



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 06:01 am GMT

PDB ID : 6RW9
EMDB ID : EMD-10035
Title : Cryo-EM structure of Morganella morganii TcdA4
Authors : Roderer, D.; Leidreiter, F.; Gatsogiannis, C.; Meusch, D.; Benz, R.; Raunser, S.
Deposited on : 2019-06-04
Resolution : 3.27 Å(reported)
Based on initial model : 1VW1

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

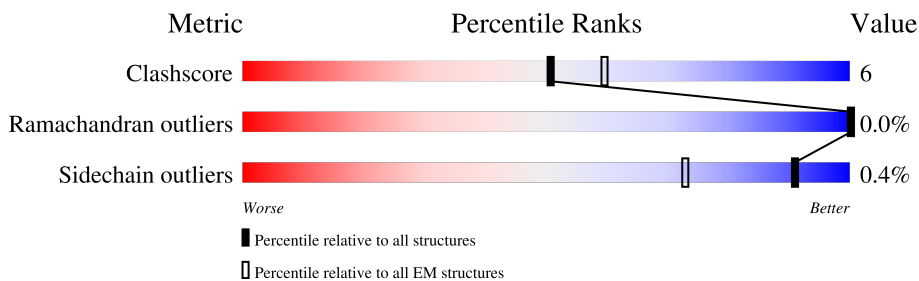
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	2469	
1	B	2469	
1	C	2469	
1	D	2469	
1	E	2469	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 88700 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.

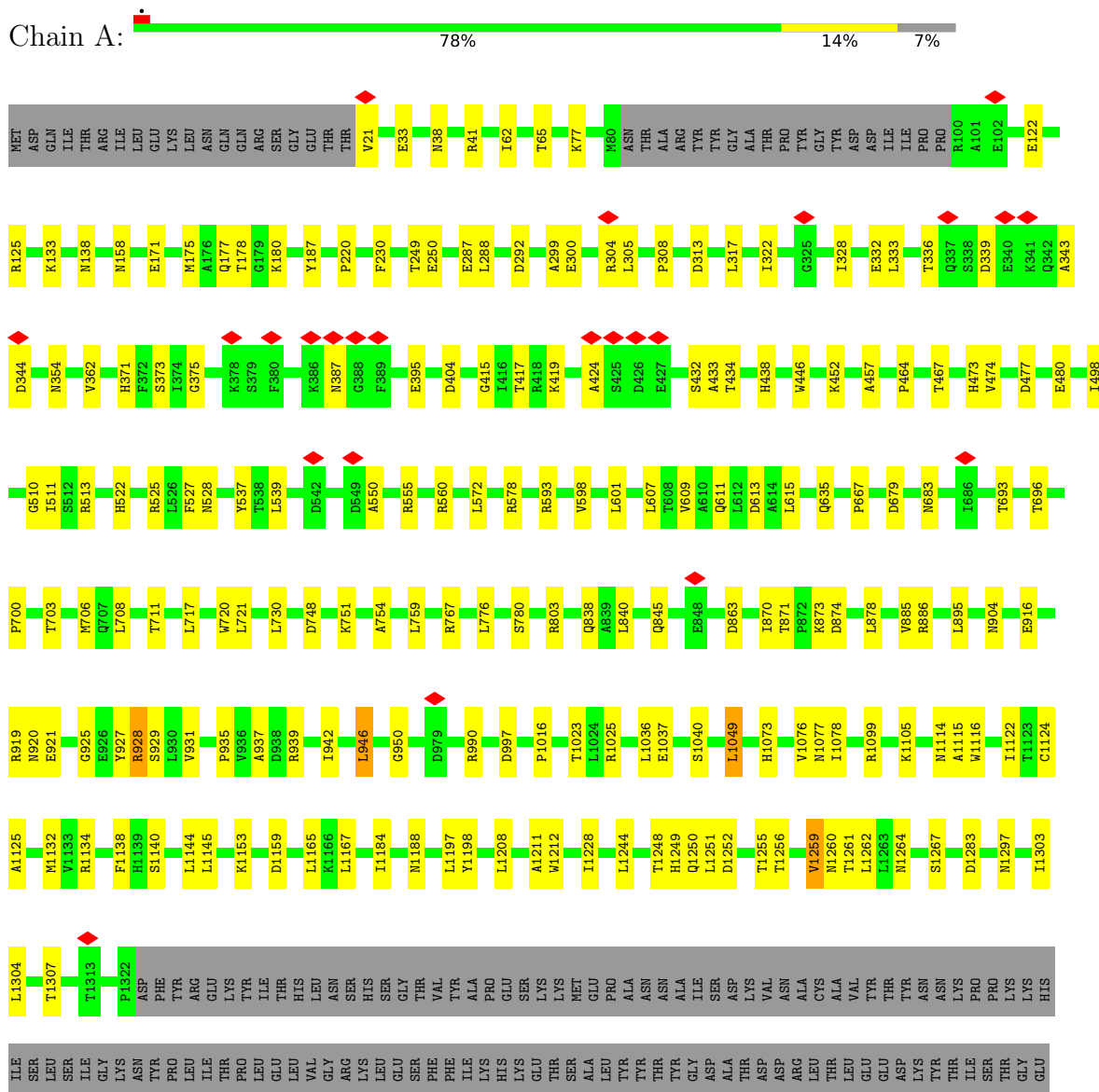
- Molecule 1 is a protein called Insecticidal toxin protein TcdA4.

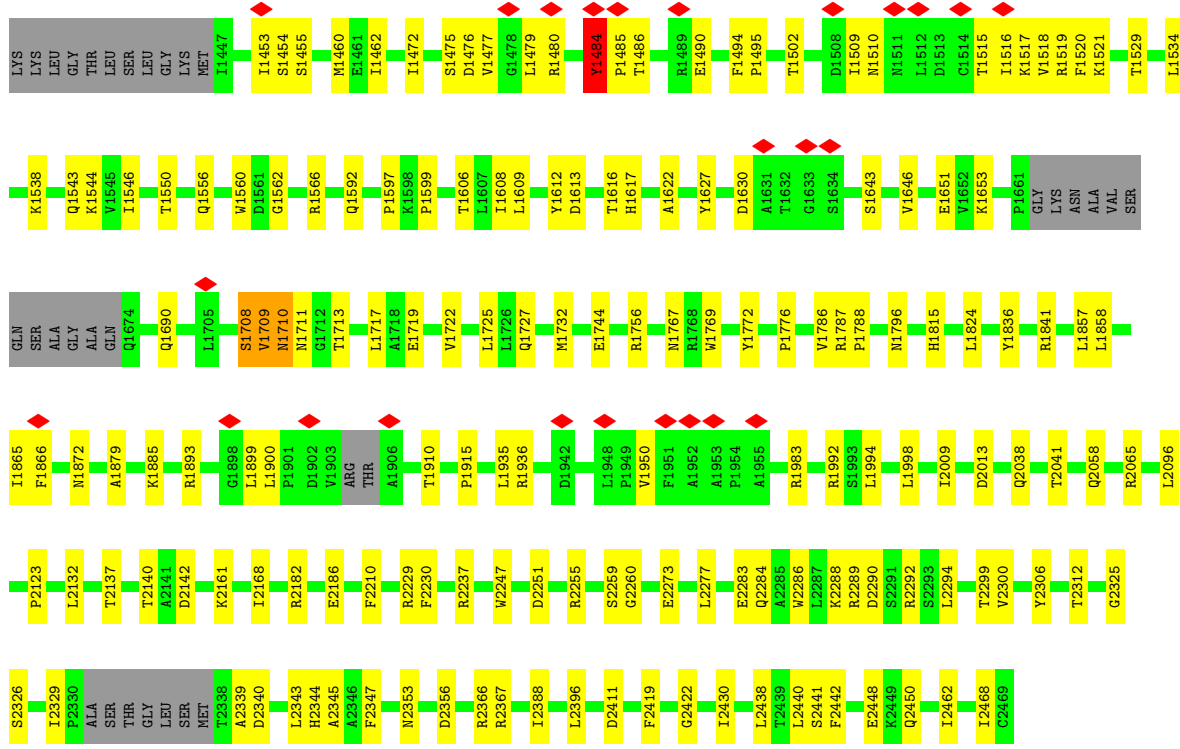
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	B	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	C	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	D	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	E	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0

3 Residue-property plots [i](#)

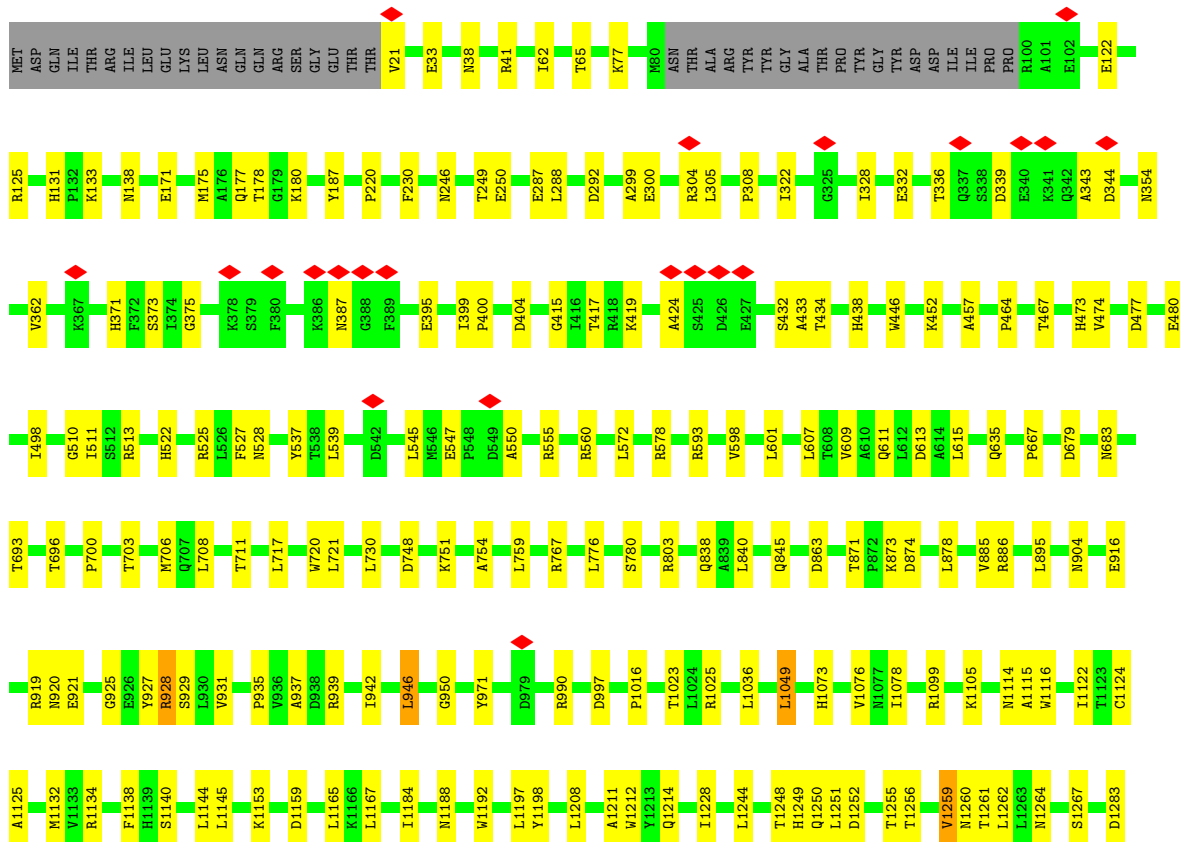
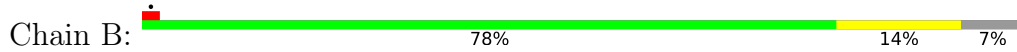
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

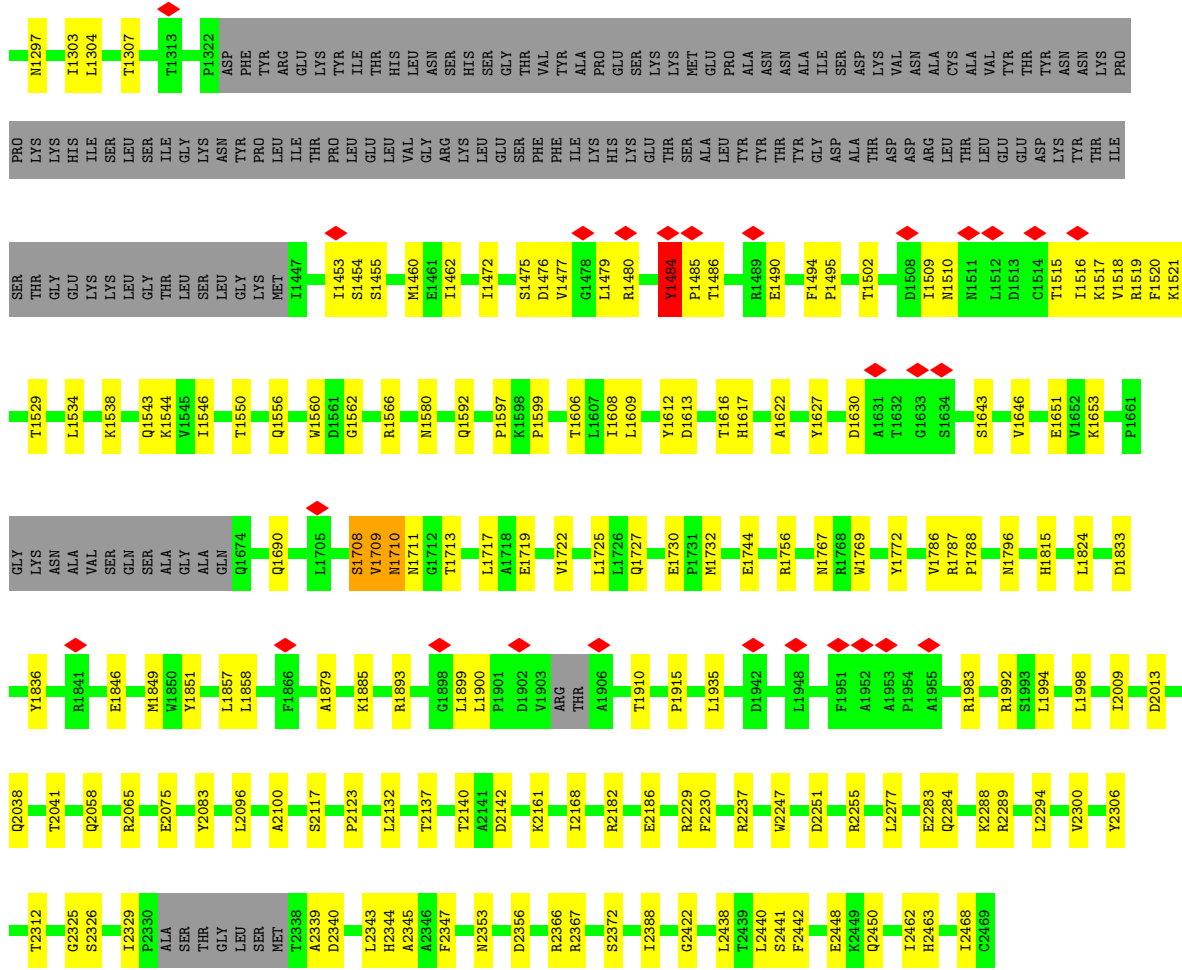
- Molecule 1: Insecticidal toxin protein TcdA4



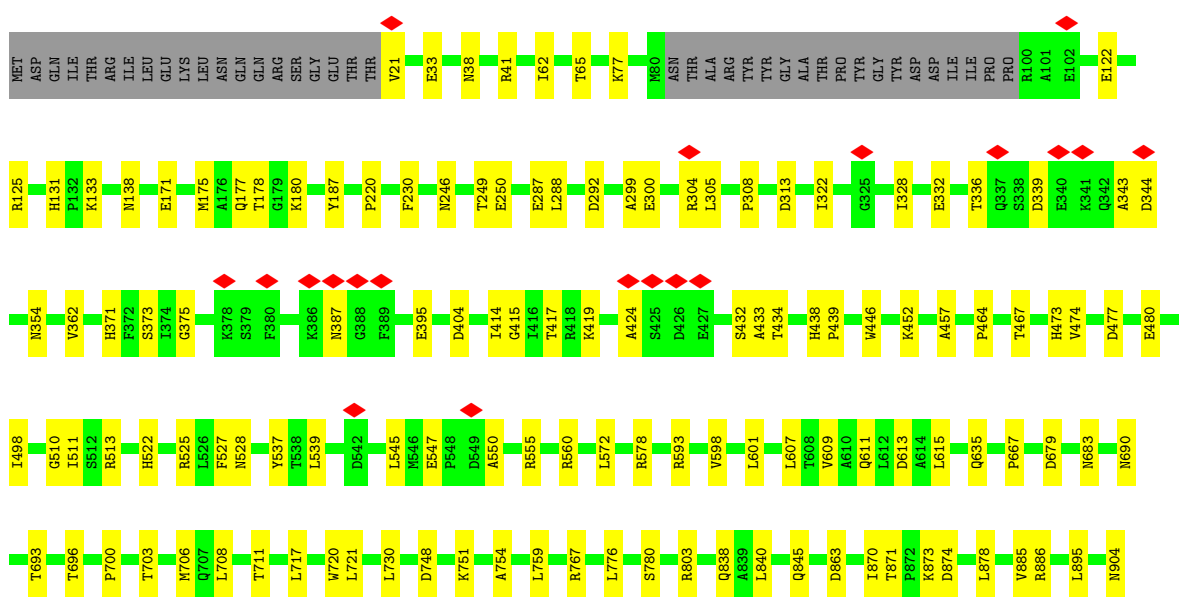
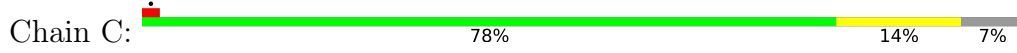


