



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 10:43 PM UTC

PDB ID : 8YHX / pdb_00008yhx
EMDB ID : EMD-39302
Title : Cryo-EM structure of the trimeric HerA
Authors : Zhen, X.; Zhou, B.; Xiong, X.
Deposited on : 2024-02-28
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

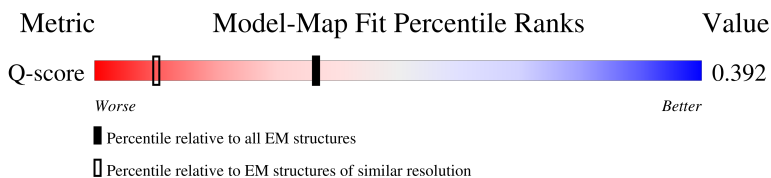
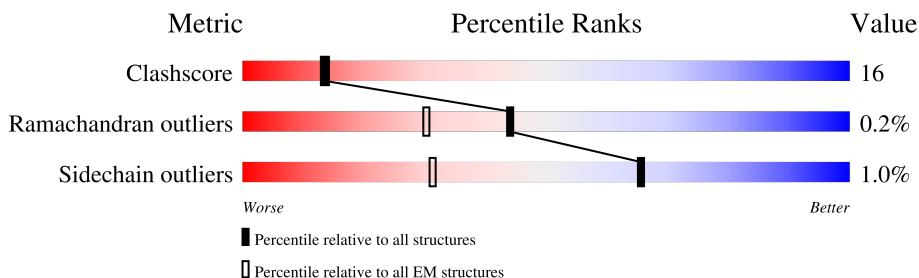
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11740 (2.31 - 3.31)

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

Mol	Chain	Length	Quality of chain
1	A	562	19% 62% 38%
1	B	562	13% 65% 35%
1	C	562	14% 65% 34% .
1	D	562	32% 62% 38% .

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Mol	Chain	Length	Quality of chain
1	E	562	
1	F	562	
2	G	428	
2	H	428	
2	I	428	
2	J	428	
2	K	428	
2	L	428	
2	M	428	
2	N	428	
2	O	428	
2	P	428	
2	Q	428	
2	R	428	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	APR	H	501	-	-	X	-
3	APR	J	501	-	-	X	-
3	APR	L	501	-	-	X	-
3	APR	N	501	-	-	X	-
3	APR	P	501	-	-	X	-
3	APR	R	501	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 69979 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 DUF87 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4601	2957	751	880	13		
1	B	562	Total	C	N	O	S	0	0
			4601	2957	751	880	13		
1	C	562	Total	C	N	O	S	0	0
			4601	2957	751	880	13		
1	D	562	Total	C	N	O	S	0	0
			4593	2952	750	878	13		
1	E	562	Total	C	N	O	S	0	0
			4601	2957	751	880	13		
1	F	562	Total	C	N	O	S	0	0
			4601	2957	751	880	13		

- Molecule 2 is a protein called SIR2 family protein.

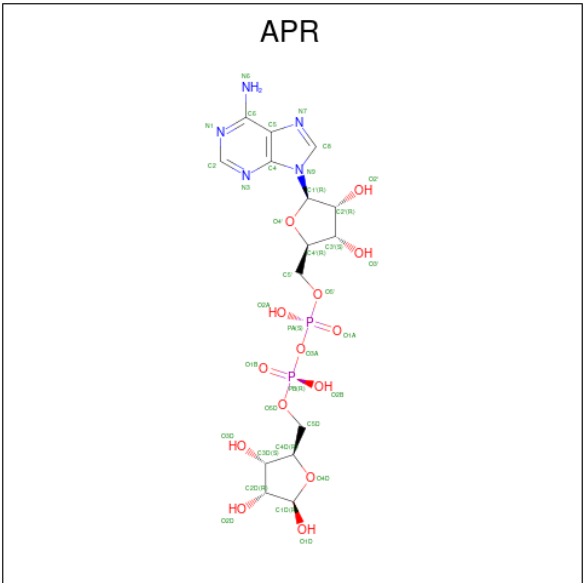
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	408	Total	C	N	O	S	0	0
			3392	2162	549	672	9		
2	H	427	Total	C	N	O	S	0	0
			3568	2276	583	700	9		
2	I	428	Total	C	N	O	S	0	0
			3579	2282	587	701	9		
2	J	425	Total	C	N	O	S	0	0
			3545	2264	575	697	9		
2	K	428	Total	C	N	O	S	0	0
			3579	2282	587	701	9		
2	L	425	Total	C	N	O	S	0	0
			3545	2264	575	697	9		
2	M	428	Total	C	N	O	S	0	0
			3579	2282	587	701	9		
2	N	425	Total	C	N	O	S	0	0
			3545	2264	575	697	9		
2	O	428	Total	C	N	O	S	0	0
			3579	2282	587	701	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	425	Total	C	N	O	S	0	0
			3545	2264	575	697	9		
2	Q	418	Total	C	N	O	S	0	0
			3479	2225	561	684	9		
2	R	390	Total	C	N	O	S	0	0
			3230	2065	522	636	7		

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	H	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	J	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	L	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	N	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	P	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	R	1	Total	C	N	O	P	0
			36	15	5	14	2	

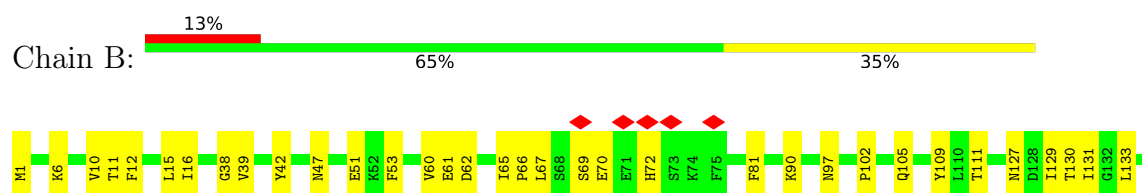
3 Residue-property plots

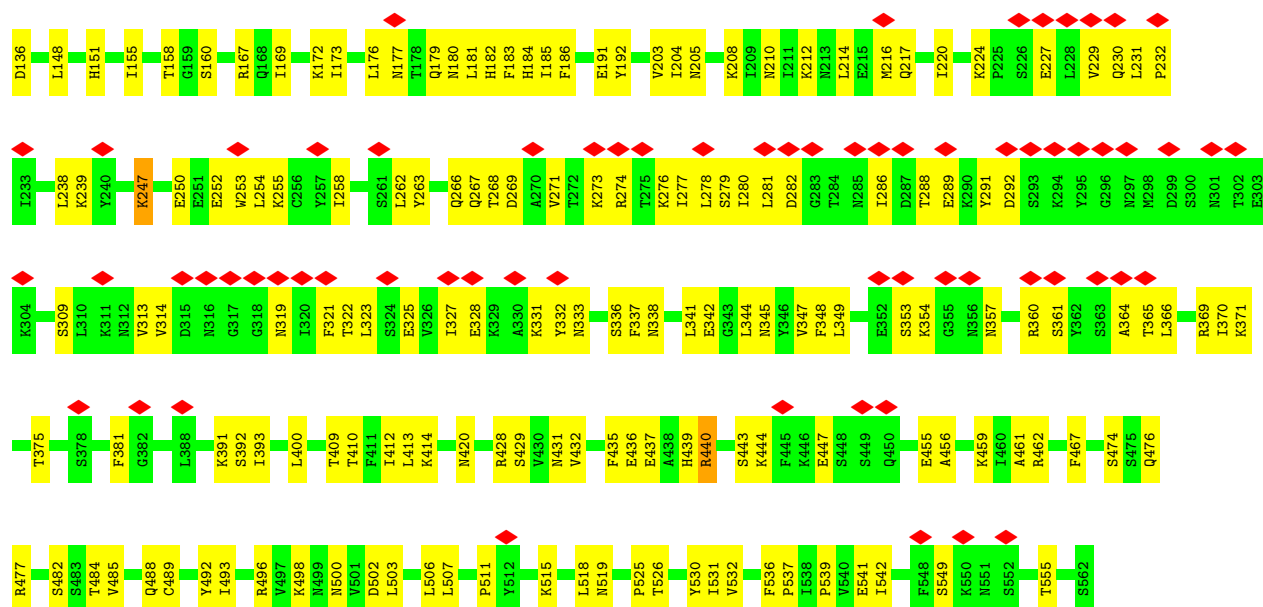
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DUF87 domain-containing protein

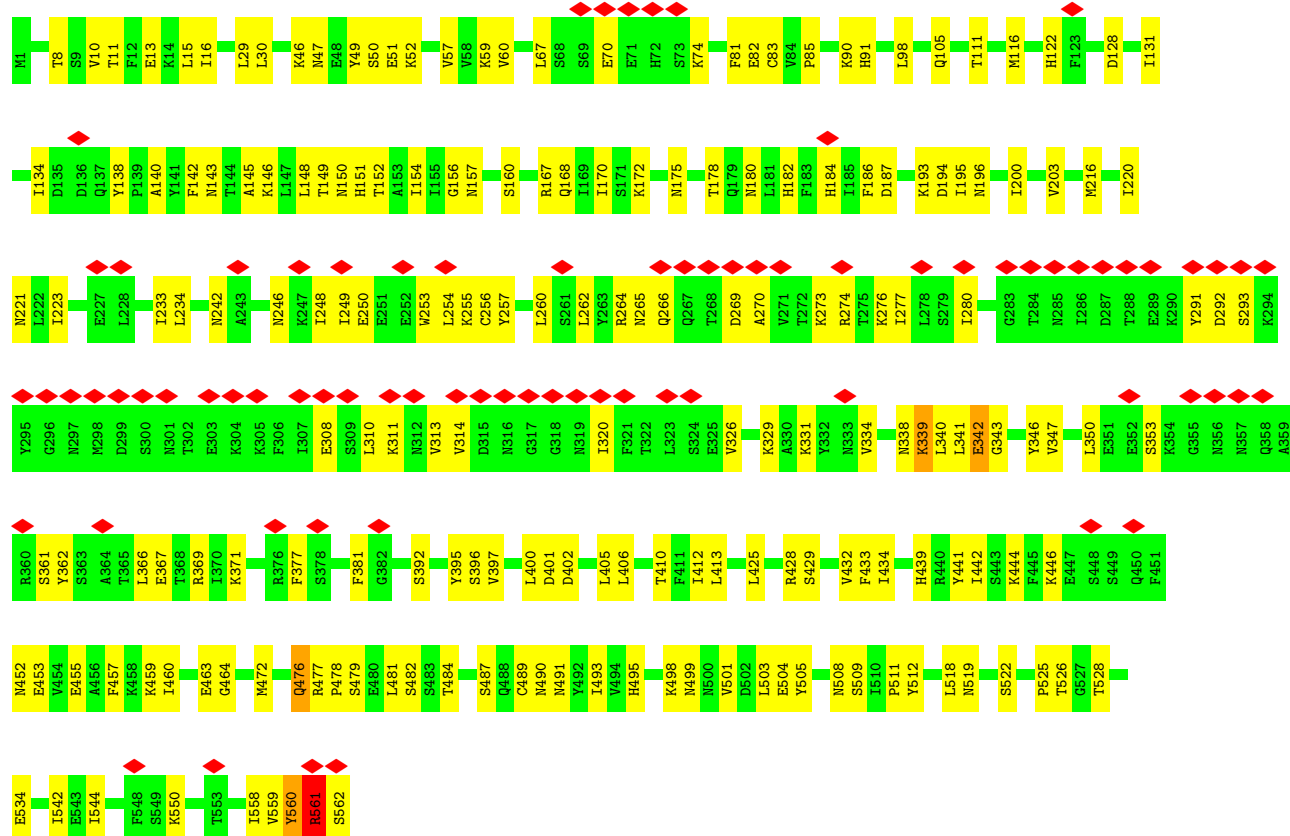


• Molecule 1: DUF87 domain-containing protein



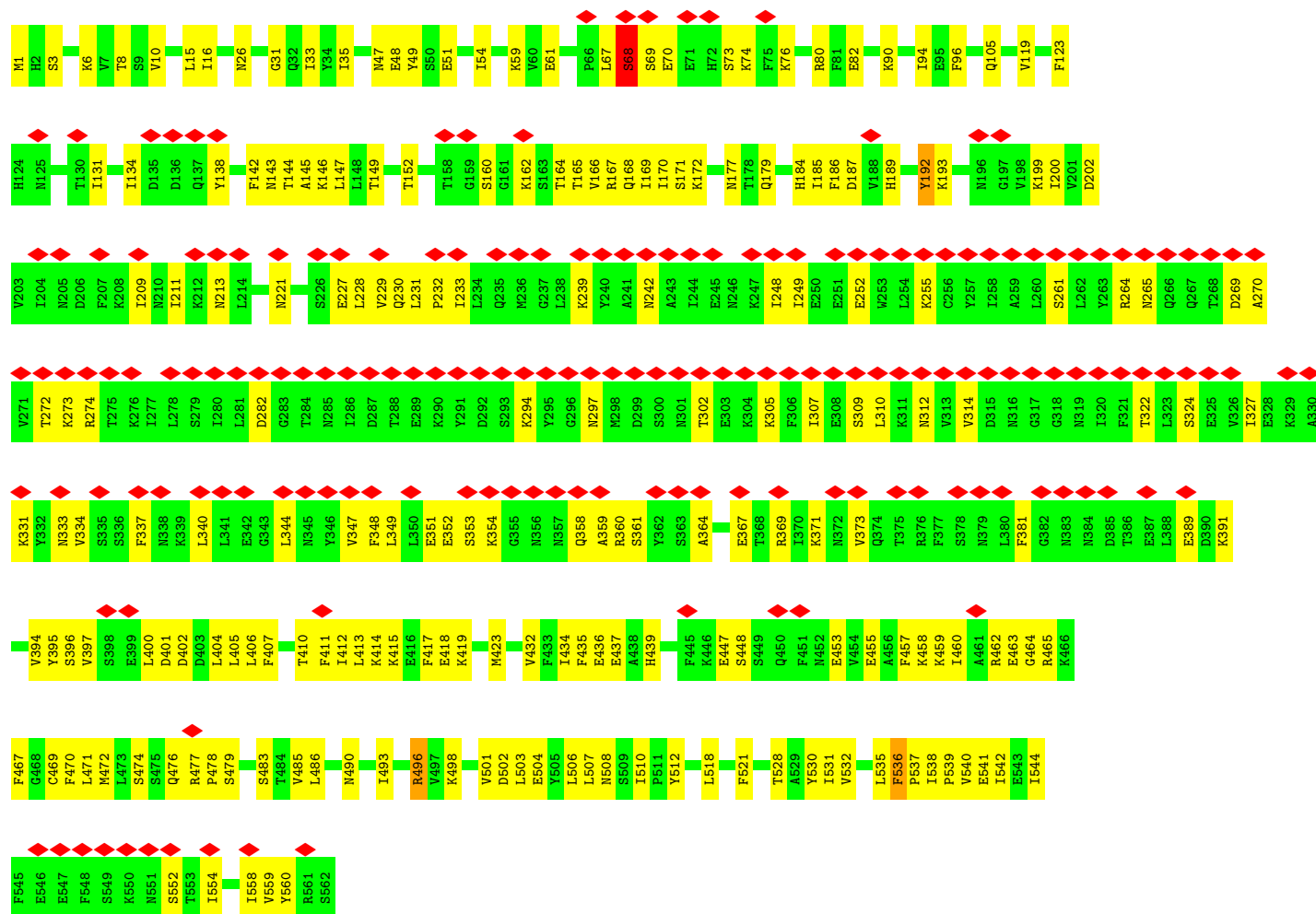


• Molecule 1: DUF87 domain-containing protein

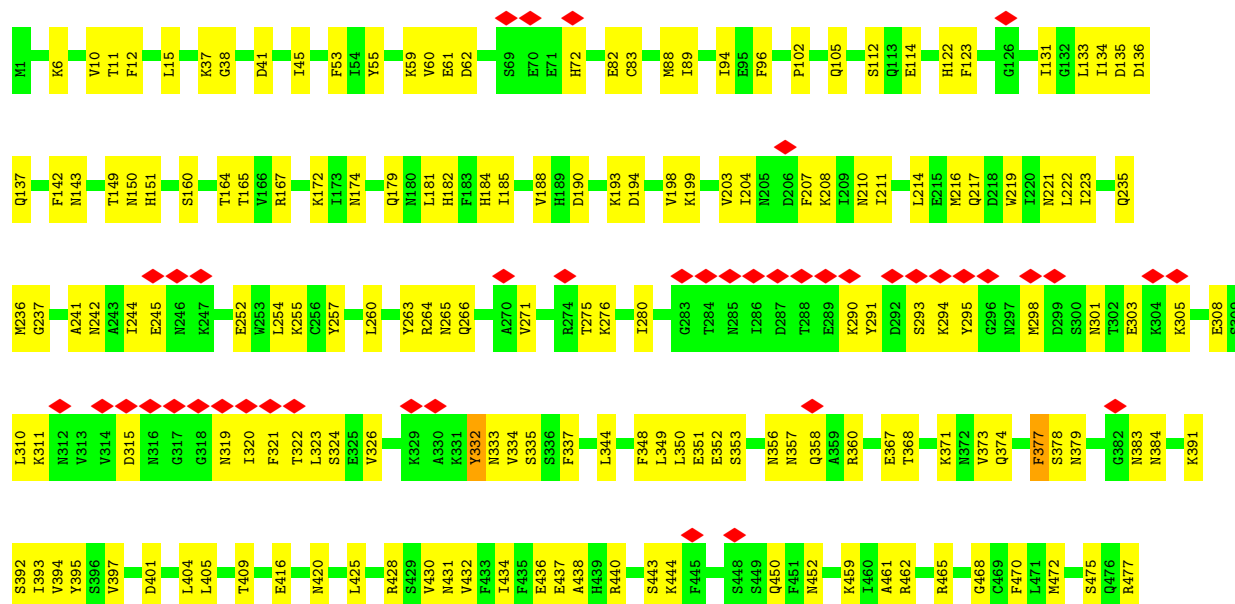


• Molecule 1: DUF87 domain-containing protein



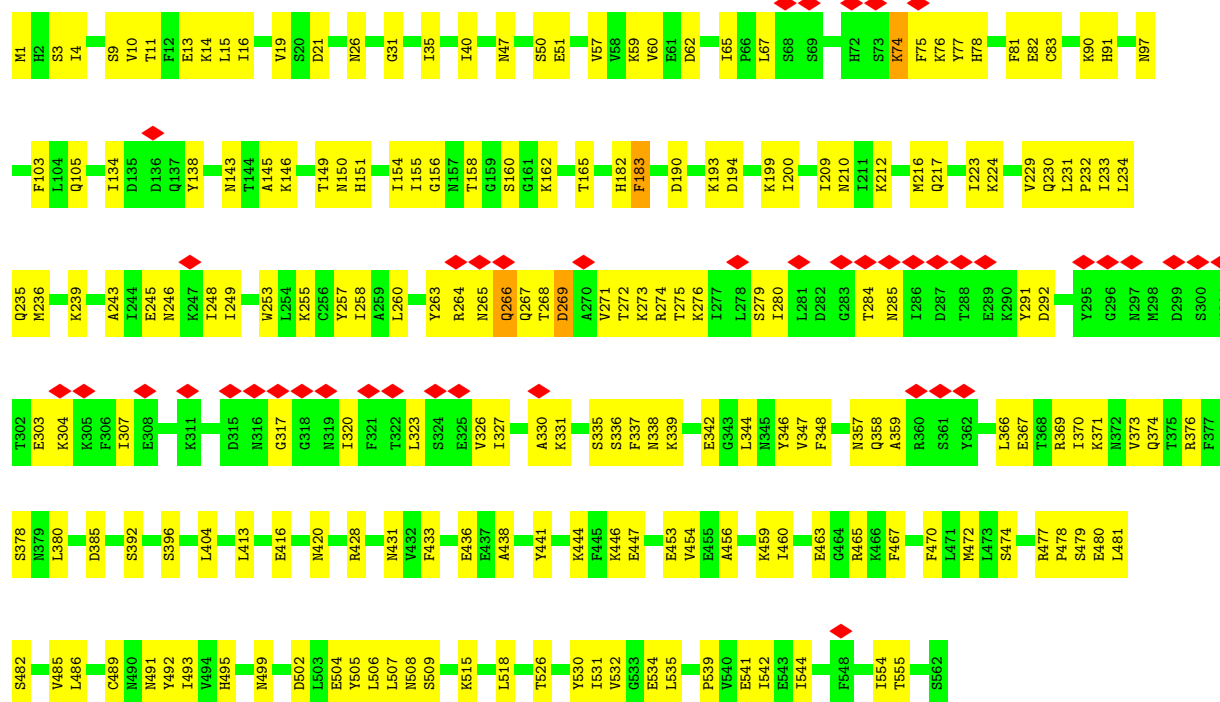


• Molecule 1: DUF87 domain-containing protein

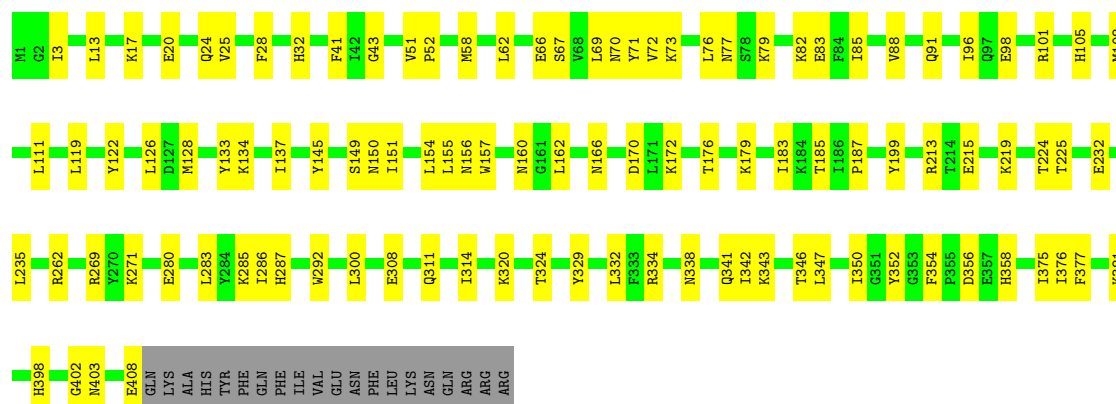




• Molecule 1: DUF87 domain-containing protein

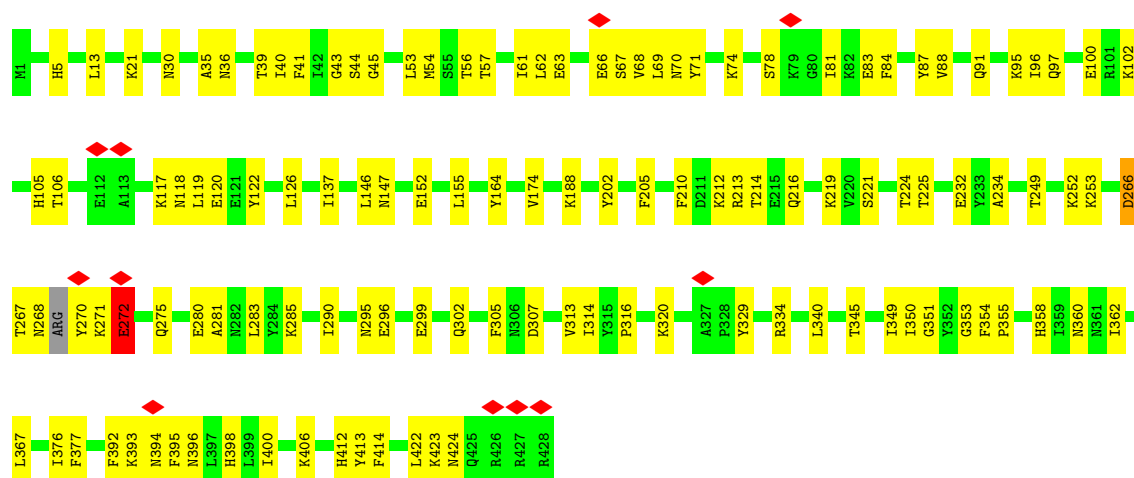


• Molecule 2: SIR2 family protein

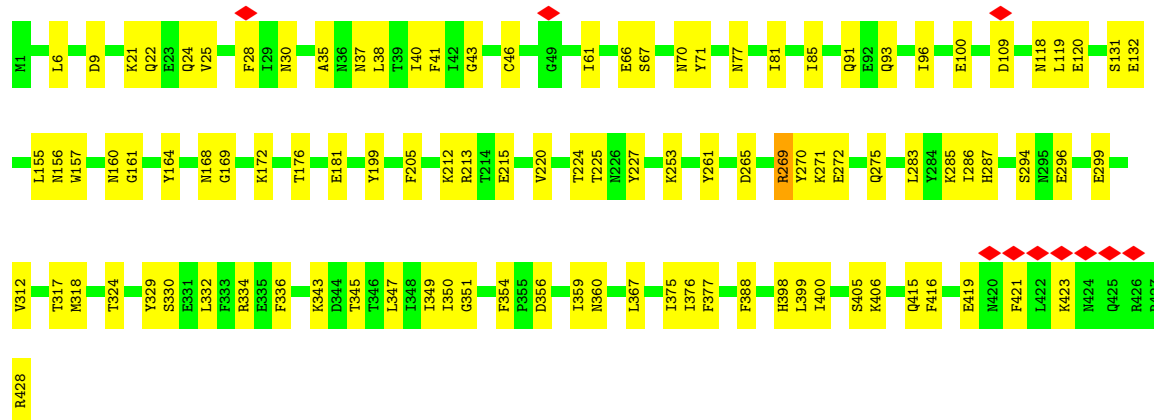


• Molecule 2: SIR2 family protein

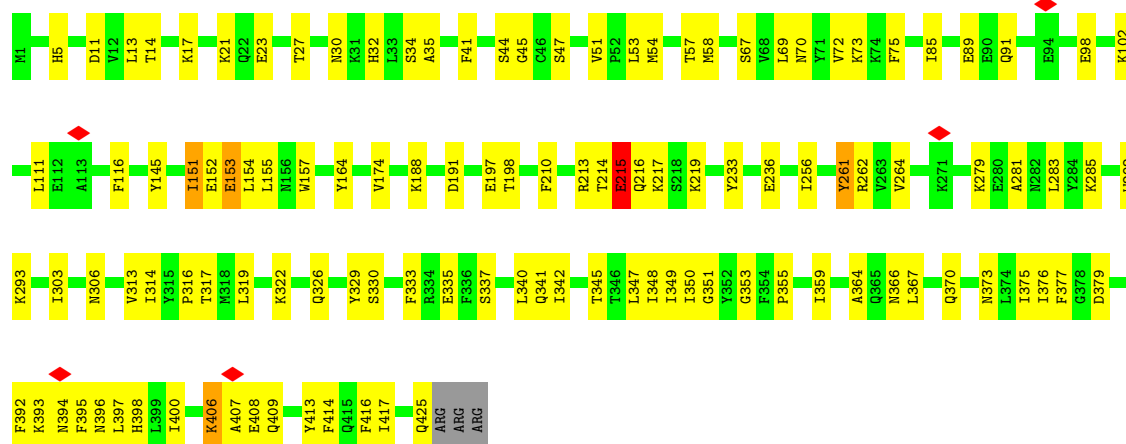




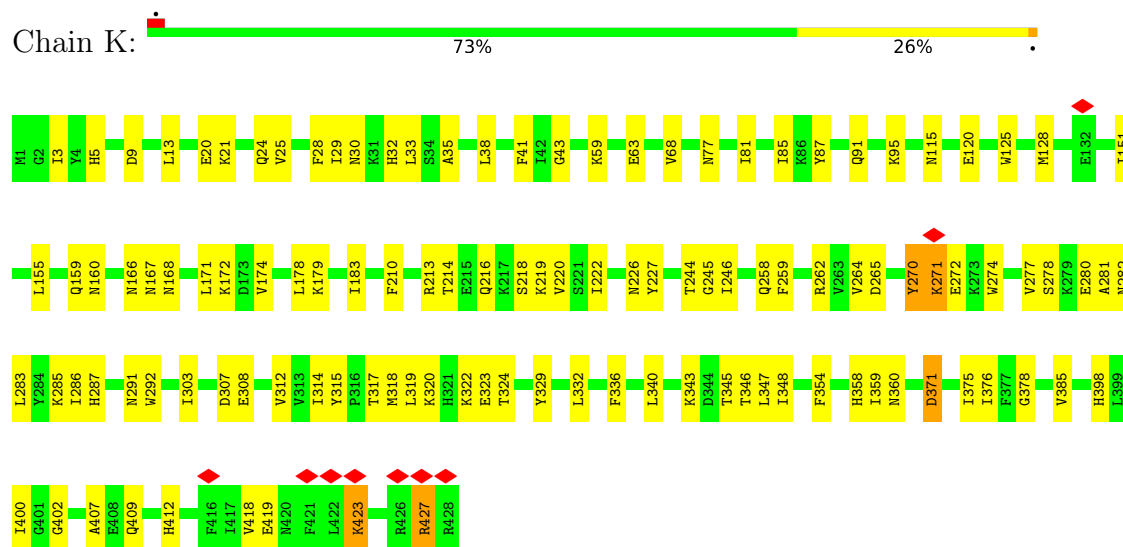
• Molecule 2: SIR2 family protein



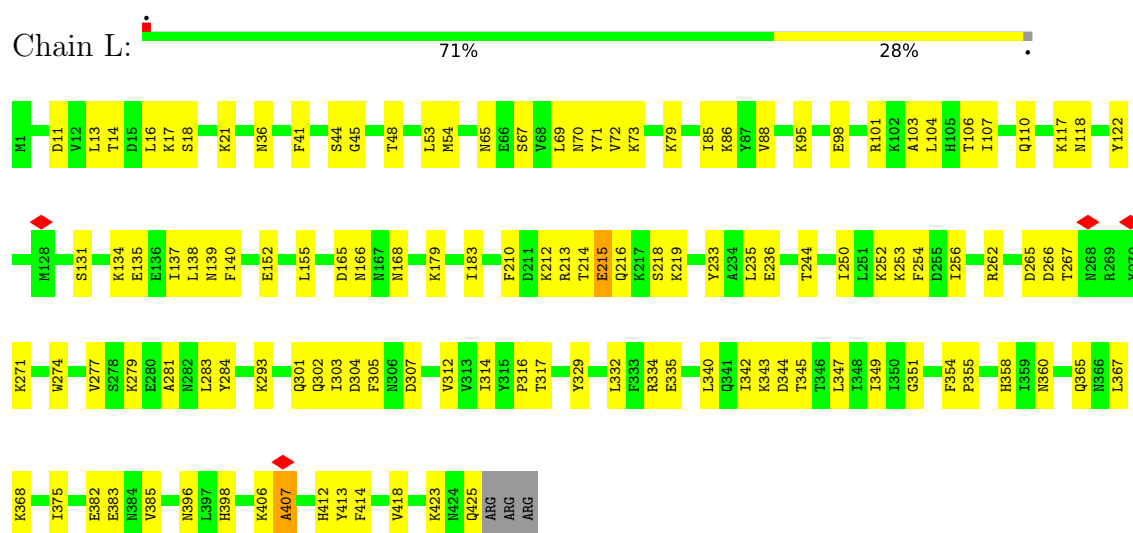
• Molecule 2: SIR2 family protein



• Molecule 2: SIR2 family protein



• Molecule 2: SIR2 family protein

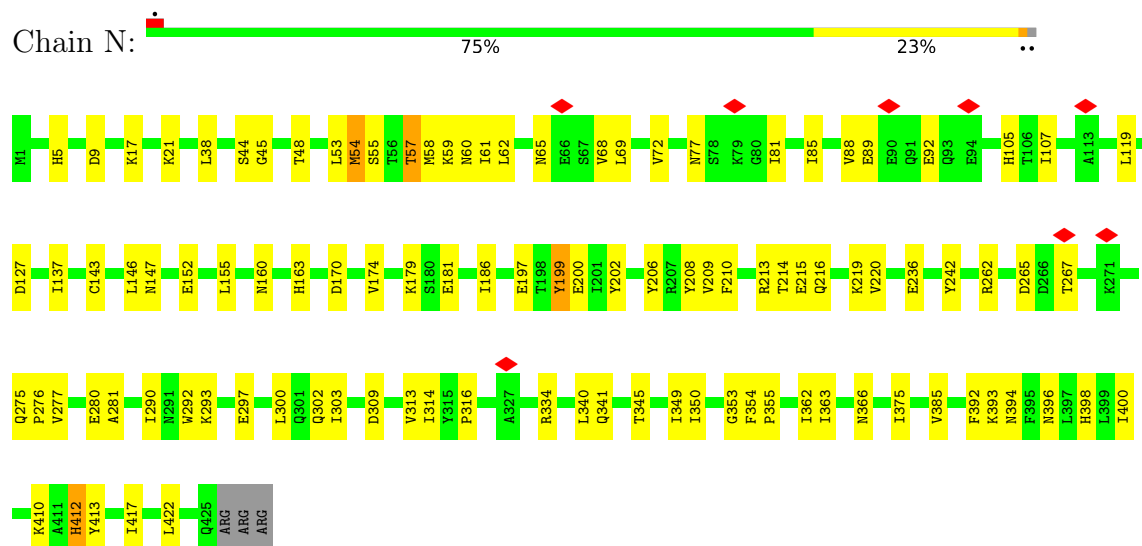


• Molecule 2: SIR2 family protein

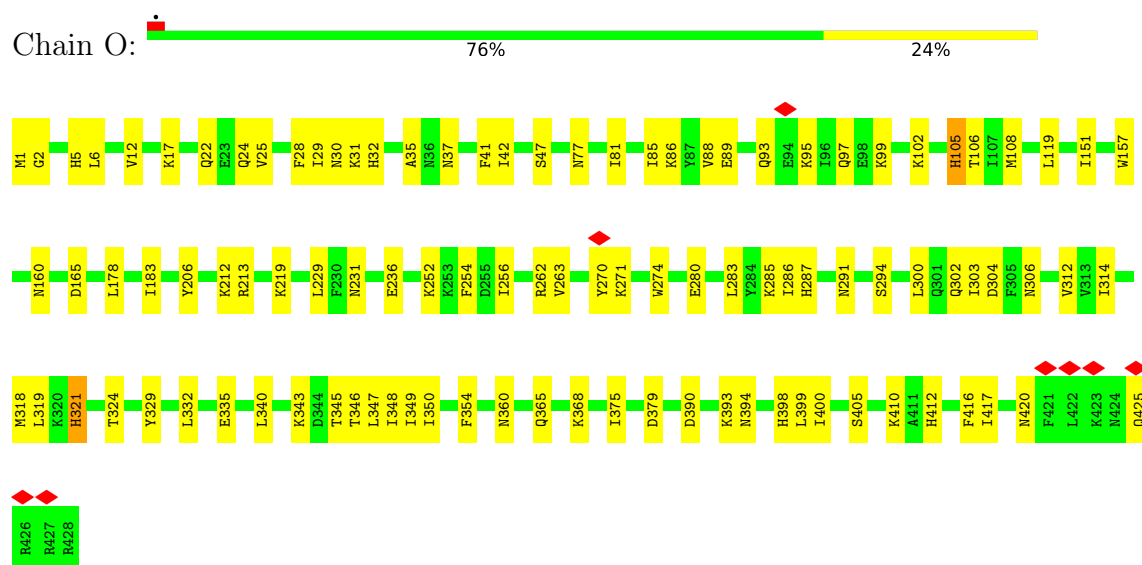




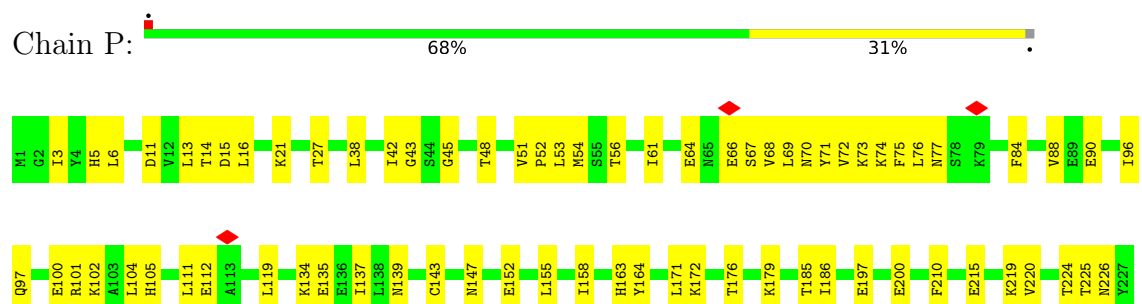
• Molecule 2: SIR2 family protein

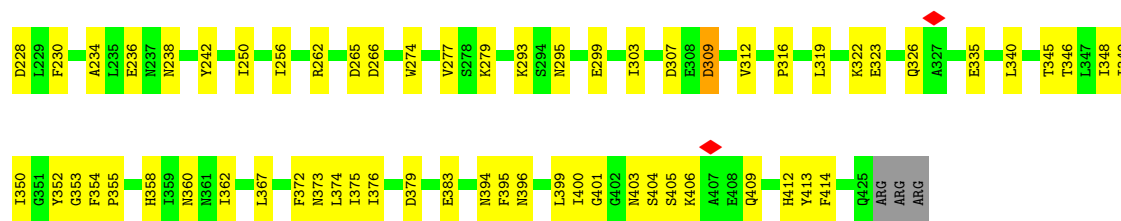


• Molecule 2: SIR2 family protein



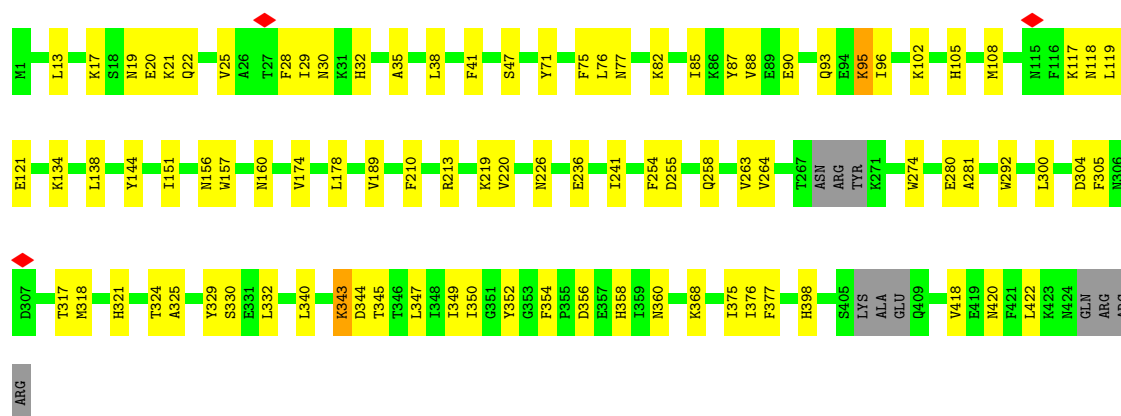
• Molecule 2: SIR2 family protein





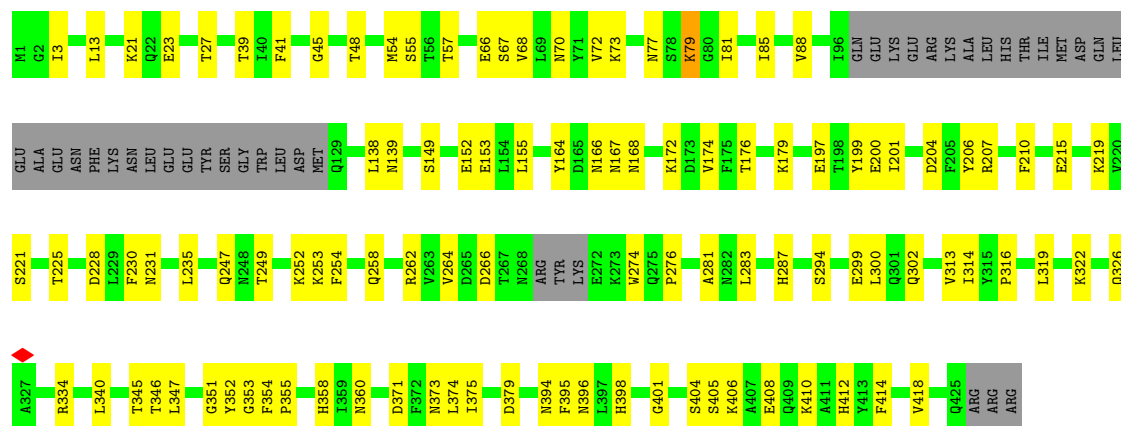
• Molecule 2: SIR2 family protein

Chain Q: 76% 21%



• Molecule 2: SIR2 family protein

Chain R: 66% 25% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79232	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.424	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	363.52, 363.52, 363.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/4691	0.41	1/6324 (0.0%)
1	B	0.16	0/4691	0.41	0/6324
1	C	0.16	0/4691	0.41	0/6324
1	D	0.17	0/4683	0.48	3/6313 (0.0%)
1	E	0.14	0/4691	0.40	0/6324
1	F	0.14	0/4691	0.40	0/6324
2	G	0.12	0/3460	0.36	0/4666
2	H	0.15	0/3640	0.40	1/4903 (0.0%)
2	I	0.13	0/3652	0.38	0/4920
2	J	0.14	0/3618	0.38	1/4878 (0.0%)
2	K	0.13	0/3652	0.37	0/4920
2	L	0.13	0/3618	0.36	0/4878
2	M	0.13	0/3652	0.37	0/4920
2	N	0.15	0/3618	0.40	0/4878
2	O	0.13	0/3652	0.36	0/4920
2	P	0.14	0/3618	0.40	0/4878
2	Q	0.12	0/3549	0.35	0/4783
2	R	0.12	0/3295	0.35	0/4445
All	All	0.14	0/71162	0.39	6/95922 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	H	0	1
2	I	0	1
2	J	0	1
2	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1
2	N	0	1
All	All	0	7

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	SER	N-CA-C	-8.45	104.11	114.75
2	H	272	GLU	N-CA-C	-7.80	104.65	114.56
1	D	501	VAL	N-CA-C	-6.36	107.04	113.47
1	D	68	SER	CA-C-N	-5.77	115.57	122.44
1	D	68	SER	C-N-CA	-5.77	115.57	122.44
2	J	151	ILE	N-CA-C	5.32	115.53	110.53

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	561	ARG	Sidechain
2	H	393	LYS	Peptide
2	I	343	LYS	Peptide
2	J	393	LYS	Peptide
2	L	407	ALA	Peptide
2	M	249	THR	Peptide
2	N	393	LYS	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	4601	0	4599	207	0
1	B	4601	0	4599	222	0
1	C	4601	0	4599	184	0
1	D	4593	0	4581	259	0
1	E	4601	0	4599	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4601	0	4599	183	0
2	G	3392	0	3285	71	0
2	H	3568	0	3457	105	0
2	I	3579	0	3471	77	0
2	J	3545	0	3432	113	0
2	K	3579	0	3471	81	0
2	L	3545	0	3432	137	0
2	M	3579	0	3471	103	0
2	N	3545	0	3432	99	0
2	O	3579	0	3471	79	0
2	P	3545	0	3432	124	0
2	Q	3479	0	3366	66	0
2	R	3230	0	3114	99	0
3	H	36	0	21	17	0
3	J	36	0	21	23	0
3	L	36	0	18	45	0
3	N	36	0	18	25	0
3	P	36	0	18	32	0
3	R	36	0	18	39	0
All	All	69979	0	68524	2196	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 16.

