Full wwPDB EM Validation Report ⓘ

May 19, 2022 – 10:34 pm BST

PDB ID	:	7ZW6
EMDB ID	:	EMD-14993
Title	:	Oligomeric structure of SynDLP
Deposited on	:	2022-05-18
Resolution	:	3.70 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

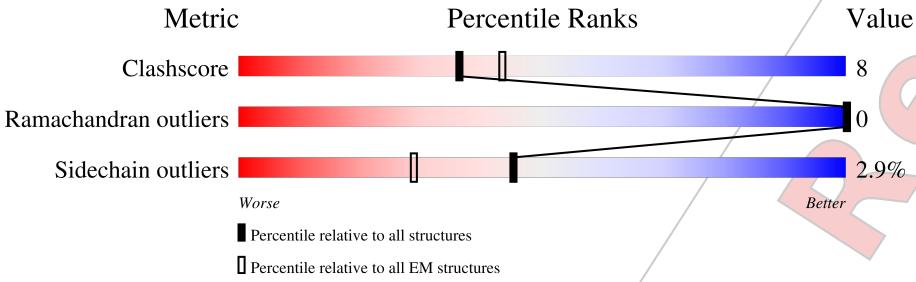
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.70 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	820	28% 75% 21%
1	B	820	43% 76% 20%
1	C	820	43% 77% 19%
1	D	820	26% 76% 19%
1	E	820	41% 77% 19%
1	F	820	29% 76% 19%
1	G	820	35% 76% 20%
1	H	820	27% 76% 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 101416 atoms, of which 50480 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 Slr0869 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	E	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		
1	A	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		
1	B	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		
1	C	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		
1	D	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		
1	F	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		
1	G	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		
1	H	793	Total	C	H	N	O	S	0	0
			12677	3998	6310	1111	1237	21		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	813	LEU	-	expression tag	UNP P73765
E	814	GLU	-	expression tag	UNP P73765
E	815	HIS	-	expression tag	UNP P73765
E	816	HIS	-	expression tag	UNP P73765
E	817	HIS	-	expression tag	UNP P73765
E	818	HIS	-	expression tag	UNP P73765
E	819	HIS	-	expression tag	UNP P73765
E	820	HIS	-	expression tag	UNP P73765
A	813	LEU	-	expression tag	UNP P73765
A	814	GLU	-	expression tag	UNP P73765
A	815	HIS	-	expression tag	UNP P73765
A	816	HIS	-	expression tag	UNP P73765
A	817	HIS	-	expression tag	UNP P73765
A	818	HIS	-	expression tag	UNP P73765

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Chain	Residue	Modelled	Actual	Comment	Reference
A	819	HIS	-	expression tag	UNP P73765
A	820	HIS	-	expression tag	UNP P73765
B	813	LEU	-	expression tag	UNP P73765
B	814	GLU	-	expression tag	UNP P73765
B	815	HIS	-	expression tag	UNP P73765
B	816	HIS	-	expression tag	UNP P73765
B	817	HIS	-	expression tag	UNP P73765
B	818	HIS	-	expression tag	UNP P73765
B	819	HIS	-	expression tag	UNP P73765
B	820	HIS	-	expression tag	UNP P73765
C	813	LEU	-	expression tag	UNP P73765
C	814	GLU	-	expression tag	UNP P73765
C	815	HIS	-	expression tag	UNP P73765
C	816	HIS	-	expression tag	UNP P73765
C	817	HIS	-	expression tag	UNP P73765
C	818	HIS	-	expression tag	UNP P73765
C	819	HIS	-	expression tag	UNP P73765
C	820	HIS	-	expression tag	UNP P73765
D	813	LEU	-	expression tag	UNP P73765
D	814	GLU	-	expression tag	UNP P73765
D	815	HIS	-	expression tag	UNP P73765
D	816	HIS	-	expression tag	UNP P73765
D	817	HIS	-	expression tag	UNP P73765
D	818	HIS	-	expression tag	UNP P73765
D	819	HIS	-	expression tag	UNP P73765
D	820	HIS	-	expression tag	UNP P73765
F	813	LEU	-	expression tag	UNP P73765
F	814	GLU	-	expression tag	UNP P73765
F	815	HIS	-	expression tag	UNP P73765
F	816	HIS	-	expression tag	UNP P73765
F	817	HIS	-	expression tag	UNP P73765
F	818	HIS	-	expression tag	UNP P73765
F	819	HIS	-	expression tag	UNP P73765
F	820	HIS	-	expression tag	UNP P73765
G	813	LEU	-	expression tag	UNP P73765
G	814	GLU	-	expression tag	UNP P73765
G	815	HIS	-	expression tag	UNP P73765
G	816	HIS	-	expression tag	UNP P73765
G	817	HIS	-	expression tag	UNP P73765
G	818	HIS	-	expression tag	UNP P73765
G	819	HIS	-	expression tag	UNP P73765
G	820	HIS	-	expression tag	UNP P73765

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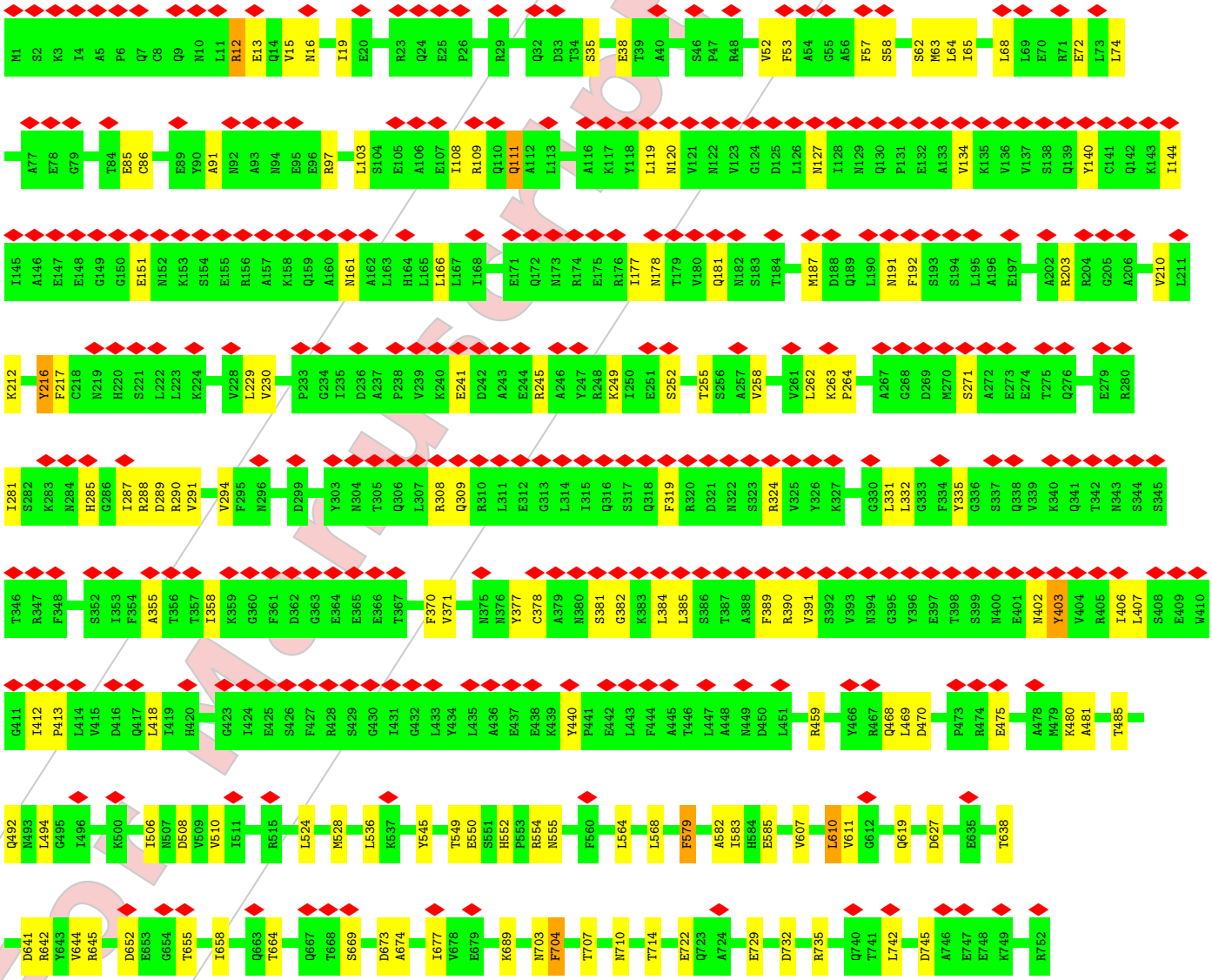
Chain	Residue	Modelled	Actual	Comment	Reference
H	813	LEU	-	expression tag	UNP P73765
H	814	GLU	-	expression tag	UNP P73765
H	815	HIS	-	expression tag	UNP P73765
H	816	HIS	-	expression tag	UNP P73765
H	817	HIS	-	expression tag	UNP P73765
H	818	HIS	-	expression tag	UNP P73765
H	819	HIS	-	expression tag	UNP P73765
H	820	HIS	-	expression tag	UNP P73765

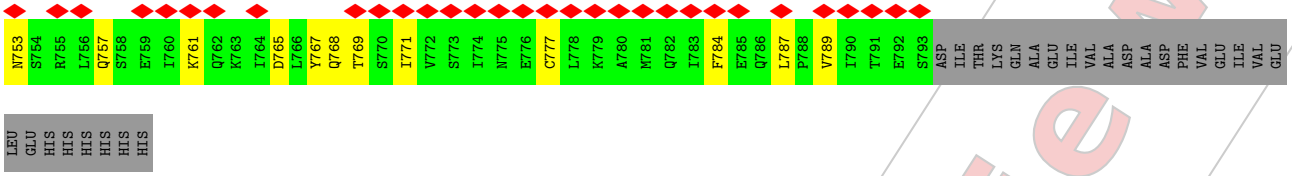
3 Residue-property plots (i)

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: Slr0869 protein

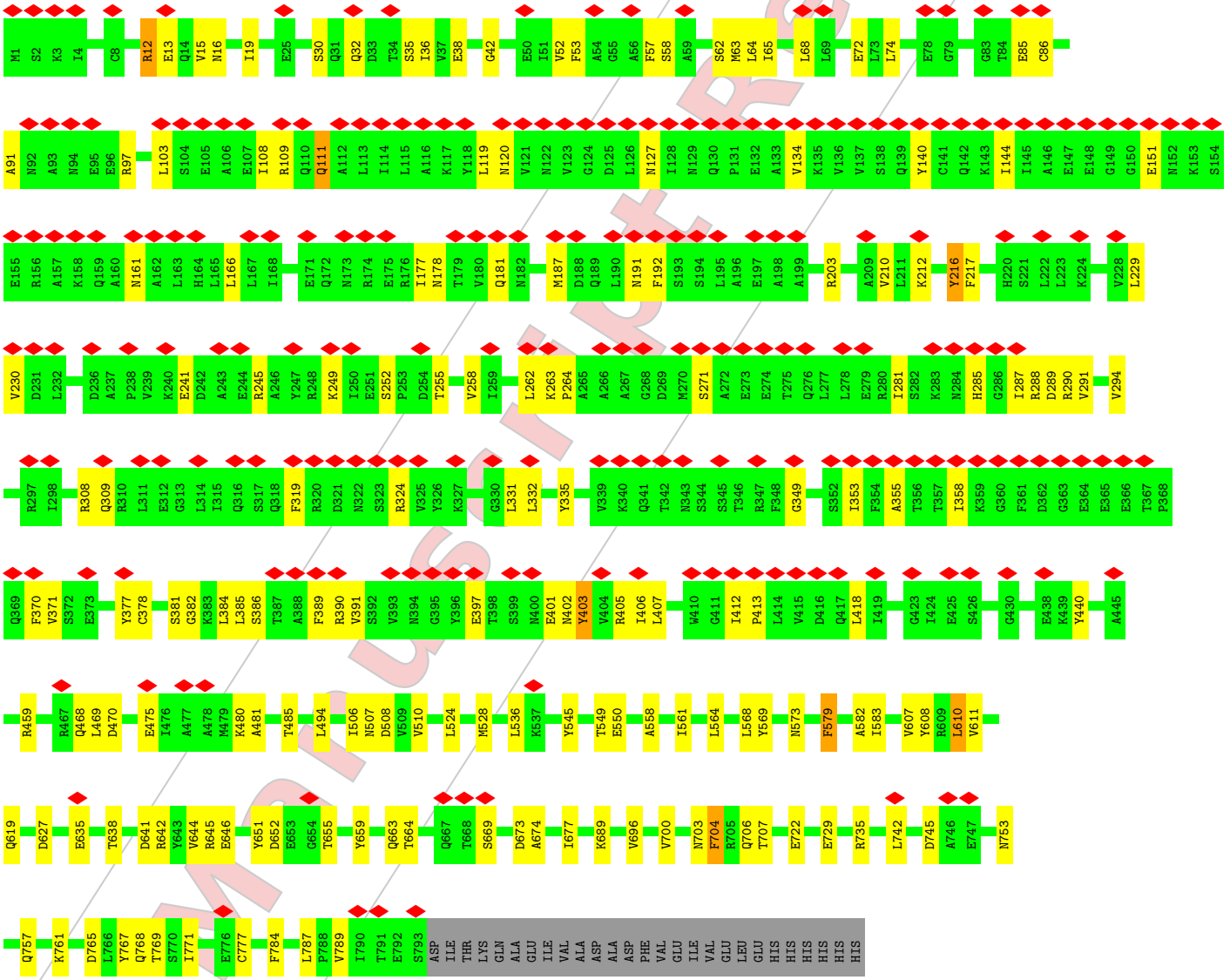
Chain E:





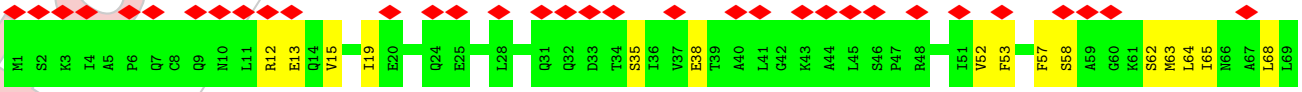
• Molecule 1: Slr0869 protein

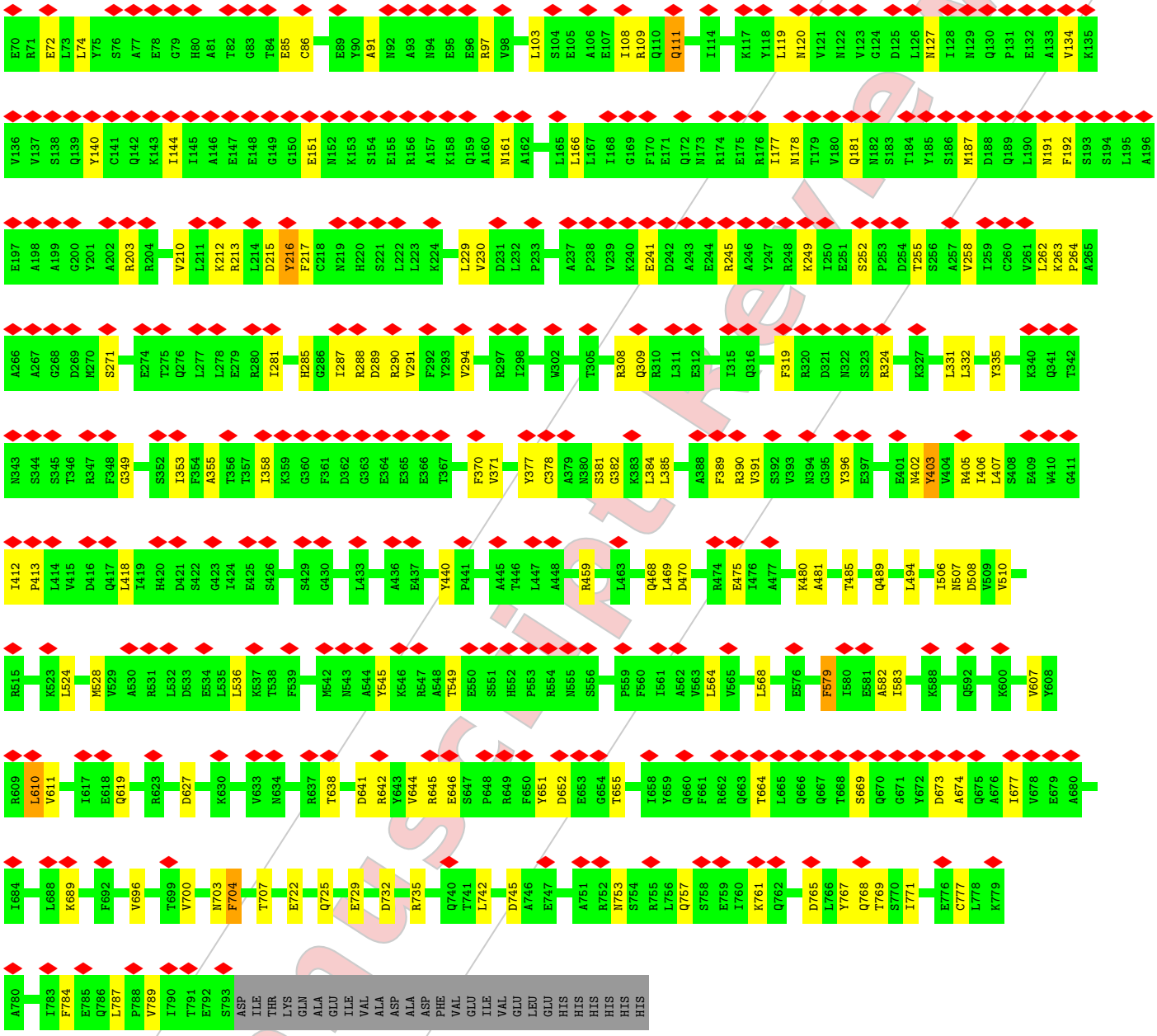
Chain A:



• Molecule 1: Slr0869 protein

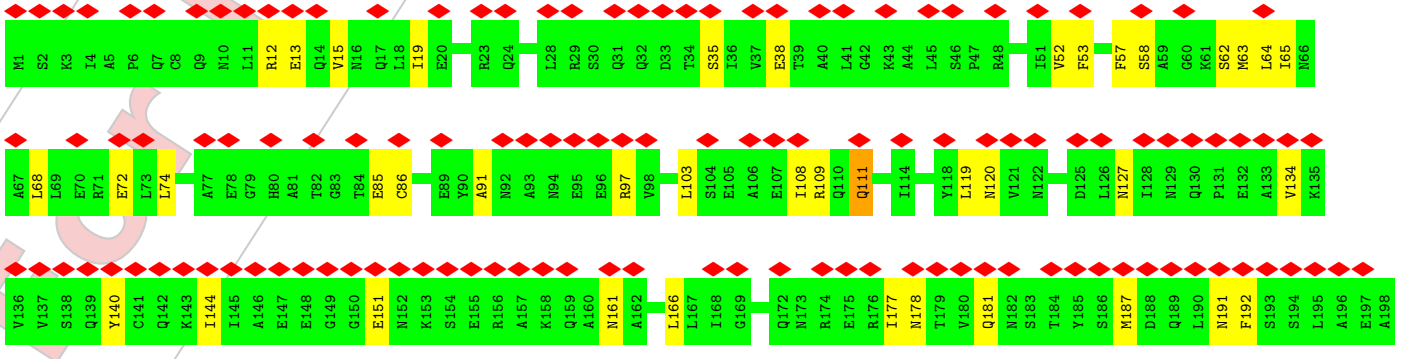
Chain B:

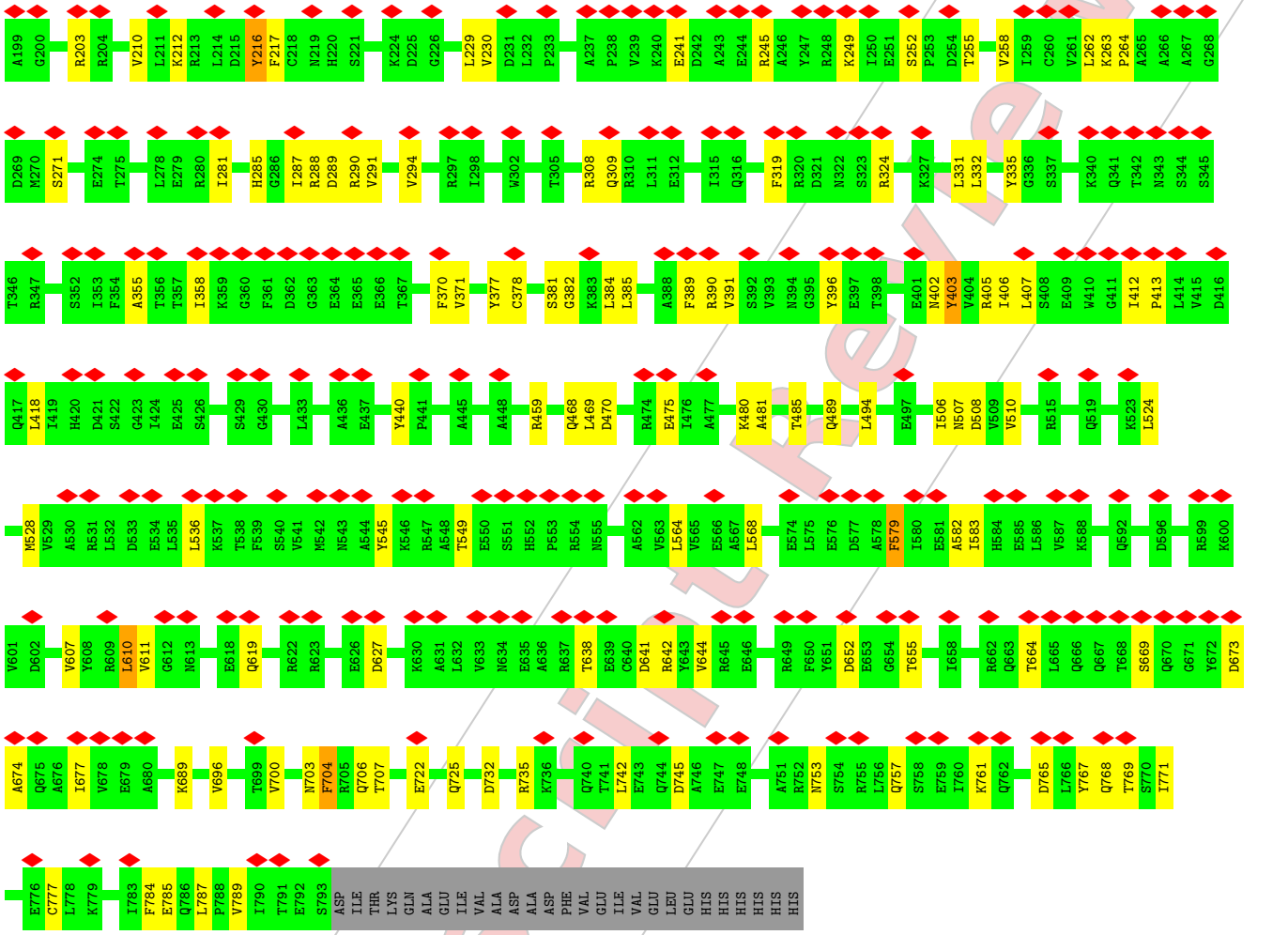




• Molecule 1: Slr0869 protein

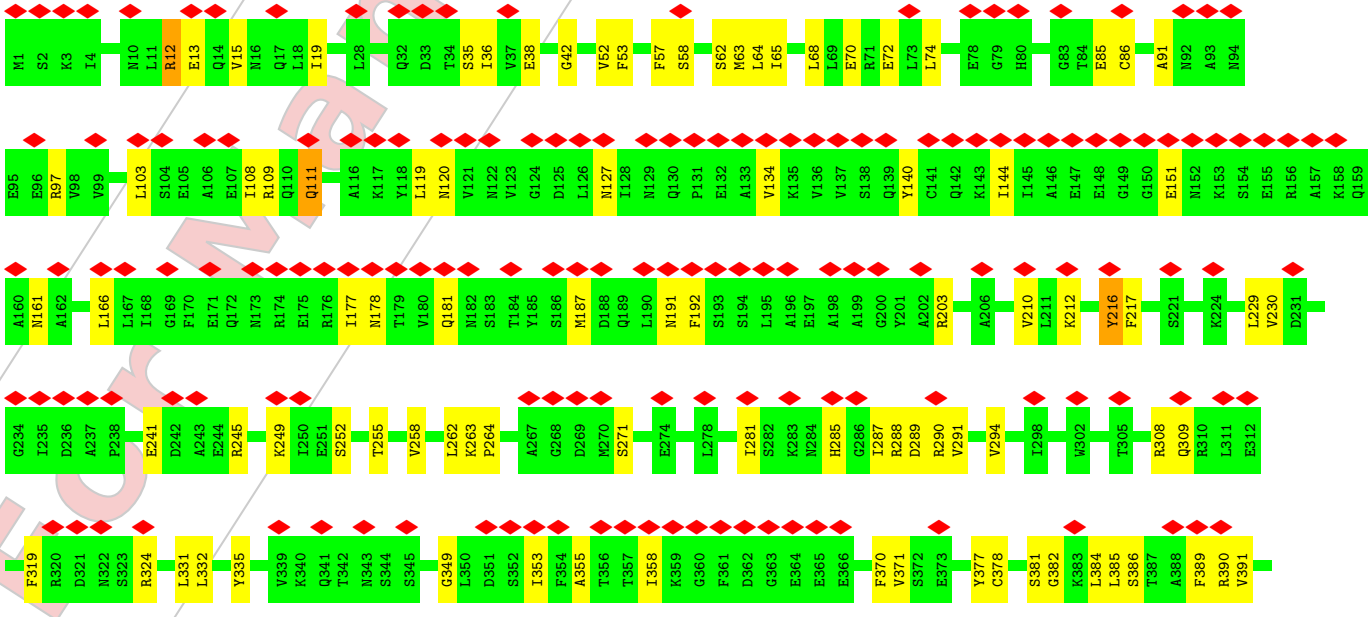
Chain C:

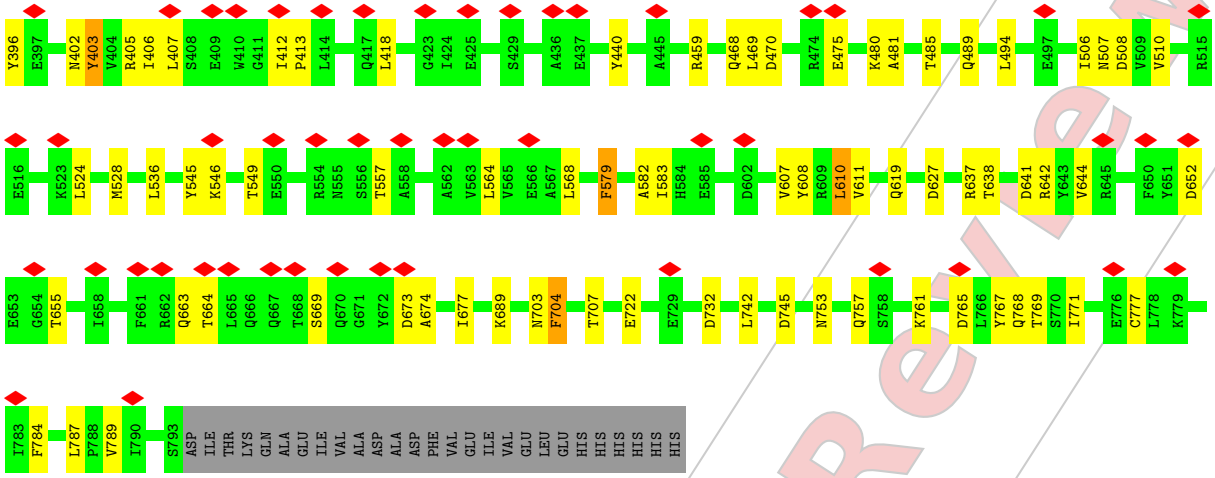




• Molecule 1: Slr0869 protein

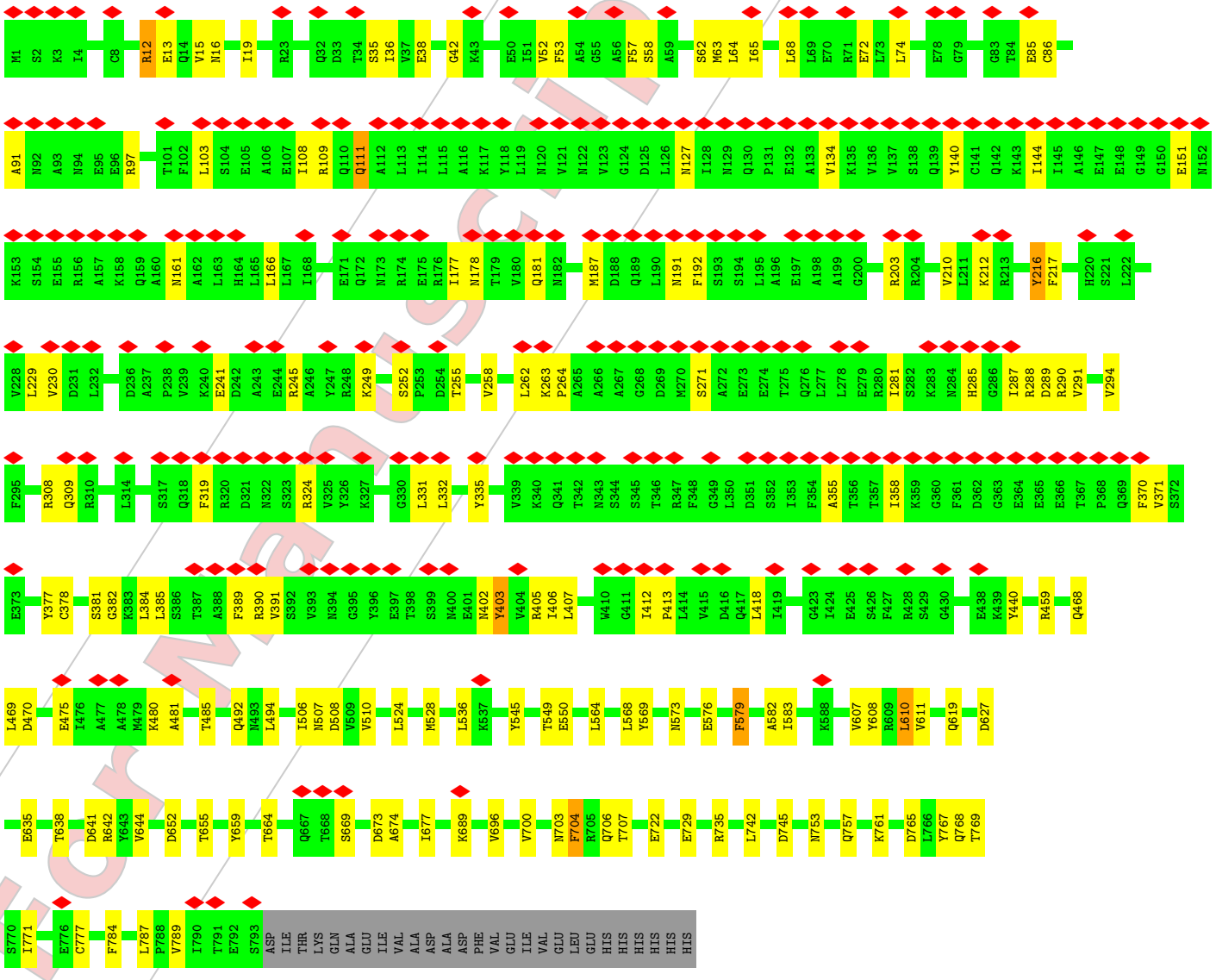
Chain D:





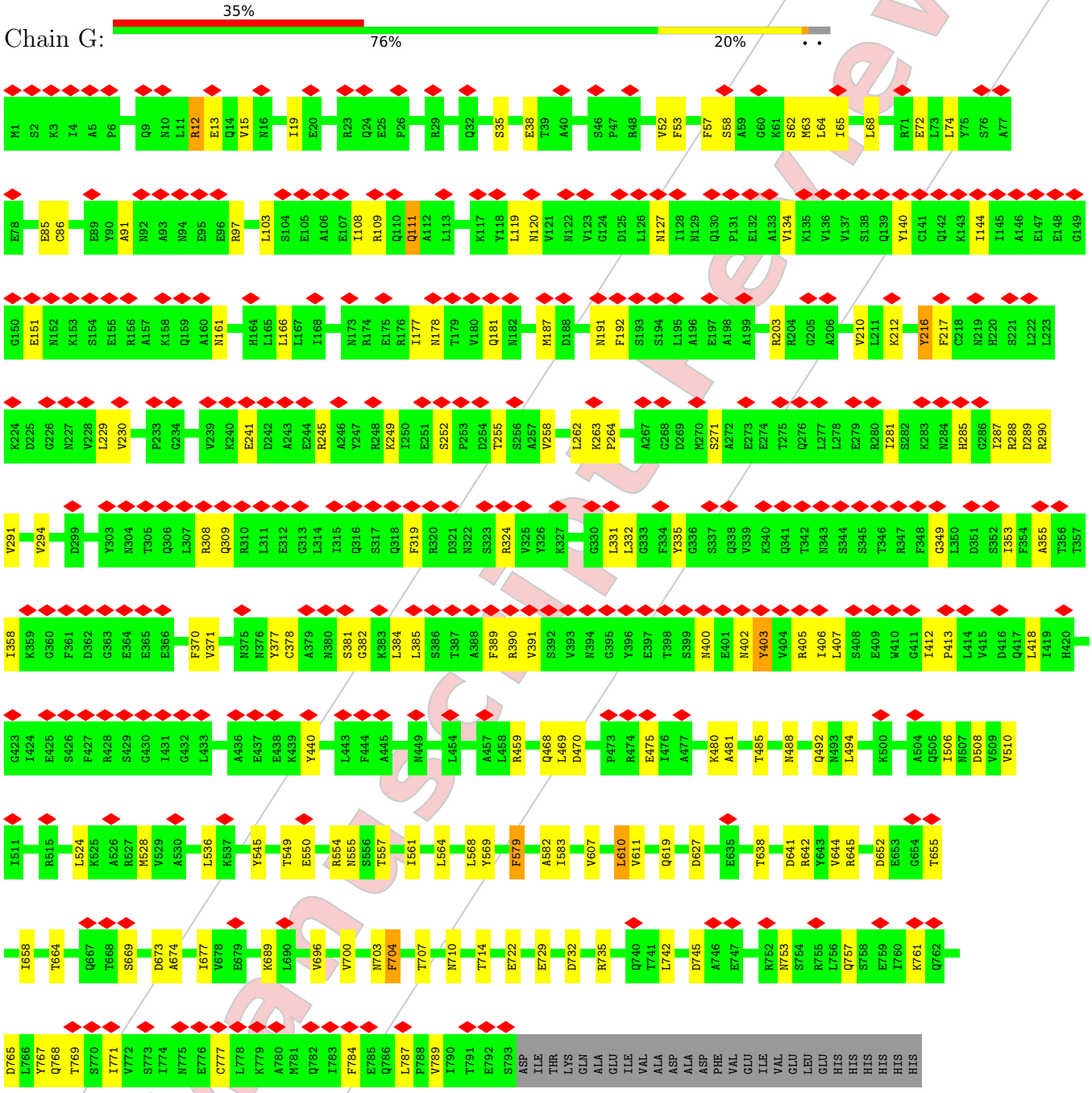
• Molecule 1: Slr0869 protein

Chain F:



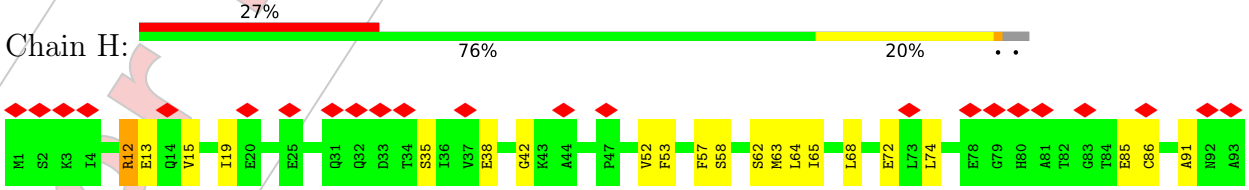
• Molecule 1: Slr0869 protein

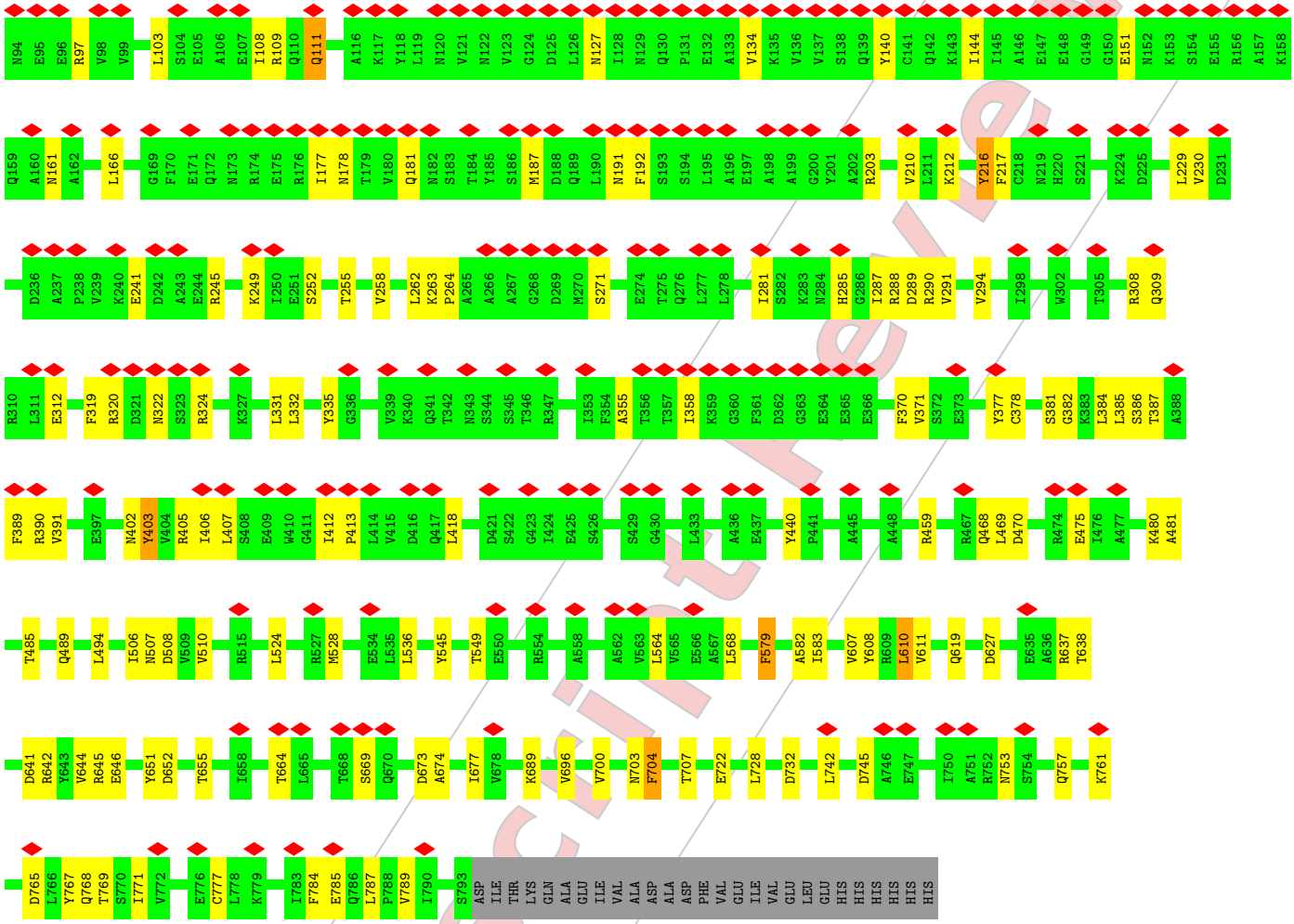
Chain G:



• Molecule 1: Slr0869 protein

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	977199	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	26.5	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	49000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.779	Depositor
Minimum map value	-0.404	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	391.05002, 391.05002, 391.05002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	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	0.26	0/6467	0.49	0/8733
1	B	0.26	0/6467	0.50	0/8733
1	C	0.26	0/6467	0.50	0/8733
1	D	0.26	0/6467	0.50	0/8733
1	E	0.26	0/6467	0.50	0/8733
1	F	0.26	0/6467	0.50	0/8733
1	G	0.26	0/6467	0.50	0/8733
1	H	0.26	0/6467	0.50	0/8733
All	All	0.26	0/51736	0.50	0/69864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6367	6310	6310	132	0
1	B	6367	6310	6310	114	0
1	C	6367	6310	6310	113	0
1	D	6367	6310	6310	129	0
1	E	6367	6310	6310	110	0
1	F	6367	6310	6310	114	0
1	G	6367	6310	6310	121	0
1	H	6367	6310	6310	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	50936	50480	50480	847	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 (847) 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:732:ASP:OD1	1:G:735:ARG:NH1	1.93	1.00
1:F:308:ARG:NH1	1:G:35:SER:OG	1.99	0.95
1:E:735:ARG:NH1	1:C:732:ASP:OD1	2.01	0.93
1:E:555:ASN:ND2	1:F:641:ASP:OD1	2.03	0.91
1:E:35:SER:OG	1:A:308:ARG:NH1	2.06	0.88
1:F:729:GLU:OE1	1:H:489:GLN:NE2	2.11	0.84
1:F:385:LEU:HD23	1:F:385:LEU:O	1.80	0.82
1:A:36:ILE:HG13	1:H:308:ARG:NH2	1.94	0.82
1:F:652:ASP:OD1	1:F:655:THR:OG1	1.97	0.82
1:H:385:LEU:O	1:H:385:LEU:HD23	1.79	0.82
1:A:652:ASP:OD1	1:A:655:THR:OG1	1.98	0.82
1:H:652:ASP:OD1	1:H:655:THR:OG1	1.97	0.82
1:D:652:ASP:OD1	1:D:655:THR:OG1	1.98	0.82
1:B:652:ASP:OD1	1:B:655:THR:OG1	1.98	0.82
1:D:385:LEU:HD23	1:D:385:LEU:O	1.80	0.82
1:A:573:ASN:OD1	1:G:554:ARG:NH1	2.13	0.81
1:C:385:LEU:O	1:C:385:LEU:HD23	1.79	0.81
1:B:385:LEU:HD23	1:B:385:LEU:O	1.80	0.81
1:E:385:LEU:O	1:E:385:LEU:HD23	1.80	0.81
1:A:641:ASP:OD1	1:G:555:ASN:ND2	2.12	0.81
1:B:489:GLN:NE2	1:G:729:GLU:OE1	2.12	0.81
1:G:385:LEU:HD23	1:G:385:LEU:O	1.80	0.81
1:E:652:ASP:OD1	1:E:655:THR:OG1	1.97	0.80
1:A:42:GLY:N	1:H:385:LEU:HD21	1.96	0.80
1:A:385:LEU:HD23	1:A:385:LEU:O	1.79	0.80
1:G:151:GLU:OE1	1:G:161:ASN:ND2	2.14	0.80
1:G:652:ASP:OD1	1:G:655:THR:OG1	1.98	0.80
1:A:151:GLU:OE1	1:A:161:ASN:ND2	2.14	0.80
1:D:151:GLU:OE1	1:D:161:ASN:ND2	2.14	0.80
1:B:151:GLU:OE1	1:B:161:ASN:ND2	2.14	0.80
1:C:652:ASP:OD1	1:C:655:THR:OG1	1.97	0.80
1:F:151:GLU:OE1	1:F:161:ASN:ND2	2.14	0.80
1:H:151:GLU:OE1	1:H:161:ASN:ND2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLU:OE1	1:C:161:ASN:ND2	2.14	0.79
1:E:151:GLU:OE1	1:E:161:ASN:ND2	2.14	0.79
1:F:308:ARG:CZ	1:G:35:SER:OG	2.30	0.79
1:A:332:LEU:HD12	1:A:418:LEU:HD21	1.67	0.77
1:C:332:LEU:HD12	1:C:418:LEU:HD21	1.67	0.77
1:G:332:LEU:HD12	1:G:418:LEU:HD21	1.67	0.77
1:H:470:ASP:OD1	1:H:757:GLN:NE2	2.18	0.77
1:G:470:ASP:OD1	1:G:757:GLN:NE2	2.18	0.76
1:E:470:ASP:OD1	1:E:757:GLN:NE2	2.18	0.76
1:D:470:ASP:OD1	1:D:757:GLN:NE2	2.18	0.76
1:E:332:LEU:HD12	1:E:418:LEU:HD21	1.67	0.76
1:F:470:ASP:OD1	1:F:757:GLN:NE2	2.18	0.76
1:B:470:ASP:OD1	1:B:757:GLN:NE2	2.18	0.76
1:H:332:LEU:HD12	1:H:418:LEU:HD21	1.67	0.76
1:A:470:ASP:OD1	1:A:757:GLN:NE2	2.18	0.76
1:F:332:LEU:HD12	1:F:418:LEU:HD21	1.67	0.76
1:C:470:ASP:OD1	1:C:757:GLN:NE2	2.18	0.75
1:A:729:GLU:OE1	1:D:489:GLN:NE2	2.19	0.75
1:C:178:ASN:OD1	1:C:181:GLN:N	2.20	0.75
1:D:178:ASN:OD1	1:D:181:GLN:N	2.20	0.75
1:G:178:ASN:OD1	1:G:181:GLN:N	2.20	0.75
1:A:16:ASN:OD1	1:H:386:SER:O	2.05	0.75
1:F:178:ASN:OD1	1:F:181:GLN:N	2.20	0.75
1:E:554:ARG:NH1	1:F:573:ASN:OD1	2.20	0.75
1:A:42:GLY:HA3	1:H:385:LEU:HD11	1.69	0.75
1:B:332:LEU:HD12	1:B:418:LEU:HD21	1.67	0.75
1:D:332:LEU:HD12	1:D:418:LEU:HD21	1.67	0.74
1:E:35:SER:OG	1:A:308:ARG:CZ	2.36	0.74
1:A:178:ASN:OD1	1:A:181:GLN:N	2.20	0.74
1:B:178:ASN:OD1	1:B:181:GLN:N	2.20	0.74
1:E:729:GLU:OE1	1:C:489:GLN:NE2	2.19	0.74
1:H:178:ASN:OD1	1:H:181:GLN:N	2.20	0.74
1:E:178:ASN:OD1	1:E:181:GLN:N	2.20	0.73
1:D:765:ASP:O	1:D:769:THR:HG23	1.88	0.73
1:E:765:ASP:O	1:E:769:THR:HG23	1.89	0.73
1:C:765:ASP:O	1:C:769:THR:HG23	1.89	0.73
1:C:787:LEU:HD11	1:D:608:TYR:CE1	2.23	0.73
1:A:765:ASP:O	1:A:769:THR:HG23	1.88	0.73
1:B:765:ASP:O	1:B:769:THR:HG23	1.89	0.72
1:F:765:ASP:O	1:F:769:THR:HG23	1.88	0.72
1:G:765:ASP:O	1:G:769:THR:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:765:ASP:O	1:H:769:THR:HG23	1.88	0.72
1:A:36:ILE:HG13	1:H:308:ARG:HH22	1.54	0.72
1:F:377:TYR:O	1:F:381:SER:OG	2.09	0.71
1:B:377:TYR:O	1:B:381:SER:OG	2.09	0.71
1:G:377:TYR:O	1:G:381:SER:OG	2.09	0.70
1:G:707:THR:HG22	1:H:642:ARG:NH2	2.07	0.70
1:D:377:TYR:O	1:D:381:SER:OG	2.09	0.70
1:E:377:TYR:O	1:E:381:SER:OG	2.09	0.70
1:E:761:LYS:NZ	1:E:765:ASP:OD2	2.20	0.70
1:H:377:TYR:O	1:H:381:SER:OG	2.09	0.70
1:A:249:LYS:O	1:A:252:SER:OG	2.09	0.69
1:B:787:LEU:HD11	1:H:608:TYR:CE1	2.28	0.69
1:A:459:ARG:HD3	1:A:787:LEU:HD13	1.75	0.69
1:A:12:ARG:NH1	1:H:385:LEU:O	2.26	0.69
1:B:249:LYS:O	1:B:252:SER:OG	2.09	0.68
1:G:459:ARG:HD3	1:G:787:LEU:HD13	1.75	0.68
1:A:377:TYR:O	1:A:381:SER:OG	2.09	0.68
1:A:761:LYS:NZ	1:A:765:ASP:OD2	2.20	0.68
1:B:459:ARG:HD3	1:B:787:LEU:HD13	1.75	0.68
1:C:377:TYR:O	1:C:381:SER:OG	2.09	0.68
1:A:659:TYR:OH	1:G:658:ILE:HG22	1.94	0.68
1:D:385:LEU:HD21	1:F:42:GLY:N	2.08	0.68
1:G:249:LYS:O	1:G:252:SER:OG	2.09	0.68
1:C:494:LEU:HD21	1:C:607:VAL:HG22	1.76	0.67
1:G:710:ASN:ND2	1:H:641:ASP:OD2	2.27	0.67
1:E:459:ARG:HD3	1:E:787:LEU:HD13	1.75	0.67
1:C:249:LYS:O	1:C:252:SER:OG	2.08	0.67
1:D:459:ARG:HD3	1:D:787:LEU:HD13	1.75	0.67
1:F:735:ARG:NH1	1:H:732:ASP:OD1	2.27	0.67
1:A:494:LEU:HD21	1:A:607:VAL:HG22	1.76	0.67
1:F:494:LEU:HD21	1:F:607:VAL:HG22	1.76	0.67
1:G:761:LYS:NZ	1:G:765:ASP:OD2	2.20	0.67
1:B:494:LEU:HD21	1:B:607:VAL:HG22	1.76	0.67
1:E:494:LEU:HD21	1:E:607:VAL:HG22	1.76	0.67
1:H:494:LEU:HD21	1:H:607:VAL:HG22	1.76	0.67
1:H:459:ARG:HD3	1:H:787:LEU:HD13	1.75	0.67
1:H:761:LYS:NZ	1:H:765:ASP:OD2	2.20	0.67
1:C:481:ALA:O	1:C:485:THR:HG23	1.95	0.67
1:F:459:ARG:HD3	1:F:787:LEU:HD13	1.75	0.67
1:F:481:ALA:O	1:F:485:THR:HG23	1.95	0.66
1:A:481:ALA:O	1:A:485:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:481:ALA:O	1:H:485:THR:HG23	1.95	0.66
1:F:507:ASN:ND2	1:G:550:GLU:OE2	2.28	0.66
1:B:481:ALA:O	1:B:485:THR:HG23	1.95	0.66
1:C:459:ARG:HD3	1:C:787:LEU:HD13	1.75	0.66
1:G:494:LEU:HD21	1:G:607:VAL:HG22	1.76	0.66
1:D:494:LEU:HD21	1:D:607:VAL:HG22	1.76	0.66
1:E:481:ALA:O	1:E:485:THR:HG23	1.95	0.66
1:D:481:ALA:O	1:D:485:THR:HG23	1.95	0.66
1:D:524:LEU:HD12	1:D:582:ALA:HB1	1.79	0.65
1:F:761:LYS:NZ	1:F:765:ASP:OD2	2.20	0.65
1:F:249:LYS:O	1:F:252:SER:OG	2.08	0.65
1:E:249:LYS:O	1:E:252:SER:OG	2.09	0.65
1:A:38:GLU:OE2	1:H:382:GLY:C	2.33	0.65
1:G:481:ALA:O	1:G:485:THR:HG23	1.95	0.65
1:B:761:LYS:NZ	1:B:765:ASP:OD2	2.20	0.65
1:B:524:LEU:HD12	1:B:582:ALA:HB1	1.79	0.65
1:E:550:GLU:OE2	1:A:507:ASN:ND2	2.31	0.64
1:A:524:LEU:HD12	1:A:582:ALA:HB1	1.79	0.64
1:D:249:LYS:O	1:D:252:SER:OG	2.09	0.64
1:A:177:ILE:HD11	1:A:210:VAL:HG11	1.80	0.64
1:D:385:LEU:HD21	1:F:42:GLY:CA	2.28	0.64
1:F:177:ILE:HD11	1:F:210:VAL:HG11	1.80	0.64
1:H:524:LEU:HD12	1:H:582:ALA:HB1	1.79	0.64
1:D:761:LYS:NZ	1:D:765:ASP:OD2	2.20	0.64
1:G:524:LEU:HD12	1:G:582:ALA:HB1	1.79	0.64
1:H:177:ILE:HD11	1:H:210:VAL:HG11	1.80	0.64
1:C:761:LYS:NZ	1:C:765:ASP:OD2	2.20	0.64
1:D:177:ILE:HD11	1:D:210:VAL:HG11	1.80	0.64
1:F:524:LEU:HD12	1:F:582:ALA:HB1	1.79	0.64
1:E:524:LEU:HD12	1:E:582:ALA:HB1	1.79	0.63
1:H:249:LYS:O	1:H:252:SER:OG	2.09	0.63
1:C:524:LEU:HD12	1:C:582:ALA:HB1	1.79	0.63
1:C:787:LEU:HD21	1:D:608:TYR:CD1	2.33	0.63
1:H:35:SER:HA	1:H:38:GLU:HB3	1.81	0.63
1:D:308:ARG:NH2	1:F:36:ILE:HG13	2.14	0.63
1:F:35:SER:HA	1:F:38:GLU:HB3	1.81	0.63
1:B:177:ILE:HD11	1:B:210:VAL:HG11	1.80	0.62
1:G:177:ILE:HD11	1:G:210:VAL:HG11	1.80	0.62
1:G:35:SER:HA	1:G:38:GLU:HB3	1.81	0.62
1:E:177:ILE:HD11	1:E:210:VAL:HG11	1.80	0.62
1:C:177:ILE:HD11	1:C:210:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:707:THR:HG22	1:H:642:ARG:HH22	1.65	0.62
1:C:35:SER:HA	1:C:38:GLU:HB3	1.81	0.62
1:C:255:THR:O	1:C:290:ARG:NH2	2.33	0.62
1:E:35:SER:HA	1:E:38:GLU:HB3	1.81	0.62
1:E:255:THR:O	1:E:290:ARG:NH2	2.33	0.62
1:B:35:SER:HA	1:B:38:GLU:HB3	1.81	0.62
1:A:608:TYR:CE1	1:H:787:LEU:HD11	2.35	0.62
1:A:35:SER:HA	1:A:38:GLU:HB3	1.81	0.61
1:D:35:SER:HA	1:D:38:GLU:HB3	1.81	0.61
1:B:255:THR:O	1:B:290:ARG:NH2	2.33	0.61
1:F:255:THR:O	1:F:290:ARG:NH2	2.33	0.61
1:G:255:THR:O	1:G:290:ARG:NH2	2.33	0.61
1:A:255:THR:O	1:A:290:ARG:NH2	2.33	0.61
1:D:255:THR:O	1:D:290:ARG:NH2	2.33	0.61
1:A:42:GLY:CA	1:H:385:LEU:HD21	2.31	0.61
1:D:382:GLY:C	1:F:38:GLU:OE2	2.38	0.61
1:H:255:THR:O	1:H:290:ARG:NH2	2.33	0.60
1:E:658:ILE:HG22	1:F:659:TYR:OH	2.02	0.60
1:B:308:ARG:NH1	1:H:35:SER:OG	2.35	0.60
1:E:610:LEU:CD1	1:E:611:VAL:HG23	2.32	0.60
1:F:610:LEU:CD1	1:F:611:VAL:HG23	2.32	0.60
1:C:507:ASN:OD1	1:D:549:THR:OG1	2.19	0.59
1:D:610:LEU:CD1	1:D:611:VAL:HG23	2.32	0.59
1:A:12:ARG:NE	1:H:387:THR:O	2.30	0.59
1:D:308:ARG:HH22	1:F:36:ILE:HG13	1.68	0.59
1:H:583:ILE:HD11	1:H:704:PHE:HZ	1.68	0.59
1:B:787:LEU:HD21	1:H:608:TYR:CD1	2.38	0.59
1:C:610:LEU:CD1	1:C:611:VAL:HG23	2.32	0.59
1:B:583:ILE:HD11	1:B:704:PHE:HZ	1.68	0.59
1:A:583:ILE:HD11	1:A:704:PHE:HZ	1.68	0.59
1:D:583:ILE:HD11	1:D:704:PHE:HZ	1.68	0.59
1:F:583:ILE:HD11	1:F:704:PHE:HZ	1.68	0.59
1:A:610:LEU:CD1	1:A:611:VAL:HG23	2.32	0.59
1:G:610:LEU:CD1	1:G:611:VAL:HG23	2.32	0.59
1:H:610:LEU:CD1	1:H:611:VAL:HG23	2.32	0.59
1:B:610:LEU:CD1	1:B:611:VAL:HG23	2.32	0.58
1:H:140:TYR:CE2	1:H:144:ILE:HD11	2.38	0.58
1:E:140:TYR:CE2	1:E:144:ILE:HD11	2.39	0.58
1:C:140:TYR:CE2	1:C:144:ILE:HD11	2.38	0.58
1:G:127:ASN:O	1:G:134:VAL:HG23	2.04	0.58
1:D:140:TYR:CE2	1:D:144:ILE:HD11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ASN:O	1:F:134:VAL:HG23	2.04	0.58
1:F:140:TYR:CE2	1:F:144:ILE:HD11	2.38	0.58
1:E:583:ILE:HD11	1:E:704:PHE:HZ	1.68	0.58
1:C:127:ASN:O	1:C:134:VAL:HG23	2.04	0.58
1:H:127:ASN:O	1:H:134:VAL:HG23	2.03	0.58
1:G:140:TYR:CE2	1:G:144:ILE:HD11	2.39	0.58
1:A:127:ASN:O	1:A:134:VAL:HG23	2.03	0.58
1:C:385:LEU:O	1:D:12:ARG:NH1	2.37	0.58
1:H:86:CYS:HG	1:H:216:TYR:HE1	1.50	0.58
1:E:127:ASN:O	1:E:134:VAL:HG23	2.04	0.58
1:D:127:ASN:O	1:D:134:VAL:HG23	2.04	0.58
1:G:583:ILE:HD11	1:G:704:PHE:HZ	1.68	0.58
1:E:707:THR:HG22	1:D:642:ARG:NH2	2.18	0.58
1:A:140:TYR:CE2	1:A:144:ILE:HD11	2.38	0.58
1:C:583:ILE:HD11	1:C:704:PHE:HZ	1.68	0.58
1:D:86:CYS:HG	1:D:216:TYR:HE1	1.51	0.58
1:E:86:CYS:HG	1:E:216:TYR:HE1	1.51	0.57
1:A:735:ARG:NH1	1:D:732:ASP:OD1	2.36	0.57
1:B:140:TYR:CE2	1:B:144:ILE:HD11	2.38	0.57
1:B:127:ASN:O	1:B:134:VAL:HG23	2.03	0.57
1:D:475:GLU:OE2	1:D:475:GLU:N	2.38	0.57
1:G:86:CYS:HG	1:G:216:TYR:HE1	1.51	0.57
1:F:86:CYS:HG	1:F:216:TYR:HE1	1.52	0.57
1:B:308:ARG:CZ	1:H:35:SER:OG	2.53	0.56
1:H:475:GLU:OE2	1:H:475:GLU:N	2.38	0.56
1:G:475:GLU:OE2	1:G:475:GLU:N	2.38	0.56
1:C:507:ASN:CG	1:D:549:THR:HG1	2.09	0.55
1:B:475:GLU:OE2	1:B:475:GLU:N	2.38	0.55
1:E:111:GLN:HG2	1:E:166:LEU:HD22	1.89	0.55
1:E:475:GLU:N	1:E:475:GLU:OE2	2.38	0.55
1:C:308:ARG:NH1	1:D:35:SER:OG	2.39	0.55
1:E:710:ASN:ND2	1:D:641:ASP:OD2	2.38	0.55
1:C:475:GLU:N	1:C:475:GLU:OE2	2.38	0.55
1:E:289:ASP:O	1:E:324:ARG:NH1	2.40	0.55
1:C:396:TYR:CG	1:D:97:ARG:NH1	2.75	0.55
1:G:289:ASP:O	1:G:324:ARG:NH1	2.40	0.55
1:D:289:ASP:O	1:D:324:ARG:NH1	2.40	0.55
1:A:111:GLN:HG2	1:A:166:LEU:HD22	1.89	0.54
1:A:289:ASP:O	1:A:324:ARG:NH1	2.40	0.54
1:F:768:GLN:NE2	1:F:789:VAL:O	2.40	0.54
1:D:385:LEU:O	1:F:12:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:768:GLN:NE2	1:G:789:VAL:O	2.40	0.54
1:H:768:GLN:NE2	1:H:789:VAL:O	2.41	0.54
1:A:550:GLU:OE2	1:H:507:ASN:ND2	2.41	0.54
1:A:768:GLN:NE2	1:A:789:VAL:O	2.40	0.54
1:B:187:MET:HB3	1:B:192:PHE:HB2	1.90	0.54
1:C:768:GLN:NE2	1:C:789:VAL:O	2.40	0.54
1:D:187:MET:HB3	1:D:192:PHE:HB2	1.90	0.54
1:H:289:ASP:O	1:H:324:ARG:NH1	2.40	0.54
1:E:187:MET:HB3	1:E:192:PHE:HB2	1.90	0.54
1:A:187:MET:HB3	1:A:192:PHE:HB2	1.90	0.54
1:G:187:MET:HB3	1:G:192:PHE:HB2	1.90	0.54
1:B:768:GLN:NE2	1:B:789:VAL:O	2.40	0.54
1:H:111:GLN:HG2	1:H:166:LEU:HD22	1.89	0.54
1:E:768:GLN:NE2	1:E:789:VAL:O	2.40	0.54
1:A:608:TYR:CD1	1:H:787:LEU:HD11	2.43	0.54
1:C:308:ARG:CZ	1:D:35:SER:OG	2.55	0.54
1:G:111:GLN:HG2	1:G:166:LEU:HD22	1.89	0.54
1:C:187:MET:HB3	1:C:192:PHE:HB2	1.90	0.53
1:A:38:GLU:OE2	1:H:381:SER:O	2.27	0.53
1:B:289:ASP:O	1:B:324:ARG:NH1	2.40	0.53
1:B:111:GLN:HG2	1:B:166:LEU:HD22	1.89	0.53
1:D:768:GLN:NE2	1:D:789:VAL:O	2.40	0.53
1:F:475:GLU:N	1:F:475:GLU:OE2	2.38	0.53
1:C:111:GLN:HG2	1:C:166:LEU:HD22	1.89	0.53
1:C:289:ASP:O	1:C:324:ARG:NH1	2.40	0.53
1:F:111:GLN:HG2	1:F:166:LEU:HD22	1.89	0.53
1:F:308:ARG:NH1	1:G:35:SER:HG	2.05	0.53
1:H:403:TYR:CE1	1:H:407:LEU:HD12	2.44	0.53
1:B:287:ILE:O	1:B:291:VAL:HG13	2.09	0.53
1:D:111:GLN:HG2	1:D:166:LEU:HD22	1.89	0.53
1:F:287:ILE:O	1:F:291:VAL:HG13	2.09	0.53
1:A:403:TYR:CE1	1:A:407:LEU:HD12	2.44	0.52
