



Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 04:19 PM EDT

PDB ID : 8TXB / pdb_00008txb
EMDB ID : EMD-41679
Title : Characterization of the Chlamydomonas Flagellar Mastigoneme Filament Structure at 3.9Å
Authors : Yue, W.; Kai, Z.
Deposited on : 2023-08-23
Resolution : 3.90 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

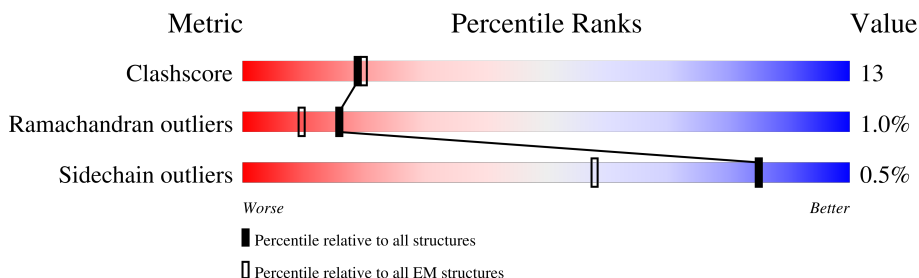
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1987	
1	B	1987	
1	C	1987	
1	D	1987	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 54748 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 Mastigoneme-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		
1	B	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		
1	C	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		
1	D	1894	Total	C	N	O	S	0	0
			13687	8643	2234	2727	83		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	VAL	conflict	UNP Q8LRM7
A	142	LEU	THR	conflict	UNP Q8LRM7
A	143	ALA	GLY	conflict	UNP Q8LRM7
A	144	SER	LEU	conflict	UNP Q8LRM7
A	145	LYS	GLU	conflict	UNP Q8LRM7
A	146	THR	ASP	conflict	UNP Q8LRM7
A	147	VAL	GLY	conflict	UNP Q8LRM7
A	149	ILE	HIS	conflict	UNP Q8LRM7
A	150	TYR	LEU	conflict	UNP Q8LRM7
A	151	VAL	CYS	conflict	UNP Q8LRM7
A	517	ARG	LYS	conflict	UNP Q8LRM7
A	530	GLU	GLY	conflict	UNP Q8LRM7
A	619	THR	ALA	conflict	UNP Q8LRM7
A	800	SER	THR	conflict	UNP Q8LRM7
A	820	SER	PHE	conflict	UNP Q8LRM7
A	?	-	GLY	deletion	UNP Q8LRM7
A	?	-	THR	deletion	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	GLY	deletion	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	TYR	deletion	UNP Q8LRM7
A	?	-	PHE	deletion	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q8LRM7
A	1399	LYS	ARG	conflict	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	GLU	deletion	UNP Q8LRM7
A	1868	PRO	ALA	conflict	UNP Q8LRM7
A	1897	PRO	GLN	conflict	UNP Q8LRM7
A	1914	PRO	ARG	conflict	UNP Q8LRM7
A	1915	PRO	ARG	conflict	UNP Q8LRM7
A	1917	PRO	HIS	conflict	UNP Q8LRM7
A	1919	SER	ALA	conflict	UNP Q8LRM7
A	1920	PRO	ARG	conflict	UNP Q8LRM7
A	1921	PRO	ARG	conflict	UNP Q8LRM7
A	1924	ASN	THR	conflict	UNP Q8LRM7
A	1925	ARG	ALA	conflict	UNP Q8LRM7
A	1926	SER	LEU	conflict	UNP Q8LRM7
A	1935	SER	PRO	conflict	UNP Q8LRM7
A	1978	ASP	-	expression tag	UNP Q8LRM7
A	1979	ALA	-	expression tag	UNP Q8LRM7
A	1980	GLU	-	expression tag	UNP Q8LRM7
A	1981	MET	-	expression tag	UNP Q8LRM7
A	1982	GLN	-	expression tag	UNP Q8LRM7
A	1983	PRO	-	expression tag	UNP Q8LRM7
A	1984	GLN	-	expression tag	UNP Q8LRM7
A	1985	ASP	-	expression tag	UNP Q8LRM7
A	1986	ASP	-	expression tag	UNP Q8LRM7
A	1987	GLU	-	expression tag	UNP Q8LRM7
B	141	LEU	VAL	conflict	UNP Q8LRM7
B	142	LEU	THR	conflict	UNP Q8LRM7
B	143	ALA	GLY	conflict	UNP Q8LRM7
B	144	SER	LEU	conflict	UNP Q8LRM7
B	145	LYS	GLU	conflict	UNP Q8LRM7
B	146	THR	ASP	conflict	UNP Q8LRM7
B	147	VAL	GLY	conflict	UNP Q8LRM7
B	149	ILE	HIS	conflict	UNP Q8LRM7
B	150	TYR	LEU	conflict	UNP Q8LRM7
B	151	VAL	CYS	conflict	UNP Q8LRM7
B	517	ARG	LYS	conflict	UNP Q8LRM7
B	530	GLU	GLY	conflict	UNP Q8LRM7
B	619	THR	ALA	conflict	UNP Q8LRM7
B	800	SER	THR	conflict	UNP Q8LRM7
B	820	SER	PHE	conflict	UNP Q8LRM7
B	?	-	GLY	deletion	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q8LRM7
B	?	-	PRO	deletion	UNP Q8LRM7
B	?	-	GLY	deletion	UNP Q8LRM7
B	?	-	PRO	deletion	UNP Q8LRM7
B	?	-	TYR	deletion	UNP Q8LRM7
B	?	-	PHE	deletion	UNP Q8LRM7
B	?	-	LEU	deletion	UNP Q8LRM7
B	1399	LYS	ARG	conflict	UNP Q8LRM7
B	?	-	PRO	deletion	UNP Q8LRM7
B	?	-	GLU	deletion	UNP Q8LRM7
B	1868	PRO	ALA	conflict	UNP Q8LRM7
B	1897	PRO	GLN	conflict	UNP Q8LRM7
B	1914	PRO	ARG	conflict	UNP Q8LRM7
B	1915	PRO	ARG	conflict	UNP Q8LRM7
B	1917	PRO	HIS	conflict	UNP Q8LRM7
B	1919	SER	ALA	conflict	UNP Q8LRM7
B	1920	PRO	ARG	conflict	UNP Q8LRM7
B	1921	PRO	ARG	conflict	UNP Q8LRM7
B	1924	ASN	THR	conflict	UNP Q8LRM7
B	1925	ARG	ALA	conflict	UNP Q8LRM7
B	1926	SER	LEU	conflict	UNP Q8LRM7
B	1935	SER	PRO	conflict	UNP Q8LRM7
B	1978	ASP	-	expression tag	UNP Q8LRM7
B	1979	ALA	-	expression tag	UNP Q8LRM7
B	1980	GLU	-	expression tag	UNP Q8LRM7
B	1981	MET	-	expression tag	UNP Q8LRM7
B	1982	GLN	-	expression tag	UNP Q8LRM7
B	1983	PRO	-	expression tag	UNP Q8LRM7
B	1984	GLN	-	expression tag	UNP Q8LRM7
B	1985	ASP	-	expression tag	UNP Q8LRM7
B	1986	ASP	-	expression tag	UNP Q8LRM7
B	1987	GLU	-	expression tag	UNP Q8LRM7
C	141	LEU	VAL	conflict	UNP Q8LRM7
C	142	LEU	THR	conflict	UNP Q8LRM7
C	143	ALA	GLY	conflict	UNP Q8LRM7
C	144	SER	LEU	conflict	UNP Q8LRM7
C	145	LYS	GLU	conflict	UNP Q8LRM7
C	146	THR	ASP	conflict	UNP Q8LRM7
C	147	VAL	GLY	conflict	UNP Q8LRM7
C	149	ILE	HIS	conflict	UNP Q8LRM7
C	150	TYR	LEU	conflict	UNP Q8LRM7
C	151	VAL	CYS	conflict	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	517	ARG	LYS	conflict	UNP Q8LRM7
C	530	GLU	GLY	conflict	UNP Q8LRM7
C	619	THR	ALA	conflict	UNP Q8LRM7
C	800	SER	THR	conflict	UNP Q8LRM7
C	820	SER	PHE	conflict	UNP Q8LRM7
C	?	-	GLY	deletion	UNP Q8LRM7
C	?	-	THR	deletion	UNP Q8LRM7
C	?	-	PRO	deletion	UNP Q8LRM7
C	?	-	GLY	deletion	UNP Q8LRM7
C	?	-	PRO	deletion	UNP Q8LRM7
C	?	-	TYR	deletion	UNP Q8LRM7
C	?	-	PHE	deletion	UNP Q8LRM7
C	?	-	LEU	deletion	UNP Q8LRM7
C	1399	LYS	ARG	conflict	UNP Q8LRM7
C	?	-	PRO	deletion	UNP Q8LRM7
C	?	-	GLU	deletion	UNP Q8LRM7
C	1868	PRO	ALA	conflict	UNP Q8LRM7
C	1897	PRO	GLN	conflict	UNP Q8LRM7
C	1914	PRO	ARG	conflict	UNP Q8LRM7
C	1915	PRO	ARG	conflict	UNP Q8LRM7
C	1917	PRO	HIS	conflict	UNP Q8LRM7
C	1919	SER	ALA	conflict	UNP Q8LRM7
C	1920	PRO	ARG	conflict	UNP Q8LRM7
C	1921	PRO	ARG	conflict	UNP Q8LRM7
C	1924	ASN	THR	conflict	UNP Q8LRM7
C	1925	ARG	ALA	conflict	UNP Q8LRM7
C	1926	SER	LEU	conflict	UNP Q8LRM7
C	1935	SER	PRO	conflict	UNP Q8LRM7
C	1978	ASP	-	expression tag	UNP Q8LRM7
C	1979	ALA	-	expression tag	UNP Q8LRM7
C	1980	GLU	-	expression tag	UNP Q8LRM7
C	1981	MET	-	expression tag	UNP Q8LRM7
C	1982	GLN	-	expression tag	UNP Q8LRM7
C	1983	PRO	-	expression tag	UNP Q8LRM7
C	1984	GLN	-	expression tag	UNP Q8LRM7
C	1985	ASP	-	expression tag	UNP Q8LRM7
C	1986	ASP	-	expression tag	UNP Q8LRM7
C	1987	GLU	-	expression tag	UNP Q8LRM7
D	141	LEU	VAL	conflict	UNP Q8LRM7
D	142	LEU	THR	conflict	UNP Q8LRM7
D	143	ALA	GLY	conflict	UNP Q8LRM7
D	144	SER	LEU	conflict	UNP Q8LRM7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	145	LYS	GLU	conflict	UNP Q8LRM7
D	146	THR	ASP	conflict	UNP Q8LRM7
D	147	VAL	GLY	conflict	UNP Q8LRM7
D	149	ILE	HIS	conflict	UNP Q8LRM7
D	150	TYR	LEU	conflict	UNP Q8LRM7
D	151	VAL	CYS	conflict	UNP Q8LRM7
D	517	ARG	LYS	conflict	UNP Q8LRM7
D	530	GLU	GLY	conflict	UNP Q8LRM7
D	619	THR	ALA	conflict	UNP Q8LRM7
D	800	SER	THR	conflict	UNP Q8LRM7
D	820	SER	PHE	conflict	UNP Q8LRM7
D	?	-	GLY	deletion	UNP Q8LRM7
D	?	-	THR	deletion	UNP Q8LRM7
D	?	-	PRO	deletion	UNP Q8LRM7
D	?	-	GLY	deletion	UNP Q8LRM7
D	?	-	PRO	deletion	UNP Q8LRM7
D	?	-	TYR	deletion	UNP Q8LRM7
D	?	-	PHE	deletion	UNP Q8LRM7
D	?	-	LEU	deletion	UNP Q8LRM7
D	1399	LYS	ARG	conflict	UNP Q8LRM7
D	?	-	PRO	deletion	UNP Q8LRM7
D	?	-	GLU	deletion	UNP Q8LRM7
D	1868	PRO	ALA	conflict	UNP Q8LRM7
D	1897	PRO	GLN	conflict	UNP Q8LRM7
D	1914	PRO	ARG	conflict	UNP Q8LRM7
D	1915	PRO	ARG	conflict	UNP Q8LRM7
D	1917	PRO	HIS	conflict	UNP Q8LRM7
D	1919	SER	ALA	conflict	UNP Q8LRM7
D	1920	PRO	ARG	conflict	UNP Q8LRM7
D	1921	PRO	ARG	conflict	UNP Q8LRM7
D	1924	ASN	THR	conflict	UNP Q8LRM7
D	1925	ARG	ALA	conflict	UNP Q8LRM7
D	1926	SER	LEU	conflict	UNP Q8LRM7
D	1935	SER	PRO	conflict	UNP Q8LRM7
D	1978	ASP	-	expression tag	UNP Q8LRM7
D	1979	ALA	-	expression tag	UNP Q8LRM7
D	1980	GLU	-	expression tag	UNP Q8LRM7
D	1981	MET	-	expression tag	UNP Q8LRM7
D	1982	GLN	-	expression tag	UNP Q8LRM7
D	1983	PRO	-	expression tag	UNP Q8LRM7
D	1984	GLN	-	expression tag	UNP Q8LRM7
D	1985	ASP	-	expression tag	UNP Q8LRM7

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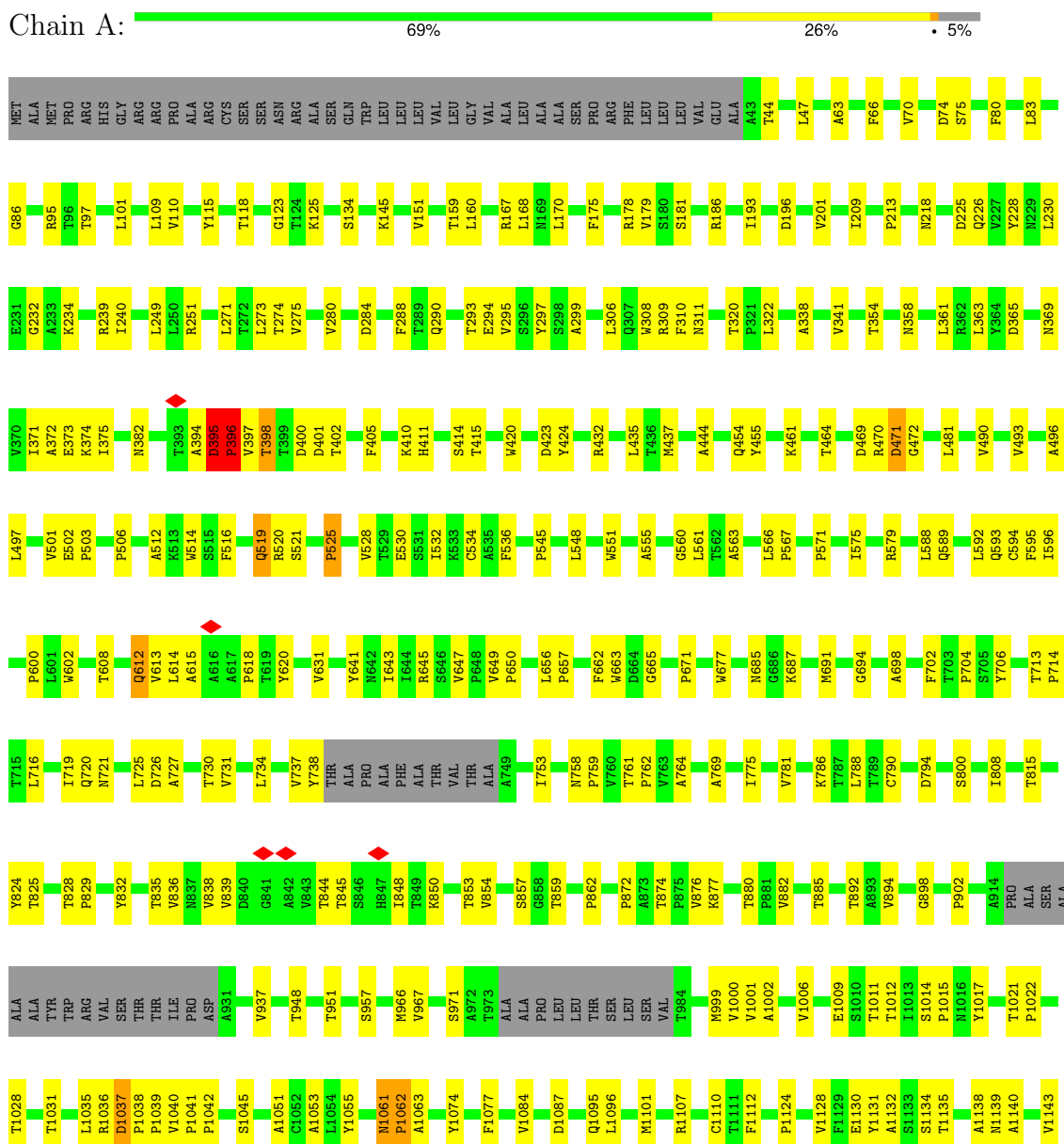
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1986	ASP	-	expression tag	UNP Q8LRM7
D	1987	GLU	-	expression tag	UNP Q8LRM7

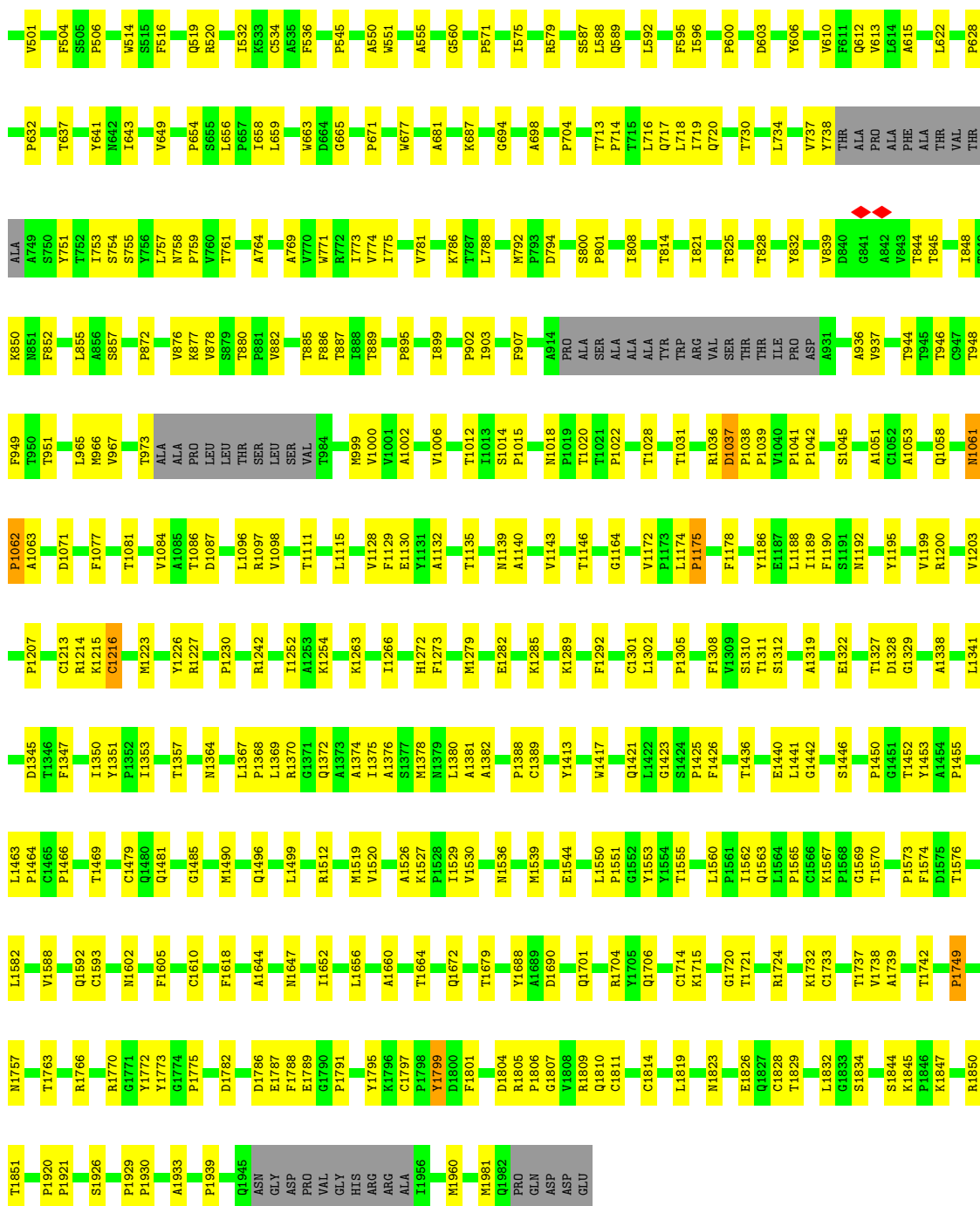
3 Residue-property plots

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: Mastigoneme-like protein









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70074	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.733	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.0728	Depositor
Map size (\AA)	229.8, 229.8, 919.2	wwPDB
Map dimensions	200, 200, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.149, 1.149, 1.149	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	6/14067 (0.0%)	0.59	15/19393 (0.1%)
1	B	0.44	10/14067 (0.1%)	0.68	28/19393 (0.1%)
1	C	0.34	6/14067 (0.0%)	0.55	13/19393 (0.1%)
1	D	0.34	6/14067 (0.0%)	0.60	18/19393 (0.1%)
All	All	0.36	28/56268 (0.0%)	0.61	74/77572 (0.1%)

