Full wwPDB EM Validation Report ⓘ

Sep 2, 2024 – 12:20 PM JST

PDB ID	:	8Y3Y
EMDB ID	:	EMD-38907
Title	:	The Cryo-EM structure of anti-phage defense associated DSR2 tetramer bound with two DSAD1 inhibitors (opposite side)
Authors	:	Wang, R.W.; Xu, Q.; Wu, Z.X.; Li, J.L.; Shi, Z.B.; Li, F.X.
Deposited on	:	2024-01-29
Resolution	:	3.33 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:

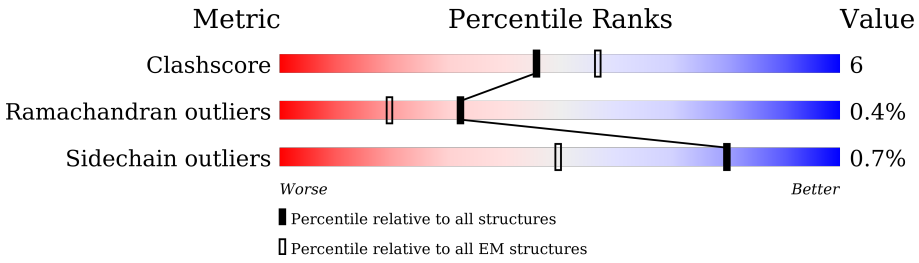
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 3.33 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1005	43% 79% 15% • 5%
1	B	1005	• 80% 15% 5%
1	D	1005	54% 80% 15% 5%
1	E	1005	19% 79% 15% 5%
2	C	120	5% 67% 18% 15%
2	F	120	30% 68% 18% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33586 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	957	Total	C	N	O	S	0	0
			7968	5155	1282	1499	32		
1	B	958	Total	C	N	O	S	0	0
			7996	5178	1290	1497	31		
1	D	957	Total	C	N	O	S	0	0
			7968	5155	1282	1499	32		
1	E	958	Total	C	N	O	S	0	0
			7996	5178	1290	1497	31		

- Molecule 2 is a protein called DSR anti-defence 1.

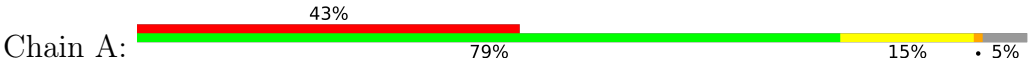
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	102	Total	C	N	O	S	0	0
			829	544	133	150	2		
2	F	102	Total	C	N	O	S	0	0
			829	544	133	150	2		

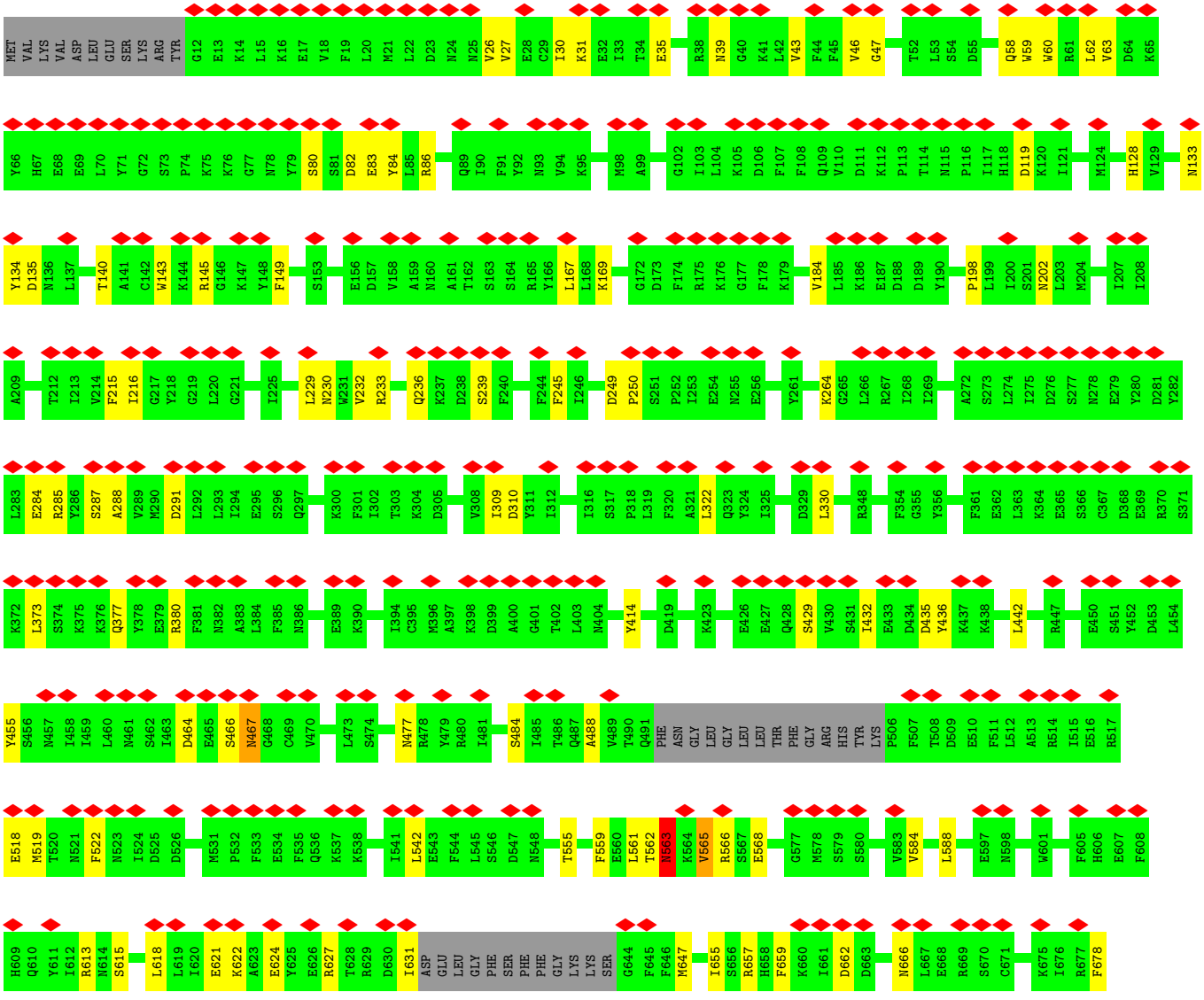
3 Residue-property plots (i)

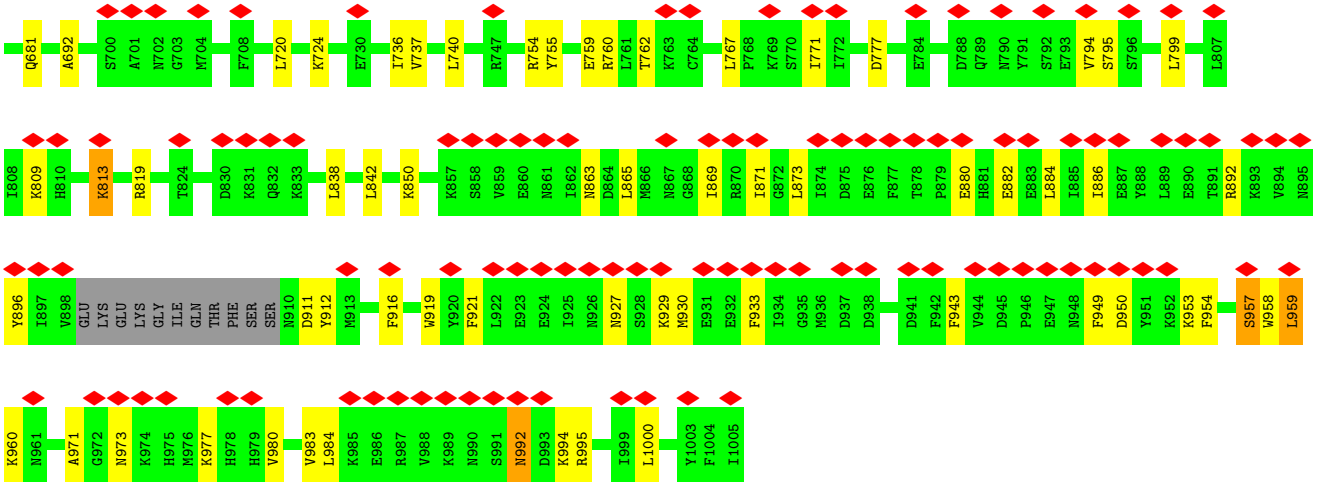
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SIR2-like domain-containing protein

Chain A:

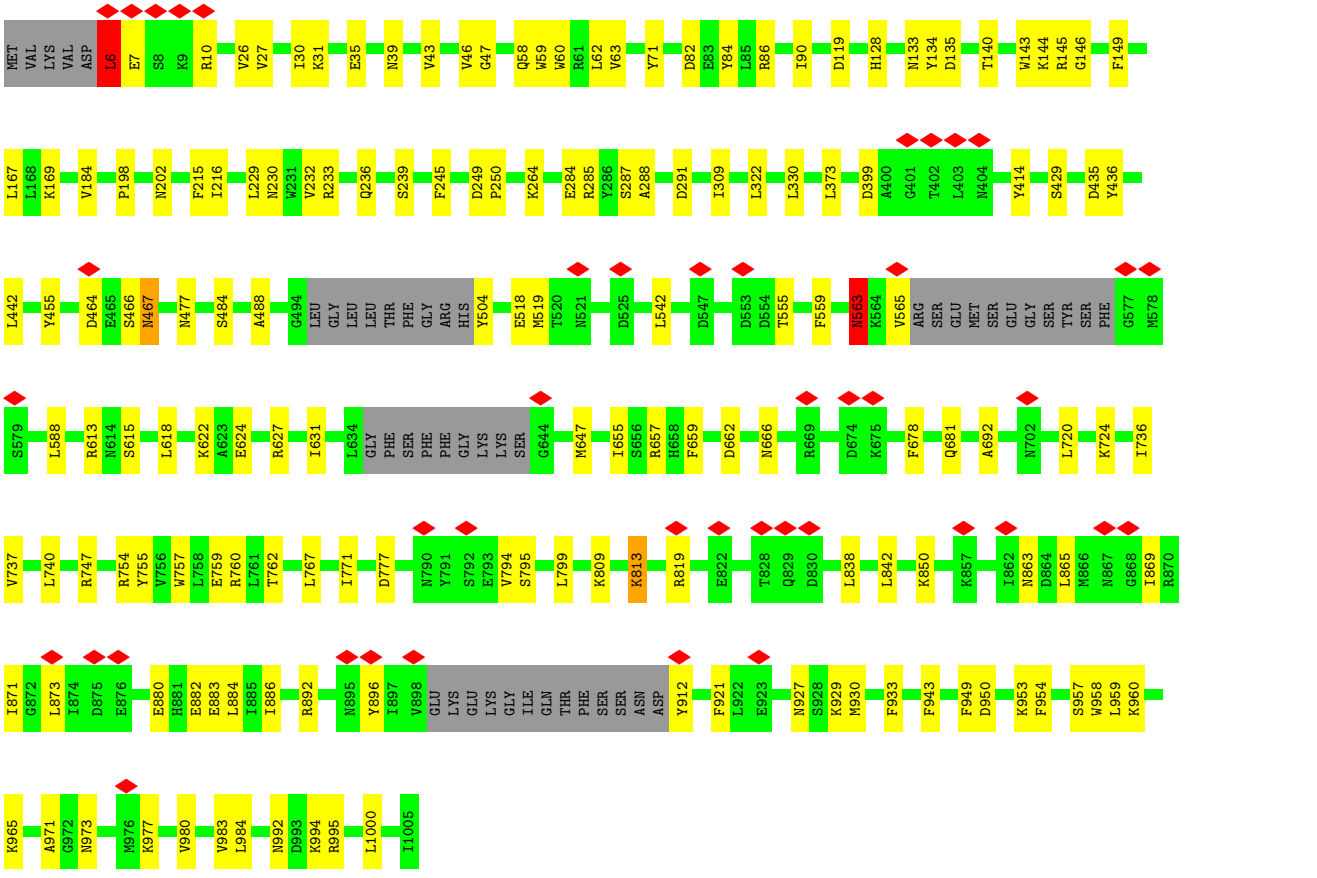






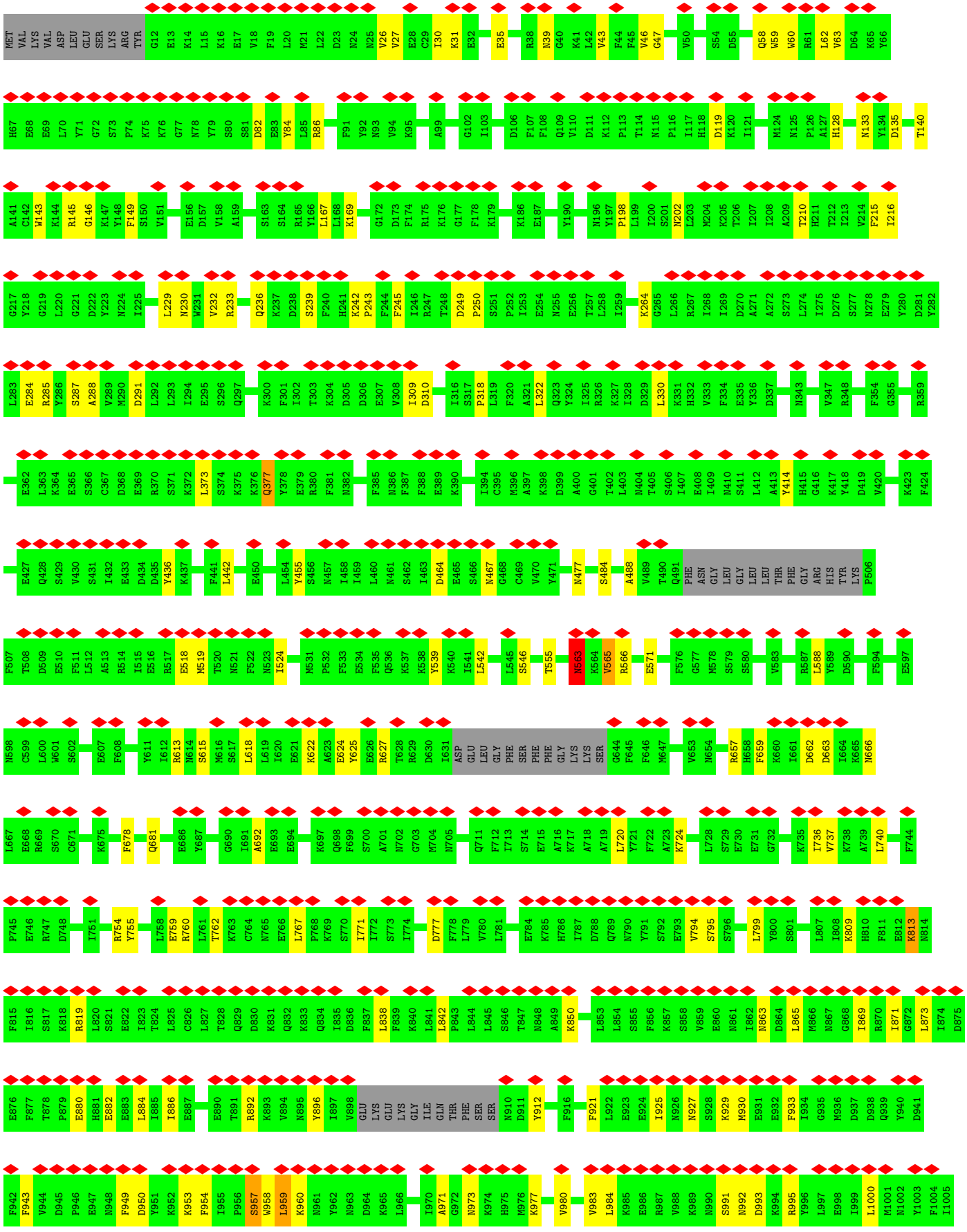
• Molecule 1: SIR2-like domain-containing protein

Chain B:



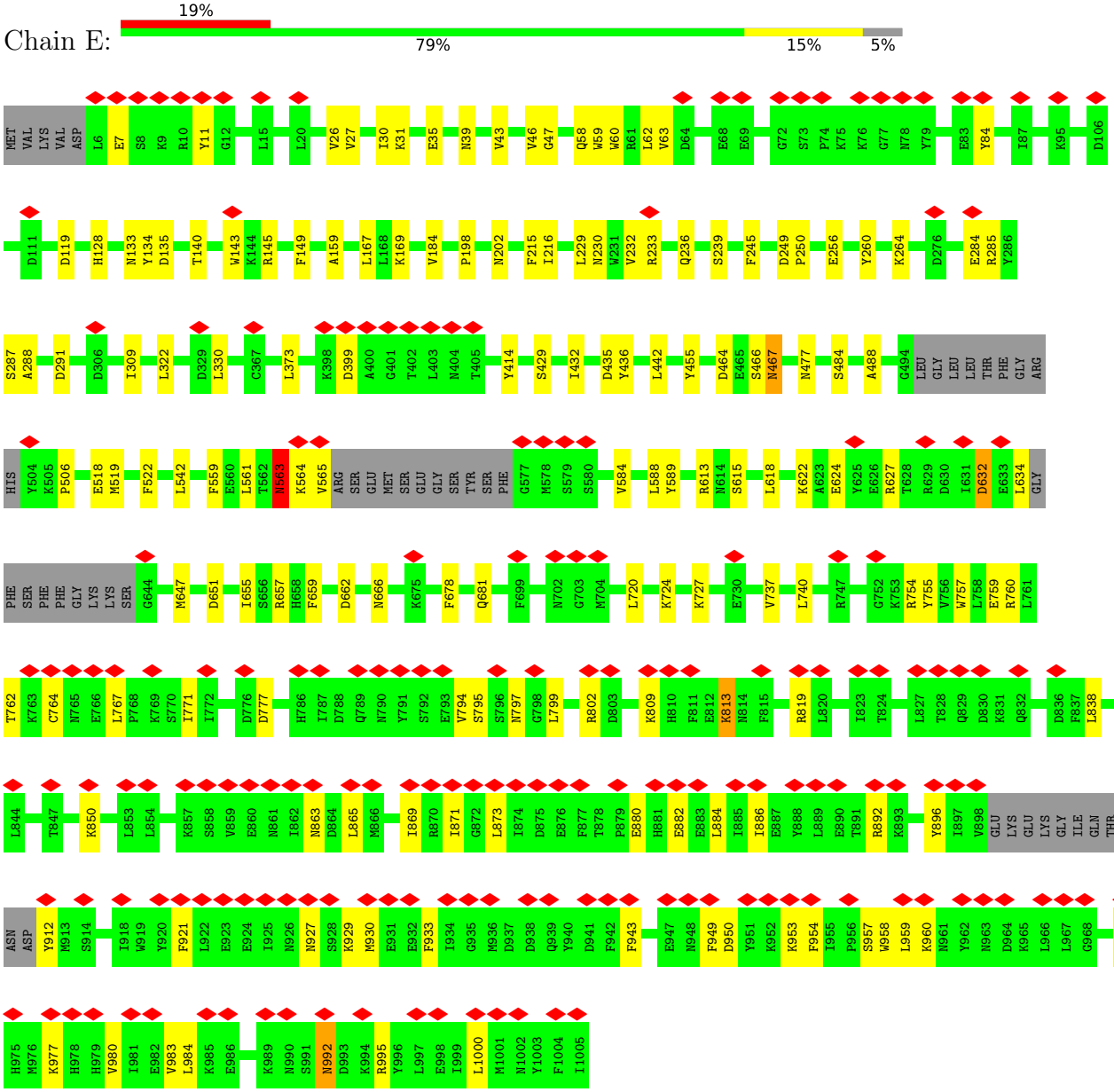
• Molecule 1: SIR2-like domain-containing protein

Chain D:


MET VAL LYS VAL ASP LEU GLU SER LYS ARG TYR G12 E13 K14 L15 K16 E17 V18 F19 L20 M21 L22 D23 N24 N25 V26 V27 E28 C29 I30 K31 E32 E35 R38 N39 G40 K41 L42 V43 F44 F45 V46 G47 V50 S54 D55 Q58 W59 W60 R61 L62 V63 D64 K65 Y66
H67 E68 E69 L70 Y71 G72 S73 P74 K75 K76 G77 N78 Y79 S80 S81 D82 E83 Y84 L85 R86 F91 Y92 N93 V94 K95 A99 G102 I103 D106 F107 F108 Q109 V110 D111 K112 P113 T114 N115 P116 I117 H118 D119 K120 I121 M124 N125 P126 A127 H128 N133 Y134 D135 T140
A141 C142 W143 K144 R145 G146 K147 Y148 F149 S150 V151 E156 D157 V158 A159 S163 S164 R165 Y166 L167 L168 K169 G172 D173 F174 R175 K176 G177 F178 K179 K186 E187 Y190 N196 Y197 P198 L199 I200 S201 N202 L203 M204 K205 T206 I207 I208 A209 T210 H211 T212 I213 V214 F215 I216
G217 Y218 G219 L220 G221 D222 Y223 N224 I225 L229 N230 W231 V232 R233 Q236 K237 D238 S239 F240 H241 K242 P243 F244 F245 I246 R247 T248 D249 P250 S251 P252 I253 E254 N255 E256 T257 L258 I259 K264 G265 L266 R267 I268 I269 D270 A271 A272 S273 L274 I275 D276 S277 N278 E279 Y280 D281 Y282
L283 E284 R285 Y286 S287 A288 V289 M290 D291 L292 L293 I294 E295 S296 Q297 K300 F301 I302 T303 K304 D305 D306 E307 V308 I309 D310 I316 S317 P318 L319 F320 A321 L322 Q323 Y324 I325 R326 K327 I328 D329 L330 K331 H332 V333 F334 E335 Y336 D337 N343 V347 R348 F354 G355 R359
E362 L363 K364 E365 S366 C367 D368 E369 R370 S371 K372 L373 S374 K375 K376 Q377 Y378 E379 R380 F381 N382 F385 N386 F387 F388 E389 K390 I394 C395 M396 A397 K398 D399 A400 G401 T402 L403 N404 T405 S406 I407 E408 I409 N410 S411 L412 A413 Y414 H415 G416 K417 Y418 D419 V420 K423 F424
E427 Q428 S429 V430 S431 I432 E433 D434 D435 Y436 K437 F441 L442 E450 L454 Y455 S456 N457 I458 I459 L460 N461 S462 I463 D464 E465 S466 N467 G468 C469 V470 Y471 N477 S484 A488 V489 T490 Q491 PHE ASN GLY LEU GLY LEU LEU THR PHE GLY ARG HIS TYR LYS P506
F507 T508 D509 E510 F511 L512 A513 R514 I515 E516 R517 E518 M519 T520 N521 F522 N523 I524 M531 P532 F533 E534 F535 Q536 K537 K538 Y539 K540 I541 L542 L545 S546 T555 N563 K564 V565 R566 E571 F576 G577 M578 S579 S580 V583 R587 L588 Y589 D590 F594 E597
N598 C599 L600 W601 S602 E607 F608 Y611 I612 R613 N614 S615 M616 S617 L618 L619 I620 E621 K622 A623 E624 Y625 E626 R627 T628 R629 D630 I631 ASP GLU LEU GLY PHE SER PHE PHE GLY LYS LYS SER G644 F645 F646 M647 V653 N654 R657 H658 F659 K660 I661 D662 D663 I664 K665 N666
L667 E668 R669 S670 C671 K675 F678 Q681 E686 Y687 G690 I691 A692 E693 E694 K697 Q698 F699 S700 A701 N702 G703 M704 N705 Q711 F712 I713 S714 E715 A716 K717 A718 A719 L720 Y721 F722 A723 K724 L728 S729 E730 E731 G732 K735 I736 V737 K738 A739 L740 F744
P745 E746 R747 D748 I751 R754 Y755 L758 E759 R760 L761 T762 K763 C764 N765 E766 L767 P768 K769 S770 I771 I772 S773 I774 D777 F778 L779 V780 L781 E784 K785 H786 I787 D788 Q789 N790 Y791 S792 E793 V794 S795 S796 L799 Y800 S801 L807 I808 K809 H810 F811 E812 K813 N814
F815 I816 S817 K818 R819 L820 S821 E822 I823 T824 L825 C826 L827 T828 Q829 D830 K831 Q832 K833 Q834 I835 D836 F837 L838 F839 K840 L841 L842 P843 L844 L845 S846 T847 N848 A849 K850 L853 L854 S855 F856 K857 S858 V859 E860 N861 I862 N863 D864 L865 M866 N867 G868 I869 R870 I871 G872 L873 I874 D875
E876 F877 T878 P879 E880 H881 E882 E883 L884 I885 I886 E887 E890 T891 R892 K893 V894 N895 Y896 I897 V898 GLU LYS GLU LYS GLY ILE GLN THR PHE SER SER N910 D911 Y912 F916 F921 L922 E923 E924 I925 N926 N927 S928 K929 M930 E931 E932 F933 I934 G935 M936 D937 D938 Q939 Y940 D941
F942 F943 V944 D945 P946 E947 N948 F949 D950 Y951 K952 K953 F954 I955 P956 S957 W958 L959 K960 N961 Y962 N963 D964 K965 L966 I970 A971 G972 N973 K974 H975 M976 K977 V980 V983 L984 K985 E986 R987 V988 K989 N990 S991 N992 D993 K994 R995 Y996 L997 E998 I999 L1000 M1001 N1002 Y1003 F1004 I1005

