



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 10:13 AM JST

PDB ID : 5GRS
EMDB ID : EMD-9537
Title : Complex structure of the fission yeast SREBP-SCAP binding domains
Authors : Gong, X.; Qian, H.W.; Wu, J.P.; Yan, N.
Deposited on : 2016-08-12
Resolution : 5.40 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.dev113
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) : 2.39

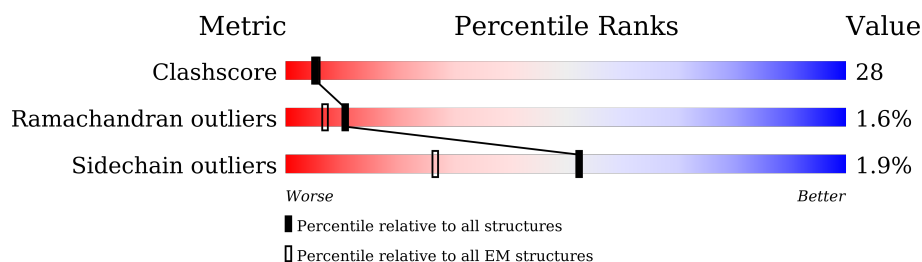
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div>19%</div> <div>43%</div> <div>51%</div> <div>• 5%</div> </div>
1	B	396	<div> <div>19%</div> <div>42%</div> <div>52%</div> <div>• 5%</div> </div>
1	C	396	<div> <div>18%</div> <div>43%</div> <div>51%</div> <div>• 5%</div> </div>
1	D	396	<div> <div>19%</div> <div>43%</div> <div>51%</div> <div>• 5%</div> </div>
2	I	103	<div> <div>12%</div> <div>29%</div> <div>31%</div> <div>40%</div> </div>
2	J	103	<div> <div>11%</div> <div>28%</div> <div>32%</div> <div>40%</div> </div>
2	K	103	<div> <div>11%</div> <div>28%</div> <div>32%</div> <div>40%</div> </div>
2	L	103	<div> <div>12%</div> <div>29%</div> <div>31%</div> <div>40%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	272	<div><div></div><div>12%</div><div>47%</div><div>21%</div><div>31%</div></div>
3	F	272	<div><div></div><div>11%</div><div>44%</div><div>21%</div><div>5%</div><div>30%</div></div>
3	G	272	<div><div></div><div>13%</div><div>49%</div><div>17%</div><div>31%</div></div>
3	H	272	<div><div></div><div>11%</div><div>43%</div><div>22%</div><div>5%</div><div>30%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19489 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 Sterol regulatory element-binding protein cleavage-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	1	0
			2986	1908	489	577	12		
1	B	375	Total	C	N	O	S	1	0
			2986	1908	489	577	12		
1	C	375	Total	C	N	O	S	1	0
			2982	1906	488	576	12		
1	D	375	Total	C	N	O	S	1	0
			2986	1908	489	577	12		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	MET	-	expression tag	UNP O43043
A	671	SER	CYS	engineered mutation	UNP O43043
A	873	SER	CYS	engineered mutation	UNP O43043
A	901	SER	CYS	engineered mutation	UNP O43043
A	920	SER	CYS	engineered mutation	UNP O43043
A	941	SER	CYS	engineered mutation	UNP O43043
B	566	MET	-	expression tag	UNP O43043
B	671	SER	CYS	engineered mutation	UNP O43043
B	873	SER	CYS	engineered mutation	UNP O43043
B	901	SER	CYS	engineered mutation	UNP O43043
B	920	SER	CYS	engineered mutation	UNP O43043
B	941	SER	CYS	engineered mutation	UNP O43043
C	566	MET	-	expression tag	UNP O43043
C	671	SER	CYS	engineered mutation	UNP O43043
C	873	SER	CYS	engineered mutation	UNP O43043
C	901	SER	CYS	engineered mutation	UNP O43043
C	920	SER	CYS	engineered mutation	UNP O43043
C	941	SER	CYS	engineered mutation	UNP O43043
D	566	MET	-	expression tag	UNP O43043
D	671	SER	CYS	engineered mutation	UNP O43043
D	873	SER	CYS	engineered mutation	UNP O43043

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Chain	Residue	Modelled	Actual	Comment	Reference
D	901	SER	CYS	engineered mutation	UNP O43043
D	920	SER	CYS	engineered mutation	UNP O43043
D	941	SER	CYS	engineered mutation	UNP O43043

- Molecule 2 is a protein called Sterol regulatory element-binding protein cleavage-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	62	Total	C	N	O	S	0	0
			489	315	80	91	3		
2	J	62	Total	C	N	O	S	0	0
			489	315	80	91	3		
2	K	62	Total	C	N	O	S	0	0
			489	315	80	91	3		
2	L	62	Total	C	N	O	S	0	0
			489	315	80	91	3		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	983	ALA	-	expression tag	UNP O43043
I	984	HIS	-	expression tag	UNP O43043
I	985	MET	-	expression tag	UNP O43043
I	1010	SER	CYS	engineered mutation	UNP O43043
J	983	ALA	-	expression tag	UNP O43043
J	984	HIS	-	expression tag	UNP O43043
J	985	MET	-	expression tag	UNP O43043
J	1010	SER	CYS	engineered mutation	UNP O43043
K	983	ALA	-	expression tag	UNP O43043
K	984	HIS	-	expression tag	UNP O43043
K	985	MET	-	expression tag	UNP O43043
K	1010	SER	CYS	engineered mutation	UNP O43043
L	983	ALA	-	expression tag	UNP O43043
L	984	HIS	-	expression tag	UNP O43043
L	985	MET	-	expression tag	UNP O43043
L	1010	SER	CYS	engineered mutation	UNP O43043

- Molecule 3 is a protein called Sterol regulatory element-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	189	Total	C	N	O	S	0	0
			1394	890	224	272	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	191	Total	C	N	O	S	0	0
			1406	901	227	270	8		
3	G	187	Total	C	N	O	S	0	0
			1383	884	222	269	8		
3	H	191	Total	C	N	O	S	0	0
			1410	904	228	270	8		

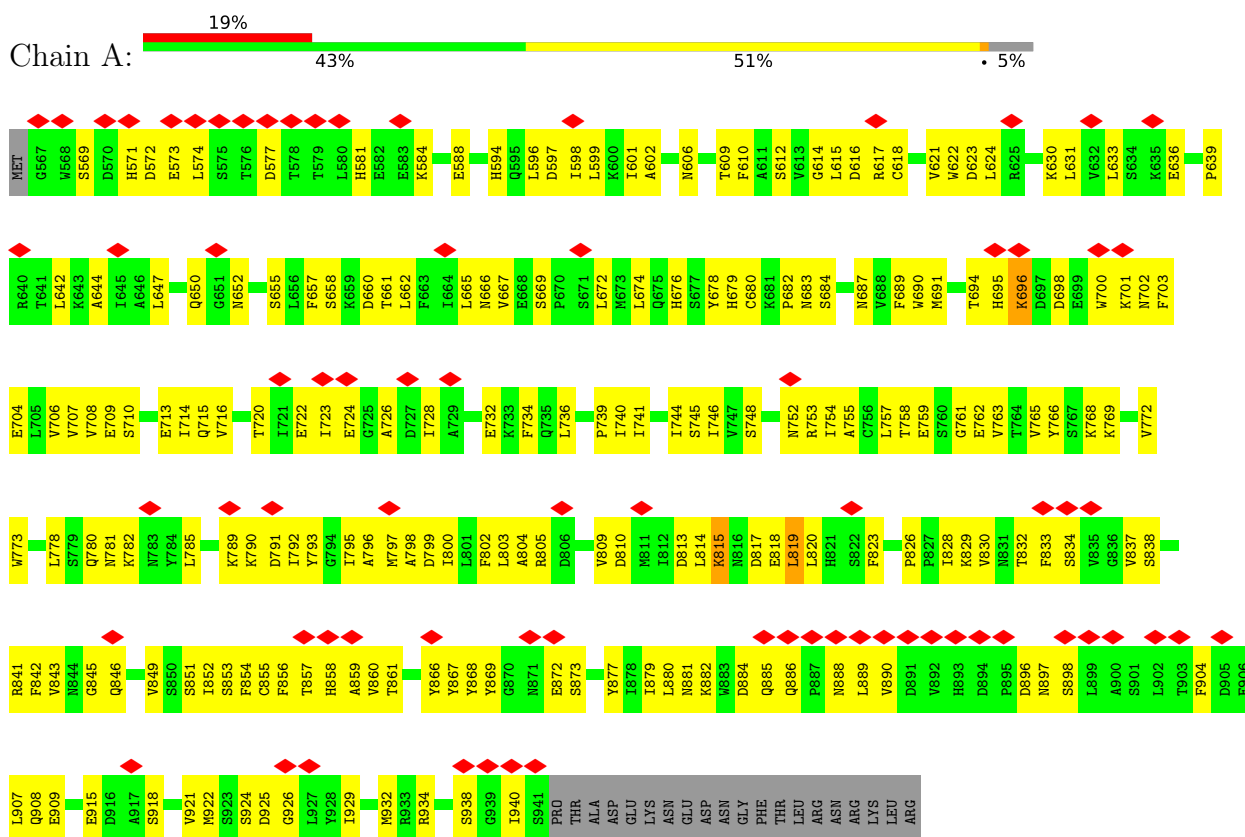
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	625	ALA	-	expression tag	UNP Q9UUD1
E	626	HIS	-	expression tag	UNP Q9UUD1
E	627	MET	-	expression tag	UNP Q9UUD1
E	644	SER	CYS	engineered mutation	UNP Q9UUD1
E	672	SER	CYS	engineered mutation	UNP Q9UUD1
F	625	ALA	-	expression tag	UNP Q9UUD1
F	626	HIS	-	expression tag	UNP Q9UUD1
F	627	MET	-	expression tag	UNP Q9UUD1
F	644	SER	CYS	engineered mutation	UNP Q9UUD1
F	672	SER	CYS	engineered mutation	UNP Q9UUD1
G	625	ALA	-	expression tag	UNP Q9UUD1
G	626	HIS	-	expression tag	UNP Q9UUD1
G	627	MET	-	expression tag	UNP Q9UUD1
G	644	SER	CYS	engineered mutation	UNP Q9UUD1
G	672	SER	CYS	engineered mutation	UNP Q9UUD1
H	625	ALA	-	expression tag	UNP Q9UUD1
H	626	HIS	-	expression tag	UNP Q9UUD1
H	627	MET	-	expression tag	UNP Q9UUD1
H	644	SER	CYS	engineered mutation	UNP Q9UUD1
H	672	SER	CYS	engineered mutation	UNP Q9UUD1

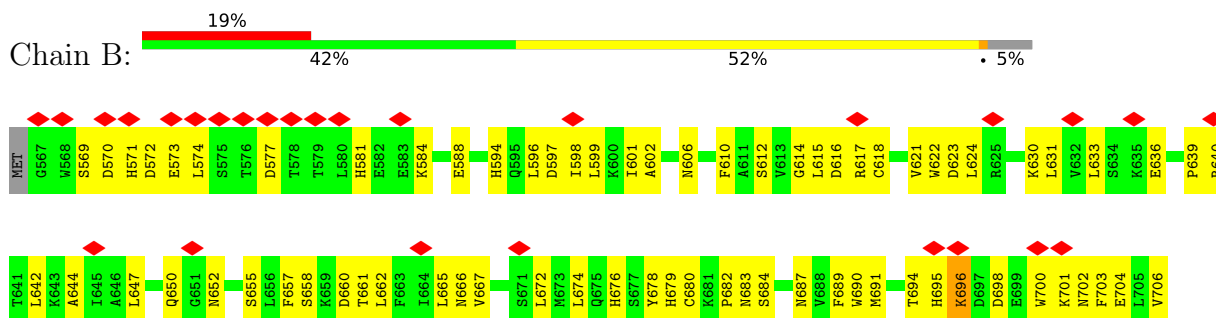
3 Residue-property plots

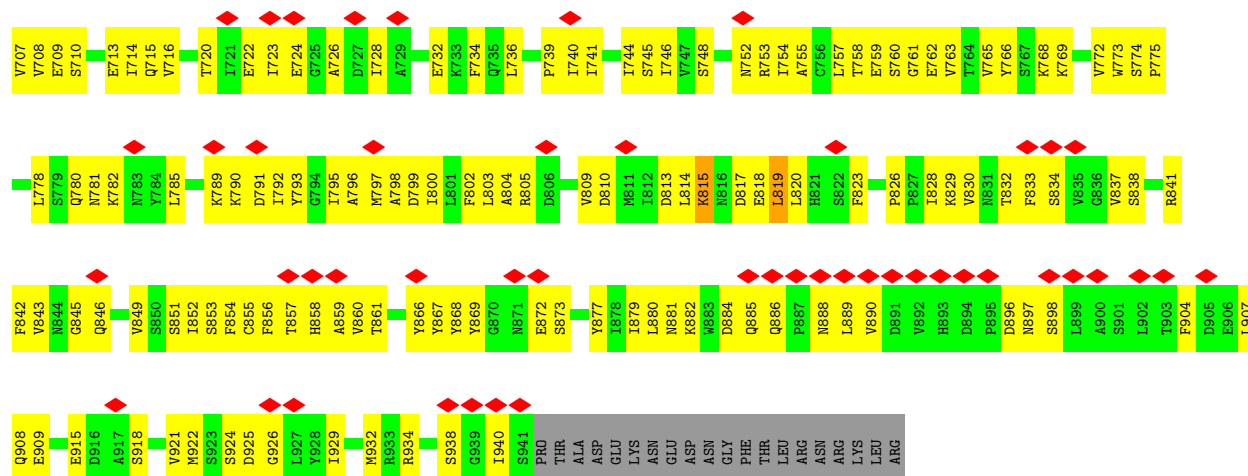
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Sterol regulatory element-binding protein cleavage-activating protein

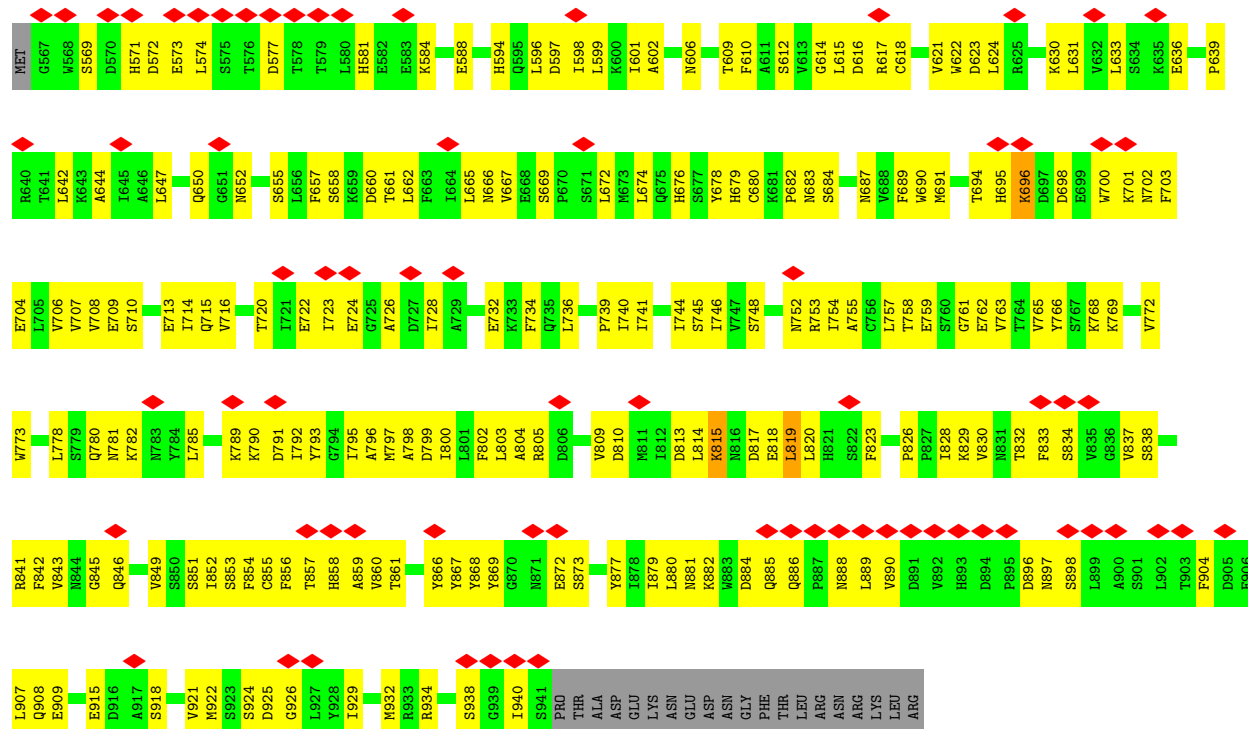


- Molecule 1: Sterol regulatory element-binding protein cleavage-activating protein

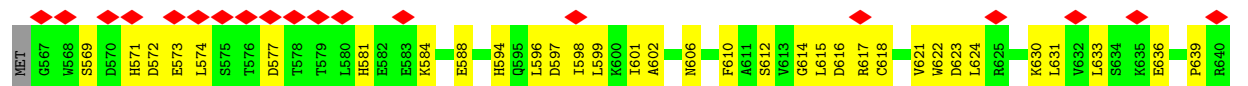


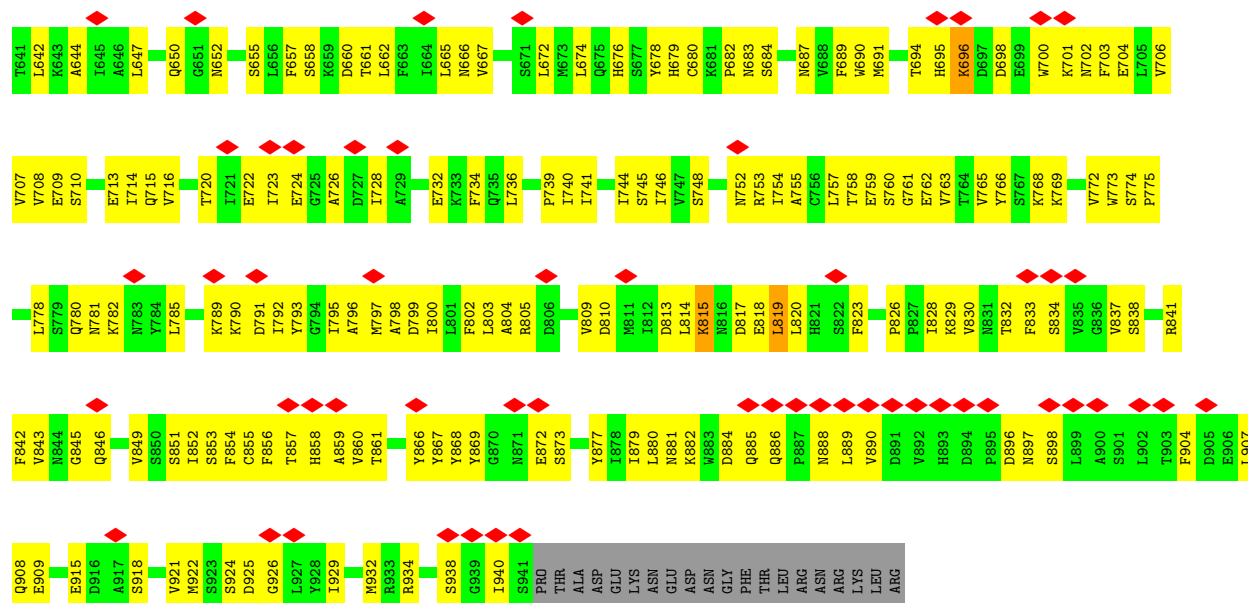


- Molecule 1: Sterol regulatory element-binding protein cleavage-activating protein