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	10
1	C	0	1
1	D	0	2
All	All	0	17

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	396	PRO	CG-CD	-28.56	0.53	1.50
1	C	396	PRO	CG-CD	-26.53	0.60	1.50
1	D	1769	PRO	CG-CD	-20.89	0.79	1.50
1	B	1769	PRO	CG-CD	-20.21	0.82	1.50
1	A	396	PRO	CB-CG	19.48	2.47	1.49
1	D	1883	PRO	CG-CD	-17.27	0.92	1.50
1	B	1769	PRO	CB-CG	17.12	2.35	1.49
1	A	396	PRO	CG-CD	-14.15	1.02	1.50
1	B	396	PRO	CB-CG	13.30	2.16	1.49
1	D	1769	PRO	CB-CG	11.61	2.07	1.49
1	C	396	PRO	CB-CG	11.38	2.06	1.49
1	B	396	PRO	N-CD	9.74	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	396	PRO	N-CD	9.13	1.60	1.47
1	B	1062	PRO	CG-CD	-8.57	1.21	1.50
1	A	1062	PRO	CG-CD	-8.55	1.21	1.50
1	C	1062	PRO	CG-CD	-8.52	1.21	1.50
1	D	1062	PRO	CG-CD	-8.38	1.22	1.50
1	D	1883	PRO	N-CD	8.04	1.59	1.47
1	A	396	PRO	N-CA	-7.97	1.37	1.47
1	B	1769	PRO	CA-CB	-7.15	1.43	1.53
1	C	396	PRO	N-CA	-6.95	1.40	1.47
1	D	1769	PRO	CA-CB	-6.91	1.44	1.53
1	B	396	PRO	CA-C	6.20	1.61	1.52
1	A	396	PRO	N-CD	5.63	1.55	1.47
1	B	396	PRO	N-CA	-5.48	1.40	1.47
1	B	1062	PRO	N-CD	5.29	1.55	1.47
1	A	1062	PRO	N-CD	5.27	1.55	1.47
1	C	1062	PRO	N-CD	5.26	1.55	1.47

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	PRO	CB-CG-CD	-33.14	0.04	106.10
1	D	1769	PRO	N-CD-CG	-26.92	62.81	103.20
1	B	1769	PRO	CB-CG-CD	-21.61	36.95	106.10
1	D	1769	PRO	CA-CB-CG	-20.80	64.99	104.50
1	B	1769	PRO	N-CD-CG	-19.02	74.66	103.20
1	B	396	PRO	CB-CG-CD	-19.00	45.31	106.10
1	B	1769	PRO	CA-CB-CG	-18.60	69.16	104.50
1	C	396	PRO	N-CA-CB	-18.27	92.69	102.92
1	D	1883	PRO	N-CD-CG	-18.03	76.15	103.20
1	C	396	PRO	N-CD-CG	-17.52	76.93	103.20
1	B	1769	PRO	N-CA-CB	-17.44	84.94	103.25
1	A	396	PRO	CA-N-CD	-16.08	89.48	112.00
1	B	396	PRO	N-CD-CG	-15.19	80.41	103.20
1	D	1769	PRO	N-CA-CB	-14.90	87.60	103.25
1	C	1062	PRO	CA-N-CD	-14.83	91.24	112.00
1	A	1062	PRO	CA-N-CD	-14.81	91.26	112.00
1	B	1062	PRO	CA-N-CD	-14.75	91.35	112.00
1	A	396	PRO	N-CA-CB	-14.26	88.28	103.25
1	B	1769	PRO	CA-N-CD	-14.21	92.10	112.00
1	B	396	PRO	CA-N-CD	-13.01	93.78	112.00
1	A	213	PRO	CA-N-CD	-12.75	94.15	112.00
1	B	394	ALA	CA-C-N	12.71	152.82	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	ALA	C-N-CA	12.71	152.82	121.80
1	C	396	PRO	CA-N-CD	-11.90	95.34	112.00
1	B	1798	PRO	CA-N-CD	-11.83	95.44	112.00
1	D	829	PRO	CA-N-CD	-11.81	95.47	112.00
1	C	1749	PRO	CA-N-CD	-11.57	95.81	112.00
1	B	1749	PRO	CA-N-CD	-11.27	96.22	112.00
1	D	1749	PRO	CA-N-CD	-11.26	96.24	112.00
1	B	396	PRO	CA-CB-CG	-11.13	83.35	104.50
1	D	1769	PRO	CB-CG-CD	-11.07	70.69	106.10
1	A	525	PRO	CA-N-CD	-10.96	96.66	112.00
1	D	1883	PRO	CA-CB-CG	-10.74	84.10	104.50
1	C	396	PRO	CA-CB-CG	-10.72	84.13	104.50
1	B	396	PRO	N-CA-CB	-10.72	92.00	103.25
1	C	396	PRO	CB-CG-CD	-10.65	72.02	106.10
1	D	1883	PRO	CA-N-CD	-10.62	97.13	112.00
1	D	1062	PRO	CA-N-CD	-9.52	98.67	112.00
1	D	1769	PRO	CA-N-CD	-9.32	98.96	112.00
1	D	1062	PRO	N-CD-CG	-9.23	89.36	103.20
1	B	1389	CYS	CA-C-N	9.20	133.55	120.49
1	B	1389	CYS	C-N-CA	9.20	133.55	120.49
1	B	1062	PRO	N-CD-CG	-9.15	89.47	103.20
1	C	1062	PRO	N-CD-CG	-9.15	89.47	103.20
1	A	1062	PRO	N-CD-CG	-9.13	89.51	103.20
1	B	1856	PRO	CA-N-CD	-8.90	99.54	112.00
1	B	1061	ASN	C-N-CD	-8.41	90.51	125.00
1	D	1255	PRO	CA-N-CD	-8.36	100.29	112.00
1	A	1061	ASN	C-N-CD	-8.29	91.02	125.00
1	C	1061	ASN	C-N-CD	-8.25	91.16	125.00
1	A	396	PRO	CA-CB-CG	-8.10	89.10	104.50
1	B	105	PRO	CA-N-CD	-8.09	100.68	112.00
1	A	1462	CYS	CA-C-N	7.87	131.22	120.67
1	A	1462	CYS	C-N-CA	7.87	131.22	120.67
1	D	1939	PRO	N-CA-CB	7.61	111.24	103.25
1	B	396	PRO	CB-CA-C	7.52	123.96	111.56
1	B	1939	PRO	N-CA-CB	6.96	110.56	103.25
1	D	1061	ASN	C-N-CD	-6.87	96.84	125.00
1	B	394	ALA	N-CA-C	6.84	125.36	110.80
1	A	1255	PRO	CA-N-CD	-6.72	102.59	112.00
1	B	396	PRO	CA-C-O	6.32	132.10	120.60
1	C	1749	PRO	N-CD-CG	-6.12	94.01	103.20
1	C	1939	PRO	N-CA-CB	6.10	110.36	102.86
1	A	1939	PRO	N-CA-CB	6.03	110.28	102.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	PRO	N-CD-CG	-5.95	94.27	103.20
1	D	1786	ASP	N-CA-C	-5.91	104.67	112.24
1	C	632	PRO	CA-N-CD	-5.88	103.77	112.00
1	C	1062	PRO	CA-CB-CG	-5.60	93.85	104.50
1	B	1062	PRO	CA-CB-CG	-5.60	93.86	104.50
1	A	1062	PRO	CA-CB-CG	-5.60	93.87	104.50
1	D	829	PRO	N-CD-CG	-5.41	95.09	103.20
1	B	396	PRO	N-CA-C	5.37	123.53	112.47
1	D	1749	PRO	N-CD-CG	-5.30	95.25	103.20
1	B	1749	PRO	N-CD-CG	-5.03	95.66	103.20

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1527	LYS	Peptide
1	A	395	ASP	Peptide
1	A	397	VAL	Peptide
1	A	398	THR	Peptide
1	B	1527	LYS	Peptide
1	B	1798	PRO	Peptide
1	B	392	THR	Peptide
1	B	393	THR	Mainchain,Peptide
1	B	394	ALA	Mainchain,Peptide
1	B	395	ASP	Peptide
1	B	396	PRO	Peptide
1	B	398	THR	Peptide
1	C	1527	LYS	Peptide
1	D	1061	ASN	Peptide
1	D	1527	LYS	Peptide

5.2 Too-close contacts ⓘ

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	13687	0	13241	374	0
1	B	13687	0	13241	344	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	13687	0	13241	353	0
1	D	13687	0	13241	323	0
All	All	54748	0	52964	1354	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 13.