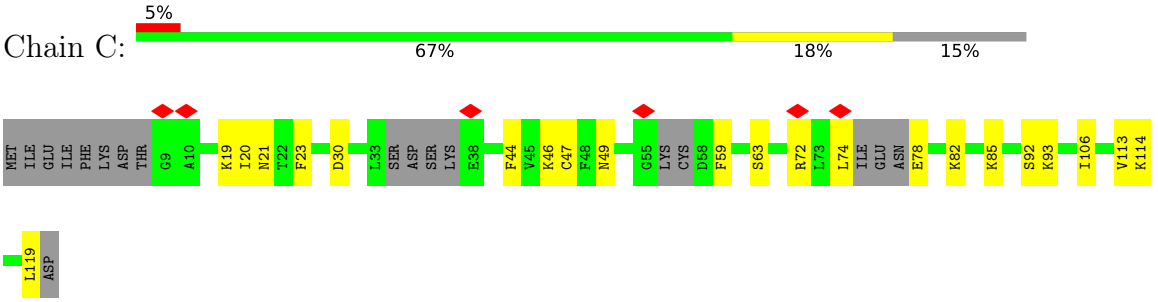
• Molecule 1: SIR2-like domain-containing protein

Chain E:



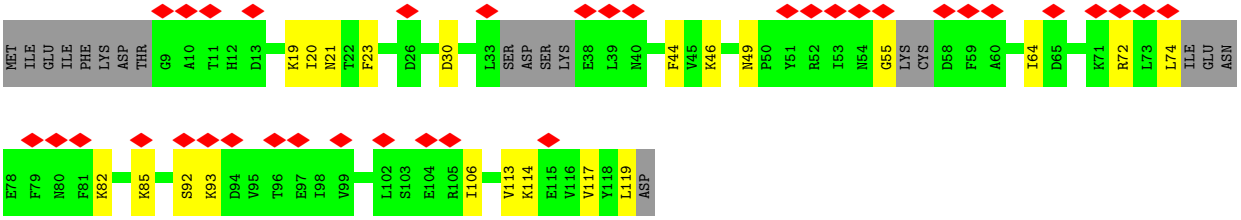
• Molecule 2: DSR anti-defence 1

Chain C:



• Molecule 2: DSR anti-defence 1

Chain F:


MET ILE GLU ILE PHE LYS ASP THR G9 A10 T11 H12 D13 K19 I20 N21 T22 F23 D26 D30 L33 SER ASP SER LYS E38 L39 N40 F44 V45 K46 N49 P50 Y51 R52 I53 N54 G55 LYS CYS D58 F59 A60 I64 D65 K71 R72 L73 L74 ILE GLU ASN
E78 F79 N80 F81 K82 K85 S92 K93 D94 V95 T96 E97 I98 V99 L102 S103 E104 R105 I106 V113 K114 E115 V116 V117 Y118 L119 ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	13000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.660	Depositor
Minimum map value	-0.368	Depositor
Average map value	0.031	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	430.91998, 430.91998, 430.91998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	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	0.39	0/8150	0.55	2/10979 (0.0%)
1	B	0.38	0/8178	0.55	3/11014 (0.0%)
1	D	0.39	0/8150	0.55	3/10979 (0.0%)
1	E	0.39	0/8178	0.55	2/11014 (0.0%)
2	C	0.44	0/847	0.63	0/1144
2	F	0.44	0/847	0.63	0/1144
All	All	0.39	0/34350	0.55	10/46274 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	3
1	D	0	4
1	E	0	4
2	C	0	1
2	F	0	1
All	All	0	19

