:648:ILE:HB	1:I:672:VAL:HA	1.90	0.53
3:K:443:LEU:HD12	3:K:446:LYS:HD2	1.90	0.53
1:M:268:HIS:O	1:M:300:THR:HA	2.07	0.53
1:M:440:CYS:SG	1:M:441:ASN:N	2.81	0.53
1:M:676:ASP:OD1	1:M:676:ASP:N	2.40	0.53
4:P:135:ILE:HG12	4:P:203:ILE:HB	1.91	0.53
3:G:443:LEU:HD12	3:G:446:LYS:HD2	1.90	0.53
3:K:141:CYS:SG	3:K:142:ALA:N	2.81	0.53
1:M:480:LEU:HD11	1:M:485:LEU:HD12	1.90	0.53
1:A:676:ASP:OD1	1:A:676:ASP:N	2.40	0.53
3:C:481:SER:OG	3:C:543:ASN:OD1	2.22	0.53
3:G:31:SER:OG	3:G:424:ARG:NH1	2.41	0.53
3:G:385:SER:OG	3:G:386:SER:N	2.42	0.53
2:J:367:ARG:NH1	3:K:628:ARG:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:31:SER:OG	3:K:424:ARG:NH1	2.41	0.53
2:N:367:ARG:NH1	3:O:628:ARG:O	2.41	0.53
2:N:681:ASN:HA	2:N:684:ILE:HD12	1.91	0.53
3:O:481:SER:OG	3:O:543:ASN:OD1	2.22	0.53
1:A:268:HIS:O	1:A:300:THR:HA	2.08	0.53
3:C:218:ASP:N	3:C:218:ASP:OD1	2.40	0.53
4:D:283:ASP:OD1	4:D:283:ASP:N	2.41	0.53
4:D:296:VAL:O	4:D:300:GLU:N	2.42	0.53
1:E:648:ILE:HB	1:E:672:VAL:HA	1.90	0.53
3:K:385:SER:OG	3:K:386:SER:N	2.42	0.53
4:P:283:ASP:OD1	4:P:283:ASP:N	2.41	0.53
4:P:296:VAL:O	4:P:300:GLU:N	2.42	0.53
2:B:367:ARG:NH1	3:C:628:ARG:O	2.41	0.53
3:C:175:ASN:O	3:C:177:LYS:NZ	2.42	0.53
3:K:98:ARG:O	3:K:102:ARG:NH1	2.42	0.53
4:L:296:VAL:O	4:L:300:GLU:N	2.42	0.53
2:N:70:ALA:O	2:N:167:ASN:ND2	2.41	0.53
3:O:175:ASN:O	3:O:177:LYS:NZ	2.42	0.53
2:F:190:GLU:OE2	2:F:232:TYR:OH	2.27	0.53
3:G:98:ARG:O	3:G:102:ARG:NH1	2.42	0.53
4:H:296:VAL:O	4:H:300:GLU:N	2.42	0.53
2:J:190:GLU:OE2	2:J:232:TYR:OH	2.27	0.53
2:J:652:ASN:ND2	2:J:676:ASP:O	2.36	0.53
3:O:218:ASP:N	3:O:218:ASP:OD1	2.40	0.53
4:P:473:THR:HG23	4:P:561:ILE:HD13	1.90	0.53
4:D:473:THR:HG23	4:D:561:ILE:HD13	1.90	0.53
1:E:480:LEU:HD11	1:E:485:LEU:HD12	1.91	0.53
2:F:367:ARG:NH1	3:G:628:ARG:O	2.42	0.53
4:H:473:THR:HG23	4:H:561:ILE:HD13	1.90	0.53
3:K:175:ASN:O	3:K:177:LYS:NZ	2.42	0.53
4:L:473:THR:HG23	4:L:561:ILE:HD13	1.90	0.53
3:O:446:LYS:HZ1	3:O:577:LYS:HD2	1.73	0.53
1:A:636:GLU:HG3	1:I:666:ARG:HH11	1.73	0.53
3:C:147:SER:OG	3:C:148:ILE:N	2.40	0.53
3:C:443:LEU:HD12	3:C:446:LYS:HD2	1.90	0.53
4:L:58:ARG:O	4:L:62:THR:OG1	2.25	0.53
2:B:70:ALA:O	2:B:167:ASN:ND2	2.41	0.52
2:B:190:GLU:OE2	2:B:232:TYR:OH	2.27	0.52
3:G:175:ASN:O	3:G:177:LYS:NZ	2.42	0.52
3:O:443:LEU:HD12	3:O:446:LYS:HD2	1.90	0.52
2:B:114:LEU:HD22	2:B:118:MET:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:LEU:HD22	2:F:118:MET:HB2	1.91	0.52
4:L:422:ILE:HG21	4:L:621:LEU:HD11	1.91	0.52
2:N:190:GLU:OE2	2:N:232:TYR:OH	2.27	0.52
3:O:147:SER:OG	3:O:148:ILE:N	2.40	0.52
4:P:198:ARG:HB3	4:P:222:TYR:HB3	1.91	0.52
1:A:351:THR:HG21	1:A:403:PRO:HG2	1.91	0.52
3:C:446:LYS:HZ1	3:C:577:LYS:HD2	1.73	0.52
4:D:198:ARG:HB3	4:D:222:TYR:HB3	1.91	0.52
3:G:429:LEU:HD12	3:G:595:LEU:HG	1.91	0.52
4:H:135:ILE:HG12	4:H:203:ILE:HB	1.91	0.52
2:J:114:LEU:HD22	2:J:118:MET:HB2	1.91	0.52
3:K:121:GLN:O	3:K:125:SER:OG	2.27	0.52
3:K:429:LEU:HD12	3:K:595:LEU:HG	1.91	0.52
1:M:351:THR:HG21	1:M:403:PRO:HG2	1.91	0.52
3:O:62:THR:OG1	3:O:63:HIS:N	2.43	0.52
3:C:62:THR:OG1	3:C:63:HIS:N	2.42	0.52
3:C:400:TYR:O	3:C:438:LYS:NZ	2.42	0.52
3:G:62:THR:OG1	3:G:63:HIS:N	2.43	0.52
4:H:58:ARG:O	4:H:62:THR:OG1	2.26	0.52
4:H:422:ILE:HG21	4:H:621:LEU:HD11	1.91	0.52
3:K:62:THR:OG1	3:K:63:HIS:N	2.43	0.52
1:M:408:ASP:O	2:N:433:ARG:NH2	2.42	0.52
1:M:466:GLN:OE1	1:M:488:ASN:ND2	2.40	0.52
3:O:400:TYR:O	3:O:438:LYS:NZ	2.42	0.52
4:L:198:ARG:HB3	4:L:222:TYR:HB3	1.91	0.52
3:O:98:ARG:O	3:O:102:ARG:NH1	2.42	0.52
3:O:429:LEU:HD12	3:O:595:LEU:HG	1.91	0.52
4:P:315:LYS:NZ	4:P:316:GLN:O	2.39	0.52
1:A:408:ASP:O	2:B:433:ARG:NH2	2.42	0.52
1:A:466:GLN:OE1	1:A:488:ASN:ND2	2.40	0.52
3:C:98:ARG:O	3:C:102:ARG:NH1	2.42	0.52
3:C:429:LEU:HD12	3:C:595:LEU:HG	1.91	0.52
4:D:422:ILE:HG21	4:D:621:LEU:HD11	1.91	0.52
3:G:481:SER:OG	3:G:543:ASN:OD1	2.22	0.52
2:J:651:ASN:HB3	2:J:654:HIS:HB2	1.92	0.52
4:P:422:ILE:HG21	4:P:621:LEU:HD11	1.91	0.52
1:A:577:TRP:HA	1:A:581:ILE:HD12	1.91	0.52
3:C:120:ASN:O	3:C:124:ASN:ND2	2.43	0.52
1:E:666:ARG:HH11	1:M:636:GLU:HG3	1.73	0.52
3:K:400:TYR:O	3:K:438:LYS:NZ	2.42	0.52
3:K:481:SER:OG	3:K:543:ASN:OD1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:135:ILE:HG12	4:L:203:ILE:HB	1.91	0.52
2:N:114:LEU:HD22	2:N:118:MET:HB2	1.92	0.52
3:G:400:TYR:O	3:G:438:LYS:NZ	2.42	0.52
3:O:120:ASN:O	3:O:124:ASN:ND2	2.43	0.52
3:O:624:SER:OG	3:O:624:SER:O	2.27	0.52
3:C:624:SER:OG	3:C:624:SER:O	2.27	0.52
2:F:41:GLN:NE2	4:H:321:ASP:OD1	2.43	0.52
2:N:651:ASN:HB3	2:N:654:HIS:HB2	1.92	0.52
1:A:633:LEU:O	1:I:666:ARG:NH2	2.40	0.52
1:E:351:THR:HG21	1:E:403:PRO:HG2	1.91	0.52
1:E:493:THR:HB	1:E:496:ILE:HD13	1.91	0.52
1:E:666:ARG:NH2	1:M:633:LEU:O	2.40	0.52
4:H:198:ARG:HB3	4:H:222:TYR:HB3	1.91	0.52
1:I:351:THR:HG21	1:I:403:PRO:HG2	1.91	0.52
1:M:577:TRP:HA	1:M:581:ILE:HD12	1.91	0.51
1:I:149:MET:O	4:L:66:LYS:NZ	2.44	0.51
2:B:573:LEU:HB3	2:B:605:LEU:HD22	1.93	0.51
2:B:610:ASP:OD1	2:B:612:ARG:NH2	2.44	0.51
1:I:440:CYS:SG	1:I:441:ASN:N	2.81	0.51
4:L:211:THR:HA	4:L:216:ILE:HD13	1.92	0.51
2:N:610:ASP:OD1	2:N:612:ARG:NH2	2.44	0.51
2:B:41:GLN:NE2	4:D:321:ASP:OD1	2.44	0.51
2:B:103:ILE:HG23	2:B:114:LEU:HG	1.92	0.51
3:C:121:GLN:O	3:C:125:SER:OG	2.27	0.51
3:C:385:SER:OG	3:C:386:SER:N	2.42	0.51
1:E:440:CYS:SG	1:E:441:ASN:N	2.81	0.51
4:H:211:THR:HA	4:H:216:ILE:HD13	1.92	0.51
3:K:19:THR:HG23	3:K:22:GLN:H	1.76	0.51
3:O:385:SER:OG	3:O:386:SER:N	2.42	0.51
4:D:131:THR:OG1	4:D:132:GLU:N	2.44	0.51
3:G:67:THR:HG22	3:G:68:LEU:HB3	1.93	0.51
3:G:120:ASN:O	3:G:124:ASN:ND2	2.43	0.51
4:H:32:TRP:NE1	4:H:309:PRO:O	2.31	0.51
4:H:131:THR:OG1	4:H:132:GLU:N	2.44	0.51
4:L:131:THR:OG1	4:L:132:GLU:N	2.43	0.51
1:M:493:THR:HB	1:M:496:ILE:HD13	1.91	0.51
2:N:573:LEU:HB3	2:N:605:LEU:HD22	1.93	0.51
1:A:493:THR:HB	1:A:496:ILE:HD13	1.91	0.51
4:D:573:GLU:HA	4:D:576:ASN:HD22	1.76	0.51
4:D:575:GLN:HA	4:D:578:LEU:HD12	1.93	0.51
1:E:302:PRO:HG2	1:E:412:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:610:ASP:OD1	2:F:612:ARG:NH2	2.43	0.51
3:G:19:THR:HG23	3:G:22:GLN:H	1.76	0.51
1:I:302:PRO:HG2	1:I:412:GLU:HB3	1.93	0.51
1:I:493:THR:HB	1:I:496:ILE:HD13	1.92	0.51
3:K:120:ASN:O	3:K:124:ASN:ND2	2.43	0.51
3:O:114:HIS:HA	3:O:117:GLN:HG3	1.93	0.51
3:C:67:THR:HG22	3:C:68:LEU:HB3	1.93	0.51
4:H:573:GLU:HA	4:H:576:ASN:HD22	1.76	0.51
2:J:103:ILE:HG23	2:J:114:LEU:HG	1.92	0.51
3:K:67:THR:HG22	3:K:68:LEU:HB3	1.93	0.51
2:N:103:ILE:HG23	2:N:114:LEU:HG	1.93	0.51
4:P:131:THR:OG1	4:P:132:GLU:N	2.44	0.51
4:P:575:GLN:HA	4:P:578:LEU:HD12	1.93	0.51
3:C:114:HIS:HA	3:C:117:GLN:HG3	1.93	0.51
4:D:211:THR:HA	4:D:216:ILE:HD13	1.92	0.51
3:G:296:SER:OG	3:G:299:HIS:N	2.44	0.51
4:H:39:LEU:HA	4:H:42:LYS:HG3	1.93	0.51
1:I:78:GLU:HA	1:I:81:ASP:HB2	1.93	0.51
2:J:610:ASP:OD1	2:J:612:ARG:NH2	2.44	0.51
3:K:110:ILE:HG22	3:K:116:PHE:HB3	1.93	0.51
4:L:39:LEU:HA	4:L:42:LYS:HG3	1.93	0.51
4:L:573:GLU:HA	4:L:576:ASN:HD22	1.76	0.51
3:O:67:THR:HG22	3:O:68:LEU:HB3	1.93	0.51
4:P:211:THR:HA	4:P:216:ILE:HD13	1.92	0.51
4:P:573:GLU:HA	4:P:576:ASN:HD22	1.76	0.51
1:E:425:SER:OG	1:E:437:ASN:ND2	2.43	0.51
3:G:110:ILE:HG22	3:G:116:PHE:HB3	1.93	0.51
3:K:296:SER:OG	3:K:299:HIS:N	2.44	0.51
3:O:121:GLN:O	3:O:125:SER:OG	2.27	0.51
3:C:102:ARG:HD3	3:C:173:LEU:HD11	1.93	0.50
1:E:48:MET:SD	1:E:48:MET:N	2.76	0.50
1:M:425:SER:OG	1:M:437:ASN:ND2	2.43	0.50
1:A:425:SER:OG	1:A:437:ASN:ND2	2.43	0.50
1:I:425:SER:OG	1:I:437:ASN:ND2	2.44	0.50
1:M:469:LEU:O	1:M:473:PHE:HB2	2.11	0.50
1:M:687:ARG:NH1	1:M:690:GLU:OE1	2.44	0.50
3:O:102:ARG:HD3	3:O:173:LEU:HD11	1.93	0.50
3:O:110:ILE:HG22	3:O:116:PHE:HB3	1.92	0.50
4:P:284:LEU:HA	4:P:287:ILE:HD12	1.93	0.50
1:A:687:ARG:NH1	1:A:690:GLU:OE1	2.44	0.50
2:B:651:ASN:HB3	2:B:654:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:ILE:HG22	3:C:116:PHE:HB3	1.93	0.50
1:E:577:TRP:HA	1:E:581:ILE:HD12	1.91	0.50
2:J:573:LEU:HB3	2:J:605:LEU:HD22	1.93	0.50
2:J:651:ASN:ND2	2:J:653:SER:OG	2.41	0.50
4:L:129:TYR:O	4:L:175:SER:OG	2.29	0.50
2:F:103:ILE:HG23	2:F:114:LEU:HG	1.93	0.50
2:F:573:LEU:HB3	2:F:605:LEU:HD22	1.93	0.50
2:F:652:ASN:OD1	2:F:674:ARG:NE	2.45	0.50
1:I:48:MET:SD	1:I:48:MET:N	2.76	0.50
2:J:505:VAL:HG12	2:J:593:ILE:HB	1.94	0.50
1:A:113:ASP:N	1:A:113:ASP:OD1	2.41	0.50
1:A:363:LYS:NZ	1:A:393:VAL:O	2.39	0.50
1:A:678:ASP:O	1:A:682:ASN:ND2	2.45	0.50
4:D:284:LEU:HA	4:D:287:ILE:HD12	1.93	0.50
1:E:678:ASP:O	1:E:682:ASN:ND2	2.45	0.50
2:F:505:VAL:HG12	2:F:593:ILE:HB	1.93	0.50
1:I:577:TRP:HA	1:I:581:ILE:HD12	1.92	0.50
1:M:113:ASP:N	1:M:113:ASP:OD1	2.41	0.50
1:M:363:LYS:NZ	1:M:393:VAL:O	2.39	0.50
1:M:678:ASP:O	1:M:682:ASN:ND2	2.45	0.50
2:N:505:VAL:HG12	2:N:593:ILE:HB	1.93	0.50
1:A:469:LEU:O	1:A:473:PHE:HB2	2.12	0.50
1:A:668:LYS:NZ	1:I:636:GLU:OE2	2.45	0.50
4:D:124:ASN:OD1	4:D:153:ASN:ND2	2.44	0.50
3:G:121:GLN:O	3:G:125:SER:OG	2.27	0.50
4:H:408:VAL:HA	4:H:631:LEU:HD21	1.94	0.50
1:I:469:LEU:O	1:I:473:PHE:HB2	2.11	0.50
1:I:678:ASP:O	1:I:682:ASN:ND2	2.45	0.50
4:L:408:VAL:HA	4:L:631:LEU:HD21	1.94	0.50
1:E:636:GLU:OE2	1:M:668:LYS:NZ	2.45	0.50
4:H:129:TYR:O	4:H:175:SER:OG	2.29	0.50
4:L:32:TRP:NE1	4:L:309:PRO:O	2.31	0.50
4:P:124:ASN:OD1	4:P:153:ASN:ND2	2.44	0.50
3:C:98:ARG:NH2	4:H:129:TYR:OH	2.45	0.50
4:D:224:ARG:HH12	4:D:232:TYR:H	1.59	0.50
4:H:575:GLN:HA	4:H:578:LEU:HD12	1.93	0.50
4:L:575:GLN:HA	4:L:578:LEU:HD12	1.93	0.50
3:O:103:MET:O	3:O:624:SER:OG	2.25	0.50
1:E:469:LEU:O	1:E:473:PHE:HB2	2.12	0.50
4:H:124:ASN:OD1	4:H:153:ASN:ND2	2.44	0.50
3:K:114:HIS:HA	3:K:117:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:224:ARG:HH12	4:P:232:TYR:H	1.59	0.50
2:B:505:VAL:HG12	2:B:593:ILE:HB	1.94	0.49
4:D:129:TYR:O	4:D:175:SER:OG	2.29	0.49
1:E:539:LYS:NZ	2:F:450:ILE:O	2.39	0.49
2:F:651:ASN:ND2	2:F:653:SER:OG	2.42	0.49
3:G:102:ARG:HD3	3:G:173:LEU:HD11	1.93	0.49
3:G:114:HIS:HA	3:G:117:GLN:HG3	1.93	0.49
2:J:103:ILE:HG22	2:J:105:ASP:H	1.77	0.49
2:J:257:TYR:OH	2:J:286:GLN:NE2	2.45	0.49
3:K:102:ARG:HD3	3:K:173:LEU:HD11	1.93	0.49
4:L:284:LEU:HA	4:L:287:ILE:HD12	1.93	0.49
4:P:129:TYR:O	4:P:175:SER:OG	2.29	0.49
1:A:666:ARG:NH2	1:I:633:LEU:O	2.40	0.49
3:C:103:MET:O	3:C:624:SER:OG	2.25	0.49
3:G:295:ASN:HD21	3:G:375:LEU:HD22	1.77	0.49
1:I:486:PRO:O	1:I:489:THR:OG1	2.28	0.49
4:P:186:ILE:HD12	4:P:215:ASP:HB2	1.94	0.49
2:B:257:TYR:OH	2:B:286:GLN:NE2	2.45	0.49
2:B:478:LEU:HB3	2:B:490:VAL:HG23	1.94	0.49
4:D:186:ILE:HD12	4:D:215:ASP:HB2	1.94	0.49
1:E:633:LEU:O	1:M:666:ARG:NH2	2.40	0.49
2:F:169:ASP:H	3:G:568:ARG:HH22	1.60	0.49
2:F:257:TYR:OH	2:F:286:GLN:NE2	2.45	0.49
4:H:284:LEU:HA	4:H:287:ILE:HD12	1.93	0.49
1:I:539:LYS:NZ	2:J:450:ILE:O	2.39	0.49
3:K:295:ASN:HD21	3:K:375:LEU:HD22	1.77	0.49
4:L:124:ASN:OD1	4:L:153:ASN:ND2	2.44	0.49
2:B:635:ASP:HB2	2:B:638:LEU:HD13	1.95	0.49
2:F:103:ILE:HG22	2:F:105:ASP:H	1.78	0.49
3:C:19:THR:HG23	3:C:22:GLN:H	1.76	0.49
1:I:408:ASP:O	2:J:433:ARG:NH2	2.42	0.49
2:J:646:SER:OG	2:J:670:GLY:O	2.30	0.49
3:K:446:LYS:HZ1	3:K:577:LYS:HD2	1.78	0.49
1:M:53:TYR:HB3	2:N:397:GLU:HG3	1.94	0.49
1:M:302:PRO:HG2	1:M:412:GLU:HB3	1.93	0.49
4:P:39:LEU:HA	4:P:42:LYS:HG3	1.93	0.49
2:F:646:SER:OG	2:F:670:GLY:O	2.31	0.49
1:I:227:ASN:O	1:I:231:ASN:ND2	2.42	0.49
2:J:169:ASP:H	3:K:568:ARG:HH22	1.60	0.49
2:N:257:TYR:OH	2:N:286:GLN:NE2	2.45	0.49
3:O:19:THR:HG23	3:O:22:GLN:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PRO:HG2	1:A:412:GLU:HB3	1.93	0.49
4:D:39:LEU:HA	4:D:42:LYS:HG3	1.93	0.49
1:E:486:PRO:O	1:E:489:THR:OG1	2.29	0.49
2:F:462:ARG:NH2	2:F:489:THR:O	2.45	0.49
3:G:624:SER:OG	3:G:624:SER:O	2.27	0.49
2:J:478:LEU:HB3	2:J:490:VAL:HG23	1.95	0.49
2:N:651:ASN:ND2	2:N:653:SER:OG	2.41	0.49
4:P:408:VAL:HA	4:P:631:LEU:HD21	1.94	0.49
1:A:53:TYR:HB3	2:B:397:GLU:HG3	1.94	0.49
1:A:234:GLU:HA	1:A:237:ARG:HH21	1.78	0.49
2:B:103:ILE:HG22	2:B:105:ASP:H	1.78	0.49
4:D:120:ARG:NH1	4:D:121:ASP:OD1	2.46	0.49
4:D:408:VAL:HA	4:D:631:LEU:HD21	1.94	0.49
1:E:227:ASN:O	1:E:231:ASN:ND2	2.42	0.49
1:E:408:ASP:O	2:F:433:ARG:NH2	2.42	0.49
2:F:478:LEU:HB3	2:F:490:VAL:HG23	1.95	0.49
3:K:624:SER:OG	3:K:624:SER:O	2.27	0.49
4:P:120:ARG:NH1	4:P:121:ASP:OD1	2.46	0.49
1:M:234:GLU:HA	1:M:237:ARG:HH21	1.77	0.49
2:N:478:LEU:HB3	2:N:490:VAL:HG23	1.95	0.49
2:N:635:ASP:HB2	2:N:638:LEU:HD13	1.95	0.49
4:D:275:ASP:OD1	4:D:275:ASP:N	2.45	0.49
1:I:338:ASP:N	1:I:338:ASP:OD1	2.46	0.49
3:O:106:THR:OG1	3:O:107:GLU:OE1	2.30	0.49
3:O:257:ASP:OD1	3:O:257:ASP:N	2.42	0.49
1:A:486:PRO:O	1:A:489:THR:OG1	2.29	0.48
2:B:169:ASP:H	3:C:568:ARG:HH22	1.60	0.48
3:C:106:THR:OG1	3:C:107:GLU:OE1	2.30	0.48
3:C:257:ASP:OD1	3:C:257:ASP:N	2.42	0.48
3:C:505:ASN:ND2	4:D:530:GLN:OE1	2.45	0.48
4:H:224:ARG:HH12	4:H:232:TYR:H	1.59	0.48
1:I:53:TYR:HB3	2:J:397:GLU:HG3	1.94	0.48
2:J:652:ASN:OD1	2:J:674:ARG:NE	2.46	0.48
1:M:486:PRO:O	1:M:489:THR:OG1	2.29	0.48
1:A:409:PRO:O	2:B:433:ARG:NH2	2.46	0.48
2:B:651:ASN:ND2	2:B:653:SER:OG	2.41	0.48
3:G:446:LYS:HZ1	3:G:577:LYS:HD2	1.78	0.48
4:L:120:ARG:NH1	4:L:121:ASP:OD1	2.46	0.48
1:E:409:PRO:O	2:F:433:ARG:NH2	2.46	0.48
3:G:488:ALA:O	3:G:492:SER:OG	2.25	0.48
4:H:255:PHE:HB2	4:H:262:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:409:PRO:O	2:J:433:ARG:NH2	2.46	0.48
4:L:255:PHE:HB2	4:L:262:TYR:HB2	1.95	0.48
1:M:409:PRO:O	2:N:433:ARG:NH2	2.47	0.48
2:N:618:VAL:O	2:N:646:SER:HA	2.14	0.48
4:P:275:ASP:OD1	4:P:275:ASP:N	2.46	0.48
1:A:636:GLU:OE2	1:I:668:LYS:NZ	2.45	0.48
1:E:53:TYR:HB3	2:F:397:GLU:HG3	1.94	0.48
1:E:234:GLU:HA	1:E:237:ARG:HH21	1.77	0.48
1:E:338:ASP:OD1	1:E:338:ASP:N	2.46	0.48
3:G:106:THR:OG1	3:G:107:GLU:OE1	2.30	0.48
4:H:120:ARG:NH1	4:H:121:ASP:OD1	2.46	0.48
4:H:186:ILE:HD12	4:H:215:ASP:HB2	1.94	0.48
2:J:635:ASP:HB2	2:J:638:LEU:HD13	1.95	0.48
3:K:106:THR:OG1	3:K:107:GLU:OE1	2.30	0.48
3:K:488:ALA:O	3:K:492:SER:OG	2.25	0.48
1:M:527:SER:HB2	2:N:558:PHE:HB2	1.95	0.48
2:N:652:ASN:OD1	2:N:674:ARG:NE	2.46	0.48
2:B:646:SER:OG	2:B:670:GLY:O	2.30	0.48
2:B:652:ASN:OD1	2:B:674:ARG:NE	2.46	0.48
1:I:687:ARG:NH1	1:I:690:GLU:OE1	2.44	0.48
2:J:462:ARG:NH2	2:J:489:THR:O	2.46	0.48
4:L:186:ILE:HD12	4:L:215:ASP:HB2	1.94	0.48
4:L:224:ARG:HH12	4:L:232:TYR:H	1.59	0.48
1:M:338:ASP:OD1	1:M:338:ASP:N	2.45	0.48
2:N:169:ASP:H	3:O:568:ARG:HH22	1.61	0.48
