Full wwPDB EM Validation Report ⓘ

Feb 2, 2025 – 02:13 am GMT

PDB ID	:	8PVY
EMDB ID	:	EMD-17980
Title	:	Cryo-EM structure of the human BRISC dimer complex bound to compound FX-171-C
Authors	:	Chandler, F.; Zeqiraj, E.
Deposited on	:	2023-07-18
Resolution	:	3.02 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:

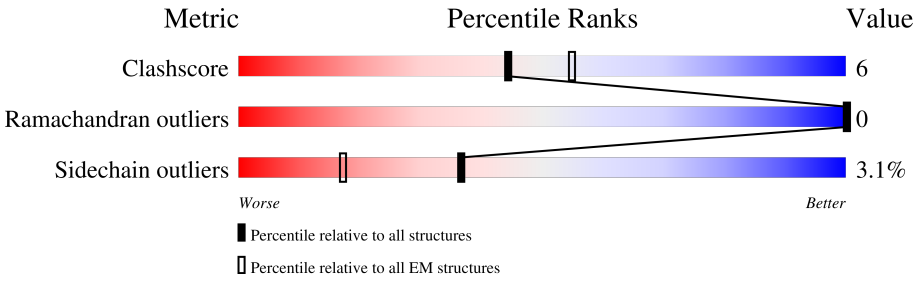
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	312	68% 13% 19%
1	C	312	65% 14% 19%
1	G	312	64% 16% 19%
1	I	312	67% 13% 19%
2	B	267	80% 8% 11%
2	D	267	70% 18% 11%
2	H	267	5% 73% 14% 11%
2	J	267	76% 12% 11%

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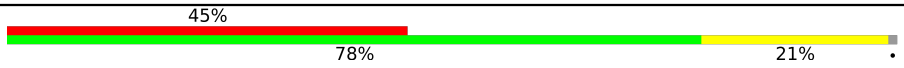
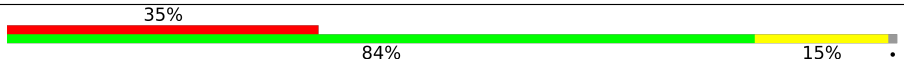
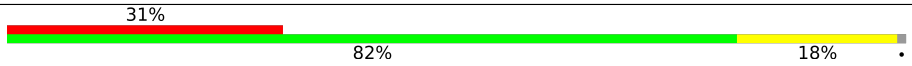
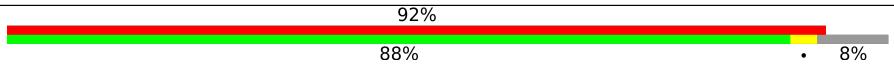
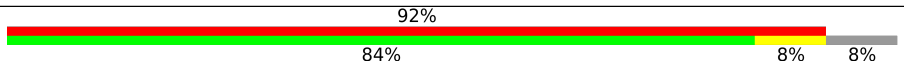
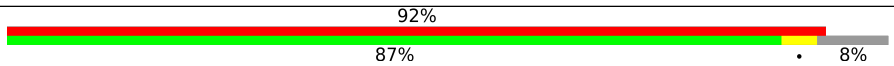
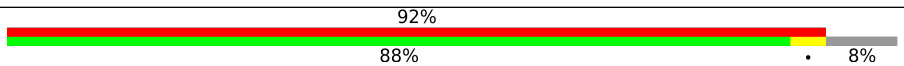
Mol	Chain	Length	Quality of chain
3	E	385	
3	F	385	
3	K	385	
3	L	385	
4	M	259	
4	N	259	
4	O	259	
4	P	259	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35736 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	C	N	O	S	0	0
			2027	1272	363	378	14		
1	C	252	Total	C	N	O	S	0	0
			2026	1272	363	377	14		
1	G	252	Total	C	N	O	S	0	0
			2027	1272	363	378	14		
1	I	252	Total	C	N	O	S	0	0
			2027	1272	363	378	14		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	383	Total	C	N	O	S	0	0
			3063	1980	503	566	14		
3	F	383	Total	C	N	O	S	0	0
			3065	1981	504	567	13		
3	K	383	Total	C	N	O	S	0	0
			3072	1987	504	567	14		
3	L	383	Total	C	N	O	S	0	0
			3071	1989	503	566	13		

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
			1879	1200	302	359	18		
4	N	237	Total	C	N	O	S	0	0
			1889	1206	306	359	18		
4	O	237	Total	C	N	O	S	0	0
			1889	1206	306	359	18		
4	P	237	Total	C	N	O	S	0	0
			1879	1199	305	357	18		

There are 4 discrepancies between the modelled and reference sequences:

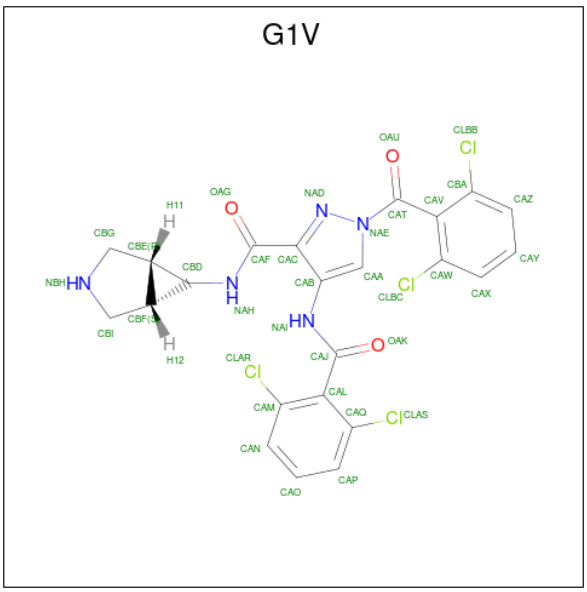
Chain	Residue	Modelled	Actual	Comment	Reference
M	71	MET	-	initiating methionine	UNP Q9NWV8
N	71	MET	-	initiating methionine	UNP Q9NWV8
O	71	MET	-	initiating methionine	UNP Q9NWV8
P	71	MET	-	initiating methionine	UNP Q9NWV8

- 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 N-[(1R,5S)-3-azabicyclo[3.1.0]hexan-6-yl]-1-[2,6-bis(chloranyl)phenyl]carbonyl-4-[[2,6-bis(chloranyl)phenyl]carbonylamino]pyrazole-3-carboxamide (three-letter code:

G1V) (formula: $C_{23}H_{17}Cl_4N_5O_3$) (labeled as "Ligand of Interest" by depositor).



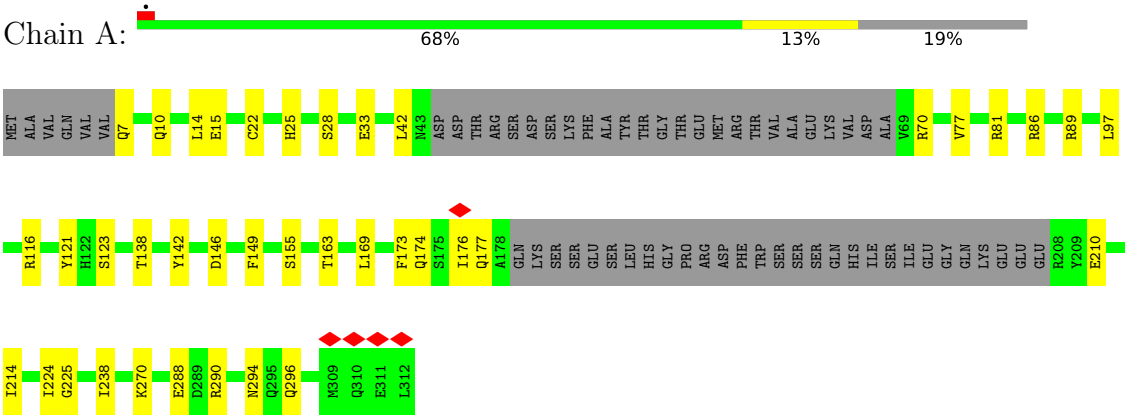
Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	Cl	N	O	0
			35	23	4	5	3	
6	I	1	Total	C	Cl	N	O	0
			35	23	4	5	3	

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.

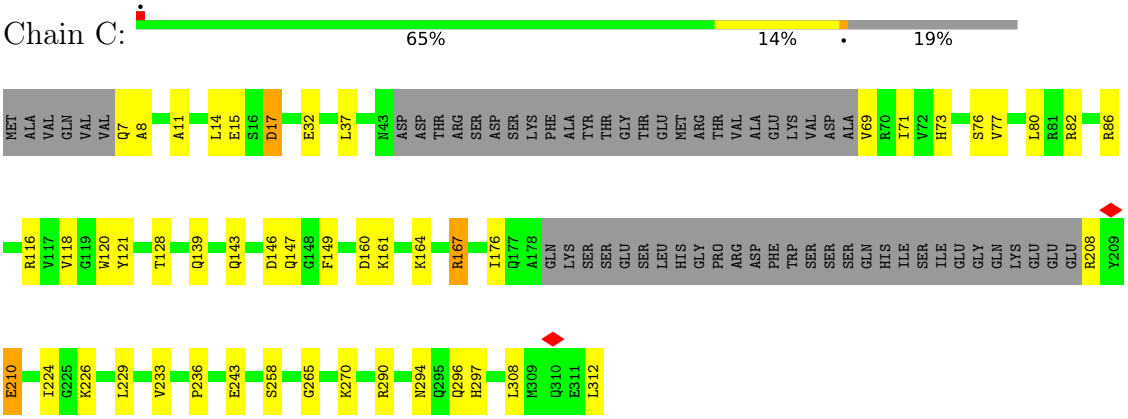
• Molecule 1: Lys-63-specific deubiquitinase BRCC36

Chain A:



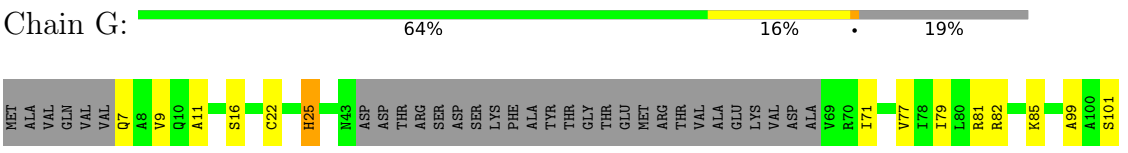
• Molecule 1: Lys-63-specific deubiquitinase BRCC36

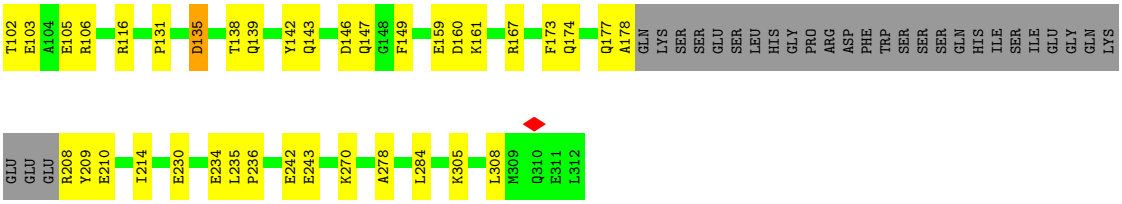
Chain C:



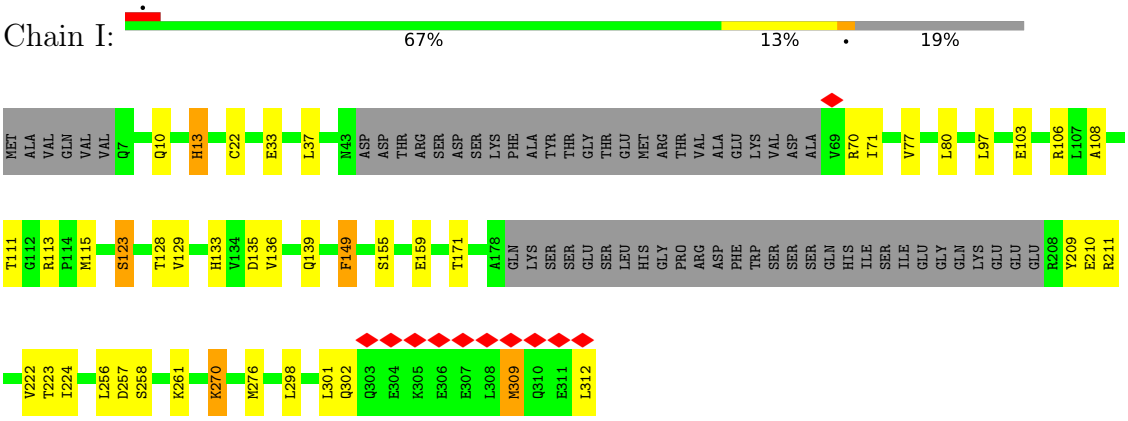
• Molecule 1: Lys-63-specific deubiquitinase BRCC36