1:D:287:ILE:O	1:D:291:VAL:HG13	2.09	0.52
1:H:187:MET:HB3	1:H:192:PHE:HB2	1.90	0.52
1:H:287:ILE:O	1:H:291:VAL:HG13	2.09	0.52
1:C:403:TYR:CE1	1:C:407:LEU:HD12	2.44	0.52
1:F:403:TYR:CE1	1:F:407:LEU:HD12	2.44	0.52
1:G:403:TYR:CE1	1:G:407:LEU:HD12	2.44	0.52
1:E:403:TYR:CE1	1:E:407:LEU:HD12	2.44	0.52
1:B:403:TYR:CE1	1:B:407:LEU:HD12	2.44	0.52
1:A:475:GLU:N	1:A:475:GLU:OE2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:LEU:HD21	1:D:42:GLY:CA	2.40	0.52
1:F:289:ASP:O	1:F:324:ARG:NH1	2.40	0.52
1:E:287:ILE:O	1:E:291:VAL:HG13	2.09	0.52
1:E:332:LEU:HD12	1:E:418:LEU:HD11	1.92	0.52
1:C:703:ASN:O	1:C:707:THR:HG23	2.10	0.52
1:F:332:LEU:HD12	1:F:418:LEU:HD11	1.92	0.52
1:G:332:LEU:HD12	1:G:418:LEU:HD11	1.92	0.52
1:H:703:ASN:O	1:H:707:THR:HG23	2.10	0.52
1:A:332:LEU:HD12	1:A:418:LEU:HD11	1.91	0.52
1:D:403:TYR:CE1	1:D:407:LEU:HD12	2.44	0.52
1:F:187:MET:HB3	1:F:192:PHE:HB2	1.90	0.52
1:H:63:MET:HG2	1:H:331:LEU:HD22	1.92	0.52
1:A:63:MET:HG2	1:A:331:LEU:HD22	1.92	0.52
1:A:545:TYR:O	1:A:549:THR:HG23	2.10	0.52
1:G:545:TYR:O	1:G:549:THR:HG23	2.10	0.52
1:G:703:ASN:O	1:G:707:THR:HG23	2.10	0.52
1:E:703:ASN:O	1:E:707:THR:HG23	2.10	0.52
1:B:507:ASN:OD1	1:H:549:THR:OG1	2.28	0.52
1:F:63:MET:HG2	1:F:331:LEU:HD22	1.92	0.52
1:F:187:MET:O	1:F:191:ASN:N	2.43	0.52
1:C:63:MET:HG2	1:C:331:LEU:HD22	1.92	0.51
1:C:287:ILE:O	1:C:291:VAL:HG13	2.09	0.51
1:D:545:TYR:O	1:D:549:THR:HG23	2.10	0.51
1:H:187:MET:O	1:H:191:ASN:N	2.43	0.51
1:A:187:MET:O	1:A:191:ASN:N	2.43	0.51
1:B:332:LEU:HD12	1:B:418:LEU:HD11	1.91	0.51
1:G:187:MET:O	1:G:191:ASN:N	2.43	0.51
1:A:287:ILE:O	1:A:291:VAL:HG13	2.09	0.51
1:B:15:VAL:O	1:B:19:ILE:HG12	2.11	0.51
1:D:63:MET:HG2	1:D:331:LEU:HD22	1.92	0.51
1:D:385:LEU:HD11	1:F:42:GLY:HA3	1.92	0.51
1:G:288:ARG:NH1	1:G:289:ASP:OD1	2.44	0.51
1:B:545:TYR:O	1:B:549:THR:HG23	2.10	0.51
1:B:703:ASN:O	1:B:707:THR:HG23	2.10	0.51
1:E:63:MET:HG2	1:E:331:LEU:HD22	1.92	0.51
1:C:288:ARG:NH1	1:C:289:ASP:OD1	2.44	0.51
1:D:703:ASN:O	1:D:707:THR:HG23	2.10	0.51
1:E:545:TYR:O	1:E:549:THR:HG23	2.10	0.51
1:A:36:ILE:H	1:H:308:ARG:HH22	1.57	0.51
1:A:703:ASN:O	1:A:707:THR:HG23	2.10	0.51
1:G:287:ILE:O	1:G:291:VAL:HG13	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:288:ARG:NH1	1:H:289:ASP:OD1	2.44	0.51
1:H:545:TYR:O	1:H:549:THR:HG23	2.10	0.51
1:E:187:MET:O	1:E:191:ASN:N	2.43	0.51
1:A:15:VAL:O	1:A:19:ILE:HG12	2.11	0.51
1:C:332:LEU:HD12	1:C:418:LEU:HD11	1.91	0.51
1:C:545:TYR:O	1:C:549:THR:HG23	2.10	0.51
1:D:187:MET:O	1:D:191:ASN:N	2.43	0.51
1:D:288:ARG:NH1	1:D:289:ASP:OD1	2.44	0.51
1:F:15:VAL:O	1:F:19:ILE:HG12	2.11	0.51
1:F:703:ASN:O	1:F:707:THR:HG23	2.10	0.51
1:E:15:VAL:O	1:E:19:ILE:HG12	2.11	0.51
1:E:288:ARG:NH1	1:E:289:ASP:OD1	2.44	0.51
1:B:735:ARG:HH12	1:G:735:ARG:HH22	1.59	0.51
1:C:187:MET:O	1:C:191:ASN:N	2.43	0.51
1:D:332:LEU:HD12	1:D:418:LEU:HD11	1.91	0.51
1:G:63:MET:HG2	1:G:331:LEU:HD22	1.92	0.51
1:D:15:VAL:O	1:D:19:ILE:HG12	2.11	0.51
1:G:13:GLU:OE1	1:G:13:GLU:N	2.43	0.51
1:E:57:PHE:O	1:E:58:SER:OG	2.27	0.51
1:B:63:MET:HG2	1:B:331:LEU:HD22	1.92	0.51
1:B:187:MET:O	1:B:191:ASN:N	2.43	0.51
1:B:332:LEU:CD1	1:B:418:LEU:HD21	2.40	0.51
1:H:332:LEU:HD12	1:H:418:LEU:HD11	1.91	0.51
1:C:86:CYS:HG	1:C:216:TYR:HE1	1.59	0.50
1:F:288:ARG:NH1	1:F:289:ASP:OD1	2.44	0.50
1:F:545:TYR:O	1:F:549:THR:HG23	2.10	0.50
1:C:15:VAL:O	1:C:19:ILE:HG12	2.11	0.50
1:D:787:LEU:HD11	1:F:608:TYR:CE1	2.45	0.50
1:H:13:GLU:OE1	1:H:13:GLU:N	2.43	0.50
1:H:15:VAL:O	1:H:19:ILE:HG12	2.11	0.50
1:E:263:LYS:N	1:E:264:PRO:CD	2.75	0.50
1:A:263:LYS:N	1:A:264:PRO:CD	2.75	0.50
1:A:335:TYR:CD1	1:A:370:PHE:HB2	2.47	0.50
1:C:263:LYS:N	1:C:264:PRO:CD	2.75	0.50
1:C:787:LEU:HD11	1:D:608:TYR:CD1	2.46	0.50
1:A:86:CYS:HG	1:A:216:TYR:HE1	1.59	0.50
1:A:288:ARG:NH1	1:A:289:ASP:OD1	2.44	0.50
1:B:263:LYS:N	1:B:264:PRO:CD	2.75	0.50
1:B:288:ARG:NH1	1:B:289:ASP:OD1	2.44	0.50
1:D:263:LYS:N	1:D:264:PRO:CD	2.75	0.50
1:G:15:VAL:O	1:G:19:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:LYS:N	1:G:264:PRO:CD	2.75	0.50
1:D:335:TYR:CD1	1:D:370:PHE:HB2	2.47	0.50
1:H:664:THR:O	1:H:669:SER:N	2.45	0.50
1:A:36:ILE:N	1:H:308:ARG:HH12	2.10	0.50
1:F:335:TYR:CD1	1:F:370:PHE:HB2	2.47	0.50
1:G:57:PHE:O	1:G:58:SER:OG	2.27	0.50
1:H:332:LEU:CD1	1:H:418:LEU:HD21	2.40	0.50
1:E:610:LEU:HD12	1:E:611:VAL:HG23	1.94	0.49
1:C:13:GLU:OE1	1:C:13:GLU:N	2.43	0.49
1:C:384:LEU:HD22	1:C:389:PHE:HB2	1.95	0.49
1:A:642:ARG:NH1	1:F:706:GLN:HG3	2.28	0.49
1:A:384:LEU:HD22	1:A:389:PHE:HB2	1.95	0.49
1:A:635:GLU:OE2	1:F:635:GLU:OE2	2.30	0.49
1:C:335:TYR:CD1	1:C:370:PHE:HB2	2.47	0.49
1:F:57:PHE:O	1:F:58:SER:OG	2.27	0.49
1:B:335:TYR:CD1	1:B:370:PHE:HB2	2.47	0.49
1:C:332:LEU:CD1	1:C:418:LEU:HD21	2.41	0.49
1:H:263:LYS:N	1:H:264:PRO:CD	2.75	0.49
1:H:335:TYR:CD1	1:H:370:PHE:HB2	2.47	0.49
1:C:402:ASN:OD1	1:C:405:ARG:NH2	2.44	0.49
1:G:335:TYR:CD1	1:G:370:PHE:HB2	2.47	0.49
1:E:335:TYR:CD1	1:E:370:PHE:HB2	2.47	0.49
1:E:707:THR:HG22	1:D:642:ARG:HH22	1.77	0.49
1:D:610:LEU:HD12	1:D:611:VAL:HG23	1.94	0.49
1:F:263:LYS:N	1:F:264:PRO:CD	2.75	0.49
1:C:371:VAL:HG13	1:C:403:TYR:HB2	1.95	0.49
1:G:402:ASN:OD1	1:G:405:ARG:NH2	2.43	0.49
1:A:57:PHE:O	1:A:58:SER:OG	2.27	0.49
1:H:57:PHE:O	1:H:58:SER:OG	2.27	0.49
1:H:384:LEU:HD22	1:H:389:PHE:HB2	1.95	0.49
1:H:391:VAL:HG23	1:H:406:ILE:HG23	1.95	0.49
1:B:13:GLU:OE1	1:B:13:GLU:N	2.43	0.48
1:B:371:VAL:HG13	1:B:403:TYR:HB2	1.95	0.48
1:C:664:THR:O	1:C:669:SER:N	2.45	0.48
1:D:384:LEU:HD22	1:D:389:PHE:HB2	1.95	0.48
1:F:371:VAL:HG13	1:F:403:TYR:HB2	1.95	0.48
1:F:610:LEU:HD12	1:F:611:VAL:HG23	1.94	0.48
1:B:384:LEU:HD22	1:B:389:PHE:HB2	1.95	0.48
1:B:664:THR:O	1:B:669:SER:N	2.45	0.48
1:G:391:VAL:HG23	1:G:406:ILE:HG23	1.95	0.48
1:B:57:PHE:O	1:B:58:SER:OG	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:VAL:HG23	1:D:406:ILE:HG23	1.95	0.48
1:F:13:GLU:OE1	1:F:13:GLU:N	2.43	0.48
1:G:610:LEU:HD12	1:G:611:VAL:HG23	1.94	0.48
1:H:97:ARG:O	1:H:217:PHE:N	2.47	0.48
1:C:57:PHE:O	1:C:58:SER:OG	2.27	0.48
1:C:97:ARG:O	1:C:217:PHE:N	2.47	0.48
1:C:391:VAL:HG23	1:C:406:ILE:HG23	1.95	0.48
1:C:610:LEU:HD12	1:C:611:VAL:HG23	1.94	0.48
1:D:97:ARG:O	1:D:217:PHE:N	2.47	0.48
1:B:97:ARG:O	1:B:217:PHE:N	2.47	0.48
1:G:97:ARG:O	1:G:217:PHE:N	2.47	0.48
1:E:480:LYS:HG2	1:E:742:LEU:HD13	1.96	0.48
1:A:638:THR:O	1:A:642:ARG:NH1	2.47	0.48
1:B:385:LEU:O	1:H:12:ARG:NH1	2.47	0.48
1:B:391:VAL:HG23	1:B:406:ILE:HG23	1.95	0.48
1:C:507:ASN:ND2	1:D:546:LYS:HG3	2.28	0.48
1:F:384:LEU:HD22	1:F:389:PHE:HB2	1.95	0.48
1:G:384:LEU:HD22	1:G:389:PHE:HB2	1.95	0.48
1:H:610:LEU:HD12	1:H:611:VAL:HG23	1.94	0.48
1:E:371:VAL:HG13	1:E:403:TYR:HB2	1.95	0.48
1:E:638:THR:O	1:E:642:ARG:NH1	2.47	0.48
1:C:308:ARG:NH2	1:D:36:ILE:HG13	2.28	0.48
1:D:57:PHE:O	1:D:58:SER:OG	2.27	0.48
1:A:64:LEU:O	1:A:68:LEU:HG	2.14	0.48
1:H:638:THR:O	1:H:642:ARG:NH1	2.47	0.48
1:E:382:GLY:O	1:E:385:LEU:HB3	2.14	0.48
1:A:610:LEU:HD12	1:A:611:VAL:HG23	1.94	0.48
1:B:64:LEU:O	1:B:68:LEU:HG	2.14	0.48
1:B:610:LEU:HD12	1:B:611:VAL:HG23	1.94	0.48
1:G:480:LYS:HG2	1:G:742:LEU:HD13	1.95	0.48
1:H:480:LYS:HG2	1:H:742:LEU:HD13	1.95	0.48
1:F:64:LEU:O	1:F:68:LEU:HG	2.14	0.47
1:G:382:GLY:O	1:G:385:LEU:HB3	2.14	0.47
1:G:664:THR:O	1:G:669:SER:N	2.45	0.47
1:E:391:VAL:HG23	1:E:406:ILE:HG23	1.95	0.47
1:A:97:ARG:O	1:A:217:PHE:N	2.47	0.47
1:B:638:THR:O	1:B:642:ARG:NH1	2.47	0.47
1:C:412:ILE:N	1:C:413:PRO:CD	2.78	0.47
1:D:507:ASN:ND2	1:F:550:GLU:OE2	2.47	0.47
1:D:610:LEU:HD13	1:D:611:VAL:HG23	1.96	0.47
1:F:382:GLY:O	1:F:385:LEU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ILE:N	1:E:413:PRO:CD	2.78	0.47
1:D:64:LEU:O	1:D:68:LEU:HG	2.14	0.47
1:F:391:VAL:HG23	1:F:406:ILE:HG23	1.95	0.47
1:H:64:LEU:O	1:H:68:LEU:HG	2.14	0.47
1:A:72:GLU:O	1:A:203:ARG:NH2	2.48	0.47
1:A:391:VAL:HG23	1:A:406:ILE:HG23	1.95	0.47
1:B:412:ILE:N	1:B:413:PRO:CD	2.78	0.47
1:D:371:VAL:HG13	1:D:403:TYR:HB2	1.95	0.47
1:G:412:ILE:N	1:G:413:PRO:CD	2.78	0.47
1:E:384:LEU:HD22	1:E:389:PHE:HB2	1.95	0.47
1:A:64:LEU:HD21	1:A:294:VAL:HG11	1.97	0.47
1:A:412:ILE:N	1:A:413:PRO:CD	2.78	0.47
1:A:610:LEU:HD13	1:A:611:VAL:HG23	1.96	0.47
1:D:72:GLU:O	1:D:203:ARG:NH2	2.48	0.47
1:G:332:LEU:CD1	1:G:418:LEU:HD21	2.40	0.47
1:G:371:VAL:HG13	1:G:403:TYR:HB2	1.95	0.47
1:H:371:VAL:HG13	1:H:403:TYR:HB2	1.95	0.47
1:E:97:ARG:O	1:E:217:PHE:N	2.47	0.47
1:A:371:VAL:HG13	1:A:403:TYR:HB2	1.95	0.47
1:A:706:GLN:HG3	1:F:642:ARG:NH1	2.29	0.47
1:F:97:ARG:O	1:F:217:PHE:N	2.47	0.47
1:G:64:LEU:O	1:G:68:LEU:HG	2.14	0.47
1:E:610:LEU:HD13	1:E:611:VAL:HG23	1.96	0.47
1:B:610:LEU:HD13	1:B:611:VAL:HG23	1.96	0.47
1:C:480:LYS:HG2	1:C:742:LEU:HD13	1.96	0.47
1:D:382:GLY:O	1:D:385:LEU:HB3	2.14	0.47
1:D:480:LYS:HG2	1:D:742:LEU:HD13	1.95	0.47
1:F:64:LEU:HD21	1:F:294:VAL:HG11	1.97	0.47
1:F:72:GLU:O	1:F:203:ARG:NH2	2.48	0.47
1:F:412:ILE:N	1:F:413:PRO:CD	2.78	0.47
1:F:468:GLN:OE1	1:F:469:LEU:HD12	2.15	0.47
1:F:480:LYS:HG2	1:F:742:LEU:HD13	1.96	0.47
1:G:638:THR:O	1:G:642:ARG:NH1	2.47	0.47
1:E:64:LEU:O	1:E:68:LEU:HG	2.14	0.47
1:E:72:GLU:O	1:E:203:ARG:NH2	2.48	0.47
1:A:480:LYS:HG2	1:A:742:LEU:HD13	1.95	0.47
1:B:382:GLY:O	1:B:385:LEU:HB3	2.14	0.47
1:B:396:TYR:CG	1:H:97:ARG:NH1	2.82	0.47
1:D:638:THR:O	1:D:642:ARG:NH1	2.47	0.47
1:F:638:THR:O	1:F:642:ARG:NH1	2.47	0.47
1:G:72:GLU:O	1:G:203:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:GLY:O	1:C:385:LEU:HB3	2.14	0.47
1:C:507:ASN:ND2	1:D:546:LYS:CG	2.77	0.47
1:C:638:THR:O	1:C:642:ARG:NH1	2.47	0.47
1:C:787:LEU:HD11	1:D:608:TYR:CZ	2.50	0.47
1:D:641:ASP:O	1:D:644:VAL:HG22	2.15	0.47
1:F:664:THR:O	1:F:669:SER:N	2.45	0.47
1:G:610:LEU:HD13	1:G:611:VAL:HG23	1.96	0.47
1:G:710:ASN:HD21	1:H:641:ASP:CB	2.28	0.47
1:D:468:GLN:OE1	1:D:469:LEU:HD12	2.15	0.47
1:F:385:LEU:O	1:G:12:ARG:CZ	2.63	0.47
1:F:641:ASP:O	1:F:644:VAL:HG22	2.15	0.47
1:H:382:GLY:O	1:H:385:LEU:HB3	2.14	0.47
1:A:468:GLN:OE1	1:A:469:LEU:HD12	2.15	0.46
1:B:72:GLU:O	1:B:203:ARG:NH2	2.48	0.46
1:B:480:LYS:HG2	1:B:742:LEU:HD13	1.96	0.46
1:H:72:GLU:O	1:H:203:ARG:NH2	2.48	0.46
1:A:641:ASP:O	1:A:644:VAL:HG22	2.15	0.46
1:B:64:LEU:HD21	1:B:294:VAL:HG11	1.97	0.46
1:B:468:GLN:OE1	1:B:469:LEU:HD12	2.15	0.46
1:C:64:LEU:HD21	1:C:294:VAL:HG11	1.97	0.46
1:D:85:GLU:OE1	1:D:245:ARG:NH1	2.49	0.46
1:D:664:THR:O	1:D:669:SER:N	2.45	0.46
1:F:332:LEU:CD1	1:F:418:LEU:HD21	2.40	0.46
1:A:85:GLU:OE1	1:A:245:ARG:NH1	2.49	0.46
1:A:332:LEU:CD1	1:A:418:LEU:HD21	2.40	0.46
1:C:64:LEU:O	1:C:68:LEU:HG	2.14	0.46
1:D:64:LEU:HD21	1:D:294:VAL:HG11	1.97	0.46
1:D:412:ILE:N	1:D:413:PRO:CD	2.78	0.46
1:G:64:LEU:HD21	1:G:294:VAL:HG11	1.97	0.46
1:H:64:LEU:HD21	1:H:294:VAL:HG11	1.97	0.46
1:H:402:ASN:OD1	1:H:405:ARG:NH2	2.44	0.46
1:E:64:LEU:HD21	1:E:294:VAL:HG11	1.97	0.46
1:E:468:GLN:OE1	1:E:469:LEU:HD12	2.15	0.46
1:C:468:GLN:OE1	1:C:469:LEU:HD12	2.15	0.46
1:C:641:ASP:O	1:C:644:VAL:HG22	2.15	0.46
1:F:610:LEU:HD13	1:F:611:VAL:HG23	1.96	0.46
1:H:610:LEU:HD13	1:H:611:VAL:HG23	1.96	0.46
1:E:714:THR:OG1	1:D:637:ARG:HD3	2.15	0.46
1:A:722:GLU:HA	1:A:722:GLU:OE1	2.16	0.46
1:B:641:ASP:O	1:B:644:VAL:HG22	2.15	0.46
1:B:722:GLU:OE1	1:B:722:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLU:O	1:C:203:ARG:NH2	2.48	0.46
1:C:610:LEU:HD13	1:C:611:VAL:HG23	1.96	0.46
1:D:674:ALA:O	1:D:677:ILE:HG22	2.16	0.46
1:G:85:GLU:OE1	1:G:245:ARG:NH1	2.49	0.46
1:G:714:THR:OG1	1:H:637:ARG:HD3	2.16	0.46
1:H:722:GLU:OE1	1:H:722:GLU:HA	2.16	0.46
1:E:85:GLU:OE1	1:E:245:ARG:NH1	2.49	0.46
1:E:332:LEU:CD1	1:E:418:LEU:HD21	2.40	0.46
1:E:722:GLU:OE1	1:E:722:GLU:HA	2.16	0.46
1:B:85:GLU:OE1	1:B:245:ARG:NH1	2.49	0.46
1:H:641:ASP:O	1:H:644:VAL:HG22	2.15	0.46
1:C:385:LEU:O	1:D:12:ARG:CZ	2.63	0.46
1:G:674:ALA:O	1:G:677:ILE:HG22	2.16	0.46
1:H:412:ILE:N	1:H:413:PRO:CD	2.78	0.46
1:H:506:ILE:O	1:H:510:VAL:HG23	2.16	0.46
1:A:32:GLN:O	1:H:312:GLU:OE1	2.34	0.46
1:A:382:GLY:O	1:A:385:LEU:HB3	2.14	0.46
1:B:674:ALA:O	1:B:677:ILE:HG22	2.16	0.46
1:C:536:LEU:O	1:C:536:LEU:HD23	2.16	0.46
1:G:641:ASP:O	1:G:644:VAL:HG22	2.15	0.46
1:E:13:GLU:OE1	1:E:13:GLU:N	2.43	0.46
1:A:38:GLU:OE2	1:H:382:GLY:CA	2.64	0.46
1:D:506:ILE:O	1:D:510:VAL:HG23	2.16	0.46
1:H:468:GLN:OE1	1:H:469:LEU:HD12	2.15	0.46
1:E:506:ILE:O	1:E:510:VAL:HG23	2.16	0.46
1:A:258:VAL:HB	1:A:291:VAL:HG12	1.98	0.46
1:B:402:ASN:OD1	1:B:405:ARG:NH2	2.44	0.46
1:D:258:VAL:HB	1:D:291:VAL:HG12	1.98	0.46
1:G:722:GLU:OE1	1:G:722:GLU:HA	2.16	0.46
1:E:641:ASP:O	1:E:644:VAL:HG22	2.15	0.45
1:C:506:ILE:O	1:C:510:VAL:HG23	2.16	0.45
1:G:468:GLN:OE1	1:G:469:LEU:HD12	2.15	0.45
1:E:536:LEU:O	1:E:536:LEU:HD23	2.16	0.45
1:E:664:THR:O	1:E:669:SER:N	2.45	0.45
1:C:85:GLU:OE1	1:C:245:ARG:NH1	2.49	0.45
1:D:308:ARG:NH1	1:F:35:SER:OG	2.50	0.45
1:F:722:GLU:HA	1:F:722:GLU:OE1	2.16	0.45
1:A:506:ILE:O	1:A:510:VAL:HG23	2.16	0.45
1:B:536:LEU:HD23	1:B:536:LEU:O	2.16	0.45
1:B:646:GLU:OE1	1:B:651:TYR:OH	2.22	0.45
1:D:536:LEU:HD23	1:D:536:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:CYS:HG	1:B:216:TYR:HE1	1.65	0.45
1:D:108:ILE:HD11	1:D:210:VAL:CG1	2.47	0.45
1:F:85:GLU:OE1	1:F:245:ARG:NH1	2.49	0.45
1:F:258:VAL:HB	1:F:291:VAL:HG12	1.98	0.45
1:G:506:ILE:O	1:G:510:VAL:HG23	2.16	0.45
