



Full wwPDB EM Validation Report ⓘ

Jan 29, 2025 – 12:26 pm GMT

PDB ID : 8PY2
EMDB ID : EMD-18009
Title : Cryo-EM structure of the human BRISC dimer complex bound to compound JMS-175-2
Authors : Chandler, F.; Zeqiraj, E.
Deposited on : 2023-07-24
Resolution : 3.32 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
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.40

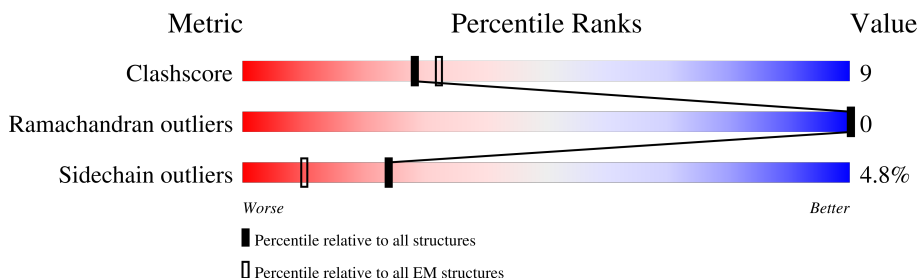
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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	316	<div> <div>8%</div> <div>56%</div> <div>23%</div> <div>•</div> <div>20%</div> </div>
1	C	316	<div> <div>•</div> <div>57%</div> <div>22%</div> <div>•</div> <div>20%</div> </div>
1	G	316	<div> <div>9%</div> <div>55%</div> <div>23%</div> <div>•</div> <div>20%</div> </div>
1	I	316	<div> <div>10%</div> <div>53%</div> <div>26%</div> <div>•</div> <div>20%</div> </div>
2	B	267	<div> <div>6%</div> <div>69%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>
2	D	267	<div> <div>6%</div> <div>67%</div> <div>21%</div> <div>•</div> <div>11%</div> </div>
2	H	267	<div> <div>15%</div> <div>63%</div> <div>24%</div> <div>•</div> <div>11%</div> </div>
2	J	267	<div> <div>7%</div> <div>64%</div> <div>24%</div> <div>•</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	385	<div><div><div>64%</div><div>74%</div><div>25%</div><div>..</div></div></div>
3	F	385	<div><div><div>51%</div><div>83%</div><div>15%</div><div>..</div></div></div>
3	K	385	<div><div><div>43%</div><div>76%</div><div>23%</div><div>.</div></div></div>
3	L	385	<div><div><div>84%</div><div>74%</div><div>24%</div><div>..</div></div></div>
4	M	259	<div><div><div>92%</div><div>85%</div><div>6%</div><div>8%</div></div></div>
4	N	259	<div><div><div>92%</div><div>85%</div><div>6%</div><div>8%</div></div></div>
4	O	259	<div><div><div>92%</div><div>85%</div><div>6%</div><div>8%</div></div></div>
4	P	259	<div><div><div>92%</div><div>84%</div><div>7%</div><div>8%</div></div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 35730 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 Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	252	Total 2023	C 1269	N 362	O 378	S 14	0	0
1	C	252	Total 2022	C 1269	N 362	O 377	S 14	0	0
1	G	252	Total 2027	C 1272	N 363	O 378	S 14	0	0
1	I	252	Total 2027	C 1272	N 363	O 378	S 14	0	0

- Molecule 2 is a protein called BRISC complex subunit Abraxas 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	237	Total 1937	C 1217	N 353	O 360	S 7	0	0
2	D	237	Total 1937	C 1217	N 353	O 360	S 7	0	0
2	H	237	Total 1937	C 1217	N 353	O 360	S 7	0	0
2	J	237	Total 1937	C 1217	N 353	O 360	S 7	0	0

- Molecule 3 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	383	Total 3078	C 1993	N 504	O 567	S 14	0	0
3	F	383	Total 3072	C 1990	N 501	O 567	S 14	0	0
3	K	383	Total 3078	C 1993	N 504	O 567	S 14	0	0
3	L	383	Total 3060	C 1978	N 501	O 567	S 14	0	0

There are 8 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
K	-1	GLY	-	expression tag	UNP Q9NXR7
K	0	ALA	-	expression tag	UNP Q9NXR7
L	-1	GLY	-	expression tag	UNP Q9NXR7
L	0	ALA	-	expression tag	UNP Q9NXR7

- Molecule 4 is a protein called BRISC and BRCA1-A complex member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	237	Total	C	N	O	S	0	0
			1888	1206	306	358	18		
4	N	237	Total	C	N	O	S	0	0
			1876	1196	306	356	18		
4	O	237	Total	C	N	O	S	0	0
			1870	1194	301	357	18		
4	P	237	Total	C	N	O	S	0	0
			1887	1206	306	357	18		

There are 4 discrepancies between the modelled and reference sequences:

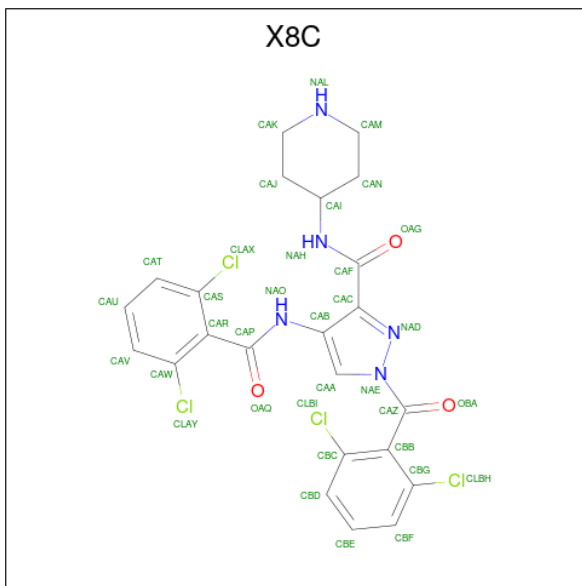
Chain	Residue	Modelled	Actual	Comment	Reference
M	71	MET	-	initiating methionine	UNP Q9NWX8
N	71	MET	-	initiating methionine	UNP Q9NWX8
O	71	MET	-	initiating methionine	UNP Q9NWX8
P	71	MET	-	initiating methionine	UNP Q9NWX8

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	

- Molecule 6 is 1-[2,6-bis(chloranyl)phenyl]carbonyl-4-[[2,6-bis(chloranyl)phenyl]carbo
nylamino]-N-piperidin-4-yl-pyrazole-3-carboxamide (three-letter code: X8C) (formula:

C₂₃H₁₉Cl₄N₅O₃) (labeled as "Ligand of Interest" by depositor).

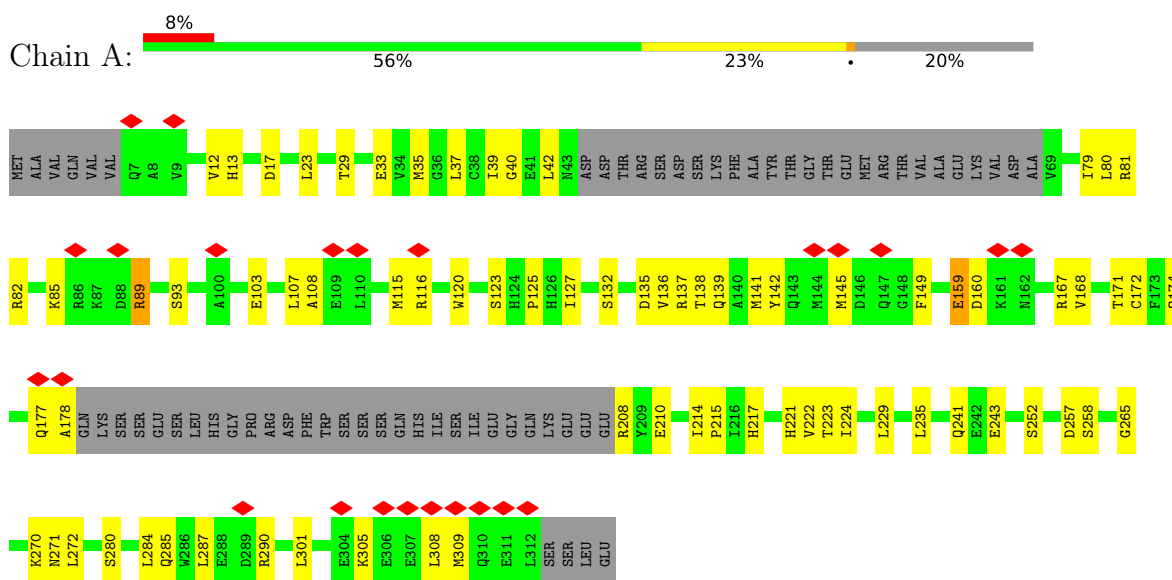


Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total 35	C 23	Cl 4	N 5	O 3	0
6	F	1	Total 35	C 23	Cl 4	N 5	O 3	0

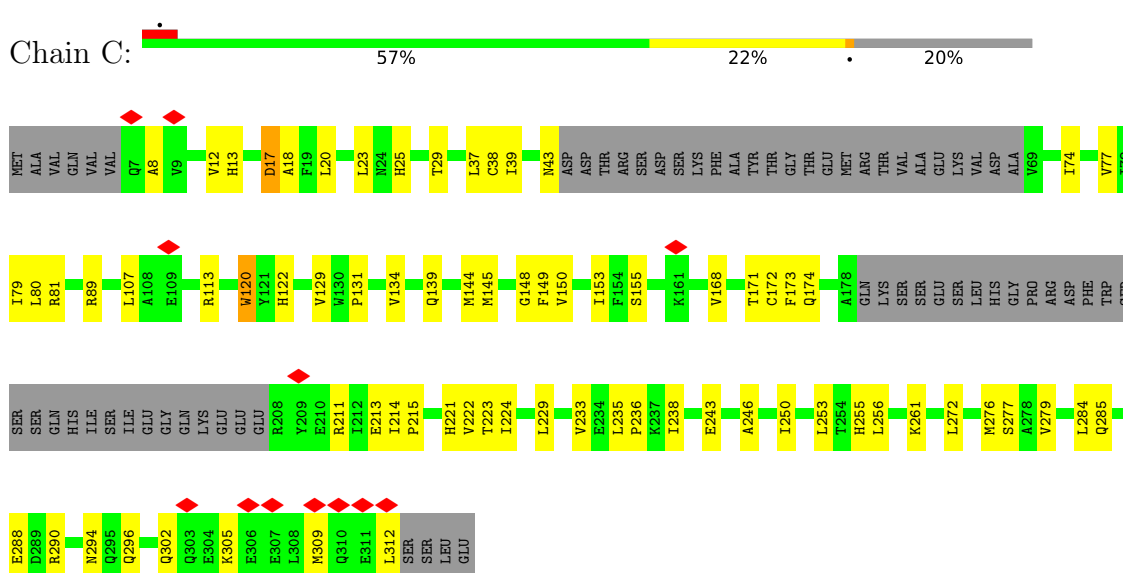
3 Residue-property plots

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.

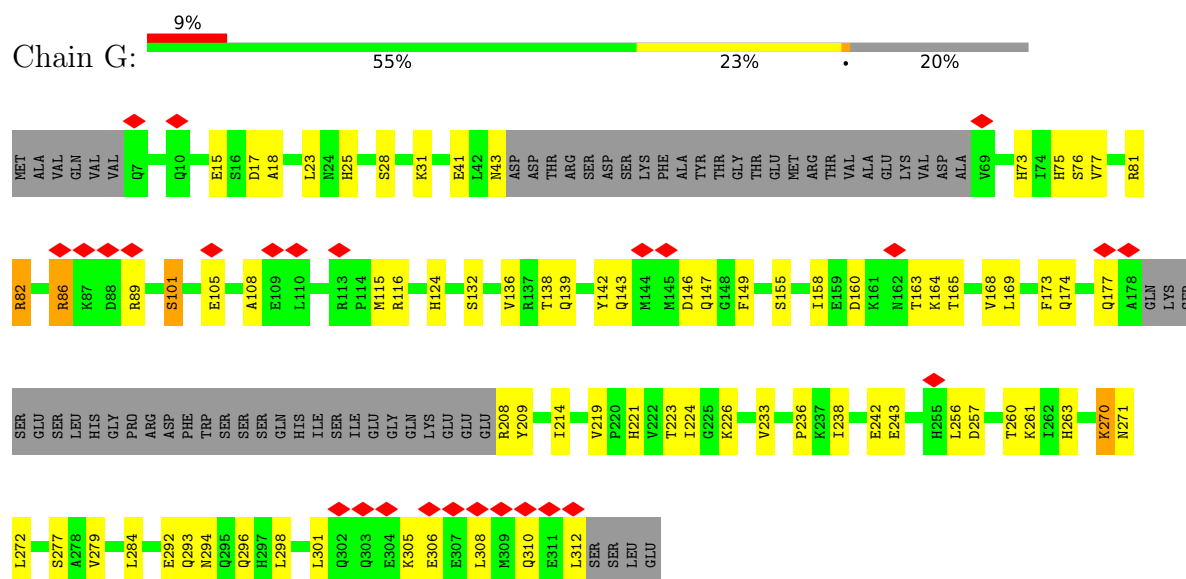
- Molecule 1: Lys-63-specific deubiquitinase BRCC36



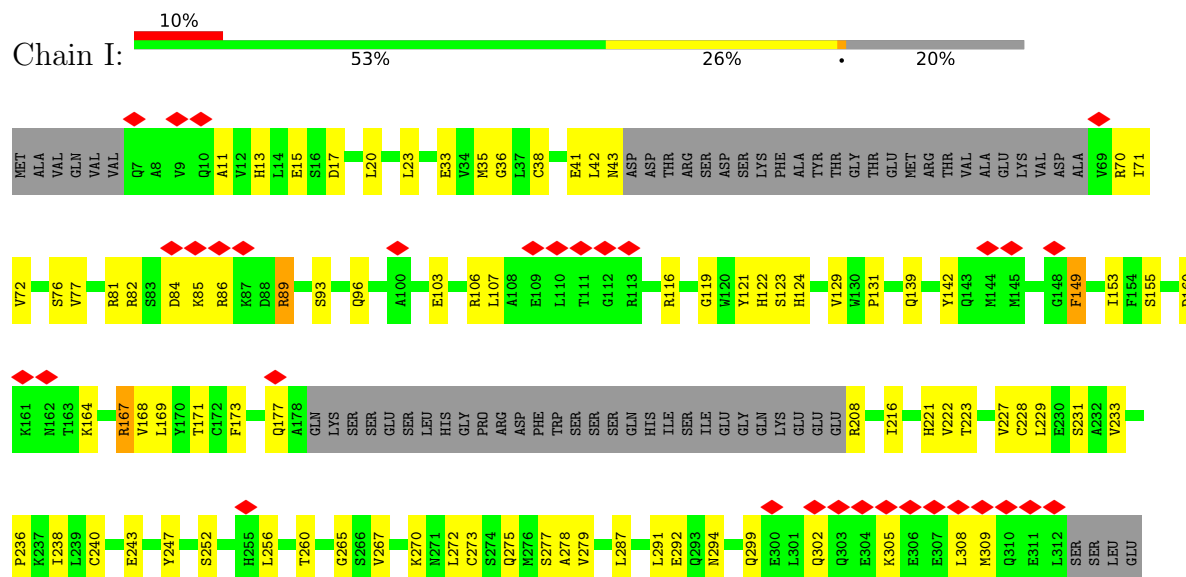
- Molecule 1: Lys-63-specific deubiquitinase BRCC36



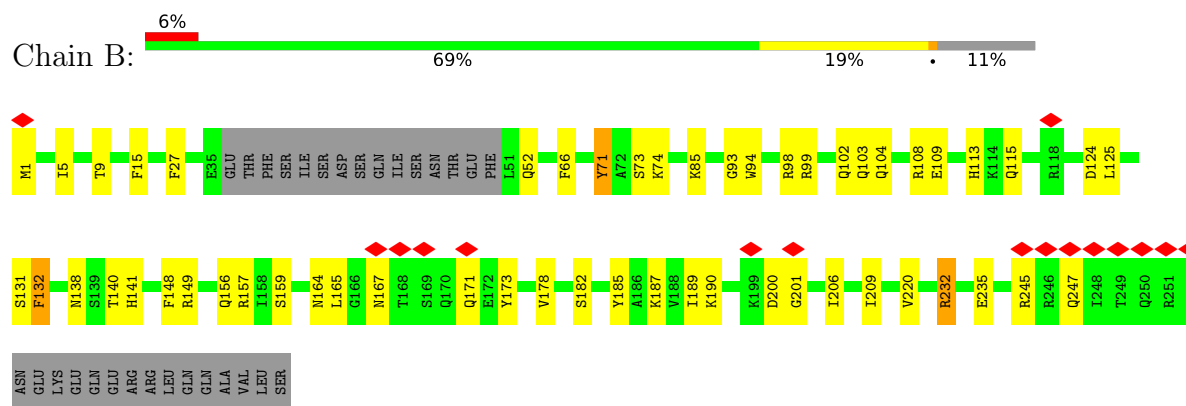
- Molecule 1: Lys-63-specific deubiquitinase BRCC36



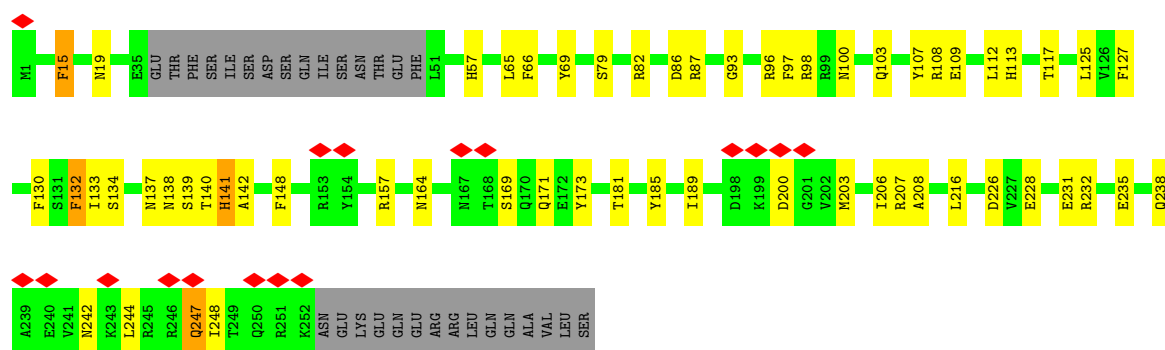
• Molecule 1: Lys-63-specific deubiquitinase BRCC36



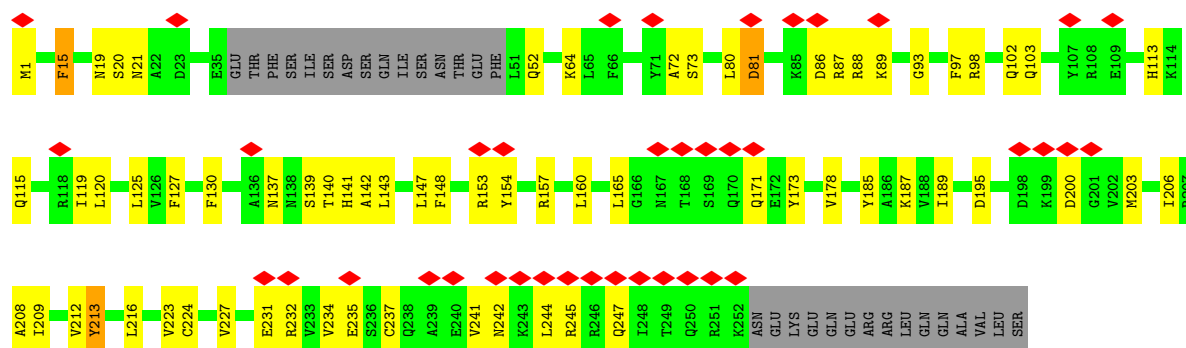
• Molecule 2: BRISC complex subunit Abraxas 2