All (1354) 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:532:ILE:HD11	1:A:594:CYS:HB3	1.47	0.97
1:A:1515:THR:HG21	1:C:1192:ASN:HD22	1.40	0.85
1:C:659:LEU:HB2	1:C:719:ILE:O	1.76	0.85
1:C:401:ASP:OD1	1:C:402:THR:N	2.10	0.85
1:A:358:ASN:HB3	1:A:375:ILE:HD11	1.58	0.84
1:C:792:MET:HE1	1:C:801:PRO:HD2	1.57	0.84
1:D:999:MET:HE3	1:D:1000:VAL:H	1.42	0.84
1:D:659:LEU:HB2	1:D:719:ILE:O	1.77	0.83
1:B:401:ASP:OD2	1:B:402:THR:N	2.11	0.83
1:A:178:ARG:HD2	1:A:218:ASN:HD22	1.43	0.83
1:A:566:LEU:HD12	1:A:567:PRO:HD2	1.59	0.83
1:C:999:MET:HE3	1:C:1000:VAL:H	1.43	0.82
1:C:168:LEU:O	1:C:170:LEU:N	2.12	0.82
1:D:168:LEU:O	1:D:170:LEU:N	2.13	0.81
1:A:829:PRO:HA	1:A:854:VAL:O	1.80	0.81
1:C:1801:PHE:HB3	1:C:1811:CYS:HB3	1.63	0.80
1:B:168:LEU:O	1:B:170:LEU:N	2.14	0.80
1:C:415:THR:HB	1:C:437:MET:HG3	1.63	0.80
1:B:108:ASN:OD1	1:B:109:LEU:N	2.15	0.79
1:B:614:LEU:HD22	1:B:650:PRO:HD2	1.65	0.79
1:C:713:THR:HG21	1:C:737:VAL:H	1.47	0.79
1:B:1805:ARG:O	1:B:1807:GLY:N	2.15	0.78
1:B:755:SER:HB2	1:B:771:TRP:HE1	1.48	0.78
1:B:1493:ARG:NH2	1:B:1549:ASN:O	2.17	0.78
1:C:755:SER:HB2	1:C:771:TRP:HE1	1.49	0.78
1:D:178:ARG:HD2	1:D:218:ASN:HD22	1.49	0.77
1:B:1180:THR:HG23	1:B:1181:THR:HG23	1.66	0.77
1:D:903:ILE:HD11	1:D:938:MET:HB2	1.66	0.77
1:D:506:PRO:HG3	1:D:588:LEU:HD11	1.67	0.77
1:B:166:PRO:HG2	1:B:261:VAL:HG13	1.65	0.77
1:D:656:LEU:HB2	1:D:691:MET:HE3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1036:ARG:HD3	1:D:1041:PRO:HD3	1.67	0.77
1:D:957:SER:HB3	1:D:1001:VAL:H	1.48	0.76
1:C:83:LEU:HD11	1:C:109:LEU:HD11	1.68	0.76
1:C:1805:ARG:O	1:C:1807:GLY:N	2.19	0.75
1:D:1569:GLY:H	1:D:1602:ASN:HB3	1.51	0.75
1:C:1289:LYS:HG2	1:C:1312:SER:H	1.52	0.75
1:B:1817:LEU:HD21	1:B:1839:PRO:HB3	1.67	0.74
1:B:764:ALA:HA	1:B:825:THR:HB	1.70	0.74
1:C:506:PRO:HG3	1:C:588:LEU:HD11	1.69	0.74
1:B:230:LEU:HB3	1:B:234:LYS:HE2	1.68	0.74
1:A:228:TYR:HD2	1:A:234:LYS:HE3	1.52	0.73
1:D:1733:CYS:HB3	1:D:1737:THR:HG23	1.71	0.73
1:A:1775:PRO:HA	1:A:1809:ARG:HD3	1.71	0.73
1:C:419:TRP:HB2	1:C:468:TYR:O	1.89	0.73
1:A:966:MET:HE3	1:A:967:VAL:H	1.53	0.72
1:A:1757:ASN:OD1	1:A:1766:ARG:NH2	2.22	0.72
1:D:1051:ALA:HB1	1:D:1096:LEU:HD11	1.71	0.72
1:C:401:ASP:O	1:C:454:GLN:NE2	2.23	0.71
1:D:1289:LYS:HG2	1:D:1312:SER:H	1.53	0.71
1:A:1186:TYR:HA	1:A:1214:ARG:O	1.90	0.71
1:C:1130:GLU:OE2	1:C:1130:GLU:N	2.22	0.71
1:D:762:PRO:HD2	1:D:857:SER:H	1.56	0.71
1:A:181:SER:HG	1:A:186:ARG:HH21	1.39	0.71
1:A:401:ASP:CG	1:A:402:THR:H	1.99	0.71
1:B:1826:GLU:OE2	1:B:1826:GLU:N	2.24	0.71
1:C:506:PRO:HD2	1:C:615:ALA:HA	1.71	0.70
1:C:885:THR:HG22	1:C:948:THR:HG22	1.71	0.70
1:B:506:PRO:HG3	1:B:588:LEU:HD21	1.71	0.70
1:C:1223:MET:HE1	1:C:1981:MET:HE1	1.74	0.70
1:B:1668:MET:SD	1:B:1668:MET:N	2.60	0.70
1:C:588:LEU:HD12	1:C:613:VAL:HB	1.74	0.70
1:A:1466:PRO:HA	1:C:1227:ARG:HB3	1.74	0.70
1:D:1493:ARG:NH2	1:D:1549:ASN:O	2.25	0.70
1:C:168:LEU:HD22	1:C:231:GLU:HB3	1.74	0.70
1:A:1037:ASP:OD1	1:A:1038:PRO:HD2	1.92	0.69
1:D:1239:GLU:OE2	1:D:1239:GLU:N	2.24	0.69
1:A:395:ASP:N	1:A:396:PRO:HG3	2.07	0.69
1:A:1733:CYS:HB3	1:A:1737:THR:HG23	1.74	0.69
1:B:1757:ASN:OD1	1:B:1766:ARG:NH2	2.25	0.69
1:D:1760:ASP:OD1	1:D:1761:SER:N	2.24	0.69
1:A:1826:GLU:N	1:A:1826:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:MET:HE3	1:B:1000:VAL:H	1.56	0.69
1:A:1709:ILE:HD12	1:A:1709:ILE:H	1.57	0.69
1:D:506:PRO:HD2	1:D:615:ALA:HA	1.75	0.69
1:D:1022:PRO:HB2	1:D:1028:THR:HG21	1.74	0.69
1:C:1826:GLU:OE2	1:C:1826:GLU:N	2.25	0.69
1:C:1338:ALA:HB3	1:C:1353:ILE:HG23	1.74	0.69
1:C:360:ARG:HB3	1:C:375:ILE:HG13	1.73	0.68
1:C:1006:VAL:HG12	1:C:1036:ARG:HA	1.75	0.68
1:B:866:VAL:HG12	1:B:888:ILE:HG13	1.75	0.68
1:B:1174:LEU:HD22	1:B:1178:PHE:HD1	1.59	0.68
1:B:1252:ILE:HD11	1:B:1301:CYS:HB2	1.74	0.68
1:B:790:CYS:HA	1:B:836:VAL:HG13	1.74	0.68
1:D:1421:GLN:HB2	1:D:1436:THR:HB	1.76	0.68
1:A:999:MET:HE3	1:A:1000:VAL:H	1.59	0.68
1:A:828:THR:O	1:A:832:TYR:OH	2.11	0.67
1:D:681:ALA:HA	1:D:686:GLY:HA3	1.75	0.67
1:A:1164:GLY:O	1:C:1481:GLN:NE2	2.26	0.67
1:B:1036:ARG:HD3	1:B:1041:PRO:HD3	1.74	0.67
1:C:536:PHE:O	1:C:579:ARG:NH2	2.28	0.67
1:D:1685:VAL:HG23	1:D:1707:ASN:HA	1.77	0.67
1:A:1563:GLN:OE1	1:A:1563:GLN:N	2.16	0.67
1:B:193:ILE:HD13	1:B:226:GLN:HE21	1.59	0.67
1:A:1537:PHE:HB2	1:C:1189:ILE:HG23	1.77	0.67
1:A:1685:VAL:HG23	1:A:1707:ASN:HA	1.76	0.67
1:B:195:LEU:HD11	1:B:226:GLN:HB2	1.77	0.67
1:B:1130:GLU:OE1	1:B:1130:GLU:N	2.21	0.67
1:B:1195:TYR:HA	1:B:1200:ARG:HA	1.77	0.67
1:B:1706:GLN:HE21	1:B:1711:GLN:HB2	1.59	0.67
1:B:1798:PRO:O	1:B:1800:ASP:N	2.28	0.67
1:D:1084:VAL:HG12	1:D:1087:ASP:HB3	1.78	0.66
1:D:1634:THR:OG1	1:D:1663:PRO:O	2.12	0.66
1:B:1037:ASP:OD1	1:B:1038:PRO:HD2	1.95	0.66
1:B:1757:ASN:ND2	1:B:1763:THR:OG1	2.28	0.66
1:C:63:ALA:HB2	1:C:118:THR:HG22	1.77	0.66
1:B:1364:ASN:N	1:B:1398:SER:OG	2.25	0.66
1:B:1733:CYS:HB3	1:B:1737:THR:HG23	1.77	0.66
1:A:294:GLU:HB3	1:A:338:ALA:HB1	1.78	0.66
1:B:1796:LYS:HD2	1:B:1832:LEU:HB3	1.78	0.66
1:A:1690:ASP:OD2	1:A:1691:GLN:N	2.28	0.66
1:D:1805:ARG:O	1:D:1807:GLY:N	2.29	0.66
1:A:193:ILE:HG21	1:A:226:GLN:HE21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1469:THR:HG22	1:B:1481:GLN:HA	1.77	0.66
1:C:189:MET:HE3	1:C:209:ILE:HD11	1.77	0.66
1:A:1012:THR:OG1	1:A:1031:THR:OG1	2.14	0.65
1:B:109:LEU:HG	1:B:110:VAL:HG23	1.78	0.65
1:B:1471:ALA:HB2	1:B:1479:CYS:HB2	1.77	0.65
1:A:1728:GLU:OE2	1:A:1729:LEU:HG	1.95	0.65
1:B:874:THR:HA	1:B:999:MET:HE1	1.78	0.65
1:C:663:TRP:O	1:C:714:PRO:HA	1.95	0.65
1:D:570:ILE:HD12	1:D:571:PRO:HD2	1.79	0.65
1:D:588:LEU:O	1:D:612:GLN:NE2	2.28	0.65
1:A:1195:TYR:OH	1:A:1200:ARG:NH2	2.28	0.65
1:C:1749:PRO:HD2	1:C:1749:PRO:O	1.96	0.65
1:C:1960:MET:SD	1:C:1960:MET:N	2.69	0.65
1:D:968:PHE:HA	1:D:988:LEU:HD23	1.76	0.65
1:A:506:PRO:HD2	1:A:615:ALA:HA	1.76	0.65
1:A:1817:LEU:HD21	1:A:1839:PRO:HB3	1.79	0.65
1:A:614:LEU:HD22	1:A:650:PRO:HD2	1.78	0.65
1:A:726:ASP:OD2	1:A:727:ALA:N	2.29	0.65
1:A:1562:ILE:HB	1:C:1188:LEU:HD21	1.77	0.65
1:C:757:LEU:HD11	1:C:769:ALA:HB1	1.79	0.65
1:D:1709:ILE:HD12	1:D:1709:ILE:H	1.61	0.65
1:A:109:LEU:HG	1:A:110:VAL:H	1.61	0.64
1:D:1453:TYR:HD1	1:D:1455:PRO:HD3	1.62	0.64
1:D:420:TRP:O	1:D:433:THR:OG1	2.15	0.64
1:B:228:TYR:HD1	1:B:234:LYS:HE3	1.62	0.64
1:D:161:LEU:HD11	1:D:178:ARG:HH22	1.62	0.64
1:A:649:VAL:HB	1:A:694:GLY:H	1.62	0.64
1:B:194:GLN:OE1	1:B:239:ARG:NH2	2.31	0.64
1:A:1414:ARG:NH2	1:A:1445:CYS:SG	2.70	0.64
1:B:662:PHE:HE2	1:B:687:LYS:HG2	1.63	0.64
1:A:1036:ARG:HD3	1:A:1041:PRO:HD3	1.79	0.64
1:D:415:THR:HB	1:D:437:MET:HG3	1.80	0.64
1:D:999:MET:HE3	1:D:1000:VAL:N	2.13	0.64
1:A:423:ASP:HB3	1:A:464:THR:HB	1.80	0.64
1:C:470:ARG:HG2	1:C:478:GLY:HA2	1.79	0.64
1:D:1452:THR:HG22	1:D:1464:PRO:HA	1.78	0.64
1:D:1616:GLY:O	1:D:1636:THR:OG1	2.16	0.64
1:C:161:LEU:HD11	1:C:178:ARG:HH22	1.63	0.64
1:C:1706:GLN:HE21	1:C:1714:CYS:HA	1.63	0.64
1:D:828:THR:O	1:D:832:TYR:OH	2.12	0.64
1:D:532:ILE:HG12	1:D:596:ILE:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:ASP:HB3	1:D:464:THR:HB	1.80	0.63
1:D:1773:TYR:HB2	1:D:1809:ARG:HA	1.79	0.63
1:A:1634:THR:OG1	1:A:1663:PRO:O	2.16	0.63
1:D:401:ASP:O	1:D:454:GLN:NE2	2.31	0.63
1:A:534:CYS:HB3	1:A:592:LEU:HD11	1.79	0.63
1:C:1042:PRO:HG2	1:C:1045:SER:HB2	1.81	0.63
1:C:1301:CYS:N	1:C:1351:TYR:OH	2.30	0.63
1:D:410:LYS:HB3	1:D:444:ALA:HA	1.79	0.63
1:D:1440:GLU:OE1	1:D:1443:SER:N	2.29	0.63
1:A:1130:GLU:OE2	1:A:1130:GLU:N	2.23	0.63
1:A:1340:SER:O	1:A:1344:THR:OG1	2.16	0.63
1:B:516:PHE:HB2	1:B:575:ILE:HG23	1.79	0.63
1:C:1036:ARG:HD3	1:C:1041:PRO:HD3	1.79	0.63
1:A:1721:THR:HG23	1:A:1732:LYS:HA	1.79	0.63
1:B:1749:PRO:HD2	1:B:1749:PRO:O	1.98	0.63
1:A:63:ALA:HB2	1:A:118:THR:HG22	1.81	0.63
1:A:1184:ASP:OD2	1:A:1184:ASP:N	2.31	0.63
1:A:271:LEU:HD22	1:A:295:VAL:HA	1.81	0.62
1:B:536:PHE:O	1:B:579:ARG:NH2	2.32	0.62
1:A:432:ARG:CZ	1:A:472:GLY:HA3	2.29	0.62
1:A:1015:PRO:HG2	1:A:1028:THR:HG22	1.82	0.62
1:B:656:LEU:HB3	1:B:691:MET:HB2	1.81	0.62
1:D:614:LEU:HD22	1:D:650:PRO:HD2	1.81	0.62
1:A:1808:VAL:HG13	1:A:1810:GLN:H	1.65	0.62
1:A:530:GLU:HB3	1:A:596:ILE:HD11	1.82	0.62
1:C:839:VAL:HG13	1:C:844:THR:HG23	1.80	0.62
1:D:1285:LYS:HD3	1:D:1285:LYS:H	1.64	0.62
1:A:874:THR:HA	1:A:999:MET:HE1	1.80	0.62
1:B:1012:THR:OG1	1:B:1031:THR:OG1	2.17	0.62
1:B:402:THR:HG22	1:B:454:GLN:HB2	1.82	0.62
1:B:517:ARG:HH21	1:B:574:ILE:HD11	1.65	0.62
1:B:775:ILE:O	1:B:814:THR:HA	1.98	0.62
1:C:794:ASP:HB2	1:C:800:SER:HB2	1.82	0.62
1:C:1308:PHE:HD2	1:C:1319:ALA:HA	1.65	0.62
1:D:1186:TYR:HB3	1:D:1213:CYS:HB2	1.82	0.62
1:A:83:LEU:HD22	1:A:109:LEU:HD11	1.82	0.62
1:A:1195:TYR:HA	1:A:1200:ARG:HA	1.82	0.62
1:B:828:THR:O	1:B:832:TYR:OH	2.11	0.62
1:A:1171:ARG:NH2	1:A:1966:GLU:OE2	2.33	0.61
1:B:1661:GLN:OE1	1:B:1661:GLN:N	2.22	0.61
1:C:1452:THR:HG22	1:C:1464:PRO:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:ILE:HG22	1:B:945:THR:HB	1.82	0.61
1:C:178:ARG:HD2	1:C:218:ASN:HD22	1.64	0.61
1:C:480:LEU:HD11	1:C:483:SER:HB2	1.82	0.61
1:D:362:ARG:HE	1:D:370:VAL:HG11	1.65	0.61
1:D:470:ARG:HG2	1:D:478:GLY:HA2	1.82	0.61
1:D:1084:VAL:HG13	1:D:1086:THR:H	1.65	0.61
1:A:1188:LEU:HD21	1:C:1562:ILE:HB	1.81	0.61
1:B:1582:LEU:HD22	1:B:1586:LEU:HD11	1.83	0.61
1:A:401:ASP:O	1:A:454:GLN:NE2	2.33	0.61
1:D:762:PRO:HG2	1:D:856:ALA:HA	1.80	0.61
1:B:1721:THR:HG21	1:B:1730:CYS:HB3	1.82	0.61
1:D:1503:ASN:HD22	1:D:1506:ASN:HD22	1.48	0.61
1:A:167:ARG:HD3	1:A:170:LEU:HD13	1.83	0.61
1:A:1378:MET:HE2	1:A:1378:MET:HA	1.81	0.61
1:B:1573:PRO:HD2	1:B:1588:VAL:HG11	1.80	0.61
1:D:1293:GLN:NE2	1:D:1295:ASN:OD1	2.33	0.61
1:A:1209:PRO:O	1:C:1553:TYR:OH	2.16	0.61
1:C:966:MET:SD	1:C:967:VAL:N	2.74	0.61
1:C:1733:CYS:HB3	1:C:1737:THR:HG23	1.83	0.61
1:A:496:ALA:HB3	1:A:519:GLN:HB2	1.82	0.61
1:B:649:VAL:HB	1:B:694:GLY:H	1.66	0.61
1:C:43:ALA:N	1:C:74:ASP:OD2	2.34	0.61
1:C:1012:THR:OG1	1:C:1031:THR:OG1	2.17	0.61
1:A:643:ILE:HB	1:A:698:ALA:HB3	1.81	0.60
1:C:1327:THR:OG1	1:C:1328:ASP:N	2.32	0.60
1:A:109:LEU:HG	1:A:110:VAL:HG23	1.82	0.60
1:A:1459:MET:SD	1:A:1459:MET:N	2.74	0.60
1:B:525:PRO:HB2	1:B:528:VAL:HG22	1.82	0.60
1:B:999:MET:HE3	1:B:1000:VAL:N	2.15	0.60
1:B:1396:THR:O	1:B:1414:ARG:NH1	2.34	0.60
1:B:1512:ARG:NH2	1:B:1531:THR:O	2.34	0.60
1:C:226:GLN:OE1	1:C:226:GLN:N	2.34	0.60
1:C:229:ASN:O	1:C:230:LEU:HD23	2.01	0.60
1:B:482:ALA:O	1:B:483:SER:OG	2.19	0.60
1:C:496:ALA:HB3	1:C:519:GLN:HB2	1.83	0.60
1:C:1037:ASP:OD1	1:C:1038:PRO:HD2	2.01	0.60
1:C:1819:LEU:HB2	1:C:1823:ASN:HB2	1.84	0.60
1:D:167:ARG:HD3	1:D:371:ILE:HG22	1.83	0.60
1:A:520:ARG:HB2	1:A:571:PRO:HD2	1.83	0.60
1:A:536:PHE:O	1:A:579:ARG:NH2	2.35	0.60
1:A:902:PRO:HB3	1:A:937:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1282:GLU:OE2	1:B:1282:GLU:N	2.24	0.60
1:A:631:VAL:HG11	1:A:706:TYR:HE1	1.66	0.60
1:B:109:LEU:HG	1:B:110:VAL:H	1.66	0.60
1:D:294:GLU:HB3	1:D:338:ALA:HB1	1.84	0.60
1:D:1012:THR:OG1	1:D:1031:THR:OG1	2.20	0.60
1:D:1378:MET:HE3	1:D:1378:MET:HA	1.84	0.60
1:A:414:SER:O	1:A:414:SER:OG	2.20	0.60
1:A:764:ALA:HA	1:A:825:THR:HB	1.84	0.60
1:C:687:LYS:HD3	1:C:687:LYS:N	2.17	0.60
1:B:522:LYS:HG2	1:B:523:ALA:H	1.67	0.59
1:C:193:ILE:HD12	1:C:194:GLN:H	1.67	0.59
1:C:1037:ASP:CG	1:C:1038:PRO:HD2	2.28	0.59
1:C:1022:PRO:HB2	1:C:1028:THR:HG21	1.83	0.59
1:C:1305:PRO:HG2	1:C:1308:PHE:HD1	1.67	0.59
1:D:166:PRO:HG2	1:D:261:VAL:HG13	1.83	0.59
1:B:460:THR:HG22	1:B:489:THR:HA	1.84	0.59
1:C:1252:ILE:HD13	1:C:1347:PHE:HE2	1.67	0.59
1:C:1282:GLU:OE2	1:C:1282:GLU:N	2.28	0.59
1:D:1220:THR:HA	1:D:1230:PRO:HA	1.83	0.59
1:A:1186:TYR:HB3	1:A:1213:CYS:HB3	1.84	0.59
1:A:1809:ARG:HG2	1:A:1810:GLN:NE2	2.17	0.59
1:B:1503:ASN:ND2	1:B:1506:ASN:HB2	2.18	0.59
1:D:1749:PRO:HD2	1:D:1749:PRO:O	2.02	0.59
1:D:1485:GLY:O	1:D:1555:THR:OG1	2.21	0.59
1:A:588:LEU:HD12	1:A:613:VAL:HB	1.83	0.59
1:A:1616:GLY:O	1:A:1636:THR:OG1	2.20	0.59
1:B:43:ALA:N	1:B:74:ASP:OD2	2.36	0.59
1:D:83:LEU:HD21	1:D:109:LEU:HD11	1.83	0.59
1:D:418:VAL:HB	1:D:435:LEU:HD23	1.84	0.59
1:A:1011:THR:HG21	1:A:1150:LEU:HD21	1.85	0.59
1:B:470:ARG:HB2	1:B:478:GLY:HA2	1.84	0.59
1:C:902:PRO:HA	1:C:937:VAL:HA	1.83	0.59
1:D:874:THR:HA	1:D:999:MET:HE1	1.85	0.59
1:A:839:VAL:HG13	1:A:844:THR:HG23	1.84	0.58
1:C:1453:TYR:HD1	1:C:1455:PRO:HD3	1.67	0.58
1:A:374:LYS:HD3	1:A:374:LYS:N	2.19	0.58
1:A:1724:ARG:NH1	1:A:1745:SER:O	2.36	0.58
1:B:294:GLU:HB3	1:B:338:ALA:HB1	1.85	0.58
1:B:839:VAL:HG13	1:B:844:THR:HG23	1.83	0.58
1:D:63:ALA:HB2	1:D:118:THR:HG22	1.84	0.58
1:A:999:MET:HE3	1:A:1000:VAL:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HG	1:C:169:ASN:OD1	2.02	0.58
1:D:1798:PRO:O	1:D:1800:ASP:N	2.36	0.58
1:B:1130:GLU:H	1:B:1130:GLU:CD	2.11	0.58
1:B:1604:GLU:N	1:B:1604:GLU:OE2	2.37	0.58
1:A:95:ARG:NH1	1:A:134:SER:O	2.35	0.58
1:D:1489:LEU:HD13	1:D:1539:MET:HE1	1.86	0.58
1:A:273:LEU:HG	1:A:275:VAL:HG13	1.86	0.58
1:A:1564:LEU:HD13	1:C:1172:VAL:HG21	1.86	0.58
1:D:468:TYR:HB3	1:D:478:GLY:HA3	1.86	0.58
1:A:415:THR:HB	1:A:437:MET:HB3	1.85	0.58
1:B:902:PRO:HA	1:B:937:VAL:HA	1.85	0.58
1:B:1006:VAL:HG12	1:B:1036:ARG:HA	1.86	0.58
1:D:1661:GLN:OE1	1:D:1661:GLN:N	2.22	0.58
1:A:502:GLU:N	1:A:502:GLU:OE2	2.35	0.58
1:A:1227:ARG:NH2	1:C:1453:TYR:OH	2.36	0.58
1:B:530:GLU:HB3	1:B:596:ILE:HD11	1.86	0.58
1:B:532:ILE:HG12	1:B:596:ILE:HD13	1.86	0.58
1:B:618:PRO:HB3	1:B:647:VAL:HG12	1.86	0.58
1:D:1466:PRO:O	1:D:1469:THR:OG1	2.17	0.58
1:B:1644:ALA:HB2	1:B:1656:LEU:HB2	1.86	0.58
1:C:1014:SER:OG	1:C:1015:PRO:HD3	2.04	0.58
1:A:1644:ALA:HB2	1:A:1656:LEU:HB2	1.84	0.58
1:B:588:LEU:HD12	1:B:613:VAL:HB	1.85	0.58
1:B:1394:ASP:OD1	1:B:1416:THR:N	2.37	0.58
1:B:1801:PHE:HA	1:B:1813:ALA:HA	1.84	0.58
1:C:761:THR:HB	1:C:857:SER:HB3	1.85	0.58
1:C:828:THR:O	1:C:832:TYR:OH	2.16	0.58
1:D:713:THR:HB	1:D:736:PRO:HB3	1.85	0.58
1:C:882:VAL:HB	1:C:951:THR:HG22	1.85	0.57
1:D:168:LEU:HD22	1:D:231:GLU:HB3	1.84	0.57
1:A:109:LEU:HG	1:A:110:VAL:N	2.18	0.57
1:A:761:THR:HG21	1:A:862:PRO:HG3	1.86	0.57
1:A:1493:ARG:NH1	1:A:1549:ASN:O	2.37	0.57
1:B:1459:MET:SD	1:B:1459:MET:N	2.76	0.57
1:D:1609:VAL:HG13	1:D:1656:LEU:HD22	1.86	0.57
1:A:469:ASP:HB2	1:A:481:LEU:HD11	1.85	0.57
1:B:273:LEU:HA	1:B:293:THR:HG22	1.86	0.57
1:C:294:GLU:HB3	1:C:338:ALA:HB1	1.85	0.57
1:D:1006:VAL:HG12	1:D:1036:ARG:HA	1.85	0.57
1:A:1189:ILE:HD11	1:A:1214:ARG:HD3	1.86	0.57
1:C:271:LEU:O	1:C:374:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1721:THR:HG23	1:C:1732:LYS:HA	1.86	0.57
1:D:829:PRO:O	1:D:829:PRO:HD2	2.02	0.57
1:A:872:PRO:HG3	1:A:882:VAL:HA	1.86	0.57
1:A:876:VAL:HB	1:A:999:MET:HE2	1.86	0.57
1:A:1378:MET:N	1:C:1328:ASP:OD1	2.33	0.57
1:C:420:TRP:CD1	1:C:435:LEU:HB2	2.40	0.57
1:D:439:ASN:HB2	1:D:446:ASN:HD21	1.70	0.57
1:D:1724:ARG:NH1	1:D:1745:SER:O	2.37	0.57
1:A:1801:PHE:HA	1:A:1813:ALA:HA	1.87	0.57
1:A:1805:ARG:O	1:A:1807:GLY:N	2.31	0.57
1:A:836:VAL:HG23	1:A:850:LYS:HZ3	1.70	0.57
1:B:283:ALA:HA	1:B:470:ARG:HH12	1.69	0.57
1:C:128:THR:HG23	1:C:146:THR:HG22	1.85	0.57
1:A:1711:GLN:NE2	1:B:1931:PRO:O	2.38	0.57
1:B:168:LEU:HG	1:B:169:ASN:OD1	2.05	0.57
1:B:618:PRO:HG3	1:B:645:ARG:CZ	2.34	0.57
1:C:1485:GLY:O	1:C:1555:THR:OG1	2.23	0.57
1:D:421:THR:OG1	1:D:466:ARG:O	2.22	0.57
1:A:719:ILE:HG12	1:A:730:THR:HG22	1.87	0.56
1:A:1754:PHE:HA	1:A:1767:ALA:HA	1.85	0.56
1:B:506:PRO:HD2	1:B:615:ALA:HA	1.87	0.56
1:C:877:LYS:HD2	1:C:1002:ALA:HB3	1.87	0.56
1:D:536:PHE:O	1:D:579:ARG:NH2	2.38	0.56
1:A:1773:TYR:HB2	1:A:1809:ARG:HA	1.88	0.56
1:D:178:ARG:HD2	1:D:218:ASN:ND2	2.18	0.56
1:D:1223:MET:HA	1:D:1223:MET:HE2	1.86	0.56
1:A:394:ALA:C	1:A:396:PRO:HG3	2.31	0.56
1:A:525:PRO:HD2	1:A:525:PRO:O	2.05	0.56
1:A:1130:GLU:H	1:A:1130:GLU:CD	2.12	0.56
1:A:1335:PRO:HB2	1:A:1337:GLU:HG2	1.87	0.56
1:B:1014:SER:OG	1:B:1015:PRO:HD3	2.05	0.56
1:B:1487:ASN:HD22	1:B:1549:ASN:HA	1.70	0.56
1:C:1051:ALA:HB1	1:C:1096:LEU:HD11	1.87	0.56
1:A:1192:ASN:ND2	1:A:1193:ASP:OD1	2.39	0.56
1:B:716:LEU:HD12	1:B:734:LEU:HD12	1.86	0.56
1:D:49:LEU:HD13	1:D:68:ALA:HB2	1.87	0.56
1:A:1408:CYS:SG	1:A:1414:ARG:NH2	2.79	0.56
1:B:238:LEU:HB3	1:B:253:PHE:HB3	1.87	0.56
1:B:1769:PRO:HB2	1:B:1772:TYR:CD2	2.41	0.56
1:D:43:ALA:N	1:D:74:ASP:OD2	2.38	0.56
1:D:496:ALA:HB3	1:D:519:GLN:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1011:THR:HG21	1:D:1150:LEU:HD21	1.87	0.56
1:C:1186:TYR:HB3	1:C:1213:CYS:HB3	1.86	0.56
1:D:1042:PRO:HG2	1:D:1045:SER:HB2	1.87	0.56
1:A:373:GLU:C	1:A:374:LYS:HD3	2.31	0.56
1:A:762:PRO:O	1:A:857:SER:OG	2.24	0.56
1:D:161:LEU:HD11	1:D:178:ARG:HH12	1.71	0.56
1:D:420:TRP:CD1	1:D:435:LEU:HB2	2.41	0.56
1:D:839:VAL:HG13	1:D:844:THR:HG23	1.87	0.56
1:B:752:THR:OG1	1:B:776:THR:OG1	2.24	0.56
1:C:589:GLN:N	1:C:589:GLN:OE1	2.39	0.56
1:C:1084:VAL:HG12	1:C:1087:ASP:HB3	1.88	0.56
1:D:692:ALA:HB3	1:D:695:SER:HB2	1.88	0.56
1:A:1328:ASP:OD2	1:C:1378:MET:N	2.39	0.55
1:B:628:PRO:HD2	1:B:637:THR:HG23	1.88	0.55
1:D:1769:PRO:HB2	1:D:1772:TYR:CE2	2.41	0.55
1:B:459:GLY:O	1:B:461:LYS:NZ	2.23	0.55
1:B:643:ILE:HB	1:B:698:ALA:HB3	1.88	0.55
1:C:877:LYS:HB2	1:C:880:THR:HG21	1.88	0.55
1:C:1810:GLN:N	1:C:1810:GLN:OE1	2.39	0.55
1:B:1430:ASP:O	1:B:1506:ASN:ND2	2.39	0.55
1:C:54:PRO:HD2	1:C:64:VAL:HG12	1.88	0.55
1:C:81:PHE:HB2	1:C:129:LEU:HD11	1.88	0.55
1:C:1544:GLU:N	1:C:1544:GLU:OE1	2.40	0.55
1:B:175:PHE:HB3	1:B:223:ILE:HD12	1.88	0.55
1:B:1293:GLN:NE2	1:B:1298:GLY:HA2	2.22	0.55
1:C:110:VAL:HG22	1:C:115:TYR:HD2	1.72	0.55
1:C:501:VAL:HG13	1:C:504:PHE:HA	1.89	0.55
1:D:306:LEU:HD23	1:D:365:ASP:HB2	1.88	0.55
1:A:1051:ALA:HB1	1:A:1096:LEU:HD11	1.88	0.55
1:A:240:ILE:HD12	1:A:251:ARG:HB3	1.88	0.55
1:A:401:ASP:CG	1:A:402:THR:N	2.63	0.55
1:D:1721:THR:HG23	1:D:1732:LYS:HA	1.89	0.55
1:A:181:SER:OG	1:A:186:ARG:NH2	2.30	0.55
1:A:618:PRO:HG3	1:A:645:ARG:CZ	2.36	0.55
1:A:734:LEU:HB3	1:C:738:TYR:OH	2.07	0.55
1:C:1378:MET:HE3	1:C:1378:MET:HA	1.89	0.55
1:D:790:CYS:HA	1:D:836:VAL:HG13	1.88	0.55
1:D:1282:GLU:H	1:D:1282:GLU:CD	2.13	0.55
1:A:179:VAL:HG21	1:A:209:ILE:HD12	1.88	0.55
1:B:63:ALA:HB2	1:B:118:THR:HG22	1.89	0.55
1:D:497:LEU:HD11	1:D:516:PHE:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1439:THR:OG1	1:D:1445:CYS:O	2.22	0.55
1:A:74:ASP:OD1	1:A:75:SER:N	2.40	0.55
1:A:1128:VAL:HG13	1:A:1140:ALA:HB3	1.89	0.55
1:A:1265:SER:C	1:A:1266:ILE:HD13	2.32	0.55
1:B:1597:GLN:O	1:B:1600:THR:OG1	2.24	0.55
1:D:1706:GLN:OE1	1:D:1715:LYS:NZ	2.40	0.55
1:A:1567:LYS:O	1:A:1570:THR:OG1	2.25	0.54
1:B:1051:ALA:HB1	1:B:1096:LEU:HD11	1.89	0.54
1:C:719:ILE:HG12	1:C:730:THR:HG22	1.87	0.54
1:A:1323:GLY:HA2	1:A:1367:LEU:HB2	1.90	0.54
1:A:1611:LYS:HB3	1:A:1643:ASN:HD22	1.72	0.54
1:B:1550:LEU:H	1:B:1563:GLN:HE22	1.55	0.54
1:B:1801:PHE:HB3	1:B:1811:CYS:HB3	1.90	0.54
1:B:167:ARG:HD3	1:B:371:ILE:HG22	1.90	0.54
1:B:872:PRO:HG3	1:B:882:VAL:HA	1.90	0.54
1:C:1374:ALA:HA	1:C:1388:PRO:HD3	1.88	0.54
1:A:663:TRP:O	1:A:714:PRO:HA	2.08	0.54
1:B:1084:VAL:HG12	1:B:1087:ASP:HB3	1.89	0.54
1:D:1423:GLY:HA3	1:D:1450:PRO:HG2	1.89	0.54
1:B:1703:GLY:H	1:B:1723:SER:HB3	1.71	0.54
1:C:801:PRO:HG2	1:C:821:ILE:HG12	1.88	0.54
1:C:1576:THR:HG22	1:C:1588:VAL:H	1.72	0.54
1:A:86:GLY:HA3	1:A:125:LYS:HB3	1.89	0.54
1:A:1539:MET:HE3	1:A:1539:MET:HA	1.89	0.54
1:B:239:ARG:HG2	1:B:249:LEU:HD11	1.90	0.54
1:D:1061:ASN:HB3	1:D:1062:PRO:HD3	1.90	0.54
1:A:1685:VAL:HG21	1:A:1728:GLU:HG2	1.89	0.54
1:B:109:LEU:HG	1:B:110:VAL:N	2.21	0.54
1:B:1015:PRO:HG2	1:B:1028:THR:HG22	1.90	0.54
1:B:1439:THR:OG1	1:B:1445:CYS:O	2.24	0.54
1:C:876:VAL:O	1:C:1002:ALA:N	2.39	0.54
1:C:889:THR:HG22	1:C:944:THR:HG22	1.90	0.54
1:C:1672:GLN:NE2	1:C:1679:THR:O	2.41	0.54
1:D:1327:THR:HG22	1:D:1328:ASP:H	1.72	0.54
1:A:877:LYS:HD2	1:A:1002:ALA:HB3	1.89	0.54
1:A:1239:GLU:OE2	1:A:1239:GLU:N	2.40	0.54
1:D:1014:SER:OG	1:D:1015:PRO:HD3	2.08	0.54
1:A:1042:PRO:HG2	1:A:1045:SER:HB2	1.90	0.54
1:B:1218:GLY:HA2	1:B:1239:GLU:H	1.72	0.54
1:C:49:LEU:HD13	1:C:68:ALA:HB2	1.88	0.54
1:C:532:ILE:HG12	1:C:596:ILE:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1592:GLN:NE2	1:C:1593:CYS:O	2.40	0.54
1:D:1254:LYS:O	1:D:1285:LYS:NZ	2.40	0.54
1:B:1453:TYR:HD2	1:B:1479:CYS:HB3	1.73	0.53
1:C:1084:VAL:HG13	1:C:1086:THR:H	1.74	0.53
1:D:1364:ASN:HD21	1:D:1414:ARG:NH1	2.06	0.53
1:B:719:ILE:HG12	1:B:730:THR:HG22	1.89	0.53
1:B:1399:LYS:HA	1:B:1399:LYS:HE2	1.90	0.53
1:C:190:TRP:CZ2	1:C:244:PRO:HG3	2.43	0.53
1:C:643:ILE:HB	1:C:698:ALA:HB3	1.90	0.53
1:C:1174:LEU:HB3	1:C:1178:PHE:HB3	1.90	0.53
1:A:239:ARG:HG2	1:A:249:LEU:HD11	1.90	0.53
1:A:1282:GLU:OE2	1:A:1282:GLU:N	2.24	0.53
1:B:280:VAL:HB	1:B:284:ASP:HB2	1.91	0.53