1:H:85:GLU:OE1	1:H:245:ARG:NH1	2.49	0.45
1:H:258:VAL:HB	1:H:291:VAL:HG12	1.98	0.45
1:E:108:ILE:HD11	1:E:210:VAL:CG1	2.47	0.45
1:A:536:LEU:HD23	1:A:536:LEU:O	2.16	0.45
1:B:506:ILE:O	1:B:510:VAL:HG23	2.16	0.45
1:C:619:GLN:HA	1:C:619:GLN:OE1	2.17	0.45
1:D:402:ASN:OD1	1:D:405:ARG:NH2	2.44	0.45
1:F:108:ILE:HD11	1:F:210:VAL:CG1	2.47	0.45
1:F:506:ILE:O	1:F:510:VAL:HG23	2.16	0.45
1:A:619:GLN:OE1	1:A:619:GLN:HA	2.17	0.45
1:B:507:ASN:CG	1:H:549:THR:HG1	2.20	0.45
1:D:619:GLN:OE1	1:D:619:GLN:HA	2.17	0.45
1:F:674:ALA:O	1:F:677:ILE:HG22	2.16	0.45
1:G:536:LEU:O	1:G:536:LEU:HD23	2.16	0.45
1:H:619:GLN:HA	1:H:619:GLN:OE1	2.17	0.45
1:E:674:ALA:O	1:E:677:ILE:HG22	2.16	0.45
1:D:722:GLU:HA	1:D:722:GLU:OE1	2.16	0.45
1:E:524:LEU:CD1	1:E:582:ALA:HB1	2.46	0.45
1:A:674:ALA:O	1:A:677:ILE:HG22	2.16	0.45
1:B:108:ILE:HD11	1:B:210:VAL:CG1	2.47	0.45
1:B:385:LEU:HD21	1:H:42:GLY:CA	2.47	0.45
1:D:386:SER:O	1:F:16:ASN:OD1	2.35	0.45
1:F:619:GLN:OE1	1:F:619:GLN:HA	2.17	0.45
1:H:674:ALA:O	1:H:677:ILE:HG22	2.16	0.45
1:E:258:VAL:HB	1:E:291:VAL:HG12	1.98	0.45
1:A:561:ILE:HG21	1:G:561:ILE:CG2	2.47	0.45
1:C:722:GLU:OE1	1:C:722:GLU:HA	2.16	0.45
1:G:108:ILE:HD11	1:G:210:VAL:CG1	2.47	0.45
1:H:536:LEU:HD23	1:H:536:LEU:O	2.16	0.45
1:C:674:ALA:O	1:C:677:ILE:HG22	2.16	0.45
1:D:332:LEU:CD1	1:D:418:LEU:HD21	2.40	0.45
1:F:524:LEU:CD1	1:F:582:ALA:HB1	2.46	0.45
1:A:108:ILE:HD11	1:A:210:VAL:CG1	2.47	0.44
1:A:402:ASN:OD1	1:A:405:ARG:NH2	2.44	0.44
1:C:52:VAL:HG22	1:C:230:VAL:HB	1.99	0.44
1:D:52:VAL:HG22	1:D:230:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:VAL:HB	1:G:291:VAL:HG12	1.98	0.44
1:G:524:LEU:CD1	1:G:582:ALA:HB1	2.46	0.44
1:B:619:GLN:OE1	1:B:619:GLN:HA	2.17	0.44
1:C:258:VAL:HB	1:C:291:VAL:HG12	1.98	0.44
1:H:108:ILE:HD11	1:H:210:VAL:CG1	2.47	0.44
1:E:528:MET:HE1	1:E:579:PHE:HA	2.00	0.44
1:C:108:ILE:HD11	1:C:210:VAL:CG1	2.47	0.44
1:B:258:VAL:HB	1:B:291:VAL:HG12	1.99	0.44
1:H:524:LEU:CD1	1:H:582:ALA:HB1	2.46	0.44
1:C:706:GLN:OE1	1:D:557:THR:CG2	2.66	0.44
1:D:396:TYR:CG	1:F:97:ARG:NH1	2.86	0.44
1:F:536:LEU:HD23	1:F:536:LEU:O	2.16	0.44
1:G:528:MET:HE1	1:G:579:PHE:HA	2.00	0.44
1:E:552:HIS:ND1	1:F:569:TYR:CE2	2.84	0.44
1:G:52:VAL:HG22	1:G:230:VAL:HB	1.99	0.44
1:E:619:GLN:HA	1:E:619:GLN:OE1	2.17	0.44
1:A:91:ALA:HB2	1:A:217:PHE:HB3	2.00	0.44
1:D:13:GLU:OE1	1:D:13:GLU:N	2.43	0.44
1:B:91:ALA:HB2	1:B:217:PHE:HB3	2.00	0.44
1:D:91:ALA:HB2	1:D:217:PHE:HB3	2.00	0.44
1:F:52:VAL:HG22	1:F:230:VAL:HB	1.99	0.44
1:B:528:MET:HE1	1:B:579:PHE:HA	2.00	0.43
1:A:52:VAL:HG22	1:A:230:VAL:HB	1.99	0.43
1:A:659:TYR:CZ	1:G:658:ILE:HG22	2.52	0.43
1:E:735:ARG:HH22	1:C:735:ARG:HH12	1.67	0.43
1:A:35:SER:OG	1:H:308:ARG:NH1	2.50	0.43
1:A:646:GLU:OE1	1:A:651:TYR:OH	2.22	0.43
1:B:52:VAL:HG22	1:B:230:VAL:HB	1.99	0.43
1:B:524:LEU:CD1	1:B:582:ALA:HB1	2.46	0.43
1:G:619:GLN:HA	1:G:619:GLN:OE1	2.17	0.43
1:A:13:GLU:OE1	1:A:13:GLU:N	2.43	0.43
1:A:664:THR:O	1:A:669:SER:N	2.45	0.43
1:A:761:LYS:O	1:A:765:ASP:OD1	2.37	0.43
1:H:52:VAL:HG22	1:H:230:VAL:HB	1.99	0.43
1:B:761:LYS:O	1:B:765:ASP:OD1	2.37	0.43
1:C:528:MET:HE1	1:C:579:PHE:HA	2.00	0.43
1:A:558:ALA:HA	1:G:569:TYR:OH	2.19	0.43
1:B:787:LEU:HD11	1:H:608:TYR:CD1	2.53	0.43
1:F:528:MET:HE1	1:F:579:PHE:HA	2.01	0.43
1:C:761:LYS:O	1:C:765:ASP:OD1	2.37	0.43
1:E:52:VAL:HG22	1:E:230:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ALA:HB2	1:E:217:PHE:HB3	2.00	0.43
1:A:355:ALA:HA	1:A:358:ILE:HG22	2.01	0.43
1:B:349:GLY:O	1:B:353:ILE:N	2.52	0.43
1:C:91:ALA:HB2	1:C:217:PHE:HB3	2.00	0.43
1:C:524:LEU:CD1	1:C:582:ALA:HB1	2.46	0.43
1:D:761:LYS:O	1:D:765:ASP:OD1	2.37	0.43
1:G:91:ALA:HB2	1:G:217:PHE:HB3	2.00	0.43
1:H:91:ALA:HB2	1:H:217:PHE:HB3	2.00	0.43
1:E:12:ARG:CZ	1:A:385:LEU:O	2.67	0.42
1:B:355:ALA:HA	1:B:358:ILE:HG22	2.01	0.42
1:D:355:ALA:HA	1:D:358:ILE:HG22	2.01	0.42
1:G:402:ASN:O	1:G:406:ILE:HG13	2.19	0.42
1:D:281:ILE:CG2	1:D:291:VAL:HG11	2.50	0.42
1:F:402:ASN:O	1:F:406:ILE:HG13	2.19	0.42
1:G:53:PHE:HZ	1:G:229:LEU:HD22	1.84	0.42
1:H:761:LYS:O	1:H:765:ASP:OD1	2.37	0.42
1:A:528:MET:HE1	1:A:579:PHE:HA	2.01	0.42
1:B:402:ASN:O	1:B:406:ILE:HG13	2.19	0.42
1:D:262:LEU:HB3	1:D:264:PRO:HD2	2.02	0.42
1:D:524:LEU:CD1	1:D:582:ALA:HB1	2.46	0.42
1:G:355:ALA:HA	1:G:358:ILE:HG22	2.01	0.42
1:H:564:LEU:O	1:H:568:LEU:HG	2.20	0.42
1:E:281:ILE:CG2	1:E:291:VAL:HG11	2.49	0.42
1:E:390:ARG:NE	1:E:390:ARG:HA	2.35	0.42
1:E:564:LEU:O	1:E:568:LEU:HG	2.20	0.42
1:B:725:GLN:HG3	1:G:492:GLN:NE2	2.34	0.42
1:D:390:ARG:HA	1:D:390:ARG:NE	2.35	0.42
1:D:528:MET:HE1	1:D:579:PHE:HA	2.01	0.42
1:F:761:LYS:O	1:F:765:ASP:OD1	2.37	0.42
1:G:281:ILE:CG2	1:G:291:VAL:HG11	2.49	0.42
1:E:262:LEU:HB3	1:E:264:PRO:HD2	2.02	0.42
1:E:402:ASN:O	1:E:406:ILE:HG13	2.19	0.42
1:E:761:LYS:O	1:E:765:ASP:OD1	2.37	0.42
1:A:103:LEU:HD23	1:A:212:LYS:HD3	2.02	0.42
1:A:349:GLY:O	1:A:353:ILE:N	2.52	0.42
1:B:262:LEU:HB3	1:B:264:PRO:HD2	2.01	0.42
1:B:281:ILE:CG2	1:B:291:VAL:HG11	2.49	0.42
1:D:564:LEU:O	1:D:568:LEU:HG	2.20	0.42
1:F:53:PHE:HZ	1:F:229:LEU:HD22	1.84	0.42
1:F:281:ILE:CG2	1:F:291:VAL:HG11	2.49	0.42
1:G:390:ARG:NE	1:G:390:ARG:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HB3	1:A:264:PRO:HD2	2.02	0.42
1:A:281:ILE:CG2	1:A:291:VAL:HG11	2.50	0.42
1:A:524:LEU:CD1	1:A:582:ALA:HB1	2.46	0.42
1:B:729:GLU:HA	1:G:488:ASN:HD22	1.84	0.42
1:H:103:LEU:HD23	1:H:212:LYS:HD3	2.02	0.42
1:H:390:ARG:HA	1:H:390:ARG:NE	2.35	0.42
1:B:103:LEU:HD23	1:B:212:LYS:HD3	2.02	0.42
1:D:402:ASN:O	1:D:406:ILE:HG13	2.19	0.42
1:G:564:LEU:O	1:G:568:LEU:HG	2.20	0.42
1:G:761:LYS:O	1:G:765:ASP:OD1	2.37	0.42
1:E:378:CYS:HB3	1:E:391:VAL:HG21	2.02	0.42
1:A:402:ASN:O	1:A:406:ILE:HG13	2.19	0.42
1:A:645:ARG:NH2	1:G:557:THR:HB	2.35	0.42
1:B:787:LEU:HD11	1:H:608:TYR:CZ	2.54	0.42
1:C:53:PHE:HZ	1:C:229:LEU:HD22	1.84	0.42
1:C:355:ALA:HA	1:C:358:ILE:HG22	2.01	0.42
1:F:91:ALA:HB2	1:F:217:PHE:HB3	2.00	0.42
1:F:564:LEU:O	1:F:568:LEU:HG	2.20	0.42
1:E:103:LEU:HD23	1:E:212:LYS:HD3	2.02	0.42
1:E:308:ARG:HD3	1:E:309:GLN:OE1	2.20	0.42
1:E:554:ARG:NH2	1:F:576:GLU:OE2	2.53	0.42
1:F:308:ARG:HD3	1:F:309:GLN:OE1	2.20	0.42
1:F:402:ASN:OD1	1:F:405:ARG:NH2	2.44	0.42
1:H:262:LEU:HB3	1:H:264:PRO:HD2	2.02	0.42
1:A:378:CYS:HB3	1:A:391:VAL:HG21	2.02	0.42
1:B:308:ARG:HD3	1:B:309:GLN:OE1	2.20	0.42
1:C:308:ARG:HH22	1:D:36:ILE:H	1.68	0.42
1:D:308:ARG:HD3	1:D:309:GLN:OE1	2.20	0.42
1:F:262:LEU:HB3	1:F:264:PRO:HD2	2.01	0.42
1:E:492:GLN:HE22	1:C:725:GLN:HG3	1.85	0.41
1:A:30:SER:HB3	1:H:322:ASN:OD1	2.20	0.41
1:B:729:GLU:HA	1:G:488:ASN:ND2	2.35	0.41
1:C:281:ILE:CG2	1:C:291:VAL:HG11	2.50	0.41
1:C:308:ARG:HD3	1:C:309:GLN:OE1	2.20	0.41
1:C:706:GLN:HE22	1:D:557:THR:HG23	1.85	0.41
1:A:53:PHE:HZ	1:A:229:LEU:HD22	1.84	0.41
1:B:489:GLN:HG2	1:G:729:GLU:OE1	2.19	0.41
1:C:402:ASN:O	1:C:406:ILE:HG13	2.19	0.41
1:C:564:LEU:O	1:C:568:LEU:HG	2.20	0.41
1:D:53:PHE:HZ	1:D:229:LEU:HD22	1.84	0.41
1:D:349:GLY:O	1:D:353:ILE:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:ALA:HA	1:F:358:ILE:HG22	2.01	0.41
1:G:696:VAL:O	1:G:700:VAL:HG12	2.21	0.41
1:H:528:MET:HE1	1:H:579:PHE:HA	2.00	0.41
1:E:355:ALA:HA	1:E:358:ILE:HG22	2.01	0.41
1:E:536:LEU:HD11	1:E:689:LYS:N	2.36	0.41
1:B:53:PHE:HZ	1:B:229:LEU:HD22	1.84	0.41
1:B:735:ARG:NH1	1:G:732:ASP:OD1	2.53	0.41
1:C:536:LEU:HD11	1:C:689:LYS:N	2.35	0.41
1:F:767:TYR:O	1:F:771:ILE:HG12	2.21	0.41
1:G:308:ARG:HD3	1:G:309:GLN:OE1	2.20	0.41
1:G:710:ASN:HD21	1:H:641:ASP:CG	2.20	0.41
1:H:308:ARG:HD3	1:H:309:GLN:OE1	2.20	0.41
1:H:402:ASN:O	1:H:406:ILE:HG13	2.19	0.41
1:A:564:LEU:O	1:A:568:LEU:HG	2.20	0.41
1:A:696:VAL:O	1:A:700:VAL:HG12	2.21	0.41
1:B:536:LEU:HD11	1:B:689:LYS:N	2.36	0.41
1:G:262:LEU:HB3	1:G:264:PRO:HD2	2.02	0.41
1:H:281:ILE:CG2	1:H:291:VAL:HG11	2.49	0.41
1:F:696:VAL:O	1:F:700:VAL:HG12	2.21	0.41
1:E:16:ASN:ND2	1:A:386:SER:O	2.53	0.41
1:E:53:PHE:HZ	1:E:229:LEU:HD22	1.84	0.41
1:E:585:GLU:HG3	1:H:320:ARG:HH22	1.85	0.41
1:A:308:ARG:HD3	1:A:309:GLN:OE1	2.20	0.41
1:A:663:GLN:OE1	1:A:663:GLN:N	2.42	0.41
1:C:385:LEU:HD21	1:D:42:GLY:N	2.36	0.41
1:C:767:TYR:O	1:C:771:ILE:HG12	2.21	0.41
1:D:767:TYR:O	1:D:771:ILE:HG12	2.21	0.41
1:F:103:LEU:HD23	1:F:212:LYS:HD3	2.02	0.41
1:F:378:CYS:HB3	1:F:391:VAL:HG21	2.02	0.41
1:F:492:GLN:OE1	1:H:728:LEU:HD23	2.20	0.41
1:H:536:LEU:HD11	1:H:689:LYS:N	2.36	0.41
1:H:646:GLU:OE1	1:H:651:TYR:OH	2.22	0.41
1:H:696:VAL:O	1:H:700:VAL:HG12	2.21	0.41
1:E:62:SER:HB2	1:E:74:LEU:HD13	2.03	0.41
1:E:119:LEU:O	1:E:120:ASN:ND2	2.54	0.41
1:A:390:ARG:NE	1:A:390:ARG:HA	2.35	0.41
1:A:569:TYR:HE2	1:G:555:ASN:HB2	1.85	0.41
1:B:287:ILE:HD12	1:B:290:ARG:HB2	2.03	0.41
1:B:385:LEU:O	1:H:12:ARG:CZ	2.69	0.41
1:B:645:ARG:HE	1:B:645:ARG:HA	1.85	0.41
1:C:378:CYS:HB3	1:C:391:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:ARG:HA	1:C:390:ARG:NE	2.35	0.41
1:H:355:ALA:HA	1:H:358:ILE:HG22	2.01	0.41
1:E:287:ILE:HD12	1:E:290:ARG:HB2	2.03	0.41
1:E:710:ASN:HD21	1:D:641:ASP:CB	2.34	0.41
1:E:732:ASP:OD1	1:C:735:ARG:NH1	2.54	0.41
1:A:536:LEU:HD11	1:A:689:LYS:N	2.36	0.41
1:B:767:TYR:O	1:B:771:ILE:HG12	2.21	0.41
1:C:119:LEU:O	1:C:120:ASN:ND2	2.54	0.41
1:C:696:VAL:O	1:C:700:VAL:HG12	2.20	0.41
1:F:65:ILE:HA	1:F:68:LEU:HD12	2.03	0.41
1:G:62:SER:HB2	1:G:74:LEU:HD13	2.03	0.41
1:H:53:PHE:HZ	1:H:229:LEU:HD22	1.84	0.41
1:H:62:SER:HB2	1:H:74:LEU:HD13	2.03	0.41
1:H:645:ARG:HE	1:H:645:ARG:HA	1.85	0.41
1:E:65:ILE:HA	1:E:68:LEU:HD12	2.03	0.41
1:E:767:TYR:O	1:E:771:ILE:HG12	2.21	0.41
1:A:65:ILE:HA	1:A:68:LEU:HD12	2.03	0.41
1:A:645:ARG:HE	1:A:645:ARG:HA	1.85	0.41
1:A:767:TYR:O	1:A:771:ILE:HG12	2.21	0.41
1:B:65:ILE:HA	1:B:68:LEU:HD12	2.03	0.41
1:C:103:LEU:HD23	1:C:212:LYS:HD3	2.02	0.41
1:C:262:LEU:HB3	1:C:264:PRO:HD2	2.02	0.41
1:D:62:SER:HB2	1:D:74:LEU:HD13	2.03	0.41
1:D:287:ILE:HD12	1:D:290:ARG:HB2	2.03	0.41
1:D:378:CYS:HB3	1:D:391:VAL:HG21	2.02	0.41
1:F:536:LEU:HD11	1:F:689:LYS:N	2.36	0.41
1:G:103:LEU:HD23	1:G:212:LYS:HD3	2.02	0.41
1:G:119:LEU:O	1:G:120:ASN:ND2	2.54	0.41
1:G:349:GLY:O	1:G:353:ILE:N	2.52	0.41
1:H:65:ILE:HA	1:H:68:LEU:HD12	2.03	0.41
1:H:378:CYS:HB3	1:H:391:VAL:HG21	2.02	0.41
1:A:119:LEU:O	1:A:120:ASN:ND2	2.54	0.41
1:B:390:ARG:NE	1:B:390:ARG:HA	2.35	0.41
1:D:103:LEU:HD23	1:D:212:LYS:HD3	2.02	0.41
1:G:65:ILE:HA	1:G:68:LEU:HD12	2.03	0.41
1:G:287:ILE:HD12	1:G:290:ARG:HB2	2.03	0.41
1:G:378:CYS:HB3	1:G:391:VAL:HG21	2.02	0.41
1:B:564:LEU:O	1:B:568:LEU:HG	2.20	0.40
1:B:696:VAL:O	1:B:700:VAL:HG12	2.21	0.40
1:F:390:ARG:NE	1:F:390:ARG:HA	2.35	0.40
1:G:645:ARG:HE	1:G:645:ARG:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:652:ASP:OD1	1:G:652:ASP:O	2.40	0.40
1:H:287:ILE:HD12	1:H:290:ARG:HB2	2.03	0.40
1:E:645:ARG:HE	1:E:645:ARG:HA	1.85	0.40
1:A:287:ILE:HD12	1:A:290:ARG:HB2	2.03	0.40
1:B:378:CYS:HB3	1:B:391:VAL:HG21	2.02	0.40
1:C:65:ILE:HA	1:C:68:LEU:HD12	2.03	0.40
1:C:652:ASP:OD1	1:C:652:ASP:O	2.40	0.40
1:D:65:ILE:HA	1:D:68:LEU:HD12	2.03	0.40
1:E:585:GLU:CG	1:H:320:ARG:HH22	2.35	0.40
1:A:536:LEU:HD11	1:A:689:LYS:HA	2.03	0.40
1:B:119:LEU:O	1:B:120:ASN:ND2	2.54	0.40
1:B:536:LEU:HD11	1:B:689:LYS:HA	2.04	0.40
1:B:725:GLN:HG3	1:G:492:GLN:HE22	1.85	0.40
1:C:785:GLU:OE1	1:C:785:GLU:HA	2.22	0.40
1:F:62:SER:HB2	1:F:74:LEU:HD13	2.03	0.40
1:G:767:TYR:O	1:G:771:ILE:HG12	2.21	0.40
1:H:652:ASP:OD1	1:H:652:ASP:O	2.40	0.40
1:B:213:ARG:NH1	1:B:215:ASP:OD1	2.48	0.40
1:D:97:ARG:HG2	1:D:187:MET:SD	2.62	0.40
1:D:536:LEU:HD11	1:D:689:LYS:HA	2.03	0.40
1:D:663:GLN:OE1	1:D:663:GLN:N	2.42	0.40
1:G:371:VAL:HG11	1:G:400:ASN:HA	2.04	0.40
1:H:785:GLU:OE1	1:H:785:GLU:HA	2.22	0.40
1:E:403:TYR:C	1:E:403:TYR:CD1	2.95	0.40
1:A:62:SER:HB2	1:A:74:LEU:HD13	2.03	0.40
1:A:397:GLU:HB3	1:A:401:GLU:OE1	2.22	0.40
1:A:652:ASP:OD1	1:A:652:ASP:O	2.40	0.40
1:B:62:SER:HB2	1:B:74:LEU:HD13	2.03	0.40
1:C:62:SER:HB2	1:C:74:LEU:HD13	2.03	0.40
1:D:70:GLU:N	1:D:70:GLU:OE1	2.55	0.40
1:D:119:LEU:O	1:D:120:ASN:ND2	2.54	0.40
1:G:536:LEU:HD11	1:G:689:LYS:N	2.36	0.40
1:G:710:ASN:HD21	1:H:641:ASP:HB3	1.85	0.40
1:H:97:ARG:HG2	1:H:187:MET:SD	2.62	0.40
1:H:767:TYR:O	1:H:771:ILE:HG12	2.21	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	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
1	B	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
1	C	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
1	D	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
1	E	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
1	F	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
1	G	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
1	H	791/820 (96%)	770 (97%)	21 (3%)	0	100	100
All	All	6328/6560 (96%)	6160 (97%)	168 (3%)	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	690/714 (97%)	670 (97%)	20 (3%)	42	66
1	B	690/714 (97%)	670 (97%)	20 (3%)	42	66
1	C	690/714 (97%)	670 (97%)	20 (3%)	42	66
1	D	690/714 (97%)	670 (97%)	20 (3%)	42	66
1	E	690/714 (97%)	670 (97%)	20 (3%)	42	66
1	F	690/714 (97%)	670 (97%)	20 (3%)	42	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	690/714 (97%)	670 (97%)	20 (3%)	42	66
1	H	690/714 (97%)	670 (97%)	20 (3%)	42	66
All	All	5520/5712 (97%)	5360 (97%)	160 (3%)	45	66

