Full wwPDB EM Validation Report

Aug 19, 2026 – 10:26 pm BST

PDB ID	:	9SQY / pdb_00009sqy
EMDB ID	:	EMD-55122
Title	:	Cryo-EM structure of the ARISC(E33A)-RAP80:K63-Ub7 complex (Composite map)
Authors	:	Foglizzo, M.; Zeqiraj, E.
Deposited on	:	2025-09-23
Resolution	:	2.92 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:

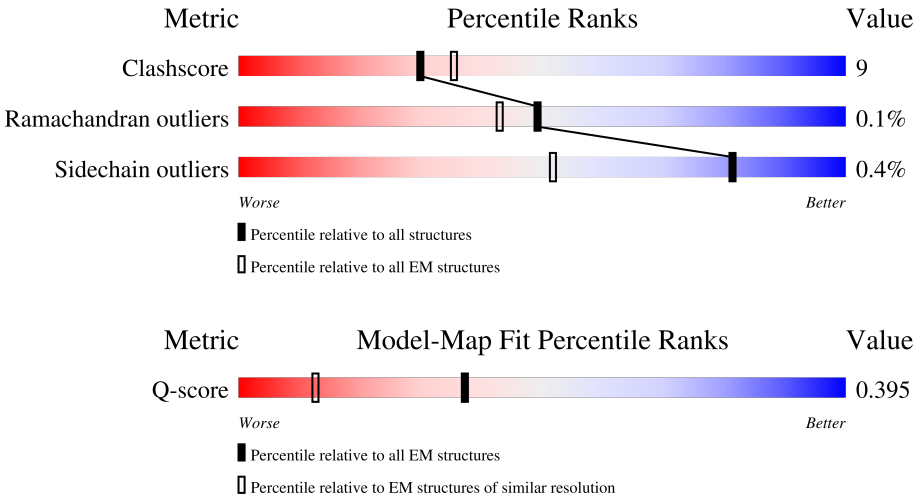
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.92 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.



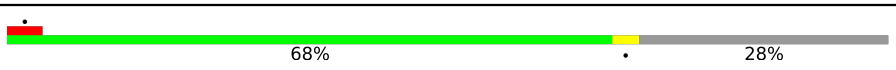
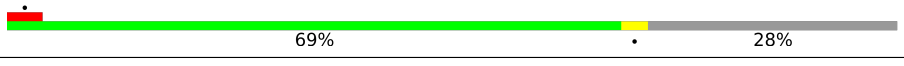
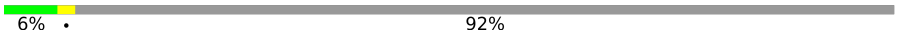
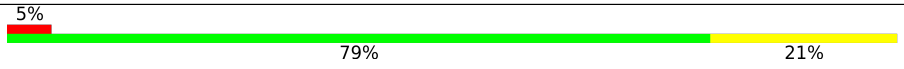
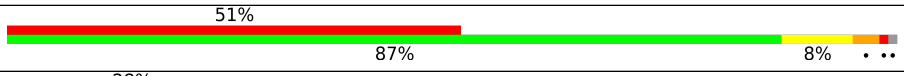
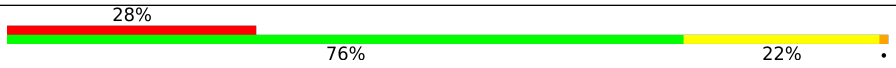
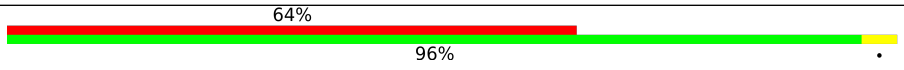
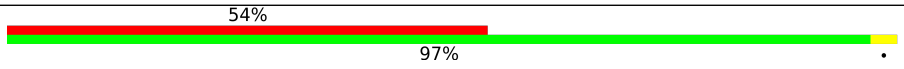
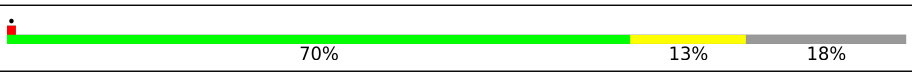
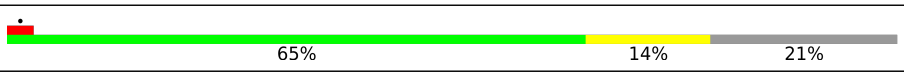
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 (2.42 - 3.42)

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	C	446	61% 9% 30%
1	D	446	6% 67% 7% 26%
2	E	385	80% 19%
2	F	385	78% 21%

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Mol	Chain	Length	Quality of chain
3	G	329	
3	H	329	
4	I	724	
4	J	724	
5	K	76	
5	L	76	
5	M	76	
5	N	76	
5	O	76	
5	P	76	
6	A	316	
6	B	316	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23659 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 BRCA1-A complex subunit Abraxas 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	329	Total	C	N	O	S	0	0
			2639	1657	462	506	14		
1	C	310	Total	C	N	O	S	0	0
			2494	1575	438	468	13		

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-36	MET	-	initiating methionine	UNP Q6UWZ7
D	-35	TRP	-	expression tag	UNP Q6UWZ7
D	-34	SER	-	expression tag	UNP Q6UWZ7
D	-33	HIS	-	expression tag	UNP Q6UWZ7
D	-32	PRO	-	expression tag	UNP Q6UWZ7
D	-31	GLN	-	expression tag	UNP Q6UWZ7
D	-30	PHE	-	expression tag	UNP Q6UWZ7
D	-29	GLU	-	expression tag	UNP Q6UWZ7
D	-28	LYS	-	expression tag	UNP Q6UWZ7
D	-27	GLY	-	expression tag	UNP Q6UWZ7
D	-26	GLY	-	expression tag	UNP Q6UWZ7
D	-25	GLY	-	expression tag	UNP Q6UWZ7
D	-24	SER	-	expression tag	UNP Q6UWZ7
D	-23	GLY	-	expression tag	UNP Q6UWZ7
D	-22	GLY	-	expression tag	UNP Q6UWZ7
D	-21	GLY	-	expression tag	UNP Q6UWZ7
D	-20	SER	-	expression tag	UNP Q6UWZ7
D	-19	GLY	-	expression tag	UNP Q6UWZ7
D	-18	GLY	-	expression tag	UNP Q6UWZ7
D	-17	SER	-	expression tag	UNP Q6UWZ7
D	-16	ALA	-	expression tag	UNP Q6UWZ7
D	-15	TRP	-	expression tag	UNP Q6UWZ7
D	-14	SER	-	expression tag	UNP Q6UWZ7
D	-13	HIS	-	expression tag	UNP Q6UWZ7
D	-12	PRO	-	expression tag	UNP Q6UWZ7
D	-11	GLN	-	expression tag	UNP Q6UWZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	PHE	-	expression tag	UNP Q6UWZ7
D	-9	GLU	-	expression tag	UNP Q6UWZ7
D	-8	LYS	-	expression tag	UNP Q6UWZ7
D	-7	LEU	-	expression tag	UNP Q6UWZ7
D	-6	GLU	-	expression tag	UNP Q6UWZ7
D	-5	VAL	-	expression tag	UNP Q6UWZ7
D	-4	LEU	-	expression tag	UNP Q6UWZ7
D	-3	PHE	-	expression tag	UNP Q6UWZ7
D	-2	GLN	-	expression tag	UNP Q6UWZ7
D	-1	GLY	-	expression tag	UNP Q6UWZ7
D	0	THR	-	expression tag	UNP Q6UWZ7
C	-36	MET	-	initiating methionine	UNP Q6UWZ7
C	-35	TRP	-	expression tag	UNP Q6UWZ7
C	-34	SER	-	expression tag	UNP Q6UWZ7
C	-33	HIS	-	expression tag	UNP Q6UWZ7
C	-32	PRO	-	expression tag	UNP Q6UWZ7
C	-31	GLN	-	expression tag	UNP Q6UWZ7
C	-30	PHE	-	expression tag	UNP Q6UWZ7
C	-29	GLU	-	expression tag	UNP Q6UWZ7
C	-28	LYS	-	expression tag	UNP Q6UWZ7
C	-27	GLY	-	expression tag	UNP Q6UWZ7
C	-26	GLY	-	expression tag	UNP Q6UWZ7
C	-25	GLY	-	expression tag	UNP Q6UWZ7
C	-24	SER	-	expression tag	UNP Q6UWZ7
C	-23	GLY	-	expression tag	UNP Q6UWZ7
C	-22	GLY	-	expression tag	UNP Q6UWZ7
C	-21	GLY	-	expression tag	UNP Q6UWZ7
C	-20	SER	-	expression tag	UNP Q6UWZ7
C	-19	GLY	-	expression tag	UNP Q6UWZ7
C	-18	GLY	-	expression tag	UNP Q6UWZ7
C	-17	SER	-	expression tag	UNP Q6UWZ7
C	-16	ALA	-	expression tag	UNP Q6UWZ7
C	-15	TRP	-	expression tag	UNP Q6UWZ7
C	-14	SER	-	expression tag	UNP Q6UWZ7
C	-13	HIS	-	expression tag	UNP Q6UWZ7
C	-12	PRO	-	expression tag	UNP Q6UWZ7
C	-11	GLN	-	expression tag	UNP Q6UWZ7
C	-10	PHE	-	expression tag	UNP Q6UWZ7
C	-9	GLU	-	expression tag	UNP Q6UWZ7
C	-8	LYS	-	expression tag	UNP Q6UWZ7
C	-7	LEU	-	expression tag	UNP Q6UWZ7
C	-6	GLU	-	expression tag	UNP Q6UWZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	expression tag	UNP Q6UWZ7
C	-4	LEU	-	expression tag	UNP Q6UWZ7
C	-3	PHE	-	expression tag	UNP Q6UWZ7
C	-2	GLN	-	expression tag	UNP Q6UWZ7
C	-1	GLY	-	expression tag	UNP Q6UWZ7
C	0	THR	-	expression tag	UNP Q6UWZ7

- Molecule 2 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	381	Total	C	N	O	S	0	0
			3061	1982	502	564	13		
2	F	380	Total	C	N	O	S	0	0
			3052	1976	500	563	13		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q9NXR7
E	0	ALA	-	expression tag	UNP Q9NXR7
F	-1	GLY	-	expression tag	UNP Q9NXR7
F	0	ALA	-	expression tag	UNP Q9NXR7

- Molecule 3 is a protein called BRISC and BRCA1-A complex member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	236	Total	C	N	O	S	0	0
			1880	1201	305	356	18		
3	H	238	Total	C	N	O	S	0	0
			1896	1211	307	360	18		

- Molecule 4 is a protein called BRCA1-A complex subunit RAP80.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	58	Total	C	N	O	S	0	0
			466	305	78	80	3		
4	J	58	Total	C	N	O	S	0	0
			466	305	78	80	3		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	GLY	-	expression tag	UNP Q96RL1
I	-3	ALA	-	expression tag	UNP Q96RL1
I	-2	MET	-	expression tag	UNP Q96RL1
I	-1	GLY	-	expression tag	UNP Q96RL1
I	0	SER	-	expression tag	UNP Q96RL1
J	-4	GLY	-	expression tag	UNP Q96RL1
J	-3	ALA	-	expression tag	UNP Q96RL1
J	-2	MET	-	expression tag	UNP Q96RL1
J	-1	GLY	-	expression tag	UNP Q96RL1
J	0	SER	-	expression tag	UNP Q96RL1