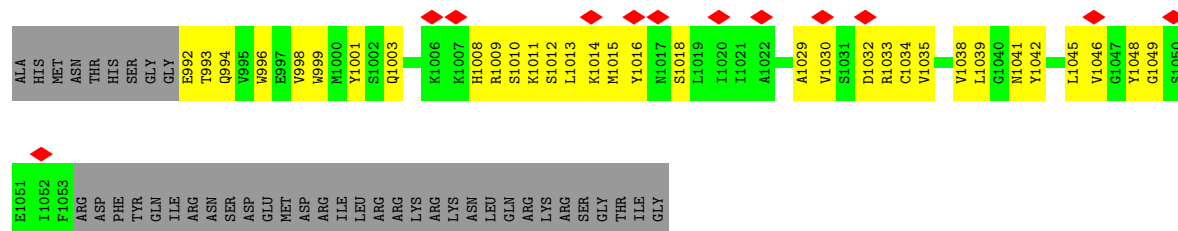
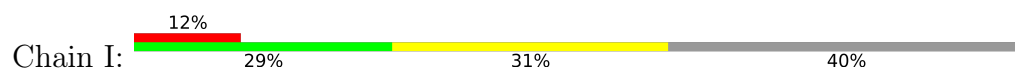


- Molecule 1: Sterol regulatory element-binding protein cleavage-activating protein

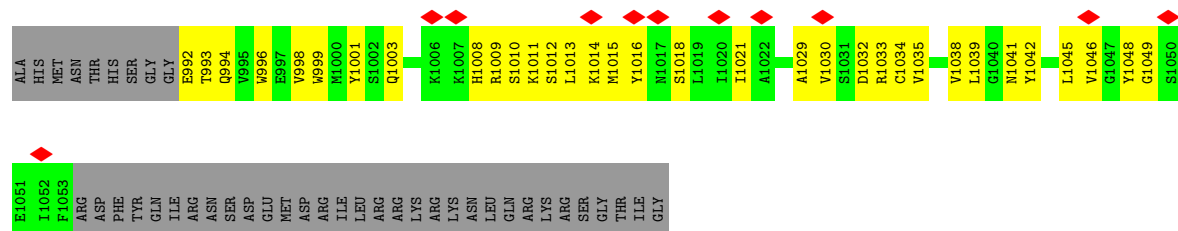
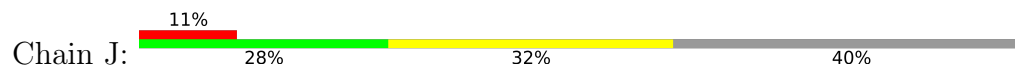




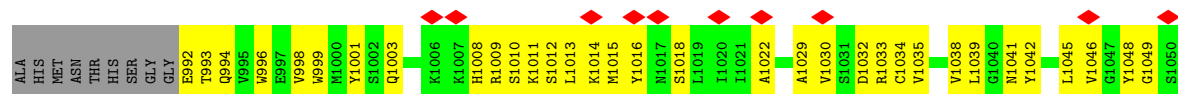
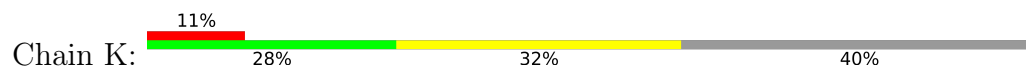
• Molecule 2: Sterol regulatory element-binding protein cleavage-activating protein

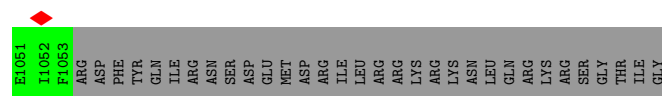


• Molecule 2: Sterol regulatory element-binding protein cleavage-activating protein

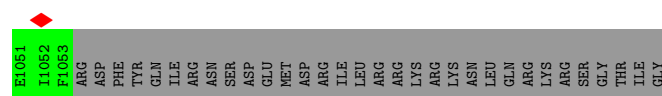
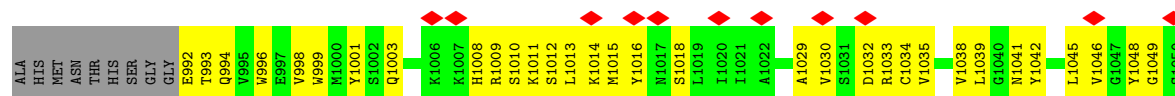
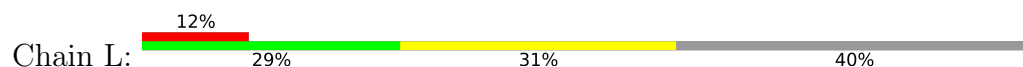


• Molecule 2: Sterol regulatory element-binding protein cleavage-activating protein

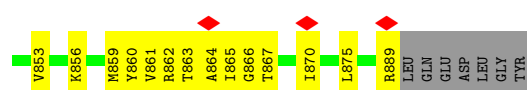
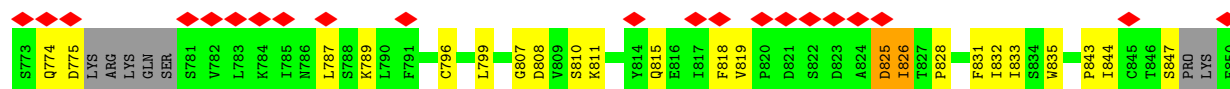
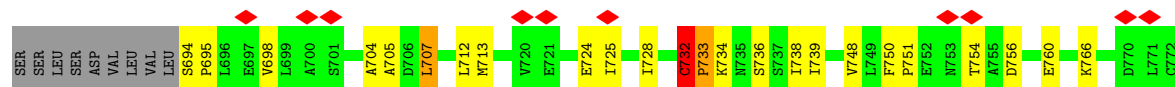
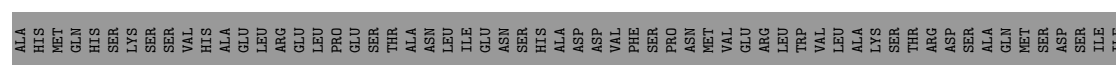




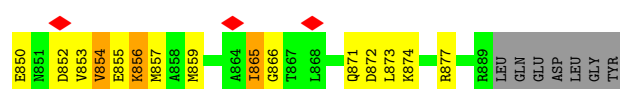
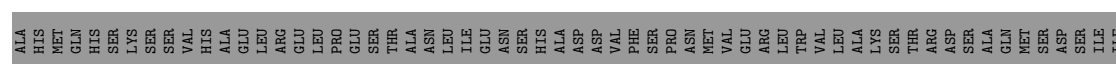
• Molecule 2: Sterol regulatory element-binding protein cleavage-activating protein



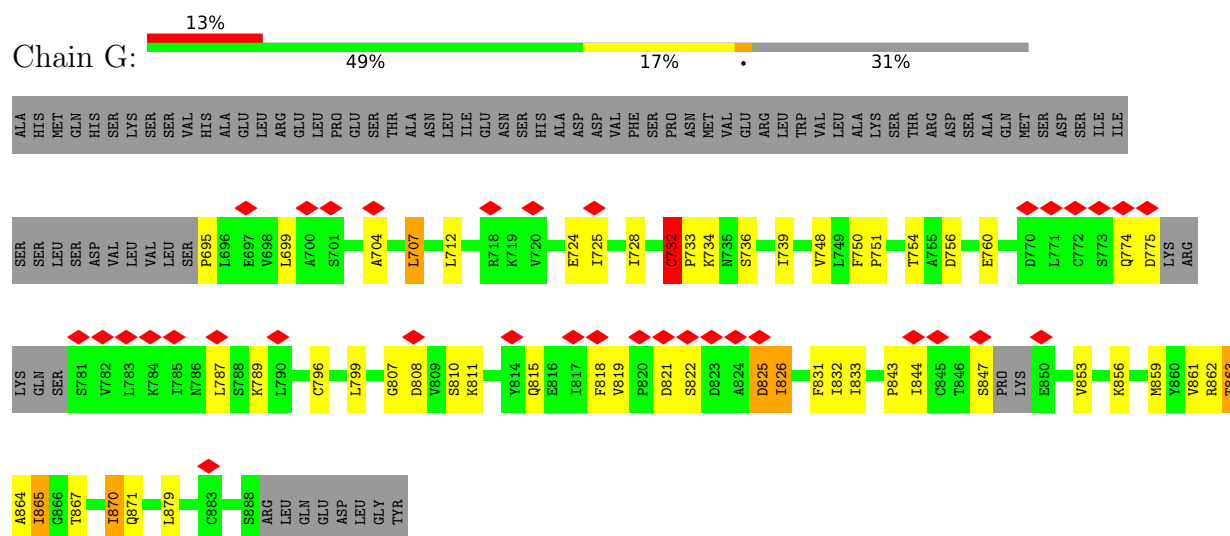
• Molecule 3: Sterol regulatory element-binding protein 1



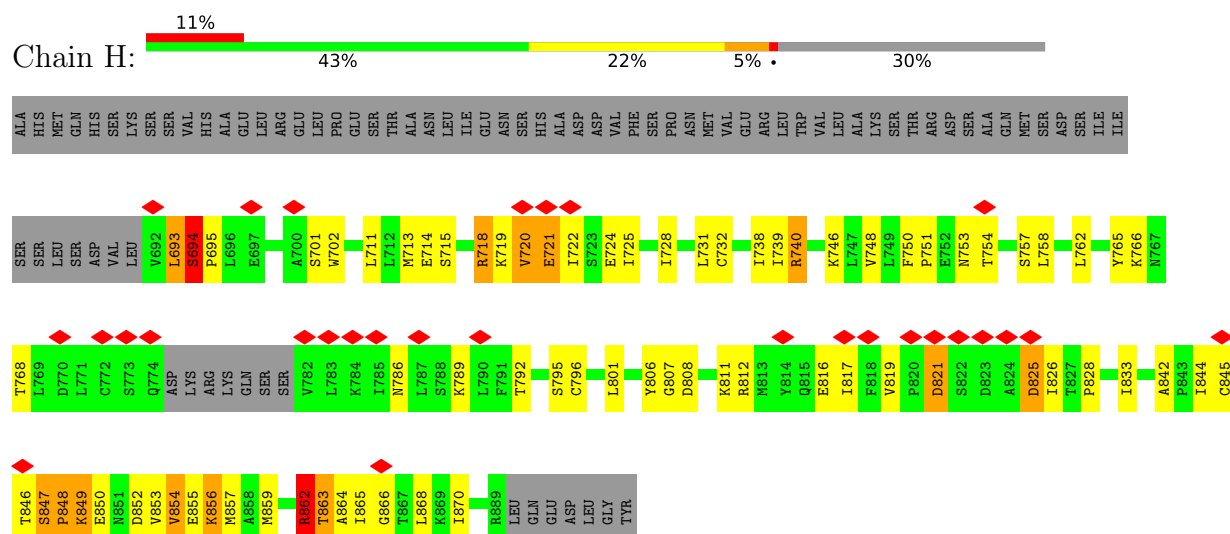
• Molecule 3: Sterol regulatory element-binding protein 1



• Molecule 3: Sterol regulatory element-binding protein 1



• Molecule 3: Sterol regulatory element-binding protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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	0.32	0/3054	0.60	0/4147
1	B	0.32	0/3054	0.61	0/4147
1	C	0.32	0/3050	0.61	0/4142
1	D	0.32	0/3054	0.60	0/4147
2	I	0.28	0/500	0.50	0/677
2	J	0.28	0/500	0.50	0/677
2	K	0.28	0/500	0.50	0/677
2	L	0.28	0/500	0.51	0/677
3	E	0.33	1/1413 (0.1%)	0.48	1/1925 (0.1%)
3	F	0.60	6/1427 (0.4%)	0.57	3/1948 (0.2%)
3	G	0.33	0/1402	0.51	1/1909 (0.1%)
3	H	0.60	5/1431 (0.3%)	0.57	3/1952 (0.2%)
All	All	0.37	12/19885 (0.1%)	0.58	8/27025 (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
3	H	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	740	ARG	NE-CZ	-9.46	1.20	1.33
3	H	740	ARG	NE-CZ	-9.43	1.20	1.33
3	F	740	ARG	CZ-NH2	-9.01	1.21	1.33
3	H	740	ARG	CZ-NH2	-8.87	1.21	1.33
3	H	740	ARG	CD-NE	-8.00	1.32	1.46
3	F	740	ARG	CD-NE	-7.88	1.33	1.46
3	H	740	ARG	CZ-NH1	-7.25	1.23	1.33
3	F	740	ARG	CZ-NH1	-7.20	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	848	PRO	N-CD	5.39	1.55	1.47
3	H	848	PRO	N-CD	5.21	1.55	1.47
3	F	695	PRO	N-CD	5.15	1.55	1.47
3	E	733	PRO	N-CD	5.01	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	694	SER	C-N-CD	6.06	141.13	128.40
3	G	732	CYS	C-N-CD	6.04	141.08	128.40
3	F	694	SER	C-N-CD	6.04	141.07	128.40
3	E	732	CYS	C-N-CD	6.02	141.04	128.40
3	H	847	SER	C-N-CD	5.65	140.26	128.40
3	F	847	SER	C-N-CD	5.57	140.09	128.40
3	H	740	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	F	740	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	862	ARG	Mainchain

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	2986	0	2934	175	0
1	B	2986	0	2934	187	0
1	C	2982	0	2928	183	0
1	D	2986	0	2933	178	0
2	I	489	0	487	36	0
2	J	489	0	487	40	0
2	K	489	0	487	39	0
2	L	489	0	487	36	0
3	E	1394	0	1349	84	0
3	F	1406	0	1364	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1383	0	1343	49	0
3	H	1410	0	1377	109	0
All	All	19489	0	19110	1086	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 28.