1:A:338:ASP:OD1	1:A:338:ASP:N	2.46	0.48
3:C:295:ASN:HD21	3:C:375:LEU:HD22	1.77	0.48
4:D:255:PHE:HB2	4:D:262:TYR:HB2	1.95	0.48
1:E:687:ARG:NH1	1:E:690:GLU:OE1	2.44	0.48
2:F:635:ASP:HB2	2:F:638:LEU:HD13	1.95	0.48
3:O:295:ASN:HD21	3:O:375:LEU:HD22	1.76	0.48
3:C:167:ARG:HG2	3:C:169:SER:H	1.79	0.48
3:C:296:SER:OG	3:C:299:HIS:N	2.44	0.48
3:G:167:ARG:HG2	3:G:169:SER:H	1.79	0.48
2:J:618:VAL:O	2:J:646:SER:HA	2.14	0.48
2:N:646:SER:OG	2:N:670:GLY:O	2.30	0.48
4:P:255:PHE:HB2	4:P:262:TYR:HB2	1.95	0.48
1:A:448:ASP:OD1	1:A:448:ASP:N	2.42	0.48
4:H:321:ASP:O	4:H:325:SER:OG	2.30	0.48
3:K:98:ARG:NH2	4:P:129:TYR:OH	2.47	0.48
2:N:103:ILE:HG22	2:N:105:ASP:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:167:ARG:HG2	3:O:169:SER:H	1.79	0.48
3:O:505:ASN:ND2	4:P:530:GLN:OE1	2.46	0.48
1:A:318:VAL:HG21	1:A:417:ILE:HD11	1.95	0.48
2:B:618:VAL:O	2:B:646:SER:HA	2.14	0.48
1:E:57:LYS:HE3	1:E:119:LEU:HB2	1.96	0.48
1:E:245:ASP:OD1	1:E:247:HIS:ND1	2.43	0.48
3:K:167:ARG:HG2	3:K:169:SER:H	1.79	0.48
2:B:80:ILE:HD13	3:C:469:LYS:HD3	1.95	0.48
3:C:158:ILE:HA	3:C:161:LYS:HD2	1.96	0.48
3:G:478:ILE:HG13	3:G:550:LEU:HD22	1.95	0.48
3:G:505:ASN:ND2	4:H:530:GLN:OE1	2.46	0.48
1:I:234:GLU:HA	1:I:237:ARG:HH21	1.78	0.48
1:I:269:ARG:NH2	1:I:271:GLU:OE2	2.43	0.48
2:J:624:ASP:OD1	2:J:624:ASP:N	2.42	0.48
1:M:57:LYS:HE3	1:M:119:LEU:HB2	1.96	0.48
3:O:158:ILE:HA	3:O:161:LYS:HD2	1.96	0.48
1:A:57:LYS:HE3	1:A:119:LEU:HB2	1.96	0.47
1:E:269:ARG:NH2	1:E:271:GLU:OE2	2.44	0.47
4:H:484:LEU:HD21	4:H:550:MET:HB3	1.95	0.47
1:I:57:LYS:HE3	1:I:119:LEU:HB2	1.96	0.47
1:I:318:VAL:HG21	1:I:417:ILE:HD11	1.95	0.47
4:L:484:LEU:HD21	4:L:550:MET:HB3	1.95	0.47
1:M:269:ARG:NH2	1:M:271:GLU:OE2	2.43	0.47
3:O:296:SER:OG	3:O:299:HIS:N	2.44	0.47
1:A:269:ARG:NH2	1:A:271:GLU:OE2	2.43	0.47
3:C:478:ILE:HG13	3:C:550:LEU:HD22	1.95	0.47
1:E:318:VAL:HG21	1:E:417:ILE:HD11	1.95	0.47
1:E:448:ASP:OD1	1:E:448:ASP:N	2.42	0.47
3:G:325:SER:OG	3:G:326:GLN:N	2.47	0.47
4:L:571:LEU:HA	4:L:574:LYS:HD2	1.96	0.47
1:M:448:ASP:OD1	1:M:448:ASP:N	2.42	0.47
2:B:381:ASP:OD2	2:B:381:ASP:N	2.47	0.47
2:F:618:VAL:O	2:F:646:SER:HA	2.14	0.47
1:I:527:SER:HB2	2:J:558:PHE:HB2	1.95	0.47
3:K:325:SER:OG	3:K:326:GLN:N	2.47	0.47
3:K:478:ILE:HG13	3:K:550:LEU:HD22	1.95	0.47
4:L:275:ASP:N	4:L:275:ASP:OD1	2.45	0.47
4:L:321:ASP:O	4:L:325:SER:OG	2.30	0.47
1:M:318:VAL:HG21	1:M:417:ILE:HD11	1.95	0.47
3:O:478:ILE:HG13	3:O:550:LEU:HD22	1.95	0.47
4:H:571:LEU:HA	4:H:574:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:245:ASP:OD1	1:I:247:HIS:ND1	2.43	0.47
4:P:129:TYR:HB3	4:P:131:THR:HG22	1.97	0.47
4:P:484:LEU:HD21	4:P:550:MET:HB3	1.95	0.47
1:A:502:ILE:HG12	1:A:547:GLY:HA3	1.96	0.47
4:D:129:TYR:HB3	4:D:131:THR:HG22	1.97	0.47
4:D:484:LEU:HD21	4:D:550:MET:HB3	1.95	0.47
4:H:275:ASP:OD1	4:H:275:ASP:N	2.45	0.47
1:I:448:ASP:OD1	1:I:448:ASP:N	2.42	0.47
1:M:502:ILE:HG12	1:M:547:GLY:HA3	1.95	0.47
2:N:381:ASP:OD2	2:N:381:ASP:N	2.47	0.47
4:H:275:ASP:OD2	4:H:276:ARG:NH1	2.48	0.47
4:H:405:SER:OG	4:H:635:ARG:NH2	2.46	0.47
2:N:584:PHE:HB2	2:N:587:VAL:HB	1.97	0.47
3:O:488:ALA:O	3:O:492:SER:OG	2.25	0.47
1:A:527:SER:HB2	2:B:558:PHE:HB2	1.96	0.47
3:C:488:ALA:O	3:C:492:SER:OG	2.25	0.47
4:H:129:TYR:HB3	4:H:131:THR:HG22	1.97	0.47
1:I:502:ILE:HG12	1:I:547:GLY:HA3	1.95	0.47
4:L:275:ASP:OD2	4:L:276:ARG:NH1	2.48	0.47
2:F:624:ASP:OD1	2:F:624:ASP:N	2.42	0.47
3:G:158:ILE:HA	3:G:161:LYS:HD2	1.96	0.47
1:I:308:ASP:OD1	1:I:308:ASP:N	2.48	0.47
3:K:158:ILE:HA	3:K:161:LYS:HD2	1.96	0.47
1:E:308:ASP:OD1	1:E:308:ASP:N	2.48	0.47
1:E:502:ILE:HG12	1:E:547:GLY:HA3	1.96	0.47
1:E:668:LYS:NZ	1:M:636:GLU:OE2	2.46	0.47
1:A:245:ASP:OD1	1:A:247:HIS:ND1	2.43	0.47
2:B:584:PHE:HB2	2:B:587:VAL:HB	1.97	0.47
1:E:329:ASP:O	1:E:369:ASN:ND2	2.36	0.47
1:E:527:SER:HB2	2:F:558:PHE:HB2	1.96	0.47
4:L:129:TYR:HB3	4:L:131:THR:HG22	1.97	0.47
4:L:405:SER:OG	4:L:635:ARG:NH2	2.47	0.47
1:M:245:ASP:OD1	1:M:247:HIS:ND1	2.43	0.47
3:O:398:LEU:HD21	3:O:428:ARG:HH22	1.80	0.47
4:P:321:ASP:O	4:P:325:SER:OG	2.30	0.47
3:C:398:LEU:HD21	3:C:428:ARG:HH22	1.80	0.46
4:D:321:ASP:O	4:D:325:SER:OG	2.30	0.46
4:D:630:ASN:HA	4:D:633:ILE:HG22	1.97	0.46
2:F:80:ILE:HD13	3:G:469:LYS:HD3	1.96	0.46
2:F:584:PHE:HB2	2:F:587:VAL:HB	1.97	0.46
3:G:463:SER:HA	3:G:466:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:630:ASN:HA	4:H:633:ILE:HG22	1.97	0.46
3:C:325:SER:OG	3:C:326:GLN:N	2.47	0.46
4:D:239:VAL:HG23	4:D:245:ASP:HB3	1.97	0.46
1:E:507:HIS:O	1:E:552:ASN:HA	2.15	0.46
2:F:671:ARG:HG2	2:F:673:LEU:HD21	1.96	0.46
4:H:617:LEU:HD12	4:H:617:LEU:HA	1.82	0.46
3:K:398:LEU:HD21	3:K:428:ARG:HH22	1.80	0.46
3:K:463:SER:HA	3:K:466:LEU:HD12	1.97	0.46
3:O:325:SER:OG	3:O:326:GLN:N	2.47	0.46
4:P:630:ASN:HA	4:P:633:ILE:HG22	1.97	0.46
3:G:398:LEU:HD21	3:G:428:ARG:HH22	1.80	0.46
1:I:507:HIS:O	1:I:552:ASN:HA	2.15	0.46
2:J:537:PHE:O	2:J:541:GLY:N	2.46	0.46
4:L:630:ASN:HA	4:L:633:ILE:HG22	1.97	0.46
4:P:239:VAL:HG23	4:P:245:ASP:HB3	1.97	0.46
1:E:78:GLU:HA	1:E:81:ASP:HB2	1.96	0.46
2:F:537:PHE:O	2:F:541:GLY:N	2.46	0.46
3:K:69:SER:H	3:K:72:GLN:HE21	1.64	0.46
3:G:69:SER:H	3:G:72:GLN:HE21	1.64	0.46
1:I:329:ASP:O	1:I:369:ASN:ND2	2.35	0.46
2:N:80:ILE:HD13	3:O:469:LYS:HD3	1.97	0.46
4:P:275:ASP:OD2	4:P:276:ARG:NH1	2.48	0.46
3:C:69:SER:H	3:C:72:GLN:HE21	1.64	0.46
3:C:266:PRO:HA	3:C:290:LYS:HD3	1.97	0.46
3:C:463:SER:HA	3:C:466:LEU:HD12	1.97	0.46
2:N:671:ARG:HG2	2:N:673:LEU:HD21	1.96	0.46
3:O:69:SER:H	3:O:72:GLN:HE21	1.64	0.46
3:O:266:PRO:HA	3:O:290:LYS:HD3	1.97	0.46
4:P:571:LEU:HA	4:P:574:LYS:HD2	1.96	0.46
4:D:275:ASP:OD2	4:D:276:ARG:NH1	2.48	0.46
4:D:571:LEU:HA	4:D:574:LYS:HD2	1.96	0.46
1:I:484:ASP:OD1	1:I:484:ASP:N	2.41	0.46
3:O:463:SER:HA	3:O:466:LEU:HD12	1.97	0.46
4:D:80:ASN:HA	4:D:83:LEU:HD12	1.98	0.46
1:M:78:GLU:HA	1:M:81:ASP:HB2	1.96	0.46
4:P:80:ASN:HA	4:P:83:LEU:HD12	1.98	0.46
1:A:78:GLU:HA	1:A:81:ASP:HB2	1.96	0.46
2:J:80:ILE:HD13	3:K:469:LYS:HD3	1.97	0.46
2:J:671:ARG:HG2	2:J:673:LEU:HD21	1.97	0.46
1:A:507:HIS:O	1:A:552:ASN:HA	2.15	0.45
4:H:80:ASN:HA	4:H:83:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:671:ARG:HG2	2:B:673:LEU:HD21	1.97	0.45
1:E:524:ASP:OD2	1:E:527:SER:N	2.48	0.45
4:H:158:LYS:HG2	4:H:194:LYS:HE3	1.98	0.45
4:L:80:ASN:HA	4:L:83:LEU:HD12	1.98	0.45
4:L:158:LYS:HG2	4:L:194:LYS:HE3	1.98	0.45
1:M:507:HIS:O	1:M:552:ASN:HA	2.15	0.45
1:M:539:LYS:NZ	2:N:450:ILE:O	2.39	0.45
4:L:239:VAL:HG23	4:L:245:ASP:HB3	1.97	0.45
1:A:539:LYS:NZ	2:B:450:ILE:O	2.39	0.45
1:E:388:LEU:HD11	1:E:392:LYS:HE3	1.99	0.45
4:H:239:VAL:HG23	4:H:245:ASP:HB3	1.97	0.45
1:I:388:LEU:HD11	1:I:392:LYS:HE3	1.99	0.45
4:L:315:LYS:NZ	4:L:316:GLN:O	2.39	0.45
4:P:295:LEU:HD11	4:P:308:LEU:HD11	1.98	0.45
4:D:158:LYS:HG2	4:D:194:LYS:HE3	1.98	0.45
4:D:295:LEU:HD11	4:D:308:LEU:HD11	1.98	0.45
3:G:266:PRO:HA	3:G:290:LYS:HD3	1.97	0.45
2:J:381:ASP:OD2	2:J:381:ASP:N	2.47	0.45
3:K:432:ILE:HG21	3:K:595:LEU:HD23	1.99	0.45
1:M:388:LEU:HD11	1:M:392:LYS:HE3	1.99	0.45
1:A:388:LEU:HD11	1:A:392:LYS:HE3	1.99	0.45
2:F:381:ASP:OD2	2:F:381:ASP:N	2.48	0.45
3:G:30:ILE:O	3:G:34:ALA:HB2	2.16	0.45
3:G:405:LEU:HD23	3:G:405:LEU:HA	1.88	0.45
4:H:295:LEU:HD11	4:H:308:LEU:HD11	1.98	0.45
3:K:30:ILE:O	3:K:34:ALA:HB2	2.17	0.45
2:N:429:ASN:HA	2:N:432:ARG:HH21	1.82	0.45
2:B:429:ASN:HA	2:B:432:ARG:HH21	1.82	0.45
3:C:30:ILE:O	3:C:34:ALA:HB2	2.17	0.45
3:G:432:ILE:HG21	3:G:595:LEU:HD23	1.99	0.45
2:J:30:ASN:HD21	2:J:32:LEU:HD12	1.82	0.45
3:K:266:PRO:HA	3:K:290:LYS:HD3	1.97	0.45
3:K:405:LEU:HD23	3:K:405:LEU:HA	1.88	0.45
2:N:462:ARG:NH2	2:N:489:THR:O	2.46	0.45
3:O:30:ILE:O	3:O:34:ALA:HB2	2.16	0.45
4:P:158:LYS:HG2	4:P:194:LYS:HE3	1.98	0.45
2:B:462:ARG:NH2	2:B:489:THR:O	2.46	0.45
4:L:129:TYR:OH	3:O:98:ARG:NH2	2.50	0.45
3:C:429:LEU:HA	3:C:432:ILE:HG22	1.99	0.44
2:F:583:TYR:HB3	4:H:445:LEU:HD22	1.99	0.44
4:H:315:LYS:NZ	4:H:316:GLN:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:496:ILE:HG12	1:I:549:ILE:HD11	1.98	0.44
1:I:624:ASP:OD1	1:I:624:ASP:N	2.50	0.44
4:L:295:LEU:HD11	4:L:308:LEU:HD11	1.98	0.44
4:H:404:ASN:OD1	4:H:404:ASN:N	2.50	0.44
2:J:89:ARG:NH2	2:J:376:GLY:O	2.50	0.44
3:O:429:LEU:HA	3:O:432:ILE:HG22	1.99	0.44
1:E:624:ASP:OD1	1:E:624:ASP:N	2.50	0.44
2:J:429:ASN:HA	2:J:432:ARG:HH21	1.82	0.44
1:A:496:ILE:HG12	1:A:549:ILE:HD11	1.98	0.44
3:C:432:ILE:HG21	3:C:595:LEU:HD23	1.99	0.44
2:F:429:ASN:HA	2:F:432:ARG:HH21	1.82	0.44
3:K:405:LEU:HA	3:K:406:PRO:HD3	1.85	0.44
4:L:404:ASN:OD1	4:L:404:ASN:N	2.50	0.44
1:E:178:CYS:O	1:E:182:ILE:N	2.49	0.44
1:E:496:ILE:HG12	1:E:549:ILE:HD11	1.99	0.44
2:F:89:ARG:NH2	2:F:376:GLY:O	2.51	0.44
2:F:682:ASN:O	2:F:686:GLU:HB2	2.17	0.44
4:L:600:ILE:HA	4:L:603:LEU:HB2	2.00	0.44
2:N:30:ASN:HD21	2:N:32:LEU:HD12	1.82	0.44
3:O:432:ILE:HG21	3:O:595:LEU:HD23	1.99	0.44
4:H:600:ILE:HA	4:H:603:LEU:HB2	2.00	0.44
1:I:457:LEU:HD22	2:J:530:ILE:HG21	2.00	0.44
4:P:404:ASN:N	4:P:404:ASN:OD1	2.50	0.44
2:B:89:ARG:NH2	2:B:376:GLY:O	2.50	0.44
2:B:578:ASP:OD1	2:B:582:LYS:NZ	2.44	0.44
3:C:268:LEU:H	3:C:290:LYS:HZ3	1.65	0.44
3:C:511:ASN:OD1	3:C:511:ASN:N	2.51	0.44
4:D:404:ASN:N	4:D:404:ASN:OD1	2.50	0.44
1:I:97:LEU:HD23	1:I:97:LEU:HA	1.87	0.44
3:O:511:ASN:OD1	3:O:511:ASN:N	2.51	0.44
2:B:578:ASP:HA	2:B:582:LYS:HD2	2.00	0.44
3:G:429:LEU:HA	3:G:432:ILE:HG22	1.99	0.44
1:I:229:LEU:HD23	1:I:229:LEU:HA	1.83	0.44
3:K:429:LEU:HA	3:K:432:ILE:HG22	1.99	0.44
1:M:496:ILE:HG12	1:M:549:ILE:HD11	1.98	0.44
2:N:578:ASP:HA	2:N:582:LYS:HD2	2.00	0.44
3:C:25:LEU:HD23	3:C:25:LEU:HA	1.89	0.43
1:E:97:LEU:HD23	1:E:97:LEU:HA	1.87	0.43
3:G:405:LEU:HA	3:G:406:PRO:HD3	1.85	0.43
3:G:454:GLN:HA	3:G:457:LEU:HD12	2.00	0.43
4:H:215:ASP:OD1	4:H:215:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:454:GLN:HA	3:K:457:LEU:HD12	2.00	0.43
1:M:457:LEU:HD22	2:N:530:ILE:HG21	2.00	0.43
2:B:388:LEU:HD11	2:B:392:LYS:HE3	2.01	0.43
3:C:102:ARG:HB3	3:C:173:LEU:HD21	2.01	0.43
1:E:457:LEU:HD22	2:F:530:ILE:HG21	2.00	0.43
4:L:215:ASP:OD1	4:L:215:ASP:N	2.50	0.43
1:M:624:ASP:N	1:M:624:ASP:OD1	2.50	0.43
2:N:578:ASP:OD1	2:N:582:LYS:NZ	2.44	0.43
3:O:102:ARG:HB3	3:O:173:LEU:HD21	2.01	0.43
4:P:87:HIS:HD2	4:P:89:TYR:H	1.66	0.43
1:A:457:LEU:HD22	2:B:530:ILE:HG21	2.00	0.43
1:A:624:ASP:N	1:A:624:ASP:OD1	2.50	0.43
4:D:547:LYS:HD3	4:D:547:LYS:HA	1.85	0.43
1:E:229:LEU:HD23	1:E:229:LEU:HA	1.83	0.43
1:E:417:ILE:HD12	1:E:417:ILE:HA	1.91	0.43
3:G:71:ARG:HG2	3:G:328:TYR:CZ	2.54	0.43
1:I:333:ILE:HB	1:I:372:VAL:HG22	1.99	0.43
1:I:360:HIS:CD2	2:J:364:SER:HB2	2.53	0.43
2:J:578:ASP:HA	2:J:582:LYS:HD2	1.99	0.43
2:N:388:LEU:HD11	2:N:392:LYS:HE3	2.01	0.43
2:N:687:ARG:HA	2:N:687:ARG:HD3	1.83	0.43
4:P:32:TRP:HA	4:P:237:ARG:HB2	2.01	0.43
4:D:87:HIS:HD2	4:D:89:TYR:H	1.66	0.43
1:E:180:GLY:O	1:E:183:GLU:HB2	2.18	0.43
1:E:333:ILE:HB	1:E:372:VAL:HG22	1.99	0.43
2:F:388:LEU:HD11	2:F:392:LYS:HE3	2.01	0.43
1:I:417:ILE:HD12	1:I:417:ILE:HA	1.92	0.43
4:D:32:TRP:HA	4:D:237:ARG:HB2	2.01	0.43
1:E:360:HIS:CD2	2:F:364:SER:HB2	2.53	0.43
3:G:470:LYS:HB3	3:G:553:LEU:HD21	2.00	0.43
1:I:180:GLY:O	1:I:183:GLU:HB2	2.18	0.43
2:J:388:LEU:HD11	2:J:392:LYS:HE3	2.01	0.43
3:K:71:ARG:HG2	3:K:328:TYR:CZ	2.54	0.43
1:A:180:GLY:O	1:A:183:GLU:HB2	2.18	0.43
3:C:470:LYS:HB3	3:C:553:LEU:HD21	2.00	0.43
1:I:524:ASP:OD2	1:I:527:SER:N	2.49	0.43
2:J:162:ASP:OD1	2:J:162:ASP:N	2.39	0.43
2:J:584:PHE:HB2	2:J:587:VAL:HB	2.00	0.43
3:K:470:LYS:HB3	3:K:553:LEU:HD21	2.01	0.43
3:K:551:LYS:HD3	3:K:551:LYS:HA	1.83	0.43
3:O:25:LEU:HD23	3:O:25:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:470:LYS:HB3	3:O:553:LEU:HD21	2.01	0.43
1:A:586:SER:O	1:A:586:SER:OG	2.34	0.43
1:E:408:ASP:HB3	2:F:433:ARG:HE	1.84	0.43
2:F:30:ASN:HD21	2:F:32:LEU:HD12	1.84	0.43
2:F:162:ASP:N	2:F:162:ASP:OD1	2.39	0.43
3:G:10:LYS:HA	3:G:10:LYS:HD3	1.84	0.43
4:H:422:ILE:HD12	4:H:422:ILE:HA	1.93	0.43
1:M:635:ASP:OD2	1:M:637:THR:OG1	2.33	0.43
4:P:606:GLU:HA	4:P:609:LEU:HD12	2.01	0.43
1:A:333:ILE:HB	1:A:372:VAL:HG22	1.99	0.43
4:D:600:ILE:HA	4:D:603:LEU:HB2	2.00	0.43
4:D:606:GLU:HA	4:D:609:LEU:HD12	2.01	0.43
2:F:269:ARG:NH1	2:F:346:GLY:O	2.51	0.43
3:G:551:LYS:HD3	3:G:551:LYS:HA	1.83	0.43
4:H:547:LYS:HA	4:H:547:LYS:HD3	1.85	0.43
4:H:606:GLU:HA	4:H:609:LEU:HD12	2.01	0.43
4:L:422:ILE:HD12	4:L:422:ILE:HA	1.93	0.43
4:P:600:ILE:HA	4:P:603:LEU:HB2	2.00	0.43
3:C:71:ARG:HG2	3:C:328:TYR:CZ	2.54	0.43
3:C:420:GLU:HA	3:C:423:HIS:CE1	2.53	0.43
3:C:454:GLN:HA	3:C:457:LEU:HD12	2.00	0.43
3:G:413:ASP:O	3:G:417:TYR:N	2.43	0.43
4:H:87:HIS:HD2	4:H:89:TYR:H	1.66	0.43
4:L:87:HIS:HD2	4:L:89:TYR:H	1.66	0.43
1:M:360:HIS:CD2	2:N:364:SER:HB2	2.53	0.43
3:O:71:ARG:HG2	3:O:328:TYR:CZ	2.54	0.43
3:G:257:ASP:N	3:G:257:ASP:OD1	2.42	0.43
3:G:560:LYS:HD2	3:G:560:LYS:HA	1.84	0.43
1:I:96:ILE:HD12	1:I:96:ILE:HA	1.94	0.43
3:K:75:TYR:O	3:K:79:SER:OG	2.34	0.43
3:K:445:GLU:HA	3:K:448:LEU:HD12	2.00	0.43
3:K:560:LYS:HA	3:K:560:LYS:HD2	1.84	0.43
4:L:244:ILE:HA	4:L:247:CYS:HB3	2.01	0.43
1:M:333:ILE:HB	1:M:372:VAL:HG22	2.00	0.43
1:M:535:LEU:HA	1:M:538:ILE:HD12	2.01	0.43
1:M:586:SER:O	1:M:586:SER:OG	2.34	0.43
3:O:420:GLU:HA	3:O:423:HIS:CE1	2.53	0.43
3:O:445:GLU:HA	3:O:448:LEU:HD12	2.00	0.43
3:O:454:GLN:HA	3:O:457:LEU:HD12	2.00	0.43
4:P:547:LYS:HD3	4:P:547:LYS:HA	1.85	0.43
1:A:360:HIS:CD2	2:B:364:SER:HB2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LEU:HA	1:A:538:ILE:HD12	2.01	0.42
2:B:687:ARG:HA	2:B:687:ARG:HD3	1.83	0.42
3:C:445:GLU:HA	3:C:448:LEU:HD12	2.00	0.42
1:E:241:ILE:HG23	1:E:264:TYR:HA	2.01	0.42
3:G:445:GLU:HA	3:G:448:LEU:HD12	2.00	0.42
1:I:635:ASP:OD2	1:I:637:THR:OG1	2.33	0.42
4:L:608:LYS:HD3	4:L:608:LYS:HA	1.79	0.42
1:M:180:GLY:O	1:M:183:GLU:HB2	2.18	0.42
1:M:227:ASN:O	1:M:231:ASN:ND2	2.43	0.42
1:M:524:ASP:OD2	1:M:527:SER:N	2.49	0.42
1:A:227:ASN:O	1:A:231:ASN:ND2	2.43	0.42
1:E:96:ILE:HD12	1:E:96:ILE:HA	1.94	0.42
2:F:578:ASP:HA	2:F:582:LYS:HD2	2.00	0.42
4:H:244:ILE:HA	4:H:247:CYS:HB3	2.01	0.42
1:I:90:ILE:HD13	1:I:201:ARG:HG2	2.01	0.42
2:J:260:ASP:OD1	2:J:260:ASP:N	2.42	0.42
3:K:10:LYS:HA	3:K:10:LYS:HD3	1.84	0.42
3:K:35:LYS:HA	3:K:35:LYS:HD2	1.87	0.42
3:K:413:ASP:O	3:K:417:TYR:N	2.43	0.42
4:L:606:GLU:HA	4:L:609:LEU:HD12	2.01	0.42
1:A:90:ILE:HD13	1:A:201:ARG:HG2	2.01	0.42
