Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 06:40 AM EST

PDB ID	:	6O2M
EMDB ID	:	EMD-0608
Title	:	CDTb Double Heptamer Long Form Modeled from Cryo-EM Map Reconstructed using C7 Symmetry
Authors	:	Lacy, D.B.; Sheedlo, M.J.; Anderson, D.M.
Deposited on	:	2019-02-24
Resolution	:	6.30 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:

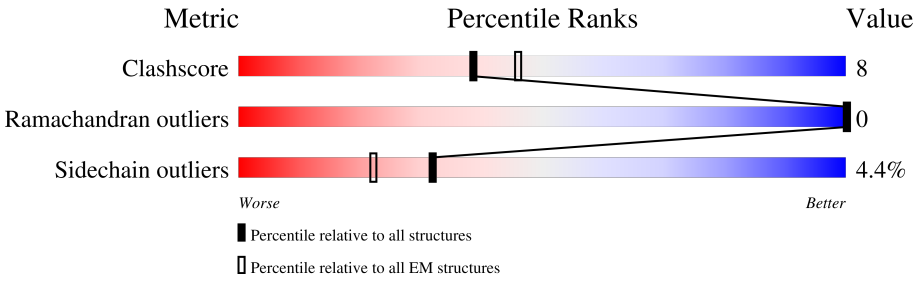
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	876	36% 55% 15% • 29%
1	B	876	15% 54% 16% • 29%
1	C	876	17% 54% 15% • 29%
1	D	876	11% 55% 15% • 29%
1	E	876	18% 55% 15% • 29%
1	F	876	25% 55% 15% • 29%
1	G	876	40% 55% 15% • 29%
1	T	876	9% 54% 16% • 29%

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Mol	Chain	Length	Quality of chain
1	U	876	10% 55% 15% 29%
1	V	876	15% 53% 16% 29%
1	W	876	20% 54% 16% 29%
1	X	876	8% 55% 15% 29%
1	Y	876	8% 55% 15% 29%
1	Z	876	11% 54% 16% 29%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 68446 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 ADP-ribosyltransferase binding component.

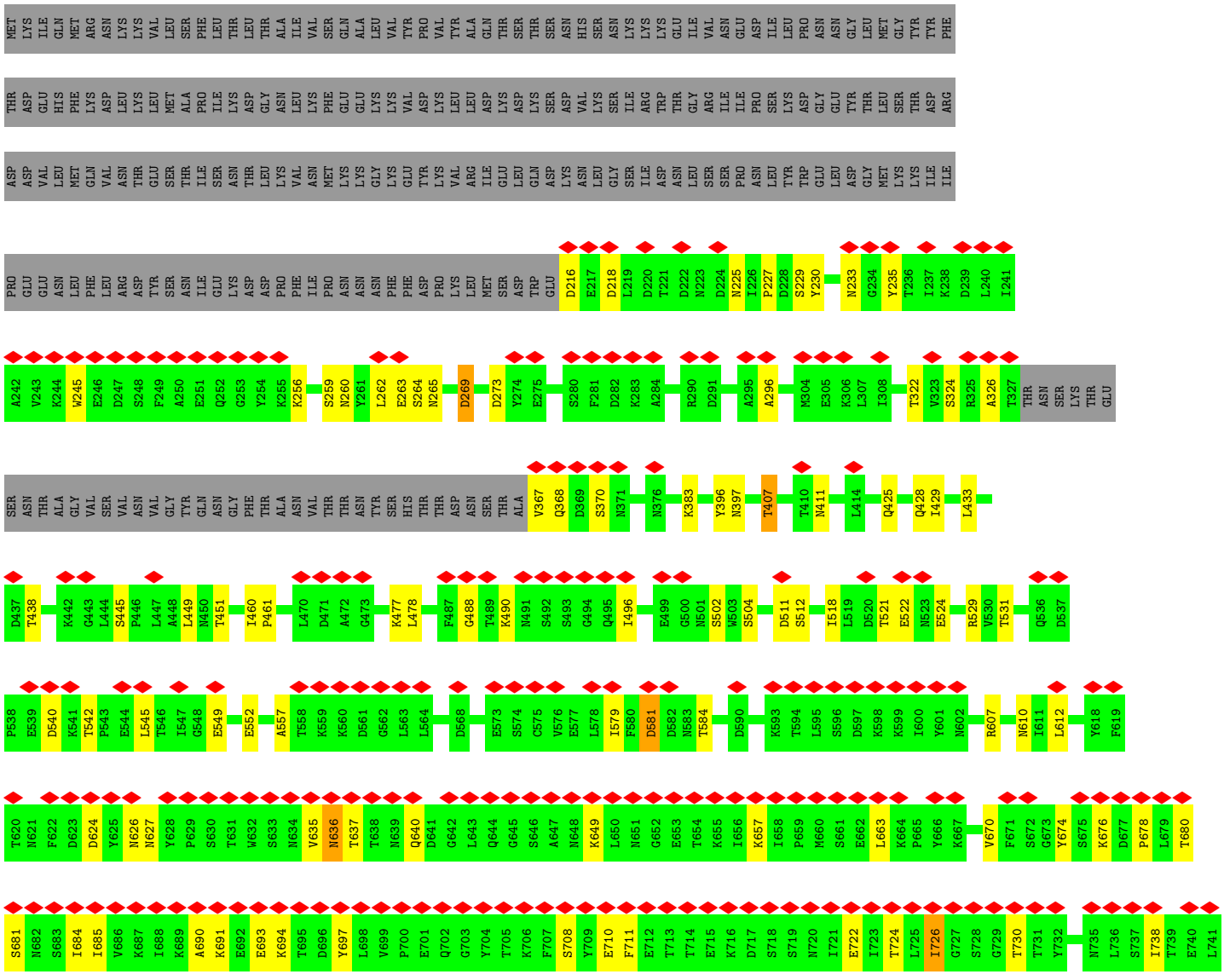
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	B	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	C	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	D	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	E	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	F	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	G	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	T	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	U	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	V	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	W	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	X	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	Y	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		
1	Z	618	Total	C	N	O	S	0	0
			4889	3071	791	1017	10		

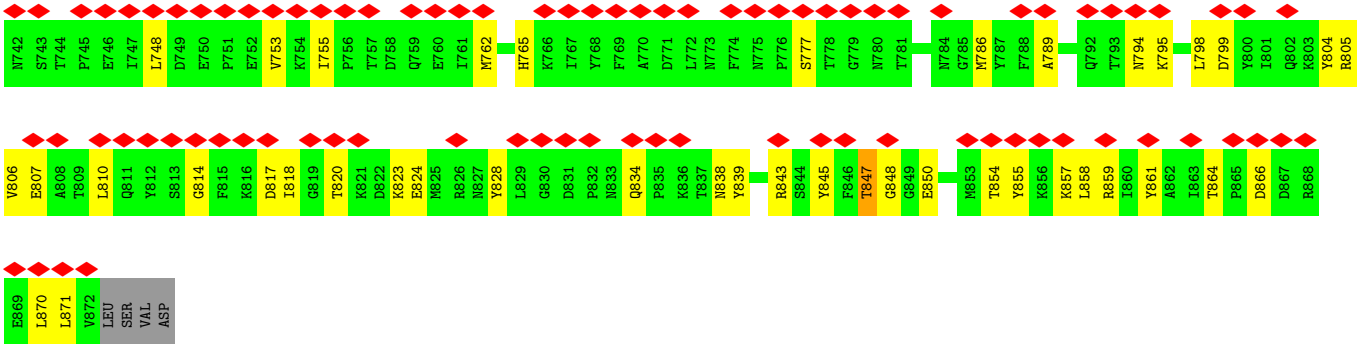
3 Residue-property plots (i)

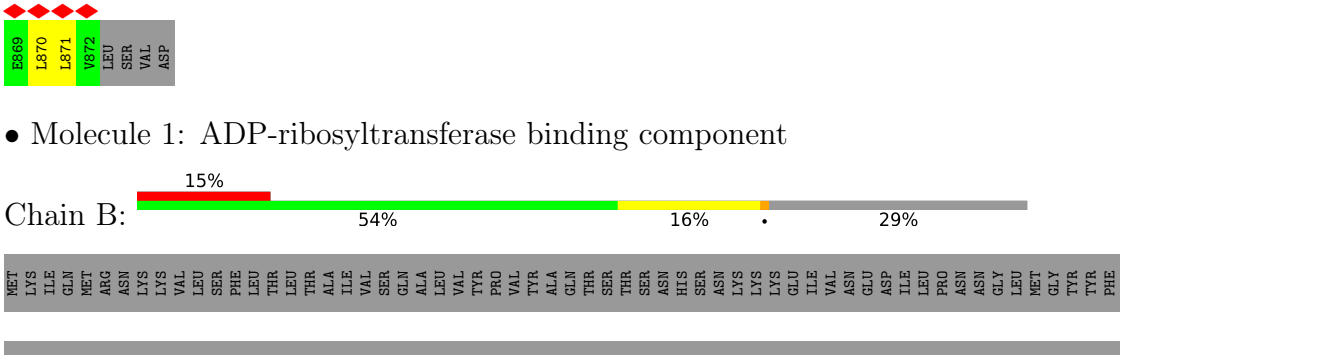
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: ADP-ribosyltransferase binding component

Chain A:

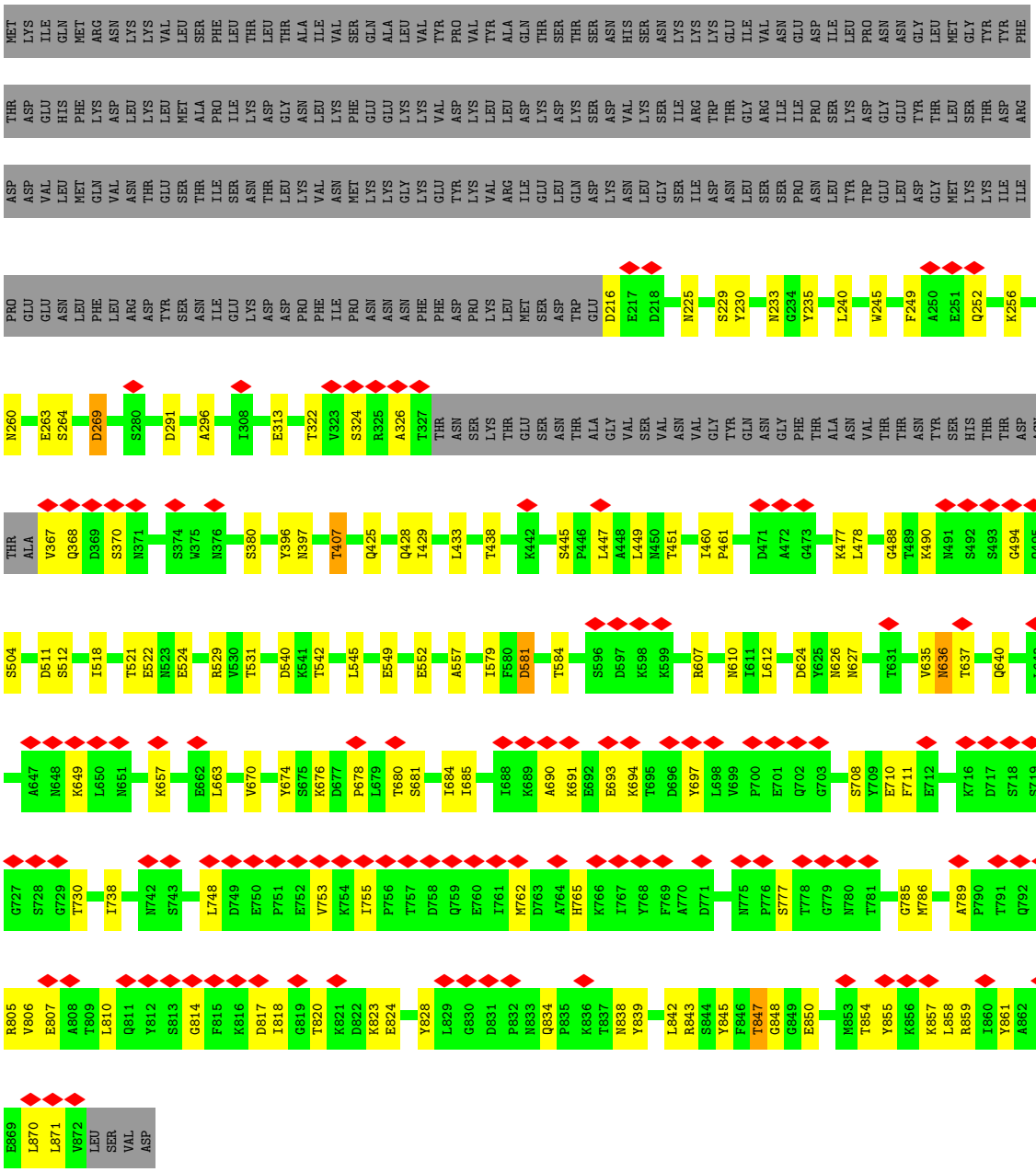






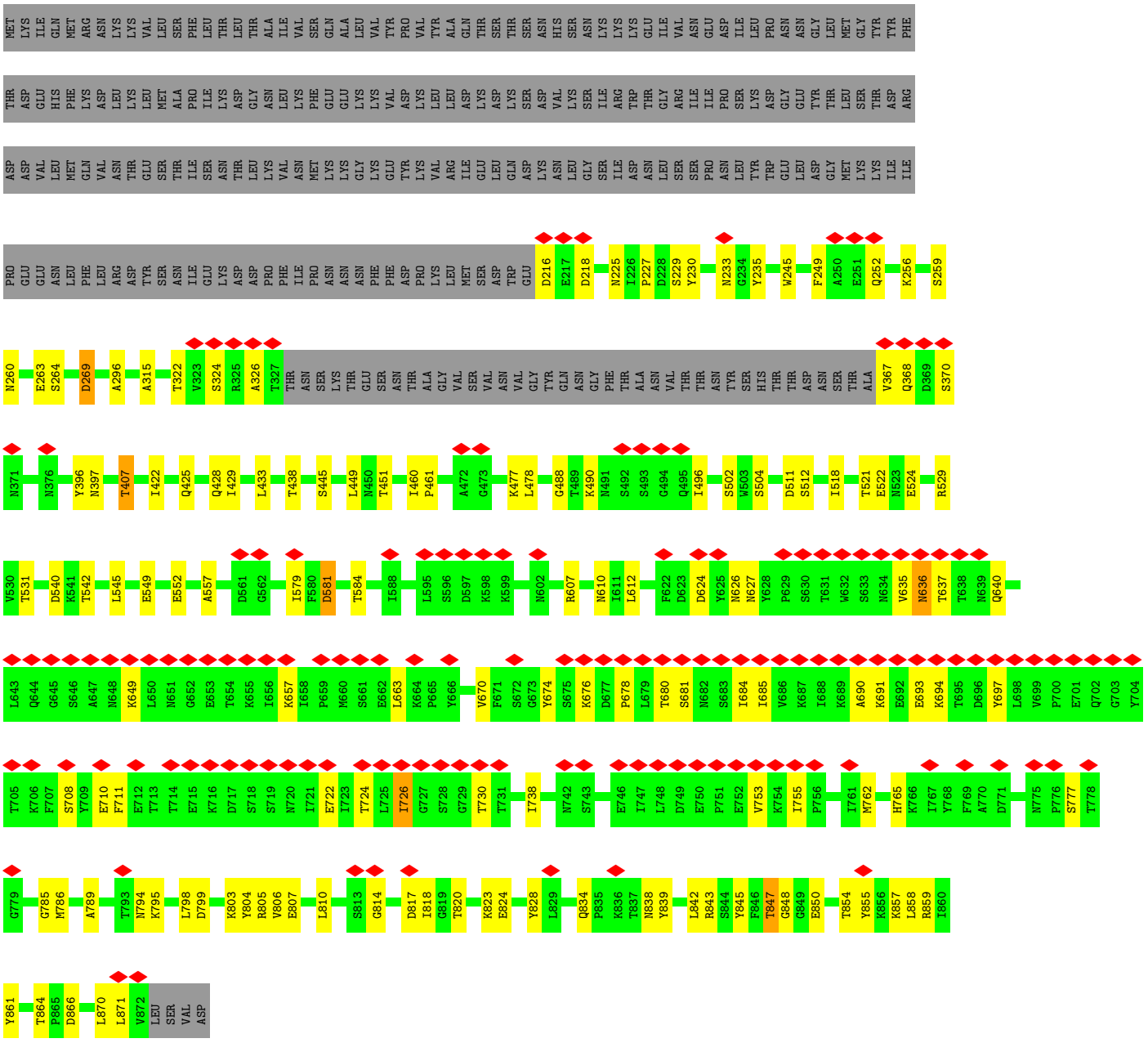
• Molecule 1: ADP-ribosyltransferase binding component

Chain B:



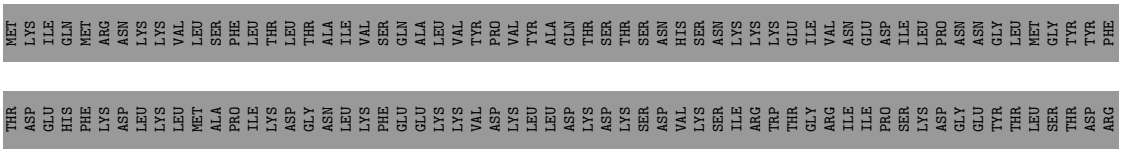
• Molecule 1: ADP-ribosyltransferase binding component

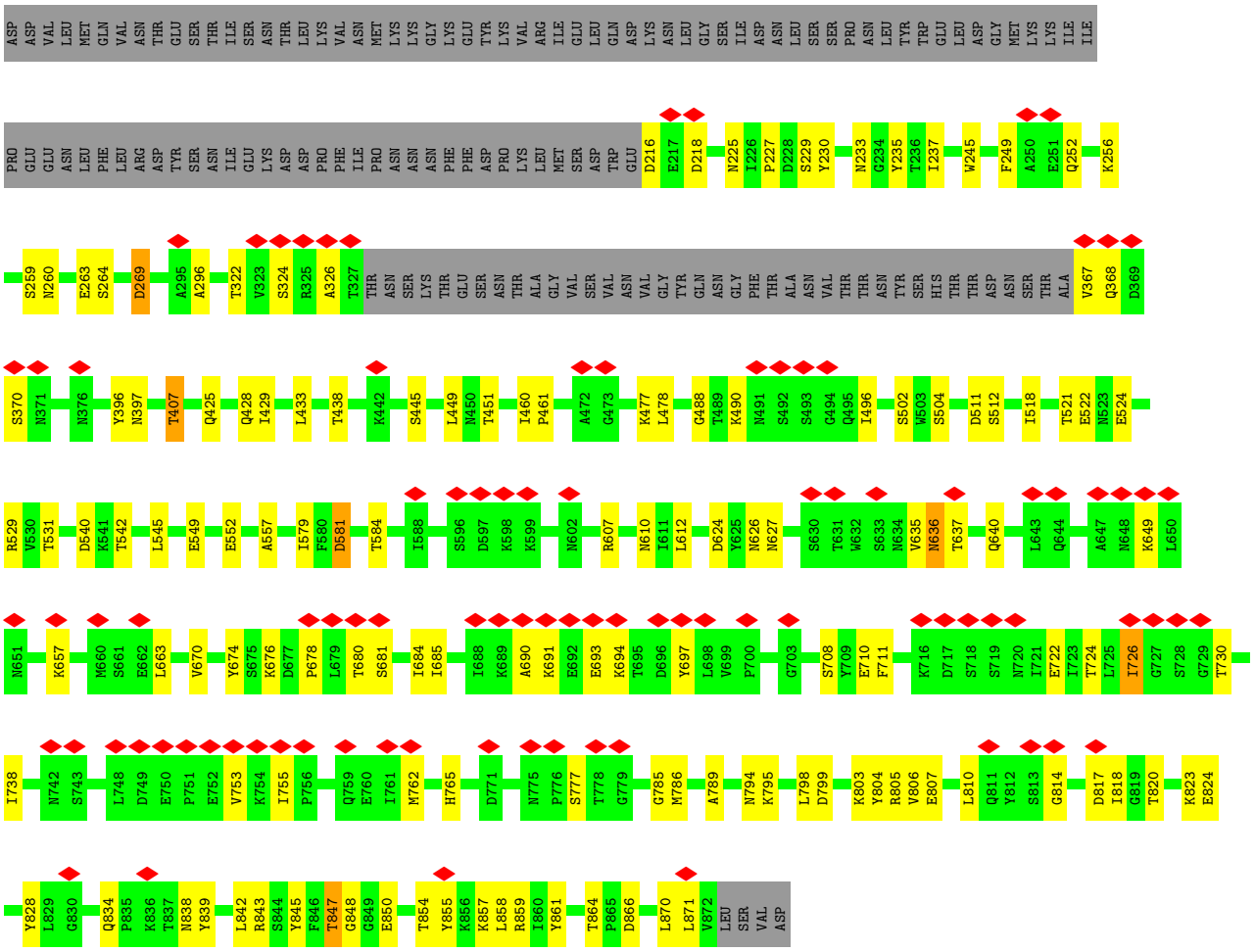
Chain C:



• Molecule 1: ADP-ribosyltransferase binding component

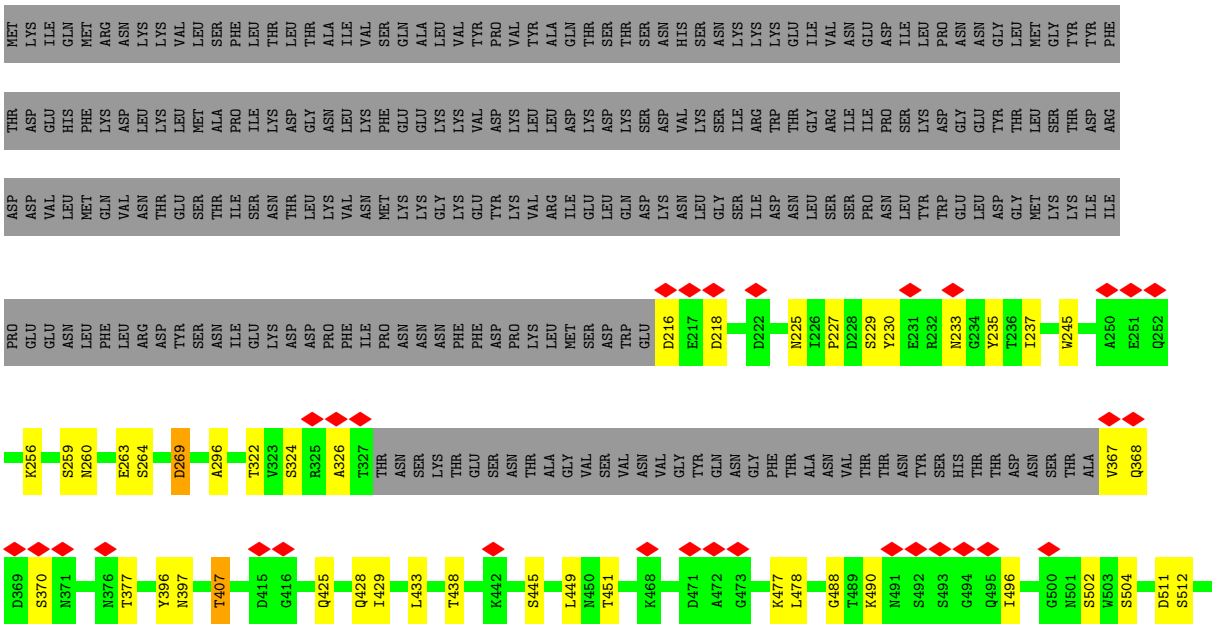
Chain D:

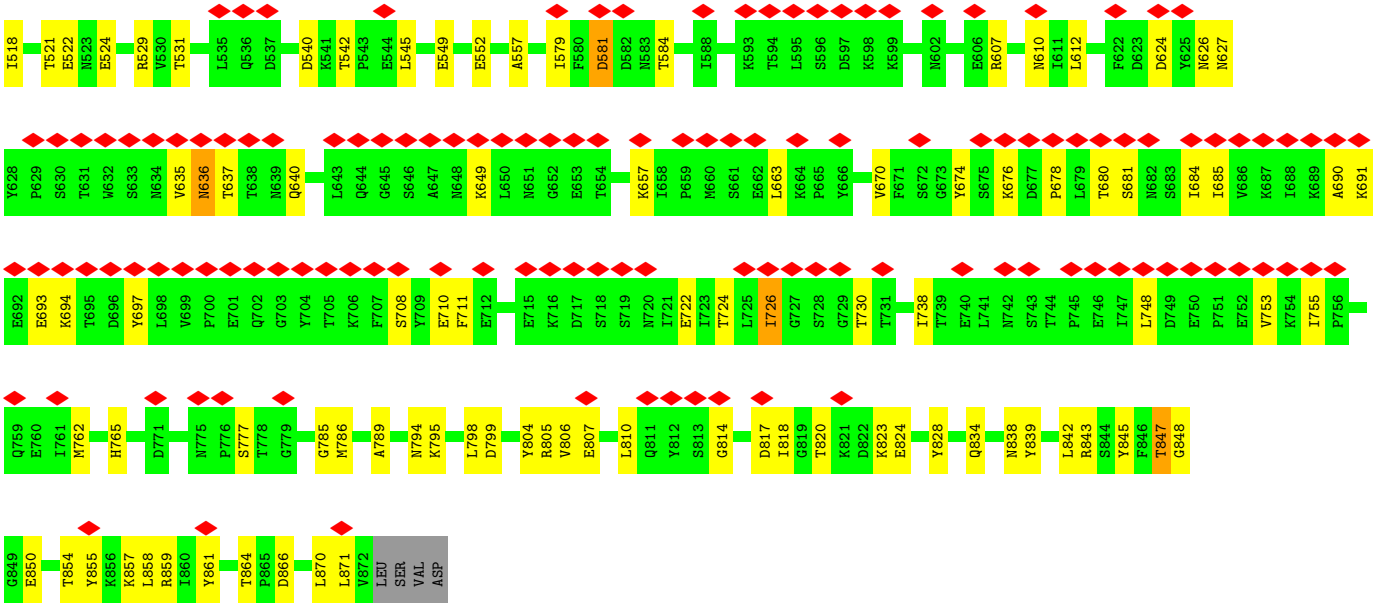




• Molecule 1: ADP-ribosyltransferase binding component

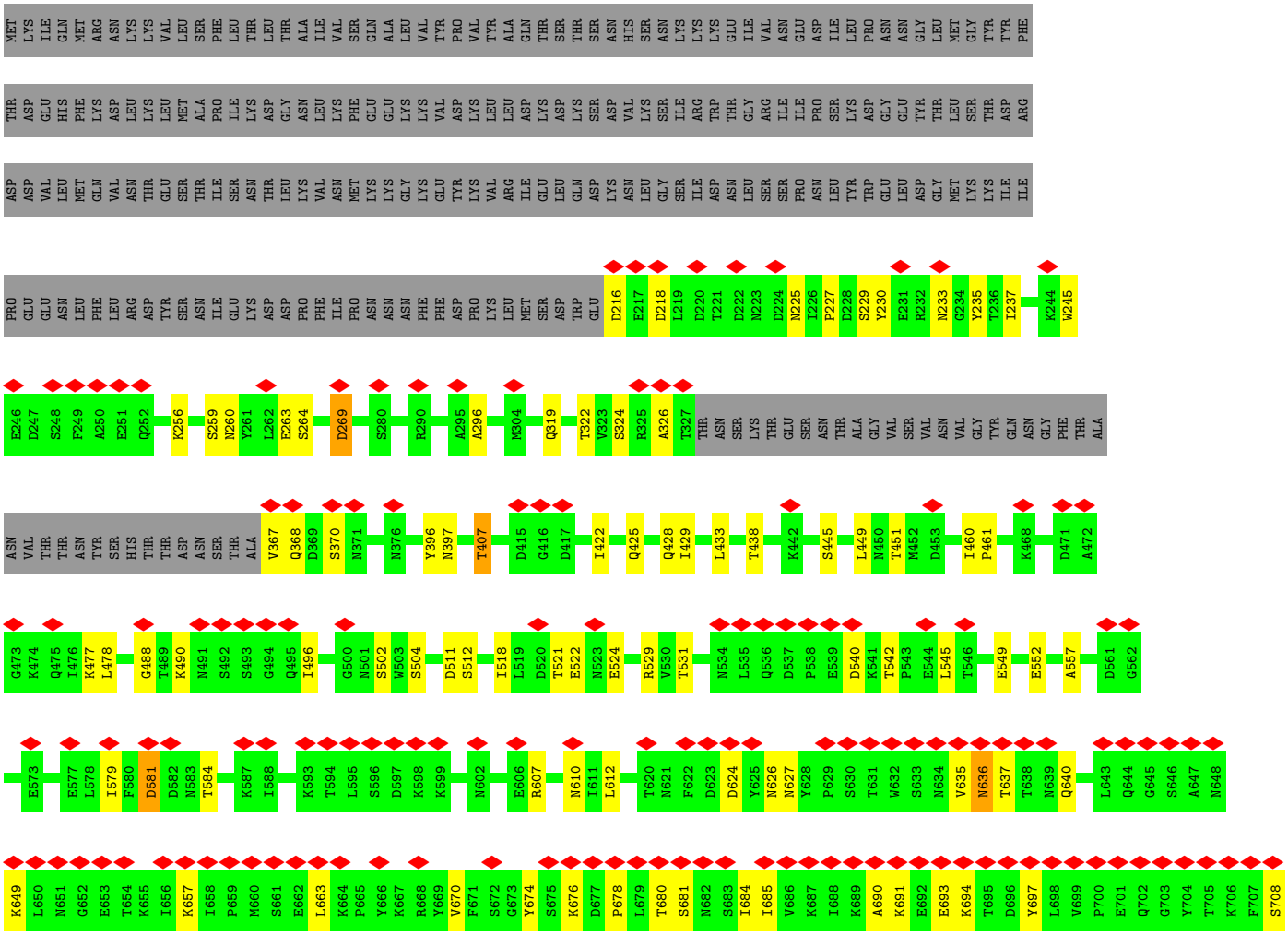
Chain E:

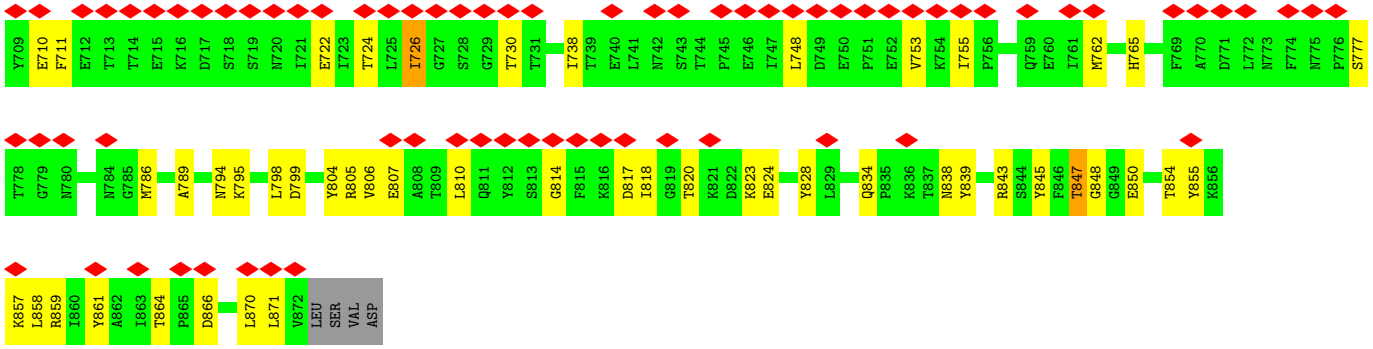




• Molecule 1: ADP-ribosyltransferase binding component

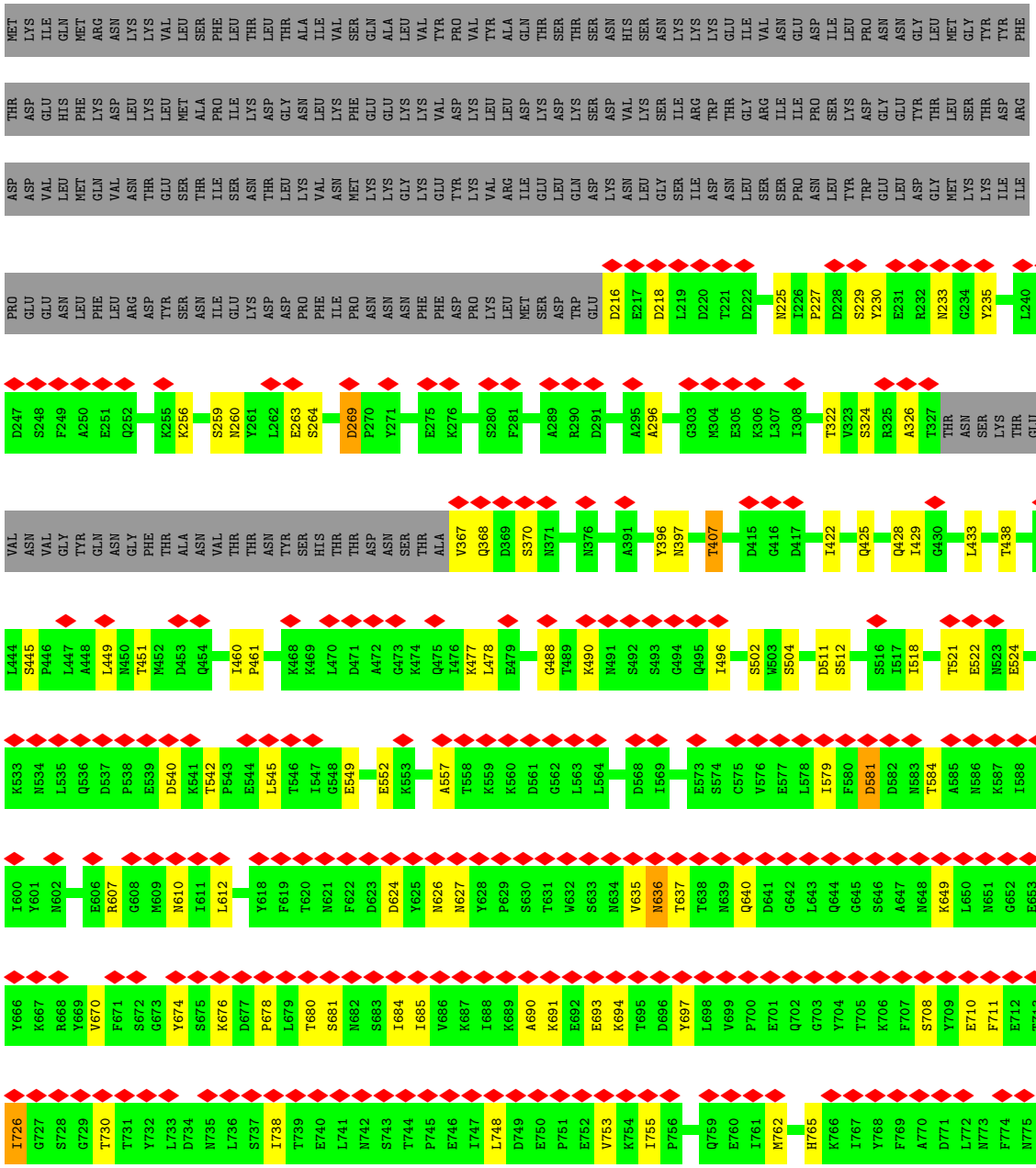
Chain F: 25% 55% 15% 29%

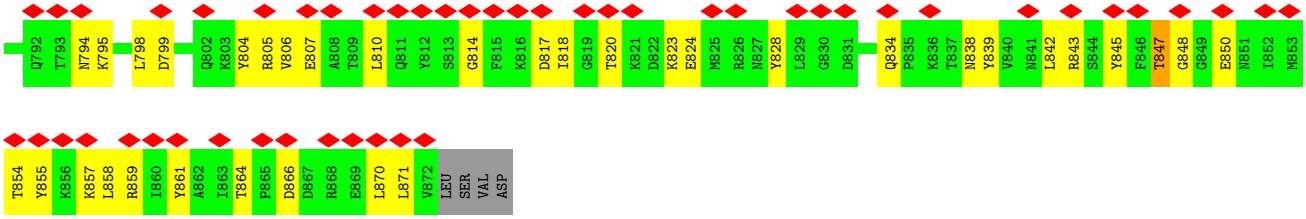




• Molecule 1: ADP-ribosyltransferase binding component

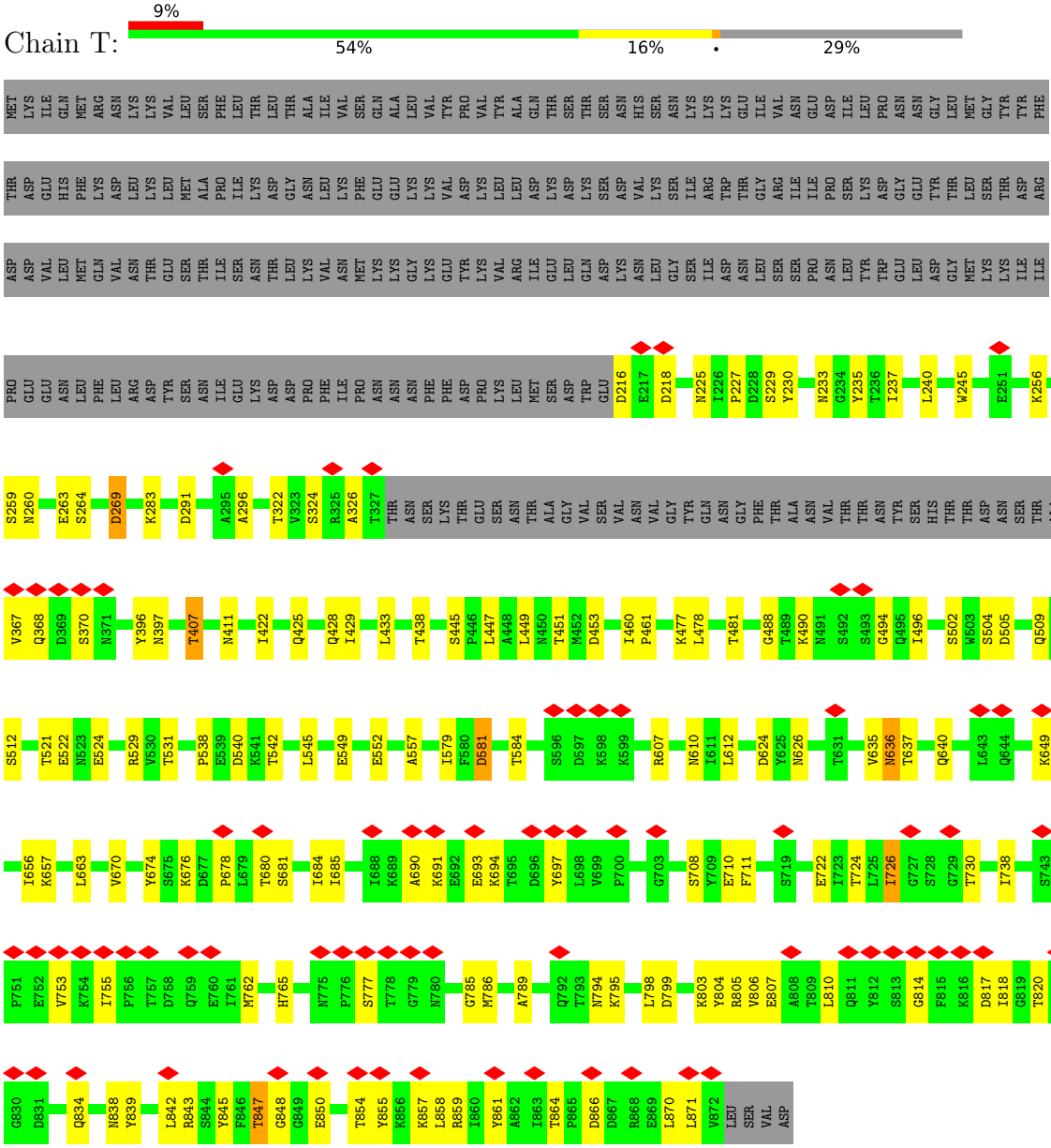
Chain G:





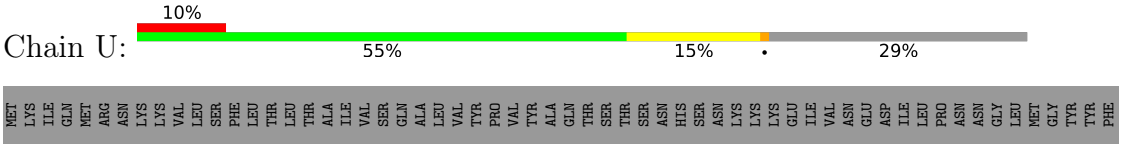
• Molecule 1: ADP-ribosyltransferase binding component

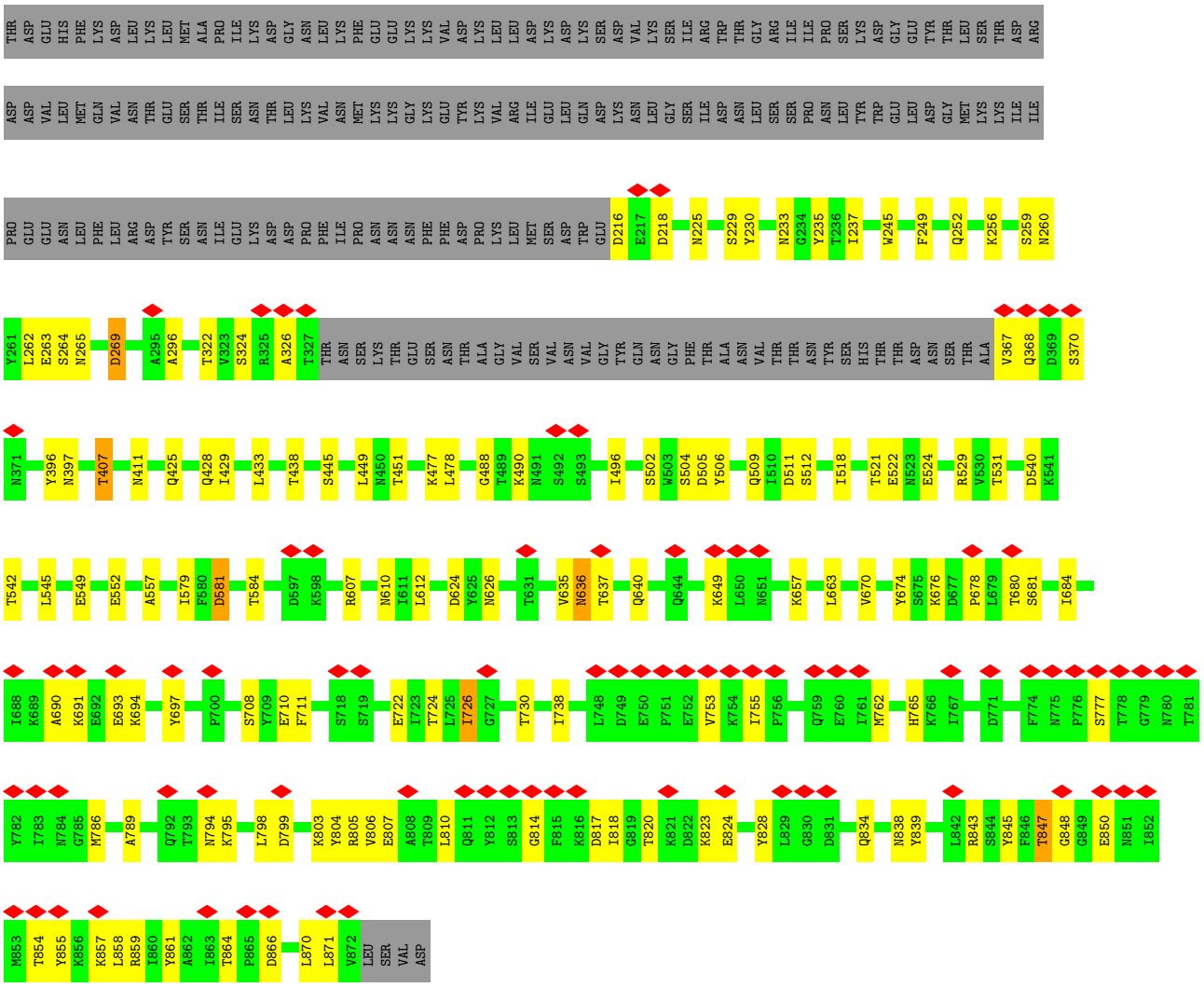
Chain T:



• Molecule 1: ADP-ribosyltransferase binding component

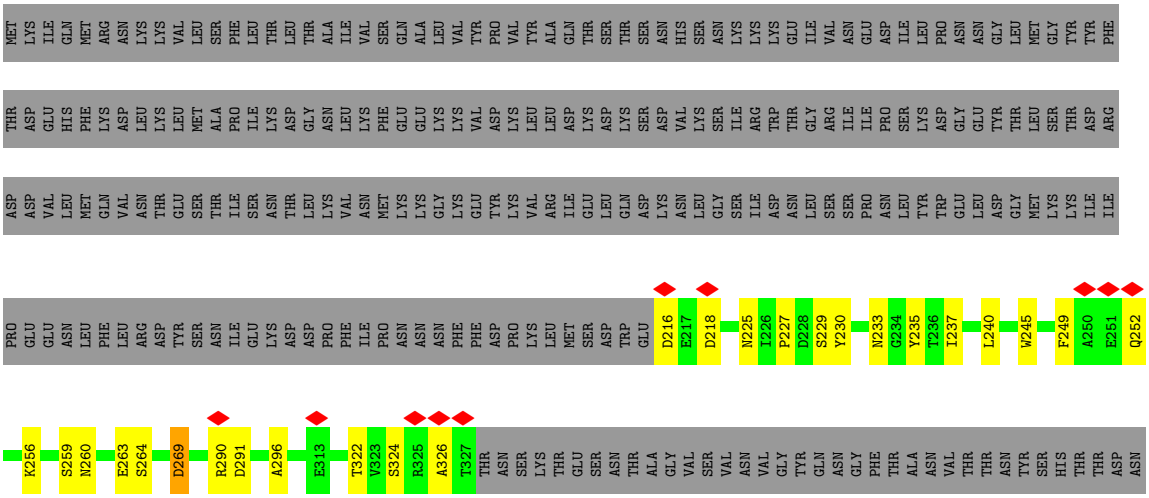
Chain U:

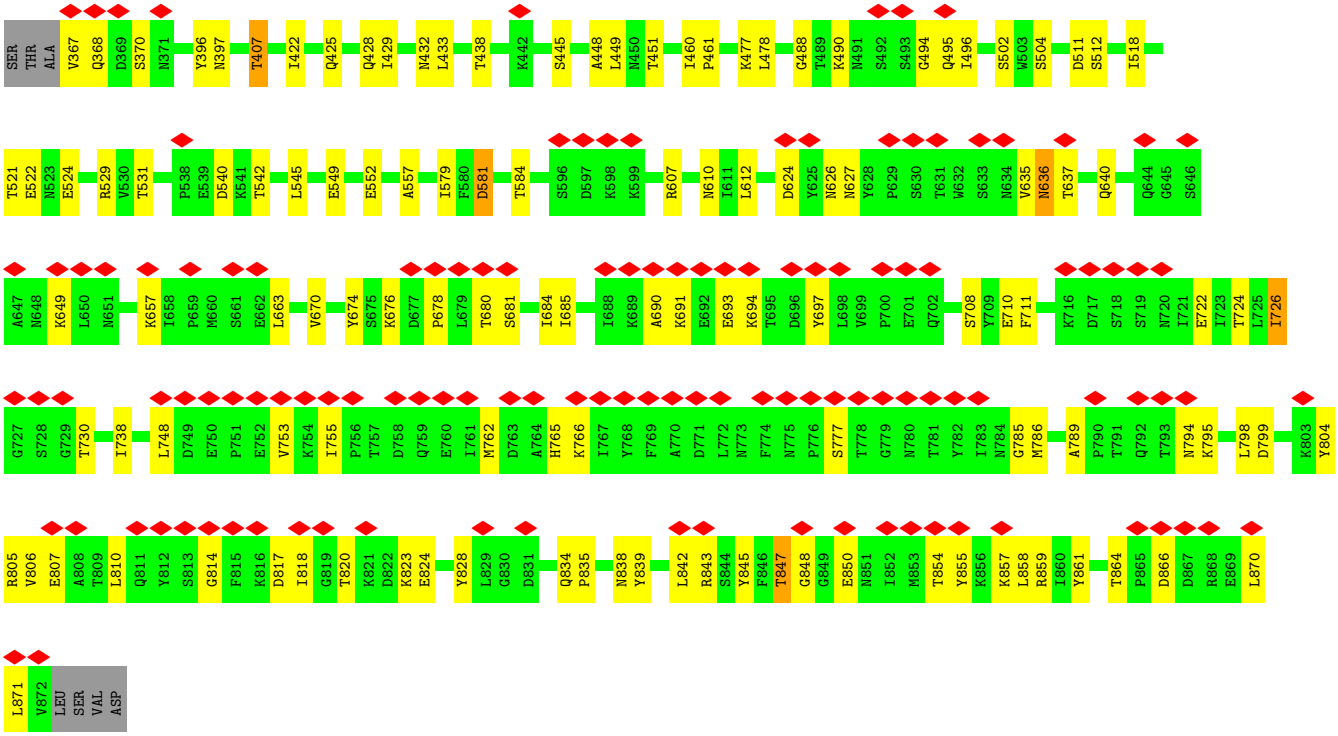




• Molecule 1: ADP-ribosyltransferase binding component

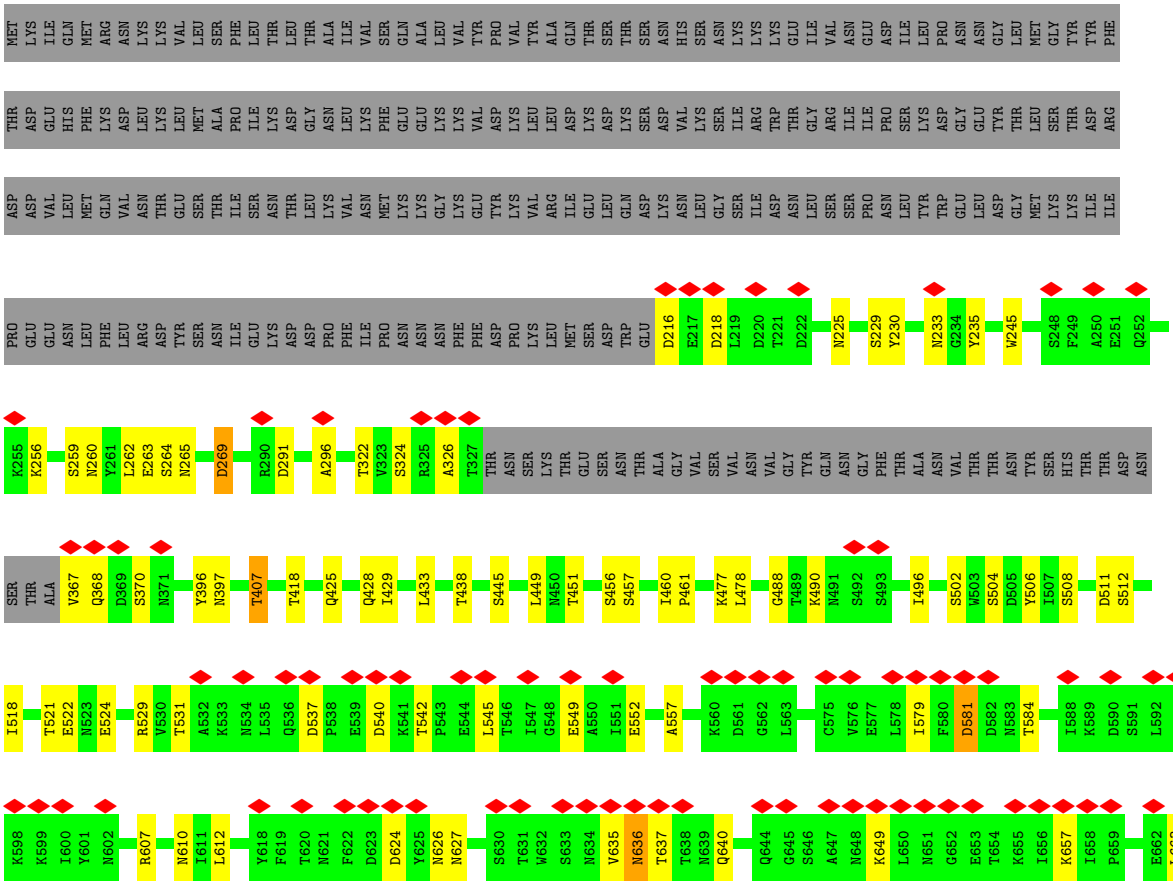
Chain V:

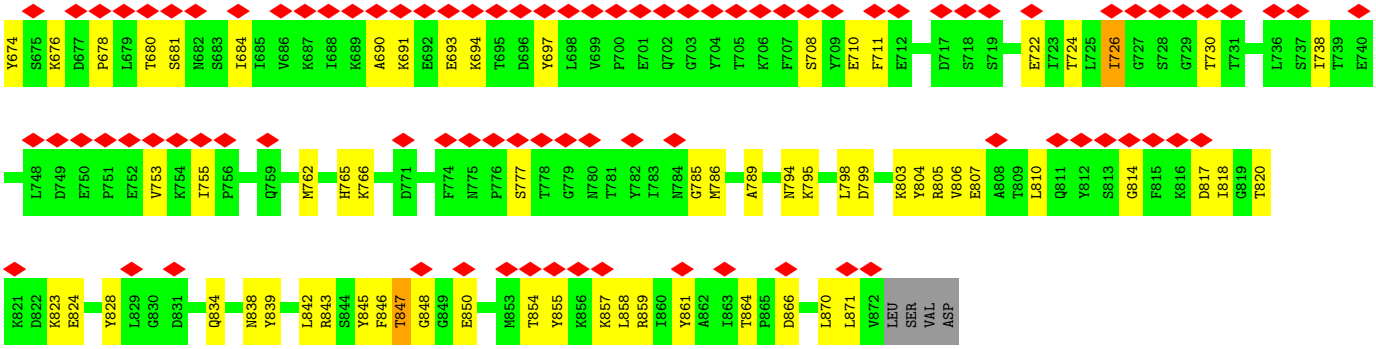




• Molecule 1: ADP-ribosyltransferase binding component

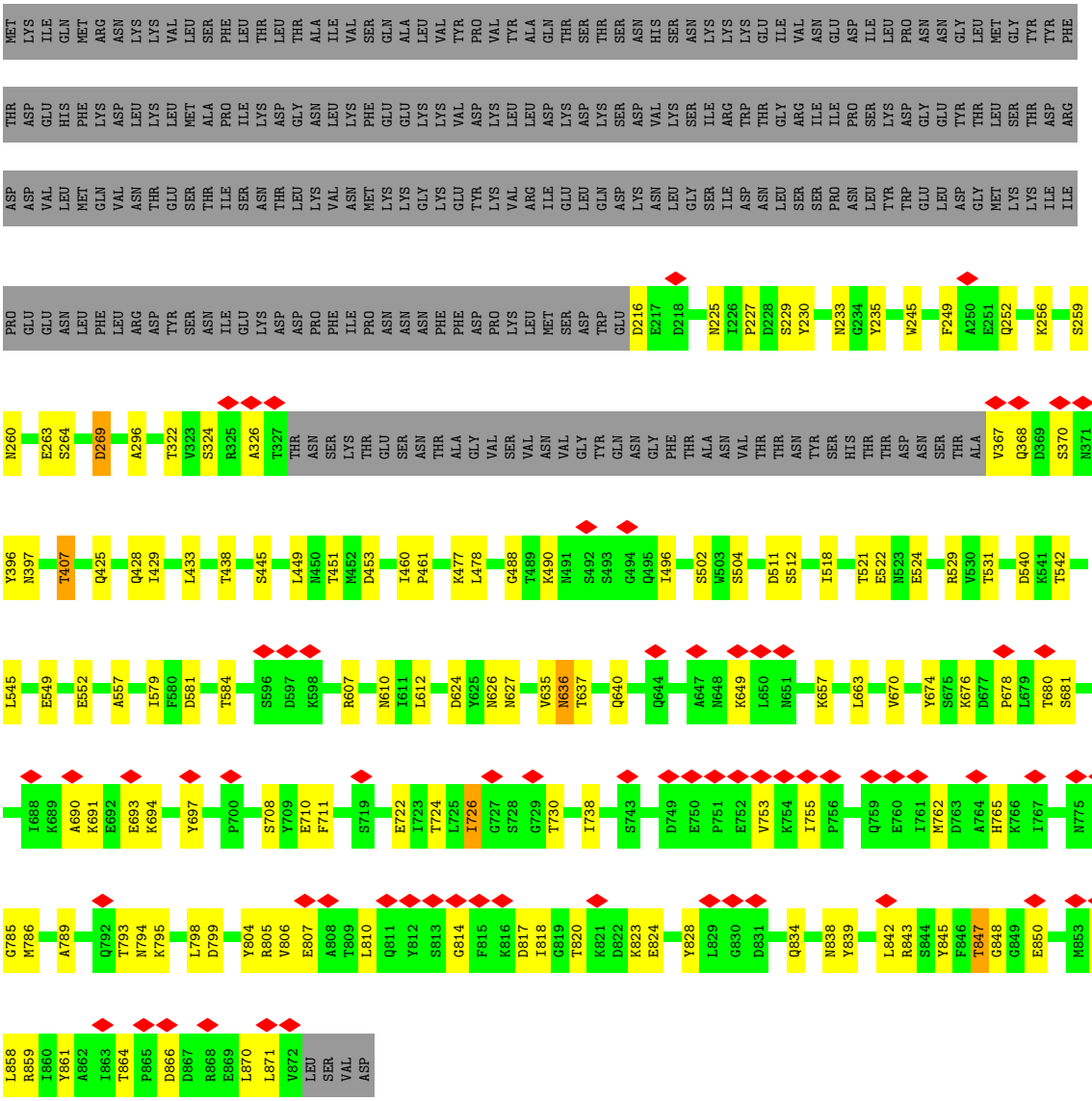
Chain W:





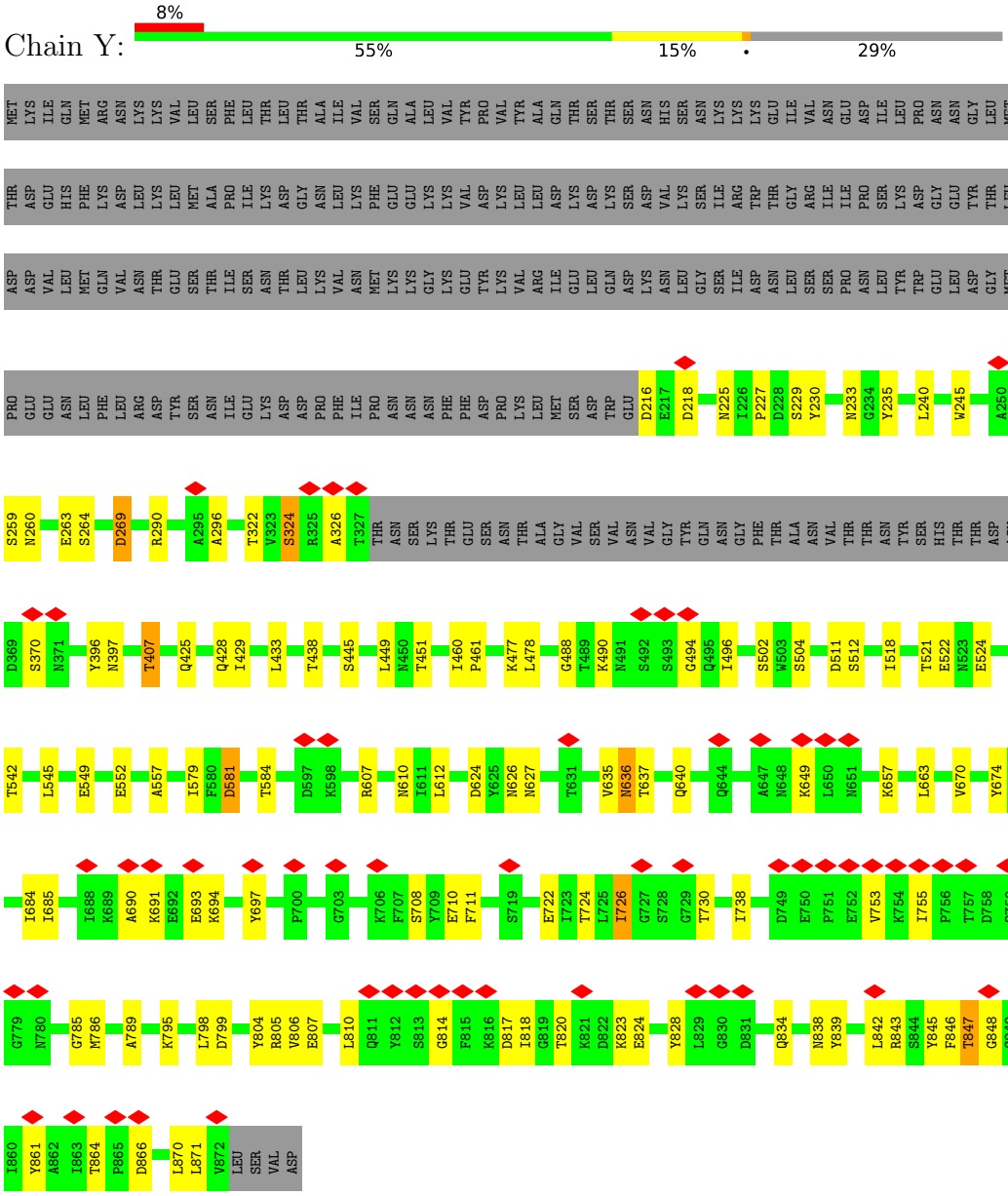
• Molecule 1: ADP-ribosyltransferase binding component

Chain X:



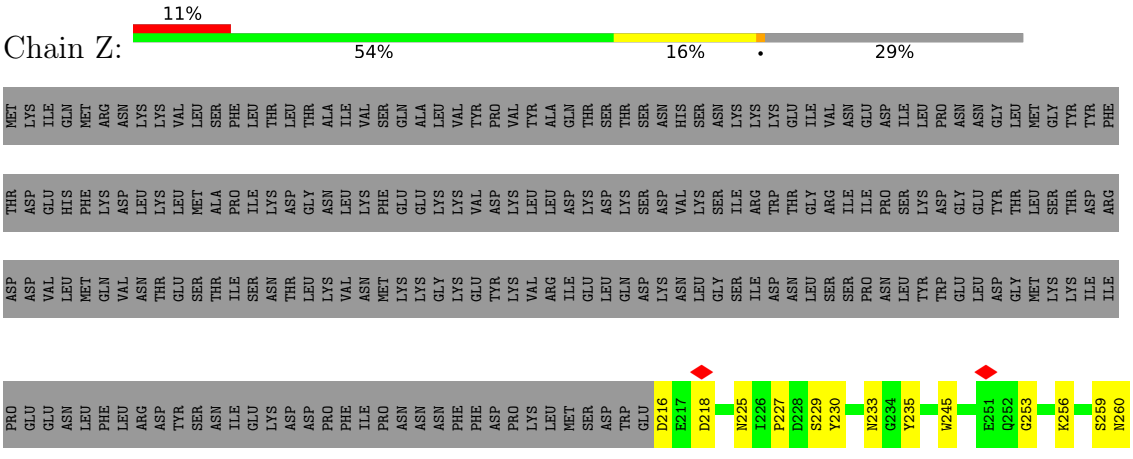
• Molecule 1: ADP-ribosyltransferase binding component

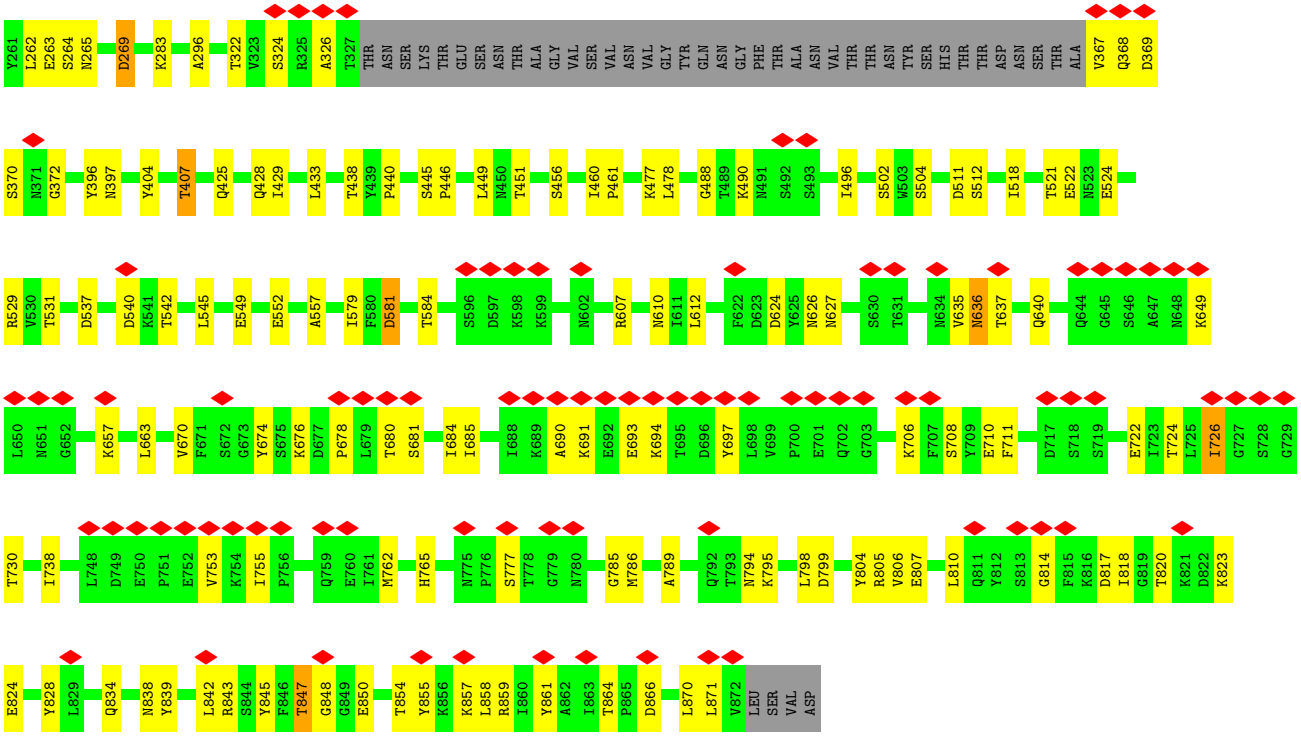
Chain Y:



- Molecule 1: ADP-ribosyltransferase binding component

Chain Z:




Y261 L262 E263 S264 N265 D269 K283 A296 T322 V323 S324 R325 A326 T327 THR ASN SER LYS THR GLU SER ASN THR ALA GLY VAL SER VAL ASN VAL GLY TYR GLN ASN GLY PHE THR ALA ASN VAL THR THR ASN TYR SER HIS THR THR ASP ASN SER THR ALA V367 Q368 D369
S370 N371 G372 Y396 N397 Y404 T407 Q425 Q428 I429 L433 T438 Y439 P440 S445 P446 L449 N450 T451 S456 I460 P461 K477 L478 G488 T489 K490 N491 S492 S493 I496 S502 W503 S504 D511 S512 I518 T521 E522 N523 E524
R529 W530 T531 D537 D540 K541 T542 L545 E549 E552 A557 I579 F580 D581 T584 S596 D597 K598 K599 M602 R607 N610 I611 L612 F622 D623 D624 Y625 N626 N627 S630 T631 N634 V635 N636 T637 Q640 Q644 G645 S646 A647 N648 K649
L650 N651 G652 K657 L663 V670 F671 S672 G673 Y674 S675 K676 D677 P678 L679 T680 S681 I684 I685 I688 K689 A690 K691 E692 E693 K694 T695 D696 Y697 L698 V699 P700 E701 Q702 G703 K706 F707 S708 Y709 E710 F711 D717 S718 S719 E722 I723 T724 L725 I726 G727 S728 G729
T730 I738 L748 D749 E750 P751 E752 V753 K754 I755 P756 Q759 E760 I761 M762 H765 N775 P776 S777 T778 G779 N780 G785 M786 A789 Q792 T793 N794 K795 L798 D799 Y804 R805 V806 E807 L810 Q811 Y812 S813 G814 F815 K816 D817 I818 G819 T820 K821 D822 K823
E824 Y828 L829 Q834 N838 Y839 L842 R843 S844 Y845 F846 T847 G848 G849 E850 T854 Y855 K856 K857 L858 R859 I860 Y861 A862 I863 T864 P865 D866 L870 L871 V872 LEU SER VAL ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	13266	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	110.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	20.781	Depositor
Minimum map value	-10.302	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.890	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	362.5, 362.5, 362.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	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	0.29	0/4980	0.54	0/6753
1	B	0.29	0/4980	0.54	0/6753
1	C	0.29	0/4980	0.54	0/6753
1	D	0.29	0/4980	0.54	0/6753
1	E	0.29	0/4980	0.54	0/6753
1	F	0.29	0/4980	0.54	0/6753
1	G	0.29	0/4980	0.54	0/6753
1	T	0.29	0/4980	0.54	0/6753
1	U	0.29	0/4980	0.54	0/6753
1	V	0.29	0/4980	0.54	0/6753
1	W	0.29	0/4980	0.54	0/6753
1	X	0.29	0/4980	0.54	0/6753
1	Y	0.29	0/4980	0.54	0/6753
1	Z	0.29	0/4980	0.54	0/6753
All	All	0.29	0/69720	0.54	0/94542