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	12	ARG
1	E	109	ARG
1	E	111	GLN
1	E	216	TYR
1	E	241	GLU
1	E	271	SER
1	E	285	HIS
1	E	319	PHE
1	E	403	TYR
1	E	440	TYR
1	E	508	ASP
1	E	579	PHE
1	E	610	LEU
1	E	627	ASP
1	E	673	ASP
1	E	704	PHE
1	E	745	ASP
1	E	753	ASN
1	E	777	CYS
1	E	784	PHE
1	A	12	ARG
1	A	109	ARG
1	A	111	GLN
1	A	216	TYR
1	A	241	GLU
1	A	271	SER
1	A	285	HIS
1	A	319	PHE
1	A	403	TYR
1	A	440	TYR
1	A	508	ASP
1	A	579	PHE
1	A	610	LEU
1	A	627	ASP

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Mol	Chain	Res	Type
1	A	673	ASP
1	A	704	PHE
1	A	745	ASP
1	A	753	ASN
1	A	777	CYS
1	A	784	PHE
1	B	12	ARG
1	B	109	ARG
1	B	111	GLN
1	B	216	TYR
1	B	241	GLU
1	B	271	SER
1	B	285	HIS
1	B	319	PHE
1	B	403	TYR
1	B	440	TYR
1	B	508	ASP
1	B	579	PHE
1	B	610	LEU
1	B	627	ASP
1	B	673	ASP
1	B	704	PHE
1	B	745	ASP
1	B	753	ASN
1	B	777	CYS
1	B	784	PHE
1	C	12	ARG
1	C	109	ARG
1	C	111	GLN
1	C	216	TYR
1	C	241	GLU
1	C	271	SER
1	C	285	HIS
1	C	319	PHE
1	C	403	TYR
1	C	440	TYR
1	C	508	ASP
1	C	579	PHE
1	C	610	LEU
1	C	627	ASP
1	C	673	ASP
1	C	704	PHE

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Mol	Chain	Res	Type
1	C	745	ASP
1	C	753	ASN
1	C	777	CYS
1	C	784	PHE
1	D	12	ARG
1	D	109	ARG
1	D	111	GLN
1	D	216	TYR
1	D	241	GLU
1	D	271	SER
1	D	285	HIS
1	D	319	PHE
1	D	403	TYR
1	D	440	TYR
1	D	508	ASP
1	D	579	PHE
1	D	610	LEU
1	D	627	ASP
1	D	673	ASP
1	D	704	PHE
1	D	745	ASP
1	D	753	ASN
1	D	777	CYS
1	D	784	PHE
1	F	12	ARG
1	F	109	ARG
1	F	111	GLN
1	F	216	TYR
1	F	241	GLU
1	F	271	SER
1	F	285	HIS
1	F	319	PHE
1	F	403	TYR
1	F	440	TYR
1	F	508	ASP
1	F	579	PHE
1	F	610	LEU
1	F	627	ASP
1	F	673	ASP
1	F	704	PHE
1	F	745	ASP
1	F	753	ASN

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Mol	Chain	Res	Type
1	F	777	CYS
1	F	784	PHE
1	G	12	ARG
1	G	109	ARG
1	G	111	GLN
1	G	216	TYR
1	G	241	GLU
1	G	271	SER
1	G	285	HIS
1	G	319	PHE
1	G	403	TYR
1	G	440	TYR
1	G	508	ASP
1	G	579	PHE
1	G	610	LEU
1	G	627	ASP
1	G	673	ASP
1	G	704	PHE
1	G	745	ASP
1	G	753	ASN
1	G	777	CYS
1	G	784	PHE
1	H	12	ARG
1	H	109	ARG
1	H	111	GLN
1	H	216	TYR
1	H	241	GLU
1	H	271	SER
1	H	285	HIS
1	H	319	PHE
1	H	403	TYR
1	H	440	TYR
1	H	508	ASP
1	H	579	PHE
1	H	610	LEU
1	H	627	ASP
1	H	673	ASP
1	H	704	PHE
1	H	745	ASP
1	H	753	ASN
1	H	777	CYS
1	H	784	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	120	ASN
1	E	584	HIS
1	E	710	ASN
1	A	16	ASN
1	A	120	ASN
1	A	507	ASN
1	A	710	ASN
1	B	120	ASN
1	B	507	ASN
1	B	725	GLN
1	C	120	ASN
1	C	725	GLN
1	D	16	ASN
1	D	120	ASN
1	D	507	ASN
1	D	584	HIS
1	D	725	GLN
1	F	16	ASN
1	F	120	ASN
1	F	710	ASN
1	G	16	ASN
1	G	120	ASN
1	G	584	HIS
1	G	710	ASN
1	H	120	ASN
1	H	507	ASN
1	H	584	HIS
1	H	725	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

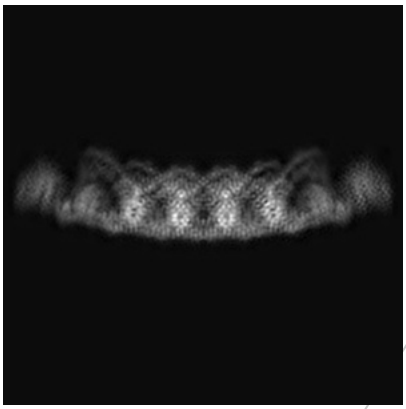
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14993. These allow visual inspection of the internal detail of the map and identification of artifacts.

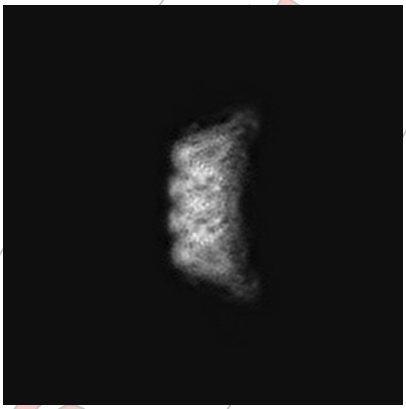
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

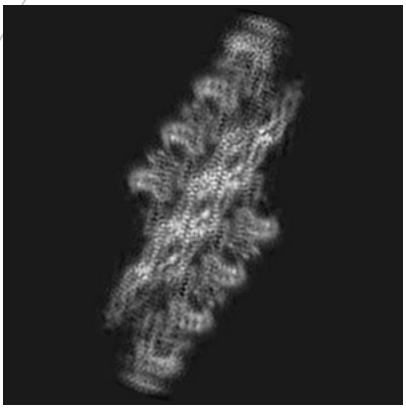
6.1.1 Primary map



X

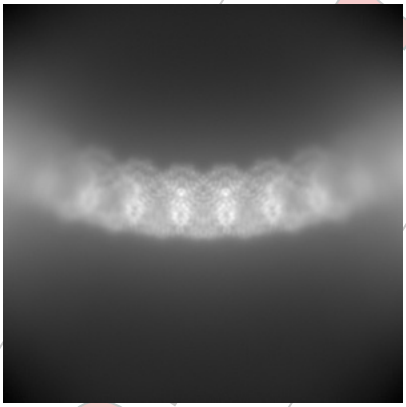


Y

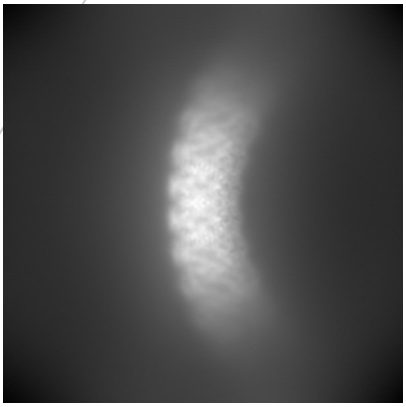


Z

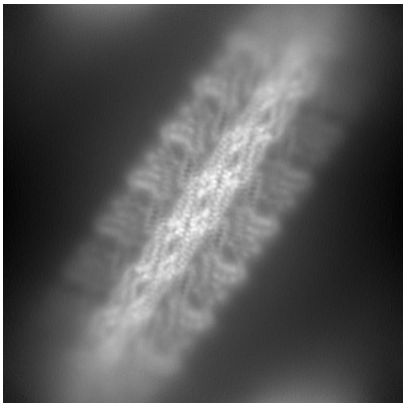
6.1.2 Raw map



X



Y

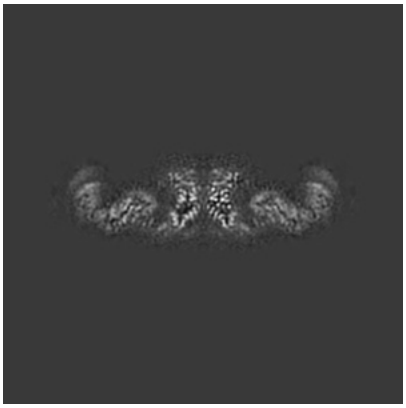


Z

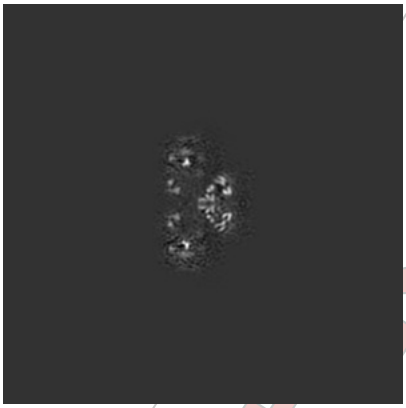
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

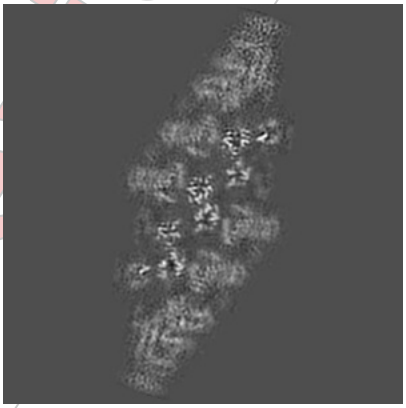
6.2.1 Primary map



X Index: 225

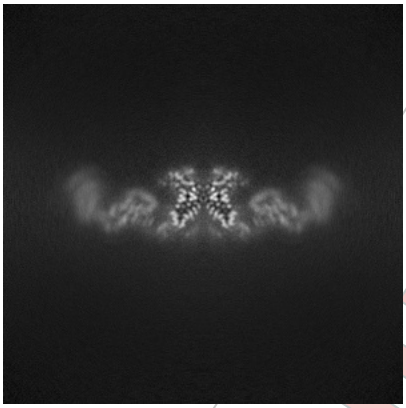


Y Index: 225

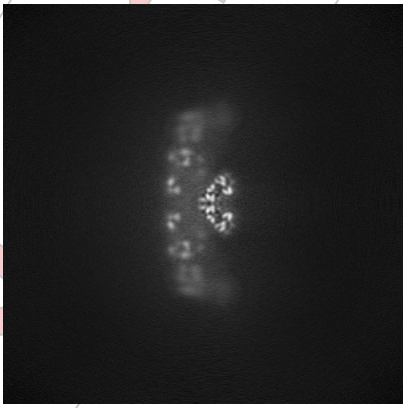


Z Index: 225

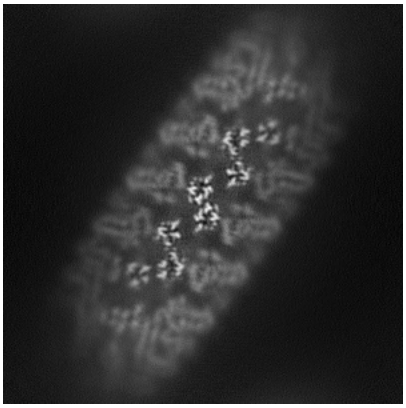
6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

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

6.3 Largest variance slices (i)

6.3.1 Primary map

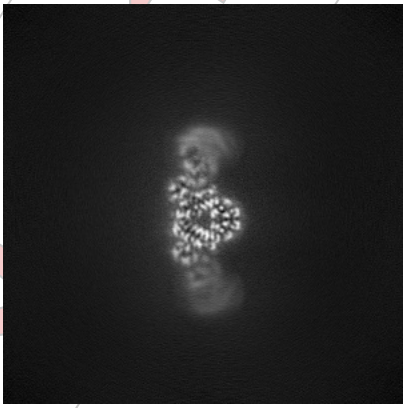
X Index: 201

Y Index: 249

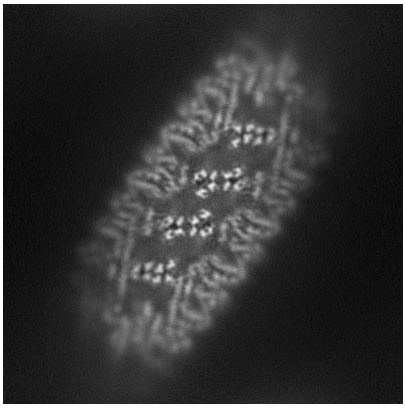
Z Index: 208

6.3.2 Raw map

X Index: 212



Y Index: 201



Z Index: 214

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

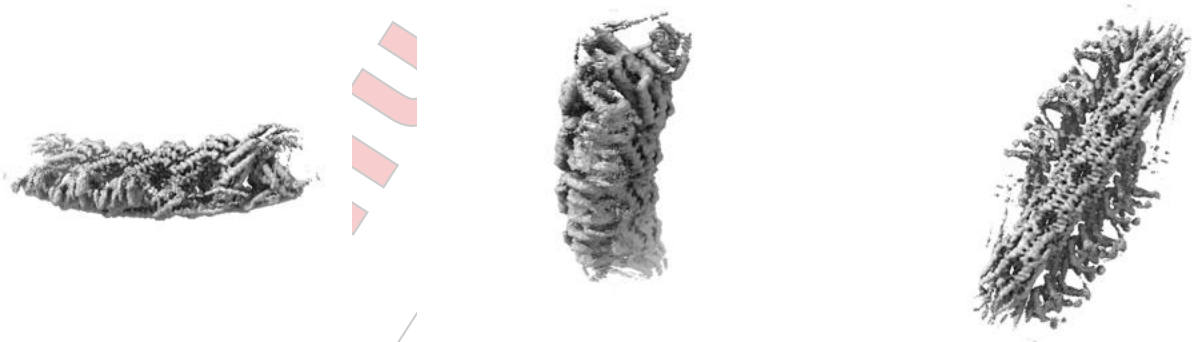
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

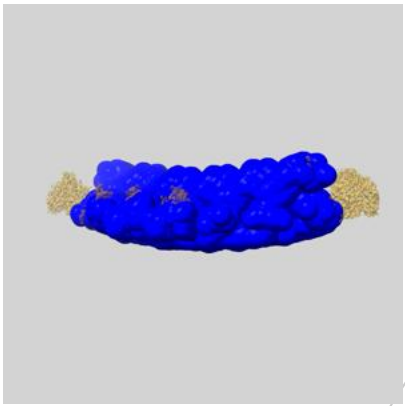
6.5 Mask visualisation

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

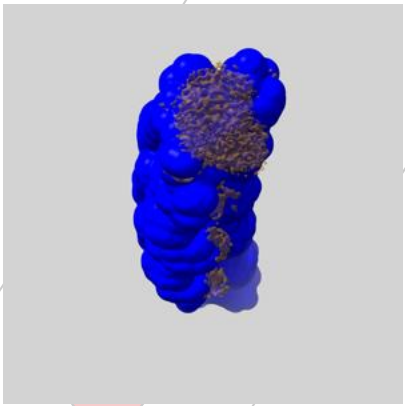
A mask typically either:

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

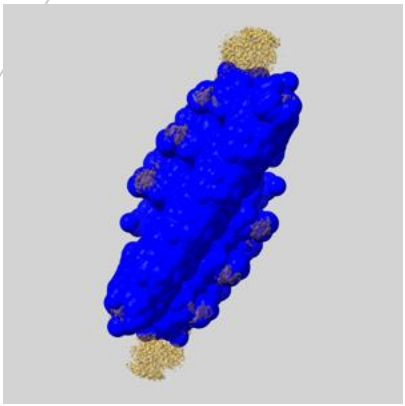
6.5.1 D_1292123101_em-mask-volume_P1.map.V2