All (2196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:LEU:HD11	1:D:405:LEU:CD2	1.34	1.56
1:B:507:LEU:HD12	1:B:518:LEU:CD1	1.26	1.54
1:B:507:LEU:HD11	1:B:518:LEU:CG	1.36	1.53
2:N:92:GLU:OE2	2:N:105:HIS:CE1	1.67	1.46
1:B:507:LEU:CD1	1:B:518:LEU:CD1	1.90	1.45
2:L:79:LYS:NZ	2:L:118:ASN:HD21	0.96	1.40
2:L:412:HIS:CD2	3:L:501:APR:O2'	1.75	1.39
1:D:506:LEU:CD1	1:D:510:ILE:HD12	1.54	1.37
1:C:67:LEU:CD2	1:C:74:LYS:HG3	1.58	1.33
1:D:400:LEU:CD1	1:D:405:LEU:CD2	2.07	1.31
1:D:401:ASP:O	1:D:405:LEU:HG	1.29	1.30
1:D:349:LEU:HA	1:D:352:GLU:OE1	1.28	1.30
2:M:254:PHE:CB	2:M:300:LEU:HD23	1.63	1.29
2:L:79:LYS:NZ	2:L:118:ASN:ND2	1.78	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:167:ASN:OD1	2:L:117:LYS:NZ	1.62	1.28
1:B:507:LEU:CD1	1:B:518:LEU:HD11	1.53	1.28
2:L:351:GLY:O	3:L:501:APR:H'4	1.24	1.25
1:E:15:LEU:HD22	1:E:83:CYS:SG	1.76	1.25
3:P:501:APR:O4'	3:P:501:APR:C1'	1.66	1.25
2:R:352:TYR:HE1	3:R:501:APR:C2D	1.48	1.25
1:D:400:LEU:CD1	1:D:405:LEU:HD23	1.63	1.24
2:N:65:ASN:ND2	2:N:69:LEU:HD23	1.50	1.24
2:L:267:THR:CG2	2:L:271:LYS:HA	1.66	1.24
3:L:501:APR:C1'	3:L:501:APR:O4'	1.65	1.21
1:D:186:PHE:HA	1:D:436:GLU:OE1	1.40	1.20
1:F:182:HIS:HB2	1:F:431:ASN:OD1	1.39	1.20
1:D:186:PHE:CA	1:D:436:GLU:OE1	1.91	1.18
1:E:188:VAL:HG21	1:E:437:GLU:HG2	1.25	1.18
1:F:65:ILE:HD12	1:F:74:LYS:HD2	1.22	1.17
1:D:67:LEU:HD23	1:D:73:SER:CB	1.72	1.17
1:D:349:LEU:CA	1:D:352:GLU:OE1	1.93	1.17
1:B:507:LEU:CD1	1:B:518:LEU:HG	1.69	1.17
2:L:412:HIS:NE2	3:L:501:APR:O2'	1.75	1.17
1:B:254:LEU:HD12	1:B:323:LEU:CD2	1.76	1.16
1:B:254:LEU:HD12	1:B:323:LEU:HD21	1.28	1.16
2:L:54:MET:SD	3:L:501:APR:O4D	2.05	1.15
1:B:507:LEU:CD1	1:B:518:LEU:CG	2.12	1.15
2:R:54:MET:HE1	3:R:501:APR:HR'4	1.22	1.15
3:R:501:APR:C1'	3:R:501:APR:O4'	1.65	1.14
3:N:501:APR:C1'	3:N:501:APR:O4'	1.66	1.14
2:J:32:HIS:CD2	2:J:373:ASN:ND2	2.15	1.14
1:F:65:ILE:CD1	1:F:74:LYS:HD2	1.76	1.13
2:K:244:THR:HG23	2:K:246:ILE:HG12	1.14	1.13
1:E:15:LEU:CD2	1:E:83:CYS:SG	2.35	1.13
2:I:96:ILE:HD12	2:I:100:GLU:HB2	1.31	1.11
2:L:351:GLY:O	3:L:501:APR:C4'	1.98	1.11
1:D:221:ASN:HD21	1:D:406:LEU:HD23	1.15	1.11
1:D:348:PHE:O	1:D:352:GLU:OE1	1.65	1.11
2:L:351:GLY:C	3:L:501:APR:H'4	1.74	1.10
2:L:48:THR:HG21	3:L:501:APR:N1	1.65	1.10
2:R:352:TYR:CE1	3:R:501:APR:C2D	2.35	1.10
1:B:169:ILE:O	1:B:173:ILE:HG12	1.52	1.09
2:M:254:PHE:HB2	2:M:300:LEU:HD23	1.31	1.08
2:N:65:ASN:HD22	2:N:69:LEU:HD23	1.03	1.08
1:D:221:ASN:ND2	1:D:406:LEU:HD23	1.68	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:392:PHE:HB3	2:J:394:ASN:ND2	1.68	1.07
2:N:48:THR:HG21	3:N:501:APR:N6	1.70	1.06
1:E:89:ILE:HG12	1:E:94:ILE:HD13	1.34	1.06
2:L:267:THR:HG22	2:L:271:LYS:HA	1.26	1.06
1:A:440:ARG:NE	1:D:460:ILE:HD13	1.71	1.05
2:I:96:ILE:HD12	2:I:100:GLU:CB	1.86	1.05
2:R:152:GLU:OE2	3:R:501:APR:H5R1	1.54	1.05
1:D:506:LEU:HD11	1:D:510:ILE:HD12	1.11	1.05
2:K:244:THR:CG2	2:K:246:ILE:HG12	1.86	1.05
2:L:413:TYR:CE1	3:L:501:APR:C4	2.39	1.04
1:D:131:ILE:HD12	1:D:172:LYS:HZ1	1.16	1.04
1:F:532:VAL:HG12	1:F:539:PRO:HB3	1.38	1.04
2:L:79:LYS:HZ1	2:L:118:ASN:ND2	1.44	1.03
2:N:48:THR:HG21	3:N:501:APR:H61	1.16	1.03
2:N:413:TYR:CD1	3:N:501:APR:N3	2.25	1.03
1:D:131:ILE:HD12	1:D:172:LYS:NZ	1.72	1.03
1:B:341:LEU:HD13	1:B:370:ILE:HD13	1.38	1.03
1:C:57:VAL:HG22	1:C:83:CYS:SG	1.98	1.03
1:A:148:LEU:HD22	1:A:432:VAL:HG21	1.36	1.02
1:B:281:LEU:O	1:B:281:LEU:HD12	1.58	1.02
1:C:140:ALA:CB	1:C:542:ILE:HD12	1.90	1.02
1:D:67:LEU:HG	1:D:68:SER:H	1.20	1.02
2:N:355:PRO:HG3	3:N:501:APR:O4D	1.56	1.01
1:A:278:LEU:HD21	1:A:306:PHE:HE1	1.24	1.01
2:R:152:GLU:OE2	3:R:501:APR:C5D	2.07	1.01
2:R:352:TYR:HE1	3:R:501:APR:O2D	1.42	1.01
1:D:67:LEU:CD2	1:D:73:SER:OG	2.08	1.00
2:R:54:MET:HE3	3:R:501:APR:O5D	1.61	1.00
1:C:67:LEU:HD22	1:C:74:LYS:CG	1.91	1.00
2:L:413:TYR:CE1	3:L:501:APR:N3	2.29	1.00
1:E:188:VAL:HG21	1:E:437:GLU:CG	1.91	1.00
1:A:554:ILE:HD12	1:D:464:GLY:O	1.61	1.00
1:D:221:ASN:OD1	1:D:406:LEU:HD22	1.63	0.99
1:E:349:LEU:HD23	1:E:352:GLU:OE2	1.61	0.99
2:R:352:TYR:CE1	3:R:501:APR:O2D	2.15	0.99
1:B:507:LEU:HD12	1:B:518:LEU:HD12	1.44	0.99
1:D:227:GLU:HA	1:D:231:LEU:HD23	1.45	0.98
1:F:57:VAL:HA	1:F:83:CYS:SG	2.03	0.98
2:P:355:PRO:HG2	3:P:501:APR:HR'3	1.45	0.98
2:N:413:TYR:CE1	3:N:501:APR:C4	2.47	0.98
1:D:186:PHE:HA	1:D:436:GLU:CD	1.88	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:LEU:HD11	1:F:366:LEU:HD11	1.46	0.97
1:A:216:MET:O	1:A:220:ILE:HG12	1.62	0.97
1:D:221:ASN:OD1	1:D:406:LEU:CD2	2.13	0.97
2:R:352:TYR:CE1	3:R:501:APR:HR'2	1.99	0.97
2:R:152:GLU:OE2	3:R:501:APR:C4D	2.14	0.96
2:N:65:ASN:HD22	2:N:69:LEU:CD2	1.78	0.96
1:B:254:LEU:CD1	1:B:323:LEU:CD2	2.43	0.96
1:C:140:ALA:CB	1:C:542:ILE:CD1	2.43	0.95
1:B:409:THR:O	1:B:413:LEU:HD13	1.64	0.95
1:C:67:LEU:CD2	1:C:74:LYS:CG	2.42	0.95
1:D:506:LEU:CD1	1:D:510:ILE:CD1	2.45	0.95
2:L:54:MET:CE	3:L:501:APR:O1D	2.13	0.95
2:L:267:THR:HG21	2:L:271:LYS:HA	1.45	0.95
1:A:262:LEU:HD11	1:A:353:SER:OG	1.65	0.95
1:A:276:LYS:O	1:A:280:ILE:HD12	1.65	0.95
2:L:412:HIS:CD2	3:L:501:APR:H'1	2.02	0.94
1:C:140:ALA:HB2	1:C:542:ILE:HD12	1.45	0.94
1:A:507:LEU:HG	1:A:518:LEU:CD2	1.96	0.94
2:R:54:MET:HE1	3:R:501:APR:C4D	1.96	0.94
1:A:484:THR:HG22	1:A:488:GLN:NE2	1.83	0.94
1:C:67:LEU:HD22	1:C:74:LYS:HG3	0.95	0.94
2:L:79:LYS:HZ3	2:L:118:ASN:ND2	1.65	0.93
2:L:412:HIS:NE2	3:L:501:APR:H'1	1.83	0.93
1:F:65:ILE:HG21	1:F:78:HIS:CG	2.03	0.93
2:N:355:PRO:HG3	3:N:501:APR:H5R2	1.51	0.93
1:D:211:ILE:HG21	1:D:333:ASN:CG	1.93	0.93
2:R:45:GLY:O	3:R:501:APR:C6	2.16	0.92
2:O:254:PHE:CB	2:O:300:LEU:HD11	2.00	0.92
1:D:400:LEU:CD1	1:D:405:LEU:HD21	1.99	0.92
1:B:254:LEU:CD1	1:B:323:LEU:HD23	1.99	0.92
2:O:102:LYS:O	2:O:106:THR:HG23	1.70	0.91
1:A:440:ARG:CZ	1:D:460:ILE:HD13	2.01	0.91
1:B:216:MET:HG3	1:B:238:LEU:CD1	2.01	0.90
2:J:32:HIS:CD2	2:J:373:ASN:HD22	1.89	0.90
2:N:413:TYR:HE1	3:N:501:APR:C4	1.82	0.90
1:F:57:VAL:HG22	1:F:83:CYS:SG	2.12	0.90
1:C:248:ILE:HD12	1:C:329:LYS:HE3	1.53	0.89
1:F:531:ILE:O	1:F:539:PRO:HA	1.73	0.89
2:O:300:LEU:O	2:O:300:LEU:HD12	1.72	0.89
1:D:67:LEU:HD23	1:D:73:SER:OG	1.70	0.88
1:D:360:ARG:NH1	1:E:319:ASN:OD1	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:244:THR:HG23	2:K:246:ILE:CG1	2.01	0.88
1:D:186:PHE:CB	1:D:436:GLU:OE1	2.20	0.88
1:D:506:LEU:HD12	1:D:510:ILE:HD12	1.52	0.88
1:A:503:LEU:O	1:A:518:LEU:HD21	1.73	0.88
1:F:416:GLU:CG	1:F:431:ASN:HD22	1.85	0.88
2:P:96:ILE:HG22	2:P:97:GLN:H	1.38	0.88
1:E:525:PRO:O	1:E:528:THR:HG22	1.74	0.88
2:P:54:MET:HB2	3:P:501:APR:O2B	1.74	0.88
2:R:54:MET:CE	3:R:501:APR:O5D	2.22	0.88
2:N:413:TYR:CE1	3:N:501:APR:N3	2.40	0.87
1:F:65:ILE:CG2	1:F:78:HIS:HB2	2.04	0.87
2:G:314:ILE:HD11	2:G:329:TYR:CD2	2.08	0.87
1:D:402:ASP:HA	1:D:405:LEU:HD12	1.55	0.87
2:Q:343:LYS:O	2:Q:344:ASP:OD1	1.92	0.87
2:M:254:PHE:HB2	2:M:300:LEU:CD2	2.05	0.87
2:N:44:SER:OG	3:N:501:APR:O3D	1.92	0.87
2:M:254:PHE:HB3	2:M:300:LEU:HD23	1.54	0.87
1:A:440:ARG:CZ	1:D:460:ILE:CD1	2.53	0.86
2:R:54:MET:HE3	3:R:501:APR:C5D	2.05	0.86
2:R:54:MET:CE	3:R:501:APR:C4D	2.53	0.86
1:C:57:VAL:HA	1:C:83:CYS:SG	2.16	0.86
1:D:349:LEU:HA	1:D:352:GLU:CD	2.00	0.86
1:D:211:ILE:HG21	1:D:333:ASN:OD1	1.76	0.85
2:H:224:THR:O	2:H:225:THR:HG22	1.75	0.85
2:R:54:MET:CE	3:R:501:APR:HR'4	2.05	0.85
2:R:355:PRO:HG2	3:R:501:APR:HR'3	1.56	0.85
1:A:271:VAL:HG13	1:D:264:ARG:O	1.75	0.85
1:E:431:ASN:OD1	1:E:431:ASN:O	1.94	0.85
2:H:96:ILE:HG22	2:H:100:GLU:HB2	1.59	0.85
2:L:79:LYS:HZ3	2:L:118:ASN:HD21	1.17	0.85
2:P:38:LEU:HB3	2:P:220:VAL:HG23	1.57	0.85
1:D:221:ASN:CG	1:D:406:LEU:HD23	2.00	0.84
1:D:67:LEU:HD22	1:D:73:SER:OG	1.75	0.84
1:E:368:THR:HG21	1:F:232:PRO:HB3	1.59	0.84
1:D:221:ASN:CG	1:D:406:LEU:CD2	2.51	0.84
2:P:224:THR:O	2:P:225:THR:HG22	1.77	0.84
2:H:122:TYR:CE2	2:H:126:LEU:HD11	2.12	0.83
1:C:67:LEU:HD21	1:C:74:LYS:HE3	1.59	0.83
1:D:67:LEU:HD23	1:D:73:SER:HB2	1.60	0.83
1:F:26:ASN:CG	1:F:35:ILE:HG12	2.03	0.83
1:D:400:LEU:HD11	1:D:405:LEU:HD21	1.54	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:418:VAL:HG12	2:Q:422:LEU:HD12	1.58	0.83
2:J:32:HIS:HD2	2:J:373:ASN:HD22	1.21	0.83
1:D:401:ASP:O	1:D:405:LEU:CG	2.23	0.83
2:L:54:MET:HE3	3:L:501:APR:O1D	1.79	0.83
1:A:507:LEU:HG	1:A:518:LEU:HD22	1.60	0.83
1:B:341:LEU:HD13	1:B:370:ILE:CD1	2.08	0.83
1:D:165:THR:HB	1:D:544:ILE:HD13	1.61	0.83
1:E:15:LEU:HD23	1:E:83:CYS:SG	2.17	0.83
2:H:270:TYR:N	2:O:270:TYR:HH	1.77	0.83
2:N:413:TYR:CD1	3:N:501:APR:C2	2.61	0.82
1:D:221:ASN:ND2	1:D:406:LEU:CD2	2.42	0.82
2:L:412:HIS:NE2	3:L:501:APR:C2'	2.42	0.82
2:M:25:VAL:HG12	2:M:25:VAL:O	1.79	0.82
1:F:182:HIS:CB	1:F:431:ASN:OD1	2.27	0.82
2:P:355:PRO:CG	3:P:501:APR:HR'3	2.09	0.82
1:F:344:LEU:CD1	1:F:366:LEU:HD11	2.08	0.82
2:H:422:LEU:HD12	2:H:422:LEU:O	1.78	0.82
2:R:54:MET:CE	3:R:501:APR:C5D	2.58	0.81
2:R:152:GLU:OE2	3:R:501:APR:C3D	2.28	0.81
2:L:54:MET:HE1	3:L:501:APR:O1D	1.79	0.81
2:L:45:GLY:O	2:L:48:THR:HG23	1.81	0.81
1:F:268:THR:OG1	1:F:272:THR:HG21	1.80	0.81
1:D:69:SER:O	1:D:70:GLU:HG3	1.81	0.81
2:H:54:MET:HG3	3:H:501:APR:HR'4	1.63	0.81
1:F:65:ILE:CG2	1:F:78:HIS:CG	2.64	0.81
1:A:226:SER:OG	1:A:229:VAL:HG22	1.81	0.80
2:L:413:TYR:HE1	3:L:501:APR:C4	1.92	0.80
2:K:159:GLN:NE2	2:K:319:LEU:HD12	1.95	0.80
2:J:303:ILE:CD1	2:J:306:ASN:HB2	2.11	0.80
2:P:355:PRO:HG3	3:P:501:APR:H5R2	1.63	0.80
2:P:412:HIS:NE2	3:P:501:APR:H'2	1.96	0.80
1:B:254:LEU:CD1	1:B:323:LEU:HD21	2.08	0.80
2:J:32:HIS:NE2	2:J:373:ASN:ND2	2.29	0.80
1:B:216:MET:HG3	1:B:238:LEU:HD11	1.62	0.80
2:L:44:SER:HB3	3:L:501:APR:O1D	1.80	0.80
2:P:90:GLU:OE2	2:P:383:GLU:OE1	2.00	0.79
1:C:131:ILE:O	1:C:542:ILE:HD11	1.82	0.79
2:R:355:PRO:CG	3:R:501:APR:HR'3	2.13	0.79
2:J:355:PRO:HG3	3:J:501:APR:HR'3	1.63	0.79
1:C:140:ALA:HB3	1:C:542:ILE:CD1	2.12	0.79
1:B:254:LEU:HD12	1:B:323:LEU:HD23	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:LEU:CD1	1:B:518:LEU:HD12	2.05	0.79
1:E:405:LEU:O	1:E:409:THR:HG22	1.83	0.79
2:P:51:VAL:HG23	2:P:185:THR:O	1.82	0.78
1:F:416:GLU:CG	1:F:431:ASN:ND2	2.46	0.78
1:D:67:LEU:HG	1:D:68:SER:N	1.98	0.78
2:L:267:THR:HG22	2:L:271:LYS:CA	2.12	0.78
1:D:348:PHE:C	1:D:352:GLU:OE1	2.26	0.78
2:J:32:HIS:CD2	2:J:373:ASN:HD21	1.98	0.78
2:N:355:PRO:HG3	3:N:501:APR:C5D	2.13	0.77
2:N:355:PRO:CG	3:N:501:APR:O4D	2.32	0.77
1:A:554:ILE:CD1	1:D:465:ARG:HA	2.14	0.77
1:A:237:GLY:HA2	1:A:347:VAL:HG21	1.67	0.77
2:L:412:HIS:NE2	3:L:501:APR:C1'	2.46	0.77
1:A:554:ILE:CD1	1:D:464:GLY:O	2.31	0.77
2:P:355:PRO:HG2	3:P:501:APR:C3D	2.14	0.77
1:B:531:ILE:HD11	1:B:542:ILE:HD11	1.67	0.77
1:C:254:LEU:HD22	1:C:346:TYR:CD2	2.20	0.77
2:M:254:PHE:CG	2:M:300:LEU:HD23	2.20	0.77
1:D:211:ILE:CG2	1:D:333:ASN:CG	2.57	0.77
1:E:315:ASP:OD1	1:E:319:ASN:OD1	2.03	0.77
2:O:254:PHE:HB2	2:O:300:LEU:HD11	1.66	0.77
1:D:400:LEU:HD12	1:D:405:LEU:CD2	2.12	0.76
2:M:24:GLN:OE1	2:M:417:ILE:CD1	2.33	0.76
1:B:216:MET:HG3	1:B:238:LEU:CD2	2.15	0.76
2:L:48:THR:HG21	3:L:501:APR:C2	2.14	0.76
2:J:215:GLU:HG2	2:J:279:LYS:HG3	1.66	0.76
2:J:367:LEU:HD13	2:J:394:ASN:HD22	1.49	0.76
2:L:413:TYR:CD1	3:L:501:APR:N3	2.52	0.76
2:L:412:HIS:CD2	3:L:501:APR:C1'	2.68	0.76
1:B:461:ALA:HB1	1:B:488:GLN:HG2	1.67	0.75
2:J:392:PHE:CB	2:J:394:ASN:ND2	2.48	0.75
2:Q:352:TYR:OH	2:Q:356:ASP:OD1	2.04	0.75
2:R:355:PRO:HG3	3:R:501:APR:H5R2	1.68	0.75
1:A:278:LEU:HD21	1:A:306:PHE:CE1	2.17	0.75
1:C:262:LEU:HA	1:C:265:ASN:HB2	1.69	0.75
1:D:400:LEU:CD1	1:D:405:LEU:CG	2.64	0.75
2:L:44:SER:OG	3:L:501:APR:HR'3	1.87	0.75
2:L:79:LYS:HZ3	2:L:118:ASN:CG	1.94	0.75
1:A:228:LEU:CD1	1:B:361:SER:HA	2.17	0.75
2:K:246:ILE:HD11	2:K:292:TRP:CZ2	2.21	0.75
2:M:249:THR:OG1	2:P:242:TYR:OH	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HD11	1:B:323:LEU:HD23	1.68	0.74
1:D:67:LEU:HD23	1:D:73:SER:CA	2.17	0.74
2:L:351:GLY:O	3:L:501:APR:C5'	2.35	0.74
2:P:354:PHE:HB3	2:P:360:ASN:HD21	1.53	0.74
1:B:507:LEU:HD12	1:B:518:LEU:HD11	0.74	0.74
1:E:525:PRO:HD2	1:E:528:THR:HG21	1.70	0.74
1:D:230:GLN:HA	1:D:233:ILE:HD12	1.67	0.74
2:H:267:THR:O	2:H:268:ASN:O	2.06	0.74
1:A:554:ILE:HD12	1:D:465:ARG:HA	1.70	0.74
1:D:67:LEU:CD2	1:D:73:SER:CB	2.58	0.74
1:B:357:ASN:HB2	1:E:357:ASN:H	1.53	0.74
1:B:391:LYS:HE3	1:C:560:TYR:HB3	1.68	0.74
1:F:200:ILE:HD11	1:F:396:SER:OG	1.88	0.74
1:F:416:GLU:HG3	1:F:431:ASN:HD22	1.52	0.73
1:E:482:SER:OG	1:E:485:VAL:HG23	1.87	0.73
2:J:341:GLN:HG3	2:J:366:ASN:OD1	1.89	0.73
1:B:531:ILE:HD13	1:B:542:ILE:HD12	1.71	0.73
1:D:67:LEU:CG	1:D:68:SER:H	2.00	0.73
1:F:284:THR:HG22	1:F:285:ASN:N	2.03	0.73
2:N:355:PRO:HG3	3:N:501:APR:C4D	2.19	0.73
1:B:274:ARG:HG3	1:B:291:TYR:HB3	1.69	0.73
1:B:507:LEU:HD11	1:B:518:LEU:HG	0.73	0.73
2:Q:356:ASP:OD2	2:Q:358:HIS:CE1	2.42	0.72
1:B:179:GLN:HB3	1:C:561:ARG:HB3	1.71	0.72
1:D:261:SER:HA	1:D:264:ARG:HE	1.53	0.72
1:B:370:ILE:HD12	1:B:371:LYS:HD2	1.71	0.72
2:J:413:TYR:CD1	3:J:501:APR:C5	2.72	0.72
1:A:228:LEU:HD13	1:B:361:SER:HA	1.69	0.72
2:K:214:THR:HG22	2:K:214:THR:O	1.89	0.72
2:N:92:GLU:OE2	2:N:105:HIS:HE1	1.64	0.72
1:F:284:THR:HG22	1:F:285:ASN:H	1.54	0.72
1:F:57:VAL:CA	1:F:83:CYS:SG	2.76	0.72
2:L:355:PRO:HG3	3:L:501:APR:O3D	1.90	0.71
2:L:412:HIS:CD2	3:L:501:APR:C2'	2.72	0.71
1:A:157:ASN:ND2	1:A:497:VAL:HA	2.05	0.71
2:P:96:ILE:HG22	2:P:97:GLN:N	2.05	0.71
2:K:244:THR:CG2	2:K:246:ILE:CG1	2.64	0.71
1:C:67:LEU:HD21	1:C:74:LYS:HG3	1.69	0.71
2:I:334:ARG:HH12	2:J:342:ILE:HD13	1.56	0.71
2:I:96:ILE:HD12	2:I:100:GLU:HB3	1.71	0.70
2:L:79:LYS:HZ1	2:L:118:ASN:HD21	0.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:ILE:HD11	2:H:117:LYS:HA	1.71	0.70
1:D:227:GLU:CA	1:D:231:LEU:HD23	2.20	0.70
1:E:280:ILE:HG12	1:E:349:LEU:HD13	1.73	0.70
1:E:425:LEU:HD12	1:E:428:ARG:HD2	1.73	0.70
2:H:91:GLN:O	2:H:95:LYS:NZ	2.24	0.70
2:R:346:THR:HG23	2:R:373:ASN:HD22	1.56	0.70
1:F:65:ILE:HD12	1:F:74:LYS:CD	2.13	0.70
1:C:140:ALA:HB2	1:C:542:ILE:CD1	2.15	0.70
1:E:242:ASN:HD21	1:E:333:ASN:H	1.39	0.70
2:M:24:GLN:CD	2:M:417:ILE:CD1	2.65	0.70
1:B:176:LEU:HB3	1:C:562:SER:HA	1.74	0.69
2:J:303:ILE:HD11	2:J:306:ASN:HB2	1.73	0.69
2:R:352:TYR:HE1	3:R:501:APR:C1D	2.01	0.69
1:D:221:ASN:HD21	1:D:406:LEU:CD2	1.98	0.69
1:E:351:GLU:HG3	1:E:356:ASN:HB2	1.74	0.69
1:E:494:VAL:HG23	1:E:530:TYR:HB3	1.73	0.69
2:H:54:MET:HG3	3:H:501:APR:C4D	2.22	0.69
1:D:348:PHE:O	1:D:352:GLU:CD	2.35	0.69
1:F:284:THR:HG22	1:F:285:ASN:OD1	1.92	0.69
1:E:89:ILE:CG1	1:E:94:ILE:HD13	2.19	0.69
2:N:92:GLU:CD	2:N:105:HIS:CE1	2.67	0.69
1:A:503:LEU:C	1:A:518:LEU:HD21	2.17	0.69
1:C:57:VAL:CG2	1:C:83:CYS:SG	2.80	0.69
2:L:414:PHE:O	2:L:418:VAL:HG23	1.93	0.69
1:A:532:VAL:HG23	1:A:539:PRO:HB3	1.75	0.68
2:H:267:THR:HG21	2:H:275:GLN:HB2	1.73	0.68
2:K:68:VAL:HG22	2:K:174:VAL:HG13	1.75	0.68
2:H:106:THR:HG23	2:H:137:ILE:HD11	1.74	0.68
1:A:280:ILE:HG12	1:A:349:LEU:HD21	1.75	0.68
1:E:89:ILE:HG12	1:E:94:ILE:CD1	2.16	0.68
2:M:25:VAL:HG11	2:M:419:GLU:H	1.58	0.68
2:Q:292:TRP:HB3	2:Q:300:LEU:HD11	1.74	0.68
2:L:54:MET:HE1	3:L:501:APR:C1D	2.22	0.68
2:L:79:LYS:HZ2	2:L:118:ASN:HD21	1.32	0.68
1:B:204:ILE:HG23	1:B:205:ASN:H	1.57	0.68
2:L:351:GLY:O	3:L:501:APR:H5'1	1.94	0.68
1:A:554:ILE:HD12	1:D:464:GLY:C	2.18	0.68
1:F:65:ILE:CG2	1:F:78:HIS:CB	2.71	0.68
2:J:45:GLY:O	3:J:501:APR:C5	2.41	0.68
1:C:248:ILE:CD1	1:C:329:LYS:HE3	2.23	0.68
1:E:219:TRP:O	1:E:223:ILE:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:155:LEU:HB3	2:J:316:PRO:HB3	1.76	0.68
2:R:45:GLY:O	3:R:501:APR:C5	2.42	0.68
2:I:155:LEU:CB	2:I:317:THR:HG22	2.24	0.67
1:D:400:LEU:HD12	1:D:405:LEU:HD21	1.75	0.67
1:D:187:ASP:N	1:D:436:GLU:OE1	2.27	0.67
1:F:532:VAL:HG12	1:F:539:PRO:CB	2.21	0.67
2:I:354:PHE:HD1	2:I:360:ASN:OD1	1.77	0.67
1:D:123:PHE:O	1:D:143:ASN:ND2	2.28	0.67
1:F:374:GLN:O	1:F:378:SER:OG	2.09	0.67
2:P:413:TYR:CE1	3:P:501:APR:C6	2.77	0.67
1:A:156:GLY:HA2	1:A:495:HIS:HB2	1.74	0.67
2:H:96:ILE:CG2	2:H:100:GLU:CB	2.72	0.67
2:I:35:ALA:O	2:I:213:ARG:NH1	2.26	0.67
2:N:355:PRO:CG	3:N:501:APR:H5R2	2.23	0.67
1:A:14:LYS:HA	1:A:83:CYS:O	1.95	0.67
2:G:13:LEU:HB3	2:G:20:GLU:HG2	1.77	0.67
2:K:32:HIS:HB3	2:K:346:THR:HG21	1.75	0.67
1:D:147:LEU:HB2	1:D:535:LEU:HD13	1.76	0.67
2:Q:47:SER:OG	2:Q:226:ASN:ND2	2.28	0.67
2:Q:354:PHE:HB3	2:Q:360:ASN:HD21	1.59	0.67
2:J:72:VAL:O	2:J:75:PHE:HB2	1.93	0.67
1:D:344:LEU:CD1	1:D:348:PHE:HE2	2.08	0.67
2:L:54:MET:CE	3:L:501:APR:C1D	2.72	0.67
1:B:181:LEU:HB2	1:C:561:ARG:HG3	1.77	0.67
2:N:152:GLU:OE2	3:N:501:APR:HR'2	1.95	0.67
1:A:267:GLN:NE2	1:E:264:ARG:O	2.28	0.66
2:O:274:TRP:HB3	2:R:264:VAL:HG11	1.76	0.66
2:Q:340:LEU:HA	2:Q:345:THR:HG21	1.77	0.66
1:A:440:ARG:CZ	1:D:460:ILE:HD11	2.24	0.66
1:D:406:LEU:HD11	1:D:453:GLU:OE2	1.96	0.66
1:F:416:GLU:HG2	1:F:431:ASN:HD22	1.58	0.66
2:M:24:GLN:OE1	2:M:417:ILE:HD11	1.95	0.66
1:D:221:ASN:OD1	1:D:406:LEU:HD23	1.90	0.66
1:E:15:LEU:HD22	1:E:83:CYS:HG	1.59	0.66
1:D:186:PHE:HB2	1:D:436:GLU:OE1	1.93	0.66
2:J:11:ASP:HB3	2:J:14:THR:HG23	1.76	0.66
2:N:292:TRP:HD1	2:N:302:GLN:HG3	1.61	0.66
1:C:57:VAL:CA	1:C:83:CYS:SG	2.84	0.66
1:C:256:CYS:SG	1:C:257:TYR:N	2.69	0.66
1:D:186:PHE:C	1:D:436:GLU:OE1	2.37	0.66
1:A:334:VAL:CG1	1:A:340:LEU:HD11	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:LEU:HD11	1:D:405:LEU:HD23	0.70	0.66
2:P:102:LYS:HA	2:P:105:HIS:CD2	2.31	0.66
2:Q:77:ASN:HA	2:Q:119:LEU:HB3	1.76	0.66
1:D:503:LEU:HB3	1:D:518:LEU:HD21	1.76	0.66
1:D:506:LEU:HD12	1:D:510:ILE:CD1	2.18	0.66
2:J:392:PHE:HB3	2:J:394:ASN:HD21	1.55	0.66
1:A:440:ARG:CD	1:D:460:ILE:HD13	2.26	0.65
2:M:24:GLN:CD	2:M:417:ILE:HD13	2.21	0.65
1:C:67:LEU:HG	1:C:67:LEU:O	1.95	0.65
1:D:413:LEU:HD23	1:D:435:PHE:CZ	2.30	0.65
2:H:96:ILE:HG22	2:H:97:GLN:N	2.11	0.65
2:I:41:PHE:HB3	2:I:349:ILE:HG12	1.77	0.65
2:M:80:GLY:HA2	2:M:118:ASN:HA	1.79	0.65
2:Q:41:PHE:HB2	2:Q:347:LEU:HD11	1.77	0.65
1:E:263:TYR:OH	1:E:303:GLU:OE1	2.13	0.65
2:L:354:PHE:HB3	2:L:360:ASN:HD21	1.61	0.65
2:N:92:GLU:HG2	2:N:92:GLU:O	1.96	0.65
2:N:413:TYR:CE1	3:N:501:APR:C2	2.79	0.65
2:O:5:HIS:O	2:O:12:VAL:HG12	1.96	0.65
1:A:157:ASN:HD21	1:A:497:VAL:HA	1.62	0.65
1:D:47:ASN:HD21	1:D:51:GLU:HB2	1.61	0.65
1:D:239:LYS:HG3	1:D:327:ILE:HA	1.78	0.65
1:D:364:ALA:HB2	1:E:326:VAL:HG12	1.77	0.65
1:D:506:LEU:HD11	1:D:510:ILE:CD1	2.06	0.65
1:A:188:VAL:CG1	1:D:460:ILE:HD12	2.26	0.65
1:C:254:LEU:HD22	1:C:346:TYR:CG	2.32	0.65
1:D:228:LEU:HD13	1:D:229:VAL:HG12	1.77	0.65
2:P:48:THR:OG1	3:P:501:APR:N6	2.30	0.65
1:F:371:LYS:HA	1:F:374:GLN:HB2	1.78	0.65
2:I:77:ASN:HA	2:I:119:LEU:HB2	1.79	0.65
1:B:278:LEU:HD11	1:B:289:GLU:HA	1.79	0.65
1:B:536:PHE:HD2	1:B:537:PRO:HD2	1.62	0.65
1:D:349:LEU:C	1:D:352:GLU:OE1	2.40	0.65
1:E:11:THR:HG22	1:E:12:PHE:N	2.11	0.65
2:I:269:ARG:HG3	2:I:271:LYS:HB2	1.78	0.65
2:J:293:LYS:HE2	2:J:303:ILE:HD13	1.78	0.65
2:M:160:ASN:OD1	2:N:160:ASN:ND2	2.30	0.65
1:A:531:ILE:O	1:A:539:PRO:HA	1.96	0.64
1:A:374:GLN:O	1:A:378:SER:OG	2.13	0.64
1:D:67:LEU:HD22	1:D:73:SER:HG	1.62	0.64
1:D:507:LEU:HB3	1:D:518:LEU:HD13	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:35:ALA:O	2:O:213:ARG:NH1	2.31	0.64
2:P:413:TYR:CD1	3:P:501:APR:C6	2.80	0.64
1:B:216:MET:HG3	1:B:238:LEU:HD21	1.78	0.64
1:F:507:LEU:HB2	1:F:518:LEU:HD11	1.80	0.64
2:P:355:PRO:CG	3:P:501:APR:HR'2	2.28	0.64
1:D:211:ILE:HG22	1:D:333:ASN:ND2	2.12	0.64
1:F:447:GLU:HA	1:F:454:VAL:HG11	1.80	0.64
2:G:314:ILE:HG21	2:G:320:LYS:HG3	1.80	0.64
2:I:354:PHE:CD1	2:I:360:ASN:OD1	2.50	0.64
1:B:274:ARG:NH1	1:B:292:ASP:O	2.30	0.64
1:E:322:THR:HG22	1:E:323:LEU:H	1.63	0.64
1:F:532:VAL:CG1	1:F:539:PRO:HB3	2.22	0.64
2:G:24:GLN:HG3	2:G:25:VAL:HG13	1.80	0.64
2:K:35:ALA:O	2:K:213:ARG:NH1	2.31	0.64
1:A:263:TYR:HA	1:A:273:LYS:HD2	1.80	0.64
1:D:131:ILE:CD1	1:D:172:LYS:NZ	2.56	0.64
1:B:216:MET:CB	1:B:238:LEU:HD22	2.29	0.63
2:J:303:ILE:HD12	2:J:306:ASN:HB2	1.79	0.63
2:O:97:GLN:HE22	2:O:99:LYS:HB3	1.63	0.63
1:E:15:LEU:HB3	1:E:83:CYS:SG	2.39	0.63
2:K:24:GLN:HA	2:K:28:PHE:HB2	1.81	0.63
2:M:249:THR:HG1	2:P:242:TYR:HH	1.41	0.63
1:A:440:ARG:NH1	1:D:460:ILE:HD11	2.13	0.63
1:C:167:ARG:NH1	1:C:550:LYS:O	2.30	0.63
2:O:254:PHE:HB3	2:O:300:LEU:HD11	1.80	0.63
1:A:228:LEU:CD2	1:B:361:SER:HB2	2.28	0.63
1:B:428:ARG:O	1:C:558:ILE:HG23	1.99	0.63
1:C:67:LEU:HD21	1:C:74:LYS:CG	2.28	0.63
1:A:148:LEU:CD2	1:A:432:VAL:HG21	2.20	0.63
2:L:355:PRO:HG3	3:L:501:APR:HR'4	1.81	0.63
1:A:203:VAL:O	1:A:203:VAL:HG12	1.97	0.63
2:P:69:LEU:HA	2:P:72:VAL:HG12	1.80	0.63
1:B:239:LYS:HG3	1:B:327:ILE:HG23	1.81	0.63
1:D:400:LEU:CD1	1:D:405:LEU:HG	2.28	0.63
1:C:140:ALA:HB3	1:C:542:ILE:HD11	1.78	0.63
2:M:25:VAL:HG11	2:M:419:GLU:N	2.13	0.63
1:A:303:GLU:O	1:A:307:ILE:HG12	1.99	0.62
1:F:258:ILE:HD11	1:F:346:TYR:HE1	1.64	0.62
1:B:413:LEU:HD11	1:B:435:PHE:CZ	2.34	0.62
2:O:254:PHE:CB	2:O:300:LEU:CD1	2.76	0.62
1:A:507:LEU:CG	1:A:518:LEU:CD2	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:SER:HA	1:C:558:ILE:HG21	1.80	0.62
1:F:428:ARG:NH1	1:F:428:ARG:O	2.31	0.62
2:H:355:PRO:HG3	3:H:501:APR:HR'3	1.80	0.62
2:L:131:SER:HA	2:L:134:LYS:HG3	1.81	0.62
2:P:111:LEU:HD12	2:P:112:GLU:N	2.14	0.62
1:A:219:TRP:CZ3	1:A:222:LEU:CD2	2.83	0.62
2:O:291:ASN:O	2:O:303:ILE:N	2.32	0.62
1:A:8:THR:HA	1:B:62:ASP:OD2	1.99	0.62
1:A:273:LYS:O	1:A:277:ILE:HG12	1.98	0.62
1:B:531:ILE:CD1	1:B:542:ILE:CD1	2.76	0.62
1:F:255:LYS:HA	1:F:258:ILE:HD12	1.81	0.62
1:B:167:ARG:NH1	1:B:191:GLU:O	2.32	0.62
1:D:167:ARG:HE	1:D:192:TYR:HB3	1.64	0.62
2:H:188:LYS:HD3	2:H:290:ILE:HD12	1.80	0.62
2:L:79:LYS:NZ	2:L:118:ASN:CG	2.54	0.62
2:L:215:GLU:HG2	2:L:279:LYS:HG3	1.82	0.62
1:C:505:TYR:O	1:C:509:SER:HB3	2.00	0.62
2:L:95:LYS:O	2:L:101:ARG:NH2	2.31	0.62
2:N:68:VAL:HG22	2:N:174:VAL:HG13	1.81	0.62
1:F:65:ILE:HG21	1:F:78:HIS:CB	2.30	0.62
2:H:353:GLY:N	3:H:501:APR:H'4	2.14	0.62
2:H:354:PHE:HB3	2:H:360:ASN:HD21	1.65	0.62
2:K:159:GLN:CD	2:K:319:LEU:HD12	2.25	0.62
2:R:79:LYS:NZ	2:R:153:GLU:OE1	2.32	0.62
1:B:532:VAL:HG12	1:B:539:PRO:HB3	1.82	0.61
1:D:16:ILE:HG12	1:D:82:GLU:HG2	1.81	0.61
1:D:413:LEU:HD23	1:D:435:PHE:HZ	1.65	0.61
2:I:286:ILE:HG22	2:I:332:LEU:HB3	1.81	0.61
2:J:53:LEU:HD11	3:J:501:APR:H8	1.81	0.61
2:M:22:GLN:O	2:M:26:ALA:HB2	2.00	0.61
2:O:271:LYS:HD3	2:Q:343:LYS:HZ2	1.65	0.61
1:D:233:ILE:HG23	1:D:347:VAL:HG12	1.80	0.61
2:H:96:ILE:HG22	2:H:100:GLU:CB	2.28	0.61
2:O:354:PHE:HB3	2:O:360:ASN:HD21	1.64	0.61
1:B:183:PHE:O	1:B:392:SER:HA	2.00	0.61
2:G:157:TRP:NE1	2:H:164:TYR:O	2.31	0.61
1:A:334:VAL:HG12	1:A:340:LEU:HD11	1.80	0.61
1:E:401:ASP:O	1:E:405:LEU:N	2.30	0.61
2:K:286:ILE:HG22	2:K:332:LEU:HB3	1.81	0.61
1:C:67:LEU:HD21	1:C:74:LYS:CE	2.29	0.61
2:K:371:ASP:OD1	2:K:371:ASP:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:155:LEU:HB3	2:L:316:PRO:HB3	1.82	0.61
2:O:25:VAL:O	2:O:30:ASN:ND2	2.34	0.61
2:R:287:HIS:HE1	3:R:501:APR:O3D	1.83	0.61
2:H:96:ILE:CG2	2:H:100:GLU:HB2	2.30	0.61
2:J:210:PHE:HA	2:J:213:ARG:HG2	1.82	0.61
2:O:286:ILE:HG22	2:O:332:LEU:HB3	1.83	0.61
1:C:410:THR:HA	1:C:413:LEU:HG	1.82	0.61
1:C:478:PRO:HA	1:C:481:LEU:HD23	1.83	0.61
2:H:96:ILE:HG21	2:H:100:GLU:HB3	1.81	0.61
2:P:349:ILE:HD12	2:P:376:ILE:HG12	1.82	0.61
1:E:210:ASN:ND2	1:E:383:ASN:O	2.32	0.61
2:I:6:LEU:HB2	2:I:399:LEU:HB3	1.81	0.61
2:L:86:LYS:NZ	2:L:383:GLU:OE2	2.34	0.61
2:L:210:PHE:HA	2:L:213:ARG:HG2	1.82	0.61
2:N:61:ILE:HG22	2:N:69:LEU:HD13	1.82	0.61
2:O:254:PHE:HB2	2:O:300:LEU:CD1	2.30	0.61
1:A:434:ILE:HA	1:A:472:MET:HB3	1.82	0.61
1:D:270:ALA:HA	1:D:273:LYS:HG3	1.82	0.61
2:I:155:LEU:HB3	2:I:317:THR:HG22	1.82	0.61
2:J:54:MET:HA	2:J:57:THR:HG22	1.83	0.61
1:B:484:THR:OG1	1:C:501:VAL:HG11	2.00	0.61
1:D:152:THR:HG23	1:D:152:THR:O	1.99	0.60
2:H:39:THR:HG22	2:H:221:SER:HB2	1.83	0.60
2:M:25:VAL:O	2:M:25:VAL:CG1	2.47	0.60
2:R:352:TYR:CE1	3:R:501:APR:C1D	2.81	0.60
1:A:440:ARG:NE	1:D:460:ILE:CD1	2.57	0.60
1:B:216:MET:HB2	1:B:238:LEU:CD2	2.31	0.60
1:C:122:HIS:CE1	1:C:143:ASN:HD22	2.19	0.60
2:L:69:LEU:HD12	2:L:72:VAL:HB	1.83	0.60
2:Q:105:HIS:HA	2:Q:108:MET:HG2	1.82	0.60
1:A:278:LEU:HA	1:A:281:LEU:HB2	1.82	0.60
1:B:67:LEU:H	1:B:70:GLU:HG3	1.66	0.60
1:B:507:LEU:CG	1:B:518:LEU:HD11	2.30	0.60
1:C:10:VAL:HG13	1:C:15:LEU:HD12	1.83	0.60
2:G:133:TYR:HB3	2:G:137:ILE:HD13	1.84	0.60
2:K:155:LEU:HB3	2:K:317:THR:HB	1.84	0.60
2:L:71:TYR:OH	2:L:168:ASN:ND2	2.33	0.60
1:A:276:LYS:HD2	1:A:277:ILE:HG23	1.83	0.60
1:A:503:LEU:O	1:A:518:LEU:CD2	2.48	0.60
1:B:281:LEU:O	1:B:281:LEU:CD1	2.44	0.60
1:F:416:GLU:OE2	1:F:431:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:392:PHE:HB3	2:J:394:ASN:CG	2.27	0.60
2:K:151:ILE:HD11	2:K:178:LEU:HD22	1.83	0.60
2:N:143:CYS:SG	2:N:147:ASN:ND2	2.75	0.60
2:P:51:VAL:HG21	2:P:186:ILE:HG13	1.84	0.60
1:C:187:ASP:N	1:C:395:TYR:O	2.30	0.60
1:E:134:ILE:HG12	1:E:542:ILE:HG13	1.84	0.60
2:I:96:ILE:CD1	2:I:100:GLU:HB2	2.21	0.60
2:J:11:ASP:HB3	2:J:14:THR:CG2	2.32	0.60
2:M:200:GLU:HA	2:M:203:LYS:HG2	1.82	0.60
1:B:409:THR:O	1:B:413:LEU:CD1	2.46	0.60
1:C:277:ILE:HD11	1:C:291:TYR:HB2	1.84	0.60
2:L:13:LEU:O	2:L:21:LYS:NZ	2.32	0.60
2:P:96:ILE:CG2	2:P:97:GLN:H	2.12	0.60
1:B:204:ILE:HG23	1:B:205:ASN:N	2.17	0.60
1:F:373:VAL:HA	1:F:376:ARG:HG2	1.84	0.60
2:J:69:LEU:O	2:J:73:LYS:N	2.34	0.60
2:J:413:TYR:CD1	3:J:501:APR:C6	2.85	0.60
2:K:160:ASN:ND2	2:K:318:MET:SD	2.64	0.60
2:L:79:LYS:HZ2	2:L:117:LYS:HE2	1.66	0.60
2:M:24:GLN:CD	2:M:417:ILE:HD11	2.27	0.60
2:P:355:PRO:CG	3:P:501:APR:H5R2	2.30	0.60
2:R:152:GLU:OE2	3:R:501:APR:HR'3	2.00	0.60
1:E:174:ASN:O	1:E:179:GLN:NE2	2.35	0.60
1:F:231:LEU:HG	1:F:232:PRO:HD3	1.83	0.60
2:H:66:GLU:O	2:H:70:ASN:ND2	2.35	0.60
1:A:146:LYS:O	1:A:491:ASN:ND2	2.35	0.60
1:E:188:VAL:HG22	1:E:436:GLU:HB3	1.84	0.59
2:O:32:HIS:HB3	2:O:346:THR:HG21	1.83	0.59
1:A:192:TYR:HD2	1:A:394:VAL:HG21	1.67	0.59
1:E:11:THR:HG22	1:E:12:PHE:H	1.67	0.59
2:L:219:LYS:HG3	2:L:262:ARG:HD3	1.84	0.59
1:F:47:ASN:HD21	1:F:51:GLU:HB2	1.68	0.59
2:M:35:ALA:O	2:M:213:ARG:NH1	2.35	0.59
1:C:157:ASN:HA	1:C:476:GLN:HB2	1.84	0.59
1:C:254:LEU:CD2	1:C:346:TYR:CG	2.86	0.59
1:D:67:LEU:O	1:D:68:SER:C	2.45	0.59
1:E:199:LYS:HB3	1:E:393:ILE:HG22	1.84	0.59
2:P:340:LEU:HA	2:P:345:THR:HG21	1.85	0.59
1:A:348:PHE:HE2	1:A:367:GLU:HB2	1.66	0.59
1:D:74:LYS:HG3	1:D:76:LYS:H	1.65	0.59
2:J:341:GLN:CG	2:J:366:ASN:OD1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:HA	1:A:254:LEU:HD12	1.84	0.59
1:F:271:VAL:HA	1:F:274:ARG:HG2	1.84	0.59
2:I:24:GLN:HA	2:I:28:PHE:HB2	1.83	0.59
2:J:70:ASN:O	2:J:73:LYS:HB2	2.03	0.59
2:O:206:TYR:OH	2:O:231:ASN:ND2	2.35	0.59
2:M:22:GLN:HG3	2:M:421:PHE:HB3	1.84	0.59
2:N:410:LYS:HB3	2:N:412:HIS:CE1	2.37	0.59
2:P:355:PRO:HG2	3:P:501:APR:HR'2	1.84	0.59
1:B:345:ASN:HA	1:B:348:PHE:CE2	2.37	0.59
1:B:391:LYS:O	1:B:391:LYS:NZ	2.33	0.59
2:G:162:LEU:O	2:G:166:ASN:ND2	2.27	0.59
2:R:45:GLY:O	3:R:501:APR:N1	2.36	0.59
1:A:258:ILE:HD12	1:A:350:LEU:HD12	1.83	0.59
1:B:531:ILE:CD1	1:B:542:ILE:HD12	2.33	0.59
1:D:145:ALA:O	1:D:149:THR:OG1	2.21	0.59
1:F:284:THR:CG2	1:F:285:ASN:H	2.15	0.59
2:I:272:GLU:HB3	2:I:275:GLN:HB2	1.85	0.59
2:L:340:LEU:HA	2:L:345:THR:HG21	1.83	0.59
1:A:228:LEU:HD12	1:A:229:VAL:HG13	1.85	0.59
1:C:338:ASN:HA	1:C:341:LEU:HB2	1.83	0.59
2:J:13:LEU:O	2:J:21:LYS:NZ	2.35	0.59
2:J:413:TYR:HD1	3:J:501:APR:C5	2.14	0.59
2:M:254:PHE:CB	2:M:300:LEU:CD2	2.57	0.59
1:A:9:SER:HA	1:B:61:GLU:HA	1.84	0.58
1:D:165:THR:CB	1:D:544:ILE:HD13	2.33	0.58
1:F:224:LYS:O	1:F:369:ARG:NH1	2.36	0.58
2:L:165:ASP:O	2:L:166:ASN:ND2	2.36	0.58
2:O:314:ILE:O	2:O:314:ILE:HG13	2.03	0.58
1:B:11:THR:HB	1:C:59:LYS:HG3	1.84	0.58
2:P:355:PRO:CG	3:P:501:APR:C3D	2.77	0.58
1:A:217:GLN:O	1:A:221:ASN:ND2	2.36	0.58
1:A:361:SER:HA	1:D:229:VAL:HB	1.86	0.58
1:E:61:GLU:HA	1:F:9:SER:HA	1.83	0.58
2:J:319:LEU:HB2	2:J:322:LYS:HB2	1.84	0.58
2:M:324:THR:O	2:M:330:SER:OG	2.17	0.58
1:A:355:GLY:O	1:B:267:GLN:NE2	2.36	0.58
1:A:484:THR:HG22	1:A:488:GLN:HE21	1.64	0.58
1:C:477:ARG:HE	1:C:479:SER:HB2	1.68	0.58
1:F:267:GLN:NE2	1:F:268:THR:HG23	2.18	0.58
2:H:35:ALA:O	2:H:213:ARG:NH1	2.31	0.58
2:I:350:ILE:HA	2:I:377:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:VAL:HG12	1:C:560:TYR:N	2.19	0.58
1:E:478:PRO:HG2	1:E:502:ASP:HB3	1.84	0.58
2:G:219:LYS:HE3	2:G:280:GLU:HG2	1.84	0.58
2:Q:160:ASN:ND2	2:Q:318:MET:SD	2.72	0.58
1:F:404:LEU:HD23	1:F:404:LEU:H	1.68	0.58
1:E:188:VAL:CG2	1:E:437:GLU:HG2	2.17	0.58
2:G:43:GLY:HA3	2:G:352:TYR:HB2	1.85	0.58
2:N:45:GLY:HA2	2:N:53:LEU:HD11	1.84	0.58
1:A:158:THR:O	1:D:512:TYR:OH	2.22	0.58
1:D:170:ILE:O	1:D:391:LYS:NZ	2.29	0.58
1:D:344:LEU:CD1	1:D:348:PHE:CE2	2.86	0.58
2:N:413:TYR:HD1	3:N:501:APR:N3	1.95	0.58
2:P:13:LEU:O	2:P:21:LYS:NZ	2.36	0.58
2:R:287:HIS:CE1	3:R:501:APR:O3D	2.56	0.58
1:B:266:GLN:HG2	1:B:273:LYS:HE3	1.85	0.58
1:C:131:ILE:O	1:C:542:ILE:CD1	2.52	0.58
1:D:228:LEU:CD1	1:D:229:VAL:HG12	2.34	0.58
1:A:438:ALA:HB1	1:A:442:ILE:HD12	1.86	0.58
1:C:441:TYR:HB2	1:C:442:ILE:HD12	1.85	0.58
2:G:314:ILE:HD11	2:G:329:TYR:CE2	2.37	0.58
2:L:70:ASN:O	2:L:73:LYS:HB2	2.03	0.58
2:P:13:LEU:HB3	2:P:21:LYS:HG2	1.85	0.58
1:A:507:LEU:HG	1:A:518:LEU:HD23	1.82	0.57
1:B:314:VAL:CG1	1:B:319:ASN:HA	2.34	0.57
1:A:428:ARG:NH2	1:B:555:THR:OG1	2.36	0.57
2:M:21:LYS:NZ	2:M:422:LEU:O	2.30	0.57
1:C:152:THR:HB	1:C:472:MET:HG3	1.87	0.57
1:D:228:LEU:HD12	1:D:229:VAL:N	2.18	0.57
1:D:412:ILE:HA	1:D:415:LYS:HG2	1.87	0.57
1:E:368:THR:HG21	1:F:232:PRO:CB	2.33	0.57
2:H:96:ILE:CG2	2:H:97:GLN:N	2.67	0.57
2:H:96:ILE:HG21	2:H:100:GLU:CB	2.35	0.57
1:A:549:SER:O	1:A:551:ASN:ND2	2.36	0.57
1:B:133:LEU:HG	1:B:136:ASP:HA	1.85	0.57
2:P:367:LEU:HB3	2:P:394:ASN:ND2	2.19	0.57
1:B:455:GLU:O	1:B:459:LYS:N	2.37	0.57
1:E:150:ASN:HB3	1:E:490:ASN:HB2	1.86	0.57
2:K:312:VAL:O	2:K:329:TYR:OH	2.19	0.57
2:N:92:GLU:OE2	2:N:105:HIS:ND1	2.27	0.57
1:D:166:VAL:HA	1:D:169:ILE:HD12	1.86	0.57
1:D:228:LEU:HD12	1:D:230:GLN:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ILE:HG12	1:F:82:GLU:HG2	1.85	0.57
1:F:156:GLY:HA3	1:F:495:HIS:HB2	1.86	0.57
2:R:340:LEU:HA	2:R:345:THR:HG21	1.87	0.57
2:J:355:PRO:CG	3:J:501:APR:HR'3	2.31	0.57
2:K:219:LYS:HD2	2:K:262:ARG:HG2	1.86	0.57
2:Q:219:LYS:HG2	2:Q:280:GLU:HG3	1.86	0.57
1:C:561:ARG:O	1:C:562:SER:HB2	2.03	0.57
1:E:164:THR:HG23	1:E:547:GLU:HB3	1.86	0.57
1:F:239:LYS:HD2	1:F:330:ALA:HB3	1.86	0.57
2:H:102:LYS:HA	2:H:105:HIS:CD2	2.40	0.57
2:P:355:PRO:HG2	3:P:501:APR:C2D	2.34	0.57
2:R:319:LEU:HB2	2:R:322:LYS:HB2	1.86	0.57
2:R:353:GLY:N	3:R:501:APR:H'4	2.20	0.57
1:B:269:ASP:HB3	1:B:271:VAL:HG12	1.86	0.57
1:C:223:ILE:HG21	1:C:234:LEU:HD11	1.87	0.57
1:D:211:ILE:HD13	1:D:334:VAL:N	2.19	0.57
1:E:420:ASN:ND2	1:E:428:ARG:O	2.38	0.57
2:O:22:GLN:HA	2:O:25:VAL:HG22	1.86	0.57
2:O:42:ILE:HG22	2:O:350:ILE:HB	1.87	0.57
2:Q:25:VAL:HA	2:Q:29:ILE:HG22	1.86	0.57
1:C:334:VAL:HG11	1:C:340:LEU:HD22	1.87	0.56
1:F:268:THR:OG1	1:F:272:THR:CG2	2.51	0.56
2:J:69:LEU:HD12	2:J:72:VAL:HB	1.86	0.56
2:P:135:GLU:O	2:P:139:ASN:ND2	2.37	0.56
1:C:178:THR:OG1	1:C:180:ASN:OD1	2.20	0.56
1:C:242:ASN:O	1:C:246:ASN:N	2.37	0.56
1:D:349:LEU:N	1:D:352:GLU:OE1	2.38	0.56
2:H:68:VAL:HG12	2:H:174:VAL:HG13	1.88	0.56
2:H:414:PHE:N	3:H:501:APR:N1	2.53	0.56
2:K:324:THR:HA	2:K:329:TYR:HD1	1.70	0.56
2:L:303:ILE:HG13	2:L:305:PHE:H	1.70	0.56
2:M:414:PHE:HA	2:M:417:ILE:HG22	1.87	0.56
1:B:420:ASN:ND2	1:B:467:PHE:O	2.38	0.56
1:B:492:TYR:HB2	1:B:532:VAL:HG22	1.87	0.56
1:E:350:LEU:HA	1:E:353:SER:HB3	1.86	0.56
1:F:57:VAL:CG2	1:F:83:CYS:SG	2.91	0.56
2:H:41:PHE:HB3	2:H:349:ILE:HG23	1.88	0.56
2:I:46:CYS:HB2	2:I:351:GLY:HA3	1.85	0.56
2:J:69:LEU:HD11	2:J:145:TYR:HB3	1.86	0.56
2:J:355:PRO:HG3	3:J:501:APR:C3D	2.35	0.56
2:K:245:GLY:HA2	2:K:258:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:134:LYS:O	2:L:138:LEU:HG	2.05	0.56
2:M:324:THR:HA	2:M:329:TYR:HB2	1.88	0.56
2:R:375:ILE:HA	2:R:398:HIS:HB2	1.87	0.56
1:B:263:TYR:HA	1:B:273:LYS:HD2	1.87	0.56
1:B:484:THR:HG23	1:B:485:VAL:N	2.21	0.56
1:F:13:GLU:HG2	1:F:14:LYS:HG2	1.87	0.56
1:F:554:ILE:HG23	1:F:555:THR:HG23	1.86	0.56
2:J:367:LEU:HD22	2:J:394:ASN:HB3	1.88	0.56
2:K:315:TYR:HB2	2:K:317:THR:HG22	1.86	0.56
2:O:85:ILE:HA	2:O:88:VAL:HG22	1.87	0.56
2:P:64:GLU:HB3	2:P:68:VAL:HB	1.87	0.56
2:Q:329:TYR:HA	2:Q:332:LEU:HD12	1.88	0.56
2:R:225:THR:HG21	3:R:501:APR:O2D	2.05	0.56
1:A:104:LEU:HD13	1:B:62:ASP:OD1	2.06	0.56
1:F:209:ILE:HG22	1:F:380:LEU:HD12	1.88	0.56
2:M:267:THR:O	2:M:268:ASN:ND2	2.39	0.56
2:Q:156:ASN:OD1	2:Q:318:MET:N	2.39	0.56
2:Q:418:VAL:HA	2:Q:422:LEU:HB2	1.86	0.56
1:B:477:ARG:NH2	1:B:502:ASP:OD2	2.39	0.56
1:E:188:VAL:HG11	1:E:437:GLU:HB2	1.88	0.56
2:J:314:ILE:HG22	2:J:316:PRO:HD2	1.87	0.56
2:O:165:ASP:O	2:P:77:ASN:ND2	2.37	0.56
2:P:219:LYS:HG2	2:P:262:ARG:HH11	1.70	0.56
2:Q:35:ALA:O	2:Q:213:ARG:NH1	2.38	0.56