- Molecule 5 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	76	Total	C	N	O	S	0	0
			602	378	105	118	1		
5	L	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
5	M	75	Total	C	N	O		0	0
			589	371	103	115			
5	N	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
5	O	76	Total	C	N	O	S	0	0
			602	378	105	118	1		
5	P	76	Total	C	N	O	S	0	0
			602	378	105	118	1		

- Molecule 6 is a protein called Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	260	Total	C	N	O	S	1	0
			2099	1314	376	395	14		
6	B	251	Total	C	N	O	S	0	0
			2007	1259	358	376	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ALA	GLU	engineered mutation	UNP P46736
B	33	ALA	GLU	engineered mutation	UNP P46736

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

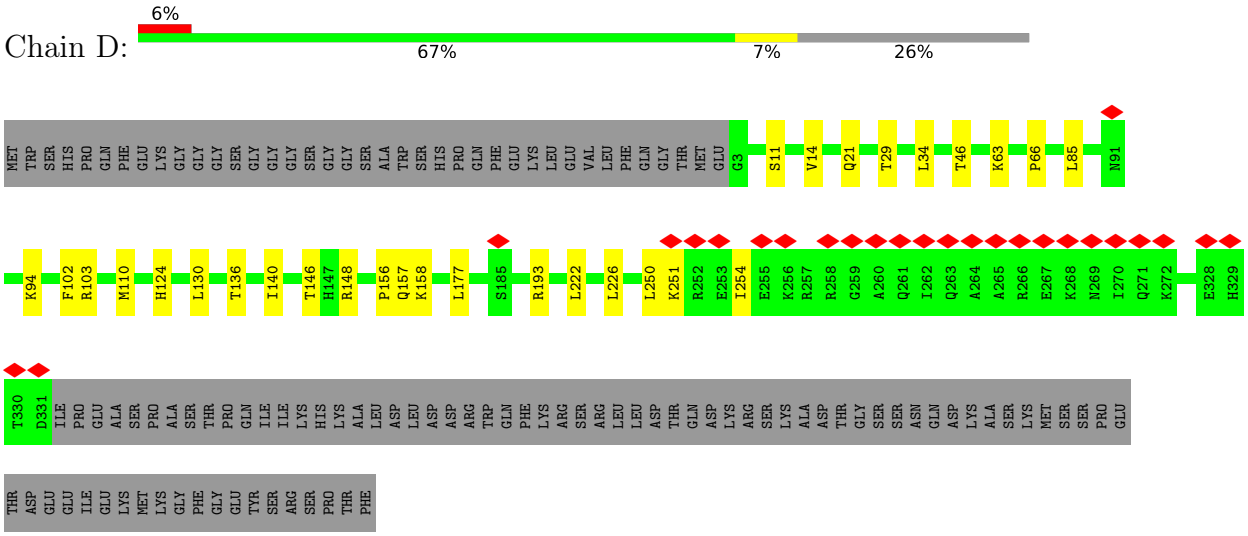
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Zn 1 1	0
7	B	1	Total Zn 1 1	0

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.

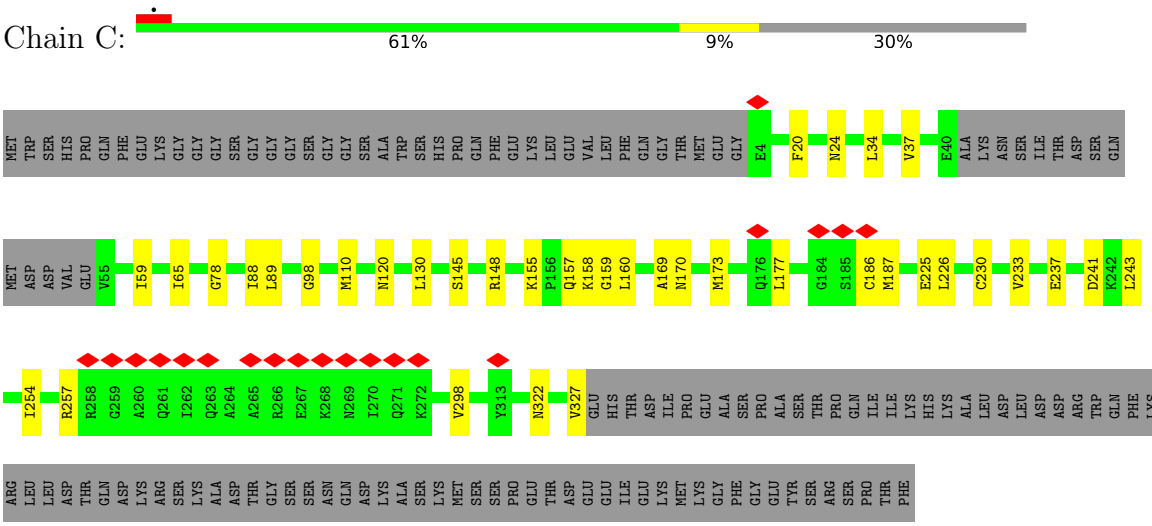
• Molecule 1: BRCA1-A complex subunit Abraxas 1

Chain D:



• Molecule 1: BRCA1-A complex subunit Abraxas 1

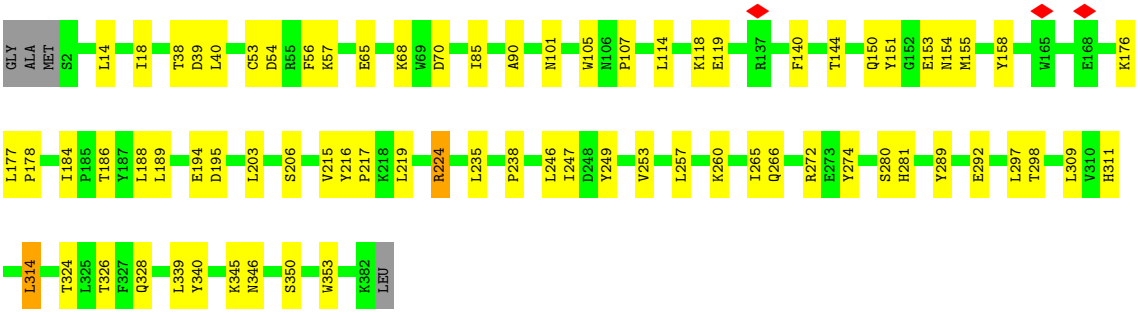
Chain C:



• Molecule 2: BRISC and BRCA1-A complex member 2

Chain E:

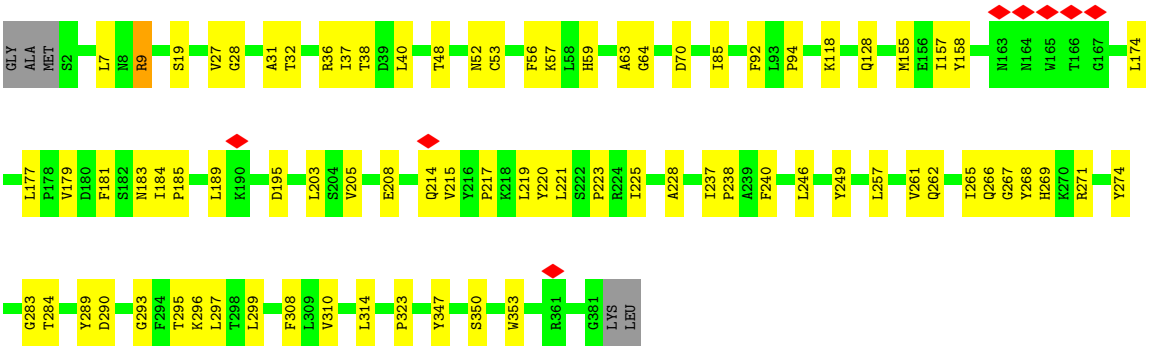




• Molecule 2: BRISC and BRCA1-A complex member 2

Chain F:

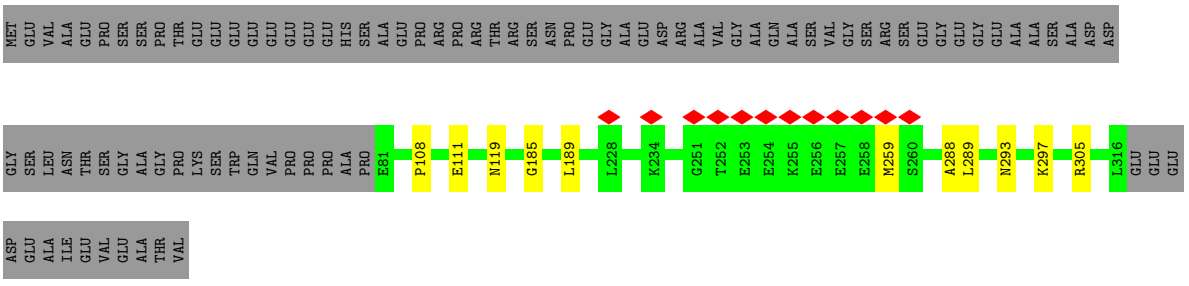




• Molecule 3: BRISC and BRCA1-A complex member 1

Chain G:

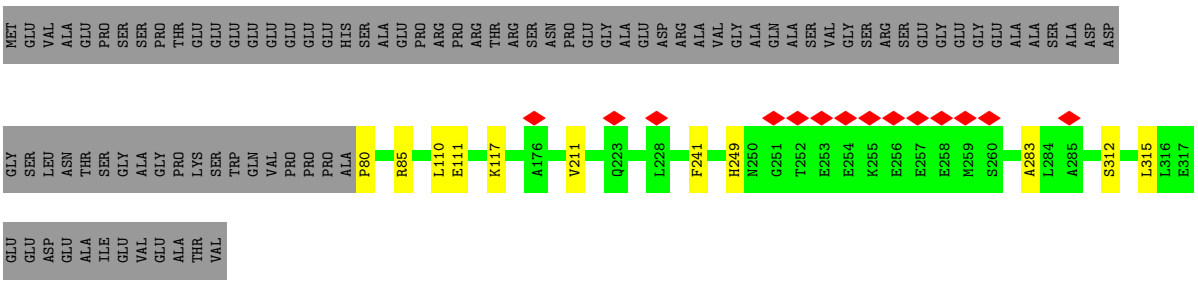




• Molecule 3: BRISC and BRCA1-A complex member 1

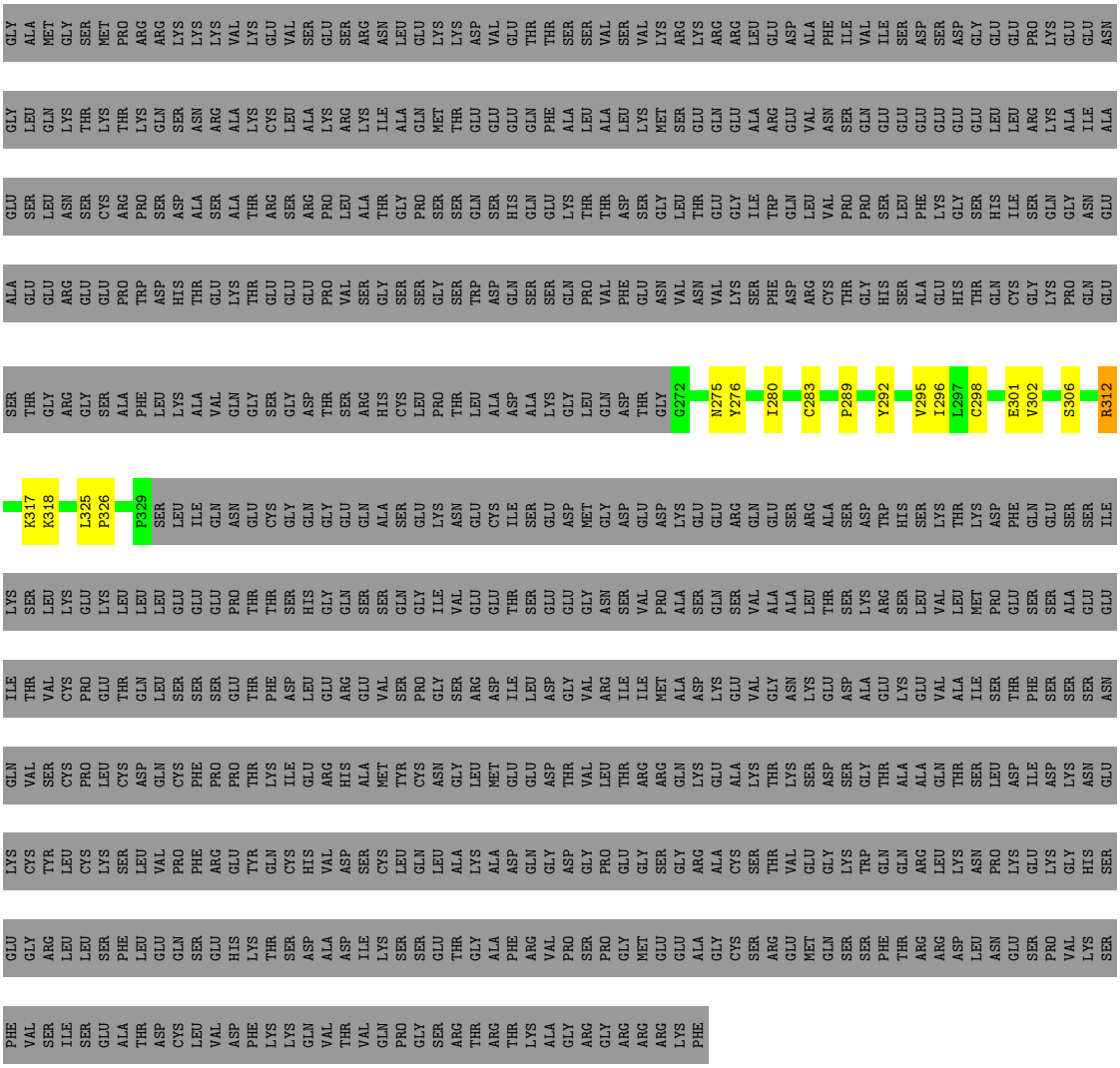
Chain H:





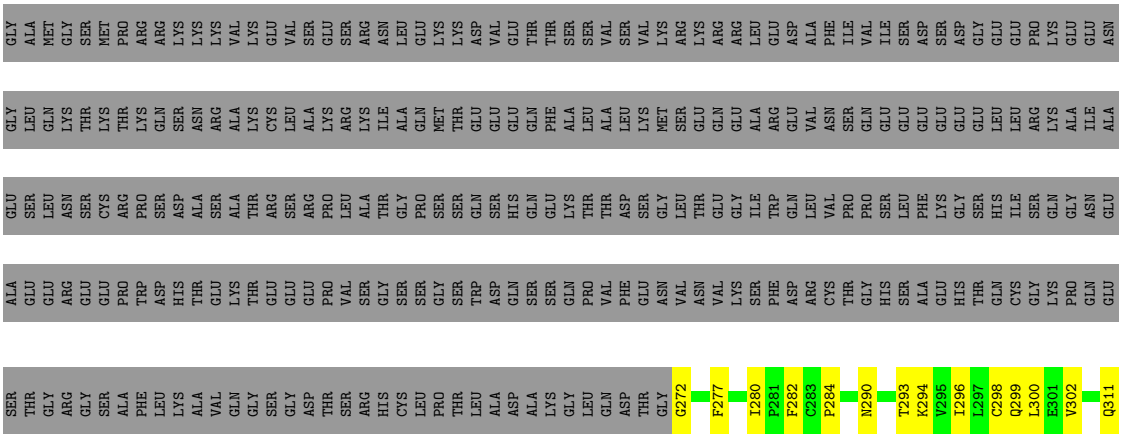
• Molecule 4: BRCA1-A complex subunit RAP80

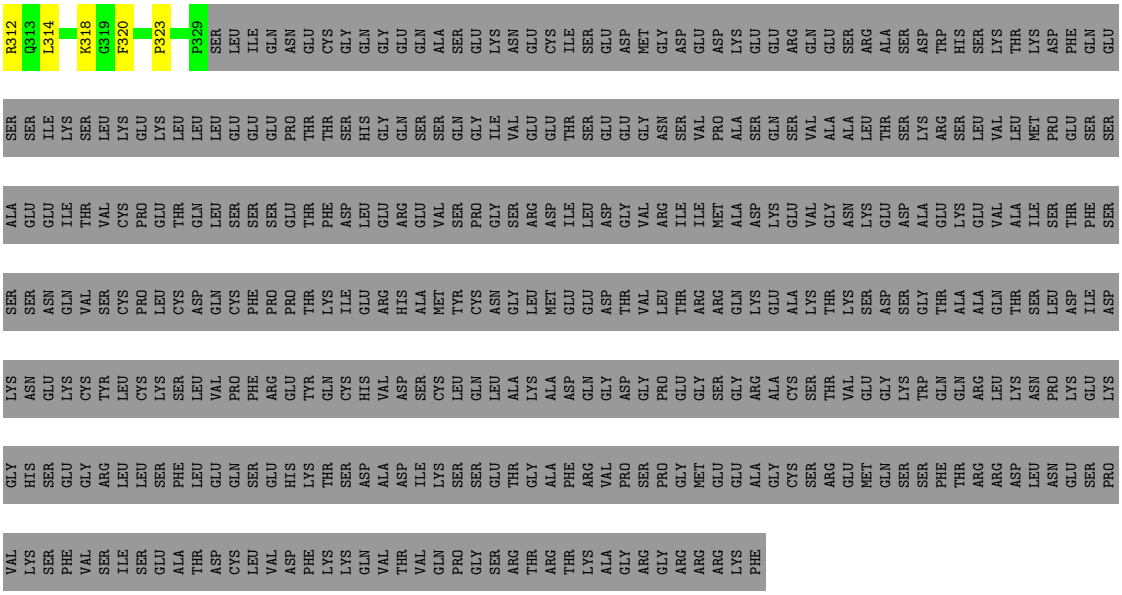
Chain I: 6% 92%



• Molecule 4: BRCA1-A complex subunit RAP80

Chain J: 5% 92%

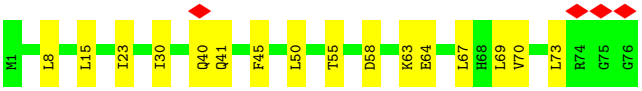




• Molecule 5: Ubiquitin

Chain K:





• Molecule 5: Ubiquitin

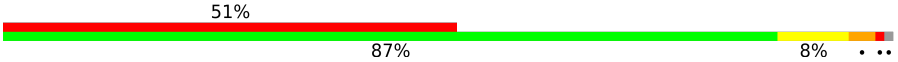
Chain L:

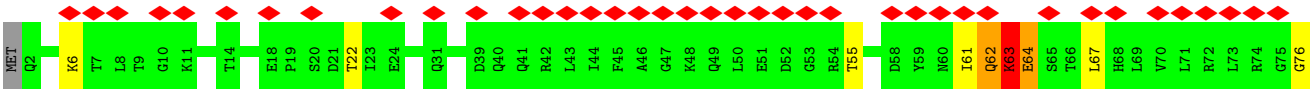




• Molecule 5: Ubiquitin

Chain M:

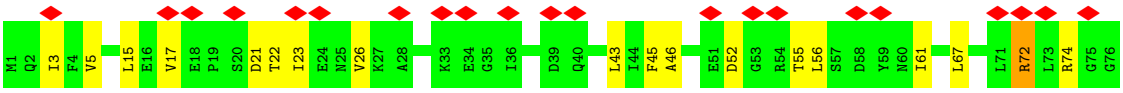




• Molecule 5: Ubiquitin

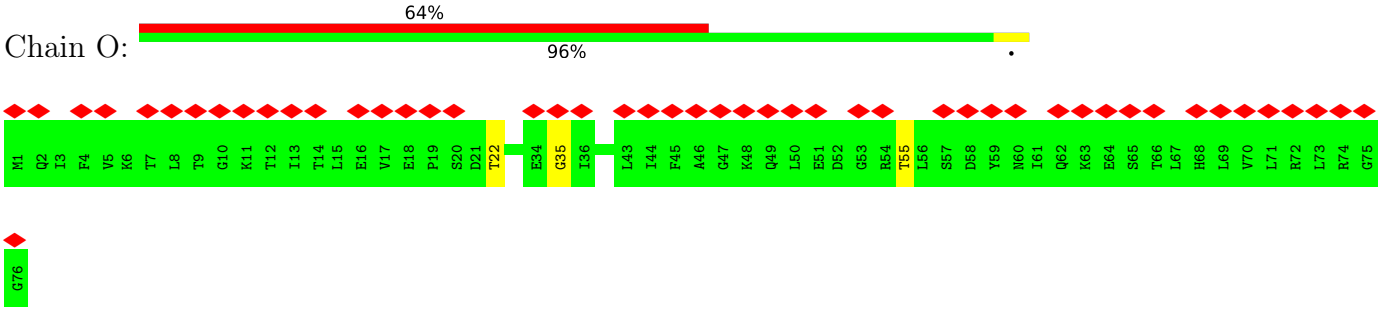
Chain N:





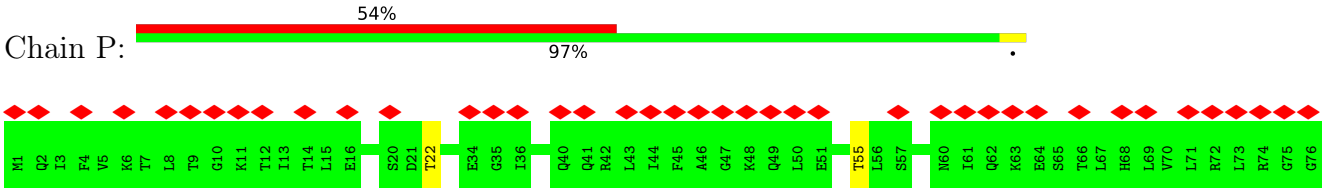
• Molecule 5: Ubiquitin

Chain O:



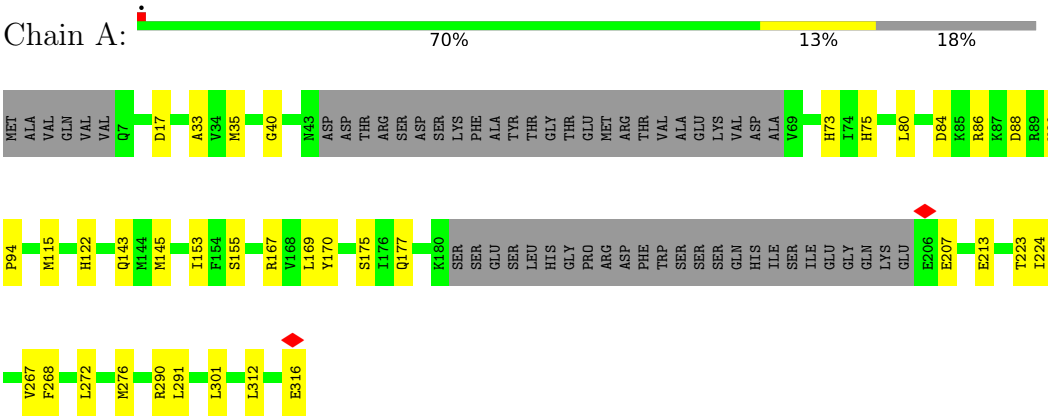
• Molecule 5: Ubiquitin

Chain P:



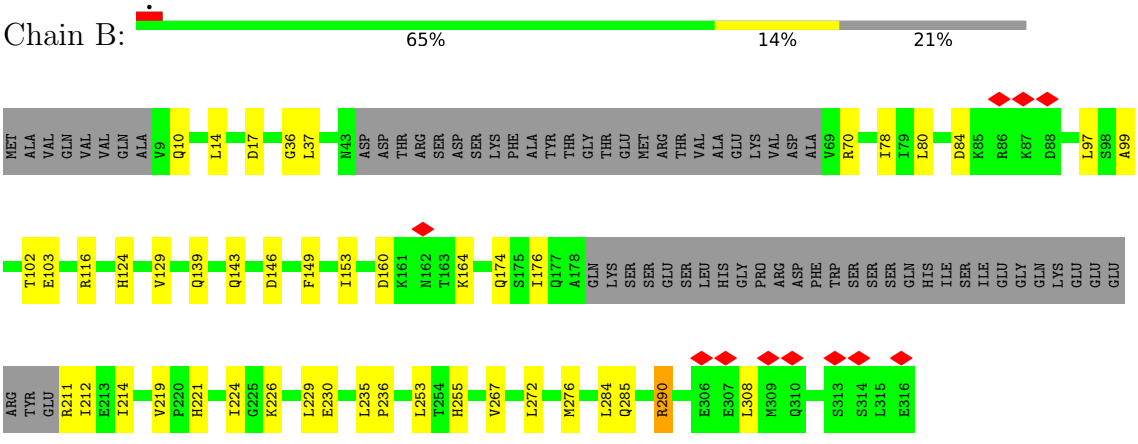
• Molecule 6: Lys-63-specific deubiquitinase BRCC36

Chain A:



• Molecule 6: Lys-63-specific deubiquitinase BRCC36

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	214650	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.5	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.527	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.0482	Depositor
Map size (Å)	344.84, 345.58002, 345.58002	wwPDB
Map dimensions	466, 467, 467	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	C	0.24	0/2539	0.42	1/3414 (0.0%)
1	D	0.23	0/2686	0.41	1/3614 (0.0%)
2	E	0.17	0/3152	0.37	0/4289
2	F	0.15	0/3143	0.38	0/4278
3	G	0.22	0/1925	0.52	0/2611
3	H	0.17	0/1942	0.46	0/2634
4	I	0.26	0/480	0.43	0/652
4	J	0.28	0/480	0.46	0/652
5	K	0.08	0/608	0.22	0/816
5	L	0.18	0/607	0.30	0/816
5	M	0.33	0/595	0.44	0/801
5	N	0.26	0/607	0.32	0/816
5	O	0.05	0/608	0.17	0/816
5	P	0.06	0/608	0.20	0/816
6	A	0.19	0/2136	0.35	0/2884
6	B	0.23	0/2042	0.34	0/2759
All	All	0.20	0/24158	0.39	2/32668 (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
2	E	0	1
2	F	0	1
4	I	0	1
5	N	0	1
6	B	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	158	LYS	N-CA-CB	-5.74	102.82	110.57
1	C	159	GLY	CA-C-O	-5.21	117.71	122.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	290	ARG	Sidechain
2	E	224	ARG	Sidechain
2	F	9	ARG	Sidechain
4	I	312	ARG	Sidechain
5	N	72	ARG	Sidechain

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	C	2494	0	2488	38	0
1	D	2639	0	2615	31	0
2	E	3061	0	2978	72	0
2	F	3052	0	2964	58	0
3	G	1880	0	1864	4	0
3	H	1896	0	1877	6	0
4	I	466	0	472	17	0
4	J	466	0	472	17	0
5	K	602	0	626	13	0
5	L	601	0	628	16	0
5	M	589	0	609	13	0
5	N	601	0	629	21	0
5	O	602	0	629	2	0
5	P	602	0	629	1	0
6	A	2099	0	2087	44	0
6	B	2007	0	2007	34	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23659	0	23574	335	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 9.