Chain G:

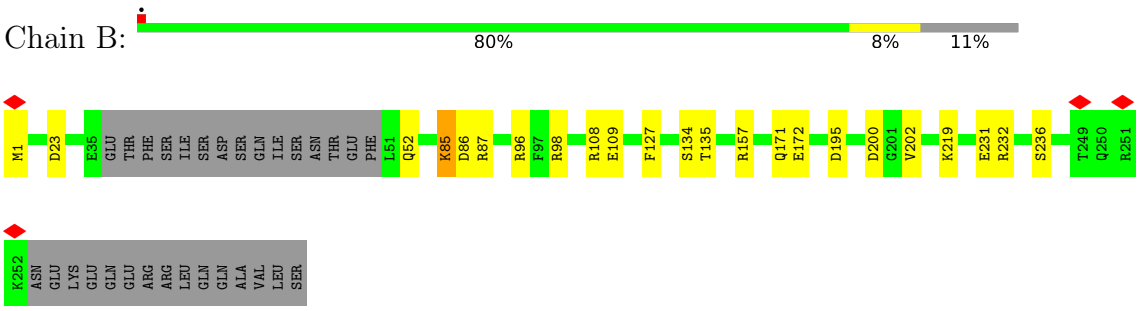




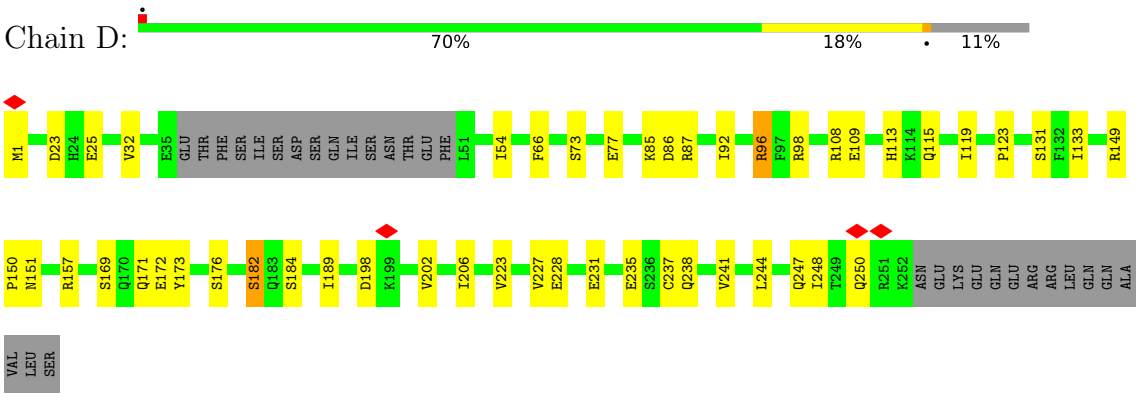
• Molecule 1: Lys-63-specific deubiquitinase BRCC36



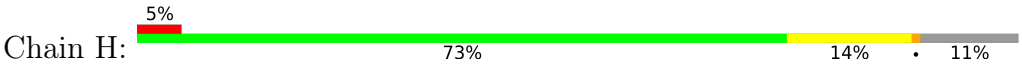
• Molecule 2: BRISC complex subunit Abraxas 2