1:B:1647:ASN:HD21	1:B:1652:ILE:HG22	1.73	0.53
1:C:754:SER:HA	1:C:850:LYS:NZ	2.23	0.53
1:C:1128:VAL:HG13	1:C:1140:ALA:HB3	1.90	0.53
1:D:308:TRP:CE2	1:D:341:VAL:HB	2.43	0.53
1:A:1130:GLU:OE1	1:A:1138:ALA:N	2.39	0.53
1:A:1850:ARG:HG2	1:A:1851:THR:N	2.23	0.53
1:B:230:LEU:O	1:B:231:GLU:HG3	2.08	0.53
1:B:1607:GLN:OE1	1:B:1608:PRO:HD2	2.08	0.53
1:C:1573:PRO:HG3	1:C:1582:LEU:HD11	1.90	0.53
1:D:903:ILE:HD13	1:D:945:THR:HG21	1.90	0.53
1:D:1195:TYR:HA	1:D:1200:ARG:HA	1.90	0.53
1:A:1006:VAL:HG12	1:A:1036:ARG:HA	1.90	0.53
1:A:1252:ILE:HD11	1:A:1301:CYS:HB2	1.89	0.53
1:A:1618:PHE:HB3	1:A:1636:THR:HG21	1.90	0.53
1:B:308:TRP:CE2	1:B:341:VAL:HB	2.44	0.53
1:D:555:ALA:HA	1:D:560:GLY:HA3	1.89	0.53
1:D:1037:ASP:HB3	1:D:1038:PRO:HD2	1.90	0.53
1:B:1569:GLY:H	1:B:1602:ASN:HB3	1.74	0.53
1:C:1569:GLY:H	1:C:1602:ASN:HB3	1.74	0.53
1:D:910:GLY:HA3	1:D:961:PHE:HB3	1.91	0.53
1:A:620:TYR:HE2	1:A:731:VAL:HG21	1.74	0.53
1:A:1805:ARG:O	1:A:1805:ARG:HG2	2.08	0.53
1:B:196:ASP:HB3	1:B:201:VAL:HG11	1.91	0.53
1:C:308:TRP:CE2	1:C:341:VAL:HB	2.44	0.53
1:A:1757:ASN:HD22	1:A:1763:THR:HB	1.74	0.53
1:A:592:LEU:HD12	1:A:593:GLN:N	2.24	0.53
1:A:1306:SER:HA	1:C:1375:ILE:HD11	1.91	0.53
1:A:1562:ILE:HD11	1:C:1190:PHE:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1706:GLN:NE2	1:A:1711:GLN:HG3	2.23	0.53
1:B:877:LYS:O	1:B:880:THR:HG22	2.09	0.53
1:B:1178:PHE:HD2	1:B:1211:GLY:H	1.57	0.53
1:A:1489:LEU:HD13	1:A:1539:MET:HE1	1.91	0.52
1:D:1527:LYS:HD3	1:D:1527:LYS:N	2.24	0.52
1:A:704:PRO:HG3	1:A:714:PRO:HG2	1.91	0.52
1:A:1390:ARG:HH11	1:C:1302:LEU:HD21	1.74	0.52
1:B:1361:CYS:HB3	1:B:1365:THR:HG23	1.90	0.52
1:C:445:PRO:C	1:C:446:ASN:HD22	2.17	0.52
1:C:1350:ILE:HG13	1:C:1351:TYR:CD1	2.45	0.52
1:C:1368:PRO:HG2	1:C:1369:LEU:HD12	1.90	0.52
1:D:844:THR:HG22	1:D:845:THR:HG23	1.90	0.52
1:A:1573:PRO:HD2	1:A:1588:VAL:HG11	1.90	0.52
1:A:1801:PHE:HB3	1:A:1811:CYS:HB3	1.90	0.52
1:B:1332:THR:HG23	1:B:1359:ARG:HE	1.74	0.52
1:C:280:VAL:HB	1:C:284:ASP:HB2	1.91	0.52
1:D:80:PHE:HD1	1:D:97:THR:HA	1.74	0.52
1:D:761:THR:HG22	1:D:894:VAL:HG21	1.91	0.52
1:A:167:ARG:HH12	1:A:369:ASN:HD22	1.56	0.52
1:B:161:LEU:HD11	1:B:178:ARG:HH11	1.74	0.52
1:B:581:TYR:HE1	1:B:588:LEU:HD22	1.74	0.52
1:B:1055:TYR:HD1	1:B:1094:GLN:HB3	1.74	0.52
1:B:1599:GLY:HA2	1:B:1619:ALA:HB3	1.92	0.52
1:B:1850:ARG:HG2	1:B:1851:THR:N	2.25	0.52
1:D:1829:THR:HB	1:D:1834:SER:HB3	1.91	0.52
1:A:1009:GLU:OE2	1:A:1107:ARG:NH1	2.42	0.52
1:A:1053:ALA:HB2	1:A:1096:LEU:HD13	1.91	0.52
1:B:1215:LYS:O	1:B:1216:CYS:HB2	2.08	0.52
1:C:628:PRO:HD2	1:C:637:THR:HG23	1.90	0.52
1:C:1644:ALA:HB2	1:C:1656:LEU:HB2	1.91	0.52
1:D:81:PHE:HB2	1:D:129:LEU:HD11	1.91	0.52
1:A:534:CYS:O	1:A:560:GLY:CA	2.58	0.52
1:A:1014:SER:OG	1:A:1015:PRO:HD3	2.09	0.52
1:B:1293:GLN:OE1	1:B:1295:ASN:N	2.43	0.52
1:D:1769:PRO:HB2	1:D:1772:TYR:CD2	2.45	0.52
1:A:1215:LYS:O	1:A:1216:CYS:HB2	2.10	0.52
1:C:555:ALA:HA	1:C:560:GLY:HA3	1.92	0.52
1:D:109:LEU:HG	1:D:110:VAL:HG23	1.91	0.52
1:D:110:VAL:HG22	1:D:115:TYR:CD2	2.45	0.52
1:D:297:TYR:CZ	1:D:299:ALA:HB3	2.44	0.52
1:D:1187:GLU:HB2	1:D:1228:CYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1397:TRP:N	1:D:1406:GLN:O	2.33	0.52
1:A:80:PHE:HD1	1:A:97:THR:HA	1.74	0.52
1:A:363:LEU:HD12	1:A:371:ILE:HD11	1.91	0.52
1:A:1329:GLY:HA3	1:A:1357:THR:HG21	1.92	0.52
1:B:170:LEU:HG	1:C:1203:VAL:HG13	1.91	0.52
1:C:178:ARG:HD2	1:C:218:ASN:HB3	1.91	0.52
1:A:1736:GLY:HA2	1:A:1780:TYR:HB3	1.91	0.52
1:C:1466:PRO:O	1:C:1469:THR:OG1	2.28	0.52
1:D:1644:ALA:HB2	1:D:1656:LEU:HB2	1.91	0.52
1:A:1516:ILE:HD11	1:A:1608:PRO:HD3	1.92	0.51
1:B:1492:ASP:OD2	1:B:1494:THR:N	2.40	0.51
1:A:354:THR:HG21	1:A:382:ASN:HB3	1.91	0.51
1:B:757:LEU:HD11	1:B:769:ALA:HB1	1.91	0.51
1:C:420:TRP:O	1:C:433:THR:OG1	2.26	0.51
1:C:1499:LEU:HD22	1:C:1512:ARG:HG2	1.92	0.51
1:A:790:CYS:HA	1:A:836:VAL:HG13	1.92	0.51
1:A:1515:THR:HA	1:A:1530:VAL:HB	1.92	0.51
1:A:1669:GLY:H	1:A:1689:ALA:HB3	1.75	0.51
1:C:1199:VAL:O	1:C:1200:ARG:HB3	2.11	0.51
1:D:432:ARG:CZ	1:D:472:GLY:HA3	2.40	0.51
1:D:437:MET:HE2	1:D:437:MET:HA	1.93	0.51
1:D:1515:THR:HG22	1:D:1515:THR:O	2.10	0.51
1:B:902:PRO:HB3	1:B:937:VAL:HG12	1.93	0.51
1:B:1125:LYS:NZ	1:B:1149:SER:OG	2.42	0.51
1:C:758:ASN:HD22	1:C:759:PRO:HA	1.75	0.51
1:D:62:ASP:OD1	1:D:63:ALA:N	2.44	0.51
1:D:1772:TYR:CD1	1:D:1796:LYS:HG2	2.45	0.51
1:A:493:VAL:HG23	1:A:521:SER:HB2	1.93	0.51
1:A:1490:MET:SD	1:A:1536:ASN:HB3	2.51	0.51
1:B:410:LYS:HD2	1:B:410:LYS:C	2.36	0.51
1:B:877:LYS:HD2	1:B:1002:ALA:HB3	1.92	0.51
1:C:1195:TYR:OH	1:C:1200:ARG:NH2	2.33	0.51
1:D:1174:LEU:HD13	1:D:1178:PHE:HB3	1.93	0.51
1:D:1773:TYR:CE1	1:D:1797:CYS:HB3	2.46	0.51
1:C:832:TYR:HB2	1:C:852:PHE:CE2	2.46	0.51
1:D:1299:THR:HG23	1:D:1300:VAL:HG22	1.93	0.51
1:D:1722:TYR:HD1	1:D:1747:CYS:SG	2.34	0.51
1:A:1463:LEU:H	1:A:1463:LEU:HD12	1.74	0.51
1:B:1263:LYS:HB2	1:B:1266:ILE:HG22	1.92	0.51
1:B:1720:GLY:HA2	1:B:1739:ALA:HB3	1.92	0.51
1:D:1257:ALA:HA	1:D:1276:HIS:HD2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1453:TYR:CD1	1:D:1455:PRO:HD3	2.45	0.51
1:A:1035:LEU:HG	1:A:1037:ASP:H	1.76	0.51
1:D:228:TYR:HD1	1:D:234:LYS:HE3	1.76	0.51
1:D:957:SER:HB3	1:D:1001:VAL:N	2.21	0.51
1:A:1235:TYR:HD1	1:A:1246:ALA:HA	1.76	0.51
1:C:423:ASP:HB3	1:C:464:THR:HB	1.93	0.51
1:C:1539:MET:H	1:C:1539:MET:HE2	1.75	0.51
1:A:1600:THR:HB	1:A:1610:CYS:HB2	1.93	0.51
1:A:1796:LYS:HD2	1:A:1832:LEU:HB3	1.93	0.51
1:C:1015:PRO:HG2	1:C:1028:THR:HG22	1.93	0.51
1:C:1453:TYR:CD1	1:C:1455:PRO:HD3	2.45	0.51
1:C:1520:VAL:HG12	1:C:1529:ILE:HG12	1.92	0.51
1:A:308:TRP:HB2	1:A:361:LEU:HD11	1.91	0.50
1:A:1466:PRO:HB3	1:C:1227:ARG:HD3	1.93	0.50
1:C:534:CYS:HB3	1:C:592:LEU:HD11	1.92	0.50
1:D:689:THR:HG21	1:D:700:CYS:HB2	1.92	0.50
1:C:195:LEU:HD22	1:C:228:TYR:CZ	2.46	0.50
1:C:1647:ASN:HD21	1:C:1652:ILE:HG22	1.76	0.50
1:D:59:THR:N	1:D:62:ASP:OD2	2.42	0.50
1:D:1285:LYS:HD3	1:D:1285:LYS:N	2.27	0.50
1:A:1452:THR:HG22	1:A:1464:PRO:HA	1.93	0.50
1:A:1850:ARG:HG2	1:A:1851:THR:H	1.77	0.50
1:B:1721:THR:HG23	1:B:1732:LYS:HA	1.93	0.50
1:C:1844:SER:HB2	1:C:1847:LYS:HZ1	1.76	0.50
1:A:1132:ALA:O	1:A:1135:THR:OG1	2.26	0.50
1:C:1289:LYS:HG2	1:C:1312:SER:N	2.22	0.50
1:C:1724:ARG:HA	1:C:1724:ARG:NE	2.27	0.50
1:D:280:VAL:HB	1:D:284:ASP:HB2	1.94	0.50
1:D:1539:MET:HA	1:D:1539:MET:HE3	1.93	0.50
1:B:293:THR:O	1:B:340:ALA:HA	2.12	0.50
1:D:1199:VAL:O	1:D:1200:ARG:HB3	2.11	0.50
1:D:1255:PRO:HD2	1:D:1255:PRO:O	2.12	0.50
1:B:155:THR:HB	1:B:182:SER:HB3	1.93	0.50
1:B:555:ALA:HA	1:B:560:GLY:HA3	1.94	0.50
1:B:1672:GLN:NE2	1:B:1679:THR:O	2.44	0.50
1:C:1289:LYS:HZ3	1:C:1289:LYS:HB2	1.75	0.50
1:D:110:VAL:HG22	1:D:115:TYR:HD2	1.77	0.50
1:A:1022:PRO:HB2	1:A:1028:THR:HG21	1.92	0.50
1:A:1321:SER:O	1:A:1324:THR:OG1	2.28	0.50
1:A:1844:SER:HB2	1:A:1847:LYS:NZ	2.26	0.50
1:A:506:PRO:HG3	1:A:588:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:VAL:HB	1:D:951:THR:HG22	1.93	0.50
1:A:47:LEU:HD23	1:A:70:VAL:HG22	1.94	0.49
1:A:721:ASN:HD22	1:A:725:LEU:HD13	1.77	0.49
1:B:761:THR:HB	1:B:857:SER:HB3	1.94	0.49
1:B:1515:THR:HA	1:B:1530:VAL:HB	1.94	0.49
1:C:656:LEU:HD23	1:C:658:ILE:HD11	1.93	0.49
1:C:1539:MET:HE2	1:C:1539:MET:N	2.27	0.49
1:B:287:THR:HG22	1:B:348:THR:HG22	1.92	0.49
1:C:470:ARG:NE	1:C:477:THR:O	2.36	0.49
1:D:1379:ASN:OD1	1:D:1379:ASN:N	2.43	0.49
1:D:1816:PRO:HB2	1:D:1824:LEU:HD21	1.93	0.49
1:A:957:SER:HB3	1:A:1001:VAL:O	2.12	0.49
1:A:1481:GLN:NE2	1:C:1164:GLY:O	2.46	0.49
1:B:1392:CYS:SG	1:B:1396:THR:OG1	2.61	0.49
1:B:1757:ASN:HD21	1:B:1764:SER:HB3	1.78	0.49
1:D:659:LEU:HB3	1:D:681:ALA:HB1	1.95	0.49
1:A:702:PHE:HE2	1:A:704:PRO:HB3	1.77	0.49
1:B:161:LEU:HD11	1:B:178:ARG:NH1	2.27	0.49
1:B:625:SER:HB3	1:B:640:THR:HG22	1.93	0.49
1:B:1496:GLN:HA	1:B:1511:LEU:HD11	1.94	0.49
1:B:1672:GLN:HG2	1:B:1677:THR:HG21	1.95	0.49
1:A:290:GLN:O	1:A:293:THR:OG1	2.29	0.49
1:A:656:LEU:HB3	1:A:691:MET:HB3	1.95	0.49
1:A:1737:THR:OG1	1:A:1738:VAL:N	2.45	0.49
1:B:876:VAL:HB	1:B:999:MET:HE2	1.94	0.49
1:C:516:PHE:HB2	1:C:575:ILE:HG22	1.94	0.49
1:C:545:PRO:HB3	1:C:550:ALA:HB3	1.95	0.49
1:C:781:VAL:HG13	1:C:786:LYS:HE2	1.95	0.49
1:D:1586:LEU:HD13	1:D:1594:TYR:CZ	2.48	0.49
1:B:290:GLN:HG3	1:B:345:ALA:HB3	1.95	0.49
1:B:458:GLY:HA3	1:B:492:PRO:HD3	1.94	0.49
1:B:1192:ASN:OD1	1:B:1192:ASN:N	2.44	0.49
1:B:1844:SER:O	1:B:1847:LYS:HE3	2.12	0.49
1:B:1220:THR:OG1	1:B:1229:ILE:O	2.29	0.49
1:B:1466:PRO:O	1:B:1469:THR:OG1	2.24	0.49
1:B:1549:ASN:OD1	1:B:1549:ASN:N	2.46	0.49
1:C:1469:THR:HB	1:C:1479:CYS:HB3	1.94	0.49
1:A:470:ARG:NH2	1:A:471:ASP:OD2	2.37	0.49
1:B:517:ARG:HG2	1:B:517:ARG:HH11	1.78	0.49
1:B:1035:LEU:HG	1:B:1037:ASP:H	1.77	0.49
1:B:1440:GLU:OE2	1:B:1442:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1195:TYR:HA	1:C:1200:ARG:HA	1.93	0.49
1:C:1850:ARG:HD3	1:C:1851:THR:O	2.13	0.49
1:D:1289:LYS:HZ3	1:D:1289:LYS:HB2	1.78	0.49
1:A:534:CYS:O	1:A:560:GLY:HA2	2.13	0.49
1:A:1421:GLN:HB2	1:A:1436:THR:HB	1.95	0.49
1:B:393:THR:O	1:B:394:ALA:HB2	2.13	0.49
1:B:775:ILE:HB	1:B:815:THR:HG22	1.95	0.49
1:B:1573:PRO:HG2	1:B:1588:VAL:HG21	1.94	0.49
1:C:420:TRP:HD1	1:C:435:LEU:HB2	1.76	0.49
1:C:677:TRP:CD1	1:C:717:GLN:HE21	2.31	0.49
1:A:297:TYR:CZ	1:A:299:ALA:HB3	2.48	0.48
1:A:420:TRP:CD1	1:A:435:LEU:HB2	2.48	0.48
1:B:1042:PRO:HG2	1:B:1045:SER:HB2	1.94	0.48
1:B:1326:HIS:NE2	1:B:1355:PRO:O	2.33	0.48
1:B:1614:TRP:O	1:B:1614:TRP:CD1	2.66	0.48
1:D:1683:CYS:SG	1:D:1687:THR:OG1	2.65	0.48
1:B:274:THR:O	1:B:274:THR:OG1	2.28	0.48
1:D:1668:MET:SD	1:D:1668:MET:N	2.68	0.48
1:A:758:ASN:HD22	1:A:759:PRO:HA	1.78	0.48
1:A:1569:GLY:H	1:A:1602:ASN:HB3	1.77	0.48
1:B:420:TRP:CD1	1:B:435:LEU:HB2	2.48	0.48
1:B:1452:THR:HG22	1:B:1464:PRO:HA	1.94	0.48
1:C:167:ARG:HD3	1:C:371:ILE:HG22	1.95	0.48
1:C:1272:HIS:CD2	1:C:1273:PHE:N	2.81	0.48
1:D:618:PRO:HG3	1:D:645:ARG:CZ	2.43	0.48
1:A:519:GLN:HA	1:A:519:GLN:NE2	2.27	0.48
1:A:593:GLN:HE22	1:A:608:THR:HG22	1.78	0.48
1:A:738:TYR:OH	1:C:734:LEU:HB3	2.13	0.48
1:C:1380:LEU:HD23	1:C:1381:ALA:H	1.78	0.48
1:D:1465:CYS:SG	1:D:1469:THR:OG1	2.71	0.48
1:A:877:LYS:HB2	1:A:880:THR:HG21	1.96	0.48
1:A:1809:ARG:HG2	1:A:1810:GLN:HE22	1.78	0.48
1:A:1844:SER:HB2	1:A:1847:LYS:HZ1	1.77	0.48
1:C:1844:SER:HB2	1:C:1847:LYS:NZ	2.28	0.48
1:D:620:TYR:HA	1:D:644:ILE:O	2.13	0.48
1:B:1798:PRO:HB3	1:B:1832:LEU:HD23	1.96	0.48
1:A:400:ASP:OD1	1:A:401:ASP:N	2.43	0.48
1:B:451:LEU:HD12	1:B:452:SER:N	2.29	0.48
1:B:1324:THR:HB	1:B:1358:CYS:HB3	1.94	0.48
1:C:1425:PRO:HG2	1:C:1426:PHE:CE1	2.49	0.48
1:C:1519:MET:HE3	1:C:1519:MET:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:758:ASN:HD21	1:D:988:LEU:HD11	1.78	0.48
1:A:1037:ASP:CG	1:A:1038:PRO:HD2	2.37	0.48
1:B:202:PHE:CG	1:C:1279:MET:HE1	2.49	0.48
1:B:686:GLY:C	1:B:687:LYS:HD3	2.39	0.48
1:B:1586:LEU:HD13	1:B:1594:TYR:CZ	2.49	0.48
1:B:1769:PRO:HB2	1:B:1772:TYR:CE2	2.48	0.48
1:C:1081:THR:HB	1:C:1098:VAL:H	1.78	0.48
1:D:517:ARG:HH21	1:D:723:PHE:HB3	1.79	0.48
1:D:673:THR:HG23	1:D:675:ALA:H	1.79	0.48
1:D:889:THR:HG22	1:D:944:THR:HG22	1.95	0.48
1:D:1647:ASN:HD21	1:D:1652:ILE:HG22	1.79	0.48
1:A:966:MET:HE3	1:A:967:VAL:N	2.25	0.48
1:C:1512:ARG:HB3	1:C:1530:VAL:HG11	1.96	0.48
1:C:1706:GLN:OE1	1:C:1715:LYS:NZ	2.47	0.48
1:D:254:THR:HG22	1:D:255:PRO:HD2	1.96	0.48
1:D:1304:CYS:SG	1:D:1310:SER:HB3	2.54	0.48
1:D:1486:THR:HG22	1:D:1548:THR:HA	1.94	0.48
1:A:1798:PRO:O	1:A:1800:ASP:N	2.47	0.47
1:B:687:LYS:HD3	1:B:687:LYS:N	2.29	0.47
1:C:1791:PRO:O	1:C:1795:TYR:OH	2.22	0.47
1:D:1130:GLU:OE2	1:D:1138:ALA:N	2.46	0.47
1:D:1215:LYS:O	1:D:1216:CYS:HB2	2.14	0.47
1:D:1603:ASP:OD1	1:D:1603:ASP:N	2.47	0.47
1:A:1227:ARG:HB3	1:C:1466:PRO:HA	1.96	0.47
1:A:1671:PHE:HD2	1:A:1696:ALA:HA	1.79	0.47
1:B:1011:THR:HG21	1:B:1150:LEU:HD21	1.94	0.47
1:B:1423:GLY:HA3	1:B:1450:PRO:HG2	1.96	0.47
1:C:966:MET:HA	1:C:966:MET:HE2	1.96	0.47
1:D:1350:ILE:HG12	1:D:1351:TYR:CD1	2.49	0.47
1:D:1803:ALA:O	1:D:1805:ARG:HD3	2.14	0.47
1:B:663:TRP:CZ2	1:B:665:GLY:HA2	2.50	0.47
1:B:1058:GLN:NE2	1:B:1115:LEU:O	2.33	0.47
1:B:1196:THR:O	1:B:1198:GLY:N	2.47	0.47
1:B:1453:TYR:CD2	1:B:1479:CYS:HB3	2.50	0.47
1:D:190:TRP:CZ2	1:D:244:PRO:HG3	2.48	0.47
1:A:1440:GLU:OE1	1:A:1443:SER:HB2	2.14	0.47
1:B:469:ASP:OD2	1:B:470:ARG:HG2	2.15	0.47
1:C:659:LEU:HB3	1:C:681:ALA:HB1	1.95	0.47
1:C:764:ALA:HA	1:C:825:THR:HB	1.94	0.47
1:D:1817:LEU:HD21	1:D:1839:PRO:HB3	1.97	0.47
1:A:762:PRO:HG3	1:A:824:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PHE:HB2	1:B:129:LEU:HD11	1.97	0.47
1:B:496:ALA:HB3	1:B:519:GLN:HB3	1.96	0.47
1:B:1131:TYR:OH	1:B:1134:SER:HA	2.14	0.47
1:B:1490:MET:SD	1:B:1536:ASN:HB3	2.54	0.47
1:B:1615:SER:OG	1:B:1616:GLY:N	2.46	0.47
1:C:308:TRP:HB2	1:C:361:LEU:HD11	1.96	0.47
1:C:1254:LYS:HB3	1:C:1285:LYS:NZ	2.29	0.47
1:C:1292:PHE:CZ	1:C:1302:LEU:HD23	2.49	0.47
1:C:1772:TYR:OH	1:C:1789:GLU:OE2	2.25	0.47
1:A:536:PHE:HD1	1:A:592:LEU:HB2	1.80	0.47
1:B:392:THR:O	1:B:393:THR:O	2.32	0.47
1:D:517:ARG:HD3	1:D:574:ILE:HG12	1.97	0.47
1:A:159:THR:OG1	1:A:178:ARG:NH1	2.48	0.47
1:A:288:PHE:CE1	1:A:290:GLN:HG2	2.50	0.47
1:A:1192:ASN:HA	1:A:1209:PRO:HA	1.97	0.47
1:B:423:ASP:HB3	1:B:464:THR:HB	1.97	0.47
1:B:1189:ILE:O	1:B:1211:GLY:HA2	2.14	0.47
1:B:1257:ALA:HA	1:B:1276:HIS:HD2	1.79	0.47
1:B:1374:ALA:HA	1:B:1388:PRO:HD3	1.96	0.47
1:C:80:PHE:HD1	1:C:97:THR:HA	1.80	0.47
1:C:455:TYR:CD2	1:C:461:LYS:HD2	2.50	0.47
1:C:755:SER:HB3	1:C:773:ILE:HG12	1.95	0.47
1:C:1018:ASN:HD21	1:C:1020:THR:HB	1.80	0.47
1:C:1551:PRO:HG3	1:C:1574:PHE:HD1	1.79	0.47
1:D:565:ILE:HG23	1:D:571:PRO:HB3	1.96	0.47
1:D:656:LEU:HD23	1:D:658:ILE:HD11	1.97	0.47
1:A:882:VAL:HB	1:A:951:THR:HG22	1.97	0.47
1:A:1139:ASN:ND2	1:A:1146:THR:H	2.12	0.47
1:A:1456:THR:O	1:A:1459:MET:HE1	2.15	0.47
1:A:1683:CYS:SG	1:A:1687:THR:OG1	2.68	0.47
1:B:166:PRO:HG3	1:B:172:PHE:CE2	2.49	0.47
1:B:885:THR:HG22	1:B:948:THR:HG22	1.95	0.47
1:B:1031:THR:HA	1:B:1110:CYS:O	2.14	0.47
1:B:1037:ASP:OD2	1:B:1039:PRO:HD2	2.15	0.47
1:D:1492:ASP:OD2	1:D:1494:THR:N	2.46	0.47
1:D:1842:LEU:HB3	1:D:1843:LEU:HD22	1.96	0.47
1:A:44:THR:N	1:A:74:ASP:OD2	2.47	0.47
1:A:168:LEU:C	1:A:170:LEU:H	2.22	0.47
1:A:1301:CYS:N	1:A:1351:TYR:OH	2.48	0.47
1:B:876:VAL:O	1:B:1002:ALA:N	2.48	0.47
1:C:622:LEU:HD11	1:C:718:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:LYS:HB3	1:A:1528:PRO:HD3	1.97	0.47
1:A:1647:ASN:HD21	1:A:1652:ILE:HG22	1.80	0.47
1:B:872:PRO:HG2	1:B:882:VAL:HG13	1.96	0.47
1:B:1601:PHE:CE1	1:B:1611:LYS:HB2	2.50	0.47
1:B:1737:THR:OG1	1:B:1738:VAL:N	2.48	0.47
1:C:156:LEU:HD12	1:C:250:LEU:HB3	1.97	0.47
1:C:788:LEU:HG	1:C:808:ILE:HD11	1.97	0.47
1:C:1061:ASN:O	1:C:1063:ALA:N	2.48	0.47
1:D:671:PRO:HD2	1:D:677:TRP:CH2	2.50	0.47
1:D:1035:LEU:HG	1:D:1037:ASP:H	1.79	0.47
1:A:196:ASP:HB3	1:A:201:VAL:HG11	1.97	0.46
1:A:532:ILE:HG23	1:A:563:ALA:HB3	1.96	0.46
1:A:1334:THR:O	1:A:1334:THR:OG1	2.33	0.46
1:B:1186:TYR:HB3	1:B:1213:CYS:HB3	1.97	0.46
1:B:1279:MET:HE1	1:C:202:PHE:CG	2.50	0.46
1:C:297:TYR:CZ	1:C:299:ALA:HB3	2.50	0.46
1:C:622:LEU:HB2	1:C:734:LEU:HD11	1.98	0.46
1:C:1370:ARG:O	1:C:1372:GLN:NE2	2.48	0.46
1:D:385:TYR:CD2	1:D:481:LEU:HD13	2.50	0.46
1:D:419:TRP:HD1	1:D:432:ARG:HB3	1.80	0.46
1:D:938:MET:HE1	1:D:940:PRO:HA	1.98	0.46
1:D:1055:TYR:OH	1:D:1059:ASN:OD1	2.34	0.46
1:A:123:GLY:H	1:A:151:VAL:HB	1.81	0.46
1:A:788:LEU:HD22	1:A:838:VAL:HG13	1.97	0.46
1:B:592:LEU:HD12	1:B:593:GLN:N	2.30	0.46
1:B:1573:PRO:HG3	1:B:1582:LEU:HD11	1.96	0.46
1:C:1724:ARG:HA	1:C:1724:ARG:CZ	2.45	0.46
1:D:195:LEU:HD21	1:D:226:GLN:HG3	1.98	0.46
1:D:1719:MET:SD	1:D:1720:GLY:N	2.89	0.46
1:A:759:PRO:HD2	1:A:769:ALA:HA	1.97	0.46
1:A:1551:PRO:HG3	1:A:1574:PHE:HD1	1.80	0.46
1:B:1304:CYS:SG	1:B:1310:SER:HB3	2.55	0.46
1:B:1308:PHE:HD1	1:B:1319:ALA:HA	1.80	0.46
1:B:1421:GLN:HB2	1:B:1436:THR:HB	1.96	0.46
1:B:1519:MET:HE3	1:B:1520:VAL:O	2.16	0.46
1:D:155:THR:HB	1:D:182:SER:HB3	1.97	0.46
1:B:308:TRP:HB2	1:B:361:LEU:HD11	1.97	0.46
1:B:1485:GLY:O	1:B:1555:THR:OG1	2.34	0.46
1:B:1772:TYR:CD1	1:B:1796:LYS:HG2	2.50	0.46
1:B:1801:PHE:CE2	1:B:1813:ALA:HB2	2.51	0.46
1:C:903:ILE:HD12	1:C:903:ILE:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1618:PHE:HB2	1:C:1660:ALA:O	2.15	0.46
1:C:1724:ARG:HG2	1:C:1724:ARG:HH11	1.80	0.46
1:D:141:LEU:HD12	1:D:141:LEU:H	1.80	0.46
1:D:360:ARG:HB3	1:D:375:ILE:HG23	1.97	0.46
1:D:877:LYS:HD2	1:D:1002:ALA:HB3	1.97	0.46
1:A:193:ILE:HD13	1:A:226:GLN:NE2	2.31	0.46
1:A:308:TRP:CE2	1:A:341:VAL:HB	2.50	0.46
1:C:401:ASP:CG	1:C:402:THR:N	2.73	0.46
1:C:753:ILE:HG12	1:C:775:ILE:HG12	1.96	0.46
1:D:530:GLU:OE2	1:D:530:GLU:N	2.48	0.46
1:D:595:PHE:CE2	1:D:600:PRO:HB3	2.51	0.46
1:D:1009:GLU:N	1:D:1033:THR:O	2.45	0.46
1:A:1189:ILE:CD1	1:A:1214:ARG:HD3	2.44	0.46
1:B:1558:ASP:OD1	1:B:1558:ASP:N	2.46	0.46
1:B:1721:THR:HG22	1:B:1722:TYR:H	1.80	0.46
1:C:207:ILE:HD12	1:C:208:PHE:H	1.80	0.46
1:C:753:ILE:HG12	1:C:775:ILE:HG23	1.98	0.46
1:C:907:PHE:HB2	1:C:949:PHE:CD2	2.50	0.46
1:D:362:ARG:NE	1:D:370:VAL:HG11	2.31	0.46
1:D:877:LYS:HB2	1:D:880:THR:HG21	1.97	0.46
1:A:1017:TYR:CD1	1:A:1156:GLN:HG3	2.50	0.46
1:A:1061:ASN:O	1:A:1063:ALA:N	2.49	0.46
1:A:1282:GLU:H	1:A:1282:GLU:CD	2.14	0.46
1:A:1707:ASN:OD1	1:A:1707:ASN:N	2.49	0.46
1:B:545:PRO:HB3	1:B:550:ALA:HB3	1.97	0.46
1:B:620:TYR:HE2	1:B:731:VAL:HG21	1.81	0.46
1:C:193:ILE:HD12	1:C:194:GLN:N	2.31	0.46
1:C:1490:MET:O	1:C:1496:GLN:NE2	2.45	0.46
1:A:1084:VAL:HG13	1:A:1087:ASP:HB3	1.98	0.46
1:C:1742:THR:HG21	1:D:1165:PRO:HG2	1.98	0.46
1:D:439:ASN:HB2	1:D:446:ASN:ND2	2.31	0.46
1:D:794:ASP:HB2	1:D:800:SER:HB2	1.97	0.46
1:D:855:LEU:HD11	1:D:894:VAL:HB	1.97	0.46
1:D:1672:GLN:NE2	1:D:1680:CYS:HA	2.30	0.46
1:A:271:LEU:HD13	1:A:295:VAL:HG12	1.97	0.46
1:B:470:ARG:HA	1:B:470:ARG:CZ	2.46	0.46
1:B:497:LEU:HD11	1:B:516:PHE:HB3	1.98	0.46
1:C:110:VAL:HG22	1:C:115:TYR:CD2	2.51	0.46
1:C:1720:GLY:HA2	1:C:1739:ALA:HB3	1.98	0.46
1:D:189:MET:HE3	1:D:209:ILE:HD11	1.97	0.46
1:D:193:ILE:HD12	1:D:194:GLN:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:641:TYR:CD1	1:D:716:LEU:HD11	2.51	0.46
1:D:902:PRO:HB3	1:D:937:VAL:HG22	1.98	0.46
1:A:514:TRP:CZ3	1:A:613:VAL:HG21	2.51	0.46
1:A:844:THR:HG22	1:A:845:THR:HG23	1.99	0.46
1:B:306:LEU:HD23	1:B:365:ASP:HB2	1.98	0.46
1:B:520:ARG:HB2	1:B:571:PRO:HD2	1.97	0.46
1:B:1279:MET:HE1	1:C:202:PHE:CD2	2.51	0.46
1:B:1603:ASP:OD1	1:B:1603:ASP:N	2.49	0.46
1:D:1292:PHE:CD2	1:D:1294:PRO:HD3	2.51	0.46
1:D:1826:GLU:OE2	1:D:1826:GLU:N	2.47	0.46
1:A:862:PRO:HB3	1:A:892:THR:HG21	1.97	0.45
1:A:1037:ASP:OD2	1:A:1039:PRO:HD2	2.16	0.45
1:A:1576:THR:HG22	1:A:1588:VAL:H	1.81	0.45
1:A:1667:GLY:HA3	1:B:1936:ALA:O	2.16	0.45
1:B:832:TYR:HB2	1:B:852:PHE:CZ	2.51	0.45
1:B:1187:GLU:OE2	1:B:1228:CYS:HB3	2.16	0.45
1:C:1367:LEU:HA	1:C:1367:LEU:HD23	1.74	0.45
1:C:1372:GLN:CD	1:C:1372:GLN:N	2.74	0.45
1:A:589:GLN:N	1:A:589:GLN:OE1	2.49	0.45
1:B:821:ILE:HB	1:B:824:TYR:HB2	1.97	0.45
1:C:311:ASN:HB2	1:C:319:GLU:HG3	1.99	0.45
1:C:363:LEU:HD12	1:C:372:ALA:HB3	1.98	0.45
1:C:504:PHE:CZ	1:C:720:GLN:HG2	2.51	0.45
1:C:872:PRO:HG2	1:C:882:VAL:HG13	1.98	0.45
1:C:1341:LEU:HA	1:C:1345:ASP:OD1	2.16	0.45
1:C:1413:TYR:O	1:C:1446:SER:N	2.49	0.45
1:C:1423:GLY:HA3	1:C:1450:PRO:HG2	1.99	0.45
1:C:1441:LEU:H	1:C:1441:LEU:HD23	1.80	0.45
1:C:1770:ARG:NH2	1:C:1804:ASP:O	2.49	0.45
1:C:1786:ASP:O	1:C:1788:PHE:N	2.49	0.45
1:D:1497:MET:HE1	1:D:1574:PHE:CE1	2.52	0.45
1:D:1719:MET:HE1	1:D:1740:SER:C	2.40	0.45
1:A:555:ALA:HA	1:A:560:GLY:HA3	1.97	0.45
1:A:1417:TRP:CH2	1:C:1254:LYS:HD2	2.51	0.45
1:A:1617:SER:HB2	1:A:1627:CYS:HB3	1.97	0.45
1:A:1782:ASP:O	1:A:1784:LEU:N	2.45	0.45
1:B:411:HIS:HB3	1:B:415:THR:HG22	1.98	0.45
1:A:280:VAL:HB	1:A:284:ASP:HB2	1.99	0.45
1:A:593:GLN:OE1	1:A:602:TRP:HB2	2.17	0.45
1:B:1814:CYS:HB3	1:B:1827:GLN:HB2	1.98	0.45
1:C:663:TRP:CZ2	1:C:665:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:PHE:HB2	1:C:899:ILE:HD11	1.98	0.45
1:C:1567:LYS:O	1:C:1570:THR:OG1	2.25	0.45
1:C:1757:ASN:OD1	1:C:1766:ARG:NH1	2.49	0.45
1:D:702:PHE:HE2	1:D:704:PRO:HB3	1.81	0.45
1:D:713:THR:HG21	1:D:737:VAL:H	1.81	0.45
1:D:1573:PRO:HG2	1:D:1588:VAL:HG21	1.98	0.45
1:A:1629:ILE:HD13	1:A:1629:ILE:HA	1.87	0.45
1:B:548:LEU:HD21	1:B:600:PRO:HG3	1.98	0.45
1:B:755:SER:HB2	1:B:771:TRP:NE1	2.24	0.45
1:C:757:LEU:HD22	1:C:771:TRP:CE3	2.51	0.45
1:D:1520:VAL:HG12	1:D:1526:ALA:H	1.82	0.45
1:A:902:PRO:HG2	1:A:971:SER:HB3	1.98	0.45
1:A:1708:SER:OG	1:B:1930:PRO:HB2	2.17	0.45
1:C:275:VAL:HG12	1:C:288:PHE:HA	1.99	0.45
1:C:1053:ALA:HB2	1:C:1096:LEU:HD13	1.99	0.45