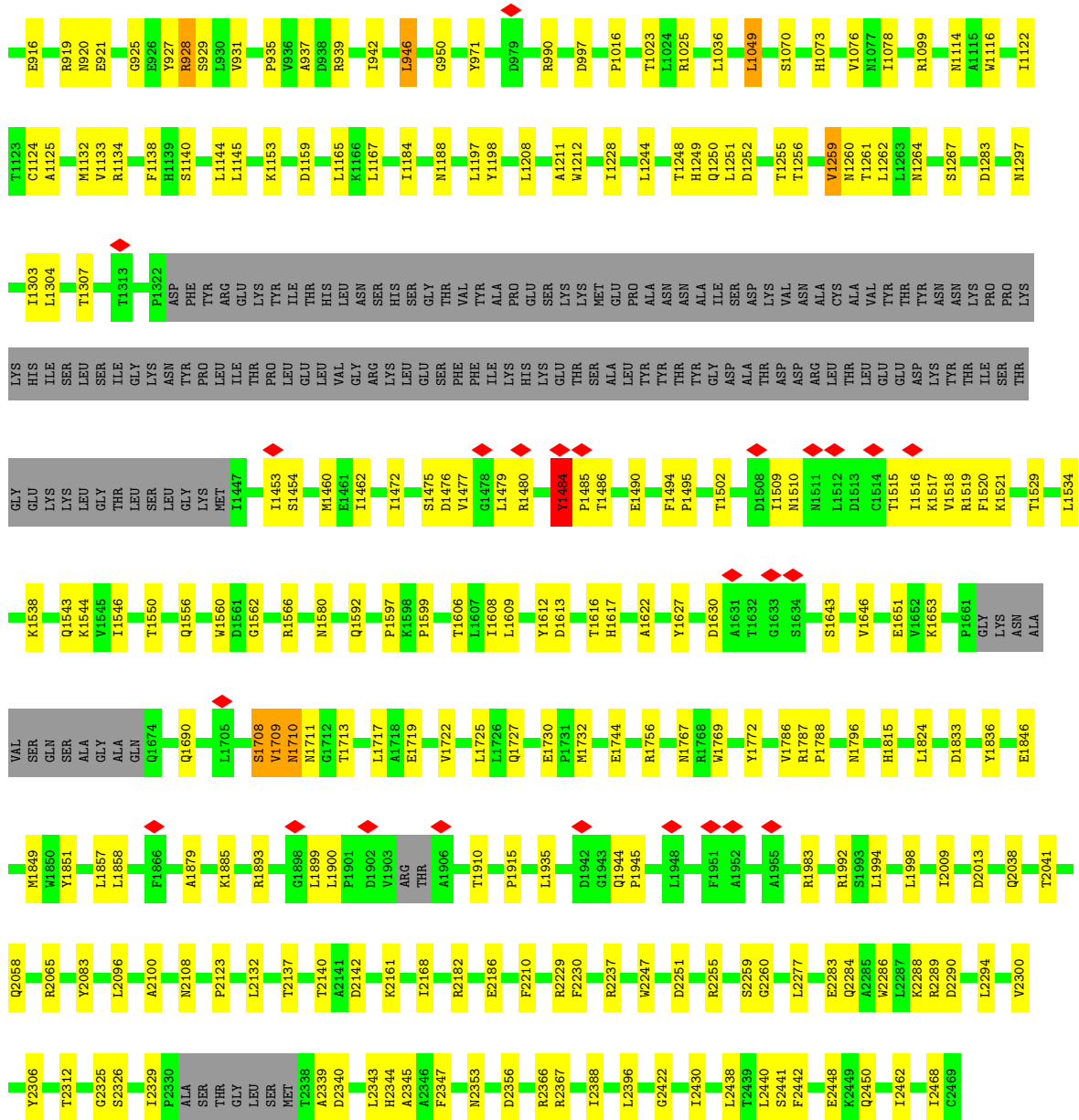
● Molecule 1: Insecticidal toxin protein TcdA4



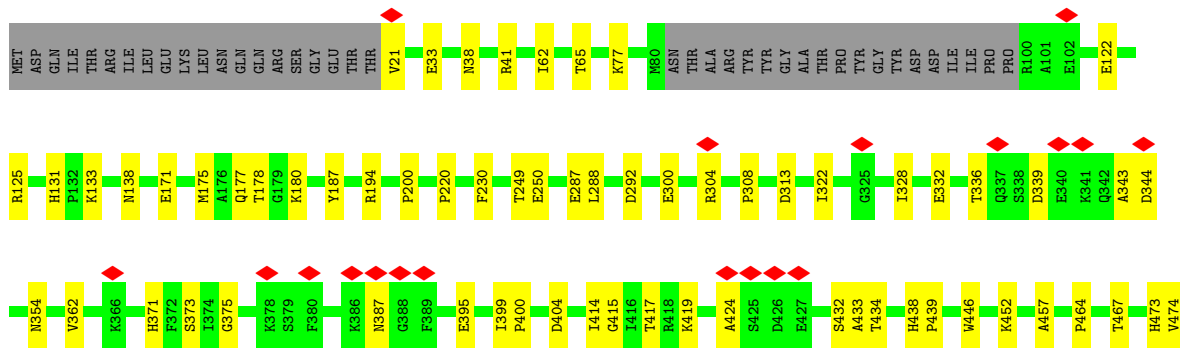
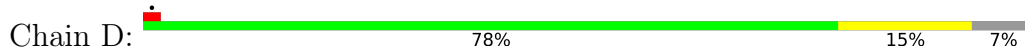


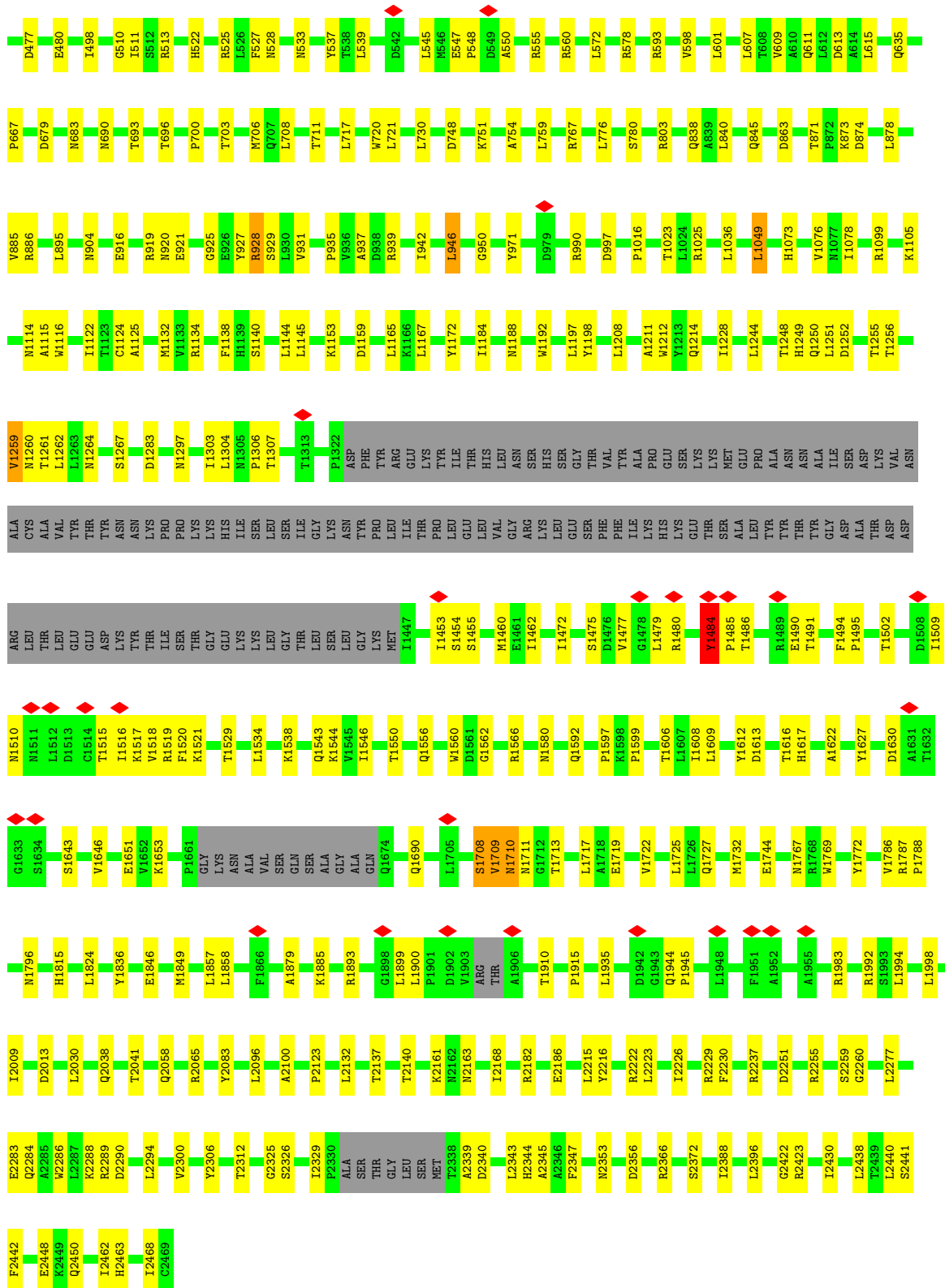
• Molecule 1: Insecticidal toxin protein TcdA4



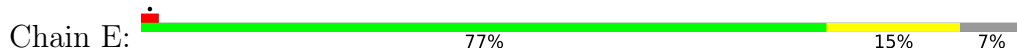


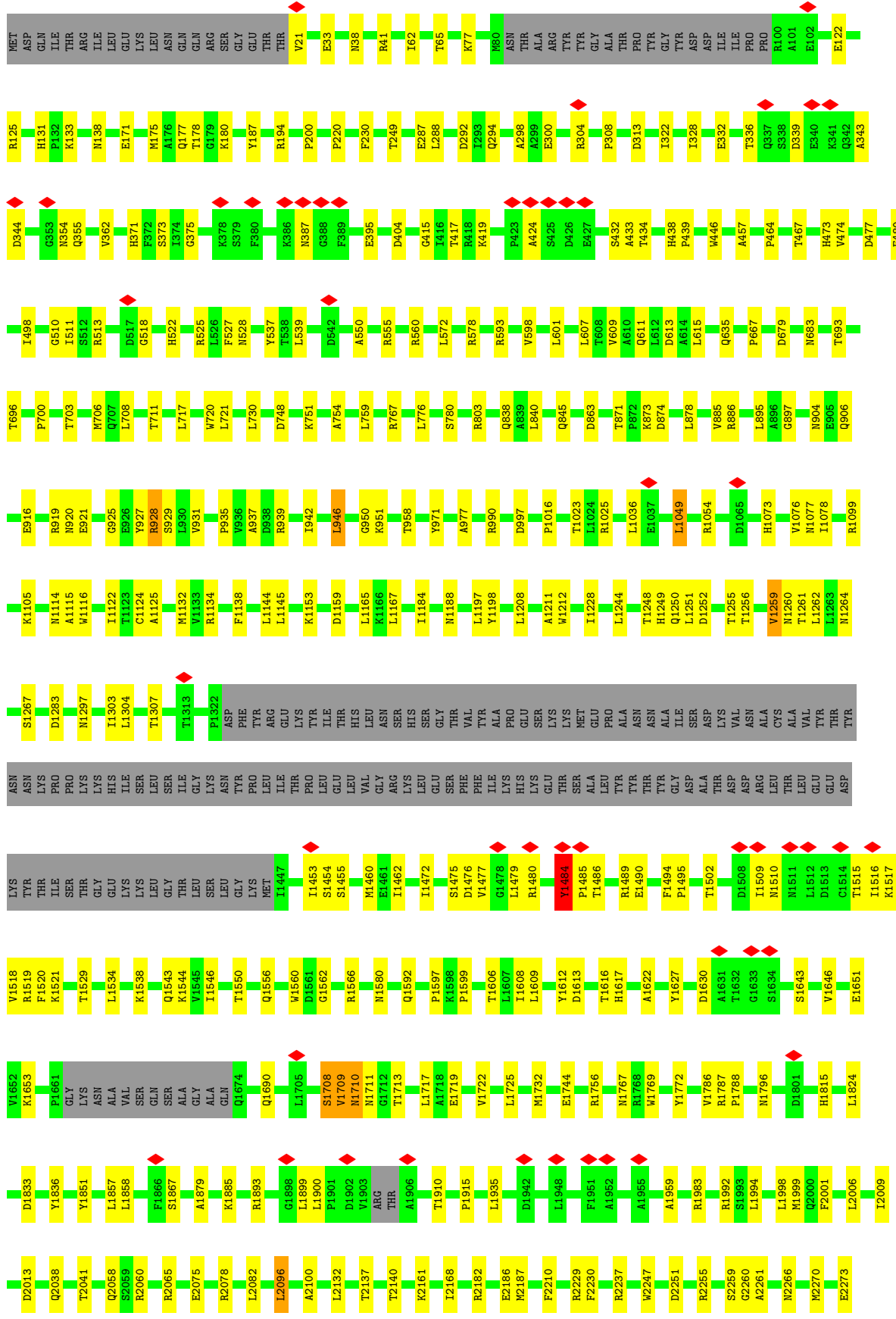
● Molecule 1: Insecticidal toxin protein TcdA4

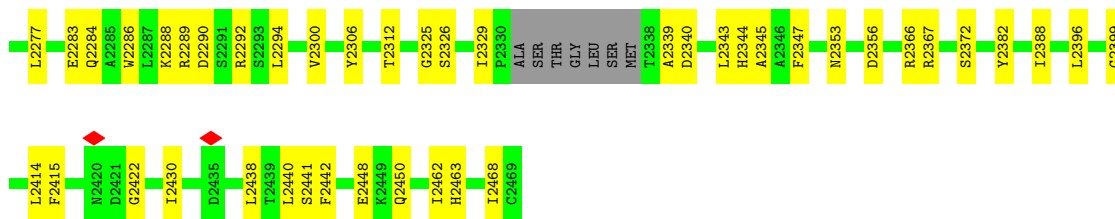




• Molecule 1: Insecticidal toxin protein TcdA4







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	247513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/18078	0.61	11/24569 (0.0%)
1	B	0.38	0/18078	0.61	11/24569 (0.0%)
1	C	0.38	0/18078	0.61	11/24569 (0.0%)
1	D	0.38	0/18078	0.61	11/24569 (0.0%)
1	E	0.38	0/18078	0.61	11/24569 (0.0%)
All	All	0.38	0/90390	0.61	55/122845 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
All	All	0	20

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	748	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	748	ASP	CB-CG-OD1	7.23	124.81	118.30
1	E	748	ASP	CB-CG-OD1	7.23	124.81	118.30
1	D	748	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	748	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	2096	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	D	2096	LEU	CB-CG-CD2	-6.46	100.02	111.00
1	C	2096	LEU	CB-CG-CD2	-6.46	100.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2096	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	B	2096	LEU	CB-CG-CD2	-6.43	100.06	111.00
1	B	946	LEU	CA-CB-CG	6.28	129.74	115.30
1	C	946	LEU	CA-CB-CG	6.28	129.74	115.30
1	D	946	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	946	LEU	CA-CB-CG	6.27	129.72	115.30
1	E	946	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	2132	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	C	2132	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	B	2132	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	D	2132	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	E	2132	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	C	1725	LEU	CB-CG-CD2	-5.44	101.76	111.00
1	D	1725	LEU	CB-CG-CD2	-5.44	101.76	111.00
1	E	1725	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	B	1725	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	A	1725	LEU	CB-CG-CD2	-5.40	101.81	111.00
1	D	1484	TYR	C-N-CD	-5.40	108.72	120.60
1	B	1484	TYR	C-N-CD	-5.39	108.75	120.60
1	E	1484	TYR	C-N-CD	-5.38	108.76	120.60
1	C	1484	TYR	C-N-CD	-5.38	108.76	120.60
1	A	1484	TYR	C-N-CD	-5.36	108.81	120.60
1	A	1262	LEU	CA-CB-CG	5.33	127.56	115.30
1	D	1262	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	1262	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	1262	LEU	CA-CB-CG	5.32	127.53	115.30
1	E	1262	LEU	CA-CB-CG	5.32	127.52	115.30
1	D	840	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	E	840	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	C	1049	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	840	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	1049	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	840	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	C	840	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	E	1049	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	1049	LEU	CA-CB-CG	5.21	127.29	115.30
1	D	1049	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	498	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	D	498	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	A	498	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	C	498	ILE	CG1-CB-CG2	-5.17	100.02	111.40
1	E	498	ILE	CG1-CB-CG2	-5.17	100.02	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2132	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	2132	LEU	CA-CB-CG	5.05	126.91	115.30
1	D	2132	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	2132	LEU	CA-CB-CG	5.04	126.88	115.30
1	E	2132	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1484	TYR	Peptide
1	A	1708	SER	Peptide
1	A	1722	VAL	Peptide
1	A	845	GLN	Peptide
1	B	1484	TYR	Peptide
1	B	1708	SER	Peptide
1	B	1722	VAL	Peptide
1	B	845	GLN	Peptide
1	C	1484	TYR	Peptide
1	C	1708	SER	Peptide
1	C	1722	VAL	Peptide
1	C	845	GLN	Peptide
1	D	1484	TYR	Peptide
1	D	1708	SER	Peptide
1	D	1722	VAL	Peptide
1	D	845	GLN	Peptide
1	E	1484	TYR	Peptide
1	E	1708	SER	Peptide
1	E	1722	VAL	Peptide
1	E	845	GLN	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	17740	0	17523	224	0
1	B	17740	0	17523	210	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	17740	0	17523	211	0
1	D	17740	0	17523	222	0
1	E	17740	0	17523	234	0
All	All	88700	0	87615	1037	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 6.