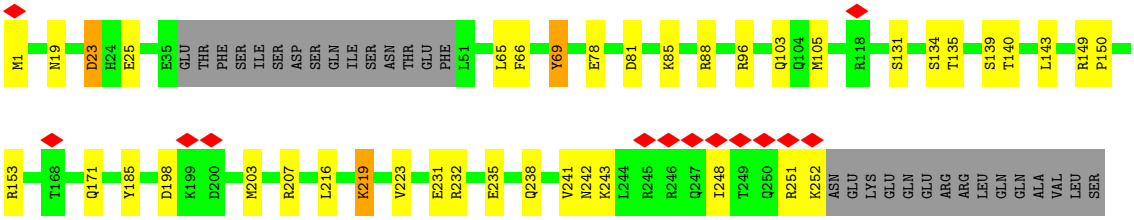


• Molecule 2: BRISC complex subunit Abraxas 2

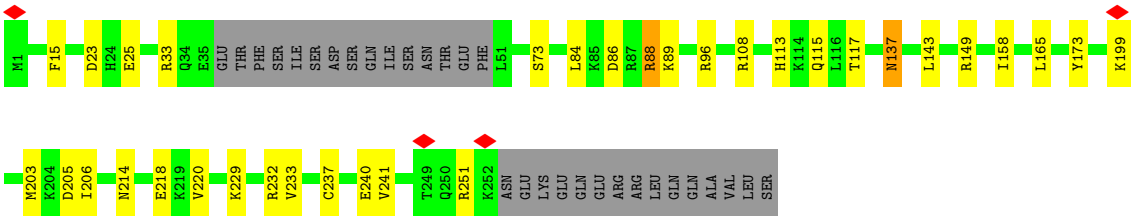


• Molecule 2: BRISC complex subunit Abraxas 2

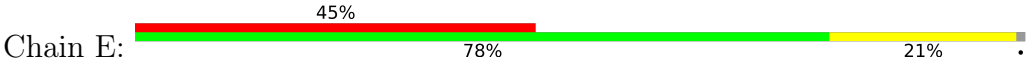


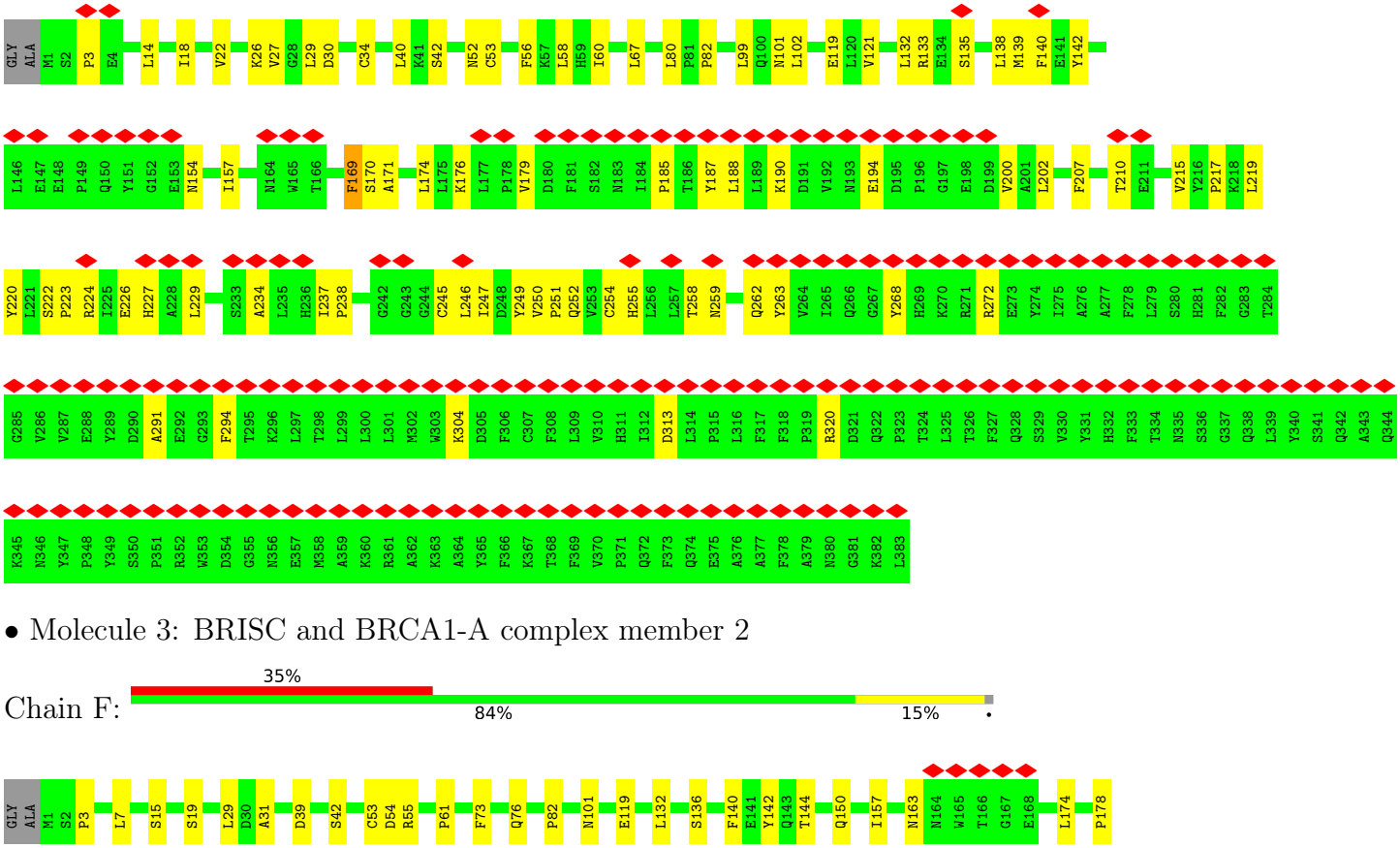


• Molecule 2: BRISC complex subunit Abraxas 2

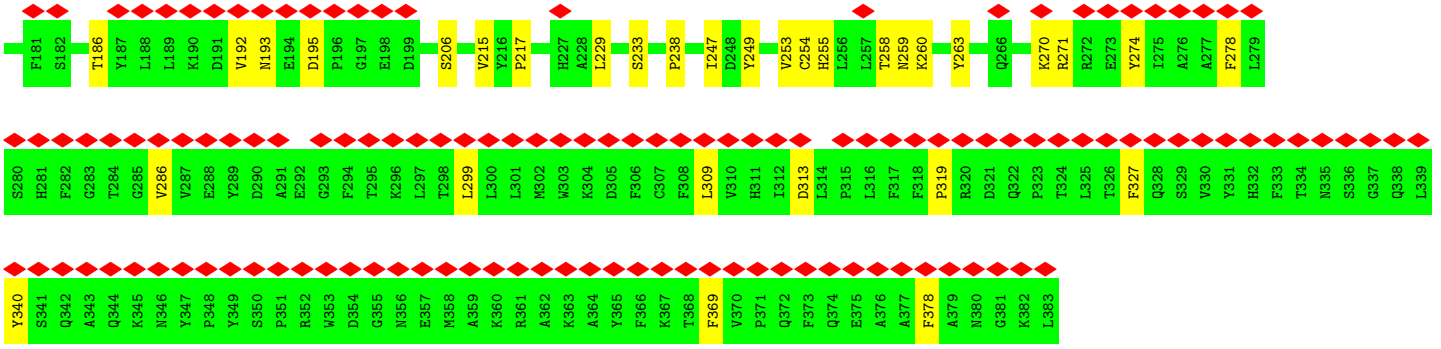


• Molecule 3: BRISC and BRCA1-A complex member 2



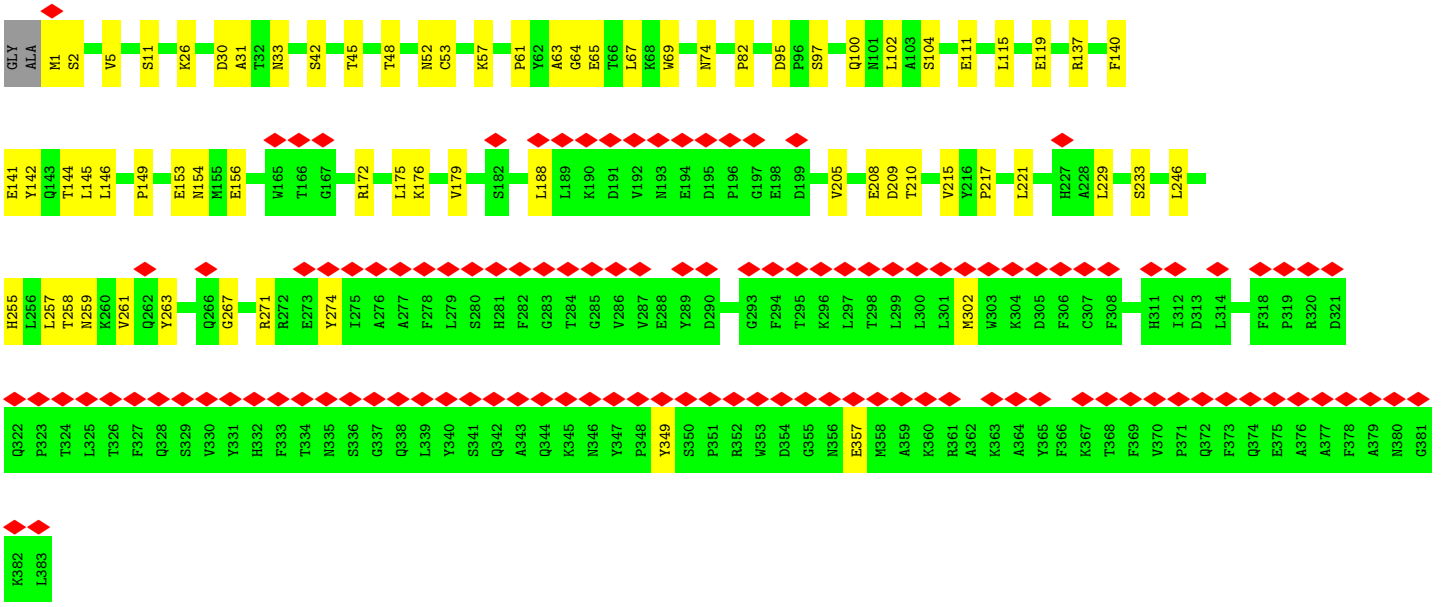


• Molecule 3: BRISC and BRCA1-A complex member 2



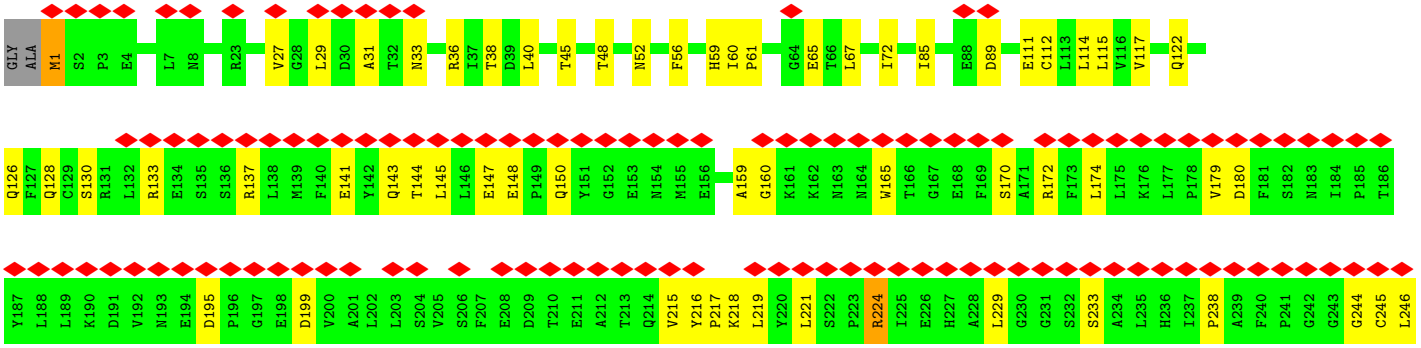
• Molecule 3: BRISC and BRCA1-A complex member 2

Chain K:



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

Chain L:



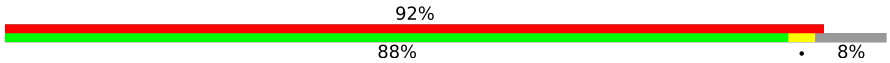
I247 D248 Y249 V250 P251 Q252 V253 C254 H255 L256 L257 T258 N259 K260 V261 Q262 Y263 V264 I265 Q266 G267 Y268 H269 K270 R271 R272 E273 Y274 I275 A276 A277 F278 L279 S280 H281 F282 G283 T284 G285 V286 V287 E288 Y289 D290 A291 E292 G293 F294 T295 K296 L297 T298 L299 L300 L301 M302 W303 K304 D305 F306

C307 F308 L309 V310 H311 I312 D313 L314 P315 L316 F317 F318 P319 R320 D321 Q322 P323 T324 L325 T326 F327 Q328 S329 V330 Y331 H332 F333 T334 N335 S336 G337 Q338 L339 Y340 S341 Q342 A343 Q344 K345 N346 Y347 P348 Y349 S350 P351 R352 W353 D354 G355 N356 E357 M358 A359 K360 R361 A362 K363 A364 Y365 F366

K367 T368 F369 V370 P371 Q372 F373 Q374 E375 A376 A377 F378 A379 N380 G381 K382 L383

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

Chain M:



MET SER TRP GLN VAL PRO PRO PRO ALA PRO E81 V82 Q83 I84 R85 T86 P87 R88 V89 N90 C91 P92 E93 K94 V95 I96 I97 C98 L99 D100 L101 S102 E103 E104 M105 S106 L107 P108 K109 L110 E111 S112 F113 N114 G115 S116 K117 T118 N119 A120 L121 N122 V123 S124 Q125 K126 M127 I128 E129 M130

F131 V132 R133 T134 K135 H136 K137 I138 D139 K140 S141 H142 E143 F144 A145 L146 V147 V148 V149 N150 D151 D152 T153 A154 W155 L156 S157 G158 L159 T160 S161 D162 P163 R164 E165 L166 C167 S168 C169 L170 Y171 D172 L173 E174 T175 A176 S177 C178 S179 T180 F181 N182 L183 E184 G185 L186 F187 S188 L189 I190

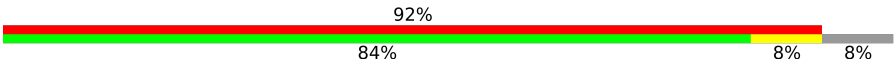
Q191 Q192 K193 T194 E195 L196 P197 V198 T199 E200 N201 V202 Q203 T204 I205 P206 P207 P208 Y209 V210 V211 R212 T213 I214 L215 V216 Y217 S218 R219 P220 P221 C222 Q223 P224 Q225 F226 S227 L228 T229 E230 P231 M232 K233 K234 M235 F236 Q237 C238 P239 Y240 F241 F242 F243 D244 V245 V246 Y247 I248 H249 N250

G251 T252 E253 E254 K255 E256 E257 E258 M259 S260 W261 K262 D263 M264 F265 A266 F267 M268 G269 S270 L271 D272 T273 K274 G275 T276 S277 Y278 K279 Y280 E281 V282 A283 L284 A285 G286 P287 A288 L289 E290 L291 H292 N293 C294 M295 A296 K297 L298 L299 A300 H301 P302 L303 Q304 R305 P306 C307 Q308 S309 H310

A311 S312 Y313 S314 L315 L316 E317 GLU GLU ASP GLU ALA ILE GLU VAL GLU ALA THR VAL

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

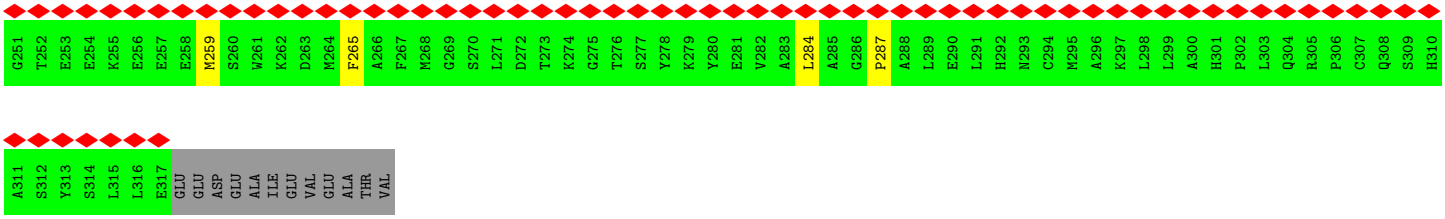
Chain N:



MET SER TRP GLN VAL PRO PRO PRO ALA PRO E81 V82 Q83 I84 R85 T86 P87 R88 V89 N90 C91 P92 E93 K94 V95 I96 I97 C98 L99 D100 L101 S102 E103 E104 M105 S106 L107 P108 K109 L110 E111 S112 F113 N114 G115 S116 K117 T118 N119 A120 L121 N122 V123 S124 Q125 K126 M127 I128 E129 M130

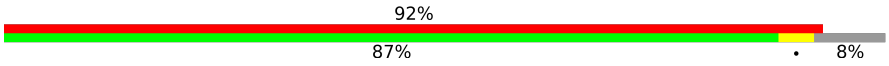
F131 V132 R133 T134 K135 H136 K137 I138 D139 K140 S141 H142 E143 F144 A145 L146 V147 V148 V149 N150 D151 D152 T153 A154 W155 L156 S157 G158 L159 T160 S161 D162 P163 R164 E165 L166 C167 S168 C169 L170 Y171 D172 L173 E174 T175 A176 S177 C178 S179 T180 F181 N182 L183 E184 G185 L186 F187 S188 L189 I190

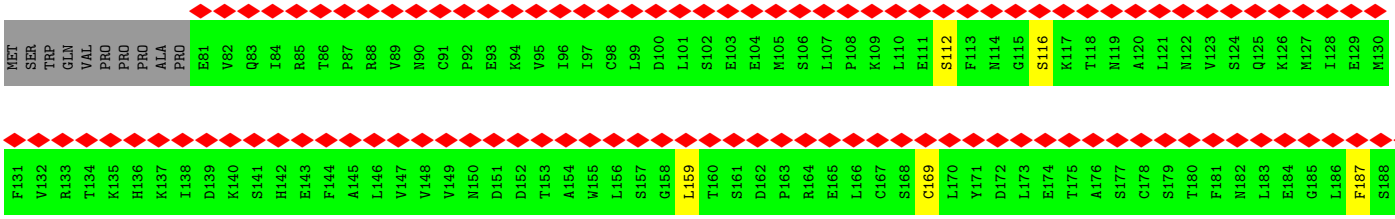
Q191 Q192 K193 T194 E195 L196 P197 V198 T199 E200 N201 V202 Q203 T204 I205 P206 P207 P208 Y209 V210 V211 R212 T213 I214 L215 V216 Y217 S218 R219 P220 P221 C222 Q223 P224 Q225 F226 S227 L228 T229 E230 P231 M232 K233 K234 M235 F236 Q237 C238 P239 Y240 F241 F242 F243 D244 V245 V246 Y247 I248 H249 N250



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

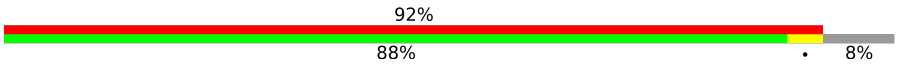
Chain O:

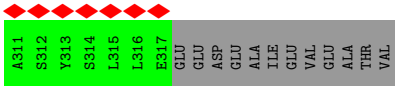




• Molecule 4: BRISC and BRCA1-A complex member 1

Chain P:




A311
S312
Y313
S314
L315
L316
E317
GLU
GLU
ASP
GLU
ALA
ILE
GLU
VAL
GLU
ALA
THR
VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	632988	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 ($e^-/Å^2$)	34.97	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	272.60162, 272.60162, 272.60162	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7099001, 0.7099001, 0.7099001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G1V, 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	A	0.24	0/2063	0.48	0/2788
1	C	0.25	0/2062	0.50	0/2787
1	G	0.25	0/2063	0.49	0/2788
1	I	0.24	0/2063	0.49	0/2788
2	B	0.26	0/1972	0.49	0/2655
2	D	0.27	0/1972	0.52	0/2655
2	H	0.25	0/1972	0.49	0/2655
2	J	0.26	0/1972	0.50	0/2655
3	E	0.26	0/3152	0.50	0/4288
3	F	0.25	0/3154	0.49	0/4291
3	K	0.25	0/3162	0.47	0/4301
3	L	0.26	0/3162	0.50	1/4302 (0.0%)
4	M	0.25	0/1922	0.49	0/2607
4	N	0.29	0/1934	0.59	2/2623 (0.1%)
4	O	0.25	0/1934	0.52	1/2623 (0.0%)
4	P	0.24	0/1923	0.50	1/2608 (0.0%)
All	All	0.25	0/36482	0.50	5/49414 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	232	MET	CA-CB-CG	7.15	125.46	113.30
4	O	159	LEU	CA-CB-CG	6.94	131.26	115.30
4	P	284	LEU	CA-CB-CG	6.88	131.12	115.30
3	L	145	LEU	CA-CB-CG	6.68	130.67	115.30
4	N	284	LEU	CA-CB-CG	6.52	130.29	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2027	0	2022	24	0
1	C	2026	0	2019	28	0
1	G	2027	0	2022	30	0
1	I	2027	0	2022	28	0
2	B	1937	0	1924	21	0
2	D	1937	0	1924	38	0
2	H	1937	0	1924	28	0
2	J	1937	0	1924	22	0
3	E	3063	0	2983	49	0
3	F	3065	0	2984	30	0
3	K	3072	0	2994	41	0
3	L	3071	0	2988	45	0
4	M	1879	0	1861	2	0
4	N	1889	0	1871	7	0
4	O	1889	0	1871	2	0
4	P	1879	0	1860	0	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	5	0
6	I	35	0	0	7	0
All	All	35736	0	35193	354	0