1:C:1797:CYS:HB2	1:C:1801:PHE:HB2	1.99	0.45
1:A:764:ALA:HB3	1:A:859:THR:HG22	1.97	0.45
1:A:1236:TRP:O	1:A:1245:THR:OG1	2.31	0.45
1:B:1722:TYR:HD2	1:B:1724:ARG:HH11	1.64	0.45
1:C:418:VAL:HB	1:C:435:LEU:HD23	1.98	0.45
1:C:1799:TYR:HA	1:C:1829:THR:OG1	2.17	0.45
1:D:362:ARG:HG3	1:D:364:TYR:CE1	2.51	0.45
1:D:389:LEU:HA	1:D:407:ALA:HA	1.98	0.45
1:A:410:LYS:HB3	1:A:444:ALA:HA	1.99	0.45
1:C:371:ILE:HG13	1:C:372:ALA:N	2.31	0.45
1:C:420:TRP:HB2	1:C:465:LEU:HD11	1.99	0.45
1:D:519:GLN:OE1	1:D:519:GLN:HA	2.17	0.45
1:D:1497:MET:HG3	1:D:1514:TYR:HD2	1.81	0.45
1:A:411:HIS:HB3	1:A:415:THR:HG22	1.98	0.45
1:A:503:PRO:HD2	1:A:512:ALA:HA	1.98	0.45
1:B:424:TYR:CZ	1:B:453:ASN:HB2	2.52	0.45
1:B:1253:ALA:HA	1:B:1283:SER:O	2.17	0.45
1:B:1782:ASP:O	1:B:1784:LEU:N	2.49	0.45
1:D:987:GLN:C	1:D:988:LEU:HD22	2.42	0.45
1:A:110:VAL:HG22	1:A:115:TYR:HB2	1.97	0.45
1:A:1036:ARG:HB2	1:A:1101:MET:HE1	1.99	0.45
1:C:1421:GLN:HB2	1:C:1436:THR:HB	1.98	0.45
1:D:1070:THR:OG1	1:D:1145:ASP:OD2	2.28	0.45
1:A:525:PRO:HD2	1:A:528:VAL:HB	1.99	0.44
1:A:853:THR:HB	1:A:898:GLY:HA2	1.98	0.44
1:A:1534:ASP:OD2	1:C:1192:ASN:N	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1604:GLU:HG2	1:B:1607:GLN:HB2	1.99	0.44
1:C:1071:ASP:HB2	1:C:1129:PHE:HE1	1.82	0.44
1:C:1372:GLN:N	1:C:1372:GLN:OE1	2.50	0.44
1:C:1550:LEU:HD23	1:C:1563:GLN:HE22	1.82	0.44
1:C:1773:TYR:CD1	1:C:1797:CYS:HB3	2.52	0.44
1:D:432:ARG:NH2	1:D:471:ASP:O	2.50	0.44
1:D:533:LYS:HD3	1:D:556:ASN:HA	2.00	0.44
1:D:759:PRO:HD2	1:D:769:ALA:HA	1.98	0.44
1:A:506:PRO:HG3	1:A:588:LEU:HD11	1.98	0.44
1:A:1339:THR:OG1	1:A:1342:ASP:OD2	2.35	0.44
1:B:195:LEU:HD22	1:B:228:TYR:CZ	2.53	0.44
1:B:1022:PRO:HB2	1:B:1028:THR:HG21	1.99	0.44
1:D:497:LEU:HD21	1:D:592:LEU:HD23	1.99	0.44
1:D:764:ALA:HB3	1:D:859:THR:HG22	2.00	0.44
1:B:758:ASN:HD22	1:B:759:PRO:HA	1.83	0.44
1:B:844:THR:HG22	1:B:845:THR:HG23	2.00	0.44
1:C:158:ALA:HA	1:C:178:ARG:O	2.17	0.44
1:C:297:TYR:CE2	1:C:299:ALA:HB3	2.52	0.44
1:D:1694:LEU:HD23	1:D:1694:LEU:HA	1.79	0.44
1:A:309:ARG:HD2	1:A:322:LEU:HG	2.00	0.44
1:A:1370:ARG:O	1:A:1372:GLN:NE2	2.50	0.44
1:A:1467:ALA:HB3	1:C:1226:TYR:HB3	2.00	0.44
1:B:592:LEU:HD12	1:B:593:GLN:H	1.82	0.44
1:B:762:PRO:O	1:B:857:SER:OG	2.32	0.44
1:B:1218:GLY:HA2	1:B:1239:GLU:N	2.32	0.44
1:B:1426:PHE:CE1	1:B:1490:MET:HB2	2.52	0.44
1:B:1616:GLY:O	1:B:1630:ALA:HB2	2.18	0.44
1:C:1573:PRO:HG2	1:C:1588:VAL:HG21	1.98	0.44
1:D:719:ILE:HG12	1:D:730:THR:HG22	2.00	0.44
1:D:1537:PHE:O	1:D:1537:PHE:CG	2.71	0.44
1:D:1549:ASN:ND2	1:D:1555:THR:OG1	2.45	0.44
1:D:1606:SER:O	1:D:1607:GLN:HG2	2.17	0.44
1:D:1722:TYR:HE1	1:D:1734:PRO:HD3	1.83	0.44
1:A:1604:GLU:OE1	1:A:1604:GLU:N	2.51	0.44
1:B:792:MET:HG3	1:B:801:PRO:HD2	1.99	0.44
1:B:862:PRO:HB3	1:B:892:THR:HG21	2.00	0.44
1:B:1465:CYS:SG	1:B:1469:THR:OG1	2.76	0.44
1:C:189:MET:O	1:C:209:ILE:HG12	2.17	0.44
1:C:398:THR:HG21	1:C:492:PRO:HA	1.98	0.44
1:C:514:TRP:CH2	1:C:613:VAL:HG21	2.53	0.44
1:C:1031:THR:HG22	1:C:1111:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1503:ASN:ND2	1:D:1506:ASN:HB2	2.32	0.44
1:A:405:PHE:HZ	1:A:424:TYR:HE1	1.64	0.44
1:D:775:ILE:O	1:D:814:THR:HA	2.18	0.44
1:D:876:VAL:HB	1:D:999:MET:HE2	2.00	0.44
1:D:1247:CYS:SG	1:D:1253:ALA:HB2	2.58	0.44
1:D:1361:CYS:HB3	1:D:1365:THR:HG23	1.99	0.44
1:A:1255:PRO:HB2	1:A:1276:HIS:HB3	1.99	0.44
1:A:1355:PRO:HG2	1:C:1375:ILE:HG22	1.99	0.44
1:A:1779:ALA:HB1	1:A:1793:GLY:HA2	2.00	0.44
1:C:288:PHE:CD1	1:C:290:GLN:HG2	2.53	0.44
1:C:1189:ILE:CD1	1:C:1214:ARG:HB2	2.47	0.44
1:A:561:LEU:HD12	1:A:575:ILE:HD11	1.99	0.44
1:A:1021:THR:HG22	1:A:1153:PHE:HB2	1.99	0.44
1:B:410:LYS:HB3	1:B:444:ALA:O	2.17	0.44
1:C:306:LEU:HD23	1:C:365:ASP:HB2	2.00	0.44
1:C:903:ILE:HG22	1:C:936:ALA:O	2.18	0.44
1:C:1329:GLY:HA3	1:C:1357:THR:HG21	1.99	0.44
1:D:1195:TYR:OH	1:D:1200:ARG:NH2	2.51	0.44
1:D:1399:LYS:O	1:D:1399:LYS:HG3	2.18	0.44
1:D:1415:ASN:OD1	1:D:1418:PHE:N	2.28	0.44
1:A:753:ILE:HG21	1:A:850:LYS:HE2	2.00	0.44
1:A:1560:LEU:HD23	1:A:1560:LEU:HA	1.89	0.44
1:A:1694:LEU:HD23	1:A:1694:LEU:HA	1.85	0.44
1:B:514:TRP:CZ3	1:B:613:VAL:HG21	2.53	0.44
1:B:593:GLN:HE22	1:B:608:THR:HG22	1.82	0.44
1:C:1453:TYR:CE1	1:C:1463:LEU:HD21	2.53	0.44
1:D:1618:PHE:O	1:D:1628:GLU:N	2.47	0.44
1:A:160:LEU:HD21	1:A:175:PHE:HE1	1.83	0.43
1:A:306:LEU:HD23	1:A:365:ASP:HB2	2.00	0.43
1:B:161:LEU:HD21	1:B:178:ARG:HH12	1.82	0.43
1:C:480:LEU:HD12	1:C:481:LEU:N	2.33	0.43
1:C:1737:THR:OG1	1:C:1738:VAL:N	2.51	0.43
1:D:534:CYS:HB3	1:D:592:LEU:HD11	1.99	0.43
1:D:876:VAL:O	1:D:1002:ALA:N	2.50	0.43
1:D:1569:GLY:N	1:D:1602:ASN:HB3	2.28	0.43
1:D:1737:THR:OG1	1:D:1738:VAL:N	2.50	0.43
1:A:786:LYS:HB2	1:A:808:ILE:HD13	2.00	0.43
1:A:1031:THR:HA	1:A:1110:CYS:O	2.17	0.43
1:A:1265:SER:O	1:A:1266:ILE:HD13	2.18	0.43
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.82	0.43
1:B:455:TYR:CD2	1:B:461:LYS:HE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:PHE:CE2	1:C:600:PRO:HB3	2.54	0.43
1:D:762:PRO:O	1:D:857:SER:OG	2.36	0.43
1:D:1770:ARG:HA	1:D:1806:PRO:CD	2.48	0.43
1:A:788:LEU:HD12	1:A:815:THR:HG21	2.00	0.43
1:A:1036:ARG:O	1:A:1037:ASP:HB3	2.18	0.43
1:A:1293:GLN:HE21	1:A:1301:CYS:HA	1.82	0.43
1:A:1413:TYR:O	1:A:1446:SER:N	2.52	0.43
1:A:1819:LEU:HB3	1:A:1823:ASN:HB2	1.99	0.43
1:B:79:VAL:O	1:B:98:THR:OG1	2.36	0.43
1:B:1390:ARG:HA	1:B:1391:PRO:HD3	1.90	0.43
1:B:1501:VAL:HG23	1:B:1509:PRO:HD2	2.00	0.43
1:C:362:ARG:HB2	1:C:364:TYR:CE1	2.54	0.43
1:C:1322:GLU:OE1	1:C:1322:GLU:N	2.41	0.43
1:D:464:THR:C	1:D:465:LEU:HD23	2.44	0.43
1:D:886:PHE:CD2	1:D:965:LEU:HD22	2.53	0.43
1:D:965:LEU:HD12	1:D:965:LEU:HA	1.80	0.43
1:A:775:ILE:HB	1:A:815:THR:HG22	2.01	0.43
1:A:1708:SER:HB2	1:A:1711:GLN:HG3	2.01	0.43
1:B:277:PRO:HB2	1:B:280:VAL:HG13	2.00	0.43
1:B:1453:TYR:HD1	1:B:1455:PRO:HD3	1.83	0.43
1:B:1724:ARG:NH1	1:B:1745:SER:O	2.50	0.43
1:B:1772:TYR:CE1	1:B:1796:LYS:HG2	2.54	0.43
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.76	0.43
1:C:1223:MET:HE3	1:C:1242:ARG:HH12	1.84	0.43
1:C:1664:THR:HG23	1:C:1664:THR:O	2.19	0.43
1:D:311:ASN:HB2	1:D:319:GLU:HG3	2.01	0.43
1:A:193:ILE:HD13	1:A:226:GLN:HE22	1.83	0.43
1:A:271:LEU:HG	1:A:374:LYS:HE2	2.00	0.43
1:A:835:THR:HA	1:A:848:ILE:O	2.19	0.43
1:C:603:ASP:OD1	1:C:606:TYR:HB2	2.18	0.43
1:C:649:VAL:HB	1:C:694:GLY:H	1.82	0.43
1:D:909:ASN:HB2	1:D:953:TYR:CZ	2.53	0.43
1:D:1071:ASP:HB2	1:D:1129:PHE:CE1	2.54	0.43
1:D:1110:CYS:HB3	1:D:1112:PHE:CE2	2.54	0.43
1:D:1754:PHE:HA	1:D:1767:ALA:HA	2.00	0.43
1:A:1372:GLN:N	1:A:1372:GLN:CD	2.76	0.43
1:B:882:VAL:HB	1:B:951:THR:HG22	2.00	0.43
1:B:1132:ALA:O	1:B:1135:THR:OG1	2.31	0.43
1:B:1489:LEU:O	1:B:1542:LYS:NZ	2.37	0.43
1:B:1527:LYS:HG3	1:B:1528:PRO:CD	2.49	0.43
1:D:393:THR:HG23	1:D:404:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ASN:N	1:A:685:ASN:OD1	2.52	0.43
1:A:1148:THR:HG23	1:A:1148:THR:O	2.18	0.43
1:A:1867:PRO:HA	1:A:1868:PRO:HD3	1.91	0.43
1:B:297:TYR:CE2	1:B:299:ALA:HB3	2.54	0.43
1:B:1758:ALA:HB1	1:B:1759:PRO:HD2	2.00	0.43
1:C:774:VAL:HG23	1:C:814:THR:HG23	2.00	0.43
1:C:878:VAL:O	1:C:1039:PRO:HB3	2.18	0.43
1:C:1037:ASP:OD2	1:C:1039:PRO:HD2	2.19	0.43
1:C:1096:LEU:HD12	1:C:1097:ARG:N	2.33	0.43
1:C:1844:SER:O	1:C:1847:LYS:HG2	2.18	0.43
1:D:1819:LEU:HB2	1:D:1823:ASN:HB2	2.01	0.43
1:A:193:ILE:HG21	1:A:226:GLN:NE2	2.32	0.43
1:A:497:LEU:HD11	1:A:516:PHE:HB3	2.01	0.43
1:A:1814:CYS:HB3	1:A:1827:GLN:HB2	2.00	0.43
1:B:1239:GLU:CG	1:B:1240:GLY:N	2.80	0.43
1:C:293:THR:O	1:C:340:ALA:HA	2.19	0.43
1:C:514:TRP:CZ3	1:C:613:VAL:HG21	2.54	0.43
1:D:193:ILE:HD12	1:D:194:GLN:N	2.33	0.43
1:D:1499:LEU:HD22	1:D:1512:ARG:HG2	2.00	0.43
1:D:1618:PHE:HB2	1:D:1660:ALA:O	2.17	0.43
1:D:1826:GLU:N	1:D:1826:GLU:CD	2.77	0.43
1:D:1867:PRO:HA	1:D:1868:PRO:HD3	1.93	0.43
1:A:1131:TYR:OH	1:A:1134:SER:HA	2.18	0.43
1:A:1832:LEU:HD21	1:A:1850:ARG:HD2	1.99	0.43
1:B:1707:ASN:N	1:B:1707:ASN:OD1	2.51	0.43
1:C:170:LEU:HA	1:C:170:LEU:HD23	1.72	0.43
1:C:671:PRO:O	1:C:677:TRP:NE1	2.52	0.43
1:C:1688:TYR:HE2	1:C:1690:ASP:HB2	1.84	0.43
1:C:1775:PRO:HB3	1:C:1809:ARG:HD3	2.01	0.43
1:D:132:TYR:CE2	1:D:141:LEU:HG	2.54	0.43
1:D:673:THR:HG23	1:D:675:ALA:N	2.34	0.43
1:A:1528:PRO:HG3	1:C:1207:PRO:HA	2.00	0.43
1:B:482:ALA:C	1:B:483:SER:HG	2.25	0.43
1:B:1237:SER:OG	1:B:1238:ASN:N	2.51	0.43
1:B:1672:GLN:HE21	1:B:1680:CYS:HA	1.84	0.43
1:C:1757:ASN:HD22	1:C:1763:THR:HB	1.84	0.43
1:D:753:ILE:HG23	1:D:773:ILE:HG23	2.00	0.43
1:D:1672:GLN:HE21	1:D:1680:CYS:HA	1.84	0.43
1:A:1370:ARG:C	1:A:1372:GLN:HE22	2.27	0.42
1:A:1461:VAL:HG11	1:C:1230:PRO:HG2	2.00	0.42
1:C:1263:LYS:HE3	1:C:1263:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:PHE:HE1	1:D:422:ILE:HD11	1.84	0.42
1:D:1459:MET:HE2	1:D:1459:MET:HB3	1.80	0.42
1:A:1770:ARG:CZ	1:A:1806:PRO:HD2	2.49	0.42
1:B:1037:ASP:CG	1:B:1038:PRO:HD2	2.43	0.42
1:B:1239:GLU:HG2	1:B:1240:GLY:H	1.84	0.42
1:B:1255:PRO:HB3	1:B:1277:LEU:C	2.44	0.42
1:B:1415:ASN:OD1	1:B:1418:PHE:N	2.34	0.42
1:B:1551:PRO:HG3	1:B:1574:PHE:HD1	1.85	0.42
1:B:1845:LYS:N	1:B:1846:PRO:HD2	2.34	0.42
1:C:1139:ASN:HD21	1:C:1146:THR:H	1.67	0.42
1:D:1722:TYR:HB2	1:D:1745:SER:O	2.19	0.42
1:D:1920:PRO:HA	1:D:1921:PRO:HD3	1.95	0.42
1:A:612:GLN:N	1:A:612:GLN:CD	2.77	0.42
1:A:662:PHE:HE2	1:A:687:LYS:HG2	1.85	0.42
1:A:663:TRP:CZ2	1:A:665:GLY:HA2	2.55	0.42
1:A:902:PRO:HA	1:A:937:VAL:HA	2.01	0.42
1:A:1491:GLY:O	1:A:1496:GLN:NE2	2.52	0.42
1:A:1687:THR:HB	1:A:1697:CYS:HB3	2.00	0.42
1:B:595:PHE:CE2	1:B:600:PRO:HB3	2.54	0.42
1:B:1018:ASN:HD21	1:B:1020:THR:HB	1.84	0.42
1:C:195:LEU:HD13	1:C:228:TYR:CD1	2.53	0.42
1:C:255:PRO:HB3	1:C:260:ALA:HA	2.01	0.42
1:C:973:THR:O	1:C:973:THR:OG1	2.30	0.42
1:C:1701:GLN:OE1	1:C:1704:ARG:NH1	2.52	0.42
1:C:1829:THR:HB	1:C:1834:SER:HB3	2.00	0.42
1:A:501:VAL:HG13	1:A:503:PRO:O	2.19	0.42
1:A:1162:ILE:HD12	1:C:1481:GLN:HG3	2.02	0.42
1:A:1724:ARG:CZ	1:A:1724:ARG:HA	2.50	0.42
1:A:1772:TYR:HB3	1:A:1794:CYS:HB3	2.02	0.42
1:B:751:TYR:HB2	1:B:848:ILE:HD11	2.00	0.42
1:C:79:VAL:O	1:C:98:THR:OG1	2.32	0.42
1:C:231:GLU:HA	1:C:263:VAL:HB	2.00	0.42
1:C:358:ASN:HB3	1:C:375:ILE:HD11	2.01	0.42
1:C:1920:PRO:HA	1:C:1921:PRO:HD3	1.92	0.42
1:D:1080:VAL:HG12	1:D:1083:ALA:HB2	2.01	0.42
1:D:1128:VAL:HG13	1:D:1140:ALA:HB3	2.00	0.42
1:B:957:SER:HB3	1:B:1001:VAL:O	2.20	0.42
1:C:1440:GLU:OE2	1:C:1442:GLY:N	2.52	0.42
1:D:308:TRP:HB2	1:D:361:LEU:HD11	2.02	0.42
1:D:631:VAL:HG11	1:D:706:TYR:CE2	2.55	0.42
1:D:1366:TYR:CG	1:D:1405:CYS:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:PRO:HD2	1:A:551:TRP:CZ2	2.55	0.42
1:A:618:PRO:HB3	1:A:647:VAL:HB	2.02	0.42
1:A:1902:PRO:HA	1:A:1903:PRO:HD3	1.93	0.42
1:B:621:THR:OG1	1:B:644:ILE:HB	2.20	0.42
1:B:1036:ARG:O	1:B:1037:ASP:HB3	2.17	0.42
1:B:1222:THR:HG22	1:B:1225:GLY:HA2	2.02	0.42
1:B:1672:GLN:NE2	1:B:1680:CYS:HA	2.34	0.42
1:C:497:LEU:HD21	1:C:592:LEU:HD23	2.01	0.42
1:C:613:VAL:HG12	1:C:613:VAL:O	2.18	0.42
1:C:641:TYR:CD2	1:C:716:LEU:HD11	2.54	0.42
1:C:734:LEU:HD23	1:C:734:LEU:HA	1.92	0.42
1:C:1310:SER:OG	1:C:1311:THR:N	2.52	0.42
1:C:1565:PRO:HB2	1:C:1605:PHE:HB3	2.01	0.42
1:D:1574:PHE:HD2	1:D:1578:THR:HG21	1.84	0.42
1:A:1599:GLY:HA2	1:A:1619:ALA:HB3	2.02	0.42
1:B:1497:MET:HG3	1:B:1514:TYR:HD2	1.84	0.42
1:C:206:ARG:NE	1:C:244:PRO:O	2.52	0.42
1:C:887:THR:HG22	1:C:946:THR:HG22	2.01	0.42
1:D:1049:GLN:HG3	1:D:1131:TYR:HB3	2.02	0.42
1:A:310:PHE:N	1:A:320:THR:OG1	2.49	0.42
1:A:1074:TYR:HA	1:A:1077:PHE:CZ	2.55	0.42
1:A:1582:LEU:HD23	1:A:1582:LEU:HA	1.86	0.42
1:B:230:LEU:HG	1:B:232:GLY:N	2.34	0.42
1:B:671:PRO:O	1:B:677:TRP:NE1	2.53	0.42
1:B:1048:VAL:HG13	1:B:1101:MET:HB3	2.01	0.42
1:B:1061:ASN:O	1:B:1063:ALA:N	2.53	0.42
1:B:1759:PRO:O	1:B:1761:SER:N	2.52	0.42
1:C:188:ASP:HB3	1:C:208:PHE:HE1	1.85	0.42
1:C:1189:ILE:HD11	1:C:1214:ARG:HB2	2.01	0.42
1:C:1520:VAL:HG11	1:C:1526:ALA:HB3	2.00	0.42
1:D:288:PHE:CD1	1:D:290:GLN:HG2	2.55	0.42
1:D:1770:ARG:NH2	1:D:1805:ARG:HA	2.35	0.42
1:A:1786:ASP:C	1:A:1786:ASP:OD2	2.63	0.42
1:C:876:VAL:HG23	1:C:999:MET:HE2	2.01	0.42
1:C:1058:GLN:NE2	1:C:1115:LEU:O	2.31	0.42
1:C:1828:CYS:SG	1:C:1845:LYS:HE2	2.59	0.42
1:D:723:PHE:CD1	1:D:723:PHE:N	2.87	0.42
1:D:1201:VAL:HG23	1:D:1202:ALA:N	2.35	0.42
1:D:1453:TYR:O	1:D:1462:CYS:HB2	2.20	0.42
1:D:1492:ASP:CG	1:D:1493:ARG:N	2.78	0.42
1:D:1512:ARG:HB3	1:D:1530:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1608:PRO:HG2	1:D:1646:PHE:HE2	1.85	0.42
1:A:47:LEU:O	1:A:145:LYS:HE2	2.20	0.42
1:A:371:ILE:HG13	1:A:372:ALA:N	2.33	0.42
1:A:788:LEU:HG	1:A:808:ILE:HD11	2.01	0.42
1:A:1492:ASP:OD1	1:A:1494:THR:OG1	2.37	0.42
1:A:1507:ASP:HB3	1:C:1263:LYS:O	2.20	0.42
1:B:395:ASP:N	1:B:396:PRO:HG3	2.34	0.42
1:B:631:VAL:HG11	1:B:706:TYR:CE1	2.55	0.42
1:B:786:LYS:H	1:B:808:ILE:HD11	1.85	0.42
1:B:1093:ASP:OD1	1:B:1093:ASP:N	2.52	0.42
1:C:671:PRO:HD2	1:C:677:TRP:CH2	2.54	0.42
1:C:886:PHE:CG	1:C:965:LEU:HD22	2.55	0.42
1:D:50:ASP:N	1:D:50:ASP:OD1	2.52	0.42
1:D:109:LEU:HG	1:D:110:VAL:N	2.35	0.42
1:D:1251:THR:HA	1:D:1286:LYS:HA	2.02	0.42
1:A:230:LEU:HD22	1:A:232:GLY:HA3	2.02	0.41
1:A:1327:THR:HG22	1:A:1359:ARG:HG3	2.02	0.41
1:B:1543:SER:O	1:B:1543:SER:OG	2.37	0.41
1:C:421:THR:CG2	1:C:432:ARG:HG2	2.50	0.41
1:C:458:GLY:HA2	1:C:490:VAL:HG23	2.02	0.41
1:C:587:SER:HB2	1:C:612:GLN:HE22	1.84	0.41
1:D:1758:ALA:HB1	1:D:1759:PRO:HD2	2.02	0.41
1:A:641:TYR:CG	1:A:716:LEU:HD11	2.56	0.41
1:A:1174:LEU:HD11	1:A:1180:THR:HG23	2.02	0.41
1:B:230:LEU:HG	1:B:232:GLY:H	1.85	0.41
1:B:437:MET:HB3	1:B:437:MET:HE3	1.83	0.41
1:B:772:ARG:HH21	1:B:986:SER:HB3	1.85	0.41
1:B:886:PHE:CD2	1:B:965:LEU:HD22	2.56	0.41
1:B:1267:ASP:OD2	1:B:1267:ASP:C	2.62	0.41
1:C:1490:MET:CE	1:C:1536:ASN:HB3	2.50	0.41
1:A:516:PHE:HB2	1:A:575:ILE:HG23	2.02	0.41
1:A:548:LEU:HD21	1:A:600:PRO:HG3	2.01	0.41
1:C:1602:ASN:HB2	1:C:1610:CYS:HB3	2.02	0.41
1:D:504:PHE:CZ	1:D:720:GLN:HG2	2.56	0.41
1:D:788:LEU:HD22	1:D:838:VAL:HG13	2.02	0.41
1:A:595:PHE:CE2	1:A:600:PRO:HB3	2.55	0.41
1:A:761:THR:HG22	1:A:894:VAL:HG21	2.03	0.41
1:A:1220:THR:O	1:A:1237:SER:OG	2.25	0.41
1:A:1376:ALA:HB2	1:C:1376:ALA:HA	2.02	0.41
1:B:420:TRP:O	1:B:433:THR:OG1	2.38	0.41
1:B:1263:LYS:O	1:B:1264:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:PRO:HB3	1:C:937:VAL:HG12	2.01	0.41
1:D:87:ASP:OD1	1:D:87:ASP:N	2.54	0.41
1:D:207:ILE:HD13	1:D:224:PRO:HG3	2.01	0.41
1:D:612:GLN:O	1:D:654:PRO:HD2	2.20	0.41
1:A:410:LYS:HB3	1:A:444:ALA:O	2.21	0.41
1:A:781:VAL:HG13	1:A:786:LYS:HE2	2.01	0.41
1:A:1930:PRO:HA	1:A:1931:PRO:HD3	1.92	0.41
1:B:1456:THR:HG22	1:B:1457:PHE:H	1.85	0.41
1:C:178:ARG:CZ	1:C:178:ARG:HB2	2.50	0.41
1:C:1132:ALA:O	1:C:1135:THR:OG1	2.38	0.41
1:D:1706:GLN:OE1	1:D:1706:GLN:HA	2.20	0.41
1:A:1254:LYS:HD2	1:C:1417:TRP:CH2	2.55	0.41
1:B:170:LEU:HD23	1:C:1200:ARG:HG2	2.03	0.41
1:B:179:VAL:HG21	1:B:209:ILE:HD12	2.02	0.41
1:B:713:THR:HB	1:B:736:PRO:HB3	2.01	0.41
1:B:882:VAL:O	1:B:950:THR:HA	2.21	0.41
1:C:108:ASN:CG	1:C:109:LEU:H	2.27	0.41
1:C:335:PRO:HG2	1:C:339:THR:HG21	2.02	0.41
1:C:419:TRP:CB	1:C:468:TYR:O	2.64	0.41
1:C:575:ILE:HD12	1:C:575:ILE:HA	1.81	0.41
1:D:253:PHE:CG	1:D:254:THR:N	2.89	0.41
1:A:66:PHE:O	1:A:110:VAL:HB	2.20	0.41
1:A:1162:ILE:HG13	1:C:1481:GLN:HB2	2.02	0.41
1:A:1515:THR:HG23	1:A:1530:VAL:O	2.20	0.41
1:A:1760:ASP:OD2	1:A:1760:ASP:C	2.63	0.41
1:B:545:PRO:HD2	1:B:551:TRP:CZ2	2.56	0.41
1:B:909:ASN:HB2	1:B:953:TYR:CZ	2.56	0.41
1:B:1055:TYR:CD1	1:B:1094:GLN:HB3	2.55	0.41
1:B:1258:LEU:HD12	1:B:1258:LEU:O	2.21	0.41
1:B:1336:GLY:O	1:B:1356:ASN:HB3	2.20	0.41
1:B:1773:TYR:CD1	1:B:1797:CYS:HB3	2.55	0.41
1:C:844:THR:HG22	1:C:845:THR:HG23	2.03	0.41
1:D:167:ARG:CZ	1:D:170:LEU:HD13	2.50	0.41
1:A:461:LYS:HE3	1:A:490:VAL:HG21	2.02	0.41
1:A:1187:GLU:OE1	1:A:1187:GLU:N	2.46	0.41
1:A:1305:PRO:HG2	1:A:1308:PHE:CD2	2.56	0.41
1:A:1361:CYS:HB3	1:A:1365:THR:HG23	2.02	0.41
1:C:253:PHE:CG	1:C:254:THR:N	2.89	0.41
1:C:1773:TYR:CE1	1:C:1797:CYS:HB3	2.56	0.41
1:D:677:TRP:CD1	1:D:717:GLN:HE21	2.39	0.41
1:D:832:TYR:HE2	1:D:854:VAL:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:PRO:O	1:A:720:GLN:HG3	2.21	0.41
1:A:663:TRP:CH2	1:A:665:GLY:HA2	2.56	0.41
1:B:786:LYS:HG3	1:B:840:ASP:OD2	2.21	0.41
1:B:1053:ALA:HB2	1:B:1096:LEU:HD13	2.03	0.41
1:B:1181:THR:HG22	1:B:1226:TYR:HE2	1.86	0.41
1:B:1503:ASN:HD22	1:B:1506:ASN:HB2	1.86	0.41
1:B:1791:PRO:O	1:B:1795:TYR:OH	2.30	0.41
1:C:362:ARG:HG2	1:C:373:GLU:HB2	2.03	0.41
1:C:545:PRO:HD2	1:C:551:TRP:CZ2	2.56	0.41
1:C:855:LEU:HD11	1:C:895:PRO:HA	2.03	0.41
1:C:1139:ASN:ND2	1:C:1146:THR:H	2.18	0.41
1:D:76:THR:HG22	1:D:102:SER:HA	2.02	0.41
1:D:161:LEU:HD11	1:D:178:ARG:NH2	2.32	0.41
1:D:360:ARG:CZ	1:D:362:ARG:HH11	2.33	0.41
1:D:545:PRO:HD2	1:D:551:TRP:CZ2	2.55	0.41
1:D:663:TRP:CZ2	1:D:665:GLY:HA2	2.56	0.41
1:D:872:PRO:HG2	1:D:882:VAL:HG13	2.02	0.41
1:D:884:TYR:HB3	1:D:886:PHE:CE1	2.56	0.41
1:D:1081:THR:HG23	1:D:1082:THR:HG23	2.02	0.41
1:D:1178:PHE:HA	1:D:1211:GLY:H	1.85	0.41
1:D:1604:GLU:N	1:D:1604:GLU:OE1	2.54	0.41
1:D:1773:TYR:HE1	1:D:1797:CYS:HB3	1.86	0.41
1:D:1805:ARG:O	1:D:1806:PRO:C	2.64	0.41
1:A:225:ASP:OD1	1:A:225:ASP:N	2.54	0.41
1:A:455:TYR:CD2	1:A:461:LYS:HD2	2.56	0.41
1:B:581:TYR:N	1:B:581:TYR:CD2	2.89	0.41
1:B:677:TRP:HB3	1:B:717:GLN:HG2	2.03	0.41
1:C:225:ASP:OD1	1:C:225:ASP:N	2.54	0.41
1:C:1215:LYS:O	1:C:1216:CYS:HB2	2.21	0.41
1:C:1367:LEU:HD21	1:C:1389:CYS:HA	2.03	0.41
1:C:1782:ASP:N	1:C:1782:ASP:OD2	2.52	0.41
1:D:1081:THR:HA	1:D:1097:ARG:HG2	2.03	0.41
1:A:274:THR:O	1:A:274:THR:OG1	2.35	0.40
1:A:1367:LEU:HD23	1:A:1367:LEU:HA	1.73	0.40
1:A:1844:SER:O	1:A:1847:LYS:NZ	2.49	0.40
1:B:623:SER:O	1:B:641:TYR:HA	2.21	0.40
1:B:777:ARG:HB3	1:B:813:THR:HB	2.03	0.40
1:C:446:ASN:HD22	1:C:446:ASN:N	2.16	0.40
1:C:520:ARG:HB2	1:C:571:PRO:HD2	2.02	0.40
1:C:612:GLN:O	1:C:654:PRO:HD2	2.21	0.40
1:C:704:PRO:HG3	1:C:714:PRO:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:PRO:HD2	1:D:551:TRP:CE2	2.54	0.40
1:D:1062:PRO:HD3	1:D:1093:ASP:OD1	2.20	0.40
1:D:1410:PRO:HD3	1:D:1457:PHE:CD2	2.56	0.40
1:D:1766:ARG:HH11	1:D:1766:ARG:HG2	1.85	0.40
1:D:1902:PRO:HA	1:D:1903:PRO:HD3	1.93	0.40
1:A:461:LYS:HZ2	1:A:490:VAL:HG11	1.85	0.40
1:A:520:ARG:NH1	1:A:530:GLU:OE2	2.54	0.40
1:A:1095:GLN:NE2	1:A:1112:PHE:HB3	2.37	0.40
1:B:398:THR:HB	1:B:399:THR:HG23	2.03	0.40
1:B:522:LYS:HG2	1:B:523:ALA:N	2.33	0.40
1:B:561:LEU:HD12	1:B:575:ILE:HD11	2.03	0.40
1:B:832:TYR:HB2	1:B:852:PHE:CE2	2.56	0.40
1:B:1582:LEU:HD23	1:B:1582:LEU:HA	1.93	0.40
1:C:387:LEU:HD22	1:C:465:LEU:HG	2.03	0.40
1:C:389:LEU:HA	1:C:407:ALA:HA	2.03	0.40
1:C:589:GLN:HB3	1:C:610:VAL:HG13	2.03	0.40
1:C:751:TYR:HB2	1:C:848:ILE:HD11	2.02	0.40
1:C:1036:ARG:O	1:C:1037:ASP:HB3	2.21	0.40
1:C:1263:LYS:HB2	1:C:1266:ILE:HG22	2.03	0.40
1:C:1929:PRO:HA	1:C:1930:PRO:HD3	1.91	0.40
1:D:271:LEU:HD11	1:D:372:ALA:HB1	2.03	0.40
1:D:970:GLU:N	1:D:970:GLU:OE1	2.55	0.40
1:D:1603:ASP:N	1:D:1604:GLU:OE1	2.54	0.40
1:A:713:THR:HG21	1:A:737:VAL:C	2.46	0.40
1:A:1038:PRO:O	1:A:1040:VAL:N	2.53	0.40
1:A:1055:TYR:O	1:A:1124:PRO:HA	2.22	0.40
1:B:641:TYR:CG	1:B:716:LEU:HD11	2.56	0.40
1:B:1551:PRO:O	1:B:1572:MET:HB3	2.21	0.40
1:C:1285:LYS:HB2	1:C:1285:LYS:HE2	1.81	0.40
1:C:1560:LEU:HD23	1:C:1560:LEU:HA	1.82	0.40
1:D:122:ILE:HD12	1:D:153:ASP:HB2	2.03	0.40
1:D:623:SER:OG	1:D:642:ASN:HB2	2.22	0.40
1:D:764:ALA:N	1:D:858:GLY:O	2.46	0.40
1:D:1058:GLN:NE2	1:D:1115:LEU:O	2.52	0.40
1:D:1786:ASP:O	1:D:1786:ASP:OD2	2.39	0.40
1:A:885:THR:HG22	1:A:948:THR:HG22	2.04	0.40
1:C:1071:ASP:HB2	1:C:1129:PHE:CE1	2.57	0.40
1:C:1192:ASN:OD1	1:C:1192:ASN:C	2.64	0.40
1:D:1282:GLU:CD	1:D:1282:GLU:N	2.79	0.40
1:D:1805:ARG:O	1:D:1805:ARG:HG2	2.21	0.40
1:A:596:ILE:HD12	1:A:596:ILE:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:PRO:HD2	1:A:677:TRP:CH2	2.57	0.40
1:A:753:ILE:HG12	1:A:775:ILE:HG12	2.03	0.40
1:A:794:ASP:HB2	1:A:800:SER:HB2	2.03	0.40
1:A:1605:PHE:CD1	1:C:1175:PRO:HB3	2.57	0.40
1:A:1799:TYR:O	1:A:1829:THR:HG23	2.21	0.40
1:B:759:PRO:HD2	1:B:769:ALA:HA	2.03	0.40
1:B:808:ILE:CG2	1:B:815:THR:HB	2.51	0.40
1:B:1183:PHE:C	1:B:1184:ASP:OD1	2.64	0.40
1:D:680:LEU:HD11	1:D:685:ASN:HD22	1.87	0.40
1:D:1325:TYR:O	1:D:1358:CYS:HA	2.22	0.40
1:D:1519:MET:SD	1:D:1520:VAL:N	2.93	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	1884/1987 (95%)	1738 (92%)	132 (7%)	14 (1%)	19	54
1	B	1884/1987 (95%)	1725 (92%)	133 (7%)	26 (1%)	9	39
1	C	1884/1987 (95%)	1727 (92%)	139 (7%)	18 (1%)	13	46
1	D	1884/1987 (95%)	1726 (92%)	137 (7%)	21 (1%)	12	45
All	All	7536/7948 (95%)	6916 (92%)	541 (7%)	79 (1%)	16	46