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	442	LEU	CA-CB-CG	6.87	131.09	115.30
1	B	442	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	442	LEU	CA-CB-CG	6.84	131.04	115.30
1	E	442	LEU	CA-CB-CG	6.83	131.01	115.30
1	E	959	LEU	CA-CB-CG	5.54	128.04	115.30
1	D	959	LEU	CA-CB-CG	5.54	128.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	959	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	959	LEU	CA-CB-CG	5.52	127.99	115.30
1	D	377	GLN	CA-CB-CG	-5.27	101.81	113.40
1	B	6	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	563	ASN	Peptide
1	A	565	VAL	Peptide
1	A	568	GLU	Peptide
1	A	794	VAL	Peptide
1	A	911	ASP	Peptide
1	A	957	SER	Peptide
1	B	563	ASN	Peptide
1	B	794	VAL	Peptide
1	B	957	SER	Peptide
2	C	92	SER	Peptide
1	D	563	ASN	Peptide
1	D	565	VAL	Peptide
1	D	794	VAL	Peptide
1	D	957	SER	Peptide
1	E	563	ASN	Peptide
1	E	632	ASP	Peptide
1	E	794	VAL	Peptide
1	E	957	SER	Peptide
2	F	92	SER	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	7968	0	7798	101	0
1	B	7996	0	7845	102	0
1	D	7968	0	7798	93	0
1	E	7996	0	7845	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	829	0	820	15	0
2	F	829	0	820	14	0
All	All	33586	0	32926	397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (397) 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:B:912:TYR:HH	2:C:78:GLU:N	1.50	1.10
1:A:562:THR:O	1:A:566:ARG:HB2	1.61	0.99
1:D:892:ARG:O	1:D:896:TYR:HB2	1.73	0.88
1:B:892:ARG:O	1:B:896:TYR:HB2	1.73	0.88
1:A:892:ARG:O	1:A:896:TYR:HB2	1.73	0.88
1:E:892:ARG:O	1:E:896:TYR:HB2	1.73	0.87
1:A:563:ASN:O	1:A:566:ARG:N	2.17	0.76
1:A:559:PHE:HE2	1:B:555:THR:HG23	1.55	0.71
1:E:802:ARG:HH22	2:F:55:GLY:HA2	1.55	0.70
1:D:146:GLY:H	1:E:522:PHE:HA	1.56	0.70
1:D:284:GLU:O	1:D:288:ALA:HB2	1.93	0.69
1:A:284:GLU:O	1:A:288:ALA:HB2	1.93	0.69
1:A:618:LEU:HD11	1:B:559:PHE:HE1	1.58	0.69
1:E:284:GLU:O	1:E:288:ALA:HB2	1.93	0.68
1:B:284:GLU:O	1:B:288:ALA:HB2	1.93	0.67
1:A:886:ILE:HG12	1:A:929:LYS:HG2	1.77	0.67
1:D:886:ILE:HG12	1:D:929:LYS:HG2	1.77	0.67
1:E:886:ILE:HG12	1:E:929:LYS:HG2	1.77	0.66
1:D:563:ASN:O	1:D:566:ARG:N	2.24	0.66
1:B:886:ILE:HG12	1:B:929:LYS:HG2	1.77	0.65
1:B:504:TYR:OH	1:B:747:ARG:NH1	2.33	0.62
1:B:912:TYR:OH	2:C:78:GLU:N	2.29	0.61
1:D:146:GLY:N	1:E:522:PHE:HA	2.14	0.61
1:E:565:VAL:O	1:E:622:LYS:NZ	2.33	0.61
1:D:755:TYR:O	1:D:759:GLU:HB2	2.01	0.61
1:A:559:PHE:CE2	1:B:555:THR:HG23	2.36	0.61
1:A:994:LYS:HB2	1:B:631:ILE:HG12	1.80	0.61
1:A:755:TYR:O	1:A:759:GLU:HB2	2.01	0.61
1:A:565:VAL:O	1:A:622:LYS:NZ	2.33	0.61
1:B:755:TYR:O	1:B:759:GLU:HB2	2.01	0.61
1:E:755:TYR:O	1:E:759:GLU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:VAL:O	1:D:622:LYS:NZ	2.33	0.61
1:B:565:VAL:O	1:B:622:LYS:NZ	2.33	0.60
1:B:414:TYR:O	1:B:657:ARG:NH2	2.35	0.60
1:B:6:LEU:HD13	1:B:7:GLU:H	1.66	0.60
1:A:414:TYR:O	1:A:657:ARG:NH2	2.34	0.60
1:E:414:TYR:O	1:E:657:ARG:NH2	2.34	0.60
2:C:46:LYS:HE3	2:C:113:VAL:HG21	1.83	0.60
1:E:484:SER:O	1:E:488:ALA:HB2	2.02	0.59
1:B:484:SER:O	1:B:488:ALA:HB2	2.02	0.59
1:E:7:GLU:O	1:E:11:TYR:CB	2.50	0.59
1:A:149:PHE:HB3	1:A:167:LEU:HB2	1.85	0.59
1:B:149:PHE:HB3	1:B:167:LEU:HB2	1.85	0.59
1:D:484:SER:O	1:D:488:ALA:HB2	2.02	0.59
1:A:484:SER:O	1:A:488:ALA:HB2	2.02	0.59
1:D:149:PHE:HB3	1:D:167:LEU:HB2	1.85	0.59
1:D:414:TYR:O	1:D:657:ARG:NH2	2.34	0.59
2:F:46:LYS:HE3	2:F:113:VAL:HG21	1.83	0.59
1:B:236:GLN:OE1	1:B:239:SER:OG	2.21	0.58
2:C:72:ARG:HH21	2:C:74:LEU:HD21	1.68	0.58
1:D:236:GLN:OE1	1:D:239:SER:OG	2.21	0.58
1:B:7:GLU:HA	1:B:10:ARG:HB2	1.85	0.58
2:C:44:PHE:H	2:C:114:LYS:HD3	1.69	0.58
1:E:236:GLN:OE1	1:E:239:SER:OG	2.21	0.58
1:E:149:PHE:HB3	1:E:167:LEU:HB2	1.85	0.58
2:F:72:ARG:HH21	2:F:74:LEU:HD21	1.68	0.58
1:B:613:ARG:HA	1:B:659:PHE:HE1	1.69	0.58
1:A:613:ARG:HA	1:A:659:PHE:HE1	1.69	0.57
1:B:863:ASN:HD22	1:B:912:TYR:HD1	1.52	0.57
1:D:863:ASN:HD22	1:D:912:TYR:HD1	1.52	0.57
1:A:436:TYR:OH	1:A:477:ASN:ND2	2.38	0.57
1:A:624:GLU:OE2	1:A:627:ARG:NH2	2.38	0.57
1:B:43:VAL:HG22	1:B:128:HIS:H	1.70	0.57
1:E:588:LEU:HD11	1:E:615:SER:HB3	1.87	0.57
2:F:44:PHE:H	2:F:114:LYS:HD3	1.68	0.57
1:B:436:TYR:OH	1:B:477:ASN:ND2	2.38	0.57
1:E:624:GLU:OE2	1:E:627:ARG:NH2	2.38	0.57
1:A:980:VAL:HA	1:A:983:VAL:HG22	1.87	0.57
1:A:236:GLN:OE1	1:A:239:SER:OG	2.21	0.57
1:D:436:TYR:OH	1:D:477:ASN:ND2	2.38	0.57
1:D:624:GLU:OE2	1:D:627:ARG:NH2	2.38	0.57
1:E:436:TYR:OH	1:E:477:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LEU:HD11	1:A:615:SER:HB3	1.87	0.56
1:D:980:VAL:HA	1:D:983:VAL:HG22	1.87	0.56
1:B:624:GLU:OE2	1:B:627:ARG:NH2	2.38	0.56
1:E:43:VAL:HG22	1:E:128:HIS:H	1.70	0.56
1:D:588:LEU:HD11	1:D:615:SER:HB3	1.87	0.56
1:D:613:ARG:HA	1:D:659:PHE:HE1	1.69	0.56
1:D:230:ASN:OD1	1:D:233:ARG:NH2	2.37	0.56
1:A:43:VAL:HG22	1:A:128:HIS:H	1.70	0.56
1:D:43:VAL:HG22	1:D:128:HIS:H	1.70	0.56
1:E:613:ARG:HA	1:E:659:PHE:HE1	1.69	0.56
1:E:980:VAL:HA	1:E:983:VAL:HG22	1.87	0.56
1:B:980:VAL:HA	1:B:983:VAL:HG22	1.87	0.56
1:B:198:PRO:O	1:B:202:ASN:ND2	2.39	0.56
1:E:198:PRO:O	1:E:202:ASN:ND2	2.39	0.56
1:D:35:GLU:OE2	1:D:39:ASN:ND2	2.40	0.55
1:B:35:GLU:OE2	1:B:39:ASN:ND2	2.40	0.55
1:E:863:ASN:HD22	1:E:912:TYR:HD1	1.52	0.55
1:A:35:GLU:OE2	1:A:39:ASN:ND2	2.40	0.55
1:B:588:LEU:HD11	1:B:615:SER:HB3	1.87	0.55
1:D:198:PRO:O	1:D:202:ASN:ND2	2.39	0.55
1:E:35:GLU:OE2	1:E:39:ASN:ND2	2.40	0.55
1:A:863:ASN:HD22	1:A:912:TYR:HD1	1.52	0.55
1:B:762:THR:HB	1:B:767:LEU:HD21	1.89	0.55
1:A:198:PRO:O	1:A:202:ASN:ND2	2.39	0.54
1:A:566:ARG:HH22	1:A:621:GLU:HB2	1.72	0.54
1:B:950:ASP:OD2	1:B:953:LYS:NZ	2.40	0.54
1:D:950:ASP:OD2	1:D:953:LYS:NZ	2.40	0.54
1:E:230:ASN:OD1	1:E:233:ARG:NH2	2.37	0.54
1:A:871:ILE:HG13	1:A:873:LEU:HD23	1.90	0.54
1:E:762:THR:HB	1:E:767:LEU:HD21	1.89	0.54
1:D:871:ILE:HG13	1:D:873:LEU:HD23	1.90	0.54
1:A:842:LEU:HD22	1:A:871:ILE:HD12	1.90	0.54
1:A:950:ASP:OD2	1:A:953:LYS:NZ	2.40	0.54
1:D:842:LEU:HD22	1:D:871:ILE:HD12	1.90	0.54
1:E:871:ILE:HG13	1:E:873:LEU:HD23	1.90	0.54
1:E:797:ASN:HA	2:F:117:VAL:HG21	1.90	0.54
1:E:842:LEU:HD22	1:E:871:ILE:HD12	1.90	0.54
1:E:950:ASP:OD2	1:E:953:LYS:NZ	2.40	0.54
1:A:762:THR:HB	1:A:767:LEU:HD21	1.89	0.54
1:E:518:GLU:HG2	1:E:519:MET:HE2	1.91	0.53
1:A:310:ASP:OD1	1:A:377:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASN:OD1	1:B:233:ARG:NH2	2.37	0.53
2:F:20:ILE:HD12	2:F:46:LYS:HD2	1.90	0.53
1:D:762:THR:HB	1:D:767:LEU:HD21	1.89	0.53
1:D:518:GLU:HG2	1:D:519:MET:HE2	1.91	0.53
1:A:229:LEU:HA	1:A:232:VAL:HG22	1.91	0.53
2:C:20:ILE:HD12	2:C:46:LYS:HD2	1.90	0.53
1:A:230:ASN:OD1	1:A:233:ARG:NH2	2.37	0.52
1:B:229:LEU:HA	1:B:232:VAL:HG22	1.91	0.52
1:B:518:GLU:HG2	1:B:519:MET:HE2	1.92	0.52
1:B:842:LEU:HD22	1:B:871:ILE:HD12	1.90	0.52
1:D:755:TYR:O	1:D:759:GLU:CB	2.58	0.52
1:A:631:ILE:HG12	1:B:994:LYS:HB2	1.91	0.52
1:A:755:TYR:O	1:A:759:GLU:CB	2.58	0.52
1:D:777:ASP:OD1	1:D:819:ARG:NH2	2.43	0.52
1:E:740:LEU:O	1:E:754:ARG:NH1	2.43	0.52
1:A:777:ASP:OD1	1:A:819:ARG:NH2	2.43	0.52
1:D:863:ASN:HD22	1:D:912:TYR:HA	1.75	0.52
2:F:49:ASN:HB2	2:F:119:LEU:HD12	1.91	0.52
1:A:740:LEU:O	1:A:754:ARG:NH1	2.43	0.52
1:A:863:ASN:HD22	1:A:912:TYR:HA	1.75	0.52
1:B:755:TYR:O	1:B:759:GLU:CB	2.58	0.52
1:B:777:ASP:OD1	1:B:819:ARG:NH2	2.43	0.52
1:D:229:LEU:HA	1:D:232:VAL:HG22	1.90	0.52
1:E:7:GLU:O	1:E:11:TYR:HB3	2.10	0.52
1:E:755:TYR:O	1:E:759:GLU:CB	2.58	0.52
1:E:7:GLU:O	1:E:11:TYR:HB2	2.08	0.52
1:E:229:LEU:HA	1:E:232:VAL:HG22	1.91	0.52
1:B:871:ILE:HG13	1:B:873:LEU:HD23	1.90	0.52
2:C:49:ASN:HB2	2:C:119:LEU:HD12	1.91	0.52
2:C:47:CYS:HG	2:C:63:SER:HG	1.58	0.51
1:D:740:LEU:O	1:D:754:ARG:NH1	2.43	0.51
1:E:662:ASP:O	1:E:666:ASN:ND2	2.44	0.51
1:B:662:ASP:O	1:B:666:ASN:ND2	2.44	0.51
1:B:740:LEU:O	1:B:754:ARG:NH1	2.43	0.51
1:D:229:LEU:HD22	1:D:264:LYS:HG2	1.93	0.51
1:B:229:LEU:HD22	1:B:264:LYS:HG2	1.93	0.51
1:D:250:PRO:HA	1:D:285:ARG:HH12	1.76	0.51
1:E:777:ASP:OD1	1:E:819:ARG:NH2	2.43	0.51
1:A:250:PRO:HA	1:A:285:ARG:HH12	1.76	0.51
1:B:863:ASN:HD22	1:B:912:TYR:HA	1.75	0.50
1:A:518:GLU:HG2	1:A:519:MET:HE2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ASP:O	1:A:666:ASN:ND2	2.44	0.50
1:D:662:ASP:O	1:D:666:ASN:ND2	2.44	0.50
1:E:863:ASN:HD22	1:E:912:TYR:HA	1.75	0.50
1:E:724:LYS:HB2	1:E:760:ARG:HB3	1.94	0.50
2:F:30:ASP:HB2	2:F:85:LYS:HB3	1.93	0.50
1:A:229:LEU:HD22	1:A:264:LYS:HG2	1.93	0.50
1:B:250:PRO:HA	1:B:285:ARG:HH12	1.76	0.50
1:E:229:LEU:HD22	1:E:264:LYS:HG2	1.93	0.50
1:D:566:ARG:HA	1:D:625:TYR:CE2	2.46	0.49
1:D:892:ARG:O	1:D:896:TYR:CB	2.55	0.49
1:E:135:ASP:O	1:E:169:LYS:NZ	2.45	0.49
1:E:250:PRO:HA	1:E:285:ARG:HH12	1.76	0.49
1:B:921:PHE:HB2	1:B:943:PHE:HB3	1.94	0.49
1:E:119:ASP:OD1	1:E:145:ARG:NH2	2.42	0.49
1:B:58:GLN:OE1	1:B:60:TRP:NE1	2.38	0.49
2:C:30:ASP:HB2	2:C:85:LYS:HB3	1.93	0.49
1:D:993:ASP:HB2	1:E:634:LEU:HD11	1.94	0.49
1:A:724:LYS:HB2	1:A:760:ARG:HB3	1.94	0.49
1:B:724:LYS:HB2	1:B:760:ARG:HB3	1.94	0.49
1:D:921:PHE:HB2	1:D:943:PHE:HB3	1.94	0.49
1:B:135:ASP:O	1:B:169:LYS:NZ	2.45	0.49
1:D:724:LYS:HB2	1:D:760:ARG:HB3	1.94	0.49
1:A:921:PHE:HB2	1:A:943:PHE:HB3	1.94	0.48
1:D:310:ASP:OD1	1:D:377:GLN:NE2	2.46	0.48
1:E:921:PHE:HB2	1:E:943:PHE:HB3	1.94	0.48
1:D:949:PHE:HE2	1:D:954:PHE:HB2	1.78	0.48
1:B:949:PHE:HE2	1:B:954:PHE:HB2	1.78	0.48
1:D:135:ASP:O	1:D:169:LYS:NZ	2.45	0.48
1:A:949:PHE:HE2	1:A:954:PHE:HB2	1.78	0.48
1:D:618:LEU:O	1:D:622:LYS:HB2	2.14	0.48
1:A:618:LEU:HD11	1:B:559:PHE:CE1	2.44	0.48
1:B:63:VAL:HG21	1:B:84:TYR:HA	1.96	0.48
1:A:755:TYR:HD2	1:A:799:LEU:HD13	1.79	0.48
1:D:555:THR:HG23	1:E:559:PHE:HE2	1.78	0.48