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

All (354) 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)
6:I:402:G1V:CLAR	6:I:402:G1V:NAI	2.46	0.84
1:G:305:LYS:HZ1	2:J:241:VAL:HA	1.45	0.82
1:C:128:THR:HA	6:D:301:G1V:CLAS	2.20	0.79
6:D:301:G1V:CLAR	6:D:301:G1V:NAI	2.54	0.77
1:A:294:ASN:HD21	2:B:231:GLU:HG2	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:73:SER:O	2:J:115:GLN:NE2	2.21	0.73
3:L:274:TYR:OH	3:L:358:MET:SD	2.43	0.73
2:H:150:PRO:O	2:H:153:ARG:NH1	2.22	0.73
1:C:294:ASN:ND2	2:D:231:GLU:OE2	2.21	0.73
1:C:160:ASP:OD2	1:C:167:ARG:NH1	2.22	0.73
3:K:31:ALA:HB1	3:K:64:GLY:H	1.52	0.73
3:K:145:LEU:HD13	3:K:175:LEU:HD21	1.72	0.72
3:E:174:LEU:HD11	3:E:202:LEU:HD23	1.71	0.72
1:I:128:THR:HA	6:I:402:G1V:CLAS	2.27	0.72
1:I:309:MET:SD	1:I:309:MET:N	2.61	0.71
3:K:2:SER:HB2	3:K:5:VAL:HG12	1.73	0.71
3:L:1:MET:HG2	3:L:36:ARG:HH21	1.55	0.71
3:E:223:PRO:HD2	3:E:224:ARG:H	1.54	0.71
1:A:174:GLN:HB2	1:A:214:ILE:HD11	1.71	0.71
3:L:33:ASN:HB2	3:L:61:PRO:HB3	1.73	0.70
3:F:286:VAL:N	4:N:225:GLN:O	2.25	0.70
1:G:116:ARG:NH2	1:G:146:ASP:OD1	2.24	0.70
3:E:40:LEU:HD23	3:E:56:PHE:HB3	1.74	0.69
6:D:301:G1V:CLBB	6:D:301:G1V:NAD	2.63	0.68
1:C:296:GLN:OE1	2:D:87:ARG:NH2	2.27	0.68
2:D:73:SER:O	2:D:115:GLN:NE2	2.22	0.68
3:E:60:ILE:HB	3:E:67:LEU:HD12	1.76	0.67
2:D:108:ARG:NH2	3:E:82:PRO:O	2.28	0.67
3:F:136:SER:OG	1:I:211:ARG:NH2	2.22	0.67
1:I:139:GLN:NE2	1:I:149:PHE:O	2.27	0.67
2:J:86:ASP:O	2:J:89:LYS:NZ	2.27	0.67
1:G:174:GLN:HB2	1:G:214:ILE:HD11	1.77	0.66
3:L:130:SER:HA	3:L:133:ARG:HG3	1.76	0.66
2:B:1:MET:N	2:B:52:GLN:O	2.28	0.66
1:G:178:ALA:O	1:G:208:ARG:N	2.29	0.66
1:A:116:ARG:NH2	1:A:146:ASP:OD2	2.28	0.66
6:I:402:G1V:CLBB	6:I:402:G1V:NAD	2.66	0.66
3:L:29:LEU:HD11	3:L:174:LEU:HD21	1.76	0.66
3:E:190:LYS:NZ	3:E:223:PRO:O	2.29	0.66
1:C:265:GLY:HA2	2:D:206:ILE:HD11	1.77	0.66
2:B:108:ARG:NH2	3:F:82:PRO:O	2.29	0.65
3:K:97:SER:O	3:K:100:GLN:NE2	2.28	0.65
1:C:139:GLN:NE2	1:C:149:PHE:O	2.21	0.65
2:B:171:GLN:NE2	2:D:169:SER:O	2.30	0.65
3:E:229:LEU:HB2	3:E:234:ALA:HB2	1.79	0.64
3:E:101:ASN:ND2	3:E:119:GLU:OE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:LYS:HD3	2:D:184:SER:HB3	1.79	0.63
2:B:171:GLN:HG2	1:C:270:LYS:HE3	1.80	0.63
3:E:133:ARG:HH22	3:E:142:TYR:HE2	1.46	0.62
2:H:23:ASP:HB3	2:H:65:LEU:HD21	1.81	0.62
1:I:111:THR:HG23	1:I:113:ARG:H	1.64	0.62
1:I:129:VAL:N	6:I:402:G1V:CLAS	2.70	0.62
3:L:215:VAL:HG23	3:L:217:PRO:HD3	1.80	0.62
1:G:270:LYS:HE3	2:H:171:GLN:HE21	1.65	0.61
2:D:123:PRO:O	2:D:151:ASN:ND2	2.31	0.61
1:I:256:LEU:O	1:I:261:LYS:NZ	2.33	0.61
1:A:177:GLN:HB2	1:A:210:GLU:HG2	1.83	0.60
3:L:263:TYR:HA	3:L:266:GLN:HB2	1.82	0.60
3:E:247:ILE:HD12	3:E:247:ILE:H	1.66	0.60
3:L:112:CYS:HA	3:L:115:LEU:HD12	1.83	0.60
2:J:108:ARG:NH2	3:K:82:PRO:O	2.32	0.59
3:F:144:THR:HG23	3:F:247:ILE:HD11	1.83	0.59
3:L:229:LEU:O	3:L:233:SER:OG	2.20	0.59
3:L:38:THR:OG1	3:L:59:HIS:NE2	2.32	0.59
1:C:229:LEU:HD23	2:D:228:GLU:HG2	1.86	0.58
1:A:288:GLU:OE1	2:D:182:SER:OG	2.20	0.58
3:K:229:LEU:O	3:K:233:SER:OG	2.21	0.58
3:F:299:LEU:HA	4:N:229:THR:O	2.03	0.58
2:H:105:MET:HE1	2:H:150:PRO:HG3	1.85	0.58
3:L:40:LEU:HD23	3:L:56:PHE:HB3	1.86	0.57
3:K:154:ASN:HD22	3:K:176:LYS:HB3	1.69	0.57
1:C:226:LYS:HD2	2:D:228:GLU:OE1	2.04	0.57
2:D:32:VAL:HG23	2:D:92:ILE:HG13	1.85	0.57
3:L:144:THR:HB	3:L:247:ILE:HD12	1.87	0.57
3:F:247:ILE:HD12	3:F:247:ILE:H	1.70	0.56
2:H:103:GLN:OE1	2:H:131:SER:OG	2.15	0.56
3:E:3:PRO:HB3	3:E:22:VAL:HG21	1.87	0.56
3:E:238:PRO:O	3:E:249:TYR:OH	2.20	0.56
2:H:171:GLN:HE22	1:I:270:LYS:HE3	1.69	0.56
3:L:195:ASP:N	3:L:195:ASP:OD1	2.36	0.56
4:O:265:PHE:O	4:O:269:GLY:N	2.39	0.56
3:L:31:ALA:HB3	3:L:61:PRO:HB2	1.88	0.55
1:G:82:ARG:O	1:G:85:LYS:NZ	2.39	0.55
3:E:245:CYS:SG	3:E:246:LEU:N	2.78	0.55
1:G:160:ASP:OD1	1:G:167:ARG:NH2	2.38	0.55
2:J:137:ASN:O	2:J:137:ASN:ND2	2.40	0.55
3:L:238:PRO:O	3:L:249:TYR:OH	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:42:SER:HA	3:E:53:CYS:HA	1.88	0.55
2:H:81:ASP:OD1	2:H:88:ARG:NH1	2.38	0.55
3:E:272:ARG:HG2	3:E:291:ALA:HA	1.88	0.55
3:E:135:SER:HB3	3:E:138:LEU:HB2	1.88	0.55
3:L:72:ILE:HD11	3:L:85:ILE:HD11	1.87	0.55
3:L:179:VAL:HG13	3:L:258:THR:HG23	1.87	0.55
2:H:1:MET:SD	2:H:149:ARG:NH1	2.73	0.55
1:C:11:ALA:HB3	1:C:71:ILE:HG12	1.88	0.55
1:C:312:LEU:HD21	2:D:248:ILE:HD11	1.89	0.55
1:I:298:LEU:O	1:I:302:GLN:HG2	2.07	0.55
1:A:296:GLN:OE1	2:B:87:ARG:NH2	2.41	0.54
3:E:185:PRO:HG2	3:E:187:TYR:HE2	1.73	0.54
1:G:284:LEU:HD23	2:H:185:TYR:HB2	1.88	0.54
3:L:45:THR:OG1	3:L:48:THR:OG1	2.24	0.54
1:C:243:GLU:OE1	2:D:173:TYR:OH	2.25	0.54
1:A:22:CYS:SG	1:A:77:VAL:HG21	2.48	0.54
2:D:98:ARG:NH1	2:D:109:GLU:OE2	2.41	0.54
3:F:29:LEU:HD23	3:F:174:LEU:HD23	1.90	0.54
3:F:140:PHE:O	3:F:144:THR:HG22	2.08	0.54
2:J:25:GLU:HG3	2:J:96:ARG:HG2	1.90	0.54
3:L:27:VAL:HG21	3:L:117:VAL:HG12	1.89	0.54
2:H:235:GLU:HB2	1:I:223:THR:HG21	1.90	0.53
2:J:214:ASN:O	2:J:218:GLU:HG3	2.08	0.53
3:E:202:LEU:HB2	3:E:220:TYR:HB3	1.89	0.53
2:J:203:MET:HB2	2:J:206:ILE:HD12	1.90	0.53
3:F:31:ALA:HB3	3:F:61:PRO:HB2	1.90	0.53
1:G:139:GLN:NE2	1:G:149:PHE:O	2.41	0.53
1:A:225:GLY:HA2	2:B:232:ARG:HH22	1.73	0.53
3:E:169:PHE:HD1	3:E:170:SER:H	1.57	0.53
3:F:192:VAL:HA	3:F:195:ASP:HB2	1.92	0.52
1:A:270:LYS:NZ	2:D:171:GLN:HG3	2.23	0.52
3:E:132:LEU:HD12	3:E:157:ILE:HD11	1.91	0.52
1:G:159:GLU:OE2	1:G:161:LYS:NZ	2.41	0.52
2:H:231:GLU:OE2	1:I:224:ILE:N	2.36	0.52
3:E:250:VAL:HG13	3:E:251:PRO:HD3	1.91	0.52
3:L:65:GLU:HG2	3:L:172:ARG:HH11	1.75	0.52
3:L:259:ASN:OD1	3:L:263:TYR:OH	2.25	0.52
2:H:135:THR:HG22	6:I:402:G1V:CAX	2.39	0.52
1:A:294:ASN:ND2	2:B:231:GLU:HG2	2.22	0.52
4:O:112:SER:N	4:O:116:SER:O	2.35	0.52
3:E:185:PRO:HG2	3:E:187:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:26:LYS:HD2	3:K:30:ASP:HB2	1.91	0.51
1:A:25:HIS:O	1:A:28:SER:OG	2.27	0.51
3:E:215:VAL:HG23	3:E:217:PRO:HD3	1.93	0.51
2:H:25:GLU:N	2:H:25:GLU:OE2	2.44	0.51
2:D:133:ILE:HD11	6:D:301:G1V:CLBB	2.47	0.51
3:F:319:PRO:C	3:L:165:TRP:HE1	2.13	0.51
2:J:237:CYS:O	2:J:241:VAL:HG23	2.11	0.51
2:H:23:ASP:OD2	2:H:96:ARG:NH1	2.43	0.51
3:L:160:GLY:N	3:L:170:SER:O	2.44	0.51
3:F:309:LEU:HA	4:N:230:GLU:H	1.75	0.51
1:I:257:ASP:OD1	1:I:258:SER:N	2.43	0.51
1:G:305:LYS:NZ	2:J:241:VAL:HG22	2.26	0.50
2:J:23:ASP:OD2	3:K:74:ASN:ND2	2.32	0.50
2:D:235:GLU:O	2:D:238:GLN:HG3	2.12	0.50
3:L:271:ARG:HA	3:L:274:TYR:CZ	2.47	0.50
1:C:76:SER:OG	1:C:77:VAL:N	2.44	0.50
3:F:132:LEU:HD22	3:F:157:ILE:HG21	1.93	0.50
3:K:255:HIS:HA	3:K:258:THR:HG22	1.93	0.50
2:D:54:ILE:HG23	2:D:92:ILE:HD11	1.94	0.50
1:G:11:ALA:HB3	1:G:71:ILE:HG12	1.92	0.50
3:L:271:ARG:HA	3:L:274:TYR:CE1	2.47	0.50
1:I:210:GLU:OE1	1:I:210:GLU:N	2.45	0.50
3:E:251:PRO:HA	3:E:254:CYS:SG	2.51	0.49
3:F:247:ILE:HD12	3:F:247:ILE:N	2.27	0.49
1:G:278:ALA:HB3	2:J:165:LEU:HD13	1.94	0.49
2:J:113:HIS:O	2:J:117:THR:OG1	2.24	0.49
2:D:1:MET:HG3	2:D:149:ARG:HH22	1.76	0.49
3:F:101:ASN:ND2	3:F:119:GLU:OE1	2.46	0.49
3:L:219:LEU:HG	3:L:221:LEU:HD22	1.95	0.49
1:G:143:GLN:HG2	1:G:147:GLN:HA	1.94	0.49
1:I:37:LEU:HD12	1:I:80:LEU:HD11	1.93	0.49
2:B:96:ARG:HG3	2:B:127:PHE:CE1	2.48	0.49
1:C:8:ALA:H	1:C:69:VAL:HG13	1.77	0.49
3:E:179:VAL:HG13	3:E:258:THR:HG22	1.95	0.49
1:G:22:CYS:SG	1:G:77:VAL:HG21	2.53	0.49
4:N:223:GLN:O	4:N:225:GLN:N	2.45	0.49
3:L:180:ASP:O	3:L:262:GLN:NE2	2.45	0.49
1:A:81:ARG:HG2	1:A:238:ILE:HG23	1.94	0.49
1:I:108:ALA:HB2	1:I:115:MET:HB2	1.94	0.48
2:J:229:LYS:O	2:J:233:VAL:HG13	2.13	0.48
2:D:66:PHE:HD2	3:E:80:LEU:HD13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:GLN:HB2	1:G:9:VAL:HG23	1.95	0.48
3:E:171:ALA:HB3	3:E:207:PHE:HB2	1.95	0.48
2:H:19:ASN:HD21	1:I:222:VAL:HA	1.79	0.48
2:H:134:SER:OG	2:H:135:THR:N	2.47	0.48
1:A:42:LEU:HD21	1:A:70:ARG:H	1.78	0.48
4:N:126:LYS:O	4:N:129:GLU:N	2.47	0.48
2:B:98:ARG:NH1	2:B:109:GLU:OE2	2.44	0.48
1:C:37:LEU:HD12	1:C:80:LEU:HD11	1.96	0.48
1:C:77:VAL:HG13	1:C:121:TYR:HE2	1.79	0.48
3:K:257:LEU:O	3:K:261:VAL:HG12	2.14	0.48
1:A:14:LEU:HD12	1:A:15:GLU:H	1.79	0.47
1:A:86:ARG:HH21	1:A:89:ARG:HD2	1.80	0.47
2:D:77:GLU:HG2	2:D:119:ILE:HD13	1.97	0.47
3:K:154:ASN:ND2	3:K:176:LYS:HB3	2.29	0.47
3:K:205:VAL:HG13	3:K:215:VAL:HG13	1.95	0.47
4:N:97:ILE:O	4:N:147:VAL:N	2.46	0.47
3:L:141:GLU:O	3:L:144:THR:OG1	2.25	0.47
2:B:200:ASP:HB3	2:B:202:VAL:HG12	1.97	0.47
3:F:142:TYR:CE1	3:F:157:ILE:HD11	2.48	0.47
1:G:177:GLN:N	1:G:210:GLU:OE1	2.47	0.47
2:H:248:ILE:HD12	1:I:312:LEU:HD22	1.96	0.47
1:G:243:GLU:OE2	2:J:173:TYR:OH	2.28	0.47
1:I:103:GLU:OE1	1:I:106:ARG:NH2	2.47	0.47
3:K:33:ASN:HB2	3:K:61:PRO:HB3	1.96	0.47
2:D:23:ASP:HB3	2:D:96:ARG:HH21	1.79	0.47