1:E:90:ILE:HD13	1:E:201:ARG:HG2	2.01	0.42
1:E:108:LEU:O	2:F:40:ARG:NH2	2.52	0.42
1:E:535:LEU:HA	1:E:538:ILE:HD12	2.01	0.42
1:E:635:ASP:OD2	1:E:637:THR:OG1	2.33	0.42
4:H:155:VAL:HG22	4:H:176:CYS:HB3	2.02	0.42
4:H:257:LYS:HA	4:H:257:LYS:HD3	1.74	0.42
4:H:480:ARG:O	4:H:484:LEU:HB2	2.19	0.42
3:K:272:LEU:HB2	3:K:275:LEU:HD12	2.01	0.42
2:B:269:ARG:NH1	2:B:346:GLY:O	2.52	0.42
4:D:129:TYR:OH	3:G:98:ARG:NH2	2.52	0.42
3:G:102:ARG:HB3	3:G:173:LEU:HD21	2.00	0.42
3:G:272:LEU:HB2	3:G:275:LEU:HD12	2.01	0.42
4:H:32:TRP:HA	4:H:237:ARG:HB2	2.01	0.42
4:H:608:LYS:HD3	4:H:608:LYS:HA	1.79	0.42
3:K:257:ASP:N	3:K:257:ASP:OD1	2.42	0.42
3:K:603:LEU:HD13	3:K:610:SER:HA	2.02	0.42
4:L:480:ARG:O	4:L:484:LEU:HB2	2.19	0.42
2:N:110:GLY:O	3:O:447:ARG:NH1	2.52	0.42
4:P:559:ASP:OD1	4:P:562:ARG:NH2	2.47	0.42
2:B:167:ASN:OD1	3:C:568:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:428:TRP:O	1:E:432:ARG:NH1	2.52	0.42
1:E:508:ASP:OD1	1:E:508:ASP:N	2.41	0.42
2:F:260:ASP:OD1	2:F:260:ASP:N	2.41	0.42
3:G:35:LYS:HA	3:G:35:LYS:HD2	1.87	0.42
3:G:420:GLU:HA	3:G:423:HIS:CE1	2.53	0.42
3:K:102:ARG:HB3	3:K:173:LEU:HD21	2.01	0.42
4:L:155:VAL:HG22	4:L:176:CYS:HB3	2.02	0.42
4:L:257:LYS:HA	4:L:257:LYS:HD3	1.74	0.42
1:M:327:LYS:HE2	1:M:327:LYS:HB2	1.94	0.42
2:N:167:ASN:OD1	3:O:568:ARG:NH2	2.53	0.42
1:A:241:ILE:HG23	1:A:264:TYR:HA	2.02	0.42
2:B:93:ILE:HG21	2:B:199:VAL:HG11	2.01	0.42
2:B:227:ASN:OD1	2:B:231:ASN:ND2	2.53	0.42
4:D:405:SER:OG	4:D:635:ARG:NH2	2.47	0.42
2:F:453:LYS:H	2:F:453:LYS:HG2	1.60	0.42
1:I:535:LEU:HA	1:I:538:ILE:HD12	2.02	0.42
3:K:420:GLU:HA	3:K:423:HIS:CE1	2.54	0.42
1:M:90:ILE:HD13	1:M:201:ARG:HG2	2.01	0.42
2:N:89:ARG:NH2	2:N:376:GLY:O	2.52	0.42
2:N:227:ASN:OD1	2:N:231:ASN:ND2	2.53	0.42
2:N:583:TYR:HB3	4:P:445:LEU:HD22	2.01	0.42
1:A:108:LEU:O	2:B:40:ARG:NH2	2.52	0.42
1:A:408:ASP:HB3	2:B:433:ARG:HE	1.85	0.42
4:D:155:VAL:HG22	4:D:176:CYS:HB3	2.02	0.42
4:D:156:HIS:HB2	4:D:177:THR:HG22	2.02	0.42
4:D:215:ASP:N	4:D:215:ASP:OD1	2.50	0.42
4:D:559:ASP:OD1	4:D:562:ARG:NH2	2.47	0.42
3:G:603:LEU:HD13	3:G:610:SER:HA	2.02	0.42
1:I:241:ILE:HG23	1:I:264:TYR:HA	2.02	0.42
1:M:108:LEU:O	2:N:40:ARG:NH2	2.52	0.42
2:N:624:ASP:OD1	2:N:624:ASP:N	2.42	0.42
1:A:248:HIS:NE2	1:A:253:GLN:OE1	2.43	0.42
3:C:413:ASP:O	3:C:417:TYR:N	2.43	0.42
2:F:75:SER:OG	2:F:76:TYR:N	2.53	0.42
1:I:428:TRP:O	1:I:432:ARG:NH1	2.53	0.42
2:J:75:SER:OG	2:J:76:TYR:N	2.53	0.42
4:L:32:TRP:HA	4:L:237:ARG:HB2	2.01	0.42
4:P:155:VAL:HG22	4:P:176:CYS:HB3	2.02	0.42
4:P:156:HIS:HB2	4:P:177:THR:HG22	2.02	0.42
4:P:215:ASP:N	4:P:215:ASP:OD1	2.50	0.42
2:F:307:GLY:H	2:F:310:GLU:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:408:ASP:HB3	2:J:433:ARG:HE	1.85	0.42
1:I:508:ASP:N	1:I:508:ASP:OD1	2.41	0.42
3:K:272:LEU:HD23	3:K:272:LEU:HA	1.89	0.42
1:M:241:ILE:HG23	1:M:264:TYR:HA	2.02	0.42
1:M:333:ILE:HD11	1:M:362:LEU:HD12	2.01	0.42
1:M:408:ASP:HB3	2:N:433:ARG:HE	1.85	0.42
2:N:594:GLY:HA3	2:N:599:TYR:HD1	1.85	0.42
3:O:513:ASN:HD21	3:O:515:LEU:HB2	1.85	0.42
4:P:480:ARG:O	4:P:484:LEU:HB2	2.19	0.42
1:A:230:LYS:HE3	1:A:230:LYS:HB3	1.88	0.42
1:A:333:ILE:HD11	1:A:362:LEU:HD12	2.01	0.42
3:C:513:ASN:HD21	3:C:515:LEU:HB2	1.85	0.42
4:D:244:ILE:HA	4:D:247:CYS:HB3	2.01	0.42
4:D:480:ARG:O	4:D:484:LEU:HB2	2.19	0.42
2:F:167:ASN:OD1	3:G:568:ARG:NH2	2.52	0.42
3:G:430:ARG:NH2	3:G:609:GLU:OE2	2.53	0.42
1:I:108:LEU:O	2:J:40:ARG:NH2	2.53	0.42
3:K:371:PRO:HA	3:K:373:LEU:HD13	2.02	0.42
3:K:430:ARG:NH2	3:K:609:GLU:OE2	2.53	0.42
4:P:244:ILE:HA	4:P:247:CYS:HB3	2.01	0.42
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.83	0.41
1:A:250:ASN:OD1	1:A:250:ASN:N	2.53	0.41
1:A:428:TRP:O	1:A:432:ARG:NH1	2.53	0.41
1:A:524:ASP:OD2	1:A:527:SER:N	2.49	0.41
2:B:682:ASN:O	2:B:686:GLU:HB2	2.20	0.41
3:C:430:ARG:NH2	3:C:609:GLU:OE2	2.53	0.41
4:D:466:GLU:HA	4:D:469:THR:HG22	2.02	0.41
1:E:267:LEU:HG	1:E:299:ILE:HB	2.02	0.41
2:F:267:LEU:HD23	2:F:301:TRP:HZ2	1.85	0.41
1:I:267:LEU:HG	1:I:299:ILE:HB	2.02	0.41
2:J:227:ASN:OD1	2:J:231:ASN:ND2	2.53	0.41
4:L:430:MET:O	4:L:434:VAL:HG12	2.20	0.41
4:P:405:SER:OG	4:P:635:ARG:NH2	2.47	0.41
4:P:422:ILE:HD12	4:P:422:ILE:HA	1.93	0.41
4:P:466:GLU:HA	4:P:469:THR:HG22	2.02	0.41
2:F:227:ASN:OD1	2:F:231:ASN:ND2	2.53	0.41
4:H:430:MET:O	4:H:434:VAL:HG12	2.20	0.41
1:I:285:ASP:OD1	1:I:285:ASP:N	2.45	0.41
1:I:476:VAL:N	1:I:492:CYS:O	2.46	0.41
1:I:676:ASP:OD1	1:I:676:ASP:N	2.40	0.41
2:J:269:ARG:NH1	2:J:346:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:250:ASN:OD1	1:M:250:ASN:N	2.53	0.41
1:M:428:TRP:O	1:M:432:ARG:NH1	2.53	0.41
2:N:269:ARG:NH1	2:N:346:GLY:O	2.52	0.41
3:O:413:ASP:O	3:O:417:TYR:N	2.43	0.41
1:A:267:LEU:HG	1:A:299:ILE:HB	2.02	0.41
2:B:75:SER:OG	2:B:76:TYR:N	2.53	0.41
2:B:583:TYR:HB3	4:D:445:LEU:HD22	2.01	0.41
4:D:420:LYS:HE3	4:D:420:LYS:HB3	1.95	0.41
1:E:250:ASN:OD1	1:E:250:ASN:N	2.53	0.41
3:G:371:PRO:HA	3:G:373:LEU:HD13	2.02	0.41
2:J:96:ILE:HD13	2:J:96:ILE:HA	1.91	0.41
2:J:167:ASN:OD1	3:K:568:ARG:NH2	2.53	0.41
2:J:267:LEU:HD23	2:J:301:TRP:HZ2	1.85	0.41
1:M:53:TYR:CZ	1:M:194:LYS:HB3	2.56	0.41
1:M:248:HIS:NE2	1:M:253:GLN:OE1	2.43	0.41
3:O:371:PRO:HA	3:O:373:LEU:HD13	2.02	0.41
3:O:415:LYS:HB3	3:O:415:LYS:HE3	1.88	0.41
3:O:430:ARG:NH2	3:O:609:GLU:OE2	2.53	0.41
2:B:30:ASN:HD21	2:B:32:LEU:HD12	1.85	0.41
2:B:624:ASP:OD1	2:B:624:ASP:N	2.42	0.41
3:C:371:PRO:HA	3:C:373:LEU:HD13	2.02	0.41
1:E:315:PHE:HE2	1:E:358:MET:HG2	1.85	0.41
4:H:522:ALA:O	4:H:526:THR:OG1	2.29	0.41
1:I:53:TYR:CZ	1:I:194:LYS:HB3	2.56	0.41
1:I:644:LYS:HB2	1:I:644:LYS:HE3	1.88	0.41
2:J:594:GLY:HA3	2:J:599:TYR:HD1	1.85	0.41
1:M:267:LEU:HG	1:M:299:ILE:HB	2.02	0.41
2:N:75:SER:OG	2:N:76:TYR:N	2.53	0.41
2:N:130:GLU:H	2:N:130:GLU:HG2	1.71	0.41
4:P:517:SER:OG	4:P:518:LYS:N	2.53	0.41
1:A:53:TYR:CZ	1:A:194:LYS:HB3	2.56	0.41
2:B:110:GLY:O	3:C:447:ARG:NH1	2.53	0.41
3:C:32:LEU:HD22	3:C:421:LEU:HD13	2.02	0.41
3:C:272:LEU:HB2	3:C:275:LEU:HD12	2.01	0.41
4:D:422:ILE:HD12	4:D:422:ILE:HA	1.93	0.41
4:D:517:SER:OG	4:D:518:LYS:N	2.53	0.41
1:E:503:ILE:HD12	1:E:591:ALA:HB3	2.03	0.41
2:F:96:ILE:HD13	2:F:96:ILE:HA	1.90	0.41
2:F:110:GLY:O	3:G:447:ARG:NH1	2.53	0.41
3:G:32:LEU:HD22	3:G:421:LEU:HD13	2.02	0.41
3:G:87:HIS:CD2	3:G:89:SER:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:272:LEU:HD23	3:G:272:LEU:HA	1.89	0.41
4:H:156:HIS:HB2	4:H:177:THR:HG22	2.02	0.41
1:I:315:PHE:HE2	1:I:358:MET:HG2	1.85	0.41
1:I:333:ILE:HD11	1:I:362:LEU:HD12	2.01	0.41
3:K:87:HIS:CD2	3:K:89:SER:HB2	2.56	0.41
4:L:559:ASP:OD1	4:L:562:ARG:NH2	2.47	0.41
3:O:272:LEU:HB2	3:O:275:LEU:HD12	2.01	0.41
2:B:594:GLY:HA3	2:B:599:TYR:HD1	1.86	0.41
3:C:354:ILE:H	3:C:354:ILE:HG13	1.72	0.41
3:C:415:LYS:HB3	3:C:415:LYS:HE3	1.87	0.41
4:D:491:LYS:HE3	4:D:491:LYS:HB3	1.93	0.41
1:E:333:ILE:HD11	1:E:362:LEU:HD12	2.01	0.41
1:I:503:ILE:HD12	1:I:591:ALA:HB3	2.03	0.41
2:J:595:ILE:O	2:J:598:SER:OG	2.38	0.41
2:J:620:ASN:HB3	2:J:648:ILE:HG12	2.03	0.41
4:L:156:HIS:HB2	4:L:177:THR:HG22	2.01	0.41
1:M:315:PHE:HE2	1:M:358:MET:HG2	1.86	0.41
1:M:503:ILE:HD12	1:M:591:ALA:HB3	2.03	0.41
3:O:32:LEU:HD22	3:O:421:LEU:HD13	2.02	0.41
1:A:315:PHE:HE2	1:A:358:MET:HG2	1.85	0.41
1:E:53:TYR:CZ	1:E:194:LYS:HB3	2.56	0.41
2:F:595:ILE:O	2:F:598:SER:OG	2.38	0.41
3:G:577:LYS:HE3	3:G:577:LYS:HB3	1.96	0.41
1:I:250:ASN:OD1	1:I:250:ASN:N	2.53	0.41
2:J:307:GLY:H	2:J:310:GLU:CD	2.24	0.41
1:M:229:LEU:HA	1:M:229:LEU:HD23	1.84	0.41
1:M:230:LYS:HE3	1:M:230:LYS:HB3	1.88	0.41
2:N:192:ARG:HD3	3:O:623:GLN:HE22	1.86	0.41
2:N:336:GLY:HA2	2:N:376:GLY:H	1.85	0.41
4:P:491:LYS:HE3	4:P:491:LYS:HB3	1.93	0.41
1:A:503:ILE:HD12	1:A:591:ALA:HB3	2.03	0.41
1:E:676:ASP:OD1	1:E:676:ASP:N	2.40	0.41
3:G:19:THR:OG1	3:G:20:GLN:N	2.54	0.41
3:G:513:ASN:HD21	3:G:515:LEU:HB2	1.85	0.41
4:H:559:ASP:OD1	4:H:562:ARG:NH2	2.47	0.41
3:K:32:LEU:HD22	3:K:421:LEU:HD13	2.02	0.41
2:N:307:GLY:H	2:N:310:GLU:CD	2.24	0.41
2:N:620:ASN:HB3	2:N:648:ILE:HG12	2.03	0.41
1:A:496:ILE:HD12	1:A:496:ILE:HA	1.94	0.41
2:B:192:ARG:HD3	3:C:623:GLN:HE22	1.86	0.41
2:B:307:GLY:H	2:B:310:GLU:CD	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:GLY:HA2	2:B:376:GLY:H	1.85	0.41
3:C:603:LEU:HD13	3:C:610:SER:HA	2.02	0.41
4:D:430:MET:O	4:D:434:VAL:HG12	2.20	0.41
4:D:572:ASN:O	4:D:576:ASN:ND2	2.54	0.41
2:F:192:ARG:HD3	3:G:623:GLN:HE22	1.85	0.41
2:F:594:GLY:HA3	2:F:599:TYR:HD1	1.86	0.41
3:K:19:THR:OG1	3:K:20:GLN:N	2.54	0.41
4:L:572:ASN:O	4:L:576:ASN:ND2	2.54	0.41
1:M:496:ILE:HD12	1:M:496:ILE:HA	1.94	0.41
3:O:10:LYS:HD3	3:O:10:LYS:HA	1.84	0.41
3:O:325:SER:N	3:O:327:GLU:OE2	2.54	0.41
3:O:354:ILE:H	3:O:354:ILE:HG13	1.72	0.41
3:O:603:LEU:HD13	3:O:610:SER:HA	2.02	0.41
4:P:421:LEU:HD12	4:P:421:LEU:HA	1.94	0.41
4:P:572:ASN:O	4:P:576:ASN:ND2	2.54	0.41
2:B:684:ILE:O	2:B:688:PHE:HB2	2.21	0.41
3:C:325:SER:N	3:C:327:GLU:OE2	2.54	0.41
2:F:684:ILE:O	2:F:688:PHE:HB2	2.21	0.41
3:G:325:SER:N	3:G:327:GLU:OE2	2.54	0.41
3:G:427:ILE:HD12	3:G:430:ARG:HB2	2.03	0.41
2:J:185:CYS:HB3	2:J:228:ILE:HD11	2.03	0.41
3:K:513:ASN:HD21	3:K:515:LEU:HB2	1.85	0.41
4:P:72:GLU:O	4:P:76:THR:OG1	2.35	0.41
4:P:430:MET:O	4:P:434:VAL:HG12	2.20	0.41
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.93	0.40
2:B:267:LEU:HD23	2:B:301:TRP:HZ2	1.85	0.40
2:B:595:ILE:O	2:B:598:SER:OG	2.37	0.40
3:C:10:LYS:HA	3:C:10:LYS:HD3	1.84	0.40
3:C:70:GLN:HA	3:C:73:LEU:HD12	2.03	0.40
4:D:498:LEU:HB2	4:D:536:GLU:HG2	2.03	0.40
2:F:301:TRP:HA	2:F:302:PRO:HD3	1.95	0.40
3:G:69:SER:H	3:G:72:GLN:NE2	2.18	0.40
3:G:70:GLN:HA	3:G:73:LEU:HD12	2.03	0.40
4:H:425:MET:HA	4:H:428:VAL:HG12	2.04	0.40
4:H:466:GLU:HA	4:H:469:THR:HG22	2.02	0.40
4:H:572:ASN:O	4:H:576:ASN:ND2	2.54	0.40
1:I:387:ALA:HA	1:I:390:VAL:HG12	2.03	0.40
2:J:301:TRP:HA	2:J:302:PRO:HD3	1.94	0.40
3:K:69:SER:H	3:K:72:GLN:NE2	2.18	0.40
3:K:70:GLN:HA	3:K:73:LEU:HD12	2.03	0.40
3:K:325:SER:N	3:K:327:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:427:ILE:HD12	3:K:430:ARG:HB2	2.03	0.40
3:K:577:LYS:HE3	3:K:577:LYS:HB3	1.96	0.40
4:L:425:MET:HA	4:L:428:VAL:HG12	2.04	0.40
4:L:466:GLU:HA	4:L:469:THR:HG22	2.02	0.40
2:N:86:ASP:OD1	2:N:86:ASP:N	2.54	0.40
3:O:70:GLN:HA	3:O:73:LEU:HD12	2.03	0.40
1:A:259:ASP:OD1	1:A:260:ASP:N	2.54	0.40
2:B:537:PHE:O	2:B:541:GLY:N	2.46	0.40
1:E:259:ASP:OD1	1:E:260:ASP:N	2.54	0.40
1:E:387:ALA:HA	1:E:390:VAL:HG12	2.03	0.40
4:H:517:SER:OG	4:H:518:LYS:N	2.53	0.40
2:J:422:ARG:HA	2:J:422:ARG:HD3	1.92	0.40
2:J:447:ASN:OD1	2:J:448:ASP:N	2.54	0.40
4:L:517:SER:OG	4:L:518:LYS:N	2.53	0.40
1:M:259:ASP:OD1	1:M:260:ASP:N	2.54	0.40
2:N:267:LEU:HD23	2:N:301:TRP:HZ2	1.85	0.40
2:B:185:CYS:HB3	2:B:228:ILE:HD11	2.03	0.40
2:B:524:ASP:OD1	2:B:526:SER:OG	2.35	0.40
3:C:35:LYS:HG2	3:C:409:ASP:HA	2.03	0.40
3:C:427:ILE:HD12	3:C:430:ARG:HB2	2.03	0.40
4:D:160:TYR:CE1	4:D:179:HIS:HB3	2.56	0.40
4:D:421:LEU:HD12	4:D:421:LEU:HA	1.94	0.40
4:D:425:MET:HA	4:D:428:VAL:HG12	2.04	0.40
2:F:447:ASN:OD1	2:F:448:ASP:N	2.54	0.40
3:G:511:ASN:OD1	3:G:511:ASN:N	2.51	0.40
1:I:259:ASP:OD1	1:I:260:ASP:N	2.54	0.40
1:M:96:ILE:HD12	1:M:96:ILE:HA	1.94	0.40
2:N:606:LEU:HD23	2:N:606:LEU:HA	1.94	0.40
3:O:19:THR:OG1	3:O:20:GLN:N	2.54	0.40
3:O:560:LYS:HD2	3:O:560:LYS:HA	1.83	0.40
4:P:425:MET:HA	4:P:428:VAL:HG12	2.04	0.40
1:A:642:TYR:O	1:A:646:SER:OG	2.29	0.40
2:B:620:ASN:HB3	2:B:648:ILE:HG12	2.03	0.40
3:C:19:THR:OG1	3:C:20:GLN:N	2.54	0.40
3:C:87:HIS:CD2	3:C:89:SER:HB2	2.56	0.40
3:C:551:LYS:HD3	3:C:551:LYS:HA	1.83	0.40
3:C:560:LYS:HD2	3:C:560:LYS:HA	1.84	0.40
1:E:269:ARG:HG2	1:E:301:TRP:HB2	2.04	0.40
1:E:394:LEU:HD23	1:E:394:LEU:HA	1.93	0.40
1:I:195:ASN:N	1:I:195:ASN:OD1	2.55	0.40
1:M:308:ASP:N	1:M:308:ASP:OD1	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:537:PHE:O	2:N:541:GLY:N	2.46	0.40
3:O:35:LYS:HG2	3:O:409:ASP:HA	2.04	0.40
3:O:87:HIS:CD2	3:O:89:SER:HB2	2.56	0.40
3:O:427:ILE:HD12	3:O:430:ARG:HB2	2.03	0.40
4:P:274:ARG:HA	4:P:277:LEU:HD23	2.03	0.40
4:P:498:LEU:HB2	4:P:536:GLU:HG2	2.03	0.40
4:P:617:LEU:HA	4:P:617:LEU:HD12	1.82	0.40
2:B:606:LEU:HD23	2:B:606:LEU:HA	1.94	0.40
3:C:25:LEU:HD23	3:C:28:ILE:HD12	2.03	0.40
4:D:274:ARG:HA	4:D:277:LEU:HD23	2.03	0.40
1:E:421:ILE:HD12	1:E:421:ILE:HA	1.95	0.40
2:F:167:ASN:O	2:F:170:SER:OG	2.32	0.40
2:F:336:GLY:HA2	2:F:376:GLY:H	1.85	0.40
2:J:110:GLY:O	3:K:447:ARG:NH1	2.55	0.40
2:J:682:ASN:O	2:J:686:GLU:HB2	2.21	0.40
3:K:511:ASN:OD1	3:K:511:ASN:N	2.51	0.40
3:O:25:LEU:HD23	3:O:28:ILE:HD12	2.03	0.40
3:O:551:LYS:HD3	3:O:551:LYS:HA	1.83	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	652/661 (99%)	591 (91%)	61 (9%)	0	100	100
1	E	652/661 (99%)	591 (91%)	61 (9%)	0	100	100
1	I	652/661 (99%)	591 (91%)	61 (9%)	0	100	100
1	M	652/661 (99%)	590 (90%)	62 (10%)	0	100	100
2	B	655/672 (98%)	602 (92%)	53 (8%)	0	100	100
2	F	655/672 (98%)	603 (92%)	52 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	655/672 (98%)	605 (92%)	50 (8%)	0	100	100
2	N	655/672 (98%)	603 (92%)	52 (8%)	0	100	100
3	C	534/629 (85%)	490 (92%)	44 (8%)	0	100	100
3	G	534/629 (85%)	490 (92%)	44 (8%)	0	100	100
3	K	534/629 (85%)	490 (92%)	44 (8%)	0	100	100
3	O	534/629 (85%)	490 (92%)	44 (8%)	0	100	100
4	D	538/542 (99%)	507 (94%)	31 (6%)	0	100	100
4	H	538/542 (99%)	507 (94%)	31 (6%)	0	100	100
4	L	538/542 (99%)	508 (94%)	30 (6%)	0	100	100
4	P	538/542 (99%)	507 (94%)	31 (6%)	0	100	100
All	All	9516/10016 (95%)	8765 (92%)	751 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/585 (99%)	580 (100%)	0	100	100
1	E	580/585 (99%)	580 (100%)	0	100	100
1	I	580/585 (99%)	580 (100%)	0	100	100
1	M	580/585 (99%)	580 (100%)	0	100	100
2	B	586/596 (98%)	584 (100%)	2 (0%)	91	92
2	F	586/596 (98%)	585 (100%)	1 (0%)	92	94
2	J	586/596 (98%)	584 (100%)	2 (0%)	91	92
2	N	586/596 (98%)	584 (100%)	2 (0%)	91	92
3	C	511/582 (88%)	508 (99%)	3 (1%)	84	88
3	G	511/582 (88%)	508 (99%)	3 (1%)	84	88
3	K	511/582 (88%)	508 (99%)	3 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	511/582 (88%)	508 (99%)	3 (1%)	84	88
4	D	510/510 (100%)	500 (98%)	10 (2%)	50	68
4	H	510/510 (100%)	499 (98%)	11 (2%)	47	64
4	L	510/510 (100%)	500 (98%)	10 (2%)	50	68
4	P	510/510 (100%)	500 (98%)	10 (2%)	50	68
All	All	8748/9092 (96%)	8688 (99%)	60 (1%)	80	86