1:B:322:LEU:HD11	1:B:542:LEU:HD11	1.96	0.48
1:B:618:LEU:O	1:B:622:LYS:HB2	2.14	0.48
1:D:322:LEU:HD11	1:D:542:LEU:HD11	1.96	0.48
1:E:322:LEU:HD11	1:E:542:LEU:HD11	1.96	0.48
1:E:618:LEU:O	1:E:622:LYS:HB2	2.14	0.48
1:A:322:LEU:HD11	1:A:542:LEU:HD11	1.96	0.48
1:E:755:TYR:HD2	1:E:799:LEU:HD13	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:TYR:HD2	1:B:799:LEU:HD13	1.79	0.47
1:D:119:ASP:OD1	1:D:145:ARG:NH2	2.42	0.47
1:E:455:TYR:CZ	1:E:477:ASN:HB3	2.49	0.47
2:C:23:PHE:HE2	2:C:106:ILE:HG13	1.79	0.47
1:D:809:LYS:NZ	1:D:813:LYS:O	2.39	0.47
1:A:464:ASP:OD1	1:A:464:ASP:N	2.47	0.47
1:D:991:SER:HB2	1:E:634:LEU:HD22	1.95	0.47
1:A:135:ASP:O	1:A:169:LYS:NZ	2.45	0.47
1:A:455:TYR:CZ	1:A:477:ASN:HB3	2.49	0.47
1:E:429:SER:OG	1:E:435:ASP:OD1	2.25	0.47
2:F:23:PHE:HE2	2:F:106:ILE:HG13	1.79	0.47
1:B:455:TYR:CZ	1:B:477:ASN:HB3	2.49	0.47
1:B:464:ASP:OD1	1:B:464:ASP:N	2.47	0.47
1:D:755:TYR:HD2	1:D:799:LEU:HD13	1.79	0.47
1:E:63:VAL:HG21	1:E:84:TYR:HA	1.96	0.47
1:A:63:VAL:HG21	1:A:84:TYR:HA	1.96	0.47
1:A:618:LEU:O	1:A:622:LYS:HB2	2.14	0.47
1:D:63:VAL:HG21	1:D:84:TYR:HA	1.96	0.47
1:D:455:TYR:CZ	1:D:477:ASN:HB3	2.49	0.47
1:D:957:SER:O	1:D:959:LEU:N	2.41	0.47
1:E:892:ARG:O	1:E:896:TYR:CB	2.55	0.47
1:E:949:PHE:HE2	1:E:954:PHE:HB2	1.78	0.47
2:C:44:PHE:O	2:C:114:LYS:N	2.47	0.47
1:D:464:ASP:N	1:D:464:ASP:OD1	2.47	0.47
1:E:215:PHE:HB2	1:E:245:PHE:HA	1.98	0.46
1:B:90:ILE:HG12	1:E:260:TYR:CG	2.51	0.46
1:E:678:PHE:O	1:E:681:GLN:NE2	2.48	0.46
1:B:119:ASP:OD1	1:B:145:ARG:NH2	2.42	0.46
1:A:215:PHE:HB2	1:A:245:PHE:HA	1.98	0.46
1:A:647:MET:HE1	1:A:655:ILE:HD12	1.98	0.46
1:B:892:ARG:O	1:B:896:TYR:CB	2.55	0.46
1:D:215:PHE:HB2	1:D:245:PHE:HA	1.98	0.46
1:A:377:GLN:OE1	1:A:380:ARG:NH1	2.49	0.46
1:A:882:GLU:HG2	1:A:927:ASN:HB2	1.98	0.46
1:B:618:LEU:O	1:B:622:LYS:CB	2.64	0.46
1:E:618:LEU:O	1:E:622:LYS:CB	2.64	0.46
1:E:865:LEU:O	1:E:869:ILE:HB	2.15	0.46
1:B:134:TYR:OH	1:B:184:VAL:O	2.28	0.46
1:A:678:PHE:O	1:A:681:GLN:NE2	2.48	0.46
1:A:618:LEU:O	1:A:622:LYS:CB	2.64	0.46
1:B:865:LEU:O	1:B:869:ILE:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:971:ALA:HA	1:D:977:LYS:HG3	1.98	0.46
1:A:47:GLY:O	1:A:133:ASN:ND2	2.49	0.46
1:A:865:LEU:O	1:A:869:ILE:HB	2.16	0.46
1:B:215:PHE:HB2	1:B:245:PHE:HA	1.98	0.46
1:D:678:PHE:O	1:D:681:GLN:NE2	2.48	0.46
1:A:892:ARG:O	1:A:896:TYR:CB	2.55	0.45
1:E:647:MET:HE1	1:E:655:ILE:HD12	1.98	0.45
1:B:647:MET:HE1	1:B:655:ILE:HD12	1.99	0.45
1:E:971:ALA:HA	1:E:977:LYS:HG3	1.98	0.45
1:D:865:LEU:O	1:D:869:ILE:HB	2.16	0.45
1:E:249:ASP:O	1:E:285:ARG:NH1	2.50	0.45
1:E:984:LEU:HB3	1:E:1000:LEU:HD12	1.99	0.45
1:A:992:ASN:OD1	1:B:627:ARG:NH1	2.49	0.45
1:B:249:ASP:O	1:B:285:ARG:NH1	2.50	0.45
1:B:287:SER:O	1:B:291:ASP:HB2	2.17	0.45
1:D:140:THR:HA	1:D:143:TRP:HD1	1.82	0.45
1:E:287:SER:O	1:E:291:ASP:HB2	2.17	0.45
1:D:287:SER:O	1:D:291:ASP:HB2	2.17	0.45
1:E:882:GLU:HG2	1:E:927:ASN:HB2	1.98	0.45
1:A:287:SER:O	1:A:291:ASP:HB2	2.17	0.45
1:A:971:ALA:HA	1:A:977:LYS:HG3	1.98	0.45
1:B:882:GLU:HG2	1:B:927:ASN:HB2	1.98	0.45
1:A:58:GLN:OE1	1:A:60:TRP:NE1	2.38	0.45
1:A:559:PHE:HE1	1:B:618:LEU:HD11	1.82	0.45
1:D:249:ASP:O	1:D:285:ARG:NH1	2.50	0.45
1:D:618:LEU:O	1:D:622:LYS:CB	2.64	0.45
1:A:119:ASP:OD1	1:A:145:ARG:NH2	2.42	0.45
1:A:140:THR:HA	1:A:143:TRP:HD1	1.82	0.45
1:B:46:VAL:HG12	1:B:216:ILE:HG23	2.00	0.45
1:B:971:ALA:HA	1:B:977:LYS:HG3	1.98	0.45
2:F:44:PHE:O	2:F:114:LYS:N	2.47	0.45
1:A:249:ASP:O	1:A:285:ARG:NH1	2.50	0.44
1:D:882:GLU:HG2	1:D:927:ASN:HB2	1.98	0.44
1:E:58:GLN:OE1	1:E:60:TRP:NE1	2.38	0.44
1:A:957:SER:O	1:A:959:LEU:N	2.41	0.44
1:B:563:ASN:O	1:B:565:VAL:N	2.50	0.44
1:D:46:VAL:HG12	1:D:216:ILE:HG23	2.00	0.44
1:E:563:ASN:O	1:E:565:VAL:N	2.50	0.44
1:A:563:ASN:O	1:A:565:VAL:N	2.50	0.44
1:A:720:LEU:HD13	1:A:740:LEU:HD12	2.00	0.44
1:B:678:PHE:O	1:B:681:GLN:NE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:LEU:HB3	1:B:1000:LEU:HD12	1.99	0.44
1:D:720:LEU:HD13	1:D:740:LEU:HD12	2.00	0.44
1:A:930:MET:SD	1:A:930:MET:N	2.91	0.44
1:D:563:ASN:O	1:D:565:VAL:N	2.50	0.44
1:B:720:LEU:HD13	1:B:740:LEU:HD12	2.00	0.44
1:D:930:MET:SD	1:D:930:MET:N	2.91	0.44
1:B:880:GLU:O	1:B:884:LEU:N	2.50	0.44
1:B:929:LYS:HG3	1:B:933:PHE:HE2	1.83	0.44
1:B:930:MET:SD	1:B:930:MET:N	2.91	0.44
1:E:464:ASP:OD1	1:E:464:ASP:N	2.47	0.44
1:E:484:SER:O	1:E:488:ALA:CB	2.66	0.44
1:A:80:SER:OG	1:A:83:GLU:OE1	2.27	0.44
1:A:929:LYS:HG3	1:A:933:PHE:HE2	1.83	0.44
1:A:984:LEU:HB3	1:A:1000:LEU:HD12	1.99	0.44
1:B:82:ASP:O	1:B:86:ARG:N	2.40	0.44
1:D:929:LYS:HG3	1:D:933:PHE:HE2	1.83	0.44
1:A:555:THR:HG23	1:B:559:PHE:HE2	1.82	0.43
1:A:880:GLU:O	1:A:884:LEU:N	2.50	0.43
1:D:58:GLN:OE1	1:D:60:TRP:NE1	2.38	0.43
1:D:484:SER:O	1:D:488:ALA:CB	2.66	0.43
1:D:627:ARG:NH1	1:E:992:ASN:OD1	2.51	0.43
1:E:140:THR:HA	1:E:143:TRP:HD1	1.82	0.43
1:A:46:VAL:HG12	1:A:216:ILE:HG23	2.00	0.43
1:A:809:LYS:NZ	1:A:813:LYS:O	2.39	0.43
1:E:11:TYR:OH	1:E:291:ASP:OD2	2.36	0.43
1:A:724:LYS:HD3	1:A:760:ARG:HG2	2.01	0.43
1:B:724:LYS:HD3	1:B:760:ARG:HG2	2.01	0.43
1:D:984:LEU:HB3	1:D:1000:LEU:HD12	1.99	0.43
1:E:930:MET:N	1:E:930:MET:SD	2.91	0.43
1:B:140:THR:HA	1:B:143:TRP:HD1	1.82	0.43
1:E:47:GLY:O	1:E:133:ASN:ND2	2.49	0.43
1:B:47:GLY:O	1:B:133:ASN:ND2	2.49	0.43
1:A:309:ILE:HG13	1:A:373:LEU:HD21	2.01	0.43
1:E:46:VAL:HG12	1:E:216:ILE:HG23	2.00	0.43
1:E:880:GLU:O	1:E:884:LEU:N	2.50	0.43
1:E:724:LYS:HD3	1:E:760:ARG:HG2	2.01	0.43
1:E:929:LYS:HG3	1:E:933:PHE:HE2	1.83	0.43
1:A:82:ASP:O	1:A:86:ARG:N	2.40	0.42
1:A:134:TYR:OH	1:A:184:VAL:O	2.28	0.42
1:D:663:ASP:OD1	1:E:564:LYS:HE2	2.19	0.42
1:D:724:LYS:HD3	1:D:760:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:632:ASP:OD1	1:E:632:ASP:N	2.49	0.42
1:E:720:LEU:HD13	1:E:740:LEU:HD12	2.00	0.42
1:D:880:GLU:O	1:D:884:LEU:N	2.50	0.42
1:D:47:GLY:O	1:D:133:ASN:ND2	2.49	0.42
1:D:242:LYS:HA	1:D:243:PRO:HD3	1.92	0.42
1:E:309:ILE:HG13	1:E:373:LEU:HD21	2.00	0.42
2:F:23:PHE:CE2	2:F:106:ILE:HG13	2.54	0.42
1:A:466:SER:OG	1:A:467:ASN:N	2.53	0.42
1:A:484:SER:O	1:A:488:ALA:CB	2.66	0.42
1:B:965:LYS:HD2	2:C:59:PHE:HE1	1.85	0.42
1:E:466:SER:OG	1:E:467:ASN:N	2.53	0.42
1:E:809:LYS:NZ	1:E:813:LYS:O	2.39	0.42
1:A:518:GLU:HG3	1:B:144:LYS:HD2	2.01	0.42
1:D:309:ILE:HG13	1:D:373:LEU:HD21	2.00	0.42
1:B:90:ILE:HG12	1:E:260:TYR:CD2	2.54	0.42
1:B:309:ILE:HG13	1:B:373:LEU:HD21	2.00	0.42
1:D:950:ASP:OD1	1:D:950:ASP:N	2.53	0.42
1:E:589:TYR:OH	1:E:651:ASP:OD1	2.37	0.42
1:D:82:ASP:O	1:D:86:ARG:N	2.40	0.41
1:A:27:VAL:HG12	1:A:31:LYS:HE2	2.02	0.41
2:C:23:PHE:CE2	2:C:106:ILE:HG13	2.54	0.41
1:D:571:GLU:HA	2:F:19:LYS:HE2	2.02	0.41
1:E:134:TYR:OH	1:E:184:VAL:O	2.28	0.41
1:A:692:ALA:HB2	1:A:736:ILE:HG13	2.03	0.41
1:D:27:VAL:HG12	1:D:31:LYS:HE2	2.02	0.41
1:E:26:VAL:O	1:E:30:ILE:HG12	2.20	0.41
1:E:950:ASP:N	1:E:950:ASP:OD1	2.53	0.41
1:D:737:VAL:HG11	1:D:771:ILE:HG23	2.03	0.41
1:D:842:LEU:HD21	1:D:850:LYS:HE3	2.02	0.41
2:F:82:LYS:HE2	2:F:82:LYS:HB3	1.86	0.41
1:A:631:ILE:HG22	2:C:19:LYS:HG2	2.03	0.41
1:A:960:LYS:HG2	1:A:995:ARG:HG2	2.03	0.41
1:B:429:SER:OG	1:B:435:ASP:OD1	2.25	0.41
1:B:484:SER:O	1:B:488:ALA:CB	2.66	0.41
1:A:842:LEU:HD21	1:A:850:LYS:HE3	2.02	0.41
1:D:26:VAL:O	1:D:30:ILE:HG12	2.20	0.41
1:E:432:ILE:HD12	1:E:432:ILE:HA	1.98	0.41
1:B:737:VAL:HG11	1:B:771:ILE:HG23	2.03	0.41
2:C:82:LYS:HB3	2:C:82:LYS:HE2	1.86	0.41
1:D:925:ILE:H	1:D:925:ILE:HG13	1.79	0.41
1:E:737:VAL:HG11	1:E:771:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:842:LEU:HD21	1:E:850:LYS:HE3	2.02	0.41
1:B:26:VAL:O	1:B:30:ILE:HG12	2.20	0.41
1:B:27:VAL:HG12	1:B:31:LYS:HE2	2.02	0.41
1:B:950:ASP:OD1	1:B:950:ASP:N	2.53	0.41
1:D:692:ALA:HB2	1:D:736:ILE:HG13	2.02	0.41
1:A:429:SER:OG	1:A:435:ASP:OD1	2.25	0.41
1:A:432:ILE:HD12	1:A:432:ILE:HA	1.98	0.41
1:A:522:PHE:HA	1:B:146:GLY:H	1.86	0.41
1:A:737:VAL:HG11	1:A:771:ILE:HG23	2.03	0.41
1:A:950:ASP:OD1	1:A:950:ASP:N	2.53	0.41
1:B:466:SER:OG	1:B:467:ASN:N	2.53	0.41
1:E:27:VAL:HG12	1:E:31:LYS:HE2	2.02	0.41
1:E:561:LEU:HD11	1:E:584:VAL:HG21	2.03	0.41
1:E:740:LEU:HD11	1:E:757:TRP:HB3	2.03	0.41
1:B:71:TYR:CE1	1:E:256:GLU:HB2	2.56	0.41
1:E:960:LYS:HG2	1:E:995:ARG:HG2	2.03	0.41
1:B:399:ASP:OD1	1:B:399:ASP:N	2.55	0.40
1:B:692:ALA:HB2	1:B:736:ILE:HG13	2.02	0.40
1:B:809:LYS:NZ	1:B:813:LYS:O	2.39	0.40
1:E:399:ASP:OD1	1:E:399:ASP:N	2.54	0.40
1:E:727:LYS:NZ	1:E:764:CYS:SG	2.82	0.40
1:B:59:TRP:CZ3	1:B:62:LEU:HD22	2.57	0.40
1:D:318:PRO:O	1:D:539:TYR:OH	2.29	0.40
1:E:59:TRP:CZ3	1:E:62:LEU:HD22	2.57	0.40
1:A:561:LEU:HD11	1:A:584:VAL:HG21	2.03	0.40
1:D:960:LYS:HG2	1:D:995:ARG:HG2	2.03	0.40
2:F:44:PHE:HB3	2:F:64:ILE:HD11	2.03	0.40
1:A:26:VAL:O	1:A:30:ILE:HG12	2.20	0.40
1:B:842:LEU:HD21	1:B:850:LYS:HE3	2.02	0.40
1:B:883:GLU:HA	1:B:886:ILE:HD12	2.04	0.40
1:B:960:LYS:HG2	1:B:995:ARG:HG2	2.03	0.40
1:D:59:TRP:CZ3	1:D:62:LEU:HD22	2.57	0.40
1:D:210:THR:HG22	1:E:159:ALA:HA	2.04	0.40
1:D:555:THR:HG23	1:E:559:PHE:CE2	2.57	0.40
1:A:59:TRP:CZ3	1:A:62:LEU:HD22	2.57	0.40
1:A:916:PHE:HA	1:A:919:TRP:HB2	2.04	0.40
1:B:740:LEU:HD11	1:B:757:TRP:HB3	2.03	0.40
1:D:524:ILE:HG13	1:D:546:SER:HB2	2.04	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	949/1005 (94%)	872 (92%)	74 (8%)	3 (0%)	37	66
1	B	948/1005 (94%)	871 (92%)	74 (8%)	3 (0%)	37	66
1	D	949/1005 (94%)	870 (92%)	76 (8%)	3 (0%)	37	66
1	E	948/1005 (94%)	870 (92%)	74 (8%)	4 (0%)	30	61
2	C	94/120 (78%)	74 (79%)	19 (20%)	1 (1%)	12	41
2	F	94/120 (78%)	74 (79%)	19 (20%)	1 (1%)	12	41
All	All	3982/4260 (94%)	3631 (91%)	336 (8%)	15 (0%)	32	61