1:A:278:LEU:CD2	1:A:306:PHE:HE1	2.10	0.56
2:H:296:GLU:HA	2:H:320:LYS:HD3	1.88	0.56
2:L:351:GLY:C	3:L:501:APR:C4'	2.63	0.56
2:P:353:GLY:H	3:P:501:APR:H'4	1.70	0.56
2:R:81:ILE:HG22	2:R:81:ILE:O	2.06	0.56
1:C:46:LYS:HG2	1:C:52:LYS:HG2	1.87	0.56
2:G:219:LYS:HD2	2:G:262:ARG:HG2	1.87	0.56
2:J:41:PHE:HB2	2:J:347:LEU:HD11	1.87	0.56
2:P:307:ASP:OD2	2:P:307:ASP:N	2.35	0.56
2:Q:21:LYS:HD2	2:Q:420:ASN:HB3	1.87	0.56
1:B:167:ARG:NH2	1:B:549:SER:OG	2.38	0.56
2:J:413:TYR:HD1	3:J:501:APR:C6	2.18	0.56
2:L:16:LEU:O	2:L:21:LYS:NZ	2.38	0.56
2:O:294:SER:HA	2:O:300:LEU:HA	1.88	0.56
2:P:309:ASP:OD1	2:P:309:ASP:N	2.36	0.56
2:Q:210:PHE:HZ	2:Q:281:ALA:HB2	1.71	0.56
1:A:148:LEU:HD21	1:A:183:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD11	1:A:353:SER:HG	1.68	0.56
1:F:65:ILE:HG22	1:F:78:HIS:CD2	2.41	0.56
1:F:210:ASN:N	1:F:385:ASP:OD1	2.36	0.56
2:L:98:GLU:HA	2:L:101:ARG:HG2	1.88	0.56
2:O:375:ILE:HG12	2:O:398:HIS:HB2	1.88	0.56
1:D:211:ILE:HG22	1:D:211:ILE:O	2.04	0.55
1:E:94:ILE:HG23	1:E:96:PHE:CE1	2.40	0.55
1:F:216:MET:HE3	1:F:235:GLN:HG3	1.89	0.55
2:I:155:LEU:HB2	2:I:317:THR:HG22	1.88	0.55
2:N:54:MET:O	2:N:57:THR:HG22	2.05	0.55
2:O:219:LYS:HD2	2:O:262:ARG:HG2	1.87	0.55
1:E:165:THR:HG21	1:E:495:HIS:HE1	1.70	0.55
1:D:302:THR:HA	1:D:305:LYS:HB3	1.89	0.55
1:D:554:ILE:HG13	1:E:425:LEU:HD23	1.89	0.55
2:G:91:GLN:HE21	2:G:96:ILE:HD11	1.71	0.55
2:K:77:ASN:HB3	2:K:120:GLU:HG2	1.87	0.55
2:O:6:LEU:HD12	2:O:399:LEU:HD23	1.89	0.55
1:A:252:GLU:HA	1:A:255:LYS:HE3	1.89	0.55
1:A:252:GLU:HA	1:A:255:LYS:HG2	1.88	0.55
2:I:81:ILE:H	2:I:81:ILE:HD12	1.71	0.55
2:R:138:LEU:O	2:R:139:ASN:ND2	2.39	0.55
1:D:231:LEU:HD12	1:D:232:PRO:HD3	1.88	0.55
1:D:233:ILE:HA	1:D:347:VAL:HG11	1.88	0.55
2:K:41:PHE:HB2	2:K:347:LEU:HD11	1.88	0.55
2:L:41:PHE:HB2	2:L:347:LEU:HD11	1.88	0.55
2:L:382:GLU:OE2	3:L:501:APR:H'2	2.06	0.55
2:Q:28:PHE:O	2:Q:32:HIS:ND1	2.33	0.55
1:B:216:MET:CB	1:B:238:LEU:CD2	2.85	0.55
2:K:418:VAL:HG23	2:K:418:VAL:O	2.07	0.55
2:L:342:ILE:HG22	2:L:343:LYS:N	2.22	0.55
2:P:224:THR:O	2:P:225:THR:CG2	2.54	0.55
2:R:206:TYR:OH	2:R:231:ASN:ND2	2.38	0.55
1:A:365:THR:HG23	1:D:231:LEU:HD11	1.87	0.55
1:C:508:ASN:O	1:F:477:ARG:NH2	2.38	0.55
1:D:436:GLU:HA	1:D:474:SER:HB2	1.88	0.55
1:E:10:VAL:HG22	1:E:15:LEU:HD12	1.89	0.55
2:G:105:HIS:HA	2:G:108:MET:HG2	1.89	0.55
2:J:326:GLN:O	2:J:330:SER:OG	2.23	0.55
2:K:3:ILE:HA	2:K:402:GLY:HA3	1.89	0.55
1:A:166:VAL:HA	1:A:169:ILE:HD12	1.88	0.55
1:A:182:HIS:ND1	1:A:390:ASP:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:HIS:HB2	1:C:489:CYS:HA	1.89	0.55
1:C:248:ILE:HD12	1:C:329:LYS:CE	2.31	0.55
1:F:264:ARG:HA	1:F:273:LYS:HD3	1.89	0.55
2:N:179:LYS:NZ	2:N:309:ASP:O	2.39	0.55
2:P:346:THR:HG23	2:P:373:ASN:HD22	1.71	0.55
2:R:210:PHE:HZ	2:R:281:ALA:HB2	1.72	0.55
1:A:400:LEU:HD12	1:A:404:LEU:HB3	1.87	0.55
1:F:223:ILE:HG12	1:F:370:ILE:HG12	1.87	0.55
2:I:157:TRP:NE1	2:J:164:TYR:O	2.35	0.55
2:J:406:LYS:HG3	2:J:407:ALA:H	1.72	0.55
2:N:413:TYR:CE1	3:N:501:APR:C5	2.89	0.55
2:Q:317:THR:OG1	2:Q:318:MET:N	2.40	0.55
2:R:394:ASN:O	2:R:396:ASN:N	2.39	0.55
1:A:228:LEU:HD21	1:B:361:SER:HB2	1.89	0.55
1:B:179:GLN:O	1:C:559:VAL:HA	2.07	0.55
1:B:531:ILE:CD1	1:B:542:ILE:HD11	2.36	0.55
1:C:343:GLY:O	1:C:347:VAL:HG23	2.07	0.55
1:F:336:SER:HB3	1:F:339:LYS:HE3	1.88	0.55
2:R:13:LEU:O	2:R:21:LYS:NZ	2.34	0.55
2:R:294:SER:HB2	2:R:319:LEU:HD23	1.88	0.55
1:E:211:ILE:HA	1:E:214:LEU:HD13	1.88	0.54
2:G:3:ILE:H	2:G:17:LYS:HZ3	1.55	0.54
1:A:501:VAL:HG11	1:D:508:ASN:HA	1.90	0.54
1:D:67:LEU:HD23	1:D:73:SER:HA	1.87	0.54
1:E:165:THR:HG22	1:E:544:ILE:HG13	1.89	0.54
2:H:62:LEU:HD12	2:H:63:GLU:HG3	1.89	0.54
2:I:155:LEU:HB3	2:I:317:THR:CG2	2.37	0.54
2:K:375:ILE:HG12	2:K:398:HIS:HB2	1.89	0.54
2:L:135:GLU:O	2:L:139:ASN:ND2	2.41	0.54
2:O:77:ASN:HA	2:O:119:LEU:HB2	1.89	0.54
2:O:417:ILE:O	2:O:417:ILE:HG22	2.07	0.54
1:D:131:ILE:CD1	1:D:172:LYS:HZ1	2.05	0.54
2:H:53:LEU:HB3	2:H:56:THR:HG23	1.89	0.54
2:H:253:LYS:HG2	2:H:299:GLU:HB3	1.90	0.54
2:J:394:ASN:O	2:J:396:ASN:N	2.40	0.54
1:A:229:VAL:HG23	1:A:230:GLN:HG3	1.88	0.54
1:B:181:LEU:HD11	1:B:183:PHE:CD1	2.43	0.54
1:D:69:SER:O	1:D:70:GLU:CG	2.53	0.54
1:E:432:VAL:HG12	1:E:470:PHE:HB2	1.89	0.54
1:F:284:THR:CG2	1:F:285:ASN:N	2.68	0.54
2:K:222:ILE:HB	2:K:283:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:340:LEU:HA	2:K:345:THR:HG21	1.88	0.54
2:R:172:LYS:O	2:R:176:THR:HG23	2.08	0.54
1:B:462:ARG:HD2	1:C:477:ARG:HH11	1.71	0.54
2:M:247:GLN:HE21	2:M:255:ASP:HB2	1.73	0.54
1:B:443:SER:OG	1:B:444:LYS:N	2.41	0.54
1:C:170:ILE:HG22	1:C:195:ILE:HG21	1.89	0.54
1:D:164:THR:HG1	1:D:192:TYR:HH	1.52	0.54
1:D:477:ARG:HB3	1:E:462:ARG:HE	1.73	0.54
2:M:135:GLU:O	2:M:139:ASN:ND2	2.40	0.54
2:Q:93:GLN:HE21	2:Q:95:LYS:HD3	1.73	0.54
1:A:505:TYR:O	1:A:509:SER:OG	2.18	0.54
2:J:313:VAL:HG23	2:J:313:VAL:O	2.07	0.54
2:L:266:ASP:C	2:L:267:THR:HG23	2.33	0.54
1:A:61:GLU:HG3	1:A:80:ARG:HB2	1.90	0.54
1:B:227:GLU:HG3	1:B:231:LEU:HD22	1.88	0.54
1:E:217:GLN:NE2	1:E:452:ASN:O	2.41	0.54
2:Q:41:PHE:HB3	2:Q:349:ILE:HG12	1.89	0.54
1:A:8:THR:O	1:B:62:ASP:N	2.38	0.54
1:A:477:ARG:NH2	1:D:508:ASN:O	2.35	0.54
1:A:496:ARG:NH2	1:D:512:TYR:OH	2.40	0.54
1:B:151:HIS:HB2	1:B:489:CYS:HA	1.90	0.54
1:B:345:ASN:O	1:B:349:LEU:HG	2.08	0.54
1:B:414:LYS:HZ2	1:B:456:ALA:HB1	1.73	0.54
1:C:310:LEU:HA	1:C:313:VAL:HG12	1.89	0.54
1:E:59:LYS:HB3	1:E:82:GLU:HB3	1.90	0.54
1:E:477:ARG:NH2	1:F:508:ASN:O	2.41	0.54
1:F:21:ASP:HA	1:F:76:LYS:HD2	1.89	0.54
2:G:213:ARG:NH2	2:G:215:GLU:OE2	2.41	0.54
2:N:340:LEU:HA	2:N:345:THR:HG21	1.90	0.54
1:A:507:LEU:CG	1:A:518:LEU:HD22	2.37	0.53
1:D:134:ILE:HB	1:D:138:TYR:HB2	1.89	0.53
1:E:367:GLU:O	1:E:371:LYS:HG2	2.08	0.53
2:H:96:ILE:CG2	2:H:100:GLU:CD	2.81	0.53
2:K:277:VAL:HG13	2:K:277:VAL:O	2.08	0.53
2:M:216:GLN:HB3	2:M:277:VAL:HA	1.90	0.53
2:Q:85:ILE:HA	2:Q:88:VAL:HG22	1.88	0.53
1:C:402:ASP:OD1	1:C:402:ASP:N	2.41	0.53
1:D:242:ASN:ND2	1:D:331:LYS:O	2.41	0.53
1:E:260:LEU:HB3	1:E:310:LEU:HD11	1.90	0.53
2:I:205:PHE:HB2	2:I:415:GLN:HE22	1.73	0.53
2:N:313:VAL:HG23	2:N:313:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:413:TYR:CD1	3:P:501:APR:C5	2.91	0.53
2:R:351:GLY:O	3:R:501:APR:O4'	2.26	0.53
1:C:134:ILE:N	1:C:138:TYR:O	2.40	0.53
1:C:511:PRO:HA	1:F:499:ASN:HB2	1.91	0.53
1:D:160:SER:O	1:D:160:SER:OG	2.23	0.53
2:I:6:LEU:HD12	2:I:399:LEU:HD23	1.90	0.53
2:N:210:PHE:HA	2:N:213:ARG:HG2	1.91	0.53
2:O:41:PHE:HB2	2:O:347:LEU:HD11	1.90	0.53
1:B:39:VAL:HG12	1:B:60:VAL:HG13	1.90	0.53
1:B:365:THR:OG1	1:B:369:ARG:HG2	2.07	0.53
1:B:531:ILE:O	1:B:539:PRO:HA	2.09	0.53
2:G:342:ILE:HG22	2:G:343:LYS:N	2.23	0.53
2:I:38:LEU:HB3	2:I:220:VAL:HG12	1.89	0.53
2:N:81:ILE:HG22	2:N:85:ILE:HG23	1.91	0.53
2:N:155:LEU:HB3	2:N:316:PRO:HB3	1.90	0.53
2:P:11:ASP:HB3	2:P:14:THR:HG23	1.90	0.53
2:P:403:ASN:HB3	2:P:409:GLN:HB3	1.89	0.53
1:A:294:LYS:HB2	1:D:307:ILE:HD11	1.89	0.53
1:F:65:ILE:HG22	1:F:78:HIS:CG	2.43	0.53
2:G:85:ILE:HA	2:G:88:VAL:HG22	1.91	0.53
2:H:340:LEU:HA	2:H:345:THR:HG21	1.89	0.53
2:P:158:ILE:HG23	2:P:171:LEU:HD22	1.89	0.53
2:Q:321:HIS:ND1	2:R:326:GLN:OE1	2.38	0.53
2:R:73:LYS:O	2:R:77:ASN:ND2	2.41	0.53
1:A:228:LEU:HD22	1:B:361:SER:HB2	1.91	0.53
1:D:193:LYS:HE3	1:D:200:ILE:HG12	1.90	0.53
1:E:59:LYS:HG3	1:F:11:THR:HB	1.90	0.53
1:F:413:LEU:HG	1:F:460:ILE:HG13	1.89	0.53
2:H:30:ASN:O	2:H:212:LYS:NZ	2.41	0.53
2:H:67:SER:O	2:H:70:ASN:HB2	2.08	0.53
2:J:355:PRO:CG	3:J:501:APR:HR'2	2.38	0.53
2:R:152:GLU:OE2	3:R:501:APR:HR'4	2.05	0.53
2:R:215:GLU:HB3	2:R:276:PRO:HB2	1.91	0.53
1:A:16:ILE:HG12	1:A:82:GLU:HG2	1.90	0.53
1:A:255:LYS:HB2	1:A:280:ILE:HG22	1.90	0.53
1:D:404:LEU:HA	1:D:407:PHE:HB3	1.91	0.53
1:F:145:ALA:O	1:F:149:THR:OG1	2.19	0.53
2:M:41:PHE:HB2	2:M:347:LEU:HD11	1.90	0.53
2:N:214:THR:O	2:N:216:GLN:N	2.41	0.53
2:N:262:ARG:HH21	2:N:280:GLU:HG3	1.72	0.53
2:P:355:PRO:HG3	3:P:501:APR:C5D	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD11	1:B:361:SER:HA	1.90	0.53
1:B:216:MET:CG	1:B:238:LEU:CD2	2.87	0.53
1:E:203:VAL:HG13	1:E:204:ILE:HG13	1.91	0.53
2:G:235:LEU:HD12	2:G:283:LEU:HD22	1.90	0.53
2:I:71:TYR:OH	2:I:168:ASN:OD1	2.27	0.53
2:I:283:LEU:HG	2:I:285:LYS:HD3	1.90	0.53
2:L:267:THR:HG21	2:L:271:LYS:CA	2.31	0.53
2:L:413:TYR:HE1	3:L:501:APR:N9	2.06	0.53
1:F:304:LYS:HA	1:F:307:ILE:HG22	1.91	0.53
1:E:459:LYS:HG2	1:E:462:ARG:HH12	1.74	0.53
2:G:292:TRP:HB3	2:G:300:LEU:HD11	1.91	0.53
2:L:85:ILE:HA	2:L:88:VAL:HG22	1.90	0.53
2:M:375:ILE:HG12	2:M:398:HIS:HB2	1.90	0.53
2:P:394:ASN:O	2:P:396:ASN:N	2.42	0.53
2:R:201:ILE:HG23	2:R:418:VAL:HG21	1.91	0.53
1:D:397:VAL:HG12	1:D:400:LEU:HD21	1.91	0.52
1:F:465:ARG:HD2	1:F:470:PHE:HE1	1.74	0.52
2:L:375:ILE:HA	2:L:398:HIS:HB2	1.91	0.52
2:M:189:VAL:CG2	2:P:250:ILE:CG2	2.87	0.52
2:R:155:LEU:HB3	2:R:316:PRO:HB3	1.91	0.52
2:R:355:PRO:CD	3:R:501:APR:HR'2	2.39	0.52
1:A:507:LEU:CG	1:A:518:LEU:HD23	2.39	0.52
2:H:214:THR:HG22	2:H:216:GLN:H	1.74	0.52
2:J:370:GLN:HA	2:J:396:ASN:HD21	1.74	0.52
2:N:375:ILE:HA	2:N:398:HIS:HB2	1.92	0.52
1:A:185:ILE:HG12	1:A:434:ILE:HD12	1.90	0.52
1:B:180:ASN:C	1:C:561:ARG:HB2	2.34	0.52
1:D:532:VAL:HG22	1:D:539:PRO:HB3	1.92	0.52
1:E:241:ALA:O	1:E:245:GLU:HG2	2.10	0.52
2:G:308:GLU:O	2:G:311:GLN:NE2	2.42	0.52
2:H:62:LEU:HB3	2:H:146:LEU:HD11	1.91	0.52
2:H:413:TYR:HA	3:H:501:APR:C6	2.38	0.52
2:N:300:LEU:HD11	2:N:313:VAL:HG11	1.90	0.52
2:Q:157:TRP:NE1	2:R:164:TYR:O	2.41	0.52
2:Q:254:PHE:HB2	2:Q:300:LEU:HD23	1.91	0.52
1:C:187:ASP:HB3	1:C:396:SER:HA	1.91	0.52
1:C:250:GLU:HB3	1:C:253:TRP:HB2	1.92	0.52
1:C:460:ILE:O	1:C:464:GLY:N	2.38	0.52
1:E:525:PRO:HA	1:F:97:ASN:HB2	1.91	0.52
2:J:350:ILE:HA	2:J:377:PHE:HB2	1.91	0.52
2:L:253:LYS:HG2	2:L:301:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:SER:O	1:C:50:SER:OG	2.24	0.52
1:D:496:ARG:HB3	1:D:498:LYS:HE3	1.91	0.52
1:F:65:ILE:CG2	1:F:78:HIS:CD2	2.92	0.52
2:I:172:LYS:O	2:I:176:THR:HG23	2.09	0.52
2:K:265:ASP:OD1	2:K:265:ASP:N	2.40	0.52
2:L:179:LYS:HE3	2:L:312:VAL:HG12	1.91	0.52
2:N:216:GLN:OE1	2:N:275:GLN:NE2	2.43	0.52
2:P:215:GLU:O	2:P:262:ARG:NH2	2.41	0.52
1:C:270:ALA:HA	1:C:273:LYS:HE2	1.91	0.52
1:C:444:LYS:NZ	1:C:479:SER:O	2.32	0.52
1:D:26:ASN:HB2	1:D:35:ILE:HG23	1.92	0.52
1:D:400:LEU:HD12	1:D:400:LEU:C	2.35	0.52
1:E:165:THR:HG21	1:E:495:HIS:CE1	2.45	0.52
1:E:323:LEU:HD22	1:E:324:SER:H	1.75	0.52
1:E:383:ASN:ND2	1:E:384:ASN:H	2.07	0.52
1:F:31:GLY:O	2:H:398:HIS:NE2	2.40	0.52
2:P:53:LEU:HB3	2:P:56:THR:HG22	1.91	0.52
1:B:344:LEU:HA	1:B:347:VAL:HG22	1.91	0.52
1:D:493:ILE:HD13	1:D:531:ILE:HG22	1.91	0.52
1:F:265:ASN:H	1:F:273:LYS:HG2	1.75	0.52
2:K:319:LEU:O	2:K:323:GLU:N	2.43	0.52
2:L:18:SER:HA	2:L:21:LYS:HE2	1.91	0.52
2:M:189:VAL:HG21	2:P:250:ILE:CG2	2.40	0.52
1:A:547:GLU:HG3	1:A:549:SER:H	1.74	0.52
1:C:150:ASN:HB3	1:C:490:ASN:HB2	1.92	0.52
1:F:234:LEU:HD11	1:F:366:LEU:HD22	1.91	0.52
1:F:478:PRO:HB2	1:F:502:ASP:HB3	1.92	0.52
2:N:127:ASP:OD1	2:N:127:ASP:N	2.39	0.52
2:P:412:HIS:CD2	3:P:501:APR:C2'	2.92	0.52
2:R:252:LYS:HB3	2:R:302:GLN:HB3	1.92	0.52
1:A:503:LEU:CA	1:A:518:LEU:HD21	2.39	0.52
1:F:331:LYS:H	1:F:331:LYS:HD3	1.75	0.52
2:G:314:ILE:CD1	2:G:329:TYR:CD2	2.89	0.52
2:H:13:LEU:O	2:H:21:LYS:NZ	2.43	0.52
2:I:161:GLY:HA2	2:I:164:TYR:HB3	1.91	0.52
2:N:61:ILE:CG2	2:N:69:LEU:HD13	2.40	0.52
1:A:147:LEU:HB2	1:A:535:LEU:HD13	1.92	0.51
1:B:507:LEU:HG	1:B:518:LEU:HD21	1.92	0.51
1:C:248:ILE:HG13	1:C:326:VAL:HG13	1.91	0.51
2:G:156:ASN:O	2:G:160:ASN:ND2	2.43	0.51
2:O:390:ASP:HA	2:O:393:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TRP:CE3	1:A:222:LEU:CD2	2.93	0.51
2:G:52:PRO:HD2	2:G:185:THR:HB	1.92	0.51
2:I:270:TYR:CD1	2:M:342:ILE:HG12	2.46	0.51
2:N:44:SER:CB	3:N:501:APR:O3D	2.58	0.51
2:P:96:ILE:O	2:P:101:ARG:NH1	2.39	0.51
1:B:322:THR:N	1:C:361:SER:O	2.39	0.51
1:C:193:LYS:HG2	1:C:200:ILE:HG12	1.91	0.51
1:C:341:LEU:HD11	1:C:371:LYS:HD3	1.91	0.51
1:D:410:THR:HA	1:D:413:LEU:HG	1.93	0.51
1:F:160:SER:HA	1:F:526:THR:HG22	1.90	0.51
1:F:416:GLU:HG2	1:F:431:ASN:ND2	2.21	0.51
2:I:261:TYR:CE1	2:N:277:VAL:HG11	2.45	0.51
2:J:44:SER:HB3	3:J:501:APR:O4D	2.10	0.51
2:J:413:TYR:CE1	3:J:501:APR:C5	2.94	0.51
2:Q:375:ILE:HA	2:Q:398:HIS:HB2	1.90	0.51
1:A:439:HIS:CG	1:A:477:ARG:HB3	2.46	0.51
1:B:97:ASN:HB2	1:C:525:PRO:HG3	1.92	0.51
1:D:252:GLU:HA	1:D:255:LYS:HB3	1.92	0.51
1:F:65:ILE:HD11	1:F:74:LYS:HD2	1.81	0.51
1:F:420:ASN:ND2	1:F:467:PHE:O	2.35	0.51
1:F:459:LYS:O	1:F:463:GLU:N	2.35	0.51
2:H:351:GLY:HA2	3:H:501:APR:N3	2.24	0.51
2:J:406:LYS:HA	2:J:409:GLN:HB3	1.92	0.51
2:L:67:SER:O	2:L:70:ASN:HB2	2.09	0.51
2:O:340:LEU:HA	2:O:345:THR:HG21	1.91	0.51
1:A:94:ILE:CD1	1:A:119:VAL:HG22	2.40	0.51
1:D:351:GLU:HA	1:D:354:LYS:HG3	1.92	0.51
2:G:338:ASN:ND2	2:G:341:GLN:OE1	2.43	0.51
2:I:41:PHE:HB2	2:I:347:LEU:HD11	1.92	0.51
2:L:266:ASP:O	2:L:267:THR:HG23	2.11	0.51
2:L:267:THR:HG21	2:L:271:LYS:HD3	1.92	0.51
2:M:21:LYS:HB2	2:M:421:PHE:HA	1.92	0.51
1:B:252:GLU:HA	1:B:255:LYS:HB2	1.91	0.51
1:C:140:ALA:CB	1:C:542:ILE:HD11	2.33	0.51
1:D:200:ILE:HA	1:D:394:VAL:HG13	1.93	0.51
2:G:286:ILE:HG13	2:G:332:LEU:HB3	1.92	0.51
2:H:268:ASN:HD21	2:H:271:LYS:HE2	1.75	0.51
2:R:13:LEU:HB3	2:R:21:LYS:HG2	1.91	0.51
1:A:120:PHE:HE1	1:A:538:ILE:HD11	1.75	0.51
1:D:269:ASP:O	1:D:272:THR:OG1	2.25	0.51
1:E:6:LYS:HB3	1:E:105:GLN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:TYR:OH	2:H:147:ASN:ND2	2.43	0.51
2:M:81:ILE:HG22	2:M:85:ILE:HG23	1.91	0.51
2:R:70:ASN:HA	2:R:73:LYS:HG2	1.92	0.51
1:A:52:LYS:HB2	1:A:89:ILE:HB	1.92	0.51
1:A:271:VAL:O	1:A:275:THR:HG23	2.10	0.51
1:A:554:ILE:HD13	1:D:465:ARG:HA	1.93	0.51
1:B:507:LEU:HD11	1:B:518:LEU:CD2	2.31	0.51
1:D:54:ILE:HG21	1:D:119:VAL:HG21	1.92	0.51
1:E:217:GLN:O	1:E:221:ASN:ND2	2.43	0.51
1:E:465:ARG:HD2	1:E:470:PHE:HE1	1.76	0.51
1:F:416:GLU:HG3	1:F:431:ASN:ND2	2.19	0.51
2:G:41:PHE:HB2	2:G:347:LEU:HD11	1.93	0.51
2:G:314:ILE:CD1	2:G:329:TYR:CE2	2.94	0.51
2:L:65:ASN:HA	2:L:69:LEU:HB3	1.92	0.51
2:L:265:ASP:HB2	2:L:277:VAL:HG12	1.92	0.51
2:N:265:ASP:CG	2:N:277:VAL:HG12	2.36	0.51
2:P:69:LEU:O	2:P:72:VAL:HG12	2.10	0.51
1:B:181:LEU:N	1:C:560:TYR:O	2.44	0.51
1:C:154:ILE:HG12	1:C:493:ILE:HD12	1.93	0.51
2:P:48:THR:HG21	3:P:501:APR:N1	2.25	0.51
2:Q:324:THR:OG1	2:R:334:ARG:NH2	2.42	0.51
1:A:214:LEU:HD13	1:A:218:ASP:HB2	1.93	0.51
1:C:131:ILE:HD11	1:C:544:ILE:HD12	1.93	0.51
1:C:156:GLY:HA3	1:C:495:HIS:HB2	1.93	0.51
1:E:443:SER:OG	1:E:444:LYS:N	2.44	0.51
2:H:270:TYR:O	2:H:272:GLU:HG3	2.11	0.51
2:I:270:TYR:HB2	2:M:342:ILE:HA	1.92	0.51
1:A:507:LEU:HD11	1:A:515:LYS:HG3	1.93	0.50
1:B:6:LYS:HB3	1:B:105:GLN:HA	1.91	0.50
1:B:474:SER:O	1:B:474:SER:OG	2.27	0.50
1:E:185:ILE:HB	1:E:394:VAL:HG22	1.92	0.50
1:F:236:MET:HA	1:F:239:LYS:HG2	1.93	0.50
2:K:81:ILE:O	2:K:85:ILE:HG13	2.11	0.50
2:M:50:ALA:HB1	2:M:193:GLU:HB3	1.93	0.50
2:O:41:PHE:HB3	2:O:349:ILE:HG12	1.92	0.50
2:P:179:LYS:HZ1	2:P:312:VAL:HG13	1.76	0.50
2:R:197:GLU:O	2:R:200:GLU:HB2	2.12	0.50
2:R:355:PRO:HD2	3:R:501:APR:HR'2	1.91	0.50
1:A:16:ILE:HA	1:A:81:PHE:O	2.11	0.50
1:B:131:ILE:HB	1:B:172:LYS:HD3	1.92	0.50
1:E:135:ASP:OD2	1:E:137:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:GLU:OE1	1:E:431:ASN:ND2	2.44	0.50
2:G:334:ARG:NH1	2:G:338:ASN:OD1	2.41	0.50
2:I:24:GLN:HE22	2:I:400:ILE:HD13	1.76	0.50
2:L:104:LEU:HD21	2:L:140:PHE:CE2	2.46	0.50
2:M:354:PHE:HZ	2:M:376:ILE:HD13	1.76	0.50
2:N:9:ASP:OD2	2:N:9:ASP:N	2.42	0.50
2:P:45:GLY:O	3:P:501:APR:N7	2.44	0.50
2:Q:13:LEU:HB3	2:Q:20:GLU:HG2	1.92	0.50
1:E:142:PHE:HB3	1:E:535:LEU:HD11	1.94	0.50
2:Q:343:LYS:HE2	2:Q:343:LYS:HA	1.93	0.50
1:A:216:MET:O	1:A:220:ILE:CG1	2.50	0.50
1:B:230:GLN:HB3	1:B:366:LEU:HD22	1.93	0.50
2:P:52:PRO:HD2	2:P:185:THR:HB	1.94	0.50
1:F:357:ASN:HD21	1:F:359:ALA:HB3	1.77	0.50
2:K:324:THR:OG1	2:L:334:ARG:NH2	2.40	0.50
2:O:37:ASN:H	2:O:213:ARG:HH22	1.60	0.50
2:O:254:PHE:HB3	2:O:300:LEU:CD1	2.39	0.50
1:C:264:ARG:NH1	1:F:292:ASP:OD1	2.45	0.50
1:C:405:LEU:HG	1:C:441:TYR:HE1	1.76	0.50
1:C:405:LEU:HG	1:C:441:TYR:CE1	2.46	0.50
1:D:1:MET:HG3	1:D:3:SER:H	1.77	0.50
1:F:263:TYR:OH	1:F:303:GLU:OE1	2.27	0.50
1:F:367:GLU:O	1:F:371:LYS:HG3	2.12	0.50
2:G:58:MET:HG3	2:G:149:SER:HA	1.94	0.50
2:H:96:ILE:HG21	2:H:100:GLU:CD	2.37	0.50
2:N:55:SER:HA	2:N:58:MET:HG2	1.93	0.50
2:P:15:ASP:OD1	2:P:15:ASP:N	2.45	0.50
1:C:11:THR:HB	1:F:59:LYS:HG3	1.93	0.50
1:D:506:LEU:HD12	1:D:510:ILE:CG1	2.40	0.50
1:E:55:TYR:HD2	1:E:83:CYS:HG	1.55	0.50
2:I:265:ASP:O	2:I:269:ARG:NH1	2.45	0.50
2:J:58:MET:HE2	2:J:151:ILE:HB	1.92	0.50
2:M:5:HIS:HE1	2:M:398:HIS:HB3	1.76	0.50
2:O:394:ASN:OD1	2:O:394:ASN:N	2.44	0.50
1:B:217:GLN:O	1:B:220:ILE:HG12	2.12	0.50
2:G:126:LEU:O	2:G:134:LYS:NZ	2.44	0.50
2:K:13:LEU:HB3	2:K:20:GLU:HG2	1.93	0.50
2:N:206:TYR:HA	2:N:209:VAL:HB	1.93	0.50
2:N:410:LYS:HB3	2:N:412:HIS:NE2	2.27	0.50
2:Q:38:LEU:HB3	2:Q:220:VAL:HG13	1.94	0.50
2:Q:134:LYS:HG3	2:Q:138:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:TYR:HD1	1:A:541:GLU:HG2	1.77	0.50
1:E:235:GLN:HE21	1:E:236:MET:HG3	1.77	0.50
2:H:78:SER:O	2:H:78:SER:OG	2.21	0.50
2:H:350:ILE:HA	2:H:377:PHE:HB2	1.94	0.50
2:I:9:ASP:OD2	2:I:9:ASP:N	2.45	0.50
2:N:350:ILE:HD11	2:N:417:ILE:HG21	1.94	0.50
2:Q:95:LYS:HG3	2:Q:96:ILE:HG23	1.94	0.50
1:A:62:ASP:N	1:D:8:THR:O	2.42	0.49
1:A:444:LYS:HA	1:A:447:GLU:HB2	1.93	0.49
1:B:266:GLN:HE22	1:B:268:THR:HG22	1.77	0.49
1:E:149:THR:O	1:E:465:ARG:NH1	2.45	0.49
1:E:500:ASN:HD21	1:F:515:LYS:HG3	1.77	0.49
1:F:274:ARG:HB2	1:F:291:TYR:HE2	1.77	0.49
2:H:392:PHE:HB3	2:H:394:ASN:OD1	2.11	0.49
2:J:348:ILE:HG12	2:J:375:ILE:HD12	1.94	0.49
2:P:405:SER:HB2	2:P:406:LYS:HG2	1.93	0.49
1:A:269:ASP:HB3	1:D:265:ASN:OD1	2.11	0.49
1:A:481:LEU:O	1:A:505:TYR:OH	2.22	0.49
1:B:127:ASN:HD21	1:C:561:ARG:HH12	1.59	0.49
1:D:209:ILE:HB	1:D:411:PHE:HZ	1.76	0.49
1:D:369:ARG:O	1:D:373:VAL:HG23	2.12	0.49
2:G:62:LEU:HB3	2:G:69:LEU:HD13	1.94	0.49
2:I:61:ILE:HG12	2:I:181:GLU:HG2	1.93	0.49
2:O:405:SER:OG	2:O:425:GLN:O	2.30	0.49
2:P:71:TYR:O	2:P:74:LYS:HB3	2.11	0.49
2:H:40:ILE:HG21	2:H:205:PHE:HZ	1.78	0.49
2:H:118:ASN:O	2:H:120:GLU:N	2.45	0.49
2:H:355:PRO:CG	3:H:501:APR:HR'3	2.42	0.49
2:O:303:ILE:HG21	2:O:306:ASN:HB2	1.94	0.49
1:A:97:ASN:OD1	1:B:496:ARG:NH1	2.46	0.49
1:A:204:ILE:HG23	1:A:205:ASN:ND2	2.28	0.49
2:M:111:LEU:O	2:M:111:LEU:HD23	2.12	0.49
2:P:355:PRO:CG	3:P:501:APR:C2D	2.90	0.49
2:R:48:THR:OG1	3:R:501:APR:N6	2.45	0.49
1:A:492:TYR:HB2	1:A:532:VAL:HG12	1.94	0.49
1:B:493:ILE:HG23	1:B:531:ILE:HG22	1.95	0.49
1:C:292:ASP:OD1	1:C:293:SER:N	2.43	0.49
1:D:261:SER:HB3	1:D:353:SER:OG	2.13	0.49
2:G:172:LYS:O	2:G:176:THR:HG23	2.12	0.49
2:J:262:ARG:N	2:K:264:VAL:O	2.39	0.49
2:M:417:ILE:O	2:M:417:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:38:LEU:HB3	2:N:220:VAL:HG13	1.94	0.49
2:N:355:PRO:CB	3:N:501:APR:H5R2	2.43	0.49
2:P:172:LYS:O	2:P:176:THR:HG23	2.11	0.49
2:P:319:LEU:HB2	2:P:322:LYS:HB2	1.95	0.49
2:Q:376:ILE:N	2:Q:398:HIS:O	2.38	0.49
1:B:16:ILE:HA	1:B:81:PHE:O	2.13	0.49
1:B:179:GLN:HG3	1:C:562:SER:C	2.36	0.49
1:B:511:PRO:HB3	1:C:522:SER:HB2	1.95	0.49
1:C:29:LEU:HG	1:C:30:LEU:HG	1.95	0.49
1:C:559:VAL:CG1	1:C:560:TYR:N	2.75	0.49
1:E:266:GLN:HE22	1:E:276:LYS:HD3	1.77	0.49
1:E:383:ASN:HD22	1:E:384:ASN:H	1.59	0.49
2:J:413:TYR:CE1	3:J:501:APR:N7	2.80	0.49
2:N:219:LYS:HG2	2:N:280:GLU:HB2	1.94	0.49
2:P:66:GLU:O	2:P:70:ASN:ND2	2.45	0.49
1:A:147:LEU:HD13	1:A:535:LEU:HD22	1.95	0.49
1:C:203:VAL:HG21	1:C:400:LEU:HD11	1.95	0.49
1:C:350:LEU:HA	1:C:353:SER:HB3	1.95	0.49
1:D:211:ILE:CG2	1:D:333:ASN:ND2	2.74	0.49
1:F:266:GLN:HE22	1:F:357:ASN:HB2	1.77	0.49
2:I:271:LYS:HG2	2:M:343:LYS:HE3	1.93	0.49
2:L:256:ILE:HD11	2:L:335:GLU:HG3	1.94	0.49
2:M:287:HIS:HA	2:M:314:ILE:HD12	1.93	0.49
2:P:84:PHE:O	2:P:88:VAL:HG23	2.13	0.49
1:B:336:SER:OG	1:B:337:PHE:N	2.45	0.49
1:C:260:LEU:HD22	1:C:311:LYS:HZ1	1.77	0.49
1:D:6:LYS:HB3	1:D:105:GLN:HA	1.94	0.49
1:E:241:ALA:O	1:E:244:ILE:HG12	2.13	0.49
1:F:267:GLN:HE21	1:F:268:THR:HG23	1.78	0.49
2:G:77:ASN:HA	2:G:119:LEU:HB3	1.94	0.49
2:H:96:ILE:CG2	2:H:97:GLN:H	2.25	0.49
2:N:155:LEU:HD22	2:N:316:PRO:HG3	1.95	0.49
2:R:85:ILE:HA	2:R:88:VAL:HG22	1.94	0.49
2:R:155:LEU:HD22	2:R:316:PRO:HG3	1.95	0.49
1:E:11:THR:CG2	1:E:12:PHE:N	2.76	0.49
1:E:174:ASN:HD21	1:E:392:SER:HB3	1.78	0.49
2:I:131:SER:OG	2:I:132:GLU:N	2.45	0.49
2:I:324:THR:HA	2:I:329:TYR:HD2	1.78	0.49
2:K:218:SER:HA	2:K:262:ARG:HH12	1.77	0.49
2:Q:87:TYR:O	2:Q:90:GLU:HG3	2.13	0.49
1:B:180:ASN:HD21	1:C:561:ARG:HH21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD22	1:B:182:HIS:H	1.77	0.49
1:C:122:HIS:H	1:C:122:HIS:CD2	2.31	0.49
1:D:400:LEU:HD12	1:D:405:LEU:HG	1.94	0.49
2:H:224:THR:O	2:H:225:THR:CG2	2.54	0.49
2:H:305:PHE:HB3	2:Q:305:PHE:HZ	1.78	0.49
2:R:355:PRO:HG3	3:R:501:APR:HR'3	1.93	0.49
1:A:356:ASN:HB2	1:A:359:ALA:HB2	1.95	0.48
1:B:155:ILE:HG21	1:B:506:LEU:HD11	1.94	0.48
1:C:150:ASN:ND2	1:C:534:GLU:OE1	2.46	0.48
1:C:256:CYS:HA	1:C:310:LEU:HD11	1.95	0.48
1:C:406:LEU:HD12	1:C:441:TYR:HA	1.95	0.48
1:E:133:LEU:HD21	1:E:136:ASP:HA	1.95	0.48
2:I:30:ASN:HD22	2:I:212:LYS:HG2	1.78	0.48
2:L:423:LYS:O	2:L:425:GLN:NE2	2.46	0.48
1:A:562:SER:HA	1:D:177:ASN:HA	1.96	0.48
1:B:357:ASN:HB2	1:E:357:ASN:N	2.25	0.48
1:D:359:ALA:HB1	1:E:322:THR:C	2.38	0.48
1:D:413:LEU:CD2	1:D:435:PHE:HZ	2.27	0.48
1:F:134:ILE:N	1:F:138:TYR:O	2.46	0.48
2:G:28:PHE:O	2:G:32:HIS:ND1	2.46	0.48
2:J:30:ASN:HD22	2:J:425:GLN:HE21	1.61	0.48
2:K:219:LYS:HG2	2:K:280:GLU:HG3	1.93	0.48
2:L:79:LYS:NZ	2:L:117:LYS:HE2	2.28	0.48
2:R:179:LYS:HG3	2:R:314:ILE:HG13	1.95	0.48
2:R:204:ASP:O	2:R:207:ARG:HB3	2.13	0.48
1:A:368:THR:HG21	1:D:231:LEU:HD12	1.95	0.48
1:B:496:ARG:HD2	1:B:498:LYS:HE2	1.95	0.48
1:D:273:LYS:HD2	1:D:274:ARG:HH22	1.78	0.48
2:I:66:GLU:O	2:I:70:ASN:ND2	2.46	0.48
1:A:219:TRP:CE3	1:A:222:LEU:HD22	2.48	0.48
1:A:418:GLU:HA	1:A:421:LYS:HB3	1.95	0.48
1:C:439:HIS:CE1	1:C:476:GLN:HE22	2.31	0.48
2:G:149:SER:OG	2:G:150:ASN:N	2.46	0.48
2:K:25:VAL:O	2:K:30:ASN:ND2	2.46	0.48
2:K:348:ILE:HD13	2:K:375:ILE:HB	1.95	0.48
2:P:51:VAL:HG23	2:P:185:THR:C	2.39	0.48
1:A:193:LYS:HD3	1:A:553:THR:HG21	1.94	0.48
1:D:167:ARG:O	1:D:171:SER:OG	2.27	0.48
1:E:123:PHE:HB3	1:E:143:ASN:ND2	2.28	0.48
2:J:317:THR:O	2:J:329:TYR:OH	2.30	0.48
2:L:367:LEU:O	2:L:396:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:GLN:HA	2:O:28:PHE:HB2	1.96	0.48
2:O:93:GLN:HB2	2:O:95:LYS:HD2	1.95	0.48
2:P:413:TYR:HD1	3:P:501:APR:C5	2.27	0.48
1:A:405:LEU:O	1:A:409:THR:HG23	2.13	0.48
1:B:212:LYS:O	1:B:333:ASN:ND2	2.47	0.48
1:B:276:LYS:O	1:B:280:ILE:HG13	2.13	0.48
1:C:145:ALA:O	1:C:149:THR:OG1	2.23	0.48
1:C:501:VAL:O	1:C:504:GLU:HG2	2.12	0.48
1:F:257:TYR:HA	1:F:260:LEU:HD12	1.94	0.48
1:F:267:GLN:NE2	1:F:268:THR:CG2	2.76	0.48
2:G:85:ILE:HG22	2:G:111:LEU:HD13	1.96	0.48
2:J:256:ILE:HD11	2:J:335:GLU:HG3	1.95	0.48
2:L:412:HIS:CE1	3:L:501:APR:HO'2	2.25	0.48
1:A:250:GLU:HB2	1:A:253:TRP:HB2	1.94	0.48
1:B:255:LYS:HE3	1:B:280:ILE:HG22	1.94	0.48
1:D:48:GLU:HG2	2:N:214:THR:HG21	1.96	0.48
1:E:94:ILE:HG23	1:E:94:ILE:O	2.13	0.48
1:E:374:GLN:O	1:E:378:SER:OG	2.17	0.48
2:L:266:ASP:O	2:L:267:THR:CG2	2.61	0.48
1:B:238:LEU:HD21	1:B:332:TYR:HD1	1.79	0.48
1:D:389:GLU:CD	1:D:419:LYS:NZ	2.72	0.48
1:D:401:ASP:H	1:D:404:LEU:HD21	1.78	0.48
1:E:131:ILE:HB	1:E:172:LYS:HD2	1.95	0.48
2:G:172:LYS:HE2	2:G:172:LYS:HB3	1.67	0.48
2:H:5:HIS:CD2	2:H:400:ILE:HG12	2.49	0.48
2:H:224:THR:HG23	2:H:225:THR:N	2.28	0.48
2:K:5:HIS:CD2	2:K:400:ILE:HG12	2.49	0.48
2:N:179:LYS:HE2	2:N:314:ILE:HG12	1.94	0.48
1:A:203:VAL:O	1:A:203:VAL:CG1	2.60	0.48
1:B:179:GLN:H	1:C:560:TYR:H	1.61	0.48
1:C:47:ASN:HD21	1:C:51:GLU:HB2	1.79	0.48
1:C:111:THR:HB	1:C:116:MET:HE2	1.96	0.48
1:D:211:ILE:CG2	1:D:211:ILE:O	2.62	0.48
1:D:413:LEU:HD12	1:D:414:LYS:N	2.29	0.48
2:G:324:THR:OG1	2:H:334:ARG:NH2	2.47	0.48
2:J:34:SER:O	2:J:217:LYS:NZ	2.45	0.48
2:N:152:GLU:OE2	3:N:501:APR:C2D	2.61	0.48
1:B:429:SER:HA	1:C:558:ILE:CG2	2.43	0.48
1:C:273:LYS:O	1:C:277:ILE:HG23	2.13	0.48
1:C:339:LYS:O	1:C:342:GLU:HG3	2.13	0.48
1:D:496:ARG:NH1	1:D:528:THR:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:ALA:HB3	1:E:475:SER:HB2	1.96	0.48
2:K:214:THR:O	2:K:214:THR:CG2	2.62	0.48
1:D:143:ASN:HB3	1:D:146:LYS:HB2	1.96	0.47
2:I:21:LYS:HB2	2:I:421:PHE:HE2	1.79	0.47
2:R:66:GLU:O	2:R:70:ASN:ND2	2.47	0.47
1:A:327:ILE:HA	1:A:330:ALA:HB3	1.96	0.47
1:D:31:GLY:O	2:J:398:HIS:NE2	2.45	0.47
1:D:400:LEU:HD12	1:D:405:LEU:CG	2.41	0.47
1:F:491:ASN:HB3	1:F:535:LEU:HB2	1.96	0.47
2:G:67:SER:HA	2:G:70:ASN:HD21	1.79	0.47
2:I:270:TYR:CE1	2:M:342:ILE:HG12	2.49	0.47
2:L:214:THR:O	2:L:216:GLN:N	2.47	0.47
2:N:77:ASN:O	2:N:77:ASN:ND2	2.47	0.47
2:P:70:ASN:O	2:P:73:LYS:HB2	2.14	0.47
2:P:367:LEU:HD11	2:P:374:LEU:HD22	1.96	0.47
2:P:412:HIS:CD2	3:P:501:APR:H'2	2.49	0.47
2:P:412:HIS:HD2	3:P:501:APR:C8	2.27	0.47
1:A:262:LEU:HD21	1:A:353:SER:HA	1.96	0.47
1:A:451:PHE:HB2	1:A:453:GLU:HG2	1.96	0.47
2:G:329:TYR:HA	2:G:332:LEU:HD12	1.97	0.47
2:J:414:PHE:N	3:J:501:APR:N1	2.58	0.47
2:M:270:TYR:O	2:O:343:LYS:NZ	2.45	0.47
2:N:69:LEU:O	2:N:72:VAL:HG12	2.14	0.47
1:A:223:ILE:HD11	1:A:369:ARG:HG2	1.97	0.47
1:A:369:ARG:O	1:A:373:VAL:HG23	2.14	0.47
1:C:10:VAL:H	1:F:60:VAL:HG23	1.79	0.47
1:C:401:ASP:OD2	1:C:401:ASP:N	2.43	0.47
1:D:389:GLU:CD	1:D:419:LYS:HZ2	2.22	0.47
2:L:244:THR:HG22	2:L:283:LEU:HB3	1.96	0.47
2:L:355:PRO:HG3	3:L:501:APR:C4D	2.44	0.47
1:F:269:ASP:OD1	1:F:269:ASP:N	2.35	0.47
2:I:406:LYS:HG3	2:I:428:ARG:HD3	1.96	0.47
2:J:340:LEU:HA	2:J:345:THR:HG21	1.97	0.47
2:K:354:PHE:HD2	2:K:385:VAL:HG22	1.80	0.47
2:M:134:LYS:HE2	2:M:138:LEU:HD12	1.96	0.47
2:O:157:TRP:NE1	2:P:164:TYR:O	2.44	0.47
2:P:45:GLY:O	3:P:501:APR:C5	2.62	0.47
2:P:53:LEU:HD11	3:P:501:APR:C5'	2.44	0.47
1:A:6:LYS:HB3	1:A:105:GLN:HA	1.97	0.47
1:B:254:LEU:O	1:B:258:ILE:HG12	2.14	0.47
1:D:413:LEU:CD2	1:D:435:PHE:CZ	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:VAL:HG11	1:E:181:LEU:HD21	1.95	0.47
1:E:185:ILE:HG23	1:E:434:ILE:HB	1.95	0.47
1:E:254:LEU:HA	1:E:257:TYR:HB3	1.96	0.47
1:E:430:VAL:HG22	1:E:468:GLY:HA2	1.96	0.47
2:H:152:GLU:OE1	3:H:501:APR:O2D	2.30	0.47
2:I:37:ASN:HB3	2:I:345:THR:HB	1.97	0.47
2:I:294:SER:OG	2:I:312:VAL:CG2	2.63	0.47
2:N:65:ASN:ND2	2:N:69:LEU:CD2	2.43	0.47
2:N:219:LYS:HD2	2:N:262:ARG:HG2	1.96	0.47
2:O:1:MET:HA	2:O:2:GLY:HA3	1.58	0.47
2:O:102:LYS:HA	2:O:105:HIS:NE2	2.30	0.47
1:A:103:PHE:HD1	1:B:38:GLY:HA2	1.80	0.47
1:A:131:ILE:HA	1:A:172:LYS:HE2	1.97	0.47
1:A:239:LYS:HE3	1:A:330:ALA:HB3	1.97	0.47
1:A:397:VAL:HG22	1:A:400:LEU:HB2	1.96	0.47
1:A:554:ILE:HD12	1:D:465:ARG:CA	2.41	0.47
1:B:160:SER:HA	1:B:526:THR:HG22	1.96	0.47
1:B:216:MET:SD	1:B:238:LEU:HD13	2.55	0.47
1:B:247:LYS:HE2	1:B:250:GLU:HA	1.96	0.47
1:D:538:ILE:O	1:D:540:VAL:HG13	2.14	0.47
1:D:560:TYR:OH	1:E:391:LYS:NZ	2.38	0.47
2:G:71:TYR:HE2	2:G:170:ASP:HB3	1.80	0.47
2:I:376:ILE:HD11	2:I:388:PHE:HE2	1.80	0.47
2:L:54:MET:SD	3:L:501:APR:H5R1	2.54	0.47
2:L:413:TYR:CE1	3:L:501:APR:C2	2.96	0.47
2:N:210:PHE:HZ	2:N:281:ALA:HB2	1.80	0.47
2:O:283:LEU:HG	2:O:285:LYS:HD3	1.97	0.47
1:C:148:LEU:HD12	1:C:432:VAL:HG21	1.97	0.47
1:D:179:GLN:HB3	1:D:467:PHE:HE2	1.80	0.47
1:E:37:LYS:N	1:E:41:ASP:OD2	2.47	0.47
2:K:427:ARG:HD3	2:K:427:ARG:HA	1.69	0.47
2:O:151:ILE:HD11	2:O:178:LEU:HD22	1.96	0.47
2:O:416:PHE:HA	2:O:420:ASN:HD22	1.80	0.47
2:R:39:THR:HG22	2:R:221:SER:HB2	1.96	0.47
1:B:10:VAL:HG13	1:B:15:LEU:HD12	1.97	0.47
1:B:410:THR:O	1:B:414:LYS:HE2	2.14	0.47
1:C:49:TYR:HE1	1:F:35:ILE:HG21	1.80	0.47
1:D:297:ASN:OD1	1:D:297:ASN:N	2.46	0.47
2:H:355:PRO:HG3	3:H:501:APR:C3D	2.43	0.47
2:Q:241:ILE:HG21	2:Q:263:VAL:HG21	1.97	0.47
1:A:148:LEU:HD21	1:A:183:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HA	1:A:313:VAL:HG22	1.97	0.47
1:B:322:THR:HG22	1:B:325:GLU:H	1.80	0.47
1:B:488:GLN:OE1	1:C:499:ASN:ND2	2.47	0.47
1:C:160:SER:HA	1:C:526:THR:HG23	1.96	0.47
1:C:248:ILE:CD1	1:C:326:VAL:HG13	2.44	0.47
1:D:309:SER:HA	1:D:312:ASN:OD1	2.15	0.47
1:D:486:LEU:HD11	1:D:510:ILE:HD11	1.97	0.47
2:G:224:THR:O	2:G:225:THR:HG22	2.15	0.47
2:J:214:THR:O	2:J:216:GLN:N	2.48	0.47
3:L:501:APR:H'2	3:L:501:APR:H8	1.70	0.47
2:N:197:GLU:HA	2:N:200:GLU:HB2	1.95	0.47
2:R:68:VAL:HG12	2:R:174:VAL:HG13	1.97	0.47
2:R:253:LYS:HE2	2:R:299:GLU:HG3	1.96	0.47
1:A:187:ASP:OD2	1:A:190:ASP:N	2.48	0.46
1:B:503:LEU:HD22	1:B:518:LEU:HD22	1.98	0.46
1:F:233:ILE:HA	1:F:236:MET:HE3	1.96	0.46
2:I:77:ASN:HB3	2:I:120:GLU:HB3	1.97	0.46
2:L:41:PHE:HB3	2:L:349:ILE:HG12	1.97	0.46
2:M:411:ALA:HA	2:M:414:PHE:HB2	1.97	0.46
2:P:100:GLU:O	2:P:104:LEU:HG	2.15	0.46
2:P:293:LYS:HB2	2:P:303:ILE:HG12	1.97	0.46
2:Q:304:ASP:OD1	2:Q:304:ASP:N	2.48	0.46
1:A:63:LYS:HB2	1:A:80:ARG:HG3	1.97	0.46
1:B:179:GLN:HE21	1:C:561:ARG:CZ	2.27	0.46
1:C:128:ASP:HB3	1:C:142:PHE:O	2.16	0.46
1:E:237:GLY:HA3	1:E:344:LEU:HD22	1.97	0.46
1:F:337:PHE:HB3	1:F:374:GLN:NE2	2.30	0.46
2:J:44:SER:HB3	3:J:501:APR:O1D	2.15	0.46
2:J:47:SER:HB3	2:J:51:VAL:HB	1.95	0.46
1:A:222:LEU:HD13	1:A:407:PHE:CZ	2.49	0.46
1:A:377:PHE:CZ	1:A:400:LEU:HD11	2.51	0.46
1:A:406:LEU:O	1:A:410:THR:HG22	2.14	0.46
1:B:53:PHE:CG	1:B:102:PRO:HG3	2.50	0.46
1:B:158:THR:HA	1:B:476:GLN:HE22	1.81	0.46
1:B:325:GLU:HA	1:B:328:GLU:HB2	1.98	0.46
1:D:360:ARG:HH22	1:E:311:LYS:HE3	1.80	0.46
1:F:50:SER:HB3	2:L:212:LYS:HD3	1.96	0.46
2:L:155:LEU:HD22	2:L:316:PRO:HG3	1.97	0.46
2:L:213:ARG:NH2	2:L:218:SER:O	2.41	0.46
2:L:314:ILE:O	2:L:329:TYR:OH	2.34	0.46
2:M:219:LYS:HB3	2:M:280:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:92:GLU:OE2	2:N:105:HIS:NE2	2.34	0.46
1:A:248:ILE:HG21	1:A:326:VAL:HG13	1.96	0.46
1:C:194:ASP:OD1	1:C:194:ASP:N	2.48	0.46
1:C:425:LEU:HA	1:C:428:ARG:HD2	1.96	0.46
1:D:131:ILE:HD12	1:D:172:LYS:HZ2	1.71	0.46
2:G:70:ASN:HA	2:G:73:LYS:HD2	1.96	0.46
2:I:336:PHE:HE2	2:I:359:ILE:HG23	1.81	0.46
2:M:86:LYS:O	2:M:90:GLU:HG2	2.14	0.46
2:N:48:THR:CG2	3:N:501:APR:N6	2.60	0.46
2:N:236:GLU:HG3	2:N:242:TYR:HE1	1.79	0.46
2:P:412:HIS:CD2	3:P:501:APR:C1'	2.98	0.46
2:R:371:ASP:OD1	2:R:371:ASP:N	2.46	0.46
1:A:272:THR:HA	1:D:264:ARG:HB3	1.98	0.46
1:B:216:MET:HB2	1:B:238:LEU:HD21	1.97	0.46
1:C:85:PRO:HB3	1:C:98:LEU:HD13	1.97	0.46
1:C:269:ASP:O	1:C:273:LYS:HG3	2.15	0.46
1:E:290:LYS:HB2	1:E:290:LYS:HE3	1.70	0.46
1:E:500:ASN:HD21	1:F:515:LYS:H	1.64	0.46
2:K:43:GLY:C	2:K:226:ASN:HD21	2.24	0.46
2:P:155:LEU:HD22	2:P:316:PRO:HG3	1.97	0.46
2:P:266:ASP:OD1	2:P:274:TRP:NE1	2.36	0.46
1:D:209:ILE:HB	1:D:411:PHE:CZ	2.50	0.46
1:D:532:VAL:HA	1:D:539:PRO:HB3	1.97	0.46
1:E:123:PHE:HB3	1:E:143:ASN:HD21	1.80	0.46
2:H:71:TYR:HA	2:H:74:LYS:HB2	1.98	0.46
2:J:151:ILE:O	2:J:152:GLU:C	2.59	0.46
2:P:76:LEU:HD22	2:P:119:LEU:HB3	1.98	0.46
2:Q:82:LYS:O	2:Q:85:ILE:HG13	2.15	0.46
1:A:332:TYR:HE2	1:B:375:THR:HG21	1.80	0.46
1:C:412:ILE:HG22	1:C:433:PHE:HE1	1.80	0.46
1:C:512:TYR:OH	1:F:158:THR:O	2.31	0.46
1:D:15:LEU:O	1:D:82:GLU:HA	2.16	0.46
1:D:59:LYS:HE3	1:D:61:GLU:HB3	1.98	0.46
1:D:185:ILE:HG12	1:D:395:TYR:HB2	1.97	0.46
1:E:55:TYR:HD2	1:E:83:CYS:SG	2.38	0.46
2:G:286:ILE:HG23	2:G:287:HIS:CD2	2.51	0.46
2:N:85:ILE:HA	2:N:88:VAL:HG22	1.97	0.46
2:O:410:LYS:HG3	2:O:412:HIS:H	1.80	0.46
2:Q:325:ALA:HA	2:Q:330:SER:OG	2.15	0.46
1:A:299:ASP:N	1:A:299:ASP:OD1	2.49	0.46
1:B:185:ILE:HG21	1:B:192:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:HG21	1:B:400:LEU:HD21	1.97	0.46
1:C:143:ASN:HB3	1:C:146:LYS:HB2	1.98	0.46
1:D:447:GLU:HG3	1:D:448:SER:H	1.79	0.46
1:F:150:ASN:ND2	1:F:534:GLU:OE1	2.49	0.46
2:H:295:ASN:HB3	2:H:299:GLU:H	1.80	0.46
2:N:107:ILE:HD11	2:N:137:ILE:HG12	1.97	0.46
2:P:3:ILE:HD11	2:P:404:SER:HB3	1.98	0.46
2:R:374:LEU:O	2:R:398:HIS:N	2.48	0.46
1:A:440:ARG:CD	1:D:460:ILE:CD1	2.93	0.46
1:B:227:GLU:HA	1:B:231:LEU:HB3	1.97	0.46
1:E:352:GLU:HB3	1:E:360:ARG:HH22	1.80	0.46
1:E:367:GLU:OE2	1:E:368:THR:HG23	2.16	0.46
2:I:213:ARG:HG3	2:I:215:GLU:HG2	1.98	0.46
2:J:364:ALA:HA	2:J:367:LEU:HD12	1.98	0.46
2:K:167:ASN:OD1	2:L:117:LYS:CE	2.55	0.46
2:L:235:LEU:HD12	2:L:283:LEU:HD22	1.98	0.46
2:M:165:ASP:OD1	2:M:168:ASN:ND2	2.48	0.46
2:O:25:VAL:HA	2:O:29:ILE:HB	1.98	0.46
2:Q:17:LYS:HG3	2:Q:19:ASN:H	1.80	0.46
1:B:180:ASN:H	1:C:561:ARG:HB3	1.81	0.46
1:C:168:GLN:OE1	1:C:172:LYS:NZ	2.40	0.46
1:D:231:LEU:CD1	1:D:232:PRO:HD3	2.46	0.46
2:I:160:ASN:ND2	2:I:318:MET:SD	2.82	0.46
2:K:125:TRP:HA	2:K:128:MET:HE2	1.98	0.46
2:P:220:VAL:HG13	2:P:220:VAL:O	2.16	0.46
2:P:256:ILE:HD11	2:P:335:GLU:HG3	1.98	0.46
2:R:166:ASN:O	2:R:168:ASN:N	2.49	0.46
1:A:274:ARG:HD3	1:A:291:TYR:HE2	1.81	0.45
1:B:216:MET:CG	1:B:238:LEU:HD21	2.45	0.45
1:B:530:TYR:HD1	1:B:541:GLU:HG3	1.80	0.45