All (1086) 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)
3:E:713:MET:CE	3:E:867:THR:HG21	1.08	1.50
3:E:713:MET:CE	3:E:867:THR:CG2	2.04	1.34
3:E:860:TYR:O	3:E:864:ALA:HB3	1.11	1.28
3:E:713:MET:HE3	3:E:867:THR:CG2	1.60	1.27
3:E:860:TYR:O	3:E:864:ALA:CB	1.86	1.23
3:F:702:TRP:CH2	3:G:695:PRO:HB3	1.77	1.19
1:B:640:ARG:NH1	3:H:849:LYS:NZ	1.91	1.16
3:E:859:MET:O	3:E:863:THR:HG22	1.48	1.13
3:H:715:SER:CB	3:H:720:VAL:HG21	1.78	1.12
3:E:695:PRO:HB3	3:H:702:TRP:CH2	1.84	1.12
3:F:702:TRP:HH2	3:G:695:PRO:HB3	1.06	1.12
3:F:715:SER:CB	3:F:720:VAL:HG21	1.77	1.11
3:E:733:PRO:HG2	3:E:736:SER:HB3	1.36	1.08
3:H:842:ALA:O	3:H:846:THR:HG23	1.55	1.07
3:G:733:PRO:HG2	3:G:736:SER:HB3	1.36	1.07
3:E:713:MET:HE1	3:E:867:THR:HG21	1.10	1.07
3:F:842:ALA:O	3:F:846:THR:HG23	1.55	1.07
1:B:640:ARG:NH1	3:H:849:LYS:HZ3	1.51	1.05
3:E:861:VAL:O	3:E:865:ILE:CD1	2.05	1.03
3:H:842:ALA:O	3:H:846:THR:CG2	2.07	1.03
3:F:842:ALA:O	3:F:846:THR:CG2	2.07	1.03
3:E:774:GLN:O	3:E:775:ASP:OD1	1.74	1.03
3:G:774:GLN:O	3:G:775:ASP:OD1	1.74	1.02
1:B:872:GLU:HG2	1:B:873:SER:HA	1.41	1.01
3:F:715:SER:HA	3:F:720:VAL:CG2	1.90	1.01
1:D:872:GLU:HG2	1:D:873:SER:HA	1.41	1.01
3:H:715:SER:HA	3:H:720:VAL:CG2	1.90	1.01
1:A:872:GLU:HG2	1:A:873:SER:HA	1.41	1.00
1:C:872:GLU:HG2	1:C:873:SER:HA	1.41	1.00
3:G:733:PRO:HD2	3:G:736:SER:OG	1.64	0.98
3:E:733:PRO:HD2	3:E:736:SER:OG	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:859:MET:O	3:G:863:THR:HG22	1.63	0.97
1:B:640:ARG:HH12	3:H:849:LYS:NZ	1.55	0.96
3:E:695:PRO:HB3	3:H:702:TRP:HH2	1.23	0.96
3:F:758:LEU:HD23	3:F:762:LEU:CD1	1.98	0.94
2:J:1034:CYS:SG	2:J:1046:VAL:O	2.26	0.94
2:L:1034:CYS:SG	2:L:1046:VAL:O	2.25	0.94
2:I:1034:CYS:SG	2:I:1046:VAL:O	2.26	0.93
1:B:640:ARG:HH12	3:H:849:LYS:HZ3	0.93	0.93
2:K:1034:CYS:SG	2:K:1046:VAL:O	2.26	0.93
3:H:758:LEU:HD23	3:H:762:LEU:CD1	1.98	0.93
3:F:715:SER:HB3	3:F:720:VAL:HG21	1.48	0.93
3:E:713:MET:HE1	3:E:867:THR:CG2	1.83	0.93
3:H:819:VAL:HG11	3:H:856:LYS:HB3	1.48	0.93
3:H:715:SER:HB3	3:H:720:VAL:HG21	1.48	0.92
3:H:714:GLU:OE1	3:H:718:ARG:NH1	2.02	0.92
3:H:758:LEU:HD23	3:H:762:LEU:HD13	1.50	0.92
3:F:714:GLU:OE1	3:F:718:ARG:NH1	2.03	0.91
3:E:859:MET:O	3:E:863:THR:CG2	2.19	0.91
3:F:819:VAL:HG11	3:F:856:LYS:HB3	1.48	0.91
3:F:758:LEU:HD23	3:F:762:LEU:HD13	1.50	0.90
1:A:678:TYR:CE1	1:A:680:CYS:SG	2.65	0.90
1:C:678:TYR:CE1	1:C:680:CYS:SG	2.65	0.90
1:D:678:TYR:CE1	1:D:680:CYS:SG	2.65	0.90
1:B:678:TYR:CE1	1:B:680:CYS:SG	2.65	0.90
3:F:722:ILE:HG13	3:F:750:PHE:CD1	2.06	0.89
3:H:722:ILE:HG13	3:H:750:PHE:CD1	2.06	0.89
3:G:748:VAL:HG21	3:G:833:ILE:HG12	1.55	0.89
3:E:748:VAL:HG21	3:E:833:ILE:HG12	1.55	0.88
3:E:713:MET:HE3	3:E:867:THR:HG21	0.88	0.87
3:F:711:LEU:HD11	3:F:720:VAL:CG1	2.05	0.86
3:H:711:LEU:HD11	3:H:720:VAL:CG1	2.05	0.86
1:C:594:HIS:HD1	1:C:618:CYS:HG	1.19	0.86
3:F:715:SER:CA	3:F:720:VAL:HG21	2.05	0.86
3:H:715:SER:CA	3:H:720:VAL:HG21	2.05	0.85
1:B:594:HIS:HD1	1:B:618:CYS:HG	1.23	0.85
1:B:640:ARG:NH1	3:H:849:LYS:HZ1	1.71	0.84
1:A:594:HIS:HD1	1:A:618:CYS:HG	1.21	0.84
3:E:825:ASP:O	3:E:826:ILE:HG23	1.78	0.83
1:D:594:HIS:HD1	1:D:618:CYS:HG	1.24	0.83
3:E:733:PRO:HG2	3:E:736:SER:CB	2.08	0.83
3:G:733:PRO:HG2	3:G:736:SER:CB	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:862:ARG:O	3:H:865:ILE:HG13	1.79	0.82
3:G:825:ASP:O	3:G:826:ILE:HG23	1.78	0.82
3:H:724:GLU:O	3:H:728:ILE:HG13	1.80	0.81
3:F:724:GLU:O	3:F:728:ILE:HG13	1.80	0.81
1:A:691:MET:HB2	1:A:704:GLU:HB2	1.63	0.81
3:E:733:PRO:CG	3:E:736:SER:HB3	2.09	0.81
1:C:691:MET:HB2	1:C:704:GLU:HB2	1.63	0.81
3:F:722:ILE:HG13	3:F:750:PHE:CE1	2.15	0.81
3:H:722:ILE:HG13	3:H:750:PHE:CE1	2.15	0.81
3:G:733:PRO:CG	3:G:736:SER:HB3	2.10	0.81
3:H:811:LYS:HD3	3:H:844:ILE:HG22	1.62	0.80
1:C:594:HIS:ND1	1:C:618:CYS:SG	2.55	0.79
3:F:811:LYS:HD3	3:F:844:ILE:HG22	1.63	0.79
1:A:594:HIS:ND1	1:A:618:CYS:SG	2.55	0.79
1:B:640:ARG:HH11	3:H:849:LYS:HZ1	1.28	0.79
1:D:594:HIS:ND1	1:D:618:CYS:SG	2.55	0.79
1:B:594:HIS:ND1	1:B:618:CYS:SG	2.55	0.79
3:E:733:PRO:CD	3:E:736:SER:OG	2.31	0.79
3:E:861:VAL:O	3:E:865:ILE:HG12	1.83	0.79
3:G:733:PRO:CD	3:G:736:SER:OG	2.31	0.79
1:B:691:MET:HB2	1:B:704:GLU:HB2	1.63	0.79
1:D:691:MET:HB2	1:D:704:GLU:HB2	1.63	0.78
3:F:715:SER:CA	3:F:720:VAL:CG2	2.60	0.78
1:B:769:LYS:HB3	1:B:772:VAL:HB	1.66	0.78
3:H:715:SER:CA	3:H:720:VAL:CG2	2.60	0.78
1:D:769:LYS:HB3	1:D:772:VAL:HB	1.66	0.78
3:G:864:ALA:O	3:G:865:ILE:HD13	1.84	0.78
2:L:994:GLN:HB2	2:L:1015:MET:HB2	1.67	0.77
2:J:994:GLN:HB2	2:J:1015:MET:HB2	1.67	0.77
3:F:715:SER:CB	3:F:720:VAL:CG2	2.63	0.76
3:F:849:LYS:HE2	3:F:849:LYS:HA	1.66	0.76
3:H:721:GLU:C	3:H:750:PHE:CE1	2.58	0.76
3:E:861:VAL:O	3:E:865:ILE:CG1	2.32	0.76
1:C:804:ALA:HA	1:C:809:VAL:HG12	1.68	0.76
1:A:804:ALA:HA	1:A:809:VAL:HG12	1.68	0.76
3:H:715:SER:CB	3:H:720:VAL:CG2	2.63	0.76
3:F:694:SER:HB2	3:F:695:PRO:CD	2.15	0.76
3:H:694:SER:HB2	3:H:695:PRO:CD	2.15	0.76
3:H:849:LYS:HA	3:H:849:LYS:HE2	1.66	0.76
2:I:994:GLN:HB2	2:I:1015:MET:HB2	1.67	0.76
3:E:861:VAL:O	3:E:865:ILE:HD13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:758:LEU:CD2	3:F:762:LEU:CD1	2.64	0.76
1:C:615:LEU:HD13	3:E:859:MET:HE3	1.66	0.75
1:C:769:LYS:HB3	1:C:772:VAL:HB	1.66	0.75
3:F:721:GLU:C	3:F:750:PHE:CE1	2.58	0.75
3:H:862:ARG:HH21	3:H:863:THR:HG22	1.50	0.75
2:K:994:GLN:HB2	2:K:1015:MET:HB2	1.67	0.75
1:A:769:LYS:HB3	1:A:772:VAL:HB	1.66	0.75
1:D:803:LEU:HB3	1:D:810:ASP:HB2	1.68	0.75
1:D:804:ALA:HA	1:D:809:VAL:HG12	1.68	0.75
3:H:758:LEU:CD2	3:H:762:LEU:CD1	2.64	0.75
1:B:804:ALA:HA	1:B:809:VAL:HG12	1.68	0.75
1:B:803:LEU:HB3	1:B:810:ASP:HB2	1.69	0.75
3:F:849:LYS:HA	3:F:849:LYS:CE	2.16	0.75
1:B:755:ALA:HA	1:B:765:VAL:HG22	1.68	0.75
1:D:755:ALA:HA	1:D:765:VAL:HG22	1.68	0.75
1:D:678:TYR:HE1	1:D:680:CYS:SG	2.10	0.74
3:H:849:LYS:HA	3:H:849:LYS:CE	2.16	0.74
1:A:755:ALA:HA	1:A:765:VAL:HG22	1.68	0.74
1:B:678:TYR:HE1	1:B:680:CYS:SG	2.10	0.74
1:A:644:ALA:HB3	1:A:657:PHE:HB2	1.70	0.74
1:A:803:LEU:HB3	1:A:810:ASP:HB2	1.69	0.74
1:C:707:VAL:HB	1:C:715:GLN:HB2	1.69	0.74
3:H:842:ALA:O	3:H:846:THR:HG21	1.88	0.74
1:C:644:ALA:HB3	1:C:657:PHE:HB2	1.70	0.74
1:C:755:ALA:HA	1:C:765:VAL:HG22	1.68	0.74
1:C:803:LEU:HB3	1:C:810:ASP:HB2	1.69	0.73
1:A:707:VAL:HB	1:A:715:GLN:HB2	1.69	0.73
1:A:678:TYR:HE1	1:A:680:CYS:SG	2.10	0.73
1:D:644:ALA:HB3	1:D:657:PHE:HB2	1.70	0.73
1:B:644:ALA:HB3	1:B:657:PHE:HB2	1.70	0.73
1:C:678:TYR:HE1	1:C:680:CYS:SG	2.10	0.73
3:F:842:ALA:O	3:F:846:THR:HG21	1.88	0.72
1:A:872:GLU:CG	1:A:873:SER:HA	2.19	0.72
2:J:1021:ILE:CD1	3:H:866:GLY:HA3	2.19	0.72
3:H:849:LYS:HE2	3:H:849:LYS:CA	2.18	0.72
1:B:707:VAL:HB	1:B:715:GLN:HB2	1.69	0.72
1:B:698:ASP:OD1	1:B:701:LYS:NZ	2.23	0.71
1:A:837:VAL:HG12	1:A:852:ILE:HG12	1.72	0.71
1:D:569:SER:OG	1:D:572:ASP:OD1	2.08	0.71
1:B:569:SER:OG	1:B:572:ASP:OD1	2.08	0.71
1:C:837:VAL:HG12	1:C:852:ILE:HG12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:ASP:OD1	1:D:701:LYS:NZ	2.23	0.71
1:D:707:VAL:HB	1:D:715:GLN:HB2	1.69	0.71
3:F:711:LEU:HD11	3:F:720:VAL:HG11	1.72	0.71
3:H:711:LEU:HD11	3:H:720:VAL:HG11	1.73	0.71
1:D:781:ASN:OD1	1:D:782:LYS:N	2.20	0.71
3:E:713:MET:HE2	3:E:828:PRO:HB3	1.71	0.71
3:H:721:GLU:C	3:H:750:PHE:HE1	1.94	0.71
1:B:872:GLU:CG	1:B:873:SER:HA	2.19	0.71
3:F:849:LYS:HE2	3:F:849:LYS:CA	2.18	0.71
1:B:781:ASN:OD1	1:B:782:LYS:N	2.20	0.71
3:F:714:GLU:CD	3:F:718:ARG:NH1	2.44	0.71
3:H:714:GLU:CD	3:H:718:ARG:NH1	2.44	0.70
1:D:872:GLU:CG	1:D:873:SER:HA	2.20	0.70
3:E:811:LYS:NZ	3:E:847:SER:OG	2.24	0.70
1:B:837:VAL:HG12	1:B:852:ILE:HG12	1.72	0.70
1:D:837:VAL:HG12	1:D:852:ILE:HG12	1.72	0.70
3:G:811:LYS:NZ	3:G:847:SER:OG	2.24	0.70
1:A:698:ASP:OD1	1:A:701:LYS:NZ	2.23	0.70
1:C:698:ASP:OD1	1:C:701:LYS:NZ	2.23	0.70
1:A:781:ASN:OD1	1:A:782:LYS:N	2.20	0.70
1:B:924:SER:OG	2:J:1032:ASP:OD1	2.10	0.70
3:E:861:VAL:O	3:E:865:ILE:HD11	1.90	0.70
1:C:615:LEU:HD13	3:E:859:MET:CE	2.22	0.69
1:D:924:SER:OG	2:L:1032:ASP:OD1	2.10	0.69
3:H:758:LEU:CD2	3:H:762:LEU:HD11	2.22	0.69
1:C:781:ASN:OD1	1:C:782:LYS:N	2.20	0.69
3:E:860:TYR:O	3:E:864:ALA:CA	2.39	0.69
3:F:702:TRP:CZ3	3:G:695:PRO:HB3	2.27	0.69
3:E:860:TYR:C	3:E:864:ALA:HB3	2.08	0.69
3:F:721:GLU:C	3:F:750:PHE:HE1	1.94	0.69
1:C:569:SER:OG	1:C:572:ASP:OD1	2.08	0.69
1:D:855:CYS:HA	1:D:866:TYR:HD1	1.58	0.69
1:A:569:SER:OG	1:A:572:ASP:OD1	2.08	0.69
1:B:855:CYS:HA	1:B:866:TYR:HD1	1.58	0.69
3:E:825:ASP:O	3:E:826:ILE:CG2	2.41	0.69
1:B:748:SER:OG	1:B:753:ARG:NH1	2.26	0.69
1:C:748:SER:OG	1:C:753:ARG:NH1	2.26	0.69
1:D:748:SER:OG	1:D:753:ARG:NH1	2.26	0.69
3:E:787:LEU:HD21	3:E:818:PHE:HD2	1.58	0.69
3:G:787:LEU:HD21	3:G:818:PHE:HD2	1.58	0.69
1:A:748:SER:OG	1:A:753:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:714:GLU:CD	3:F:718:ARG:HH12	1.94	0.69
3:G:825:ASP:O	3:G:826:ILE:CG2	2.40	0.68
1:C:872:GLU:CG	1:C:873:SER:HA	2.19	0.68
1:C:924:SER:OG	2:K:1032:ASP:OD1	2.10	0.68
3:H:714:GLU:CD	3:H:718:ARG:HH12	1.95	0.68
2:J:1021:ILE:HD11	3:H:866:GLY:HA3	1.76	0.68
1:A:758:THR:OG1	1:A:762:GLU:N	2.27	0.68
1:C:758:THR:OG1	1:C:762:GLU:N	2.27	0.68
3:F:758:LEU:CD2	3:F:762:LEU:HD11	2.22	0.68
1:A:924:SER:OG	2:I:1032:ASP:OD1	2.10	0.68
1:B:758:THR:OG1	1:B:762:GLU:N	2.27	0.67
1:D:758:THR:OG1	1:D:762:GLU:N	2.27	0.67
1:C:683:ASN:CG	3:E:889:ARG:O	2.32	0.67
1:A:855:CYS:HA	1:A:866:TYR:HD1	1.58	0.67
3:E:861:VAL:HG12	3:E:865:ILE:HD11	1.76	0.67
1:C:855:CYS:HA	1:C:866:TYR:HD1	1.58	0.67
1:C:882:LYS:HE3	1:C:885:GLN:HA	1.78	0.66
3:H:748:VAL:HG21	3:H:833:ILE:HG12	1.77	0.66
1:A:882:LYS:HE3	1:A:885:GLN:HA	1.78	0.66
1:B:790:LYS:NZ	1:B:828:ILE:O	2.26	0.66
1:C:792:ILE:HG22	1:C:803:LEU:HG	1.78	0.66
1:D:790:LYS:NZ	1:D:828:ILE:O	2.26	0.66
3:F:748:VAL:HG21	3:F:833:ILE:HG12	1.77	0.66
1:D:792:ILE:HG22	1:D:803:LEU:HG	1.78	0.66
3:E:695:PRO:HB3	3:H:702:TRP:CZ3	2.29	0.66
1:A:598:ILE:HA	1:A:614:GLY:HA2	1.78	0.66
1:B:792:ILE:HG22	1:B:803:LEU:HG	1.78	0.66
3:F:693:LEU:N	3:F:693:LEU:HD12	2.11	0.66
3:H:693:LEU:N	3:H:693:LEU:HD12	2.10	0.66
1:A:792:ILE:HG22	1:A:803:LEU:HG	1.78	0.65
1:C:763:VAL:HG13	1:C:778:LEU:HB2	1.78	0.65
1:D:882:LYS:HE3	1:D:885:GLN:HA	1.78	0.65
1:B:882:LYS:HE3	1:B:885:GLN:HA	1.78	0.65
2:J:993:THR:HA	2:J:1016:TYR:HA	1.79	0.65
1:C:598:ILE:HA	1:C:614:GLY:HA2	1.78	0.65
2:L:993:THR:HA	2:L:1016:TYR:HA	1.79	0.65
1:A:763:VAL:HG13	1:A:778:LEU:HB2	1.78	0.65
1:B:640:ARG:HH11	3:H:849:LYS:NZ	1.81	0.65
3:F:758:LEU:CD2	3:F:762:LEU:HD13	2.23	0.65
3:E:826:ILE:CD1	3:E:865:ILE:O	2.45	0.65
1:B:598:ILE:HA	1:B:614:GLY:HA2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:ILE:HA	1:D:614:GLY:HA2	1.77	0.65
1:D:658:SER:OG	1:D:661:THR:O	2.14	0.65
3:H:758:LEU:CD2	3:H:762:LEU:HD13	2.23	0.65
1:B:658:SER:OG	1:B:661:THR:O	2.14	0.64
1:D:763:VAL:HG13	1:D:778:LEU:HB2	1.78	0.64
1:B:932:MET:HG2	2:J:998:VAL:HA	1.79	0.64
1:B:763:VAL:HG13	1:B:778:LEU:HB2	1.78	0.64
3:F:847:SER:HB3	3:F:848:PRO:HD3	1.78	0.64
3:F:758:LEU:O	3:F:762:LEU:HD13	1.97	0.64
1:D:932:MET:HG2	2:L:998:VAL:HA	1.79	0.64
3:H:847:SER:HB3	3:H:848:PRO:HD3	1.78	0.64
1:C:658:SER:OG	1:C:661:THR:O	2.14	0.64
3:H:758:LEU:O	3:H:762:LEU:HD13	1.97	0.64
1:A:658:SER:OG	1:A:661:THR:O	2.14	0.64
1:B:682:PRO:HB2	1:B:683:ASN:OD1	1.98	0.64
2:K:993:THR:HA	2:K:1016:TYR:HA	1.79	0.64
1:D:682:PRO:HB2	1:D:683:ASN:OD1	1.98	0.63
2:I:993:THR:HA	2:I:1016:TYR:HA	1.79	0.63
2:K:992:GLU:N	2:K:1018:SER:O	2.31	0.63
3:E:831:PHE:HE1	3:E:861:VAL:HG13	1.64	0.63
2:I:992:GLU:N	2:I:1018:SER:O	2.31	0.63
3:H:701:SER:HB2	3:H:738:ILE:HD13	1.79	0.63
1:C:932:MET:HG2	2:K:998:VAL:HA	1.79	0.63
1:D:623:ASP:HB2	1:D:630:LYS:HD2	1.81	0.63
3:F:701:SER:HB2	3:F:738:ILE:HD13	1.79	0.63
3:G:831:PHE:HE1	3:G:861:VAL:HG13	1.64	0.63
1:A:932:MET:HG2	2:I:998:VAL:HA	1.79	0.63
1:A:682:PRO:HB2	1:A:683:ASN:OD1	1.98	0.63
1:B:623:ASP:HB2	1:B:630:LYS:HD2	1.81	0.63
1:D:746:ILE:HG23	1:D:796:ALA:HA	1.80	0.63
1:C:682:PRO:HB2	1:C:683:ASN:OD1	1.98	0.63
1:D:819:LEU:HD12	1:D:820:LEU:H	1.63	0.63
3:F:845:CYS:O	3:F:852:ASP:OD2	2.17	0.63
1:B:746:ILE:HG23	1:B:796:ALA:HA	1.80	0.63
1:B:819:LEU:HD12	1:B:820:LEU:H	1.63	0.63
1:D:754:ILE:HD11	1:D:766:TYR:HB2	1.81	0.62
3:H:845:CYS:O	3:H:852:ASP:OD2	2.17	0.62
1:A:606:ASN:ND2	1:A:650:GLN:O	2.31	0.62
1:A:746:ILE:HG23	1:A:796:ALA:HA	1.80	0.62
2:J:992:GLU:N	2:J:1018:SER:O	2.31	0.62
1:C:606:ASN:ND2	1:C:650:GLN:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ASN:ND2	1:D:650:GLN:O	2.31	0.62
1:A:832:THR:HB	1:A:857:THR:H	1.64	0.62
1:C:623:ASP:HB2	1:C:630:LYS:HD2	1.81	0.62
1:C:832:THR:HB	1:C:857:THR:H	1.64	0.62
2:L:992:GLU:N	2:L:1018:SER:O	2.31	0.62
3:H:801:LEU:HD22	3:H:806:TYR:CE2	2.34	0.62
1:A:623:ASP:HB2	1:A:630:LYS:HD2	1.81	0.62
1:A:819:LEU:HD12	1:A:820:LEU:H	1.63	0.62
1:B:606:ASN:ND2	1:B:650:GLN:O	2.31	0.62
1:B:754:ILE:HD11	1:B:766:TYR:HB2	1.82	0.62
1:C:746:ILE:HG23	1:C:796:ALA:HA	1.80	0.62
1:C:813:ASP:HB3	1:C:818:GLU:H	1.64	0.62
1:C:819:LEU:HD12	1:C:820:LEU:H	1.63	0.62
1:A:813:ASP:HB3	1:A:818:GLU:H	1.64	0.62
1:C:683:ASN:ND2	3:E:889:ARG:O	2.33	0.62
3:F:801:LEU:HD22	3:F:806:TYR:CE2	2.34	0.62
3:G:865:ILE:HG22	3:G:867:THR:H	1.64	0.62
1:C:683:ASN:OD1	3:E:889:ARG:O	2.18	0.62
1:A:754:ILE:HD11	1:A:766:TYR:HB2	1.81	0.62
1:C:754:ILE:HD11	1:C:766:TYR:HB2	1.81	0.62
1:B:597:ASP:O	1:B:615:LEU:N	2.30	0.61
1:B:938:SER:O	2:J:993:THR:N	2.33	0.61
1:D:596:LEU:HD12	1:D:616:ASP:HB3	1.82	0.61
3:H:715:SER:HA	3:H:720:VAL:HG21	1.69	0.61
1:D:938:SER:O	2:L:993:THR:N	2.33	0.61
1:D:597:ASP:O	1:D:615:LEU:N	2.30	0.61
1:A:790:LYS:NZ	1:A:828:ILE:O	2.26	0.61
1:B:596:LEU:HD12	1:B:616:ASP:HB3	1.82	0.61
1:B:832:THR:HB	1:B:857:THR:H	1.64	0.61
1:C:790:LYS:NZ	1:C:828:ILE:O	2.26	0.61
1:D:832:THR:HB	1:D:857:THR:H	1.64	0.61
3:E:860:TYR:O	3:E:864:ALA:N	2.33	0.61
1:B:813:ASP:HB3	1:B:818:GLU:H	1.64	0.61
1:D:813:ASP:HB3	1:D:818:GLU:H	1.64	0.61
3:E:733:PRO:CG	3:E:736:SER:CB	2.76	0.61
3:G:864:ALA:O	3:G:865:ILE:CD1	2.48	0.61
3:H:852:ASP:HB3	3:H:854:VAL:HG22	1.82	0.61
1:C:674:LEU:HB2	1:C:726:ALA:HB3	1.83	0.61
1:C:938:SER:O	2:K:993:THR:N	2.33	0.61
1:A:674:LEU:HB2	1:A:726:ALA:HB3	1.83	0.60
3:G:733:PRO:CG	3:G:736:SER:CB	2.76	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:SER:O	2:I:993:THR:N	2.33	0.60
3:F:812:ARG:NH1	3:F:816:GLU:OE1	2.34	0.60
3:H:693:LEU:HD12	3:H:693:LEU:H	1.66	0.60
1:B:577:ASP:OD1	2:J:1011:LYS:HE2	2.01	0.60
1:C:758:THR:HG1	1:C:762:GLU:H	1.49	0.60
1:D:674:LEU:HB2	1:D:726:ALA:HB3	1.83	0.60
1:B:687:ASN:HB3	1:B:708:VAL:HB	1.84	0.60
1:D:577:ASP:OD1	2:L:1011:LYS:HE2	2.01	0.60
3:F:693:LEU:HD12	3:F:693:LEU:H	1.66	0.60
1:A:596:LEU:HD12	1:A:616:ASP:HB3	1.82	0.60
1:A:869:TYR:CZ	1:A:909:GLU:HB3	2.37	0.60
1:B:674:LEU:HB2	1:B:726:ALA:HB3	1.83	0.60
1:D:687:ASN:HB3	1:D:708:VAL:HB	1.84	0.60
3:F:852:ASP:HB3	3:F:854:VAL:HG22	1.82	0.60
3:H:812:ARG:NH1	3:H:816:GLU:OE1	2.34	0.60
1:A:758:THR:HG1	1:A:762:GLU:H	1.49	0.60
1:C:869:TYR:CZ	1:C:909:GLU:HB3	2.37	0.60
1:C:596:LEU:HD12	1:C:616:ASP:HB3	1.82	0.60
1:A:577:ASP:OD1	2:I:1011:LYS:HE2	2.01	0.60
1:A:882:LYS:N	1:A:885:GLN:HE22	2.00	0.60
1:A:687:ASN:HB3	1:A:708:VAL:HB	1.84	0.59
1:C:597:ASP:O	1:C:615:LEU:N	2.30	0.59
1:C:687:ASN:HB3	1:C:708:VAL:HB	1.84	0.59
1:A:702:ASN:OD1	1:A:703:PHE:N	2.35	0.59
1:C:702:ASN:OD1	1:C:703:PHE:N	2.35	0.59
1:B:702:ASN:OD1	1:B:703:PHE:N	2.35	0.59
1:C:577:ASP:OD1	2:K:1011:LYS:HE2	2.01	0.59
1:C:882:LYS:N	1:C:885:GLN:HE22	2.00	0.59
3:E:766:LYS:NZ	3:F:816:GLU:OE2	2.27	0.59
1:A:597:ASP:O	1:A:615:LEU:N	2.30	0.59
1:D:702:ASN:OD1	1:D:703:PHE:N	2.35	0.59
1:D:869:TYR:CZ	1:D:909:GLU:HB3	2.37	0.59
3:H:853:VAL:HG12	3:H:853:VAL:O	2.03	0.59
3:F:853:VAL:HG12	3:F:853:VAL:O	2.02	0.59
1:B:869:TYR:CZ	1:B:909:GLU:HB3	2.37	0.59
1:B:882:LYS:N	1:B:885:GLN:HE22	2.00	0.58
1:D:882:LYS:N	1:D:885:GLN:HE22	2.01	0.58
3:H:826:ILE:O	3:H:868:LEU:HD11	2.03	0.58
1:B:598:ILE:HG13	2:J:1041:ASN:HA	1.86	0.58
1:D:598:ILE:HG13	2:L:1041:ASN:HA	1.86	0.58
1:C:689:PHE:CZ	1:C:744:ILE:HA	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:819:VAL:HG21	3:E:856:LYS:HB3	1.85	0.57
3:E:865:ILE:HG22	3:E:867:THR:H	1.68	0.57
3:G:819:VAL:HG21	3:G:856:LYS:HB3	1.85	0.57
1:A:689:PHE:CZ	1:A:744:ILE:HA	2.40	0.57
3:E:695:PRO:CB	3:H:702:TRP:CH2	2.75	0.57
1:C:621:VAL:HG22	1:C:631:LEU:HB3	1.87	0.57
3:F:715:SER:HB2	3:F:720:VAL:HG21	1.81	0.57