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	T	0	1
1	U	0	1
1	V	0	1
1	W	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1
1	Y	0	1
1	Z	0	1
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	864	THR	Peptide
1	B	864	THR	Peptide
1	C	864	THR	Peptide
1	D	864	THR	Peptide
1	E	864	THR	Peptide
1	F	864	THR	Peptide
1	G	864	THR	Peptide
1	T	864	THR	Peptide
1	U	864	THR	Peptide
1	V	864	THR	Peptide
1	W	864	THR	Peptide
1	X	864	THR	Peptide
1	Y	864	THR	Peptide
1	Z	864	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4889	0	4756	78	0
1	B	4889	0	4756	81	0
1	C	4889	0	4756	77	0
1	D	4889	0	4756	74	0
1	E	4889	0	4756	73	0
1	F	4889	0	4756	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4889	0	4756	73	0
1	T	4889	0	4756	88	0
1	U	4889	0	4756	78	0
1	V	4889	0	4756	86	0
1	W	4889	0	4756	86	0
1	X	4889	0	4756	75	0
1	Y	4889	0	4756	78	0
1	Z	4889	0	4756	85	0
All	All	68446	0	66584	1068	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1068) 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:411:ASN:HD21	1:B:447:LEU:HA	1.50	0.74
1:A:262:LEU:HD22	1:B:240:LEU:HD13	1.70	0.74
1:T:411:ASN:ND2	1:Z:446:PRO:O	2.20	0.74
1:V:494:GLY:O	1:W:265:ASN:ND2	2.28	0.67
1:Y:290:ARG:NH2	1:Z:537:ASP:OD2	2.28	0.66
1:V:290:ARG:NH2	1:W:537:ASP:OD2	2.30	0.65
1:D:397:ASN:HB2	1:D:433:LEU:HG	1.80	0.63
1:G:397:ASN:HB2	1:G:433:LEU:HG	1.80	0.63
1:A:397:ASN:HB2	1:A:433:LEU:HG	1.80	0.63
1:E:397:ASN:HB2	1:E:433:LEU:HG	1.80	0.63
1:Y:397:ASN:HB2	1:Y:433:LEU:HG	1.80	0.63
1:U:397:ASN:HB2	1:U:433:LEU:HG	1.80	0.62
1:Z:397:ASN:HB2	1:Z:433:LEU:HG	1.80	0.62
1:V:397:ASN:HB2	1:V:433:LEU:HG	1.80	0.62
1:B:397:ASN:HB2	1:B:433:LEU:HG	1.80	0.62
1:X:397:ASN:HB2	1:X:433:LEU:HG	1.80	0.62
1:C:397:ASN:HB2	1:C:433:LEU:HG	1.80	0.62
1:F:397:ASN:HB2	1:F:433:LEU:HG	1.80	0.62
1:T:397:ASN:HB2	1:T:433:LEU:HG	1.80	0.61
1:E:579:ILE:HB	1:E:612:LEU:HB3	1.83	0.61
1:V:579:ILE:HB	1:V:612:LEU:HB3	1.83	0.61
1:B:579:ILE:HB	1:B:612:LEU:HB3	1.83	0.61
1:C:579:ILE:HB	1:C:612:LEU:HB3	1.83	0.61
1:W:397:ASN:HB2	1:W:433:LEU:HG	1.80	0.61
1:W:579:ILE:HB	1:W:612:LEU:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:579:ILE:HB	1:U:612:LEU:HB3	1.83	0.61
1:D:579:ILE:HB	1:D:612:LEU:HB3	1.83	0.61
1:F:579:ILE:HB	1:F:612:LEU:HB3	1.83	0.61
1:T:579:ILE:HB	1:T:612:LEU:HB3	1.83	0.60
1:X:579:ILE:HB	1:X:612:LEU:HB3	1.83	0.60
1:A:579:ILE:HB	1:A:612:LEU:HB3	1.83	0.60
1:G:579:ILE:HB	1:G:612:LEU:HB3	1.83	0.60
1:D:804:TYR:OH	1:D:838:ASN:ND2	2.35	0.60
1:W:804:TYR:OH	1:W:838:ASN:ND2	2.35	0.60
1:Y:579:ILE:HB	1:Y:612:LEU:HB3	1.83	0.60
1:Z:579:ILE:HB	1:Z:612:LEU:HB3	1.83	0.60
1:C:804:TYR:OH	1:C:838:ASN:ND2	2.35	0.59
1:X:804:TYR:OH	1:X:838:ASN:ND2	2.35	0.59
1:U:804:TYR:OH	1:U:838:ASN:ND2	2.35	0.59
1:V:804:TYR:OH	1:V:838:ASN:ND2	2.35	0.59
1:B:804:TYR:OH	1:B:838:ASN:ND2	2.35	0.59
1:E:804:TYR:OH	1:E:838:ASN:ND2	2.35	0.59
1:Z:804:TYR:OH	1:Z:838:ASN:ND2	2.35	0.59
1:F:804:TYR:OH	1:F:838:ASN:ND2	2.35	0.58
1:Y:804:TYR:OH	1:Y:838:ASN:ND2	2.35	0.58
1:F:512:SER:O	1:F:607:ARG:NH2	2.37	0.58
1:G:512:SER:O	1:G:607:ARG:NH2	2.36	0.58
1:G:804:TYR:OH	1:G:838:ASN:ND2	2.35	0.58
1:Y:512:SER:O	1:Y:607:ARG:NH2	2.37	0.58
1:A:804:TYR:OH	1:A:838:ASN:ND2	2.35	0.58
1:T:512:SER:O	1:T:607:ARG:NH2	2.36	0.58
1:X:512:SER:O	1:X:607:ARG:NH2	2.37	0.58
1:B:512:SER:O	1:B:607:ARG:NH2	2.36	0.58
1:T:804:TYR:OH	1:T:838:ASN:ND2	2.35	0.58
1:A:512:SER:O	1:A:607:ARG:NH2	2.37	0.57
1:Z:512:SER:O	1:Z:607:ARG:NH2	2.37	0.57
1:E:259:SER:OG	1:E:260:ASN:N	2.38	0.57
1:U:259:SER:OG	1:U:260:ASN:N	2.38	0.57
1:Y:259:SER:OG	1:Y:260:ASN:N	2.38	0.57
1:B:259:SER:OG	1:B:260:ASN:N	2.38	0.57
1:D:512:SER:O	1:D:607:ARG:NH2	2.37	0.57
1:V:512:SER:O	1:V:607:ARG:NH2	2.36	0.57
1:F:259:SER:OG	1:F:260:ASN:N	2.38	0.57
1:V:259:SER:OG	1:V:260:ASN:N	2.38	0.57
1:X:259:SER:OG	1:X:260:ASN:N	2.38	0.57
1:T:229:SER:HB3	1:T:235:TYR:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:512:SER:O	1:U:607:ARG:NH2	2.36	0.57
1:E:512:SER:O	1:E:607:ARG:NH2	2.37	0.57
1:F:229:SER:HB3	1:F:235:TYR:HB3	1.87	0.57
1:G:229:SER:HB3	1:G:235:TYR:HB3	1.87	0.57
1:Z:229:SER:HB3	1:Z:235:TYR:HB3	1.87	0.57
1:A:670:VAL:HG22	1:A:710:GLU:HG2	1.88	0.56
1:W:259:SER:OG	1:W:260:ASN:N	2.38	0.56
1:Y:229:SER:HB3	1:Y:235:TYR:HB3	1.87	0.56
1:C:259:SER:OG	1:C:260:ASN:N	2.38	0.56
1:E:229:SER:HB3	1:E:235:TYR:HB3	1.87	0.56
1:E:670:VAL:HG22	1:E:710:GLU:HG2	1.88	0.56
1:F:670:VAL:HG22	1:F:710:GLU:HG2	1.87	0.56
1:U:229:SER:HB3	1:U:235:TYR:HB3	1.87	0.56
1:B:670:VAL:HG22	1:B:710:GLU:HG2	1.88	0.56
1:G:670:VAL:HG22	1:G:710:GLU:HG2	1.88	0.56
1:T:259:SER:OG	1:T:260:ASN:N	2.38	0.56
1:W:670:VAL:HG22	1:W:710:GLU:HG2	1.88	0.56
1:G:259:SER:OG	1:G:260:ASN:N	2.38	0.56
1:T:670:VAL:HG22	1:T:710:GLU:HG2	1.88	0.56
1:V:670:VAL:HG22	1:V:710:GLU:HG2	1.88	0.56
1:W:512:SER:O	1:W:607:ARG:NH2	2.36	0.56
1:Y:670:VAL:HG22	1:Y:710:GLU:HG2	1.88	0.56
1:Z:259:SER:OG	1:Z:260:ASN:N	2.38	0.56
1:A:229:SER:HB3	1:A:235:TYR:HB3	1.87	0.56
1:T:798:LEU:O	1:T:823:LYS:NZ	2.39	0.56
1:D:670:VAL:HG22	1:D:710:GLU:HG2	1.88	0.56
1:U:670:VAL:HG22	1:U:710:GLU:HG2	1.88	0.56
1:C:670:VAL:HG22	1:C:710:GLU:HG2	1.88	0.56
1:V:229:SER:HB3	1:V:235:TYR:HB3	1.87	0.56
1:Z:798:LEU:O	1:Z:823:LYS:NZ	2.39	0.56
1:D:229:SER:HB3	1:D:235:TYR:HB3	1.87	0.56
1:X:229:SER:HB3	1:X:235:TYR:HB3	1.87	0.56
1:X:670:VAL:HG22	1:X:710:GLU:HG2	1.88	0.56
1:C:512:SER:O	1:C:607:ARG:NH2	2.36	0.56
1:U:798:LEU:O	1:U:823:LYS:NZ	2.39	0.56
1:W:229:SER:HB3	1:W:235:TYR:HB3	1.87	0.56
1:Z:670:VAL:HG22	1:Z:710:GLU:HG2	1.88	0.56
1:A:259:SER:OG	1:A:260:ASN:N	2.38	0.55
1:G:798:LEU:O	1:G:823:LYS:NZ	2.39	0.55
1:C:229:SER:HB3	1:C:235:TYR:HB3	1.87	0.55
1:E:805:ARG:NH1	1:E:817:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:805:ARG:NH1	1:V:817:ASP:OD1	2.39	0.55
1:A:805:ARG:NH1	1:A:817:ASP:OD1	2.39	0.55
1:D:805:ARG:NH1	1:D:817:ASP:OD1	2.39	0.55
1:F:798:LEU:O	1:F:823:LYS:NZ	2.39	0.55
1:B:229:SER:HB3	1:B:235:TYR:HB3	1.87	0.55
1:B:407:THR:HG23	1:B:429:ILE:HG13	1.89	0.55
1:C:798:LEU:O	1:C:823:LYS:NZ	2.39	0.55
1:T:538:PRO:HG3	1:Z:253:GLY:HA3	1.88	0.55
1:V:407:THR:HG23	1:V:429:ILE:HG13	1.89	0.55
1:W:407:THR:HG23	1:W:429:ILE:HG13	1.89	0.55
1:W:805:ARG:NH1	1:W:817:ASP:OD1	2.39	0.55
1:Y:798:LEU:O	1:Y:823:LYS:NZ	2.39	0.55
1:Z:805:ARG:NH1	1:Z:817:ASP:OD1	2.39	0.55
1:D:407:THR:HG23	1:D:429:ILE:HG13	1.89	0.55
1:D:798:LEU:O	1:D:823:LYS:NZ	2.39	0.55
1:U:407:THR:HG23	1:U:429:ILE:HG13	1.89	0.55
1:V:798:LEU:O	1:V:823:LYS:NZ	2.39	0.55
1:X:805:ARG:NH1	1:X:817:ASP:OD1	2.39	0.55
1:C:407:THR:HG23	1:C:429:ILE:HG13	1.89	0.55
1:A:798:LEU:O	1:A:823:LYS:NZ	2.39	0.55
1:B:798:LEU:O	1:B:823:LYS:NZ	2.39	0.55
1:D:259:SER:OG	1:D:260:ASN:N	2.38	0.55
1:E:798:LEU:O	1:E:823:LYS:NZ	2.39	0.55
1:V:448:ALA:HB2	1:W:418:THR:HB	1.89	0.55
1:W:690:ALA:HB1	1:W:711:PHE:HB2	1.89	0.55
1:X:407:THR:HG23	1:X:429:ILE:HG13	1.89	0.55
1:Y:805:ARG:NH1	1:Y:817:ASP:OD1	2.39	0.55
1:U:805:ARG:NH1	1:U:817:ASP:OD1	2.39	0.55
1:X:690:ALA:HB1	1:X:711:PHE:HB2	1.89	0.55
1:B:805:ARG:NH1	1:B:817:ASP:OD1	2.39	0.54
1:G:690:ALA:HB1	1:G:711:PHE:HB2	1.89	0.54
1:T:690:ALA:HB1	1:T:711:PHE:HB2	1.89	0.54
1:E:407:THR:HG23	1:E:429:ILE:HG13	1.89	0.54
1:G:805:ARG:NH1	1:G:817:ASP:OD1	2.39	0.54
1:A:407:THR:HG23	1:A:429:ILE:HG13	1.89	0.54
1:E:674:TYR:O	1:E:697:TYR:OH	2.26	0.54
1:W:674:TYR:O	1:W:697:TYR:OH	2.26	0.54
1:C:674:TYR:O	1:C:697:TYR:OH	2.26	0.54
1:D:674:TYR:O	1:D:697:TYR:OH	2.26	0.54
1:V:674:TYR:O	1:V:697:TYR:OH	2.26	0.54
1:A:690:ALA:HB1	1:A:711:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:218:ASP:OD1	1:T:218:ASP:N	2.40	0.54
1:T:805:ARG:NH1	1:T:817:ASP:OD1	2.39	0.54
1:U:674:TYR:O	1:U:697:TYR:OH	2.26	0.54
1:U:690:ALA:HB1	1:U:711:PHE:HB2	1.89	0.54
1:X:674:TYR:O	1:X:697:TYR:OH	2.26	0.54
1:Y:425:GLN:NE2	1:Y:451:THR:OG1	2.41	0.54
1:B:674:TYR:O	1:B:697:TYR:OH	2.26	0.54
1:D:425:GLN:NE2	1:D:451:THR:OG1	2.41	0.54
1:F:690:ALA:HB1	1:F:711:PHE:HB2	1.89	0.54
1:U:218:ASP:OD1	1:U:218:ASP:N	2.39	0.54
1:V:690:ALA:HB1	1:V:711:PHE:HB2	1.89	0.54
1:W:798:LEU:O	1:W:823:LYS:NZ	2.39	0.54
1:C:690:ALA:HB1	1:C:711:PHE:HB2	1.89	0.54
1:E:425:GLN:NE2	1:E:451:THR:OG1	2.41	0.54
1:F:425:GLN:NE2	1:F:451:THR:OG1	2.41	0.54
1:F:805:ARG:NH1	1:F:817:ASP:OD1	2.39	0.54
1:T:674:TYR:O	1:T:697:TYR:OH	2.26	0.54
1:Z:690:ALA:HB1	1:Z:711:PHE:HB2	1.89	0.54
1:A:674:TYR:O	1:A:697:TYR:OH	2.26	0.54
1:C:425:GLN:NE2	1:C:451:THR:OG1	2.41	0.54
1:F:674:TYR:O	1:F:697:TYR:OH	2.26	0.54
1:X:798:LEU:O	1:X:823:LYS:NZ	2.39	0.54
1:Y:407:THR:HG23	1:Y:429:ILE:HG13	1.89	0.54
1:U:425:GLN:NE2	1:U:451:THR:OG1	2.41	0.53
1:W:477:LYS:NZ	1:W:478:LEU:O	2.42	0.53
1:Y:674:TYR:O	1:Y:697:TYR:OH	2.26	0.53
1:Y:690:ALA:HB1	1:Y:711:PHE:HB2	1.89	0.53
1:Z:407:THR:HG23	1:Z:429:ILE:HG13	1.89	0.53
1:Z:425:GLN:NE2	1:Z:451:THR:OG1	2.41	0.53
1:A:425:GLN:NE2	1:A:451:THR:OG1	2.41	0.53
1:C:818:ILE:HG22	1:C:845:TYR:HB3	1.91	0.53
1:D:818:ILE:HG22	1:D:845:TYR:HB3	1.91	0.53
1:G:477:LYS:NZ	1:G:478:LEU:O	2.42	0.53
1:T:494:GLY:O	1:U:265:ASN:ND2	2.38	0.53
1:V:818:ILE:HG22	1:V:845:TYR:HB3	1.91	0.53
1:X:477:LYS:NZ	1:X:478:LEU:O	2.42	0.53
1:G:407:THR:HG23	1:G:429:ILE:HG13	1.89	0.53
1:G:674:TYR:O	1:G:697:TYR:OH	2.26	0.53
1:T:407:THR:HG23	1:T:429:ILE:HG13	1.89	0.53
1:U:818:ILE:HG22	1:U:845:TYR:HB3	1.91	0.53
1:X:425:GLN:NE2	1:X:451:THR:OG1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:477:LYS:NZ	1:Z:478:LEU:O	2.42	0.53
1:A:477:LYS:NZ	1:A:478:LEU:O	2.42	0.53
1:B:690:ALA:HB1	1:B:711:PHE:HB2	1.89	0.53
1:C:805:ARG:NH1	1:C:817:ASP:OD1	2.39	0.53
1:Y:324:SER:HA	1:Z:372:GLY:HA2	1.89	0.53
1:B:425:GLN:NE2	1:B:451:THR:OG1	2.41	0.53
1:E:690:ALA:HB1	1:E:711:PHE:HB2	1.89	0.53
1:F:407:THR:HG23	1:F:429:ILE:HG13	1.89	0.53
1:W:425:GLN:NE2	1:W:451:THR:OG1	2.41	0.53
1:Z:674:TYR:O	1:Z:697:TYR:OH	2.26	0.53
1:C:477:LYS:NZ	1:C:478:LEU:O	2.42	0.53
1:D:690:ALA:HB1	1:D:711:PHE:HB2	1.89	0.53
1:B:477:LYS:NZ	1:B:478:LEU:O	2.42	0.53
1:D:477:LYS:NZ	1:D:478:LEU:O	2.42	0.53
1:E:818:ILE:HG22	1:E:845:TYR:HB3	1.90	0.53
1:G:425:GLN:NE2	1:G:451:THR:OG1	2.41	0.53
1:T:477:LYS:NZ	1:T:478:LEU:O	2.42	0.53
1:B:818:ILE:HG22	1:B:845:TYR:HB3	1.90	0.53
1:W:818:ILE:HG22	1:W:845:TYR:HB3	1.91	0.53
1:B:428:GLN:HE21	1:B:449:LEU:HA	1.74	0.53
1:E:477:LYS:NZ	1:E:478:LEU:O	2.42	0.53
1:T:425:GLN:NE2	1:T:451:THR:OG1	2.41	0.53
1:V:425:GLN:NE2	1:V:451:THR:OG1	2.41	0.53
1:Y:511:ASP:OD1	1:Y:529:ARG:NH1	2.42	0.53
1:F:428:GLN:HE21	1:F:449:LEU:HA	1.74	0.52
1:B:511:ASP:OD1	1:B:529:ARG:NH1	2.42	0.52
1:E:428:GLN:HE21	1:E:449:LEU:HA	1.74	0.52
1:F:818:ILE:HG22	1:F:845:TYR:HB3	1.90	0.52
1:X:428:GLN:HE21	1:X:449:LEU:HA	1.74	0.52
1:Y:477:LYS:NZ	1:Y:478:LEU:O	2.42	0.52
1:A:511:ASP:OD1	1:A:529:ARG:NH1	2.42	0.52
1:F:477:LYS:NZ	1:F:478:LEU:O	2.42	0.52
1:T:511:ASP:OD1	1:T:529:ARG:NH1	2.42	0.52
1:U:428:GLN:HE21	1:U:449:LEU:HA	1.74	0.52
1:V:511:ASP:OD1	1:V:529:ARG:NH1	2.42	0.52
1:Z:428:GLN:HE21	1:Z:449:LEU:HA	1.74	0.52
1:T:818:ILE:HG22	1:T:845:TYR:HB3	1.90	0.52
1:U:477:LYS:NZ	1:U:478:LEU:O	2.42	0.52
1:W:511:ASP:OD1	1:W:529:ARG:NH1	2.42	0.52
1:X:511:ASP:OD1	1:X:529:ARG:NH1	2.42	0.52
1:Y:326:ALA:HB1	1:Z:369:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:OD1	1:A:218:ASP:N	2.39	0.52
1:G:818:ILE:HG22	1:G:845:TYR:HB3	1.90	0.52
1:T:428:GLN:HE21	1:T:449:LEU:HA	1.74	0.52
1:X:818:ILE:HG22	1:X:845:TYR:HB3	1.91	0.52
1:D:428:GLN:HE21	1:D:449:LEU:HA	1.74	0.52
1:E:511:ASP:OD1	1:E:529:ARG:NH1	2.42	0.52
1:Z:818:ILE:HG22	1:Z:845:TYR:HB3	1.90	0.52
1:A:818:ILE:HG22	1:A:845:TYR:HB3	1.90	0.52
1:U:511:ASP:OD1	1:U:529:ARG:NH1	2.42	0.52
1:F:511:ASP:OD1	1:F:529:ARG:NH1	2.42	0.52
1:V:477:LYS:NZ	1:V:478:LEU:O	2.42	0.52
1:W:428:GLN:HE21	1:W:449:LEU:HA	1.74	0.52
1:Y:818:ILE:HG22	1:Y:845:TYR:HB3	1.91	0.52
1:A:428:GLN:HE21	1:A:449:LEU:HA	1.74	0.52
1:A:859:ARG:NH2	1:A:861:TYR:OH	2.43	0.52
1:G:218:ASP:OD1	1:G:218:ASP:N	2.39	0.52
1:G:859:ARG:NH2	1:G:861:TYR:OH	2.43	0.52
1:Z:511:ASP:OD1	1:Z:529:ARG:NH1	2.42	0.52
1:G:428:GLN:HE21	1:G:449:LEU:HA	1.74	0.52
1:T:496:ILE:O	1:U:506:TYR:OH	2.20	0.52
1:V:428:GLN:HE21	1:V:449:LEU:HA	1.74	0.52
1:X:859:ARG:NH2	1:X:861:TYR:OH	2.43	0.52
1:Y:859:ARG:NH2	1:Y:861:TYR:OH	2.43	0.52
1:C:428:GLN:HE21	1:C:449:LEU:HA	1.74	0.51
1:E:859:ARG:NH2	1:E:861:TYR:OH	2.43	0.51
1:D:511:ASP:OD1	1:D:529:ARG:NH1	2.42	0.51
1:D:859:ARG:NH2	1:D:861:TYR:OH	2.43	0.51
1:G:511:ASP:OD1	1:G:529:ARG:NH1	2.42	0.51
1:Z:859:ARG:NH2	1:Z:861:TYR:OH	2.43	0.51
1:C:843:ARG:NH2	1:C:850:GLU:OE2	2.42	0.51
1:V:843:ARG:NH2	1:V:850:GLU:OE2	2.42	0.51
1:C:511:ASP:OD1	1:C:529:ARG:NH1	2.42	0.51
1:F:521:THR:HG23	1:F:524:GLU:H	1.76	0.51
1:V:859:ARG:NH2	1:V:861:TYR:OH	2.43	0.51
1:X:521:THR:HG23	1:X:524:GLU:H	1.76	0.51
1:Y:521:THR:HG23	1:Y:524:GLU:H	1.76	0.51
1:W:859:ARG:NH2	1:W:861:TYR:OH	2.43	0.51
1:Y:428:GLN:HE21	1:Y:449:LEU:HA	1.74	0.51
1:F:859:ARG:NH2	1:F:861:TYR:OH	2.43	0.51
1:G:521:THR:HG23	1:G:524:GLU:H	1.76	0.51
1:B:762:MET:O	1:B:765:HIS:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:MET:O	1:C:765:HIS:NE2	2.44	0.51
1:V:762:MET:O	1:V:765:HIS:NE2	2.44	0.51
1:B:859:ARG:NH2	1:B:861:TYR:OH	2.43	0.51
1:T:545:LEU:HD13	1:T:549:GLU:HB3	1.94	0.51
1:Z:521:THR:HG23	1:Z:524:GLU:H	1.76	0.51
1:C:521:THR:HG23	1:C:524:GLU:H	1.76	0.50
1:E:521:THR:HG23	1:E:524:GLU:H	1.76	0.50
1:T:859:ARG:NH2	1:T:861:TYR:OH	2.43	0.50
1:U:859:ARG:NH2	1:U:861:TYR:OH	2.43	0.50
1:V:545:LEU:HD13	1:V:549:GLU:HB3	1.94	0.50
1:W:762:MET:O	1:W:765:HIS:NE2	2.44	0.50
1:W:795:LYS:HZ3	1:W:798:LEU:HD11	1.75	0.50
1:Y:490:LYS:HB3	1:Y:496:ILE:HG22	1.93	0.50
1:Z:762:MET:O	1:Z:765:HIS:NE2	2.44	0.50
1:A:691:LYS:HE2	1:A:693:GLU:HB3	1.93	0.50
1:C:859:ARG:NH2	1:C:861:TYR:OH	2.43	0.50
1:E:545:LEU:HD13	1:E:549:GLU:HB3	1.94	0.50
1:F:545:LEU:HD13	1:F:549:GLU:HB3	1.94	0.50
1:U:521:THR:HG23	1:U:524:GLU:H	1.76	0.50
1:X:762:MET:O	1:X:765:HIS:NE2	2.44	0.50
1:Z:490:LYS:HB3	1:Z:496:ILE:HG22	1.94	0.50
1:Z:545:LEU:HD13	1:Z:549:GLU:HB3	1.93	0.50
1:A:762:MET:O	1:A:765:HIS:NE2	2.44	0.50
1:B:521:THR:HG23	1:B:524:GLU:H	1.76	0.50
1:D:762:MET:O	1:D:765:HIS:NE2	2.44	0.50
1:F:762:MET:O	1:F:765:HIS:NE2	2.44	0.50
1:C:545:LEU:HD13	1:C:549:GLU:HB3	1.94	0.50
1:D:545:LEU:HD13	1:D:549:GLU:HB3	1.94	0.50
1:T:490:LYS:HB3	1:T:496:ILE:HG22	1.94	0.50
1:Y:691:LYS:HE2	1:Y:693:GLU:HB3	1.94	0.50
1:Y:762:MET:O	1:Y:765:HIS:NE2	2.44	0.50
1:D:521:THR:HG23	1:D:524:GLU:H	1.76	0.50
1:G:691:LYS:HE2	1:G:693:GLU:HB3	1.94	0.50
1:G:762:MET:O	1:G:765:HIS:NE2	2.44	0.50
1:T:521:THR:HG23	1:T:524:GLU:H	1.76	0.50
1:U:762:MET:O	1:U:765:HIS:NE2	2.44	0.50
1:X:490:LYS:HB3	1:X:496:ILE:HG22	1.94	0.50
1:Y:545:LEU:HD13	1:Y:549:GLU:HB3	1.94	0.50
1:B:545:LEU:HD13	1:B:549:GLU:HB3	1.94	0.50
1:E:762:MET:O	1:E:765:HIS:NE2	2.44	0.50
1:U:545:LEU:HD13	1:U:549:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:521:THR:HG23	1:V:524:GLU:H	1.76	0.50
1:W:545:LEU:HD13	1:W:549:GLU:HB3	1.94	0.50
1:W:799:ASP:OD1	1:W:799:ASP:N	2.45	0.50
1:X:545:LEU:HD13	1:X:549:GLU:HB3	1.94	0.50
1:B:691:LYS:HE2	1:B:693:GLU:HB3	1.94	0.50
1:G:545:LEU:HD13	1:G:549:GLU:HB3	1.93	0.50
1:T:762:MET:O	1:T:765:HIS:NE2	2.44	0.50
1:V:448:ALA:HB2	1:W:418:THR:CB	2.42	0.50
1:Z:691:LYS:HE2	1:Z:693:GLU:HB3	1.93	0.50
1:W:490:LYS:HB3	1:W:496:ILE:HG22	1.93	0.50
1:X:691:LYS:HE2	1:X:693:GLU:HB3	1.94	0.50
1:X:799:ASP:OD1	1:X:799:ASP:N	2.45	0.50
1:Y:799:ASP:OD1	1:Y:799:ASP:N	2.45	0.50
1:Z:799:ASP:OD1	1:Z:799:ASP:N	2.45	0.50
1:A:521:THR:HG23	1:A:524:GLU:H	1.76	0.49
1:C:824:GLU:HB2	1:C:839:TYR:HD2	1.77	0.49
1:D:824:GLU:HB2	1:D:839:TYR:HD2	1.77	0.49
1:G:799:ASP:OD1	1:G:799:ASP:N	2.45	0.49
1:V:824:GLU:HB2	1:V:839:TYR:HD2	1.77	0.49
1:B:799:ASP:OD1	1:B:799:ASP:N	2.45	0.49
1:G:490:LYS:HB3	1:G:496:ILE:HG22	1.93	0.49
1:Y:824:GLU:HB2	1:Y:839:TYR:HD2	1.77	0.49
1:A:490:LYS:HB3	1:A:496:ILE:HG22	1.94	0.49
1:G:824:GLU:HB2	1:G:839:TYR:HD2	1.77	0.49
1:W:521:THR:HG23	1:W:524:GLU:H	1.76	0.49
1:W:691:LYS:HE2	1:W:693:GLU:HB3	1.94	0.49
1:E:490:LYS:HB3	1:E:496:ILE:HG22	1.93	0.49
1:F:490:LYS:HB3	1:F:496:ILE:HG22	1.93	0.49
1:F:691:LYS:HE2	1:F:693:GLU:HB3	1.94	0.49
1:U:824:GLU:HB2	1:U:839:TYR:HD2	1.78	0.49
1:W:552:GLU:HA	1:W:557:ALA:HB3	1.94	0.49
1:A:545:LEU:HD13	1:A:549:GLU:HB3	1.94	0.49
1:B:552:GLU:HA	1:B:557:ALA:HB3	1.95	0.49
1:E:824:GLU:HB2	1:E:839:TYR:HD2	1.78	0.49
1:C:552:GLU:HA	1:C:557:ALA:HB3	1.94	0.49
1:C:799:ASP:OD1	1:C:799:ASP:N	2.45	0.49
1:D:490:LYS:HB3	1:D:496:ILE:HG22	1.93	0.49
1:V:552:GLU:HA	1:V:557:ALA:HB3	1.95	0.49
1:W:805:ARG:HB2	1:W:820:THR:HG22	1.95	0.49
1:W:824:GLU:HB2	1:W:839:TYR:HD2	1.77	0.49
1:X:552:GLU:HA	1:X:557:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLU:HA	1:A:557:ALA:HB3	1.94	0.49
1:T:691:LYS:HE2	1:T:693:GLU:HB3	1.93	0.49
1:V:799:ASP:OD1	1:V:799:ASP:N	2.45	0.49
1:X:805:ARG:HB2	1:X:820:THR:HG22	1.95	0.49
1:A:824:GLU:HB2	1:A:839:TYR:HD2	1.77	0.49
1:B:824:GLU:HB2	1:B:839:TYR:HD2	1.78	0.49
1:E:396:TYR:HA	1:E:438:THR:HA	1.95	0.49
1:E:691:LYS:HE2	1:E:693:GLU:HB3	1.94	0.49
1:F:396:TYR:HA	1:F:438:THR:HA	1.95	0.49
1:T:396:TYR:HA	1:T:438:THR:HA	1.95	0.49
1:T:824:GLU:HB2	1:T:839:TYR:HD2	1.77	0.49
1:Y:805:ARG:HB2	1:Y:820:THR:HG22	1.95	0.49
1:Z:824:GLU:HB2	1:Z:839:TYR:HD2	1.77	0.49
1:C:490:LYS:HB3	1:C:496:ILE:HG22	1.94	0.49
1:C:691:LYS:HE2	1:C:693:GLU:HB3	1.94	0.49
1:V:691:LYS:HE2	1:V:693:GLU:HB3	1.94	0.49
1:W:456:SER:HB2	1:X:453:ASP:HA	1.95	0.49
1:Z:396:TYR:HA	1:Z:438:THR:HA	1.95	0.49
1:A:805:ARG:HB2	1:A:820:THR:HG22	1.95	0.48
1:B:805:ARG:HB2	1:B:820:THR:HG22	1.95	0.48
1:Y:857:LYS:HG3	1:Y:871:LEU:HD11	1.95	0.48
1:D:552:GLU:HA	1:D:557:ALA:HB3	1.94	0.48
1:D:636:ASN:O	1:D:640:GLN:NE2	2.46	0.48
1:D:857:LYS:HG3	1:D:871:LEU:HD11	1.96	0.48
1:G:396:TYR:HA	1:G:438:THR:HA	1.95	0.48
1:G:857:LYS:HG3	1:G:871:LEU:HD11	1.96	0.48
1:Z:857:LYS:HG3	1:Z:871:LEU:HD11	1.96	0.48
1:A:636:ASN:O	1:A:640:GLN:NE2	2.46	0.48
1:C:857:LYS:HG3	1:C:871:LEU:HD11	1.96	0.48
1:D:691:LYS:HE2	1:D:693:GLU:HB3	1.94	0.48
1:U:552:GLU:HA	1:U:557:ALA:HB3	1.95	0.48
1:U:691:LYS:HE2	1:U:693:GLU:HB3	1.94	0.48
1:V:857:LYS:HG3	1:V:871:LEU:HD11	1.96	0.48
1:X:843:ARG:NH2	1:X:850:GLU:OE2	2.42	0.48
1:Z:805:ARG:HB2	1:Z:820:THR:HG22	1.95	0.48
1:E:805:ARG:HB2	1:E:820:THR:HG22	1.95	0.48
1:V:805:ARG:HB2	1:V:820:THR:HG22	1.95	0.48
1:W:857:LYS:HG3	1:W:871:LEU:HD11	1.95	0.48
1:Y:552:GLU:HA	1:Y:557:ALA:HB3	1.94	0.48
1:A:857:LYS:HG3	1:A:871:LEU:HD11	1.95	0.48
1:B:396:TYR:HA	1:B:438:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:LYS:HB3	1:D:678:PRO:HD3	1.95	0.48
1:F:857:LYS:HG3	1:F:871:LEU:HD11	1.95	0.48
1:G:805:ARG:HB2	1:G:820:THR:HG22	1.95	0.48
1:Y:396:TYR:HA	1:Y:438:THR:HA	1.95	0.48
1:C:396:TYR:HA	1:C:438:THR:HA	1.95	0.48
1:C:636:ASN:O	1:C:640:GLN:NE2	2.46	0.48
1:C:676:LYS:HB3	1:C:678:PRO:HD3	1.95	0.48
1:C:866:ASP:OD2	1:C:866:ASP:N	2.47	0.48
1:D:866:ASP:OD2	1:D:866:ASP:N	2.47	0.48
1:E:636:ASN:O	1:E:640:GLN:NE2	2.46	0.48
1:T:857:LYS:HG3	1:T:871:LEU:HD11	1.96	0.48
1:U:490:LYS:HB3	1:U:496:ILE:HG22	1.93	0.48
1:W:396:TYR:HA	1:W:438:THR:HA	1.95	0.48
1:B:490:LYS:HB3	1:B:496:ILE:HG22	1.94	0.48
1:B:636:ASN:O	1:B:640:GLN:NE2	2.46	0.48
1:B:857:LYS:HG3	1:B:871:LEU:HD11	1.96	0.48
1:B:866:ASP:OD2	1:B:866:ASP:N	2.47	0.48
1:F:824:GLU:HB2	1:F:839:TYR:HD2	1.77	0.48
1:T:636:ASN:O	1:T:640:GLN:NE2	2.46	0.48
1:U:799:ASP:OD1	1:U:799:ASP:N	2.45	0.48
1:U:857:LYS:HG3	1:U:871:LEU:HD11	1.96	0.48
1:V:490:LYS:HB3	1:V:496:ILE:HG22	1.94	0.48
1:Y:636:ASN:O	1:Y:640:GLN:NE2	2.46	0.48
1:D:858:LEU:HD23	1:D:870:LEU:HB3	1.96	0.48
1:U:396:TYR:HA	1:U:438:THR:HA	1.95	0.48
1:U:636:ASN:O	1:U:640:GLN:NE2	2.46	0.48
1:U:866:ASP:OD2	1:U:866:ASP:N	2.47	0.48
1:V:676:LYS:HB3	1:V:678:PRO:HD3	1.95	0.48
1:W:684:ILE:HB	1:W:724:THR:HB	1.96	0.48
1:X:857:LYS:HG3	1:X:871:LEU:HD11	1.96	0.48
1:Z:636:ASN:O	1:Z:640:GLN:NE2	2.46	0.48
1:A:684:ILE:HB	1:A:724:THR:HB	1.96	0.48
1:C:805:ARG:HB2	1:C:820:THR:HG22	1.95	0.48
1:C:858:LEU:HD23	1:C:870:LEU:HB3	1.96	0.48
1:D:805:ARG:HB2	1:D:820:THR:HG22	1.95	0.48
1:E:857:LYS:HG3	1:E:871:LEU:HD11	1.96	0.48
1:F:636:ASN:O	1:F:640:GLN:NE2	2.46	0.48
1:U:676:LYS:HB3	1:U:678:PRO:HD3	1.95	0.48
1:V:636:ASN:O	1:V:640:GLN:NE2	2.46	0.48
1:X:824:GLU:HB2	1:X:839:TYR:HD2	1.77	0.48
1:T:496:ILE:HD11	1:U:505:ASP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:396:TYR:HA	1:V:438:THR:HA	1.95	0.48
1:W:636:ASN:O	1:W:640:GLN:NE2	2.46	0.48
1:X:396:TYR:HA	1:X:438:THR:HA	1.95	0.48
1:X:866:ASP:OD2	1:X:866:ASP:N	2.47	0.48
1:Y:240:LEU:HD13	1:Z:262:LEU:HD22	1.96	0.48
1:D:584:THR:HG21	1:D:610:ASN:H	1.79	0.47
1:D:799:ASP:OD1	1:D:799:ASP:N	2.45	0.47
1:E:866:ASP:OD2	1:E:866:ASP:N	2.47	0.47
1:F:805:ARG:HB2	1:F:820:THR:HG22	1.95	0.47
1:G:552:GLU:HA	1:G:557:ALA:HB3	1.94	0.47
1:T:805:ARG:HB2	1:T:820:THR:HG22	1.95	0.47
1:V:866:ASP:OD2	1:V:866:ASP:N	2.47	0.47
1:W:866:ASP:OD2	1:W:866:ASP:N	2.47	0.47
1:A:396:TYR:HA	1:A:438:THR:HA	1.95	0.47
1:B:684:ILE:HB	1:B:724:THR:HB	1.96	0.47
1:D:624:ASP:OD1	1:D:624:ASP:N	2.47	0.47
1:E:552:GLU:HA	1:E:557:ALA:HB3	1.94	0.47
1:E:858:LEU:HD23	1:E:870:LEU:HB3	1.96	0.47
1:T:447:LEU:HA	1:U:411:ASN:HD21	1.79	0.47
1:Y:494:GLY:O	1:Z:265:ASN:ND2	2.46	0.47
1:Y:584:THR:HG21	1:Y:610:ASN:H	1.79	0.47
1:Z:552:GLU:HA	1:Z:557:ALA:HB3	1.94	0.47
1:Z:676:LYS:HB3	1:Z:678:PRO:HD3	1.95	0.47
1:C:540:ASP:OD1	1:C:542:THR:OG1	2.32	0.47
1:U:805:ARG:HB2	1:U:820:THR:HG22	1.95	0.47
1:V:858:LEU:HD23	1:V:870:LEU:HB3	1.95	0.47
1:X:636:ASN:O	1:X:640:GLN:NE2	2.46	0.47
1:X:684:ILE:HB	1:X:724:THR:HB	1.96	0.47
1:D:396:TYR:HA	1:D:438:THR:HA	1.95	0.47
1:G:584:THR:HG21	1:G:610:ASN:H	1.79	0.47
1:T:866:ASP:OD2	1:T:866:ASP:N	2.47	0.47
1:W:540:ASP:OD1	1:W:542:THR:OG1	2.32	0.47
1:W:676:LYS:HB3	1:W:678:PRO:HD3	1.95	0.47
1:X:624:ASP:OD1	1:X:624:ASP:N	2.48	0.47
1:B:843:ARG:NH2	1:B:850:GLU:OE2	2.42	0.47
1:E:684:ILE:HB	1:E:724:THR:HB	1.96	0.47
1:U:584:THR:HG21	1:U:610:ASN:H	1.79	0.47
1:V:684:ILE:HB	1:V:724:THR:HB	1.96	0.47
1:W:457:SER:HB3	1:X:453:ASP:OD1	2.14	0.47
1:B:858:LEU:HD23	1:B:870:LEU:HB3	1.96	0.47
1:E:676:LYS:HB3	1:E:678:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:552:GLU:HA	1:F:557:ALA:HB3	1.94	0.47
1:F:858:LEU:HD23	1:F:870:LEU:HB3	1.96	0.47
1:F:866:ASP:OD2	1:F:866:ASP:N	2.47	0.47
1:G:636:ASN:O	1:G:640:GLN:NE2	2.46	0.47
1:T:584:THR:HG21	1:T:610:ASN:H	1.79	0.47
1:U:858:LEU:HD23	1:U:870:LEU:HB3	1.96	0.47
1:W:584:THR:HG21	1:W:610:ASN:H	1.79	0.47
1:A:584:THR:HG21	1:A:610:ASN:H	1.79	0.47
1:B:676:LYS:HB3	1:B:678:PRO:HD3	1.95	0.47
1:E:624:ASP:OD1	1:E:624:ASP:N	2.47	0.47
1:F:684:ILE:HB	1:F:724:THR:HB	1.96	0.47
1:G:540:ASP:OD1	1:G:542:THR:OG1	2.32	0.47
1:G:676:LYS:HB3	1:G:678:PRO:HD3	1.95	0.47
1:G:684:ILE:HB	1:G:724:THR:HB	1.96	0.47
1:T:552:GLU:HA	1:T:557:ALA:HB3	1.95	0.47
1:T:676:LYS:HB3	1:T:678:PRO:HD3	1.95	0.47
1:T:858:LEU:HD23	1:T:870:LEU:HB3	1.96	0.47
1:W:843:ARG:NH2	1:W:850:GLU:OE2	2.42	0.47
1:Z:540:ASP:OD1	1:Z:542:THR:OG1	2.32	0.47
1:B:584:THR:HG21	1:B:610:ASN:H	1.79	0.47
1:E:806:VAL:HG23	1:E:818:ILE:HB	1.97	0.47
1:G:806:VAL:HG23	1:G:818:ILE:HB	1.97	0.47
1:Z:584:THR:HG21	1:Z:610:ASN:H	1.79	0.47
1:Z:806:VAL:HG23	1:Z:818:ILE:HB	1.97	0.47
1:A:676:LYS:HB3	1:A:678:PRO:HD3	1.95	0.47
1:C:584:THR:HG21	1:C:610:ASN:H	1.79	0.47
1:F:676:LYS:HB3	1:F:678:PRO:HD3	1.95	0.47
1:T:684:ILE:HB	1:T:724:THR:HB	1.96	0.47
1:Y:540:ASP:OD1	1:Y:542:THR:OG1	2.32	0.47
1:Y:676:LYS:HB3	1:Y:678:PRO:HD3	1.95	0.47
1:Y:866:ASP:N	1:Y:866:ASP:OD2	2.47	0.47
1:A:858:LEU:HD23	1:A:870:LEU:HB3	1.96	0.47
1:F:584:THR:HG21	1:F:610:ASN:H	1.79	0.47
1:T:624:ASP:N	1:T:624:ASP:OD1	2.48	0.47
1:V:624:ASP:OD1	1:V:624:ASP:N	2.48	0.47
1:Y:806:VAL:HG23	1:Y:818:ILE:HB	1.97	0.47
1:Z:843:ARG:NH2	1:Z:850:GLU:OE2	2.42	0.47
1:A:540:ASP:OD1	1:A:542:THR:OG1	2.32	0.46
1:D:684:ILE:HB	1:D:724:THR:HB	1.96	0.46
1:F:789:ALA:O	1:F:795:LYS:NZ	2.48	0.46
1:F:806:VAL:HG23	1:F:818:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:806:VAL:HG23	1:T:818:ILE:HB	1.97	0.46
1:V:584:THR:HG21	1:V:610:ASN:H	1.79	0.46
1:Z:624:ASP:OD1	1:Z:624:ASP:N	2.48	0.46
1:B:624:ASP:OD1	1:B:624:ASP:N	2.48	0.46
1:D:789:ALA:O	1:D:795:LYS:NZ	2.48	0.46
1:G:843:ARG:NH2	1:G:850:GLU:OE2	2.42	0.46
1:G:858:LEU:HD23	1:G:870:LEU:HB3	1.96	0.46
1:T:509:GLN:HG3	1:Z:283:LYS:HB2	1.97	0.46
1:U:806:VAL:HG23	1:U:818:ILE:HB	1.97	0.46
1:V:789:ALA:O	1:V:795:LYS:NZ	2.48	0.46
1:X:676:LYS:HB3	1:X:678:PRO:HD3	1.95	0.46
1:Z:866:ASP:OD2	1:Z:866:ASP:N	2.47	0.46
1:D:269:ASP:OD1	1:D:296:ALA:N	2.49	0.46
1:D:806:VAL:HG23	1:D:818:ILE:HB	1.97	0.46
1:E:584:THR:HG21	1:E:610:ASN:H	1.79	0.46
1:F:269:ASP:OD1	1:F:296:ALA:N	2.49	0.46
1:G:269:ASP:OD1	1:G:296:ALA:N	2.49	0.46
1:T:269:ASP:OD1	1:T:296:ALA:N	2.49	0.46
1:X:858:LEU:HD23	1:X:870:LEU:HB3	1.96	0.46
1:Z:858:LEU:HD23	1:Z:870:LEU:HB3	1.96	0.46
1:B:789:ALA:O	1:B:795:LYS:NZ	2.48	0.46
1:G:789:ALA:O	1:G:795:LYS:NZ	2.48	0.46
1:G:866:ASP:OD2	1:G:866:ASP:N	2.47	0.46