1:C:457:PHE:O	1:C:460:ILE:HG12	2.16	0.45
1:D:33:ILE:HD12	2:J:35:ALA:HB2	1.98	0.45
2:J:233:TYR:HA	2:J:236:GLU:HG2	1.99	0.45
2:M:24:GLN:NE2	2:M:417:ILE:HD13	2.30	0.45
2:N:353:GLY:HA3	3:N:501:APR:O2A	2.16	0.45
1:C:366:LEU:HG	1:C:369:ARG:HH21	1.81	0.45
1:E:211:ILE:HG23	1:E:214:LEU:HD22	1.99	0.45
1:F:162:LYS:NZ	1:F:474:SER:OG	2.44	0.45
2:G:155:LEU:HD13	2:G:179:LYS:HE2	1.99	0.45
2:I:91:GLN:O	2:I:93:GLN:NE2	2.49	0.45
2:K:59:LYS:NZ	2:K:63:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:LYS:O	2:L:21:LYS:HG3	2.16	0.45
2:P:61:ILE:HB	2:P:69:LEU:HD13	1.97	0.45
1:B:456:ALA:O	1:B:459:LYS:HB3	2.17	0.45
1:C:406:LEU:HA	1:C:441:TYR:HD1	1.81	0.45
1:D:402:ASP:HA	1:D:405:LEU:CD1	2.38	0.45
1:E:194:ASP:OD1	1:E:194:ASP:N	2.45	0.45
1:F:492:TYR:HB2	1:F:532:VAL:CG2	2.46	0.45
2:H:45:GLY:O	3:H:501:APR:C6	2.64	0.45
2:M:5:HIS:CE1	2:M:398:HIS:HB3	2.51	0.45
2:Q:22:GLN:HA	2:Q:25:VAL:HG22	1.98	0.45
1:B:127:ASN:HD21	1:C:561:ARG:NH1	2.14	0.45
1:B:216:MET:CG	1:B:238:LEU:CD1	2.86	0.45
1:D:233:ILE:HG23	1:D:347:VAL:CG1	2.43	0.45
1:E:38:GLY:HA2	1:F:103:PHE:HD1	1.80	0.45
2:G:375:ILE:HA	2:G:398:HIS:HB2	1.98	0.45
2:H:314:ILE:O	2:H:329:TYR:OH	2.26	0.45
2:O:304:ASP:OD1	2:O:304:ASP:N	2.50	0.45
1:A:167:ARG:HA	1:A:170:ILE:HD12	1.97	0.45
1:A:554:ILE:HG22	1:A:554:ILE:O	2.17	0.45
1:B:216:MET:HB2	1:B:238:LEU:HD22	1.95	0.45
1:C:276:LYS:O	1:C:280:ILE:HG13	2.16	0.45
1:D:51:GLU:HG2	1:D:90:LYS:HD2	1.98	0.45
1:E:208:LYS:HE2	1:E:383:ASN:HB2	1.99	0.45
1:F:182:HIS:HB2	1:F:431:ASN:CG	2.31	0.45
1:F:416:GLU:CD	1:F:431:ASN:ND2	2.73	0.45
2:H:424:ASN:OD1	2:H:424:ASN:N	2.48	0.45
2:J:102:LYS:HB3	2:J:102:LYS:HE2	1.74	0.45
2:K:210:PHE:HZ	2:K:281:ALA:HB2	1.82	0.45
1:A:29:LEU:HG	1:A:30:LEU:HG	1.98	0.45
1:C:487:SER:OG	1:F:477:ARG:NH1	2.50	0.45
1:D:199:LYS:HE2	1:D:199:LYS:HB2	1.68	0.45
1:F:155:ILE:HD11	1:F:486:LEU:HD21	1.98	0.45
2:K:271:LYS:HB2	2:K:271:LYS:HE3	1.57	0.45
2:N:44:SER:HG	3:N:501:APR:C3D	2.19	0.45
2:P:72:VAL:O	2:P:75:PHE:HB3	2.15	0.45
2:Q:117:LYS:NZ	2:Q:121:GLU:OE2	2.48	0.45
2:R:379:ASP:N	2:R:379:ASP:OD1	2.48	0.45
1:F:444:LYS:HG2	1:F:480:GLU:HA	1.99	0.45
2:H:355:PRO:HG3	3:H:501:APR:H5R1	1.99	0.45
2:J:303:ILE:CD1	2:J:306:ASN:CB	2.90	0.45
2:Q:118:ASN:CG	2:Q:120:GLU:OE2	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:219:LYS:HG3	2:R:262:ARG:HD3	1.98	0.45
1:A:560:TYR:HH	1:D:144:THR:HG1	1.60	0.45
1:B:186:PHE:HZ	1:B:412:ILE:HB	1.82	0.45
1:C:11:THR:HG23	1:C:13:GLU:H	1.80	0.45
1:D:434:ILE:HA	1:D:472:MET:HB2	1.97	0.45
1:F:16:ILE:HA	1:F:81:PHE:O	2.17	0.45
2:G:72:VAL:HG23	2:G:154:LEU:HD13	1.99	0.45
2:H:253:LYS:HD2	2:Q:236:GLU:OE2	2.17	0.45
2:L:342:ILE:CG2	2:L:343:LYS:N	2.79	0.45
2:L:406:LYS:HZ3	2:L:406:LYS:H	1.65	0.45
2:O:81:ILE:O	2:O:85:ILE:HG13	2.17	0.45
2:P:5:HIS:HD2	2:P:400:ILE:HG12	1.82	0.45
2:Q:151:ILE:HD11	2:Q:178:LEU:HD22	1.99	0.45
2:Q:264:VAL:HG11	2:Q:274:TRP:HA	1.97	0.45
2:R:67:SER:HA	2:R:70:ASN:HD21	1.82	0.45
1:A:135:ASP:O	1:A:137:GLN:HG3	2.16	0.45
1:C:377:PHE:HD2	1:C:381:PHE:HE2	1.65	0.45
1:D:361:SER:H	1:E:320:ILE:HB	1.81	0.45
1:E:290:LYS:NZ	1:E:305:LYS:HB2	2.32	0.45
2:I:225:THR:HG23	2:I:287:HIS:CD2	2.51	0.45
2:M:307:ASP:OD1	2:M:307:ASP:N	2.48	0.45
2:M:330:SER:HB2	2:N:341:GLN:HE22	1.82	0.45
2:P:197:GLU:O	2:P:200:GLU:HB2	2.17	0.45
1:A:101:TYR:HB2	1:B:39:VAL:HG22	1.98	0.45
1:B:262:LEU:N	1:B:353:SER:OG	2.50	0.45
1:C:452:ASN:HD21	1:C:455:GLU:HB2	1.81	0.45
1:E:188:VAL:HG21	1:E:437:GLU:HG3	1.92	0.45
1:F:155:ILE:HG21	1:F:506:LEU:HD11	1.98	0.45
1:F:481:LEU:O	1:F:505:TYR:OH	2.27	0.45
2:I:40:ILE:HG21	2:I:205:PHE:HZ	1.81	0.45
2:I:296:GLU:H	2:I:296:GLU:HG3	1.62	0.45
2:K:179:LYS:O	2:K:183:ILE:HG13	2.17	0.45
2:L:365:GLN:O	2:L:368:LYS:NZ	2.50	0.45
2:O:324:THR:HA	2:O:329:TYR:HB2	1.99	0.45
1:B:10:VAL:H	1:C:60:VAL:HG23	1.82	0.44
1:C:367:GLU:O	1:C:371:LYS:HG2	2.17	0.44
1:D:10:VAL:HG13	1:D:15:LEU:HD12	1.99	0.44
1:D:94:ILE:HG23	1:D:94:ILE:O	2.16	0.44
1:D:360:ARG:NH1	1:E:319:ASN:CG	2.72	0.44
1:E:112:SER:OG	1:E:114:GLU:OE1	2.36	0.44
1:F:474:SER:OG	1:F:474:SER:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:377:PHE:O	2:H:412:HIS:HB2	2.17	0.44
2:K:423:LYS:HD3	2:K:423:LYS:O	2.17	0.44
2:L:11:ASP:HB3	2:L:14:THR:HG23	1.98	0.44
2:M:25:VAL:HG11	2:M:419:GLU:HG3	1.98	0.44
2:M:358:HIS:CD2	2:N:334:ARG:HH22	2.35	0.44
2:M:408:GLU:HB3	2:M:413:TYR:CD2	2.52	0.44
2:P:69:LEU:HD12	2:P:72:VAL:CG1	2.46	0.44
2:P:72:VAL:O	2:P:75:PHE:CB	2.65	0.44
2:P:412:HIS:CD2	3:P:501:APR:N9	2.85	0.44
2:R:23:GLU:O	2:R:27:THR:HG23	2.17	0.44
2:R:235:LEU:HD12	2:R:283:LEU:HD22	1.99	0.44
2:R:355:PRO:CG	3:R:501:APR:C3D	2.92	0.44
2:R:404:SER:OG	2:R:405:SER:N	2.50	0.44
1:B:204:ILE:CG2	1:B:205:ASN:H	2.28	0.44
1:B:437:GLU:HG3	1:B:439:HIS:CD2	2.53	0.44
1:C:460:ILE:HA	1:C:463:GLU:HB2	1.98	0.44
1:D:367:GLU:O	1:D:371:LYS:HG2	2.17	0.44
1:D:437:GLU:HG2	1:D:476:GLN:HB3	1.98	0.44
1:F:40:ILE:HG13	1:F:40:ILE:O	2.16	0.44
1:F:65:ILE:HD11	1:F:74:LYS:HB2	1.99	0.44
1:F:253:TRP:CE2	1:F:320:ILE:HG12	2.53	0.44
1:F:276:LYS:O	1:F:280:ILE:HG13	2.18	0.44
2:H:406:LYS:HE2	2:H:406:LYS:HB2	1.82	0.44
2:J:283:LEU:HG	2:J:285:LYS:HD3	1.98	0.44
2:J:349:ILE:HB	2:J:376:ILE:HA	1.98	0.44
2:K:216:GLN:NE2	2:K:278:SER:O	2.42	0.44
2:M:25:VAL:CG1	2:M:419:GLU:H	2.30	0.44
2:M:254:PHE:CG	2:M:300:LEU:CD2	2.98	0.44
2:M:340:LEU:HB3	2:M:372:PHE:HE1	1.83	0.44
2:O:160:ASN:OD1	2:P:163:HIS:ND1	2.50	0.44
2:P:179:LYS:NZ	2:P:309:ASP:O	2.36	0.44
2:P:346:THR:HG23	2:P:373:ASN:HB3	1.99	0.44
2:Q:102:LYS:HA	2:Q:105:HIS:ND1	2.32	0.44
2:Q:318:MET:HE3	2:R:326:GLN:HE21	1.82	0.44
1:A:255:LYS:HB2	1:A:280:ILE:CG2	2.47	0.44
1:A:364:ALA:O	1:A:368:THR:HG22	2.17	0.44
1:C:184:HIS:NE2	1:C:392:SER:HB2	2.31	0.44
1:C:479:SER:OG	1:C:501:VAL:HG22	2.17	0.44
1:E:184:HIS:ND1	1:E:393:ILE:HD11	2.32	0.44
1:E:459:LYS:HB3	1:E:459:LYS:HE3	1.69	0.44
1:F:194:ASP:OD2	1:F:194:ASP:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:TRP:CD1	1:F:317:GLY:HA3	2.52	0.44
2:G:314:ILE:HG13	2:G:329:TYR:CE2	2.53	0.44
2:H:367:LEU:HB3	2:H:394:ASN:CG	2.43	0.44
2:I:224:THR:HG21	2:I:285:LYS:NZ	2.32	0.44
2:I:356:ASP:OD1	2:I:356:ASP:N	2.40	0.44
2:J:413:TYR:HE1	3:J:501:APR:C8	2.30	0.44
2:K:307:ASP:OD1	2:K:308:GLU:N	2.50	0.44
2:M:224:THR:HG23	2:M:225:THR:N	2.32	0.44
2:N:199:TYR:HA	2:N:202:TYR:HB2	1.99	0.44
1:A:457:PHE:HA	1:A:460:ILE:HG22	1.98	0.44
1:C:152:THR:HA	1:C:491:ASN:HB2	1.99	0.44
1:C:266:GLN:HB2	1:C:273:LYS:HD3	1.99	0.44
1:C:310:LEU:O	1:C:314:VAL:HG23	2.17	0.44
1:D:518:LEU:HA	1:D:521:PHE:CD2	2.53	0.44
1:E:88:MET:C	1:E:94:ILE:HD12	2.42	0.44
1:E:198:VAL:HG11	1:E:394:VAL:HG23	1.99	0.44
1:E:337:PHE:HB2	1:E:374:GLN:HE21	1.82	0.44
2:G:346:THR:O	2:G:346:THR:OG1	2.35	0.44
2:H:252:LYS:HB2	2:H:302:GLN:H	1.82	0.44
2:N:354:PHE:HD2	2:N:385:VAL:HG22	1.81	0.44
2:P:42:ILE:HD13	2:P:350:ILE:HG13	1.98	0.44
1:A:10:VAL:HB	1:B:60:VAL:HG22	2.00	0.44
1:B:322:THR:HG22	1:B:325:GLU:N	2.32	0.44
1:B:357:ASN:HB3	1:E:358:GLN:H	1.83	0.44
1:C:446:LYS:O	1:C:452:ASN:HB2	2.18	0.44
1:D:211:ILE:HD13	1:D:334:VAL:H	1.83	0.44
1:D:233:ILE:HA	1:D:347:VAL:CG1	2.46	0.44
1:F:151:HIS:HB2	1:F:489:CYS:HA	2.00	0.44
1:F:478:PRO:HB3	1:F:506:LEU:HD11	1.99	0.44
2:H:54:MET:CG	3:H:501:APR:HR'4	2.41	0.44
2:K:259:PHE:O	2:K:282:ASN:ND2	2.44	0.44
2:L:347:LEU:HG	2:L:349:ILE:HG13	1.99	0.44
2:N:394:ASN:O	2:N:396:ASN:N	2.49	0.44
2:O:47:SER:O	2:O:47:SER:OG	2.30	0.44
2:P:348:ILE:HG12	2:P:375:ILE:HD12	1.98	0.44
1:A:201:VAL:HG11	1:A:207:PHE:HD1	1.82	0.44
1:A:348:PHE:CE2	1:A:367:GLU:HB2	2.51	0.44
1:A:498:LYS:HG3	1:D:512:TYR:HD1	1.82	0.44
1:B:130:THR:O	1:B:130:THR:OG1	2.34	0.44
1:B:136:ASP:HB3	2:P:27:THR:HG21	2.00	0.44
1:B:288:THR:OG1	1:B:289:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HA	1:C:81:PHE:O	2.18	0.44
1:E:151:HIS:CE1	1:E:461:ALA:HA	2.53	0.44
2:H:349:ILE:HD12	2:H:376:ILE:HG12	2.00	0.44
2:I:416:PHE:CE2	2:I:423:LYS:HB3	2.52	0.44
2:M:107:ILE:HG13	2:M:137:ILE:HD12	2.00	0.44
2:N:60:ASN:HD21	2:N:181:GLU:HB3	1.83	0.44
1:D:479:SER:HB3	1:E:462:ARG:CZ	2.48	0.44
1:E:167:ARG:NH1	1:E:549:SER:O	2.50	0.44
1:F:4:ILE:HB	1:F:19:VAL:HG13	1.99	0.44
1:F:344:LEU:HA	1:F:347:VAL:HG12	2.00	0.44
2:G:51:VAL:HG12	2:G:187:PRO:HD3	2.00	0.44
2:N:62:LEU:HD13	2:N:146:LEU:HD22	2.00	0.44
2:O:252:LYS:HD2	2:O:302:GLN:HB3	1.98	0.44
2:R:41:PHE:HB2	2:R:347:LEU:HD11	1.98	0.44
1:B:42:TYR:HB2	1:B:111:THR:HG21	1.99	0.44
1:B:484:THR:OG1	1:C:501:VAL:CG1	2.66	0.44
1:C:91:HIS:ND1	2:H:423:LYS:O	2.50	0.44
1:F:348:PHE:HB2	1:F:358:GLN:NE2	2.32	0.44
2:G:98:GLU:HA	2:G:101:ARG:HB3	1.99	0.44
2:H:232:GLU:OE2	2:H:285:LYS:NZ	2.36	0.44
2:I:25:VAL:HB	2:I:419:GLU:HG2	1.98	0.44
2:I:253:LYS:HG3	2:I:299:GLU:HB3	2.00	0.44
2:K:21:LYS:O	2:K:25:VAL:HG23	2.18	0.44
2:K:287:HIS:HA	2:K:314:ILE:HD11	2.00	0.44
2:L:354:PHE:HD2	2:L:385:VAL:HG22	1.83	0.44
2:M:354:PHE:HD2	2:M:385:VAL:HG22	1.82	0.44
1:A:168:GLN:NE2	1:A:545:PHE:O	2.51	0.44
1:A:192:TYR:HD2	1:A:394:VAL:CG2	2.30	0.44
1:A:220:ILE:HG21	1:A:231:LEU:CD1	2.48	0.44
1:B:51:GLU:HG3	1:B:90:LYS:HB2	2.00	0.44
1:B:286:ILE:H	1:B:286:ILE:HD12	1.83	0.44
1:C:175:ASN:OD1	1:C:196:ASN:ND2	2.51	0.44
1:C:561:ARG:O	1:C:561:ARG:HG2	2.17	0.44
1:D:61:GLU:OE2	1:D:80:ARG:NH1	2.45	0.44
1:D:147:LEU:HD13	1:D:535:LEU:HD22	2.00	0.44
1:E:11:THR:CG2	1:E:12:PHE:H	2.27	0.44
1:E:547:GLU:H	1:E:547:GLU:HG3	1.59	0.44
1:F:266:GLN:H	1:F:273:LYS:HE3	1.81	0.44
2:H:67:SER:OG	2:H:174:VAL:HG22	2.17	0.44
2:L:250:ILE:HD13	2:L:250:ILE:HA	1.88	0.44
2:Q:71:TYR:CD2	2:Q:174:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:HG2	1:B:364:ALA:HB1	2.00	0.43
1:B:266:GLN:HE22	1:B:268:THR:CG2	2.31	0.43
1:B:354:LYS:HB2	1:B:354:LYS:HE2	1.65	0.43
1:D:184:HIS:CE1	1:D:186:PHE:HB3	2.53	0.43
1:F:1:MET:HG3	1:F:3:SER:H	1.83	0.43
1:F:15:LEU:O	1:F:82:GLU:HA	2.18	0.43
2:I:318:MET:HE3	2:I:318:MET:HB2	1.95	0.43
2:J:197:GLU:HG2	2:J:198:THR:N	2.33	0.43
2:J:264:VAL:HG11	2:K:274:TRP:HB3	1.99	0.43
2:L:233:TYR:HA	2:L:236:GLU:HG2	2.00	0.43
2:M:115:ASN:OD1	2:M:115:ASN:N	2.51	0.43
2:M:125:TRP:HA	2:M:128:MET:HE3	1.99	0.43
2:N:54:MET:O	2:N:58:MET:HG2	2.18	0.43
1:A:151:HIS:HB2	1:A:489:CYS:HA	2.00	0.43
1:A:249:ILE:HD12	1:A:249:ILE:HA	1.86	0.43
1:B:192:TYR:OH	1:B:436:GLU:OE2	2.28	0.43
1:B:309:SER:O	1:B:313:VAL:HG23	2.17	0.43
1:C:70:GLU:N	1:C:70:GLU:OE1	2.50	0.43
1:D:67:LEU:HB3	1:D:73:SER:HB2	1.99	0.43
1:D:310:LEU:O	1:D:314:VAL:HG13	2.18	0.43
1:D:344:LEU:HD13	1:D:348:PHE:CE2	2.53	0.43
2:H:249:THR:HG21	2:Q:236:GLU:HG2	2.00	0.43
2:J:353:GLY:N	3:J:501:APR:H'4	2.33	0.43
2:J:413:TYR:O	2:J:417:ILE:HG12	2.18	0.43
2:K:115:ASN:OD1	2:K:115:ASN:N	2.50	0.43
2:L:252:LYS:HB3	2:L:302:GLN:HB3	1.99	0.43
2:M:235:LEU:HD22	2:M:240:ILE:HG21	2.00	0.43
2:O:254:PHE:CG	2:O:300:LEU:HD11	2.52	0.43
2:P:295:ASN:HB3	2:P:299:GLU:H	1.82	0.43
2:R:55:SER:HB2	2:R:149:SER:HB3	1.99	0.43
1:A:547:GLU:HB3	1:A:551:ASN:ND2	2.34	0.43
1:B:413:LEU:HD11	1:B:435:PHE:HZ	1.78	0.43
1:B:429:SER:HA	1:C:558:ILE:HD13	2.00	0.43
1:D:458:LYS:HE3	1:D:463:GLU:HG3	2.00	0.43
1:E:551:ASN:HB2	1:E:554:ILE:HG12	2.01	0.43
1:F:150:ASN:OD1	1:F:465:ARG:NH1	2.49	0.43
1:F:446:LYS:NZ	1:F:453:GLU:OE2	2.48	0.43
2:J:326:GLN:HB2	2:J:329:TYR:HD2	1.83	0.43
2:L:44:SER:HG	3:L:501:APR:HR'3	1.83	0.43
2:M:73:LYS:HG2	2:M:145:TYR:CD2	2.52	0.43
2:M:160:ASN:HB3	2:N:163:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:271:LYS:HB2	2:O:271:LYS:HE3	1.67	0.43
1:A:148:LEU:CD2	1:A:183:PHE:CE2	3.01	0.43
1:B:176:LEU:HD22	1:B:177:ASN:H	1.83	0.43
1:B:186:PHE:CD2	1:B:409:THR:HG22	2.53	0.43
1:B:447:GLU:HG2	1:B:482:SER:HB3	2.01	0.43
1:D:96:PHE:CD1	1:D:537:PRO:HB3	2.54	0.43
1:E:271:VAL:O	1:E:275:THR:OG1	2.25	0.43
1:F:50:SER:O	1:F:50:SER:OG	2.34	0.43
2:H:394:ASN:O	2:H:396:ASN:N	2.51	0.43
2:J:219:LYS:HG2	2:J:262:ARG:HD3	1.99	0.43
2:K:168:ASN:HB3	2:K:171:LEU:HD12	1.99	0.43
2:L:107:ILE:HD11	2:L:137:ILE:HG23	2.00	0.43
2:L:152:GLU:OE2	3:L:501:APR:O4D	2.36	0.43
2:P:66:GLU:HG3	2:P:67:SER:H	1.82	0.43
1:A:188:VAL:HG11	1:D:460:ILE:HD12	2.00	0.43
1:A:484:THR:C	1:A:488:GLN:HE21	2.26	0.43
1:B:65:ILE:HD12	1:B:66:PRO:HD2	2.01	0.43
1:B:254:LEU:HD11	1:B:323:LEU:CD2	2.33	0.43
1:B:369:ARG:HA	1:B:369:ARG:HD3	1.75	0.43
1:D:162:LYS:HG2	1:D:552:SER:HA	2.00	0.43
1:F:230:GLN:NE2	1:F:366:LEU:HD23	2.34	0.43
1:F:266:GLN:N	1:F:273:LYS:HE3	2.34	0.43
1:F:479:SER:OG	1:F:480:GLU:N	2.51	0.43
2:G:66:GLU:O	2:G:70:ASN:ND2	2.51	0.43
2:G:122:TYR:CZ	2:G:126:LEU:HD11	2.53	0.43
2:J:379:ASP:N	2:J:379:ASP:OD1	2.49	0.43
2:K:270:TYR:C	2:K:272:GLU:H	2.26	0.43
2:K:407:ALA:HB1	2:K:409:GLN:HG2	1.99	0.43
1:B:266:GLN:CD	1:B:268:THR:H	2.25	0.43
1:B:273:LYS:HD3	1:B:277:ILE:HD13	1.99	0.43
1:B:440:ARG:H	1:B:440:ARG:HG2	1.56	0.43
1:C:482:SER:HB2	1:C:484:THR:HG22	2.00	0.43
1:C:519:ASN:O	1:C:522:SER:OG	2.36	0.43
1:D:67:LEU:CD2	1:D:73:SER:HB2	2.40	0.43
1:D:282:ASP:OD2	1:D:282:ASP:N	2.52	0.43
1:D:458:LYS:NZ	1:D:471:LEU:HD11	2.34	0.43
1:E:222:LEU:HD11	1:E:373:VAL:HG21	2.01	0.43
2:G:3:ILE:HA	2:G:402:GLY:HA3	2.00	0.43
2:H:155:LEU:HD13	2:H:316:PRO:HG3	2.00	0.43
2:J:111:LEU:HD23	2:J:116:PHE:HD2	1.84	0.43
2:K:13:LEU:HD13	2:K:20:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:208:TYR:HB2	2:N:422:LEU:HD23	2.01	0.43
2:N:275:GLN:NE2	2:N:276:PRO:HD2	2.34	0.43
2:O:229:LEU:HD11	2:O:291:ASN:HB3	2.00	0.43
2:P:219:LYS:HG2	2:P:262:ARG:HD3	2.01	0.43
2:Q:325:ALA:HB3	2:R:358:HIS:CE1	2.53	0.43
1:B:184:HIS:HA	1:B:393:ILE:O	2.18	0.43
1:E:334:VAL:HG12	1:E:335:SER:H	1.84	0.43
2:G:82:LYS:O	2:G:85:ILE:HG13	2.18	0.43
2:J:17:LYS:O	2:J:21:LYS:HG3	2.19	0.43
2:K:29:ILE:HG23	2:K:33:LEU:HD13	2.00	0.43
2:L:179:LYS:NZ	2:L:317:THR:OG1	2.37	0.43
2:L:210:PHE:HZ	2:L:281:ALA:HB2	1.83	0.43
2:M:205:PHE:HB2	2:M:415:GLN:NE2	2.33	0.43
2:M:300:LEU:O	2:M:300:LEU:HG	2.18	0.43
2:M:325:ALA:HB1	2:N:362:ILE:HG12	2.01	0.43
2:N:297:GLU:OE2	2:N:297:GLU:N	2.50	0.43
2:P:16:LEU:O	2:P:21:LYS:NZ	2.42	0.43
1:A:148:LEU:HD22	1:A:183:PHE:CE2	2.54	0.43
1:A:255:LYS:CB	1:A:280:ILE:HG22	2.49	0.43
1:D:358:GLN:H	1:D:358:GLN:HG3	1.64	0.43
2:L:355:PRO:HG3	3:L:501:APR:C3D	2.48	0.43
2:M:76:LEU:HD12	2:M:145:TYR:HD1	1.84	0.43
2:M:224:THR:C	2:M:226:ASN:H	2.26	0.43
2:P:413:TYR:CE1	3:P:501:APR:N1	2.86	0.43
2:Q:96:ILE:H	2:Q:96:ILE:HG13	1.70	0.43
2:R:81:ILE:O	2:R:81:ILE:CG2	2.67	0.43
1:B:273:LYS:HA	1:B:277:ILE:HD13	2.00	0.43
1:B:279:SER:O	1:B:282:ASP:HB2	2.19	0.43
1:D:560:TYR:HH	1:E:391:LYS:HZ3	1.61	0.43
1:E:60:VAL:HG23	1:F:10:VAL:HB	1.99	0.43
1:E:203:VAL:HA	1:E:207:PHE:HB3	2.00	0.43
1:F:276:LYS:HD2	1:F:279:SER:HB3	2.01	0.43
1:F:456:ALA:O	1:F:460:ILE:HG12	2.19	0.43
2:G:403:ASN:HB3	2:G:408:GLU:HG2	2.00	0.43
2:J:394:ASN:O	2:J:397:LEU:N	2.46	0.43
1:B:515:LYS:HA	1:B:515:LYS:HD2	1.86	0.43
1:C:182:HIS:HE1	1:C:434:ILE:HG13	1.84	0.43
1:C:233:ILE:HG13	1:C:234:LEU:N	2.34	0.43
1:D:400:LEU:HB2	1:D:404:LEU:HD21	2.01	0.43
1:D:432:VAL:HG12	1:D:470:PHE:HB2	1.99	0.43
2:G:62:LEU:HD22	2:G:69:LEU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:350:ILE:HA	2:G:377:PHE:HB2	2.01	0.43
2:O:256:ILE:HD11	2:O:335:GLU:HG3	2.01	0.43
2:O:263:VAL:H	2:O:280:GLU:CD	2.27	0.43
2:O:321:HIS:CD2	2:O:321:HIS:H	2.37	0.43
2:R:68:VAL:O	2:R:72:VAL:HG12	2.19	0.43
2:R:247:GLN:HG2	2:R:258:GLN:HE21	1.83	0.43
1:B:179:GLN:HB3	1:B:180:ASN:H	1.74	0.42
1:B:208:LYS:HG2	1:B:381:PHE:HA	2.00	0.42
1:B:531:ILE:HD11	1:B:542:ILE:CD1	2.35	0.42
1:D:162:LYS:HA	1:D:162:LYS:HD2	1.86	0.42
1:D:213:ASN:HD21	1:D:418:GLU:HB2	1.84	0.42
1:F:482:SER:HB3	1:F:485:VAL:HG12	2.00	0.42
2:H:413:TYR:HA	3:H:501:APR:N1	2.34	0.42
2:J:210:PHE:HZ	2:J:281:ALA:HB2	1.84	0.42
2:L:53:LEU:CD2	3:L:501:APR:O1A	2.67	0.42
2:L:254:PHE:HZ	2:L:332:LEU:HD21	1.83	0.42
2:M:368:LYS:HB3	2:M:368:LYS:HE3	1.76	0.42
2:O:183:ILE:HD12	2:O:183:ILE:HA	1.95	0.42
2:P:340:LEU:HD22	2:P:372:PHE:HE1	1.83	0.42
1:A:97:ASN:HB2	1:B:525:PRO:HA	2.01	0.42
1:A:228:LEU:HD12	1:A:229:VAL:CG1	2.48	0.42
1:A:372:ASN:HA	1:A:375:THR:HG22	2.01	0.42
1:B:160:SER:O	1:B:160:SER:OG	2.34	0.42
1:B:181:LEU:HB3	1:C:560:TYR:O	2.19	0.42
1:B:253:TRP:CD1	1:B:314:VAL:HA	2.54	0.42
1:D:459:LYS:HA	1:D:463:GLU:HB2	2.00	0.42
1:D:531:ILE:HD11	1:D:536:PHE:HB2	2.01	0.42
2:G:162:LEU:HD21	2:G:172:LYS:HA	2.01	0.42
2:H:61:ILE:HB	2:H:69:LEU:HD13	2.01	0.42
2:H:96:ILE:CG2	2:H:100:GLU:HB3	2.41	0.42
2:H:353:GLY:H	3:H:501:APR:H'4	1.81	0.42
2:I:375:ILE:HA	2:I:398:HIS:HB2	2.01	0.42
2:M:24:GLN:OE1	2:M:417:ILE:HD13	2.17	0.42
2:O:348:ILE:HD13	2:O:375:ILE:HB	2.01	0.42
1:A:62:ASP:OD1	1:D:105:GLN:NE2	2.52	0.42
1:C:67:LEU:HB3	1:C:70:GLU:O	2.19	0.42
1:E:294:LYS:HD2	1:E:294:LYS:HA	1.79	0.42
2:G:403:ASN:N	2:G:403:ASN:OD1	2.52	0.42
2:H:210:PHE:HZ	2:H:281:ALA:HB2	1.83	0.42
2:L:103:ALA:O	2:L:106:THR:OG1	2.32	0.42
2:O:212:LYS:HE3	2:O:212:LYS:HB3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:189:VAL:HG13	2:Q:304:ASP:O	2.19	0.42
1:C:154:ILE:HA	1:C:493:ILE:HB	2.01	0.42
1:D:337:PHE:O	1:D:340:LEU:HG	2.19	0.42
1:E:182:HIS:HB2	1:E:431:ASN:HB3	2.01	0.42
2:H:44:SER:OG	3:H:501:APR:O4D	2.38	0.42
2:H:53:LEU:O	2:H:57:THR:HG22	2.19	0.42
2:J:153:GLU:HG3	2:J:154:LEU:H	1.84	0.42
2:J:351:GLY:HA2	3:J:501:APR:N3	2.34	0.42
2:M:189:VAL:HG23	2:P:250:ILE:CG2	2.48	0.42
2:N:293:LYS:HD2	2:N:303:ILE:HD13	2.02	0.42
2:P:265:ASP:HB2	2:P:277:VAL:HG12	2.01	0.42
1:B:360:ARG:NH2	1:E:356:ASN:OD1	2.47	0.42
1:C:91:HIS:HB3	2:H:424:ASN:HB3	2.02	0.42
1:D:352:GLU:OE2	1:E:321:PHE:HA	2.20	0.42
1:E:405:LEU:HD22	1:E:440:ARG:CZ	2.50	0.42
1:F:65:ILE:HG21	1:F:78:HIS:HB2	1.87	0.42
1:F:190:ASP:HA	1:F:193:LYS:HE3	2.02	0.42
1:F:438:ALA:HA	1:F:441:TYR:CZ	2.53	0.42
2:H:307:ASP:N	2:H:307:ASP:OD1	2.51	0.42
2:I:22:GLN:HA	2:I:25:VAL:HG22	2.01	0.42
2:J:342:ILE:H	2:J:342:ILE:HG12	1.66	0.42
2:K:354:PHE:HB3	2:K:360:ASN:HD21	1.84	0.42
2:M:136:GLU:HA	2:M:139:ASN:HD21	1.84	0.42
2:M:227:TYR:OH	2:M:314:ILE:O	2.28	0.42
2:M:250:ILE:H	2:M:250:ILE:HD12	1.85	0.42
2:N:213:ARG:HD2	2:N:213:ARG:HA	1.77	0.42
2:P:143:CYS:O	2:P:147:ASN:N	2.45	0.42
2:Q:255:ASP:HB3	2:Q:258:GLN:HG2	2.02	0.42
1:A:25:LEU:HD22	1:A:36:ALA:HB2	2.00	0.42
1:D:530:TYR:CD1	1:D:541:GLU:HB2	2.55	0.42
1:E:379:ASN:OD1	1:E:379:ASN:N	2.46	0.42
2:J:333:PHE:HE1	2:J:359:ILE:HG12	1.84	0.42
2:K:271:LYS:HG3	2:K:272:GLU:HG2	2.01	0.42
2:L:13:LEU:HA	2:L:16:LEU:HD12	2.00	0.42
2:L:293:LYS:HE2	2:L:293:LYS:HB2	1.91	0.42
2:L:304:ASP:OD2	2:L:304:ASP:N	2.48	0.42
2:M:406:LYS:HB2	2:M:413:TYR:CD1	2.55	0.42
2:N:341:GLN:HG3	2:N:366:ASN:ND2	2.34	0.42
2:O:417:ILE:O	2:O:417:ILE:CG2	2.67	0.42
2:P:155:LEU:HB3	2:P:316:PRO:HB3	2.01	0.42
2:P:323:GLU:H	2:P:323:GLU:HG3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:CG2	1:A:231:LEU:HD12	2.50	0.42
1:D:483:SER:C	1:D:485:VAL:H	2.28	0.42
1:E:295:TYR:HB2	1:E:298:MET:HG3	2.01	0.42
1:E:395:TYR:HB3	1:E:397:VAL:HG13	2.01	0.42
1:E:493:ILE:HG12	1:E:531:ILE:HG23	2.01	0.42
1:F:224:LYS:HE2	1:F:224:LYS:HB2	1.90	0.42
2:G:232:GLU:OE2	2:G:285:LYS:NZ	2.51	0.42
2:H:84:PHE:O	2:H:88:VAL:HG23	2.19	0.42
2:H:95:LYS:HE2	2:H:95:LYS:HB2	1.82	0.42
2:J:13:LEU:HD13	2:J:21:LYS:HB3	2.00	0.42
2:J:408:GLU:OE2	2:J:416:PHE:N	2.53	0.42
2:K:38:LEU:HB3	2:K:220:VAL:HG12	2.00	0.42
2:M:131:SER:OG	2:M:132:GLU:N	2.53	0.42
2:N:85:ILE:O	2:N:89:GLU:HG2	2.20	0.42
2:P:412:HIS:CD2	3:P:501:APR:C8	3.03	0.42
2:Q:76:LEU:HD13	2:Q:144:TYR:CZ	2.54	0.42
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.87	0.42
1:A:142:PHE:HD1	1:A:142:PHE:HA	1.76	0.42
1:A:224:LYS:HB3	1:A:224:LYS:HE3	1.84	0.42
1:A:514:ASN:HA	1:B:500:ASN:HD21	1.83	0.42
1:B:238:LEU:HD21	1:B:332:TYR:CD1	2.54	0.42
1:B:239:LYS:HD3	1:B:239:LYS:HA	1.88	0.42
1:C:221:ASN:HD22	1:C:453:GLU:CD	2.28	0.42
1:C:308:GLU:HA	1:C:311:LYS:HG2	2.00	0.42
1:D:239:LYS:NZ	1:D:331:LYS:O	2.53	0.42
1:E:190:ASP:HB3	1:E:193:LYS:HE3	2.00	0.42
1:F:272:THR:HG1	1:F:273:LYS:HZ3	1.59	0.42
2:I:81:ILE:HG22	2:I:85:ILE:HG23	2.01	0.42
2:I:330:SER:HB3	2:J:337:SER:HB3	2.01	0.42
2:J:413:TYR:HA	3:J:501:APR:N1	2.34	0.42
2:K:329:TYR:HA	2:K:332:LEU:HD12	2.01	0.42
2:L:284:TYR:HD2	2:L:332:LEU:HD22	1.84	0.42
2:M:84:PHE:O	2:M:88:VAL:HG22	2.20	0.42
2:O:318:MET:HG3	2:O:319:LEU:HD12	2.01	0.42
2:P:43:GLY:HA3	2:P:352:TYR:HB2	2.01	0.42
2:Q:25:VAL:O	2:Q:30:ASN:ND2	2.53	0.42
2:R:54:MET:HA	2:R:57:THR:HG22	2.01	0.42
2:R:354:PHE:HB3	2:R:360:ASN:HD21	1.84	0.42
1:A:305:LYS:HA	1:A:308:GLU:HG2	2.02	0.42
1:A:309:SER:O	1:A:313:VAL:HG13	2.19	0.42
1:C:8:THR:O	1:F:62:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ASN:HA	1:C:429:SER:OG	2.20	0.42
1:D:478:PRO:HB2	1:D:502:ASP:OD2	2.20	0.42
1:F:217:GLN:HE21	1:F:217:GLN:HB3	1.73	0.42
2:G:151:ILE:HG13	2:G:155:LEU:HG	2.01	0.42
2:H:219:LYS:HE3	2:H:280:GLU:HB3	2.01	0.42
2:I:169:GLY:HA2	2:I:172:LYS:HE2	2.02	0.42
2:M:82:LYS:HE2	2:M:82:LYS:HB2	1.95	0.42
2:N:186:ILE:HB	2:N:290:ILE:HD11	2.01	0.42
2:O:86:LYS:HE2	2:O:86:LYS:HB3	1.90	0.42
2:P:111:LEU:HD12	2:P:111:LEU:C	2.45	0.42
1:B:69:SER:HB3	1:B:72:HIS:HB3	2.01	0.42
1:B:180:ASN:H	1:C:561:ARG:CB	2.33	0.42
1:B:180:ASN:HA	1:C:558:ILE:O	2.20	0.42
1:C:498:LYS:HE2	1:C:498:LYS:HB2	1.88	0.42
1:D:142:PHE:HZ	1:D:531:ILE:HG21	1.85	0.42
1:D:322:THR:HG22	1:D:324:SER:H	1.85	0.42
1:D:439:HIS:NE2	1:D:477:ARG:HB2	2.35	0.42
1:D:455:GLU:HA	1:D:458:LYS:HE2	2.02	0.42
1:D:528:THR:OG1	1:D:542:ILE:O	2.32	0.42
2:H:202:TYR:HB3	2:H:234:ALA:HB2	2.01	0.42
2:J:5:HIS:CD2	2:J:400:ILE:HG12	2.54	0.42
2:K:322:LYS:HG3	2:L:358:HIS:CG	2.55	0.42
2:M:273:LYS:HD3	2:M:273:LYS:HA	1.92	0.42
2:N:57:THR:C	2:N:59:LYS:H	2.28	0.42
2:O:365:GLN:O	2:O:368:LYS:NZ	2.41	0.42
2:Q:13:LEU:HD13	2:Q:20:GLU:HB3	2.02	0.42
2:R:201:ILE:CG2	2:R:418:VAL:HG21	2.49	0.42
1:A:158:THR:HG21	1:D:490:ASN:HD22	1.85	0.41
1:A:503:LEU:HA	1:A:518:LEU:HD11	2.02	0.41
1:F:199:LYS:HB2	1:F:199:LYS:HE2	1.77	0.41
1:F:243:ALA:HB1	1:F:249:ILE:HB	2.02	0.41
2:J:85:ILE:O	2:J:89:GLU:HG3	2.20	0.41
2:K:25:VAL:HG11	2:K:419:GLU:HA	2.01	0.41
2:L:266:ASP:HA	2:L:274:TRP:CD1	2.55	0.41
2:L:307:ASP:OD1	2:L:307:ASP:N	2.53	0.41
2:O:5:HIS:CD2	2:O:400:ILE:HG12	2.55	0.41
1:D:504:GLU:O	1:D:508:ASN:ND2	2.53	0.41
2:G:356:ASP:HB3	2:G:358:HIS:CE1	2.55	0.41
2:H:155:LEU:HB3	2:H:316:PRO:HB3	2.02	0.41
2:I:405:SER:OG	2:I:406:LYS:N	2.51	0.41
2:J:45:GLY:O	3:J:501:APR:C6	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:179:LYS:O	2:M:183:ILE:HG13	2.19	0.41
2:R:406:LYS:C	2:R:408:GLU:H	2.28	0.41
1:C:90:LYS:HE2	1:C:91:HIS:CE1	2.55	0.41
1:C:203:VAL:HG11	1:C:397:VAL:HG12	2.01	0.41
1:D:152:THR:O	1:D:152:THR:CG2	2.68	0.41
1:D:168:GLN:O	1:D:172:LYS:HB2	2.20	0.41
1:E:450:GLN:H	1:E:450:GLN:HG2	1.69	0.41
1:F:11:THR:HG23	1:F:14:LYS:H	1.85	0.41
1:F:165:THR:HA	1:F:544:ILE:HG21	2.02	0.41
1:F:246:ASN:HD21	1:F:248:ILE:HB	1.85	0.41
1:F:323:LEU:HA	1:F:326:VAL:HB	2.02	0.41
2:I:406:LYS:HA	2:I:428:ARG:HB2	2.02	0.41
2:K:128:MET:HE2	2:K:128:MET:HB2	1.89	0.41
2:N:265:ASP:OD2	2:N:267:THR:OG1	2.28	0.41
2:P:210:PHE:HB3	2:P:279:LYS:HD3	2.00	0.41
2:Q:350:ILE:HA	2:Q:377:PHE:HB2	2.01	0.41
1:B:11:THR:OG1	1:B:12:PHE:N	2.53	0.41
1:B:210:ASN:O	1:B:214:LEU:HB2	2.19	0.41
1:B:484:THR:CG2	1:B:485:VAL:N	2.82	0.41
1:D:229:VAL:O	1:D:232:PRO:HD2	2.21	0.41
1:F:338:ASN:O	1:F:342:GLU:HG2	2.20	0.41
1:F:504:GLU:O	1:F:508:ASN:ND2	2.54	0.41
2:G:269:ARG:HD2	2:G:269:ARG:HA	1.80	0.41
2:J:67:SER:HB2	2:J:174:VAL:HG22	2.02	0.41
2:K:376:ILE:HG22	2:K:378:GLY:H	1.86	0.41
2:L:36:ASN:HB2	2:L:344:ASP:HB2	2.02	0.41
2:M:25:VAL:O	2:M:30:ASN:ND2	2.53	0.41
2:O:31:LYS:O	2:O:35:ALA:N	2.54	0.41
2:P:54:MET:HB2	3:P:501:APR:PB	2.60	0.41
3:R:501:APR:H8	3:R:501:APR:H'2	1.79	0.41
1:D:239:LYS:HA	1:D:239:LYS:HD3	1.82	0.41
1:E:377:PHE:CZ	1:E:404:LEU:HD11	2.55	0.41
1:F:67:LEU:N	1:F:74:LYS:HD3	2.35	0.41
1:F:143:ASN:HD22	1:F:146:LYS:HG3	1.86	0.41
2:G:76:LEU:HD12	2:G:145:TYR:HD1	1.85	0.41
2:G:271:LYS:HE2	2:K:343:LYS:HD3	2.03	0.41
2:H:61:ILE:HD12	2:H:146:LEU:HA	2.02	0.41
2:I:67:SER:HA	2:I:70:ASN:HD21	1.85	0.41
2:J:54:MET:HE2	2:J:151:ILE:HG21	2.03	0.41
2:J:413:TYR:HA	3:J:501:APR:C2	2.50	0.41
2:M:132:GLU:H	2:M:132:GLU:CD	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:146:LEU:HD23	2:M:146:LEU:HA	1.86	0.41
2:M:217:LYS:HE2	2:M:217:LYS:HB2	1.84	0.41
2:M:408:GLU:HB3	2:M:413:TYR:HD2	1.86	0.41
2:R:406:LYS:HA	2:R:406:LYS:HD3	1.86	0.41
1:A:45:ILE:HB	1:A:53:PHE:HB2	2.02	0.41
1:A:241:ALA:O	1:A:245:GLU:HG2	2.21	0.41
1:A:425:LEU:HD13	1:A:428:ARG:HG2	2.03	0.41
1:B:229:VAL:O	1:B:232:PRO:HD2	2.21	0.41
1:D:248:ILE:HG22	1:D:249:ILE:HG22	2.02	0.41
1:E:216:MET:HB2	1:E:332:TYR:CD2	2.56	0.41
1:E:301:ASN:O	1:E:305:LYS:HD3	2.20	0.41
1:E:348:PHE:O	1:E:351:GLU:HB3	2.20	0.41
1:F:183:PHE:HB2	1:F:392:SER:HA	2.02	0.41
2:H:358:HIS:O	2:H:362:ILE:HG13	2.20	0.41
2:I:77:ASN:O	2:I:118:ASN:HB2	2.20	0.41
2:K:283:LEU:HD21	2:K:285:LYS:HE3	2.03	0.41
2:K:291:ASN:HB2	2:K:303:ILE:O	2.21	0.41
2:N:349:ILE:HD11	2:N:363:ILE:HD13	2.02	0.41
2:P:134:LYS:HD3	2:P:137:ILE:HD12	2.03	0.41
1:A:228:LEU:HD12	1:A:228:LEU:C	2.46	0.41
1:A:242:ASN:HA	1:A:245:GLU:HG2	2.02	0.41
1:B:391:LYS:HA	1:B:391:LYS:HD2	1.83	0.41
1:C:16:ILE:HG12	1:C:82:GLU:HG2	2.02	0.41
1:C:503:LEU:HD22	1:C:518:LEU:HG	2.03	0.41
1:E:160:SER:OG	1:E:495:HIS:HB3	2.21	0.41
2:G:381:LYS:HA	2:G:381:LYS:HD2	1.82	0.41
2:I:25:VAL:HG11	2:I:419:GLU:HA	2.01	0.41
2:J:44:SER:HB3	3:J:501:APR:H5R2	2.02	0.41
2:J:153:GLU:O	2:J:154:LEU:C	2.63	0.41
2:L:183:ILE:HD11	2:L:312:VAL:HG11	2.02	0.41
2:M:76:LEU:HB2	2:M:145:TYR:HE1	1.85	0.41
2:M:251:LEU:HB2	2:P:236:GLU:CD	2.46	0.41
2:P:3:ILE:HA	2:P:401:GLY:O	2.21	0.41
2:P:234:ALA:O	2:P:238:ASN:ND2	2.37	0.41
1:A:4:ILE:HB	1:A:19:VAL:HG13	2.01	0.41
1:B:1:MET:HE3	1:B:109:TYR:HE1	1.86	0.41
1:C:105:GLN:HG3	1:F:77:TYR:CD2	2.56	0.41
1:E:208:LYS:HB3	1:E:383:ASN:HB3	2.02	0.41
1:E:252:GLU:HA	1:E:255:LYS:HB2	2.02	0.41
1:E:371:LYS:HD2	1:F:327:ILE:HD11	2.02	0.41
1:F:26:ASN:HB3	2:H:36:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:THR:O	1:F:273:LYS:HE2	2.21	0.41
2:H:266:ASP:HB3	2:H:271:LYS:HB3	2.03	0.41
2:I:156:ASN:OD1	2:I:318:MET:N	2.53	0.41
2:J:23:GLU:O	2:J:27:THR:HG23	2.21	0.41
2:J:44:SER:CB	3:J:501:APR:O4D	2.69	0.41
2:J:349:ILE:HD12	2:J:376:ILE:HG12	2.03	0.41
2:M:41:PHE:HB3	2:M:349:ILE:HG12	2.01	0.41
2:N:17:LYS:O	2:N:21:LYS:HG3	2.21	0.41
2:O:286:ILE:HA	2:O:332:LEU:HD13	2.03	0.41
2:P:379:ASP:OD1	2:P:379:ASP:N	2.53	0.41
1:A:155:ILE:HG23	1:A:478:PRO:HB3	2.03	0.41
1:A:220:ILE:HG21	1:A:231:LEU:HD12	2.03	0.41
1:A:446:LYS:HB3	1:A:449:SER:HB2	2.03	0.41
1:A:447:GLU:HG3	1:A:482:SER:HB2	2.02	0.41
1:A:547:GLU:HB3	1:A:551:ASN:HD21	1.86	0.41
1:B:184:HIS:HB2	1:B:393:ILE:HB	2.02	0.41
1:B:216:MET:HG3	1:B:238:LEU:HD13	1.93	0.41
1:B:322:THR:OG1	1:C:362:TYR:HA	2.21	0.41
1:C:528:THR:HA	1:C:544:ILE:HG12	2.03	0.41
1:D:202:ASP:HB3	1:D:396:SER:HB3	2.02	0.41
1:D:417:PHE:CE1	1:D:462:ARG:HB3	2.56	0.41
1:D:458:LYS:HE2	1:D:458:LYS:HB3	1.82	0.41
1:E:62:ASP:OD2	1:F:105:GLN:NE2	2.45	0.41
1:E:290:LYS:HZ2	1:E:305:LYS:HB2	1.86	0.41
1:F:57:VAL:HG22	1:F:83:CYS:HG	1.84	0.41
1:F:446:LYS:HE3	1:F:446:LYS:HB3	1.91	0.41
2:H:53:LEU:HD11	3:H:501:APR:H5'1	2.03	0.41
2:H:283:LEU:HG	2:H:285:LYS:HD3	2.02	0.41
2:I:224:THR:O	2:I:224:THR:HG23	2.21	0.41
2:I:367:LEU:HD23	2:I:367:LEU:HA	1.93	0.41
2:K:166:ASN:OD1	2:K:172:LYS:NZ	2.49	0.41
2:K:336:PHE:HE2	2:K:359:ILE:HG23	1.85	0.41
2:K:358:HIS:HD2	2:L:334:ARG:HH12	1.66	0.41
2:M:68:VAL:HG22	2:M:174:VAL:HG13	2.03	0.41
2:M:93:GLN:H	2:M:93:GLN:HG2	1.64	0.41
2:M:337:SER:OG	2:M:362:ILE:HG23	2.21	0.41
2:N:5:HIS:CD2	2:N:400:ILE:HG12	2.56	0.41
2:N:292:TRP:CD1	2:N:302:GLN:HG3	2.49	0.41
2:O:108:MET:H	2:O:108:MET:HG3	1.72	0.41
2:Q:138:LEU:HD23	2:Q:138:LEU:HA	1.88	0.41
2:R:410:LYS:HB3	2:R:412:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:OD2	1:A:287:ASP:N	2.45	0.41
1:B:267:GLN:HB2	1:E:265:ASN:HB3	2.01	0.41
1:B:338:ASN:O	1:B:342:GLU:HG3	2.21	0.41
1:C:74:LYS:HD3	1:C:74:LYS:HA	1.89	0.41
1:C:265:ASN:HA	1:F:275:THR:OG1	2.20	0.41
1:D:152:THR:HG22	1:D:472:MET:HG2	2.03	0.41
1:D:463:GLU:OE2	1:D:469:CYS:HB2	2.21	0.41
1:D:558:ILE:H	1:D:558:ILE:HD12	1.86	0.41
2:G:79:LYS:HE3	2:G:83:GLU:HG2	2.02	0.41
2:G:342:ILE:HG22	2:G:343:LYS:H	1.85	0.41
2:J:91:GLN:HE21	2:J:91:GLN:HB2	1.69	0.41
2:K:87:TYR:O	2:K:91:GLN:HB2	2.20	0.41
2:L:44:SER:O	3:L:501:APR:H5'1	2.20	0.41
2:O:12:VAL:O	2:O:12:VAL:HG22	2.21	0.41
2:O:17:LYS:HB3	2:O:17:LYS:HE2	1.80	0.41
1:A:229:VAL:HB	1:A:362:TYR:CG	2.56	0.40
1:B:47:ASN:HD21	1:B:51:GLU:HB3	1.85	0.40
1:B:185:ILE:HG21	1:B:192:TYR:HD2	1.87	0.40
1:C:249:ILE:HD12	1:C:320:ILE:HD13	2.03	0.40
1:E:53:PHE:CG	1:E:102:PRO:HG3	2.56	0.40
1:F:216:MET:HE2	1:F:216:MET:HB2	1.83	0.40
1:F:530:TYR:CD1	1:F:541:GLU:HG3	2.57	0.40
2:H:43:GLY:HA2	2:H:224:THR:O	2.22	0.40
2:I:43:GLY:HA2	2:I:225:THR:HB	2.02	0.40
2:J:151:ILE:HG23	2:J:152:GLU:N	2.36	0.40
2:J:188:LYS:N	2:J:191:ASP:OD2	2.54	0.40
2:L:219:LYS:HG3	2:L:262:ARG:HH11	1.86	0.40
2:M:256:ILE:HD11	2:M:335:GLU:HG3	2.03	0.40
2:O:236:GLU:HG3	2:R:249:THR:HG21	2.03	0.40
2:P:358:HIS:O	2:P:362:ILE:HG13	2.21	0.40
2:Q:368:LYS:HE2	2:Q:368:LYS:HB3	1.94	0.40
1:A:503:LEU:HD22	1:A:518:LEU:CD1	2.50	0.40
1:C:216:MET:O	1:C:220:ILE:HG12	2.21	0.40
1:C:274:ARG:O	1:C:277:ILE:HG12	2.21	0.40
1:D:69:SER:OG	1:D:70:GLU:N	2.47	0.40
1:E:305:LYS:HA	1:E:308:GLU:HB3	2.04	0.40
1:F:90:LYS:HE3	1:F:91:HIS:CE1	2.56	0.40
1:F:245:GLU:OE2	1:F:335:SER:OG	2.35	0.40
1:F:515:LYS:HA	1:F:518:LEU:HB2	2.03	0.40
2:J:98:GLU:H	2:J:98:GLU:HG3	1.68	0.40
2:L:355:PRO:CG	3:L:501:APR:O3D	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:LEU:HD12	2:P:399:LEU:HD23	2.03	0.40
2:Q:82:LYS:HE3	2:Q:82:LYS:HB3	1.99	0.40
2:R:300:LEU:HD11	2:R:313:VAL:HG21	2.02	0.40
1:A:13:GLU:HG2	1:B:519:ASN:HB3	2.04	0.40
1:B:129:ILE:HG22	1:B:131:ILE:H	1.86	0.40
1:E:45:ILE:HG21	1:E:102:PRO:HB3	2.02	0.40
1:E:465:ARG:HA	1:E:470:PHE:CE1	2.56	0.40
1:F:154:ILE:HG12	1:F:493:ILE:HB	2.03	0.40
1:F:193:LYS:HD2	1:F:200:ILE:HD13	2.03	0.40
1:F:229:VAL:C	1:F:232:PRO:HD2	2.46	0.40
1:F:433:PHE:O	1:F:472:MET:N	2.50	0.40
1:F:531:ILE:HG13	1:F:542:ILE:HD12	2.04	0.40
2:G:183:ILE:HD12	2:G:183:ILE:HA	1.94	0.40
2:G:354:PHE:HZ	2:G:376:ILE:HD13	1.87	0.40
2:H:81:ILE:H	2:H:81:ILE:HD12	1.87	0.40
2:J:261:TYR:HD1	2:J:261:TYR:HA	1.77	0.40
2:M:352:TYR:C	2:M:354:PHE:H	2.28	0.40
2:O:287:HIS:CE1	2:O:314:ILE:HD11	2.57	0.40
2:P:51:VAL:HG21	2:P:186:ILE:HA	2.03	0.40
2:P:228:ASP:HB2	2:P:230:PHE:HD2	1.86	0.40
2:Q:75:PHE:HB2	2:Q:157:TRP:CE3	2.56	0.40
2:R:167:ASN:OD1	2:R:167:ASN:N	2.55	0.40
1:A:170:ILE:O	1:A:173:ILE:HG13	2.21	0.40
1:B:148:LEU:HB3	1:B:432:VAL:HG21	2.03	0.40
1:B:431:ASN:HD22	1:B:432:VAL:N	2.19	0.40
1:C:186:PHE:HB3	1:C:397:VAL:HG21	2.03	0.40
1:C:254:LEU:CD2	1:C:346:TYR:CD1	3.05	0.40
1:E:122:HIS:HB3	1:E:537:PRO:HG3	2.02	0.40
1:F:436:GLU:HA	1:F:474:SER:HB3	2.04	0.40
1:F:506:LEU:HA	1:F:509:SER:HB3	2.02	0.40
2:J:75:PHE:HE2	2:J:157:TRP:CD2	2.40	0.40
2:L:79:LYS:HD3	2:L:79:LYS:HA	1.85	0.40
2:O:86:LYS:O	2:O:89:GLU:HG3	2.20	0.40
2:O:300:LEU:HD22	2:O:312:VAL:HG11	2.03	0.40
2:P:224:THR:HG22	2:P:226:ASN:HB2	2.03	0.40
2:R:228:ASP:HB2	2:R:230:PHE:HD2	1.87	0.40
2:R:254:PHE:HB3	2:R:300:LEU:HB3	2.03	0.40
1:A:484:THR:HG22	1:A:488:GLN:HE22	1.77	0.40
1:D:229:VAL:C	1:D:232:PRO:HD2	2.46	0.40
1:E:293:SER:O	1:E:293:SER:OG	2.38	0.40
1:E:472:MET:HE3	1:E:472:MET:HB2	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:LEU:HD22	2:H:316:PRO:HG3	2.03	0.40
2:J:292:TRP:HE3	2:J:313:VAL:HG21	1.87	0.40
2:K:320:LYS:HD3	2:K:358:HIS:CE1	2.56	0.40
2:L:54:MET:CE	3:L:501:APR:O4D	2.68	0.40
2:L:110:GLN:NE2	2:L:122:TYR:OH	2.55	0.40
2:M:76:LEU:HD13	2:M:144:TYR:CZ	2.57	0.40
2:M:377:PHE:HE1	2:M:400:ILE:HD12	1.87	0.40
2:R:3:ILE:HA	2:R:401:GLY:O	2.20	0.40
2:R:266:ASP:HB2	2:R:274:TRP:CZ3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	560/562 (100%)	532 (95%)	28 (5%)	0	100	100
1	B	560/562 (100%)	531 (95%)	29 (5%)	0	100	100
1	C	560/562 (100%)	528 (94%)	30 (5%)	2 (0%)	30	58
1	D	560/562 (100%)	507 (90%)	52 (9%)	1 (0%)	43	71
1	E	560/562 (100%)	526 (94%)	34 (6%)	0	100	100
1	F	560/562 (100%)	528 (94%)	32 (6%)	0	100	100
2	G	406/428 (95%)	376 (93%)	30 (7%)	0	100	100
2	H	423/428 (99%)	385 (91%)	36 (8%)	2 (0%)	24	53
2	I	426/428 (100%)	390 (92%)	35 (8%)	1 (0%)	43	71
2	J	423/428 (99%)	392 (93%)	29 (7%)	2 (0%)	24	53
2	K	426/428 (100%)	397 (93%)	29 (7%)	0	100	100
2	L	423/428 (99%)	396 (94%)	25 (6%)	2 (0%)	24	53
2	M	426/428 (100%)	389 (91%)	36 (8%)	1 (0%)	43	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	423/428 (99%)	386 (91%)	35 (8%)	2 (0%)	24	53
2	O	426/428 (100%)	394 (92%)	32 (8%)	0	100	100
2	P	423/428 (99%)	392 (93%)	30 (7%)	1 (0%)	43	71
2	Q	412/428 (96%)	383 (93%)	28 (7%)	1 (0%)	43	71
2	R	384/428 (90%)	359 (94%)	24 (6%)	1 (0%)	36	64
All	All	8381/8508 (98%)	7791 (93%)	574 (7%)	16 (0%)	44	71