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	958	TRP
1	B	958	TRP
1	D	958	TRP
1	E	958	TRP
1	A	795	SER
1	B	795	SER
1	D	795	SER
1	E	795	SER
2	C	93	LYS
2	F	93	LYS
1	A	563	ASN
1	B	563	ASN
1	D	563	ASN
1	E	563	ASN
1	E	506	PRO

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	879/923 (95%)	873 (99%)	6 (1%)	81 88
1	B	881/923 (95%)	874 (99%)	7 (1%)	79 87
1	D	879/923 (95%)	873 (99%)	6 (1%)	81 88
1	E	881/923 (95%)	875 (99%)	6 (1%)	81 88
2	C	94/113 (83%)	93 (99%)	1 (1%)	70 82
2	F	94/113 (83%)	93 (99%)	1 (1%)	70 82
All	All	3708/3918 (95%)	3681 (99%)	27 (1%)	80 88

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	LEU
1	A	467	ASN
1	A	813	LYS
1	A	838	LEU
1	A	973	ASN
1	A	992	ASN
1	B	6	LEU
1	B	330	LEU
1	B	467	ASN
1	B	813	LYS
1	B	838	LEU
1	B	973	ASN
1	B	992	ASN
2	C	21	ASN
1	D	330	LEU
1	D	467	ASN
1	D	813	LYS
1	D	838	LEU
1	D	973	ASN
1	D	992	ASN
1	E	330	LEU
1	E	467	ASN

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Mol	Chain	Res	Type
1	E	813	LYS
1	E	838	LEU
1	E	973	ASN
1	E	992	ASN
2	F	21	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	202	ASN
1	A	477	ASN
1	A	765	ASN
1	A	863	ASN
1	B	93	ASN
1	B	202	ASN
1	B	477	ASN
1	B	765	ASN
1	B	863	ASN
1	B	992	ASN
2	C	17	HIS
2	C	21	ASN
2	C	88	HIS
1	D	93	ASN
1	D	202	ASN
1	D	477	ASN
1	D	765	ASN
1	D	863	ASN
1	E	93	ASN
1	E	202	ASN
1	E	477	ASN
1	E	765	ASN
1	E	863	ASN
2	F	17	HIS
2	F	21	ASN
2	F	88	HIS

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.

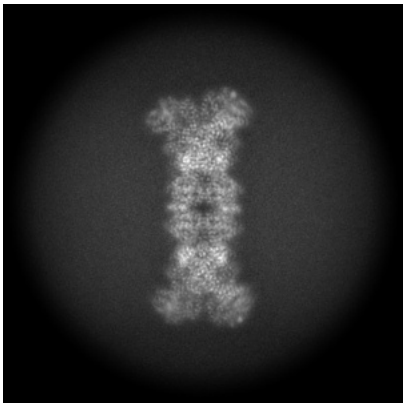
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38907. These allow visual inspection of the internal detail of the map and identification of artifacts.

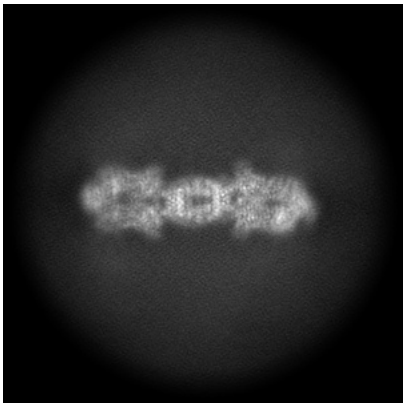
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

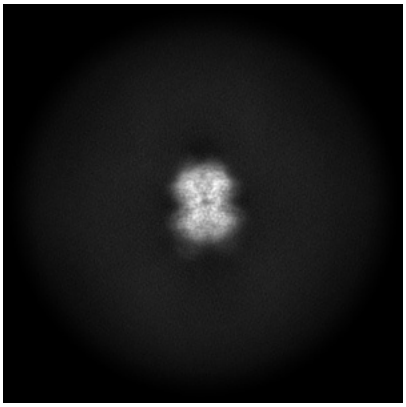
6.1.1 Primary map



X



Y

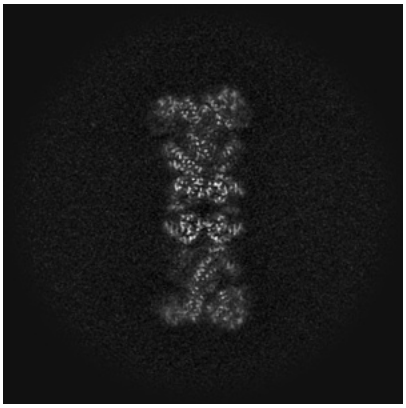


Z

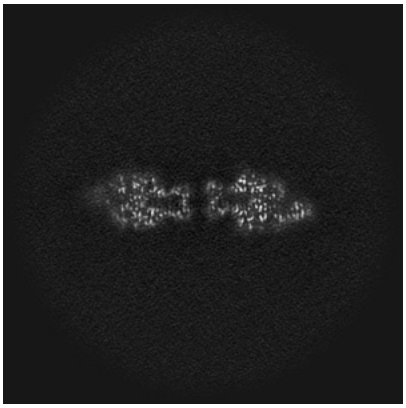
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 200