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	34	THR
2	B	35	THR
3	C	125	SER
3	C	245	HIS
3	C	546	LEU
4	D	38	SER
4	D	73	SER
4	D	129	TYR
4	D	164	SER
4	D	172	ASN
4	D	285	ARG
4	D	325	SER
4	D	497	THR
4	D	519	LEU
4	D	591	ILE
2	F	35	THR
3	G	125	SER
3	G	245	HIS
3	G	546	LEU
4	H	38	SER
4	H	73	SER
4	H	78	CYS
4	H	129	TYR
4	H	164	SER
4	H	172	ASN
4	H	285	ARG
4	H	325	SER
4	H	497	THR
4	H	519	LEU
4	H	591	ILE

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Mol	Chain	Res	Type
2	J	34	THR
2	J	35	THR
3	K	125	SER
3	K	245	HIS
3	K	546	LEU
4	L	38	SER
4	L	73	SER
4	L	129	TYR
4	L	164	SER
4	L	172	ASN
4	L	285	ARG
4	L	325	SER
4	L	497	THR
4	L	519	LEU
4	L	591	ILE
2	N	34	THR
2	N	35	THR
3	O	125	SER
3	O	245	HIS
3	O	546	LEU
4	P	38	SER
4	P	73	SER
4	P	129	TYR
4	P	164	SER
4	P	172	ASN
4	P	285	ARG
4	P	325	SER
4	P	497	THR
4	P	519	LEU
4	P	591	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	286	GLN
1	A	379	ASN
1	A	437	ASN
1	A	552	ASN
2	B	231	ASN
2	B	286	GLN
2	B	463	GLN