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	561	ARG
1	D	68	SER
2	H	119	LEU
2	I	269	ARG
2	J	395	PHE
2	N	215	GLU
2	P	395	PHE
2	R	395	PHE
2	J	215	GLU
2	L	215	GLU
1	C	560	TYR
2	H	395	PHE
2	M	249	THR
2	N	119	LEU
2	L	407	ALA
2	Q	343	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	523/523 (100%)	519 (99%)	4 (1%)	73	90
1	B	523/523 (100%)	518 (99%)	5 (1%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	523/523 (100%)	516 (99%)	7 (1%)	61	85
1	D	520/523 (99%)	511 (98%)	9 (2%)	53	81
1	E	523/523 (100%)	519 (99%)	4 (1%)	73	90
1	F	523/523 (100%)	517 (99%)	6 (1%)	65	86
2	G	380/399 (95%)	378 (100%)	2 (0%)	81	93
2	H	398/399 (100%)	394 (99%)	4 (1%)	68	88
2	I	399/399 (100%)	396 (99%)	3 (1%)	73	90
2	J	396/399 (99%)	392 (99%)	4 (1%)	68	88
2	K	399/399 (100%)	390 (98%)	9 (2%)	44	76
2	L	396/399 (99%)	396 (100%)	0	100	100
2	M	399/399 (100%)	396 (99%)	3 (1%)	73	90
2	N	396/399 (99%)	390 (98%)	6 (2%)	57	83
2	O	399/399 (100%)	396 (99%)	3 (1%)	73	90
2	P	396/399 (99%)	392 (99%)	4 (1%)	68	88
2	Q	389/399 (98%)	388 (100%)	1 (0%)	86	95
2	R	361/399 (90%)	358 (99%)	3 (1%)	73	90
All	All	7843/7926 (99%)	7766 (99%)	77 (1%)	65	88