X



Y

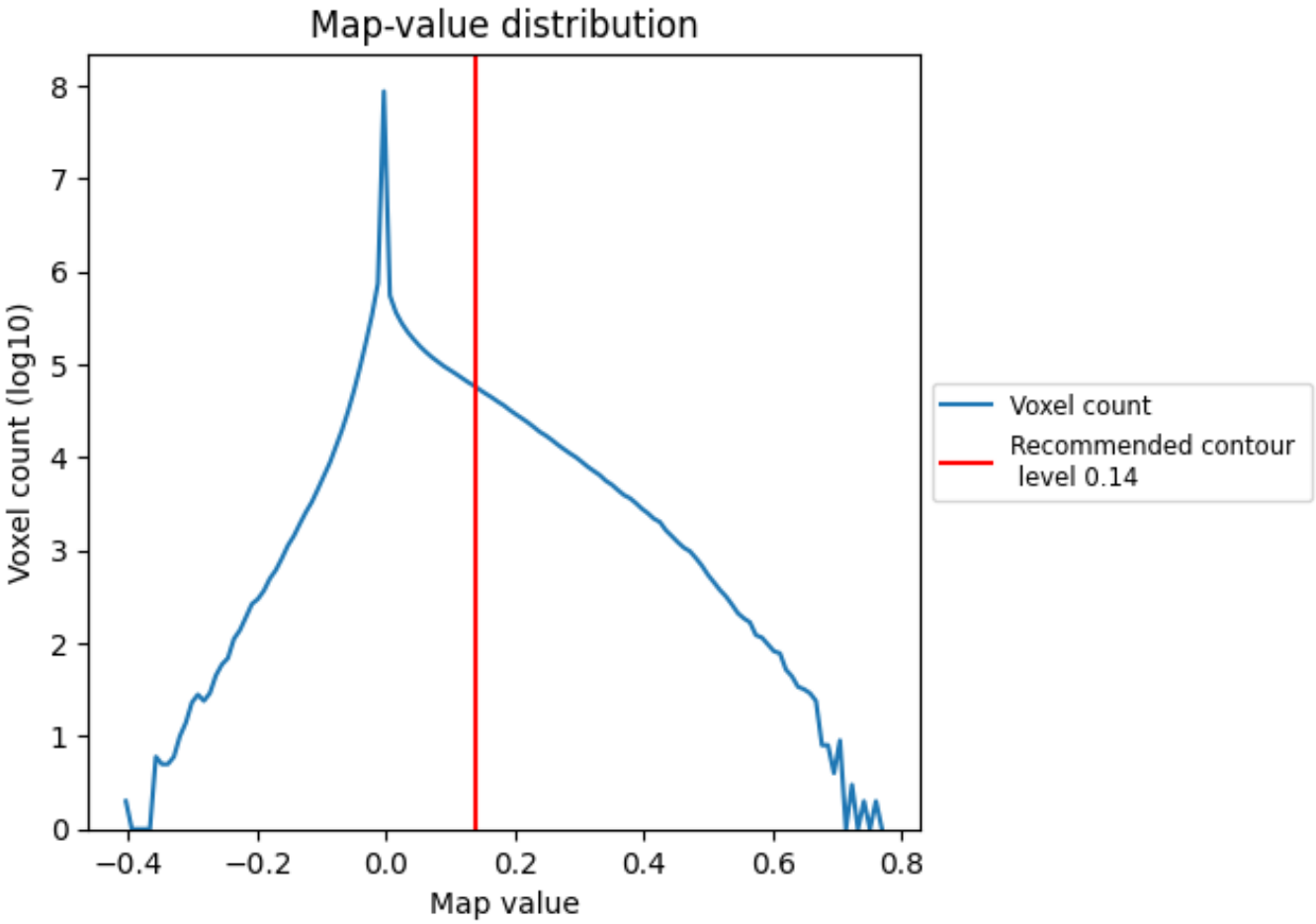


Z

7 Map analysis

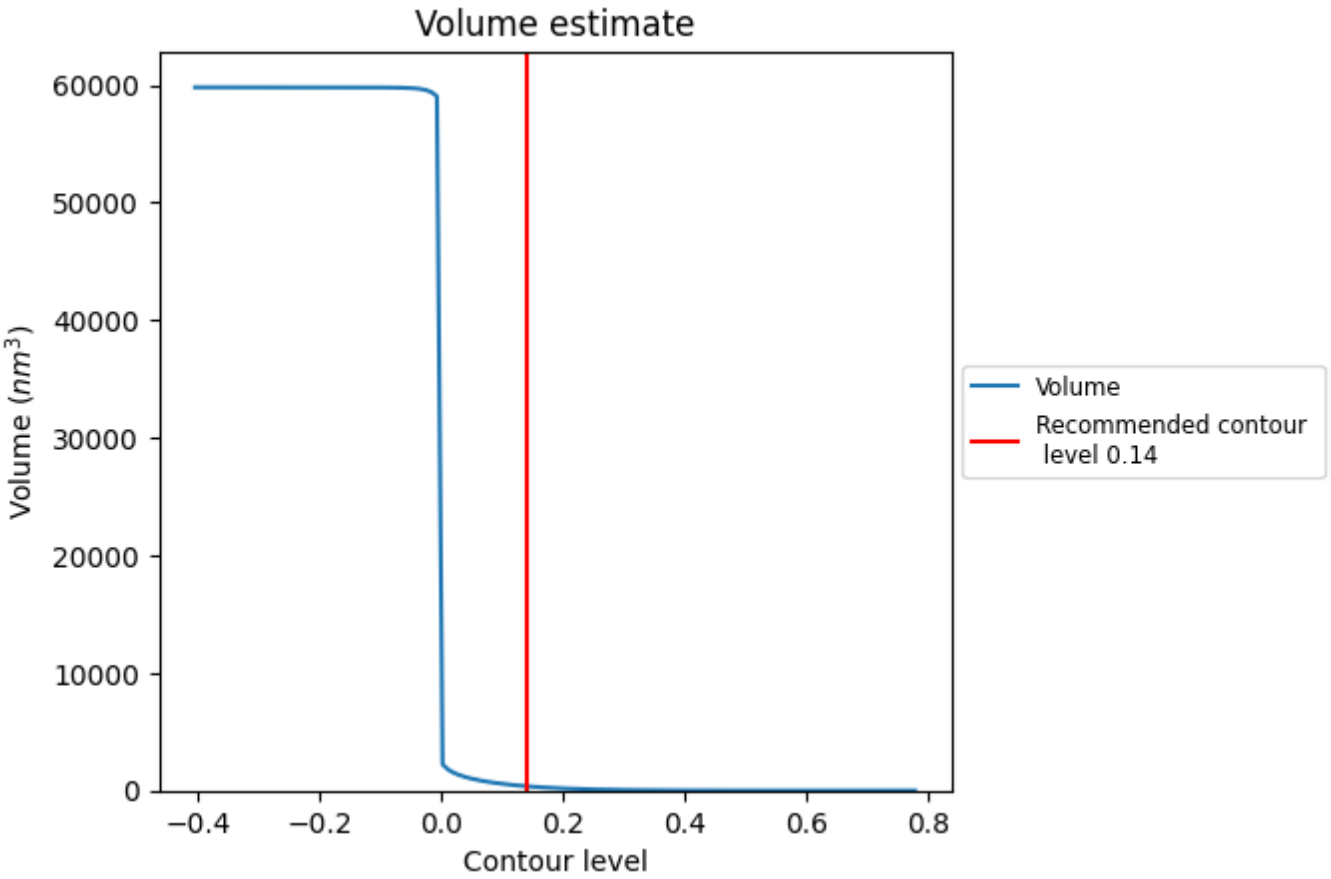
This section contains the results of statistical analysis of the map.

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.

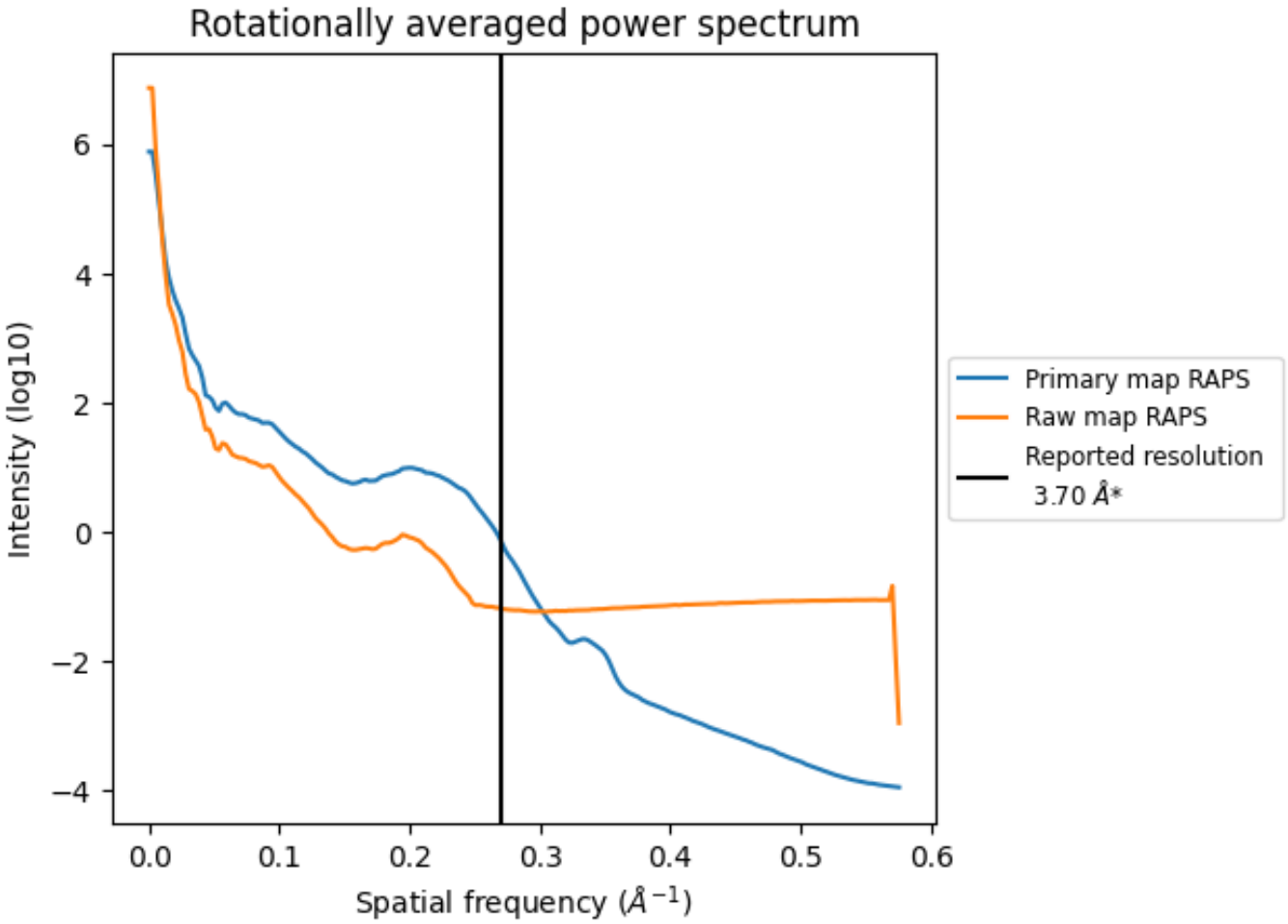
7.2 Volume estimate (i)



The volume at the recommended contour level is 371 nm^3; this corresponds to an approximate mass of 335 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)

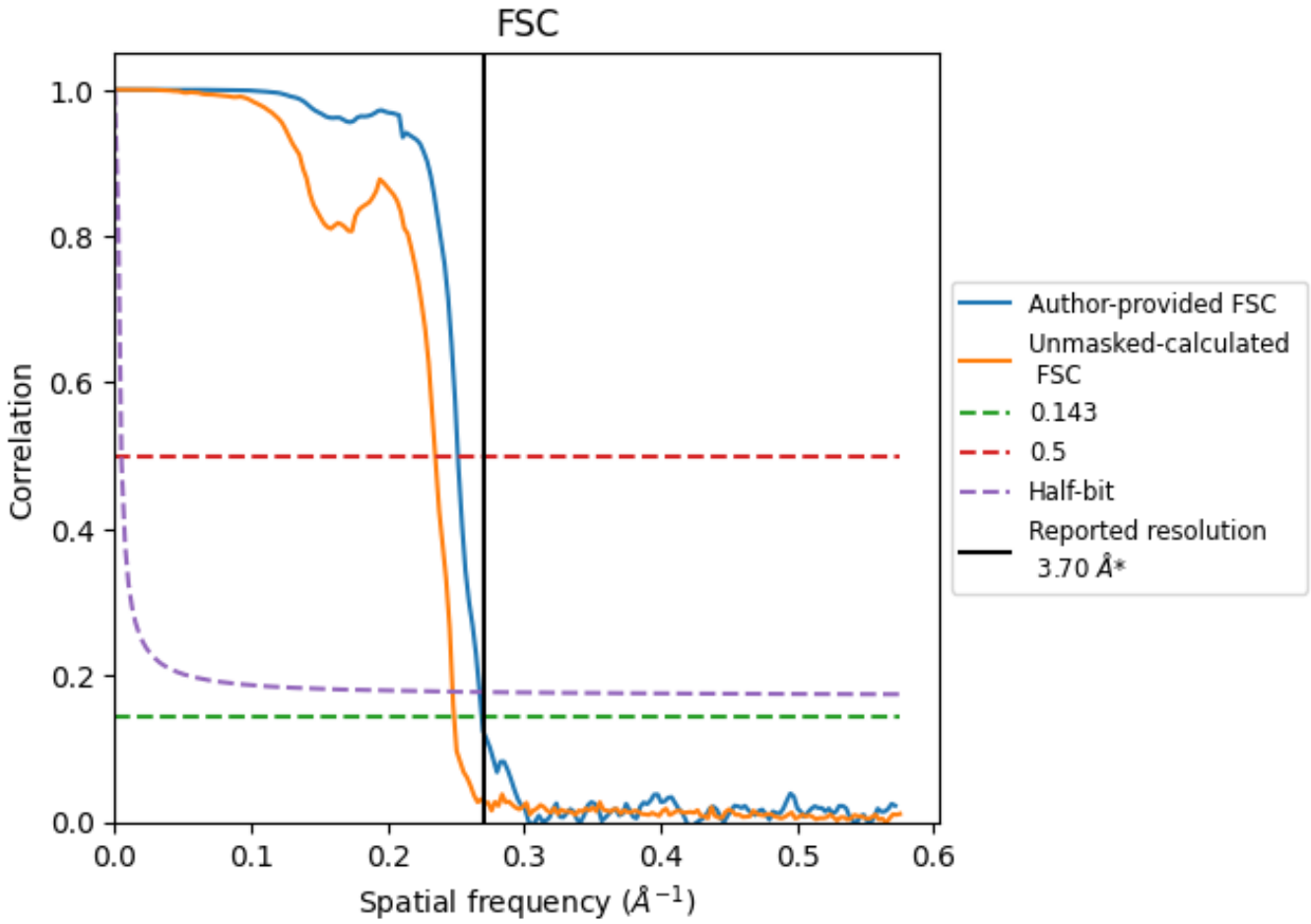


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 $Å^{-1}$

8.2 Resolution estimates (i)

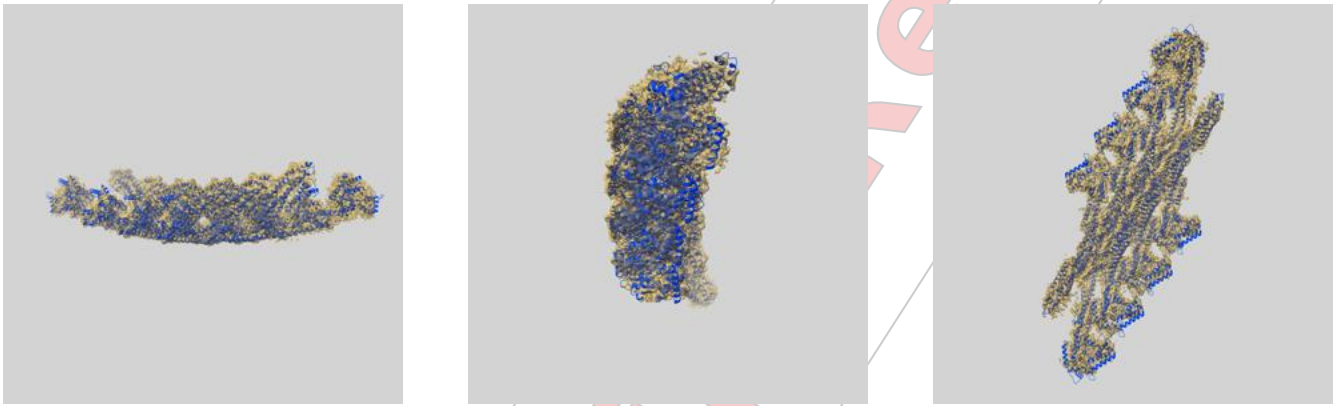
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	3.97	3.74
Unmasked-calculated*	4.02	4.26	4.04

*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-14993 and PDB model 7ZW6. Per-residue inclusion information can be found in section 3 on page 6.

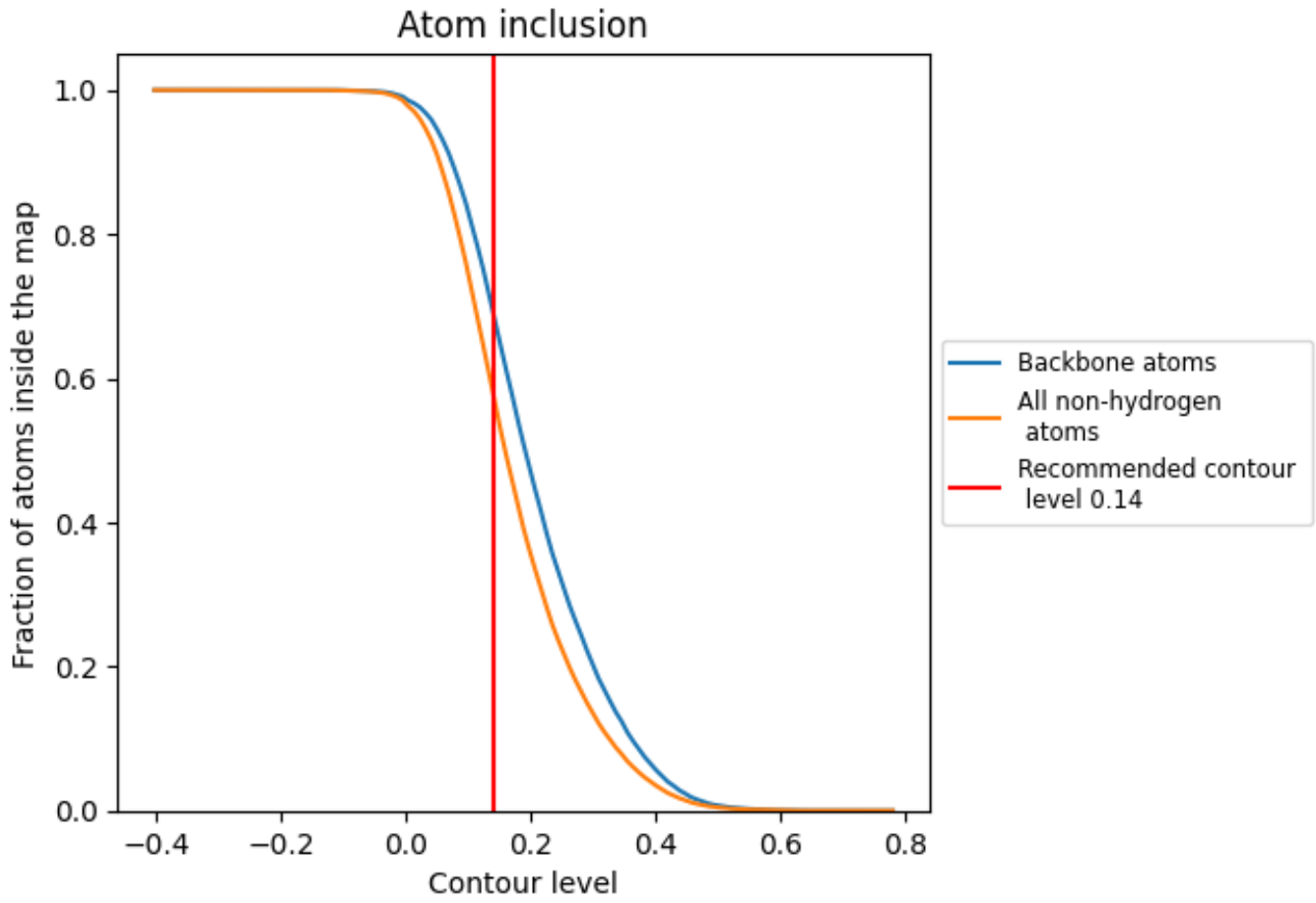
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 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 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.