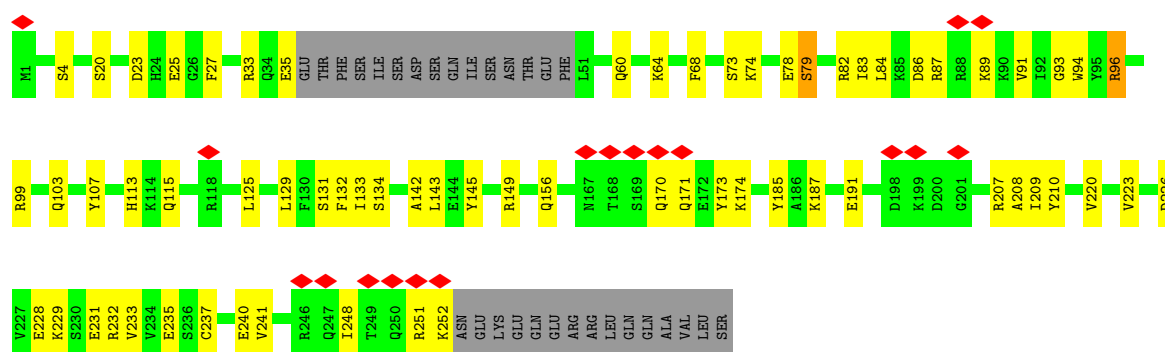
• Molecule 2: BRISC complex subunit Abraxas 2



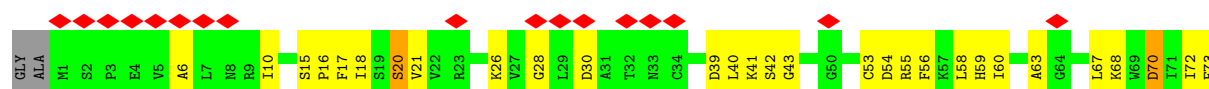
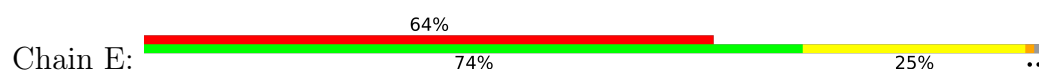
• Molecule 2: BRISC complex subunit Abraxas 2

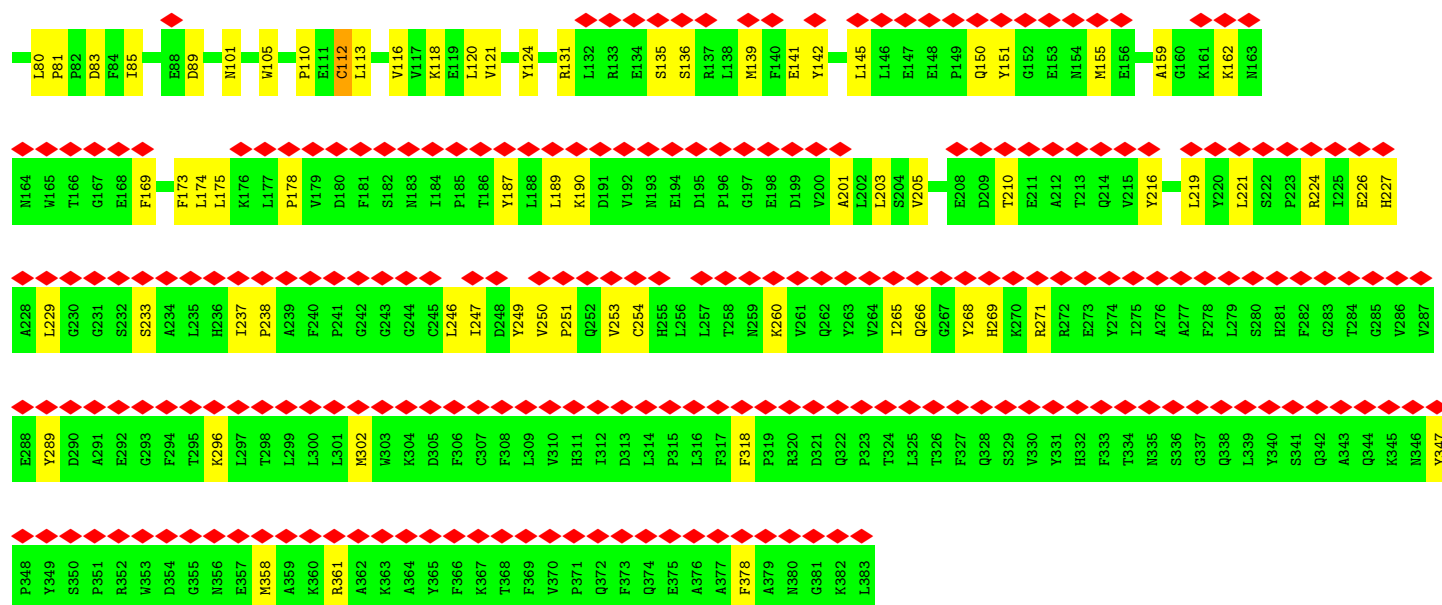


• Molecule 2: BRISC complex subunit Abraxas 2

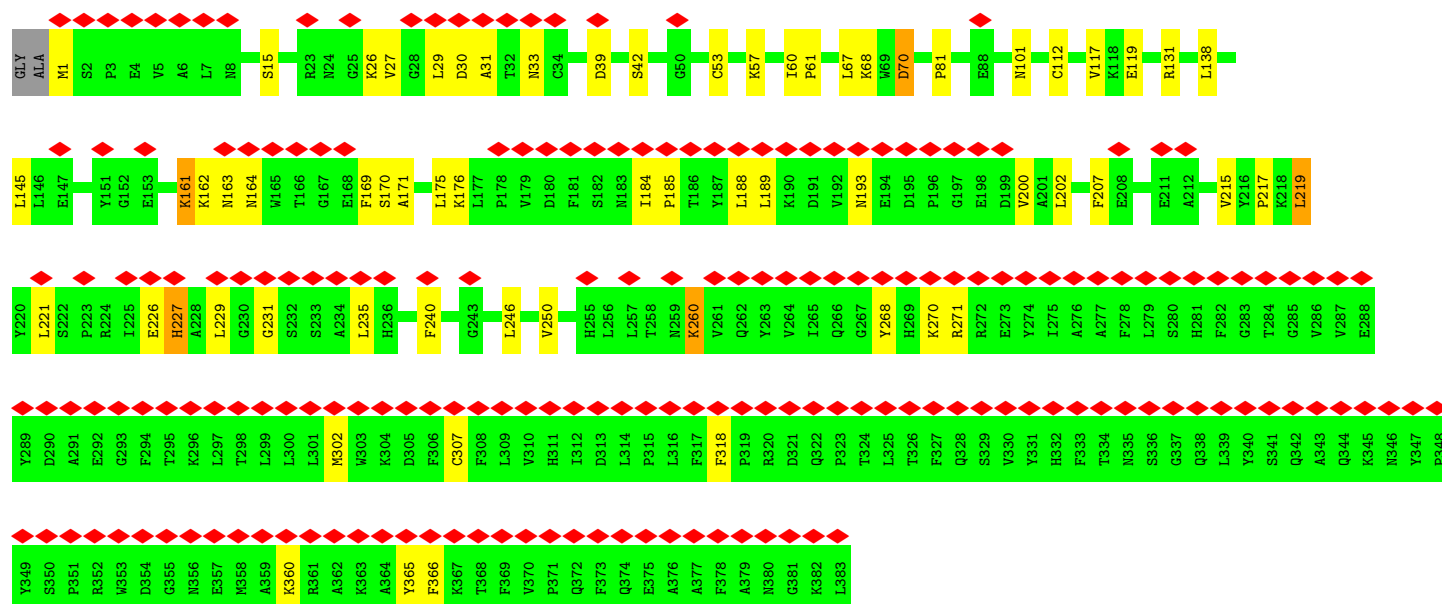
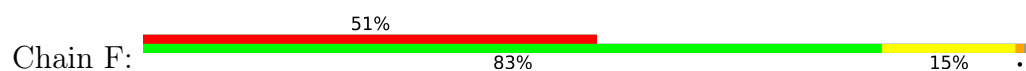


• Molecule 3: BRISC and BRCA1-A complex member 2

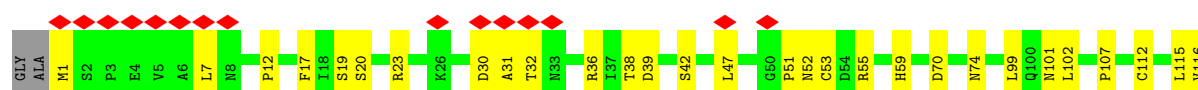
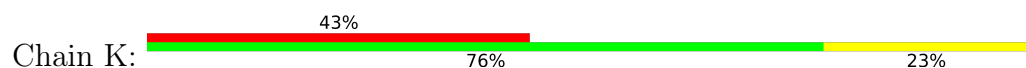


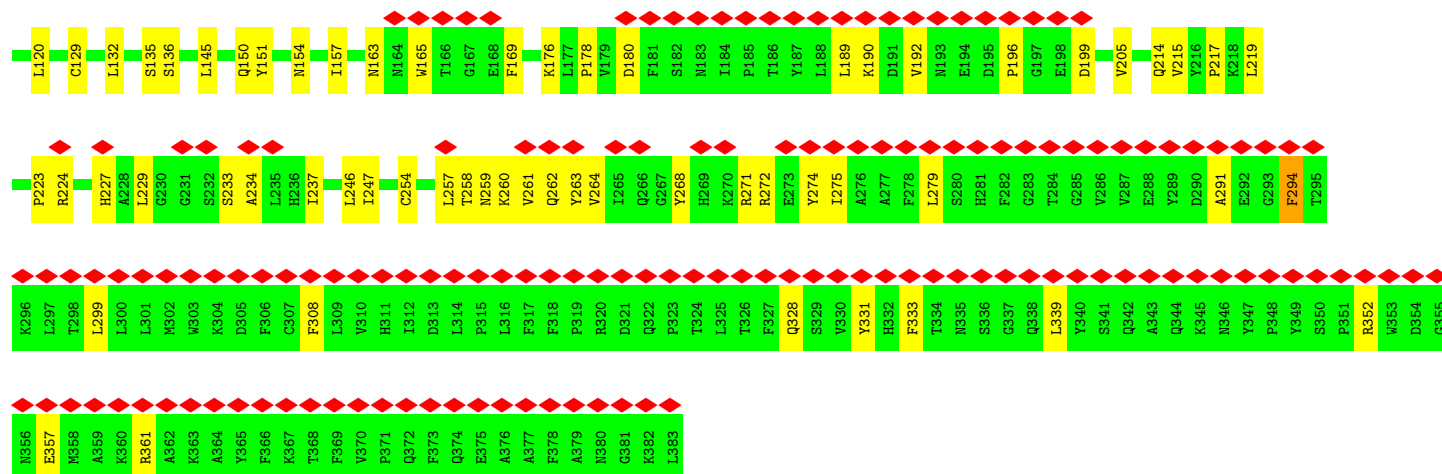


• Molecule 3: BRISC and BRCA1-A complex member 2

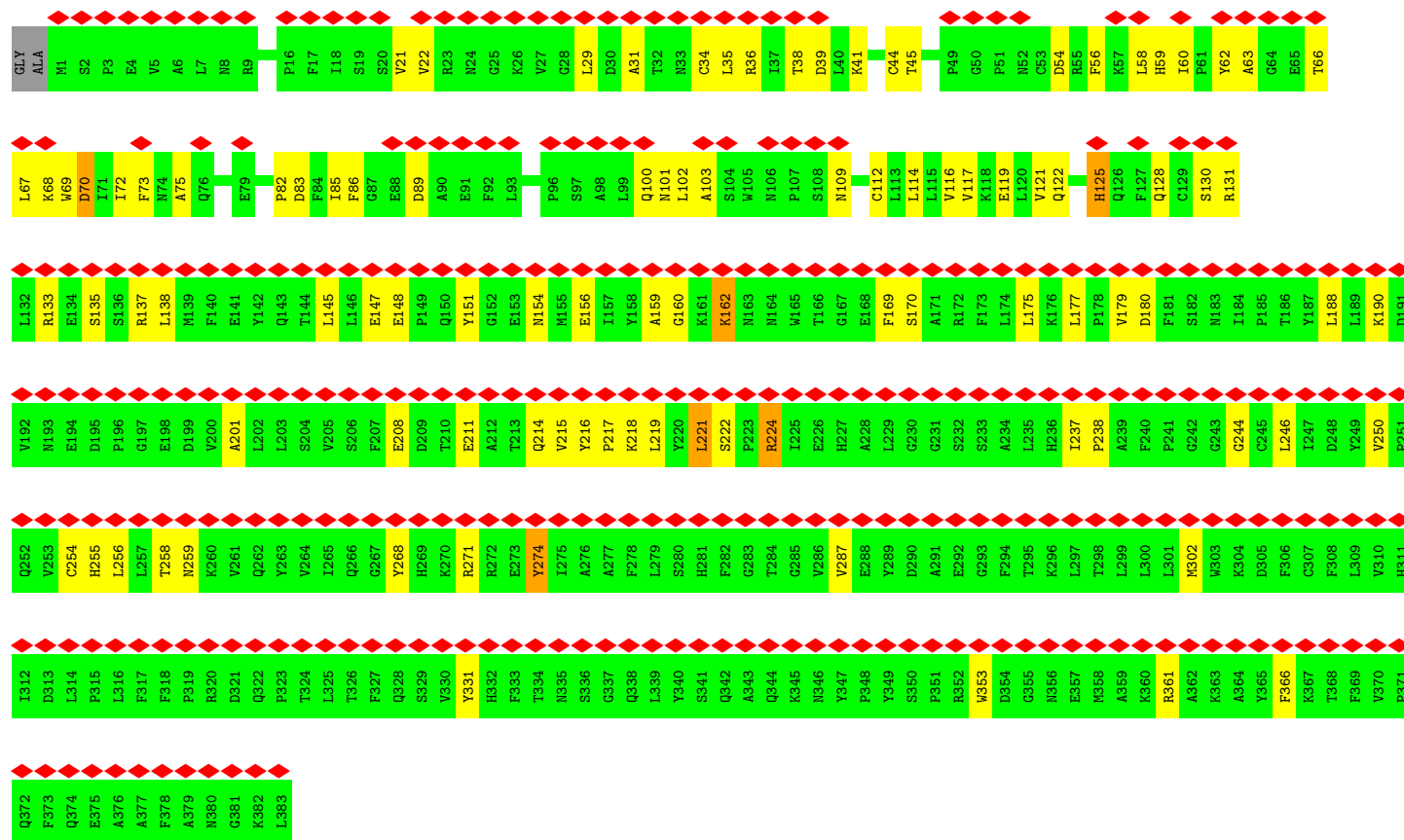
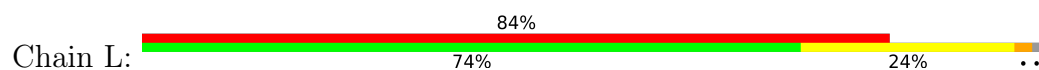


• Molecule 3: BRISC and BRCA1-A complex member 2

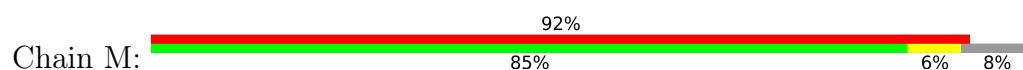


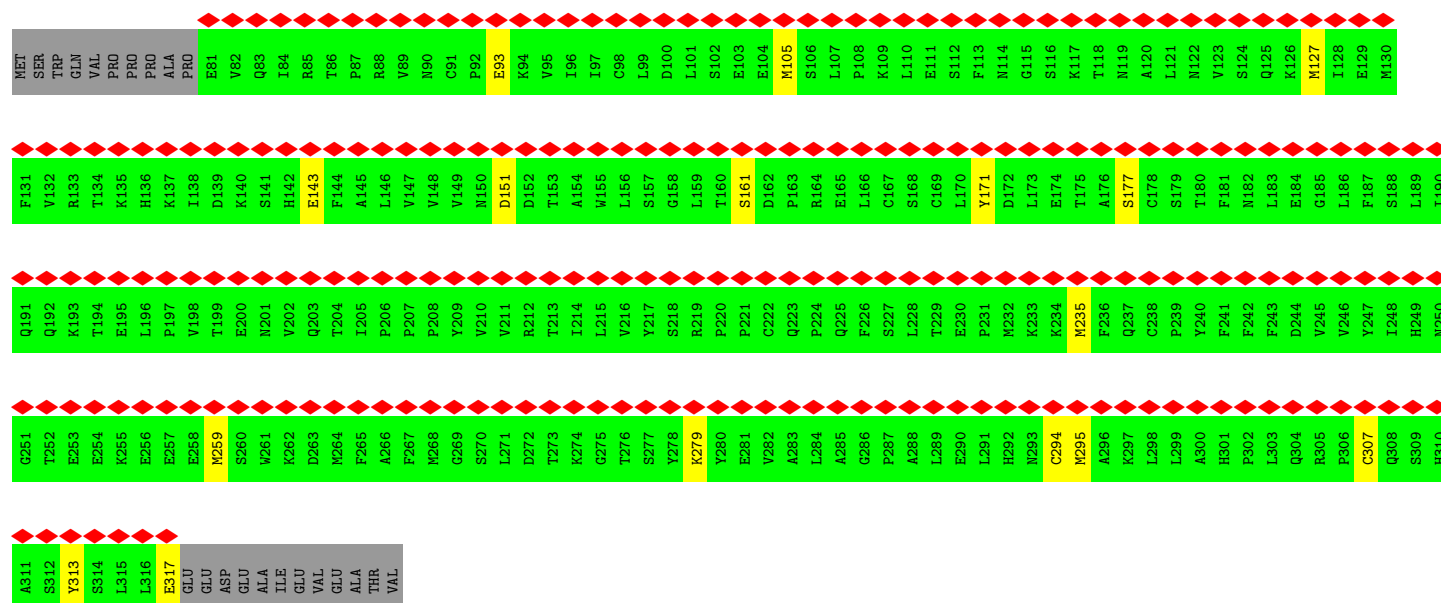


• Molecule 3: BRISC and BRCA1-A complex member 2

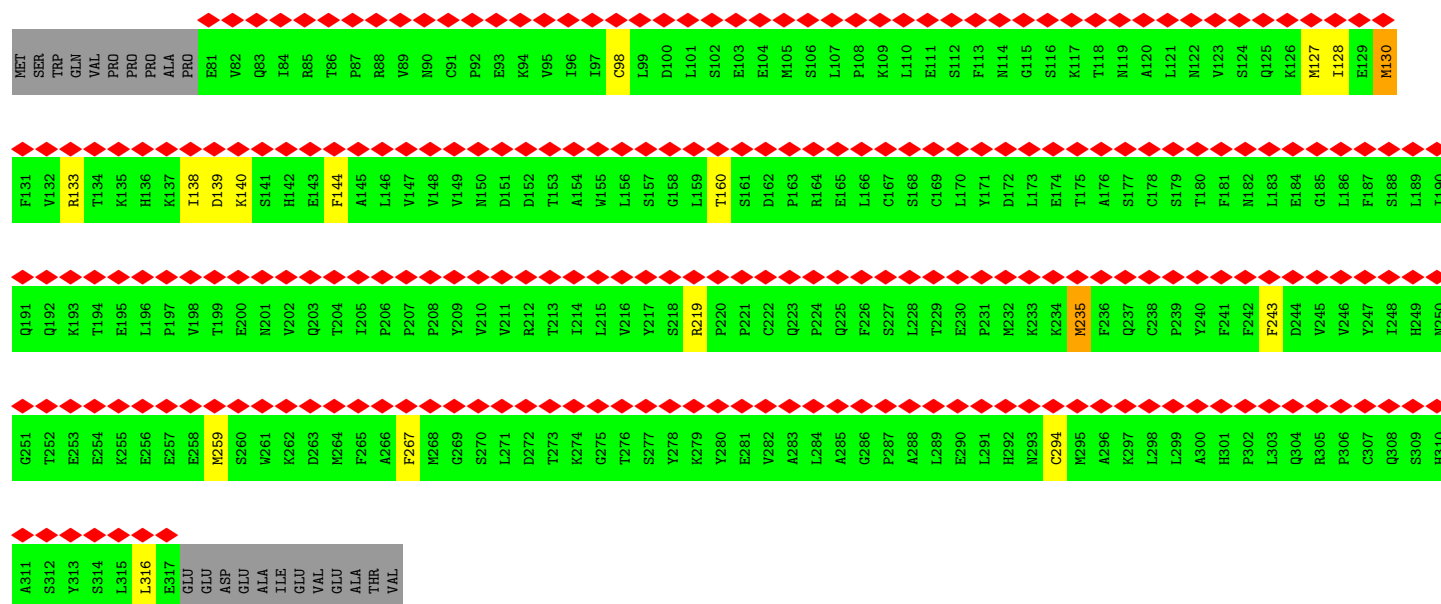
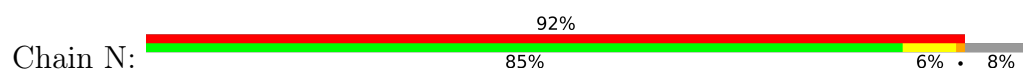