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Mol	Chain	Res	Type
2	B	517	ASN
2	B	620	ASN
3	C	72	GLN
3	C	280	ASN
3	C	295	ASN
3	C	347	ASN
3	C	367	ASN
3	C	454	GLN
3	C	505	ASN
3	C	507	GLN
3	C	513	ASN
3	C	557	ASN
3	C	589	GLN
3	C	623	GLN
4	D	41	GLN
4	D	47	GLN
4	D	87	HIS
4	D	153	ASN
4	D	172	ASN
4	D	293	HIS
4	D	316	GLN
4	D	404	ASN
4	D	449	GLN
4	D	477	ASN
4	D	488	ASN
4	D	512	GLN
4	D	530	GLN
4	D	572	ASN
4	D	576	ASN
4	D	611	ASN
1	E	268	HIS
1	E	286	GLN
1	E	379	ASN
1	E	437	ASN
1	E	552	ASN
2	F	231	ASN
2	F	286	GLN
2	F	463	GLN
2	F	517	ASN
2	F	620	ASN
3	G	72	GLN
3	G	280	ASN

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Mol	Chain	Res	Type
3	G	295	ASN
3	G	347	ASN
3	G	367	ASN
3	G	454	GLN
3	G	505	ASN
3	G	513	ASN
3	G	557	ASN
3	G	589	GLN
3	G	623	GLN
4	H	41	GLN
4	H	47	GLN
4	H	87	HIS
4	H	153	ASN
4	H	172	ASN
4	H	293	HIS
4	H	316	GLN
4	H	404	ASN
4	H	449	GLN
4	H	477	ASN
4	H	488	ASN
4	H	512	GLN
4	H	530	GLN
4	H	572	ASN
4	H	576	ASN
4	H	611	ASN
1	I	168	ASN
1	I	268	HIS
1	I	286	GLN
1	I	379	ASN
1	I	437	ASN
1	I	500	ASN
1	I	552	ASN
2	J	231	ASN
2	J	286	GLN
2	J	463	GLN
2	J	517	ASN
2	J	620	ASN
3	K	72	GLN
3	K	280	ASN
3	K	295	ASN
3	K	347	ASN
3	K	367	ASN