3:G:863:THR:O	3:G:864:ALA:HB2	2.05	0.57
1:A:598:ILE:HG13	2:I:1041:ASN:HA	1.86	0.57
1:D:780:GLN:OE1	1:D:789:LYS:NZ	2.29	0.57
3:F:702:TRP:CH2	3:G:695:PRO:CB	2.71	0.57
1:A:621:VAL:HG22	1:A:631:LEU:HB3	1.87	0.57
1:B:689:PHE:CZ	1:B:744:ILE:HA	2.40	0.57
1:D:689:PHE:CZ	1:D:744:ILE:HA	2.40	0.57
3:G:859:MET:O	3:G:863:THR:CG2	2.48	0.57
3:H:715:SER:HB2	3:H:720:VAL:HG21	1.82	0.57
1:B:780:GLN:OE1	1:B:789:LYS:NZ	2.29	0.57
1:C:598:ILE:HG13	2:K:1041:ASN:HA	1.86	0.56
1:D:741:ILE:HG13	1:D:759:GLU:HG2	1.86	0.56
1:B:741:ILE:HG13	1:B:759:GLU:HG2	1.86	0.56
3:F:738:ILE:H	3:F:738:ILE:HD12	1.69	0.56
1:D:658:SER:O	1:D:678:TYR:OH	2.16	0.56
1:D:758:THR:HG1	1:D:762:GLU:H	1.51	0.56
3:H:738:ILE:H	3:H:738:ILE:HD12	1.70	0.56
1:A:745:SER:HA	1:A:754:ILE:HG22	1.88	0.56
1:B:658:SER:O	1:B:678:TYR:OH	2.16	0.56
1:B:758:THR:HG1	1:B:762:GLU:H	1.51	0.56
1:C:745:SER:HA	1:C:754:ILE:HG22	1.88	0.56
1:D:621:VAL:HG22	1:D:631:LEU:HB3	1.87	0.56
3:G:870:ILE:H	3:G:871:GLN:C	2.09	0.56
3:F:751:PRO:HA	3:F:754:THR:HG23	1.87	0.56
3:H:751:PRO:HA	3:H:754:THR:HG23	1.87	0.56
1:A:741:ILE:HG13	1:A:759:GLU:HG2	1.86	0.55
1:B:621:VAL:HG22	1:B:631:LEU:HB3	1.87	0.55
3:E:725:ILE:HG13	3:E:750:PHE:HE2	1.69	0.55
3:E:807:GLY:HA2	3:E:810:SER:HB3	1.88	0.55
3:G:725:ILE:HG13	3:G:750:PHE:HE2	1.70	0.55
2:J:1021:ILE:HD13	3:H:866:GLY:HA3	1.87	0.55
1:C:741:ILE:HG13	1:C:759:GLU:HG2	1.86	0.55
1:B:655:SER:HB3	1:B:690:TRP:HZ2	1.72	0.55
1:B:745:SER:HA	1:B:754:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:SER:HA	1:D:754:ILE:HG22	1.88	0.55
3:F:795:SER:HB3	3:F:817:ILE:HD13	1.89	0.55
1:A:736:LEU:HD11	1:A:766:TYR:HE1	1.72	0.55
3:E:861:VAL:HG12	3:E:865:ILE:CD1	2.37	0.55
1:C:736:LEU:HD11	1:C:766:TYR:HE1	1.72	0.55
3:G:807:GLY:HA2	3:G:810:SER:HB3	1.88	0.55
1:A:655:SER:HB3	1:A:690:TRP:HZ2	1.72	0.55
1:B:674:LEU:HD21	1:B:676:HIS:HB2	1.88	0.55
1:D:819:LEU:HD12	1:D:820:LEU:N	2.22	0.55
1:D:858:HIS:CG	1:D:861:THR:HG1	2.25	0.55
3:G:844:ILE:HD12	3:G:844:ILE:H	1.70	0.55
1:A:674:LEU:HD21	1:A:676:HIS:HB2	1.88	0.55
1:A:819:LEU:HD12	1:A:820:LEU:N	2.22	0.55
1:B:702:ASN:HA	1:B:720:THR:HA	1.89	0.55
1:B:819:LEU:HD12	1:B:820:LEU:N	2.22	0.55
1:B:858:HIS:CG	1:B:861:THR:HG1	2.25	0.55
1:C:615:LEU:CD1	3:E:859:MET:CE	2.84	0.55
1:C:655:SER:HB3	1:C:690:TRP:HZ2	1.72	0.55
1:C:819:LEU:HD12	1:C:820:LEU:N	2.22	0.55
1:D:655:SER:HB3	1:D:690:TRP:HZ2	1.72	0.55
1:D:736:LEU:HD11	1:D:766:TYR:HE1	1.72	0.55
3:E:844:ILE:HD12	3:E:844:ILE:H	1.71	0.55
1:D:702:ASN:HA	1:D:720:THR:HA	1.89	0.55
1:B:736:LEU:HD11	1:B:766:TYR:HE1	1.72	0.54
1:C:674:LEU:HD21	1:C:676:HIS:HB2	1.88	0.54
3:H:713:MET:SD	3:H:828:PRO:HB3	2.47	0.54
3:H:795:SER:HB3	3:H:817:ILE:HD13	1.89	0.54
2:J:1033:ARG:NH1	2:J:1049:GLY:O	2.39	0.54
1:D:674:LEU:HD21	1:D:676:HIS:HB2	1.89	0.54
3:F:865:ILE:HD12	3:F:865:ILE:O	2.07	0.54
1:A:753:ARG:HH21	1:A:815:LYS:HB2	1.72	0.54
1:A:793:TYR:O	1:A:802:PHE:HB2	2.08	0.54
2:I:1033:ARG:NH1	2:I:1049:GLY:O	2.39	0.54
2:L:1033:ARG:NH1	2:L:1049:GLY:O	2.39	0.54
1:B:793:TYR:O	1:B:802:PHE:HB2	2.08	0.54
1:C:753:ARG:HH21	1:C:815:LYS:HB2	1.72	0.54
1:C:793:TYR:O	1:C:802:PHE:HB2	2.08	0.54
1:D:793:TYR:O	1:D:802:PHE:HB2	2.08	0.54
3:E:707:LEU:HB3	3:E:728:ILE:HD12	1.89	0.54
3:F:713:MET:SD	3:F:828:PRO:HB3	2.47	0.54
3:E:825:ASP:C	3:E:826:ILE:HG23	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:826:ILE:HD11	3:E:866:GLY:HA3	1.90	0.54
3:G:707:LEU:HB3	3:G:728:ILE:HD12	1.89	0.54
1:B:795:ILE:O	1:B:799:ASP:N	2.41	0.54
2:K:1033:ARG:NH1	2:K:1049:GLY:O	2.39	0.54
1:D:795:ILE:O	1:D:799:ASP:N	2.41	0.54
3:F:721:GLU:O	3:F:750:PHE:CZ	2.61	0.54
3:H:722:ILE:HD12	3:H:722:ILE:H	1.73	0.54
3:H:722:ILE:N	3:H:750:PHE:CE1	2.75	0.54
1:C:702:ASN:HA	1:C:720:THR:HA	1.89	0.54
3:F:806:TYR:O	3:F:808:ASP:N	2.41	0.54
1:A:702:ASN:HA	1:A:720:THR:HA	1.89	0.53
1:B:722:GLU:HB3	1:B:724:GLU:OE1	2.08	0.53
3:G:756:ASP:O	3:G:760:GLU:HG3	2.08	0.53
1:B:753:ARG:HH21	1:B:815:LYS:HB2	1.72	0.53
1:D:722:GLU:HB3	1:D:724:GLU:OE1	2.08	0.53
3:F:722:ILE:HD12	3:F:722:ILE:H	1.73	0.53
3:G:825:ASP:C	3:G:826:ILE:HG23	2.29	0.53
1:A:849:VAL:HG22	1:A:880:LEU:HD23	1.91	0.53
1:C:581:HIS:HB3	2:K:1009:ARG:NH2	2.23	0.53
1:C:739:PRO:HB2	1:C:759:GLU:OE1	2.09	0.53
3:E:756:ASP:O	3:E:760:GLU:HG3	2.08	0.53
3:H:721:GLU:O	3:H:750:PHE:CZ	2.61	0.53
1:A:581:HIS:HB3	2:I:1009:ARG:NH2	2.23	0.53
1:A:739:PRO:HB2	1:A:759:GLU:OE1	2.09	0.53
1:C:849:VAL:HG22	1:C:880:LEU:HD23	1.91	0.53
3:H:806:TYR:O	3:H:808:ASP:N	2.41	0.53
1:B:581:HIS:HB3	2:J:1009:ARG:NH2	2.23	0.53
1:C:722:GLU:HB3	1:C:724:GLU:OE1	2.08	0.53
1:C:795:ILE:O	1:C:799:ASP:N	2.41	0.53
1:D:753:ARG:HH21	1:D:815:LYS:HB2	1.72	0.53
3:F:711:LEU:CD1	3:F:720:VAL:HG11	2.37	0.53
3:F:722:ILE:N	3:F:750:PHE:CE1	2.76	0.53
1:A:722:GLU:HB3	1:A:724:GLU:OE1	2.08	0.53
1:D:581:HIS:HB3	2:L:1009:ARG:NH2	2.23	0.53
1:D:598:ILE:HD12	2:L:1038:VAL:HG13	1.91	0.53
3:E:774:GLN:C	3:E:775:ASP:OD1	2.47	0.53
1:B:598:ILE:HD12	2:J:1038:VAL:HG13	1.91	0.53
3:F:702:TRP:CZ3	3:G:695:PRO:CB	2.92	0.53
1:A:795:ILE:O	1:A:799:ASP:N	2.41	0.53
3:G:774:GLN:C	3:G:775:ASP:OD1	2.47	0.53
1:B:696:LYS:CB	1:B:700:TRP:CE2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:696:LYS:CB	1:D:700:TRP:CE2	2.92	0.52
3:H:722:ILE:HA	3:H:750:PHE:CZ	2.44	0.52
1:A:702:ASN:ND2	1:A:720:THR:OG1	2.42	0.52
1:A:752:ASN:HB2	1:A:768:LYS:HB3	1.90	0.52
1:A:598:ILE:HD12	2:I:1038:VAL:HG13	1.91	0.52
1:B:702:ASN:ND2	1:B:720:THR:OG1	2.42	0.52
1:B:740:ILE:HG23	1:B:757:LEU:O	2.10	0.52
1:D:702:ASN:ND2	1:D:720:THR:OG1	2.42	0.52
3:F:722:ILE:HA	3:F:750:PHE:CZ	2.44	0.52
3:G:724:GLU:O	3:G:728:ILE:HG12	2.10	0.52
1:A:855:CYS:HA	1:A:866:TYR:CD1	2.42	0.52
2:J:1030:VAL:H	2:J:1035:VAL:HA	1.75	0.52
1:C:666:ASN:OD1	1:C:667:VAL:N	2.43	0.52
1:C:702:ASN:ND2	1:C:720:THR:OG1	2.42	0.52
1:C:855:CYS:HA	1:C:866:TYR:CD1	2.43	0.52
1:D:740:ILE:HG23	1:D:757:LEU:O	2.10	0.52
3:E:724:GLU:O	3:E:728:ILE:HG12	2.10	0.52
3:H:862:ARG:NH2	3:H:863:THR:HG22	2.23	0.52
1:A:666:ASN:OD1	1:A:667:VAL:N	2.43	0.52
1:B:768:LYS:HD2	1:B:773:TRP:CH2	2.45	0.52
1:C:598:ILE:HD12	2:K:1038:VAL:HG13	1.91	0.52
1:D:768:LYS:HD2	1:D:773:TRP:CH2	2.45	0.52
2:L:1030:VAL:H	2:L:1035:VAL:HA	1.75	0.52
3:E:695:PRO:CB	3:H:702:TRP:CZ3	2.93	0.52
3:H:711:LEU:CD1	3:H:720:VAL:HG11	2.37	0.52
1:B:666:ASN:OD1	1:B:667:VAL:N	2.43	0.52
1:B:849:VAL:HG22	1:B:880:LEU:HD23	1.91	0.52
1:C:752:ASN:HB2	1:C:768:LYS:HB3	1.91	0.52
1:C:805:ARG:HH12	1:C:810:ASP:CG	2.13	0.52
3:F:715:SER:HA	3:F:720:VAL:HG22	1.86	0.52
1:A:805:ARG:HH12	1:A:810:ASP:CG	2.13	0.52
2:I:1030:VAL:H	2:I:1035:VAL:HA	1.75	0.52
1:B:640:ARG:HH12	3:H:849:LYS:CE	2.22	0.52
1:B:855:CYS:HA	1:B:866:TYR:CD1	2.43	0.52
1:B:915:GLU:HG3	1:B:918:SER:H	1.75	0.52
1:C:696:LYS:CB	1:C:700:TRP:CE2	2.92	0.52
1:D:855:CYS:HA	1:D:866:TYR:CD1	2.42	0.52
1:D:915:GLU:HG3	1:D:918:SER:H	1.75	0.52
3:F:872:ASP:O	3:F:874:LYS:N	2.40	0.52
1:D:666:ASN:OD1	1:D:667:VAL:N	2.43	0.52
1:D:684:SER:OG	1:D:710:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:849:VAL:HG22	1:D:880:LEU:HD23	1.91	0.52
1:B:684:SER:OG	1:B:710:SER:HB2	2.10	0.51
1:B:739:PRO:HB2	1:B:759:GLU:OE1	2.09	0.51
3:H:711:LEU:HD11	3:H:720:VAL:HG13	1.89	0.51
1:A:858:HIS:CG	1:A:861:THR:HG1	2.28	0.51
3:E:713:MET:CE	3:E:867:THR:CB	2.85	0.51
1:A:696:LYS:CB	1:A:700:TRP:CE2	2.93	0.51
1:B:793:TYR:HB3	1:B:833:PHE:CE2	2.45	0.51
1:C:780:GLN:OE1	1:C:789:LYS:NZ	2.28	0.51
2:K:1030:VAL:H	2:K:1035:VAL:HA	1.75	0.51
1:D:739:PRO:HB2	1:D:759:GLU:OE1	2.09	0.51
1:D:793:TYR:HB3	1:D:833:PHE:CE2	2.45	0.51
1:D:805:ARG:HH12	1:D:810:ASP:CG	2.13	0.51
2:L:1038:VAL:O	2:L:1039:LEU:HD12	2.10	0.51
1:A:780:GLN:OE1	1:A:789:LYS:NZ	2.29	0.51
1:B:805:ARG:HH12	1:B:810:ASP:CG	2.13	0.51
1:C:676:HIS:CG	1:C:728:ILE:HD13	2.46	0.51
1:A:676:HIS:CG	1:A:728:ILE:HD13	2.46	0.51
1:A:684:SER:OG	1:A:710:SER:HB2	2.10	0.51
1:A:791:ASP:OD1	1:A:792:ILE:N	2.43	0.51
1:B:736:LEU:HD11	1:B:766:TYR:CE1	2.45	0.51
1:B:882:LYS:H	1:B:885:GLN:HE22	1.57	0.51
2:J:1038:VAL:O	2:J:1039:LEU:HD12	2.10	0.51
1:C:791:ASP:OD1	1:C:792:ILE:N	2.43	0.51
1:D:736:LEU:HD11	1:D:766:TYR:CE1	2.45	0.51
1:D:752:ASN:HB2	1:D:768:LYS:HB3	1.91	0.51
1:A:740:ILE:HG23	1:A:757:LEU:O	2.10	0.51
1:C:793:TYR:HB3	1:C:833:PHE:CE2	2.45	0.51
1:C:829:LYS:HB2	1:C:859:ALA:HA	1.93	0.51
1:A:793:TYR:HB3	1:A:833:PHE:CE2	2.45	0.51
2:I:1038:VAL:O	2:I:1039:LEU:HD12	2.10	0.51
1:C:858:HIS:CG	1:C:861:THR:HG1	2.29	0.51
2:K:1038:VAL:O	2:K:1039:LEU:HD12	2.10	0.51
3:E:835:TRP:HH2	3:E:875:LEU:O	1.93	0.51
1:A:829:LYS:HB2	1:A:859:ALA:HA	1.93	0.51
1:A:882:LYS:H	1:A:885:GLN:HE22	1.57	0.51
1:B:752:ASN:HB2	1:B:768:LYS:HB3	1.91	0.51
1:C:740:ILE:HG23	1:C:757:LEU:O	2.10	0.51
1:C:768:LYS:HD2	1:C:773:TRP:CH2	2.45	0.51
1:D:791:ASP:OD1	1:D:792:ILE:N	2.44	0.51
1:D:798:ALA:O	1:D:800:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:711:LEU:HD11	3:F:720:VAL:HG13	1.89	0.51
3:F:721:GLU:O	3:F:750:PHE:HZ	1.94	0.51
3:H:721:GLU:O	3:H:750:PHE:HZ	1.94	0.51
1:A:768:LYS:HD2	1:A:773:TRP:CH2	2.45	0.51
1:A:882:LYS:H	1:A:885:GLN:NE2	2.09	0.51
1:B:798:ALA:O	1:B:800:ILE:HG13	2.11	0.51
1:B:882:LYS:H	1:B:885:GLN:NE2	2.09	0.51
1:A:851:SER:HB3	1:A:872:GLU:OE1	2.11	0.51
1:B:791:ASP:OD1	1:B:792:ILE:N	2.44	0.51
1:C:684:SER:OG	1:C:710:SER:HB2	2.10	0.51
1:C:851:SER:HB3	1:C:872:GLU:OE1	2.11	0.51
1:D:882:LYS:H	1:D:885:GLN:NE2	2.09	0.51
1:D:882:LYS:H	1:D:885:GLN:HE22	1.57	0.50
1:D:851:SER:HB3	1:D:872:GLU:OE1	2.11	0.50
1:A:798:ALA:O	1:A:800:ILE:HG13	2.11	0.50
1:B:851:SER:HB3	1:B:872:GLU:OE1	2.11	0.50
3:H:715:SER:HA	3:H:720:VAL:HG22	1.86	0.50
1:B:676:HIS:CG	1:B:728:ILE:HD13	2.46	0.50
1:C:798:ALA:O	1:C:800:ILE:HG13	2.11	0.50
1:C:882:LYS:H	1:C:885:GLN:NE2	2.09	0.50
1:A:915:GLU:HG3	1:A:918:SER:H	1.75	0.50
1:B:689:PHE:HB2	1:B:706:VAL:HB	1.94	0.50
1:C:736:LEU:HD11	1:C:766:TYR:CE1	2.45	0.50
1:C:915:GLU:HG3	1:C:918:SER:H	1.75	0.50
1:D:676:HIS:CG	1:D:728:ILE:HD13	2.46	0.50
3:E:712:LEU:HB3	3:E:832:ILE:HG13	1.93	0.50
1:A:736:LEU:HD11	1:A:766:TYR:CE1	2.45	0.50
1:B:829:LYS:HB2	1:B:859:ALA:HA	1.93	0.50
1:D:689:PHE:HB2	1:D:706:VAL:HB	1.94	0.50
2:K:1022:ALA:HB2	3:E:862:ARG:HH12	1.77	0.50
1:D:832:THR:HG21	1:D:857:THR:HB	1.94	0.50
3:G:712:LEU:HB3	3:G:832:ILE:HG13	1.93	0.50
1:B:601:ILE:HG22	1:B:612:SER:HA	1.94	0.50
1:B:832:THR:HG21	1:B:857:THR:HB	1.94	0.50
1:D:793:TYR:HB3	1:D:833:PHE:CD2	2.47	0.50
1:D:829:LYS:HB2	1:D:859:ALA:HA	1.93	0.50
1:B:793:TYR:HB3	1:B:833:PHE:CD2	2.47	0.49
1:C:882:LYS:H	1:C:885:GLN:HE22	1.58	0.49
2:K:1029:ALA:HA	2:K:1035:VAL:HA	1.95	0.49
1:A:689:PHE:HB2	1:A:706:VAL:HB	1.94	0.49
2:I:1029:ALA:HA	2:I:1035:VAL:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ILE:HA	1:B:796:ALA:HB1	1.95	0.49
1:B:869:TYR:HD1	1:B:907:LEU:HB3	1.78	0.49
1:C:689:PHE:HB2	1:C:706:VAL:HB	1.94	0.49
1:D:601:ILE:HG22	1:D:612:SER:HA	1.94	0.49
1:D:746:ILE:HA	1:D:796:ALA:HB1	1.95	0.49
1:B:802:PHE:HB3	1:B:833:PHE:HZ	1.77	0.49
2:K:1001:TYR:HD1	2:K:1008:HIS:HB2	1.78	0.49
1:A:869:TYR:HD1	1:A:907:LEU:HB3	1.77	0.49
1:C:842:PHE:CE2	1:C:845:GLY:HA2	2.48	0.49
1:D:877:TYR:CE2	1:D:879:ILE:HG13	2.48	0.49
3:F:718:ARG:CG	3:F:719:LYS:N	2.75	0.49
1:A:842:PHE:CE2	1:A:845:GLY:HA2	2.48	0.49
1:B:884:ASP:HB3	1:B:886:GLN:HG2	1.94	0.49
1:A:574:LEU:HD11	2:I:1013:LEU:HD12	1.95	0.49
1:A:802:PHE:HB3	1:A:833:PHE:HZ	1.77	0.49
2:I:1001:TYR:HD1	2:I:1008:HIS:HB2	1.78	0.49
1:C:802:PHE:HB3	1:C:833:PHE:HZ	1.77	0.49
1:C:832:THR:HG21	1:C:857:THR:HB	1.94	0.49
1:D:802:PHE:HB3	1:D:833:PHE:HZ	1.77	0.49
1:D:842:PHE:CE2	1:D:845:GLY:HA2	2.48	0.49
3:H:721:GLU:CA	3:H:750:PHE:HE1	2.25	0.49
1:A:832:THR:HG21	1:A:857:THR:HB	1.94	0.49
1:B:640:ARG:NH1	3:H:849:LYS:CE	2.72	0.49
1:B:842:PHE:CE2	1:B:845:GLY:HA2	2.48	0.49
1:B:877:TYR:CE2	1:B:879:ILE:HG13	2.48	0.49
1:C:869:TYR:HD1	1:C:907:LEU:HB3	1.78	0.49
1:D:869:TYR:HD1	1:D:907:LEU:HB3	1.78	0.49
1:C:574:LEU:HD11	2:K:1013:LEU:HD12	1.95	0.48
2:J:1001:TYR:HD1	2:J:1008:HIS:HB2	1.78	0.48
1:D:884:ASP:HB3	1:D:886:GLN:HG2	1.95	0.48
3:H:711:LEU:HD23	3:H:725:ILE:HD13	1.95	0.48
1:A:793:TYR:HB3	1:A:833:PHE:CD2	2.47	0.48
1:A:841:ARG:NH2	1:A:896:ASP:OD2	2.45	0.48
1:B:574:LEU:HD11	2:J:1013:LEU:HD12	1.95	0.48
1:C:793:TYR:HB3	1:C:833:PHE:CD2	2.47	0.48
2:L:1001:TYR:HD1	2:L:1008:HIS:HB2	1.78	0.48
3:H:718:ARG:CG	3:H:719:LYS:N	2.76	0.48
1:B:854:PHE:CE2	1:B:869:TYR:HD2	2.32	0.48
1:C:841:ARG:NH2	1:C:896:ASP:OD2	2.45	0.48
1:D:574:LEU:HD11	2:L:1013:LEU:HD12	1.95	0.48
1:D:841:ARG:NH2	1:D:896:ASP:OD2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:704:ALA:CB	3:E:732:CYS:SG	3.01	0.48
3:F:721:GLU:CA	3:F:750:PHE:HE1	2.25	0.48
1:C:602:ALA:HB3	1:C:647:LEU:HD13	1.95	0.48
1:C:795:ILE:HG22	1:C:798:ALA:H	1.78	0.48
1:A:795:ILE:HG22	1:A:798:ALA:H	1.78	0.48
1:B:802:PHE:HA	1:B:810:ASP:O	2.14	0.48
1:D:802:PHE:HA	1:D:810:ASP:O	2.14	0.48
1:D:854:PHE:CE2	1:D:869:TYR:HD2	2.32	0.48
2:L:1029:ALA:HA	2:L:1035:VAL:HA	1.95	0.48
3:E:826:ILE:HD13	3:E:865:ILE:O	2.13	0.48
1:A:601:ILE:HG22	1:A:612:SER:HA	1.94	0.48
1:A:746:ILE:HA	1:A:796:ALA:HB1	1.95	0.48
1:B:841:ARG:NH2	1:B:896:ASP:OD2	2.45	0.48
2:J:1029:ALA:HA	2:J:1035:VAL:HA	1.95	0.48
1:C:601:ILE:HG22	1:C:612:SER:HA	1.94	0.48
1:C:615:LEU:CD1	3:E:859:MET:HE1	2.44	0.48
1:C:746:ILE:HA	1:C:796:ALA:HB1	1.95	0.48
3:E:704:ALA:HB1	3:E:732:CYS:SG	2.54	0.48
3:G:704:ALA:CB	3:G:732:CYS:SG	3.01	0.48
1:A:602:ALA:HB3	1:A:647:LEU:HD13	1.95	0.48
1:B:753:ARG:NH2	1:B:815:LYS:HB2	2.28	0.48
3:E:811:LYS:O	3:E:815:GLN:HG3	2.14	0.48
1:D:753:ARG:NH2	1:D:815:LYS:HB2	2.28	0.48
3:G:811:LYS:O	3:G:815:GLN:HG3	2.14	0.48
1:C:877:TYR:CE2	1:C:879:ILE:HG13	2.48	0.48
3:G:704:ALA:HB1	3:G:732:CYS:SG	2.54	0.48
3:H:792:THR:HG23	3:H:833:ILE:HD12	1.94	0.48
1:A:716:VAL:CG2	1:A:732:GLU:HB2	2.44	0.47
1:B:617:ARG:HD2	1:B:642:LEU:HD12	1.96	0.47
1:A:877:TYR:CE2	1:A:879:ILE:HG13	2.48	0.47
1:B:888:ASN:OD1	1:B:889:LEU:N	2.47	0.47
1:C:615:LEU:HD12	3:E:859:MET:HE1	1.97	0.47
1:C:884:ASP:HB3	1:C:886:GLN:HG2	1.94	0.47
3:F:792:THR:HG23	3:F:833:ILE:HD12	1.94	0.47
1:A:884:ASP:HB3	1:A:886:GLN:HG2	1.95	0.47
1:B:795:ILE:HG22	1:B:798:ALA:H	1.78	0.47
1:C:716:VAL:CG2	1:C:732:GLU:HB2	2.44	0.47
1:D:888:ASN:OD1	1:D:889:LEU:N	2.47	0.47
3:F:711:LEU:HD23	3:F:725:ILE:HD13	1.95	0.47
1:A:753:ARG:NH2	1:A:815:LYS:HB2	2.29	0.47
1:B:925:ASP:OD2	2:J:1032:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:ASN:OD1	1:C:889:LEU:N	2.47	0.47
2:K:1022:ALA:HB2	3:E:862:ARG:NH1	2.28	0.47
1:D:622:TRP:C	1:D:630:LYS:HD3	2.35	0.47
1:D:795:ILE:HG22	1:D:798:ALA:H	1.78	0.47
1:A:888:ASN:OD1	1:A:889:LEU:N	2.47	0.47
1:B:622:TRP:C	1:B:630:LYS:HD3	2.35	0.47
1:C:753:ARG:NH2	1:C:815:LYS:HB2	2.29	0.47
1:D:925:ASP:OD2	2:L:1032:ASP:HB3	2.15	0.47
1:A:802:PHE:HA	1:A:810:ASP:O	2.14	0.47
1:C:802:PHE:HA	1:C:810:ASP:O	2.14	0.47
1:A:617:ARG:HD2	1:A:642:LEU:HD12	1.96	0.47
1:A:636:GLU:OE1	1:A:636:GLU:N	2.47	0.47
1:A:854:PHE:CE2	1:A:869:TYR:HD2	2.32	0.47
1:B:602:ALA:HB3	1:B:647:LEU:HD13	1.95	0.47
1:B:716:VAL:CG2	1:B:732:GLU:HB2	2.44	0.47
1:C:617:ARG:HD2	1:C:642:LEU:HD12	1.96	0.47
1:C:636:GLU:OE1	1:C:636:GLU:N	2.47	0.47
1:C:854:PHE:CE2	1:C:869:TYR:HD2	2.32	0.47
1:D:602:ALA:HB3	1:D:647:LEU:HD13	1.95	0.47
1:D:617:ARG:HD2	1:D:642:LEU:HD12	1.96	0.47
3:E:835:TRP:CH2	3:E:875:LEU:O	2.67	0.47
1:B:828:ILE:C	1:B:859:ALA:HB2	2.34	0.47
1:D:828:ILE:C	1:D:859:ALA:HB2	2.34	0.47
1:A:925:ASP:OD2	2:I:1032:ASP:HB3	2.15	0.47
1:D:814:LEU:HD13	1:D:814:LEU:HA	1.74	0.47
3:H:826:ILE:O	3:H:868:LEU:CD1	2.62	0.47
2:J:993:THR:HG1	2:J:1016:TYR:HD1	1.62	0.47
1:C:925:ASP:OD2	2:K:1032:ASP:HB3	2.15	0.47
1:D:918:SER:HB3	2:L:999:TRP:HE1	1.80	0.47
3:G:862:ARG:HE	3:G:879:LEU:CB	2.28	0.47
3:H:720:VAL:C	3:H:721:GLU:HG3	2.35	0.47
1:B:665:LEU:HD23	1:B:672:LEU:HA	1.98	0.46
1:B:868:TYR:HB2	2:J:1003:GLN:HE21	1.80	0.46
1:C:881:ASN:CG	1:C:882:LYS:H	2.19	0.46
1:D:665:LEU:HD23	1:D:672:LEU:HA	1.98	0.46
1:D:716:VAL:CG2	1:D:732:GLU:HB2	2.44	0.46
1:A:828:ILE:C	1:A:859:ALA:HB2	2.34	0.46
2:L:993:THR:HG1	2:L:1016:TYR:HD1	1.63	0.46
3:H:725:ILE:HG13	3:H:750:PHE:CE2	2.50	0.46
1:A:597:ASP:O	1:A:615:LEU:HG	2.15	0.46
1:A:622:TRP:C	1:A:630:LYS:HD3	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ASN:OD1	1:A:885:GLN:NE2	2.48	0.46
1:B:918:SER:HB3	2:J:999:TRP:HE1	1.80	0.46
1:C:828:ILE:C	1:C:859:ALA:HB2	2.34	0.46
1:C:929:ILE:HD12	2:K:1001:TYR:HB3	1.97	0.46
3:F:721:GLU:C	3:F:750:PHE:CZ	2.89	0.46
