Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 02:04 PM EDT

PDB ID	:	9NBD
EMDB ID	:	EMD-49227
Title	:	AUGMIN Dimer
Authors	:	Ashaduzzaman, M.; Al-Bassam, J.; Taheri, A.
Deposited on	:	2025-02-13
Resolution	:	8.10 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:

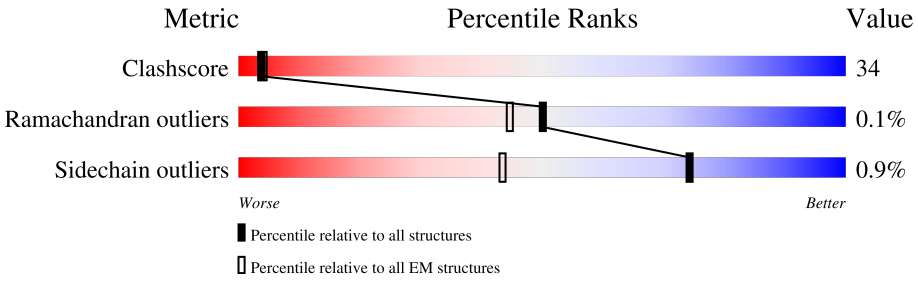
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 8.10 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 <=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	298	28% 38% 55% • 6%
1	M	298	24% 36% 57% • 6%
2	D	423	24% 35% 50% • 14%
2	N	423	22% 39% 46% • 14%
3	E	747	12% 23% 31% • 46%
3	O	747	14% 23% 31% 46%
4	C	617	25% 32% 29% 39%
4	P	617	25% 31% 29% 40%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22553 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 AUGMIN subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	280	Total	C	N	O	S	0	0
			2235	1399	389	439	8		
1	M	280	Total	C	N	O	S	0	0
			2235	1399	389	439	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP F4IK01
M	?	-	GLN	deletion	UNP F4IK01

- Molecule 2 is a protein called AUGMIN subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	363	Total	C	N	O	S	0	0
			2890	1804	505	566	15		
2	N	363	Total	C	N	O	S	0	0
			2890	1804	505	566	15		

- Molecule 3 is a protein called AUGMIN subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	405	Total	C	N	O	S	0	0
			3236	2009	587	627	13		
3	O	405	Total	C	N	O	S	0	0
			3236	2009	587	627	13		

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP Q9FMB4
E	?	-	SER	deletion	UNP Q9FMB4
E	?	-	TYR	deletion	UNP Q9FMB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLN	deletion	UNP Q9FMB4
E	?	-	PHE	deletion	UNP Q9FMB4
E	?	-	ASN	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
E	?	-	ASN	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
E	?	-	LYS	deletion	UNP Q9FMB4
E	?	-	ILE	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
E	?	-	THR	deletion	UNP Q9FMB4
E	?	-	ASP	deletion	UNP Q9FMB4
E	?	-	THR	deletion	UNP Q9FMB4
E	?	-	HIS	deletion	UNP Q9FMB4
E	?	-	PHE	deletion	UNP Q9FMB4
E	?	-	GLN	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
E	?	-	LEU	deletion	UNP Q9FMB4
E	?	-	GLU	deletion	UNP Q9FMB4
E	?	-	SER	deletion	UNP Q9FMB4
E	?	-	MET	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	ASN	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
E	?	-	SER	deletion	UNP Q9FMB4
E	?	-	THR	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
E	?	-	PRO	deletion	UNP Q9FMB4
E	?	-	GLU	deletion	UNP Q9FMB4
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	VAL	deletion	UNP Q9FMB4
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	TYR	deletion	UNP Q9FMB4
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	GLU	deletion	UNP Q9FMB4
E	?	-	LYS	deletion	UNP Q9FMB4
E	?	-	ASN	deletion	UNP Q9FMB4
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	LEU	deletion	UNP Q9FMB4
E	?	-	LEU	deletion	UNP Q9FMB4
E	?	-	THR	deletion	UNP Q9FMB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	ARG	deletion	UNP Q9FMB4
E	?	-	ALA	deletion	UNP Q9FMB4
E	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	LEU	deletion	UNP Q9FMB4
O	?	-	SER	deletion	UNP Q9FMB4
O	?	-	TYR	deletion	UNP Q9FMB4
O	?	-	GLN	deletion	UNP Q9FMB4
O	?	-	PHE	deletion	UNP Q9FMB4
O	?	-	ASN	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	ASN	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	LYS	deletion	UNP Q9FMB4
O	?	-	ILE	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	THR	deletion	UNP Q9FMB4
O	?	-	ASP	deletion	UNP Q9FMB4
O	?	-	THR	deletion	UNP Q9FMB4
O	?	-	HIS	deletion	UNP Q9FMB4
O	?	-	PHE	deletion	UNP Q9FMB4
O	?	-	GLN	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	LEU	deletion	UNP Q9FMB4
O	?	-	GLU	deletion	UNP Q9FMB4
O	?	-	SER	deletion	UNP Q9FMB4
O	?	-	MET	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	ASN	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	SER	deletion	UNP Q9FMB4
O	?	-	THR	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4
O	?	-	PRO	deletion	UNP Q9FMB4
O	?	-	GLU	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	VAL	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	TYR	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	GLU	deletion	UNP Q9FMB4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	LYS	deletion	UNP Q9FMB4
O	?	-	ASN	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	LEU	deletion	UNP Q9FMB4
O	?	-	LEU	deletion	UNP Q9FMB4
O	?	-	THR	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	ARG	deletion	UNP Q9FMB4
O	?	-	ALA	deletion	UNP Q9FMB4
O	?	-	GLY	deletion	UNP Q9FMB4

- Molecule 4 is a protein called AUGMIN subunit 3.

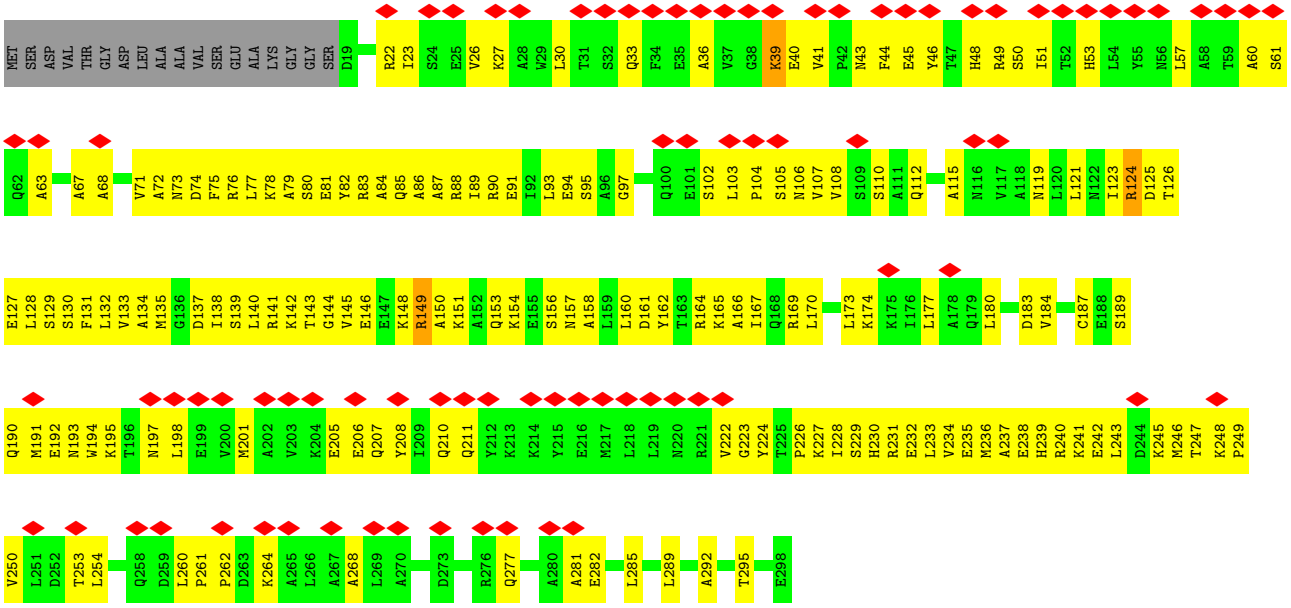
Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	375	Total	C	N	O	S	0	0
			2930	1809	535	575	11		
4	P	371	Total	C	N	O	S	0	0
			2901	1792	531	567	11		

3 Residue-property plots (i)

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.

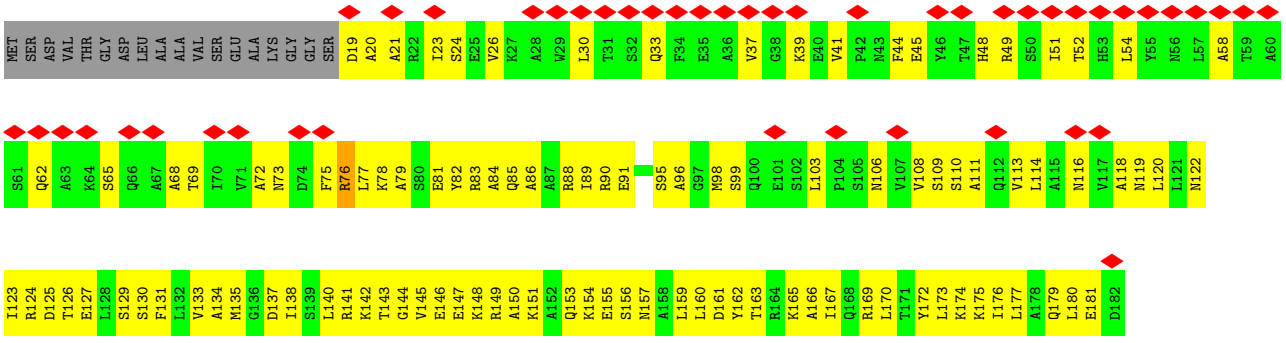
• Molecule 1: AUGMIN subunit 1

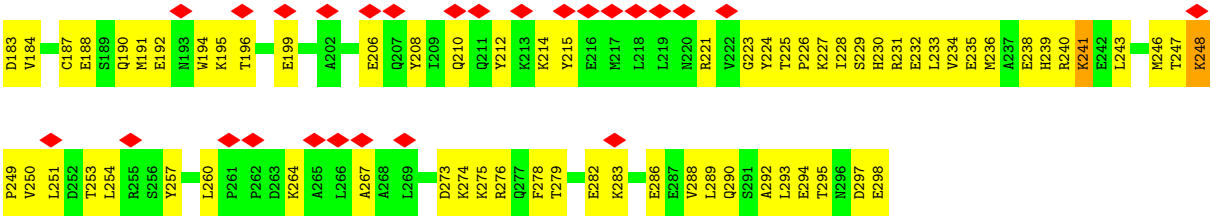
Chain A:



• Molecule 1: AUGMIN subunit 1

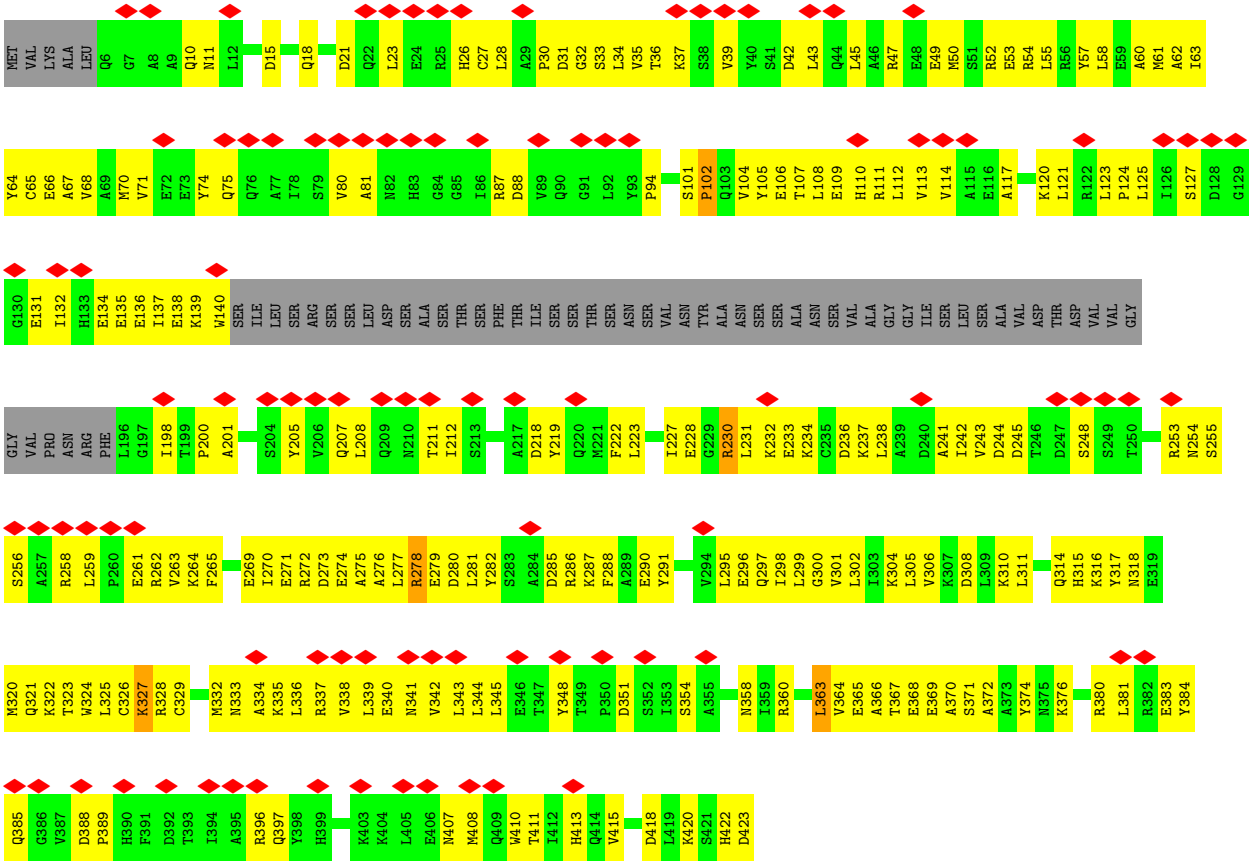
Chain M:





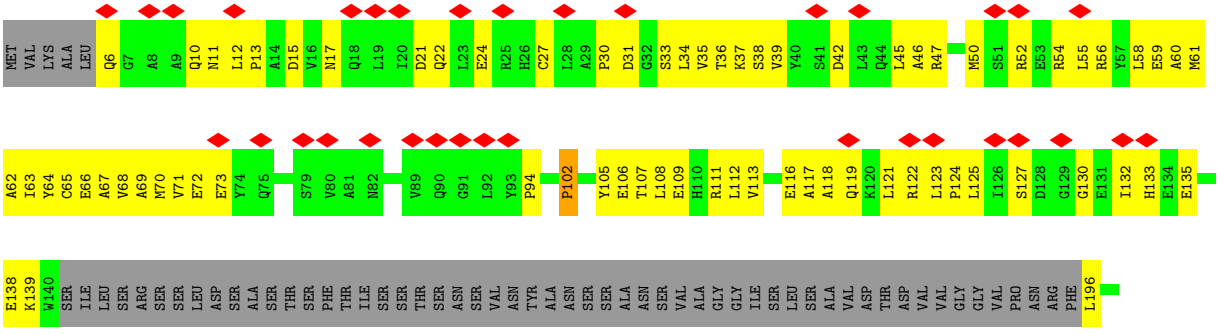
• Molecule 2: AUGMIN subunit 4

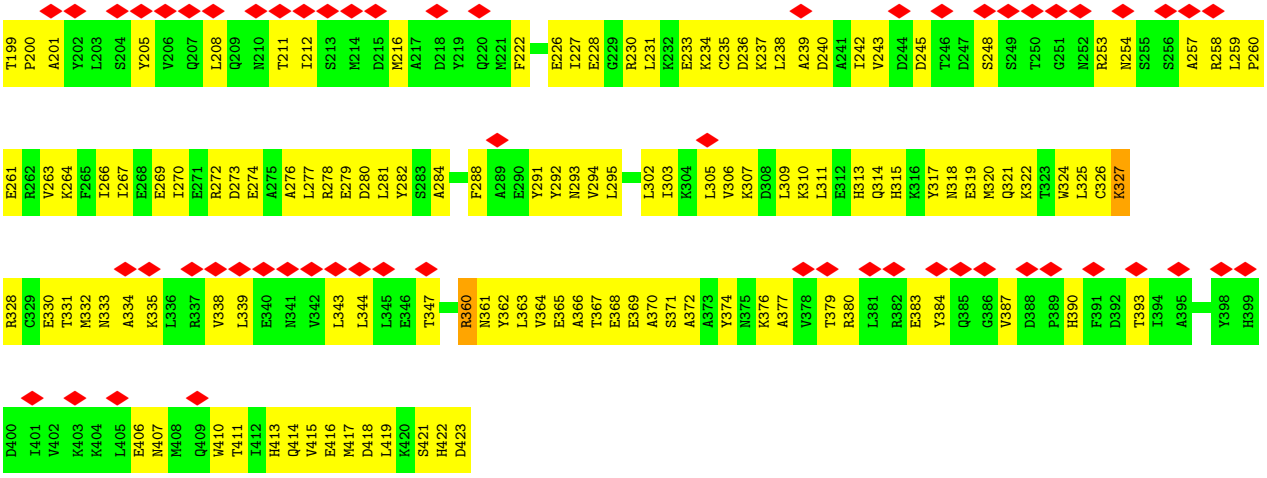
Chain D:



• Molecule 2: AUGMIN subunit 4

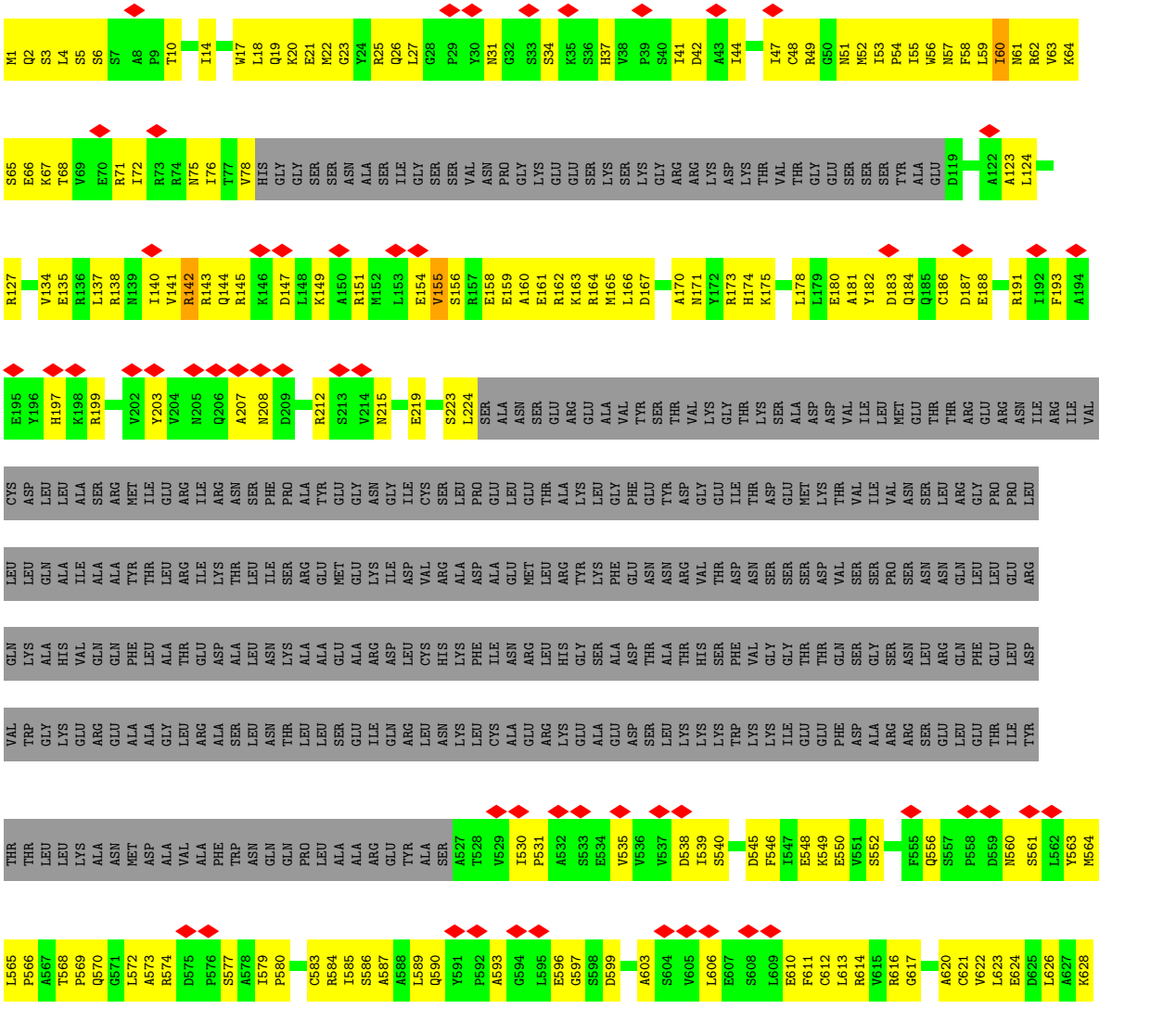
Chain N:

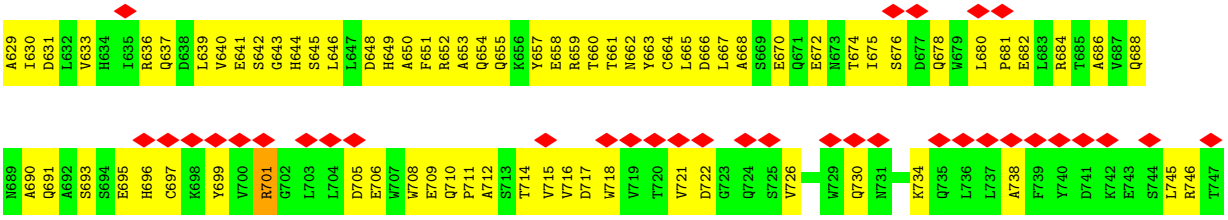




• Molecule 3: AUGMIN subunit 5

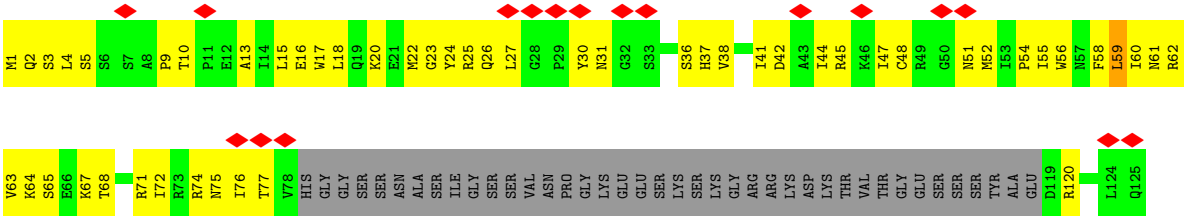
Chain E:

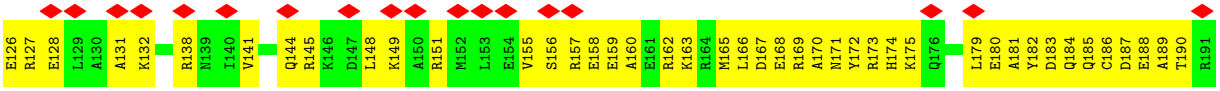


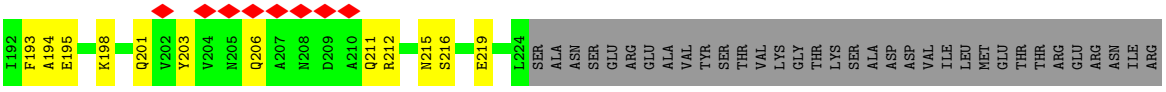


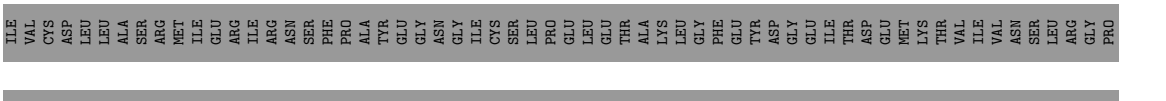
• Molecule 3: AUGMIN subunit 5

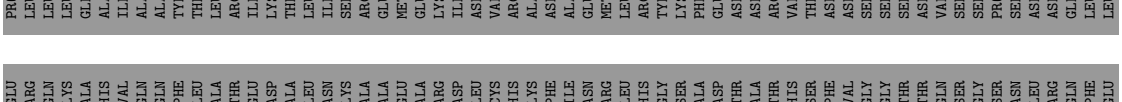
Chain O:

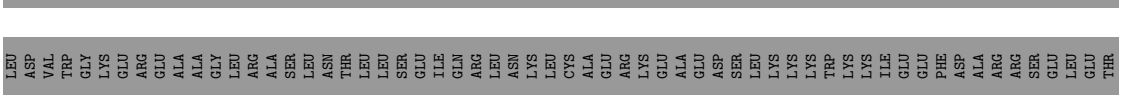


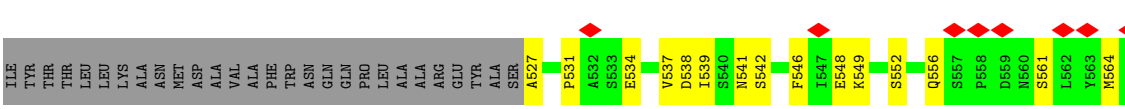


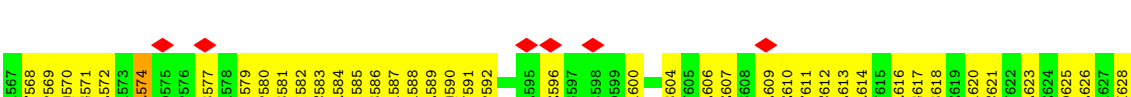






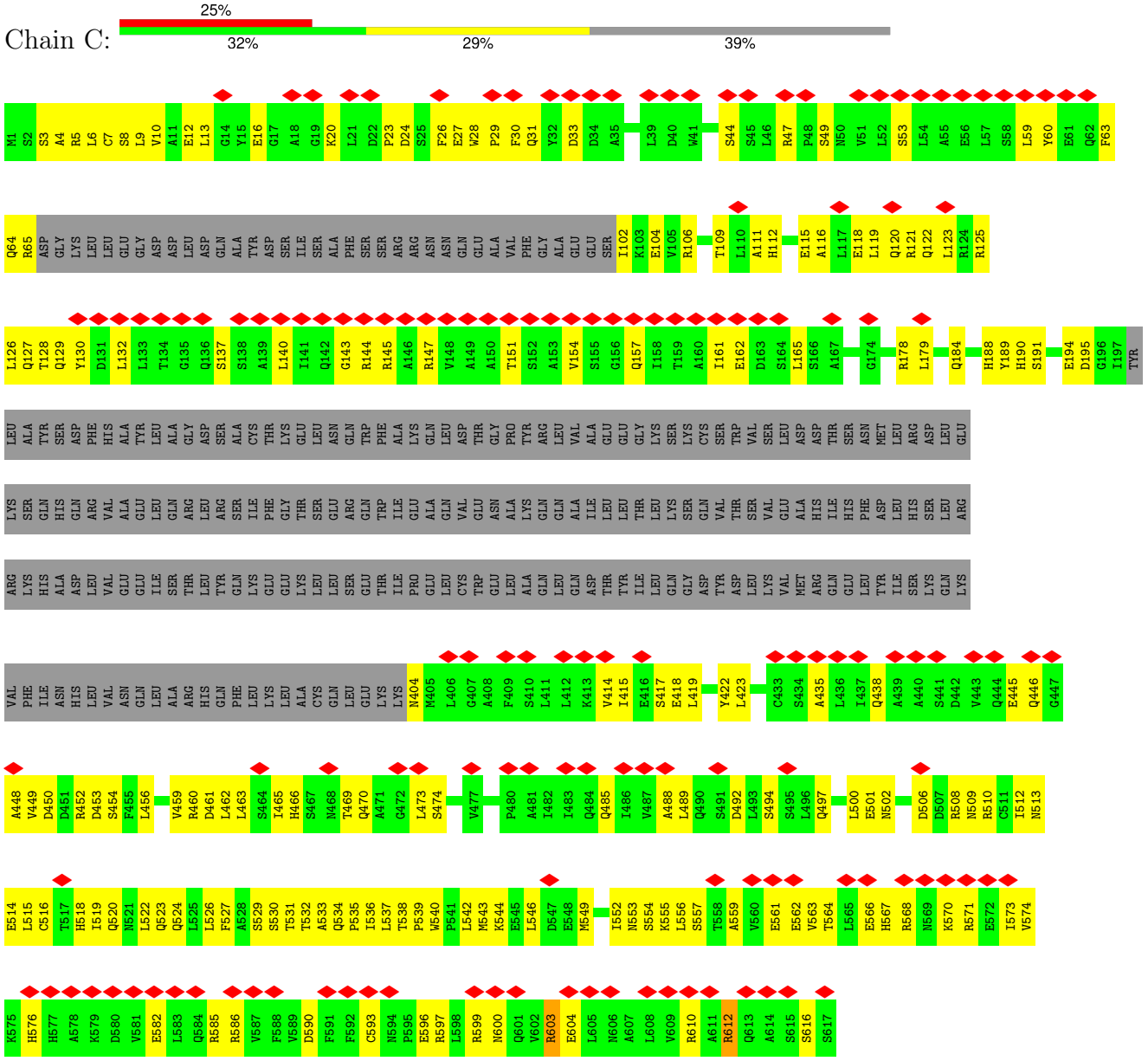






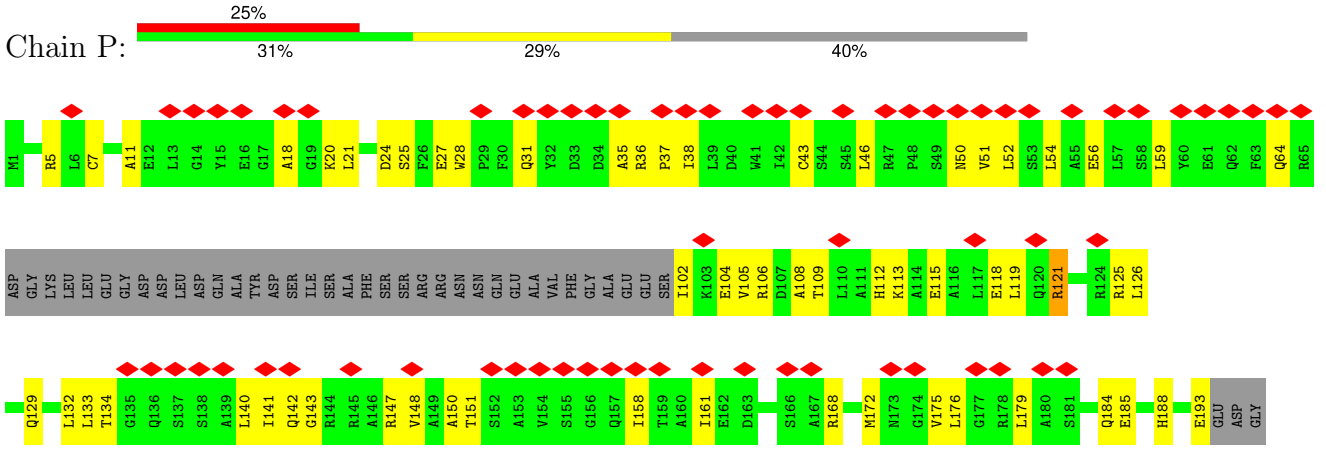
• Molecule 4: AUGMIN subunit 3

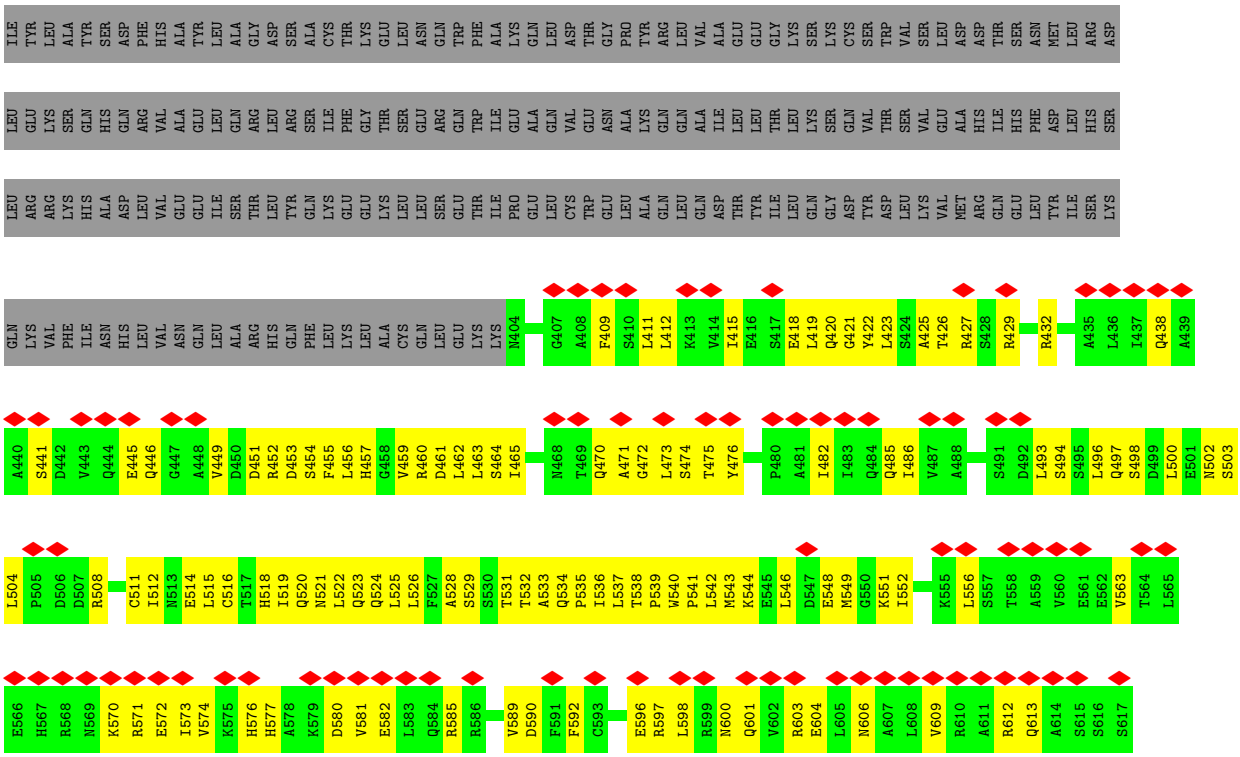
Chain C:



• Molecule 4: AUGMIN subunit 3

Chain P:




ILE TYR LEU ALA TYR SER ASP PHE HIS ALA TYR LEU ALA GLY ASP SER ALA CYS THR LYS GLU LEU ASN GLN TRP PHE ALA LYS GLN LEU ASP THR GLY PRO TYR ARG LEU VAL ALA GLU GLY SER ASP THR SER ASN MET LEU ARG ASP
LEU GLU LYS SER GLN HIS GLN ARG VAL ALA GLU GLU LEU GLN ARG LEU ARG SER ILE PHE GLY THR SER GLU ARG GLN THR ILE GLU ALA GLN VAL GLU ASN ALA LYS GLN LEU GLN GLN ALA ILE LEU LEU THR LEU LYS SER GLN VAL THR SER VAL GLU ALA HIS ILE HIS PHE ASP LEU HIS SER
LEU ARG ARG LYS HIS ALA ASP LEU VAL GLU GLU ILE SER THR LEU TYR GLN LYS GLU GLU LYS LEU LEU SER GLU ARG GLN THR ILE PRO GLU ALA LEU CYS TRP GLU LEU ALA GLN LEU GLN ASP ALA ILE LEU GLN ASP THR TYR ILE LEU GLN GLY ASP TYR ASP LEU LYS VAL MET ARG GLN GLU LEU TYR ILE SER LYS
GLN LYS VAL PHE ILE ASN HIS LEU VAL ASN GLN LEU ALA ARG HIS GLN PHE LEU LYS LEU ALA CYS GLN LEU GLU LYS LYS N404 G407 A408 F409 S410 L411 L412 K413 V414 I415 E416 S417 E418 L419 Q420 G421 Y422 L423 S424 A425 T426 R427 S428 R429 R432 A435 L436 I437 Q438 A439
A440 S441 D442 V443 Q444 E445 Q446 G447 A448 V449 D450 D451 R452 D453 S454 F455 L456 H457 G458 V459 R460 D461 L462 L463 S464 I465 N468 T469 Q470 A471 G472 L473 S474 T475 Y476 P480 A481 I482 I483 Q484 Q485 I486 V487 A488 S491 D492 L493 S494 S495 L496 Q497 S498 D499 L500 E501 N502 S503
L504 P505 D506 D507 R508 C511 I512 N513 E514 L515 C516 T517 H518 I519 Q520 N521 L522 Q523 Q524 L525 L526 F527 A528 S529 S530 T531 T532 A533 Q534 P535 I536 L537 T538 P539 W540 P541 L542 M543 K544 E545 L546 D547 E548 M549 G550 K551 I552 K555 L556 S557 T558 A559 V560 E561 E562 V563 T564 L565
E566 H567 R568 N569 K570 R571 E572 I573 V574 K575 H576 H577 A578 K579 D580 V581 E582 L583 Q584 R585 R586 V589 D590 F591 F592 C593 E596 R597 L598 R599 N600 Q601 V602 R603 E604 L605 N606 A607 L608 V609 R610 A611 R612 Q613 A614 S615 S616 S617