All (335) 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)
5:L:63:LYS:NZ	5:M:76:GLY:C	1.79	1.37
5:N:5:VAL:CG1	5:N:15:LEU:HD12	1.59	1.29
1:C:257:ARG:NH2	6:A:316:GLU:HG3	1.45	1.29
5:K:30:ILE:CG2	5:K:41:GLN:HE22	1.56	1.18
6:A:224:ILE:HG13	6:A:290:ARG:NH1	1.58	1.15
5:L:63:LYS:CE	5:M:76:GLY:C	2.20	1.15
5:K:30:ILE:HG21	5:K:41:GLN:NE2	1.62	1.12
5:N:5:VAL:HG11	5:N:15:LEU:CD1	1.81	1.10
5:N:5:VAL:CG1	5:N:15:LEU:CD1	2.31	1.07
4:J:290:ASN:O	4:J:293:THR:HG22	1.57	1.04
5:N:72:ARG:HH21	5:N:74:ARG:NH2	1.54	1.04
5:N:72:ARG:NH2	5:N:74:ARG:NH2	2.05	1.04
1:C:155:LYS:HD3	1:C:158:LYS:HD3	1.40	1.03
6:A:35:MET:HG3	6:A:122:HIS:HB3	1.46	0.98
5:L:63:LYS:HE3	5:M:76:GLY:C	1.85	0.96
5:N:72:ARG:HH21	5:N:74:ARG:CZ	1.77	0.95
5:L:63:LYS:HZ2	5:M:76:GLY:C	1.51	0.95
5:N:5:VAL:HG11	5:N:15:LEU:HD12	0.97	0.95
6:B:99:ALA:O	6:B:102:THR:HG22	1.68	0.93
2:F:215:VAL:HG21	2:F:240:PHE:CE2	2.04	0.92
2:E:57:LYS:NZ	2:E:68:LYS:HE2	1.85	0.92
5:K:30:ILE:CG2	5:K:41:GLN:NE2	2.23	0.92
2:E:150:GLN:HE21	2:E:178:PRO:CG	1.84	0.91
1:C:257:ARG:HH22	6:A:316:GLU:HG3	1.26	0.90
6:B:224:ILE:HD11	6:B:290:ARG:NH2	1.85	0.90
5:L:63:LYS:HZ1	5:M:76:GLY:C	1.73	0.90
2:F:215:VAL:HG21	2:F:240:PHE:HE2	1.35	0.89
2:E:57:LYS:HZ2	2:E:68:LYS:HE2	1.35	0.89
6:A:224:ILE:HG13	6:A:290:ARG:HH11	1.36	0.89
6:A:224:ILE:CG1	6:A:290:ARG:NH1	2.35	0.88
2:F:257:LEU:O	2:F:261:VAL:HG23	1.74	0.87
5:L:61:ILE:HG23	5:L:65:SER:OG	1.74	0.87
1:D:21:GLN:HE22	1:D:66:PRO:CB	1.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LYS:HA	1:D:254:ILE:HG22	1.57	0.84
1:D:21:GLN:HE22	1:D:66:PRO:HB2	1.42	0.84
6:B:174:GLN:HB2	6:B:214:ILE:HD11	1.59	0.84
2:E:151:TYR:CE1	2:E:178:PRO:HD3	2.14	0.83
5:L:21:ASP:OD1	5:L:25:ASN:HB3	1.79	0.83
1:C:169:ALA:HA	1:C:173:MET:SD	2.20	0.82
5:K:30:ILE:HG22	5:K:41:GLN:HE22	1.40	0.81
2:E:150:GLN:HE21	2:E:178:PRO:HG3	1.45	0.80
6:A:224:ILE:CD1	6:A:290:ARG:CZ	2.60	0.79
6:A:35:MET:HB2	6:A:90:VAL:HG11	1.64	0.78
2:F:219:LEU:HD21	2:F:221:LEU:HD21	1.66	0.77
2:E:346:ASN:OD1	2:E:346:ASN:O	2.03	0.77
5:K:30:ILE:HG21	5:K:41:GLN:HE21	1.50	0.76
2:F:237:ILE:HD12	2:F:238:PRO:HD2	1.67	0.76
5:K:40:GLN:HB2	5:K:73:LEU:HD22	1.67	0.76
5:N:5:VAL:HG13	5:N:15:LEU:HD12	1.65	0.76
6:A:224:ILE:HD11	6:A:290:ARG:CZ	2.17	0.74
2:E:90:ALA:HB1	1:C:160:LEU:HD23	1.70	0.73
2:F:284:THR:HG21	3:H:312:SER:H	1.52	0.73
4:I:295:VAL:HA	4:I:298:CYS:SG	2.29	0.72
1:C:187:MET:O	6:B:285:GLN:NE2	2.22	0.72
1:C:170:ASN:OD1	1:C:173:MET:HG3	1.88	0.72
2:F:262:GLN:HA	2:F:265:ILE:HB	1.72	0.72
6:B:176:ILE:HG22	6:B:211:ARG:C	2.14	0.72
5:N:5:VAL:HG13	5:N:15:LEU:CD1	2.17	0.71
1:D:251:LYS:HA	1:D:254:ILE:CG2	2.20	0.70
6:A:80:LEU:HB2	6:A:92:ILE:HD13	1.71	0.70
6:B:253:LEU:HD23	6:B:255:HIS:NE2	2.07	0.70
4:I:295:VAL:O	4:I:298:CYS:SG	2.49	0.70
1:D:85:LEU:HD23	1:D:124:HIS:CE1	2.27	0.69
5:M:22:THR:HA	5:M:55:THR:HA	1.75	0.69
2:F:262:GLN:O	2:F:266:GLN:HG2	1.93	0.69
1:C:145:SER:OG	6:A:213:GLU:OE1	2.12	0.68
1:D:251:LYS:CA	1:D:254:ILE:HG22	2.23	0.68
1:D:226:LEU:HG	6:B:284:LEU:HD21	1.74	0.68
1:C:243:LEU:HD22	6:A:301:LEU:HB3	1.77	0.67
2:E:150:GLN:HE21	2:E:178:PRO:HG2	1.59	0.67
2:F:290:ASP:OD2	2:F:296:LYS:HB2	1.94	0.67
1:D:21:GLN:NE2	1:D:66:PRO:HB2	2.09	0.66
2:E:40:LEU:HD22	2:E:53:CYS:HB3	1.78	0.66
5:L:44:ILE:HD11	6:A:94:PRO:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LEU:HD11	1:C:177:LEU:HD11	1.78	0.65
1:D:250:LEU:HD13	6:B:308:LEU:HD22	1.77	0.65
6:A:224:ILE:CD1	6:A:290:ARG:NH1	2.59	0.65
5:L:21:ASP:OD1	5:L:25:ASN:CB	2.45	0.65
2:E:186:THR:OG1	2:E:292:GLU:OE1	2.15	0.65
6:A:84:ASP:OD1	6:A:86:ARG:HG3	1.98	0.64
6:A:207:GLU:OE1	6:A:207:GLU:N	2.30	0.64
2:F:350:SER:HB2	5:O:35:GLY:HA2	1.79	0.64
2:F:179:VAL:HG21	2:F:257:LEU:HD23	1.79	0.63
2:F:155:MET:HE2	2:F:157:ILE:HG12	1.81	0.63
5:K:23:ILE:HD13	5:K:50:LEU:HB3	1.81	0.63
3:H:111:GLU:HA	3:H:117:LYS:HA	1.81	0.62
6:B:78:ILE:HG22	6:B:80:LEU:HD12	1.82	0.62
2:F:63:ALA:HA	2:F:174:LEU:HD22	1.80	0.62
5:N:5:VAL:CG1	5:N:15:LEU:HD13	2.29	0.61
2:F:38:THR:OG1	2:F:59:HIS:NE2	2.32	0.61
1:C:155:LYS:HD3	1:C:158:LYS:CD	2.22	0.61
1:C:78:GLY:O	1:C:120:ASN:ND2	2.34	0.61
6:B:224:ILE:HD11	6:B:290:ARG:HH21	1.65	0.61
5:M:61:ILE:O	5:M:62:GLN:C	2.44	0.61
4:J:280:ILE:HD11	4:J:284:PRO:HG3	1.81	0.60
2:E:266:GLN:NE2	1:C:327:VAL:C	2.59	0.60
2:E:272:ARG:NH1	4:I:301:GLU:OE1	2.34	0.60
2:E:289:TYR:HB3	2:E:297:LEU:HD23	1.82	0.60
5:L:56:LEU:HD22	5:L:61:ILE:HD12	1.83	0.60
5:N:17:VAL:HG11	5:N:26:VAL:HG22	1.83	0.60
5:M:63:LYS:O	5:M:64:GLU:C	2.45	0.60
3:G:185:GLY:O	3:G:189:LEU:N	2.35	0.59
1:D:34:LEU:HD12	1:D:63:LYS:HE2	1.85	0.59
2:F:308:PHE:HE1	2:F:310:VAL:CG2	2.15	0.59
2:E:114:LEU:O	2:E:118:LYS:HG3	2.03	0.59
1:D:21:GLN:NE2	1:D:66:PRO:CB	2.64	0.58
2:E:57:LYS:NZ	2:E:68:LYS:CE	2.63	0.58
5:N:5:VAL:HG12	5:N:67:LEU:HB2	1.86	0.58
1:D:177:LEU:HB2	6:B:267:VAL:HG13	1.85	0.58
2:E:101:ASN:ND2	2:E:119:GLU:OE2	2.36	0.57
2:E:151:TYR:CZ	2:E:178:PRO:HD3	2.39	0.57
5:L:45:PHE:HB3	5:L:50:LEU:HD21	1.86	0.57
6:A:17:ASP:OD1	6:A:17:ASP:N	2.37	0.57
4:J:311:GLN:HA	4:J:314:LEU:HD13	1.85	0.57
5:N:26:VAL:HG21	5:N:56:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:235:LEU:HB3	6:B:236:PRO:HD3	1.87	0.57
1:D:140:ILE:HB	1:D:146:THR:HG23	1.86	0.57
6:A:88:ASP:OD2	6:A:88:ASP:N	2.38	0.57
6:B:224:ILE:CD1	6:B:290:ARG:NH2	2.66	0.57
6:B:36:GLY:HA2	6:B:80:LEU:HD13	1.86	0.57
2:E:140:PHE:O	2:E:144:THR:HG22	2.05	0.56
2:F:308:PHE:CE1	2:F:310:VAL:CG2	2.89	0.56
6:A:177:GLN:HE22	6:A:207:GLU:HB3	1.70	0.56
1:D:251:LYS:C	1:D:254:ILE:HG22	2.30	0.56
2:E:153:GLU:O	2:E:153:GLU:HG2	2.05	0.56
1:D:251:LYS:O	1:D:254:ILE:HG22	2.05	0.56
1:C:237:GLU:OE2	6:A:290:ARG:NH1	2.37	0.56
2:F:183:ASN:OD1	2:F:269:HIS:NE2	2.30	0.55
2:F:179:VAL:HG11	2:F:181:PHE:CE1	2.42	0.55
1:C:237:GLU:OE2	6:A:290:ARG:NE	2.40	0.55
2:E:215:VAL:HG12	2:E:217:PRO:HD3	1.89	0.55
2:F:271:ARG:NH1	2:F:293:GLY:O	2.39	0.55
2:F:289:TYR:HB3	2:F:297:LEU:HD23	1.88	0.55
1:D:140:ILE:HD11	1:D:148:ARG:HD3	1.88	0.55
2:F:215:VAL:CG2	2:F:240:PHE:CE2	2.86	0.55
2:E:150:GLN:NE2	2:E:178:PRO:HG3	2.17	0.55
2:F:27:VAL:HG23	2:F:28:GLY:H	1.72	0.55
5:M:62:GLN:C	5:M:64:GLU:H	2.14	0.55
6:A:33:ALA:HB3	6:A:90:VAL:CG2	2.37	0.54
1:C:241:ASP:HB2	6:A:223:THR:HG21	1.89	0.54
4:J:296:ILE:HA	4:J:299:GLN:HB2	1.88	0.54
2:E:235:LEU:HD13	2:E:260:LYS:HZ1	1.73	0.54
1:C:177:LEU:HD13	6:A:267:VAL:HG22	1.87	0.54
6:A:75:HIS:HB2	6:A:115:MET:HE1	1.89	0.54
6:A:268:PHE:O	6:A:272:LEU:HD13	2.08	0.54
4:I:276:TYR:HD2	4:I:280:ILE:HA	1.73	0.54
2:E:70:ASP:HB2	2:E:85:ILE:HB	1.89	0.53
2:E:144:THR:HG23	2:E:247:ILE:HD11	1.90	0.53
2:E:274:TYR:CE1	2:E:314:LEU:HD11	2.43	0.53
5:K:41:GLN:HE21	5:K:69:LEU:HD11	1.72	0.53
2:E:266:GLN:CD	1:C:327:VAL:C	2.76	0.53
2:F:128:GLN:HG2	2:F:158:TYR:HA	1.90	0.53
5:K:45:PHE:HB2	5:K:67:LEU:HD22	1.90	0.53
2:E:340:TYR:O	2:E:340:TYR:CD2	2.61	0.53
1:C:257:ARG:NH2	6:A:316:GLU:CG	2.41	0.53
5:N:3:ILE:HG13	5:N:15:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:139:GLN:HE22	6:B:149:PHE:HD2	1.56	0.53
1:D:11:SER:HB3	1:D:14:VAL:HG23	1.90	0.53
2:E:281:HIS:CE1	4:I:289:PRO:HB2	2.44	0.53
2:F:283:GLY:HA3	4:J:282:PHE:HA	1.91	0.53
1:D:222:LEU:HD12	6:B:276:MET:HG2	1.90	0.52
3:H:80:PRO:O	4:J:272:GLY:N	2.42	0.52
1:C:88:ILE:HG22	1:C:89:LEU:HG	1.92	0.52
6:B:99:ALA:O	6:B:102:THR:CG2	2.52	0.52
2:E:57:LYS:HZ1	2:E:68:LYS:HE2	1.70	0.52
6:A:257:ASP:OD1	6:A:257:ASP:N	2.38	0.52
5:L:63:LYS:HG2	5:L:64:GLU:HG3	1.91	0.51
3:H:85:ARG:HA	4:J:277:PHE:HB2	1.93	0.51
2:E:150:GLN:NE2	2:E:178:PRO:CG	2.66	0.51
2:E:54:ASP:OD1	2:E:54:ASP:N	2.44	0.51
2:F:267:GLY:O	2:F:271:ARG:HB2	2.11	0.51
6:B:78:ILE:HG22	6:B:80:LEU:CD1	2.41	0.51
2:E:219:LEU:HD11	2:E:257:LEU:HD11	1.92	0.50
4:I:325:LEU:HD13	4:I:326:PRO:HD2	1.94	0.50
5:M:62:GLN:O	5:M:64:GLU:N	2.44	0.50
2:F:27:VAL:O	2:F:118:LYS:HD3	2.12	0.50
2:F:184:ILE:HG12	2:F:225:ILE:HG22	1.93	0.50
1:D:46:THR:O	5:L:72:ARG:NH2	2.38	0.50
1:D:63:LYS:HD3	1:D:94:LYS:HD2	1.93	0.50
5:N:22:THR:HA	5:N:55:THR:HA	1.92	0.50
2:F:92:PHE:CZ	2:F:94:PRO:HG3	2.47	0.50
1:C:98:GLY:HA2	1:C:130:LEU:HD22	1.94	0.50
6:B:14:LEU:O	6:B:219:VAL:N	2.35	0.50
2:E:311:HIS:HB2	2:E:326:THR:HG23	1.94	0.49
4:J:298:CYS:O	4:J:302:VAL:HG23	2.11	0.49
5:P:22:THR:HA	5:P:55:THR:HA	1.93	0.49
1:C:37:VAL:HG22	1:C:59:ILE:HG23	1.94	0.49
1:C:157:GLN:OE1	1:C:157:GLN:N	2.37	0.49
6:B:160:ASP:O	6:B:164:LYS:N	2.37	0.49
2:F:177:LEU:HD21	2:F:203:LEU:HB2	1.94	0.49
2:F:274:TYR:CE1	2:F:314:LEU:HD21	2.48	0.49
6:A:224:ILE:HD12	6:A:290:ARG:CZ	2.41	0.49
5:L:61:ILE:CG2	5:L:65:SER:OG	2.55	0.49
1:C:233:VAL:HG22	6:A:291:LEU:HG	1.95	0.49
3:H:249:HIS:O	3:H:283:ALA:HA	2.13	0.49
2:E:57:LYS:HD3	2:E:68:LYS:HE3	1.94	0.48
2:E:235:LEU:CD1	2:E:260:LYS:HZ1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:235:LEU:CD1	2:E:260:LYS:NZ	2.76	0.48
2:F:9:ARG:O	2:F:53:CYS:HB2	2.14	0.48
2:E:177:LEU:HD21	2:E:253:VAL:HG13	1.95	0.48
2:F:36:ARG:HG2	2:F:36:ARG:HH11	1.79	0.48
1:D:21:GLN:HE22	1:D:66:PRO:HB3	1.74	0.48
5:N:56:LEU:HB3	5:N:61:ILE:HD12	1.96	0.48
6:B:84:ASP:OD1	6:B:84:ASP:N	2.47	0.48
5:K:15:LEU:HD11	5:K:30:ILE:HG13	1.96	0.48
4:I:302:VAL:O	4:I:306:SER:OG	2.23	0.47
2:E:151:TYR:HE1	2:E:177:LEU:HA	1.78	0.47
2:E:324:THR:HB	2:E:345:LYS:HE2	1.96	0.47
2:F:32:THR:HG21	2:F:220:TYR:CG	2.49	0.47
6:B:226:LYS:O	6:B:230:GLU:HG3	2.15	0.47
2:E:177:LEU:HD11	2:E:203:LEU:HB2	1.96	0.47
6:B:176:ILE:CG2	6:B:211:ARG:C	2.86	0.47
2:E:184:ILE:HA	2:E:265:ILE:HD11	1.96	0.47
3:H:211:VAL:O	3:H:241:PHE:HA	2.14	0.47
4:I:275:ASN:OD1	1:C:298:VAL:HA	2.14	0.47
1:C:170:ASN:OD1	1:C:170:ASN:N	2.46	0.47
1:D:251:LYS:O	1:D:254:ILE:CG2	2.63	0.47
2:E:40:LEU:HD23	2:E:56:PHE:HB3	1.96	0.47
2:F:7:LEU:HD21	2:F:19:SER:HA	1.97	0.47
2:E:38:THR:OG1	2:E:39:ASP:N	2.48	0.47
2:F:189:LEU:HD13	4:J:318:LYS:HD2	1.97	0.47
5:K:8:LEU:HD11	5:K:70:VAL:HA	1.97	0.47
6:A:143:GLN:NE2	6:A:175:SER:O	2.32	0.46
2:E:150:GLN:NE2	2:E:178:PRO:HG2	2.30	0.46
2:E:155:MET:HE2	2:E:155:MET:HB3	1.76	0.46
2:F:223:PRO:HD3	4:J:320:PHE:CE1	2.50	0.46
6:B:143:GLN:HA	6:B:146:ASP:O	2.15	0.46
2:E:151:TYR:CZ	2:E:178:PRO:CD	2.98	0.46
5:M:6:LYS:N	5:M:67:LEU:O	2.38	0.46
5:N:23:ILE:HB	5:N:52:ASP:HA	1.98	0.46
2:F:31:ALA:HB1	2:F:64:GLY:H	1.80	0.46
2:F:174:LEU:HD12	2:F:174:LEU:HA	1.81	0.46
3:G:111:GLU:O	3:G:288:ALA:N	2.34	0.46
3:G:289:LEU:O	3:G:293:ASN:N	2.45	0.46
2:F:40:LEU:HD23	2:F:40:LEU:HA	1.79	0.45
5:M:63:LYS:HD2	5:M:63:LYS:HA	1.45	0.45
6:B:17:ASP:OD2	6:B:221:HIS:ND1	2.49	0.45
2:F:195:ASP:OD1	4:J:311:GLN:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:23:ILE:HG23	5:N:43:LEU:HD12	1.97	0.45
6:A:33:ALA:HB3	6:A:90:VAL:HG23	1.98	0.45
6:A:224:ILE:HD12	6:A:290:ARG:NE	2.31	0.45
2:E:195:ASP:OD1	4:I:317:LYS:NZ	2.50	0.45
2:E:340:TYR:O	2:E:340:TYR:CG	2.69	0.45
4:J:280:ILE:CD1	4:J:284:PRO:HG3	2.45	0.45
2:F:185:PRO:HB3	2:F:268:TYR:CE1	2.52	0.45
6:B:102:THR:HG23	6:B:103:GLU:N	2.32	0.45
6:B:116:ARG:NH2	6:B:146:ASP:OD2	2.50	0.45
2:E:151:TYR:OH	2:E:178:PRO:HD2	2.16	0.45
2:F:48:THR:HB	2:F:52:ASN:HD21	1.81	0.44
2:F:208:GLU:HB2	2:F:214:GLN:HB3	1.98	0.44
2:F:57:LYS:HA	2:F:70:ASP:HA	2.00	0.44
2:E:188:LEU:O	2:E:189:LEU:HD13	2.17	0.44
2:E:195:ASP:OD1	4:I:312:ARG:HA	2.17	0.44
2:E:324:THR:HA	2:E:345:LYS:HG2	1.99	0.44
2:F:184:ILE:HD11	2:F:228:ALA:HB3	1.99	0.44
6:A:90:VAL:HG12	6:A:91:GLU:N	2.32	0.44
4:J:293:THR:HG23	4:J:294:LYS:N	2.33	0.44
6:B:124:HIS:CG	6:B:153:ILE:HD11	2.53	0.44
2:E:246:LEU:HD23	2:E:246:LEU:HA	1.84	0.44
2:F:179:VAL:CG1	2:F:181:PHE:CE1	3.01	0.44
5:L:69:LEU:HG	6:A:145:MET:HE1	1.98	0.44
1:C:148:ARG:HD2	6:A:167:ARG:HE	1.82	0.44
2:E:280:SER:HB2	4:I:292:TYR:HD2	1.83	0.44
5:M:62:GLN:C	5:M:64:GLU:N	2.75	0.44
1:C:20:PHE:O	1:C:24:ASN:ND2	2.50	0.44
1:D:177:LEU:HD21	1:C:177:LEU:HD21	2.00	0.43
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.89	0.43
1:C:186:CYS:SG	6:A:257:ASP:HB3	2.58	0.43
6:A:153:ILE:O	6:A:170:TYR:HA	2.19	0.43
2:E:184:ILE:HD12	2:E:184:ILE:O	2.17	0.43
1:D:29:THR:OG1	1:D:102:PHE:HB2	2.18	0.43
4:I:275:ASN:OD1	1:C:298:VAL:CA	2.67	0.43
6:B:176:ILE:HG21	6:B:212:ILE:HB	2.01	0.43
2:F:179:VAL:HG11	2:F:181:PHE:CZ	2.54	0.43
5:K:63:LYS:HG2	5:K:64:GLU:HG3	1.99	0.43
1:C:110:MET:HE2	1:C:110:MET:HB3	1.91	0.43
6:A:272:LEU:O	6:A:276:MET:HG3	2.19	0.43
1:C:254:ILE:HG13	6:A:312:LEU:HD13	2.00	0.42
2:E:65:GLU:OE2	2:E:158:TYR:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:THR:HG21	2:F:220:TYR:CD1	2.54	0.42
2:F:308:PHE:CE1	2:F:310:VAL:HG23	2.53	0.42
1:C:34:LEU:HD11	1:C:65:ILE:HD11	2.00	0.42
5:L:51:GLU:OE1	5:L:54:ARG:NE	2.39	0.42
5:O:22:THR:HA	5:O:55:THR:HA	2.01	0.42
1:D:85:LEU:CD2	1:D:124:HIS:CE1	2.99	0.42
2:F:295:THR:O	2:F:314:LEU:N	2.44	0.42
5:N:72:ARG:NH2	5:N:74:ARG:HH22	2.09	0.42
2:E:154:ASN:HB3	2:E:176:LYS:HB3	2.00	0.42
6:A:35:MET:CE	6:A:92:ILE:HG13	2.50	0.42
1:D:103:ARG:O	1:D:136:THR:HA	2.19	0.42
2:E:297:LEU:HD22	2:E:298:THR:H	1.83	0.42
3:G:108:PRO:HA	3:G:119:ASN:HA	2.00	0.42
4:I:318:LYS:HE2	4:I:318:LYS:HB3	1.80	0.42
2:E:189:LEU:HG	2:E:194:GLU:HB2	2.02	0.42
2:F:70:ASP:OD2	2:F:85:ILE:HB	2.19	0.42
2:F:217:PRO:HG3	2:F:249:TYR:HE2	1.84	0.42
1:C:230:CYS:SG	6:A:233:VAL:HG11	2.59	0.42
2:E:40:LEU:HD23	2:E:40:LEU:HA	1.90	0.42
2:E:339:LEU:HD12	2:E:339:LEU:HA	1.87	0.42
2:F:299:LEU:O	2:F:310:VAL:N	2.47	0.42
4:J:300:LEU:H	4:J:300:LEU:HD22	1.84	0.42
4:I:317:LYS:HA	4:I:317:LYS:HD3	1.73	0.41
2:F:323:PRO:O	2:F:347:TYR:OH	2.17	0.41
1:C:170:ASN:OD1	1:C:173:MET:CG	2.63	0.41
6:B:37:LEU:HD21	6:B:97:LEU:HD23	2.02	0.41
2:E:309:LEU:HD23	2:E:328:GLN:OE1	2.20	0.41
4:I:292:TYR:O	4:I:296:ILE:HG22	2.20	0.41
4:J:312:ARG:HD2	4:J:312:ARG:HA	1.91	0.41
6:B:229:LEU:HD12	6:B:229:LEU:HA	1.89	0.41
2:E:280:SER:O	4:I:283:CYS:SG	2.74	0.41
2:F:195:ASP:OD1	4:J:311:GLN:HB3	2.20	0.41
5:K:55:THR:N	5:K:58:ASP:OD2	2.45	0.41
6:B:224:ILE:CD1	6:B:290:ARG:CZ	2.98	0.41
2:E:206:SER:OG	2:E:216:TYR:HB2	2.20	0.41
6:B:10:GLN:HG3	6:B:70:ARG:H	1.85	0.41
1:D:193:ARG:NH1	1:C:225:GLU:OE2	2.51	0.41
4:I:301:GLU:HG2	1:C:322:ASN:O	2.21	0.41
6:A:155:SER:HB3	6:A:169:LEU:HB2	2.01	0.41
2:E:57:LYS:HZ2	2:E:68:LYS:CE	2.19	0.41
2:F:220:TYR:CE1	4:J:323:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:MET:SD	1:D:156:PRO:HG3	2.61	0.41
1:D:156:PRO:O	1:D:157:GLN:C	2.64	0.41
2:E:14:LEU:O	2:E:18:ILE:HG12	2.21	0.41
2:E:184:ILE:HD13	2:E:224:ARG:HG2	2.02	0.41
2:E:350:SER:HB2	2:E:353:TRP:CD2	2.56	0.41
5:N:21:ASP:O	5:N:55:THR:OG1	2.31	0.41
6:A:40:GLY:HA3	6:A:73[B]:HIS:O	2.20	0.41
2:E:105:TRP:CD1	2:E:107:PRO:HG3	2.56	0.41
2:E:184:ILE:HG22	2:E:265:ILE:HD11	2.03	0.41
5:N:45:PHE:HD1	5:N:46:ALA:N	2.19	0.41
6:B:129:VAL:O	6:B:153:ILE:HD13	2.21	0.40
2:E:238:PRO:O	2:E:249:TYR:OH	2.31	0.40
2:F:37:ILE:HG23	2:F:56:PHE:HB2	2.04	0.40
2:F:205:VAL:HG21	2:F:246:LEU:HD21	2.04	0.40
2:E:235:LEU:HD13	2:E:260:LYS:NZ	2.35	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	C	306/446 (69%)	282 (92%)	24 (8%)	0	100	100
1	D	327/446 (73%)	311 (95%)	16 (5%)	0	100	100
2	E	379/385 (98%)	366 (97%)	13 (3%)	0	100	100
2	F	378/385 (98%)	362 (96%)	16 (4%)	0	100	100
3	G	234/329 (71%)	217 (93%)	17 (7%)	0	100	100
3	H	236/329 (72%)	224 (95%)	12 (5%)	0	100	100
4	I	56/724 (8%)	54 (96%)	2 (4%)	0	100	100
4	J	56/724 (8%)	53 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	K	74/76 (97%)	67 (90%)	7 (10%)	0	100 100
5	L	74/76 (97%)	73 (99%)	1 (1%)	0	100 100
5	M	73/76 (96%)	65 (89%)	5 (7%)	3 (4%)	2 8
5	N	74/76 (97%)	74 (100%)	0	0	100 100
5	O	74/76 (97%)	73 (99%)	1 (1%)	0	100 100
5	P	74/76 (97%)	72 (97%)	2 (3%)	0	100 100
6	A	255/316 (81%)	254 (100%)	1 (0%)	0	100 100
6	B	245/316 (78%)	241 (98%)	4 (2%)	0	100 100
All	All	2915/4856 (60%)	2788 (96%)	124 (4%)	3 (0%)	49 76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	M	63	LYS
5	M	62	GLN
5	M	64	GLU