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Mol	Chain	Res	Type
3	K	454	GLN
3	K	505	ASN
3	K	513	ASN
3	K	557	ASN
3	K	589	GLN
3	K	623	GLN
4	L	41	GLN
4	L	47	GLN
4	L	87	HIS
4	L	153	ASN
4	L	172	ASN
4	L	293	HIS
4	L	316	GLN
4	L	404	ASN
4	L	449	GLN
4	L	477	ASN
4	L	488	ASN
4	L	512	GLN
4	L	530	GLN
4	L	572	ASN
4	L	576	ASN
4	L	611	ASN
1	M	268	HIS
1	M	286	GLN
1	M	379	ASN
1	M	437	ASN
1	M	552	ASN
2	N	231	ASN
2	N	286	GLN
2	N	517	ASN
2	N	620	ASN
3	O	72	GLN
3	O	280	ASN
3	O	295	ASN
3	O	347	ASN
3	O	367	ASN
3	O	454	GLN
3	O	505	ASN
3	O	513	ASN
3	O	557	ASN
3	O	589	GLN
3	O	623	GLN

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Mol	Chain	Res	Type
4	P	41	GLN
4	P	47	GLN
4	P	87	HIS
4	P	153	ASN
4	P	172	ASN
4	P	293	HIS
4	P	316	GLN
4	P	404	ASN
4	P	449	GLN
4	P	477	ASN
4	P	488	ASN
4	P	512	GLN
4	P	530	GLN
4	P	572	ASN
4	P	576	ASN
4	P	611	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1
4	H	1
4	L	1
4	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	333:LYS	C	404:ASN	N	81.43
1	H	333:LYS	C	404:ASN	N	81.43
1	L	333:LYS	C	404:ASN	N	81.43
1	P	333:LYS	C	404:ASN	N	81.43

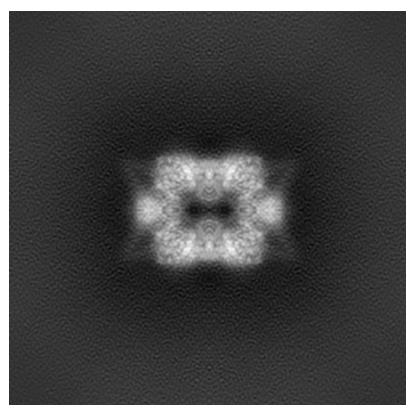
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11101. These allow visual inspection of the internal detail of the map and identification of artifacts.