• Molecule 4: BRISC and BRCA1-A complex member 1

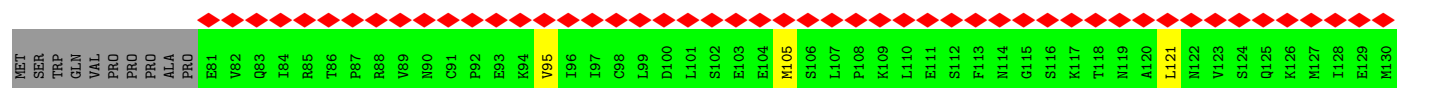
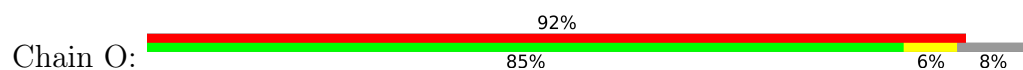


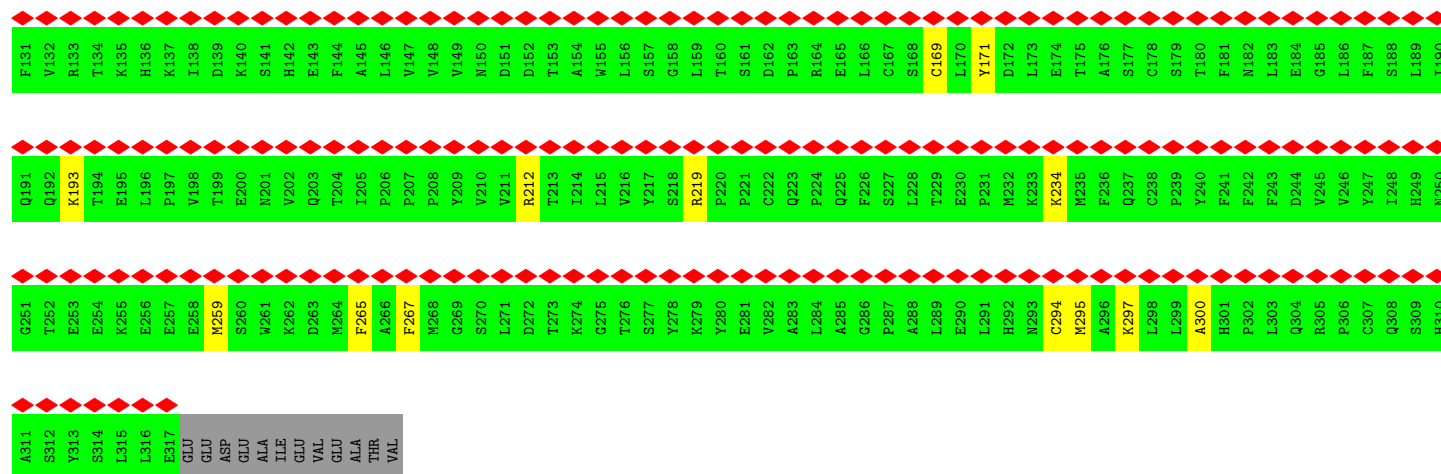


• Molecule 4: BRISC and BRCA1-A complex member 1

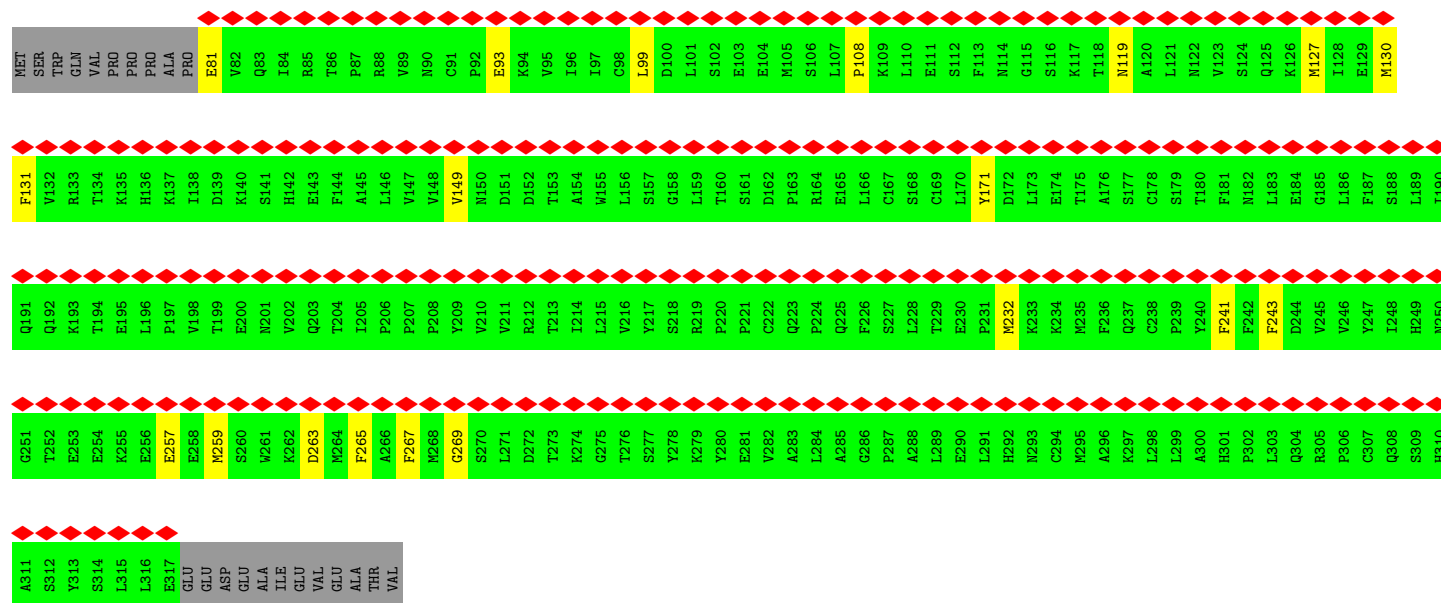
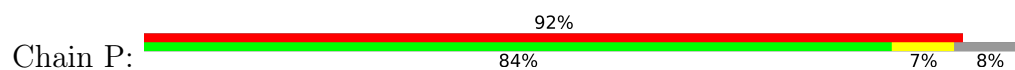


• Molecule 4: BRISC and BRCA1-A complex member 1





- Molecule 4: BRISC and BRCA1-A complex member 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371872	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 ($e^-/\text{\AA}^2$)	39.84	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0095	Depositor
Map size (Å)	289.344, 289.344, 289.344	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82199997, 0.82199997, 0.82199997	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, X8C