1:A:714:ILE:O	1:A:734:PHE:HB2	2.16	0.46
1:A:881:ASN:CG	1:A:882:LYS:H	2.19	0.46
1:A:929:ILE:HD12	2:I:1001:TYR:HB3	1.97	0.46
1:B:881:ASN:CG	1:B:882:LYS:H	2.19	0.46
1:C:622:TRP:C	1:C:630:LYS:HD3	2.35	0.46
1:D:597:ASP:O	1:D:615:LEU:HG	2.16	0.46
1:D:868:TYR:HB2	2:L:1003:GLN:HE21	1.81	0.46
1:B:929:ILE:HD12	2:J:1001:TYR:HB3	1.97	0.46
1:C:881:ASN:OD1	1:C:885:GLN:NE2	2.48	0.46
1:D:584:LYS:HB2	2:L:1048:TYR:CE1	2.51	0.46
1:D:881:ASN:CG	1:D:882:LYS:H	2.19	0.46
1:A:868:TYR:HB2	2:I:1003:GLN:HE21	1.80	0.46
1:B:584:LYS:HB2	2:J:1048:TYR:CE1	2.51	0.46
1:B:597:ASP:O	1:B:615:LEU:HG	2.16	0.46
1:C:597:ASP:O	1:C:615:LEU:HG	2.16	0.46
1:C:714:ILE:O	1:C:734:PHE:HB2	2.16	0.46
1:C:855:CYS:SG	1:C:866:TYR:HE1	2.39	0.46
1:C:868:TYR:HB2	2:K:1003:GLN:HE21	1.80	0.46
1:C:918:SER:HB3	2:K:999:TRP:HE1	1.80	0.46
1:D:929:ILE:HD12	2:L:1001:TYR:HB3	1.97	0.46
1:A:855:CYS:SG	1:A:866:TYR:HE1	2.39	0.46
1:B:814:LEU:HD13	1:B:814:LEU:HA	1.75	0.46
1:B:855:CYS:SG	1:B:866:TYR:HE1	2.39	0.46
1:D:855:CYS:SG	1:D:866:TYR:HE1	2.39	0.46
3:F:725:ILE:HG13	3:F:750:PHE:CE2	2.50	0.46
3:H:721:GLU:C	3:H:750:PHE:CZ	2.89	0.46
1:A:665:LEU:HD23	1:A:672:LEU:HA	1.98	0.46
1:A:918:SER:HB3	2:I:999:TRP:HE1	1.80	0.46
1:B:714:ILE:O	1:B:734:PHE:HB2	2.16	0.46
1:C:665:LEU:HD23	1:C:672:LEU:HA	1.98	0.46
1:D:940:ILE:HG23	2:L:1016:TYR:OH	2.16	0.46
3:F:719:LYS:HA	3:F:719:LYS:HD3	1.70	0.46
1:B:940:ILE:HG23	2:J:1016:TYR:OH	2.16	0.46
1:D:714:ILE:O	1:D:734:PHE:HB2	2.15	0.46
1:A:584:LYS:HB2	2:I:1048:TYR:CE1	2.51	0.45
1:C:584:LYS:HB2	2:K:1048:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:LEU:HG	1:D:676:HIS:O	2.17	0.45
3:H:719:LYS:HA	3:H:719:LYS:HD3	1.71	0.45
1:B:662:LEU:HG	1:B:676:HIS:O	2.17	0.45
1:B:790:LYS:O	1:B:830:VAL:HG23	2.16	0.45
1:B:921:VAL:HG22	1:B:922:MET:O	2.16	0.45
1:C:826:PRO:O	1:C:828:ILE:HG13	2.16	0.45
1:D:921:VAL:HG22	1:D:922:MET:O	2.16	0.45
1:B:573:GLU:HG2	2:J:1014:LYS:HB3	1.99	0.45
1:B:881:ASN:OD1	1:B:885:GLN:NE2	2.48	0.45
1:D:573:GLU:HG2	2:L:1014:LYS:HB3	1.99	0.45
1:D:790:LYS:O	1:D:830:VAL:HG23	2.16	0.45
1:D:881:ASN:OD1	1:D:885:GLN:NE2	2.48	0.45
3:E:736:SER:O	3:E:739:ILE:HG22	2.16	0.45
3:F:718:ARG:HG2	3:F:719:LYS:N	2.31	0.45
3:F:720:VAL:C	3:F:721:GLU:HG3	2.35	0.45
1:A:826:PRO:O	1:A:828:ILE:HG13	2.16	0.45
1:B:795:ILE:HG22	1:B:797:MET:HG2	1.99	0.45
2:J:992:GLU:OE2	2:J:994:GLN:NE2	2.40	0.45
1:C:834:SER:OG	1:C:855:CYS:HB3	2.17	0.45
1:D:858:HIS:HE1	1:D:860:VAL:HB	1.81	0.45
1:A:834:SER:OG	1:A:855:CYS:HB3	2.17	0.45
1:B:636:GLU:N	1:B:636:GLU:OE1	2.47	0.45
1:C:790:LYS:O	1:C:830:VAL:HG23	2.16	0.45
1:D:636:GLU:N	1:D:636:GLU:OE1	2.47	0.45
2:L:992:GLU:OE2	2:L:994:GLN:NE2	2.41	0.45
3:F:720:VAL:HG12	3:F:721:GLU:H	1.82	0.45
3:H:853:VAL:HG13	3:H:856:LYS:HB2	1.99	0.45
1:A:573:GLU:HG2	2:I:1014:LYS:HE3	1.98	0.45
1:A:790:LYS:O	1:A:830:VAL:HG23	2.16	0.45
1:A:921:VAL:HG22	1:A:922:MET:O	2.16	0.45
2:I:999:TRP:HA	2:I:1010:SER:HA	1.99	0.45
1:B:758:THR:HG1	1:B:760:SER:HB2	1.81	0.45
3:F:695:PRO:HB3	3:G:699:LEU:HD21	1.98	0.45
3:F:847:SER:HB3	3:F:848:PRO:CD	2.45	0.45
1:B:858:HIS:HE1	1:B:860:VAL:HB	1.81	0.45
1:C:573:GLU:HG2	2:K:1014:LYS:HE3	1.98	0.45
1:C:921:VAL:HG22	1:C:922:MET:O	2.16	0.45
2:K:999:TRP:HA	2:K:1010:SER:HA	1.99	0.45
3:G:736:SER:O	3:G:739:ILE:HG22	2.16	0.45
1:A:858:HIS:HE1	1:A:860:VAL:HB	1.81	0.45
1:A:662:LEU:HG	1:A:676:HIS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ASN:OD1	1:A:898:SER:N	2.50	0.45
1:B:897:ASN:OD1	1:B:898:SER:N	2.50	0.45
1:C:897:ASN:OD1	1:C:898:SER:N	2.50	0.45
1:D:571:HIS:CE1	2:L:1014:LYS:HE2	2.52	0.45
1:D:573:GLU:HG2	2:L:1014:LYS:HE3	1.98	0.45
1:D:795:ILE:HG22	1:D:797:MET:HG2	2.00	0.45
1:D:826:PRO:O	1:D:828:ILE:HG13	2.16	0.45
3:G:815:GLN:HA	3:G:853:VAL:HG21	1.98	0.45
1:A:940:ILE:HG23	2:I:1016:TYR:OH	2.17	0.44
1:B:573:GLU:HG2	2:J:1014:LYS:HE3	1.98	0.44
1:B:826:PRO:O	1:B:828:ILE:HG13	2.16	0.44
1:C:940:ILE:HG23	2:K:1016:TYR:OH	2.16	0.44
1:D:834:SER:OG	1:D:855:CYS:HB3	2.17	0.44
1:D:897:ASN:OD1	1:D:898:SER:N	2.50	0.44
3:F:853:VAL:HG13	3:F:856:LYS:HB2	1.99	0.44
3:H:718:ARG:HG2	3:H:719:LYS:N	2.31	0.44
3:H:720:VAL:HG12	3:H:721:GLU:H	1.82	0.44
1:B:571:HIS:CE1	2:J:1014:LYS:HE2	2.53	0.44
1:C:662:LEU:HG	1:C:676:HIS:O	2.17	0.44
1:B:834:SER:OG	1:B:855:CYS:HB3	2.17	0.44
1:C:858:HIS:HE1	1:C:860:VAL:HB	1.81	0.44
3:E:748:VAL:HG22	3:E:799:LEU:HD23	1.99	0.44
3:G:748:VAL:HG22	3:G:799:LEU:HD23	1.99	0.44
1:A:814:LEU:HD13	1:A:814:LEU:HA	1.74	0.44
1:B:679:HIS:O	1:B:680:CYS:SG	2.74	0.44
2:J:999:TRP:HA	2:J:1010:SER:HA	1.99	0.44
1:D:574:LEU:HG	2:L:1012:SER:O	2.18	0.44
1:D:714:ILE:HD12	1:D:736:LEU:HD22	1.99	0.44
3:E:751:PRO:HA	3:E:754:THR:HG23	1.99	0.44
3:E:815:GLN:HA	3:E:853:VAL:HG21	1.99	0.44
3:F:765:TYR:HA	3:F:768:THR:HG22	2.00	0.44
1:A:573:GLU:HG2	2:I:1014:LYS:HB3	1.98	0.44
1:A:682:PRO:HA	1:A:683:ASN:HA	1.67	0.44
1:B:574:LEU:HG	2:J:1012:SER:O	2.18	0.44
1:C:571:HIS:CE1	2:K:1014:LYS:HE2	2.52	0.44
1:C:573:GLU:HG2	2:K:1014:LYS:HB3	1.98	0.44
1:D:679:HIS:O	1:D:680:CYS:SG	2.74	0.44
2:L:999:TRP:HA	2:L:1010:SER:HA	1.99	0.44
1:B:868:TYR:O	1:B:909:GLU:HA	2.18	0.44
2:K:992:GLU:OE2	2:K:994:GLN:NE2	2.41	0.44
1:D:758:THR:HG1	1:D:760:SER:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:855:GLU:O	3:F:859:MET:HG3	2.18	0.44
1:A:714:ILE:HD12	1:A:736:LEU:HD22	1.99	0.44
2:I:992:GLU:OE2	2:I:994:GLN:NE2	2.41	0.44
1:B:802:PHE:HB3	1:B:833:PHE:CZ	2.52	0.44
1:C:682:PRO:HA	1:C:683:ASN:HA	1.66	0.44
1:C:714:ILE:HD12	1:C:736:LEU:HD22	1.99	0.44
1:D:868:TYR:O	1:D:909:GLU:HA	2.18	0.44
1:A:571:HIS:CE1	2:I:1014:LYS:HE2	2.53	0.43
1:A:665:LEU:CD2	1:A:672:LEU:HA	2.48	0.43
1:B:709:GLU:OE1	1:B:713:GLU:HB3	2.18	0.43
1:B:714:ILE:HD12	1:B:736:LEU:HD22	1.99	0.43
1:D:709:GLU:OE1	1:D:713:GLU:HB3	2.18	0.43
1:D:802:PHE:HB3	1:D:833:PHE:CZ	2.52	0.43
3:F:811:LYS:HD3	3:F:844:ILE:CG2	2.43	0.43
3:H:765:TYR:HA	3:H:768:THR:HG22	2.00	0.43
3:H:855:GLU:O	3:H:859:MET:HG3	2.18	0.43
1:A:795:ILE:HG22	1:A:797:MET:HG2	1.99	0.43
1:C:665:LEU:CD2	1:C:672:LEU:HA	2.48	0.43
3:G:751:PRO:HA	3:G:754:THR:HG23	1.99	0.43
3:H:786:ASN:HB3	3:H:789:LYS:HG3	2.00	0.43
1:C:802:PHE:HB3	1:C:833:PHE:CZ	2.52	0.43
1:C:814:LEU:HD13	1:C:814:LEU:HA	1.74	0.43
1:C:660:ASP:OD1	1:C:661:THR:N	2.52	0.43
1:B:934:ARG:HB3	2:J:996:TRP:CZ3	2.54	0.43
1:C:610:PHE:HB2	1:C:624:LEU:HD21	2.00	0.43
1:C:795:ILE:HG22	1:C:797:MET:HG2	1.99	0.43
1:D:934:ARG:HB3	2:L:996:TRP:CZ3	2.54	0.43
3:F:711:LEU:CD1	3:F:720:VAL:CG1	2.87	0.43
3:G:789:LYS:HD3	3:G:789:LYS:HA	1.85	0.43
1:A:802:PHE:HB3	1:A:833:PHE:CZ	2.52	0.43
1:B:639:PRO:HG2	1:B:642:LEU:HD21	2.01	0.43
1:C:868:TYR:O	1:C:909:GLU:HA	2.18	0.43
1:D:610:PHE:HB2	1:D:624:LEU:HD21	2.01	0.43
1:A:615:LEU:HD13	3:G:859:MET:CE	2.48	0.43
1:A:660:ASP:OD1	1:A:661:THR:N	2.52	0.43
1:A:868:TYR:O	1:A:909:GLU:HA	2.18	0.43
1:B:610:PHE:HB2	1:B:624:LEU:HD21	2.01	0.43
1:B:660:ASP:OD1	1:B:661:THR:N	2.52	0.43
1:C:709:GLU:OE1	1:C:713:GLU:HB3	2.18	0.43
1:D:639:PRO:HG2	1:D:642:LEU:HD21	2.01	0.43
1:D:660:ASP:OD1	1:D:661:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:PHE:HB2	1:A:624:LEU:HD21	2.01	0.43
1:A:709:GLU:OE1	1:A:713:GLU:HB3	2.18	0.43
1:B:665:LEU:CD2	1:B:672:LEU:HA	2.48	0.43
1:B:838:SER:O	1:B:849:VAL:HB	2.19	0.43
1:C:574:LEU:HG	2:K:1012:SER:O	2.18	0.43
1:C:694:THR:O	1:C:695:HIS:HB3	2.19	0.43
3:F:753:ASN:O	3:F:757:SER:OG	2.29	0.43
1:A:574:LEU:HG	2:I:1012:SER:O	2.18	0.43
1:A:888:ASN:OD1	1:A:890:VAL:HG23	2.19	0.43
1:B:882:LYS:N	1:B:885:GLN:NE2	2.65	0.43
1:C:621:VAL:CG2	1:C:631:LEU:HB3	2.49	0.43
3:E:861:VAL:CG1	3:E:865:ILE:CD1	2.96	0.43
1:A:694:THR:O	1:A:695:HIS:HB3	2.19	0.43
1:A:869:TYR:OH	1:A:909:GLU:HB3	2.19	0.43
1:B:694:THR:O	1:B:695:HIS:HB3	2.19	0.43
1:C:934:ARG:HB3	2:K:996:TRP:CZ3	2.54	0.43
1:D:838:SER:O	1:D:849:VAL:HB	2.19	0.43
1:A:690:TRP:HZ3	1:A:703:PHE:CG	2.37	0.42
1:A:818:GLU:HG2	1:A:819:LEU:O	2.20	0.42
2:I:993:THR:HG1	2:I:1016:TYR:HD1	1.64	0.42
1:B:690:TRP:HZ3	1:B:703:PHE:CG	2.37	0.42
1:C:741:ILE:HG13	1:C:759:GLU:HA	2.01	0.42
1:C:818:GLU:HG2	1:C:819:LEU:O	2.20	0.42
1:C:869:TYR:OH	1:C:909:GLU:HB3	2.19	0.42
1:C:888:ASN:OD1	1:C:890:VAL:HG23	2.19	0.42
2:K:992:GLU:O	2:K:1018:SER:N	2.48	0.42
1:D:665:LEU:CD2	1:D:672:LEU:HA	2.49	0.42
1:D:682:PRO:HA	1:D:683:ASN:HA	1.67	0.42
1:D:690:TRP:HZ3	1:D:703:PHE:CG	2.37	0.42
3:F:714:GLU:HB3	3:F:718:ARG:NH1	2.34	0.42
1:A:621:VAL:CG2	1:A:631:LEU:HB3	2.50	0.42
1:A:934:ARG:HB3	2:I:996:TRP:CZ3	2.54	0.42
1:B:571:HIS:O	2:J:1014:LYS:NZ	2.47	0.42
1:B:741:ILE:HG13	1:B:759:GLU:HA	2.01	0.42
1:B:888:ASN:OD1	1:B:890:VAL:HG23	2.19	0.42
1:C:723:ILE:HD12	1:C:723:ILE:H	1.84	0.42
1:D:694:THR:O	1:D:695:HIS:HB3	2.19	0.42
1:D:869:TYR:OH	1:D:909:GLU:HB3	2.19	0.42
3:F:732:CYS:HB2	3:F:739:ILE:HD13	2.01	0.42
1:A:723:ILE:H	1:A:723:ILE:HD12	1.85	0.42
1:A:741:ILE:HG13	1:A:759:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PRO:HA	1:B:683:ASN:HA	1.67	0.42
1:B:758:THR:OG1	1:B:761:GLY:N	2.51	0.42
1:C:690:TRP:HZ3	1:C:703:PHE:CG	2.37	0.42
1:D:621:VAL:CG2	1:D:631:LEU:HB3	2.49	0.42
1:D:882:LYS:N	1:D:885:GLN:NE2	2.65	0.42
1:A:758:THR:OG1	1:A:761:GLY:N	2.51	0.42
2:I:992:GLU:O	2:I:1018:SER:N	2.48	0.42
1:C:758:THR:OG1	1:C:761:GLY:N	2.51	0.42
1:D:758:THR:OG1	1:D:761:GLY:N	2.51	0.42
1:D:888:ASN:OD1	1:D:890:VAL:HG23	2.19	0.42
3:F:873:LEU:O	3:F:877:ARG:N	2.49	0.42
3:H:753:ASN:O	3:H:757:SER:OG	2.29	0.42
1:A:780:GLN:HG3	1:A:785:LEU:CD2	2.50	0.42
1:B:780:GLN:HG3	1:B:785:LEU:CD2	2.50	0.42
1:B:799:ASP:O	1:B:814:LEU:HD23	2.20	0.42
1:B:813:ASP:HB3	1:B:818:GLU:N	2.33	0.42
1:B:869:TYR:OH	1:B:909:GLU:HB3	2.19	0.42
1:C:780:GLN:HG3	1:C:785:LEU:CD2	2.49	0.42
1:D:571:HIS:O	2:L:1014:LYS:NZ	2.47	0.42
1:D:723:ILE:HD12	1:D:723:ILE:H	1.85	0.42
1:D:741:ILE:HG13	1:D:759:GLU:HA	2.01	0.42
1:D:799:ASP:O	1:D:814:LEU:HD23	2.20	0.42
1:D:853:SER:HB2	1:D:926:GLY:HA3	2.02	0.42
3:E:789:LYS:HD3	3:E:789:LYS:HA	1.85	0.42
3:H:714:GLU:HB3	3:H:718:ARG:NH1	2.34	0.42
1:B:621:VAL:CG2	1:B:631:LEU:HB3	2.49	0.42
1:B:723:ILE:HD12	1:B:723:ILE:H	1.85	0.42
1:B:853:SER:HB2	1:B:926:GLY:HA3	2.02	0.42
1:D:780:GLN:HG3	1:D:785:LEU:CD2	2.50	0.42
3:E:860:TYR:CD1	3:E:864:ALA:CB	3.03	0.42
3:H:732:CYS:HB2	3:H:739:ILE:HD13	2.01	0.42
3:H:711:LEU:CD1	3:H:720:VAL:CG1	2.87	0.42
1:A:882:LYS:N	1:A:885:GLN:NE2	2.65	0.42
1:D:843:VAL:O	1:D:846:GLN:N	2.52	0.42
3:E:695:PRO:CB	3:H:702:TRP:HH2	2.12	0.42
3:E:748:VAL:HG23	3:E:796:CYS:SG	2.60	0.42
3:H:715:SER:HB2	3:H:720:VAL:CG2	2.45	0.42
3:H:862:ARG:C	3:H:864:ALA:N	2.72	0.42
1:A:838:SER:O	1:A:849:VAL:HB	2.19	0.42
1:B:843:VAL:O	1:B:846:GLN:N	2.52	0.42
1:C:706:VAL:HG22	1:C:716:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:LYS:N	1:C:885:GLN:NE2	2.65	0.42
1:D:813:ASP:HB3	1:D:818:GLU:N	2.33	0.42
1:D:934:ARG:HG3	1:D:934:ARG:O	2.20	0.42
1:A:698:ASP:O	1:A:723:ILE:HD11	2.20	0.42
1:C:639:PRO:HG2	1:C:642:LEU:HD21	2.01	0.42
1:C:679:HIS:O	1:C:680:CYS:SG	2.74	0.42
1:D:856:PHE:HZ	1:D:867:TYR:CE2	2.38	0.42
1:A:588:GLU:O	2:I:1045:LEU:HB2	2.20	0.41
1:A:639:PRO:HG2	1:A:642:LEU:HD21	2.01	0.41
1:A:661:THR:HG23	1:A:676:HIS:C	2.40	0.41
1:B:698:ASP:O	1:B:723:ILE:HD11	2.20	0.41
1:B:934:ARG:HG3	1:B:934:ARG:O	2.20	0.41
1:C:661:THR:HG23	1:C:676:HIS:C	2.40	0.41
1:C:698:ASP:O	1:C:723:ILE:HD11	2.20	0.41
2:K:993:THR:HG1	2:K:1016:TYR:HD1	1.65	0.41
1:D:698:ASP:O	1:D:723:ILE:HD11	2.20	0.41
3:F:715:SER:HB2	3:F:720:VAL:CG2	2.45	0.41
3:F:865:ILE:H	3:F:865:ILE:HG13	1.53	0.41
3:H:693:LEU:N	3:H:693:LEU:CD1	2.79	0.41
1:A:679:HIS:O	1:A:680:CYS:SG	2.74	0.41
1:A:706:VAL:HG22	1:A:716:VAL:HG12	2.02	0.41
1:B:573:GLU:C	1:B:574:LEU:HD12	2.41	0.41
1:B:774:SER:HA	1:B:775:PRO:HD2	1.83	0.41
1:B:856:PHE:HZ	1:B:867:TYR:CE2	2.38	0.41
1:C:838:SER:O	1:C:849:VAL:HB	2.19	0.41
1:D:573:GLU:C	1:D:574:LEU:HD12	2.41	0.41
3:G:748:VAL:HG23	3:G:796:CYS:SG	2.60	0.41
3:H:847:SER:HB3	3:H:848:PRO:CD	2.46	0.41
1:A:573:GLU:C	1:A:574:LEU:HD12	2.41	0.41
1:A:853:SER:HB2	1:A:926:GLY:HA3	2.02	0.41
2:I:996:TRP:HB2	2:I:1013:LEU:O	2.20	0.41
1:C:588:GLU:O	2:K:1045:LEU:HB2	2.21	0.41
2:K:996:TRP:HB2	2:K:1013:LEU:O	2.20	0.41
1:D:650:GLN:HB3	1:D:652:ASN:OD1	2.20	0.41
1:D:661:THR:HG23	1:D:676:HIS:C	2.40	0.41
3:H:725:ILE:HG13	3:H:750:PHE:HE2	1.85	0.41
1:B:650:GLN:HB3	1:B:652:ASN:OD1	2.20	0.41
1:C:573:GLU:C	1:C:574:LEU:HD12	2.41	0.41
1:C:853:SER:HB2	1:C:926:GLY:HA3	2.02	0.41
1:D:588:GLU:O	2:L:1045:LEU:HB2	2.21	0.41
1:D:774:SER:HA	1:D:775:PRO:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:818:GLU:HG2	1:D:819:LEU:O	2.20	0.41
3:F:693:LEU:N	3:F:693:LEU:CD1	2.79	0.41
1:A:934:ARG:O	1:A:934:ARG:HG3	2.20	0.41
1:B:588:GLU:O	2:J:1045:LEU:HB2	2.21	0.41
1:B:818:GLU:HG2	1:B:819:LEU:O	2.20	0.41
1:C:666:ASN:ND2	1:C:669:SER:HB2	2.36	0.41
1:C:934:ARG:O	1:C:934:ARG:HG3	2.20	0.41
1:A:799:ASP:O	1:A:814:LEU:HD23	2.20	0.41
1:A:843:VAL:O	1:A:846:GLN:N	2.52	0.41
1:B:661:THR:HG23	1:B:676:HIS:C	2.40	0.41
1:C:615:LEU:CD1	3:E:859:MET:HE3	2.44	0.41
1:D:631:LEU:HD21	1:D:633:LEU:HG	2.02	0.41
3:H:715:SER:HA	3:H:720:VAL:HG23	1.93	0.41
1:A:615:LEU:HD13	3:G:859:MET:HE3	2.02	0.41
1:A:666:ASN:ND2	1:A:669:SER:HB2	2.36	0.41
1:C:799:ASP:O	1:C:814:LEU:HD23	2.20	0.41
1:C:843:VAL:O	1:C:846:GLN:N	2.52	0.41
3:H:765:TYR:O	3:H:768:THR:HG22	2.21	0.41
3:H:801:LEU:HD22	3:H:806:TYR:CD2	2.56	0.41
1:A:650:GLN:HB3	1:A:652:ASN:OD1	2.20	0.41
1:A:856:PHE:HZ	1:A:867:TYR:CE2	2.38	0.41
1:C:650:GLN:HB3	1:C:652:ASN:OD1	2.20	0.41
1:D:577:ASP:CG	2:L:1011:LYS:HZ3	2.24	0.41
3:E:694:SER:O	3:E:698:VAL:HG23	2.21	0.41
3:F:725:ILE:HG13	3:F:750:PHE:HE2	1.85	0.41
3:F:871:GLN:HA	3:F:872:ASP:HA	1.71	0.41
3:H:826:ILE:HG22	3:H:868:LEU:HD12	2.03	0.41
1:A:584:LYS:HD2	2:I:1049:GLY:HA2	2.02	0.41
1:B:631:LEU:HD21	1:B:633:LEU:HG	2.03	0.41
1:C:573:GLU:O	1:C:574:LEU:HD12	2.21	0.41
3:E:705:ALA:HB2	3:E:738:ILE:HG12	2.02	0.41
3:F:715:SER:HA	3:F:720:VAL:HG23	1.93	0.41
1:B:869:TYR:CD1	1:B:907:LEU:HB3	2.55	0.40
1:C:584:LYS:HD2	2:K:1049:GLY:HA2	2.03	0.40
2:L:1041:ASN:OD1	2:L:1042:TYR:CD2	2.75	0.40
3:F:722:ILE:CG2	3:F:746:LYS:HD2	2.52	0.40
3:F:765:TYR:O	3:F:768:THR:HG22	2.21	0.40
3:F:801:LEU:HD22	3:F:806:TYR:CD2	2.57	0.40
1:A:573:GLU:O	1:A:574:LEU:HD12	2.21	0.40
1:A:823:PHE:HE1	1:A:904:PHE:CD1	2.39	0.40
1:B:854:PHE:O	1:B:866:TYR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1041:ASN:OD1	2:J:1042:TYR:CD2	2.75	0.40
1:C:571:HIS:O	2:K:1014:LYS:NZ	2.46	0.40
1:C:856:PHE:HZ	1:C:867:TYR:CE2	2.39	0.40
1:D:706:VAL:HG22	1:D:716:VAL:HG12	2.02	0.40
2:L:996:TRP:HB2	2:L:1013:LEU:O	2.20	0.40
3:F:758:LEU:HD21	3:F:762:LEU:HD11	2.01	0.40
3:F:792:THR:O	3:F:796:CYS:HB2	2.21	0.40
3:H:722:ILE:CG2	3:H:746:LYS:HD2	2.52	0.40
3:H:766:LYS:HA	3:H:766:LYS:HD3	1.91	0.40
3:H:792:THR:O	3:H:796:CYS:HB2	2.21	0.40
1:B:570:ASP:HB2	2:J:1016:TYR:HD2	1.86	0.40
1:B:706:VAL:HG22	1:B:716:VAL:HG12	2.02	0.40
1:C:609:THR:HG23	1:C:630:LYS:NZ	2.37	0.40
1:C:823:PHE:HE1	1:C:904:PHE:CD1	2.39	0.40
3:E:713:MET:HE3	3:E:867:THR:CB	2.40	0.40
2:I:1041:ASN:OD1	2:I:1042:TYR:CD2	2.74	0.40
2:J:996:TRP:HB2	2:J:1013:LEU:O	2.20	0.40
1:D:854:PHE:O	1:D:866:TYR:HA	2.21	0.40
3:E:733:PRO:CG	3:E:736:SER:OG	2.68	0.40
1:A:609:THR:HG23	1:A:630:LYS:NZ	2.37	0.40
1:A:631:LEU:HD21	1:A:633:LEU:HG	2.03	0.40
1:B:573:GLU:O	1:B:574:LEU:HD12	2.21	0.40
1:B:823:PHE:HE1	1:B:904:PHE:CD1	2.39	0.40
2:J:992:GLU:O	2:J:1018:SER:N	2.48	0.40
1:C:631:LEU:HD21	1:C:633:LEU:HG	2.03	0.40
2:K:1041:ASN:OD1	2:K:1042:TYR:CD2	2.74	0.40
1:D:573:GLU:O	1:D:574:LEU:HD12	2.21	0.40
1:D:823:PHE:HE1	1:D:904:PHE:CD1	2.39	0.40
1:D:869:TYR:CD1	1:D:907:LEU:HB3	2.56	0.40
3:G:821:ASP:HB3	3:G:822:SER:H	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	12	46
1	B	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	12	46
1	C	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	12	46
1	D	374/396 (94%)	335 (90%)	35 (9%)	4 (1%)	12	46
2	I	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
2	J	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
2	K	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
2	L	60/103 (58%)	56 (93%)	4 (7%)	0	100	100
3	E	183/272 (67%)	163 (89%)	16 (9%)	4 (2%)	5	28
3	F	187/272 (69%)	165 (88%)	16 (9%)	6 (3%)	3	21
3	G	181/272 (66%)	160 (88%)	15 (8%)	6 (3%)	3	20
3	H	187/272 (69%)	165 (88%)	14 (8%)	8 (4%)	2	17
All	All	2474/3084 (80%)	2217 (90%)	217 (9%)	40 (2%)	10	37