All (1037) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1786:VAL:HG12	1:A:1788:PRO:HD2	1.72	0.72
1:C:1786:VAL:HG12	1:C:1788:PRO:HD2	1.72	0.72
1:E:1786:VAL:HG12	1:E:1788:PRO:HD2	1.72	0.71
1:B:1786:VAL:HG12	1:B:1788:PRO:HD2	1.72	0.70
1:D:1786:VAL:HG12	1:D:1788:PRO:HD2	1.72	0.70
1:C:1304:LEU:HB2	1:C:1494:PHE:HB2	1.75	0.68
1:D:1304:LEU:HB2	1:D:1494:PHE:HB2	1.75	0.68
1:A:1304:LEU:HB2	1:A:1494:PHE:HB2	1.75	0.68
1:E:1304:LEU:HB2	1:E:1494:PHE:HB2	1.75	0.67
1:B:1304:LEU:HB2	1:B:1494:PHE:HB2	1.75	0.67
1:C:230:PHE:HB3	1:C:635:GLN:HE21	1.62	0.65
1:D:1994:LEU:HD12	1:D:2237:ARG:HG3	1.80	0.64
1:E:1994:LEU:HD12	1:E:2237:ARG:HG3	1.80	0.64
1:B:2123:PRO:HB2	1:C:2100:ALA:HB2	1.80	0.64
1:A:1994:LEU:HD12	1:A:2237:ARG:HG3	1.80	0.64
1:B:1994:LEU:HD12	1:B:2237:ARG:HG3	1.80	0.64
1:C:1994:LEU:HD12	1:C:2237:ARG:HG3	1.80	0.64
1:E:1297:ASN:HD22	1:E:1502:THR:HG22	1.63	0.64
1:C:1297:ASN:HD22	1:C:1502:THR:HG22	1.64	0.63
1:D:1297:ASN:HD22	1:D:1502:THR:HG22	1.64	0.63
1:C:38:ASN:HB3	1:C:41:ARG:HB2	1.80	0.63
1:A:1297:ASN:HD22	1:A:1502:THR:HG22	1.64	0.63
1:D:230:PHE:HB3	1:D:635:GLN:HE21	1.62	0.63
1:B:1297:ASN:HD22	1:B:1502:THR:HG22	1.64	0.63
1:B:230:PHE:HB3	1:B:635:GLN:HE21	1.62	0.63
1:A:230:PHE:HB3	1:A:635:GLN:HE21	1.62	0.63
1:D:1073:HIS:HB3	1:D:1261:THR:HG22	1.81	0.62
1:E:38:ASN:HB3	1:E:41:ARG:HB2	1.80	0.62
1:E:1073:HIS:HB3	1:E:1261:THR:HG22	1.81	0.62
1:A:513:ARG:HH21	1:A:539:LEU:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:GLY:HA2	1:C:593:ARG:HG3	1.82	0.62
1:E:513:ARG:HH21	1:E:539:LEU:HD12	1.64	0.62
1:E:2448:GLU:HG3	1:E:2450:GLN:H	1.65	0.62
1:D:513:ARG:HH21	1:D:539:LEU:HD12	1.64	0.62
1:D:2215:LEU:HD12	1:E:2266:ASN:HD22	1.64	0.62
1:A:510:GLY:HA2	1:A:593:ARG:HG3	1.82	0.62
1:C:2123:PRO:HB2	1:D:2100:ALA:HB2	1.82	0.62
1:C:513:ARG:HH21	1:C:539:LEU:HD12	1.64	0.62
1:A:38:ASN:HB3	1:A:41:ARG:HB2	1.80	0.62
1:D:2448:GLU:HG3	1:D:2450:GLN:H	1.65	0.62
1:A:2448:GLU:HG3	1:A:2450:GLN:H	1.65	0.62
1:B:1073:HIS:HB3	1:B:1261:THR:HG22	1.81	0.62
1:E:230:PHE:HB3	1:E:635:GLN:HE21	1.62	0.62
1:A:1114:ASN:ND2	1:A:1796:ASN:OD1	2.33	0.62
1:B:1114:ASN:ND2	1:B:1796:ASN:OD1	2.33	0.62
1:D:1114:ASN:ND2	1:D:1796:ASN:OD1	2.33	0.61
1:B:510:GLY:HA2	1:B:593:ARG:HG3	1.82	0.61
1:B:38:ASN:HB3	1:B:41:ARG:HB2	1.80	0.61
1:D:38:ASN:HB3	1:D:41:ARG:HB2	1.80	0.61
1:C:1114:ASN:ND2	1:C:1796:ASN:OD1	2.33	0.61
1:D:510:GLY:HA2	1:D:593:ARG:HG3	1.82	0.61
1:A:1073:HIS:HB3	1:A:1261:THR:HG22	1.82	0.61
1:B:513:ARG:HH21	1:B:539:LEU:HD12	1.64	0.61
1:C:1073:HIS:HB3	1:C:1261:THR:HG22	1.81	0.61
1:C:2448:GLU:HG3	1:C:2450:GLN:H	1.65	0.61
1:E:1114:ASN:ND2	1:E:1796:ASN:OD1	2.33	0.61
1:B:415:GLY:HA2	1:B:432:SER:HA	1.83	0.60
1:B:1608:ILE:HG12	1:B:1651:GLU:HG2	1.83	0.60
1:C:415:GLY:HA2	1:C:432:SER:HA	1.83	0.60
1:D:1608:ILE:HG12	1:D:1651:GLU:HG2	1.83	0.60
1:E:415:GLY:HA2	1:E:432:SER:HA	1.83	0.60
1:D:131:HIS:HD1	1:D:971:TYR:HH	1.47	0.60
1:E:1608:ILE:HG12	1:E:1651:GLU:HG2	1.83	0.60
1:A:1732:MET:O	1:A:1787:ARG:NH2	2.35	0.60
1:B:2448:GLU:HG3	1:B:2450:GLN:H	1.65	0.60
1:A:1608:ILE:HG12	1:A:1651:GLU:HG2	1.83	0.60
1:B:2325:GLY:HA2	1:B:2340:ASP:HA	1.84	0.60
1:D:1732:MET:O	1:D:1787:ARG:NH2	2.35	0.60
1:C:2325:GLY:HA2	1:C:2340:ASP:HA	1.84	0.60
1:E:1732:MET:O	1:E:1787:ARG:NH2	2.35	0.60
1:C:131:HIS:HD1	1:C:971:TYR:HH	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2123:PRO:HB2	1:E:2100:ALA:HB2	1.84	0.60
1:D:2325:GLY:HA2	1:D:2340:ASP:HA	1.84	0.60
1:B:1732:MET:O	1:B:1787:ARG:NH2	2.35	0.60
1:E:510:GLY:HA2	1:E:593:ARG:HG3	1.82	0.60
1:B:131:HIS:HD1	1:B:971:TYR:HH	1.50	0.60
1:A:415:GLY:HA2	1:A:432:SER:HA	1.83	0.59
1:C:997:ASP:OD2	1:D:1767:ASN:ND2	2.35	0.59
1:C:1732:MET:O	1:C:1787:ARG:NH2	2.35	0.59
1:A:997:ASP:OD2	1:B:1767:ASN:ND2	2.35	0.59
1:A:1476:ASP:O	1:B:1727:GLN:NE2	2.35	0.59
1:A:1936:ARG:NH1	1:E:951:LYS:HD2	2.17	0.59
1:D:415:GLY:HA2	1:D:432:SER:HA	1.83	0.59
1:C:1608:ILE:HG12	1:C:1651:GLU:HG2	1.83	0.59
1:B:920:ASN:ND2	1:B:950:GLY:O	2.36	0.59
1:C:1476:ASP:O	1:D:1727:GLN:NE2	2.35	0.59
1:D:1519:ARG:HH21	1:D:1529:THR:HG21	1.68	0.59
1:E:2325:GLY:HA2	1:E:2340:ASP:HA	1.84	0.59
1:A:920:ASN:ND2	1:A:950:GLY:O	2.36	0.59
1:C:920:ASN:ND2	1:C:950:GLY:O	2.36	0.59
1:C:1519:ARG:HH21	1:C:1529:THR:HG21	1.68	0.59
1:A:2325:GLY:HA2	1:A:2340:ASP:HA	1.84	0.58
1:C:1613:ASP:H	1:C:1617:HIS:HD2	1.51	0.58
1:D:1613:ASP:H	1:D:1617:HIS:HD2	1.51	0.58
1:E:187:TYR:OH	1:E:919:ARG:NH2	2.36	0.58
1:D:920:ASN:ND2	1:D:950:GLY:O	2.36	0.58
1:A:336:THR:HG22	1:A:434:THR:H	1.68	0.58
1:C:336:THR:HG22	1:C:434:THR:H	1.68	0.58
1:D:336:THR:HG22	1:D:434:THR:H	1.68	0.58
1:E:706:MET:O	1:E:767:ARG:NH2	2.37	0.58
1:A:1992:ARG:NH2	1:A:2283:GLU:OE1	2.37	0.58
1:A:1519:ARG:HH21	1:A:1529:THR:HG21	1.68	0.58
1:B:706:MET:O	1:B:767:ARG:NH2	2.37	0.58
1:C:1992:ARG:NH2	1:C:2283:GLU:OE1	2.37	0.58
1:D:1516:ILE:HG12	1:D:1517:LYS:HG2	1.86	0.58
1:E:1519:ARG:HH21	1:E:1529:THR:HG21	1.68	0.58
1:D:1099:ARG:HH21	1:D:1116:TRP:HB3	1.69	0.58
1:E:1516:ILE:HG12	1:E:1517:LYS:HG2	1.86	0.58
1:D:2222:ARG:NH2	1:E:2261:ALA:O	2.37	0.58
1:E:920:ASN:ND2	1:E:950:GLY:O	2.36	0.58
1:A:1516:ILE:HG12	1:A:1517:LYS:HG2	1.86	0.58
1:B:1476:ASP:O	1:C:1727:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1519:ARG:HH21	1:B:1529:THR:HG21	1.68	0.58
1:B:1613:ASP:H	1:B:1617:HIS:HD2	1.51	0.58
1:D:187:TYR:OH	1:D:919:ARG:NH2	2.36	0.58
1:E:1099:ARG:HH21	1:E:1116:TRP:HB3	1.69	0.58
1:C:187:TYR:OH	1:C:919:ARG:NH2	2.36	0.58
1:A:187:TYR:OH	1:A:919:ARG:NH2	2.36	0.57
1:A:371:HIS:ND1	1:A:387:ASN:O	2.37	0.57
1:B:187:TYR:OH	1:B:919:ARG:NH2	2.36	0.57
1:D:706:MET:O	1:D:767:ARG:NH2	2.37	0.57
1:E:336:THR:HG22	1:E:434:THR:H	1.68	0.57
1:D:1025:ARG:NH2	1:D:1744:GLU:OE2	2.38	0.57
1:A:578:ARG:NH1	1:A:613:ASP:OD1	2.38	0.57
1:D:344:ASP:HB3	1:D:362:VAL:HA	1.86	0.57
1:A:706:MET:O	1:A:767:ARG:NH2	2.37	0.57
1:B:578:ARG:NH1	1:B:613:ASP:OD1	2.37	0.57
1:B:1992:ARG:NH2	1:B:2283:GLU:OE1	2.37	0.57
1:E:344:ASP:HB3	1:E:362:VAL:HA	1.86	0.57
1:E:371:HIS:ND1	1:E:387:ASN:O	2.37	0.57
1:A:1025:ARG:NH2	1:A:1744:GLU:OE2	2.38	0.57
1:A:1613:ASP:H	1:A:1617:HIS:HD2	1.51	0.57
1:A:2345:ALA:HB3	1:A:2440:LEU:HB3	1.87	0.57
1:C:1516:ILE:HG12	1:C:1517:LYS:HG2	1.86	0.57
1:E:1613:ASP:H	1:E:1617:HIS:HD2	1.51	0.57
1:B:371:HIS:ND1	1:B:387:ASN:O	2.37	0.57
1:B:1099:ARG:HH21	1:B:1116:TRP:HB3	1.69	0.57
1:B:1484:TYR:HA	1:B:1486:THR:H	1.70	0.57
1:C:578:ARG:NH1	1:C:613:ASP:OD1	2.37	0.57
1:C:706:MET:O	1:C:767:ARG:NH2	2.37	0.57
1:C:1099:ARG:HH21	1:C:1116:TRP:HB3	1.69	0.57
1:D:371:HIS:ND1	1:D:387:ASN:O	2.37	0.57
1:D:1484:TYR:HA	1:D:1486:THR:H	1.70	0.57
1:D:1992:ARG:NH2	1:D:2283:GLU:OE1	2.37	0.57
1:E:1992:ARG:NH2	1:E:2283:GLU:OE1	2.37	0.57
1:A:1767:ASN:ND2	1:E:997:ASP:OD2	2.37	0.57
1:B:336:THR:HG22	1:B:434:THR:H	1.68	0.57
1:B:1516:ILE:HG12	1:B:1517:LYS:HG2	1.86	0.57
1:E:1025:ARG:NH2	1:E:1744:GLU:OE2	2.38	0.57
1:B:344:ASP:HB3	1:B:362:VAL:HA	1.86	0.57
1:E:1484:TYR:HA	1:E:1486:THR:H	1.70	0.57
1:A:1484:TYR:HA	1:A:1486:THR:H	1.70	0.57
1:B:2366:ARG:HG2	1:B:2468:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2345:ALA:HB3	1:E:2440:LEU:HB3	1.87	0.56
1:A:1099:ARG:HH21	1:A:1116:TRP:HB3	1.69	0.56
1:A:2366:ARG:HG2	1:A:2468:ILE:HG12	1.87	0.56
1:B:997:ASP:OD2	1:C:1767:ASN:ND2	2.38	0.56
1:B:1025:ARG:NH2	1:B:1744:GLU:OE2	2.38	0.56
1:D:2366:ARG:HG2	1:D:2468:ILE:HG12	1.87	0.56
1:C:371:HIS:ND1	1:C:387:ASN:O	2.37	0.56
1:C:2345:ALA:HB3	1:C:2440:LEU:HB3	1.87	0.56
1:D:77:LYS:NZ	1:D:1858:LEU:O	2.39	0.56
1:A:77:LYS:NZ	1:A:1858:LEU:O	2.39	0.56
1:D:2345:ALA:HB3	1:D:2440:LEU:HB3	1.87	0.56
1:E:2366:ARG:HG2	1:E:2468:ILE:HG12	1.87	0.56
1:B:2345:ALA:HB3	1:B:2440:LEU:HB3	1.87	0.56
1:C:344:ASP:HB3	1:C:362:VAL:HA	1.86	0.56
1:C:1025:ARG:NH2	1:C:1744:GLU:OE2	2.38	0.56
1:C:2366:ARG:HG2	1:C:2468:ILE:HG12	1.87	0.56
1:E:308:PRO:HD2	1:E:473:HIS:H	1.71	0.56
1:D:171:GLU:OE2	1:D:919:ARG:NH2	2.39	0.56
1:E:171:GLU:OE2	1:E:919:ARG:NH2	2.39	0.56
1:A:344:ASP:HB3	1:A:362:VAL:HA	1.86	0.56
1:B:1076:VAL:HG21	1:B:1264:ASN:HD21	1.71	0.56
1:C:1244:LEU:HD22	1:C:1251:LEU:HD11	1.88	0.56
1:C:1484:TYR:HA	1:C:1486:THR:H	1.70	0.56
1:C:2343:LEU:HB3	1:C:2442:PHE:HB2	1.88	0.56
1:D:997:ASP:OD2	1:E:1767:ASN:ND2	2.39	0.56
1:B:171:GLU:OE2	1:B:919:ARG:NH2	2.39	0.56
1:C:474:VAL:HB	1:C:477:ASP:HB2	1.88	0.56
1:C:1453:ILE:HG23	1:C:1480:ARG:HH22	1.71	0.56
1:B:1566:ARG:NH2	1:B:1597:PRO:O	2.40	0.55
1:D:1453:ILE:HG23	1:D:1480:ARG:HH22	1.71	0.55
1:E:77:LYS:NZ	1:E:1858:LEU:O	2.39	0.55
1:E:578:ARG:NH1	1:E:613:ASP:OD1	2.38	0.55
1:B:77:LYS:NZ	1:B:1858:LEU:O	2.39	0.55
1:B:1453:ILE:HG23	1:B:1480:ARG:HH22	1.71	0.55
1:B:2300:VAL:HB	1:B:2462:ILE:HG22	1.89	0.55
1:C:171:GLU:OE2	1:C:919:ARG:NH2	2.39	0.55
1:C:2300:VAL:HB	1:C:2462:ILE:HG22	1.89	0.55
1:E:1453:ILE:HG23	1:E:1480:ARG:HH22	1.71	0.55
1:E:1566:ARG:NH2	1:E:1597:PRO:O	2.39	0.55
1:A:171:GLU:OE2	1:A:919:ARG:NH2	2.39	0.55
1:A:1453:ILE:HG23	1:A:1480:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2343:LEU:HB3	1:A:2442:PHE:HB2	1.88	0.55
1:C:395:GLU:OE2	1:C:513:ARG:NH2	2.40	0.55
1:D:1140:SER:HB3	1:E:1580:ASN:HD22	1.71	0.55
1:A:1566:ARG:NH2	1:A:1597:PRO:O	2.39	0.55
1:A:2277:LEU:HD21	1:E:2229:ARG:HD2	1.89	0.55
1:D:474:VAL:HB	1:D:477:ASP:HB2	1.88	0.55
1:D:572:LEU:HD12	1:D:609:VAL:HG21	1.89	0.55
1:D:2300:VAL:HB	1:D:2462:ILE:HG22	1.89	0.55
1:D:2343:LEU:HB3	1:D:2442:PHE:HB2	1.88	0.55
1:E:2300:VAL:HB	1:E:2462:ILE:HG22	1.89	0.55
1:A:308:PRO:HD2	1:A:473:HIS:H	1.71	0.55
1:A:2300:VAL:HB	1:A:2462:ILE:HG22	1.89	0.55
1:A:395:GLU:OE2	1:A:513:ARG:NH2	2.40	0.55
1:B:2294:LEU:HB2	1:B:2468:ILE:HB	1.89	0.55
1:C:77:LYS:NZ	1:C:1858:LEU:O	2.39	0.55
1:C:308:PRO:HD2	1:C:473:HIS:H	1.71	0.55
1:C:878:LEU:HA	1:C:895:LEU:HD11	1.89	0.55
1:A:1076:VAL:HG21	1:A:1264:ASN:HD21	1.71	0.55
1:B:528:ASN:HD21	1:B:537:TYR:H	1.55	0.55
1:C:528:ASN:HD21	1:C:537:TYR:H	1.55	0.55
1:C:572:LEU:HD12	1:C:609:VAL:HG21	1.89	0.55
1:C:1566:ARG:NH2	1:C:1597:PRO:O	2.39	0.55
1:C:2294:LEU:HB2	1:C:2468:ILE:HB	1.89	0.55
1:D:1566:ARG:NH2	1:D:1597:PRO:O	2.39	0.55
1:B:572:LEU:HD12	1:B:609:VAL:HG21	1.89	0.55
1:B:2343:LEU:HB3	1:B:2442:PHE:HB2	1.88	0.55
1:C:322:ILE:HG22	1:C:328:ILE:HG12	1.89	0.55
1:D:395:GLU:OE2	1:D:513:ARG:NH2	2.40	0.55
1:E:1076:VAL:HG21	1:E:1264:ASN:HD21	1.71	0.55
1:E:1244:LEU:HD22	1:E:1251:LEU:HD11	1.88	0.55
1:D:528:ASN:HD21	1:D:537:TYR:H	1.55	0.55
1:D:1244:LEU:HD22	1:D:1251:LEU:HD11	1.88	0.55
1:D:2294:LEU:HB2	1:D:2468:ILE:HB	1.89	0.55
1:A:474:VAL:HB	1:A:477:ASP:HB2	1.88	0.54
1:A:1040:SER:OG	1:E:2078:ARG:NH1	2.39	0.54
1:D:1076:VAL:HG21	1:D:1264:ASN:HD21	1.71	0.54
1:E:528:ASN:HD21	1:E:537:TYR:H	1.55	0.54
1:E:572:LEU:HD12	1:E:609:VAL:HG21	1.89	0.54
1:B:474:VAL:HB	1:B:477:ASP:HB2	1.88	0.54
1:E:395:GLU:OE2	1:E:513:ARG:NH2	2.40	0.54
1:E:878:LEU:HA	1:E:895:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LEU:HD13	1:A:759:LEU:HD23	1.90	0.54
1:B:1244:LEU:HD22	1:B:1251:LEU:HD11	1.88	0.54
1:C:1076:VAL:HG21	1:C:1264:ASN:HD21	1.71	0.54
1:B:721:LEU:HD13	1:B:759:LEU:HD23	1.90	0.54
1:D:322:ILE:HG22	1:D:328:ILE:HG12	1.90	0.54
1:E:474:VAL:HB	1:E:477:ASP:HB2	1.88	0.54
1:A:528:ASN:HD21	1:A:537:TYR:H	1.55	0.54
1:A:878:LEU:HA	1:A:895:LEU:HD11	1.89	0.54
1:B:322:ILE:HG22	1:B:328:ILE:HG12	1.89	0.54
1:B:395:GLU:OE2	1:B:513:ARG:NH2	2.40	0.54
1:E:928:ARG:NH1	1:E:937:ALA:O	2.41	0.54
1:A:1244:LEU:HD22	1:A:1251:LEU:HD11	1.88	0.54
1:C:721:LEU:HD13	1:C:759:LEU:HD23	1.90	0.54
1:D:928:ARG:NH1	1:D:937:ALA:O	2.41	0.54
1:D:871:THR:HG22	1:D:874:ASP:HB2	1.90	0.54
1:D:878:LEU:HA	1:D:895:LEU:HD11	1.89	0.54
1:E:921:GLU:HG3	1:E:939:ARG:HH22	1.73	0.54
1:A:928:ARG:NH1	1:A:937:ALA:O	2.41	0.54
1:E:721:LEU:HD13	1:E:759:LEU:HD23	1.90	0.54
1:A:322:ILE:HG22	1:A:328:ILE:HG12	1.90	0.54
1:A:1630:ASP:OD2	1:A:1690:GLN:NE2	2.41	0.54
1:A:1865:ILE:HA	1:E:294:GLN:NE2	2.23	0.54
1:B:1630:ASP:OD2	1:B:1690:GLN:NE2	2.41	0.54
1:B:308:PRO:HD2	1:B:473:HIS:H	1.71	0.54
1:B:878:LEU:HA	1:B:895:LEU:HD11	1.89	0.54
1:B:928:ARG:NH1	1:B:937:ALA:O	2.41	0.54
1:C:871:THR:HG22	1:C:874:ASP:HB2	1.90	0.54
1:D:308:PRO:HD2	1:D:473:HIS:H	1.71	0.54
1:A:572:LEU:HD12	1:A:609:VAL:HG21	1.89	0.53
1:A:2294:LEU:HB2	1:A:2468:ILE:HB	1.89	0.53
1:C:1630:ASP:OD2	1:C:1690:GLN:NE2	2.41	0.53
1:E:871:THR:HG22	1:E:874:ASP:HB2	1.90	0.53
1:E:2343:LEU:HB3	1:E:2442:PHE:HB2	1.88	0.53
1:A:158:ASN:ND2	1:E:518:GLY:O	2.41	0.53
1:D:721:LEU:HD13	1:D:759:LEU:HD23	1.90	0.53
1:D:1134:ARG:NH2	1:D:1252:ASP:OD2	2.41	0.53
1:E:322:ILE:HG22	1:E:328:ILE:HG12	1.89	0.53
1:E:942:ILE:O	1:E:946:LEU:HB3	2.09	0.53
1:B:871:THR:HG22	1:B:874:ASP:HB2	1.90	0.53
1:C:928:ARG:NH1	1:C:937:ALA:O	2.41	0.53
1:E:1078:ILE:HG12	1:E:1544:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2294:LEU:HB2	1:E:2468:ILE:HB	1.89	0.53
1:A:1134:ARG:NH2	1:A:1252:ASP:OD2	2.42	0.53
1:D:578:ARG:NH1	1:D:613:ASP:OD1	2.38	0.53
1:D:929:SER:HA	1:D:935:PRO:HG3	1.91	0.53
1:E:1134:ARG:NH2	1:E:1252:ASP:OD2	2.41	0.53
1:D:1078:ILE:HG12	1:D:1544:LYS:HD3	1.91	0.53
1:C:1134:ARG:NH2	1:C:1252:ASP:OD2	2.41	0.53
1:D:1630:ASP:OD2	1:D:1690:GLN:NE2	2.41	0.53
1:A:1078:ILE:HG12	1:A:1544:LYS:HD3	1.91	0.53
1:B:1134:ARG:NH2	1:B:1252:ASP:OD2	2.41	0.53
1:E:1630:ASP:OD2	1:E:1690:GLN:NE2	2.41	0.53
1:A:942:ILE:O	1:A:946:LEU:HB3	2.09	0.53
1:C:921:GLU:HG3	1:C:939:ARG:HH22	1.73	0.53
1:C:929:SER:HA	1:C:935:PRO:HG3	1.91	0.53
1:A:921:GLU:HG3	1:A:939:ARG:HH22	1.73	0.53
1:A:2123:PRO:HB2	1:B:2100:ALA:HB2	1.90	0.53
1:C:1078:ILE:HG12	1:C:1544:LYS:HD3	1.91	0.53
1:A:871:THR:HG22	1:A:874:ASP:HB2	1.90	0.53
1:B:921:GLU:HG3	1:B:939:ARG:HH22	1.73	0.53
1:B:929:SER:HA	1:B:935:PRO:HG3	1.91	0.53
1:B:942:ILE:O	1:B:946:LEU:HB3	2.09	0.52
1:B:373:SER:HB3	1:B:417:THR:HB	1.91	0.52
1:C:122:GLU:OE1	1:C:125:ARG:NH2	2.43	0.52
1:C:2229:ARG:HD2	1:D:2277:LEU:HD21	1.91	0.52
1:D:292:ASP:HB3	1:D:464:PRO:HD2	1.92	0.52
1:D:921:GLU:HG3	1:D:939:ARG:HH22	1.73	0.52
1:D:942:ILE:O	1:D:946:LEU:HB3	2.09	0.52
1:B:1477:VAL:HG12	1:B:1479:LEU:H	1.74	0.52
1:E:550:ALA:HB3	1:E:555:ARG:HH22	1.75	0.52
1:A:929:SER:HA	1:A:935:PRO:HG3	1.91	0.52
1:A:1727:GLN:NE2	1:E:1476:ASP:O	2.43	0.52
1:B:1138:PHE:HB2	1:B:1208:LEU:HD21	1.91	0.52
1:C:942:ILE:O	1:C:946:LEU:HB3	2.09	0.52
1:D:1167:LEU:HD22	1:D:1228:ILE:HD13	1.92	0.52
1:D:1477:VAL:HG12	1:D:1479:LEU:H	1.74	0.52
1:A:1167:LEU:HD22	1:A:1228:ILE:HD13	1.92	0.52
1:B:122:GLU:OE1	1:B:125:ARG:NH2	2.43	0.52
1:C:373:SER:HB3	1:C:417:THR:HB	1.91	0.52
1:C:1167:LEU:HD22	1:C:1228:ILE:HD13	1.92	0.52
1:D:2226:ILE:HG23	1:E:2277:LEU:HD22	1.92	0.52
1:B:1078:ILE:HG12	1:B:1544:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1167:LEU:HD22	1:E:1228:ILE:HD13	1.92	0.52
1:A:550:ALA:HB3	1:A:555:ARG:HH22	1.75	0.52
1:A:1138:PHE:HB2	1:A:1208:LEU:HD21	1.91	0.52
1:C:1138:PHE:HB2	1:C:1208:LEU:HD21	1.91	0.52
1:C:1477:VAL:HG12	1:C:1479:LEU:H	1.74	0.52
1:A:1477:VAL:HG12	1:A:1479:LEU:H	1.75	0.52
1:B:1622:ALA:HA	1:B:1643:SER:HA	1.92	0.52
1:E:1250:GLN:HB3	1:E:1260:ASN:HD22	1.75	0.52
1:E:1477:VAL:HG12	1:E:1479:LEU:H	1.75	0.52
1:B:1167:LEU:HD22	1:B:1228:ILE:HD13	1.92	0.51
1:B:2137:THR:HA	1:B:2140:THR:HG22	1.93	0.51
1:D:550:ALA:HB3	1:D:555:ARG:HH22	1.75	0.51
1:D:1138:PHE:HB2	1:D:1208:LEU:HD21	1.91	0.51
1:E:929:SER:HA	1:E:935:PRO:HG3	1.91	0.51
1:B:1566:ARG:HH21	1:B:1599:PRO:HD3	1.75	0.51
1:E:122:GLU:OE1	1:E:125:ARG:NH2	2.43	0.51
1:A:373:SER:HB3	1:A:417:THR:HB	1.91	0.51
1:A:1250:GLN:HB3	1:A:1260:ASN:HD22	1.75	0.51
1:D:122:GLU:OE1	1:D:125:ARG:NH2	2.43	0.51
1:D:373:SER:HB3	1:D:417:THR:HB	1.91	0.51
1:E:1138:PHE:HB2	1:E:1208:LEU:HD21	1.91	0.51
1:B:550:ALA:HB3	1:B:555:ARG:HH22	1.75	0.51
1:C:1165:LEU:HB2	1:C:1184:ILE:HD11	1.93	0.51
1:D:1023:THR:HG23	1:D:1036:LEU:HD21	1.93	0.51
1:D:1165:LEU:HB2	1:D:1184:ILE:HD11	1.93	0.51
1:D:2223:LEU:HB2	1:E:2270:MET:HE1	1.92	0.51
1:A:2038:GLN:HG3	1:E:2187:MET:SD	2.50	0.51
1:A:2137:THR:HA	1:A:2140:THR:HG22	1.92	0.51
1:B:2388:ILE:O	1:B:2441:SER:N	2.44	0.51
1:A:927:TYR:O	1:A:931:VAL:N	2.38	0.51
1:A:1566:ARG:HH21	1:A:1599:PRO:HD3	1.75	0.51
1:C:292:ASP:HB3	1:C:464:PRO:HD2	1.92	0.51