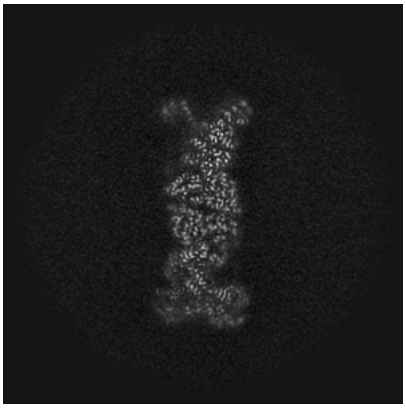
Y Index: 200

Z Index: 200

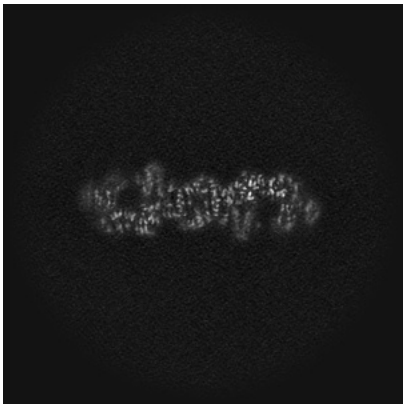
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

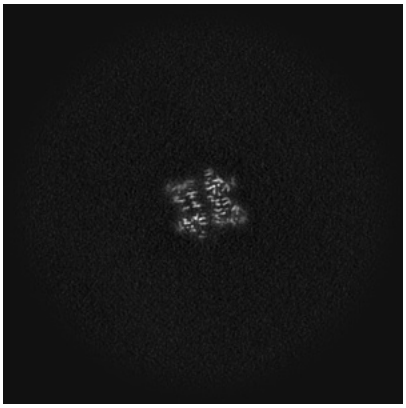
6.3.1 Primary map



X Index: 212



Y Index: 219

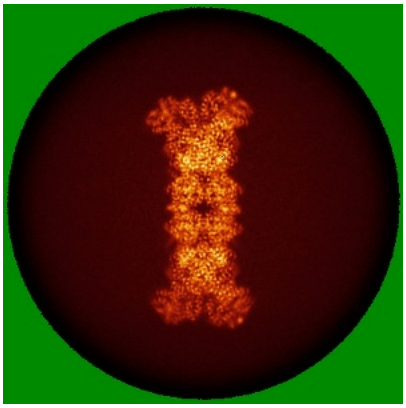


Z Index: 242

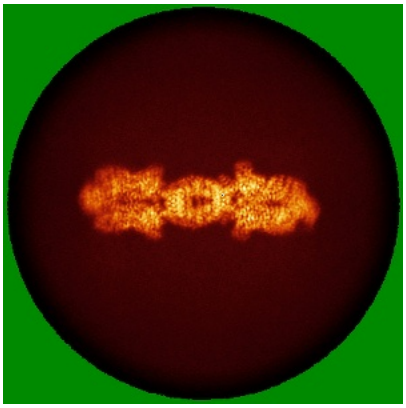
The images above show the largest variance slices of the map in three orthogonal directions.

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

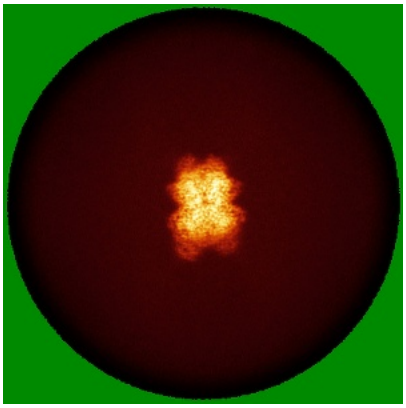
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

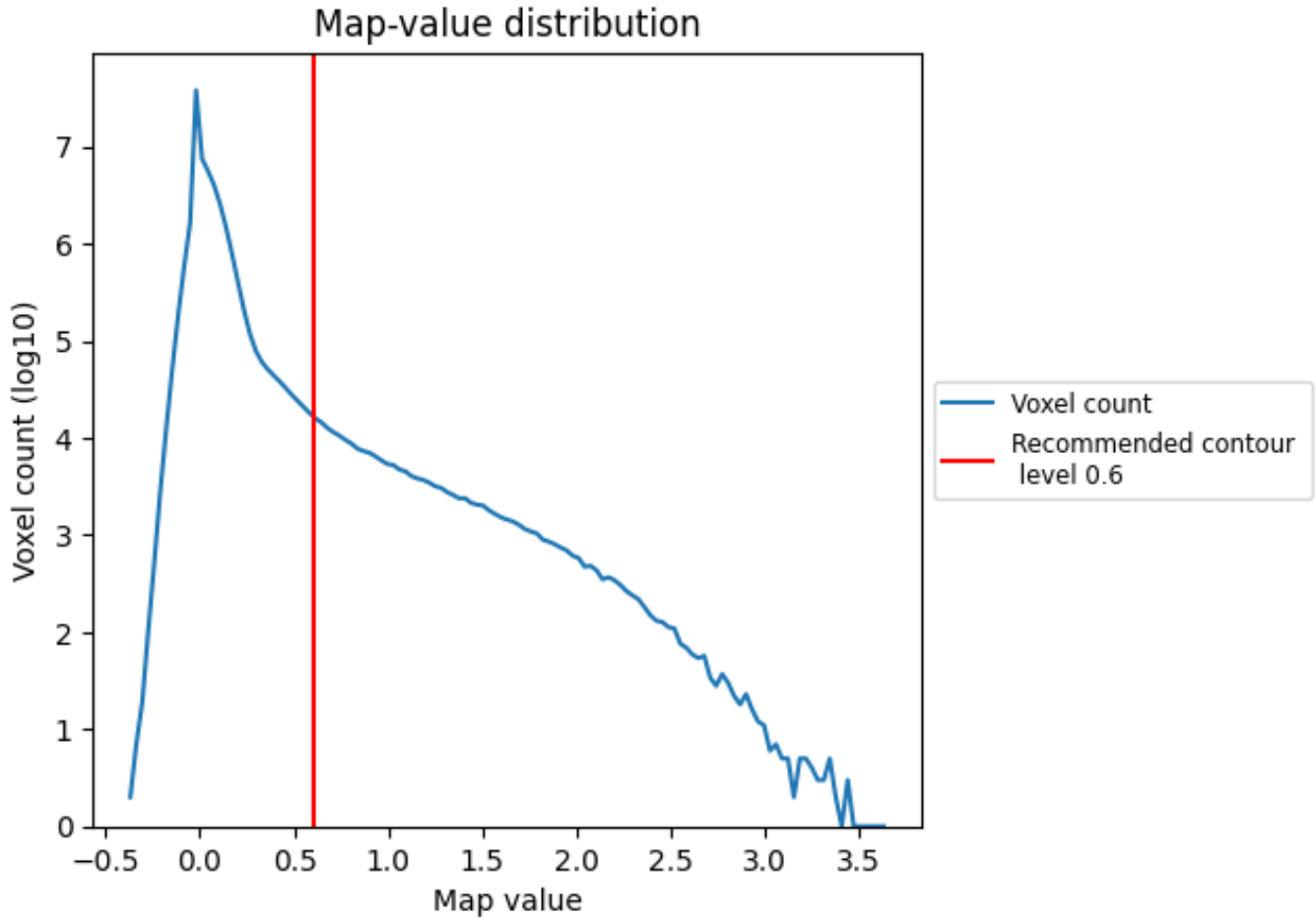
6.6 Mask visualisation (i)

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

7 Map analysis

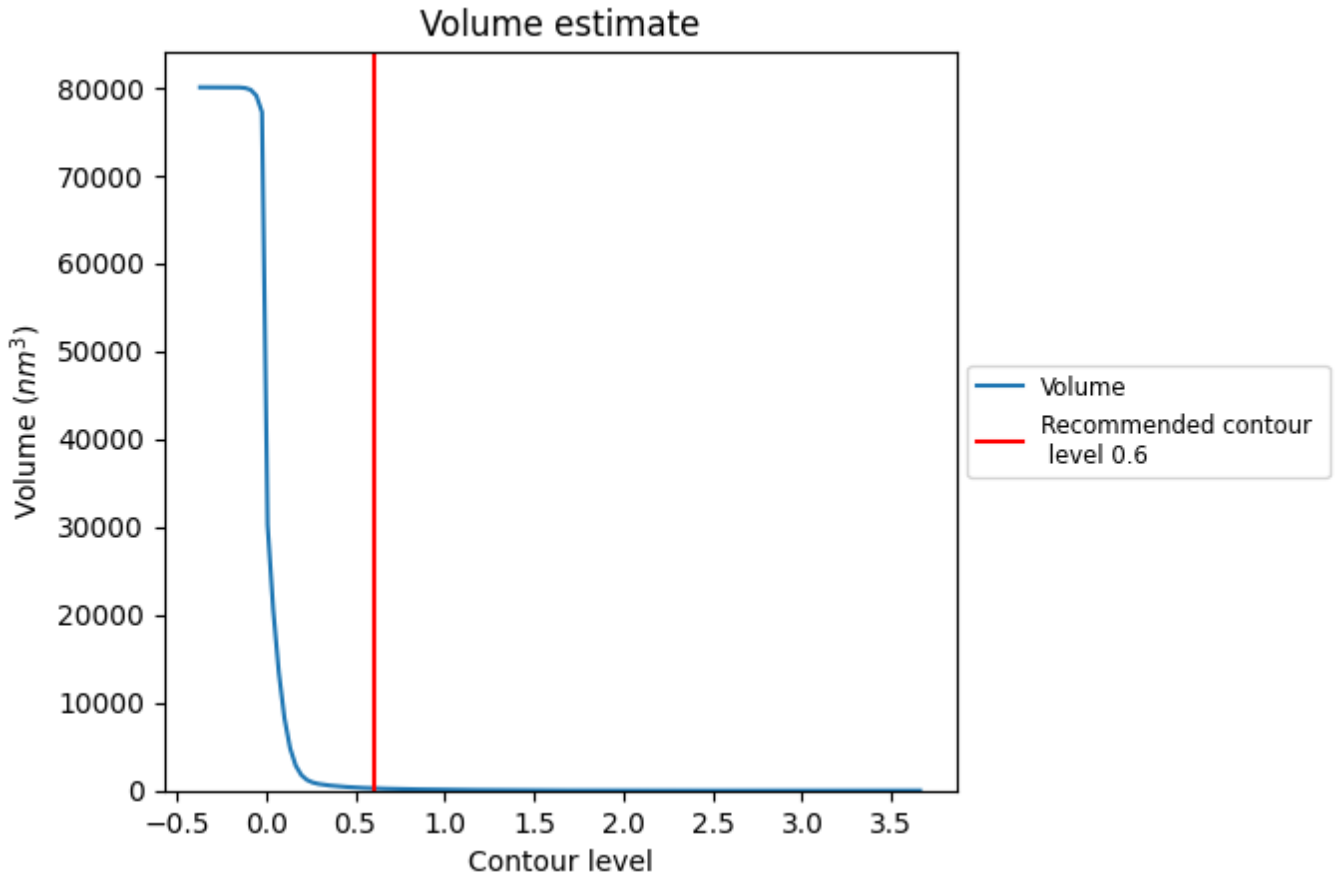
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