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	0.24	0/2059	0.49	0/2784
1	C	0.25	0/2058	0.50	0/2783
1	G	0.24	0/2063	0.48	0/2788
1	I	0.24	0/2063	0.48	0/2788
2	B	0.26	0/1972	0.49	0/2655
2	D	0.26	0/1972	0.51	0/2655
2	H	0.26	0/1972	0.48	0/2655
2	J	0.25	0/1972	0.48	0/2655
3	E	0.25	0/3169	0.47	0/4310
3	F	0.25	0/3163	0.47	0/4303
3	K	0.25	0/3169	0.47	0/4310
3	L	0.25	0/3150	0.47	0/4286
4	M	0.25	0/1933	0.48	0/2622
4	N	0.24	0/1920	0.47	0/2604
4	O	0.25	0/1913	0.48	0/2597
4	P	0.24	0/1932	0.48	0/2621
All	All	0.25	0/36480	0.48	0/49416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2023	0	2011	49	0
1	C	2022	0	2008	49	0
1	G	2027	0	2022	55	0
1	I	2027	0	2022	66	0
2	B	1937	0	1924	37	0
2	D	1937	0	1924	47	0
2	H	1937	0	1924	55	0
2	J	1937	0	1924	43	0
3	E	3078	0	3001	54	0
3	F	3072	0	2990	32	0
3	K	3078	0	3001	54	0
3	L	3060	0	2965	58	0
4	M	1888	0	1868	2	0
4	N	1876	0	1840	5	0
4	O	1870	0	1835	3	0
4	P	1887	0	1865	4	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	D	35	0	0	1	0
6	F	35	0	0	2	0
All	All	35730	0	35124	530	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 (530) 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:237:ILE:HD11	3:E:253:VAL:HG12	1.61	0.82
3:K:215:VAL:HG23	3:K:217:PRO:HD3	1.65	0.78
2:H:140:THR:HG23	1:I:171:THR:HG22	1.69	0.73
2:H:72:ALA:HB2	3:L:103:ALA:HB2	1.70	0.73
2:J:23:ASP:OD1	3:K:55:ARG:NH2	2.22	0.72
3:F:26:LYS:HD2	3:F:30:ASP:HB2	1.70	0.72
3:L:302:MET:SD	3:L:302:MET:N	2.64	0.70
3:K:145:LEU:HD11	3:K:246:LEU:HD23	1.72	0.70
1:C:139:GLN:NE2	1:C:149:PHE:O	2.24	0.69
3:K:36:ARG:HB3	3:K:59:HIS:HB2	1.72	0.69
2:D:132:PHE:HE1	2:D:141:HIS:HB3	1.58	0.69
2:J:25:GLU:HB2	2:J:96:ARG:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:THR:HG22	2:D:140:THR:HG23	1.76	0.68
1:C:223:THR:HG21	2:D:235:GLU:HB2	1.76	0.68
3:K:132:LEU:HD21	3:K:157:ILE:HD12	1.76	0.67
3:L:44:CYS:SG	3:L:45:THR:N	2.67	0.67
2:J:73:SER:O	2:J:115:GLN:NE2	2.27	0.67
2:H:173:TYR:OH	1:I:243:GLU:OE2	2.12	0.67
2:B:98:ARG:NH1	2:B:109:GLU:OE1	2.28	0.67
3:L:59:HIS:HB3	3:L:66:THR:HB	1.77	0.66
3:E:173:PHE:HB2	3:E:205:VAL:HB	1.77	0.66
2:J:93:GLY:HA2	2:J:125:LEU:HG	1.78	0.66
1:A:223:THR:HG21	2:B:235:GLU:HB2	1.77	0.66
2:H:87:ARG:HH22	1:I:292:GLU:HB3	1.60	0.65
2:D:93:GLY:HA2	2:D:125:LEU:HG	1.77	0.65
1:A:142:TYR:HB3	1:A:149:PHE:HD2	1.62	0.65
4:M:143:GLU:HA	4:M:161:SER:HA	1.79	0.65
3:L:21:VAL:HA	3:L:114:LEU:HD11	1.78	0.64
3:L:36:ARG:HB2	3:L:59:HIS:HB2	1.78	0.64
2:H:93:GLY:HA2	2:H:125:LEU:HG	1.79	0.64
2:B:93:GLY:HA2	2:B:125:LEU:HG	1.80	0.64
1:G:81:ARG:HG2	1:G:238:ILE:HG23	1.80	0.64
1:C:89:ARG:HH21	1:C:134:VAL:HG21	1.63	0.63
2:H:235:GLU:HB2	1:I:223:THR:HG21	1.78	0.63
2:B:171:GLN:NE2	2:D:169:SER:O	2.31	0.63
3:K:154:ASN:ND2	3:K:176:LYS:O	2.31	0.63
1:C:285:GLN:NE2	2:D:57:HIS:O	2.32	0.62
3:E:203:LEU:HD11	3:E:253:VAL:HG21	1.81	0.62
2:B:74:LYS:HA	2:B:115:GLN:HE22	1.64	0.62
1:C:243:GLU:OE1	2:D:173:TYR:OH	2.17	0.62
3:E:131:ARG:HE	3:E:162:LYS:HE3	1.63	0.62
1:G:219:VAL:HG22	3:K:47:LEU:HD11	1.80	0.62
3:L:162:LYS:HG2	3:L:169:PHE:HB3	1.81	0.62
2:H:21:ASN:HA	3:L:45:THR:HG23	1.81	0.62
1:G:296:GLN:OE1	2:J:87:ARG:NH2	2.33	0.61
3:F:60:ILE:HB	3:F:67:LEU:HB2	1.83	0.61
1:I:38:CYS:N	1:I:119:GLY:O	2.32	0.60
3:L:237:ILE:HD12	3:L:238:PRO:HD2	1.83	0.60
1:G:86:ARG:HE	1:G:89:ARG:HH21	1.48	0.60
2:B:164:ASN:ND2	2:B:167:ASN:OD1	2.35	0.60
6:F:401:X8C:CLAY	6:F:401:X8C:NAO	2.71	0.60
2:H:1:MET:N	2:H:52:GLN:O	2.34	0.60
1:A:222:VAL:HG23	1:A:223:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:ARG:O	2:H:153:ARG:NH1	2.32	0.60
2:J:86:ASP:O	2:J:89:LYS:NZ	2.34	0.60
3:L:102:LEU:HD13	3:L:116:VAL:HG11	1.84	0.60
1:G:17:ASP:HB3	1:G:224:ILE:HG22	1.83	0.60
1:I:17:ASP:OD2	1:I:221:HIS:ND1	2.35	0.59
3:K:229:LEU:HD21	3:K:261:VAL:HG23	1.84	0.59
1:I:142:TYR:HB3	1:I:149:PHE:HD2	1.66	0.59
1:G:41:GLU:OE2	1:G:43:ASN:ND2	2.35	0.59
2:J:84:LEU:HD13	2:J:91:VAL:HG21	1.85	0.59
2:D:228:GLU:OE2	2:D:232:ARG:NH1	2.35	0.59
1:A:108:ALA:HB2	1:A:115:MET:HB2	1.84	0.58
2:H:103:GLN:O	2:H:157:ARG:NH2	2.36	0.58
3:L:177:LEU:HD22	3:L:254:CYS:HB2	1.85	0.58
2:H:232:ARG:NH1	2:H:235:GLU:OE1	2.36	0.58
1:G:17:ASP:OD1	1:G:17:ASP:N	2.36	0.58
1:I:129:VAL:HG11	1:I:169:LEU:HB2	1.85	0.58
1:C:25:HIS:CE1	1:C:79:ILE:HG23	2.39	0.58
3:F:31:ALA:HB3	3:F:61:PRO:HB2	1.86	0.58
2:D:127:PHE:HB3	2:D:148:PHE:HB2	1.84	0.58
3:F:176:LYS:HG2	3:F:200:VAL:HG11	1.86	0.58
2:J:228:GLU:OE2	2:J:232:ARG:NH1	2.37	0.58
1:G:243:GLU:OE1	2:J:173:TYR:OH	2.21	0.58
1:I:139:GLN:NE2	1:I:149:PHE:O	2.37	0.58
3:E:43:GLY:O	3:E:55:ARG:NH2	2.37	0.57
3:L:29:LEU:HD23	3:L:154:ASN:HB3	1.87	0.57
1:A:142:TYR:HB3	1:A:149:PHE:CD2	2.38	0.57
2:B:200:ASP:OD1	2:B:201:GLY:N	2.37	0.57
4:N:127:MET:HA	4:N:130:MET:SD	2.44	0.57
3:E:70:ASP:HB2	3:E:85:ILE:HB	1.86	0.57
3:L:137:ARG:NH1	3:L:211:GLU:OE2	2.37	0.57
1:A:270:LYS:NZ	2:D:171:GLN:OE1	2.38	0.57
3:K:19:SER:OG	3:K:23:ARG:NH2	2.38	0.57
1:C:23:LEU:HD11	1:C:168:VAL:HG11	1.87	0.56
2:H:141:HIS:NE2	1:I:216:ILE:O	2.38	0.56
1:A:178:ALA:O	1:A:208:ARG:NH2	2.38	0.56
2:H:242:ASN:HA	2:H:245:ARG:HE	1.70	0.56
3:K:229:LEU:HB2	3:K:234:ALA:HB2	1.87	0.56
3:L:128:GLN:HE21	3:L:159:ALA:H	1.53	0.56
3:K:272:ARG:NH1	3:K:291:ALA:O	2.38	0.56
2:H:165:LEU:HD21	1:I:275:GLN:HA	1.88	0.56
1:I:107:LEU:HD21	1:I:227:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:190:LYS:HE2	3:L:224:ARG:HH11	1.71	0.56
3:E:189:LEU:HA	3:E:224:ARG:HD2	1.86	0.56
2:H:223:VAL:O	2:H:227:VAL:HG12	2.06	0.56
1:I:160:ASP:OD1	1:I:167:ARG:NH2	2.35	0.56
3:L:86:PHE:HB3	3:L:89:ASP:HB2	1.88	0.56
1:I:15:GLU:OE1	1:I:221:HIS:ND1	2.39	0.56
1:A:308:LEU:HD11	2:B:245:ARG:HD3	1.87	0.56
3:E:72:ILE:HB	3:E:83:ASP:HB3	1.88	0.56
2:H:113:HIS:CE1	2:H:125:LEU:HB3	2.41	0.55
4:N:127:MET:SD	4:N:128:ILE:N	2.79	0.55
1:A:243:GLU:OE1	2:B:173:TYR:OH	2.23	0.55
2:D:103:GLN:O	2:D:157:ARG:NH2	2.40	0.55
1:I:81:ARG:HG2	1:I:238:ILE:HG23	1.87	0.55
2:D:98:ARG:NH1	2:D:109:GLU:OE1	2.39	0.55
2:H:73:SER:O	2:H:115:GLN:NE2	2.39	0.55
2:B:73:SER:OG	2:B:108:ARG:NE	2.39	0.55
3:E:150:GLN:HG2	3:E:178:PRO:HG2	1.88	0.55
1:A:174:GLN:HB2	1:A:214:ILE:HD11	1.88	0.55
1:G:163:THR:HB	1:G:165:THR:HG22	1.88	0.55
3:K:219:LEU:HB2	3:K:237:ILE:HD13	1.89	0.55
3:F:1:MET:SD	3:F:1:MET:N	2.75	0.55
2:J:20:SER:O	2:J:99:ARG:NH2	2.39	0.55
1:C:79:ILE:HD13	1:C:235:LEU:HB2	1.89	0.54
1:C:81:ARG:HG2	1:C:238:ILE:HG23	1.89	0.54
3:F:229:LEU:HD21	3:F:260:LYS:HD3	1.89	0.54
2:D:66:PHE:HD2	3:E:80:LEU:HD13	1.72	0.54
1:G:305:LYS:HZ1	1:G:308:LEU:HD22	1.72	0.54
1:A:139:GLN:NE2	1:A:149:PHE:O	2.35	0.54
3:E:221:LEU:HB2	3:E:226:GLU:HG3	1.89	0.54
1:G:272:LEU:HD23	2:J:209:ILE:HG23	1.88	0.54
3:K:229:LEU:O	3:K:233:SER:OG	2.24	0.54
3:L:70:ASP:HB2	3:L:85:ILE:HB	1.89	0.54
1:A:35:MET:HG2	1:A:82:ARG:HD2	1.90	0.54
2:B:232:ARG:HE	2:B:232:ARG:HA	1.73	0.54
1:G:116:ARG:NH2	1:G:146:ASP:OD2	2.41	0.54
2:H:19:ASN:OD1	1:I:221:HIS:N	2.39	0.54
3:L:109:ASN:HD21	3:L:112:CYS:HB2	1.72	0.54
3:E:63:ALA:HA	3:E:174:LEU:HD22	1.90	0.54
1:G:260:THR:HG23	2:J:174:LYS:HE2	1.89	0.54
1:C:211:ARG:HH12	3:K:136:SER:HG	1.55	0.54
2:H:81:ASP:HB3	2:H:88:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:ASP:OD1	2:H:195:ASP:N	2.41	0.54
1:G:108:ALA:HB2	1:G:115:MET:HB2	1.88	0.54
3:L:287:VAL:HA	4:O:300:ALA:HA	1.89	0.54
2:B:98:ARG:NH2	2:B:102:GLN:O	2.41	0.53
1:G:23:LEU:HD11	1:G:168:VAL:HG11	1.89	0.53
2:J:113:HIS:CE1	2:J:125:LEU:HB3	2.44	0.53
2:D:79:SER:HA	2:D:82:ARG:HD3	1.89	0.53
3:F:162:LYS:HB2	3:F:169:PHE:CE1	2.43	0.53
1:G:43:ASN:N	1:G:43:ASN:OD1	2.41	0.53
2:J:60:GLN:NE2	2:J:83:ILE:O	2.38	0.53
3:L:56:PHE:HE1	3:L:58:LEU:HD12	1.73	0.53
4:P:127:MET:HA	4:P:130:MET:SD	2.49	0.53
3:E:135:SER:OG	3:E:136:SER:N	2.42	0.53
3:L:121:VAL:HG12	3:L:125:HIS:CE1	2.44	0.53
1:A:17:ASP:OD2	1:A:224:ILE:HA	2.09	0.53
1:A:23:LEU:HD11	1:A:168:VAL:HG11	1.91	0.53
2:D:15:PHE:O	2:D:19:ASN:HB2	2.09	0.53
1:I:82:ARG:NH2	1:I:86:ARG:O	2.23	0.53
3:K:101:ASN:ND2	3:K:115:LEU:HB3	2.24	0.53
3:K:257:LEU:O	3:K:261:VAL:HG12	2.09	0.53
2:B:182:SER:OG	1:C:288:GLU:OE1	2.26	0.52
2:B:149:ARG:N	2:B:156:GLN:O	2.42	0.52
3:E:59:HIS:CE1	3:E:68:LYS:HG2	2.44	0.52
1:G:25:HIS:O	1:G:28:SER:OG	2.26	0.52
1:I:41:GLU:OE2	1:I:43:ASN:ND2	2.43	0.52
1:A:284:LEU:HD23	2:D:185:TYR:HB2	1.91	0.52
1:C:296:GLN:OE1	2:D:87:ARG:NH2	2.43	0.52
3:L:72:ILE:N	3:L:83:ASP:O	2.42	0.52
3:L:22:VAL:HA	3:L:35:LEU:HD21	1.90	0.52
3:E:210:THR:HG21	3:K:357:GLU:H	1.74	0.52
3:K:102:LEU:HG	3:K:116:VAL:HG21	1.92	0.52
1:C:129:VAL:HG22	1:C:171:THR:HG23	1.92	0.52
3:F:57:LYS:HD3	3:F:68:LYS:HB3	1.91	0.52
3:F:215:VAL:HG22	3:F:217:PRO:HD3	1.92	0.52
2:H:241:VAL:HG13	2:H:245:ARG:HH21	1.74	0.52
3:K:189:LEU:HD23	3:K:192:VAL:HA	1.91	0.52
4:N:235:MET:SD	4:N:235:MET:N	2.76	0.52
2:D:65:LEU:HD11	2:D:96:ARG:HH22	1.75	0.52
1:G:124:HIS:HB2	1:G:155:SER:HB2	1.91	0.52
2:H:127:PHE:HB3	2:H:148:PHE:HB2	1.91	0.52
3:K:17:PHE:HZ	3:K:107:PRO:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD23	2:B:209:ILE:HG23	1.92	0.51
1:G:160:ASP:O	1:G:164:LYS:N	2.38	0.51
1:G:305:LYS:HD3	2:J:241:VAL:HG22	1.92	0.51
1:C:131:PRO:HG3	1:C:173:PHE:CG	2.45	0.51
3:F:27:VAL:HG11	3:F:117:VAL:HG12	1.91	0.51
1:G:226:LYS:HD3	2:J:228:GLU:HG2	1.92	0.51
2:H:200:ASP:OD1	2:H:200:ASP:N	2.36	0.51
3:E:6:ALA:O	3:E:10:ILE:HG12	2.10	0.51
1:G:139:GLN:NE2	1:G:149:PHE:O	2.43	0.51
1:I:77:VAL:HG11	1:I:121:TYR:HE1	1.74	0.51
2:B:99:ARG:HG2	2:B:132:PHE:HB3	1.92	0.51
3:F:184:ILE:HG13	3:F:185:PRO:HD2	1.92	0.51
3:L:255:HIS:O	3:L:259:ASN:ND2	2.44	0.51
2:H:98:ARG:NH2	2:H:102:GLN:O	2.44	0.51
2:J:33:ARG:NH1	2:J:35:GLU:O	2.44	0.51
3:K:42:SER:HA	3:K:53:CYS:HA	1.93	0.51
1:G:15:GLU:OE1	1:G:221:HIS:ND1	2.40	0.51
2:J:79:SER:OG	2:J:82:ARG:NH2	2.44	0.51
3:L:117:VAL:O	3:L:121:VAL:HG23	2.10	0.51
1:A:37:LEU:HD12	1:A:80:LEU:HD11	1.92	0.50
1:I:299:GLN:O	1:I:302:GLN:HG3	2.10	0.50
1:A:215:PRO:HB3	2:B:138:ASN:HB2	1.92	0.50
1:I:233:VAL:O	1:I:236:PRO:HD2	2.10	0.50
3:L:180:ASP:OD1	3:L:180:ASP:N	2.43	0.50
1:C:222:VAL:HG13	1:C:223:THR:HG23	1.92	0.50
3:E:201:ALA:HB1	3:E:219:LEU:HD11	1.93	0.50
3:K:52:ASN:N	3:K:52:ASN:OD1	2.43	0.50
3:K:259:ASN:O	3:K:263:TYR:HB2	2.10	0.50
1:G:177:GLN:HA	1:G:208:ARG:HE	1.76	0.50
1:G:284:LEU:HD23	2:H:185:TYR:HB2	1.94	0.50
1:C:39:ILE:HG21	1:C:107:LEU:HD12	1.94	0.50
3:F:29:LEU:HD21	3:F:202:LEU:HD13	1.93	0.50
3:F:161:LYS:NZ	3:F:163:ASN:OD1	2.40	0.50
1:G:76:SER:OG	1:G:77:VAL:N	2.44	0.50
1:G:223:THR:HG21	2:J:235:GLU:HB2	1.94	0.50
1:G:256:LEU:O	1:G:261:LYS:NZ	2.45	0.50
2:B:1:MET:N	2:B:52:GLN:O	2.45	0.50
2:H:234:VAL:HA	2:H:237:CYS:SG	2.51	0.50
3:L:69:TRP:NE1	3:L:89:ASP:OD2	2.32	0.50
3:K:154:ASN:HD22	3:K:176:LYS:HB3	1.77	0.49
3:L:148:GLU:HG3	3:L:151:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:O	1:A:141:MET:HG3	2.12	0.49
1:G:101:SER:O	1:G:105:GLU:HG2	2.12	0.49
1:G:298:LEU:HD21	2:J:233:VAL:HG13	1.94	0.49
3:F:188:LEU:HD13	3:F:227:HIS:CE1	2.47	0.49
1:A:17:ASP:OD1	1:A:221:HIS:ND1	2.46	0.49
3:E:42:SER:HA	3:E:53:CYS:HA	1.94	0.49
3:E:265:ILE:O	3:E:269:HIS:ND1	2.46	0.49
3:E:18:ILE:HA	3:E:21:VAL:HG12	1.95	0.49
3:L:271:ARG:HA	3:L:274:TYR:CE1	2.47	0.49
1:A:79:ILE:HD13	1:A:235:LEU:HB2	1.95	0.49
2:H:157:ARG:O	1:I:164:LYS:NZ	2.34	0.49
2:H:227:VAL:HG11	1:I:287:LEU:HD22	1.95	0.49
2:D:113:HIS:CE1	2:D:125:LEU:HB3	2.47	0.49
3:K:275:ILE:O	3:K:279:LEU:N	2.41	0.49
1:A:40:GLY:O	1:A:116:ARG:N	2.39	0.49
1:C:129:VAL:HG23	1:C:155:SER:HB2	1.95	0.49
3:E:26:LYS:NZ	3:E:28:GLY:O	2.40	0.49
1:I:305:LYS:O	1:I:309:MET:HG2	2.12	0.49
2:H:244:LEU:O	2:H:247:GLN:HG3	2.13	0.48
1:I:177:GLN:HA	1:I:208:ARG:HE	1.78	0.48
1:G:82:ARG:NH2	1:G:89:ARG:O	2.46	0.48
1:I:236:PRO:HG3	1:I:279:VAL:HG12	1.95	0.48
2:J:149:ARG:N	2:J:156:GLN:O	2.45	0.48
3:L:31:ALA:HB1	3:L:63:ALA:H	1.77	0.48
1:A:265:GLY:HA2	2:B:206:ILE:HD11	1.95	0.48
3:F:145:LEU:HD13	3:F:175:LEU:HD21	1.93	0.48
3:F:270:LYS:HB3	3:F:270:LYS:HE2	1.68	0.48
1:G:270:LYS:HG3	1:G:271:ASN:N	2.26	0.48
1:A:42:LEU:HD23	1:A:116:ARG:HH12	1.79	0.48
3:F:221:LEU:HD12	3:F:235:LEU:HD12	1.95	0.48
2:H:231:GLU:HG3	1:I:223:THR:HB	1.95	0.48
1:I:131:PRO:HG3	1:I:173:PHE:CD2	2.49	0.48
3:L:73:PHE:CE1	3:L:82:PRO:HB3	2.48	0.48
2:B:232:ARG:HA	2:B:232:ARG:NE	2.29	0.48
3:E:145:LEU:HD13	3:E:175:LEU:HD21	1.96	0.48
3:E:268:TYR:O	3:E:271:ARG:HG2	2.14	0.48
3:K:205:VAL:HG21	3:K:246:LEU:HD11	1.96	0.48
3:L:54:ASP:OD2	3:L:75:ALA:N	2.46	0.48
2:J:23:ASP:OD2	3:K:74:ASN:ND2	2.34	0.48
1:A:171:THR:HG22	2:B:140:THR:HA	1.95	0.48
1:C:122:HIS:CE1	1:C:153:ILE:HG12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:131:ARG:HH22	3:F:161:LYS:HA	1.79	0.48
3:L:145:LEU:HD21	3:L:246:LEU:HD11	1.96	0.48
2:B:113:HIS:CE1	2:B:125:LEU:HB3	2.48	0.47
1:C:150:VAL:HG12	1:C:214:ILE:HD13	1.96	0.47
3:L:214:GLN:NE2	3:L:216:TYR:OH	2.45	0.47
3:F:171:ALA:HB3	3:F:207:PHE:HB2	1.96	0.47
1:I:82:ARG:HG2	1:I:85:LYS:HD3	1.96	0.47
2:B:27:PHE:HA	2:B:94:TRP:HA	1.95	0.47
1:C:173:PHE:HB2	1:C:211:ARG:HG3	1.97	0.47
3:E:89:ASP:OD2	3:E:124:TYR:OH	2.19	0.47
6:F:401:X8C:CLBI	2:H:142:ALA:HB2	2.51	0.47
1:I:222:VAL:HG13	1:I:223:THR:HG23	1.95	0.47
2:J:27:PHE:HA	2:J:94:TRP:HA	1.95	0.47