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	THR
1	A	1062	PRO
1	A	1143	VAL
1	B	169	ASN

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Mol	Chain	Res	Type
1	B	393	THR
1	B	394	ALA
1	B	395	ASP
1	B	1062	PRO
1	B	1077	PHE
1	B	1143	VAL
1	B	1197	ASN
1	B	1239	GLU
1	B	1806	PRO
1	C	169	ASN
1	C	1062	PRO
1	C	1143	VAL
1	C	1382	ALA
1	C	1806	PRO
1	D	169	ASN
1	D	1062	PRO
1	D	1077	PHE
1	D	1806	PRO
1	A	1216	CYS
1	A	1393	GLU
1	B	1760	ASP
1	B	1799	TYR
1	B	1935	SER
1	C	398	THR
1	C	1077	PHE
1	C	1832	LEU
1	D	1143	VAL
1	D	1760	ASP
1	D	1799	TYR
1	D	1832	LEU
1	D	1935	SER
1	A	101	LEU
1	A	1175	PRO
1	A	1814	CYS
1	B	101	LEU
1	B	398	THR
1	B	1176	LYS
1	B	1787	GLU
1	B	1814	CYS
1	C	1175	PRO
1	C	1787	GLU
1	C	1799	TYR

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Mol	Chain	Res	Type
1	C	1933	ALA
1	D	101	LEU
1	D	398	THR
1	D	972	ALA
1	D	1224	ASP
1	A	471	ASP
1	A	1787	GLU
1	B	392	THR
1	B	471	ASP
1	C	101	LEU
1	C	471	ASP
1	C	1926	SER
1	D	1175	PRO
1	D	1787	GLU
1	A	1926	SER
1	B	1325	TYR
1	D	1037	ASP
1	D	1814	CYS
1	A	396	PRO
1	B	1216	CYS
1	B	1926	SER
1	C	1216	CYS
1	D	1606	SER
1	D	1644	ALA
1	C	1814	CYS
1	A	1037	ASP
1	B	396	PRO
1	B	1769	PRO
1	B	1037	ASP
1	C	1037	ASP
1	A	395	ASP
1	D	1769	PRO
1	D	1926	SER