1:C:1460:MET:HA	1:C:1520:PHE:HA	1.93	0.51
1:E:1023:THR:HG23	1:E:1036:LEU:HD21	1.93	0.51
1:C:2137:THR:HA	1:C:2140:THR:HG22	1.92	0.51
1:D:1250:GLN:HB3	1:D:1260:ASN:HD22	1.75	0.51
1:D:1566:ARG:HH21	1:D:1599:PRO:HD3	1.75	0.51
1:E:1566:ARG:HH21	1:E:1599:PRO:HD3	1.75	0.51
1:A:1023:THR:HG23	1:A:1036:LEU:HD21	1.93	0.51
1:C:550:ALA:HB3	1:C:555:ARG:HH22	1.75	0.51
1:D:2388:ILE:O	1:D:2441:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1622:ALA:HA	1:A:1643:SER:HA	1.92	0.51
1:B:1460:MET:HA	1:B:1520:PHE:HA	1.93	0.51
1:C:1023:THR:HG23	1:C:1036:LEU:HD21	1.93	0.51
1:D:2229:ARG:HD2	1:E:2277:LEU:HD21	1.93	0.51
1:E:177:GLN:HG3	1:E:931:VAL:HG22	1.93	0.51
1:A:1776:PRO:HB2	1:E:977:ALA:HA	1.93	0.51
1:C:1250:GLN:HB3	1:C:1260:ASN:HD22	1.75	0.51
1:C:1566:ARG:HH21	1:C:1599:PRO:HD3	1.75	0.51
1:C:2388:ILE:O	1:C:2441:SER:N	2.44	0.51
1:E:373:SER:HB3	1:E:417:THR:HB	1.91	0.51
1:A:122:GLU:OE1	1:A:125:ARG:NH2	2.43	0.50
1:D:177:GLN:HG3	1:D:931:VAL:HG22	1.93	0.50
1:E:1165:LEU:HB2	1:E:1184:ILE:HD11	1.93	0.50
1:A:1872:ASN:H	1:E:355:GLN:HE22	1.57	0.50
1:B:2326:SER:N	1:B:2339:ALA:O	2.44	0.50
1:A:177:GLN:HG3	1:A:931:VAL:HG22	1.93	0.50
1:B:1250:GLN:HB3	1:B:1260:ASN:HD22	1.75	0.50
1:B:2229:ARG:HD2	1:C:2277:LEU:HD21	1.94	0.50
1:C:1622:ALA:HA	1:C:1643:SER:HA	1.92	0.50
1:D:1622:ALA:HA	1:D:1643:SER:HA	1.92	0.50
1:E:2388:ILE:O	1:E:2441:SER:N	2.44	0.50
1:A:292:ASP:HB3	1:A:464:PRO:HD2	1.92	0.50
1:B:292:ASP:HB3	1:B:464:PRO:HD2	1.92	0.50
1:D:2326:SER:N	1:D:2339:ALA:O	2.44	0.50
1:E:703:THR:HG21	1:E:711:THR:HA	1.94	0.50
1:E:292:ASP:HB3	1:E:464:PRO:HD2	1.92	0.50
1:B:1023:THR:HG23	1:B:1036:LEU:HD21	1.93	0.50
1:E:1250:GLN:NE2	1:E:1261:THR:OG1	2.36	0.50
1:E:1622:ALA:HA	1:E:1643:SER:HA	1.92	0.50
1:A:703:THR:HG21	1:A:711:THR:HA	1.94	0.50
1:B:1165:LEU:HB2	1:B:1184:ILE:HD11	1.93	0.50
1:C:1122:ILE:HD13	1:C:1144:LEU:HD22	1.94	0.50
1:D:322:ILE:HG12	1:E:1867:SER:HB2	1.92	0.50
1:D:1460:MET:HA	1:D:1520:PHE:HA	1.93	0.50
1:E:2137:THR:HA	1:E:2140:THR:HG22	1.93	0.50
1:E:2326:SER:N	1:E:2339:ALA:O	2.44	0.50
1:C:1248:THR:HA	1:C:1251:LEU:HD13	1.94	0.50
1:E:1460:MET:HA	1:E:1520:PHE:HA	1.93	0.50
1:A:1460:MET:HA	1:A:1520:PHE:HA	1.93	0.50
1:A:2326:SER:N	1:A:2339:ALA:O	2.44	0.50
1:B:1562:GLY:O	1:B:1627:TYR:OH	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2326:SER:N	1:C:2339:ALA:O	2.44	0.50
1:D:703:THR:HG21	1:D:711:THR:HA	1.94	0.50
1:A:1165:LEU:HB2	1:A:1184:ILE:HD11	1.93	0.49
1:B:1250:GLN:NE2	1:B:1261:THR:OG1	2.36	0.49
1:A:925:GLY:HA2	1:A:928:ARG:HE	1.77	0.49
1:B:611:GLN:O	1:B:615:LEU:HB2	2.12	0.49
1:C:177:GLN:HG3	1:C:931:VAL:HG22	1.93	0.49
1:C:2286:TRP:O	1:C:2290:ASP:N	2.36	0.49
1:D:2137:THR:HA	1:D:2140:THR:HG22	1.93	0.49
1:B:177:GLN:HG3	1:B:931:VAL:HG22	1.93	0.49
1:B:925:GLY:HA2	1:B:928:ARG:HE	1.77	0.49
1:C:925:GLY:HA2	1:C:928:ARG:HE	1.77	0.49
1:D:927:TYR:O	1:D:931:VAL:N	2.38	0.49
1:A:511:ILE:HG23	1:A:522:HIS:HD2	1.78	0.49
1:A:1248:THR:HA	1:A:1251:LEU:HD13	1.94	0.49
1:E:1248:THR:HA	1:E:1251:LEU:HD13	1.94	0.49
1:A:607:LEU:HD21	1:A:615:LEU:HD22	1.95	0.49
1:A:611:GLN:O	1:A:615:LEU:HB2	2.12	0.49
1:A:1756:ARG:NH1	1:E:2075:GLU:OE2	2.46	0.49
1:C:2182:ARG:NH1	1:C:2186:GLU:OE2	2.46	0.49
1:E:607:LEU:HD21	1:E:615:LEU:HD22	1.95	0.49
1:A:1122:ILE:HD13	1:A:1144:LEU:HD22	1.94	0.49
1:B:511:ILE:HG23	1:B:522:HIS:HD2	1.78	0.49
1:B:703:THR:HG21	1:B:711:THR:HA	1.94	0.49
1:C:1521:LYS:HG3	1:C:1529:THR:HB	1.95	0.49
1:D:1122:ILE:HD13	1:D:1144:LEU:HD22	1.94	0.49
1:D:1521:LYS:HG3	1:D:1529:THR:HB	1.95	0.49
1:A:700:PRO:HA	1:A:703:THR:HG22	1.95	0.49
1:A:1836:TYR:HE1	1:A:1935:LEU:HG	1.78	0.49
1:D:611:GLN:O	1:D:615:LEU:HB2	2.12	0.49
1:D:1562:GLY:O	1:D:1627:TYR:OH	2.29	0.49
1:E:1562:GLY:O	1:E:1627:TYR:OH	2.29	0.49
1:E:1836:TYR:HE1	1:E:1935:LEU:HG	1.78	0.49
1:B:1122:ILE:HD13	1:B:1144:LEU:HD22	1.94	0.49
1:B:1248:THR:HA	1:B:1251:LEU:HD13	1.94	0.49
1:E:2286:TRP:O	1:E:2290:ASP:N	2.36	0.49
1:B:700:PRO:HA	1:B:703:THR:HG22	1.95	0.49
1:C:611:GLN:O	1:C:615:LEU:HB2	2.12	0.49
1:C:2142:ASP:OD1	1:D:2083:TYR:OH	2.28	0.49
1:E:925:GLY:HA2	1:E:928:ARG:HE	1.77	0.49
1:E:1249:HIS:HB3	1:E:1543:GLN:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2326:SER:N	1:E:2340:ASP:OD1	2.46	0.49
1:A:1249:HIS:HB3	1:A:1543:GLN:HG2	1.95	0.48
1:B:1454:SER:H	1:B:1480:ARG:HH21	1.61	0.48
1:D:607:LEU:HD21	1:D:615:LEU:HD22	1.95	0.48
1:D:700:PRO:HA	1:D:703:THR:HG22	1.95	0.48
1:D:1836:TYR:HE1	1:D:1935:LEU:HG	1.77	0.48
1:D:2182:ARG:NH1	1:D:2186:GLU:OE2	2.46	0.48
1:E:611:GLN:O	1:E:615:LEU:HB2	2.12	0.48
1:C:703:THR:HG21	1:C:711:THR:HA	1.94	0.48
1:C:927:TYR:O	1:C:931:VAL:N	2.38	0.48
1:D:21:VAL:O	1:D:1885:LYS:NZ	2.46	0.48
1:D:1910:THR:HG21	1:D:1915:PRO:HD3	1.95	0.48
1:D:2123:PRO:HB3	1:E:2096:LEU:HG	1.95	0.48
1:A:1613:ASP:HB3	1:A:1616:THR:HG22	1.96	0.48
1:B:1836:TYR:HE1	1:B:1935:LEU:HG	1.78	0.48
1:D:1249:HIS:HB3	1:D:1543:GLN:HG2	1.95	0.48
1:E:1613:ASP:HB3	1:E:1616:THR:HG22	1.96	0.48
1:A:1910:THR:HG21	1:A:1915:PRO:HD3	1.96	0.48
1:A:2326:SER:N	1:A:2340:ASP:OD1	2.46	0.48
1:B:1521:LYS:HG3	1:B:1529:THR:HB	1.95	0.48
1:C:700:PRO:HA	1:C:703:THR:HG22	1.95	0.48
1:D:419:LYS:HG3	1:D:424:ALA:HB3	1.95	0.48
1:E:1122:ILE:HD13	1:E:1144:LEU:HD22	1.94	0.48
1:E:1893:ARG:HD3	1:E:1899:LEU:HD23	1.95	0.48
1:E:2247:TRP:O	1:E:2367:ARG:NH2	2.38	0.48
1:A:1454:SER:H	1:A:1480:ARG:HH21	1.61	0.48
1:B:607:LEU:HD21	1:B:615:LEU:HD22	1.95	0.48
1:E:511:ILE:HG23	1:E:522:HIS:HD2	1.78	0.48
1:E:1910:THR:HG21	1:E:1915:PRO:HD3	1.96	0.48
1:A:1145:LEU:HD12	1:A:1167:LEU:HD13	1.95	0.48
1:A:2142:ASP:OD1	1:B:2083:TYR:OH	2.27	0.48
1:A:2419:PHE:HE2	1:E:2415:PHE:HB2	1.78	0.48
1:C:21:VAL:O	1:C:1885:LYS:NZ	2.46	0.48
1:C:1910:THR:HG21	1:C:1915:PRO:HD3	1.96	0.48
1:D:250:GLU:O	1:D:452:LYS:NZ	2.40	0.48
1:E:375:GLY:N	1:E:415:GLY:O	2.47	0.48
1:A:1893:ARG:HD3	1:A:1899:LEU:HD23	1.95	0.48
1:B:375:GLY:N	1:B:415:GLY:O	2.47	0.48
1:B:1145:LEU:HD12	1:B:1167:LEU:HD13	1.95	0.48
1:B:1613:ASP:HB3	1:B:1616:THR:HG22	1.96	0.48
1:B:2182:ARG:NH1	1:B:2186:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1249:HIS:HB3	1:C:1543:GLN:HG2	1.95	0.48
1:C:1454:SER:H	1:C:1480:ARG:HH21	1.61	0.48
1:D:1248:THR:HA	1:D:1251:LEU:HD13	1.94	0.48
1:D:2229:ARG:HG3	1:E:2277:LEU:HD11	1.96	0.48
1:D:2251:ASP:OD2	1:D:2289:ARG:NH1	2.47	0.48
1:E:419:LYS:HG3	1:E:424:ALA:HB3	1.95	0.48
1:A:2182:ARG:NH1	1:A:2186:GLU:OE2	2.46	0.48
1:B:2251:ASP:OD2	1:B:2289:ARG:NH1	2.47	0.48
1:C:607:LEU:HD21	1:C:615:LEU:HD22	1.95	0.48
1:D:1613:ASP:HB3	1:D:1616:THR:HG22	1.96	0.48
1:A:1521:LYS:HG3	1:A:1529:THR:HB	1.95	0.48
1:B:21:VAL:O	1:B:1885:LYS:NZ	2.46	0.48
1:B:927:TYR:O	1:B:931:VAL:N	2.38	0.48
1:B:1249:HIS:HB3	1:B:1543:GLN:HG2	1.95	0.48
1:C:1836:TYR:HE1	1:C:1935:LEU:HG	1.78	0.48
1:D:287:GLU:OE2	1:D:928:ARG:NH2	2.47	0.48
1:E:1145:LEU:HD12	1:E:1167:LEU:HD13	1.95	0.48
1:E:1521:LYS:HG3	1:E:1529:THR:HB	1.95	0.48
1:A:1562:GLY:O	1:A:1627:TYR:OH	2.29	0.48
1:C:2247:TRP:O	1:C:2367:ARG:NH2	2.38	0.48
1:C:2326:SER:N	1:C:2340:ASP:OD1	2.46	0.48
1:D:925:GLY:HA2	1:D:928:ARG:HE	1.77	0.48
1:A:1865:ILE:HA	1:E:294:GLN:HE22	1.78	0.47
1:B:419:LYS:HG3	1:B:424:ALA:HB3	1.95	0.47
1:B:1910:THR:HG21	1:B:1915:PRO:HD3	1.96	0.47
1:C:419:LYS:HG3	1:C:424:ALA:HB3	1.95	0.47
1:D:1893:ARG:HD3	1:D:1899:LEU:HD23	1.95	0.47
1:D:2326:SER:N	1:D:2340:ASP:OD1	2.46	0.47
1:E:700:PRO:HA	1:E:703:THR:HG22	1.95	0.47
1:C:1893:ARG:HD3	1:C:1899:LEU:HD23	1.95	0.47
1:E:2182:ARG:NH1	1:E:2186:GLU:OE2	2.46	0.47
1:C:511:ILE:HG23	1:C:522:HIS:HD2	1.78	0.47
1:E:21:VAL:O	1:E:1885:LYS:NZ	2.46	0.47
1:A:21:VAL:O	1:A:1885:LYS:NZ	2.46	0.47
1:A:1132:MET:HB3	1:A:1197:LEU:HD23	1.97	0.47
1:A:1769:TRP:HA	1:A:1772:TYR:HD2	1.80	0.47
1:A:2229:ARG:HD2	1:B:2277:LEU:HD21	1.95	0.47
1:C:375:GLY:N	1:C:415:GLY:O	2.47	0.47
1:E:287:GLU:OE2	1:E:928:ARG:NH2	2.46	0.47
1:E:1198:TYR:N	1:E:1211:ALA:O	2.46	0.47
1:B:1132:MET:HB3	1:B:1197:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1893:ARG:HD3	1:B:1899:LEU:HD23	1.95	0.47
1:C:1145:LEU:HD12	1:C:1167:LEU:HD13	1.95	0.47
1:C:1198:TYR:N	1:C:1211:ALA:O	2.46	0.47
1:C:1769:TRP:HA	1:C:1772:TYR:HD2	1.80	0.47
1:D:1198:TYR:N	1:D:1211:ALA:O	2.46	0.47
1:D:2163:ASN:OD1	1:E:2060:ARG:NH1	2.43	0.47
1:E:1454:SER:H	1:E:1480:ARG:HH21	1.61	0.47
1:B:2326:SER:N	1:B:2340:ASP:OD1	2.46	0.47
1:B:2353:ASN:HB3	1:B:2356:ASP:HB2	1.97	0.47
1:E:2251:ASP:OD2	1:E:2289:ARG:NH1	2.47	0.47
1:A:158:ASN:HD21	1:E:518:GLY:HA3	1.80	0.47
1:A:419:LYS:HG3	1:A:424:ALA:HB3	1.95	0.47
1:A:1124:CYS:SG	1:A:1125:ALA:N	2.88	0.47
1:A:1592:GLN:OE1	1:A:1787:ARG:N	2.46	0.47
1:C:171:GLU:OE2	1:C:187:TYR:OH	2.30	0.47
1:D:375:GLY:N	1:D:415:GLY:O	2.47	0.47
1:D:511:ILE:HG23	1:D:522:HIS:HD2	1.78	0.47
1:D:1454:SER:H	1:D:1480:ARG:HH21	1.61	0.47
1:E:720:TRP:HB2	1:E:780:SER:HA	1.97	0.47
1:E:1769:TRP:HA	1:E:1772:TYR:HD2	1.80	0.47
1:B:1769:TRP:HA	1:B:1772:TYR:HD2	1.80	0.47
1:C:2353:ASN:HB3	1:C:2356:ASP:HB2	1.97	0.47
1:D:1612:TYR:HB3	1:D:1646:VAL:HG12	1.97	0.47
1:E:1132:MET:HB3	1:E:1197:LEU:HD23	1.97	0.47
1:A:2251:ASP:OD2	1:A:2289:ARG:NH1	2.47	0.47
1:A:287:GLU:OE2	1:A:928:ARG:NH2	2.47	0.47
1:A:375:GLY:N	1:A:415:GLY:O	2.47	0.47
1:A:720:TRP:HB2	1:A:780:SER:HA	1.97	0.47
1:C:287:GLU:OE2	1:C:928:ARG:NH2	2.47	0.47
1:C:300:GLU:OE2	1:C:446:TRP:NE1	2.37	0.47
1:C:1132:MET:HB3	1:C:1197:LEU:HD23	1.97	0.47
1:C:2251:ASP:OD2	1:C:2289:ARG:NH1	2.47	0.47
1:A:1546:ILE:HG13	1:A:1560:TRP:HB3	1.97	0.46
1:A:2299:THR:HG21	1:E:2382:TYR:HB3	1.95	0.46
1:B:354:ASN:HD22	1:B:404:ASP:HA	1.81	0.46
1:B:1717:LEU:HD12	1:B:1719:GLU:H	1.80	0.46
1:D:533:ASN:HD21	1:E:897:GLY:H	1.62	0.46
1:D:1132:MET:HB3	1:D:1197:LEU:HD23	1.97	0.46
1:D:1145:LEU:HD12	1:D:1167:LEU:HD13	1.95	0.46
1:D:1998:LEU:HD12	1:D:2230:PHE:HD2	1.80	0.46
1:E:1612:TYR:HB3	1:E:1646:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1710:ASN:HD22	1:E:1711:ASN:H	1.63	0.46
1:E:1717:LEU:HD12	1:E:1719:GLU:H	1.80	0.46
1:A:693:THR:HA	1:A:696:THR:HG22	1.98	0.46
1:A:1998:LEU:HD12	1:A:2230:PHE:HD2	1.80	0.46
1:A:2353:ASN:HB3	1:A:2356:ASP:HB2	1.97	0.46
1:B:1283:ASP:H	1:B:1307:THR:HG23	1.81	0.46
1:C:693:THR:HA	1:C:696:THR:HG22	1.97	0.46
1:C:1124:CYS:SG	1:C:1125:ALA:N	2.88	0.46
1:C:1546:ILE:HG13	1:C:1560:TRP:HB3	1.97	0.46
1:C:1998:LEU:HD12	1:C:2230:PHE:HD2	1.80	0.46
1:D:1717:LEU:HD12	1:D:1719:GLU:H	1.80	0.46
1:E:1283:ASP:H	1:E:1307:THR:HG23	1.80	0.46
1:B:693:THR:HA	1:B:696:THR:HG22	1.97	0.46
1:B:1124:CYS:SG	1:B:1125:ALA:N	2.88	0.46
1:B:1509:ILE:HA	1:B:1510:ASN:HA	1.64	0.46
1:B:1612:TYR:HB3	1:B:1646:VAL:HG12	1.97	0.46
1:C:720:TRP:HB2	1:C:780:SER:HA	1.97	0.46
1:C:1562:GLY:O	1:C:1627:TYR:OH	2.29	0.46
1:C:1613:ASP:HB3	1:C:1616:THR:HG22	1.96	0.46
1:D:1710:ASN:HD22	1:D:1711:ASN:H	1.63	0.46
1:D:2347:PHE:H	1:D:2438:LEU:H	1.63	0.46
1:A:249:THR:HG23	1:A:480:GLU:HG2	1.98	0.46
1:A:354:ASN:HD22	1:A:404:ASP:HA	1.81	0.46
1:A:1198:TYR:N	1:A:1211:ALA:O	2.46	0.46
1:A:2292:ARG:HH12	1:E:2414:LEU:HD21	1.81	0.46
1:B:249:THR:HG23	1:B:480:GLU:HG2	1.98	0.46
1:B:1998:LEU:HD12	1:B:2230:PHE:HD2	1.80	0.46
1:B:2247:TRP:O	1:B:2367:ARG:NH2	2.38	0.46
1:D:1124:CYS:SG	1:D:1125:ALA:N	2.88	0.46
1:E:249:THR:HG23	1:E:480:GLU:HG2	1.98	0.46
1:A:1250:GLN:NE2	1:A:1261:THR:OG1	2.36	0.46
1:A:1708:SER:OG	1:A:1709:VAL:N	2.49	0.46
1:A:2388:ILE:O	1:A:2441:SER:N	2.44	0.46
1:B:2347:PHE:H	1:B:2438:LEU:H	1.63	0.46
1:C:1717:LEU:HD12	1:C:1719:GLU:H	1.80	0.46
1:D:249:THR:HG23	1:D:480:GLU:HG2	1.98	0.46
1:D:720:TRP:HB2	1:D:780:SER:HA	1.97	0.46
1:D:1283:ASP:H	1:D:1307:THR:HG23	1.80	0.46
1:E:2347:PHE:H	1:E:2438:LEU:H	1.63	0.46
1:C:2347:PHE:H	1:C:2438:LEU:H	1.63	0.46
1:D:1546:ILE:HG13	1:D:1560:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:THR:HG23	1:C:480:GLU:HG2	1.98	0.46
1:C:1250:GLN:NE2	1:C:1261:THR:OG1	2.36	0.46
1:C:1708:SER:OG	1:C:1709:VAL:N	2.49	0.46
1:D:1769:TRP:HA	1:D:1772:TYR:HD2	1.80	0.46
1:E:1713:THR:HA	1:E:1717:LEU:HD21	1.98	0.46
1:A:1509:ILE:HA	1:A:1510:ASN:HA	1.64	0.46
1:A:2247:TRP:O	1:A:2367:ARG:NH2	2.38	0.46
1:C:1613:ASP:H	1:C:1617:HIS:CD2	2.33	0.46
1:E:2353:ASN:HB3	1:E:2356:ASP:HB2	1.97	0.46
1:B:171:GLU:OE2	1:B:187:TYR:OH	2.30	0.46
1:B:287:GLU:OE2	1:B:928:ARG:NH2	2.47	0.46
1:B:720:TRP:HB2	1:B:780:SER:HA	1.97	0.46
1:B:1198:TYR:N	1:B:1211:ALA:O	2.46	0.46
1:E:693:THR:HA	1:E:696:THR:HG22	1.98	0.46
1:E:1124:CYS:SG	1:E:1125:ALA:N	2.88	0.46
1:A:1612:TYR:HB3	1:A:1646:VAL:HG12	1.97	0.46
1:A:1710:ASN:HD22	1:A:1711:ASN:H	1.64	0.46
1:A:1717:LEU:HD12	1:A:1719:GLU:H	1.80	0.46
1:B:1546:ILE:HG13	1:B:1560:TRP:HB3	1.97	0.46
1:B:1708:SER:OG	1:B:1709:VAL:N	2.49	0.46
1:B:1613:ASP:H	1:B:1617:HIS:CD2	2.33	0.45
1:C:457:ALA:HA	1:C:467:THR:HG21	1.98	0.45
1:D:693:THR:HA	1:D:696:THR:HG22	1.97	0.45
1:D:1713:THR:HA	1:D:1717:LEU:HD21	1.98	0.45
1:E:1708:SER:OG	1:E:1709:VAL:N	2.49	0.45
1:B:1713:THR:HA	1:B:1717:LEU:HD21	1.98	0.45
1:E:1646:VAL:HG11	1:E:1900:LEU:HD21	1.99	0.45
1:C:354:ASN:HD22	1:C:404:ASP:HA	1.81	0.45
1:C:1612:TYR:HB3	1:C:1646:VAL:HG12	1.97	0.45
1:C:1710:ASN:HD22	1:C:1711:ASN:H	1.64	0.45
1:E:1546:ILE:HG13	1:E:1560:TRP:HB3	1.97	0.45
1:A:1713:THR:HA	1:A:1717:LEU:HD21	1.98	0.45
1:A:2038:GLN:HA	1:A:2041:THR:HG22	1.99	0.45
1:B:2306:TYR:HB3	1:B:2312:THR:HA	1.98	0.45
1:C:679:ASP:OD1	1:C:683:ASN:ND2	2.50	0.45
1:D:2353:ASN:HB3	1:D:2356:ASP:HB2	1.97	0.45
1:A:2347:PHE:H	1:A:2438:LEU:H	1.63	0.45
1:B:1140:SER:HB3	1:C:1580:ASN:HD22	1.82	0.45
1:B:1710:ASN:HD22	1:B:1711:ASN:H	1.64	0.45
1:C:1283:ASP:H	1:C:1307:THR:HG23	1.80	0.45
1:C:1646:VAL:HG11	1:C:1900:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2306:TYR:HB3	1:C:2312:THR:HA	1.98	0.45
1:D:679:ASP:OD1	1:D:683:ASN:ND2	2.50	0.45
1:D:885:VAL:HG13	1:D:886:ARG:HD2	1.99	0.45
1:D:1250:GLN:NE2	1:D:1261:THR:OG1	2.36	0.45
1:E:885:VAL:HG13	1:E:886:ARG:HD2	1.99	0.45
1:E:1998:LEU:HD12	1:E:2230:PHE:HD2	1.80	0.45
1:A:1283:ASP:H	1:A:1307:THR:HG23	1.80	0.45
1:A:2273:GLU:HG3	1:E:2001:PHE:CE1	2.52	0.45
1:B:1016:PRO:HD2	1:B:1815:HIS:CD2	2.52	0.45
1:B:1646:VAL:HG11	1:B:1900:LEU:HD21	1.99	0.45
1:D:354:ASN:HD22	1:D:404:ASP:HA	1.81	0.45
1:E:522:HIS:HA	1:E:525:ARG:HG2	1.99	0.45
1:E:2388:ILE:HB	1:E:2441:SER:HB3	1.99	0.45
1:A:528:ASN:ND2	1:A:537:TYR:H	2.14	0.45
1:A:885:VAL:HG13	1:A:886:ARG:HD2	1.99	0.45
1:B:2038:GLN:HA	1:B:2041:THR:HG22	1.99	0.45
1:C:1259:VAL:HG13	1:C:1546:ILE:HG23	1.99	0.45
1:D:457:ALA:HA	1:D:467:THR:HG21	1.98	0.45
1:D:2306:TYR:HB3	1:D:2312:THR:HA	1.98	0.45
1:A:2292:ARG:HB2	1:E:2399:GLY:C	2.37	0.45
1:A:2388:ILE:HB	1:A:2441:SER:HB3	1.99	0.45
1:B:175:MET:HA	1:B:178:THR:HG22	1.99	0.45
1:B:528:ASN:ND2	1:B:537:TYR:H	2.14	0.45
1:C:667:PRO:HB3	1:C:754:ALA:HB2	1.99	0.45
1:C:1713:THR:HA	1:C:1717:LEU:HD21	1.98	0.45
1:D:1613:ASP:H	1:D:1617:HIS:CD2	2.33	0.45
1:D:1708:SER:OG	1:D:1709:VAL:N	2.49	0.45
1:D:2216:TYR:HE1	1:E:2006:LEU:HD21	1.82	0.45
1:E:354:ASN:HD22	1:E:404:ASP:HA	1.81	0.45
1:E:528:ASN:ND2	1:E:537:TYR:H	2.14	0.45
1:A:125:ARG:HB2	1:A:1879:ALA:HB1	1.99	0.45
1:A:171:GLU:OE2	1:A:187:TYR:OH	2.30	0.45
1:A:1037:GLU:HG2	1:E:2082:LEU:HD11	1.99	0.45
1:A:2058:GLN:HA	1:A:2168:ILE:HD11	1.99	0.45
1:B:679:ASP:OD1	1:B:683:ASN:ND2	2.50	0.45
1:D:62:ILE:HA	1:D:65:THR:HG22	1.99	0.45
1:D:438:HIS:HA	1:D:439:PRO:HD3	1.84	0.45
1:D:522:HIS:HA	1:D:525:ARG:HG2	1.99	0.45
1:D:2058:GLN:HA	1:D:2168:ILE:HD11	1.99	0.45
1:E:927:TYR:O	1:E:931:VAL:N	2.38	0.45
1:A:522:HIS:HA	1:A:525:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HB2	1:D:1879:ALA:HB1	1.99	0.45
1:D:916:GLU:HA	1:D:919:ARG:HG2	1.99	0.45
1:D:1509:ILE:HA	1:D:1510:ASN:HA	1.64	0.45
1:E:679:ASP:OD1	1:E:683:ASN:ND2	2.50	0.45
1:E:803:ARG:NH2	1:E:863:ASP:OD1	2.46	0.45
1:E:1824:LEU:HD22	1:E:1857:LEU:HD11	1.99	0.45
1:E:2306:TYR:HB3	1:E:2312:THR:HA	1.98	0.45
1:A:1824:LEU:HD22	1:A:1857:LEU:HD11	1.99	0.44
1:B:125:ARG:HB2	1:B:1879:ALA:HB1	1.99	0.44
1:B:667:PRO:HB3	1:B:754:ALA:HB2	1.99	0.44
1:C:522:HIS:HA	1:C:525:ARG:HG2	1.99	0.44
1:C:1016:PRO:HD2	1:C:1815:HIS:CD2	2.52	0.44
1:D:803:ARG:NH2	1:D:863:ASP:OD1	2.46	0.44
1:D:1016:PRO:HD2	1:D:1815:HIS:CD2	2.52	0.44
1:E:708:LEU:HD11	1:E:717:LEU:HD13	2.00	0.44