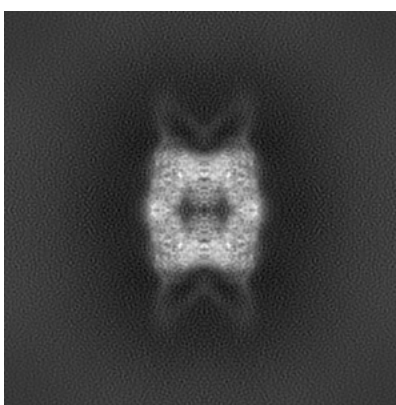
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

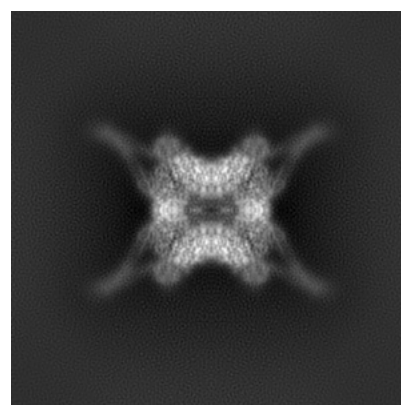
6.1.1 Primary map



X



Y

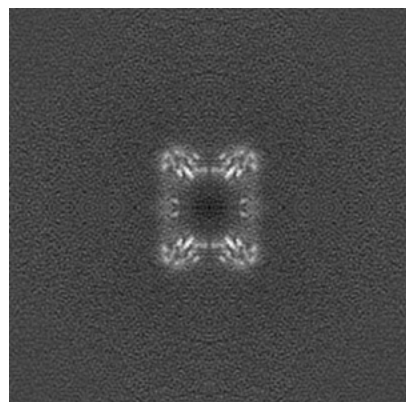


Z

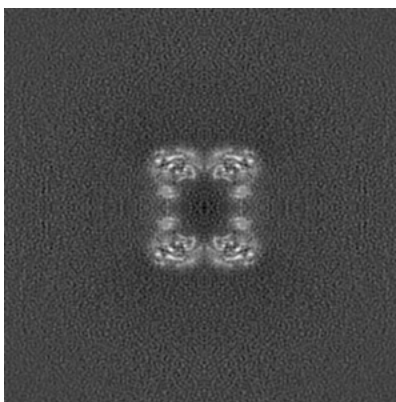
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

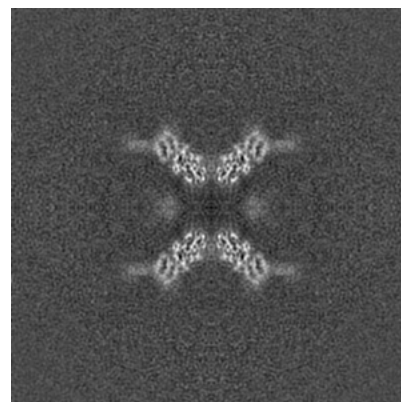
6.2.1 Primary map



X Index: 300



Y Index: 300

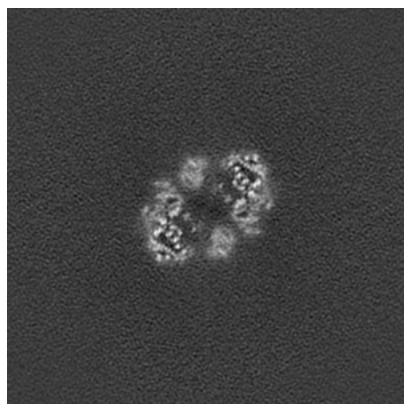


Z Index: 300

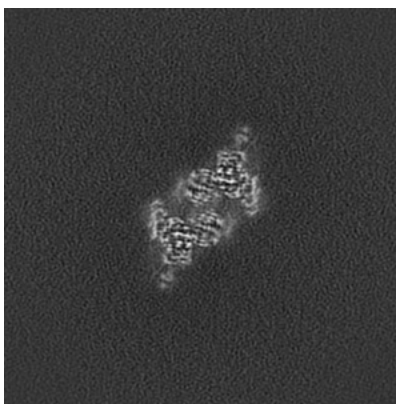
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

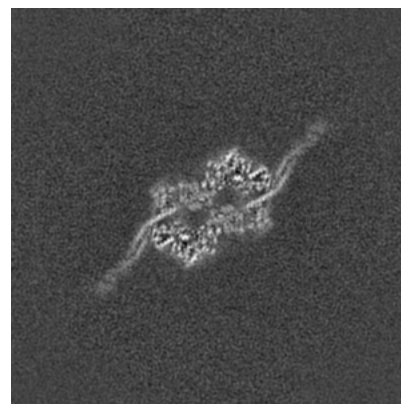
6.3.1 Primary map



X Index: 337



Y Index: 359

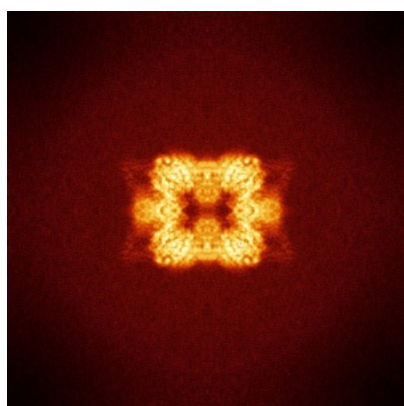


Z Index: 359

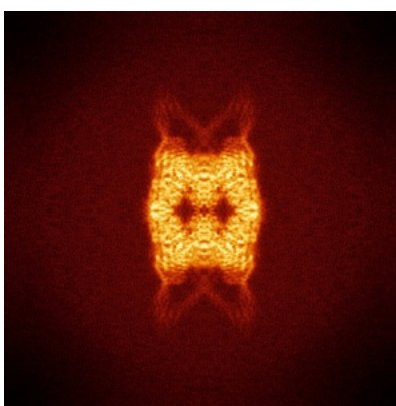
The images above show the largest variance slices of the map in three orthogonal directions.

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

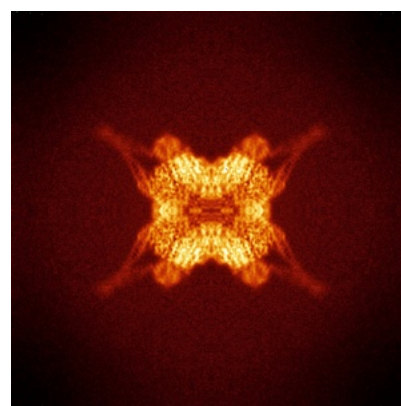
6.4.1 Primary map



X



Y

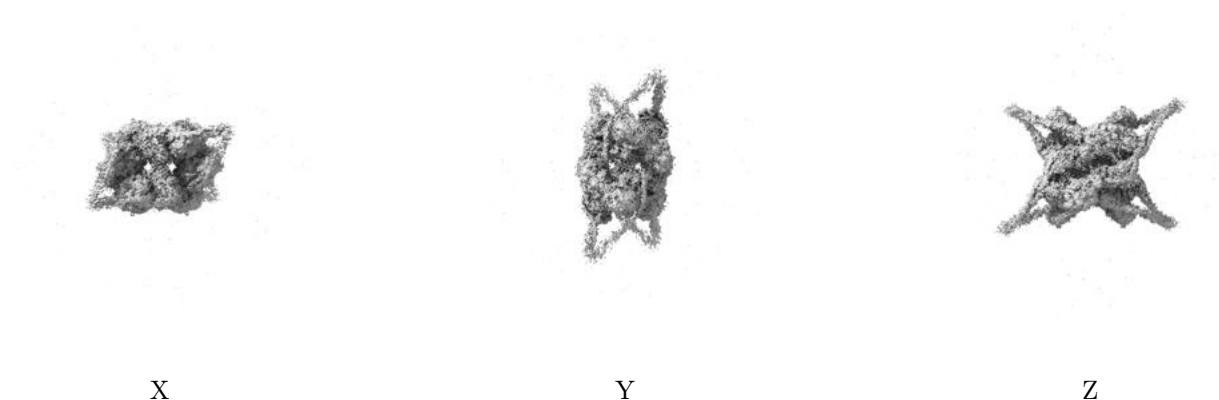


Z

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

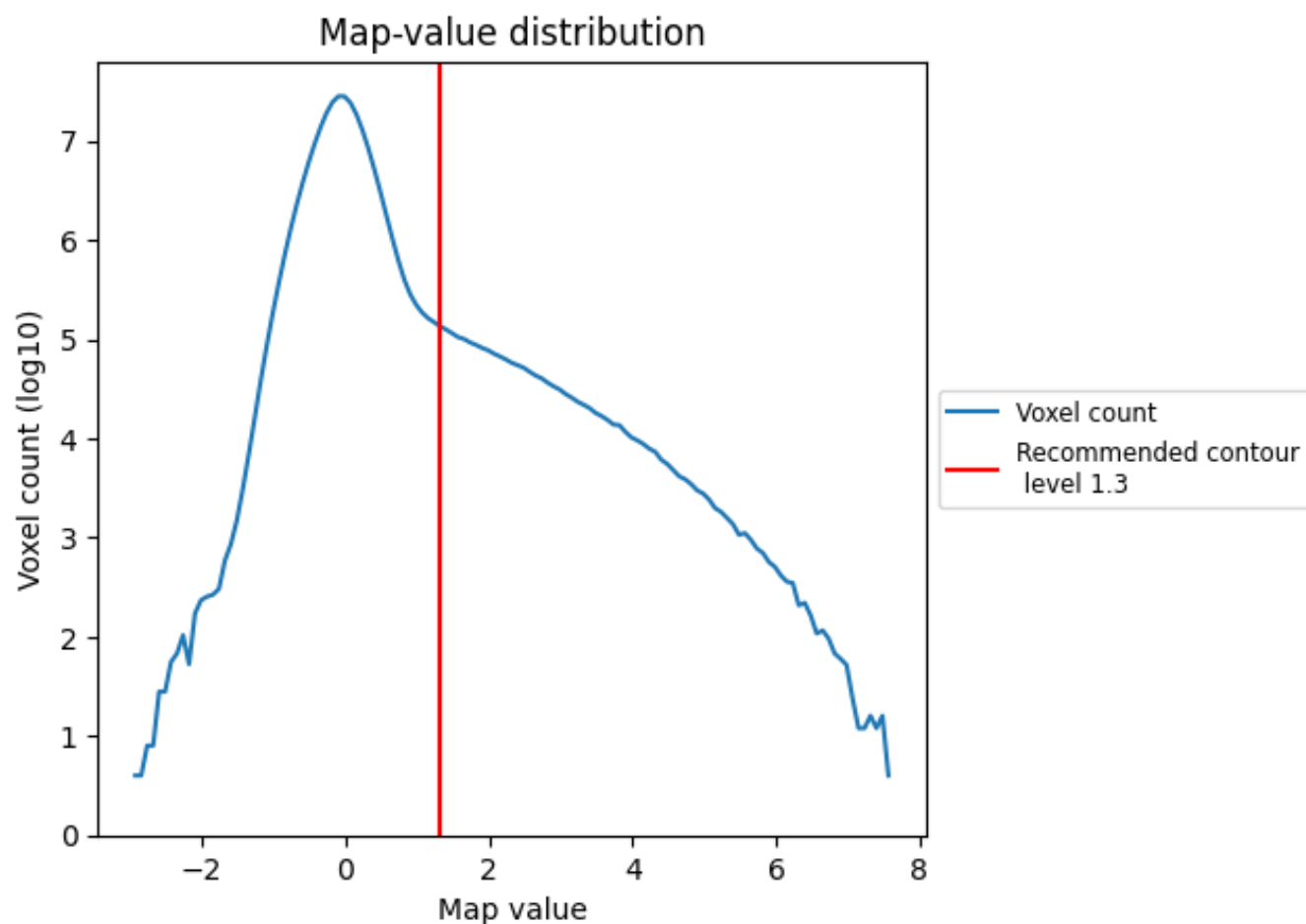
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

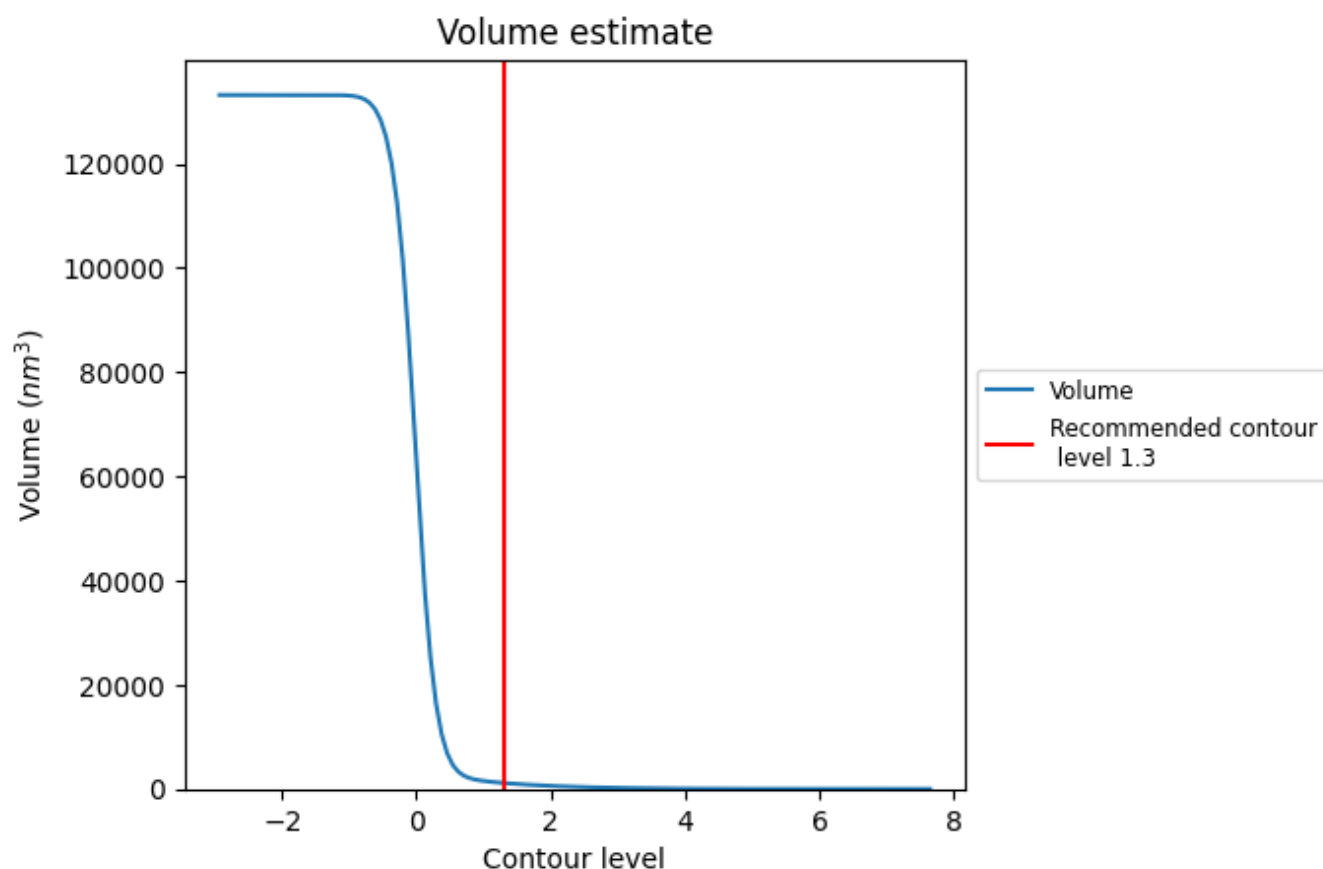
This section contains the results of statistical analysis of the map.