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	C	283/400 (71%)	282 (100%)	1 (0%)	84 94
1	D	301/400 (75%)	301 (100%)	0	100 100
2	E	335/337 (99%)	334 (100%)	1 (0%)	86 95
2	F	334/337 (99%)	333 (100%)	1 (0%)	86 95
3	G	218/290 (75%)	215 (99%)	3 (1%)	59 83
3	H	220/290 (76%)	218 (99%)	2 (1%)	70 88
4	I	52/635 (8%)	52 (100%)	0	100 100
4	J	52/635 (8%)	52 (100%)	0	100 100
5	K	68/68 (100%)	68 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	L	68/68 (100%)	68 (100%)	0	100 100
5	M	66/68 (97%)	65 (98%)	1 (2%)	57 82
5	N	68/68 (100%)	68 (100%)	0	100 100
5	O	68/68 (100%)	68 (100%)	0	100 100
5	P	68/68 (100%)	68 (100%)	0	100 100
6	A	237/285 (83%)	237 (100%)	0	100 100
6	B	228/285 (80%)	227 (100%)	1 (0%)	84 94
All	All	2666/4302 (62%)	2656 (100%)	10 (0%)	81 94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	314	LEU
2	F	353	TRP
3	G	259	MET
3	G	297	LYS
3	G	305	ARG
3	H	110	LEU
3	H	315	LEU
5	M	63	LYS
1	C	226	LEU
6	B	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	21	GLN
1	D	124	HIS
1	D	196	GLN
2	E	24	ASN
2	E	76	GLN
2	E	150	GLN
2	E	252	GLN
2	F	214	GLN
2	F	252	GLN
4	I	299	GLN
4	I	304	GLN
5	K	41	GLN