3:K:260:LYS:O	3:K:264:VAL:HB	2.14	0.47
1:C:174:GLN:HB2	1:C:214:ILE:HD11	1.96	0.47
1:I:308:LEU:HD23	1:I:309:MET:HE1	1.97	0.47
3:F:42:SER:HA	3:F:53:CYS:HA	1.95	0.47
1:A:81:ARG:HH21	1:A:241:GLN:HB3	1.78	0.47
1:A:142:TYR:HA	1:A:145:MET:HG3	1.97	0.47
2:B:185:TYR:O	2:B:189:ILE:HG12	2.14	0.47
1:C:215:PRO:HA	2:D:139:SER:HA	1.96	0.47
3:E:249:TYR:O	3:E:253:VAL:HG13	2.15	0.47
1:G:143:GLN:O	1:G:147:GLN:NE2	2.46	0.47
1:G:272:LEU:HD12	1:G:272:LEU:HA	1.77	0.47
1:G:292:GLU:OE2	2:J:87:ARG:NH1	2.47	0.47
2:H:86:ASP:O	2:H:89:LYS:NZ	2.36	0.47
1:I:89:ARG:HD2	1:I:89:ARG:N	2.29	0.47
3:L:219:LEU:HG	3:L:221:LEU:HD22	1.95	0.47
3:L:222:SER:O	3:L:224:ARG:N	2.48	0.47
1:G:86:ARG:HB3	1:G:89:ARG:HB2	1.96	0.47
3:L:60:ILE:HB	3:L:67:LEU:HB2	1.97	0.47
3:K:190:LYS:HD2	3:K:223:PRO:HB2	1.97	0.47
3:E:159:ALA:HB1	3:E:169:PHE:HZ	1.78	0.47
3:F:193:ASN:OD1	3:F:193:ASN:N	2.47	0.47
1:I:142:TYR:HB3	1:I:149:PHE:CD2	2.48	0.46
3:K:196:PRO:HG2	3:K:224:ARG:HH11	1.80	0.46
1:C:17:ASP:OD2	1:C:224:ILE:HA	2.15	0.46
1:C:18:ALA:HB1	1:C:77:VAL:HG23	1.97	0.46
1:I:240:CYS:SG	1:I:272:LEU:HD11	2.55	0.46
3:L:137:ARG:NH2	3:L:244:GLY:O	2.48	0.46
1:C:305:LYS:HZ1	2:D:244:LEU:HD13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:271:ARG:HA	3:K:274:TYR:CZ	2.50	0.46
1:C:211:ARG:NH1	3:K:136:SER:OG	2.34	0.46
1:C:221:HIS:N	2:D:19:ASN:OD1	2.32	0.46
2:D:148:PHE:HE1	2:D:157:ARG:HE	1.64	0.46
3:E:17:PHE:HB3	3:E:113:LEU:HD12	1.98	0.46
1:G:305:LYS:HD2	1:G:305:LYS:HA	1.60	0.46
2:H:216:LEU:HD21	2:J:185:TYR:HD1	1.80	0.46
1:I:93:SER:N	1:I:96:GLN:OE1	2.44	0.46
1:I:103:GLU:OE2	1:I:106:ARG:NH2	2.48	0.46
2:H:97:PHE:HD1	2:H:130:PHE:HB3	1.81	0.46
1:A:177:GLN:HA	1:A:208:ARG:HG3	1.98	0.46
3:E:229:LEU:HD23	3:E:229:LEU:HA	1.85	0.46
2:H:137:ASN:O	2:H:137:ASN:ND2	2.49	0.46
2:J:103:GLN:OE1	2:J:131:SER:OG	2.21	0.46
1:A:12:VAL:HG21	1:A:172:CYS:SG	2.56	0.46
3:E:190:LYS:HZ2	3:E:224:ARG:HA	1.81	0.46
3:L:256:LEU:HA	3:L:259:ASN:HD21	1.80	0.46
1:A:138:THR:HG22	1:A:142:TYR:CE2	2.51	0.45
1:I:11:ALA:HB3	1:I:71:ILE:HG22	1.97	0.45
1:A:285:GLN:OE1	2:D:181:THR:OG1	2.26	0.45
1:C:20:LEU:HD12	2:D:15:PHE:CG	2.51	0.45
1:C:211:ARG:NE	1:C:213:GLU:OE2	2.49	0.45
2:J:83:ILE:HG22	2:J:84:LEU:HD23	1.97	0.45
1:A:82:ARG:NH2	1:A:89:ARG:O	2.49	0.45
2:J:74:LYS:HA	2:J:115:GLN:HE22	1.81	0.45
3:K:154:ASN:HB2	3:K:176:LYS:HB3	1.98	0.45
3:E:237:ILE:HD12	3:E:238:PRO:HD2	1.98	0.45
1:I:43:ASN:O	1:I:70:ARG:NH1	2.49	0.45
1:C:215:PRO:HB3	2:D:138:ASN:HB3	1.98	0.45
1:C:236:PRO:HG3	1:C:279:VAL:HG12	1.98	0.45
1:G:312:LEU:HD21	2:J:248:ILE:HG12	1.97	0.45
2:J:99:ARG:HG3	2:J:132:PHE:HB3	1.99	0.45
3:K:271:ARG:HA	3:K:274:TYR:CE1	2.52	0.45
1:A:159:GLU:OE2	2:B:159:SER:OG	2.24	0.45
3:K:99:LEU:HD21	3:K:120:LEU:HG	1.98	0.45
3:K:180:ASP:OD1	3:K:180:ASP:N	2.44	0.45
3:L:122:GLN:HA	3:L:125:HIS:ND1	2.31	0.45
1:C:253:LEU:HD13	1:C:255:HIS:HE1	1.81	0.45
2:B:187:LYS:HB3	2:B:187:LYS:HE2	1.79	0.45
1:A:103:GLU:O	1:A:107:LEU:HG	2.16	0.45
1:A:125:PRO:O	1:A:127:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.74	0.45
2:J:251:ARG:HG3	2:J:252:LYS:HD2	1.99	0.45
3:F:215:VAL:HG11	3:F:240:PHE:CD2	2.52	0.44
1:G:155:SER:OG	1:G:158:ILE:HD11	2.17	0.44
3:K:30:ASP:OD1	3:K:30:ASP:N	2.48	0.44
1:C:305:LYS:O	1:C:309:MET:HG2	2.17	0.44
2:D:142:ALA:HB2	6:D:301:X8C:CLBI	2.54	0.44
3:F:246:LEU:HD22	3:F:250:VAL:HG23	1.99	0.44
1:A:160:ASP:OD2	1:A:167:ARG:NH2	2.46	0.44
2:B:103:GLN:OE1	2:B:131:SER:HB2	2.18	0.44
3:E:54:ASP:HB2	3:E:73:PHE:HB2	1.98	0.44
2:J:187:LYS:O	2:J:191:GLU:HG2	2.18	0.44
3:K:7:LEU:HD23	3:K:7:LEU:HA	1.85	0.44
1:C:256:LEU:O	1:C:261:LYS:NZ	2.46	0.44
2:H:15:PHE:CG	1:I:20:LEU:HD12	2.53	0.44
2:H:80:LEU:HD21	2:H:120:LEU:HD21	2.00	0.44
2:H:171:GLN:HB3	1:I:267:VAL:HG13	1.98	0.44
1:A:177:GLN:HG3	1:A:208:ARG:HD3	1.98	0.44
1:C:246:ALA:O	1:C:250:ILE:HG12	2.18	0.44
3:K:294:PHE:O	4:M:317:GLU:N	2.51	0.44
3:L:175:LEU:HD13	3:L:250:VAL:HG11	2.00	0.44
2:D:244:LEU:O	2:D:247:GLN:HG3	2.18	0.44
3:E:60:ILE:HB	3:E:67:LEU:HD12	1.99	0.44
1:A:29:THR:HG22	2:B:165:LEU:HB3	2.00	0.44
1:C:120:TRP:HD1	1:C:120:TRP:H	1.66	0.44
1:C:294:ASN:ND2	2:D:231:GLU:OE2	2.44	0.44
2:D:108:ARG:NH2	3:E:81:PRO:HB2	2.32	0.44
3:K:101:ASN:HD22	3:K:115:LEU:HB3	1.82	0.44
4:P:108:PRO:HA	4:P:119:ASN:HA	2.00	0.44
1:C:8:ALA:HB2	1:C:148:GLY:HA2	2.00	0.44
3:E:247:ILE:HD12	3:E:247:ILE:H	1.82	0.44
2:D:238:GLN:NE2	2:D:242:ASN:OD1	2.50	0.43
1:G:306:GLU:O	1:G:310:GLN:HG2	2.17	0.43
2:H:143:LEU:HB3	1:I:168:VAL:HG13	2.00	0.43
2:H:187:LYS:HA	2:H:187:LYS:HD3	1.61	0.43
1:I:272:LEU:HA	1:I:272:LEU:HD12	1.67	0.43
3:K:38:THR:OG1	3:K:59:HIS:NE2	2.49	0.43
3:L:160:GLY:HA3	3:L:170:SER:H	1.82	0.43
4:N:144:PHE:N	4:N:160:THR:O	2.36	0.43
1:A:37:LEU:HA	1:A:120:TRP:HA	2.00	0.43
2:B:66:PHE:CZ	3:F:81:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:HD21	2:D:248:ILE:HG12	2.00	0.43
1:G:236:PRO:HG3	1:G:279:VAL:HG12	2.00	0.43
1:I:77:VAL:HG11	1:I:121:TYR:CE1	2.53	0.43
1:I:256:LEU:HD22	1:I:260:THR:HG21	2.00	0.43
1:A:81:ARG:NH2	1:A:241:GLN:HB3	2.33	0.43
1:A:270:LYS:HG3	1:A:271:ASN:N	2.33	0.43
2:D:98:ARG:HE	2:D:98:ARG:HB2	1.55	0.43
3:E:20:SER:HB3	3:E:110:PRO:HB2	2.00	0.43
1:I:42:LEU:HD12	1:I:116:ARG:HH22	1.83	0.43
3:L:41:LYS:HA	3:L:41:LYS:HD3	1.84	0.43
3:L:218:LYS:HA	3:L:218:LYS:HD3	1.81	0.43
1:A:132:SER:O	1:A:136:VAL:HG23	2.17	0.43
1:G:132:SER:O	1:G:136:VAL:HG23	2.19	0.43
1:G:233:VAL:O	1:G:236:PRO:HD2	2.19	0.43
1:G:293:GLN:OE1	2:J:87:ARG:NH1	2.39	0.43
1:I:76:SER:OG	1:I:228:CYS:SG	2.67	0.43
1:C:12:VAL:HG21	1:C:172:CYS:SG	2.59	0.43
2:D:185:TYR:O	2:D:189:ILE:HG12	2.19	0.43
3:F:101:ASN:ND2	3:F:119:GLU:OE2	2.51	0.43
2:H:206:ILE:HD11	1:I:265:GLY:HA2	2.00	0.43
1:C:37:LEU:HD12	1:C:80:LEU:HD11	2.01	0.43
2:H:203:MET:HB3	2:H:206:ILE:HD13	1.99	0.43
2:H:206:ILE:HG12	1:I:247:TYR:CE2	2.54	0.43
1:I:13:HIS:N	1:I:72:VAL:O	2.51	0.43
1:A:229:LEU:HD21	1:A:287:LEU:HD21	2.00	0.43
2:D:108:ARG:HH22	3:E:81:PRO:HB2	1.84	0.43
3:E:58:LEU:HD23	3:E:58:LEU:HA	1.82	0.43
3:L:34:CYS:SG	3:L:35:LEU:N	2.90	0.43
1:I:33:GLU:HG3	1:I:123:SER:O	2.18	0.43
3:K:12:PRO:HD3	3:K:51:PRO:HG2	2.01	0.43
4:P:99:LEU:O	4:P:149:VAL:N	2.51	0.43
3:E:101:ASN:O	3:E:105:TRP:N	2.50	0.43
3:E:175:LEU:HD22	3:E:250:VAL:HG11	2.01	0.43
1:G:18:ALA:HB1	1:G:77:VAL:HG23	2.00	0.43
2:H:216:LEU:HD21	2:J:185:TYR:CD1	2.54	0.43
3:K:150:GLN:HB2	3:K:178:PRO:HG3	2.01	0.43
3:L:179:VAL:HG13	3:L:258:THR:HG23	2.01	0.43
3:K:20:SER:HA	3:K:23:ARG:HE	1.83	0.42
3:K:135:SER:HB3	3:K:169:PHE:CE1	2.54	0.42
3:L:201:ALA:HA	3:L:221:LEU:HA	2.00	0.42
3:E:229:LEU:HD21	3:E:260:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:TYR:O	2:H:189:ILE:HG12	2.19	0.42
3:L:70:ASP:OD1	3:L:70:ASP:N	2.52	0.42
2:D:133:ILE:HG22	2:D:134:SER:H	1.84	0.42
1:G:158:ILE:HD13	1:G:169:LEU:HD12	2.00	0.42
1:G:263:HIS:HB2	1:I:273:CYS:HB3	2.01	0.42
2:J:133:ILE:HB	2:J:142:ALA:HB3	2.01	0.42
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.73	0.42
1:I:122:HIS:CE1	1:I:153:ILE:HG12	2.54	0.42
3:L:101:ASN:HB3	3:L:119:GLU:OE1	2.19	0.42
3:L:162:LYS:HD3	3:L:169:PHE:HD1	1.84	0.42
1:A:284:LEU:HB2	2:B:220:VAL:HG22	2.02	0.42
1:C:276:MET:HG2	2:D:216:LEU:HD23	2.02	0.42
1:I:36:GLY:HA3	1:I:121:TYR:CE1	2.54	0.42
2:J:226:ASP:O	2:J:229:LYS:HG2	2.19	0.42
3:K:237:ILE:HD12	3:K:237:ILE:HA	1.93	0.42
2:B:5:ILE:HD11	2:B:9:THR:HG22	2.00	0.42
1:C:38:CYS:HB3	1:C:74:ILE:HG23	2.01	0.42
2:D:69:TYR:CE2	2:D:112:LEU:HD11	2.54	0.42
2:D:97:PHE:HD1	2:D:130:PHE:HB3	1.83	0.42
2:H:209:ILE:HG23	1:I:272:LEU:HD23	2.02	0.42
3:L:21:VAL:HG12	3:L:35:LEU:HD22	2.01	0.42
1:C:229:LEU:O	1:C:233:VAL:HG13	2.20	0.42
3:E:250:VAL:CG2	3:E:251:PRO:HD3	2.50	0.42
2:H:119:ILE:HD13	2:H:119:ILE:HA	1.91	0.42
4:O:95:VAL:HA	4:O:212:ARG:O	2.20	0.42
2:D:100:ASN:HB3	3:E:41:LYS:HD3	2.00	0.42
2:D:132:PHE:CE1	2:D:141:HIS:HB3	2.46	0.42
3:E:265:ILE:HG13	3:E:266:GLN:N	2.35	0.42
3:F:246:LEU:HD23	3:F:246:LEU:HA	1.78	0.42
1:G:174:GLN:HB2	1:G:214:ILE:HD11	2.00	0.42
1:G:294:ASN:ND2	2:J:231:GLU:OE2	2.48	0.42
1:I:308:LEU:HB3	1:I:309:MET:HE2	2.01	0.42
2:J:220:VAL:HA	2:J:223:VAL:HG22	2.00	0.42
2:D:207:ARG:HG3	2:D:208:ALA:N	2.35	0.42
2:D:226:ASP:OD1	2:D:226:ASP:N	2.53	0.42
3:E:18:ILE:HD11	3:E:56:PHE:CZ	2.54	0.42
1:G:73:HIS:HB3	1:G:75:HIS:CE1	2.55	0.42
1:G:233:VAL:HG23	2:J:220:VAL:HG12	2.01	0.42
2:J:237:CYS:O	2:J:240:GLU:HG3	2.20	0.42
3:K:224:ARG:H	3:K:224:ARG:HG2	1.69	0.42
3:K:258:THR:O	3:K:262:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:105:MET:O	4:O:121:LEU:N	2.53	0.42
2:D:200:ASP:OD1	2:D:200:ASP:N	2.46	0.42
3:F:70:ASP:OD1	3:F:70:ASP:N	2.53	0.42
1:I:124:HIS:O	1:I:155:SER:OG	2.29	0.42
1:A:82:ARG:NH1	1:A:85:LYS:HA	2.34	0.41
1:I:129:VAL:CG1	1:I:169:LEU:HB2	2.50	0.41
3:E:15:SER:N	3:E:16:PRO:HD2	2.35	0.41
3:E:118:LYS:O	3:E:121:VAL:HG12	2.20	0.41
3:E:250:VAL:HG23	3:E:251:PRO:HD3	2.02	0.41
3:L:121:VAL:HG12	3:L:125:HIS:NE2	2.35	0.41
4:P:265:PHE:O	4:P:269:GLY:N	2.53	0.41
2:B:132:PHE:HE1	2:B:141:HIS:HB3	1.85	0.41
1:G:31:LYS:HA	1:G:31:LYS:HD3	1.84	0.41
1:I:229:LEU:HD11	1:I:287:LEU:HD21	2.03	0.41
3:K:229:LEU:HD11	3:K:261:VAL:HB	2.03	0.41
2:B:185:TYR:HB2	1:C:284:LEU:HD23	2.02	0.41
2:H:227:VAL:HB	1:I:291:LEU:HG	2.01	0.41
1:I:23:LEU:HD23	1:I:23:LEU:HA	1.81	0.41
3:K:247:ILE:HD12	3:K:247:ILE:HA	1.82	0.41
3:L:125:HIS:CD2	3:L:156:GLU:HG2	2.55	0.41
3:E:40:LEU:HB3	3:E:53:CYS:SG	2.61	0.41
1:A:39:ILE:HG21	1:A:107:LEU:HD12	2.02	0.41
1:G:277:SER:O	2:H:178:VAL:HG21	2.21	0.41
2:H:64:LYS:HE3	2:H:64:LYS:HB2	1.78	0.41
2:H:165:LEU:HD23	1:I:278:ALA:HB3	2.02	0.41
3:K:268:TYR:OH	3:K:272:ARG:NH1	2.54	0.41
3:L:59:HIS:CE1	3:L:68:LYS:HG2	2.55	0.41
3:L:130:SER:HA	3:L:133:ARG:HD2	2.03	0.41
2:D:203:MET:HB2	2:D:206:ILE:HD13	2.02	0.41
3:E:26:LYS:HD2	3:E:30:ASP:HB2	2.03	0.41
3:E:120:LEU:HD23	3:E:120:LEU:HA	1.91	0.41
3:L:135:SER:OG	3:L:138:LEU:HB2	2.21	0.41
3:F:219:LEU:HD23	3:F:221:LEU:HG	2.03	0.41
2:H:147:LEU:HD22	2:H:160:LEU:HD13	2.03	0.41
2:H:231:GLU:OE1	1:I:294:ASN:ND2	2.47	0.41
2:J:207:ARG:HD2	2:J:208:ALA:N	2.35	0.41
2:B:71:TYR:CE1	3:F:81:PRO:HD3	2.56	0.41
2:D:113:HIS:O	2:D:117:THR:OG1	2.33	0.41
1:I:131:PRO:HG3	1:I:173:PHE:CG	2.56	0.41
2:J:129:LEU:O	2:J:145:TYR:HA	2.21	0.41
3:K:31:ALA:O	3:K:32:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:OD1	1:A:258:SER:N	2.53	0.40
2:B:148:PHE:HE1	2:B:157:ARG:HE	1.69	0.40
3:E:112:CYS:O	3:E:116:VAL:HG23	2.21	0.40
1:I:86:ARG:HB2	1:I:89:ARG:HB2	2.03	0.40
3:K:102:LEU:HD23	3:K:102:LEU:HA	1.93	0.40
3:K:129:CYS:HA	3:K:157:ILE:HD11	2.03	0.40
3:L:38:THR:OG1	3:L:39:ASP:N	2.54	0.40
4:N:138:ILE:C	4:N:140:LYS:H	2.25	0.40
1:A:33:GLU:HG3	1:A:123:SER:O	2.21	0.40
2:B:178:VAL:HG11	1:C:277:SER:O	2.21	0.40
3:E:151:TYR:HE1	3:E:254:CYS:HG	1.69	0.40
3:F:189:LEU:HD23	3:F:189:LEU:HA	1.87	0.40
2:H:213:TYR:C	2:H:213:TYR:CD1	2.95	0.40
3:E:141:GLU:OE1	3:E:246:LEU:HG	2.21	0.40
3:E:203:LEU:HD23	3:E:219:LEU:HD13	2.03	0.40
3:L:215:VAL:HG23	3:L:217:PRO:HD3	2.04	0.40
1:C:29:THR:HA	2:D:164:ASN:HD22	1.86	0.40
3:F:138:LEU:HD13	3:F:171:ALA:HB2	2.04	0.40
3:F:226:GLU:HG3	3:F:231:GLY:HA2	2.03	0.40
1:G:81:ARG:HB3	1:G:242:GLU:OE1	2.21	0.40
2:J:170:GLN:HG2	2:J:171:GLN:N	2.36	0.40
2:B:74:LYS:HA	2:B:115:GLN:NE2	2.35	0.40
1:G:138:THR:HG22	1:G:142:TYR:CE2	2.57	0.40
2:H:208:ALA:O	2:H:212:VAL:HG23	2.21	0.40
1:I:84:ASP:OD1	1:I:84:ASP:N	2.47	0.40
1:I:238:ILE:HD13	1:I:238:ILE:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/316 (78%)	243 (99%)	3 (1%)	0	100	100
1	C	246/316 (78%)	240 (98%)	6 (2%)	0	100	100
1	G	246/316 (78%)	241 (98%)	5 (2%)	0	100	100
1	I	246/316 (78%)	242 (98%)	4 (2%)	0	100	100
2	B	233/267 (87%)	226 (97%)	7 (3%)	0	100	100
2	D	233/267 (87%)	227 (97%)	6 (3%)	0	100	100
2	H	233/267 (87%)	224 (96%)	9 (4%)	0	100	100
2	J	233/267 (87%)	231 (99%)	2 (1%)	0	100	100
3	E	381/385 (99%)	351 (92%)	30 (8%)	0	100	100
3	F	381/385 (99%)	347 (91%)	34 (9%)	0	100	100
3	K	381/385 (99%)	351 (92%)	30 (8%)	0	100	100
3	L	381/385 (99%)	355 (93%)	26 (7%)	0	100	100
4	M	235/259 (91%)	214 (91%)	21 (9%)	0	100	100
4	N	235/259 (91%)	213 (91%)	22 (9%)	0	100	100
4	O	235/259 (91%)	214 (91%)	21 (9%)	0	100	100
4	P	235/259 (91%)	220 (94%)	15 (6%)	0	100	100
All	All	4380/4908 (89%)	4139 (94%)	241 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	228/286 (80%)	215 (94%)	13 (6%)	17	45
1	C	227/286 (79%)	218 (96%)	9 (4%)	27	54
1	G	229/286 (80%)	221 (96%)	8 (4%)	31	58
1	I	229/286 (80%)	221 (96%)	8 (4%)	31	58
2	B	214/243 (88%)	205 (96%)	9 (4%)	25	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	214/243 (88%)	207 (97%)	7 (3%)	33	60
2	H	214/243 (88%)	207 (97%)	7 (3%)	33	60
2	J	214/243 (88%)	204 (95%)	10 (5%)	22	51
3	E	337/337 (100%)	318 (94%)	19 (6%)	17	45
3	F	336/337 (100%)	317 (94%)	19 (6%)	17	45
3	K	337/337 (100%)	317 (94%)	20 (6%)	16	43
3	L	333/337 (99%)	316 (95%)	17 (5%)	20	48
4	M	218/238 (92%)	205 (94%)	13 (6%)	16	43
4	N	214/238 (90%)	203 (95%)	11 (5%)	20	48
4	O	213/238 (90%)	202 (95%)	11 (5%)	19	47
4	P	217/238 (91%)	206 (95%)	11 (5%)	20	48
All	All	3974/4416 (90%)	3782 (95%)	192 (5%)	24	50