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.

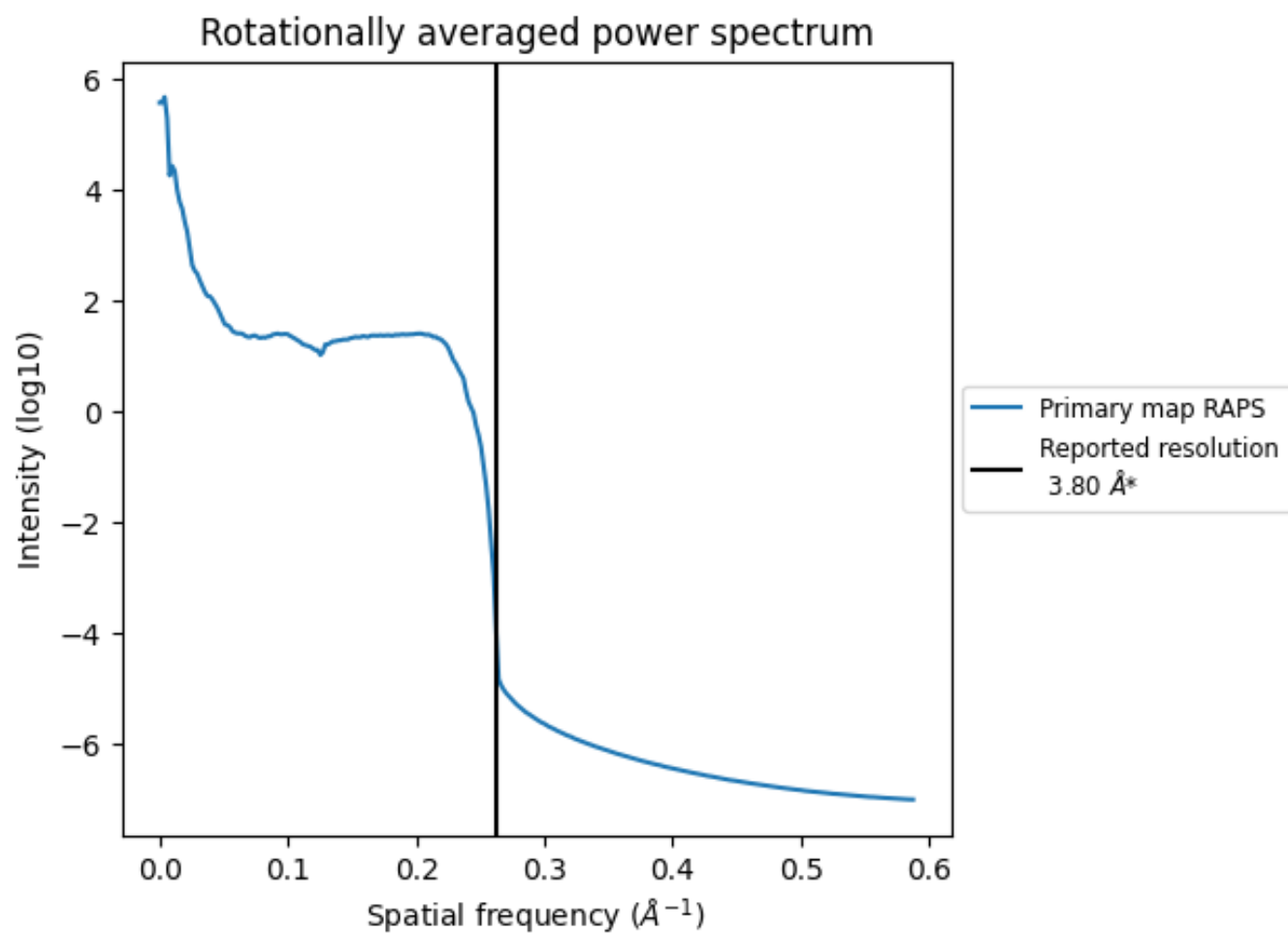
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1141 nm^3 ; this corresponds to an approximate mass of 1030 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 0.263 Å⁻¹

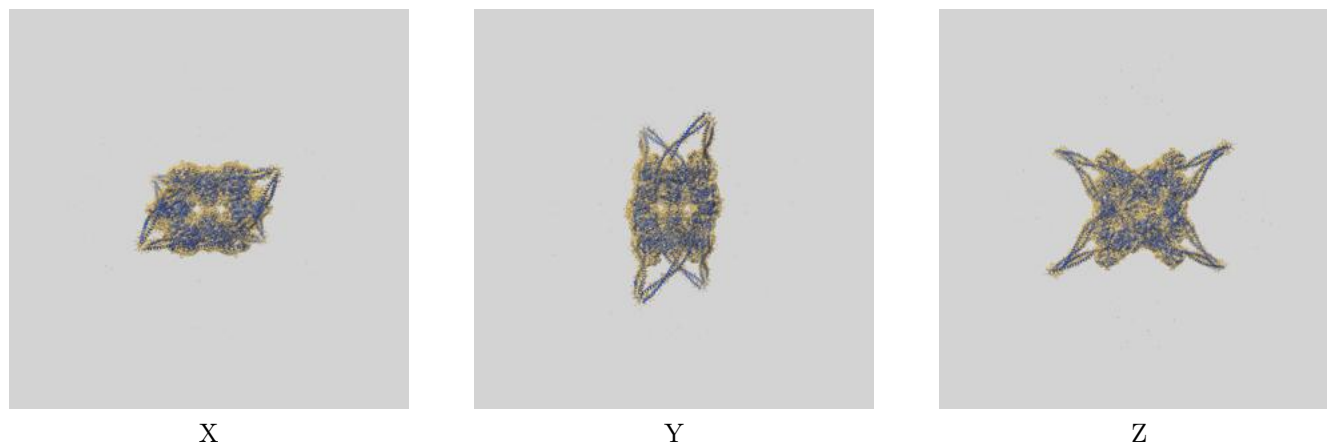
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

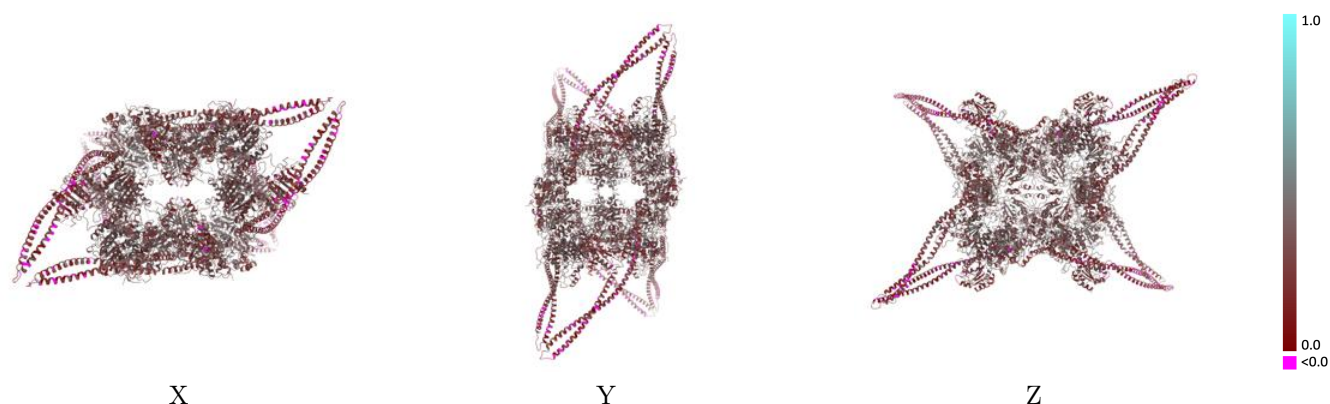
This section contains information regarding the fit between EMDB map EMD-11101 and PDB model 6Z6O. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



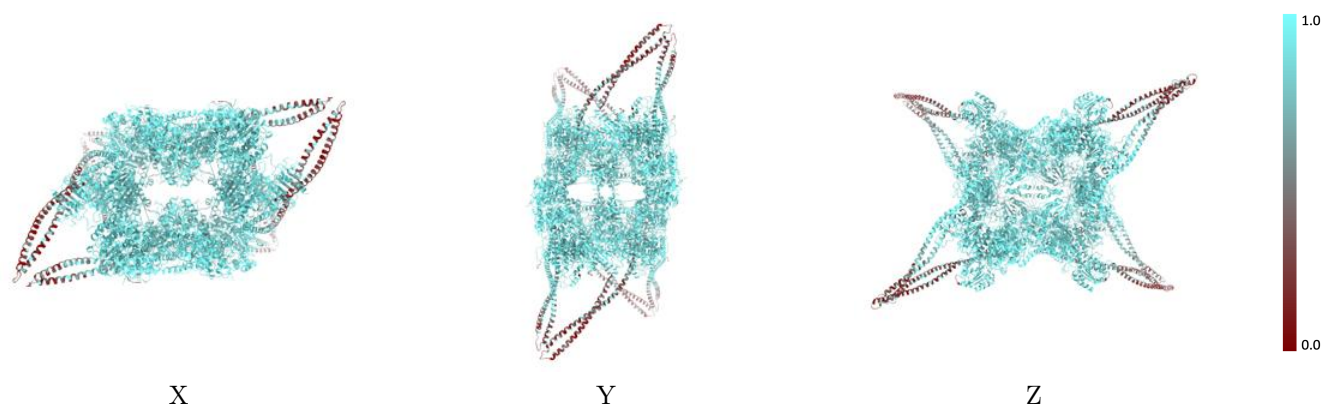
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



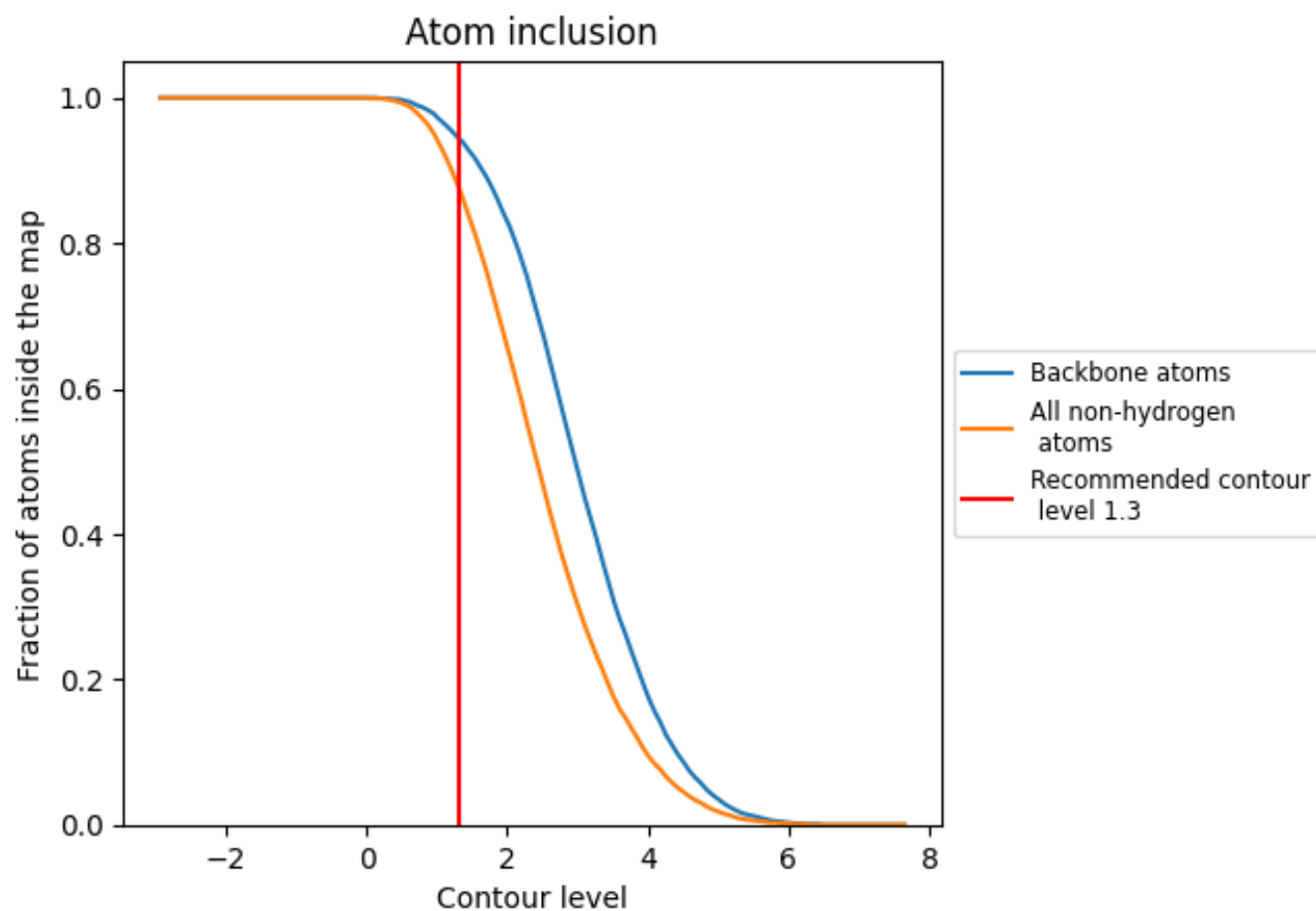
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.3).


































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8790	 0.3130
A	 0.9490	 0.3480
B	 0.9310	 0.3320
C	 0.8500	 0.2970
D	 0.7640	 0.2630
E	 0.9490	 0.3490
F	 0.9310	 0.3330
G	 0.8500	 0.2970
H	 0.7630	 0.2610
I	 0.9490	 0.3480
J	 0.9320	 0.3330
K	 0.8500	 0.2960
L	 0.7620	 0.2620
M	 0.9500	 0.3490
N	 0.9320	 0.3330
O	 0.8500	 0.2970
P	 0.7640	 0.2620