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Mol	Chain	Res	Type
5	L	25	ASN
1	C	22	HIS
1	C	24	ASN
1	C	176	GLN
1	C	248	ASN
6	A	241	GLN
6	A	244	GLN
6	A	251	HIS
6	B	174	GLN
6	B	251	HIS
6	B	275	GLN
6	B	285	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

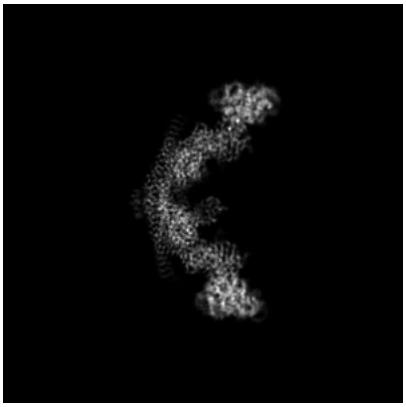
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55122. These allow visual inspection of the internal detail of the map and identification of artifacts.

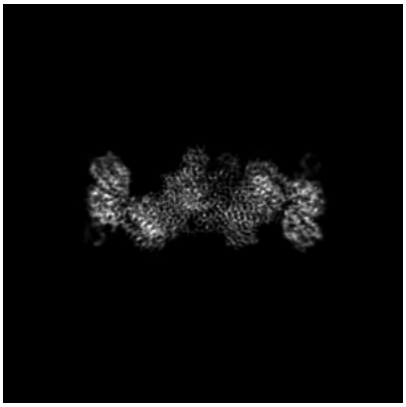
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

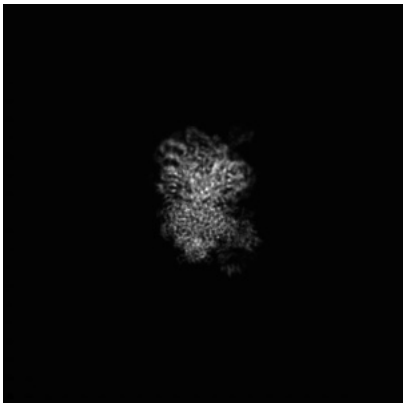
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 233



Y Index: 233



Z Index: 233

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: 225



Y Index: 268

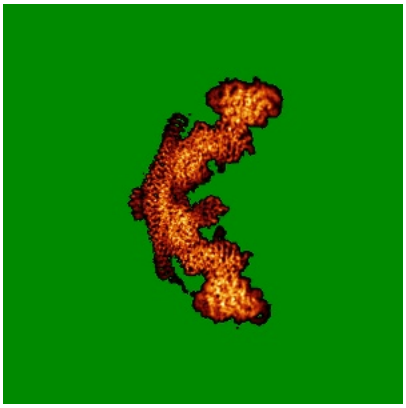


Z Index: 122

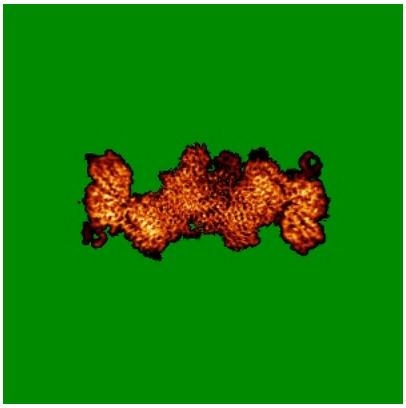
The images above show the largest variance slices of the map in three orthogonal directions.

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

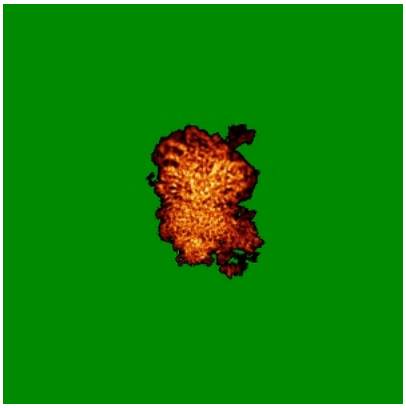
6.4.1 Primary map



X



Y

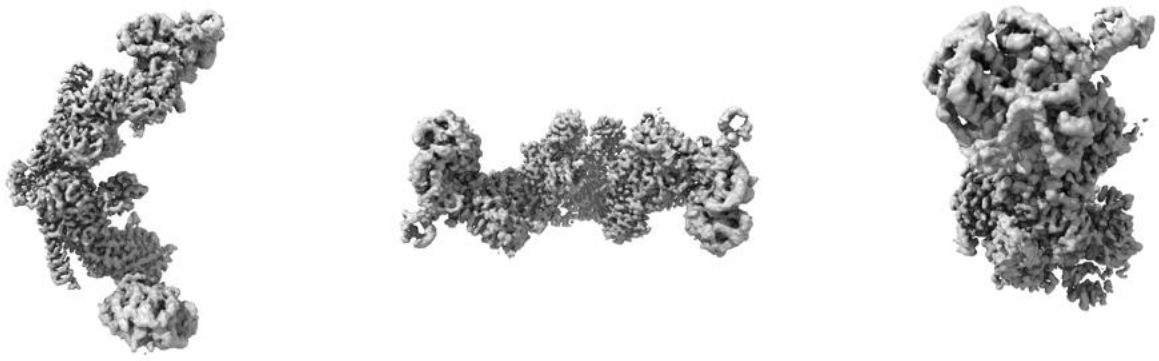


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0482. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

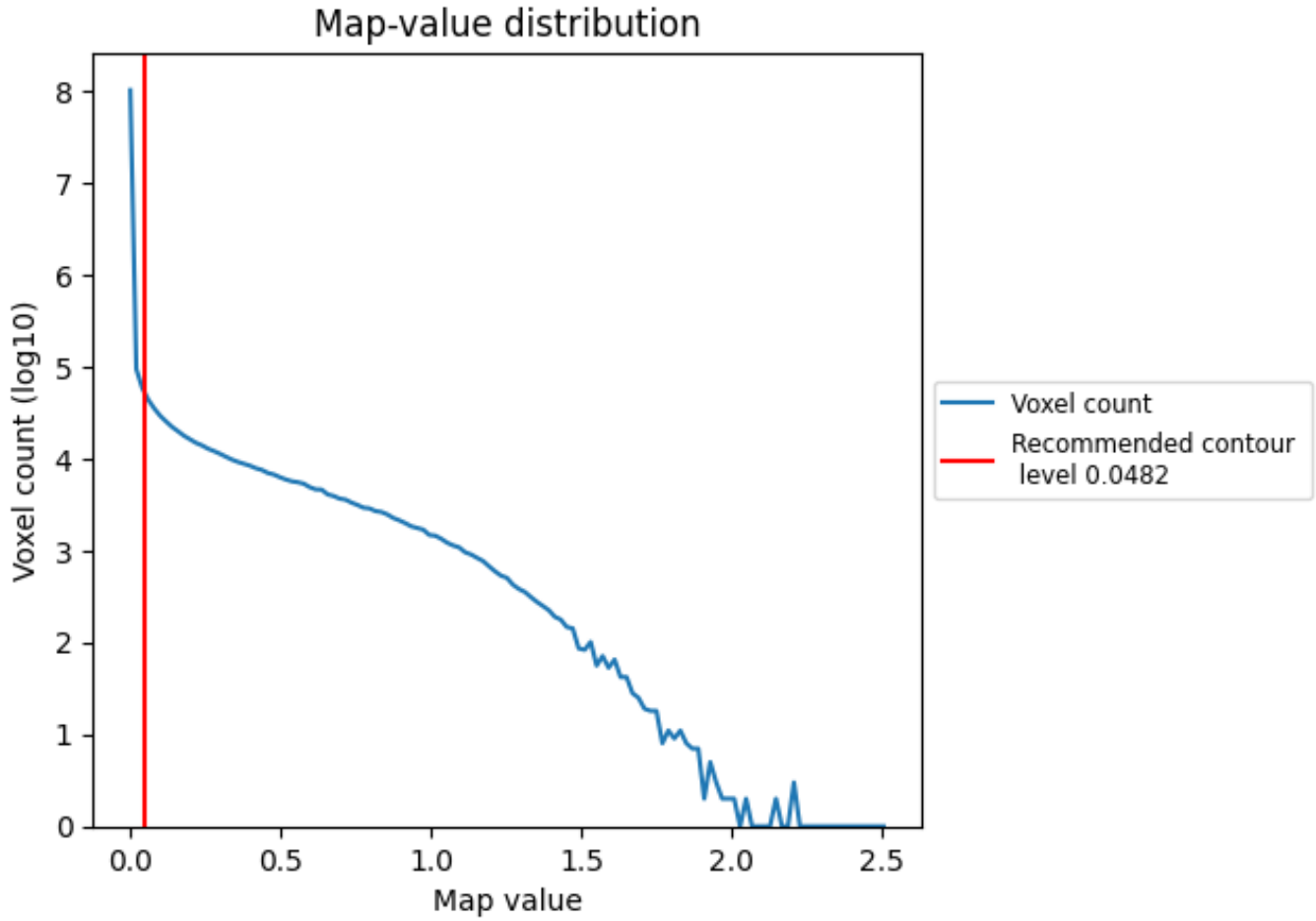
6.6 Mask visualisation (i)