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	6578	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	337.91998, 337.91998, 337.91998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87999994, 0.87999994, 0.87999994	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/2265	0.54	0/3054
1	M	0.24	0/2265	0.53	0/3054
2	D	0.26	0/2934	0.54	3/3965 (0.1%)
2	N	0.25	0/2934	0.54	2/3965 (0.1%)
3	E	0.25	0/3289	0.57	0/4447
3	O	0.25	0/3289	0.56	1/4447 (0.0%)
4	C	0.24	0/2968	0.53	0/4009
4	P	0.24	0/2939	0.54	0/3970
All	All	0.25	0/22883	0.54	6/30911 (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
2	D	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	59	LEU	CB-CG-CD2	-7.20	98.76	111.00
2	D	102	PRO	N-CA-CB	6.08	110.59	103.30
2	N	102	PRO	N-CA-CB	6.02	110.53	103.30
2	D	94	PRO	N-CA-CB	5.79	110.25	103.30
2	N	94	PRO	N-CA-CB	5.56	109.97	103.30
2	D	363	LEU	CA-CB-CG	5.23	127.32	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	326	CYS	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	2235	0	2261	230	0
1	M	2235	0	2261	242	0
2	D	2890	0	2806	272	0
2	N	2890	0	2806	278	0
3	E	3236	0	3202	310	0
3	O	3236	0	3202	303	0
4	C	2930	0	2921	214	0
4	P	2901	0	2897	217	0
All	All	22553	0	22356	1522	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 (1522) 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:N:24:GLU:HA	2:N:27:CYS:HB2	1.48	0.94
1:M:125:ASP:HB2	3:O:585:ILE:HB	1.49	0.94
2:D:422:HIS:HB2	3:E:20:LYS:HD2	1.54	0.89
1:M:239:HIS:HE2	3:O:64:LYS:HG2	1.37	0.88
2:D:314:GLN:HA	2:D:317:TYR:HB3	1.53	0.88
2:D:248:SER:HB2	4:C:132:LEU:HD23	1.58	0.85
2:D:63:ILE:HA	2:D:67:ALA:HB3	1.55	0.85
3:E:53:ILE:HA	3:E:56:TRP:HB2	1.58	0.84
1:A:233:LEU:HA	1:A:236:MET:HG2	1.61	0.83
2:D:39:VAL:HA	2:D:42:ASP:HB2	1.60	0.83
4:P:5:ARG:NH2	4:P:27:GLU:OE2	2.12	0.83
1:A:289:LEU:HB2	2:D:366:ALA:HB3	1.61	0.83
1:M:176:ILE:HA	1:M:179:GLN:HE21	1.40	0.82
1:M:236:MET:HE3	1:M:289:LEU:HD23	1.63	0.81
3:O:195:GLU:HB2	4:P:411:LEU:HD22	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:O	1:A:48:HIS:ND1	2.13	0.80
3:O:1:MET:SD	3:O:62:ARG:NH1	2.55	0.80
2:D:43:LEU:HD13	3:E:628:LYS:HE3	1.64	0.79
3:E:606:LEU:HD21	4:C:489:LEU:HD13	1.65	0.78
1:A:119:ASN:HB3	1:A:123:ILE:HB	1.65	0.78
2:N:363:LEU:HD12	2:N:366:ALA:HB2	1.65	0.78
2:N:63:ILE:HG22	2:N:68:VAL:HG23	1.65	0.78
1:M:138:ILE:HD12	3:O:623:LEU:HD21	1.66	0.78
3:O:41:ILE:HA	3:O:44:ILE:HB	1.64	0.77
1:M:120:LEU:HD22	2:N:54:ARG:HG3	1.66	0.77
3:O:579:ILE:HG21	4:P:451:ASP:HB3	1.66	0.77
1:A:78:LYS:HA	3:E:580:PRO:HB3	1.67	0.77
3:O:584:ARG:HH12	4:P:456:LEU:HD12	1.50	0.76
1:M:88:ARG:NH2	2:N:109:GLU:OE2	2.17	0.76
4:C:116:ALA:O	4:C:120:GLN:NE2	2.19	0.76
3:E:530:ILE:HG13	3:E:531:PRO:HD3	1.67	0.76
3:E:678:GLN:HB2	3:E:681:PRO:HG2	1.67	0.76
2:N:106:GLU:OE1	3:O:173:ARG:NH2	2.18	0.76
1:A:128:LEU:HD23	1:A:132:LEU:HD22	1.68	0.76
1:A:123:ILE:O	2:D:54:ARG:NH2	2.19	0.75
2:N:278:ARG:HG3	3:O:636:ARG:HD3	1.66	0.75
3:O:55:ILE:HG21	3:O:65:SER:HB3	1.68	0.75
2:D:70:MET:SD	2:D:230:ARG:NH2	2.54	0.75
3:E:149:LYS:HZ1	3:E:614:ARG:HB3	1.52	0.75
1:A:128:LEU:HD22	3:E:156:SER:HB3	1.69	0.75
2:N:63:ILE:HA	2:N:67:ALA:HB3	1.68	0.75
1:M:288:VAL:HB	2:N:363:LEU:HG	1.69	0.75
1:A:145:VAL:HB	2:D:277:LEU:HD11	1.68	0.74
1:M:248:LYS:HG3	1:M:249:PRO:HD3	1.69	0.74
3:E:539:ILE:HG22	4:C:179:LEU:HD21	1.69	0.74
1:M:124:ARG:HG3	3:O:585:ILE:HD13	1.70	0.74
2:N:39:VAL:HG12	2:N:45:LEU:HB3	1.70	0.74
2:N:309:LEU:O	2:N:315:HIS:ND1	2.20	0.74
1:M:81:GLU:O	3:O:574:ARG:NH2	2.20	0.74
2:D:71:VAL:O	2:D:75:GLN:N	2.16	0.74
2:D:49:GLU:HA	2:D:52:ARG:HE	1.53	0.73
2:D:318:ASN:ND2	4:C:534:GLN:OE1	2.21	0.73
2:N:363:LEU:HA	2:N:365:GLU:HG2	1.69	0.73
1:M:137:ASP:O	1:M:141:ARG:N	2.22	0.73
2:D:15:ASP:HA	2:D:18:GLN:HB3	1.71	0.72
1:A:230:HIS:O	3:E:71:ARG:NH1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:583:CYS:SG	4:P:453:ASP:N	2.61	0.72
4:P:536:ILE:HG23	4:P:540:TRP:HB3	1.71	0.72
4:P:516:CYS:O	4:P:520:GLN:NE2	2.21	0.72
2:N:116:GLU:OE1	2:N:119:GLN:NE2	2.20	0.72
3:E:586:SER:HA	3:E:589:LEU:HB3	1.71	0.72
3:O:712:ALA:HB3	4:P:563:VAL:HB	1.72	0.72
1:A:134:ALA:HA	1:A:138:ILE:HB	1.72	0.72
3:O:585:ILE:HG13	3:O:586:SER:H	1.54	0.72
3:E:48:CYS:O	3:E:56:TRP:NE1	2.23	0.71
3:E:171:ASN:HB3	3:E:174:HIS:HD2	1.55	0.71
1:M:58:ALA:HA	2:N:31:ASP:H	1.55	0.71
2:D:278:ARG:O	2:D:282:TYR:N	2.23	0.71
1:A:137:ASP:O	1:A:141:ARG:N	2.23	0.71
2:D:70:MET:HB3	2:D:230:ARG:HE	1.56	0.71
1:M:166:ALA:HB1	1:M:170:LEU:HB2	1.72	0.71
1:M:77:LEU:HD13	3:O:580:PRO:HG2	1.73	0.71
2:D:320:MET:O	2:D:324:TRP:N	2.22	0.71
3:O:637:GLN:HA	3:O:640:VAL:HG23	1.73	0.71
1:M:86:ALA:HB2	2:N:56:ARG:HB3	1.70	0.71
2:N:380:ARG:NH2	2:N:384:TYR:OH	2.24	0.71
1:A:142:LYS:NZ	2:D:269:GLU:OE2	2.24	0.70
3:E:62:ARG:HA	3:E:68:THR:HG21	1.71	0.70
4:P:508:ARG:NE	4:P:511:CYS:SG	2.63	0.70
1:A:80:SER:HA	1:A:83:ARG:HH21	1.55	0.70
1:A:232:GLU:OE1	3:E:61:ASN:ND2	2.24	0.70
2:N:65:CYS:SG	4:P:147:ARG:NH2	2.65	0.70
1:A:84:ALA:HB1	3:E:570:GLN:HG3	1.72	0.70
1:A:148:LYS:HB2	3:E:145:ARG:HH22	1.56	0.70
2:D:276:ALA:HA	2:D:279:GLU:HB2	1.74	0.70
3:O:62:ARG:NH1	4:P:27:GLU:OE1	2.24	0.70
1:M:99:SER:HA	2:N:216:MET:HG2	1.73	0.70
4:C:533:ALA:HA	4:C:537:LEU:HB2	1.73	0.70
2:N:423:ASP:HA	3:O:64:LYS:HG3	1.73	0.70
1:A:264:LYS:HE3	2:D:397:GLN:HE22	1.55	0.70
1:M:147:GLU:OE2	3:O:145:ARG:NH2	2.24	0.70
2:D:58:LEU:HA	2:D:61:MET:HG2	1.72	0.69
1:M:247:THR:HA	1:M:250:VAL:HB	1.73	0.69
3:E:1:MET:O	3:E:5:SER:OG	2.10	0.69
3:E:76:ILE:HD12	4:C:4:ALA:HB3	1.74	0.69
4:P:577:HIS:HA	4:P:580:ASP:HB3	1.74	0.69
2:D:244:ASP:O	2:D:248:SER:OG	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:680:LEU:HD12	3:E:684:ARG:HH12	1.58	0.69
2:N:293:ASN:OD1	2:N:294:VAL:N	2.25	0.69
4:C:10:VAL:HA	4:C:13:LEU:HB3	1.75	0.68
4:C:539:PRO:HG2	4:C:543:MET:HE3	1.76	0.68
2:D:50:MET:O	2:D:54:ARG:N	2.24	0.68
2:D:243:VAL:HA	2:D:262:ARG:HG2	1.75	0.68
2:D:271:GLU:O	2:D:275:ALA:N	2.24	0.68
1:M:129:SER:O	1:M:133:VAL:N	2.26	0.68
1:A:127:GLU:HB3	2:D:238:LEU:HD22	1.74	0.68
3:E:41:ILE:HA	3:E:44:ILE:HG22	1.74	0.68
1:A:26:VAL:O	1:A:30:LEU:N	2.23	0.68
1:A:166:ALA:HB1	2:D:298:ILE:HD13	1.76	0.68
1:M:149:ARG:NH2	4:P:118:GLU:O	2.27	0.68
3:O:566:PRO:O	3:O:572:LEU:N	2.27	0.68
1:A:237:ALA:O	1:A:241:LYS:N	2.25	0.68
1:A:292:ALA:HB2	2:D:364:VAL:HG11	1.76	0.68
2:D:396:ARG:NH1	2:D:396:ARG:O	2.27	0.68
2:D:39:VAL:HG21	3:E:630:ILE:HB	1.74	0.68
2:D:276:ALA:O	4:C:121:ARG:NH2	2.27	0.68
3:O:165:MET:HA	4:P:147:ARG:HB3	1.76	0.68
4:P:528:ALA:O	4:P:532:THR:OG1	2.10	0.68
3:O:17:TRP:HE1	3:O:63:VAL:HG21	1.59	0.67
3:O:737:LEU:HD23	4:P:582:GLU:HB3	1.76	0.67
1:A:224:TYR:O	1:A:231:ARG:NH2	2.27	0.67
2:D:102:PRO:HA	2:D:105:TYR:HB3	1.75	0.67
2:N:360:ARG:O	2:N:360:ARG:NH1	2.25	0.67
4:P:518:HIS:O	4:P:522:LEU:N	2.22	0.67
2:D:120:LYS:HA	2:D:123:LEU:HD23	1.76	0.67
3:E:653:ALA:HA	3:E:657:TYR:HB2	1.76	0.67
4:C:23:PRO:HA	4:C:26:PHE:HB3	1.75	0.67
1:M:73:ASN:ND2	2:N:42:ASP:O	2.26	0.67
3:O:175:LYS:O	3:O:179:LEU:N	2.26	0.67
2:N:281:LEU:HD22	3:O:636:ARG:HH22	1.58	0.67
3:E:590:GLN:HB3	3:E:597:GLY:HA3	1.77	0.67
3:E:641:GLU:O	3:E:645:SER:N	2.28	0.67
2:D:277:LEU:HD23	2:D:278:ARG:HH11	1.60	0.67
1:M:228:ILE:O	3:O:62:ARG:NH2	2.26	0.67
1:M:235:GLU:OE2	3:O:68:THR:OG1	2.11	0.67
3:O:539:ILE:HD11	4:P:176:LEU:HG	1.75	0.67
1:A:144:GLY:O	3:E:145:ARG:NH2	2.27	0.67
1:M:229:SER:HB2	4:P:25:SER:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:264:LYS:HB3	1:M:267:ALA:HB3	1.77	0.67
3:E:159:GLU:OE2	3:E:163:LYS:NZ	2.27	0.66
2:N:311:LEU:HD23	4:P:534:GLN:NE2	2.11	0.66
1:A:149:ARG:NH2	2:D:277:LEU:O	2.28	0.66
1:A:289:LEU:HG	2:D:364:VAL:HB	1.77	0.66
2:N:274:GLU:HB3	2:N:278:ARG:HD3	1.78	0.66
4:P:168:ARG:O	4:P:172:MET:N	2.24	0.66
1:A:81:GLU:O	1:A:85:GLN:NE2	2.29	0.66
1:M:224:TYR:O	1:M:228:ILE:N	2.27	0.66
1:M:170:LEU:HA	1:M:173:LEU:HB2	1.76	0.66
1:A:132:LEU:HD12	3:E:587:ALA:HB3	1.78	0.66
1:A:180:LEU:HD13	2:D:310:LYS:HE2	1.78	0.66
3:O:144:GLN:HB2	4:P:126:LEU:HD13	1.76	0.66
3:E:538:ASP:HB3	4:C:415:ILE:HG21	1.76	0.66
1:M:145:VAL:HG21	2:N:277:LEU:HD23	1.77	0.66
3:E:165:MET:HG3	4:C:147:ARG:HD2	1.76	0.65
3:E:127:ARG:HB2	4:C:109:THR:HG22	1.78	0.65
3:E:583:CYS:HB2	4:C:449:VAL:HG13	1.77	0.65
3:O:648:ASP:O	3:O:652:ARG:N	2.23	0.65
2:N:339:LEU:HD12	3:O:705:ASP:HB3	1.78	0.65
1:A:126:THR:HG22	3:E:159:GLU:HB2	1.77	0.65
2:D:311:LEU:HD22	4:C:534:GLN:HG3	1.78	0.65
2:D:415:VAL:O	3:E:19:GLN:NE2	2.29	0.65
3:O:163:LYS:HB3	3:O:571:GLY:HA2	1.77	0.65
3:O:613:LEU:HD13	3:O:616:ARG:HD3	1.78	0.65
4:P:504:LEU:HD13	4:P:508:ARG:HH11	1.61	0.65
1:M:21:ALA:HB2	1:M:58:ALA:HB1	1.78	0.65
4:P:522:LEU:HD23	4:P:526:LEU:HD23	1.79	0.65
2:D:62:ALA:HA	2:D:234:LYS:HB3	1.79	0.65
3:E:55:ILE:HG22	3:E:63:VAL:HA	1.79	0.65
3:E:666:ASP:O	3:E:670:GLU:N	2.30	0.65
1:A:125:ASP:HB2	3:E:159:GLU:HG2	1.78	0.65
1:A:180:LEU:HD12	2:D:310:LYS:HG2	1.79	0.65
1:A:235:GLU:HA	1:A:238:GLU:HB2	1.77	0.65
3:E:586:SER:HB3	3:E:590:GLN:HG2	1.78	0.65
1:M:278:PHE:HB3	2:N:376:LYS:HB2	1.79	0.65
1:M:90:ARG:HH12	2:N:56:ARG:HD3	1.61	0.65
3:O:158:GLU:OE2	3:O:162:ARG:NE	2.27	0.65
1:M:184:VAL:O	1:M:188:GLU:N	2.27	0.64
1:M:283:LYS:HE2	1:M:286:GLU:HG3	1.78	0.64
1:M:247:THR:O	1:M:251:LEU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HE	2:D:30:PRO:HG2	1.61	0.64
3:O:145:ARG:NH1	3:O:611:PHE:O	2.30	0.64
1:A:232:GLU:OE2	1:A:239:HIS:NE2	2.29	0.64
3:O:185:GLN:HB2	4:P:425:ALA:HB1	1.79	0.64
1:A:170:LEU:HB2	2:D:297:GLN:HB2	1.78	0.64
3:O:1:MET:N	4:P:24:ASP:OD1	2.30	0.64
1:A:112:GLN:HA	1:A:115:ALA:HB3	1.79	0.64
1:M:179:GLN:HE22	1:M:180:LEU:HG	1.62	0.64
3:O:76:ILE:HD13	4:P:5:ARG:HG3	1.80	0.64
1:A:190:GLN:HA	1:A:194:TRP:HB3	1.80	0.64
1:A:76:ARG:HA	4:C:452:ARG:HH21	1.62	0.64
1:A:154:LYS:O	1:A:158:ALA:N	2.25	0.64
4:P:590:ASP:OD1	4:P:597:ARG:NH2	2.26	0.64
1:M:239:HIS:NE2	3:O:64:LYS:HG2	2.12	0.64
1:A:145:VAL:HG12	1:A:149:ARG:HD2	1.80	0.63
2:D:344:LEU:HG	2:D:345:LEU:HD22	1.80	0.63
3:E:158:GLU:O	3:E:162:ARG:N	2.31	0.63
3:E:654:GLN:HA	3:E:658:GLU:HB3	1.80	0.63
1:A:121:LEU:HD22	2:D:47:ARG:HD2	1.79	0.63
3:E:62:ARG:NH2	4:C:8:SER:OG	2.31	0.63
4:C:529:SER:O	4:C:533:ALA:N	2.29	0.63
1:M:253:THR:OG1	2:N:407:ASN:ND2	2.32	0.63
2:N:307:LYS:HD2	3:O:660:THR:HB	1.80	0.63
2:D:344:LEU:HD22	3:E:701:ARG:HH21	1.63	0.63
1:M:120:LEU:HA	1:M:123:ILE:HB	1.80	0.63
2:N:109:GLU:HB3	3:O:173:ARG:HG3	1.78	0.63
2:N:317:TYR:O	2:N:321:GLN:N	2.31	0.63
2:N:415:VAL:O	2:N:419:LEU:HG	1.98	0.63
3:O:54:PRO:HG2	3:O:55:ILE:HD12	1.80	0.63
4:P:508:ARG:HE	4:P:511:CYS:HG	1.46	0.63
2:D:205:TYR:HA	2:D:208:LEU:HD12	1.79	0.63
3:E:6:SER:HB3	4:C:16:GLU:HG3	1.80	0.63
4:C:65:ARG:O	4:C:65:ARG:NH1	2.26	0.63
1:M:114:LEU:HD11	2:N:58:LEU:HB3	1.80	0.63
1:M:239:HIS:O	1:M:243:LEU:N	2.26	0.63
3:O:625:ASP:O	3:O:629:ALA:N	2.30	0.63
1:A:162:TYR:O	4:C:520:GLN:NE2	2.31	0.63
2:D:302:LEU:HB2	3:E:661:THR:HG22	1.81	0.63
1:M:169:ARG:HA	4:P:523:GLN:HG3	1.80	0.63
2:N:236:ASP:O	2:N:240:ASP:N	2.30	0.63
3:E:61:ASN:O	3:E:71:ARG:NH2	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1:MET:HA	3:E:60:ILE:HD11	1.80	0.63
3:O:156:SER:HA	3:O:588:ALA:HB1	1.81	0.63
3:O:679:TRP:HE1	4:P:541:PRO:HG3	1.62	0.63
2:D:340:GLU:HA	3:E:705:ASP:HB3	1.79	0.62
1:M:260:LEU:O	1:M:264:LYS:N	2.32	0.62
3:E:37:HIS:O	3:E:41:ILE:N	2.27	0.62
4:P:43:CYS:HA	4:P:46:LEU:HD23	1.80	0.62
2:D:47:ARG:NE	2:D:50:MET:SD	2.72	0.62
3:E:68:THR:OG1	3:E:71:ARG:NH2	2.33	0.62
3:E:654:GLN:NE2	4:C:514:GLU:OE2	2.32	0.62
1:M:180:LEU:HD12	2:N:310:LYS:HE2	1.82	0.62
4:P:536:ILE:O	4:P:540:TRP:N	2.33	0.62
3:E:6:SER:H	4:C:20:LYS:HE2	1.64	0.62
3:E:135:GLU:OE2	3:E:138:ARG:NH1	2.32	0.62
2:N:113:VAL:HA	2:N:139:LYS:HD2	1.81	0.62
3:E:59:LEU:O	3:E:61:ASN:N	2.30	0.62
1:M:149:ARG:HB2	1:M:153:GLN:HE22	1.64	0.62
3:O:1:MET:H2	3:O:60:ILE:HG12	1.62	0.62
3:E:165:MET:SD	3:E:166:LEU:HB2	2.40	0.62
3:E:660:THR:HA	3:E:663:TYR:HB3	1.80	0.62
1:M:156:SER:O	1:M:160:LEU:N	2.30	0.62
2:N:70:MET:HE3	2:N:226:GLU:HB3	1.80	0.62
3:O:151:ARG:HG2	4:P:134:THR:HA	1.81	0.62
1:A:130:SER:O	1:A:135:MET:N	2.29	0.62
1:M:274:LYS:HE3	2:N:379:THR:HB	1.82	0.62
4:P:457:HIS:ND1	4:P:474:SER:OG	2.29	0.62
3:E:52:MET:O	3:E:56:TRP:N	2.31	0.61
2:N:333:ASN:OD1	2:N:334:ALA:N	2.33	0.61
3:O:77:THR:HG23	4:P:52:LEU:HG	1.82	0.61
1:A:125:ASP:OD1	1:A:129:SER:N	2.32	0.61
2:D:340:GLU:OE1	3:E:696:HIS:ND1	2.34	0.61
4:C:596:GLU:HG3	4:C:599:ARG:HH11	1.65	0.61
1:M:62:GLN:HA	1:M:65:SER:HB2	1.80	0.61
3:O:71:ARG:O	3:O:75:ASN:ND2	2.32	0.61
4:P:534:GLN:HG3	4:P:535:PRO:HD3	1.81	0.61
1:A:153:GLN:NE2	4:C:501:GLU:OE2	2.33	0.61
1:M:135:MET:SD	4:P:129:GLN:NE2	2.66	0.61
3:O:630:ILE:HA	3:O:633:VAL:HG22	1.82	0.61
2:D:380:ARG:NE	2:D:383:GLU:OE1	2.32	0.61
4:C:533:ALA:O	4:C:538:THR:N	2.25	0.61
1:M:143:THR:HA	1:M:146:GLU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:MET:HB3	2:D:238:LEU:HD12	1.83	0.61
1:M:236:MET:O	1:M:240:ARG:NH1	2.33	0.61
2:D:132:ILE:O	2:D:136:GLU:N	2.30	0.61
1:M:120:LEU:HD21	2:N:58:LEU:HD22	1.82	0.61
1:M:150:ALA:O	3:O:138:ARG:NH2	2.33	0.61
1:M:157:ASN:HA	1:M:160:LEU:HB3	1.82	0.61
1:A:183:ASP:HB3	2:D:310:LYS:HZ1	1.66	0.61
1:A:227:LYS:HG2	1:A:232:GLU:HB2	1.82	0.61
3:E:186:CYS:SG	3:E:549:LYS:NZ	2.65	0.61
1:A:124:ARG:HH22	3:E:624:GLU:HB3	1.66	0.61
3:O:5:SER:HB2	3:O:59:LEU:HD23	1.81	0.61
1:M:254:LEU:HA	1:M:257:TYR:HB2	1.82	0.60
2:N:102:PRO:O	2:N:106:GLU:HG2	2.00	0.60
2:N:344:LEU:HB2	3:O:701:ARG:HD2	1.83	0.60
2:D:422:HIS:O	3:E:20:LYS:NZ	2.33	0.60
2:N:33:SER:HA	4:P:471:ALA:HB3	1.82	0.60
4:P:609:VAL:HB	4:P:613:GLN:HE22	1.65	0.60
1:A:164:ARG:NH1	2:D:287:LYS:O	2.35	0.60
1:M:123:ILE:HG23	1:M:127:GLU:HG3	1.83	0.60
1:M:231:ARG:HA	1:M:234:VAL:HG12	1.83	0.60
1:M:246:MET:HA	2:N:417:MET:HE1	1.82	0.60
2:N:278:ARG:HE	3:O:636:ARG:HB2	1.67	0.60
3:O:13:ALA:HB1	3:O:16:GLU:HB2	1.84	0.60
4:C:102:ILE:N	4:C:104:GLU:OE1	2.34	0.60
2:D:367:THR:OG1	2:D:422:HIS:O	2.19	0.60
1:M:54:LEU:HD21	2:N:27:CYS:SG	2.42	0.60
3:O:44:ILE:HA	3:O:47:ILE:HG22	1.82	0.60
3:O:542:SER:O	3:O:546:PHE:N	2.34	0.60
2:D:295:LEU:O	2:D:299:LEU:N	2.34	0.60
4:P:464:SER:HB3	4:P:470:GLN:HB2	1.83	0.60
1:A:23:ILE:HA	1:A:26:VAL:HB	1.84	0.60
1:A:245:LYS:HG2	2:D:420:LYS:HB2	1.82	0.60
2:D:242:ILE:HD11	2:D:263:VAL:HB	1.83	0.60
2:N:10:GLN:HB3	3:O:647:LEU:HG	1.84	0.60
3:O:26:GLN:NE2	3:O:48:CYS:SG	2.71	0.60
1:M:146:GLU:OE2	4:P:121:ARG:NH1	2.34	0.60
1:M:148:LYS:NZ	3:O:612:CYS:SG	2.72	0.60
2:N:259:LEU:HD23	2:N:260:PRO:HD3	1.84	0.60
3:O:59:LEU:HB2	4:P:11:ALA:HB1	1.82	0.60
3:O:215:ASN:O	3:O:219:GLU:N	2.33	0.60
2:N:111:ARG:NH1	2:N:116:GLU:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:4:ALA:O	4:C:31:GLN:NE2	2.35	0.59
2:N:314:GLN:NE2	4:P:534:GLN:O	2.34	0.59
1:A:94:GLU:OE1	2:D:111:ARG:NH2	2.33	0.59
1:A:139:SER:OG	2:D:245:ASP:OD1	2.20	0.59
1:A:164:ARG:NH2	2:D:290:GLU:OE1	2.34	0.59
2:N:240:ASP:OD1	2:N:258:ARG:NH1	2.35	0.59
3:O:652:ARG:NH1	3:O:655:GLN:OE1	2.35	0.59
2:D:261:GLU:HA	2:D:264:LYS:HE3	1.84	0.59
1:M:149:ARG:NH1	2:N:276:ALA:O	2.33	0.59
3:O:609:LEU:O	4:P:497:GLN:NE2	2.32	0.59
1:A:285:LEU:HB3	2:D:366:ALA:HB1	1.84	0.59
1:M:257:TYR:OH	2:N:383:GLU:OE2	2.21	0.59
3:E:161:GLU:O	3:E:165:MET:N	2.35	0.59
3:E:657:TYR:O	3:E:661:THR:HG23	2.03	0.59
1:A:224:TYR:OH	4:C:28:TRP:O	2.20	0.59
3:E:63:VAL:O	3:E:65:SER:N	2.34	0.59
3:E:640:VAL:HG13	4:C:500:LEU:HD13	1.84	0.59
4:C:553:ASN:HA	4:C:556:LEU:HD13	1.85	0.59
1:M:124:ARG:HH22	2:N:47:ARG:HB2	1.67	0.59
1:A:60:ALA:HA	1:A:63:ALA:HB3	1.85	0.59
1:A:89:ILE:HG21	2:D:60:ALA:HA	1.83	0.59
3:E:203:TYR:HE2	4:C:178:ARG:HB3	1.67	0.59
4:P:412:LEU:HA	4:P:415:ILE:HD12	1.85	0.59
4:P:526:LEU:HA	4:P:529:SER:HB2	1.85	0.59
2:N:423:ASP:OXT	3:O:67:LYS:NZ	2.36	0.59
3:O:27:LEU:HA	3:O:31:ASN:HB2	1.84	0.59
3:E:75:ASN:O	4:C:5:ARG:NH2	2.36	0.59
3:E:137:LEU:HD11	4:C:123:LEU:HD22	1.84	0.59
4:C:555:LYS:O	4:C:559:ALA:N	2.36	0.59
1:M:292:ALA:O	1:M:295:THR:OG1	2.19	0.59
2:N:39:VAL:HA	2:N:45:LEU:HB2	1.84	0.59
3:O:654:GLN:HA	3:O:658:GLU:HB3	1.83	0.59
4:P:415:ILE:O	4:P:419:LEU:N	2.35	0.59
1:A:102:SER:HB2	2:D:223:LEU:HD22	1.82	0.59
1:A:143:THR:O	3:E:144:GLN:NE2	2.36	0.59
1:A:157:ASN:HD21	2:D:287:LYS:HD2	1.68	0.59
1:A:201:MET:O	1:A:205:GLU:N	2.36	0.59
2:D:254:ASN:HD22	2:D:258:ARG:HE	1.48	0.59
4:P:497:GLN:O	4:P:502:ASN:N	2.35	0.59
4:P:512:ILE:O	4:P:516:CYS:N	2.28	0.59
3:E:64:LYS:O	3:E:68:THR:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:584:ARG:NH2	4:C:453:ASP:OD1	2.36	0.58
2:N:272:ARG:NH2	2:N:279:GLU:OE2	2.34	0.58
3:O:159:GLU:O	3:O:163:LYS:HG2	2.03	0.58
1:A:125:ASP:OD2	1:A:128:LEU:HB3	2.03	0.58
2:D:316:LYS:O	2:D:320:MET:N	2.33	0.58
4:C:27:GLU:HA	4:C:30:PHE:CE2	2.38	0.58
1:M:144:GLY:HA2	3:O:145:ARG:HD3	1.85	0.58
2:N:106:GLU:O	3:O:173:ARG:NH1	2.35	0.58
3:O:25:ARG:NH2	3:O:65:SER:OG	2.37	0.58
4:P:463:LEU:HD11	4:P:496:LEU:HD13	1.84	0.58
2:D:285:ASP:OD2	3:E:642:SER:OG	2.21	0.58
3:O:17:TRP:O	3:O:20:LYS:HG2	2.04	0.58
3:O:62:ARG:HB2	3:O:68:THR:HG21	1.85	0.58
3:O:184:GLN:HA	3:O:188:GLU:HB2	1.84	0.58
2:D:21:ASP:OD1	3:E:637:GLN:HG3	2.04	0.58
2:D:314:GLN:O	2:D:318:ASN:ND2	2.35	0.58
3:E:18:LEU:O	3:E:22:MET:N	2.37	0.58
3:E:650:ALA:O	3:E:654:GLN:N	2.36	0.58
4:C:519:ILE:HA	4:C:522:LEU:HD13	1.85	0.58
3:O:699:TYR:HA	3:O:701:ARG:HH21	1.67	0.58
1:A:145:VAL:HG21	3:E:636:ARG:HH22	1.68	0.58
1:M:91:GLU:O	1:M:95:SER:N	2.36	0.58
3:O:581:SER:O	3:O:586:SER:N	2.36	0.58