1:U:624:ASP:OD1	1:U:624:ASP:N	2.48	0.46
1:W:624:ASP:OD1	1:W:624:ASP:N	2.48	0.46
1:F:521:THR:OG1	1:F:522:GLU:OE1	2.34	0.46
1:T:233:ASN:N	1:T:233:ASN:OD1	2.49	0.46
1:U:810:LEU:H	1:U:814:GLY:HA2	1.81	0.46
1:V:269:ASP:OD1	1:V:296:ALA:N	2.49	0.46
1:V:432:ASN:HD22	1:W:508:SER:HB3	1.80	0.46
1:V:540:ASP:OD1	1:V:542:THR:OG1	2.32	0.46
1:W:858:LEU:HD23	1:W:870:LEU:HB3	1.96	0.46
1:Y:858:LEU:HD23	1:Y:870:LEU:HB3	1.96	0.46
1:A:624:ASP:N	1:A:624:ASP:OD1	2.47	0.46
1:A:866:ASP:OD2	1:A:866:ASP:N	2.47	0.46
1:B:810:LEU:H	1:B:814:GLY:HA2	1.81	0.46
1:C:684:ILE:HB	1:C:724:THR:HB	1.96	0.46
1:E:521:THR:OG1	1:E:522:GLU:OE1	2.34	0.46
1:F:843:ARG:NH2	1:F:850:GLU:OE2	2.42	0.46
1:G:624:ASP:OD1	1:G:624:ASP:N	2.47	0.46
1:G:810:LEU:H	1:G:814:GLY:HA2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:799:ASP:OD1	1:T:799:ASP:N	2.45	0.46
1:T:843:ARG:NH2	1:T:850:GLU:OE2	2.42	0.46
1:V:495:GLN:HB2	1:W:506:TYR:OH	2.15	0.46
1:Z:810:LEU:H	1:Z:814:GLY:HA2	1.81	0.46
1:A:810:LEU:H	1:A:814:GLY:HA2	1.81	0.46
1:B:488:GLY:HA3	1:B:496:ILE:HD12	1.97	0.46
1:D:810:LEU:H	1:D:814:GLY:HA2	1.81	0.46
1:E:233:ASN:N	1:E:233:ASN:OD1	2.49	0.46
1:E:540:ASP:OD1	1:E:542:THR:OG1	2.32	0.46
1:F:233:ASN:OD1	1:F:233:ASN:N	2.49	0.46
1:F:810:LEU:H	1:F:814:GLY:HA2	1.81	0.46
1:T:496:ILE:HG12	1:U:506:TYR:CE1	2.51	0.46
1:T:521:THR:OG1	1:T:522:GLU:OE1	2.34	0.46
1:U:269:ASP:OD1	1:U:296:ALA:N	2.49	0.46
1:U:684:ILE:HB	1:U:724:THR:HB	1.96	0.46
1:V:806:VAL:HG23	1:V:818:ILE:HB	1.97	0.46
1:W:810:LEU:H	1:W:814:GLY:HA2	1.81	0.46
1:X:269:ASP:OD1	1:X:296:ALA:N	2.49	0.46
1:X:810:LEU:H	1:X:814:GLY:HA2	1.81	0.46
1:Y:684:ILE:HB	1:Y:724:THR:HB	1.96	0.46
1:Z:269:ASP:OD1	1:Z:296:ALA:N	2.49	0.46
1:A:806:VAL:HG23	1:A:818:ILE:HB	1.97	0.46
1:C:624:ASP:N	1:C:624:ASP:OD1	2.47	0.46
1:C:810:LEU:H	1:C:814:GLY:HA2	1.81	0.46
1:F:540:ASP:OD1	1:F:542:THR:OG1	2.32	0.46
1:V:488:GLY:HA3	1:V:496:ILE:HD12	1.98	0.46
1:W:488:GLY:HA3	1:W:496:ILE:HD12	1.98	0.46
1:Y:843:ARG:NH2	1:Y:850:GLU:OE2	2.42	0.46
1:Z:684:ILE:HB	1:Z:724:THR:HB	1.96	0.46
1:A:789:ALA:O	1:A:795:LYS:NZ	2.48	0.46
1:C:269:ASP:OD1	1:C:296:ALA:N	2.49	0.46
1:E:799:ASP:OD1	1:E:799:ASP:N	2.45	0.46
1:F:624:ASP:OD1	1:F:624:ASP:N	2.48	0.46
1:W:269:ASP:OD1	1:W:296:ALA:N	2.49	0.46
1:X:584:THR:HG21	1:X:610:ASN:H	1.79	0.46
1:Y:810:LEU:H	1:Y:814:GLY:HA2	1.81	0.46
1:B:627:ASN:OD1	1:B:627:ASN:N	2.49	0.46
1:C:488:GLY:HA3	1:C:496:ILE:HD12	1.98	0.46
1:G:521:THR:OG1	1:G:522:GLU:OE1	2.34	0.46
1:U:789:ALA:O	1:U:795:LYS:NZ	2.48	0.46
1:V:218:ASP:OD1	1:V:218:ASP:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:810:LEU:H	1:V:814:GLY:HA2	1.81	0.46
1:Z:521:THR:OG1	1:Z:522:GLU:OE1	2.34	0.46
1:D:488:GLY:HA3	1:D:496:ILE:HD12	1.98	0.45
1:D:521:THR:OG1	1:D:522:GLU:OE1	2.34	0.45
1:D:540:ASP:OD1	1:D:542:THR:OG1	2.32	0.45
1:E:269:ASP:OD1	1:E:296:ALA:N	2.49	0.45
1:W:806:VAL:HG23	1:W:818:ILE:HB	1.97	0.45
1:X:806:VAL:HG23	1:X:818:ILE:HB	1.97	0.45
1:Z:233:ASN:OD1	1:Z:233:ASN:N	2.49	0.45
1:B:269:ASP:OD1	1:B:296:ALA:N	2.49	0.45
1:C:789:ALA:O	1:C:795:LYS:NZ	2.48	0.45
1:C:806:VAL:HG23	1:C:818:ILE:HB	1.97	0.45
1:E:810:LEU:H	1:E:814:GLY:HA2	1.81	0.45
1:T:283:LYS:HB2	1:U:509:GLN:HG3	1.98	0.45
1:U:233:ASN:OD1	1:U:233:ASN:N	2.49	0.45
1:W:649:LYS:HA	1:W:730:THR:HA	1.98	0.45
1:X:789:ALA:O	1:X:795:LYS:NZ	2.48	0.45
1:A:233:ASN:OD1	1:A:233:ASN:N	2.49	0.45
1:B:521:THR:OG1	1:B:522:GLU:OE1	2.34	0.45
1:B:649:LYS:HA	1:B:730:THR:HA	1.98	0.45
1:B:806:VAL:HG23	1:B:818:ILE:HB	1.97	0.45
1:C:627:ASN:OD1	1:C:627:ASN:N	2.50	0.45
1:T:488:GLY:HA3	1:T:496:ILE:HD12	1.98	0.45
1:T:540:ASP:OD1	1:T:542:THR:OG1	2.32	0.45
1:W:216:ASP:OD1	1:W:216:ASP:N	2.50	0.45
1:W:521:THR:OG1	1:W:522:GLU:OE1	2.34	0.45
1:W:627:ASN:OD1	1:W:627:ASN:N	2.49	0.45
1:X:627:ASN:N	1:X:627:ASN:OD1	2.50	0.45
1:Y:627:ASN:OD1	1:Y:627:ASN:N	2.50	0.45
1:T:626:ASN:OD1	1:T:626:ASN:N	2.50	0.45
1:U:521:THR:OG1	1:U:522:GLU:OE1	2.34	0.45
1:V:216:ASP:N	1:V:216:ASP:OD1	2.50	0.45
1:X:488:GLY:HA3	1:X:496:ILE:HD12	1.98	0.45
1:X:521:THR:OG1	1:X:522:GLU:OE1	2.34	0.45
1:D:233:ASN:OD1	1:D:233:ASN:N	2.49	0.45
1:X:233:ASN:OD1	1:X:233:ASN:N	2.49	0.45
1:Y:269:ASP:OD1	1:Y:296:ALA:N	2.49	0.45
1:A:269:ASP:OD1	1:A:296:ALA:N	2.49	0.45
1:A:521:THR:OG1	1:A:522:GLU:OE1	2.34	0.45
1:B:216:ASP:OD1	1:B:216:ASP:N	2.50	0.45
1:B:233:ASN:OD1	1:B:233:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASP:N	1:C:216:ASP:OD1	2.50	0.45
1:E:794:ASN:OD1	1:E:794:ASN:N	2.50	0.45
1:U:488:GLY:HA3	1:U:496:ILE:HD12	1.98	0.45
1:U:626:ASN:N	1:U:626:ASN:OD1	2.50	0.45
1:V:794:ASN:OD1	1:V:794:ASN:N	2.50	0.45
1:Y:218:ASP:OD1	1:Y:218:ASP:N	2.40	0.45
1:Y:521:THR:OG1	1:Y:522:GLU:OE1	2.34	0.45
1:Z:488:GLY:HA3	1:Z:496:ILE:HD12	1.98	0.45
1:A:488:GLY:HA3	1:A:496:ILE:HD12	1.97	0.45
1:F:488:GLY:HA3	1:F:496:ILE:HD12	1.97	0.45
1:G:233:ASN:OD1	1:G:233:ASN:N	2.49	0.45
1:T:649:LYS:HA	1:T:730:THR:HA	1.98	0.45
1:V:627:ASN:OD1	1:V:627:ASN:N	2.49	0.45
1:X:649:LYS:HA	1:X:730:THR:HA	1.98	0.45
1:Z:649:LYS:HA	1:Z:730:THR:HA	1.98	0.45
1:C:626:ASN:OD1	1:C:626:ASN:N	2.50	0.45
1:E:843:ARG:NH2	1:E:850:GLU:OE2	2.42	0.45
1:F:626:ASN:OD1	1:F:626:ASN:N	2.50	0.45
1:G:626:ASN:OD1	1:G:626:ASN:N	2.50	0.45
1:T:789:ALA:O	1:T:795:LYS:NZ	2.48	0.45
1:X:540:ASP:OD1	1:X:542:THR:OG1	2.33	0.45
1:A:843:ARG:NH2	1:A:850:GLU:OE2	2.42	0.45
1:C:649:LYS:HA	1:C:730:THR:HA	1.98	0.45
1:D:794:ASN:OD1	1:D:794:ASN:N	2.50	0.45
1:F:649:LYS:HA	1:F:730:THR:HA	1.98	0.45
1:F:794:ASN:OD1	1:F:794:ASN:N	2.50	0.45
1:V:233:ASN:N	1:V:233:ASN:OD1	2.49	0.45
1:V:521:THR:OG1	1:V:522:GLU:OE1	2.34	0.45
1:C:233:ASN:N	1:C:233:ASN:OD1	2.49	0.45
1:C:521:THR:OG1	1:C:522:GLU:OE1	2.34	0.45
1:D:218:ASP:OD1	1:D:218:ASP:N	2.39	0.45
1:D:626:ASN:OD1	1:D:626:ASN:N	2.50	0.45
1:Y:216:ASP:N	1:Y:216:ASP:OD1	2.50	0.45
1:A:649:LYS:HA	1:A:730:THR:HA	1.98	0.44
1:T:810:LEU:H	1:T:814:GLY:HA2	1.81	0.44
1:U:794:ASN:OD1	1:U:794:ASN:N	2.50	0.44
1:W:233:ASN:OD1	1:W:233:ASN:N	2.49	0.44
1:Z:626:ASN:OD1	1:Z:626:ASN:N	2.50	0.44
1:B:794:ASN:OD1	1:B:794:ASN:N	2.50	0.44
1:F:237:ILE:HD13	1:F:237:ILE:HA	1.87	0.44
1:F:799:ASP:OD1	1:F:799:ASP:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:488:GLY:HA3	1:G:496:ILE:HD12	1.98	0.44
1:T:481:THR:HG23	1:Z:440:PRO:HB3	1.99	0.44
1:U:216:ASP:OD1	1:U:216:ASP:N	2.50	0.44
1:V:649:LYS:HA	1:V:730:THR:HA	1.98	0.44
1:X:216:ASP:OD1	1:X:216:ASP:N	2.50	0.44
1:B:540:ASP:OD1	1:B:542:THR:OG1	2.32	0.44
1:E:218:ASP:OD1	1:E:218:ASP:N	2.39	0.44
1:E:488:GLY:HA3	1:E:496:ILE:HD12	1.98	0.44
1:E:649:LYS:HA	1:E:730:THR:HA	1.98	0.44
1:Y:624:ASP:N	1:Y:624:ASP:OD1	2.48	0.44
1:Y:649:LYS:HA	1:Y:730:THR:HA	1.98	0.44
1:A:265:ASN:ND2	1:B:494:GLY:O	2.47	0.44
1:B:657:LYS:HB3	1:B:722:GLU:HG2	2.00	0.44
1:C:794:ASN:OD1	1:C:794:ASN:N	2.50	0.44
1:E:237:ILE:HD13	1:E:237:ILE:HA	1.87	0.44
1:T:240:LEU:HD13	1:U:262:LEU:HD22	1.99	0.44
1:U:657:LYS:HB3	1:U:722:GLU:HG2	2.00	0.44
1:V:657:LYS:HB3	1:V:722:GLU:HG2	2.00	0.44
1:W:626:ASN:N	1:W:626:ASN:OD1	2.50	0.44
1:W:657:LYS:HB3	1:W:722:GLU:HG2	2.00	0.44
1:Z:260:ASN:HD22	1:Z:263:GLU:HG2	1.82	0.44
1:Z:627:ASN:OD1	1:Z:627:ASN:N	2.49	0.44
1:A:657:LYS:HB3	1:A:722:GLU:HG2	2.00	0.44
1:C:657:LYS:HB3	1:C:722:GLU:HG2	2.00	0.44
1:C:854:THR:OG1	1:C:855:TYR:N	2.51	0.44
1:G:649:LYS:HA	1:G:730:THR:HA	1.98	0.44
1:W:854:THR:OG1	1:W:855:TYR:N	2.51	0.44
1:X:657:LYS:HB3	1:X:722:GLU:HG2	2.00	0.44
1:A:260:ASN:HD22	1:A:263:GLU:HG2	1.82	0.44
1:A:854:THR:OG1	1:A:855:TYR:N	2.51	0.44
1:D:649:LYS:HA	1:D:730:THR:HA	1.98	0.44
1:D:657:LYS:HB3	1:D:722:GLU:HG2	2.00	0.44
1:T:237:ILE:HD13	1:T:237:ILE:HA	1.87	0.44
1:U:540:ASP:OD1	1:U:542:THR:OG1	2.32	0.44
1:X:626:ASN:OD1	1:X:626:ASN:N	2.50	0.44
1:Y:233:ASN:N	1:Y:233:ASN:OD1	2.49	0.44
1:Z:216:ASP:OD1	1:Z:216:ASP:N	2.50	0.44
1:A:627:ASN:OD1	1:A:627:ASN:N	2.49	0.44
1:B:626:ASN:OD1	1:B:626:ASN:N	2.50	0.44
1:V:626:ASN:OD1	1:V:626:ASN:N	2.50	0.44
1:Y:488:GLY:HA3	1:Y:496:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:626:ASN:N	1:Y:626:ASN:OD1	2.50	0.44
1:Z:789:ALA:O	1:Z:795:LYS:NZ	2.48	0.44
1:E:657:LYS:HB3	1:E:722:GLU:HG2	2.00	0.44
1:T:794:ASN:OD1	1:T:794:ASN:N	2.50	0.44
1:Y:657:LYS:HB3	1:Y:722:GLU:HG2	2.00	0.44
1:D:216:ASP:OD1	1:D:216:ASP:N	2.50	0.44
1:D:260:ASN:HD22	1:D:263:GLU:HG2	1.83	0.44
1:F:807:GLU:HB2	1:F:857:LYS:HB2	2.00	0.44
1:G:216:ASP:OD1	1:G:216:ASP:N	2.50	0.44
1:G:657:LYS:HB3	1:G:722:GLU:HG2	2.00	0.44
1:E:216:ASP:N	1:E:216:ASP:OD1	2.50	0.43
1:E:626:ASN:OD1	1:E:626:ASN:N	2.50	0.43
1:E:807:GLU:HB2	1:E:857:LYS:HB2	2.00	0.43
1:F:521:THR:OG1	1:F:522:GLU:N	2.51	0.43
1:F:657:LYS:HB3	1:F:722:GLU:HG2	2.00	0.43
1:T:657:LYS:HB3	1:T:722:GLU:HG2	2.00	0.43
1:U:854:THR:OG1	1:U:855:TYR:N	2.51	0.43
1:X:854:THR:OG1	1:X:855:TYR:N	2.51	0.43
1:Z:657:LYS:HB3	1:Z:722:GLU:HG2	2.00	0.43
1:D:807:GLU:HB2	1:D:857:LYS:HB2	2.00	0.43
1:G:260:ASN:HD22	1:G:263:GLU:HG2	1.82	0.43
1:U:260:ASN:HD22	1:U:263:GLU:HG2	1.82	0.43
1:U:807:GLU:HB2	1:U:857:LYS:HB2	2.00	0.43
1:Y:854:THR:OG1	1:Y:855:TYR:N	2.51	0.43
1:B:684:ILE:HG23	1:B:694:LYS:HE2	2.01	0.43
1:F:216:ASP:OD1	1:F:216:ASP:N	2.50	0.43
1:T:807:GLU:HB2	1:T:857:LYS:HB2	2.00	0.43
1:U:649:LYS:HA	1:U:730:THR:HA	1.98	0.43
1:X:260:ASN:HD22	1:X:263:GLU:HG2	1.82	0.43
1:A:626:ASN:OD1	1:A:626:ASN:N	2.50	0.43
1:A:799:ASP:OD1	1:A:799:ASP:N	2.45	0.43
1:B:854:THR:OG1	1:B:855:TYR:N	2.51	0.43
1:D:627:ASN:OD1	1:D:627:ASN:N	2.49	0.43
1:F:260:ASN:HD22	1:F:263:GLU:HG2	1.83	0.43
1:T:216:ASP:N	1:T:216:ASP:OD1	2.50	0.43
1:T:453:ASP:HA	1:Z:456:SER:HB2	1.99	0.43
1:V:237:ILE:HD13	1:V:237:ILE:HA	1.87	0.43
1:W:684:ILE:HG23	1:W:694:LYS:HE2	2.01	0.43
1:X:794:ASN:OD1	1:X:794:ASN:N	2.50	0.43
1:Y:260:ASN:HD22	1:Y:263:GLU:HG2	1.82	0.43
1:Z:521:THR:OG1	1:Z:522:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:807:GLU:HB2	1:Z:857:LYS:HB2	2.00	0.43
1:A:684:ILE:HG23	1:A:694:LYS:HE2	2.01	0.43
1:B:581:ASP:OD1	1:B:581:ASP:N	2.52	0.43
1:E:854:THR:OG1	1:E:855:TYR:N	2.51	0.43
1:G:794:ASN:OD1	1:G:794:ASN:N	2.50	0.43
1:G:807:GLU:HB2	1:G:857:LYS:HB2	2.00	0.43
1:V:854:THR:OG1	1:V:855:TYR:N	2.51	0.43
1:W:789:ALA:O	1:W:795:LYS:NZ	2.48	0.43
1:A:383:LYS:N	1:B:313:GLU:O	2.51	0.43
1:B:260:ASN:HD22	1:B:263:GLU:HG2	1.82	0.43
1:C:684:ILE:HG23	1:C:694:LYS:HE2	2.01	0.43
1:E:581:ASP:OD1	1:E:581:ASP:N	2.52	0.43
1:T:521:THR:OG1	1:T:522:GLU:N	2.51	0.43
1:V:684:ILE:HG23	1:V:694:LYS:HE2	2.00	0.43
1:C:433:LEU:HD12	1:C:433:LEU:HA	1.89	0.43
1:C:828:TYR:HB3	1:C:834:GLN:HG2	2.01	0.43
1:E:377:THR:OG1	1:F:319:GLN:O	2.34	0.43
1:E:789:ALA:O	1:E:795:LYS:NZ	2.48	0.43
1:U:581:ASP:OD1	1:U:581:ASP:N	2.52	0.43
1:V:807:GLU:HB2	1:V:857:LYS:HB2	2.00	0.43
1:X:684:ILE:HG23	1:X:694:LYS:HE2	2.01	0.43
1:E:748:LEU:HD23	1:E:748:LEU:HA	1.93	0.43
1:W:260:ASN:HD22	1:W:263:GLU:HG2	1.82	0.43
1:W:794:ASN:OD1	1:W:794:ASN:N	2.50	0.43
1:Y:684:ILE:HG23	1:Y:694:LYS:HE2	2.00	0.43
1:A:383:LYS:HD2	1:B:313:GLU:HB3	2.00	0.43
1:C:807:GLU:HB2	1:C:857:LYS:HB2	2.00	0.43
1:D:828:TYR:HB3	1:D:834:GLN:HG2	2.01	0.43
1:E:326:ALA:HB3	1:E:368:GLN:HG2	2.01	0.43
1:E:521:THR:OG1	1:E:522:GLU:N	2.51	0.43
1:F:326:ALA:HB3	1:F:368:GLN:HG2	2.01	0.43
1:Y:807:GLU:HB2	1:Y:857:LYS:HB2	2.00	0.43
1:Z:521:THR:HG1	1:Z:522:GLU:H	1.67	0.43
1:G:521:THR:OG1	1:G:522:GLU:N	2.51	0.42
1:G:581:ASP:OD1	1:G:581:ASP:N	2.52	0.42
1:G:627:ASN:OD1	1:G:627:ASN:N	2.50	0.42
1:C:847:THR:OG1	1:C:848:GLY:N	2.53	0.42
1:E:260:ASN:HD22	1:E:263:GLU:HG2	1.82	0.42
1:E:627:ASN:OD1	1:E:627:ASN:N	2.49	0.42
1:U:326:ALA:HB3	1:U:368:GLN:HG2	2.01	0.42
1:U:828:TYR:HB3	1:U:834:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:847:THR:OG1	1:U:848:GLY:N	2.52	0.42
1:V:326:ALA:HB3	1:V:368:GLN:HG2	2.01	0.42
1:V:828:TYR:HB3	1:V:834:GLN:HG2	2.01	0.42
1:X:847:THR:OG1	1:X:848:GLY:N	2.52	0.42
1:Y:521:THR:HG1	1:Y:522:GLU:H	1.65	0.42
1:B:828:TYR:HB3	1:B:834:GLN:HG2	2.01	0.42
1:C:843:ARG:HD3	1:C:843:ARG:HA	1.90	0.42
1:D:521:THR:OG1	1:D:522:GLU:N	2.51	0.42
1:D:581:ASP:N	1:D:581:ASP:OD1	2.52	0.42
1:F:218:ASP:OD1	1:F:218:ASP:N	2.39	0.42
1:V:581:ASP:OD1	1:V:581:ASP:N	2.52	0.42
1:Y:847:THR:OG1	1:Y:848:GLY:N	2.53	0.42
1:A:807:GLU:HB2	1:A:857:LYS:HB2	2.00	0.42
1:D:854:THR:OG1	1:D:855:TYR:N	2.51	0.42
1:G:854:THR:OG1	1:G:855:TYR:N	2.51	0.42
1:T:260:ASN:HD22	1:T:263:GLU:HG2	1.82	0.42
1:U:684:ILE:HG23	1:U:694:LYS:HE2	2.00	0.42
1:W:828:TYR:HB3	1:W:834:GLN:HG2	2.01	0.42
1:C:581:ASP:OD1	1:C:581:ASP:N	2.52	0.42
1:D:847:THR:OG1	1:D:848:GLY:N	2.52	0.42
1:G:422:ILE:HD13	1:G:422:ILE:HA	1.88	0.42
1:G:847:THR:OG1	1:G:848:GLY:N	2.53	0.42
1:T:854:THR:OG1	1:T:855:TYR:N	2.51	0.42
1:U:521:THR:OG1	1:U:522:GLU:N	2.51	0.42
1:V:260:ASN:HD22	1:V:263:GLU:HG2	1.82	0.42
1:Y:521:THR:OG1	1:Y:522:GLU:N	2.51	0.42
1:Z:681:SER:HA	1:Z:726:ILE:O	2.20	0.42
1:Z:854:THR:OG1	1:Z:855:TYR:N	2.51	0.42
1:B:807:GLU:HB2	1:B:857:LYS:HB2	2.00	0.42
1:C:260:ASN:HD22	1:C:263:GLU:HG2	1.82	0.42
1:E:681:SER:HA	1:E:726:ILE:O	2.20	0.42
1:F:854:THR:OG1	1:F:855:TYR:N	2.51	0.42
1:U:843:ARG:NH2	1:U:850:GLU:OE2	2.42	0.42
1:V:835:PRO:HG2	1:W:846:PHE:CE1	2.54	0.42
1:V:847:THR:OG1	1:V:848:GLY:N	2.52	0.42
1:W:807:GLU:HB2	1:W:857:LYS:HB2	2.00	0.42
1:X:807:GLU:HB2	1:X:857:LYS:HB2	2.00	0.42
1:X:828:TYR:HB3	1:X:834:GLN:HG2	2.01	0.42
1:Y:581:ASP:OD1	1:Y:581:ASP:N	2.52	0.42
1:Z:684:ILE:HG23	1:Z:694:LYS:HE2	2.01	0.42
1:E:684:ILE:HG23	1:E:694:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:684:ILE:HG23	1:F:694:LYS:HE2	2.01	0.42
1:G:828:TYR:HB3	1:G:834:GLN:HG2	2.01	0.42
1:T:581:ASP:OD1	1:T:581:ASP:N	2.52	0.42
1:W:521:THR:OG1	1:W:522:GLU:N	2.51	0.42
1:X:521:THR:OG1	1:X:522:GLU:N	2.51	0.42
1:Z:828:TYR:HB3	1:Z:834:GLN:HG2	2.01	0.42
1:A:521:THR:OG1	1:A:522:GLU:N	2.51	0.42
1:C:218:ASP:OD1	1:C:218:ASP:N	2.39	0.42
1:E:828:TYR:HB3	1:E:834:GLN:HG2	2.01	0.42
1:G:681:SER:HA	1:G:726:ILE:O	2.20	0.42
1:G:684:ILE:HG23	1:G:694:LYS:HE2	2.01	0.42
1:U:225:ASN:HB3	1:U:230:TYR:CE2	2.55	0.42
1:B:684:ILE:HA	1:B:694:LYS:HD2	2.02	0.42
1:D:225:ASN:HB3	1:D:230:TYR:CE2	2.55	0.42
1:F:828:TYR:HB3	1:F:834:GLN:HG2	2.01	0.42
1:F:847:THR:OG1	1:F:848:GLY:N	2.52	0.42
1:T:505:ASP:HA	1:Z:404:TYR:CE2	2.54	0.42
1:V:240:LEU:HD13	1:W:262:LEU:HD22	2.01	0.42
1:W:581:ASP:OD1	1:W:581:ASP:N	2.52	0.42
1:A:216:ASP:OD1	1:A:216:ASP:N	2.50	0.42
1:A:225:ASN:HB3	1:A:230:TYR:CE2	2.55	0.42
1:A:748:LEU:HD23	1:A:748:LEU:HA	1.93	0.42
1:D:684:ILE:HG23	1:D:694:LYS:HE2	2.01	0.42
1:T:684:ILE:HG23	1:T:694:LYS:HE2	2.00	0.42
1:U:433:LEU:HD12	1:U:433:LEU:HA	1.89	0.42
1:V:766:LYS:HE2	1:V:766:LYS:HB2	1.96	0.42
1:W:684:ILE:HA	1:W:694:LYS:HD2	2.02	0.42
1:Y:789:ALA:O	1:Y:795:LYS:NZ	2.48	0.42
1:A:326:ALA:HB3	1:A:368:GLN:HG2	2.01	0.41
1:B:847:THR:OG1	1:B:848:GLY:N	2.52	0.41
1:C:326:ALA:HB3	1:C:368:GLN:HG2	2.01	0.41
1:D:518:ILE:HG13	1:D:612:LEU:HA	2.02	0.41
1:G:225:ASN:HB3	1:G:230:TYR:CE2	2.55	0.41
1:T:681:SER:HA	1:T:726:ILE:O	2.20	0.41
1:U:681:SER:HA	1:U:726:ILE:O	2.20	0.41
1:V:291:ASP:OD1	1:V:291:ASP:N	2.53	0.41
1:W:326:ALA:HB3	1:W:368:GLN:HG2	2.01	0.41
1:W:847:THR:OG1	1:W:848:GLY:N	2.52	0.41
1:X:433:LEU:HD12	1:X:433:LEU:HA	1.89	0.41
1:Z:847:THR:OG1	1:Z:848:GLY:N	2.53	0.41
1:A:684:ILE:HA	1:A:694:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ILE:H	1:A:694:LYS:HD2	1.86	0.41
1:C:422:ILE:HD13	1:C:422:ILE:HA	1.88	0.41
1:D:237:ILE:HD13	1:D:237:ILE:HA	1.87	0.41
1:D:245:TRP:CG	1:D:256:LYS:HD3	2.56	0.41
1:D:326:ALA:HB3	1:D:368:GLN:HG2	2.01	0.41
1:D:685:ILE:H	1:D:694:LYS:HD2	1.86	0.41
1:E:225:ASN:HB3	1:E:230:TYR:CE2	2.55	0.41
1:G:326:ALA:HB3	1:G:368:GLN:HG2	2.01	0.41
1:T:291:ASP:OD1	1:T:291:ASP:N	2.53	0.41
1:T:828:TYR:HB3	1:T:834:GLN:HG2	2.01	0.41
1:V:495:GLN:HB2	1:W:506:TYR:CE1	2.55	0.41
1:V:521:THR:OG1	1:V:522:GLU:N	2.51	0.41
1:V:684:ILE:HA	1:V:694:LYS:HD2	2.02	0.41
1:W:766:LYS:HE2	1:W:766:LYS:HB2	1.95	0.41
1:X:225:ASN:HB3	1:X:230:TYR:CE2	2.55	0.41
1:Y:225:ASN:HB3	1:Y:230:TYR:CE2	2.55	0.41
1:A:245:TRP:CG	1:A:256:LYS:HD3	2.56	0.41
1:A:460:ILE:HD12	1:A:461:PRO:HD2	2.02	0.41
1:A:828:TYR:HB3	1:A:834:GLN:HG2	2.01	0.41
1:B:326:ALA:HB3	1:B:368:GLN:HG2	2.01	0.41
1:C:685:ILE:H	1:C:694:LYS:HD2	1.86	0.41
1:D:843:ARG:NH2	1:D:850:GLU:OE2	2.42	0.41
1:F:225:ASN:HB3	1:F:230:TYR:CE2	2.55	0.41
1:F:581:ASP:OD1	1:F:581:ASP:N	2.52	0.41
1:F:627:ASN:OD1	1:F:627:ASN:N	2.50	0.41
1:F:681:SER:HA	1:F:726:ILE:O	2.20	0.41
1:F:685:ILE:H	1:F:694:LYS:HD2	1.86	0.41
1:U:245:TRP:CG	1:U:256:LYS:HD3	2.56	0.41
1:W:225:ASN:HB3	1:W:230:TYR:CE2	2.55	0.41
1:W:681:SER:HA	1:W:726:ILE:O	2.20	0.41
1:X:460:ILE:HD12	1:X:461:PRO:HD2	2.03	0.41
1:X:684:ILE:HA	1:X:694:LYS:HD2	2.03	0.41
1:Y:460:ILE:HD12	1:Y:461:PRO:HD2	2.03	0.41
1:Y:828:TYR:HB3	1:Y:834:GLN:HG2	2.01	0.41
1:Z:460:ILE:HD12	1:Z:461:PRO:HD2	2.03	0.41
1:B:291:ASP:OD1	1:B:291:ASP:N	2.53	0.41
1:B:786:MET:O	1:B:839:TYR:HA	2.21	0.41
1:C:684:ILE:HA	1:C:694:LYS:HD2	2.03	0.41
1:E:685:ILE:H	1:E:694:LYS:HD2	1.86	0.41
1:F:245:TRP:CG	1:F:256:LYS:HD3	2.56	0.41
1:G:245:TRP:CG	1:G:256:LYS:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:326:ALA:HB3	1:T:368:GLN:HG2	2.01	0.41
1:T:786:MET:O	1:T:839:TYR:HA	2.21	0.41
1:V:748:LEU:HD23	1:V:748:LEU:HA	1.93	0.41
1:W:529:ARG:HA	1:W:529:ARG:HD3	1.92	0.41
1:X:786:MET:O	1:X:839:TYR:HA	2.21	0.41
1:Y:684:ILE:HA	1:Y:694:LYS:HD2	2.03	0.41
1:Y:777:SER:O	1:Y:777:SER:OG	2.39	0.41
1:Z:794:ASN:OD1	1:Z:794:ASN:N	2.50	0.41
1:A:847:THR:OG1	1:A:848:GLY:N	2.52	0.41
1:B:225:ASN:HB3	1:B:230:TYR:CE2	2.55	0.41
1:C:225:ASN:HB3	1:C:230:TYR:CE2	2.55	0.41
1:C:521:THR:OG1	1:C:522:GLU:N	2.51	0.41
1:F:748:LEU:HD23	1:F:748:LEU:HA	1.93	0.41
1:F:786:MET:O	1:F:839:TYR:HA	2.21	0.41
1:G:433:LEU:HD12	1:G:433:LEU:HA	1.89	0.41
1:G:518:ILE:HG13	1:G:612:LEU:HA	2.02	0.41
1:U:684:ILE:HA	1:U:694:LYS:HD2	2.02	0.41
1:V:225:ASN:HB3	1:V:230:TYR:CE2	2.55	0.41
1:V:227:PRO:HA	1:V:230:TYR:HD2	1.86	0.41
1:V:245:TRP:CG	1:V:256:LYS:HD3	2.56	0.41
1:V:518:ILE:HG13	1:V:612:LEU:HA	2.02	0.41
1:W:460:ILE:HD12	1:W:461:PRO:HD2	2.02	0.41
1:X:793:THR:HA	1:Y:846:PHE:CE2	2.55	0.41
1:Z:225:ASN:HB3	1:Z:230:TYR:CE2	2.55	0.41
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.95	0.41
1:B:685:ILE:H	1:B:694:LYS:HD2	1.86	0.41
1:E:245:TRP:CG	1:E:256:LYS:HD3	2.56	0.41
1:G:748:LEU:HD23	1:G:748:LEU:HA	1.93	0.41
1:T:847:THR:OG1	1:T:848:GLY:N	2.52	0.41
1:V:786:MET:O	1:V:839:TYR:HA	2.21	0.41
1:X:245:TRP:CG	1:X:256:LYS:HD3	2.56	0.41
1:X:326:ALA:HB3	1:X:368:GLN:HG2	2.01	0.41
1:X:529:ARG:HA	1:X:529:ARG:HD3	1.92	0.41
1:Y:245:TRP:CG	1:Y:256:LYS:HD3	2.56	0.41
1:Y:518:ILE:HG13	1:Y:612:LEU:HA	2.02	0.41
1:Z:218:ASP:OD1	1:Z:218:ASP:N	2.39	0.41
1:Z:326:ALA:HB3	1:Z:368:GLN:HG2	2.01	0.41
1:Z:518:ILE:HG13	1:Z:612:LEU:HA	2.02	0.41
1:Z:684:ILE:HA	1:Z:694:LYS:HD2	2.03	0.41
1:A:518:ILE:HG13	1:A:612:LEU:HA	2.02	0.41
1:B:521:THR:OG1	1:B:522:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PRO:HA	1:C:230:TYR:HD2	1.86	0.41
1:E:518:ILE:HG13	1:E:612:LEU:HA	2.02	0.41
1:F:227:PRO:HA	1:F:230:TYR:HD2	1.86	0.41
1:G:460:ILE:HD12	1:G:461:PRO:HD2	2.02	0.41
1:T:225:ASN:HB3	1:T:230:TYR:CE2	2.55	0.41
1:T:785:GLY:HA2	1:T:842:LEU:H	1.86	0.41
1:U:518:ILE:HG13	1:U:612:LEU:HA	2.02	0.41
1:Y:326:ALA:HB3	1:Y:368:GLN:HG2	2.01	0.41
1:Y:685:ILE:H	1:Y:694:LYS:HD2	1.86	0.41
1:Z:685:ILE:H	1:Z:694:LYS:HD2	1.86	0.41
1:A:227:PRO:HA	1:A:230:TYR:HD2	1.86	0.41
1:A:681:SER:HA	1:A:726:ILE:O	2.20	0.41
1:B:460:ILE:HD12	1:B:461:PRO:HD2	2.03	0.41
1:C:518:ILE:HG13	1:C:612:LEU:HA	2.02	0.41
1:C:786:MET:O	1:C:839:TYR:HA	2.21	0.41
1:T:227:PRO:HA	1:T:230:TYR:HD2	1.86	0.41
1:U:786:MET:O	1:U:839:TYR:HA	2.21	0.41
1:W:291:ASP:OD1	1:W:291:ASP:N	2.53	0.41
1:X:681:SER:HA	1:X:726:ILE:O	2.20	0.41
1:B:245:TRP:CG	1:B:256:LYS:HD3	2.56	0.41
1:B:681:SER:HA	1:B:726:ILE:O	2.20	0.41
1:C:785:GLY:HA2	1:C:842:LEU:H	1.86	0.41
1:D:684:ILE:HA	1:D:694:LYS:HD2	2.02	0.41
1:D:786:MET:O	1:D:839:TYR:HA	2.21	0.41
1:E:786:MET:O	1:E:839:TYR:HA	2.21	0.41
1:G:684:ILE:HA	1:G:694:LYS:HD2	2.02	0.41
1:T:263:GLU:OE1	1:Z:283:LYS:NZ	2.47	0.41
1:W:245:TRP:CG	1:W:256:LYS:HD3	2.56	0.41
1:W:545:LEU:HD23	1:W:545:LEU:HA	1.95	0.41
1:W:785:GLY:HA2	1:W:842:LEU:H	1.86	0.41
1:X:518:ILE:HG13	1:X:612:LEU:HA	2.02	0.41
1:X:785:GLY:HA2	1:X:842:LEU:H	1.86	0.41
1:Y:227:PRO:HA	1:Y:230:TYR:HD2	1.86	0.41
1:Y:681:SER:HA	1:Y:726:ILE:O	2.20	0.41
1:Z:786:MET:O	1:Z:839:TYR:HA	2.21	0.41
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.89	0.41
1:A:581:ASP:OD1	1:A:581:ASP:N	2.52	0.41
1:A:786:MET:O	1:A:839:TYR:HA	2.21	0.41
1:A:794:ASN:OD1	1:A:794:ASN:N	2.50	0.41
1:B:785:GLY:HA2	1:B:842:LEU:H	1.86	0.41
1:C:245:TRP:CG	1:C:256:LYS:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:PHE:HA	1:C:252:GLN:HB2	2.03	0.41
1:C:803:LYS:HB2	1:C:861:TYR:HB2	2.02	0.41
1:D:681:SER:HA	1:D:726:ILE:O	2.20	0.41
1:E:227:PRO:HA	1:E:230:TYR:HD2	1.86	0.41
1:G:227:PRO:HA	1:G:230:TYR:HD2	1.86	0.41
1:G:685:ILE:H	1:G:694:LYS:HD2	1.86	0.41
1:T:685:ILE:H	1:T:694:LYS:HD2	1.86	0.41
1:W:218:ASP:OD1	1:W:218:ASP:N	2.40	0.41
1:X:685:ILE:H	1:X:694:LYS:HD2	1.86	0.41
1:Z:227:PRO:HA	1:Z:230:TYR:HD2	1.86	0.41
1:Z:581:ASP:N	1:Z:581:ASP:OD1	2.52	0.41
1:B:249:PHE:HA	1:B:252:GLN:HB2	2.03	0.40
1:B:518:ILE:HG13	1:B:612:LEU:HA	2.02	0.40
1:C:681:SER:HA	1:C:726:ILE:O	2.20	0.40
1:E:847:THR:OG1	1:E:848:GLY:N	2.53	0.40
1:F:518:ILE:HG13	1:F:612:LEU:HA	2.02	0.40
1:T:245:TRP:CG	1:T:256:LYS:HD3	2.56	0.40
1:T:684:ILE:HA	1:T:694:LYS:HD2	2.02	0.40
1:U:237:ILE:HD13	1:U:237:ILE:HA	1.87	0.40
1:V:460:ILE:HD12	1:V:461:PRO:HD2	2.03	0.40
1:Z:245:TRP:CG	1:Z:256:LYS:HD3	2.56	0.40
1:A:259:SER:OG	1:A:273:ASP:OD2	2.36	0.40
1:B:380:SER:OG	1:C:315:ALA:O	2.31	0.40
1:D:227:PRO:HA	1:D:230:TYR:HD2	1.86	0.40
1:D:249:PHE:HA	1:D:252:GLN:HB2	2.03	0.40
1:D:785:GLY:HA2	1:D:842:LEU:H	1.86	0.40
1:F:422:ILE:HD13	1:F:422:ILE:HA	1.88	0.40
1:G:785:GLY:HA2	1:G:842:LEU:H	1.86	0.40
1:T:656:ILE:HD13	1:T:656:ILE:HA	1.93	0.40
1:V:249:PHE:HA	1:V:252:GLN:HB2	2.03	0.40
1:V:422:ILE:HD13	1:V:422:ILE:HA	1.88	0.40
1:V:685:ILE:H	1:V:694:LYS:HD2	1.86	0.40
1:X:227:PRO:HA	1:X:230:TYR:HD2	1.86	0.40
1:B:433:LEU:HD12	1:B:433:LEU:HA	1.89	0.40
1:C:460:ILE:HD12	1:C:461:PRO:HD2	2.02	0.40
1:D:803:LYS:HB2	1:D:861:TYR:HB2	2.02	0.40
1:E:785:GLY:HA2	1:E:842:LEU:H	1.86	0.40
1:F:460:ILE:HD12	1:F:461:PRO:HD2	2.03	0.40
1:T:460:ILE:HD12	1:T:461:PRO:HD2	2.03	0.40
1:U:249:PHE:HA	1:U:252:GLN:HB2	2.03	0.40
1:U:545:LEU:HD23	1:U:545:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:803:LYS:HB2	1:U:861:TYR:HB2	2.02	0.40
1:V:681:SER:HA	1:V:726:ILE:O	2.20	0.40
1:Y:785:GLY:HA2	1:Y:842:LEU:H	1.86	0.40
1:D:460:ILE:HD12	1:D:461:PRO:HD2	2.02	0.40
1:F:684:ILE:HA	1:F:694:LYS:HD2	2.02	0.40
1:V:785:GLY:HA2	1:V:842:LEU:H	1.86	0.40
1:W:518:ILE:HG13	1:W:612:LEU:HA	2.02	0.40
1:W:803:LYS:HB2	1:W:861:TYR:HB2	2.02	0.40
1:Z:785:GLY:HA2	1:Z:842:LEU:H	1.86	0.40
1:B:748:LEU:HD23	1:B:748:LEU:HA	1.93	0.40
1:B:803:LYS:HB2	1:B:861:TYR:HB2	2.03	0.40
1:E:684:ILE:HA	1:E:694:LYS:HD2	2.02	0.40
1:T:422:ILE:HD13	1:T:422:ILE:HA	1.88	0.40
1:T:803:LYS:HB2	1:T:861:TYR:HB2	2.03	0.40
1:W:786:MET:O	1:W:839:TYR:HA	2.21	0.40
1:X:249:PHE:HA	1:X:252:GLN:HB2	2.03	0.40
1:Y:786:MET:O	1:Y:839:TYR:HA	2.21	0.40
1:Z:706:LYS:HE2	1:Z:706:LYS:HB3	1.92	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	614/876 (70%)	550 (90%)	64 (10%)	0	100	100
1	B	614/876 (70%)	549 (89%)	65 (11%)	0	100	100
1	C	614/876 (70%)	550 (90%)	64 (10%)	0	100	100
1	D	614/876 (70%)	549 (89%)	65 (11%)	0	100	100
1	E	614/876 (70%)	549 (89%)	65 (11%)	0	100	100
1	F	614/876 (70%)	550 (90%)	64 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	614/876 (70%)	550 (90%)	64 (10%)	0	100	100
1	T	614/876 (70%)	551 (90%)	63 (10%)	0	100	100
1	U	614/876 (70%)	548 (89%)	66 (11%)	0	100	100
1	V	614/876 (70%)	549 (89%)	65 (11%)	0	100	100
1	W	614/876 (70%)	549 (89%)	65 (11%)	0	100	100
1	X	614/876 (70%)	550 (90%)	64 (10%)	0	100	100
1	Y	614/876 (70%)	547 (89%)	67 (11%)	0	100	100
1	Z	614/876 (70%)	551 (90%)	63 (10%)	0	100	100
All	All	8596/12264 (70%)	7692 (90%)	904 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	B	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	C	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	D	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	E	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	F	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	G	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	T	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	U	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	V	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	W	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	X	550/790 (70%)	526 (96%)	24 (4%)	28	53
1	Y	550/790 (70%)	526 (96%)	24 (4%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Z	550/790 (70%)	526 (96%)	24 (4%)	28 53
All	All	7700/11060 (70%)	7364 (96%)	336 (4%)	32 53