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	696	LYS
1	B	696	LYS
1	C	696	LYS
1	D	696	LYS
3	E	734	LYS
3	E	826	ILE
3	F	694	SER
3	F	821	ASP
3	F	850	GLU
3	G	734	LYS
3	G	826	ILE
3	G	865	ILE
3	H	694	SER
3	H	821	ASP
3	H	850	GLU
3	H	862	ARG
1	A	817	ASP
1	B	817	ASP
1	C	817	ASP

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Mol	Chain	Res	Type
1	D	817	ASP
3	E	870	ILE
3	F	807	GLY
3	F	866	GLY
3	H	807	GLY
3	H	863	THR
1	A	815	LYS
1	A	908	GLN
1	B	815	LYS
1	B	908	GLN
1	C	815	LYS
1	C	908	GLN
1	D	908	GLN
1	D	815	LYS
3	F	825	ASP
3	H	825	ASP
3	E	843	PRO
3	G	843	PRO
3	G	863	THR
3	G	870	ILE
3	H	870	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/364 (94%)	340 (99%)	2 (1%)	84	88
1	B	342/364 (94%)	340 (99%)	2 (1%)	84	88
1	C	341/364 (94%)	339 (99%)	2 (1%)	84	88
1	D	342/364 (94%)	340 (99%)	2 (1%)	84	88
2	I	54/90 (60%)	54 (100%)	0	100	100
2	J	54/90 (60%)	54 (100%)	0	100	100
2	K	54/90 (60%)	54 (100%)	0	100	100
2	L	54/90 (60%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	147/246 (60%)	143 (97%)	4 (3%)	40 59
3	F	147/246 (60%)	134 (91%)	13 (9%)	8 25
3	G	146/246 (59%)	142 (97%)	4 (3%)	40 59
3	H	148/246 (60%)	136 (92%)	12 (8%)	9 29
All	All	2171/2800 (78%)	2130 (98%)	41 (2%)	52 69