3:O:742:LYS:NZ	4:P:601:GLN:OE1	2.35	0.58
1:A:81:GLU:HG3	1:A:85:GLN:HE22	1.67	0.58
4:C:3:SER:HA	4:C:6:LEU:HB2	1.84	0.58
3:O:17:TRP:NE1	3:O:63:VAL:HG21	2.18	0.58
3:O:579:ILE:HG22	4:P:452:ARG:HG2	1.86	0.58
1:A:128:LEU:HB2	4:C:140:LEU:HD21	1.85	0.58
2:D:65:CYS:HB2	2:D:234:LYS:HG2	1.86	0.58
4:C:123:LEU:O	4:C:127:GLN:N	2.35	0.58
4:C:539:PRO:O	4:C:543:MET:N	2.35	0.58
4:P:514:GLU:O	4:P:518:HIS:ND1	2.36	0.58
3:E:6:SER:N	4:C:20:LYS:HE2	2.19	0.58
1:A:71:VAL:O	4:C:452:ARG:NH2	2.37	0.58
1:A:84:ALA:O	3:E:570:GLN:NE2	2.33	0.58
2:D:339:LEU:HB3	3:E:711:PRO:HB3	1.85	0.58
3:E:745:LEU:HD11	4:C:597:ARG:HG3	1.86	0.58
3:O:167:ASP:HA	3:O:569:PRO:HG3	1.85	0.58
2:D:28:LEU:HA	2:D:33:SER:HB2	1.86	0.58
4:C:574:VAL:HG13	4:C:612:ARG:HH22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:170:LEU:HG	1:M:173:LEU:HD22	1.85	0.58
4:P:585:ARG:NH1	4:P:590:ASP:OD2	2.30	0.58
2:N:39:VAL:HG21	3:O:626:LEU:HB3	1.85	0.57
4:P:106:ARG:O	4:P:109:THR:OG1	2.22	0.57
2:D:323:THR:O	2:D:327:LYS:N	2.37	0.57
3:E:726:VAL:O	3:E:730:GLN:N	2.37	0.57
1:M:137:ASP:OD1	1:M:138:ILE:N	2.37	0.57
1:M:165:LYS:HA	4:P:104:GLU:HB2	1.86	0.57
2:N:248:SER:HB3	4:P:132:LEU:HD22	1.85	0.57
2:D:269:GLU:O	2:D:273:ASP:N	2.31	0.57
1:M:176:ILE:HG22	2:N:310:LYS:HZ1	1.68	0.57
1:M:250:VAL:HG11	1:M:275:LYS:HE3	1.85	0.57
2:N:302:LEU:HG	2:N:305:LEU:HB2	1.86	0.57
2:N:422:HIS:O	3:O:20:LYS:NZ	2.29	0.57
3:O:55:ILE:HG13	3:O:58:PHE:CE2	2.39	0.57
3:O:165:MET:HG2	3:O:569:PRO:HB2	1.84	0.57
3:O:552:SER:O	3:O:556:GLN:N	2.31	0.57
3:E:561:SER:OG	4:C:157:GLN:NE2	2.36	0.57
4:C:463:LEU:HB3	4:C:492:ASP:HB2	1.86	0.57
1:M:154:LYS:HD2	4:P:115:GLU:HA	1.86	0.57
3:O:159:GLU:O	3:O:163:LYS:N	2.34	0.57
3:O:710:GLN:HB2	3:O:711:PRO:HD3	1.86	0.57
1:A:126:THR:HG23	1:A:127:GLU:H	1.70	0.57
2:D:410:TRP:HA	2:D:413:HIS:CE1	2.39	0.57
3:E:611:PHE:HA	3:E:614:ARG:HG3	1.85	0.57
2:N:135:GLU:OE1	3:O:171:ASN:ND2	2.37	0.57
1:M:235:GLU:HA	1:M:238:GLU:HB2	1.86	0.57
2:D:61:MET:HE2	2:D:64:TYR:HE1	1.68	0.57
3:E:565:LEU:HB3	3:E:566:PRO:HD3	1.85	0.57
1:M:123:ILE:HG13	2:N:242:ILE:HD12	1.87	0.57
2:N:135:GLU:HB2	3:O:174:HIS:HD1	1.70	0.57
3:O:165:MET:HB2	4:P:147:ARG:HD2	1.87	0.57
4:P:109:THR:O	4:P:113:LYS:N	2.23	0.57
4:P:511:CYS:SG	4:P:512:ILE:N	2.77	0.57
1:A:180:LEU:HD11	4:C:531:THR:HA	1.86	0.57
3:O:695:GLU:HA	4:P:59:LEU:HD13	1.87	0.57
1:M:131:PHE:HE2	4:P:140:LEU:HB2	1.69	0.57
3:O:585:ILE:HG13	3:O:586:SER:N	2.20	0.57
3:E:25:ARG:HH22	3:E:65:SER:HB3	1.69	0.56
3:E:610:GLU:HG3	3:E:613:LEU:HB3	1.86	0.56
4:C:459:VAL:HA	4:C:465:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:579:ILE:O	3:E:583:CYS:N	2.29	0.56
1:M:142:LYS:HB3	2:N:273:ASP:HA	1.88	0.56
1:M:148:LYS:NZ	4:P:497:GLN:OE1	2.36	0.56
2:N:314:GLN:O	2:N:318:ASN:N	2.26	0.56
3:O:160:ALA:HA	3:O:589:LEU:HD12	1.87	0.56
3:O:688:GLN:O	3:O:691:GLN:NE2	2.33	0.56
1:A:206:GLU:OE2	1:A:207:GLN:NE2	2.37	0.56
2:D:236:ASP:O	2:D:255:SER:OG	2.22	0.56
4:C:519:ILE:HG23	4:C:520:GLN:HE21	1.70	0.56
1:M:76:ARG:NH2	3:O:577:SER:OG	2.38	0.56
2:N:63:ILE:O	2:N:68:VAL:N	2.37	0.56
1:A:85:GLN:HE21	2:D:57:TYR:HD1	1.54	0.56
1:A:161:ASP:OD2	3:E:127:ARG:NH1	2.38	0.56
1:M:212:TYR:OH	2:N:330:GLU:O	2.22	0.56
3:O:61:ASN:ND2	4:P:24:ASP:OD1	2.38	0.56
3:E:560:ASN:OD1	3:E:561:SER:N	2.38	0.56
3:O:679:TRP:HA	3:O:682:GLU:HB2	1.87	0.56
1:M:232:GLU:HG3	3:O:61:ASN:HB3	1.88	0.56
3:O:646:LEU:HA	3:O:649:HIS:HB2	1.87	0.56
4:C:519:ILE:HD12	4:C:522:LEU:HD22	1.87	0.56
3:O:720:THR:O	3:O:724:GLN:N	2.36	0.56
1:A:239:HIS:HB3	1:A:289:LEU:HD11	1.87	0.56
2:D:36:THR:OG1	2:D:37:LYS:NZ	2.39	0.56
2:D:301:VAL:O	2:D:305:LEU:N	2.39	0.56
3:E:697:CYS:HB2	4:C:59:LEU:HD13	1.88	0.56
2:N:62:ALA:HB1	2:N:231:LEU:HG	1.87	0.56
3:O:587:ALA:HA	3:O:590:GLN:NE2	2.21	0.56
1:A:93:LEU:HA	1:A:107:VAL:HG11	1.86	0.56
2:D:291:TYR:O	2:D:295:LEU:HB2	2.06	0.56
1:M:116:ASN:HD21	2:N:239:ALA:HB1	1.71	0.56
2:N:111:ARG:HG3	2:N:116:GLU:HB2	1.87	0.56
3:O:654:GLN:HB2	4:P:515:LEU:HD21	1.88	0.56
2:D:112:LEU:HD21	2:D:121:LEU:HD13	1.87	0.55
2:D:278:ARG:CZ	3:E:636:ARG:HB2	2.36	0.55
3:E:21:GLU:HG2	3:E:63:VAL:O	2.07	0.55
1:M:126:THR:HG21	3:O:162:ARG:HG2	1.87	0.55
2:N:317:TYR:HD2	2:N:321:GLN:HB3	1.71	0.55
3:O:193:PHE:O	3:O:198:LYS:N	2.39	0.55
3:O:568:THR:O	3:O:574:ARG:NH1	2.38	0.55
1:A:164:ARG:HE	1:A:167:ILE:HD11	1.71	0.55
4:C:445:GLU:HG3	4:C:449:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:600:ASN:HB3	4:C:604:GLU:HB3	1.88	0.55
1:M:20:ALA:O	1:M:24:SER:OG	2.19	0.55
1:M:177:LEU:HD11	3:O:664:CYS:SG	2.46	0.55
2:N:419:LEU:HD21	3:O:23:GLY:HA3	1.87	0.55
3:O:156:SER:HB3	3:O:592:PRO:HD3	1.88	0.55
4:P:184:GLN:O	4:P:188:HIS:ND1	2.36	0.55
1:A:68:ALA:HA	1:A:72:ALA:HB3	1.88	0.55
2:D:366:ALA:O	2:D:370:ALA:N	2.38	0.55
3:E:59:LEU:H	3:E:63:VAL:HB	1.71	0.55
1:M:88:ARG:HE	3:O:170:ALA:H	1.54	0.55
1:M:133:VAL:HG22	3:O:623:LEU:HD13	1.88	0.55
3:E:51:ASN:OD1	3:E:52:MET:N	2.40	0.55
2:N:419:LEU:HD22	3:O:20:LYS:HA	1.88	0.55
4:P:419:LEU:O	4:P:423:LEU:N	2.39	0.55
2:D:105:TYR:OH	3:E:170:ALA:O	2.24	0.55
3:E:617:GLY:O	4:C:460:ARG:NE	2.40	0.55
4:C:612:ARG:O	4:C:612:ARG:NH1	2.37	0.55
1:M:169:ARG:HH21	3:O:120:ARG:HH22	1.54	0.55
3:O:527:ALA:N	4:P:193:GLU:OE1	2.40	0.55
4:P:512:ILE:HA	4:P:515:LEU:HB2	1.88	0.55
2:N:107:THR:HG21	2:N:211:THR:HG21	1.89	0.55
2:N:199:THR:HG21	4:P:421:GLY:HA2	1.89	0.55
4:P:533:ALA:HA	4:P:537:LEU:HB2	1.87	0.55
1:A:91:GLU:HG3	3:E:171:ASN:HD21	1.71	0.55
2:D:332:MET:HA	2:D:335:LYS:HB2	1.88	0.55
3:E:1:MET:N	4:C:24:ASP:OD1	2.36	0.55
4:C:469:THR:HA	4:C:473:LEU:HB2	1.88	0.55
2:N:315:HIS:ND1	4:P:534:GLN:OE1	2.40	0.55
2:N:376:LYS:O	2:N:379:THR:OG1	2.18	0.55
2:D:114:VAL:HG21	2:D:208:LEU:HB3	1.89	0.55
3:O:649:HIS:HA	3:O:652:ARG:HB2	1.89	0.55
3:E:34:SER:O	3:E:37:HIS:ND1	2.32	0.55
3:O:68:THR:HG23	3:O:71:ARG:HB3	1.88	0.55
2:D:39:VAL:HG23	3:E:631:ASP:HB2	1.88	0.55
3:E:1:MET:HE1	3:E:62:ARG:HH22	1.71	0.55
1:M:230:HIS:HA	1:M:233:LEU:HB2	1.89	0.55
1:A:93:LEU:O	1:A:97:GLY:N	2.39	0.54
2:D:245:ASP:O	4:C:125:ARG:NH1	2.39	0.54
3:E:574:ARG:HD2	3:E:577:SER:HB3	1.88	0.54
1:M:109:SER:OG	2:N:228:GLU:OE2	2.25	0.54
1:M:180:LEU:HD22	2:N:311:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:343:LEU:HB3	3:O:701:ARG:HB3	1.88	0.54
2:N:368:GLU:HB2	3:O:9:PRO:HB3	1.90	0.54
3:O:186:CYS:HA	3:O:549:LYS:HG3	1.88	0.54
3:E:212:ARG:O	3:E:215:ASN:ND2	2.40	0.54
3:E:674:THR:O	3:E:678:GLN:HG2	2.07	0.54
4:C:460:ARG:HB2	4:C:489:LEU:HD11	1.88	0.54
3:O:31:ASN:O	3:O:37:HIS:ND1	2.41	0.54
3:O:539:ILE:HG12	4:P:179:LEU:HD22	1.89	0.54
3:E:696:HIS:HA	3:E:699:TYR:HB3	1.89	0.54
4:C:184:GLN:O	4:C:188:HIS:N	2.34	0.54
3:O:148:LEU:HD12	4:P:133:LEU:HD23	1.89	0.54
3:O:548:GLU:OE1	4:P:426:THR:OG1	2.22	0.54
1:M:124:ARG:O	2:N:54:ARG:NE	2.34	0.54
4:P:539:PRO:HB2	4:P:543:MET:HE3	1.88	0.54
3:E:171:ASN:HB3	3:E:174:HIS:CD2	2.40	0.54
1:M:191:MET:O	1:M:195:LYS:N	2.41	0.54
2:N:64:TYR:HA	2:N:68:VAL:HB	1.90	0.54
1:A:230:HIS:ND1	3:E:78:VAL:O	2.39	0.54
2:D:291:TYR:HB2	2:D:295:LEU:HD23	1.90	0.54
3:E:158:GLU:HB2	4:C:144:ARG:HG3	1.88	0.54
3:E:654:GLN:O	3:E:659:ARG:N	2.34	0.54
4:C:154:VAL:O	4:C:157:GLN:NE2	2.41	0.54
4:C:509:ASN:O	4:C:513:ASN:N	2.36	0.54
3:O:3:SER:HA	4:P:18:ALA:HA	1.89	0.54
1:A:189:SER:O	1:A:194:TRP:N	2.39	0.54
3:E:49:ARG:HA	3:E:56:TRP:CE2	2.42	0.54
1:M:54:LEU:HD23	2:N:30:PRO:HG2	1.90	0.54
4:P:474:SER:HA	4:P:485:GLN:HG3	1.90	0.54
4:P:498:SER:HA	4:P:502:ASN:HB2	1.90	0.54
2:N:406:GLU:OE2	2:N:407:ASN:ND2	2.40	0.54
3:O:198:LYS:HA	3:O:201:GLN:HB3	1.89	0.54
4:P:429:ARG:NH2	4:P:432:ARG:HG3	2.23	0.54
2:D:54:ARG:HH22	2:D:57:TYR:HD2	1.55	0.54
3:O:642:SER:HA	3:O:649:HIS:NE2	2.23	0.54
2:D:101:SER:O	2:D:105:TYR:N	2.32	0.54
2:D:132:ILE:HG13	2:D:136:GLU:HG2	1.90	0.54
3:E:662:ASN:O	3:E:666:ASP:N	2.35	0.54
2:N:36:THR:HB	4:P:455:PHE:HA	1.90	0.54
3:O:539:ILE:HD13	4:P:179:LEU:HD13	1.89	0.54
1:A:149:ARG:HH12	2:D:280:ASP:HB3	1.73	0.53
1:M:131:PHE:CE2	4:P:140:LEU:HB2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:142:LYS:HD2	4:P:125:ARG:HG2	1.88	0.53
1:M:154:LYS:HD2	4:P:115:GLU:HG3	1.89	0.53
3:O:183:ASP:O	3:O:188:GLU:N	2.26	0.53
4:P:419:LEU:HA	4:P:422:TYR:HB3	1.89	0.53
1:A:166:ALA:HB1	2:D:298:ILE:HG21	1.90	0.53
2:D:270:ILE:HG21	3:E:628:LYS:HB3	1.89	0.53
2:N:21:ASP:HA	4:P:465:ILE:HG22	1.90	0.53
1:A:192:GLU:O	1:A:195:LYS:NZ	2.32	0.53
1:A:240:ARG:HG2	1:A:289:LEU:HD22	1.89	0.53
1:A:237:ALA:HB1	1:A:241:LYS:HB2	1.91	0.53
2:D:415:VAL:HG21	3:E:37:HIS:NE2	2.23	0.53
2:N:416:GLU:HB2	3:O:27:LEU:HD13	1.90	0.53
3:O:683:LEU:O	3:O:687:VAL:N	2.25	0.53
2:D:286:ARG:O	2:D:290:GLU:N	2.40	0.53
3:E:26:GLN:HG3	3:E:27:LEU:HD22	1.89	0.53
4:C:7:CYS:SG	4:C:31:GLN:NE2	2.82	0.53
4:P:582:GLU:OE1	4:P:585:ARG:NH2	2.36	0.53
3:E:186:CYS:HA	3:E:546:PHE:HE1	1.73	0.53
2:N:117:ALA:HA	2:N:121:LEU:HB3	1.91	0.53
2:N:326:CYS:HB2	4:P:542:LEU:HD21	1.89	0.53
2:N:372:ALA:HA	3:O:16:GLU:HG2	1.91	0.53
4:P:418:GLU:O	4:P:422:TYR:N	2.36	0.53
4:P:524:GLN:NE2	4:P:525:LEU:HB2	2.23	0.53
2:D:291:TYR:HD2	2:D:295:LEU:HG	1.74	0.53
1:M:83:ARG:HH21	2:N:124:PRO:HA	1.73	0.53
1:M:129:SER:O	1:M:133:VAL:HG12	2.09	0.53
1:M:147:GLU:OE1	1:M:151:LYS:NZ	2.42	0.53
1:M:235:GLU:O	1:M:239:HIS:N	2.39	0.53
3:E:566:PRO:HA	3:E:569:PRO:HG2	1.91	0.53
1:M:58:ALA:HB2	2:N:30:PRO:HB3	1.91	0.53
3:O:182:TYR:O	3:O:186:CYS:N	2.37	0.53
1:A:133:VAL:HG12	1:A:138:ILE:HG12	1.90	0.52
3:E:175:LYS:HB2	3:E:561:SER:HA	1.91	0.52
1:M:19:ASP:HA	1:M:23:ILE:HD13	1.91	0.52
1:M:206:GLU:OE2	1:M:210:GLN:NE2	2.42	0.52
3:O:2:GLN:NE2	4:P:7:CYS:O	2.42	0.52
2:D:123:LEU:HG	2:D:124:PRO:HD3	1.91	0.52
3:E:1:MET:SD	3:E:62:ARG:NH1	2.82	0.52
3:O:604:SER:HA	3:O:618:SER:HA	1.92	0.52
1:A:277:GLN:HG3	2:D:376:LYS:HG3	1.92	0.52
2:D:71:VAL:HB	3:E:166:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:147:ASP:O	3:E:151:ARG:HG3	2.10	0.52
1:M:68:ALA:HB1	1:M:72:ALA:HB3	1.91	0.52
1:A:133:VAL:O	1:A:138:ILE:N	2.32	0.52
2:D:112:LEU:O	2:D:117:ALA:N	2.42	0.52
2:D:218:ASP:O	2:D:222:PHE:N	2.42	0.52
1:M:141:ARG:HA	3:O:616:ARG:HA	1.90	0.52
1:M:170:LEU:HB3	2:N:294:VAL:HG22	1.92	0.52
4:C:6:LEU:HA	4:C:9:LEU:HD23	1.92	0.52
4:C:603:ARG:O	4:C:603:ARG:NH1	2.42	0.52
1:M:221:ARG:NH1	4:P:56:GLU:OE2	2.43	0.52
3:O:18:LEU:HD13	3:O:56:TRP:CZ3	2.44	0.52
3:O:661:THR:O	3:O:665:LEU:N	2.43	0.52
1:M:49:ARG:O	1:M:52:THR:OG1	2.23	0.52
2:N:319:GLU:O	2:N:322:LYS:NZ	2.27	0.52
3:E:563:TYR:HB2	4:C:435:ALA:HB2	1.91	0.52
1:M:283:LYS:HA	1:M:286:GLU:HB2	1.92	0.52
1:A:191:MET:HG2	2:D:316:LYS:HZ3	1.74	0.52
2:D:35:VAL:HG21	4:C:470:GLN:HB2	1.92	0.52
2:D:35:VAL:HG22	3:E:630:ILE:HG21	1.92	0.52
3:E:158:GLU:HG2	4:C:147:ARG:HG2	1.92	0.52
3:E:187:ASP:O	3:E:191:ARG:N	2.40	0.52
4:C:554:SER:O	4:C:557:SER:OG	2.26	0.52
2:N:112:LEU:HA	2:N:116:GLU:HB3	1.91	0.52
1:A:141:ARG:HA	3:E:616:ARG:HA	1.92	0.51
1:A:148:LYS:HE2	3:E:611:PHE:HE2	1.75	0.51
1:A:184:VAL:HB	2:D:310:LYS:HD3	1.92	0.51
1:A:250:VAL:HG22	1:A:254:LEU:HD13	1.93	0.51
3:E:18:LEU:HD12	3:E:19:GLN:N	2.25	0.51
2:N:68:VAL:HG13	3:O:169:ARG:HG2	1.92	0.51
2:N:243:VAL:HG21	2:N:254:ASN:HB2	1.93	0.51
3:O:607:GLU:HB2	3:O:614:ARG:HA	1.90	0.51
4:C:574:VAL:HG13	4:C:612:ARG:NH2	2.25	0.51
3:O:24:TYR:OH	3:O:25:ARG:NH1	2.43	0.51
1:A:72:ALA:O	1:A:76:ARG:NE	2.43	0.51
4:C:414:VAL:O	4:C:418:GLU:N	2.39	0.51
2:N:52:ARG:HE	2:N:56:ARG:NE	2.08	0.51
2:N:222:PHE:CE2	2:N:227:ILE:HD12	2.45	0.51
1:A:227:LYS:HB3	2:D:358:ASN:ND2	2.25	0.51
1:A:253:THR:HG22	2:D:407:ASN:ND2	2.25	0.51
2:D:371:SER:HA	2:D:422:HIS:CE1	2.44	0.51
3:E:10:THR:HG23	3:E:14:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:122:ASN:O	1:M:130:SER:N	2.43	0.51
1:M:154:LYS:NZ	2:N:280:ASP:OD1	2.32	0.51
1:M:155:GLU:OE2	4:P:504:LEU:HB3	2.10	0.51
2:D:207:GLN:O	2:D:211:THR:OG1	2.22	0.51
1:M:118:ALA:HB1	2:N:263:VAL:HB	1.93	0.51
3:O:620:ALA:HB3	4:P:459:VAL:HG21	1.92	0.51
4:P:500:LEU:O	4:P:504:LEU:N	2.37	0.51
1:A:86:ALA:O	1:A:90:ARG:HG2	2.10	0.51
3:E:672:GLU:O	3:E:676:SER:N	2.27	0.51
1:M:77:LEU:HD22	3:O:580:PRO:HD2	1.93	0.51
1:M:119:ASN:HB2	2:N:242:ILE:HD13	1.92	0.51
1:M:227:LYS:HD2	3:O:74:ARG:HH22	1.76	0.51
3:O:640:VAL:HG13	3:O:644:HIS:HB2	1.93	0.51
4:P:143:GLY:O	4:P:147:ARG:HG2	2.10	0.51
2:D:265:PHE:O	2:D:269:GLU:N	2.42	0.51
2:D:274:GLU:HB3	2:D:278:ARG:HH22	1.75	0.51
2:D:296:GLU:HG2	2:D:300:GLY:HA3	1.93	0.51
1:M:166:ALA:O	1:M:170:LEU:N	2.44	0.51
3:O:55:ILE:HA	3:O:58:PHE:CD2	2.45	0.51
4:P:548:GLU:HG2	4:P:551:LYS:HE3	1.92	0.51
1:M:72:ALA:HA	1:M:76:ARG:HB3	1.91	0.51
2:N:419:LEU:HB2	3:O:20:LYS:CB	2.41	0.51
3:O:15:LEU:HD13	3:O:42:ASP:HA	1.93	0.51
3:O:182:TYR:HA	3:O:185:GLN:HB3	1.93	0.51
3:O:190:THR:O	3:O:194:ALA:N	2.44	0.51
3:E:219:GLU:O	4:C:191:SER:OG	2.27	0.51
1:M:114:LEU:HD13	2:N:58:LEU:HD23	1.91	0.51
2:N:417:MET:O	2:N:421:SER:N	2.37	0.51
3:O:17:TRP:CE3	3:O:18:LEU:HB3	2.45	0.51
1:A:91:GLU:OE1	2:D:105:TYR:OH	2.29	0.50
1:A:106:ASN:ND2	2:D:227:ILE:O	2.45	0.50
2:D:256:SER:HA	2:D:259:LEU:HD23	1.93	0.50
2:D:315:HIS:HA	2:D:318:ASN:HD21	1.76	0.50
2:N:21:ASP:CG	3:O:637:GLN:HB3	2.32	0.50
3:O:141:VAL:O	3:O:145:ARG:HG3	2.11	0.50
1:A:53:HIS:HB3	1:A:57:LEU:HD22	1.93	0.50
1:A:124:ARG:H	1:A:129:SER:CB	2.25	0.50
3:E:2:GLN:N	4:C:24:ASP:OD1	2.42	0.50
3:O:65:SER:HB2	3:O:72:ILE:HD13	1.93	0.50
2:D:102:PRO:O	2:D:106:GLU:N	2.42	0.50
2:D:368:GLU:HB3	3:E:17:TRP:CE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:583:CYS:SG	4:C:452:ARG:HB2	2.51	0.50
2:N:423:ASP:OD1	3:O:20:LYS:HG3	2.11	0.50
2:D:111:ARG:HD2	2:D:212:ILE:HG12	1.93	0.50
3:E:599:ASP:N	3:E:599:ASP:OD1	2.44	0.50
3:E:658:GLU:HG3	4:C:515:LEU:HG	1.93	0.50
4:C:582:GLU:OE1	4:C:586:ARG:NH2	2.44	0.50
2:N:314:GLN:HA	2:N:317:TYR:CE1	2.47	0.50
2:N:377:ALA:HB3	3:O:38:VAL:HG11	1.93	0.50
3:O:662:ASN:ND2	3:O:666:ASP:OD2	2.44	0.50
2:D:27:CYS:HB3	2:D:32:GLY:HA3	1.94	0.50
2:D:125:LEU:HD22	2:D:132:ILE:HB	1.94	0.50
2:D:219:TYR:HA	2:D:222:PHE:HB3	1.94	0.50
2:D:321:GLN:HB3	2:D:325:LEU:HD23	1.93	0.50
3:E:22:MET:HG3	3:E:25:ARG:HH11	1.76	0.50
3:E:730:GLN:HG2	4:C:612:ARG:HD2	1.93	0.50
2:N:411:THR:HA	2:N:414:GLN:HB3	1.93	0.50
3:O:38:VAL:HA	3:O:41:ILE:HD12	1.94	0.50
1:A:85:GLN:HA	3:E:568:THR:O	2.11	0.50
1:A:125:ASP:CB	3:E:159:GLU:HG2	2.42	0.50
1:A:145:VAL:HG22	3:E:612:CYS:HB3	1.93	0.50
2:D:314:GLN:HB3	4:C:534:GLN:HB3	1.93	0.50
3:E:68:THR:HG23	3:E:71:ARG:HB3	1.93	0.50
1:M:227:LYS:HZ2	3:O:71:ARG:HD3	1.76	0.50
2:N:318:ASN:ND2	3:O:672:GLU:OE2	2.44	0.50
3:O:679:TRP:O	3:O:683:LEU:N	2.40	0.50
4:P:539:PRO:HA	4:P:542:LEU:HB2	1.94	0.50
1:A:57:LEU:HD23	2:D:31:ASP:HB3	1.92	0.50
1:A:154:LYS:HG3	4:C:115:GLU:HB2	1.93	0.50
3:E:47:ILE:O	3:E:51:ASN:N	2.33	0.50
1:M:85:GLN:O	1:M:89:ILE:HG12	2.12	0.50
1:M:192:GLU:HA	1:M:195:LYS:HD2	1.93	0.50
2:N:332:MET:HA	2:N:335:LYS:HG2	1.93	0.50
2:D:42:ASP:HA	2:D:45:LEU:HB3	1.93	0.50
2:D:364:VAL:HG23	3:E:60:ILE:HG21	1.92	0.50
2:N:380:ARG:NH2	2:N:384:TYR:HH	2.08	0.50
3:O:58:PHE:O	3:O:63:VAL:N	2.44	0.50
1:A:89:ILE:HG23	2:D:63:ILE:HB	1.94	0.49
2:D:74:TYR:OH	3:E:173:ARG:NH2	2.45	0.49
3:E:621:CYS:SG	4:C:460:ARG:NH1	2.85	0.49
3:E:641:GLU:HA	3:E:644:HIS:HB2	1.93	0.49
2:N:24:GLU:OE1	3:O:634:HIS:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:324:TRP:O	2:N:327:LYS:HG3	2.12	0.49
2:D:279:GLU:HB3	4:C:121:ARG:HH22	1.78	0.49
2:D:306:VAL:HG12	2:D:311:LEU:HD12	1.93	0.49
3:E:59:LEU:HD23	3:E:60:ILE:HG23	1.94	0.49
3:E:154:GLU:HB3	4:C:137:SER:HB3	1.94	0.49
1:M:146:GLU:HG2	1:M:149:ARG:CZ	2.42	0.49
1:M:232:GLU:HA	1:M:235:GLU:HB2	1.93	0.49
1:M:273:ASP:HA	1:M:276:ARG:HD3	1.93	0.49
2:N:274:GLU:OE2	3:O:616:ARG:NH2	2.45	0.49
4:P:609:VAL:O	4:P:613:GLN:NE2	2.45	0.49
1:A:97:GLY:HA2	1:A:103:LEU:HD13	1.94	0.49
2:D:288:PHE:CD1	3:E:646:LEU:HB2	2.46	0.49
3:E:5:SER:HB3	3:E:59:LEU:HD13	1.94	0.49
3:E:137:LEU:O	3:E:141:VAL:N	2.34	0.49
3:E:161:GLU:OE2	3:E:164:ARG:NH1	2.45	0.49
3:E:695:GLU:OE2	4:C:60:TYR:OH	2.25	0.49
2:N:365:GLU:HG3	2:N:369:GLU:OE2	2.12	0.49
4:P:473:LEU:HA	4:P:476:TYR:CE2	2.47	0.49
1:A:76:ARG:HG2	3:E:626:LEU:HD13	1.95	0.49
1:A:232:GLU:O	1:A:236:MET:N	2.45	0.49
3:E:6:SER:OG	4:C:12:GLU:OE1	2.19	0.49
1:M:82:TYR:OH	1:M:124:ARG:O	2.17	0.49
2:N:64:TYR:HB3	3:O:168:GLU:OE2	2.12	0.49
3:O:584:ARG:NH2	4:P:453:ASP:OD1	2.45	0.49
1:A:79:ALA:HA	1:A:82:TYR:CD2	2.47	0.49
1:A:167:ILE:HA	1:A:170:LEU:HD23	1.94	0.49
1:A:239:HIS:CE1	3:E:64:LYS:HE2	2.48	0.49
2:D:324:TRP:O	2:D:327:LYS:HG3	2.12	0.49
3:E:223:SER:HA	4:C:195:ASP:HB2	1.92	0.49
3:E:633:VAL:HG23	4:C:466:HIS:HE1	1.77	0.49
1:M:243:LEU:HD21	1:M:282:GLU:HG3	1.94	0.49
2:N:108:LEU:O	2:N:111:ARG:HG2	2.13	0.49
2:N:328:ARG:HA	2:N:331:THR:HG23	1.95	0.49
4:P:457:HIS:ND1	4:P:485:GLN:OE1	2.46	0.49
1:A:157:ASN:HA	1:A:160:LEU:HB3	1.94	0.49
2:D:277:LEU:HG	2:D:278:ARG:HD3	1.95	0.49
3:E:566:PRO:HB3	4:C:438:GLN:HG3	1.94	0.49
3:E:620:ALA:HB3	4:C:460:ARG:HH22	1.77	0.49
1:M:88:ARG:HG2	3:O:170:ALA:HB3	1.95	0.49
2:N:311:LEU:CB	2:N:314:GLN:HB3	2.43	0.49
2:N:328:ARG:HD2	4:P:549:MET:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:LEU:HB2	2:D:411:THR:HG21	1.94	0.49
3:E:178:LEU:HB3	3:E:560:ASN:HD22	1.77	0.49
3:O:52:MET:CE	3:O:55:ILE:HB	2.43	0.49
4:P:104:GLU:HG2	4:P:105:VAL:H	1.77	0.49
4:P:526:LEU:HD12	4:P:529:SER:HB2	1.94	0.49
4:P:585:ARG:HA	4:P:589:VAL:HB	1.94	0.49
1:A:128:LEU:HD12	4:C:140:LEU:HD21	1.94	0.49
1:A:195:LYS:HA	1:A:198:LEU:HD12	1.94	0.49
1:A:208:TYR:HA	1:A:211:GLN:HB2	1.95	0.49
1:M:228:ILE:HG21	4:P:27:GLU:HB3	1.93	0.49