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LYS
1	A	295	TYR
1	A	299	ASP
1	A	311	LYS
1	B	224	LYS
1	B	247	LYS
1	B	321	PHE
1	B	331	LYS
1	B	440	ARG
1	C	255	LYS
1	C	331	LYS
1	C	339	LYS
1	C	342	GLU
1	C	459	LYS
1	C	476	GLN

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Mol	Chain	Res	Type
1	C	561	ARG
1	D	49	TYR
1	D	189	HIS
1	D	192	TYR
1	D	294	LYS
1	D	381	PHE
1	D	423	MET
1	D	457	PHE
1	D	496	ARG
1	D	536	PHE
1	E	72	HIS
1	E	291	TYR
1	E	332	TYR
1	E	377	PHE
1	F	74	LYS
1	F	75	PHE
1	F	183	PHE
1	F	212	LYS
1	F	266	GLN
1	F	269	ASP
2	G	128	MET
2	G	199	TYR
2	H	83	GLU
2	H	266	ASP
2	H	272	GLU
2	H	313	VAL
2	I	109	ASP
2	I	199	TYR
2	I	227	TYR
2	J	153	GLU
2	J	215	GLU
2	J	261	TYR
2	J	406	LYS
2	K	9	ASP
2	K	95	LYS
2	K	227	TYR
2	K	270	TYR
2	K	271	LYS
2	K	371	ASP
2	K	412	HIS
2	K	423	LYS
2	K	427	ARG