2:D:171:GLN:NE2	2:D:172:GLU:O	2.48	0.47
3:K:209:ASP:OD1	3:K:210:THR:N	2.47	0.47
3:L:128:GLN:OE1	3:L:159:ALA:N	2.36	0.47
3:L:249:TYR:O	3:L:252:GLN:HG3	2.15	0.47
3:L:249:TYR:O	3:L:253:VAL:HG22	2.15	0.47
6:D:301:G1V:CLBC	6:D:301:G1V:OAU	2.69	0.47
1:A:10:GLN:OE1	1:A:70:ARG:NH1	2.48	0.47
3:F:42:SER:HA	3:F:53:CYS:HA	1.97	0.47
1:I:22:CYS:SG	1:I:77:VAL:HG21	2.55	0.47
3:L:137:ARG:NH2	3:L:244:GLY:O	2.48	0.47
4:N:94:LYS:O	4:N:212:ARG:N	2.48	0.47
1:C:17:ASP:OD2	1:C:224:ILE:HA	2.15	0.46
2:D:98:ARG:O	2:D:131:SER:HA	2.15	0.46
3:E:27:VAL:HG11	3:E:121:VAL:HG21	1.98	0.46
3:E:251:PRO:O	3:E:255:HIS:ND1	2.48	0.46
3:K:271:ARG:HG3	3:K:274:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:SER:OG	2:B:135:THR:N	2.49	0.46
3:L:251:PRO:O	3:L:255:HIS:ND1	2.27	0.46
3:K:153:GLU:HG3	3:K:154:ASN:OD1	2.15	0.46
3:L:199:ASP:OD1	3:L:224:ARG:NH2	2.45	0.46
2:B:232:ARG:HD3	2:B:232:ARG:HA	1.64	0.46
3:E:188:LEU:HD21	3:E:227:HIS:HB3	1.98	0.46
1:C:143:GLN:HA	1:C:146:ASP:O	2.15	0.46
2:D:198:ASP:OD1	2:D:202:VAL:HG12	2.15	0.46
3:E:252:GLN:HA	3:E:255:HIS:CE1	2.51	0.46
2:H:232:ARG:HA	2:H:232:ARG:HD3	1.78	0.46
2:H:238:GLN:HA	2:H:241:VAL:HG12	1.98	0.46
3:K:104:SER:O	3:K:104:SER:OG	2.26	0.46
4:M:295:MET:SD	4:M:295:MET:N	2.86	0.46
2:D:25:GLU:HB3	2:D:96:ARG:HG2	1.98	0.46
2:H:66:PHE:HA	2:H:69:TYR:CE1	2.51	0.46
6:I:402:G1V:OAU	6:I:402:G1V:CLBC	2.70	0.46
3:K:111:GLU:O	3:K:115:LEU:HG	2.16	0.46
2:B:85:LYS:HE2	2:B:85:LYS:HB2	1.60	0.46
3:E:254:CYS:SG	3:E:255:HIS:N	2.89	0.46
1:G:81:ARG:HD3	1:G:242:GLU:HG3	1.99	0.46
3:F:150:GLN:HG2	3:F:178:PRO:HB3	1.98	0.45
3:F:215:VAL:HG12	3:F:217:PRO:HD3	1.99	0.45
3:F:259:ASN:O	3:F:263:TYR:HD2	1.99	0.45
2:D:86:ASP:OD1	2:D:86:ASP:N	2.49	0.45
3:L:245:CYS:SG	3:L:246:LEU:N	2.89	0.45
1:C:82:ARG:NH2	1:C:86:ARG:O	2.49	0.45
2:H:238:GLN:OE1	1:I:301:LEU:HD11	2.16	0.45
3:E:58:LEU:HD23	3:E:58:LEU:HA	1.77	0.45
2:B:23:ASP:HB3	2:B:96:ARG:HH21	1.81	0.45
3:K:48:THR:HG23	3:K:52:ASN:ND2	2.31	0.45
3:E:29:LEU:HD11	3:E:154:ASN:HB3	1.98	0.45
3:E:219:LEU:HD23	3:E:237:ILE:HG21	1.98	0.45
3:L:60:ILE:HB	3:L:67:LEU:HB2	1.98	0.45
3:E:40:LEU:HD23	3:E:40:LEU:HA	1.76	0.45
1:A:163:THR:HG22	2:B:157:ARG:HH12	1.81	0.44
3:F:238:PRO:O	3:F:249:TYR:OH	2.27	0.44
1:G:230:GLU:O	1:G:234:GLU:HG2	2.17	0.44
3:K:45:THR:O	3:K:48:THR:HG22	2.17	0.44
3:L:216:TYR:O	3:L:218:LYS:NZ	2.50	0.44
1:C:164:LYS:NZ	2:D:157:ARG:O	2.30	0.44
3:F:193:ASN:OD1	3:F:193:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:133:HIS:O	1:I:136:VAL:HG22	2.16	0.44
1:I:301:LEU:HD12	1:I:301:LEU:HA	1.73	0.44
2:D:113:HIS:CD2	2:D:150:PRO:HG2	2.53	0.44
3:E:210:THR:HG21	3:K:357:GLU:H	1.83	0.44
3:K:259:ASN:O	3:K:263:TYR:HB2	2.18	0.44
3:K:179:VAL:HG21	3:K:257:LEU:HD23	2.00	0.44
2:B:96:ARG:HE	2:B:96:ARG:HB3	1.52	0.43
2:D:223:VAL:O	2:D:227:VAL:HG23	2.18	0.43
3:E:223:PRO:HA	3:E:226:GLU:HB2	2.00	0.43
3:K:215:VAL:HG12	3:K:217:PRO:HD3	1.99	0.43
2:H:216:LEU:HD12	1:I:276:MET:HG2	2.01	0.43
2:H:242:ASN:OD1	2:H:243:LYS:N	2.50	0.43
1:I:309:MET:HA	1:I:312:LEU:HB2	1.99	0.43
3:E:259:ASN:HB3	3:E:263:TYR:CZ	2.53	0.43
1:A:224:ILE:H	1:A:224:ILE:HG13	1.67	0.43
3:F:55:ARG:NH2	3:F:73:PHE:O	2.51	0.43
2:J:137:ASN:HD22	2:J:137:ASN:C	2.16	0.43
3:L:40:LEU:HD23	3:L:40:LEU:HA	1.82	0.43
3:L:52:ASN:OD1	3:L:52:ASN:N	2.51	0.43
2:H:219:LYS:HA	2:H:219:LYS:HD3	1.82	0.43
3:K:95:ASP:OD2	3:K:97:SER:OG	2.36	0.43
3:K:137:ARG:O	3:K:141:GLU:HG3	2.19	0.43
1:A:10:GLN:HB2	1:A:70:ARG:O	2.19	0.43
3:E:52:ASN:OD1	3:E:52:ASN:N	2.50	0.43
3:K:48:THR:HG23	3:K:52:ASN:HD22	1.84	0.43
3:K:267:GLY:O	3:K:271:ARG:HB2	2.19	0.43
3:L:143:GLN:O	3:L:147:GLU:HG2	2.19	0.43
1:I:129:VAL:HG22	1:I:171:THR:HG22	1.99	0.43
1:C:226:LYS:HE3	1:C:226:LYS:HB3	1.83	0.42
2:D:66:PHE:CD2	3:E:80:LEU:HD13	2.53	0.42
1:G:284:LEU:HD13	2:J:220:VAL:HG22	2.00	0.42
2:H:85:LYS:HE2	2:H:85:LYS:HB2	1.72	0.42
3:K:115:LEU:O	3:K:119:GLU:HG3	2.19	0.42
3:L:111:GLU:HG2	3:L:114:LEU:HD12	1.99	0.42
1:A:77:VAL:HG13	1:A:121:TYR:HE2	1.82	0.42
2:D:176:SER:O	2:D:176:SER:OG	2.33	0.42
3:E:18:ILE:HD11	3:E:56:PHE:CZ	2.54	0.42
1:G:103:GLU:OE2	1:G:106:ARG:NE	2.42	0.42
2:H:219:LYS:O	2:H:223:VAL:HG23	2.18	0.42
1:I:33:GLU:HG2	1:I:123:SER:O	2.19	0.42
2:J:137:ASN:ND2	2:J:137:ASN:C	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:142:TYR:CZ	3:K:146:LEU:HD12	2.54	0.42
4:M:94:LYS:O	4:M:212:ARG:N	2.52	0.42
3:E:99:LEU:HB3	3:E:102:LEU:HB2	2.01	0.42
3:E:250:VAL:CG1	3:E:251:PRO:HD3	2.50	0.42
3:K:63:ALA:HB2	3:K:156:GLU:HB3	2.00	0.42
3:F:249:TYR:O	3:F:253:VAL:HG23	2.20	0.42
1:G:131:PRO:HG3	1:G:173:PHE:CG	2.54	0.42
6:I:402:G1V:CLAS	6:I:402:G1V:OAK	2.75	0.42
3:K:42:SER:HA	3:K:53:CYS:HA	2.01	0.42
3:L:268:TYR:O	3:L:272:ARG:HG2	2.20	0.42
1:A:7:GLN:HB2	1:A:176:ILE:HD13	2.01	0.42
3:E:254:CYS:O	3:E:258:THR:HG23	2.19	0.42
3:L:252:GLN:NE2	3:L:253:VAL:HG13	2.34	0.42
1:C:7:GLN:OE1	1:C:147:GLN:HB3	2.19	0.42
3:K:205:VAL:HG11	3:K:246:LEU:HD21	2.01	0.42
2:B:171:GLN:HG3	2:B:172:GLU:H	1.85	0.42
1:C:116:ARG:O	1:C:118:VAL:HG13	2.20	0.42
3:K:102:LEU:HD23	3:K:102:LEU:HA	1.92	0.42
3:K:246:LEU:HD23	3:K:246:LEU:HA	1.86	0.42
1:C:233:VAL:O	1:C:236:PRO:HD2	2.19	0.42
1:G:25:HIS:NE2	1:G:79:ILE:HG23	2.35	0.42
2:H:139:SER:OG	2:H:140:THR:N	2.53	0.42
1:G:101:SER:O	1:G:105:GLU:HG2	2.20	0.41
2:J:84:LEU:O	2:J:88:ARG:HB2	2.19	0.41
2:J:232:ARG:HA	2:J:232:ARG:NE	2.33	0.41
3:E:222:SER:O	3:E:226:GLU:N	2.50	0.41
3:F:229:LEU:O	3:F:233:SER:OG	2.31	0.41
3:K:67:LEU:HD13	3:K:69:TRP:CZ2	2.55	0.41
2:D:247:GLN:O	2:D:250:GLN:HG3	2.20	0.41
3:E:259:ASN:HA	3:E:262:GLN:HB2	2.01	0.41
1:G:235:LEU:HB3	1:G:236:PRO:HD3	2.03	0.41
1:C:14:LEU:HD12	1:C:15:GLU:H	1.85	0.41
1:C:258:SER:HB3	2:D:189:ILE:HD12	2.02	0.41
1:I:13:HIS:CE1	1:I:71:ILE:HD11	2.56	0.41
3:E:26:LYS:NZ	3:E:30:ASP:H	2.19	0.41
3:E:176:LYS:HG3	3:E:200:VAL:HG23	2.03	0.41
3:F:255:HIS:HA	3:F:258:THR:HG22	2.03	0.41
1:G:99:ALA:HA	1:G:102:THR:HG22	2.03	0.41
1:A:138:THR:HG22	1:A:142:TYR:CE2	2.55	0.41
2:D:237:CYS:O	2:D:241:VAL:HG23	2.21	0.41
3:F:186:THR:O	3:F:186:THR:OG1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:149:PRO:O	3:K:153:GLU:HG2	2.21	0.41
1:A:33:GLU:HG2	1:A:123:SER:O	2.21	0.41
1:C:176:ILE:O	1:C:210:GLU:HB3	2.20	0.41
3:F:54:ASP:O	3:F:73:PHE:HB2	2.21	0.41
1:G:16:SER:HB3	2:J:15:PHE:CE1	2.56	0.41
3:K:188:LEU:HD12	3:K:188:LEU:HA	1.89	0.41
2:D:85:LYS:H	2:D:85:LYS:HG2	1.56	0.41
3:F:3:PRO:O	3:F:7:LEU:HD13	2.21	0.41
3:F:270:LYS:HE2	3:F:274:TYR:HE2	1.85	0.41
2:H:203:MET:HE3	2:H:203:MET:HB3	2.00	0.41
2:J:149:ARG:HD3	2:J:158:ILE:HD11	2.03	0.41
1:G:135:ASP:OD2	1:G:135:ASP:N	2.54	0.40
1:G:138:THR:HG22	1:G:142:TYR:CE2	2.56	0.40
3:L:122:GLN:O	3:L:126:GLN:HG2	2.21	0.40
1:I:10:GLN:HB3	1:I:70:ARG:O	2.21	0.40
2:B:96:ARG:HG3	2:B:127:PHE:HE1	1.85	0.40
1:C:308:LEU:HD22	2:D:244:LEU:HG	2.03	0.40
1:A:163:THR:HG22	2:B:157:ARG:NH1	2.36	0.40
3:K:65:GLU:OE2	3:K:172:ARG:NH1	2.53	0.40
3:K:140:PHE:O	3:K:144:THR:HG23	2.20	0.40
3:L:148:GLU:HG2	3:L:150:GLN:HG2	2.03	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	246/312 (79%)	243 (99%)	3 (1%)	0	100	100
1	C	246/312 (79%)	241 (98%)	5 (2%)	0	100	100
1	G	246/312 (79%)	237 (96%)	9 (4%)	0	100	100
1	I	246/312 (79%)	237 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/267 (87%)	229 (98%)	4 (2%)	0	100	100
2	D	233/267 (87%)	227 (97%)	6 (3%)	0	100	100
2	H	233/267 (87%)	221 (95%)	12 (5%)	0	100	100
2	J	233/267 (87%)	227 (97%)	6 (3%)	0	100	100
3	E	381/385 (99%)	342 (90%)	39 (10%)	0	100	100
3	F	381/385 (99%)	345 (91%)	36 (9%)	0	100	100
3	K	381/385 (99%)	346 (91%)	35 (9%)	0	100	100
3	L	381/385 (99%)	345 (91%)	36 (9%)	0	100	100
4	M	235/259 (91%)	207 (88%)	28 (12%)	0	100	100
4	N	235/259 (91%)	204 (87%)	31 (13%)	0	100	100
4	O	235/259 (91%)	202 (86%)	33 (14%)	0	100	100
4	P	235/259 (91%)	212 (90%)	23 (10%)	0	100	100
All	All	4380/4892 (90%)	4065 (93%)	315 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/282 (81%)	223 (97%)	6 (3%)	41	71
1	C	228/282 (81%)	218 (96%)	10 (4%)	24	56
1	G	229/282 (81%)	225 (98%)	4 (2%)	56	80
1	I	229/282 (81%)	219 (96%)	10 (4%)	24	56
2	B	214/243 (88%)	210 (98%)	4 (2%)	52	78
2	D	214/243 (88%)	212 (99%)	2 (1%)	75	89
2	H	214/243 (88%)	205 (96%)	9 (4%)	25	58
2	J	214/243 (88%)	206 (96%)	8 (4%)	29	62
3	E	334/337 (99%)	323 (97%)	11 (3%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	334/337 (99%)	319 (96%)	15 (4%)	23 56
3	K	336/337 (100%)	329 (98%)	7 (2%)	48 76
3	L	335/337 (99%)	326 (97%)	9 (3%)	40 70
4	M	217/238 (91%)	211 (97%)	6 (3%)	38 69
4	N	219/238 (92%)	211 (96%)	8 (4%)	29 62
4	O	219/238 (92%)	213 (97%)	6 (3%)	40 70
4	P	217/238 (91%)	208 (96%)	9 (4%)	26 58
All	All	3982/4400 (90%)	3858 (97%)	124 (3%)	37 67