1:M:246:MET:HG3	1:M:279:THR:HG22	1.94	0.49
3:O:17:TRP:CZ3	3:O:18:LEU:HB3	2.47	0.49
3:O:621:CYS:SG	4:P:455:PHE:HB3	2.52	0.49
1:A:73:ASN:ND2	2:D:42:ASP:OD2	2.45	0.49
4:C:454:SER:HB3	4:C:474:SER:O	2.12	0.49
1:M:96:ALA:HB2	1:M:106:ASN:HD22	1.77	0.49
1:M:154:LYS:HG3	4:P:119:LEU:HD11	1.95	0.49
1:M:240:ARG:HA	1:M:243:LEU:HB2	1.95	0.49
3:O:582:ILE:HG13	4:P:449:VAL:HG11	1.95	0.49
4:P:28:TRP:O	4:P:31:GLN:NE2	2.45	0.49
4:P:504:LEU:HD13	4:P:508:ARG:NH1	2.28	0.49
4:C:189:TYR:HB3	4:C:404:ASN:HD22	1.78	0.49
2:N:62:ALA:O	2:N:231:LEU:HA	2.13	0.49
2:N:318:ASN:HA	2:N:321:GLN:HG2	1.94	0.49
4:P:596:GLU:HG3	4:P:600:ASN:HB2	1.95	0.49
1:A:91:GLU:HA	1:A:94:GLU:HG3	1.95	0.48
4:C:122:GLN:O	4:C:126:LEU:N	2.38	0.48
1:M:75:PHE:HB3	2:N:127:SER:HB2	1.95	0.48
3:O:743:GLU:HA	3:O:746:ARG:HB3	1.95	0.48
3:E:682:GLU:O	3:E:686:ALA:N	2.46	0.48
2:N:72:GLU:OE1	4:P:150:ALA:HB2	2.13	0.48
3:O:68:THR:HG22	3:O:72:ILE:HG23	1.94	0.48
3:O:158:GLU:HB2	4:P:141:ILE:HD13	1.95	0.48
3:O:654:GLN:NE2	4:P:514:GLU:OE1	2.46	0.48
1:A:104:PRO:HA	1:A:108:VAL:HB	1.95	0.48
2:D:54:ARG:O	2:D:58:LEU:N	2.43	0.48
3:E:55:ILE:HA	3:E:58:PHE:HD2	1.79	0.48
4:C:190:HIS:NE2	4:C:194:GLU:OE1	2.46	0.48
4:C:453:ASP:O	4:C:456:LEU:HB3	2.14	0.48
1:M:180:LEU:HD11	4:P:531:THR:HA	1.96	0.48
2:N:374:TYR:HE1	2:N:415:VAL:HG13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:452:ARG:O	4:P:455:PHE:HB2	2.13	0.48
1:A:187:CYS:SG	2:D:314:GLN:NE2	2.85	0.48
2:D:136:GLU:O	2:D:140:TRP:N	2.44	0.48
1:M:208:TYR:OH	2:N:331:THR:HG21	2.13	0.48
3:O:596:GLU:OE2	4:P:446:GLN:NE2	2.44	0.48
1:A:95:SER:HB2	2:D:108:LEU:HD13	1.95	0.48
1:A:124:ARG:NH2	3:E:624:GLU:HB3	2.28	0.48
1:A:141:ARG:NH2	2:D:274:GLU:OE2	2.39	0.48
2:D:351:ASP:O	2:D:354:SER:OG	2.29	0.48
1:M:95:SER:HA	2:N:111:ARG:HH21	1.78	0.48
1:M:123:ILE:HA	1:M:127:GLU:HA	1.96	0.48
2:N:380:ARG:NH1	2:N:383:GLU:OE2	2.46	0.48
1:M:175:LYS:O	1:M:179:GLN:HG3	2.13	0.48
3:O:48:CYS:HA	3:O:51:ASN:HD21	1.79	0.48
3:O:181:ALA:HB1	4:P:425:ALA:HA	1.96	0.48
3:O:546:PHE:CE2	4:P:172:MET:HG2	2.48	0.48
3:O:649:HIS:O	3:O:653:ALA:N	2.35	0.48
1:A:131:PHE:HA	1:A:135:MET:HB3	1.96	0.48
1:A:238:GLU:OE1	1:A:238:GLU:N	2.45	0.48
4:C:461:ASP:HB3	4:C:489:LEU:HG	1.95	0.48
2:D:339:LEU:HD22	3:E:711:PRO:HG3	1.95	0.48
3:E:52:MET:C	3:E:56:TRP:HD1	2.17	0.48
4:C:162:GLU:HA	4:C:165:LEU:HD12	1.96	0.48
4:C:596:GLU:O	4:C:600:ASN:N	2.46	0.48
2:N:278:ARG:NH2	3:O:633:VAL:HG12	2.29	0.48
2:N:291:TYR:CE2	3:O:653:ALA:HB1	2.48	0.48
2:N:377:ALA:HB2	2:N:418:ASP:OD2	2.14	0.48
2:N:390:HIS:O	2:N:393:THR:OG1	2.27	0.48
4:C:506:ASP:OD1	4:C:506:ASP:N	2.46	0.48
4:C:564:THR:O	4:C:568:ARG:N	2.47	0.48
1:M:108:VAL:HA	1:M:111:ALA:HB3	1.96	0.48
2:D:113:VAL:HG22	3:E:174:HIS:CD2	2.49	0.48
1:M:249:PRO:HG2	2:N:410:TRP:NE1	2.29	0.48
2:N:240:ASP:O	2:N:243:VAL:HG22	2.13	0.48
2:N:295:LEU:HD13	3:O:657:TYR:HB2	1.96	0.48
2:N:317:TYR:HA	2:N:320:MET:HG3	1.96	0.48
3:O:3:SER:OG	3:O:4:LEU:N	2.47	0.48
3:O:17:TRP:CZ2	3:O:59:LEU:HD13	2.49	0.48
4:P:445:GLU:O	4:P:449:VAL:HG23	2.14	0.48
2:D:80:VAL:HG11	2:D:87:ARG:HB3	1.96	0.47
2:D:109:GLU:O	2:D:113:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:GLN:NE2	2:D:408:MET:SD	2.87	0.47
4:C:450:ASP:O	4:C:454:SER:N	2.47	0.47
1:M:135:MET:HB2	2:N:245:ASP:HB2	1.96	0.47
2:N:56:ARG:HH12	2:N:123:LEU:HG	1.79	0.47
1:A:151:LYS:HG2	3:E:138:ARG:HE	1.77	0.47
3:E:630:ILE:O	3:E:633:VAL:HG22	2.14	0.47
4:C:463:LEU:HD22	4:C:492:ASP:HB2	1.96	0.47
4:C:534:GLN:HA	4:C:538:THR:HB	1.96	0.47
1:M:161:ASP:HB3	4:P:112:HIS:HE2	1.79	0.47
1:M:172:TYR:O	1:M:176:ILE:HG13	2.14	0.47
2:N:201:ALA:O	2:N:205:TYR:N	2.45	0.47
2:N:374:TYR:HB2	2:N:419:LEU:HB3	1.95	0.47
1:A:227:LYS:HE2	4:C:28:TRP:HE1	1.78	0.47
2:D:23:LEU:HA	2:D:26:HIS:HB3	1.96	0.47
2:D:321:GLN:O	2:D:325:LEU:HB3	2.14	0.47
2:D:328:ARG:O	2:D:332:MET:HG2	2.14	0.47
3:E:53:ILE:N	3:E:54:PRO:HD2	2.29	0.47
4:C:122:GLN:O	4:C:126:LEU:HG	2.13	0.47
4:C:190:HIS:CE1	4:C:194:GLU:HB3	2.48	0.47
1:M:78:LYS:HD2	1:M:124:ARG:HD2	1.97	0.47
2:N:46:ALA:O	2:N:47:ARG:NE	2.23	0.47
2:N:71:VAL:HG21	2:N:109:GLU:CD	2.34	0.47
2:N:333:ASN:HD22	3:O:688:GLN:HG2	1.79	0.47
2:N:338:VAL:HG23	2:N:339:LEU:HD22	1.96	0.47
3:O:60:ILE:O	3:O:64:LYS:NZ	2.47	0.47
3:E:52:MET:SD	3:E:55:ILE:HB	2.54	0.47
4:C:26:PHE:HZ	4:C:33:ASP:HB2	1.80	0.47
4:C:485:GLN:HA	4:C:488:ALA:HB3	1.96	0.47
1:M:227:LYS:HE2	1:M:231:ARG:HG3	1.95	0.47
1:M:260:LEU:HG	1:M:264:LYS:HD2	1.96	0.47
3:E:2:GLN:HB3	4:C:20:LYS:HB2	1.97	0.47
3:E:76:ILE:HD13	4:C:5:ARG:HG2	1.97	0.47
3:E:138:ARG:HA	3:E:141:VAL:HG12	1.96	0.47
1:M:236:MET:HB2	1:M:293:LEU:HB3	1.96	0.47
1:M:248:LYS:HA	1:M:251:LEU:HD23	1.96	0.47
2:N:64:TYR:OH	3:O:162:ARG:NH1	2.47	0.47
2:N:330:GLU:HA	2:N:333:ASN:ND2	2.30	0.47
3:O:68:THR:HG22	3:O:68:THR:O	2.15	0.47
3:O:693:SER:HA	3:O:696:HIS:CD2	2.50	0.47
4:P:463:LEU:HD13	4:P:493:LEU:HA	1.96	0.47
3:E:127:ARG:HH11	4:C:112:HIS:CE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:540:SER:HA	4:C:179:LEU:HD23	1.95	0.47
3:E:620:ALA:H	4:C:460:ARG:NH2	2.13	0.47
3:O:41:ILE:O	3:O:45:ARG:N	2.44	0.47
1:A:75:PHE:O	1:A:78:LYS:HG2	2.14	0.47
1:A:157:ASN:ND2	4:C:111:ALA:HB1	2.29	0.47
1:A:240:ARG:O	1:A:243:LEU:HG	2.15	0.47
2:D:64:TYR:OH	3:E:159:GLU:OE1	2.28	0.47
4:C:537:LEU:HA	4:C:540:TRP:HB2	1.97	0.47
4:C:573:ILE:HA	4:C:576:HIS:HB2	1.97	0.47
1:M:163:THR:HA	4:P:519:ILE:HD13	1.97	0.47
2:N:34:LEU:HD22	2:N:38:SER:HA	1.97	0.47
4:P:498:SER:O	4:P:503:SER:OG	2.27	0.47
3:E:593:ALA:HB1	3:E:596:GLU:HB2	1.95	0.47
4:C:469:THR:HB	4:C:474:SER:HB2	1.96	0.47
4:C:516:CYS:HA	4:C:519:ILE:HG22	1.97	0.47
4:C:563:VAL:O	4:C:567:HIS:ND1	2.48	0.47
1:M:75:PHE:HA	1:M:79:ALA:HB3	1.97	0.47
1:M:282:GLU:O	1:M:286:GLU:HG2	2.15	0.47
2:N:361:ASN:OD1	2:N:363:LEU:HD23	2.14	0.47
2:D:304:LYS:O	2:D:308:ASP:N	2.42	0.47
3:E:193:PHE:HA	3:E:197:HIS:HB2	1.97	0.47
2:N:314:GLN:HG2	4:P:534:GLN:HB2	1.96	0.47
1:A:73:ASN:ND2	2:D:39:VAL:HG12	2.29	0.47
1:A:89:ILE:H	1:A:89:ILE:HD12	1.80	0.47
2:D:325:LEU:HD23	4:C:542:LEU:HB3	1.97	0.47
1:M:146:GLU:HG3	2:N:276:ALA:HB1	1.95	0.47
1:M:236:MET:O	1:M:240:ARG:HG2	2.14	0.47
3:O:669:SER:HB2	4:P:529:SER:O	2.15	0.47
1:A:146:GLU:HA	1:A:149:ARG:NE	2.30	0.46
1:A:231:ARG:HD3	4:C:5:ARG:HH21	1.80	0.46
2:D:23:LEU:O	2:D:27:CYS:N	2.47	0.46
2:D:66:GLU:HG2	2:D:233:GLU:HB3	1.96	0.46
2:D:198:ILE:HA	2:D:201:ALA:HB3	1.97	0.46
3:E:165:MET:HG3	4:C:147:ARG:HA	1.97	0.46
3:E:587:ALA:HB2	3:E:622:VAL:HG21	1.97	0.46
3:E:613:LEU:HD21	4:C:460:ARG:HB3	1.96	0.46
4:C:512:ILE:O	4:C:516:CYS:N	2.46	0.46
4:C:540:TRP:O	4:C:544:LYS:NZ	2.48	0.46
1:M:44:PHE:CE1	1:M:45:GLU:HG3	2.50	0.46
1:M:190:GLN:HA	1:M:194:TRP:CD2	2.50	0.46
3:O:181:ALA:O	3:O:185:GLN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:105:VAL:HA	4:P:108:ALA:HB3	1.97	0.46
4:P:148:VAL:O	4:P:151:THR:OG1	2.25	0.46
2:D:277:LEU:HD23	2:D:278:ARG:NH1	2.27	0.46
2:N:139:LYS:HD3	3:O:174:HIS:CD2	2.50	0.46
3:O:607:GLU:O	3:O:614:ARG:HB2	2.16	0.46
2:D:280:ASP:N	4:C:118:GLU:OE1	2.47	0.46
1:M:188:GLU:HA	2:N:313:HIS:CD2	2.50	0.46
2:N:11:ASN:O	2:N:15:ASP:N	2.39	0.46
2:N:324:TRP:HE3	2:N:325:LEU:HD22	1.81	0.46
1:A:105:SER:OG	1:A:106:ASN:OD1	2.33	0.46
1:A:246:MET:C	1:A:249:PRO:HD2	2.36	0.46
3:E:552:SER:O	3:E:556:GLN:N	2.48	0.46
3:E:579:ILE:N	3:E:580:PRO:HD2	2.31	0.46
3:E:580:PRO:HA	3:E:584:ARG:HB2	1.98	0.46
3:E:708:TRP:O	3:E:710:GLN:N	2.48	0.46
1:M:82:TYR:CE2	2:N:54:ARG:HD3	2.51	0.46
3:O:587:ALA:HA	3:O:590:GLN:HE21	1.80	0.46
1:A:91:GLU:HG2	2:D:112:LEU:HD13	1.98	0.46
1:A:106:ASN:HB3	2:D:227:ILE:HG22	1.96	0.46
1:A:124:ARG:HA	2:D:54:ARG:CZ	2.45	0.46
1:A:228:ILE:HA	1:A:233:LEU:H	1.81	0.46
3:E:23:GLY:N	3:E:66:GLU:OE2	2.27	0.46
1:M:76:ARG:H	2:N:47:ARG:HH12	1.62	0.46
3:O:13:ALA:O	3:O:17:TRP:N	2.39	0.46
3:O:172:TYR:HA	3:O:564:MET:SD	2.56	0.46
4:P:454:SER:HA	4:P:457:HIS:CG	2.50	0.46
2:D:134:GLU:HA	2:D:137:ILE:HG22	1.96	0.46
2:D:363:LEU:O	2:D:363:LEU:HD23	2.15	0.46
3:E:155:VAL:HG23	3:E:589:LEU:HA	1.96	0.46
1:M:84:ALA:O	2:N:132:ILE:HD11	2.16	0.46
1:M:141:ARG:HB3	2:N:273:ASP:HB3	1.98	0.46
3:O:131:ALA:HB2	4:P:112:HIS:ND1	2.31	0.46
4:P:172:MET:O	4:P:175:VAL:HG12	2.15	0.46
1:A:39:LYS:NZ	1:A:40:GLU:OE2	2.43	0.46
1:A:48:HIS:HA	1:A:51:ILE:HG13	1.96	0.46
2:D:333:ASN:OD1	3:E:691:GLN:NE2	2.46	0.46
2:D:366:ALA:HA	2:D:369:GLU:OE1	2.16	0.46
3:E:665:LEU:HD13	4:C:526:LEU:HA	1.97	0.46
3:O:22:MET:HB2	3:O:25:ARG:HB2	1.97	0.46
1:A:30:LEU:HA	1:A:33:GLN:HB2	1.97	0.46
1:A:83:ARG:HG3	2:D:53:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LYS:O	1:A:268:ALA:N	2.49	0.46
4:C:612:ARG:HH12	4:C:616:SER:HB3	1.81	0.46
2:N:130:GLY:HA2	2:N:133:HIS:HB3	1.97	0.46
2:N:322:LYS:HD2	3:O:675:ILE:HG21	1.98	0.46
2:D:374:TYR:HE1	2:D:415:VAL:HG13	1.81	0.46
4:C:126:LEU:HB3	4:C:130:TYR:CE1	2.51	0.46
1:M:143:THR:HG21	4:P:126:LEU:HG	1.98	0.46
1:M:177:LEU:HD13	2:N:310:LYS:HD2	1.97	0.46
1:M:289:LEU:HG	2:N:366:ALA:HB3	1.97	0.46
2:N:113:VAL:HA	2:N:139:LYS:CD	2.44	0.46
3:O:743:GLU:O	3:O:747:THR:OG1	2.25	0.46
1:A:50:SER:O	1:A:50:SER:OG	2.29	0.46
3:E:58:PHE:CZ	4:C:9:LEU:HB3	2.51	0.46
3:E:158:GLU:HB3	4:C:140:LEU:HD13	1.98	0.46
3:E:667:LEU:O	4:C:534:GLN:NE2	2.49	0.46
1:M:181:GLU:HA	1:M:184:VAL:HG23	1.98	0.46
1:M:196:THR:O	1:M:199:GLU:HG3	2.16	0.46
2:N:419:LEU:O	2:N:423:ASP:N	2.49	0.46
3:O:686:ALA:HA	3:O:689:ASN:HD22	1.80	0.46
3:O:721:VAL:O	3:O:725:SER:N	2.48	0.46
4:P:36:ARG:HB3	4:P:37:PRO:HD3	1.98	0.46
1:A:94:GLU:C	1:A:97:GLY:H	2.20	0.45
1:A:106:ASN:HA	2:D:232:LYS:NZ	2.31	0.45
3:E:199:ARG:HD2	3:E:203:TYR:HB2	1.98	0.45
4:C:23:PRO:O	4:C:27:GLU:N	2.49	0.45
4:C:522:LEU:HA	4:C:526:LEU:HB2	1.97	0.45
1:M:160:LEU:HG	1:M:163:THR:OG1	2.16	0.45
2:N:12:LEU:HA	2:N:15:ASP:HB2	1.98	0.45
2:N:36:THR:HG23	4:P:471:ALA:O	2.16	0.45
3:O:149:LYS:HE2	3:O:618:SER:HB2	1.97	0.45
3:O:541:ASN:HD21	4:P:419:LEU:HD11	1.80	0.45
4:P:454:SER:HB2	4:P:475:THR:HG22	1.99	0.45
1:A:227:LYS:HA	1:A:231:ARG:HE	1.81	0.45
1:A:247:THR:O	1:A:250:VAL:HG12	2.16	0.45
2:D:200:PRO:HD3	3:E:181:ALA:HB2	1.97	0.45
3:E:599:ASP:HB2	4:C:453:ASP:HB2	1.97	0.45
3:E:633:VAL:HB	4:C:462:LEU:HB2	1.99	0.45
4:C:44:SER:HB3	4:C:47:ARG:HD3	1.99	0.45
3:O:657:TYR:O	3:O:661:THR:HG23	2.16	0.45
4:P:508:ARG:HD3	4:P:512:ILE:HD11	1.98	0.45
1:A:173:LEU:HD23	4:C:527:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:VAL:HG11	2:D:208:LEU:HD13	1.98	0.45
2:D:380:ARG:NH1	2:D:384:TYR:OH	2.50	0.45
4:C:460:ARG:HB3	4:C:489:LEU:HD21	1.97	0.45
1:M:99:SER:HB2	2:N:216:MET:HA	1.98	0.45
2:N:10:GLN:HG3	3:O:651:PHE:CD2	2.52	0.45
2:N:419:LEU:HB2	3:O:20:LYS:HB2	1.99	0.45
3:O:30:TYR:CE2	3:O:44:ILE:HG12	2.51	0.45
1:A:191:MET:HE1	2:D:317:TYR:HB2	1.98	0.45
2:D:30:PRO:O	2:D:34:LEU:HG	2.16	0.45
2:D:325:LEU:O	2:D:329:CYS:HB3	2.17	0.45
3:E:734:LYS:HD3	3:E:738:ALA:HB3	1.98	0.45
2:N:66:GLU:OE1	2:N:230:ARG:NH1	2.50	0.45
2:N:278:ARG:HE	3:O:636:ARG:CB	2.29	0.45
3:O:62:ARG:HD2	4:P:5:ARG:HH22	1.81	0.45
3:O:626:LEU:HA	3:O:630:ILE:HG12	1.98	0.45
3:O:731:ASN:O	3:O:735:GLN:N	2.50	0.45
4:P:104:GLU:OE1	4:P:104:GLU:N	2.49	0.45
4:P:438:GLN:O	4:P:441:SER:OG	2.25	0.45
2:D:341:ASN:HA	3:E:699:TYR:CE2	2.52	0.45
3:E:690:ALA:HB3	4:C:63:PHE:HD1	1.81	0.45
4:C:526:LEU:O	4:C:530:SER:N	2.33	0.45
4:C:568:ARG:HA	4:C:571:ARG:HG3	1.99	0.45
1:M:282:GLU:HB2	2:N:370:ALA:HB1	1.99	0.45
2:N:291:TYR:HE2	3:O:653:ALA:HB1	1.81	0.45
3:O:1:MET:HA	3:O:60:ILE:H	1.81	0.45
3:O:647:LEU:HD13	4:P:500:LEU:HG	1.99	0.45
2:D:415:VAL:HG12	3:E:27:LEU:HD11	1.99	0.45
3:E:156:SER:OG	3:E:589:LEU:HB2	2.16	0.45
3:E:160:ALA:HB2	3:E:589:LEU:HD11	1.97	0.45
3:E:658:GLU:O	3:E:661:THR:OG1	2.16	0.45
1:M:30:LEU:HA	1:M:33:GLN:HB2	1.99	0.45
1:M:239:HIS:HE1	3:O:64:LYS:HE3	1.81	0.45
4:P:420:GLN:HA	4:P:423:LEU:HD12	1.98	0.45
4:P:482:ILE:O	4:P:486:ILE:HD13	2.17	0.45
3:E:68:THR:HG22	3:E:72:ILE:HG13	1.99	0.45
1:M:177:LEU:HD12	2:N:306:VAL:HG13	1.98	0.45
2:N:112:LEU:HD11	2:N:121:LEU:HB2	1.98	0.45
2:N:245:ASP:O	2:N:248:SER:N	2.46	0.45
3:O:52:MET:HE2	3:O:55:ILE:HB	1.98	0.45
1:A:106:ASN:ND2	2:D:228:GLU:OE1	2.45	0.45
2:D:110:HIS:NE2	3:E:173:ARG:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:LYS:HA	3:E:178:LEU:HD11	1.99	0.45
2:D:302:LEU:CD2	2:D:305:LEU:HD13	2.46	0.45
2:D:342:VAL:HB	3:E:705:ASP:OD2	2.16	0.45
2:D:345:LEU:HD13	2:D:348:TYR:HE2	1.81	0.45
4:C:446:GLN:HA	4:C:449:VAL:HB	1.98	0.45
1:M:225:THR:HA	1:M:228:ILE:HD12	1.99	0.45
2:N:68:VAL:HG12	3:O:166:LEU:HB3	1.99	0.45
2:N:117:ALA:O	2:N:122:ARG:NE	2.49	0.45
2:N:253:ARG:O	2:N:257:ALA:N	2.50	0.45
3:O:203:TYR:HA	3:O:206:GLN:HB3	1.98	0.45
4:P:574:VAL:HG13	4:P:577:HIS:HE1	1.82	0.45
1:A:148:LYS:HE3	4:C:502:ASN:HD21	1.81	0.45
2:D:18:GLN:NE2	3:E:641:GLU:OE1	2.43	0.45
3:E:680:LEU:O	3:E:684:ARG:HG2	2.17	0.45
4:C:538:THR:HB	4:C:539:PRO:HD3	1.99	0.45
1:M:233:LEU:HD21	2:N:362:TYR:HD1	1.82	0.45
3:O:1:MET:HB2	3:O:2:GLN:NE2	2.31	0.45
4:P:35:ALA:HA	4:P:38:ILE:HD12	1.98	0.45
3:E:668:ALA:HB1	4:C:533:ALA:HB3	1.98	0.45
2:N:58:LEU:HA	2:N:61:MET:HG2	1.98	0.45
2:N:266:ILE:HD12	3:O:628:LYS:HE3	1.99	0.45
2:N:303:ILE:HA	2:N:306:VAL:HG12	1.98	0.45
3:O:662:ASN:O	3:O:666:ASP:N	2.50	0.45
1:A:189:SER:HB2	1:A:193:ASN:HB2	1.99	0.44
1:A:230:HIS:O	3:E:75:ASN:ND2	2.48	0.44
1:A:235:GLU:OE2	3:E:71:ARG:NH2	2.50	0.44
3:E:714:THR:O	3:E:718:TRP:N	2.51	0.44
1:M:110:SER:HB2	2:N:59:GLU:HG3	1.99	0.44
1:M:146:GLU:CD	4:P:121:ARG:HH12	2.21	0.44
2:N:60:ALA:HB1	2:N:64:TYR:HD2	1.81	0.44
3:O:169:ARG:NH2	4:P:150:ALA:HB3	2.32	0.44
3:O:637:GLN:HG3	4:P:465:ILE:HD12	1.99	0.44
3:O:722:ASP:OD1	3:O:722:ASP:N	2.50	0.44
3:E:5:SER:OG	3:E:59:LEU:HD22	2.17	0.44
3:E:549:LYS:NZ	3:E:550:GLU:OE2	2.51	0.44
2:N:311:LEU:HB3	2:N:314:GLN:HB3	2.00	0.44
4:P:573:ILE:HA	4:P:576:HIS:ND1	2.32	0.44
1:A:57:LEU:O	1:A:61:SER:OG	2.28	0.44
1:A:194:TRP:HE1	1:A:197:ASN:HD22	1.65	0.44
1:A:281:ALA:HB1	2:D:372:ALA:HB1	2.00	0.44
2:D:314:GLN:NE2	4:C:535:PRO:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:ASP:HB2	3:E:19:GLN:OE1	2.17	0.44
3:E:57:ASN:HB3	4:C:12:GLU:HG3	1.98	0.44
1:M:51:ILE:HA	1:M:54:LEU:HB2	1.97	0.44
1:M:238:GLU:O	1:M:241:LYS:HG3	2.18	0.44
2:N:22:GLN:HA	3:O:638:ASP:HB3	2.00	0.44
3:O:1:MET:N	3:O:60:ILE:HG12	2.31	0.44
3:O:127:ARG:HD3	4:P:105:VAL:HG13	2.00	0.44
4:P:459:VAL:HB	4:P:460:ARG:HH21	1.82	0.44
4:P:521:ASN:OD1	4:P:525:LEU:HB3	2.17	0.44
2:D:10:GLN:HG3	2:D:11:ASN:H	1.81	0.44
2:D:131:GLU:HG2	3:E:574:ARG:HD3	1.98	0.44
2:D:297:GLN:HA	2:D:301:VAL:HG13	1.98	0.44
4:C:26:PHE:C	4:C:29:PRO:HD2	2.37	0.44
1:M:183:ASP:HB3	2:N:311:LEU:HD11	1.99	0.44
1:M:215:TYR:HA	2:N:338:VAL:HG12	1.98	0.44
1:M:240:ARG:HH12	1:M:289:LEU:HD22	1.82	0.44
2:N:66:GLU:HB3	2:N:230:ARG:HB3	1.99	0.44
3:O:189:ALA:HB3	3:O:549:LYS:HD2	2.00	0.44
1:A:177:LEU:HD22	2:D:301:VAL:HB	1.99	0.44
2:D:334:ALA:O	2:D:338:VAL:N	2.41	0.44
3:E:161:GLU:HA	3:E:164:ARG:HB2	1.99	0.44
1:M:214:LYS:HG3	2:N:338:VAL:HB	2.00	0.44
1:M:264:LYS:HE2	2:N:387:VAL:HG22	1.99	0.44
3:O:212:ARG:HA	3:O:215:ASN:HD21	1.83	0.44
4:P:552:ILE:HA	4:P:556:LEU:HB2	2.00	0.44
1:A:161:ASP:OD1	1:A:162:TYR:N	2.50	0.44
1:A:190:GLN:HB3	2:D:320:MET:HE2	1.99	0.44
1:A:238:GLU:HB3	1:A:242:GLU:OE2	2.18	0.44
1:M:290:GLN:HA	1:M:293:LEU:HG	2.00	0.44
2:N:413:HIS:HA	3:O:27:LEU:HD11	1.99	0.44
3:O:10:THR:HG23	3:O:17:TRP:CZ3	2.53	0.44
3:O:158:GLU:HG3	4:P:140:LEU:HG	1.99	0.44
4:P:105:VAL:O	4:P:109:THR:N	2.50	0.44
4:P:457:HIS:O	4:P:461:ASP:N	2.51	0.44
4:P:538:THR:HB	4:P:539:PRO:HD3	1.99	0.44
1:A:174:LYS:HB2	2:D:297:GLN:HB3	2.00	0.44
1:A:233:LEU:HA	1:A:236:MET:CG	2.41	0.44
2:D:10:GLN:HG3	2:D:11:ASN:N	2.33	0.44
2:D:301:VAL:HA	2:D:304:LYS:HB2	2.00	0.44
3:E:27:LEU:HA	3:E:31:ASN:HB2	1.99	0.44
4:C:49:SER:OG	4:C:53:SER:OG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:559:ALA:HA	4:C:562:GLU:HG3	1.99	0.44
1:M:26:VAL:O	1:M:30:LEU:N	2.37	0.44
1:M:187:CYS:SG	2:N:314:GLN:HB2	2.57	0.44
3:O:194:ALA:HA	3:O:198:LYS:CB	2.48	0.44
4:C:415:ILE:HA	4:C:418:GLU:HB3	2.00	0.44
1:M:96:ALA:O	1:M:103:LEU:HG	2.18	0.44
1:M:141:ARG:HG2	3:O:616:ARG:HG3	2.00	0.44
1:M:275:LYS:HG2	1:M:278:PHE:CZ	2.53	0.44
2:N:269:GLU:HA	2:N:272:ARG:HB3	1.99	0.44
3:O:211:GLN:O	3:O:215:ASN:ND2	2.51	0.44
3:O:606:LEU:HD23	3:O:607:GLU:HG3	1.99	0.44
1:A:137:ASP:O	1:A:140:LEU:N	2.49	0.44
3:E:684:ARG:HH22	4:C:64:GLN:HA	1.82	0.44
3:E:691:GLN:HB2	4:C:60:TYR:CZ	2.52	0.44
3:E:712:ALA:HB3	3:E:715:VAL:HB	2.00	0.44
4:C:128:THR:HG23	4:C:129:GLN:HG2	2.00	0.44
4:C:419:LEU:HD12	4:C:422:TYR:HD2	1.83	0.44
1:M:231:ARG:O	1:M:235:GLU:N	2.49	0.44
1:M:239:HIS:CE1	3:O:64:LYS:HE3	2.53	0.44
2:N:282:TYR:CE2	3:O:639:LEU:HD23	2.53	0.44
3:O:128:GLU:O	3:O:132:LYS:N	2.47	0.44
1:A:146:GLU:HB3	2:D:277:LEU:HD12	2.00	0.43
1:A:240:ARG:NH1	1:A:289:LEU:HD13	2.33	0.43
2:D:344:LEU:HD13	3:E:701:ARG:NE	2.32	0.43
3:E:709:GLU:OE2	4:C:555:LYS:HE2	2.18	0.43
2:N:72:GLU:HG2	3:O:166:LEU:HD22	1.99	0.43
2:N:365:GLU:O	2:N:369:GLU:HG3	2.17	0.43
2:N:414:GLN:NE2	2:N:418:ASP:OD2	2.51	0.43
3:O:538:ASP:O	3:O:542:SER:N	2.35	0.43
3:O:584:ARG:NH1	3:O:621:CYS:HB3	2.34	0.43
3:O:613:LEU:O	3:O:617:GLY:N	2.46	0.43
4:P:494:SER:HA	4:P:497:GLN:HG2	2.00	0.43
4:P:496:LEU:HD23	4:P:500:LEU:HD22	1.99	0.43
1:A:149:ARG:HH21	2:D:278:ARG:HA	1.83	0.43
2:D:138:GLU:O	3:E:178:LEU:HD21	2.17	0.43
2:D:320:MET:SD	2:D:324:TRP:HB3	2.57	0.43
3:E:21:GLU:HB3	3:E:52:MET:HE2	2.00	0.43
3:E:585:ILE:HG23	3:E:623:LEU:HD21	2.00	0.43