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	1488/1571 (95%)	1482 (100%)	6 (0%)	89	91
1	B	1488/1571 (95%)	1477 (99%)	11 (1%)	81	86
1	C	1488/1571 (95%)	1485 (100%)	3 (0%)	92	94
1	D	1488/1571 (95%)	1479 (99%)	9 (1%)	84	88
All	All	5952/6284 (95%)	5923 (100%)	29 (0%)	85	90

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	ASN
1	A	519	GLN
1	A	612	GLN
1	A	1610	CYS
1	A	1731	THR
1	A	1748	THR
1	B	290	GLN
1	B	612	GLN
1	B	824	TYR
1	B	1162	ILE
1	B	1167	ASN
1	B	1497	MET
1	B	1562	ILE
1	B	1677	THR
1	B	1748	THR
1	B	1769	PRO
1	B	1804	ASP
1	C	162	GLN
1	C	229	ASN
1	C	1364	ASN
1	D	108	ASN
1	D	156	LEU
1	D	685	ASN
1	D	1061	ASN
1	D	1497	MET
1	D	1613	CYS
1	D	1731	THR
1	D	1769	PRO
1	D	1824	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	593	GLN
1	A	758	ASN
1	A	1293	GLN
1	A	1372	GLN
1	A	1495	GLN
1	A	1496	GLN
1	A	1810	GLN
1	A	1827	GLN
1	B	185	ASN
1	B	218	ASN
1	B	229	ASN
1	B	593	GLN
1	B	791	GLN
1	B	1094	GLN
1	B	1212	GLN
1	B	1563	GLN
1	B	1672	GLN
1	B	1757	ASN
1	B	1891	ASN
1	B	1924	ASN
1	C	229	ASN
1	C	446	ASN
1	C	758	ASN
1	C	1025	ASN
1	C	1094	GLN
1	C	1095	GLN
1	C	1139	ASN
1	C	1372	GLN
1	C	1480	GLN
1	C	1672	GLN
1	D	446	ASN
1	D	847	HIS
1	D	1326	HIS
1	D	1503	ASN
1	D	1506	ASN
1	D	1672	GLN
1	D	1757	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

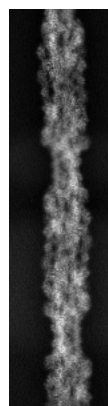
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41679. These allow visual inspection of the internal detail of the map and identification of artifacts.