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	599	LEU
1	A	819	LEU
1	B	599	LEU
1	B	819	LEU
1	C	599	LEU
1	C	819	LEU
1	D	599	LEU
1	D	819	LEU
3	E	707	LEU
3	E	732	CYS
3	E	808	ASP
3	E	825	ASP
3	F	693	LEU
3	F	718	ARG
3	F	720	VAL
3	F	721	GLU
3	F	731	LEU
3	F	740	ARG
3	F	821	ASP
3	F	825	ASP
3	F	849	LYS
3	F	854	VAL
3	F	856	LYS
3	F	857	MET
3	F	865	ILE
3	G	707	LEU
3	G	732	CYS
3	G	808	ASP
3	G	825	ASP
3	H	693	LEU
3	H	718	ARG
3	H	720	VAL

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Mol	Chain	Res	Type
3	H	721	GLU
3	H	731	LEU
3	H	740	ARG
3	H	821	ASP
3	H	825	ASP
3	H	849	LYS
3	H	854	VAL
3	H	856	LYS
3	H	857	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	844	ASN
1	A	885	GLN
2	I	1003	GLN
1	B	844	ASN
1	B	885	GLN
2	J	1003	GLN
1	C	844	ASN
1	C	885	GLN
2	K	1003	GLN
1	D	844	ASN
1	D	885	GLN
2	L	1003	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

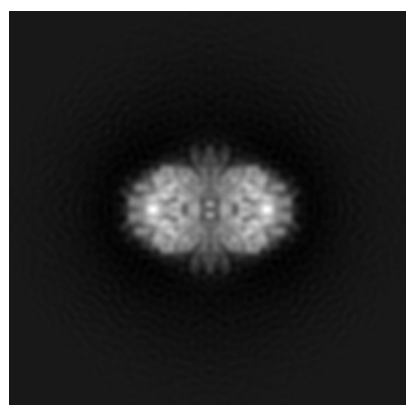
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9537. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

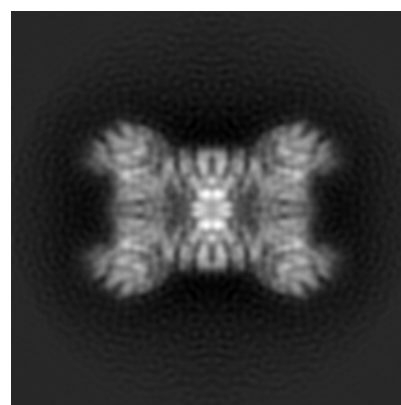
6.1.1 Primary map



X



Y



Z

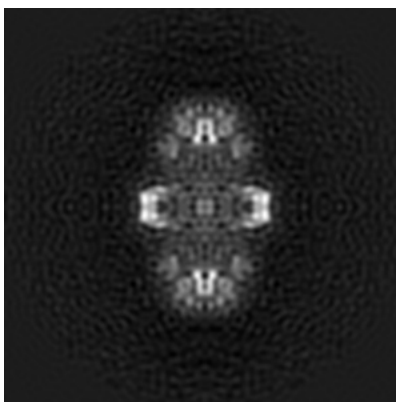
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

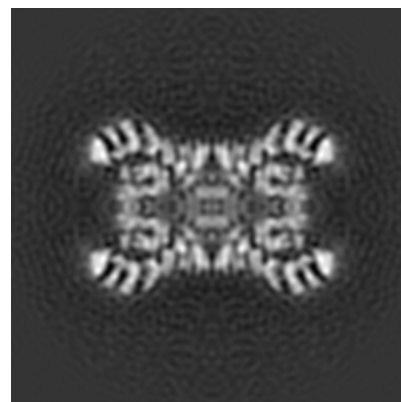
6.2.1 Primary map



X Index: 100



Y Index: 100

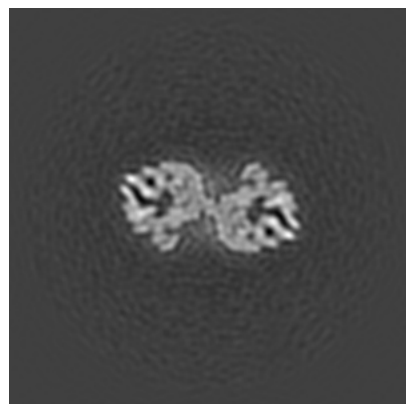


Z Index: 100

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

6.3 Largest variance slices [i](#)

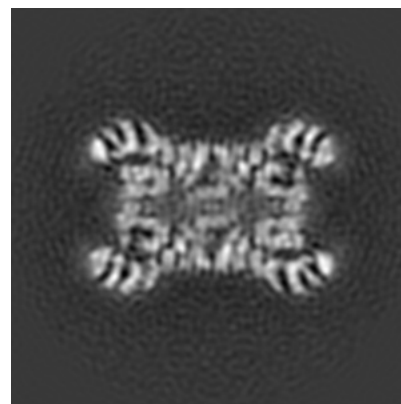
6.3.1 Primary map



X Index: 142



Y Index: 124

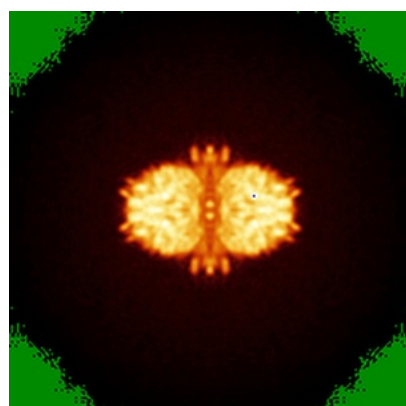


Z Index: 99

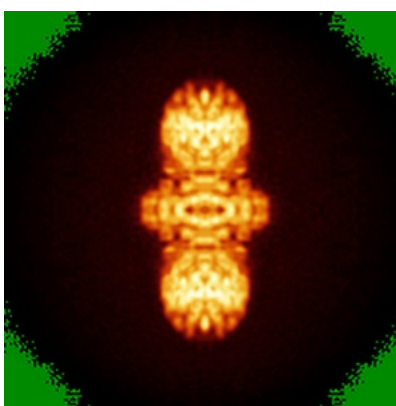
The images above show the largest variance slices of the map in three orthogonal directions.

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

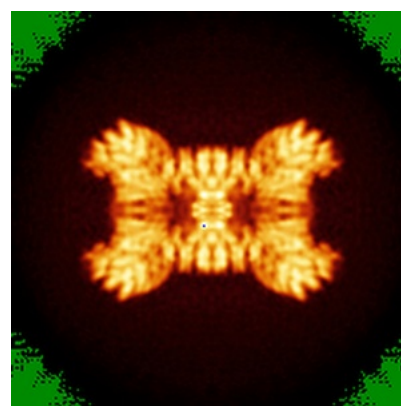
6.4.1 Primary map



X



Y

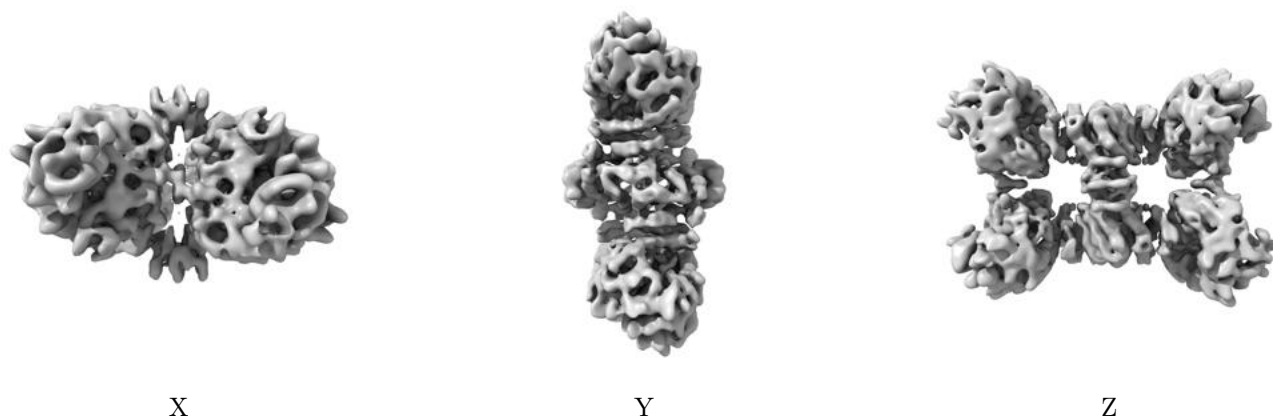


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

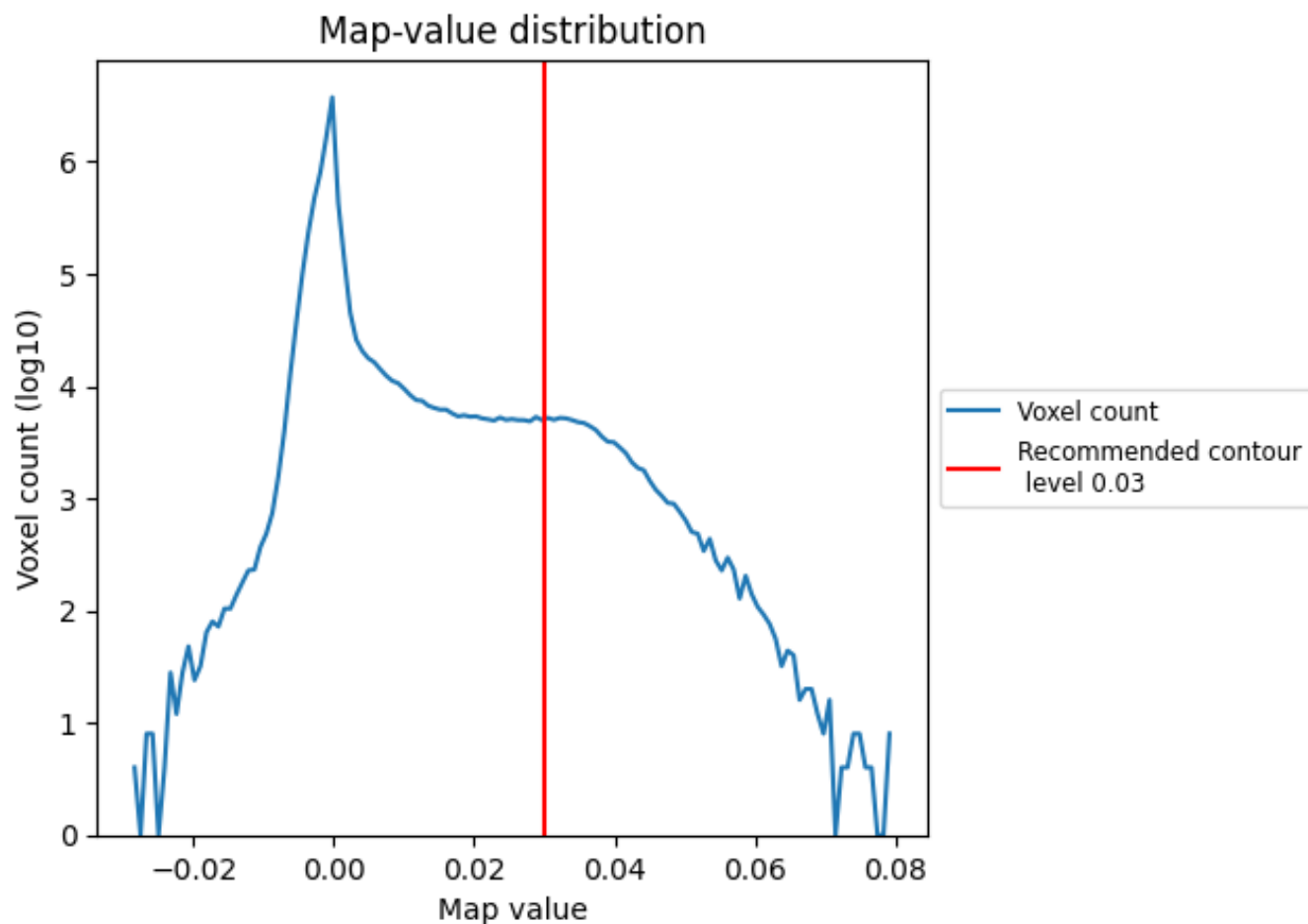
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