3:E:620:ALA:H	4:C:460:ARG:HH22	1.66	0.43
1:M:98:MET:SD	1:M:98:MET:N	2.91	0.43
2:N:135:GLU:C	2:N:139:LYS:HZ3	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:208:LEU:O	2:N:212:ILE:HD12	2.17	0.43
1:A:222:VAL:HG12	1:A:226:PRO:HG3	2.00	0.43
1:A:235:GLU:CA	1:A:238:GLU:HB2	2.45	0.43
3:E:603:ALA:HA	3:E:606:LEU:HB3	2.00	0.43
3:E:643:GLY:O	3:E:646:LEU:HG	2.18	0.43
4:C:523:GLN:HG3	4:C:524:GLN:HG2	1.99	0.43
4:C:597:ARG:NE	4:C:604:GLU:OE1	2.35	0.43
2:N:321:GLN:HA	2:N:325:LEU:HB2	2.01	0.43
1:A:165:LYS:NZ	3:E:124:LEU:HD11	2.34	0.43
2:D:228:GLU:O	2:D:232:LYS:HD3	2.19	0.43
3:E:659:ARG:O	3:E:663:TYR:N	2.45	0.43
4:C:590:ASP:HA	4:C:593:CYS:SG	2.59	0.43
1:M:184:VAL:HG22	2:N:311:LEU:HA	1.99	0.43
3:O:68:THR:CG2	3:O:71:ARG:HB3	2.49	0.43
3:O:126:GLU:OE2	4:P:106:ARG:NH1	2.46	0.43
4:P:571:ARG:HH21	4:P:574:VAL:HG11	1.83	0.43
1:A:36:ALA:O	1:A:39:LYS:HG3	2.18	0.43
1:A:261:PRO:N	1:A:262:PRO:HD2	2.33	0.43
2:D:108:LEU:HA	2:D:111:ARG:HG2	2.01	0.43
2:D:334:ALA:HA	2:D:337:ARG:HB2	2.00	0.43
2:D:372:ALA:O	2:D:376:LYS:HG2	2.19	0.43
3:E:21:GLU:HA	3:E:66:GLU:HG2	2.00	0.43
3:E:62:ARG:NH2	4:C:5:ARG:HD2	2.33	0.43
1:M:167:ILE:HG22	4:P:104:GLU:HA	2.00	0.43
2:N:196:LEU:HD13	4:P:427:ARG:O	2.18	0.43
2:N:196:LEU:HD22	4:P:427:ARG:HB3	2.01	0.43
2:N:318:ASN:OD1	2:N:319:GLU:N	2.51	0.43
4:P:589:VAL:HA	4:P:592:PHE:CZ	2.54	0.43
4:P:600:ASN:O	4:P:604:GLU:HB2	2.17	0.43
1:A:72:ALA:HA	4:C:452:ARG:HH22	1.84	0.43
1:A:123:ILE:HD11	2:D:241:ALA:HB3	2.01	0.43
2:D:310:LYS:HG3	2:D:311:LEU:HD23	2.00	0.43
2:D:388:ASP:HB2	2:D:389:PRO:HD3	2.00	0.43
3:E:164:ARG:HB3	3:E:565:LEU:HD21	2.00	0.43
4:C:539:PRO:CG	4:C:543:MET:HE3	2.48	0.43
1:M:174:LYS:NZ	2:N:294:VAL:HG23	2.33	0.43
2:N:69:ALA:O	2:N:73:GLU:HB2	2.18	0.43
2:N:112:LEU:O	2:N:117:ALA:HB2	2.19	0.43
3:O:1:MET:SD	3:O:61:ASN:ND2	2.86	0.43
4:P:7:CYS:SG	4:P:20:LYS:HG2	2.59	0.43
4:P:50:ASN:O	4:P:54:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HA	3:E:71:ARG:HH12	1.83	0.43
1:A:248:LYS:HB3	1:A:249:PRO:HD3	2.00	0.43
3:E:145:ARG:HD3	3:E:614:ARG:HD2	2.00	0.43
4:C:510:ARG:HE	4:C:513:ASN:HD22	1.66	0.43
1:M:239:HIS:CD2	2:N:422:HIS:HA	2.54	0.43
3:O:531:PRO:HG3	4:P:409:PHE:CE1	2.54	0.43
3:O:580:PRO:HA	4:P:452:ARG:HG3	2.00	0.43
3:O:735:GLN:HG2	3:O:739:PHE:CG	2.54	0.43
4:P:158:ILE:HD12	4:P:161:ILE:HD13	2.01	0.43
4:P:606:ASN:O	4:P:609:VAL:HG22	2.18	0.43
1:A:264:LYS:HE3	2:D:397:GLN:NE2	2.30	0.43
3:E:171:ASN:HB2	3:E:564:MET:CE	2.49	0.43
3:E:223:SER:OG	3:E:224:LEU:N	2.52	0.43
2:N:13:PRO:O	2:N:17:ASN:ND2	2.51	0.43
2:N:334:ALA:O	2:N:338:VAL:HG22	2.19	0.43
3:O:584:ARG:HH21	4:P:453:ASP:HA	1.84	0.43
4:P:184:GLN:NE2	4:P:185:GLU:OE2	2.48	0.43
4:P:449:VAL:HG12	4:P:449:VAL:O	2.18	0.43
1:A:232:GLU:HG3	1:A:236:MET:SD	2.59	0.43
2:D:344:LEU:HB2	3:E:701:ARG:HE	1.83	0.43
3:E:629:ALA:O	3:E:633:VAL:HG13	2.19	0.43
4:C:448:ALA:O	4:C:452:ARG:HG2	2.19	0.43
4:C:566:GLU:HA	4:C:570:LYS:NZ	2.34	0.43
1:M:179:GLN:NE2	1:M:180:LEU:HG	2.31	0.43
3:O:657:TYR:O	3:O:660:THR:OG1	2.20	0.43
4:P:574:VAL:O	4:P:577:HIS:ND1	2.52	0.43
1:A:43:ASN:HA	1:A:46:TYR:CD2	2.53	0.43
1:A:165:LYS:HB2	4:C:520:GLN:HE22	1.84	0.43
2:D:70:MET:HB3	2:D:230:ARG:NE	2.29	0.43
2:D:314:GLN:HE22	4:C:535:PRO:HB3	1.84	0.43
2:D:333:ASN:ND2	3:E:688:GLN:HE21	2.17	0.43
2:D:365:GLU:HG3	3:E:4:LEU:O	2.19	0.43
4:C:189:TYR:HB3	4:C:404:ASN:ND2	2.33	0.43
1:M:120:LEU:HB2	2:N:50:MET:HG3	1.99	0.43
2:N:314:GLN:HG3	2:N:318:ASN:HB3	2.01	0.43
2:N:343:LEU:O	2:N:347:THR:HG23	2.19	0.43
3:E:203:TYR:HA	3:E:207:ALA:HB3	2.01	0.42
3:E:651:PHE:O	3:E:655:GLN:N	2.47	0.42
4:C:561:GLU:HG2	4:C:562:GLU:N	2.34	0.42
2:N:65:CYS:HB3	2:N:234:LYS:HE2	2.00	0.42
2:N:360:ARG:HH22	3:O:4:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:55:ILE:O	3:O:63:VAL:HG23	2.19	0.42
3:O:163:LYS:HG3	3:O:589:LEU:HD12	2.00	0.42
3:O:534:GLU:HA	3:O:537:VAL:HG22	1.99	0.42
3:O:678:GLN:O	3:O:681:PRO:HD2	2.19	0.42
4:P:512:ILE:HG22	4:P:516:CYS:SG	2.59	0.42
4:P:577:HIS:O	4:P:581:VAL:HG22	2.19	0.42
1:A:177:LEU:HA	1:A:180:LEU:HD23	2.01	0.42
3:E:659:ARG:HA	3:E:659:ARG:HD3	1.74	0.42
4:C:143:GLY:O	4:C:147:ARG:HD3	2.19	0.42
1:M:86:ALA:HA	1:M:89:ILE:HG12	2.01	0.42
1:M:173:LEU:HA	1:M:176:ILE:HB	2.01	0.42
2:N:35:VAL:HB	4:P:471:ALA:O	2.19	0.42
2:N:236:ASP:OD1	2:N:237:LYS:N	2.53	0.42
2:D:374:TYR:OH	3:E:41:ILE:HD13	2.20	0.42
3:E:123:ALA:HB2	4:C:106:ARG:NH1	2.34	0.42
1:M:157:ASN:HD21	2:N:284:ALA:HB2	1.84	0.42
2:N:234:LYS:HZ2	2:N:237:LYS:HD2	1.84	0.42
2:N:237:LYS:NZ	4:P:142:GLN:HE21	2.18	0.42
2:N:266:ILE:HG13	2:N:267:ILE:N	2.34	0.42
2:N:288:PHE:O	2:N:292:TYR:N	2.45	0.42
3:O:60:ILE:HD11	4:P:24:ASP:CG	2.40	0.42
3:O:745:LEU:H	3:O:745:LEU:HD23	1.83	0.42
2:D:64:TYR:HB2	3:E:167:ASP:OD2	2.20	0.42
1:M:122:ASN:HB3	1:M:134:ALA:HB2	2.01	0.42
1:M:137:ASP:HA	1:M:140:LEU:HB2	2.01	0.42
1:M:223:GLY:O	1:M:226:PRO:HD2	2.19	0.42
1:M:234:VAL:O	1:M:238:GLU:N	2.48	0.42
3:O:155:VAL:HA	4:P:141:ILE:HD11	2.00	0.42
3:O:581:SER:O	3:O:585:ILE:HG13	2.18	0.42
3:O:591:TYR:CD1	3:O:600:ALA:HB1	2.54	0.42
3:O:679:TRP:NE1	4:P:541:PRO:HG3	2.31	0.42
1:A:154:LYS:HD2	1:A:154:LYS:HA	1.84	0.42
1:A:177:LEU:HD12	1:A:180:LEU:HB2	2.01	0.42
2:D:396:ARG:HD2	2:D:396:ARG:HA	1.80	0.42
3:E:3:SER:OG	3:E:4:LEU:N	2.52	0.42
4:C:568:ARG:HD2	4:C:571:ARG:NH1	2.35	0.42
4:C:570:LYS:O	4:C:574:VAL:HG23	2.19	0.42
1:M:77:LEU:HB2	2:N:47:ARG:NH2	2.34	0.42
2:N:36:THR:HA	4:P:455:PHE:CE1	2.54	0.42
2:N:371:SER:HA	2:N:422:HIS:CG	2.54	0.42
3:O:163:LYS:HD2	3:O:570:GLN:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD23	4:C:452:ARG:NE	2.35	0.42
1:A:223:GLY:O	1:A:229:SER:OG	2.22	0.42
2:D:296:GLU:O	2:D:301:VAL:HG13	2.20	0.42
2:D:360:ARG:HA	2:D:360:ARG:NE	2.35	0.42
3:E:163:LYS:HE3	3:E:572:LEU:HD11	2.02	0.42
4:C:585:ARG:HH12	4:C:597:ARG:NH1	2.17	0.42
1:M:140:LEU:HA	1:M:143:THR:OG1	2.19	0.42
1:M:150:ALA:O	1:M:154:LYS:HB2	2.18	0.42
1:M:159:LEU:HB3	4:P:512:ILE:HG21	2.02	0.42
1:M:250:VAL:HG13	1:M:253:THR:HB	2.02	0.42
2:N:419:LEU:HD13	3:O:20:LYS:O	2.19	0.42
3:O:187:ASP:HA	4:P:168:ARG:HH12	1.84	0.42
1:A:33:GLN:HB3	1:A:36:ALA:HB3	2.01	0.42
1:A:81:GLU:C	1:A:85:GLN:HE22	2.22	0.42
2:D:63:ILE:HA	2:D:67:ALA:CB	2.39	0.42
2:D:278:ARG:NH1	3:E:636:ARG:HD2	2.34	0.42
3:E:668:ALA:HA	4:C:534:GLN:HG2	2.01	0.42
3:E:734:LYS:HD2	4:C:604:GLU:HG3	2.01	0.42
4:C:157:GLN:O	4:C:161:ILE:HG12	2.19	0.42
2:N:35:VAL:HB	4:P:472:GLY:HA2	2.00	0.42
2:N:360:ARG:HA	4:P:21:LEU:HD21	2.01	0.42
3:O:3:SER:O	3:O:5:SER:N	2.52	0.42
3:O:716:VAL:O	3:O:719:VAL:HG22	2.20	0.42
4:P:508:ARG:HB3	4:P:512:ILE:HD12	2.02	0.42
2:D:104:VAL:O	2:D:107:THR:OG1	2.29	0.42
2:D:285:ASP:OD1	3:E:646:LEU:HD23	2.19	0.42
3:E:573:ALA:HA	4:C:438:GLN:HA	2.01	0.42
3:E:599:ASP:HB3	4:C:449:VAL:HG12	2.02	0.42
3:E:684:ARG:NH2	4:C:64:GLN:HA	2.35	0.42
2:N:62:ALA:HB2	2:N:235:CYS:SG	2.60	0.42
2:N:333:ASN:HD22	3:O:688:GLN:CG	2.33	0.42
1:A:22:ARG:HG2	1:A:43:ASN:HB3	2.01	0.42
1:A:74:ASP:OD1	2:D:50:MET:N	2.52	0.42
2:D:135:GLU:HG2	2:D:139:LYS:HZ2	1.84	0.42
2:D:311:LEU:HD22	4:C:534:GLN:CG	2.46	0.42
2:N:199:THR:HB	2:N:200:PRO:HD3	2.02	0.42
2:N:321:GLN:HB2	2:N:325:LEU:HB2	2.01	0.42
2:N:368:GLU:HA	2:N:371:SER:HB2	2.00	0.42
3:O:684:ARG:HH12	4:P:64:GLN:HA	1.84	0.42
4:P:518:HIS:O	4:P:522:LEU:HG	2.20	0.42
1:A:63:ALA:HA	1:A:67:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:LEU:HB3	3:E:664:CYS:SG	2.60	0.42
2:D:360:ARG:HH21	2:D:363:LEU:HB2	1.84	0.42
4:C:419:LEU:O	4:C:423:LEU:N	2.48	0.42
1:M:41:VAL:HA	1:M:44:PHE:CE2	2.55	0.42
1:M:162:TYR:HD2	4:P:516:CYS:HG	1.66	0.42
2:N:279:GLU:HA	2:N:282:TYR:CD2	2.55	0.42
4:P:102:ILE:N	4:P:104:GLU:OE1	2.53	0.42
1:A:90:ARG:HA	1:A:90:ARG:HD3	1.86	0.41
1:A:183:ASP:HB3	2:D:310:LYS:NZ	2.34	0.41
1:A:231:ARG:HA	3:E:71:ARG:NH1	2.35	0.41
4:C:494:SER:HA	4:C:497:GLN:HG2	2.02	0.41
1:M:160:LEU:O	1:M:163:THR:OG1	2.25	0.41
1:M:239:HIS:CE1	2:N:367:THR:HG21	2.55	0.41
3:O:211:GLN:HG3	3:O:215:ASN:HD22	1.85	0.41
3:O:216:SER:HA	3:O:219:GLU:HB2	2.02	0.41
3:O:610:GLU:CG	3:O:613:LEU:HB2	2.50	0.41
1:A:150:ALA:HB1	4:C:115:GLU:HG3	2.01	0.41
2:D:253:ARG:NH1	2:D:254:ASN:OD1	2.44	0.41
2:D:272:ARG:HH21	4:C:121:ARG:HD2	1.85	0.41
2:D:278:ARG:HG2	2:D:281:LEU:HD22	2.03	0.41
2:D:286:ARG:HH12	3:E:639:LEU:HD11	1.85	0.41
3:E:134:VAL:HG13	4:C:119:LEU:HD22	2.01	0.41
3:E:142:ARG:HH22	3:E:614:ARG:HH12	1.68	0.41
4:C:120:GLN:HA	4:C:123:LEU:HB3	2.02	0.41
1:M:138:ILE:HD11	2:N:269:GLU:HB3	2.02	0.41
1:M:233:LEU:HD21	2:N:362:TYR:CD1	2.55	0.41
2:N:270:ILE:HD11	3:O:623:LEU:HG	2.01	0.41
1:A:110:SER:OG	2:D:231:LEU:O	2.38	0.41
1:A:234:VAL:HG21	3:E:71:ARG:CZ	2.50	0.41
2:D:105:TYR:O	2:D:109:GLU:HG3	2.20	0.41
2:D:336:LEU:HG	3:E:706:GLU:HG3	2.02	0.41
2:D:423:ASP:O	3:E:67:LYS:NZ	2.35	0.41
3:E:718:TRP:O	3:E:722:ASP:N	2.53	0.41
2:N:231:LEU:O	2:N:235:CYS:HB2	2.21	0.41
2:N:321:GLN:CA	2:N:325:LEU:HB2	2.50	0.41
3:O:580:PRO:CA	4:P:452:ARG:HG3	2.50	0.41
1:A:81:GLU:HG3	1:A:85:GLN:NE2	2.34	0.41
1:A:82:TYR:HB3	2:D:57:TYR:HB2	2.03	0.41
1:A:128:LEU:HA	1:A:131:PHE:CD2	2.55	0.41
1:A:240:ARG:CZ	1:A:289:LEU:HD13	2.50	0.41
2:D:371:SER:HB2	3:E:20:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:648:ASP:O	3:E:652:ARG:HG2	2.19	0.41
4:C:596:GLU:HG2	4:C:599:ARG:HB3	2.01	0.41
1:M:180:LEU:HD23	1:M:180:LEU:HA	1.86	0.41
2:N:68:VAL:HG21	3:O:168:GLU:HA	2.01	0.41
3:O:5:SER:O	3:O:59:LEU:HD21	2.20	0.41
3:O:36:SER:O	3:O:36:SER:OG	2.37	0.41
1:A:43:ASN:HA	1:A:46:TYR:HD2	1.85	0.41
1:A:115:ALA:HB1	2:D:55:LEU:HG	2.03	0.41
3:E:59:LEU:HA	3:E:63:VAL:HB	2.01	0.41
3:E:548:GLU:OE2	4:C:422:TYR:OH	2.30	0.41
3:E:572:LEU:HB3	4:C:438:GLN:HE21	1.85	0.41
1:M:88:ARG:NH1	2:N:105:TYR:OH	2.53	0.41
1:M:169:ARG:NH1	4:P:523:GLN:OE1	2.44	0.41
1:M:175:LYS:O	1:M:179:GLN:N	2.31	0.41
3:O:58:PHE:N	3:O:58:PHE:CD1	2.89	0.41
2:D:66:GLU:HG3	2:D:230:ARG:HB2	2.03	0.41
2:D:234:LYS:HD2	2:D:238:LEU:HD21	2.03	0.41
2:D:336:LEU:HD22	3:E:693:SER:HB3	2.02	0.41
3:E:60:ILE:HA	3:E:64:LYS:HZ3	1.85	0.41
3:E:140:ILE:O	3:E:143:ARG:HG2	2.20	0.41
3:E:675:ILE:HG12	3:E:682:GLU:HG2	2.02	0.41
1:M:89:ILE:HG23	2:N:63:ILE:HG13	2.02	0.41
2:N:118:ALA:HA	2:N:122:ARG:HE	1.85	0.41
2:N:261:GLU:HB2	2:N:264:LYS:HE3	2.01	0.41
2:N:278:ARG:HH22	4:P:462:LEU:HD22	1.85	0.41
3:O:705:ASP:HA	3:O:708:TRP:HB2	2.03	0.41
4:P:462:LEU:HD12	4:P:463:LEU:N	2.35	0.41
1:A:88:ARG:HD3	3:E:170:ALA:HB3	2.02	0.41
1:A:282:GLU:OE2	2:D:370:ALA:HB1	2.21	0.41
3:E:18:LEU:HB3	3:E:56:TRP:CZ2	2.56	0.41
3:E:549:LYS:HE3	3:E:549:LYS:HB3	1.93	0.41
3:E:565:LEU:HD11	4:C:151:THR:HG23	2.01	0.41
3:E:710:GLN:HE21	3:E:716:VAL:HB	1.85	0.41
4:C:515:LEU:HD23	4:C:519:ILE:HB	2.02	0.41
4:C:532:THR:HA	4:C:535:PRO:HG2	2.03	0.41
1:M:154:LYS:HE3	4:P:115:GLU:HA	2.02	0.41
2:N:42:ASP:OD2	2:N:45:LEU:HD12	2.21	0.41
2:N:135:GLU:O	2:N:138:GLU:HB2	2.21	0.41
2:N:365:GLU:HB3	3:O:60:ILE:HB	2.02	0.41
4:P:535:PRO:C	4:P:539:PRO:HG2	2.41	0.41
1:A:180:LEU:CD1	2:D:310:LYS:HE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:O	1:A:210:GLN:NE2	2.44	0.41
2:D:365:GLU:HB3	3:E:5:SER:HA	2.03	0.41
3:E:154:GLU:N	3:E:154:GLU:OE1	2.54	0.41
3:E:180:GLU:O	3:E:184:GLN:N	2.54	0.41
4:C:26:PHE:HA	4:C:29:PRO:HD2	2.01	0.41
1:M:170:LEU:HD23	2:N:295:LEU:HA	2.03	0.41
1:M:294:GLU:O	1:M:298:GLU:N	2.53	0.41
2:N:66:GLU:HB2	2:N:234:LYS:HG3	2.03	0.41
3:O:663:TYR:HA	3:O:667:LEU:HB3	2.01	0.41
1:A:41:VAL:HA	1:A:44:PHE:CD2	2.55	0.41
1:A:72:ALA:HA	4:C:452:ARG:NH2	2.36	0.41
1:A:83:ARG:NH1	2:D:127:SER:OG	2.40	0.41
1:A:85:GLN:O	1:A:87:ALA:N	2.54	0.41
1:A:132:LEU:HG	1:A:133:VAL:HG23	2.03	0.41
1:A:235:GLU:O	1:A:239:HIS:N	2.51	0.41
2:D:81:ALA:HA	2:D:88:ASP:HB2	2.02	0.41
2:D:234:LYS:HA	2:D:234:LYS:HD3	1.79	0.41
2:D:237:LYS:HG3	2:D:238:LEU:HD23	2.03	0.41
2:D:367:THR:HA	2:D:370:ALA:HB3	2.03	0.41
3:E:165:MET:CG	4:C:147:ARG:HA	2.50	0.41
3:E:182:TYR:CZ	3:E:556:GLN:HG3	2.56	0.41
3:E:183:ASP:O	3:E:187:ASP:N	2.47	0.41
3:E:208:ASN:HD21	4:C:178:ARG:NH1	2.18	0.41
3:E:219:GLU:HB2	4:C:188:HIS:HB3	2.02	0.41
3:E:649:HIS:O	3:E:653:ALA:N	2.46	0.41
4:C:536:ILE:O	4:C:540:TRP:N	2.54	0.41
1:M:113:VAL:HG22	2:N:236:ASP:HB3	2.03	0.41
1:M:170:LEU:HA	1:M:173:LEU:HD13	2.02	0.41
1:M:236:MET:CE	1:M:292:ALA:HB3	2.51	0.41
2:N:125:LEU:HD23	2:N:125:LEU:HA	1.93	0.41
2:N:333:ASN:N	3:O:689:ASN:OD1	2.54	0.41
3:O:26:GLN:OE1	3:O:51:ASN:ND2	2.54	0.41
3:O:60:ILE:HG13	3:O:61:ASN:N	2.36	0.41
3:O:166:LEU:O	3:O:169:ARG:NE	2.54	0.41
1:A:164:ARG:HH12	2:D:287:LYS:HB2	1.86	0.41
1:A:295:THR:HB	2:D:354:SER:HB2	2.03	0.41
2:D:113:VAL:HA	3:E:174:HIS:CE1	2.56	0.41
2:D:333:ASN:HD22	3:E:688:GLN:HE21	1.68	0.41
3:E:188:GLU:OE1	4:C:417:SER:OG	2.39	0.41
1:M:240:ARG:NH2	1:M:286:GLU:OE2	2.54	0.41
1:M:240:ARG:HE	1:M:243:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:368:GLU:HG2	3:O:17:TRP:CD1	2.56	0.41
3:O:163:LYS:HZ1	3:O:586:SER:HB3	1.85	0.41
3:O:561:SER:OG	4:P:158:ILE:HD13	2.21	0.41
1:A:157:ASN:ND2	2:D:287:LYS:HD2	2.35	0.40
1:A:234:VAL:HG23	1:A:235:GLU:OE1	2.21	0.40
2:D:68:VAL:HG23	3:E:162:ARG:HH22	1.86	0.40
3:E:42:ASP:N	3:E:42:ASP:OD1	2.54	0.40
4:C:546:LEU:HD23	4:C:549:MET:HG3	2.03	0.40
1:M:23:ILE:H	1:M:23:ILE:HD12	1.85	0.40
1:M:65:SER:O	1:M:69:THR:OG1	2.39	0.40
1:M:147:GLU:HB3	3:O:141:VAL:HB	2.03	0.40
1:M:169:ARG:HB3	4:P:523:GLN:HB2	2.03	0.40
2:N:52:ARG:HE	2:N:56:ARG:HE	1.68	0.40
2:N:52:ARG:O	2:N:55:LEU:HB3	2.20	0.40
2:N:122:ARG:HA	2:N:125:LEU:HG	2.02	0.40
2:N:237:LYS:HD3	2:N:238:LEU:HD22	2.03	0.40
3:O:626:LEU:HD13	4:P:459:VAL:HG13	2.02	0.40
3:O:742:LYS:HE3	4:P:598:LEU:HD13	2.02	0.40
2:D:321:GLN:HB2	4:C:542:LEU:HD13	2.03	0.40
2:D:343:LEU:HG	3:E:705:ASP:OD2	2.21	0.40
1:M:23:ILE:HG13	1:M:44:PHE:CD1	2.57	0.40
1:M:48:HIS:HA	1:M:51:ILE:HG12	2.01	0.40
1:M:235:GLU:O	1:M:239:HIS:ND1	2.54	0.40
1:M:236:MET:HA	1:M:239:HIS:ND1	2.36	0.40
1:M:293:LEU:O	1:M:297:ASP:N	2.54	0.40
2:N:10:GLN:OE1	3:O:647:LEU:HD12	2.21	0.40
2:N:282:TYR:CZ	3:O:639:LEU:HD23	2.56	0.40
3:O:157:ARG:HG2	3:O:592:PRO:HG3	2.03	0.40
3:O:180:GLU:HA	3:O:183:ASP:HB2	2.04	0.40
4:P:542:LEU:O	4:P:546:LEU:N	2.54	0.40
4:P:544:LYS:O	4:P:548:GLU:HB3	2.22	0.40
1:A:148:LYS:HE2	3:E:611:PHE:CE2	2.55	0.40
1:A:169:ARG:HB2	2:D:298:ILE:HD12	2.03	0.40
2:D:68:VAL:HG12	3:E:170:ALA:HB2	2.03	0.40
3:E:1:MET:HE2	3:E:1:MET:HB3	1.85	0.40
3:E:44:ILE:HG12	3:E:48:CYS:SG	2.61	0.40
1:M:150:ALA:HA	1:M:154:LYS:HG2	2.03	0.40
2:N:27:CYS:C	2:N:30:PRO:HD2	2.42	0.40
2:N:33:SER:HB3	2:N:37:LYS:HD3	2.02	0.40
2:N:324:TRP:CE3	2:N:325:LEU:HD22	2.57	0.40
4:P:126:LEU:HA	4:P:126:LEU:HD23	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:572:GLU:HG3	4:P:576:HIS:CE1	2.57	0.40
1:A:107:VAL:HA	2:D:231:LEU:HD21	2.02	0.40
1:A:151:LYS:HG2	3:E:138:ARG:NE	2.35	0.40
1:A:227:LYS:HB2	4:C:28:TRP:HZ2	1.86	0.40
1:A:260:LEU:HB2	1:A:261:PRO:HD3	2.03	0.40
2:D:274:GLU:OE1	2:D:278:ARG:NH1	2.43	0.40
3:E:1:MET:HE2	3:E:2:GLN:HE22	1.87	0.40
3:E:717:ASP:O	3:E:721:VAL:HG23	2.21	0.40
4:C:518:HIS:NE2	4:C:526:LEU:HD21	2.36	0.40
1:M:37:VAL:HG22	1:M:41:VAL:HG23	2.04	0.40
1:M:153:GLN:O	1:M:157:ASN:N	2.37	0.40
2:N:230:ARG:HA	2:N:233:GLU:HG3	2.04	0.40
2:N:364:VAL:HG21	3:O:61:ASN:OD1	2.21	0.40
3:O:660:THR:O	3:O:664:CYS:N	2.49	0.40
3:O:675:ILE:HG23	3:O:678:GLN:HB3	2.03	0.40
4:P:51:VAL:HA	4:P:54:LEU:HD12	2.04	0.40
4:P:461:ASP:O	4:P:465:ILE:HG13	2.21	0.40
4:P:570:LYS:O	4:P:573:ILE:HG22	2.21	0.40
4:P:603:ARG:HG3	4:P:603:ARG:O	2.21	0.40
1:A:156:SER:OG	4:C:508:ARG:HG2	2.21	0.40
2:D:318:ASN:O	2:D:322:LYS:N	2.46	0.40
3:E:59:LEU:HD23	3:E:60:ILE:HG12	2.04	0.40
3:E:535:VAL:O	3:E:539:ILE:HG13	2.20	0.40
3:E:545:ASP:HA	3:E:548:GLU:HG2	2.04	0.40
3:E:709:GLU:OE2	4:C:552:ILE:HA	2.21	0.40
4:C:28:TRP:HB2	4:C:29:PRO:HD3	2.04	0.40
4:C:597:ARG:HD2	4:C:597:ARG:HA	1.84	0.40
2:N:6:GLN:O	2:N:10:GLN:HG2	2.22	0.40
2:N:278:ARG:CG	3:O:636:ARG:HB2	2.52	0.40
3:O:607:GLU:OE1	3:O:614:ARG:HA	2.22	0.40
4:P:536:ILE:C	4:P:539:PRO:HD2	2.42	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	278/298 (93%)	250 (90%)	28 (10%)	0	100	100
1	M	278/298 (93%)	257 (92%)	21 (8%)	0	100	100
2	D	361/423 (85%)	336 (93%)	25 (7%)	0	100	100
2	N	361/423 (85%)	320 (89%)	41 (11%)	0	100	100
3	E	399/747 (53%)	363 (91%)	34 (8%)	2 (0%)	25	64
3	O	399/747 (53%)	355 (89%)	44 (11%)	0	100	100
4	C	369/617 (60%)	346 (94%)	23 (6%)	0	100	100
4	P	365/617 (59%)	340 (93%)	25 (7%)	0	100	100
All	All	2810/4170 (67%)	2567 (91%)	241 (9%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	60	ILE
3	E	155	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/254 (95%)	238 (98%)	4 (2%)	56	72
1	M	242/254 (95%)	238 (98%)	4 (2%)	56	72
2	D	304/368 (83%)	301 (99%)	3 (1%)	73	82
2	N	304/368 (83%)	302 (99%)	2 (1%)	81	87
3	E	353/644 (55%)	350 (99%)	3 (1%)	79	85
3	O	353/644 (55%)	352 (100%)	1 (0%)	91	92
4	C	323/538 (60%)	319 (99%)	4 (1%)	67	78
4	P	320/538 (60%)	318 (99%)	2 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2441/3608 (68%)	2418 (99%)	23 (1%)	74 83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	39	LYS
1	A	124	ARG
1	A	149	ARG
2	D	230	ARG
2	D	278	ARG
2	D	327	LYS
3	E	142	ARG
3	E	701	ARG
3	E	746	ARG
4	C	145	ARG
4	C	603	ARG
4	C	610	ARG
4	C	612	ARG
1	M	39	LYS
1	M	76	ARG
1	M	241	LYS
1	M	248	LYS
2	N	327	LYS
2	N	360	ARG
3	O	574	ARG
4	P	121	ARG
4	P	612	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	157	ASN
2	D	314	GLN
2	D	318	ASN
2	D	358	ASN
2	D	361	ASN
2	D	385	GLN
2	D	397	GLN
3	E	2	GLN