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Mol	Chain	Res	Type
2	M	227	TYR
2	M	318	MET
2	M	423	LYS
2	N	54	MET
2	N	57	THR
2	N	170	ASP
2	N	199	TYR
2	N	392	PHE
2	N	412	HIS
2	O	105	HIS
2	O	321	HIS
2	O	379	ASP
2	P	152	GLU
2	P	309	ASP
2	P	326	GLN
2	P	414	PHE
2	Q	95	LYS
2	R	79	LYS
2	R	199	TYR
2	R	414	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (278) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	125	ASN
1	A	137	GLN
1	A	143	ASN
1	A	150	ASN
1	A	157	ASN
1	A	168	GLN
1	A	175	ASN
1	A	177	ASN
1	A	205	ASN
1	A	221	ASN
1	A	266	GLN
1	A	297	ASN
1	A	301	ASN
1	A	345	ASN
1	A	379	ASN
1	A	384	ASN
1	A	420	ASN

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Mol	Chain	Res	Type
1	A	488	GLN
1	B	78	HIS
1	B	122	HIS
1	B	157	ASN
1	B	168	GLN
1	B	177	ASN
1	B	179	GLN
1	B	235	GLN
1	B	265	ASN
1	B	301	ASN
1	B	333	ASN
1	B	345	ASN
1	B	356	ASN
1	B	357	ASN
1	B	431	ASN
1	B	450	GLN
1	B	500	ASN
1	B	514	ASN
1	C	2	HIS
1	C	32	GLN
1	C	97	ASN
1	C	105	GLN
1	C	122	HIS
1	C	137	GLN
1	C	150	ASN
1	C	177	ASN
1	C	182	HIS
1	C	221	ASN
1	C	235	GLN
1	C	316	ASN
1	C	333	ASN
1	C	358	GLN
1	C	379	ASN
1	C	431	ASN
1	C	452	ASN
1	C	500	ASN
1	C	551	ASN
1	D	28	ASN
1	D	32	GLN
1	D	124	HIS
1	D	127	ASN
1	D	177	ASN

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Mol	Chain	Res	Type
1	D	179	GLN
1	D	180	ASN
1	D	213	ASN
1	D	230	GLN
1	D	319	ASN
1	D	356	ASN
1	D	357	ASN
1	E	2	HIS
1	E	72	HIS
1	E	91	HIS
1	E	122	HIS
1	E	157	ASN
1	E	174	ASN
1	E	179	GLN
1	E	189	HIS
1	E	235	GLN
1	E	266	GLN
1	E	267	GLN
1	E	345	ASN
1	E	357	ASN
1	E	383	ASN
1	E	420	ASN
1	E	431	ASN
1	F	32	GLN
1	F	91	HIS
1	F	177	ASN
1	F	182	HIS
1	F	189	HIS
1	F	235	GLN
1	F	265	ASN
1	F	267	GLN
1	F	372	ASN
1	F	374	GLN
1	F	431	ASN
1	F	488	GLN
1	F	490	ASN
1	F	500	ASN
1	F	508	ASN
1	F	551	ASN
2	G	22	GLN
2	G	36	ASN
2	G	37	ASN

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Mol	Chain	Res	Type
2	G	70	ASN
2	G	91	GLN
2	G	129	GLN
2	G	139	ASN
2	G	160	ASN
2	G	168	ASN
2	G	226	ASN
2	G	238	ASN
2	G	311	GLN
2	G	365	GLN
2	G	369	ASN
2	G	396	ASN
2	H	36	ASN
2	H	60	ASN
2	H	77	ASN
2	H	93	GLN
2	H	147	ASN
2	H	167	ASN
2	H	237	ASN
2	H	238	ASN
2	H	258	GLN
2	H	321	HIS
2	H	360	ASN
2	H	361	ASN
2	H	366	ASN
2	H	396	ASN
2	H	415	GLN
2	I	22	GLN
2	I	24	GLN
2	I	30	ASN
2	I	70	ASN
2	I	105	HIS
2	I	139	ASN
2	I	150	ASN
2	I	159	GLN
2	I	238	ASN
2	I	287	HIS
2	I	301	GLN
2	I	311	GLN
2	I	326	GLN
2	I	338	ASN
2	I	360	ASN

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Mol	Chain	Res	Type
2	I	369	ASN
2	I	394	ASN
2	I	415	GLN
2	I	425	GLN
2	J	32	HIS
2	J	91	GLN
2	J	237	ASN
2	J	238	ASN
2	J	248	ASN
2	J	275	GLN
2	J	311	GLN
2	J	373	ASN
2	J	394	ASN
2	J	415	GLN
2	J	425	GLN
2	K	19	ASN
2	K	105	HIS
2	K	159	GLN
2	K	226	ASN
2	K	248	ASN
2	K	257	ASN
2	K	302	GLN
2	K	358	HIS
2	K	369	ASN
2	K	370	GLN
2	K	394	ASN
2	K	396	ASN
2	K	412	HIS
2	L	7	ASN
2	L	70	ASN
2	L	91	GLN
2	L	110	GLN
2	L	115	ASN
2	L	118	ASN
2	L	139	ASN
2	L	160	ASN
2	L	168	ASN
2	L	216	GLN
2	L	237	ASN
2	L	275	GLN
2	L	360	ASN
2	L	366	ASN

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Mol	Chain	Res	Type
2	L	391	ASN
2	L	412	HIS
2	L	424	ASN
2	L	425	GLN
2	M	22	GLN
2	M	37	ASN
2	M	139	ASN
2	M	147	ASN
2	M	150	ASN
2	M	159	GLN
2	M	226	ASN
2	M	247	GLN
2	M	268	ASN
2	M	287	HIS
2	M	306	ASN
2	M	358	HIS
2	M	365	GLN
2	M	373	ASN
2	M	384	ASN
2	M	394	ASN
2	M	425	GLN
2	N	5	HIS
2	N	32	HIS
2	N	65	ASN
2	N	105	HIS
2	N	147	ASN
2	N	216	GLN
2	N	238	ASN
2	N	275	GLN
2	N	341	GLN
2	N	361	ASN
2	N	366	ASN
2	N	391	ASN
2	N	420	ASN
2	O	97	GLN
2	O	115	ASN
2	O	226	ASN
2	O	231	ASN
2	O	239	ASN
2	O	287	HIS
2	O	301	GLN
2	O	341	GLN

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Mol	Chain	Res	Type
2	O	358	HIS
2	O	409	GLN
2	O	415	GLN
2	O	420	ASN
2	P	30	ASN
2	P	32	HIS
2	P	37	ASN
2	P	93	GLN
2	P	160	ASN
2	P	168	ASN
2	P	216	GLN
2	P	231	ASN
2	P	258	GLN
2	P	275	GLN
2	P	287	HIS
2	P	341	GLN
2	P	360	ASN
2	P	361	ASN
2	P	366	ASN
2	P	412	HIS
2	P	424	ASN
2	P	425	GLN
2	Q	65	ASN
2	Q	93	GLN
2	Q	115	ASN
2	Q	139	ASN
2	Q	150	ASN
2	Q	159	GLN
2	Q	167	ASN
2	Q	365	GLN
2	Q	373	ASN
2	Q	396	ASN
2	Q	415	GLN
2	Q	420	ASN
2	R	7	ASN
2	R	24	GLN
2	R	32	HIS
2	R	70	ASN
2	R	160	ASN
2	R	226	ASN
2	R	231	ASN
2	R	238	ASN

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Mol	Chain	Res	Type
2	R	282	ASN
2	R	287	HIS
2	R	361	ASN
2	R	366	ASN
2	R	391	ASN
2	R	394	ASN
2	R	403	ASN
2	R	420	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	APR	H	501	-	39,39,39	1.35	7 (17%)	56,60,60	1.78	12 (21%)
3	APR	L	501	-	39,39,39	5.02	14 (35%)	56,60,60	2.45	13 (23%)
3	APR	P	501	-	39,39,39	5.00	14 (35%)	56,60,60	2.56	14 (25%)
3	APR	J	501	-	39,39,39	1.29	5 (12%)	56,60,60	1.74	10 (17%)
3	APR	R	501	-	39,39,39	4.99	14 (35%)	56,60,60	2.47	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	APR	N	501	-	39,39,39	4.99	14 (35%)	56,60,60	2.45	11 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	APR	H	501	-	-	12/22/54/54	0/4/4/4
3	APR	L	501	-	-	10/22/54/54	0/4/4/4
3	APR	P	501	-	-	7/22/54/54	0/4/4/4
3	APR	J	501	-	-	10/22/54/54	0/4/4/4
3	APR	R	501	-	-	9/22/54/54	0/4/4/4
3	APR	N	501	-	-	10/22/54/54	0/4/4/4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	501	APR	O4D-C1D	16.03	1.62	1.43
3	P	501	APR	O4D-C1D	15.71	1.62	1.43
3	R	501	APR	O4D-C1D	15.66	1.62	1.43
3	N	501	APR	O4D-C1D	15.52	1.62	1.43
3	L	501	APR	C1D-C2D	-15.06	1.35	1.52
3	N	501	APR	C1D-C2D	-14.96	1.35	1.52
3	R	501	APR	C1D-C2D	-14.71	1.35	1.52
3	P	501	APR	C1D-C2D	-14.71	1.35	1.52
3	P	501	APR	PA-O3A	10.58	1.70	1.59
3	R	501	APR	PA-O3A	10.47	1.70	1.59
3	P	501	APR	O4'-C1'	10.44	1.66	1.42
3	N	501	APR	O4'-C1'	10.43	1.66	1.42
3	R	501	APR	O4'-C1'	10.35	1.65	1.42
3	L	501	APR	O4'-C1'	10.30	1.65	1.42
3	N	501	APR	PA-O3A	10.28	1.70	1.59
3	L	501	APR	PA-O3A	10.25	1.70	1.59
3	P	501	APR	PB-O3A	8.00	1.68	1.59
3	R	501	APR	PB-O3A	7.88	1.68	1.59
3	N	501	APR	PB-O3A	7.71	1.67	1.59
3	L	501	APR	PB-O3A	7.61	1.67	1.59
3	R	501	APR	C2'-C1'	-6.66	1.32	1.53
3	N	501	APR	C2'-C1'	-6.51	1.33	1.53
3	L	501	APR	C2'-C1'	-6.43	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	501	APR	C2'-C1'	-6.41	1.33	1.53
3	R	501	APR	O4D-C4D	-6.39	1.30	1.45
3	N	501	APR	O4D-C4D	-6.39	1.30	1.45
3	P	501	APR	O4D-C4D	-6.30	1.31	1.45
3	L	501	APR	O4D-C4D	-6.20	1.31	1.45
3	L	501	APR	O4'-C4'	-5.86	1.32	1.45
3	N	501	APR	O4'-C4'	-5.76	1.32	1.45
3	P	501	APR	O4'-C4'	-5.74	1.32	1.45
3	R	501	APR	O4'-C4'	-5.68	1.32	1.45
3	N	501	APR	O3D-C3D	-4.45	1.31	1.43
3	P	501	APR	C6-N6	4.45	1.45	1.34
3	N	501	APR	C6-N6	4.45	1.45	1.34
3	R	501	APR	C6-N6	4.43	1.45	1.34
3	L	501	APR	C6-N6	4.41	1.45	1.34
3	L	501	APR	O3D-C3D	-4.29	1.32	1.43
3	P	501	APR	O3D-C3D	-4.23	1.32	1.43
3	H	501	APR	C5-C4	4.21	1.46	1.39
3	R	501	APR	O3D-C3D	-4.21	1.32	1.43
3	J	501	APR	C5-C4	3.80	1.45	1.39
3	P	501	APR	O3'-C3'	-3.72	1.33	1.43
3	N	501	APR	O3'-C3'	-3.69	1.33	1.43
3	L	501	APR	O3'-C3'	-3.67	1.33	1.43
3	R	501	APR	O3'-C3'	-3.66	1.33	1.43
3	R	501	APR	C5-C4	-3.02	1.33	1.39
3	N	501	APR	C5-C4	-3.01	1.33	1.39
3	J	501	APR	C5-C6	3.00	1.49	1.41
3	L	501	APR	C5-C4	-2.98	1.33	1.39
3	R	501	APR	O2D-C2D	2.95	1.50	1.43
3	N	501	APR	O2D-C2D	2.94	1.50	1.43
3	P	501	APR	O2D-C2D	2.94	1.50	1.43
3	L	501	APR	O2D-C2D	2.92	1.50	1.43
3	H	501	APR	C3D-C4D	-2.90	1.45	1.53
3	P	501	APR	C5-C4	-2.90	1.33	1.39
3	H	501	APR	C5-C6	2.60	1.48	1.41
3	J	501	APR	C4-N9	-2.51	1.32	1.37
3	H	501	APR	C1D-C2D	-2.49	1.49	1.52
3	P	501	APR	C3D-C4D	2.43	1.59	1.53
3	R	501	APR	C3D-C4D	2.43	1.59	1.53
3	H	501	APR	C4-N9	-2.38	1.32	1.37
3	H	501	APR	C5-N7	-2.38	1.34	1.39
3	J	501	APR	C8-N7	2.28	1.36	1.31
3	L	501	APR	C3D-C4D	2.27	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	501	APR	C3D-C4D	2.25	1.58	1.53
3	H	501	APR	C8-N7	2.17	1.35	1.31
3	J	501	APR	C1D-C2D	-2.13	1.50	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	501	APR	N6-C6-N1	-10.48	95.03	118.38
3	N	501	APR	N6-C6-N1	-10.47	95.07	118.38
3	L	501	APR	N6-C6-N1	-10.45	95.11	118.38
3	R	501	APR	N6-C6-N1	-10.42	95.17	118.38
3	L	501	APR	C5-C6-N6	8.73	144.90	123.29
3	R	501	APR	C5-C6-N6	8.72	144.88	123.29
3	N	501	APR	C5-C6-N6	8.71	144.86	123.29
3	P	501	APR	C5-C6-N6	8.68	144.77	123.29
3	J	501	APR	C5-C4-N3	-5.75	118.80	126.72
3	N	501	APR	N3-C2-N1	-5.72	119.92	128.58
3	P	501	APR	N3-C2-N1	-5.72	119.93	128.58
3	L	501	APR	N3-C2-N1	-5.69	119.97	128.58
3	R	501	APR	N3-C2-N1	-5.68	119.98	128.58
3	P	501	APR	C5-C4-N3	-5.55	119.07	126.72
3	H	501	APR	C5-C4-N3	-5.25	119.48	126.72
3	L	501	APR	C5-C4-N3	-4.95	119.90	126.72
3	N	501	APR	C5-C4-N3	-4.89	119.99	126.72
3	R	501	APR	C5-C4-N3	-4.72	120.22	126.72
3	J	501	APR	N3-C4-N9	4.57	134.93	127.17
3	H	501	APR	N3-C4-N9	4.26	134.41	127.17
3	R	501	APR	N9-C8-N7	-4.21	107.96	113.94
3	N	501	APR	N9-C8-N7	-4.17	108.02	113.94
3	L	501	APR	N9-C8-N7	-4.01	108.25	113.94
3	J	501	APR	C2-N3-C4	3.87	121.28	111.83
3	J	501	APR	C4-N9-C8	3.82	109.75	105.74
3	R	501	APR	C1D-C2D-C3D	3.81	106.98	102.29
3	P	501	APR	C1D-C2D-C3D	3.81	106.98	102.29
3	P	501	APR	N9-C8-N7	-3.70	108.68	113.94
3	H	501	APR	C2-N3-C4	3.62	120.68	111.83
3	P	501	APR	C2-N3-C4	3.62	120.67	111.83
3	J	501	APR	C4-C5-N7	-3.61	106.45	110.58
3	H	501	APR	N3-C2-N1	-3.58	123.16	128.58
3	P	501	APR	N3-C4-N9	3.54	133.19	127.17
3	H	501	APR	O3D-C3D-C4D	-3.47	101.11	111.08
3	N	501	APR	C2-N3-C4	3.42	120.18	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	APR	C2-N3-C4	3.38	120.10	111.83
3	J	501	APR	N3-C2-N1	-3.34	123.52	128.58
3	R	501	APR	C2-N3-C4	3.32	119.95	111.83
3	H	501	APR	C4-C5-N7	-3.26	106.86	110.58
3	H	501	APR	C4-N9-C8	3.20	109.10	105.74
3	H	501	APR	O4D-C4D-C3D	-3.15	98.89	105.15
3	R	501	APR	C5-N7-C8	2.91	108.02	103.45
3	L	501	APR	N3-C4-N9	2.90	132.10	127.17
3	N	501	APR	C5-N7-C8	2.88	107.97	103.45
3	J	501	APR	N9-C8-N7	-2.86	109.88	113.94
3	N	501	APR	N3-C4-N9	2.82	131.97	127.17
3	L	501	APR	C5-N7-C8	2.81	107.87	103.45
3	P	501	APR	C5-N7-C8	2.72	107.73	103.45
3	L	501	APR	C3'-C2'-C1'	2.72	106.61	101.46
3	R	501	APR	N3-C4-N9	2.69	131.74	127.17
3	J	501	APR	C5-N7-C8	2.66	107.63	103.45
3	P	501	APR	C3'-C2'-C1'	2.64	106.45	101.46
3	H	501	APR	C5-N7-C8	2.44	107.29	103.45
3	P	501	APR	C1'-N9-C8	-2.39	121.80	127.09
3	N	501	APR	C4-C5-N7	-2.37	107.88	110.58
3	P	501	APR	O4D-C1D-C2D	2.36	107.95	104.67
3	R	501	APR	C4-C5-N7	-2.32	107.92	110.58
3	H	501	APR	N9-C8-N7	-2.32	110.64	113.94
3	P	501	APR	C6-C5-C4	2.27	120.28	117.18
3	H	501	APR	C2-N1-C6	2.27	122.46	118.73
3	H	501	APR	C6-C5-N7	2.25	136.42	132.09
3	J	501	APR	C6-C5-N7	2.24	136.42	132.09
3	L	501	APR	C4-C5-N7	-2.24	108.02	110.58
3	N	501	APR	C4-N9-C8	2.24	108.09	105.74
3	R	501	APR	C4-N9-C8	2.21	108.06	105.74
3	R	501	APR	O4D-C1D-C2D	2.09	107.57	104.67
3	J	501	APR	O4D-C4D-C3D	-2.06	101.07	105.15
3	N	501	APR	C5-C4-N9	2.05	108.04	105.81
3	R	501	APR	C5-C4-N9	2.04	108.04	105.81
3	L	501	APR	C4-N9-C8	2.02	107.86	105.74
3	P	501	APR	C4-C5-N7	-2.02	108.28	110.58
3	L	501	APR	C5-C4-N9	2.01	108.00	105.81
3	L	501	APR	C6-C5-C4	2.00	119.92	117.18

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	501	APR	C5'-O5'-PA-O1A
3	H	501	APR	C5D-O5D-PB-O3A
3	J	501	APR	C5'-O5'-PA-O3A
3	J	501	APR	C5D-O5D-PB-O1B
3	L	501	APR	C2'-C1'-N9-C8
3	L	501	APR	C5'-O5'-PA-O3A
3	N	501	APR	C4D-C5D-O5D-PB
3	N	501	APR	O4D-C4D-C5D-O5D
3	N	501	APR	C3D-C4D-C5D-O5D
3	P	501	APR	C4'-C5'-O5'-PA
3	P	501	APR	C5'-O5'-PA-O2A
3	P	501	APR	C5'-O5'-PA-O3A
3	P	501	APR	O4D-C4D-C5D-O5D
3	J	501	APR	C3D-C4D-C5D-O5D
3	P	501	APR	C3D-C4D-C5D-O5D
3	H	501	APR	O4'-C4'-C5'-O5'
3	J	501	APR	O4D-C4D-C5D-O5D
3	L	501	APR	O4'-C4'-C5'-O5'
3	L	501	APR	O4D-C4D-C5D-O5D
3	L	501	APR	C2'-C1'-N9-C4
3	J	501	APR	C4D-C5D-O5D-PB
3	H	501	APR	C3'-C4'-C5'-O5'
3	R	501	APR	C3D-C4D-C5D-O5D
3	H	501	APR	O4D-C4D-C5D-O5D
3	R	501	APR	C2'-C1'-N9-C8
3	L	501	APR	C3D-C4D-C5D-O5D
3	N	501	APR	C3'-C4'-C5'-O5'
3	H	501	APR	C3D-C4D-C5D-O5D
3	L	501	APR	C3'-C4'-C5'-O5'
3	L	501	APR	PA-O3A-PB-O1B
3	R	501	APR	C3'-C4'-C5'-O5'
3	R	501	APR	O4'-C4'-C5'-O5'
3	R	501	APR	O4D-C4D-C5D-O5D
3	H	501	APR	PB-O3A-PA-O5'
3	L	501	APR	PA-O3A-PB-O5D
3	N	501	APR	PA-O3A-PB-O5D
3	N	501	APR	PB-O3A-PA-O2A
3	R	501	APR	C2'-C1'-N9-C4
3	H	501	APR	C5'-O5'-PA-O2A
3	H	501	APR	C5'-O5'-PA-O3A
3	H	501	APR	C5D-O5D-PB-O1B
3	J	501	APR	C5D-O5D-PB-O3A
3	J	501	APR	C5D-O5D-PB-O2B

Continued on next page...

Continued from previous page...

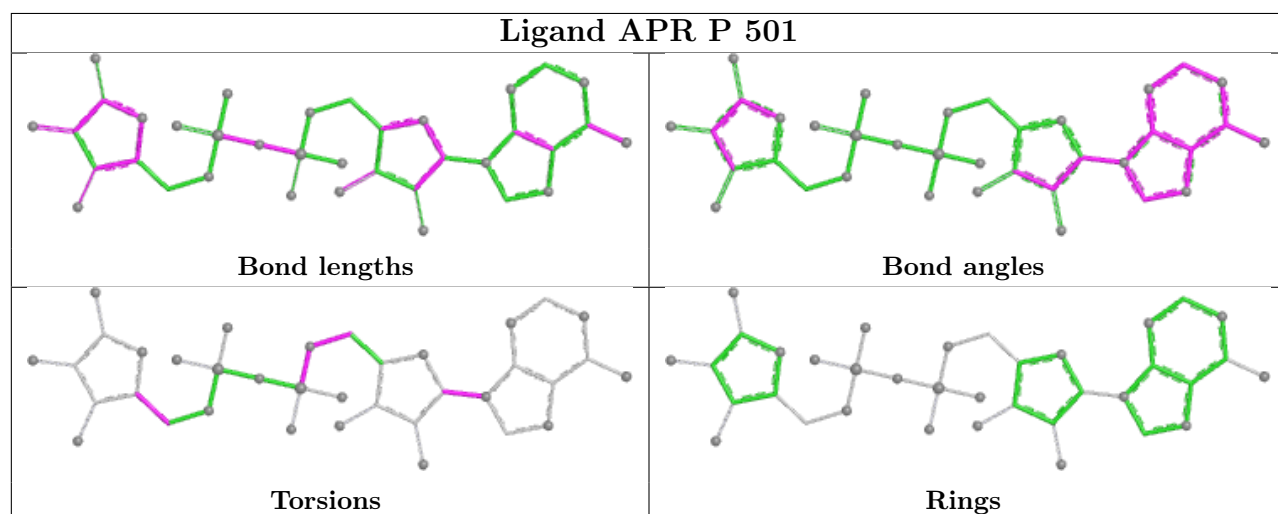
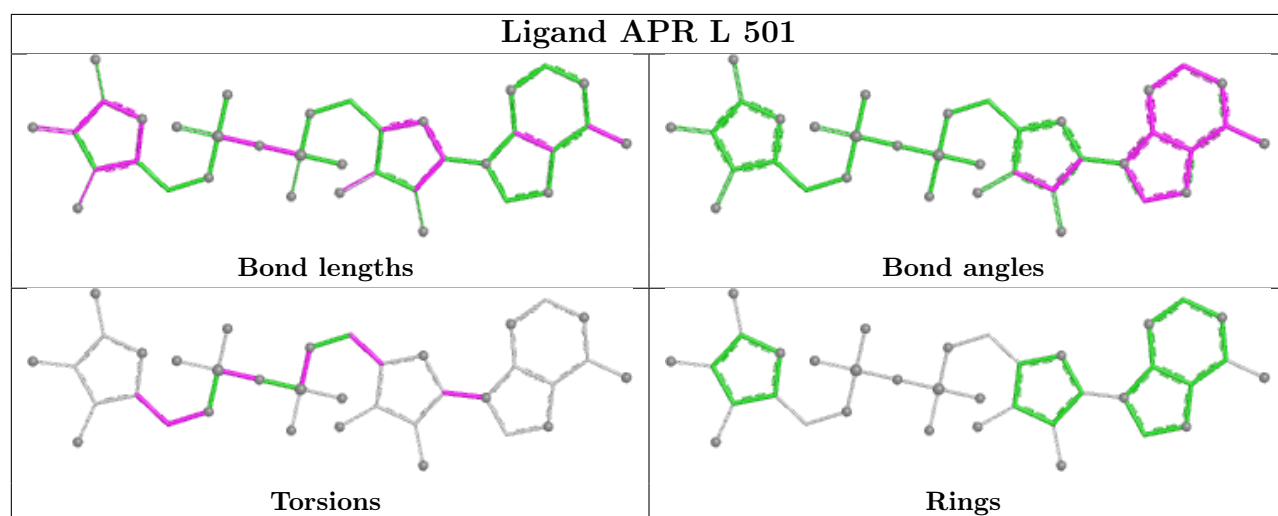
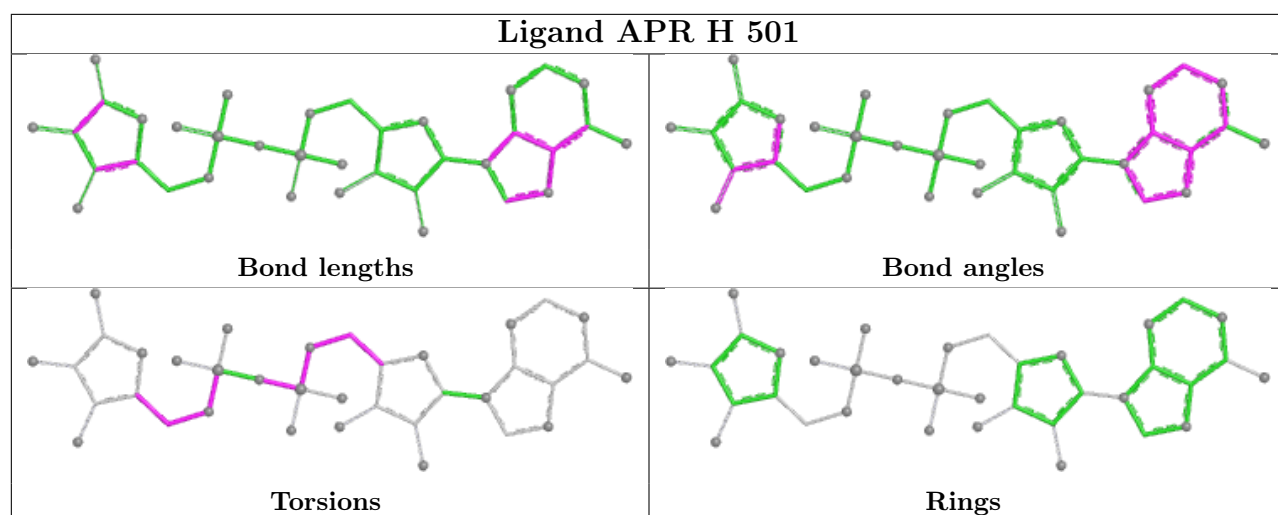
Mol	Chain	Res	Type	Atoms
3	N	501	APR	C5'-O5'-PA-O1A
3	H	501	APR	C4'-C5'-O5'-PA
3	L	501	APR	C4D-C5D-O5D-PB
3	J	501	APR	O4'-C4'-C5'-O5'
3	R	501	APR	PA-O3A-PB-O2B
3	J	501	APR	C3'-C4'-C5'-O5'
3	N	501	APR	C4'-C5'-O5'-PA
3	H	501	APR	C4D-C5D-O5D-PB
3	N	501	APR	O4'-C4'-C5'-O5'
3	R	501	APR	PA-O3A-PB-O1B
3	J	501	APR	C2'-C1'-N9-C8
3	P	501	APR	O4'-C1'-N9-C8
3	R	501	APR	O4'-C1'-N9-C8
3	P	501	APR	C2'-C1'-N9-C8
3	N	501	APR	PB-O3A-PA-O1A

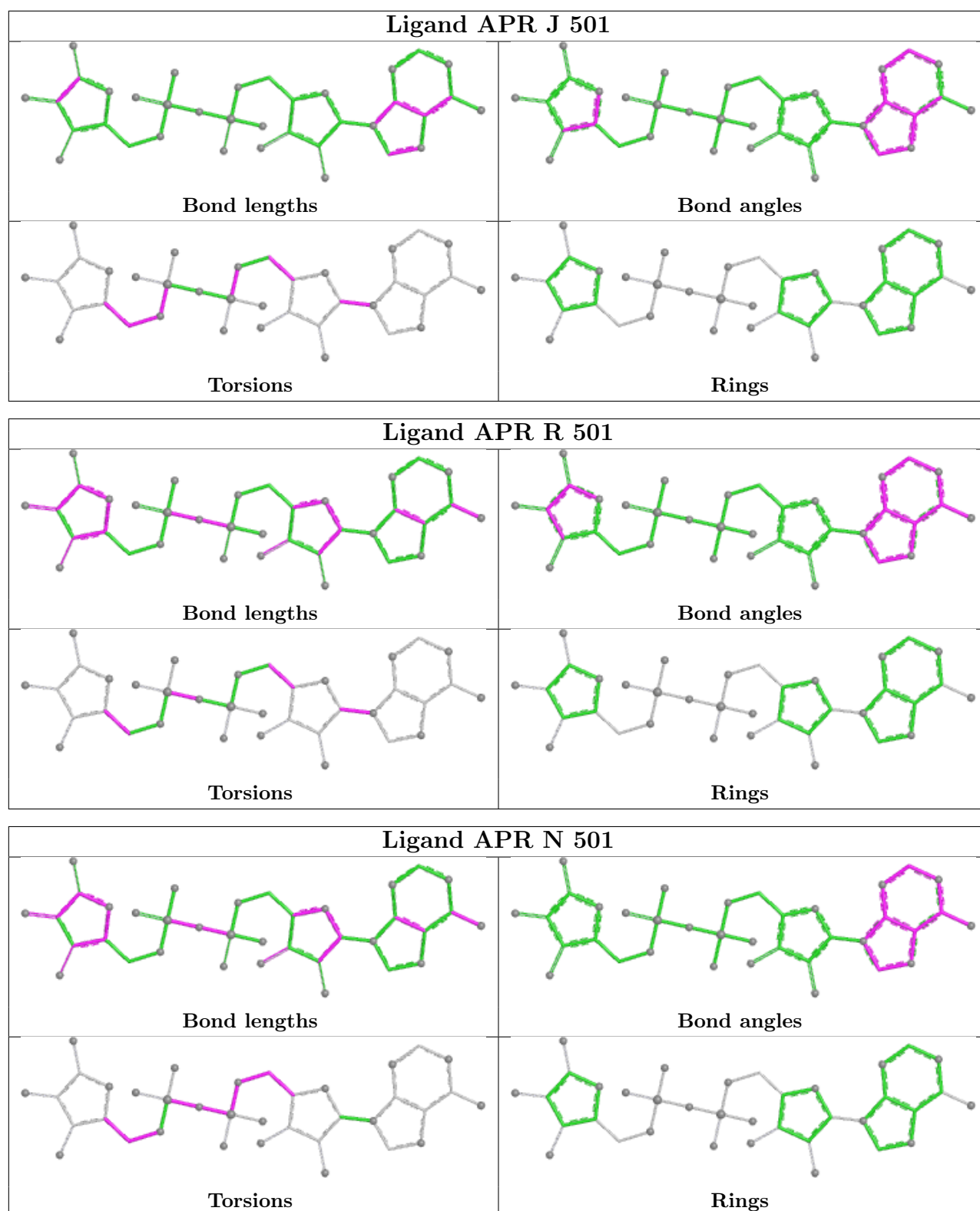
There are no ring outliers.

6 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	501	APR	17	0
3	L	501	APR	45	0
3	P	501	APR	32	0
3	J	501	APR	23	0
3	R	501	APR	39	0
3	N	501	APR	25	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

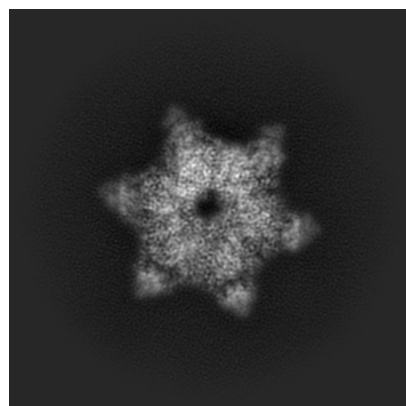
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39302. These allow visual inspection of the internal detail of the map and identification of artifacts.