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	89	ARG
1	A	93	SER
1	A	135	ASP
1	A	159	GLU
1	A	210	GLU
1	A	217	HIS
1	A	252	SER
1	A	280	SER
1	A	290	ARG
1	A	301	LEU
1	A	305	LYS
1	A	309	MET
2	B	15	PHE
2	B	71	TYR
2	B	85	LYS
2	B	104	GLN
2	B	124	ASP
2	B	132	PHE
2	B	190	LYS
2	B	232	ARG
2	B	247	GLN

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Mol	Chain	Res	Type
1	C	13	HIS
1	C	17	ASP
1	C	43	ASN
1	C	113	ARG
1	C	120	TRP
1	C	144	MET
1	C	145	MET
1	C	290	ARG
1	C	302	GLN
2	D	15	PHE
2	D	86	ASP
2	D	107	TYR
2	D	132	PHE
2	D	137	ASN
2	D	141	HIS
2	D	247	GLN
3	E	20	SER
3	E	39	ASP
3	E	70	ASP
3	E	112	CYS
3	E	139	MET
3	E	142	TYR
3	E	155	MET
3	E	187	TYR
3	E	216	TYR
3	E	227	HIS
3	E	233	SER
3	E	289	TYR
3	E	296	LYS
3	E	302	MET
3	E	318	PHE
3	E	347	TYR
3	E	358	MET
3	E	361	ARG
3	E	378	PHE
3	F	15	SER
3	F	33	ASN
3	F	39	ASP
3	F	70	ASP
3	F	112	CYS
3	F	161	LYS
3	F	164	ASN

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Mol	Chain	Res	Type
3	F	170	SER
3	F	219	LEU
3	F	227	HIS
3	F	260	LYS
3	F	268	TYR
3	F	271	ARG
3	F	302	MET
3	F	307	CYS
3	F	318	PHE
3	F	360	LYS
3	F	365	TYR
3	F	366	PHE
1	G	82	ARG
1	G	86	ARG
1	G	101	SER
1	G	173	PHE
1	G	209	TYR
1	G	257	ASP
1	G	270	LYS
1	G	301	LEU
2	H	15	PHE
2	H	20	SER
2	H	81	ASP
2	H	139	SER
2	H	154	TYR
2	H	213	TYR
2	H	224	CYS
1	I	35	MET
1	I	89	ARG
1	I	149	PHE
1	I	167	ARG
1	I	231	SER
1	I	252	SER
1	I	270	LYS
1	I	277	SER
2	J	4	SER
2	J	64	LYS
2	J	68	PHE
2	J	78	GLU
2	J	79	SER
2	J	96	ARG
2	J	107	TYR

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Mol	Chain	Res	Type
2	J	134	SER
2	J	143	LEU
2	J	210	TYR
3	K	1	MET
3	K	39	ASP
3	K	70	ASP
3	K	112	CYS
3	K	151	TYR
3	K	163	ASN
3	K	165	TRP
3	K	199	ASP
3	K	214	GLN
3	K	227	HIS
3	K	254	CYS
3	K	294	PHE
3	K	299	LEU
3	K	308	PHE
3	K	328	GLN
3	K	331	TYR
3	K	333	PHE
3	K	339	LEU
3	K	352	ARG
3	K	361	ARG
3	L	62	TYR
3	L	70	ASP
3	L	100	GLN
3	L	125	HIS
3	L	131	ARG
3	L	147	GLU
3	L	162	LYS
3	L	188	LEU
3	L	208	GLU
3	L	221	LEU
3	L	224	ARG
3	L	268	TYR
3	L	274	TYR
3	L	331	TYR
3	L	353	TRP
3	L	361	ARG
3	L	366	PHE
4	M	93	GLU
4	M	105	MET

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Mol	Chain	Res	Type
4	M	127	MET
4	M	151	ASP
4	M	171	TYR
4	M	177	SER
4	M	235	MET
4	M	259	MET
4	M	279	LYS
4	M	294	CYS
4	M	295	MET
4	M	307	CYS
4	M	313	TYR
4	N	98	CYS
4	N	130	MET
4	N	133	ARG
4	N	139	ASP
4	N	219	ARG
4	N	235	MET
4	N	243	PHE
4	N	259	MET
4	N	267	PHE
4	N	294	CYS
4	N	316	LEU
4	O	169	CYS
4	O	171	TYR
4	O	193	LYS
4	O	219	ARG
4	O	234	LYS
4	O	259	MET
4	O	265	PHE
4	O	267	PHE
4	O	294	CYS
4	O	295	MET
4	O	297	LYS
4	P	81	GLU
4	P	93	GLU
4	P	131	PHE
4	P	171	TYR
4	P	232	MET
4	P	241	PHE
4	P	243	PHE
4	P	257	GLU
4	P	259	MET

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Mol	Chain	Res	Type
4	P	263	ASP
4	P	267	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	59	HIS
2	H	113	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	X8C	D	301	-	36,38,38	1.76	10 (27%)	44,54,54	1.96	11 (25%)
6	X8C	F	401	-	36,38,38	1.75	11 (30%)	44,54,54	2.01	12 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	X8C	D	301	-	-	6/14/32/32	0/4/4/4
6	X8C	F	401	-	-	5/14/32/32	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	401	X8C	CAF-NAH	5.42	1.46	1.34
6	D	301	X8C	CAF-NAH	5.42	1.45	1.34
6	F	401	X8C	CAP-NAO	3.70	1.45	1.35
6	D	301	X8C	CAA-NAE	3.68	1.41	1.36
6	D	301	X8C	CAP-NAO	3.67	1.45	1.35
6	F	401	X8C	CAA-NAE	3.58	1.40	1.36
6	D	301	X8C	OBA-CAZ	-3.07	1.18	1.22
6	F	401	X8C	OBA-CAZ	-3.00	1.18	1.22
6	F	401	X8C	OAQ-CAP	-2.25	1.18	1.23
6	D	301	X8C	OAQ-CAP	-2.22	1.18	1.23
6	D	301	X8C	OAG-CAF	-2.21	1.18	1.23
6	F	401	X8C	OAG-CAF	-2.21	1.18	1.23
6	D	301	X8C	CBG-CLBH	2.19	1.78	1.73
6	F	401	X8C	CAW-CLAY	2.15	1.78	1.73
6	F	401	X8C	CAS-CLAX	2.15	1.78	1.73
6	F	401	X8C	CBG-CLBH	2.13	1.78	1.73
6	D	301	X8C	CAW-CLAY	2.09	1.78	1.73
6	D	301	X8C	CAS-CLAX	2.08	1.78	1.73
6	F	401	X8C	CBC-CLBI	2.08	1.78	1.73
6	D	301	X8C	CAC-CAF	2.02	1.53	1.50
6	F	401	X8C	CAC-CAF	2.00	1.53	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	401	X8C	CAM-CAN-CAI	4.86	119.07	110.50
6	F	401	X8C	CAK-CAJ-CAI	4.81	118.99	110.50
6	D	301	X8C	CAK-CAJ-CAI	4.74	118.86	110.50
6	F	401	X8C	CAA-NAE-NAD	-4.57	108.06	112.72
6	D	301	X8C	CAJ-CAK-NAL	4.54	119.82	110.64
6	D	301	X8C	CAA-NAE-NAD	-4.34	108.30	112.72
6	F	401	X8C	CAN-CAM-NAL	4.31	119.37	110.64
6	F	401	X8C	CAJ-CAK-NAL	4.19	119.12	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	301	X8C	CAM-CAN-CAI	4.10	117.73	110.50
6	D	301	X8C	CAN-CAM-NAL	3.64	118.00	110.64
6	D	301	X8C	CAA-CAB-CAC	3.26	108.09	104.91
6	F	401	X8C	CAM-NAL-CAK	3.12	119.30	110.34
6	D	301	X8C	CAM-NAL-CAK	3.06	119.14	110.34
6	F	401	X8C	CAA-CAB-CAC	3.05	107.88	104.91
6	D	301	X8C	CAF-CAC-NAD	3.02	128.15	120.57
6	D	301	X8C	CBC-CBB-CAZ	-2.70	117.95	121.19
6	F	401	X8C	CBC-CBB-CAZ	-2.53	118.16	121.19
6	F	401	X8C	CAW-CAR-CAP	-2.50	118.14	121.24
6	F	401	X8C	CBG-CBB-CBC	2.39	119.96	116.73
6	F	401	X8C	CAC-NAD-NAE	2.25	107.84	105.44
6	D	301	X8C	CBG-CBB-CBC	2.25	119.77	116.73
6	F	401	X8C	CAW-CAR-CAS	2.24	119.77	116.73
6	D	301	X8C	CAW-CAR-CAS	2.23	119.75	116.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	301	X8C	NAO-CAP-CAR-CAS
6	D	301	X8C	NAO-CAP-CAR-CAW
6	D	301	X8C	OAQ-CAP-CAR-CAS
6	D	301	X8C	OAQ-CAP-CAR-CAW
6	F	401	X8C	NAO-CAP-CAR-CAS
6	F	401	X8C	NAO-CAP-CAR-CAW
6	F	401	X8C	OAQ-CAP-CAR-CAS
6	F	401	X8C	OAQ-CAP-CAR-CAW
6	D	301	X8C	CAN-CAI-NAH-CAF
6	D	301	X8C	CAJ-CAI-NAH-CAF
6	F	401	X8C	CAJ-CAI-NAH-CAF

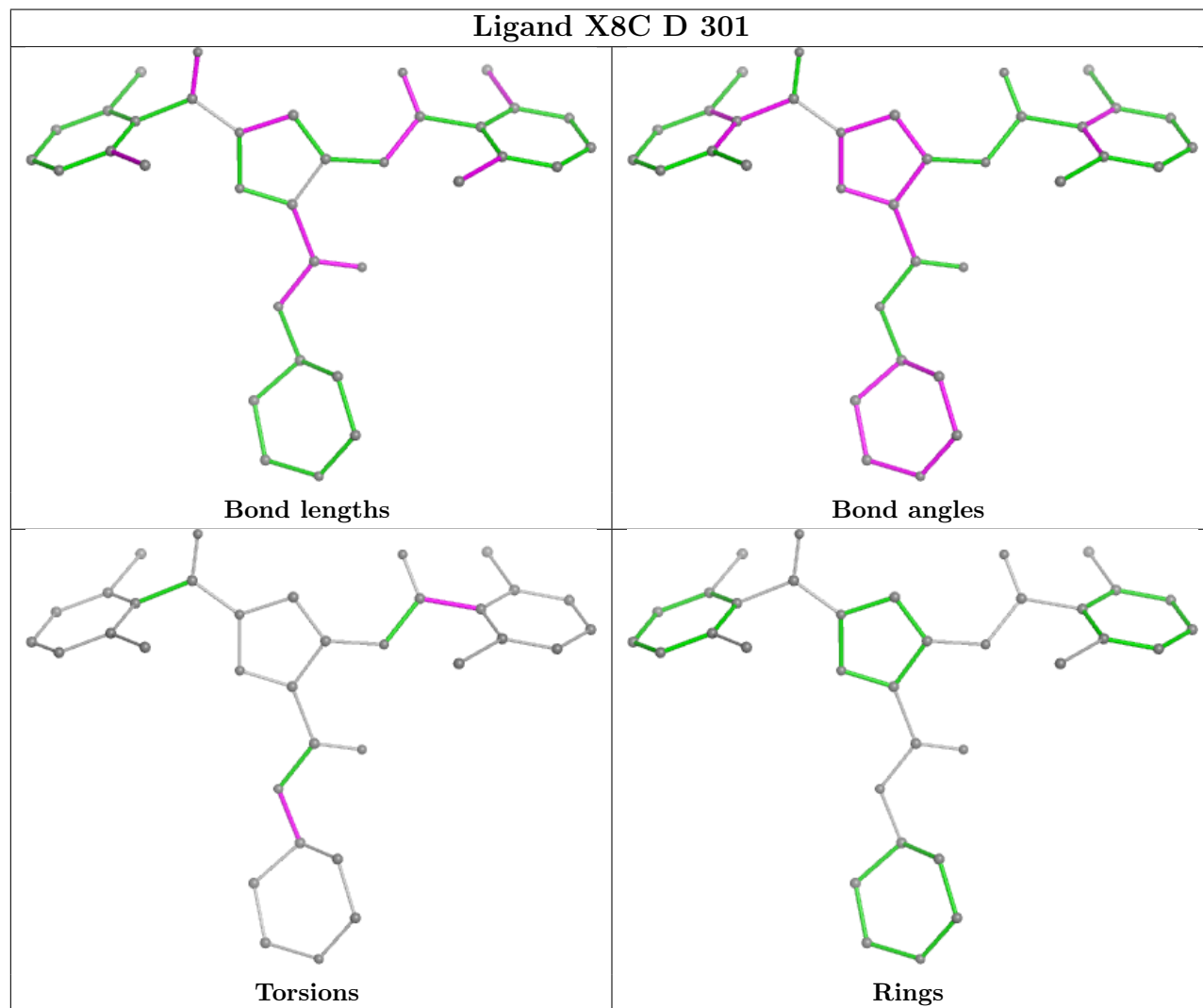
There are no ring outliers.

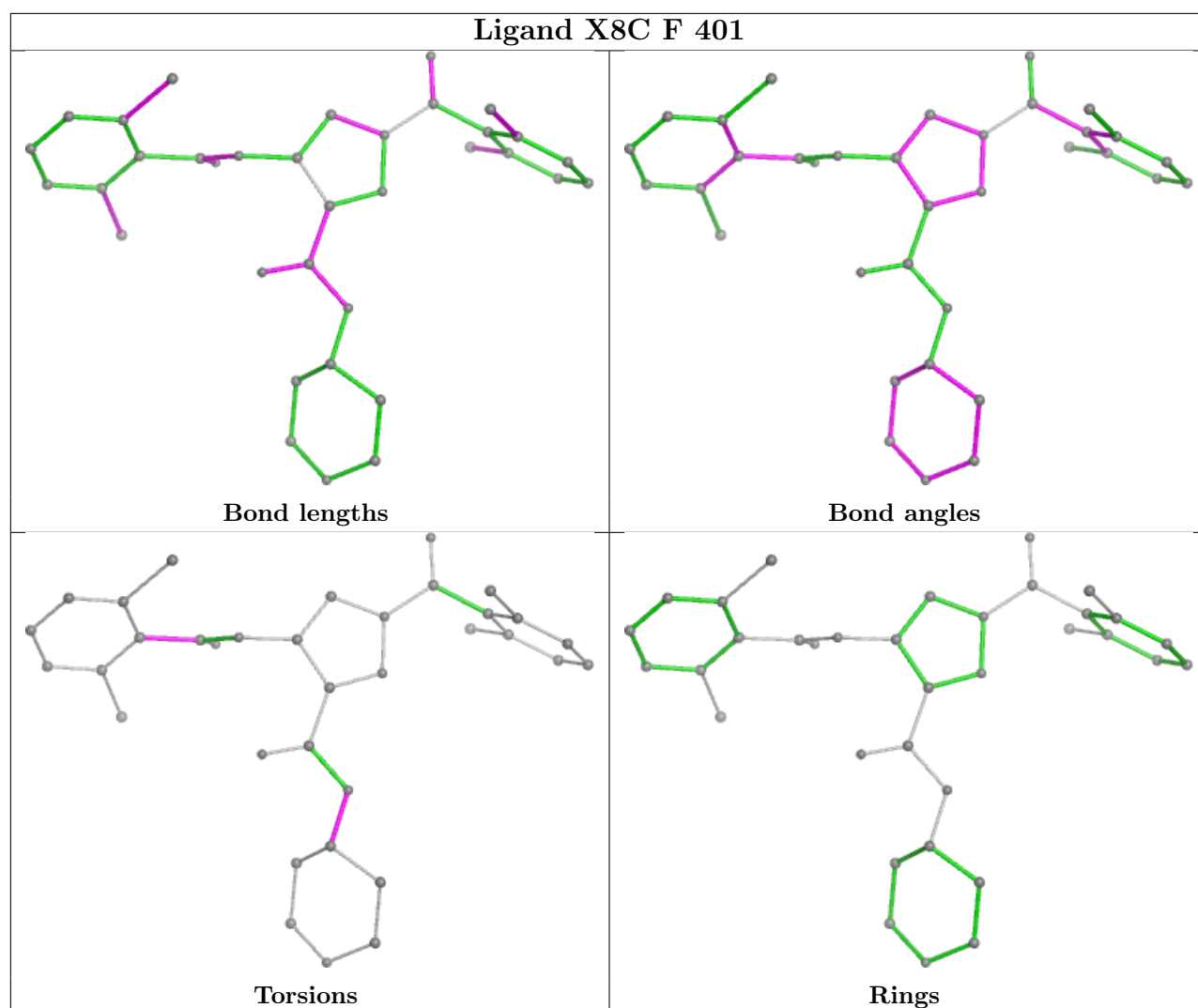
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	301	X8C	1	0
6	F	401	X8C	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

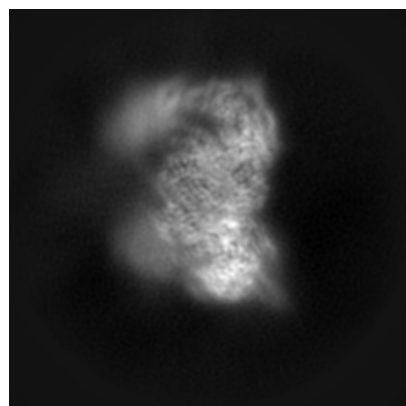
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18009. These allow visual inspection of the internal detail of the map and identification of artifacts.