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Mol	Chain	Res	Type
3	E	174	HIS
3	E	688	GLN
3	E	710	GLN
4	C	120	GLN
4	C	157	GLN
4	C	188	HIS
4	C	466	HIS
1	M	179	GLN
2	N	407	ASN
3	O	2	GLN
3	O	19	GLN
3	O	215	ASN
3	O	689	ASN
4	P	520	GLN
4	P	613	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

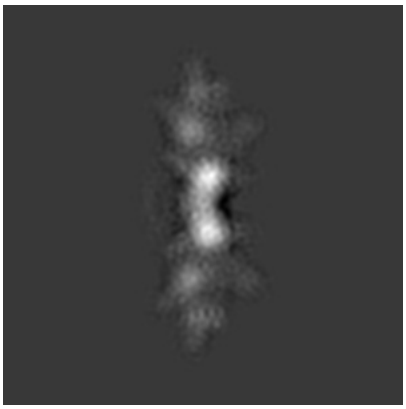
This section contains visualisations of the EMDB entry EMD-49227. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map

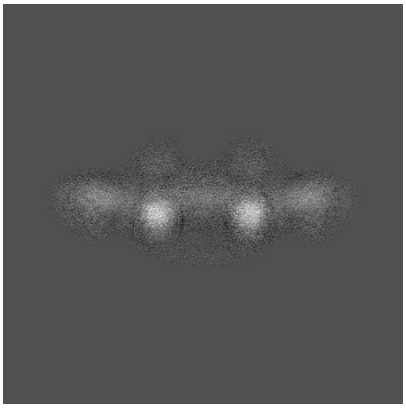
X



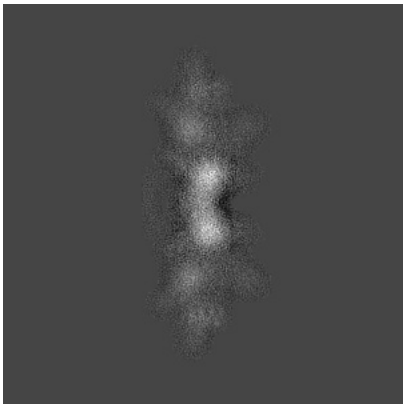
Y

Z

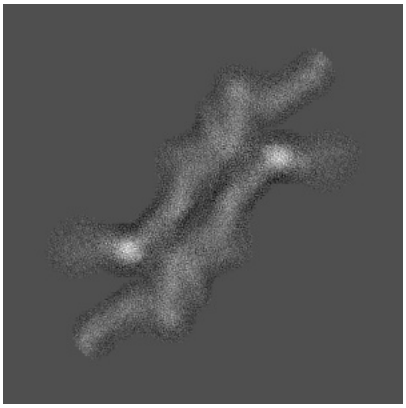
6.1.2 Raw map



X



Y

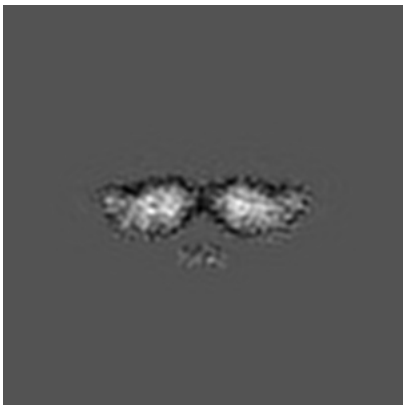


Z

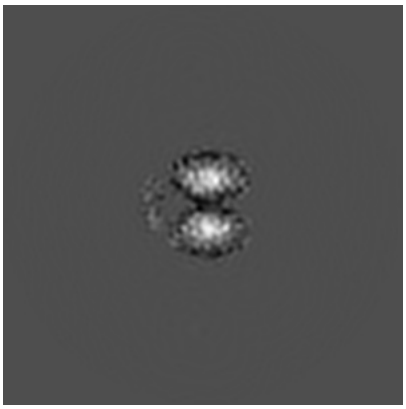
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



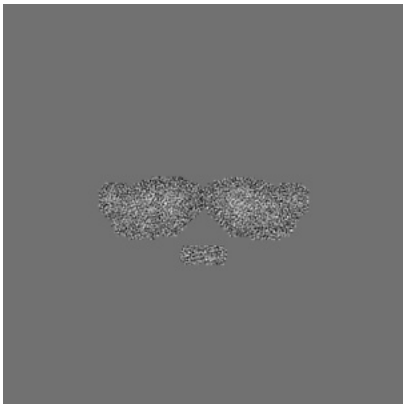
X Index: 192



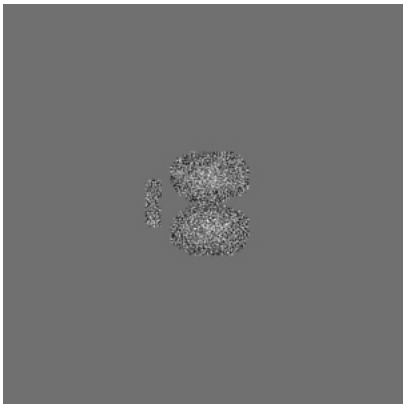
Y Index: 192

Z Index: 192

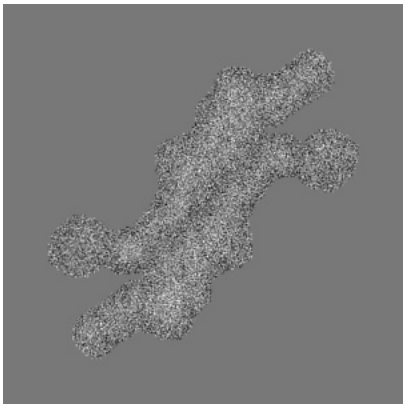
6.2.2 Raw map



X Index: 192



Y Index: 192

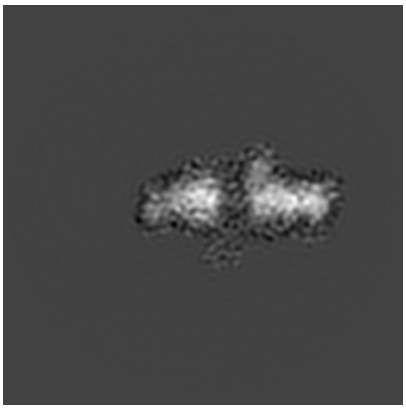


Z Index: 192

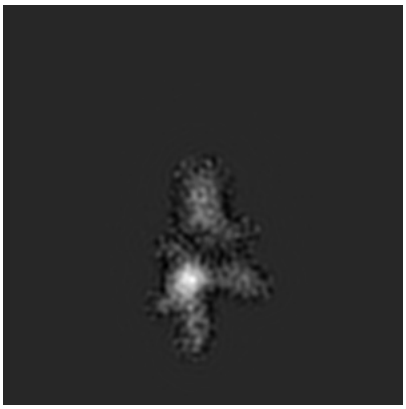
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



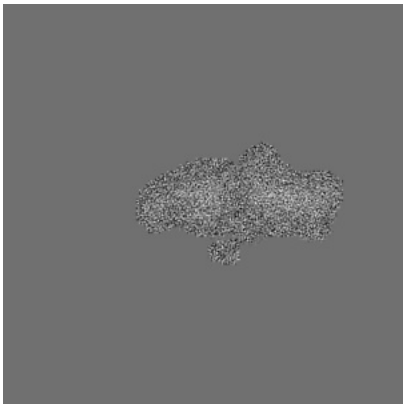
X Index: 218



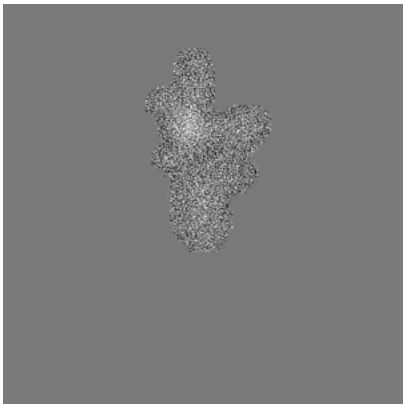
Y Index: 150

Z Index: 193

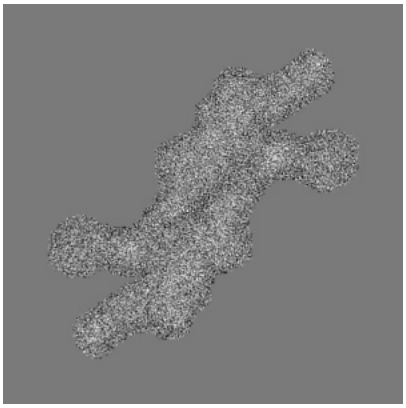
6.3.2 Raw map



X Index: 220



Y Index: 235

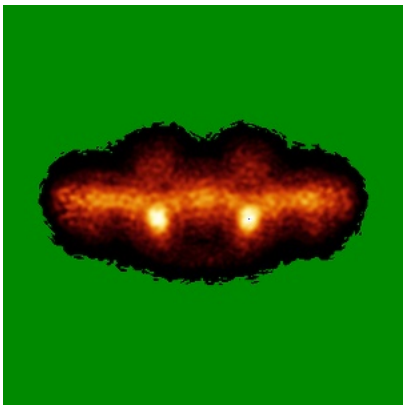


Z Index: 190

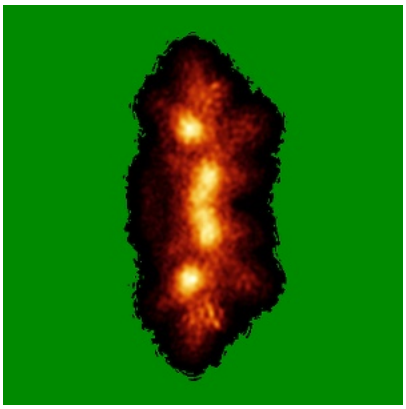
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