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LEU
1	A	149	PHE
1	A	155	SER
1	A	169	LEU
1	A	173	PHE
1	A	290	ARG
2	B	85	LYS
2	B	86	ASP
2	B	195	ASP
2	B	236	SER
1	C	17	ASP
1	C	32	GLU
1	C	73	HIS
1	C	120	TRP
1	C	161	LYS
1	C	167	ARG
1	C	208	ARG
1	C	210	GLU
1	C	290	ARG
1	C	297	HIS
2	D	96	ARG
2	D	182	SER
3	E	14	LEU
3	E	34	CYS
3	E	139	MET
3	E	140	PHE
3	E	169	PHE
3	E	194	GLU

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Mol	Chain	Res	Type
3	E	268	TYR
3	E	294	PHE
3	E	304	LYS
3	E	313	ASP
3	E	320	ARG
3	F	15	SER
3	F	19	SER
3	F	39	ASP
3	F	76	GLN
3	F	163	ASN
3	F	206	SER
3	F	254	CYS
3	F	260	LYS
3	F	271	ARG
3	F	278	PHE
3	F	313	ASP
3	F	327	PHE
3	F	340	TYR
3	F	369	PHE
3	F	378	PHE
1	G	25	HIS
1	G	135	ASP
1	G	209	TYR
1	G	308	LEU
2	H	23	ASP
2	H	69	TYR
2	H	78	GLU
2	H	143	LEU
2	H	198	ASP
2	H	207	ARG
2	H	219	LYS
2	H	251	ARG
2	H	252	LYS
1	I	13	HIS
1	I	97	LEU
1	I	123	SER
1	I	135	ASP
1	I	149	PHE
1	I	155	SER
1	I	159	GLU
1	I	209	TYR
1	I	270	LYS

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Mol	Chain	Res	Type
1	I	309	MET
2	J	33	ARG
2	J	88	ARG
2	J	137	ASN
2	J	143	LEU
2	J	199	LYS
2	J	205	ASP
2	J	240	GLU
2	J	251	ARG
3	K	1	MET
3	K	11	SER
3	K	57	LYS
3	K	208	GLU
3	K	221	LEU
3	K	302	MET
3	K	349	TYR
3	L	1	MET
3	L	89	ASP
3	L	224	ARG
3	L	256	LEU
3	L	263	TYR
3	L	307	CYS
3	L	313	ASP
3	L	331	TYR
3	L	361	ARG
4	M	101	LEU
4	M	105	MET
4	M	151	ASP
4	M	241	PHE
4	M	267	PHE
4	M	279	LYS
4	N	81	GLU
4	N	85	ARG
4	N	130	MET
4	N	131	PHE
4	N	222	CYS
4	N	259	MET
4	N	265	PHE
4	N	287	PRO
4	O	169	CYS
4	O	187	PHE
4	O	217	TYR

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Mol	Chain	Res	Type
4	O	234	LYS
4	O	256	GLU
4	O	259	MET
4	P	122	ASN
4	P	127	MET
4	P	151	ASP
4	P	178	CYS
4	P	209	TYR
4	P	234	LYS
4	P	259	MET
4	P	264	MET
4	P	287	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
2	H	52	GLN
2	J	137	ASN

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	G1V	D	301	-	37,39,39	4.05	12 (32%)	41,58,58	4.54	16 (39%)
6	G1V	I	402	-	37,39,39	4.04	13 (35%)	41,58,58	4.47	12 (29%)

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	G1V	D	301	-	-	9/14/39/39	0/5/5/5
6	G1V	I	402	-	-	9/14/39/39	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	G1V	CAC-CAF	-11.89	1.32	1.50
6	I	402	G1V	CAC-CAF	-11.65	1.33	1.50
6	I	402	G1V	CBF-CBD	11.52	1.64	1.50
6	I	402	G1V	CBE-CBD	11.25	1.64	1.50
6	D	301	G1V	CBF-CBD	11.11	1.64	1.50
6	D	301	G1V	CBE-CBD	11.01	1.63	1.50
6	D	301	G1V	CAL-CAJ	-8.28	1.38	1.51
6	I	402	G1V	CAL-CAJ	-7.80	1.39	1.51
6	I	402	G1V	CAV-CAT	-7.18	1.41	1.51
6	D	301	G1V	CAV-CAT	-6.77	1.42	1.51
6	D	301	G1V	CAC-NAD	-4.91	1.31	1.35
6	D	301	G1V	CAB-NAI	-4.67	1.32	1.41
6	I	402	G1V	CAB-NAI	-4.41	1.33	1.41
6	I	402	G1V	CAA-CAB	-4.36	1.33	1.38
6	I	402	G1V	CAC-NAD	-4.15	1.32	1.35
6	D	301	G1V	CAA-CAB	-4.13	1.33	1.38
6	I	402	G1V	CBF-CBE	-3.70	1.36	1.51
6	D	301	G1V	CBF-CBE	-3.64	1.36	1.51
6	D	301	G1V	NAD-NAE	-3.07	1.33	1.39
6	I	402	G1V	NAD-NAE	-2.55	1.34	1.39
6	D	301	G1V	CBI-CBF	2.28	1.56	1.53
6	D	301	G1V	CBG-CBE	2.22	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	402	G1V	CBI-CBF	2.19	1.56	1.53
6	I	402	G1V	CBG-CBE	2.17	1.56	1.53
6	I	402	G1V	CAA-NAE	-2.15	1.33	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	301	G1V	CBI-NBH-CBG	13.46	137.21	105.42
6	I	402	G1V	CBF-CBE-CBD	13.45	65.73	59.90
6	I	402	G1V	CBI-NBH-CBG	13.18	136.56	105.42
6	D	301	G1V	CBF-CBE-CBD	12.98	65.52	59.90
6	I	402	G1V	CBE-CBF-CBD	12.83	65.46	59.90
6	D	301	G1V	CBE-CBF-CBD	12.75	65.43	59.90
6	I	402	G1V	CBI-CBF-CBE	9.25	115.84	107.43
6	D	301	G1V	CBI-CBF-CBE	9.09	115.69	107.43
6	D	301	G1V	CBG-CBE-CBF	8.09	114.78	107.43
6	I	402	G1V	CBG-CBE-CBF	7.90	114.61	107.43
6	D	301	G1V	CAA-NAE-NAD	-6.74	105.85	112.72
6	I	402	G1V	CAA-NAE-NAD	-6.32	106.27	112.72
6	D	301	G1V	CAV-CBA-CLBB	5.40	126.64	119.59
6	D	301	G1V	CBA-CAV-CAT	4.84	126.99	121.19
6	I	402	G1V	CBA-CAV-CAT	4.32	126.36	121.19
6	I	402	G1V	CAV-CBA-CLBB	4.23	125.11	119.59
6	I	402	G1V	CAW-CAV-CAT	-4.08	116.29	121.19
6	D	301	G1V	CAW-CAV-CAT	-3.65	116.82	121.19
6	D	301	G1V	CAZ-CBA-CLBB	-3.50	111.39	118.41
6	D	301	G1V	CAV-CAW-CLBC	3.37	124.00	119.59
6	I	402	G1V	CAV-CAW-CLBC	2.94	123.43	119.59
6	D	301	G1V	CAZ-CAY-CAX	-2.79	116.28	120.25
6	I	402	G1V	CAZ-CBA-CLBB	-2.78	112.84	118.41
6	I	402	G1V	CAF-CAC-NAD	2.50	126.85	120.57
6	D	301	G1V	CAY-CAZ-CBA	2.41	123.04	119.39
6	D	301	G1V	CAQ-CAL-CAJ	-2.40	118.27	121.24
6	D	301	G1V	CAC-NAD-NAE	2.18	107.77	105.44
6	D	301	G1V	CAX-CAW-CLBC	-2.12	114.14	118.41