1:A:175:MET:HA	1:A:178:THR:HG22	1.99	0.44
1:A:916:GLU:HA	1:A:919:ARG:HG2	1.99	0.44
1:A:1259:VAL:HG13	1:A:1546:ILE:HG23	1.99	0.44
1:A:1646:VAL:HG11	1:A:1900:LEU:HD21	1.99	0.44
1:B:2388:ILE:HB	1:B:2441:SER:HB3	1.99	0.44
1:C:62:ILE:HA	1:C:65:THR:HG22	1.99	0.44
1:C:916:GLU:HA	1:C:919:ARG:HG2	1.99	0.44
1:C:1983:ARG:N	1:C:2422:GLY:O	2.51	0.44
1:E:916:GLU:HA	1:E:919:ARG:HG2	1.99	0.44
1:C:708:LEU:HD11	1:C:717:LEU:HD13	2.00	0.44
1:D:708:LEU:HD11	1:D:717:LEU:HD13	2.00	0.44
1:D:1824:LEU:HD22	1:D:1857:LEU:HD11	1.99	0.44
1:D:2286:TRP:O	1:D:2290:ASP:N	2.36	0.44
1:A:1472:ILE:HG23	1:A:1475:SER:H	1.83	0.44
1:A:2009:ILE:HG21	1:E:2210:PHE:HD2	1.82	0.44
1:B:522:HIS:HA	1:B:525:ARG:HG2	1.99	0.44
1:B:1259:VAL:HG13	1:B:1546:ILE:HG23	1.99	0.44
1:C:1756:ARG:HA	1:C:1756:ARG:HD2	1.76	0.44
1:E:62:ILE:HA	1:E:65:THR:HG22	1.99	0.44
1:E:457:ALA:HA	1:E:467:THR:HG21	1.98	0.44
1:A:679:ASP:OD1	1:A:683:ASN:ND2	2.50	0.44
1:A:1016:PRO:HD2	1:A:1815:HIS:CD2	2.52	0.44
1:B:885:VAL:HG13	1:B:886:ARG:HD2	1.99	0.44
1:C:885:VAL:HG13	1:C:886:ARG:HD2	1.99	0.44
1:E:1833:ASP:OD1	1:E:1851:TYR:OH	2.33	0.44
1:A:776:LEU:O	1:A:780:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:ILE:HD12	1:A:1560:TRP:HB2	2.00	0.44
1:A:2306:TYR:HB3	1:A:2312:THR:HA	1.98	0.44
1:B:133:LYS:HA	1:B:138:ASN:HD22	1.83	0.44
1:B:776:LEU:O	1:B:780:SER:N	2.51	0.44
1:B:1592:GLN:OE1	1:B:1787:ARG:N	2.46	0.44
1:B:1824:LEU:HD22	1:B:1857:LEU:HD11	1.99	0.44
1:D:2038:GLN:HA	1:D:2041:THR:HG22	1.99	0.44
1:E:527:PHE:O	1:E:560:ARG:NH2	2.50	0.44
1:E:2058:GLN:HA	1:E:2168:ILE:HD11	1.99	0.44
1:A:288:LEU:HD13	1:A:464:PRO:HG3	2.00	0.44
1:B:916:GLU:HA	1:B:919:ARG:HG2	1.99	0.44
1:B:2058:GLN:HA	1:B:2168:ILE:HD11	1.99	0.44
1:D:1646:VAL:HG11	1:D:1900:LEU:HD21	1.99	0.44
1:E:667:PRO:HB3	1:E:754:ALA:HB2	1.99	0.44
1:E:776:LEU:O	1:E:780:SER:N	2.51	0.44
1:E:1592:GLN:OE1	1:E:1787:ARG:N	2.46	0.44
1:E:1613:ASP:H	1:E:1617:HIS:CD2	2.33	0.44
1:A:457:ALA:HA	1:A:467:THR:HG21	1.98	0.44
1:B:62:ILE:HA	1:B:65:THR:HG22	1.99	0.44
1:B:178:THR:HG23	1:B:180:LYS:H	1.83	0.44
1:B:1472:ILE:HG23	1:B:1475:SER:H	1.83	0.44
1:C:2038:GLN:HA	1:C:2041:THR:HG22	1.99	0.44
1:D:667:PRO:HB3	1:D:754:ALA:HB2	1.99	0.44
1:E:175:MET:HA	1:E:178:THR:HG22	1.99	0.44
1:E:1016:PRO:HD2	1:E:1815:HIS:CD2	2.52	0.44
1:E:2038:GLN:HA	1:E:2041:THR:HG22	1.99	0.44
1:A:178:THR:HG23	1:A:180:LYS:H	1.83	0.44
1:B:1078:ILE:HD12	1:B:1560:TRP:HB2	2.00	0.44
1:C:133:LYS:HA	1:C:138:ASN:HD22	1.83	0.44
1:C:178:THR:HG23	1:C:180:LYS:H	1.83	0.44
1:C:1303:ILE:HG22	1:C:1495:PRO:HA	2.00	0.44
1:D:175:MET:HA	1:D:178:THR:HG22	1.99	0.44
1:D:1983:ARG:N	1:D:2422:GLY:O	2.51	0.44
1:E:288:LEU:HD13	1:E:464:PRO:HG3	2.00	0.44
1:A:667:PRO:HB3	1:A:754:ALA:HB2	1.99	0.43
1:B:457:ALA:HA	1:B:467:THR:HG21	1.98	0.43
1:B:708:LEU:HD11	1:B:717:LEU:HD13	2.00	0.43
1:B:2065:ARG:HG2	1:B:2161:LYS:HD2	2.00	0.43
1:C:175:MET:HA	1:C:178:THR:HG22	1.99	0.43
1:C:776:LEU:O	1:C:780:SER:N	2.51	0.43
1:C:1472:ILE:HG23	1:C:1475:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:THR:HG23	1:D:180:LYS:H	1.83	0.43
1:E:1078:ILE:HD12	1:E:1560:TRP:HB2	2.00	0.43
1:A:133:LYS:HA	1:A:138:ASN:HD22	1.83	0.43
1:A:313:ASP:OD1	1:A:313:ASP:N	2.51	0.43
1:C:125:ARG:HB2	1:C:1879:ALA:HB1	1.99	0.43
1:C:1078:ILE:HD12	1:C:1560:TRP:HB2	2.00	0.43
1:C:1833:ASP:OD1	1:C:1851:TYR:OH	2.33	0.43
1:D:1303:ILE:HG22	1:D:1495:PRO:HA	2.00	0.43
1:D:1472:ILE:HG23	1:D:1475:SER:H	1.83	0.43
1:D:2388:ILE:HB	1:D:2441:SER:HB3	1.99	0.43
1:E:171:GLU:OE2	1:E:187:TYR:OH	2.30	0.43
1:E:1259:VAL:HG13	1:E:1546:ILE:HG23	1.99	0.43
1:A:708:LEU:HD11	1:A:717:LEU:HD13	2.00	0.43
1:A:942:ILE:HD12	1:A:942:ILE:HA	1.74	0.43
1:A:1613:ASP:H	1:A:1617:HIS:CD2	2.33	0.43
1:C:2065:ARG:HG2	1:C:2161:LYS:HD2	2.00	0.43
1:D:527:PHE:O	1:D:560:ARG:NH2	2.50	0.43
1:E:33:GLU:HG3	1:E:990:ARG:HH21	1.83	0.43
1:E:1159:ASP:OD1	1:E:1159:ASP:N	2.51	0.43
1:E:1472:ILE:HG23	1:E:1475:SER:H	1.83	0.43
1:A:33:GLU:HG3	1:A:990:ARG:HH21	1.83	0.43
1:C:33:GLU:HG3	1:C:990:ARG:HH21	1.83	0.43
1:C:1049:LEU:HD21	1:C:1769:TRP:HE1	1.83	0.43
1:E:178:THR:HG23	1:E:180:LYS:H	1.83	0.43
1:A:339:ASP:OD1	1:A:343:ALA:N	2.41	0.43
1:A:432:SER:OG	1:A:433:ALA:N	2.52	0.43
1:A:527:PHE:O	1:A:560:ARG:NH2	2.50	0.43
1:E:125:ARG:HB2	1:E:1879:ALA:HB1	1.99	0.43
1:E:838:GLN:HG2	1:E:873:LYS:HE3	2.00	0.43
1:A:62:ILE:HA	1:A:65:THR:HG22	1.99	0.43
1:A:598:VAL:HA	1:A:601:LEU:HD12	2.01	0.43
1:B:598:VAL:HA	1:B:601:LEU:HD12	2.01	0.43
1:B:2075:GLU:OE2	1:C:1756:ARG:NH1	2.50	0.43
1:C:730:LEU:HD21	1:C:751:LYS:HD3	2.01	0.43
1:D:33:GLU:HG3	1:D:990:ARG:HH21	1.83	0.43
1:D:776:LEU:O	1:D:780:SER:N	2.51	0.43
1:E:313:ASP:OD1	1:E:313:ASP:N	2.51	0.43
1:E:1983:ARG:N	1:E:2422:GLY:O	2.51	0.43
1:B:33:GLU:HG3	1:B:990:ARG:HH21	1.83	0.43
1:B:432:SER:OG	1:B:433:ALA:N	2.52	0.43
1:B:1159:ASP:OD1	1:B:1159:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1824:LEU:HD22	1:C:1857:LEU:HD11	1.99	0.43
1:C:2388:ILE:HB	1:C:2441:SER:HB3	1.99	0.43
1:D:133:LYS:HA	1:D:138:ASN:HD22	1.83	0.43
1:D:838:GLN:HG2	1:D:873:LYS:HE3	2.00	0.43
1:D:1172:TYR:HB3	1:E:1054:ARG:HE	1.83	0.43
1:D:1259:VAL:HG13	1:D:1546:ILE:HG23	1.99	0.43
1:A:1159:ASP:N	1:A:1159:ASP:OD1	2.51	0.43
1:A:2329:ILE:HG21	1:A:2344:HIS:HB3	2.01	0.43
1:B:838:GLN:HG2	1:B:873:LYS:HE3	2.00	0.43
1:B:2142:ASP:OD1	1:C:2083:TYR:OH	2.30	0.43
1:E:1303:ILE:HG22	1:E:1495:PRO:HA	2.00	0.43
1:A:2065:ARG:HG2	1:A:2161:LYS:HD2	2.00	0.43
1:C:432:SER:OG	1:C:433:ALA:N	2.52	0.43
1:C:527:PHE:O	1:C:560:ARG:NH2	2.50	0.43
1:C:1509:ILE:HA	1:C:1510:ASN:HA	1.64	0.43
1:D:399:ILE:HA	1:D:400:PRO:HD3	1.91	0.43
1:D:1049:LEU:HD21	1:D:1769:TRP:HE1	1.83	0.43
1:D:1078:ILE:HD12	1:D:1560:TRP:HB2	2.00	0.43
1:A:1515:THR:HB	1:A:1534:LEU:HD11	2.01	0.43
1:B:250:GLU:O	1:B:452:LYS:NZ	2.40	0.43
1:B:288:LEU:HD13	1:B:464:PRO:HG3	2.00	0.43
1:C:1140:SER:HB3	1:D:1580:ASN:HD22	1.83	0.43
1:C:2058:GLN:HA	1:C:2168:ILE:HD11	1.99	0.43
1:D:288:LEU:HD13	1:D:464:PRO:HG3	2.00	0.43
1:D:598:VAL:HA	1:D:601:LEU:HD12	2.01	0.43
1:D:1306:PRO:O	1:D:1491:THR:OG1	2.31	0.43
1:E:438:HIS:HA	1:E:439:PRO:HD3	1.84	0.43
1:E:1049:LEU:HD21	1:E:1769:TRP:HE1	1.83	0.43
1:C:528:ASN:ND2	1:C:537:TYR:H	2.14	0.42
1:E:131:HIS:ND1	1:E:971:TYR:OH	2.47	0.42
1:E:598:VAL:HA	1:E:601:LEU:HD12	2.01	0.42
1:A:332:GLU:OE2	1:A:438:HIS:NE2	2.53	0.42
1:A:803:ARG:NH2	1:A:863:ASP:OD1	2.46	0.42
1:B:131:HIS:ND1	1:B:971:TYR:OH	2.47	0.42
1:C:339:ASP:OD1	1:C:343:ALA:N	2.41	0.42
1:C:598:VAL:HA	1:C:601:LEU:HD12	2.01	0.42
1:E:133:LYS:HA	1:E:138:ASN:HD22	1.83	0.42
1:E:432:SER:OG	1:E:433:ALA:N	2.52	0.42
1:E:730:LEU:HD21	1:E:751:LYS:HD3	2.01	0.42
1:E:1509:ILE:HA	1:E:1510:ASN:HA	1.64	0.42
1:B:942:ILE:HD12	1:B:942:ILE:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:THR:HB	1:B:1534:LEU:HD11	2.01	0.42
1:C:942:ILE:HA	1:C:942:ILE:HD12	1.74	0.42
1:C:2210:PHE:HD2	1:D:2009:ILE:HG21	1.83	0.42
1:E:2329:ILE:HG21	1:E:2344:HIS:HB3	2.01	0.42
1:A:730:LEU:HD21	1:A:751:LYS:HD3	2.01	0.42
1:C:838:GLN:HG2	1:C:873:LYS:HE3	2.00	0.42
1:C:1159:ASP:N	1:C:1159:ASP:OD1	2.51	0.42
1:D:528:ASN:ND2	1:D:537:TYR:H	2.14	0.42
1:D:2065:ARG:HG2	1:D:2161:LYS:HD2	2.00	0.42
1:A:1023:THR:HG21	1:E:2078:ARG:HH21	1.85	0.42
1:A:1255:THR:HG23	1:A:1256:THR:HG23	2.01	0.42
1:B:1983:ARG:N	1:B:2422:GLY:O	2.51	0.42
1:B:2347:PHE:O	1:B:2438:LEU:N	2.49	0.42
1:C:1462:ILE:HG13	1:C:1518:VAL:HG22	2.01	0.42
1:C:1592:GLN:OE1	1:C:1787:ARG:N	2.46	0.42
1:D:432:SER:OG	1:D:433:ALA:N	2.52	0.42
1:A:220:PRO:HB2	1:A:230:PHE:CE1	2.55	0.42
1:A:1049:LEU:HD21	1:A:1769:TRP:HE1	1.83	0.42
1:A:1485:PRO:HB2	1:A:1490:GLU:HG3	2.01	0.42
1:A:2347:PHE:O	1:A:2438:LEU:N	2.49	0.42
1:B:1303:ILE:HG22	1:B:1495:PRO:HA	2.00	0.42
1:C:288:LEU:HD13	1:C:464:PRO:HG3	2.00	0.42
1:C:1255:THR:HG23	1:C:1256:THR:HG23	2.01	0.42
1:C:1606:THR:HA	1:C:1653:LYS:HA	2.02	0.42
1:D:730:LEU:HD21	1:D:751:LYS:HD3	2.01	0.42
1:D:1485:PRO:HB2	1:D:1490:GLU:HG3	2.01	0.42
1:E:1255:THR:HG23	1:E:1256:THR:HG23	2.01	0.42
1:E:2259:SER:OG	1:E:2260:GLY:N	2.53	0.42
1:A:1303:ILE:HG22	1:A:1495:PRO:HA	2.00	0.42
1:A:1950:VAL:HG13	1:E:906:GLN:HE21	1.83	0.42
1:A:2286:TRP:O	1:A:2290:ASP:N	2.36	0.42
1:B:332:GLU:OE2	1:B:438:HIS:NE2	2.53	0.42
1:B:527:PHE:O	1:B:560:ARG:NH2	2.50	0.42
1:D:2030:LEU:HD21	1:E:1959:ALA:HA	2.01	0.42
1:E:332:GLU:OE2	1:E:438:HIS:NE2	2.53	0.42
1:E:1485:PRO:HB2	1:E:1490:GLU:HG3	2.01	0.42
1:A:838:GLN:HG2	1:A:873:LYS:HE3	2.00	0.42
1:B:1255:THR:HG23	1:B:1256:THR:HG23	2.01	0.42
1:B:1485:PRO:HB2	1:B:1490:GLU:HG3	2.01	0.42
1:D:300:GLU:OE2	1:D:446:TRP:NE1	2.37	0.42
1:E:220:PRO:HB2	1:E:230:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2065:ARG:HG2	1:E:2161:LYS:HD2	2.00	0.42
1:A:1866:PHE:HD2	1:E:298:ALA:HB1	1.84	0.42
1:A:2259:SER:OG	1:A:2260:GLY:N	2.53	0.42
1:C:313:ASP:OD1	1:C:313:ASP:N	2.51	0.42
1:C:332:GLU:OE2	1:C:438:HIS:NE2	2.53	0.42
1:C:545:LEU:HD23	1:C:547:GLU:H	1.85	0.42
1:D:1462:ILE:HG13	1:D:1518:VAL:HG22	2.01	0.42
1:D:2329:ILE:HG21	1:D:2344:HIS:HB3	2.01	0.42
1:A:1462:ILE:HG13	1:A:1518:VAL:HG22	2.01	0.42
1:B:299:ALA:HB1	1:B:305:LEU:HD13	2.02	0.42
1:B:300:GLU:OE2	1:B:446:TRP:NE1	2.37	0.42
1:B:339:ASP:OD1	1:B:343:ALA:N	2.41	0.42
1:C:1153:LYS:HA	1:C:1159:ASP:HA	2.02	0.42
1:D:942:ILE:HD12	1:D:942:ILE:HA	1.74	0.42
1:E:1999:MET:HE2	1:E:2273:GLU:HA	2.02	0.42
1:B:220:PRO:HB2	1:B:230:PHE:CE1	2.55	0.41
1:B:1049:LEU:HD21	1:B:1769:TRP:HE1	1.83	0.41
1:C:803:ARG:NH2	1:C:863:ASP:OD1	2.46	0.41
1:D:690:ASN:O	1:D:693:THR:OG1	2.34	0.41
1:D:1159:ASP:OD1	1:D:1159:ASP:N	2.51	0.41
1:D:1515:THR:HB	1:D:1534:LEU:HD11	2.01	0.41
1:D:1606:THR:HA	1:D:1653:LYS:HA	2.02	0.41
1:D:2372:SER:O	1:D:2463:HIS:N	2.45	0.41
1:B:399:ILE:HA	1:B:400:PRO:HD3	1.91	0.41
1:C:1070:SER:OG	1:C:1133:VAL:O	2.27	0.41
1:C:2396:LEU:HD21	1:C:2430:ILE:HG12	2.02	0.41
1:D:1105:LYS:HB2	1:D:1115:ALA:HB2	2.02	0.41
1:E:2372:SER:O	1:E:2463:HIS:N	2.45	0.41
1:A:1841:ARG:HD2	1:E:958:THR:HA	2.01	0.41
1:A:2396:LEU:HD21	1:A:2430:ILE:HG12	2.02	0.41
1:B:730:LEU:HD21	1:B:751:LYS:HD3	2.01	0.41
1:C:2284:GLN:HE21	1:C:2288:LYS:HE3	1.85	0.41
1:C:2329:ILE:HG21	1:C:2344:HIS:HB3	2.01	0.41
1:D:545:LEU:HD23	1:D:547:GLU:H	1.85	0.41
1:D:1609:LEU:HA	1:D:1717:LEU:HA	2.03	0.41
1:E:1077:ASN:OD1	1:E:1077:ASN:N	2.54	0.41
1:E:2009:ILE:O	1:E:2013:ASP:HB2	2.20	0.41
1:A:299:ALA:HB1	1:A:305:LEU:HD13	2.02	0.41
1:A:1140:SER:HB3	1:B:1580:ASN:HD22	1.84	0.41
1:B:1550:THR:HB	1:B:1556:GLN:HG2	2.02	0.41
1:B:1756:ARG:HA	1:B:1756:ARG:HD2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1515:THR:HB	1:C:1534:LEU:HD11	2.01	0.41
1:D:1255:THR:HG23	1:D:1256:THR:HG23	2.01	0.41
1:D:1267:SER:HA	1:D:1538:LYS:HA	2.03	0.41
1:D:2423:ARG:HB3	1:E:2292:ARG:HD3	2.02	0.41
1:A:2009:ILE:O	1:A:2013:ASP:HB2	2.21	0.41
1:A:2273:GLU:HG3	1:E:2001:PHE:HE1	1.86	0.41
1:B:1153:LYS:HA	1:B:1159:ASP:HA	2.02	0.41
1:B:1267:SER:HA	1:B:1538:LYS:HA	2.03	0.41
1:B:1609:LEU:HA	1:B:1717:LEU:HA	2.03	0.41
1:B:2329:ILE:HG21	1:B:2344:HIS:HB3	2.01	0.41
1:B:2372:SER:O	1:B:2463:HIS:N	2.45	0.41
1:C:1485:PRO:HB2	1:C:1490:GLU:HG3	2.01	0.41
1:C:2009:ILE:O	1:C:2013:ASP:HB2	2.21	0.41
1:D:2347:PHE:O	1:D:2438:LEU:N	2.49	0.41
1:E:1462:ILE:HG13	1:E:1518:VAL:HG22	2.01	0.41
1:A:1267:SER:HA	1:A:1538:LYS:HA	2.03	0.41
1:A:1756:ARG:HD2	1:A:1756:ARG:HA	1.76	0.41
1:B:2284:GLN:HE21	1:B:2288:LYS:HE3	1.85	0.41
1:B:2343:LEU:O	1:B:2442:PHE:N	2.54	0.41
1:C:2259:SER:OG	1:C:2260:GLY:N	2.53	0.41
1:D:332:GLU:OE2	1:D:438:HIS:NE2	2.53	0.41
1:D:339:ASP:OD1	1:D:343:ALA:N	2.41	0.41
1:D:547:GLU:HA	1:D:548:PRO:HD3	1.94	0.41
1:D:1846:GLU:O	1:D:1849:MET:HG2	2.21	0.41
1:E:339:ASP:OD1	1:E:343:ALA:N	2.41	0.41
1:E:1197:LEU:HA	1:E:1212:TRP:HA	2.03	0.41
1:E:1267:SER:HA	1:E:1538:LYS:HA	2.03	0.41
1:E:1489:ARG:HA	1:E:1489:ARG:HD2	1.93	0.41
1:A:1197:LEU:HA	1:A:1212:TRP:HA	2.03	0.41
1:A:1606:THR:HA	1:A:1653:LYS:HA	2.02	0.41
1:B:1105:LYS:HB2	1:B:1115:ALA:HB2	2.02	0.41
1:B:1197:LEU:HA	1:B:1212:TRP:HA	2.03	0.41
1:C:1267:SER:HA	1:C:1538:LYS:HA	2.03	0.41
1:A:300:GLU:OE2	1:A:446:TRP:NE1	2.37	0.41
1:B:545:LEU:HD23	1:B:547:GLU:H	1.85	0.41
1:B:1462:ILE:HG13	1:B:1518:VAL:HG22	2.01	0.41
1:B:1606:THR:HA	1:B:1653:LYS:HA	2.02	0.41
1:C:690:ASN:O	1:C:693:THR:OG1	2.34	0.41
1:C:1197:LEU:HA	1:C:1212:TRP:HA	2.03	0.41
1:C:1944:GLN:HA	1:C:1945:PRO:HD3	1.94	0.41
1:D:2259:SER:OG	1:D:2260:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:GLU:OE2	1:E:446:TRP:NE1	2.37	0.41
1:E:1606:THR:HA	1:E:1653:LYS:HA	2.02	0.41
1:A:870:ILE:HB	1:A:874:ASP:HB3	2.03	0.41
1:A:1153:LYS:HA	1:A:1159:ASP:HA	2.02	0.41
1:A:1455:SER:OG	1:A:1480:ARG:NH1	2.54	0.41
1:A:1609:LEU:HA	1:A:1717:LEU:HA	2.03	0.41
1:A:2210:PHE:HD2	1:B:2009:ILE:HG21	1.86	0.41
1:A:2284:GLN:HE21	1:A:2288:LYS:HE3	1.86	0.41
1:B:1833:ASP:OD1	1:B:1851:TYR:OH	2.33	0.41
1:B:2009:ILE:O	1:B:2013:ASP:HB2	2.21	0.41
1:C:250:GLU:O	1:C:452:LYS:NZ	2.40	0.41
1:D:220:PRO:HB2	1:D:230:PHE:CE1	2.55	0.41
1:D:313:ASP:OD1	1:D:313:ASP:N	2.51	0.41
1:D:1592:GLN:OE1	1:D:1787:ARG:N	2.46	0.41
1:D:2284:GLN:HE21	1:D:2288:LYS:HE3	1.85	0.41
1:D:2396:LEU:HD21	1:D:2430:ILE:HG12	2.02	0.41
1:E:194:ARG:HA	1:E:200:PRO:HG3	2.03	0.41
1:E:1153:LYS:HA	1:E:1159:ASP:HA	2.02	0.41
1:E:1515:THR:HB	1:E:1534:LEU:HD11	2.01	0.41
1:E:1515:THR:H	1:E:1534:LEU:HD11	1.86	0.41
1:E:1550:THR:HB	1:E:1556:GLN:HG2	2.02	0.41
1:E:1756:ARG:HD2	1:E:1756:ARG:HA	1.76	0.41
1:E:2396:LEU:HD21	1:E:2430:ILE:HG12	2.02	0.41
1:A:1550:THR:HB	1:A:1556:GLN:HG2	2.02	0.41
1:B:1515:THR:H	1:B:1534:LEU:HD11	1.86	0.41
1:C:220:PRO:HB2	1:C:230:PHE:CE1	2.55	0.41
1:C:414:ILE:N	1:C:433:ALA:O	2.53	0.41
1:C:870:ILE:HB	1:C:874:ASP:HB3	2.03	0.41
1:D:171:GLU:OE2	1:D:187:TYR:OH	2.30	0.41
1:D:1197:LEU:HA	1:D:1212:TRP:HA	2.03	0.41
1:D:1515:THR:H	1:D:1534:LEU:HD11	1.86	0.41
1:E:1105:LYS:HB2	1:E:1115:ALA:HB2	2.02	0.41
1:E:1455:SER:OG	1:E:1480:ARG:NH1	2.54	0.41
1:A:1077:ASN:OD1	1:A:1077:ASN:N	2.54	0.40
1:B:1846:GLU:O	1:B:1849:MET:HG2	2.21	0.40
1:C:299:ALA:HB1	1:C:305:LEU:HD13	2.02	0.40
1:C:438:HIS:HA	1:C:439:PRO:HD3	1.84	0.40
1:C:1550:THR:HB	1:C:1556:GLN:HG2	2.02	0.40
1:D:1153:LYS:HA	1:D:1159:ASP:HA	2.02	0.40
1:E:2284:GLN:HE21	1:E:2288:LYS:HE3	1.85	0.40
1:A:1105:LYS:HB2	1:A:1115:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:THR:H	1:A:1534:LEU:HD11	1.86	0.40
1:B:803:ARG:NH2	1:B:863:ASP:OD1	2.46	0.40
1:B:1455:SER:OG	1:B:1480:ARG:NH1	2.54	0.40
1:D:194:ARG:HA	1:D:200:PRO:HG3	2.03	0.40
1:D:1944:GLN:HA	1:D:1945:PRO:HD3	1.94	0.40
1:D:2009:ILE:O	1:D:2013:ASP:HB2	2.21	0.40
1:A:1983:ARG:N	1:A:2422:GLY:O	2.51	0.40
1:B:246:ASN:OD1	1:B:886:ARG:NH2	2.54	0.40
1:B:1566:ARG:NH1	1:B:1730:GLU:OE2	2.55	0.40
1:C:246:ASN:OD1	1:C:886:ARG:NH2	2.54	0.40
1:C:1609:LEU:HA	1:C:1717:LEU:HA	2.03	0.40
1:A:2411:ASP:OD1	1:A:2411:ASP:N	2.53	0.40
1:B:1192:TRP:CE2	1:B:1214:GLN:HB2	2.57	0.40
1:B:2117:SER:O	1:C:2108:ASN:ND2	2.41	0.40
1:D:1192:TRP:CE2	1:D:1214:GLN:HB2	2.57	0.40
1:D:1455:SER:OG	1:D:1480:ARG:NH1	2.54	0.40
1:D:1550:THR:HB	1:D:1556:GLN:HG2	2.02	0.40
1:E:1609:LEU:HA	1:E:1717:LEU:HA	2.03	0.40
1:A:250:GLU:O	1:A:452:LYS:NZ	2.40	0.40
1:A:317:LEU:HB3	1:A:333:LEU:HB2	2.04	0.40
1:C:1566:ARG:NH1	1:C:1730:GLU:OE2	2.55	0.40
1:C:1846:GLU:O	1:C:1849:MET:HG2	2.21	0.40
1:D:414:ILE:N	1:D:433:ALA:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2273/2469 (92%)	2119 (93%)	153 (7%)	1 (0%)	100	100
1	B	2273/2469 (92%)	2120 (93%)	152 (7%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	2273/2469 (92%)	2119 (93%)	153 (7%)	1 (0%)	100	100
1	D	2273/2469 (92%)	2118 (93%)	154 (7%)	1 (0%)	100	100
1	E	2273/2469 (92%)	2119 (93%)	153 (7%)	1 (0%)	100	100
All	All	11365/12345 (92%)	10595 (93%)	765 (7%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1709	VAL
1	B	1709	VAL
1	C	1709	VAL
1	D	1709	VAL
1	E	1709	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	B	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	C	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	D	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
1	E	1886/2101 (90%)	1879 (100%)	7 (0%)	91	95
All	All	9430/10505 (90%)	9395 (100%)	35 (0%)	91	95