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

7 Map analysis

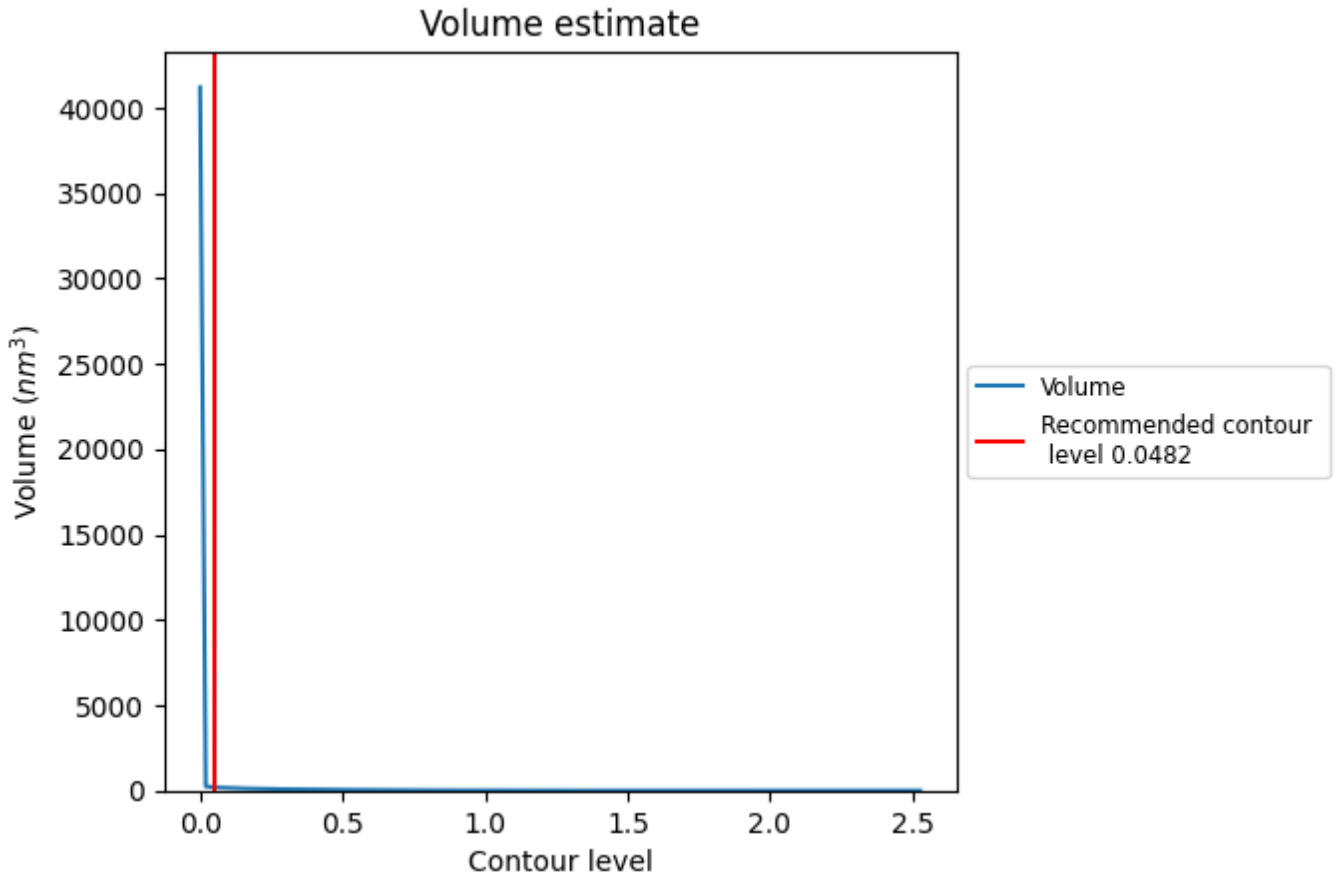
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 196 nm^3; this corresponds to an approximate mass of 177 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

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

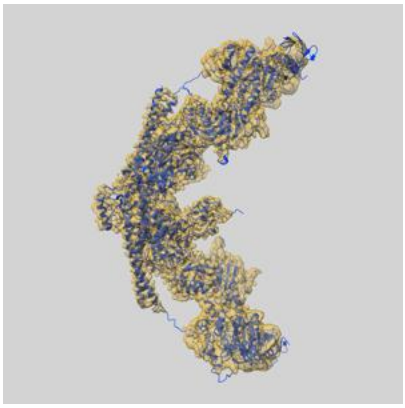
8 Fourier-Shell correlation (i)

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

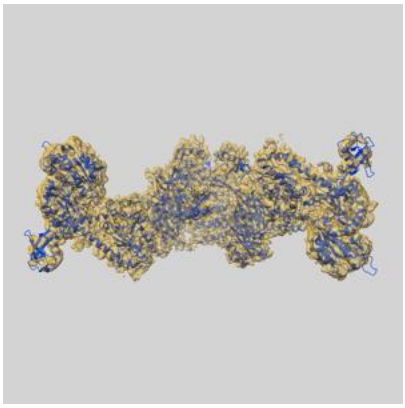
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55122 and PDB model 9SQY. Per-residue inclusion information can be found in section 3 on page 9.

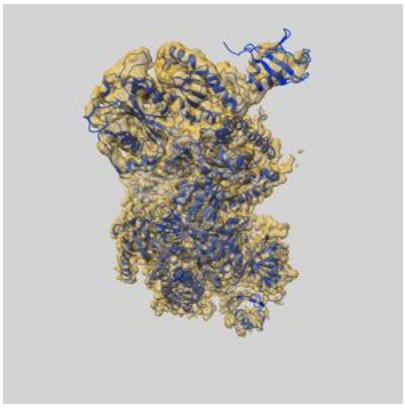
9.1 Map-model overlay



X



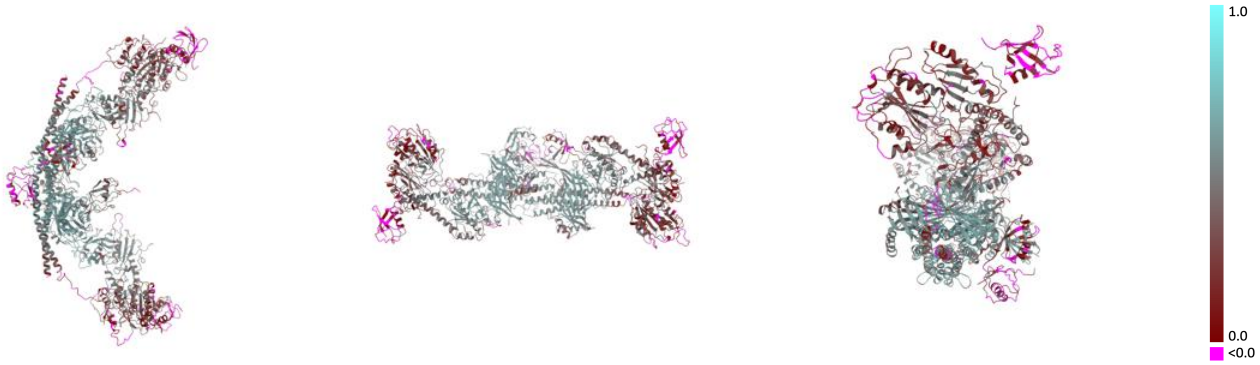
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0482 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

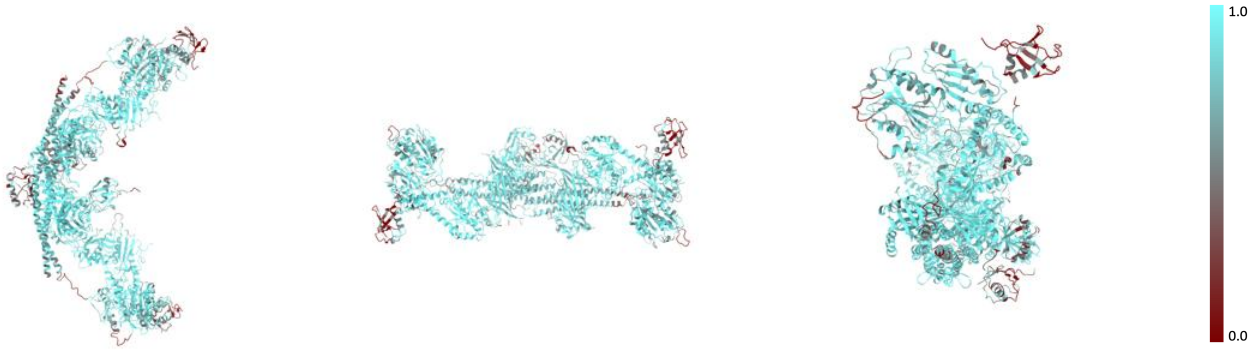
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

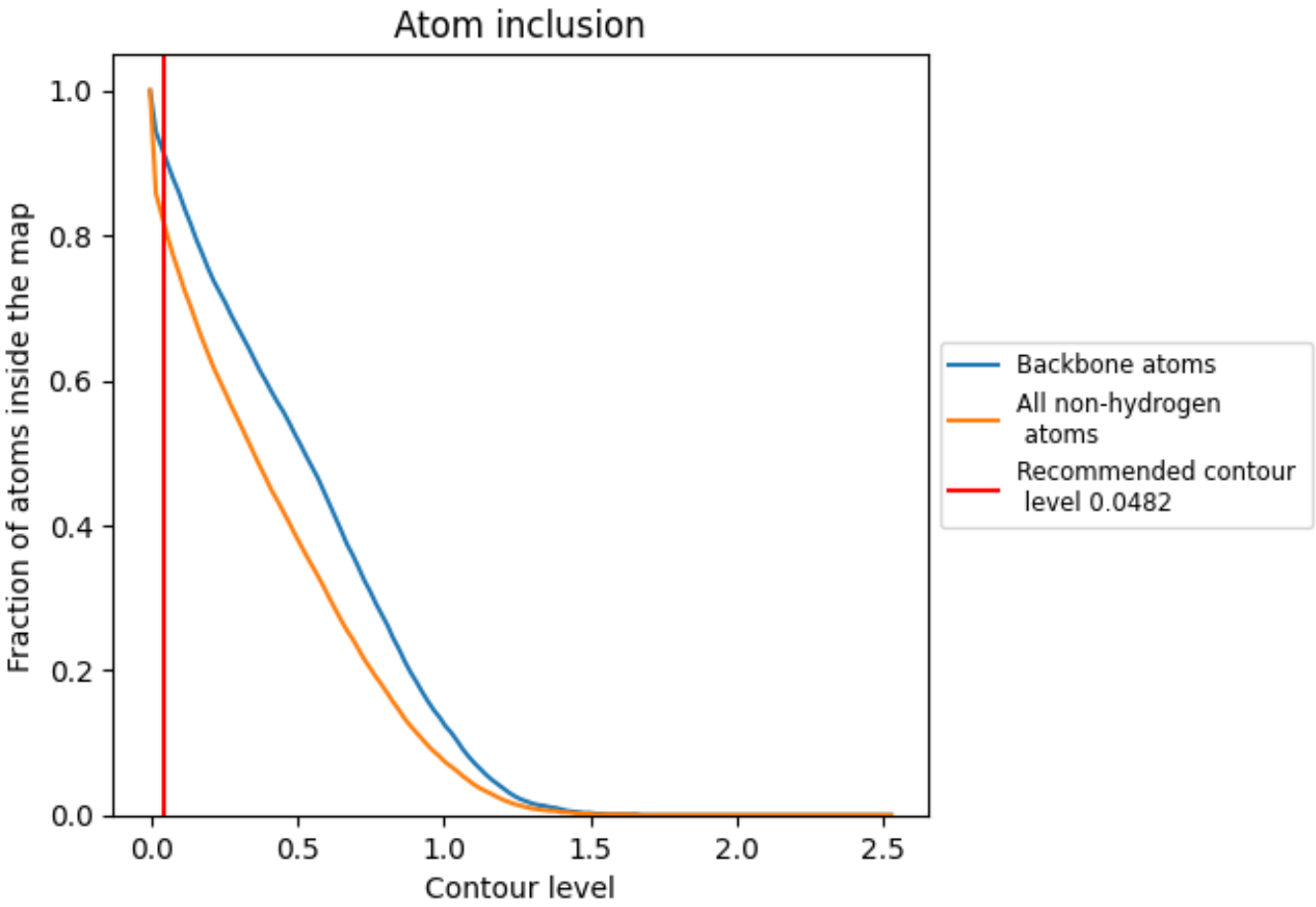
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0482).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (0.0482) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.3950
A	0.9170	0.5560
B	0.8600	0.5050
C	0.8510	0.4800
D	0.8300	0.4620
E	0.9110	0.4490
F	0.8750	0.4010
G	0.8030	0.2800
H	0.7670	0.2590
I	0.9260	0.4150
J	0.8750	0.3660
K	0.7870	0.3990
L	0.9210	0.5320
M	0.3740	0.0770
N	0.6170	0.2460
O	0.2560	0.0050
P	0.3440	0.0220