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	SER
1	A	269	ASP
1	A	322	THR
1	A	324	SER
1	A	367	VAL
1	A	370	SER
1	A	407	THR
1	A	445	SER
1	A	502	SER
1	A	504	SER
1	A	531	THR
1	A	581	ASP
1	A	635	VAL
1	A	636	ASN
1	A	637	THR
1	A	663	LEU
1	A	680	THR
1	A	708	SER
1	A	726	ILE
1	A	738	ILE
1	A	753	VAL
1	A	755	ILE
1	A	777	SER
1	A	847	THR
1	B	264	SER
1	B	269	ASP
1	B	322	THR
1	B	324	SER
1	B	367	VAL
1	B	370	SER
1	B	407	THR
1	B	445	SER
1	B	502	SER
1	B	504	SER
1	B	531	THR
1	B	581	ASP

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Mol	Chain	Res	Type
1	B	635	VAL
1	B	636	ASN
1	B	637	THR
1	B	663	LEU
1	B	680	THR
1	B	708	SER
1	B	726	ILE
1	B	738	ILE
1	B	753	VAL
1	B	755	ILE
1	B	777	SER
1	B	847	THR
1	C	264	SER
1	C	269	ASP
1	C	322	THR
1	C	324	SER
1	C	367	VAL
1	C	370	SER
1	C	407	THR
1	C	445	SER
1	C	502	SER
1	C	504	SER
1	C	531	THR
1	C	581	ASP
1	C	635	VAL
1	C	636	ASN
1	C	637	THR
1	C	663	LEU
1	C	680	THR
1	C	708	SER
1	C	726	ILE
1	C	738	ILE
1	C	753	VAL
1	C	755	ILE
1	C	777	SER
1	C	847	THR
1	D	264	SER
1	D	269	ASP
1	D	322	THR
1	D	324	SER
1	D	367	VAL
1	D	370	SER