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ARG
1	A	904	ASN
1	A	928	ARG
1	A	1188	ASN
1	A	1259	VAL

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Mol	Chain	Res	Type
1	A	1710	ASN
1	A	2255	ARG
1	B	304	ARG
1	B	904	ASN
1	B	928	ARG
1	B	1188	ASN
1	B	1259	VAL
1	B	1710	ASN
1	B	2255	ARG
1	C	304	ARG
1	C	904	ASN
1	C	928	ARG
1	C	1188	ASN
1	C	1259	VAL
1	C	1710	ASN
1	C	2255	ARG
1	D	304	ARG
1	D	904	ASN
1	D	928	ARG
1	D	1188	ASN
1	D	1259	VAL
1	D	1710	ASN
1	D	2255	ARG
1	E	304	ARG
1	E	904	ASN
1	E	928	ARG
1	E	1188	ASN
1	E	1259	VAL
1	E	1710	ASN
1	E	2255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	155	ASN
1	A	158	ASN
1	A	222	ASN
1	A	354	ASN
1	A	528	ASN
1	A	683	ASN
1	A	904	ASN

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Mol	Chain	Res	Type
1	A	1188	ASN
1	A	1222	ASN
1	A	1260	ASN
1	A	1264	ASN
1	A	1617	HIS
1	A	1710	ASN
1	A	1727	GLN
1	A	1767	ASN
1	A	1815	HIS
1	A	1883	GLN
1	A	2188	GLN
1	A	2407	HIS
1	B	38	ASN
1	B	155	ASN
1	B	158	ASN
1	B	222	ASN
1	B	354	ASN
1	B	528	ASN
1	B	683	ASN
1	B	904	ASN
1	B	1188	ASN
1	B	1222	ASN
1	B	1260	ASN
1	B	1264	ASN
1	B	1617	HIS
1	B	1710	ASN
1	B	1767	ASN
1	B	1815	HIS
1	B	1883	GLN
1	B	2188	GLN
1	B	2353	ASN
1	B	2407	HIS
1	B	2463	HIS
1	C	38	ASN
1	C	155	ASN
1	C	158	ASN
1	C	222	ASN
1	C	354	ASN
1	C	528	ASN
1	C	683	ASN
1	C	904	ASN
1	C	1188	ASN