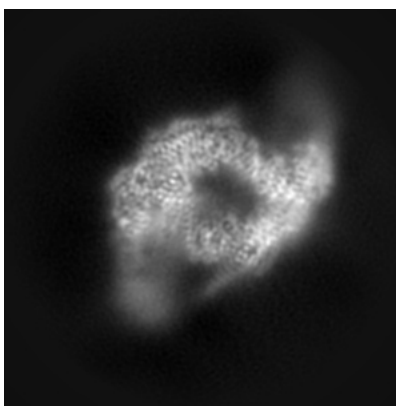
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

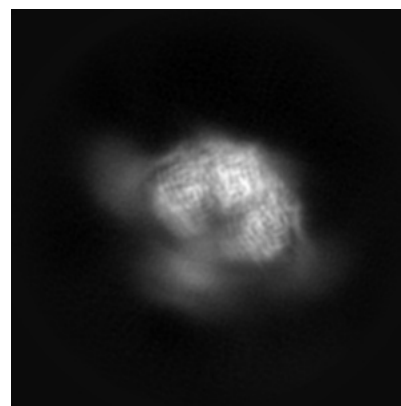
6.1.1 Primary map



X

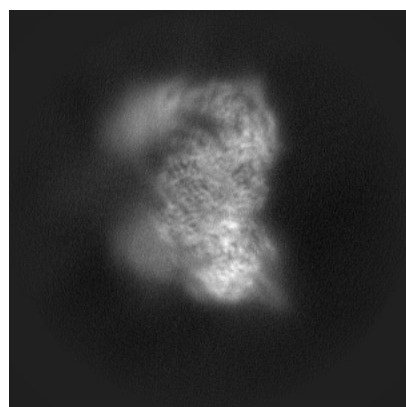


Y

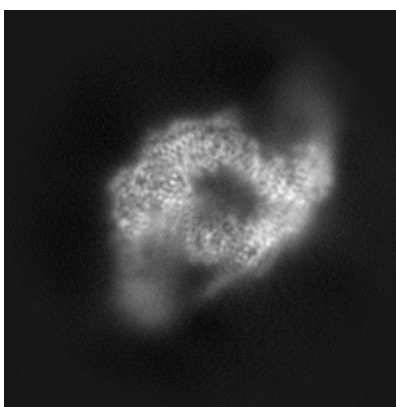


Z

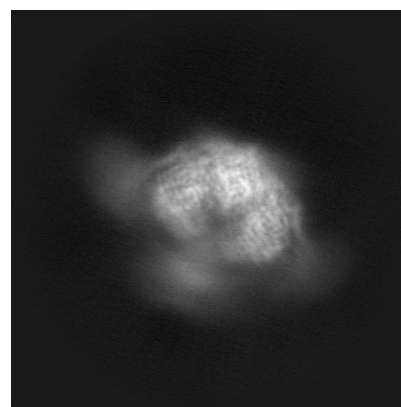
6.1.2 Raw map



X



Y

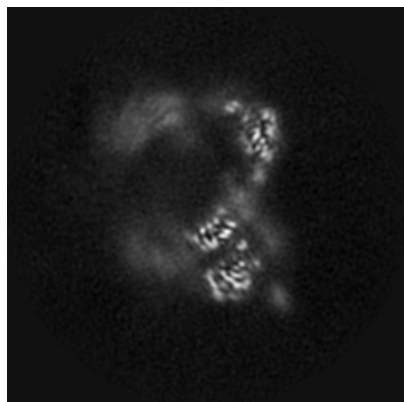


Z

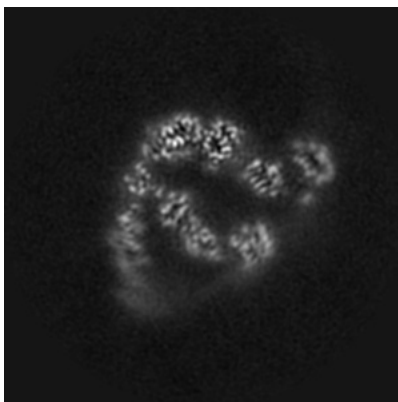
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

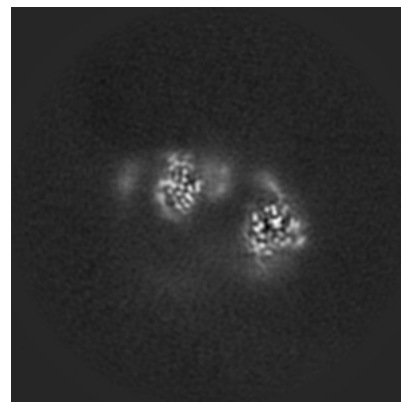
6.2.1 Primary map



X Index: 176

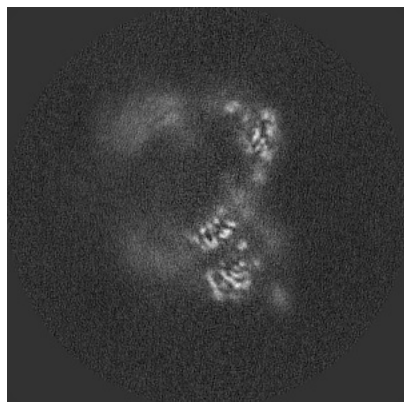


Y Index: 176

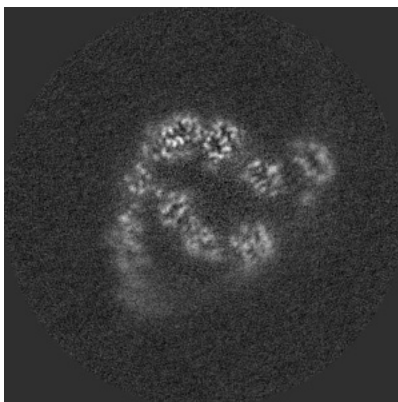


Z Index: 176

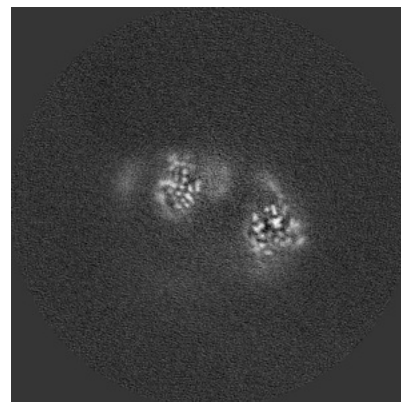
6.2.2 Raw map



X Index: 176



Y Index: 176

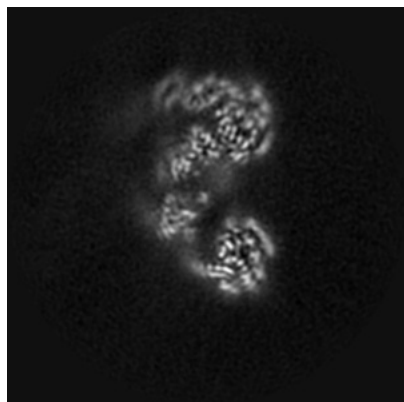


Z Index: 176

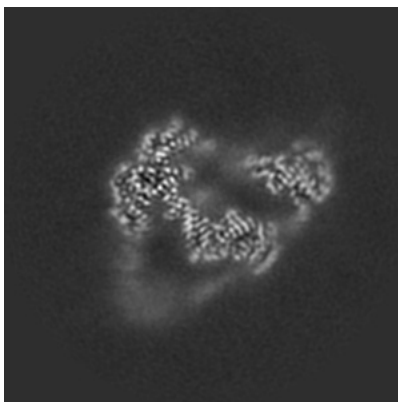
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

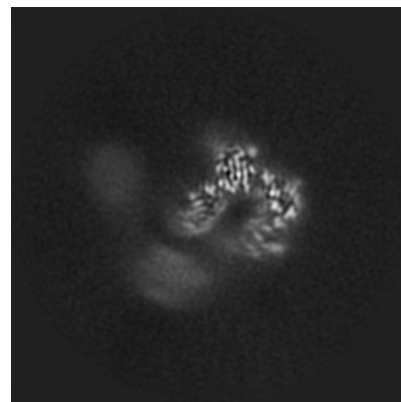
6.3.1 Primary map



X Index: 209

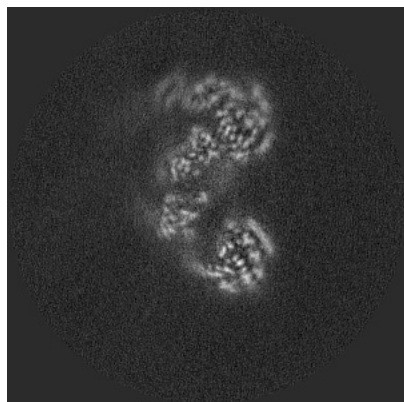


Y Index: 194

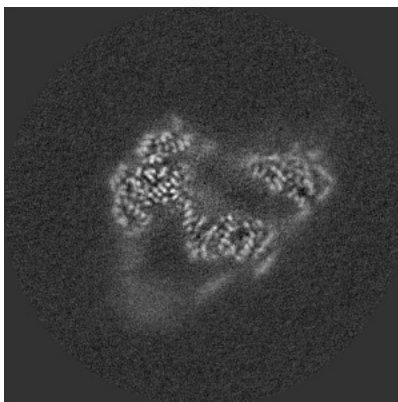


Z Index: 150

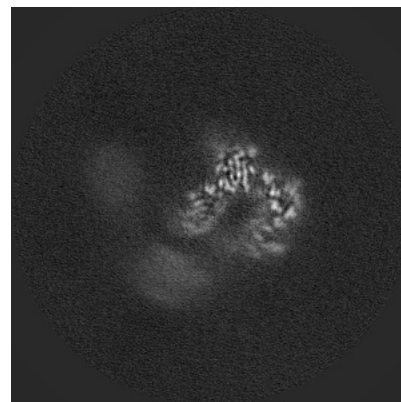
6.3.2 Raw map



X Index: 210



Y Index: 197

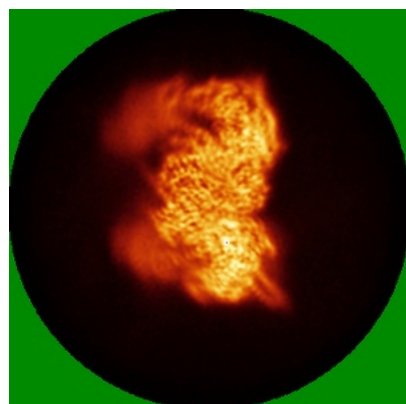


Z Index: 150

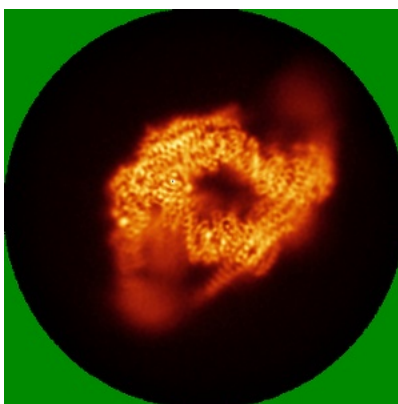
The images above show the largest variance slices of the map in three orthogonal directions.

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

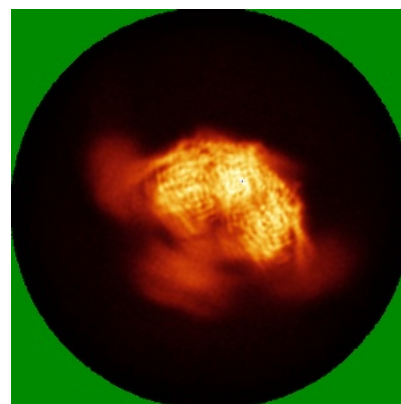
6.4.1 Primary map



X

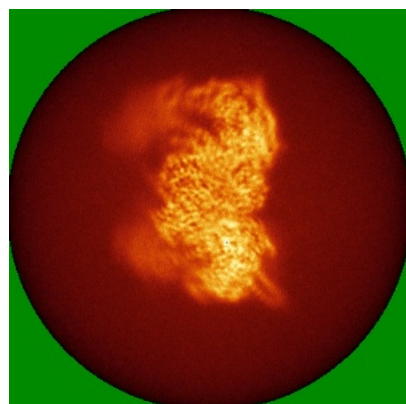


Y

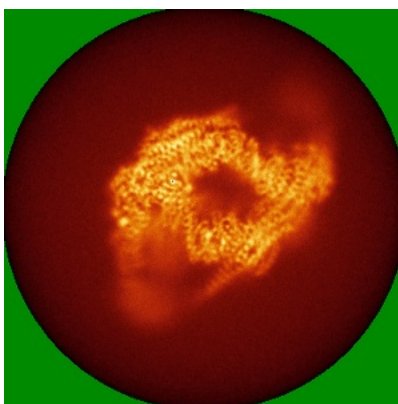


Z

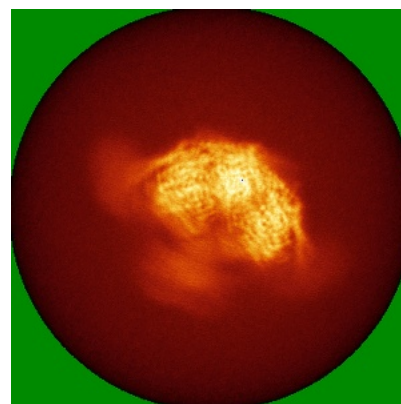
6.4.2 Raw map



X



Y

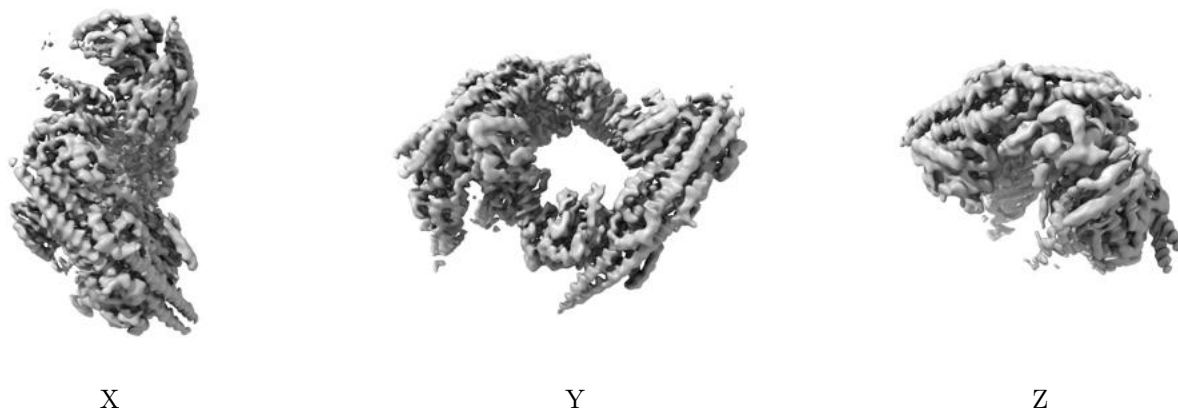


Z

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.

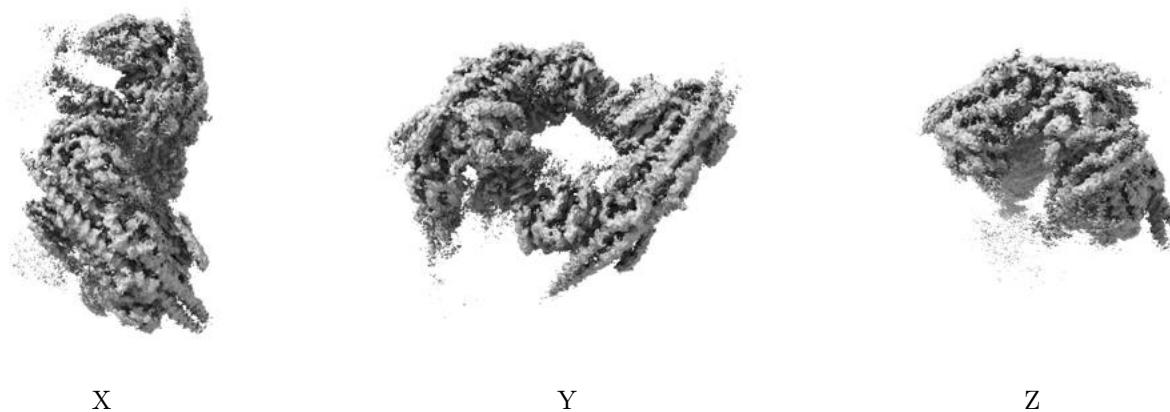
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

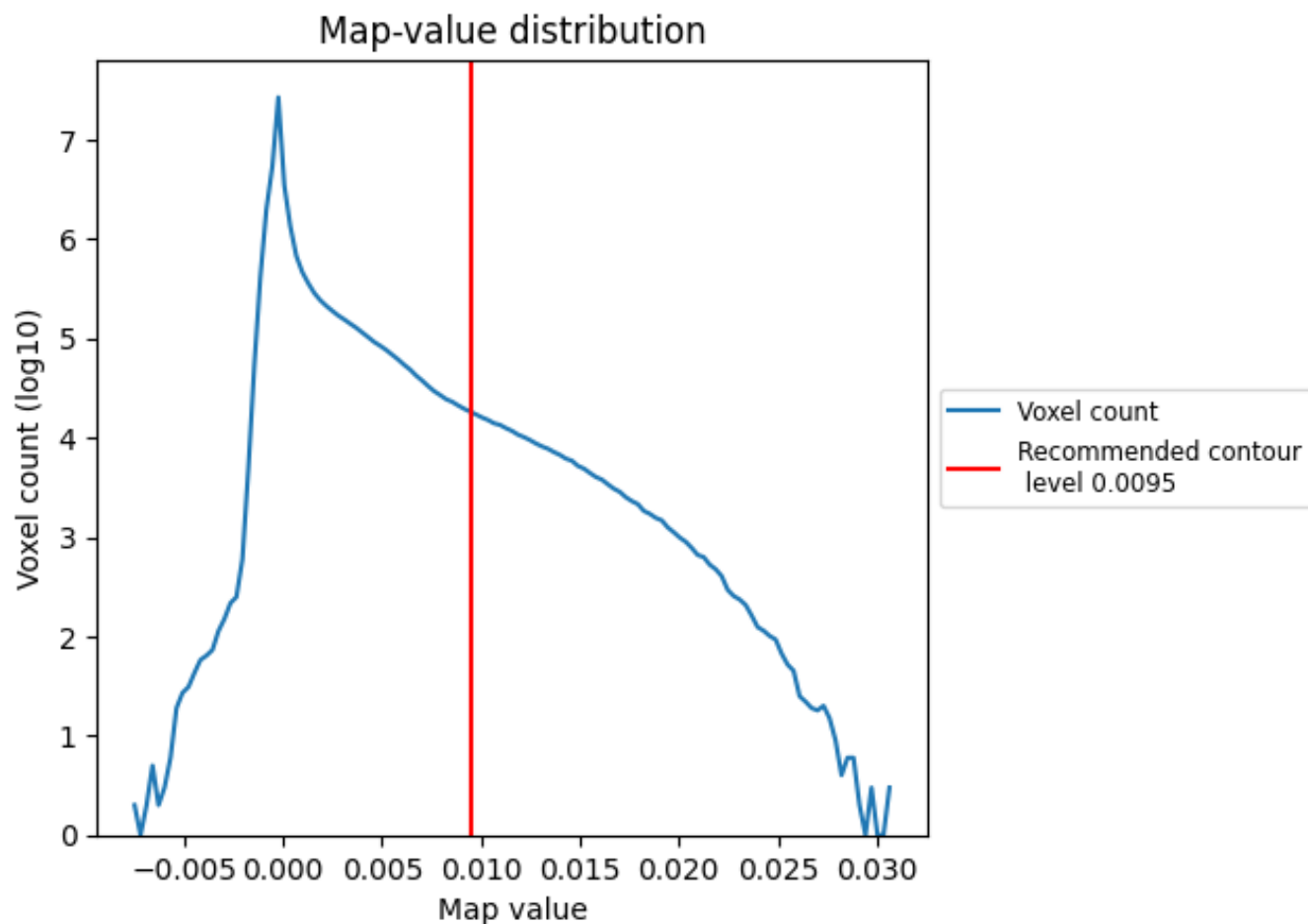
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

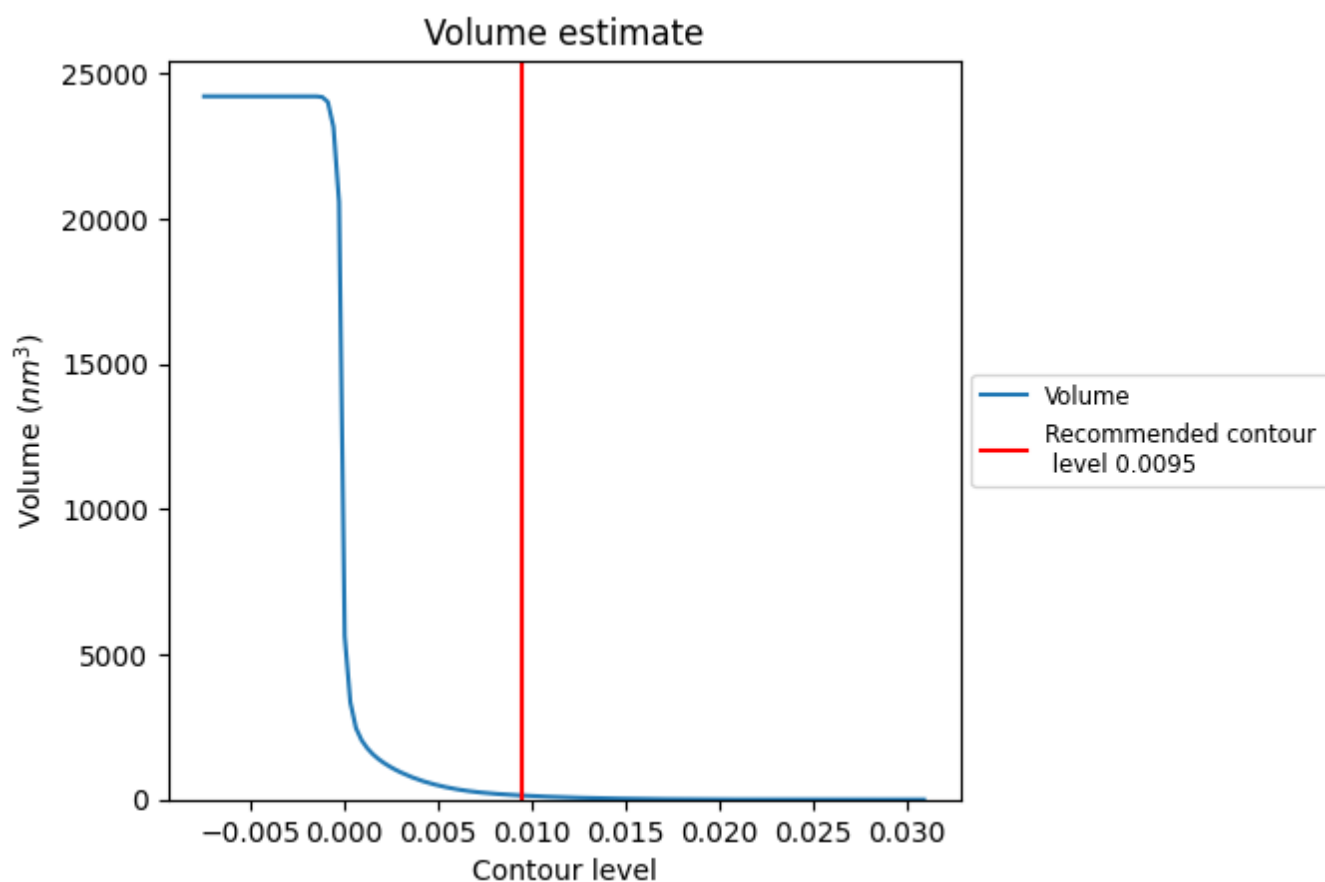
This section contains the results of statistical analysis of the map.