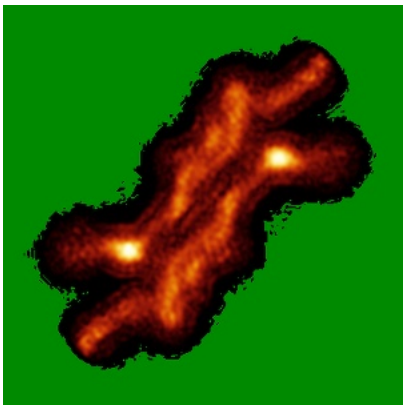
6.4.1 Primary map



X

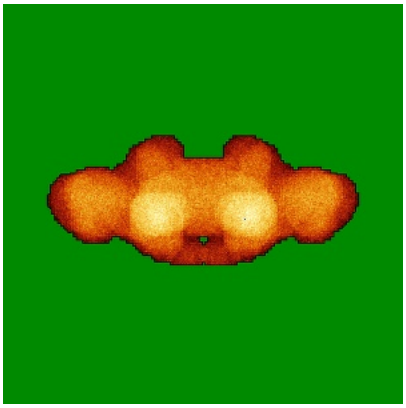


Y

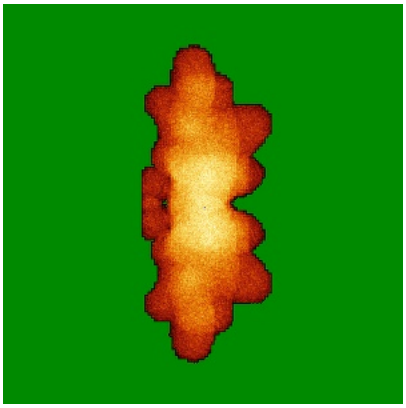


Z

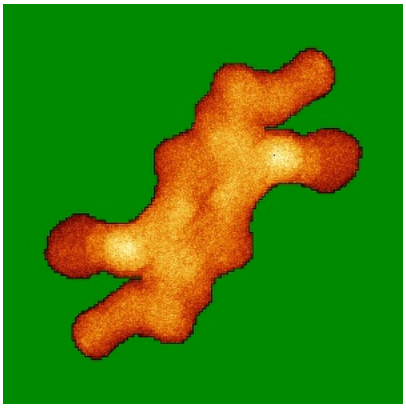
6.4.2 Raw map



X



Y

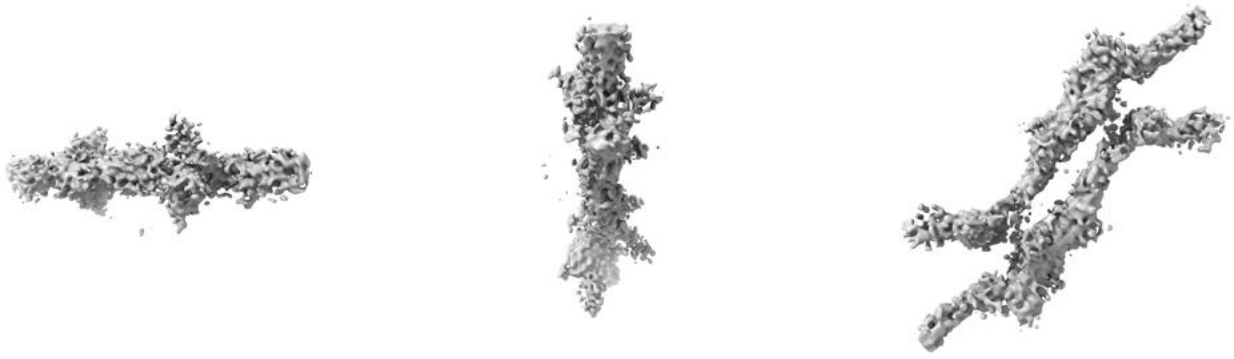


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

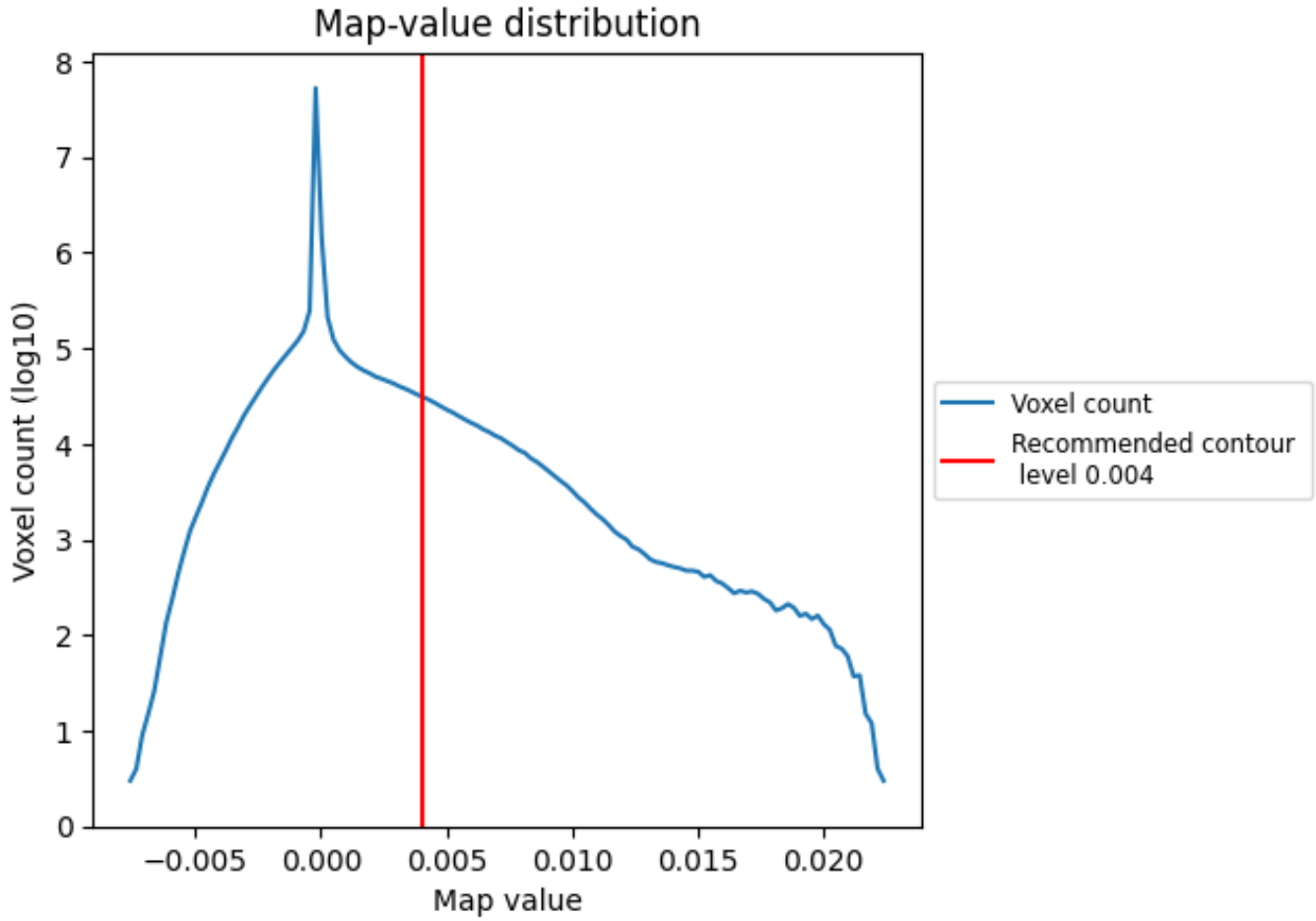
6.6 Mask visualisation (i)

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

7 Map analysis

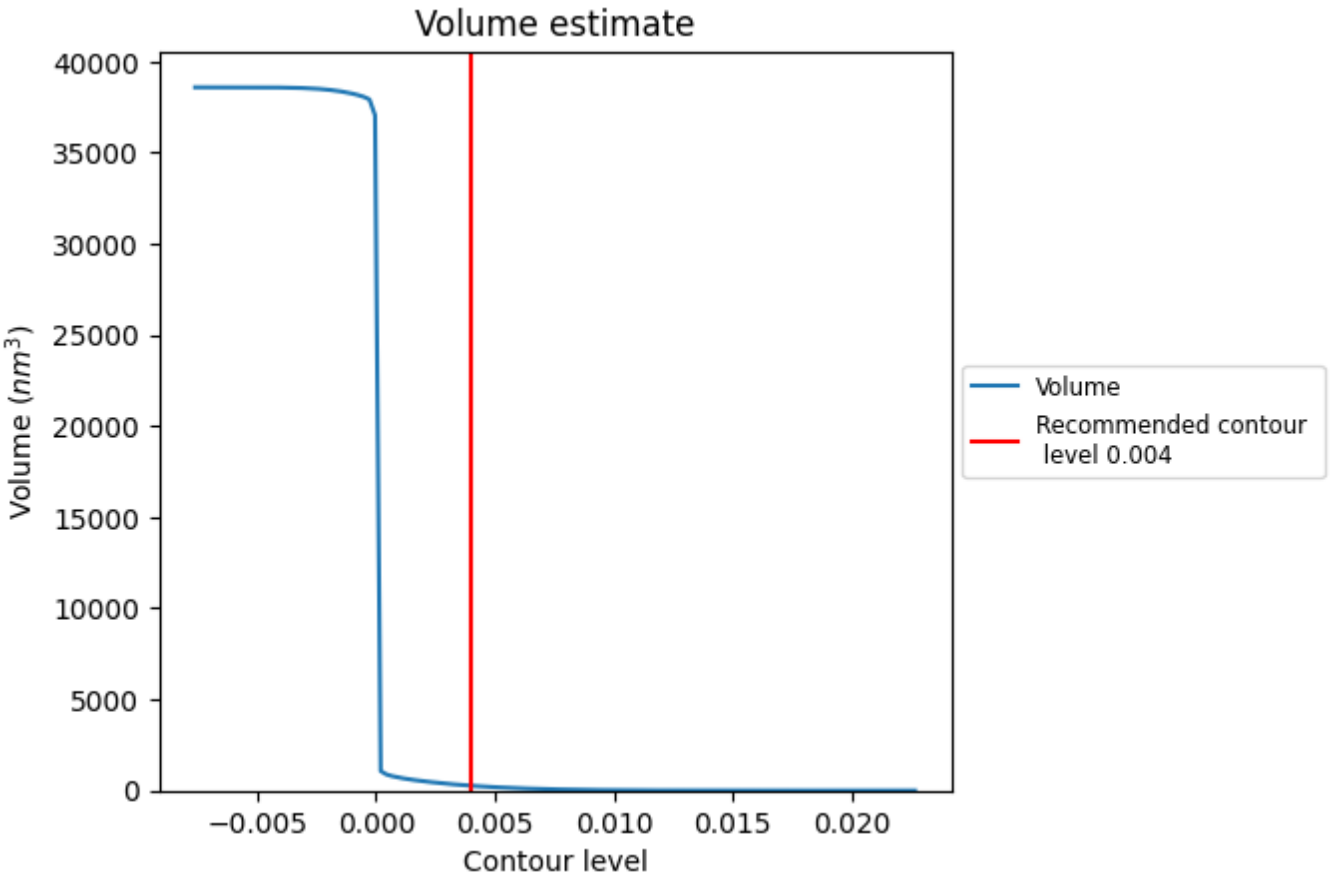
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

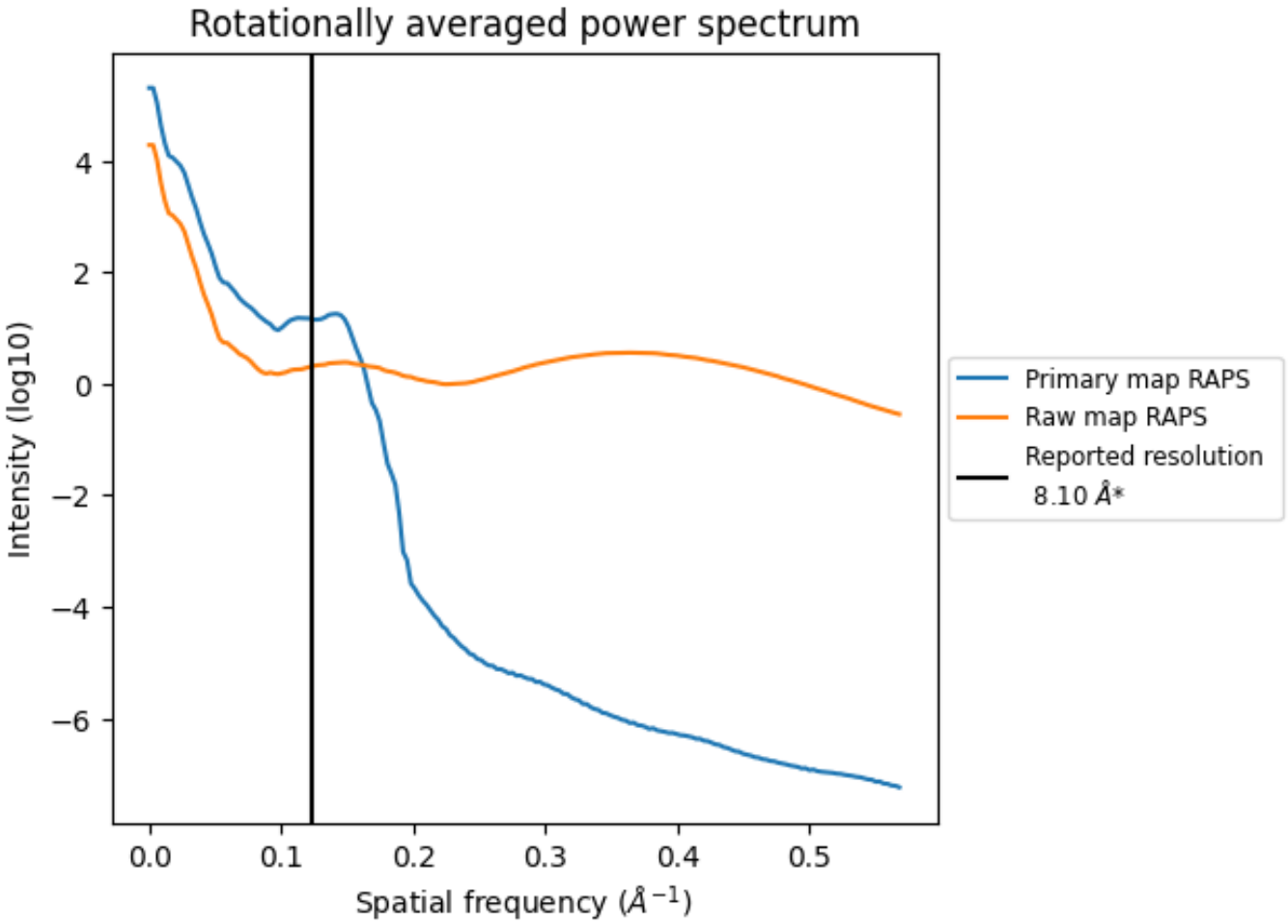
7.2 Volume estimate (i)



The volume at the recommended contour level is 266 nm^3; this corresponds to an approximate mass of 240 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 (i)

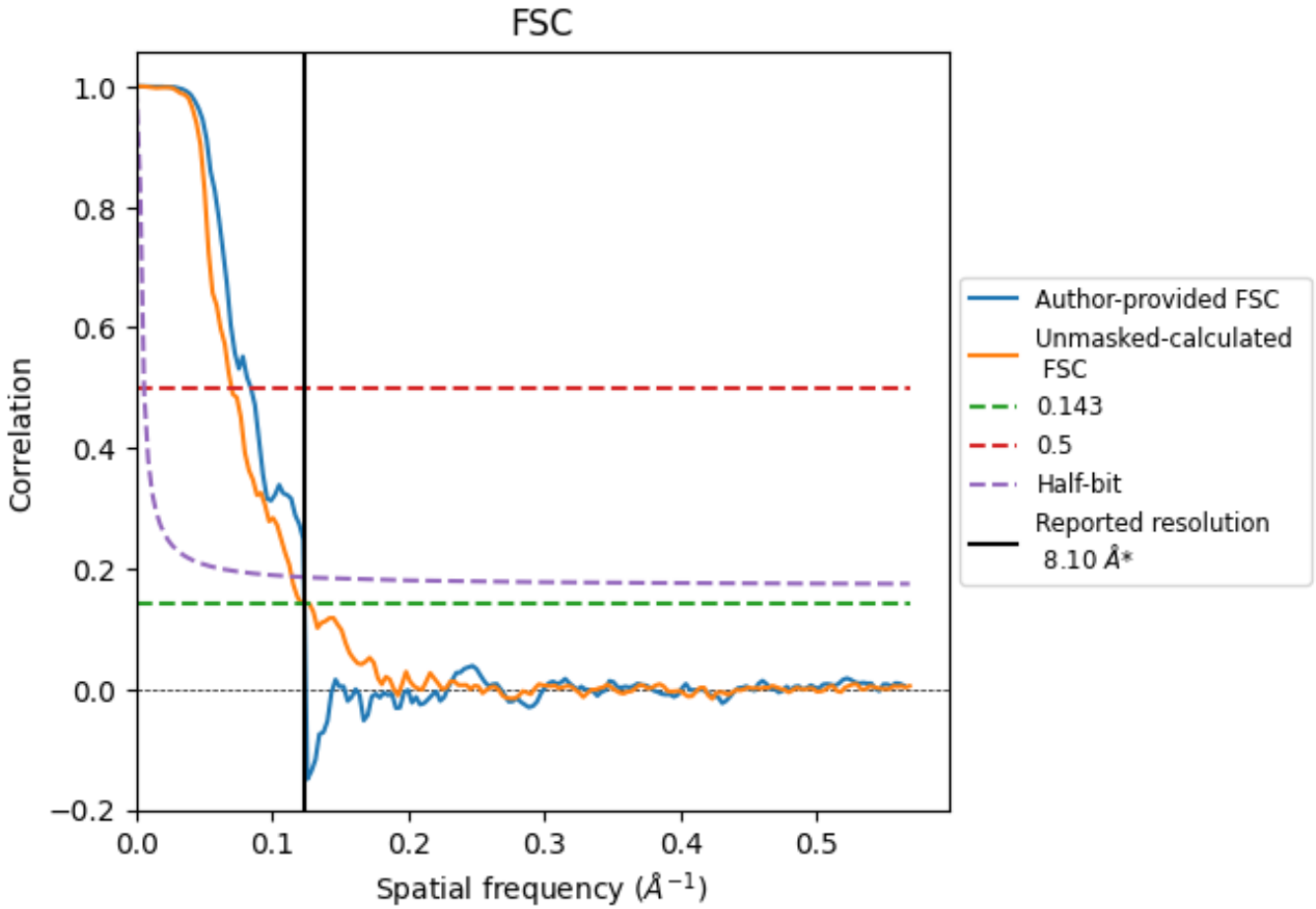


*Reported resolution corresponds to spatial frequency of 0.123 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.123 Å^{-1}

8.2 Resolution estimates (i)

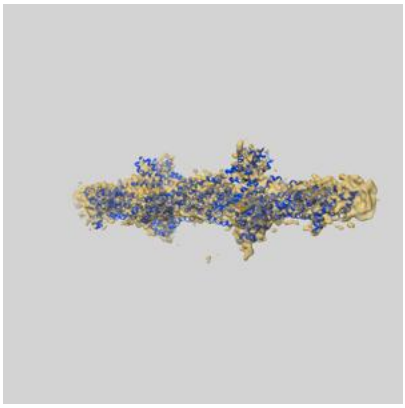
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.10	-	-
Author-provided FSC curve	8.09	11.86	8.11
Unmasked-calculated*	8.25	14.27	8.76

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

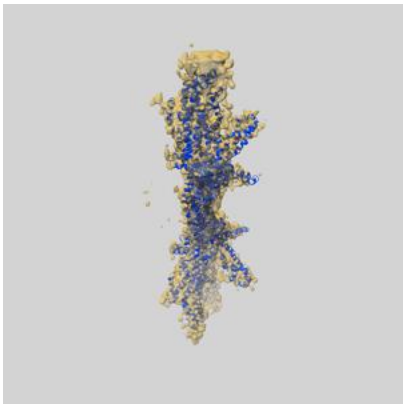
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49227 and PDB model 9NBD. Per-residue inclusion information can be found in section 3 on page 7.

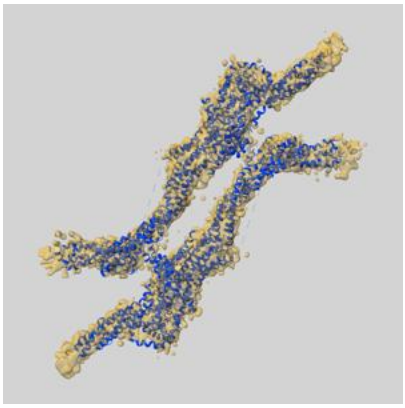
9.1 Map-model overlay



X



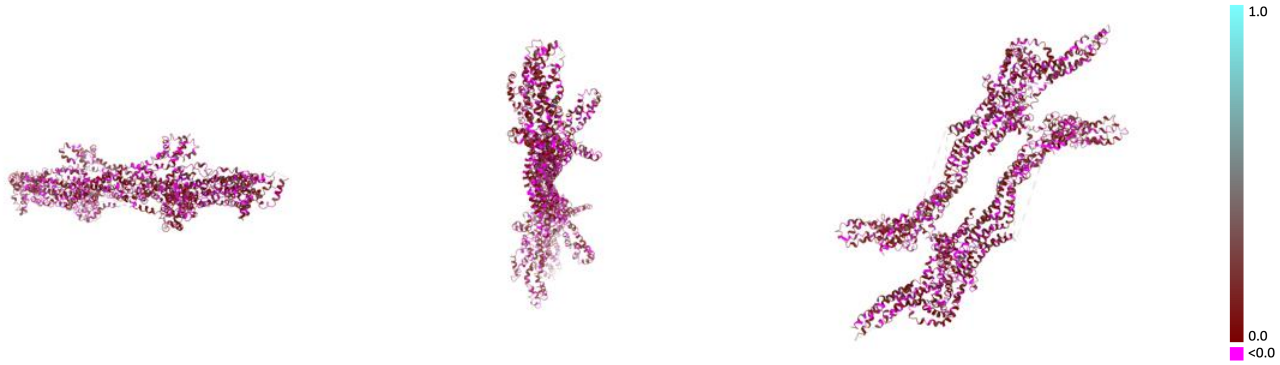
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

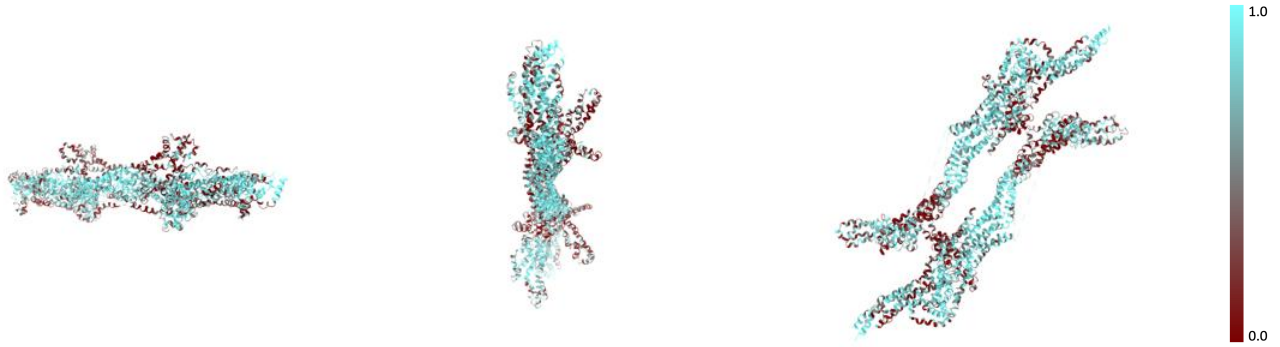
9.2 Q-score mapped to coordinate model



X Y Z

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

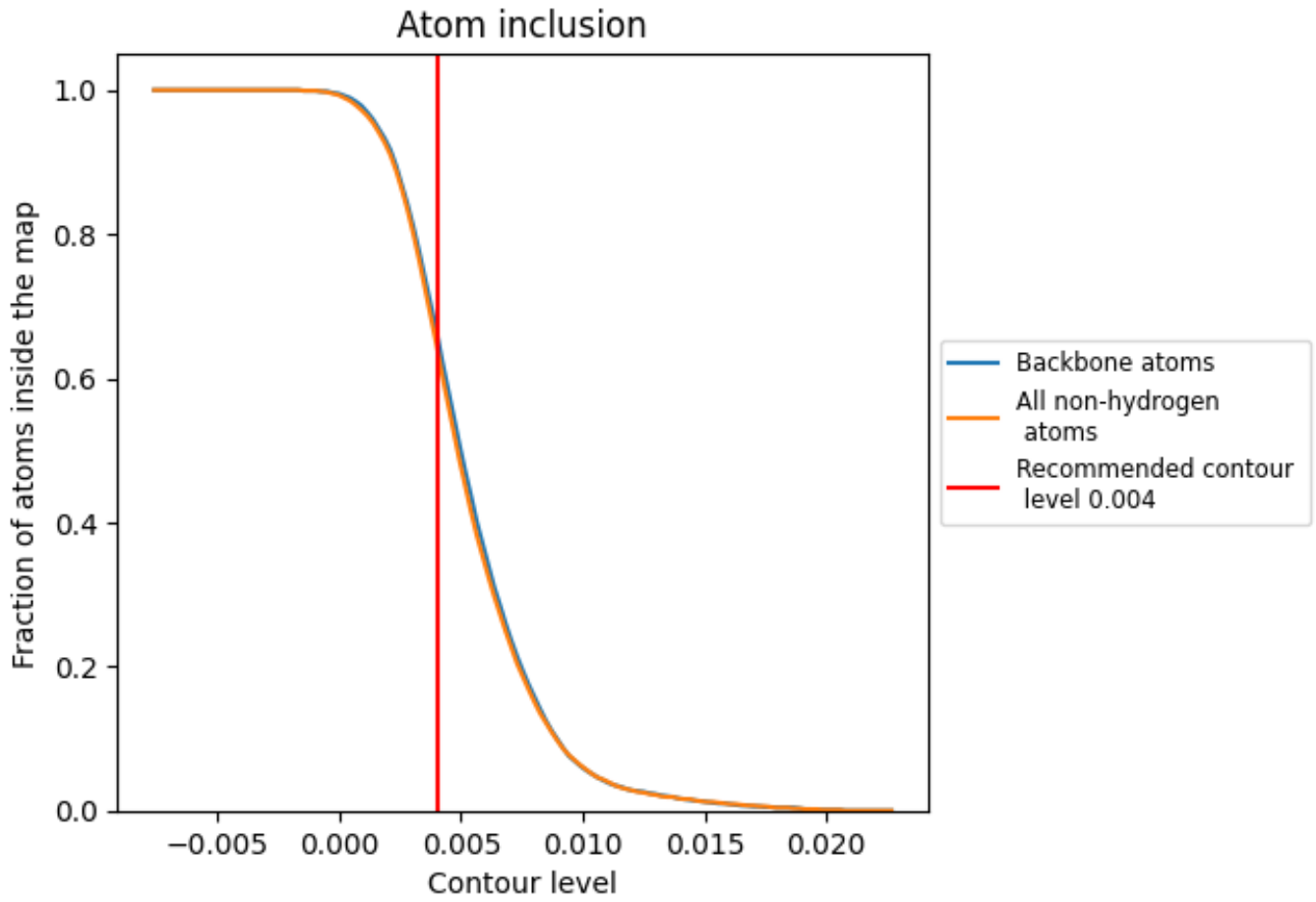
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 64% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.0910
A	0.6630	0.0940
C	0.5490	0.0930
D	0.6810	0.0930
E	0.6970	0.0900
M	0.6610	0.0940
N	0.6890	0.0870
O	0.6840	0.0810
P	0.5380	0.1010