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	301	G1V	NAI-CAJ-CAL-CAQ
6	D	301	G1V	OAK-CAJ-CAL-CAM

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Mol	Chain	Res	Type	Atoms
6	D	301	G1V	OAK-CAJ-CAL-CAQ
6	D	301	G1V	NAE-CAT-CAV-CAW
6	D	301	G1V	NAE-CAT-CAV-CBA
6	D	301	G1V	OAU-CAT-CAV-CAW
6	D	301	G1V	OAU-CAT-CAV-CBA
6	D	301	G1V	CBE-CBD-NAH-CAF
6	D	301	G1V	CBF-CBD-NAH-CAF
6	I	402	G1V	NAI-CAJ-CAL-CAQ
6	I	402	G1V	OAK-CAJ-CAL-CAQ
6	I	402	G1V	NAE-CAT-CAV-CAW
6	I	402	G1V	NAE-CAT-CAV-CBA
6	I	402	G1V	OAU-CAT-CAV-CAW
6	I	402	G1V	OAU-CAT-CAV-CBA
6	I	402	G1V	CBE-CBD-NAH-CAF
6	I	402	G1V	CBF-CBD-NAH-CAF
6	I	402	G1V	OAK-CAJ-CAL-CAM

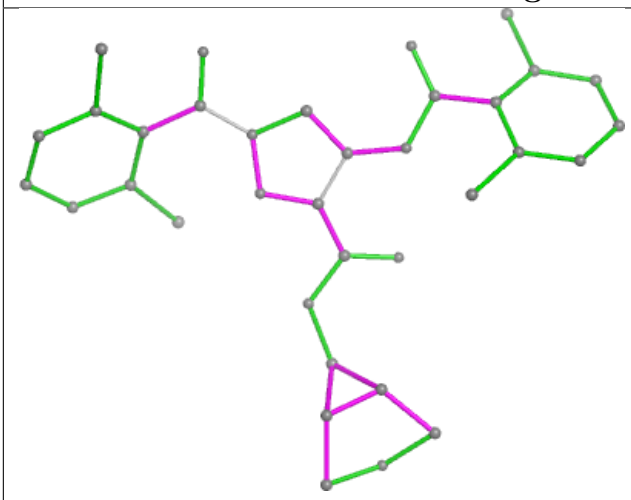
There are no ring outliers.

2 monomers are involved in 12 short contacts:

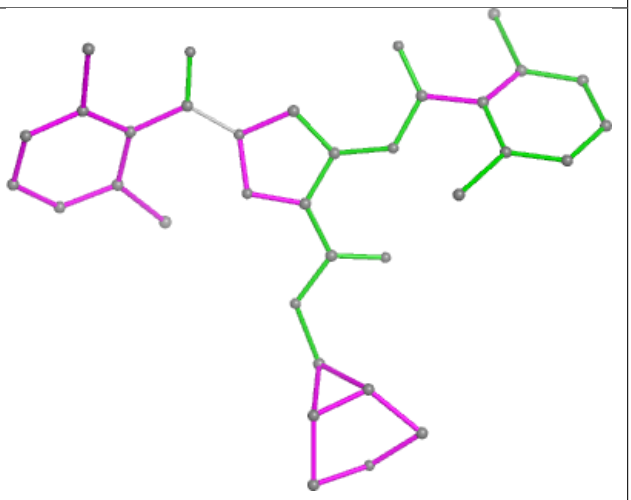
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	301	G1V	5	0
6	I	402	G1V	7	0

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 then 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.

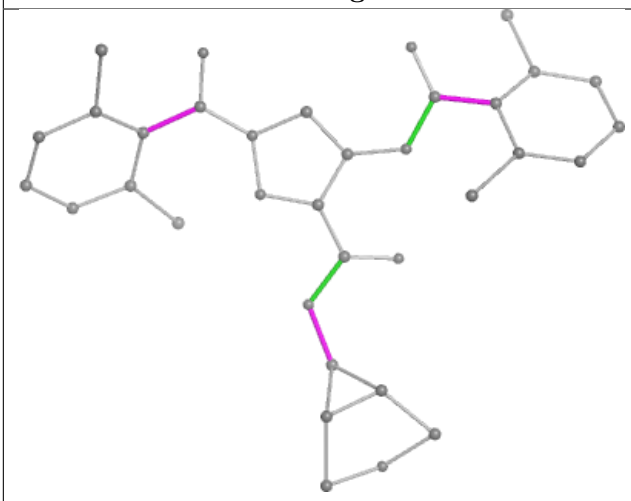
Ligand G1V D 301



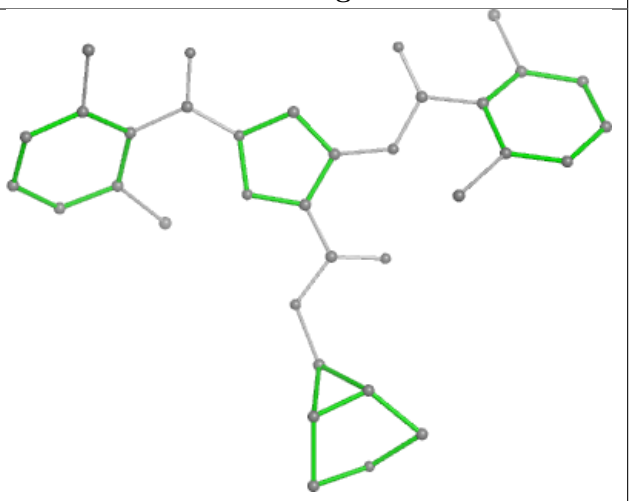
Bond lengths



Bond angles

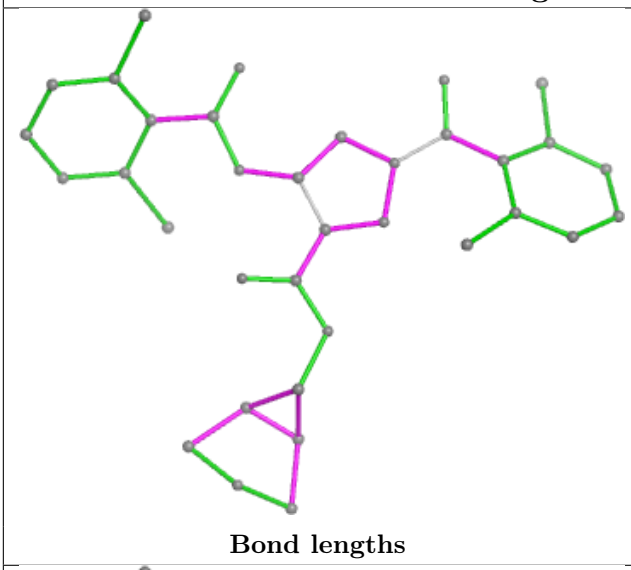


Torsions

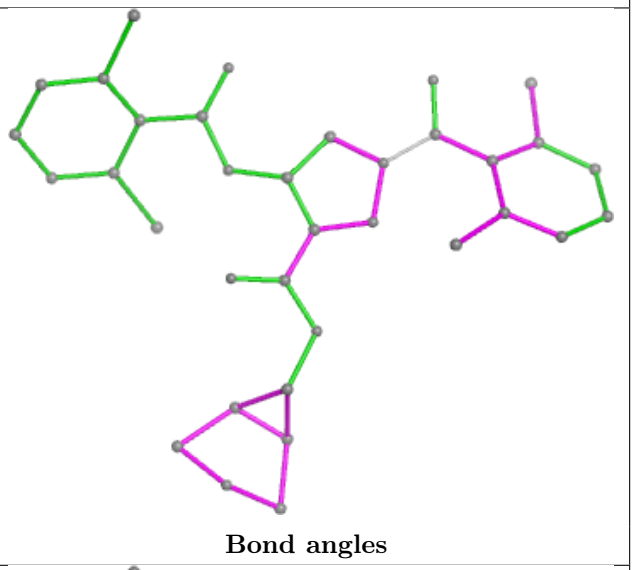


Rings

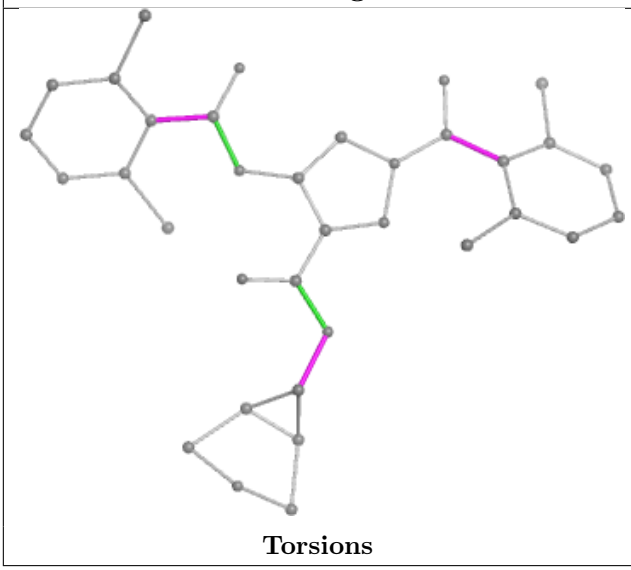
Ligand G1V I 402



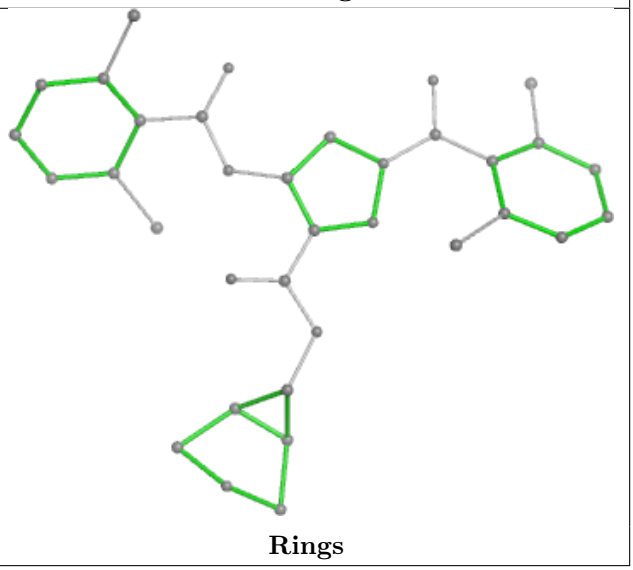
Bond lengths



Bond angles



Torsions



Rings

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.