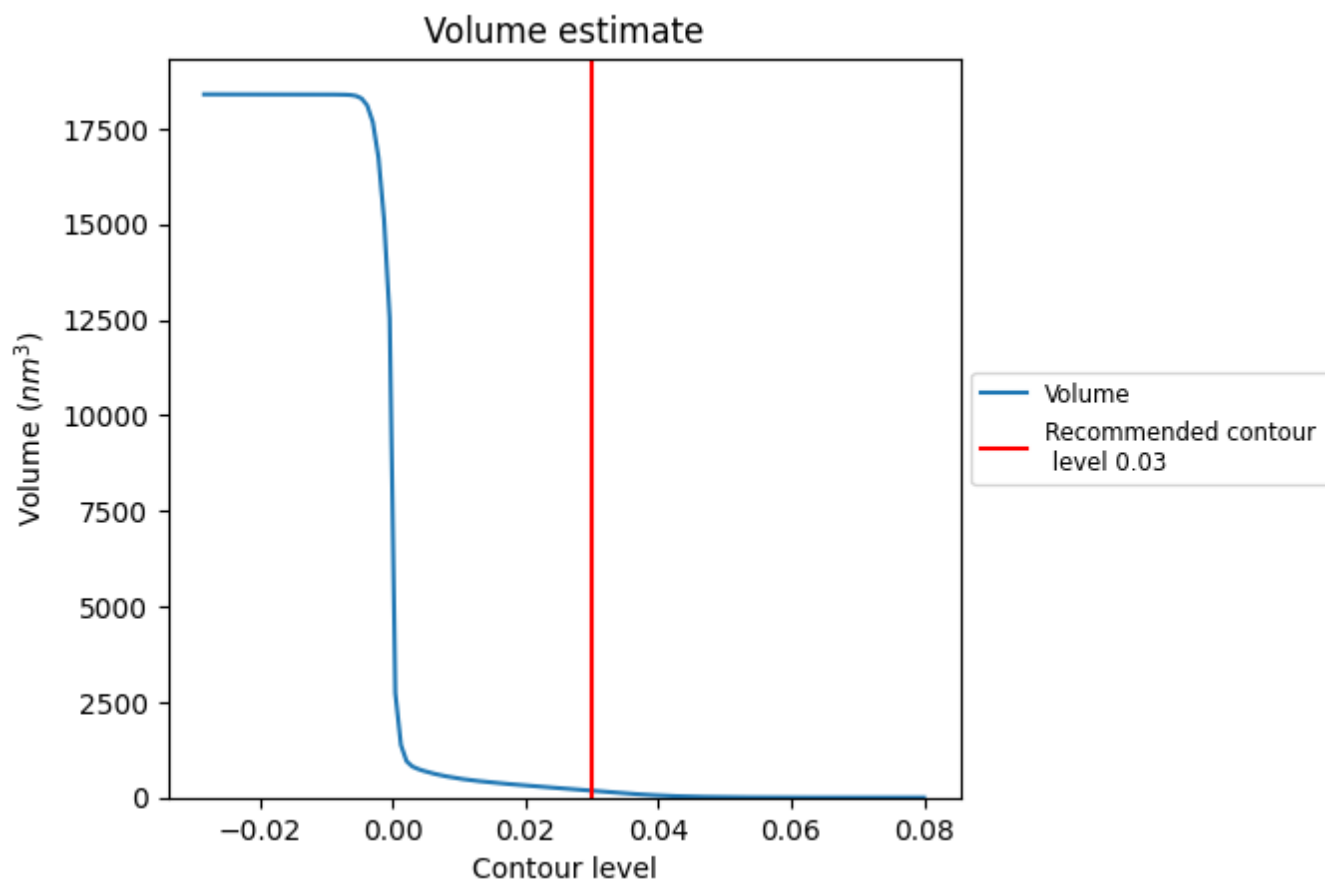
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

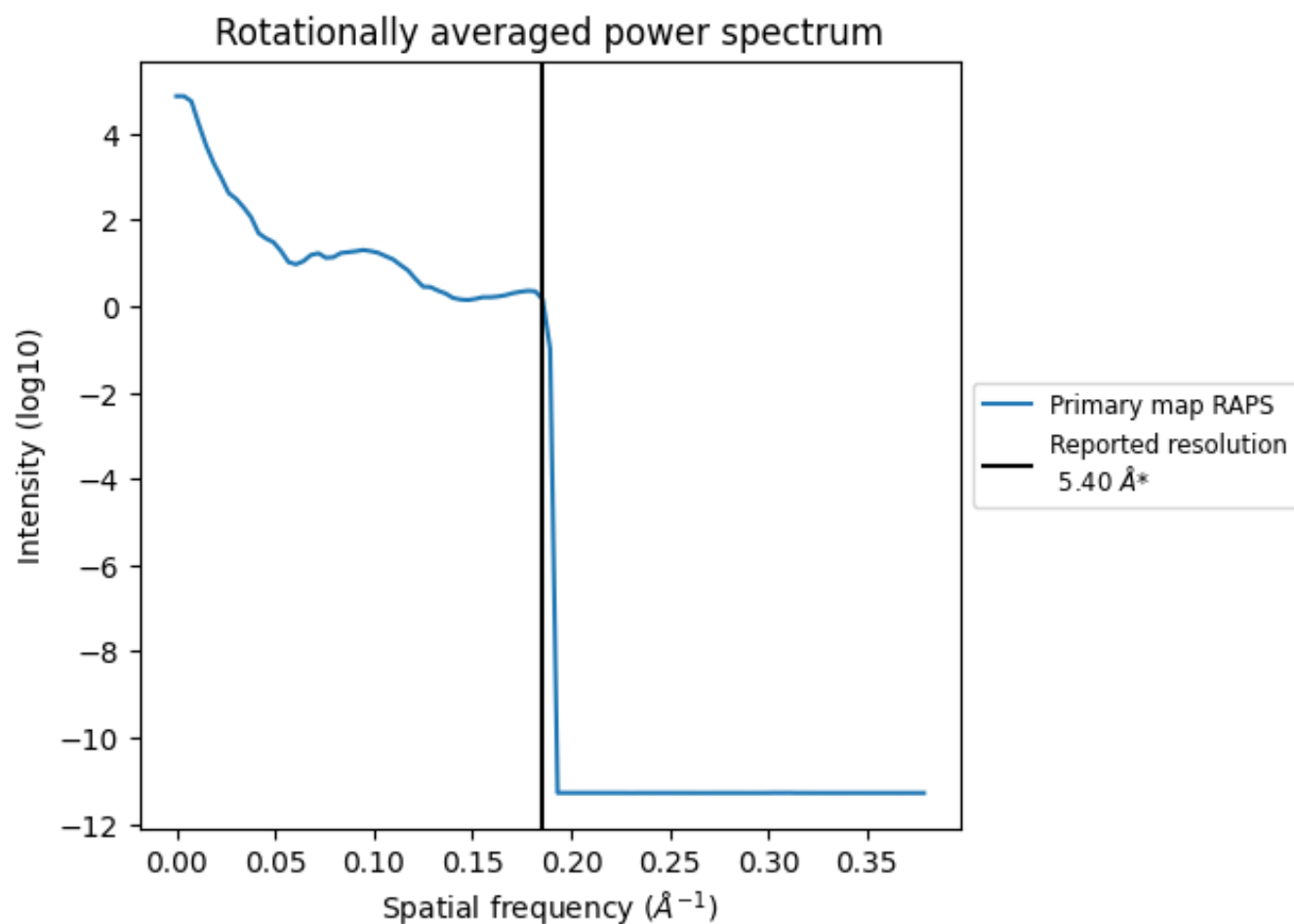
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 162 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

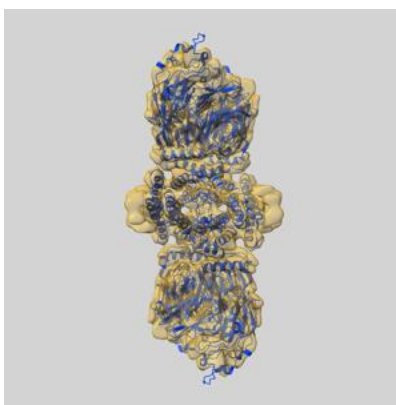
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9537 and PDB model 5GRS. Per-residue inclusion information can be found in section 3 on page 7.

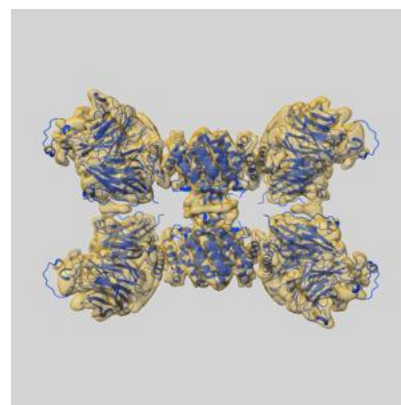
9.1 Map-model overlay [i](#)



X



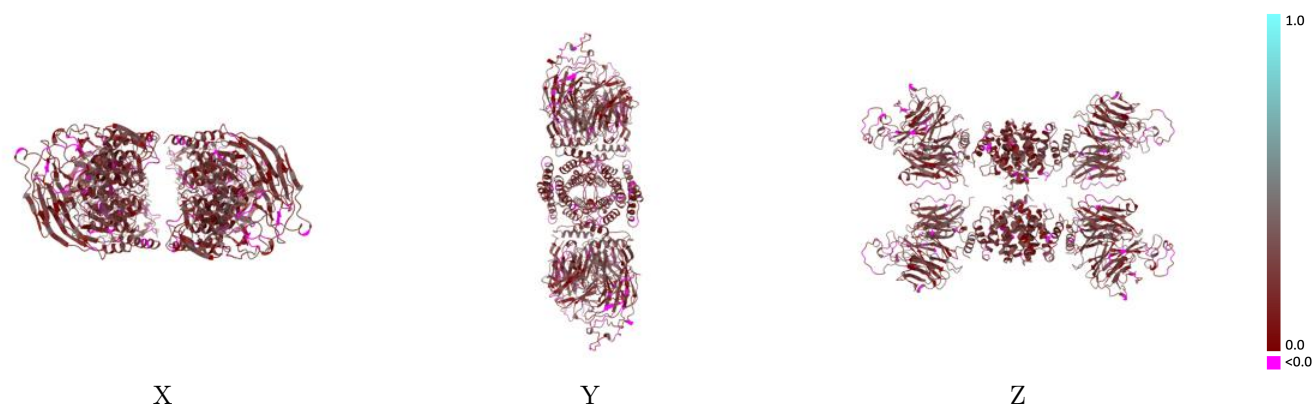
Y



Z

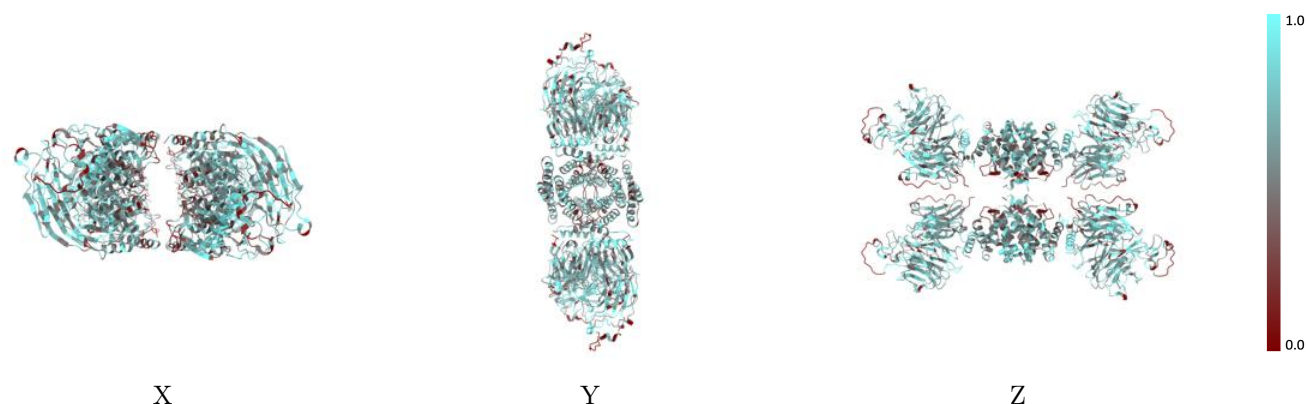
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



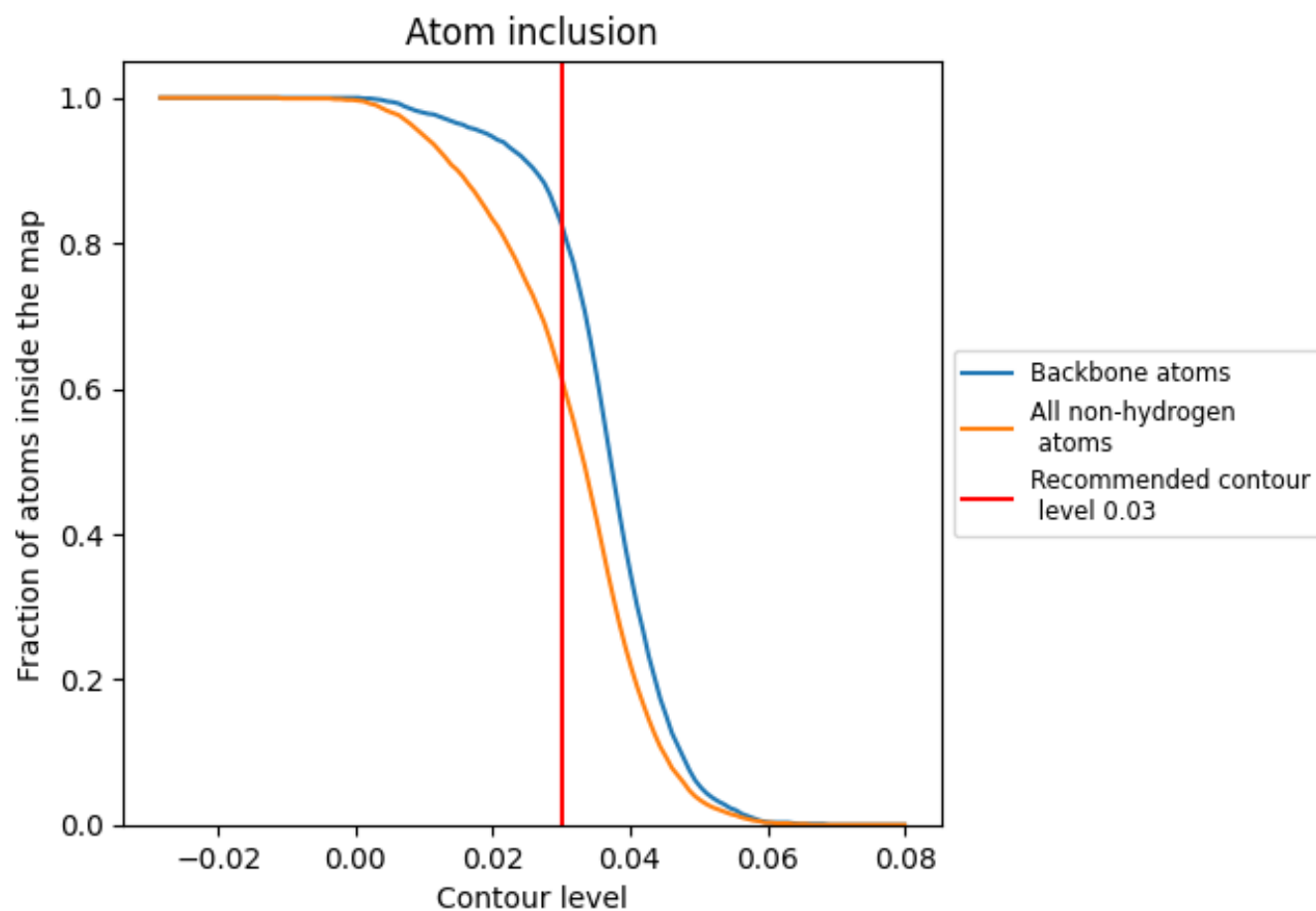
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 62% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6150	<div></div> 0.2020
A	<div></div> 0.6260	<div></div> 0.2090
B	<div></div> 0.6220	<div></div> 0.2110
C	<div></div> 0.6230	<div></div> 0.2100
D	<div></div> 0.6280	<div></div> 0.2110
E	<div></div> 0.5780	<div></div> 0.1720
F	<div></div> 0.5940	<div></div> 0.1800
G	<div></div> 0.5740	<div></div> 0.1750
H	<div></div> 0.5970	<div></div> 0.1870
I	<div></div> 0.6410	<div></div> 0.2220
J	<div></div> 0.6450	<div></div> 0.2180
K	<div></div> 0.6470	<div></div> 0.2200
L	<div></div> 0.6410	<div></div> 0.2220

1.0

0.0

<0.0