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.

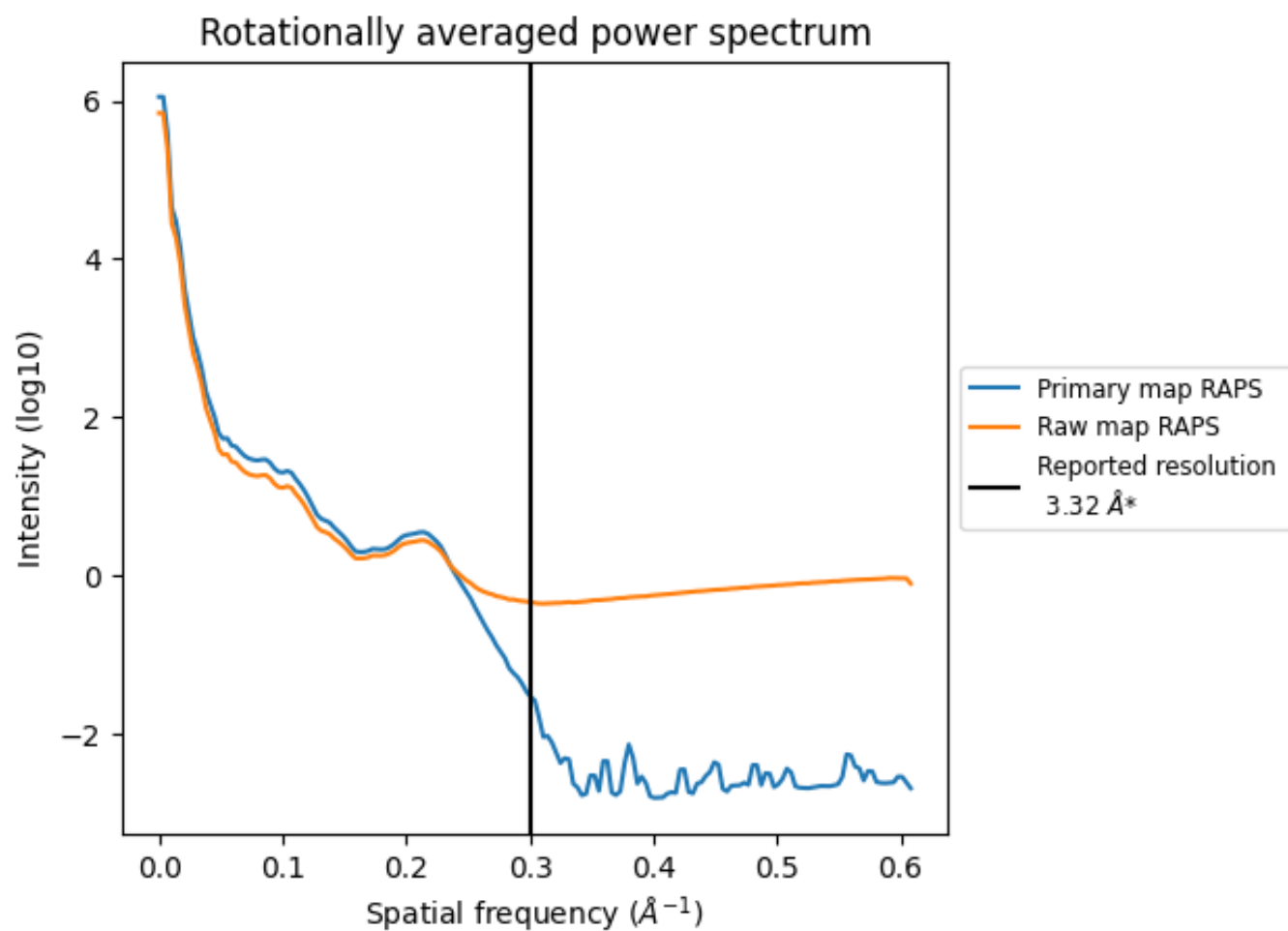
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 126 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 ⓘ

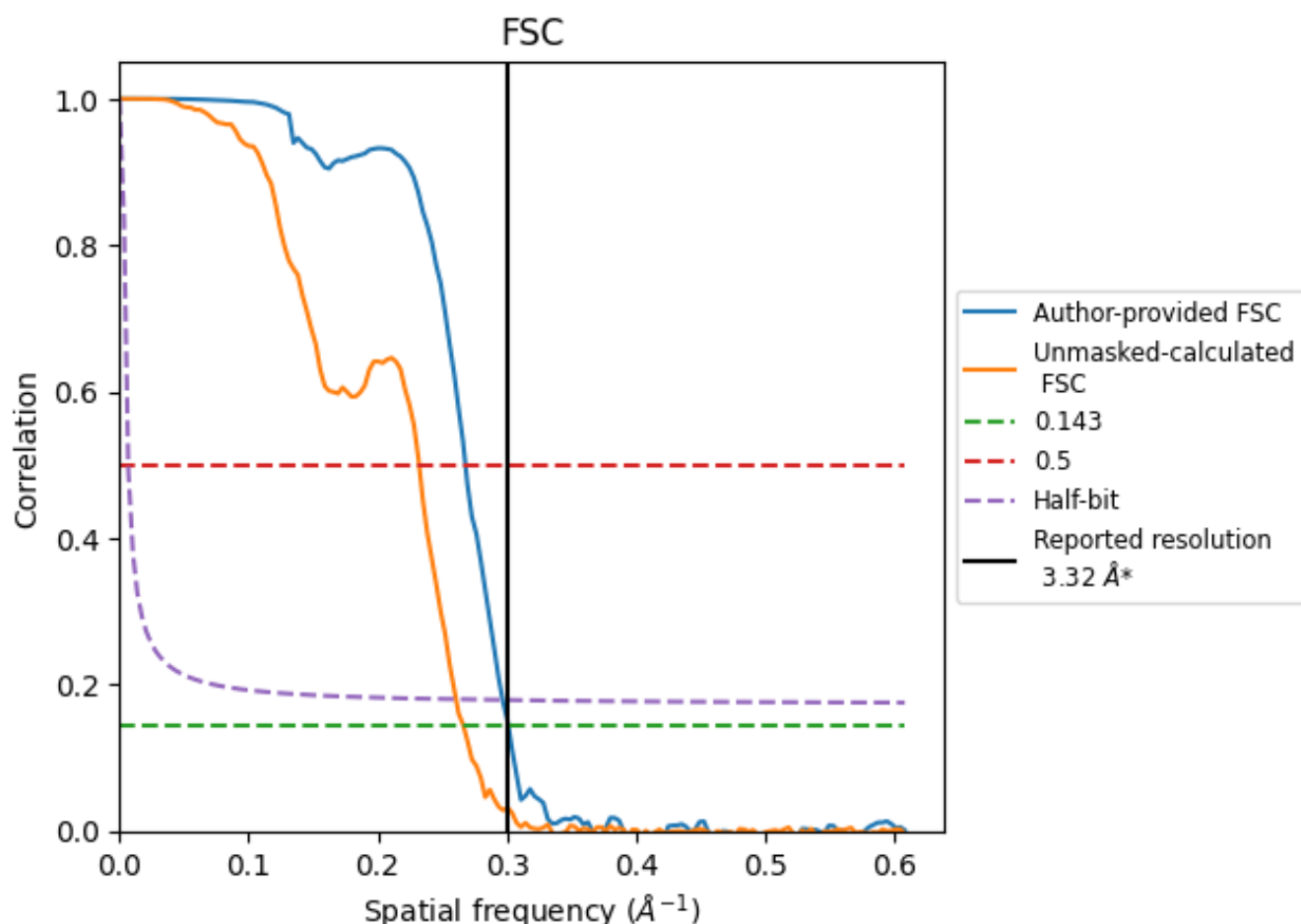


*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

8.2 Resolution estimates [i](#)

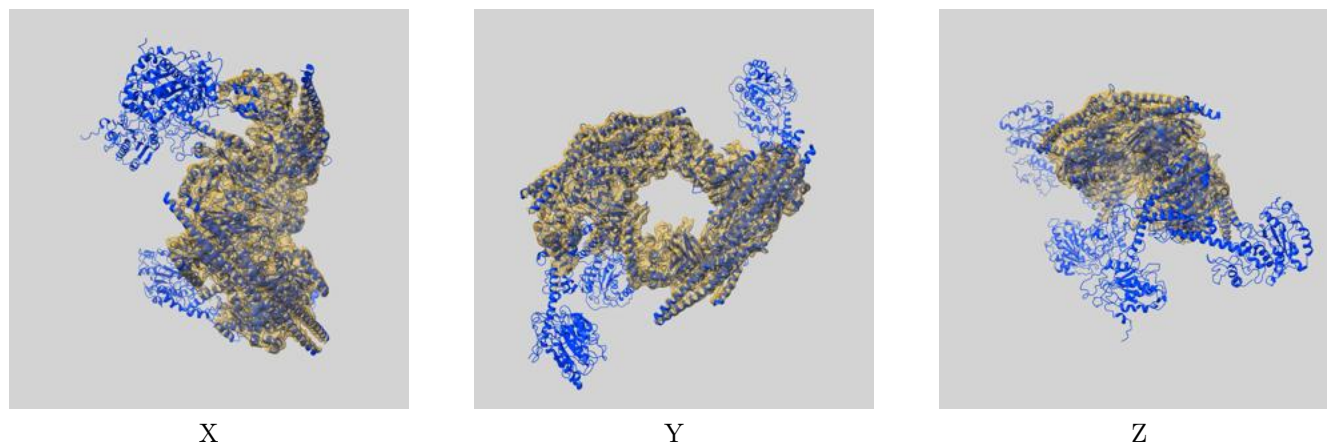
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	3.32	3.73	3.37
Unmasked-calculated*	3.75	4.31	3.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.32 by more than 10 %

9 Map-model fit [i](#)

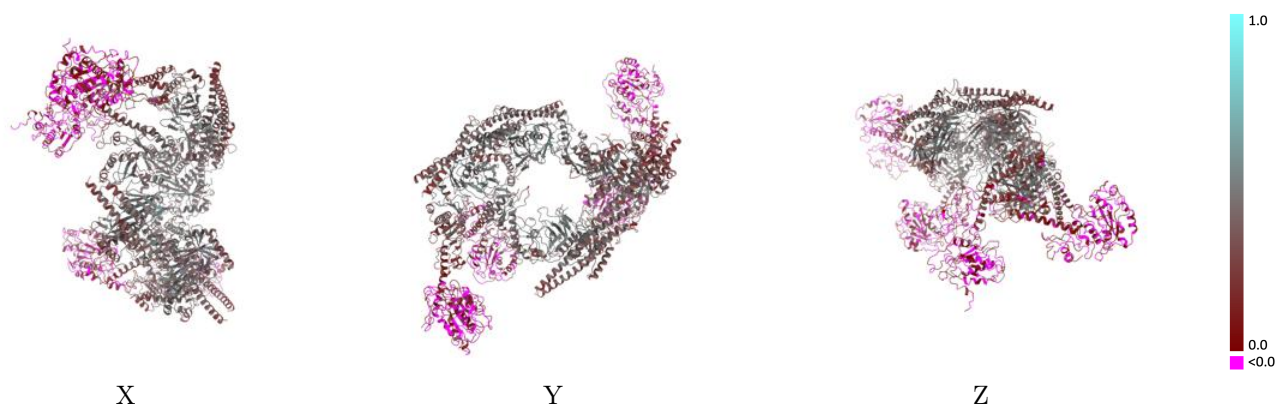
This section contains information regarding the fit between EMDB map EMD-18009 and PDB model 8PY2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



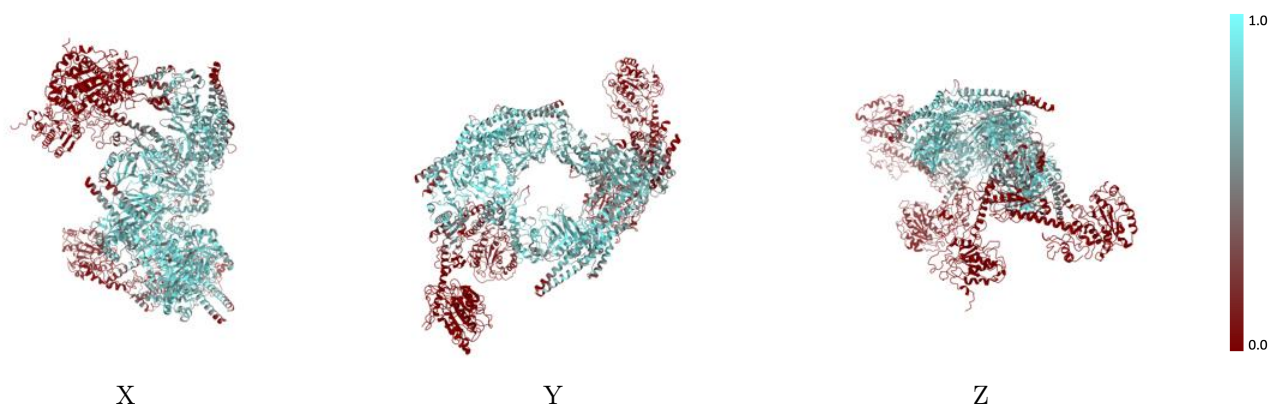
The images above show the 3D surface view of the map at the recommended contour level 0.0095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



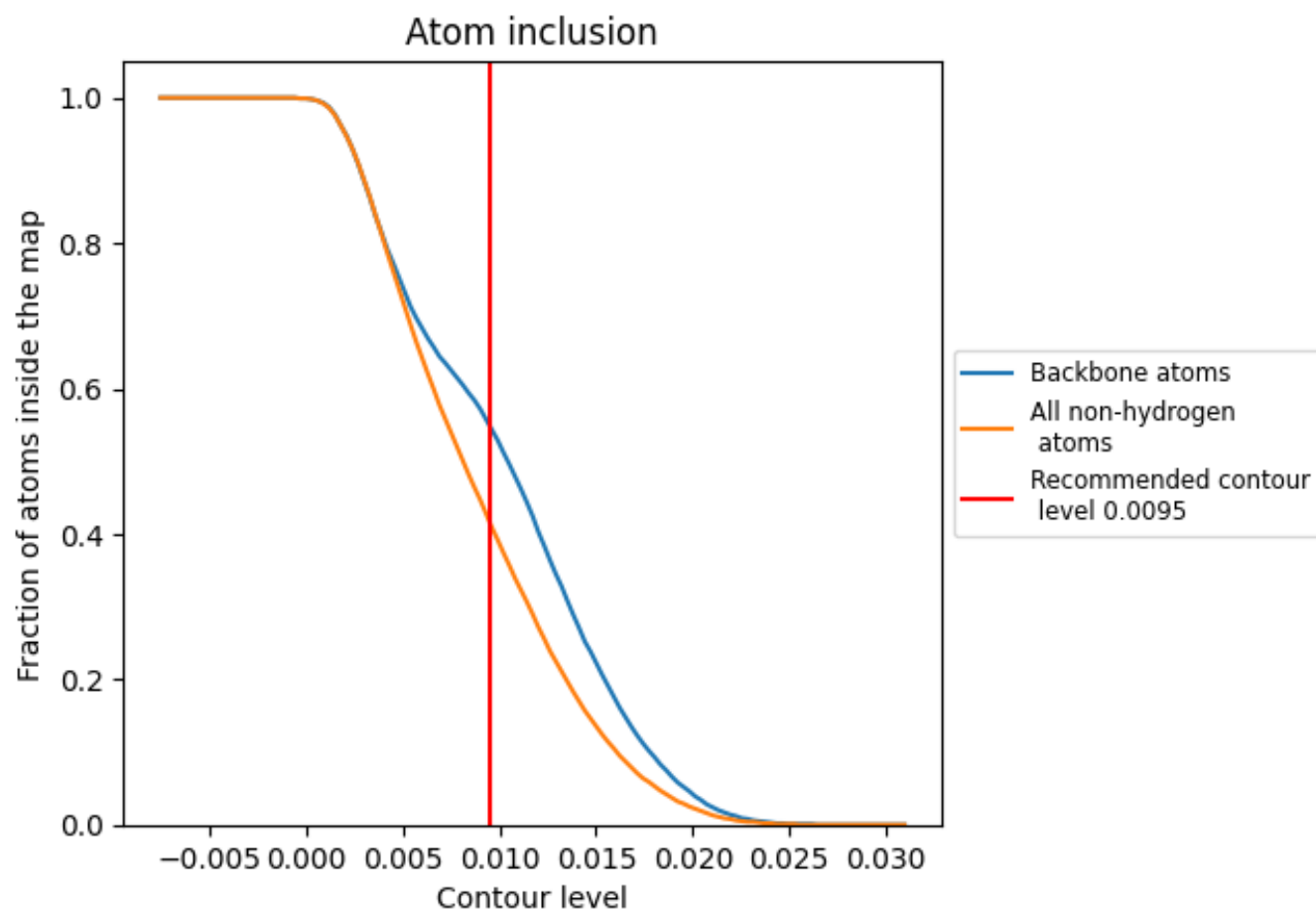
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0095).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 42% 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 (0.0095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4160	 0.2810
A	 0.7120	 0.4160
B	 0.7310	 0.4400
C	 0.7740	 0.4400
D	 0.7550	 0.4340
E	 0.2740	 0.2330
F	 0.3780	 0.3040
G	 0.6860	 0.4070
H	 0.6230	 0.3940
I	 0.6470	 0.4010
J	 0.7090	 0.4280
K	 0.4360	 0.3120
L	 0.1170	 0.1740
M	 0.0000	 0.0390
N	 0.0000	 0.0280
O	 0.0000	 0.0180
P	 0.0000	 0.0330