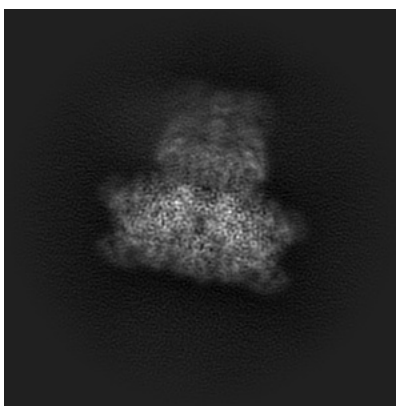
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

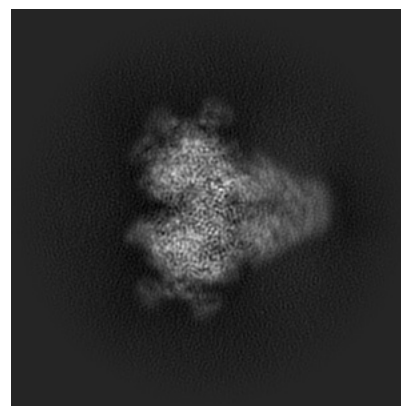
6.1.1 Primary map



X

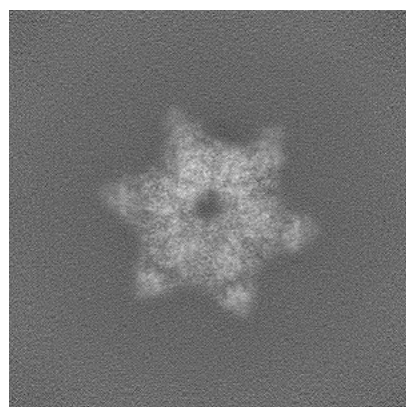


Y

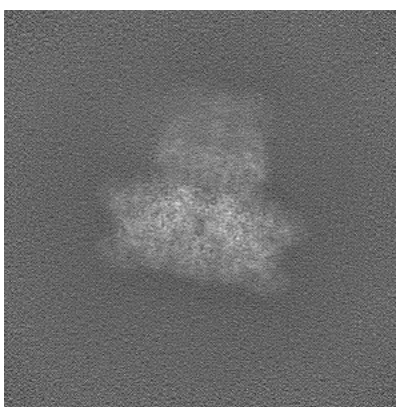


Z

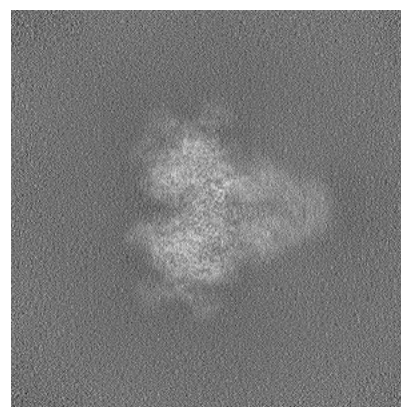
6.1.2 Raw map



X



Y

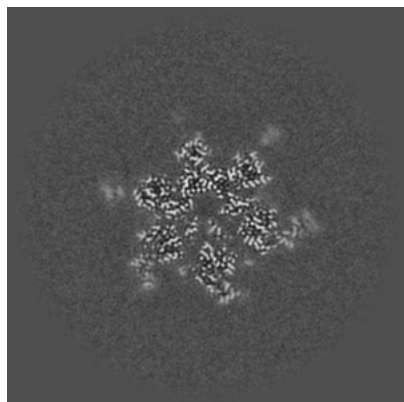


Z

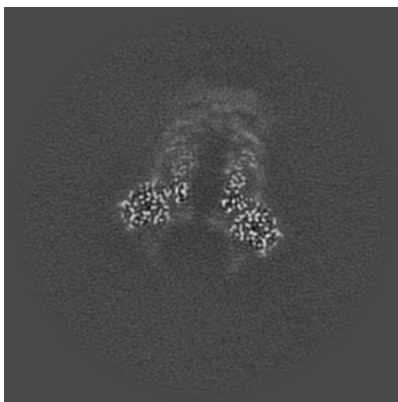
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

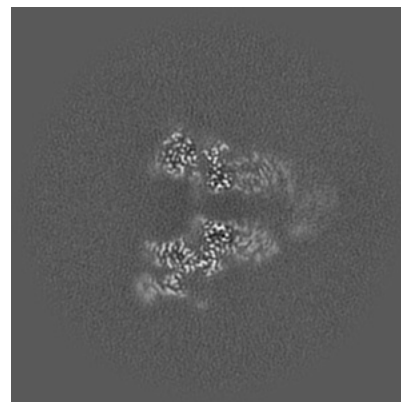
6.2.1 Primary map



X Index: 256

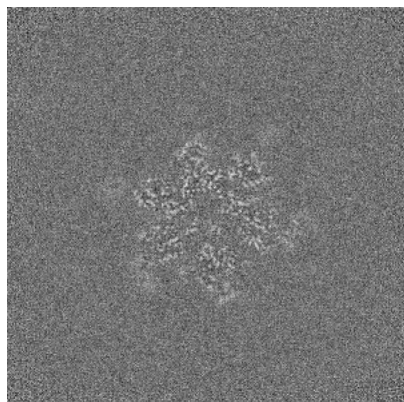


Y Index: 256

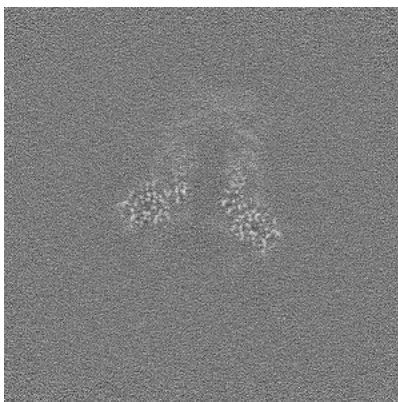


Z Index: 256

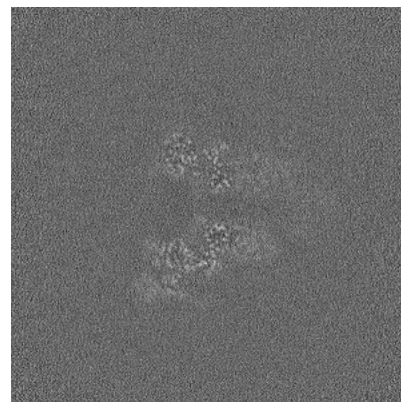
6.2.2 Raw map



X Index: 256



Y Index: 256

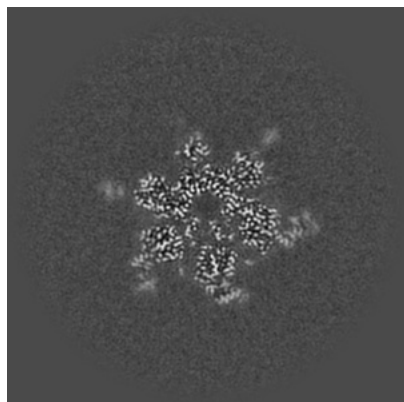


Z Index: 256

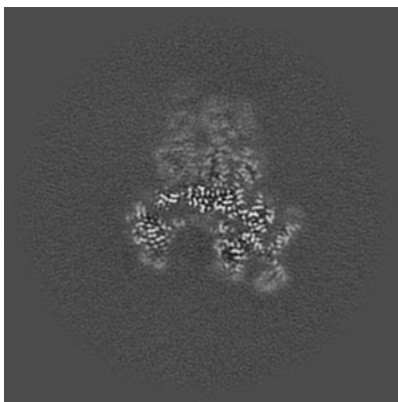
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

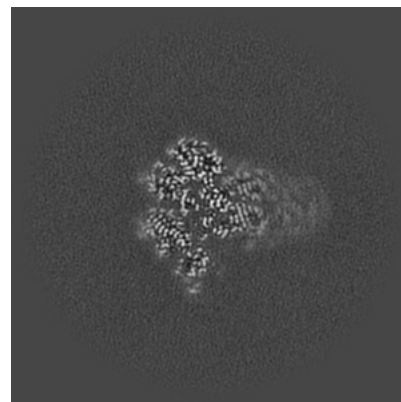
6.3.1 Primary map



X Index: 258

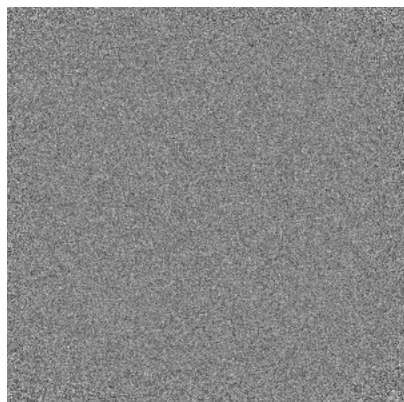


Y Index: 225

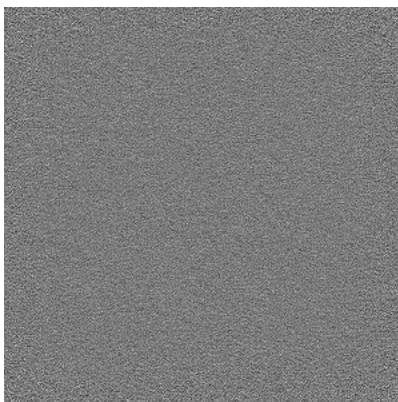


Z Index: 299

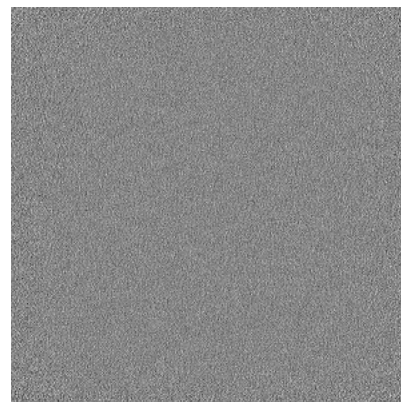
6.3.2 Raw map



X Index: 0



Y Index: 0

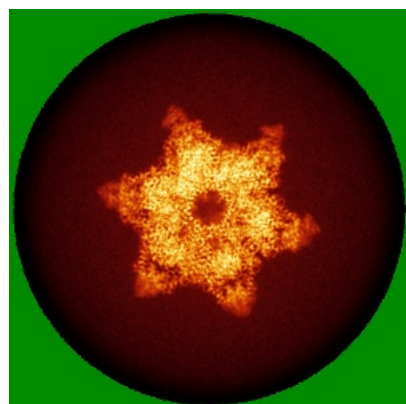


Z Index: 511

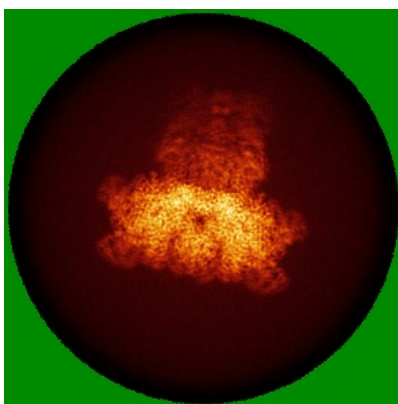
The images above show the largest variance slices of the map in three orthogonal directions.

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

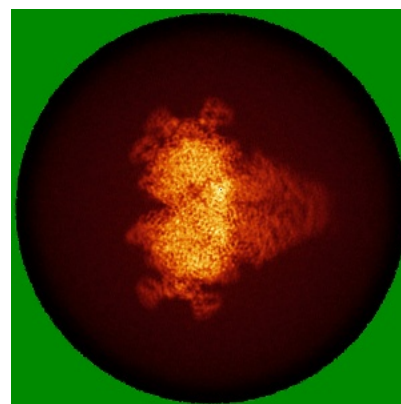
6.4.1 Primary map



X

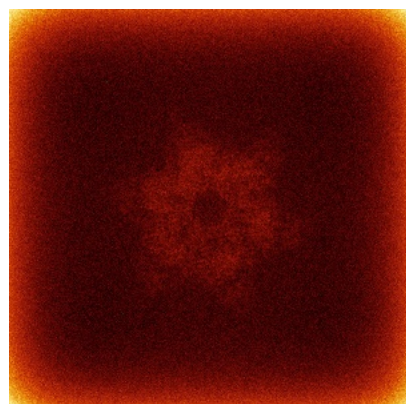


Y

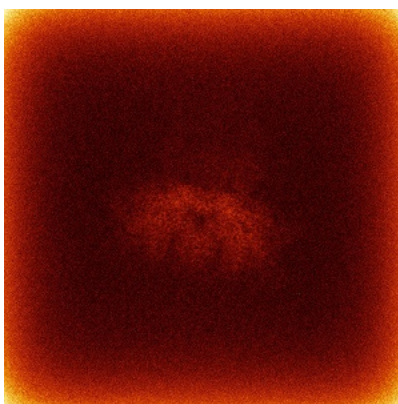


Z

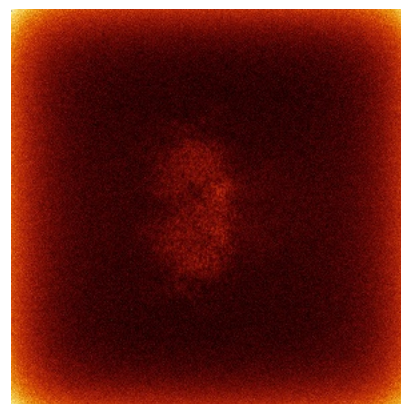
6.4.2 Raw map



X



Y

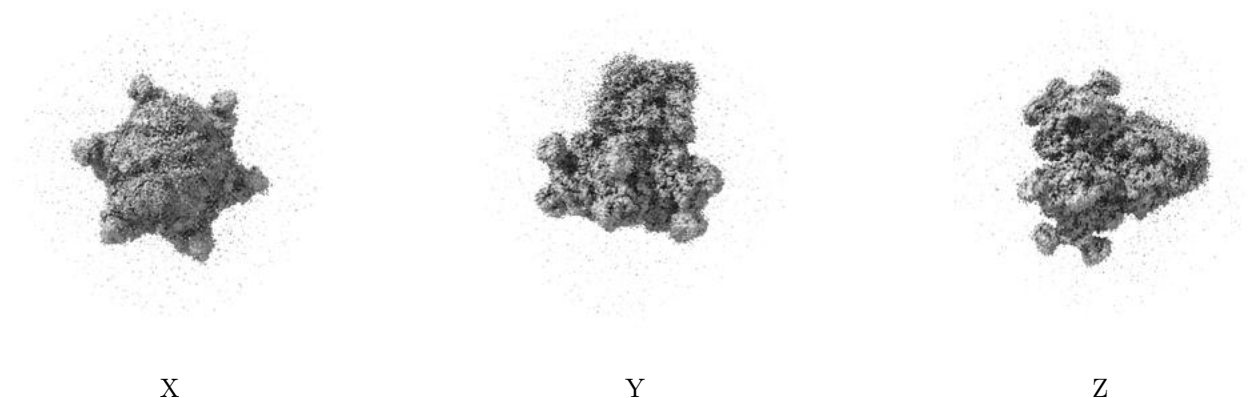


Z

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

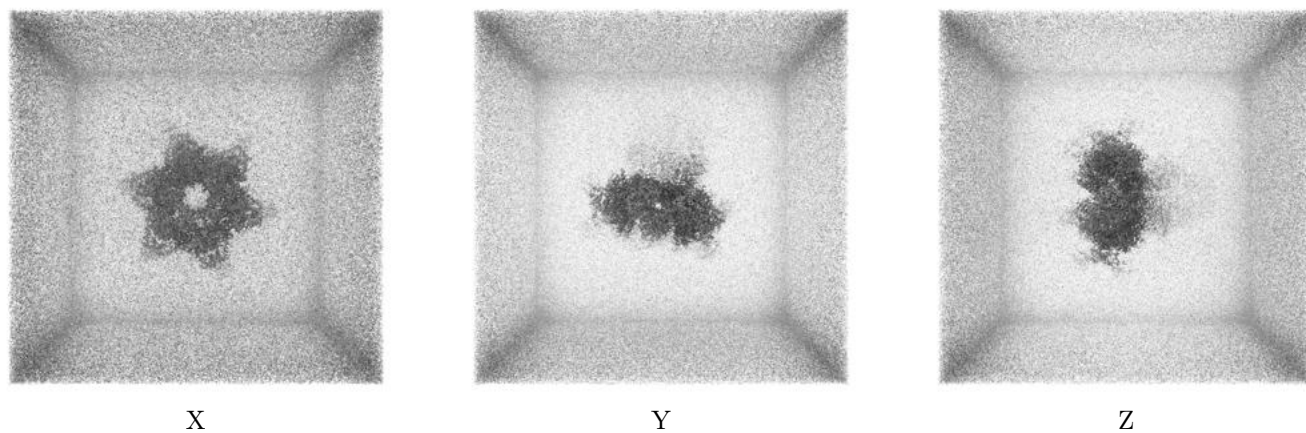
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

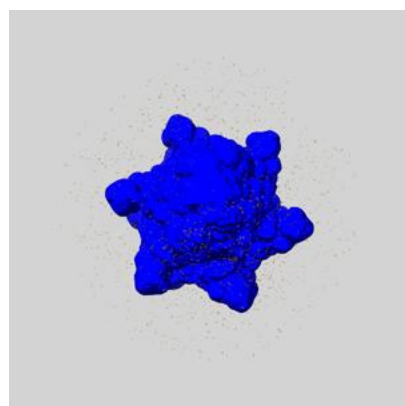
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

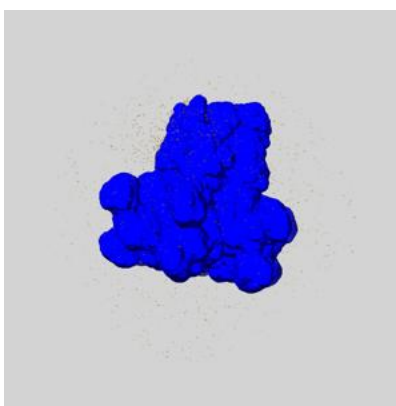
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

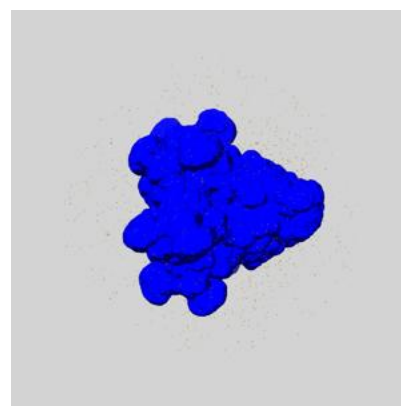
6.6.1 emd_39302_msk_1.map [i](#)



X



Y

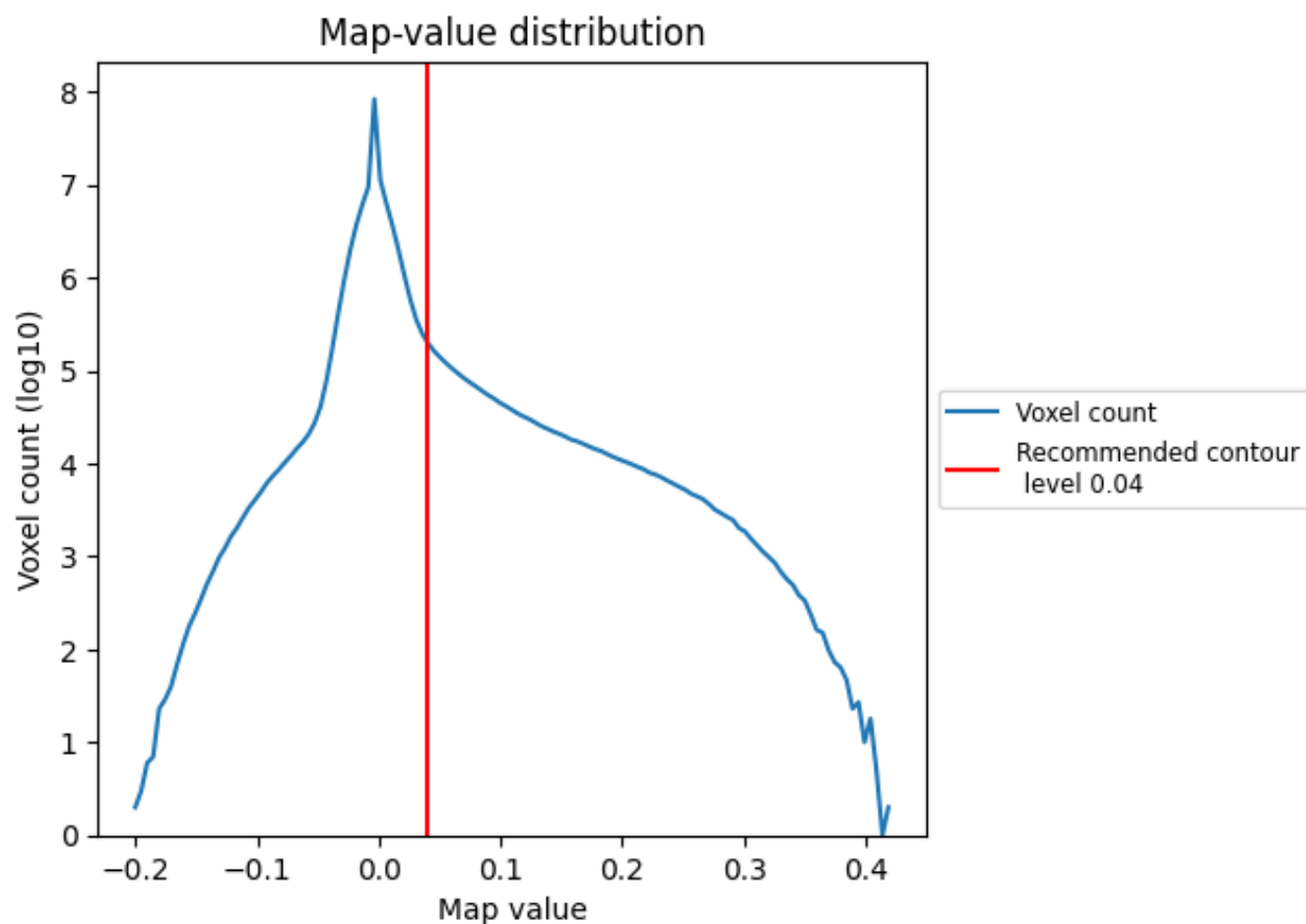


Z

7 Map analysis [i](#)

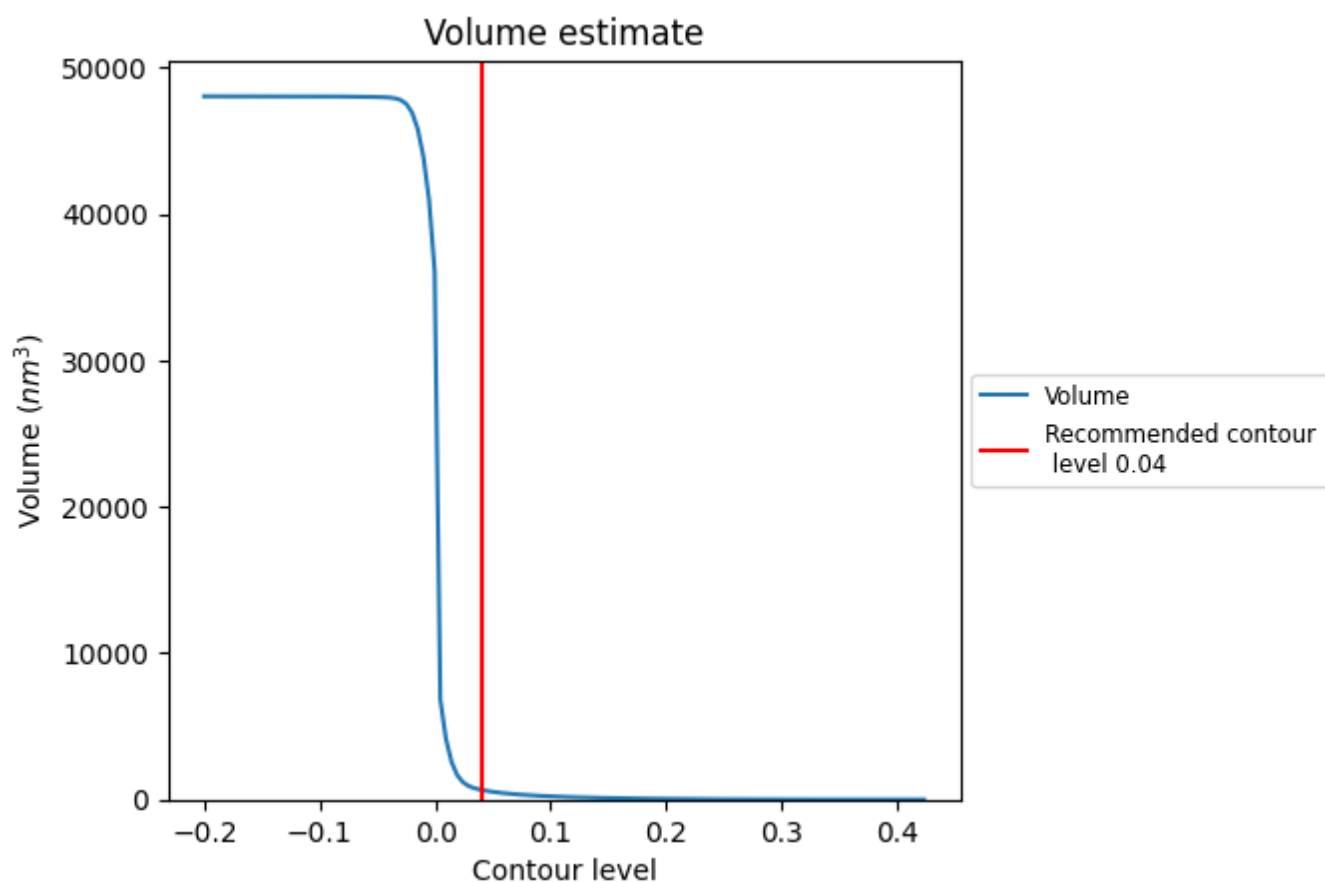
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

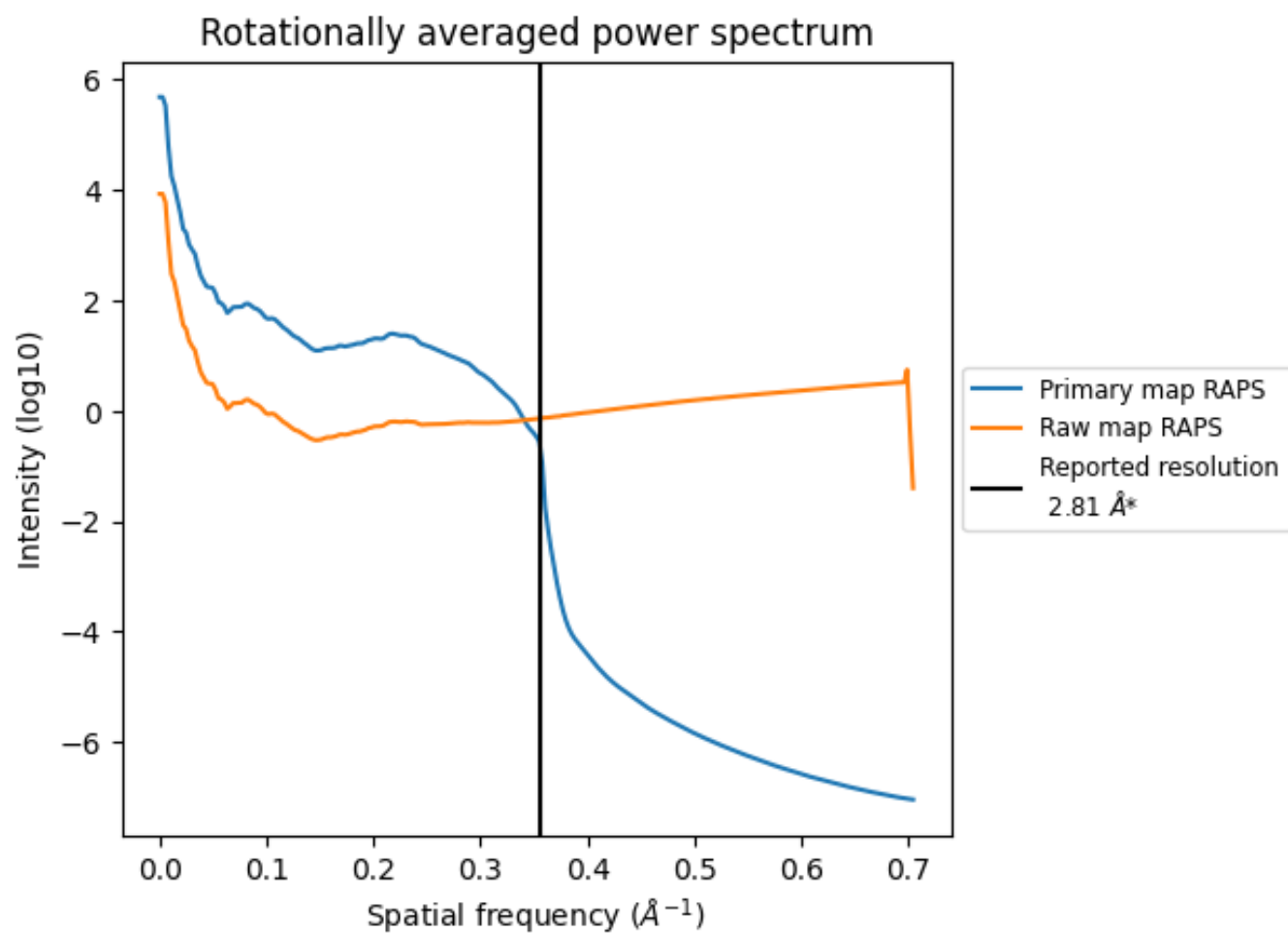
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 661 nm³; this corresponds to an approximate mass of 598 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

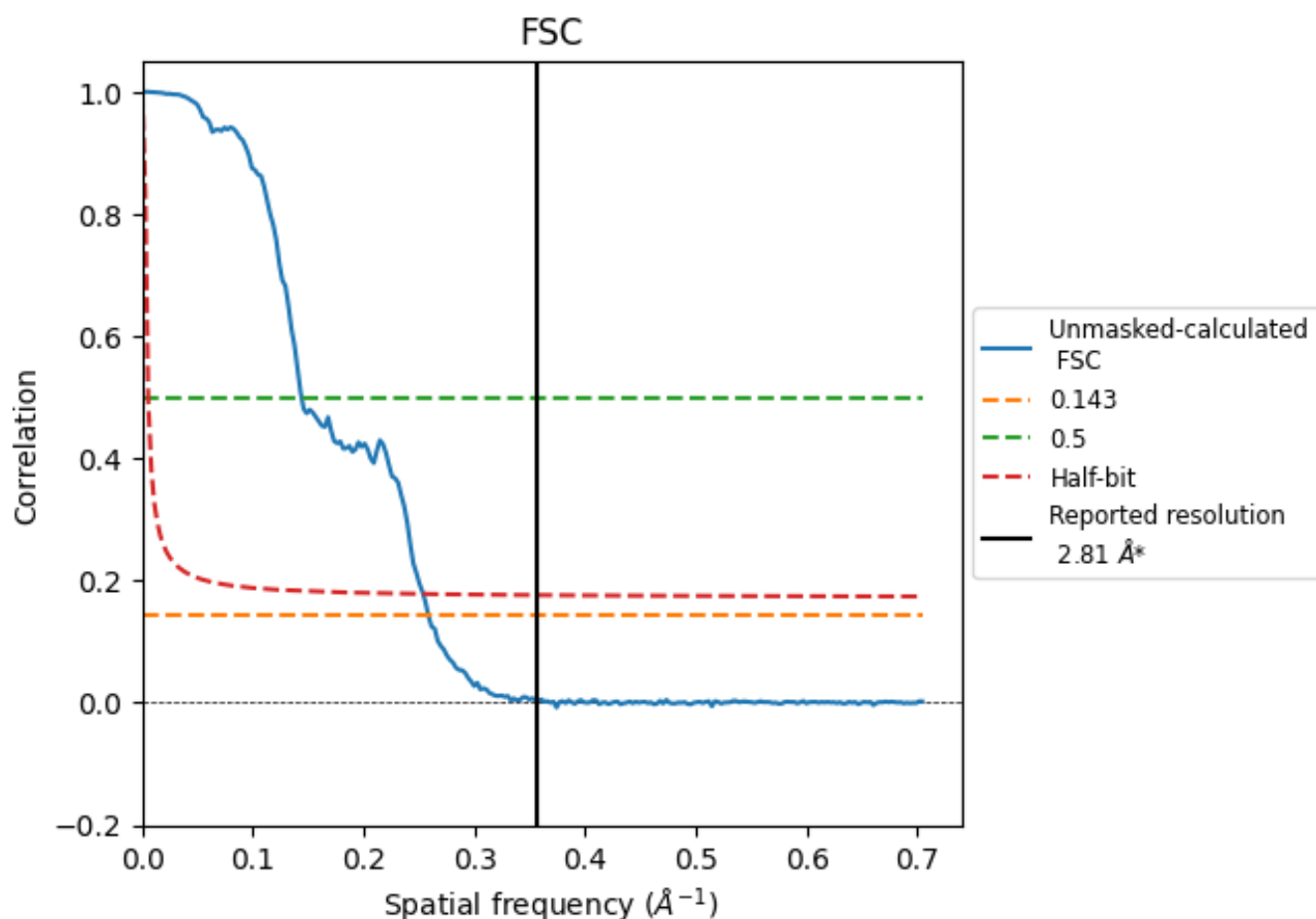


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.356 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	6.95	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.81 by more than 10 %

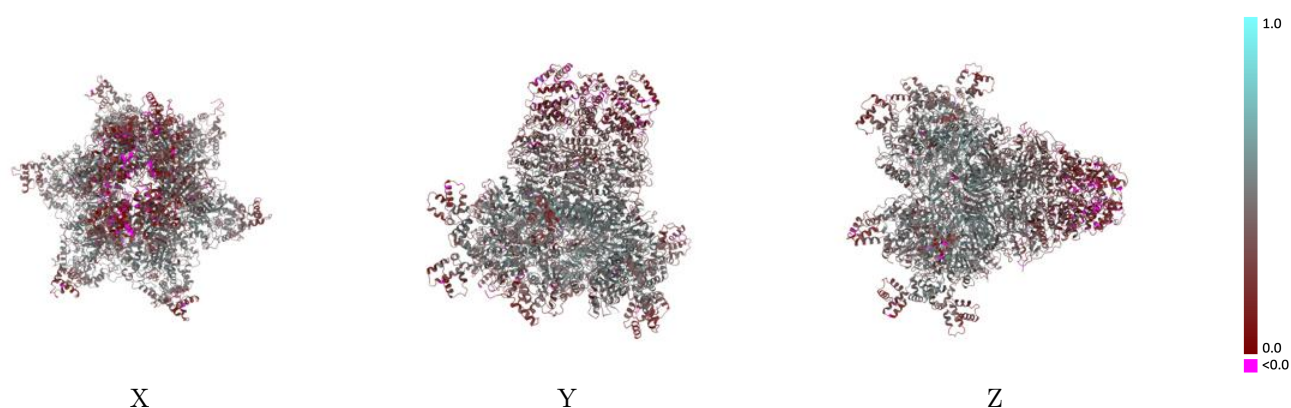
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39302 and PDB model 8YHX. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

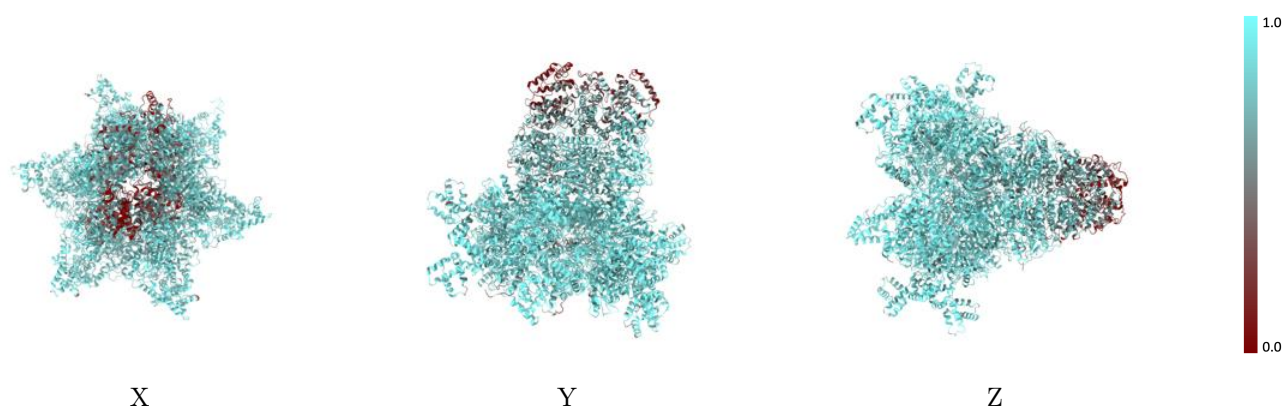
This section was not generated.

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



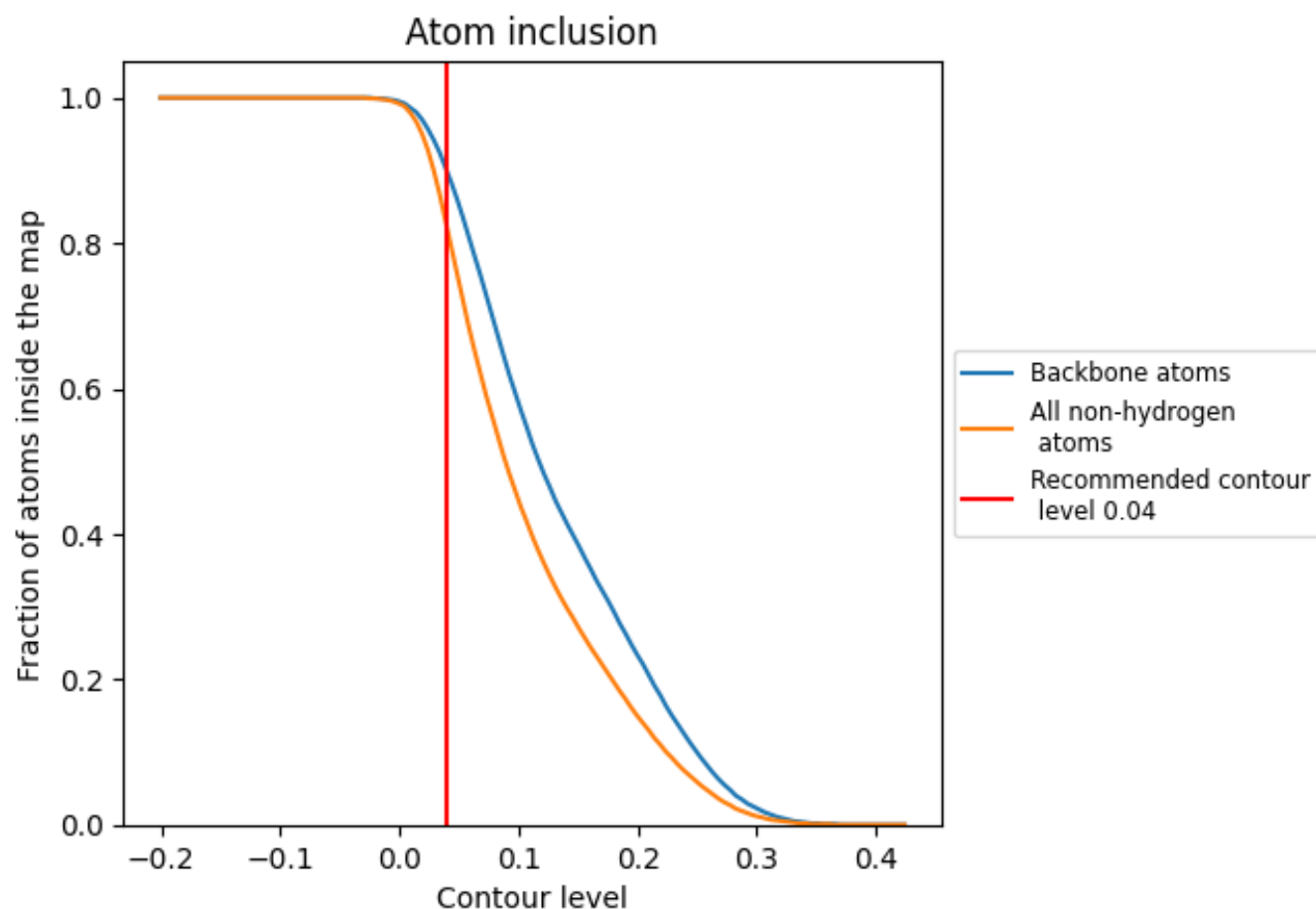
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.3920
A	 0.6800	 0.3580
B	 0.7240	 0.3460
C	 0.7450	 0.3460
D	 0.5810	 0.3040
E	 0.7920	 0.3550
F	 0.8040	 0.3770
G	 0.8960	 0.4250
H	 0.8880	 0.4320
I	 0.8690	 0.4020
J	 0.8930	 0.4270
K	 0.8680	 0.3960
L	 0.8940	 0.4330
M	 0.8670	 0.4020
N	 0.8850	 0.4250
O	 0.8820	 0.4110
P	 0.8970	 0.4290
Q	 0.8890	 0.4200
R	 0.9140	 0.4540