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Mol	Chain	Res	Type
1	C	1222	ASN
1	C	1260	ASN
1	C	1264	ASN
1	C	1617	HIS
1	C	1710	ASN
1	C	1767	ASN
1	C	1815	HIS
1	C	1883	GLN
1	C	2188	GLN
1	C	2353	ASN
1	C	2407	HIS
1	C	2463	HIS
1	D	38	ASN
1	D	155	ASN
1	D	158	ASN
1	D	222	ASN
1	D	354	ASN
1	D	528	ASN
1	D	533	ASN
1	D	683	ASN
1	D	904	ASN
1	D	1188	ASN
1	D	1222	ASN
1	D	1260	ASN
1	D	1264	ASN
1	D	1617	HIS
1	D	1710	ASN
1	D	1767	ASN
1	D	1815	HIS
1	D	1883	GLN
1	D	2188	GLN
1	D	2200	GLN
1	D	2353	ASN
1	D	2407	HIS
1	D	2463	HIS
1	E	38	ASN
1	E	155	ASN
1	E	222	ASN
1	E	294	GLN
1	E	312	ASN
1	E	354	ASN
1	E	355	GLN

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Mol	Chain	Res	Type
1	E	528	ASN
1	E	683	ASN
1	E	904	ASN
1	E	1188	ASN
1	E	1222	ASN
1	E	1260	ASN
1	E	1264	ASN
1	E	1580	ASN
1	E	1617	HIS
1	E	1710	ASN
1	E	1815	HIS
1	E	1883	GLN
1	E	2188	GLN
1	E	2266	ASN
1	E	2407	HIS
1	E	2463	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

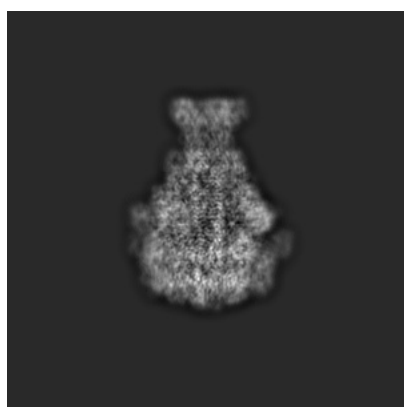
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10035. These allow visual inspection of the internal detail of the map and identification of artifacts.

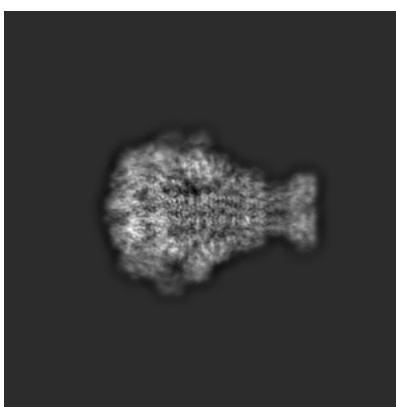
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

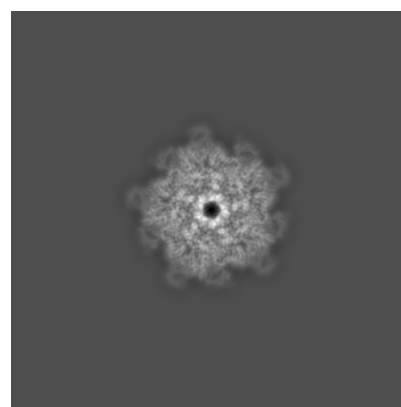
6.1.1 Primary map



X



Y

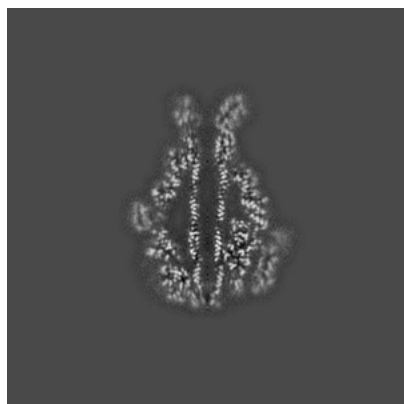


Z

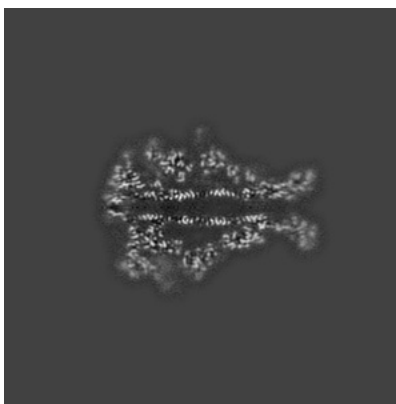
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200

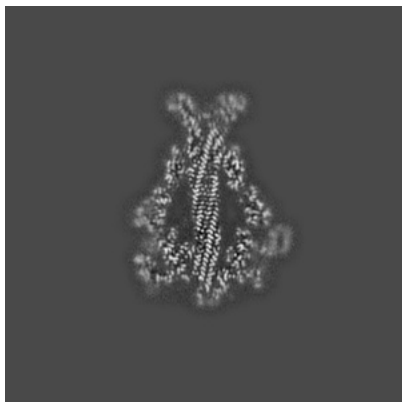


Z Index: 200

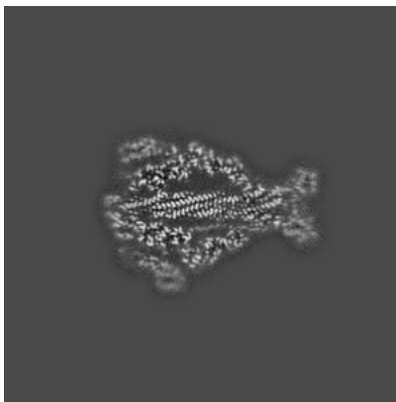
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