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Mol	Chain	Res	Type
1	D	407	THR
1	D	445	SER
1	D	502	SER
1	D	504	SER
1	D	531	THR
1	D	581	ASP
1	D	635	VAL
1	D	636	ASN
1	D	637	THR
1	D	663	LEU
1	D	680	THR
1	D	708	SER
1	D	726	ILE
1	D	738	ILE
1	D	753	VAL
1	D	755	ILE
1	D	777	SER
1	D	847	THR
1	E	264	SER
1	E	269	ASP
1	E	322	THR
1	E	324	SER
1	E	367	VAL
1	E	370	SER
1	E	407	THR
1	E	445	SER
1	E	502	SER
1	E	504	SER
1	E	531	THR
1	E	581	ASP
1	E	635	VAL
1	E	636	ASN
1	E	637	THR
1	E	663	LEU
1	E	680	THR
1	E	708	SER
1	E	726	ILE
1	E	738	ILE
1	E	753	VAL
1	E	755	ILE
1	E	777	SER
1	E	847	THR

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Mol	Chain	Res	Type
1	F	264	SER
1	F	269	ASP
1	F	322	THR
1	F	324	SER
1	F	367	VAL
1	F	370	SER
1	F	407	THR
1	F	445	SER
1	F	502	SER
1	F	504	SER
1	F	531	THR
1	F	581	ASP
1	F	635	VAL
1	F	636	ASN
1	F	637	THR
1	F	663	LEU
1	F	680	THR
1	F	708	SER
1	F	726	ILE
1	F	738	ILE
1	F	753	VAL
1	F	755	ILE
1	F	777	SER
1	F	847	THR
1	G	264	SER
1	G	269	ASP
1	G	322	THR
1	G	324	SER
1	G	367	VAL
1	G	370	SER
1	G	407	THR
1	G	445	SER
1	G	502	SER
1	G	504	SER
1	G	531	THR
1	G	581	ASP
1	G	635	VAL
1	G	636	ASN
1	G	637	THR
1	G	663	LEU
1	G	680	THR
1	G	708	SER

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Mol	Chain	Res	Type
1	G	726	ILE
1	G	738	ILE
1	G	753	VAL
1	G	755	ILE
1	G	777	SER
1	G	847	THR
1	T	264	SER
1	T	269	ASP
1	T	322	THR
1	T	324	SER
1	T	367	VAL
1	T	370	SER
1	T	407	THR
1	T	445	SER
1	T	502	SER
1	T	504	SER
1	T	531	THR
1	T	581	ASP
1	T	635	VAL
1	T	636	ASN
1	T	637	THR
1	T	663	LEU
1	T	680	THR
1	T	708	SER
1	T	726	ILE
1	T	738	ILE
1	T	753	VAL
1	T	755	ILE
1	T	777	SER
1	T	847	THR
1	U	264	SER
1	U	269	ASP
1	U	322	THR
1	U	324	SER
1	U	367	VAL
1	U	370	SER
1	U	407	THR
1	U	445	SER
1	U	502	SER
1	U	504	SER
1	U	531	THR
1	U	581	ASP

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Mol	Chain	Res	Type
1	U	635	VAL
1	U	636	ASN
1	U	637	THR
1	U	663	LEU
1	U	680	THR
1	U	708	SER
1	U	726	ILE
1	U	738	ILE
1	U	753	VAL
1	U	755	ILE
1	U	777	SER
1	U	847	THR
1	V	264	SER
1	V	269	ASP
1	V	322	THR
1	V	324	SER
1	V	367	VAL
1	V	370	SER
1	V	407	THR
1	V	445	SER
1	V	502	SER
1	V	504	SER
1	V	531	THR
1	V	581	ASP
1	V	635	VAL
1	V	636	ASN
1	V	637	THR
1	V	663	LEU
1	V	680	THR
1	V	708	SER
1	V	726	ILE
1	V	738	ILE
1	V	753	VAL
1	V	755	ILE
1	V	777	SER
1	V	847	THR
1	W	264	SER
1	W	269	ASP
1	W	322	THR
1	W	324	SER
1	W	367	VAL
1	W	370	SER

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Mol	Chain	Res	Type
1	W	407	THR
1	W	445	SER
1	W	502	SER
1	W	504	SER
1	W	531	THR
1	W	581	ASP
1	W	635	VAL
1	W	636	ASN
1	W	637	THR
1	W	663	LEU
1	W	680	THR
1	W	708	SER
1	W	726	ILE
1	W	738	ILE
1	W	753	VAL
1	W	755	ILE
1	W	777	SER
1	W	847	THR
1	X	264	SER
1	X	269	ASP
1	X	322	THR
1	X	324	SER
1	X	367	VAL
1	X	370	SER
1	X	407	THR
1	X	445	SER
1	X	502	SER
1	X	504	SER
1	X	531	THR
1	X	581	ASP
1	X	635	VAL
1	X	636	ASN
1	X	637	THR
1	X	663	LEU
1	X	680	THR
1	X	708	SER
1	X	726	ILE
1	X	738	ILE
1	X	753	VAL
1	X	755	ILE
1	X	777	SER
1	X	847	THR

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Mol	Chain	Res	Type
1	Y	264	SER
1	Y	269	ASP
1	Y	322	THR
1	Y	324	SER
1	Y	367	VAL
1	Y	370	SER
1	Y	407	THR
1	Y	445	SER
1	Y	502	SER
1	Y	504	SER
1	Y	531	THR
1	Y	581	ASP
1	Y	635	VAL
1	Y	636	ASN
1	Y	637	THR
1	Y	663	LEU
1	Y	680	THR
1	Y	708	SER
1	Y	726	ILE
1	Y	738	ILE
1	Y	753	VAL
1	Y	755	ILE
1	Y	777	SER
1	Y	847	THR
1	Z	264	SER
1	Z	269	ASP
1	Z	322	THR
1	Z	324	SER
1	Z	367	VAL
1	Z	370	SER
1	Z	407	THR
1	Z	445	SER
1	Z	502	SER
1	Z	504	SER
1	Z	531	THR
1	Z	581	ASP
1	Z	635	VAL
1	Z	636	ASN
1	Z	637	THR
1	Z	663	LEU
1	Z	680	THR
1	Z	708	SER

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Mol	Chain	Res	Type
1	Z	726	ILE
1	Z	738	ILE
1	Z	753	VAL
1	Z	755	ILE
1	Z	777	SER
1	Z	847	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	427	ASN
1	A	640	GLN
1	A	648	ASN
1	A	827	ASN
1	A	838	ASN
1	B	425	GLN
1	B	427	ASN
1	B	640	GLN
1	B	648	ASN
1	B	735	ASN
1	B	827	ASN
1	B	838	ASN
1	C	425	GLN
1	C	427	ASN
1	C	640	GLN
1	C	648	ASN
1	C	827	ASN
1	C	838	ASN
1	D	425	GLN
1	D	427	ASN
1	D	640	GLN
1	D	648	ASN
1	D	827	ASN
1	D	838	ASN
1	E	425	GLN
1	E	427	ASN
1	E	640	GLN
1	E	648	ASN
1	E	827	ASN
1	E	838	ASN
1	F	425	GLN

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Mol	Chain	Res	Type
1	F	427	ASN
1	F	640	GLN
1	F	648	ASN
1	F	827	ASN
1	F	838	ASN
1	G	425	GLN
1	G	427	ASN
1	G	640	GLN
1	G	648	ASN
1	G	827	ASN
1	G	838	ASN
1	T	425	GLN
1	T	427	ASN
1	T	640	GLN
1	T	648	ASN
1	T	827	ASN
1	T	838	ASN
1	U	425	GLN
1	U	427	ASN
1	U	640	GLN
1	U	648	ASN
1	U	827	ASN
1	U	838	ASN
1	V	425	GLN
1	V	427	ASN
1	V	640	GLN
1	V	648	ASN
1	V	827	ASN
1	V	838	ASN
1	W	265	ASN
1	W	425	GLN
1	W	427	ASN
1	W	640	GLN
1	W	648	ASN
1	W	827	ASN
1	W	838	ASN
1	X	425	GLN
1	X	427	ASN
1	X	640	GLN
1	X	648	ASN
1	X	827	ASN
1	X	838	ASN

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Mol	Chain	Res	Type
1	Y	425	GLN
1	Y	427	ASN
1	Y	640	GLN
1	Y	648	ASN
1	Y	827	ASN
1	Y	838	ASN
1	Z	425	GLN
1	Z	427	ASN
1	Z	640	GLN
1	Z	648	ASN
1	Z	827	ASN
1	Z	838	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

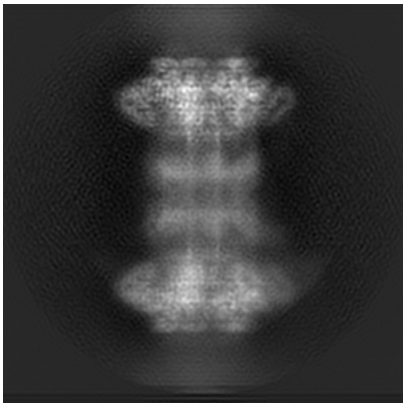
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0608. These allow visual inspection of the internal detail of the map and identification of artifacts.

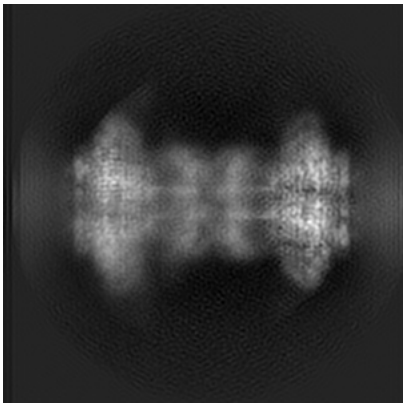
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

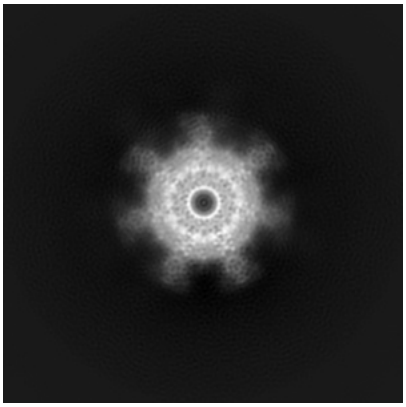
6.1.1 Primary map



X



Y

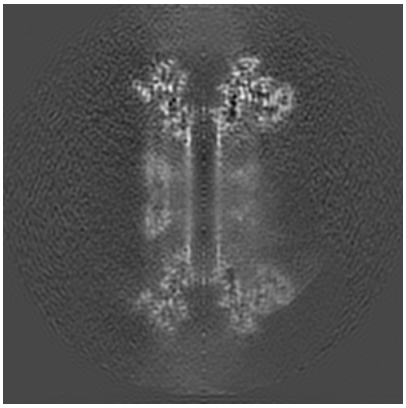


Z

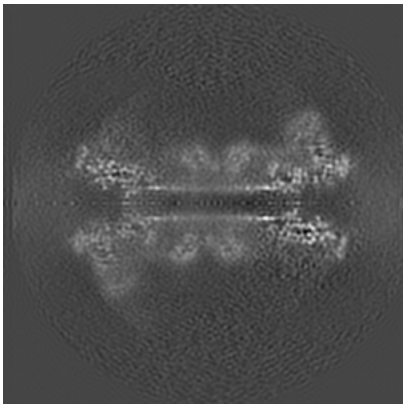
The images above show the map projected in three orthogonal directions.