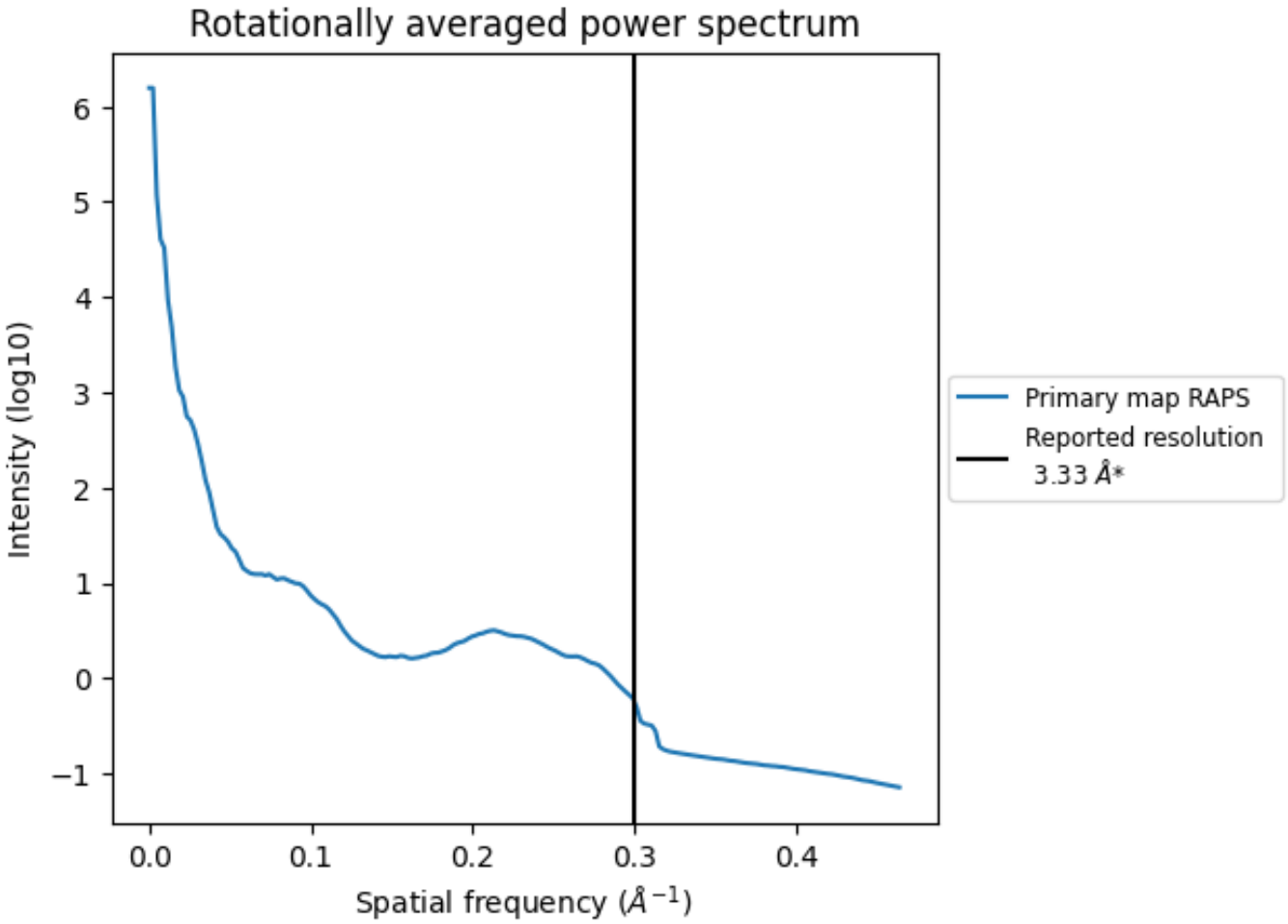
7.2 Volume estimate



The volume at the recommended contour level is 258 nm^3; this corresponds to an approximate mass of 233 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 0.300 $Å^{-1}$

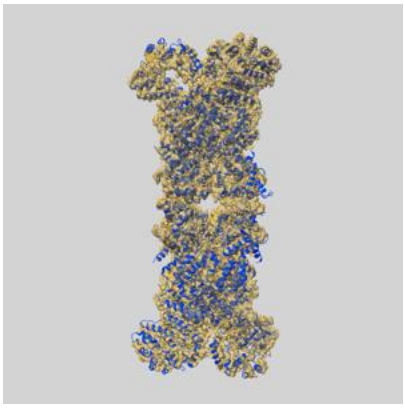
8 Fourier-Shell correlation

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

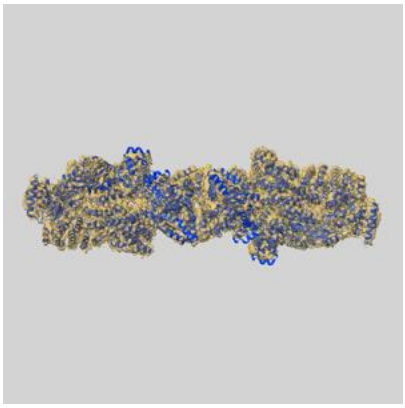
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38907 and PDB model 8Y3Y. Per-residue inclusion information can be found in section 3 on page 4.

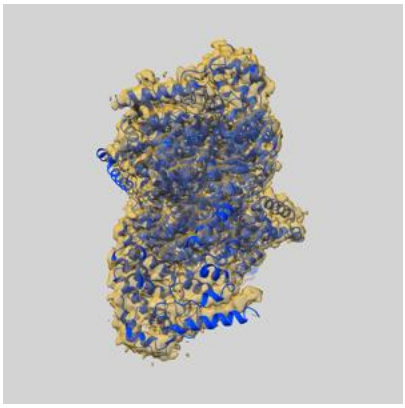
9.1 Map-model overlay



X



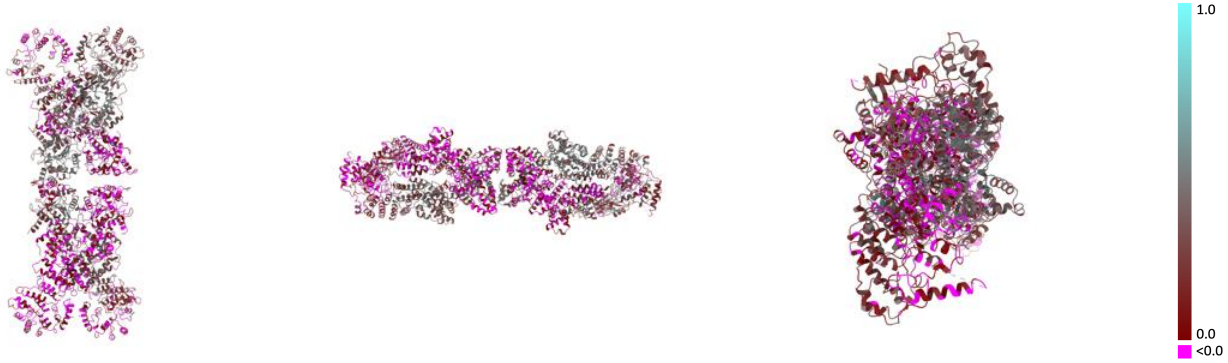
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

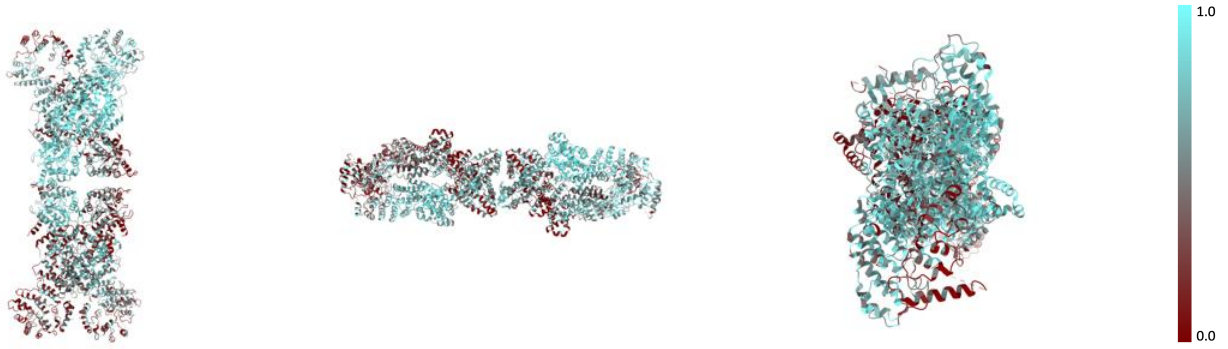
9.2 Q-score mapped to coordinate model (i)



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.

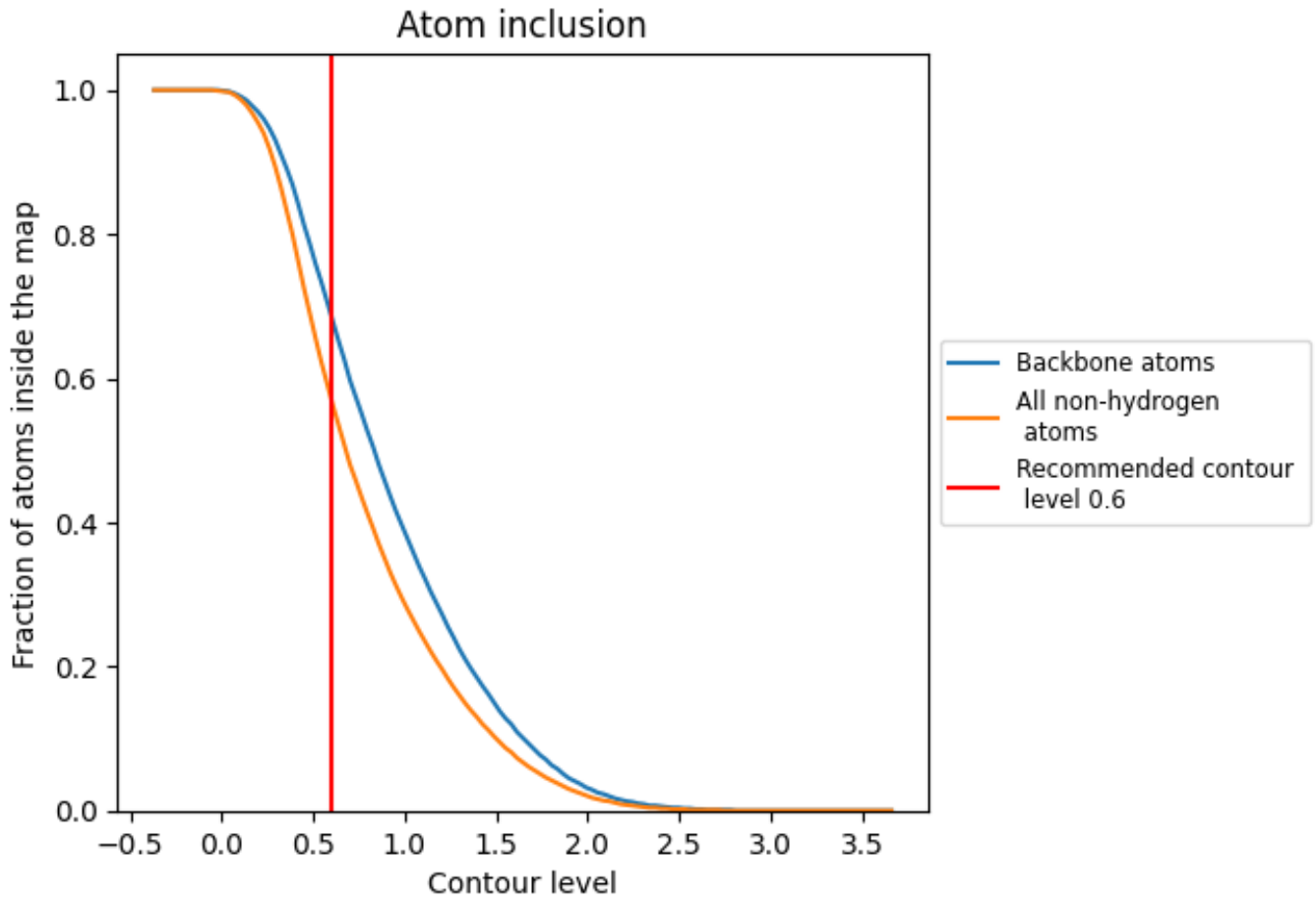
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 57% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5700	0.1840
A	0.4570	0.0680
B	0.7900	0.3750
C	0.7200	0.3560
D	0.3710	0.0170
E	0.6490	0.2540
F	0.5240	0.2310