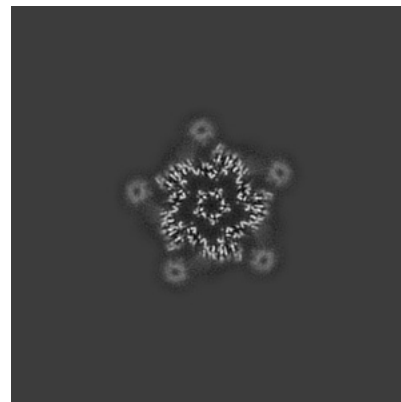
6.3.1 Primary map



X Index: 189



Y Index: 212



Z Index: 169

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

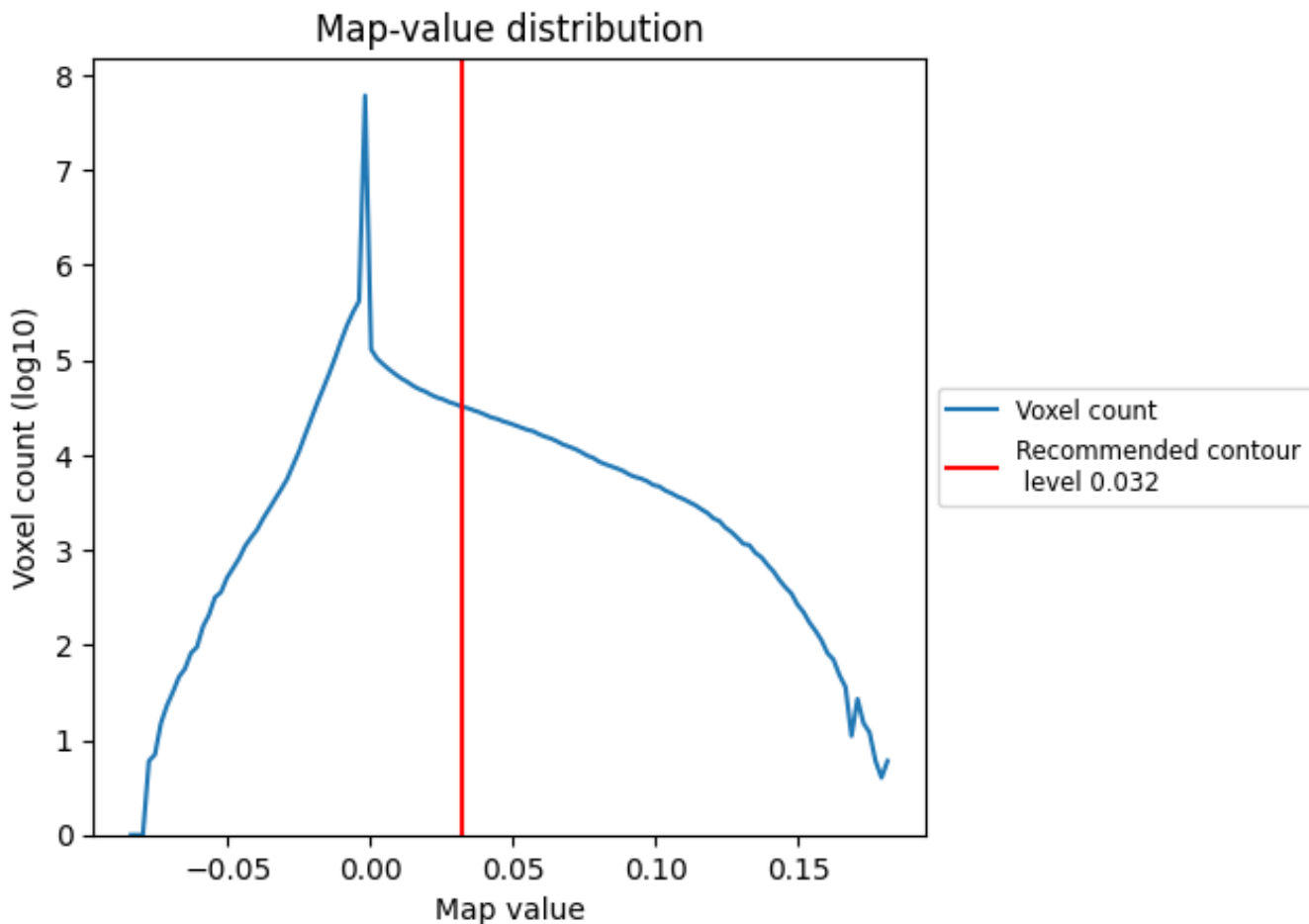
6.5 Mask visualisation

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

7 Map analysis [i](#)

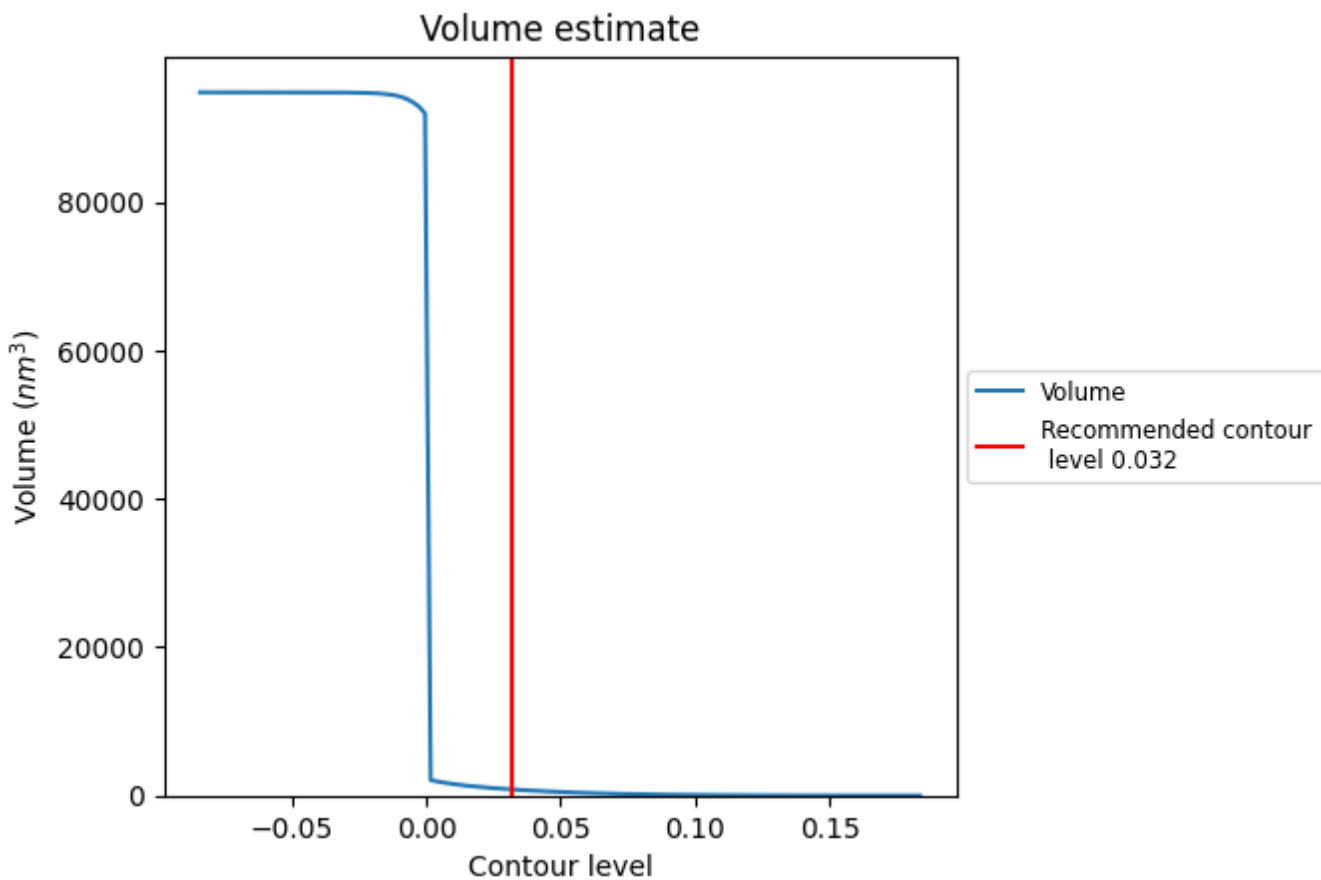
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

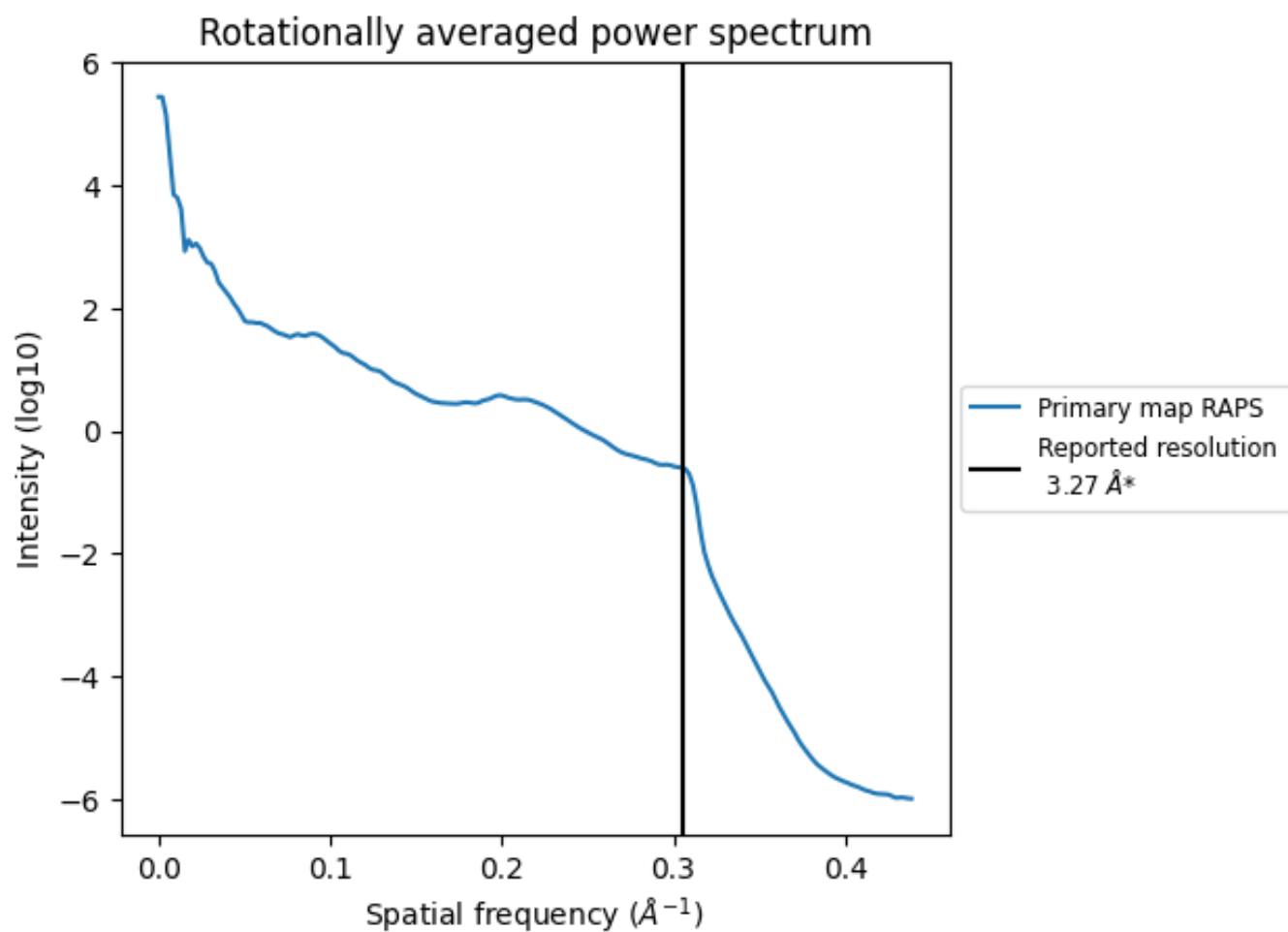
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 824 nm^3 ; this corresponds to an approximate mass of 745 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.306\AA^{-1}

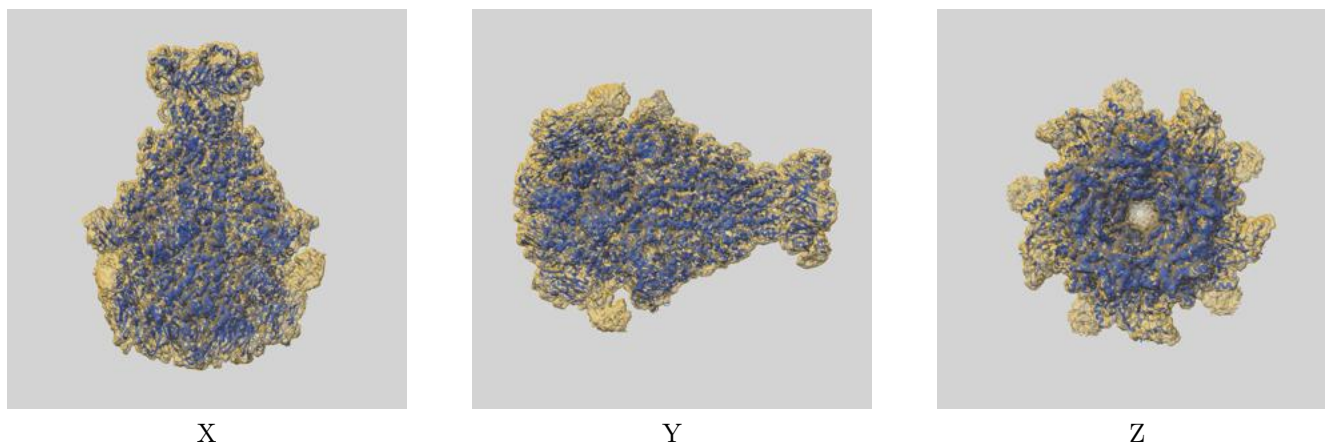
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

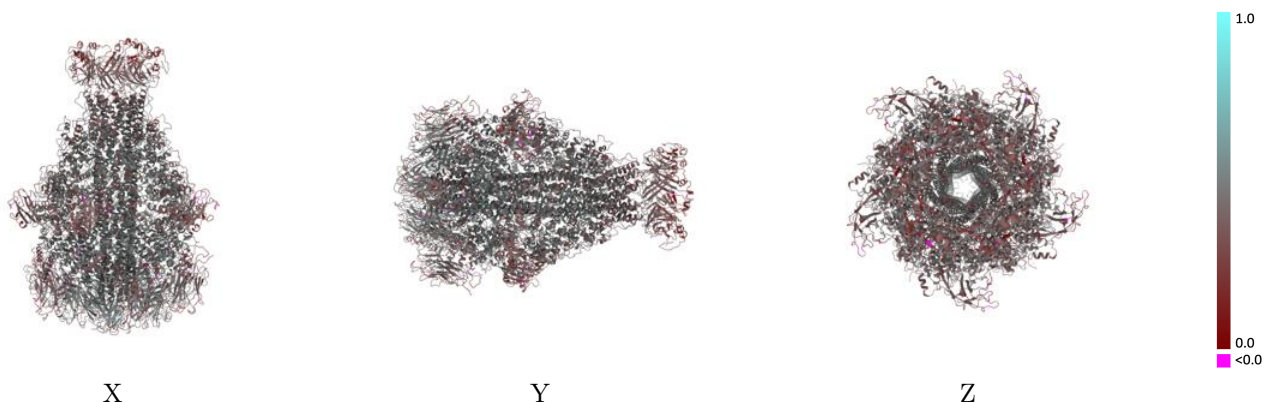
This section contains information regarding the fit between EMDB map EMD-10035 and PDB model 6RW9. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



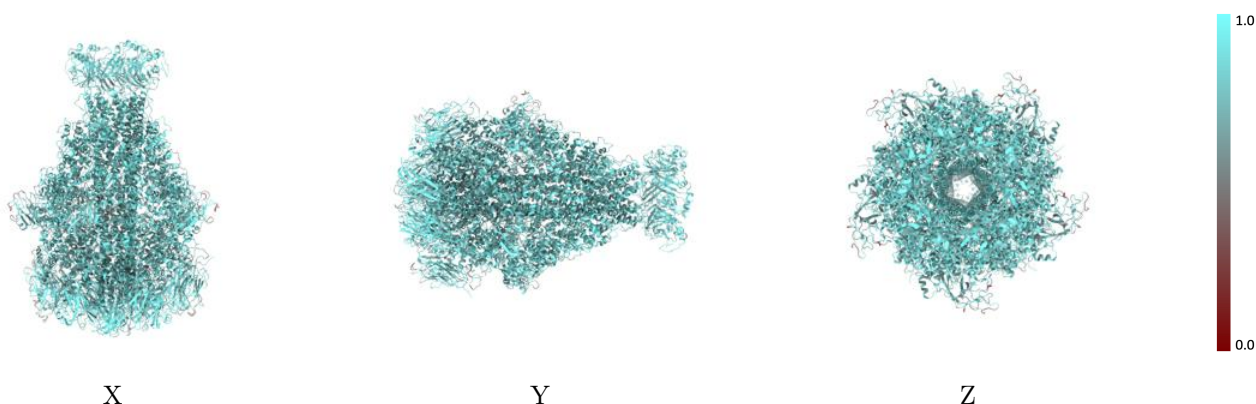
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



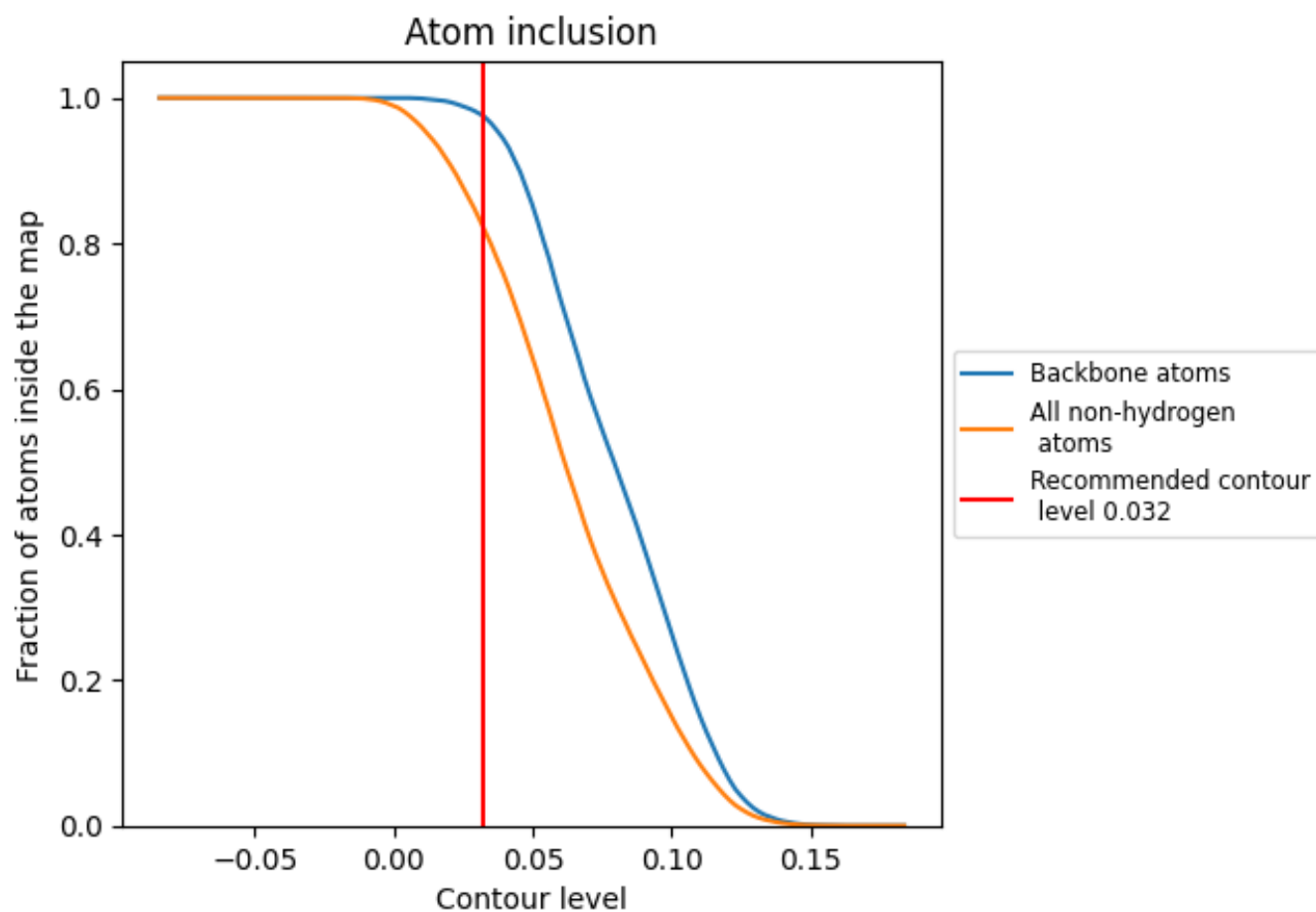
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).













9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8244	 0.4230
A	 0.8255	 0.4240
B	 0.8261	 0.4250
C	 0.8257	 0.4260
D	 0.8266	 0.4250
E	 0.8182	 0.4130