6.2 Central slices

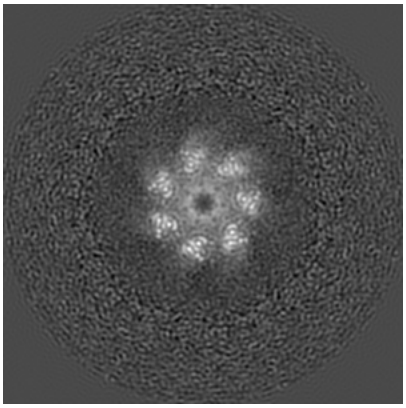
6.2.1 Primary map



X Index: 125



Y Index: 125

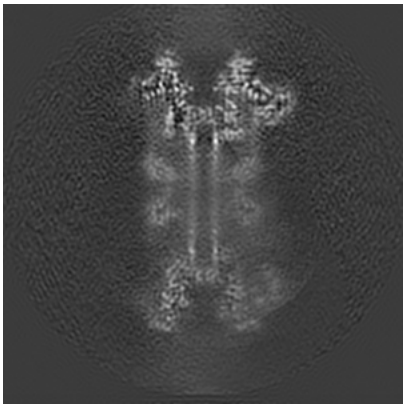


Z Index: 125

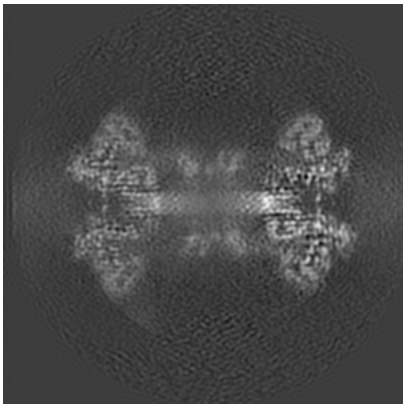
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

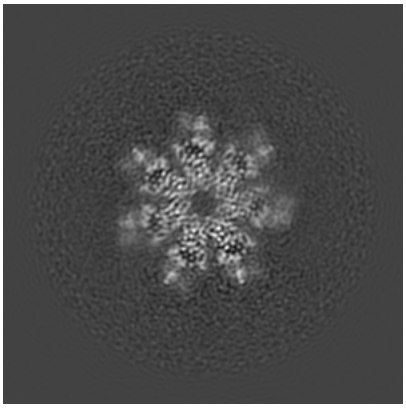
6.3.1 Primary map



X Index: 119



Y Index: 116



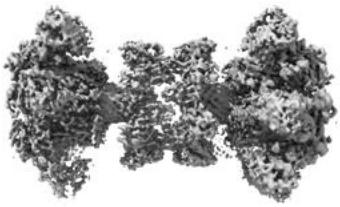
Z Index: 196

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

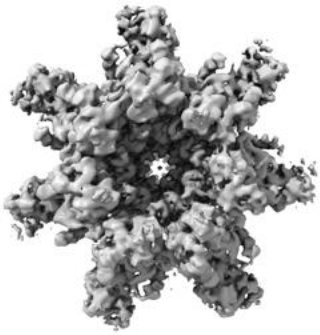
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

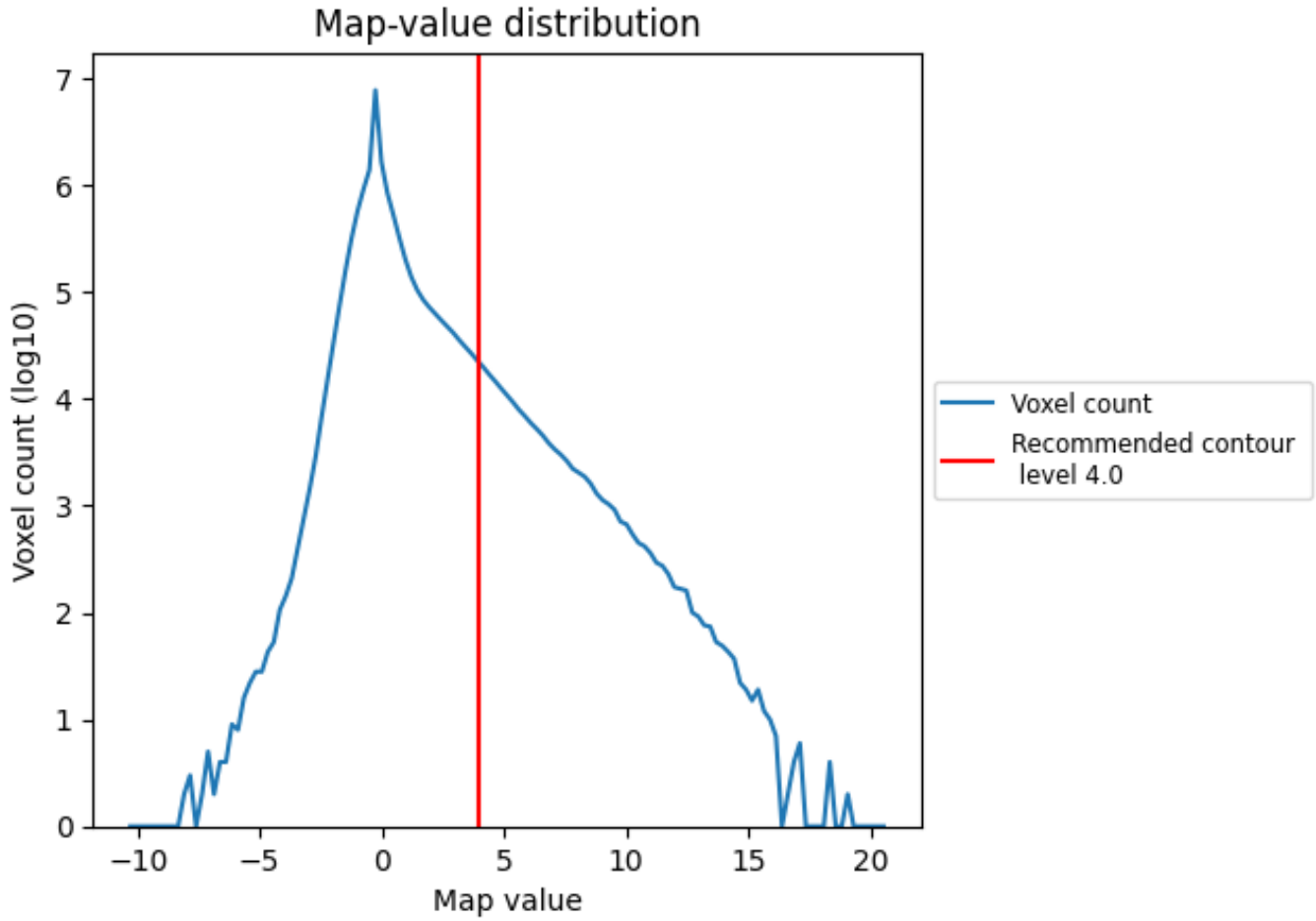
6.5 Mask visualisation (i)

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

7 Map analysis

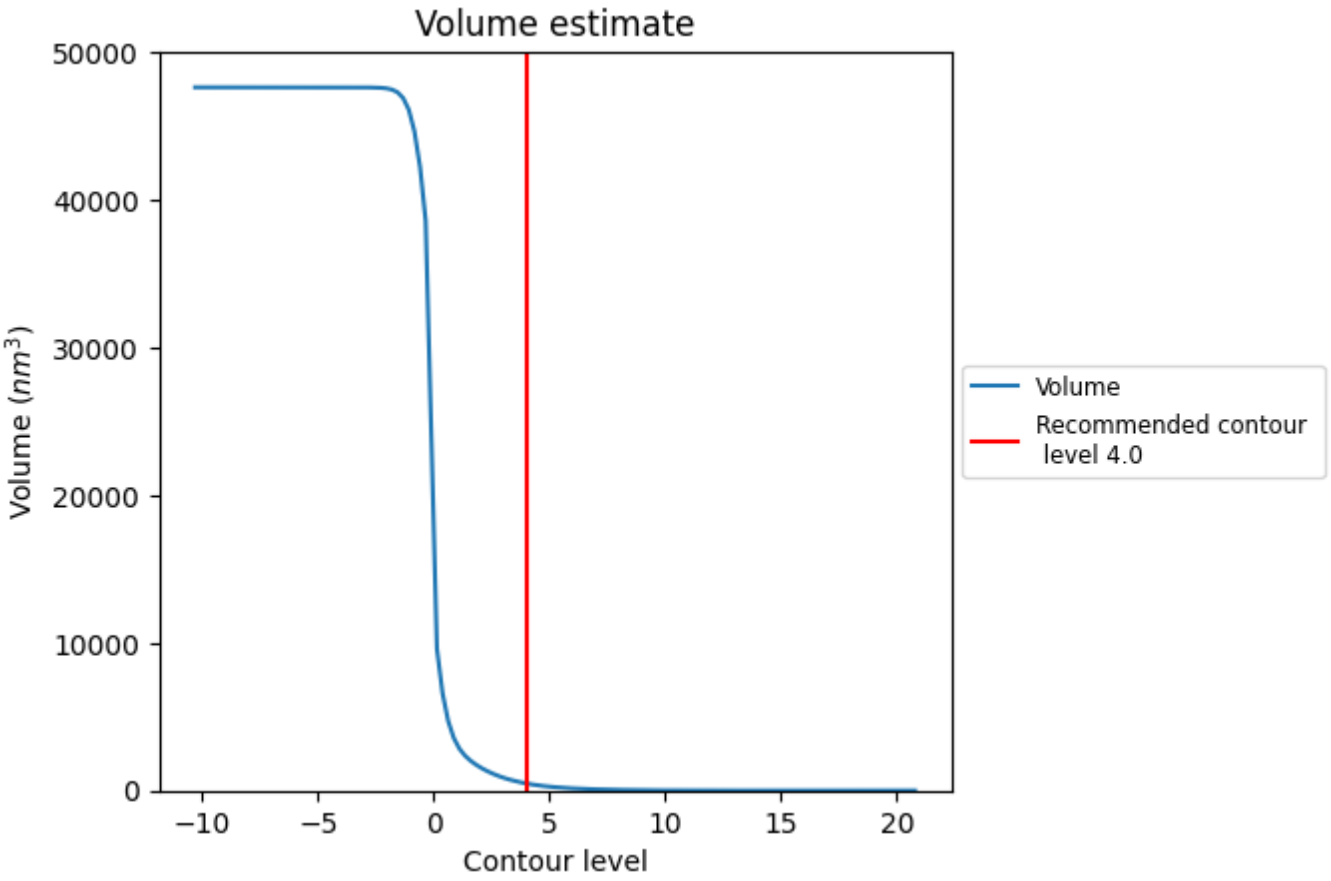
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

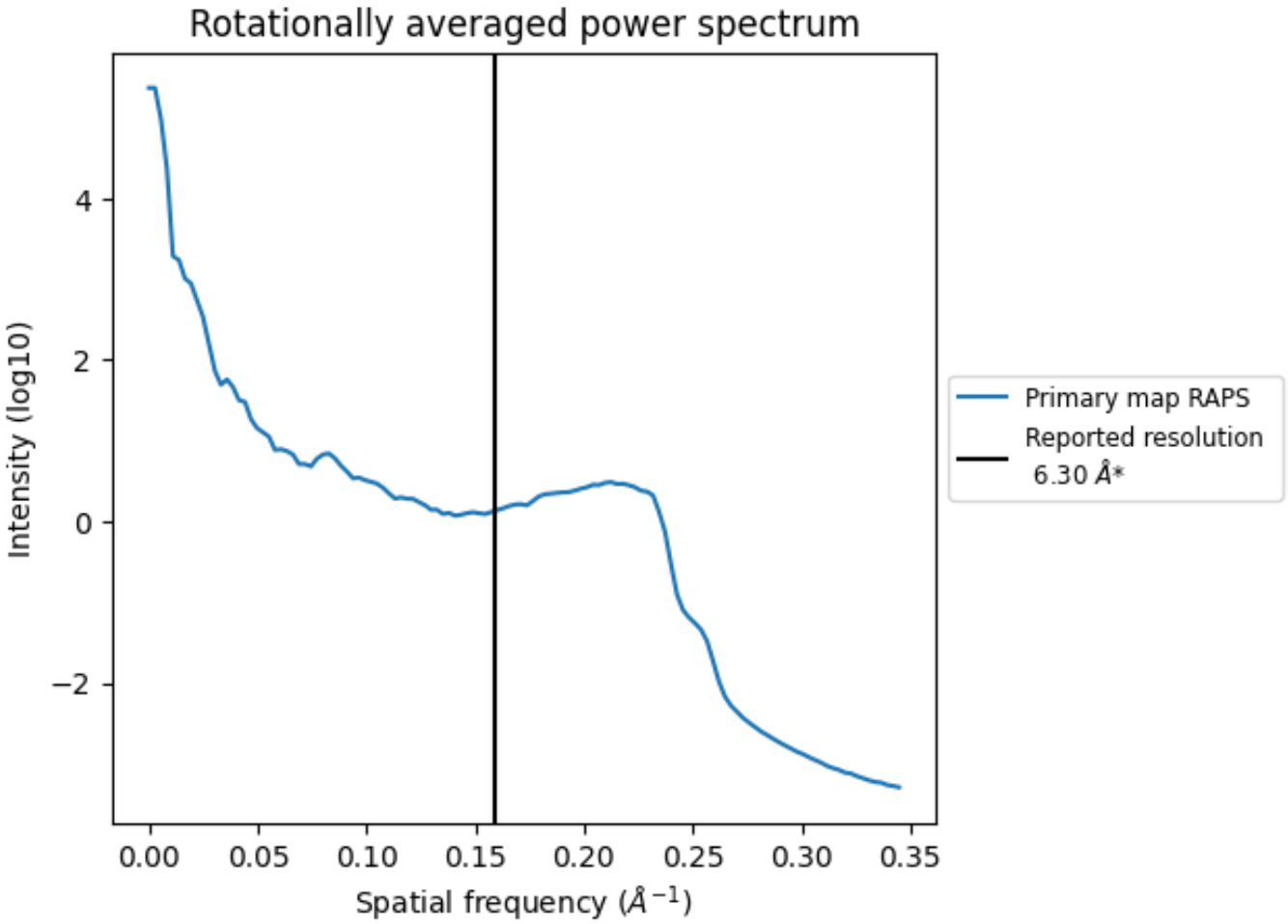
7.2 Volume estimate



The volume at the recommended contour level is 481 nm^3; this corresponds to an approximate mass of 434 kDa.

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

7.3 Rotationally averaged power spectrum (i)

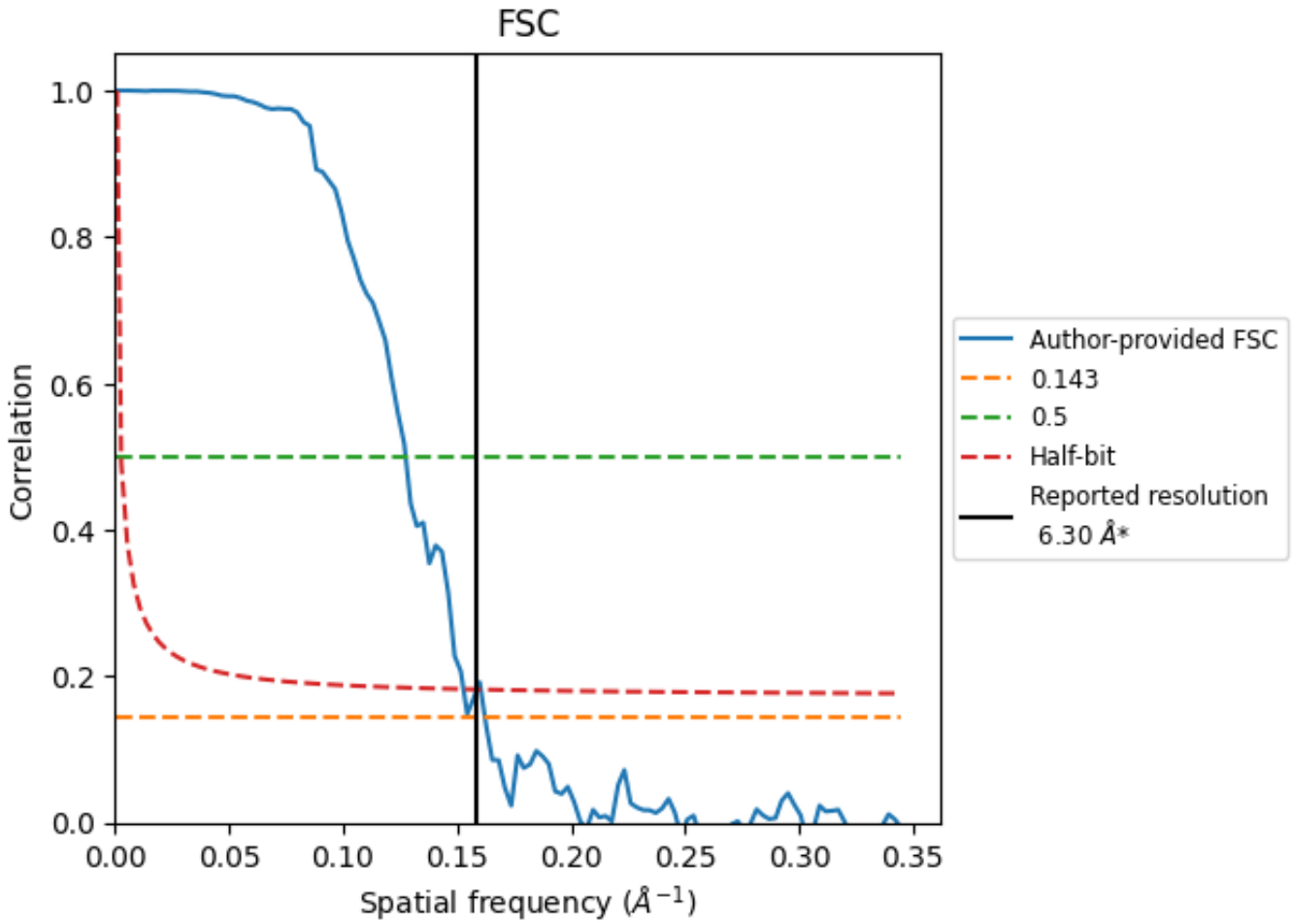


*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

8.2 Resolution estimates (i)

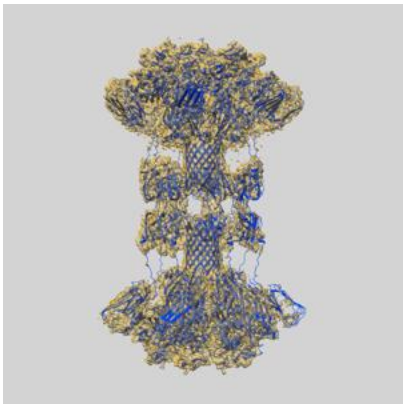
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.16	7.84	6.54
Unmasked-calculated*	-	-	-

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

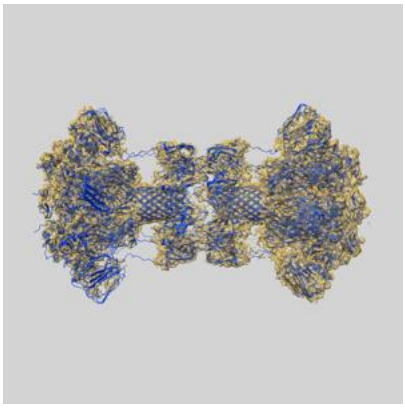
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0608 and PDB model 6O2M. Per-residue inclusion information can be found in section 3 on page 5.

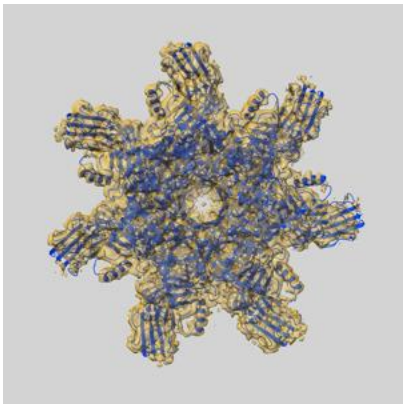
9.1 Map-model overlay



X



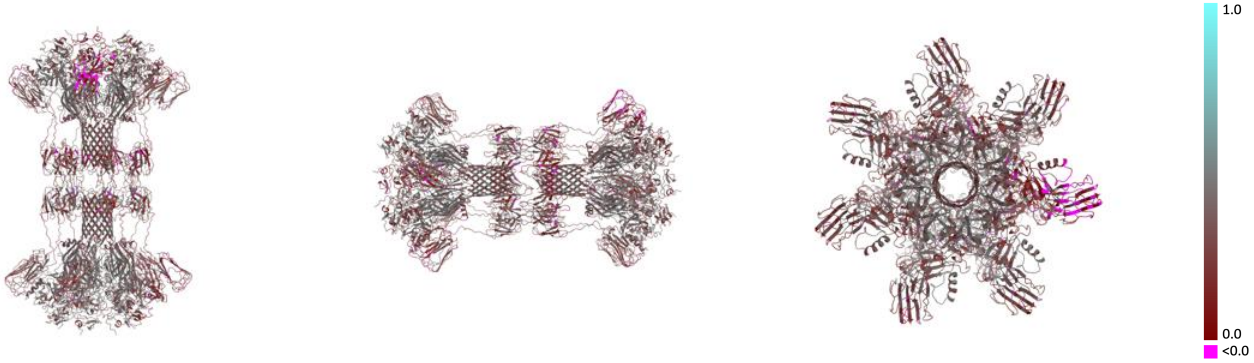
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

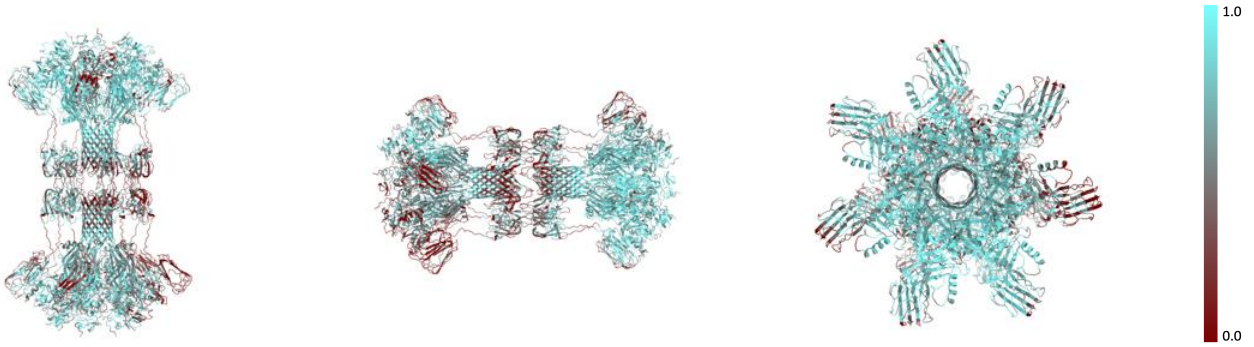
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

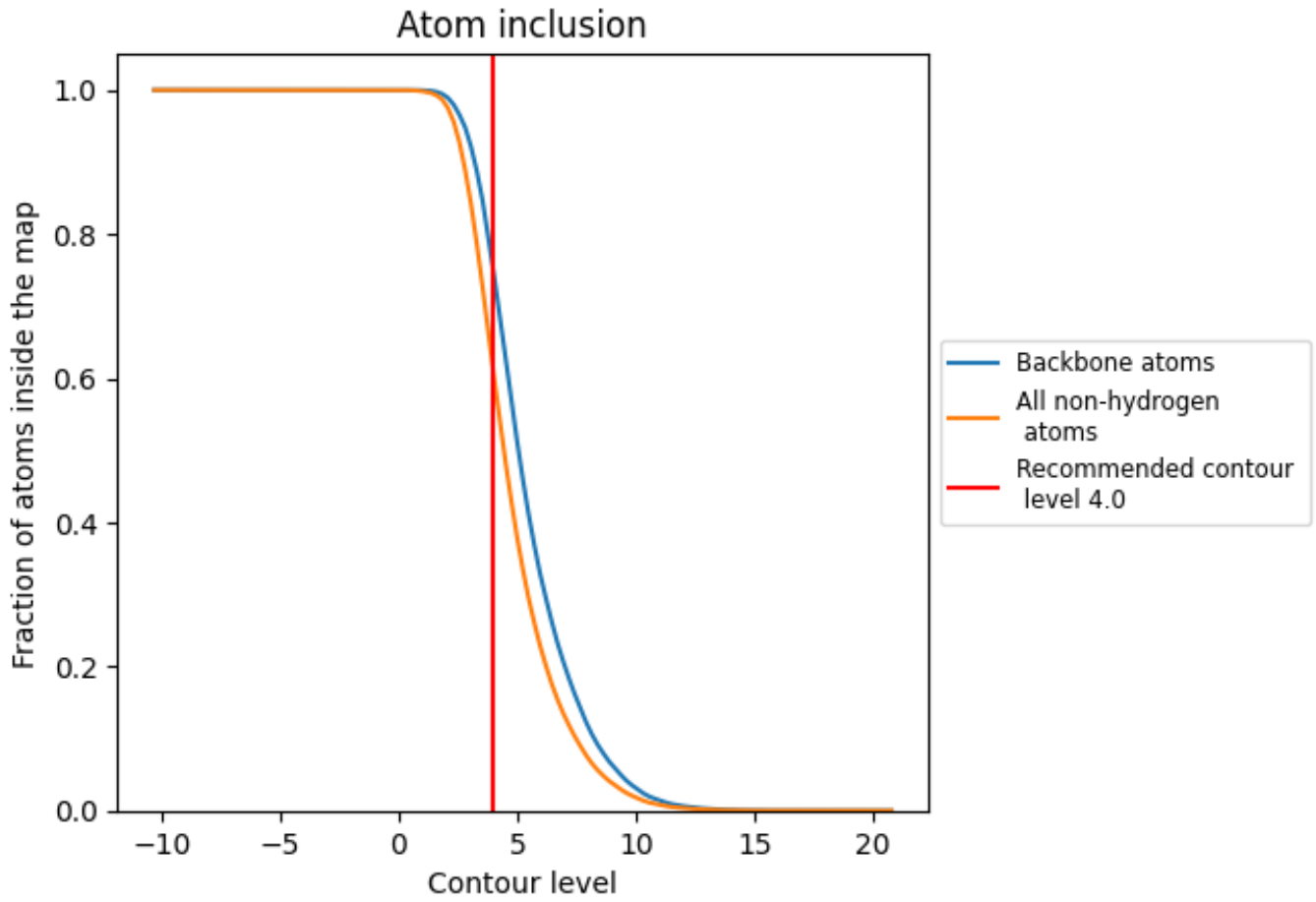
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 61% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6078	0.3360
A	0.3840	0.2940
B	0.6204	0.3640
C	0.5953	0.3620
D	0.6623	0.3650
E	0.5756	0.3610
F	0.4844	0.3590
G	0.3474	0.3280
T	0.7194	0.3360
U	0.7169	0.3370
V	0.6407	0.3180
W	0.5714	0.2390
X	0.7518	0.3530
Y	0.7493	0.3480
Z	0.6910	0.3410