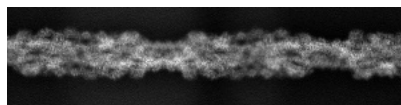
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

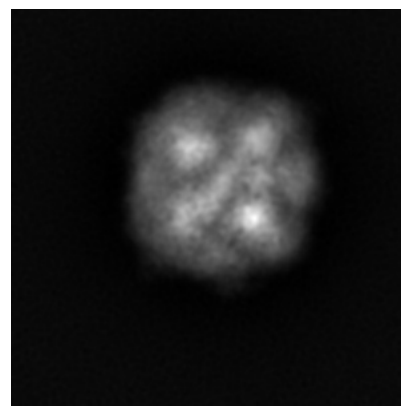
6.1.1 Primary map



X



Y

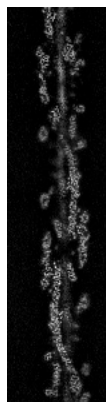


Z

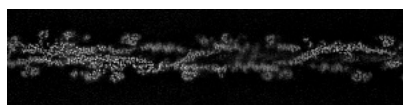
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

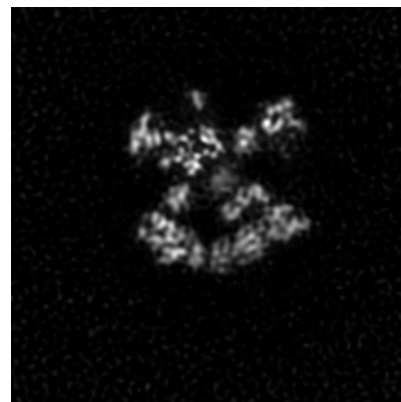
6.2.1 Primary map



X Index:
100



Y Index: 100

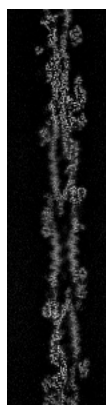


Z Index: 400

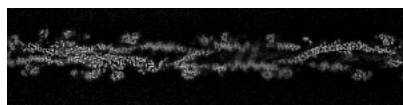
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

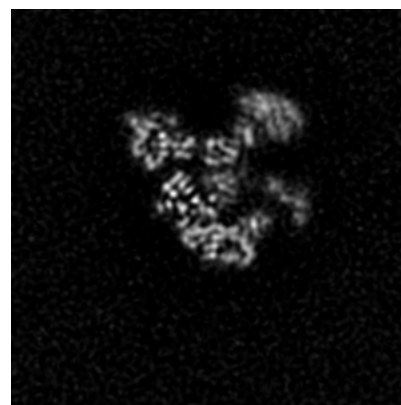
6.3.1 Primary map



X Index:
122



Y Index: 99

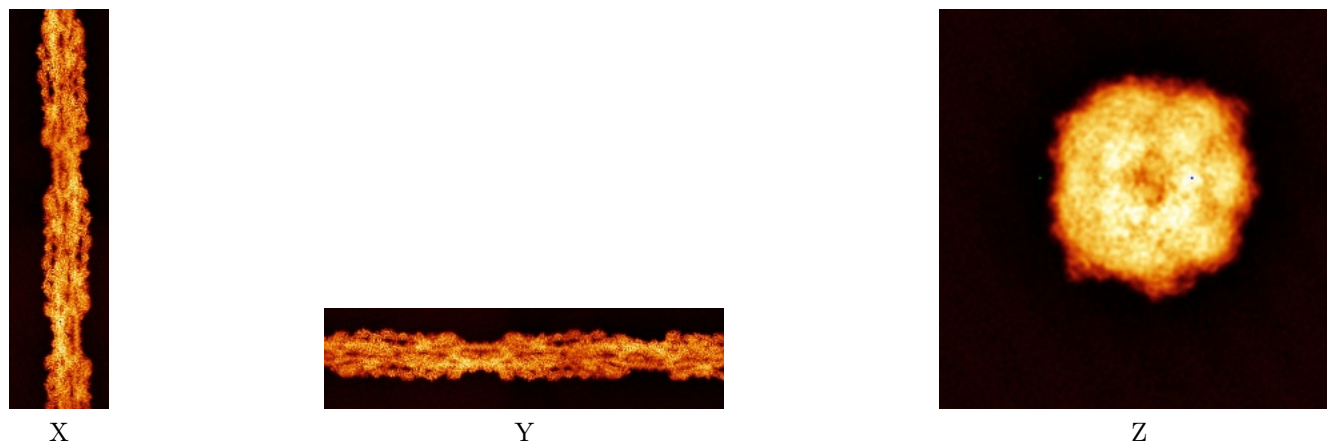


Z Index: 264

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

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

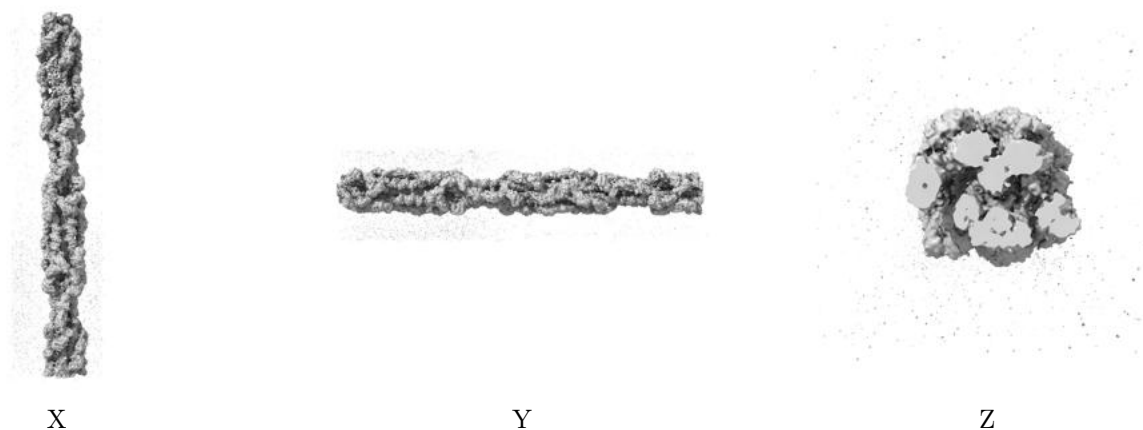
6.4.1 Primary map



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 0.0728. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

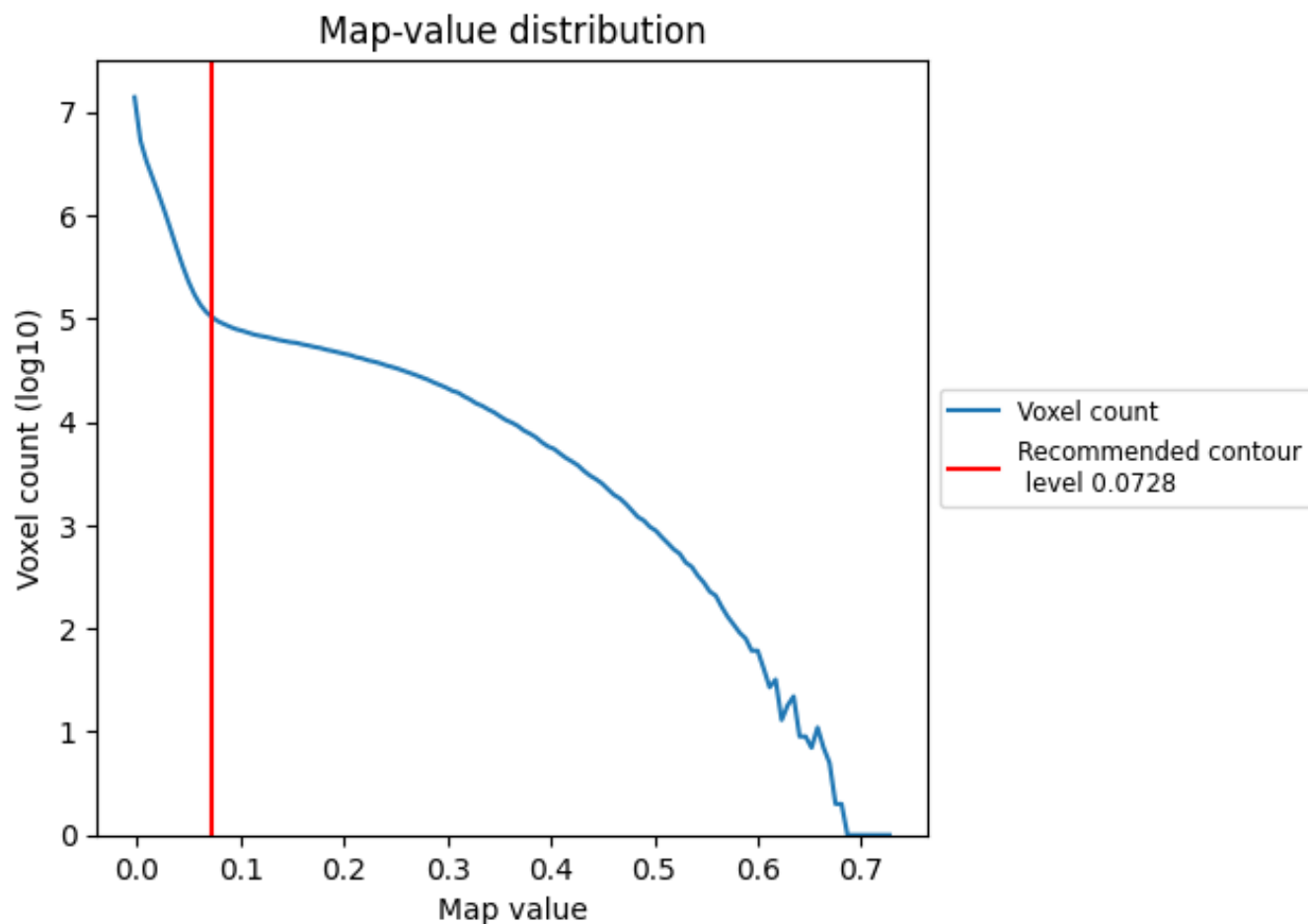
6.6 Mask visualisation

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

7 Map analysis [i](#)

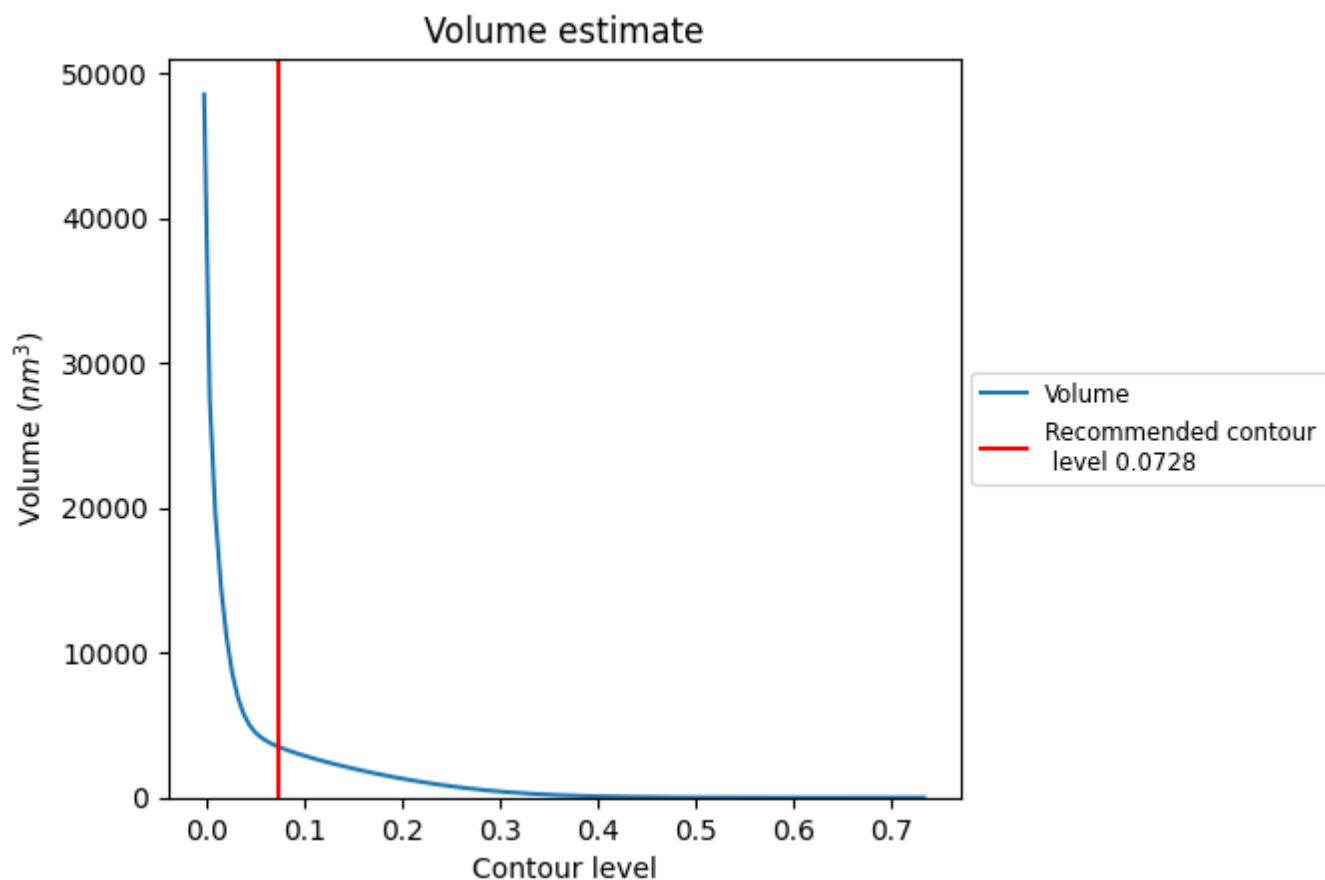
This section contains the results of statistical analysis of the map.

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 3533 nm³; this corresponds to an approximate mass of 3192 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

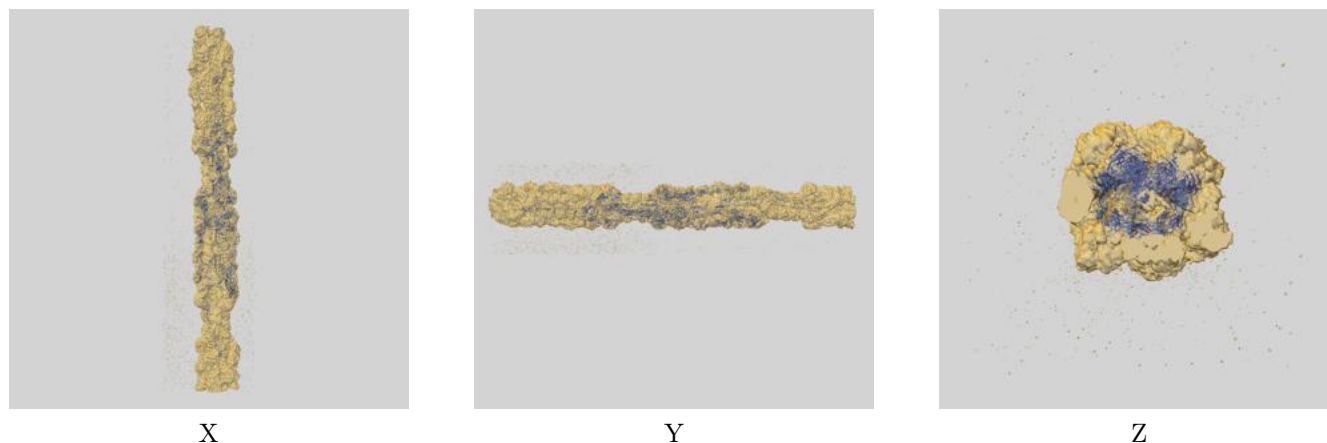
8 Fourier-Shell correlation

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-41679 and PDB model 8TXB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0728 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](#)



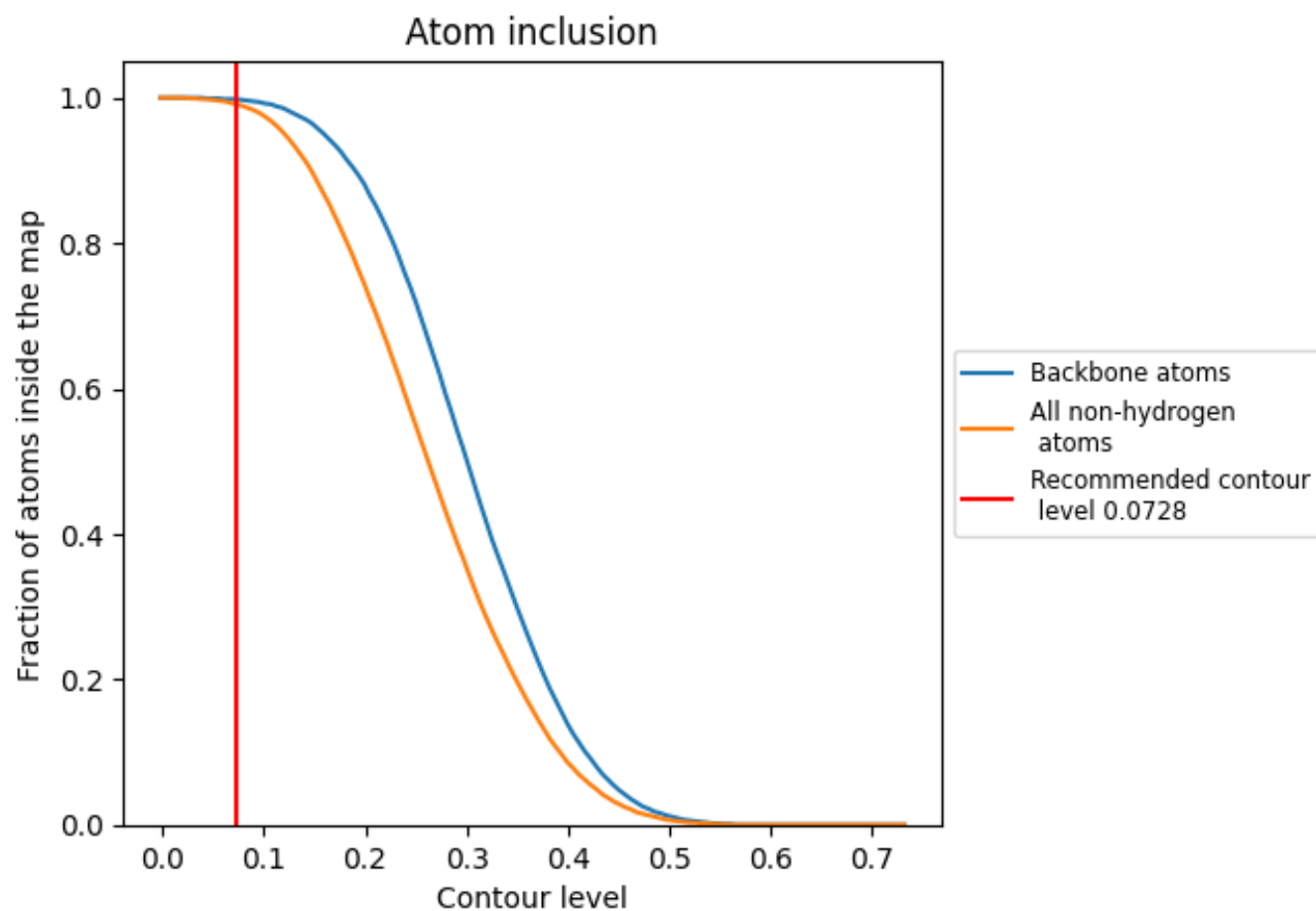
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0728).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0728) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9910	<div></div> 0.3500
A	<div></div> 0.9910	<div></div> 0.3490
B	<div></div> 0.9930	<div></div> 0.3620
C	<div></div> 0.9930	<div></div> 0.3500
D	<div></div> 0.9880	<div></div> 0.3360