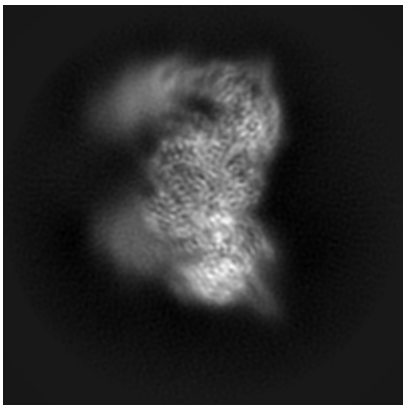
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17980. These allow visual inspection of the internal detail of the map and identification of artifacts.

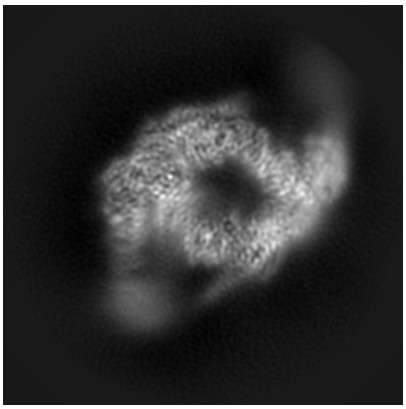
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

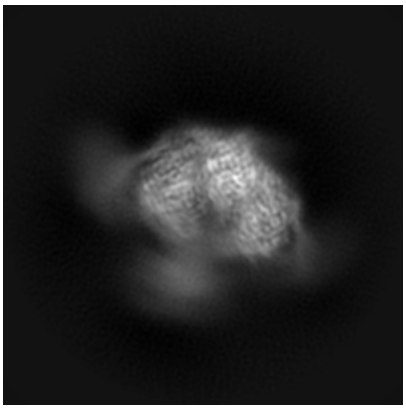
6.1.1 Primary map



X

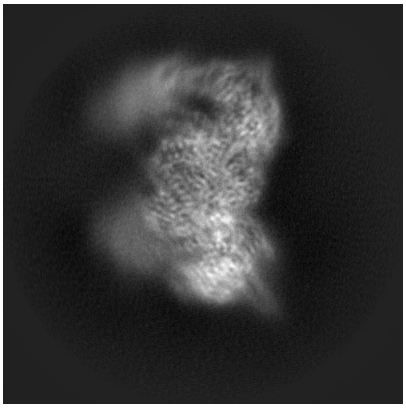


Y

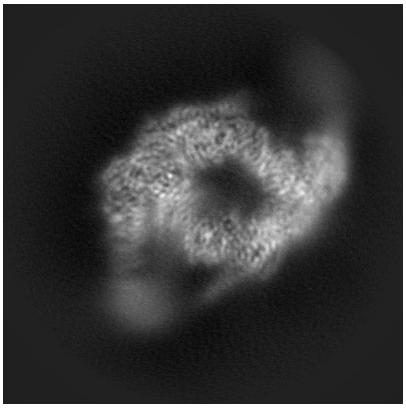


Z

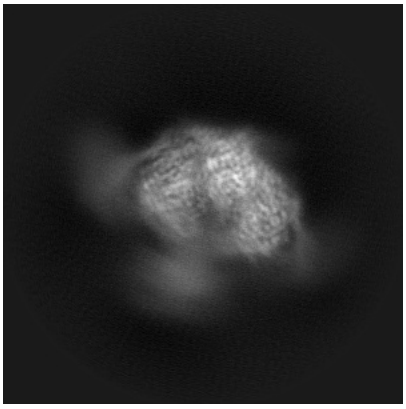
6.1.2 Raw map



X



Y

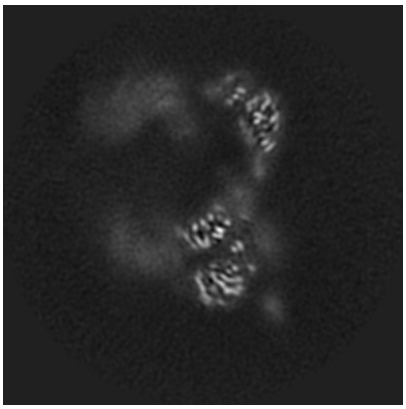


Z

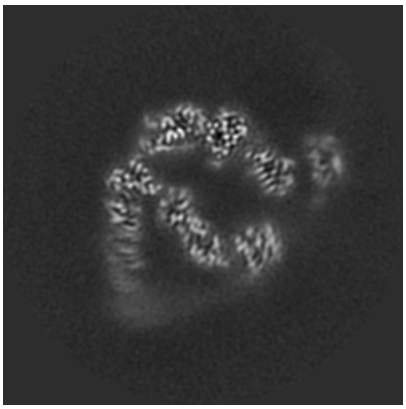
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

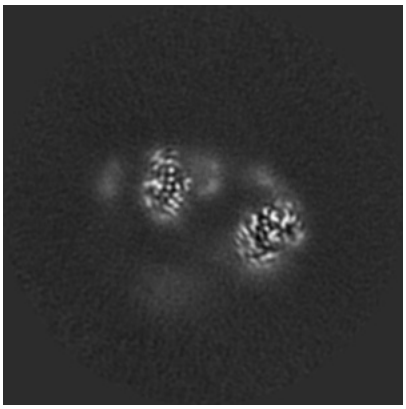
6.2.1 Primary map



X Index: 192

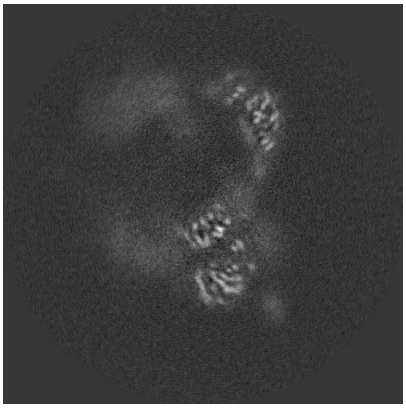


Y Index: 192

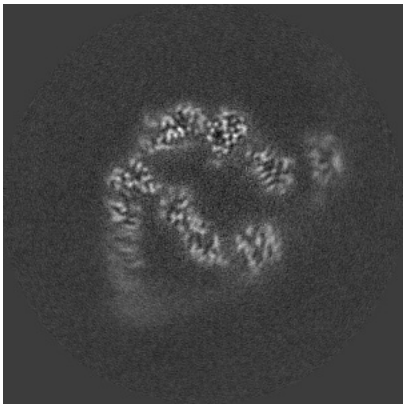


Z Index: 192

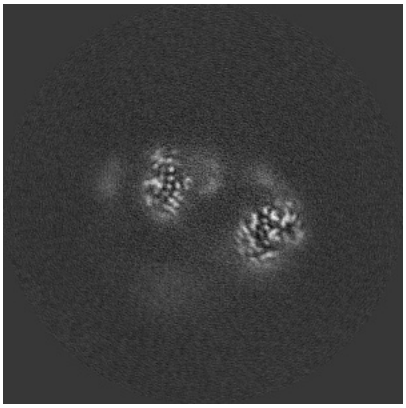
6.2.2 Raw map



X Index: 192



Y Index: 192

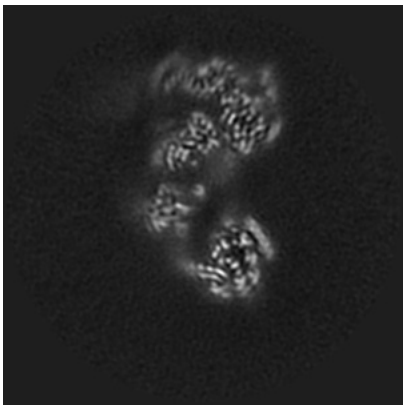


Z Index: 192

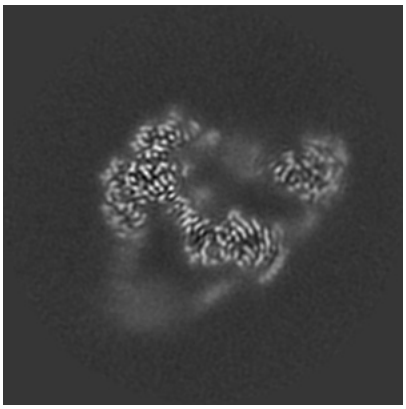
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

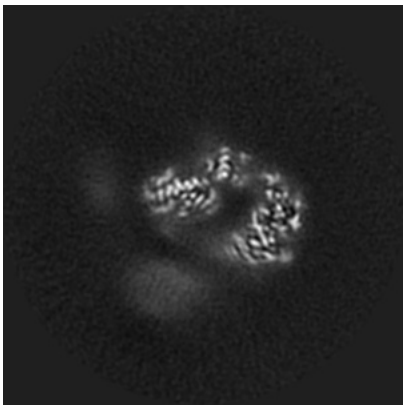
6.3.1 Primary map



X Index: 231

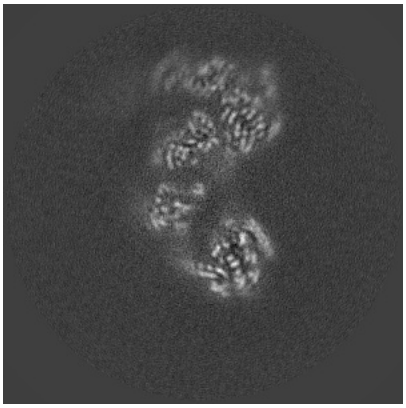


Y Index: 212

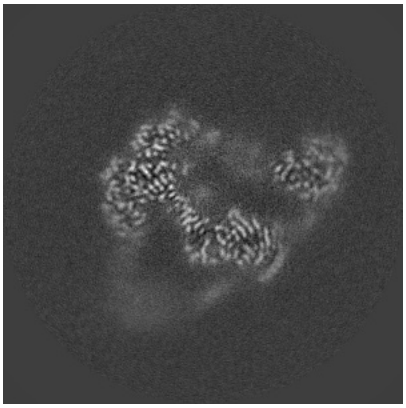


Z Index: 177

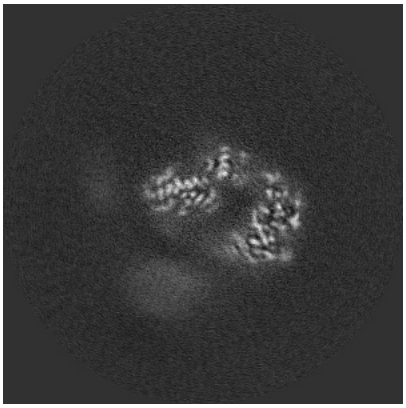
6.3.2 Raw map



X Index: 232



Y Index: 212

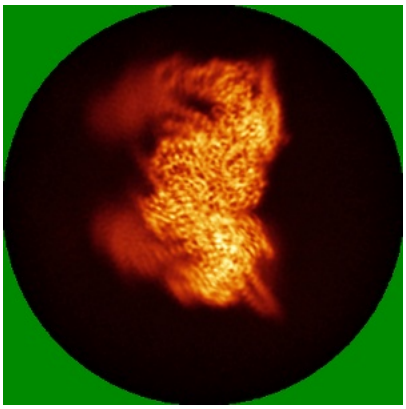


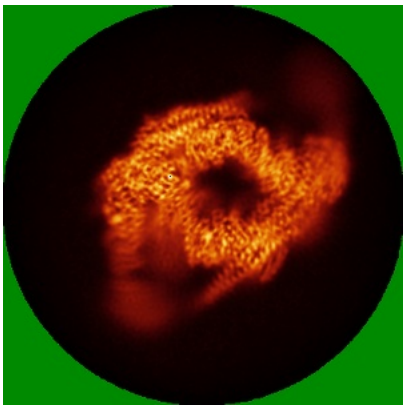
Z Index: 177

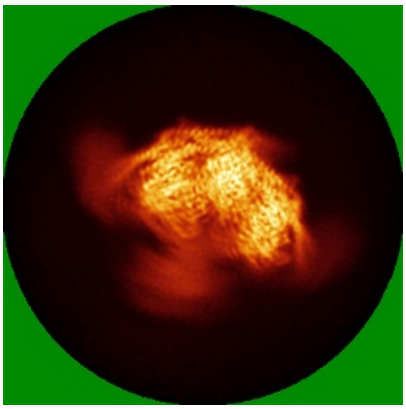
The images above show the largest variance slices of the map in three orthogonal directions.

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

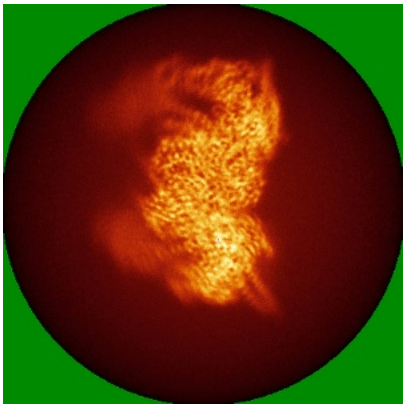
6.4.1 Primary map

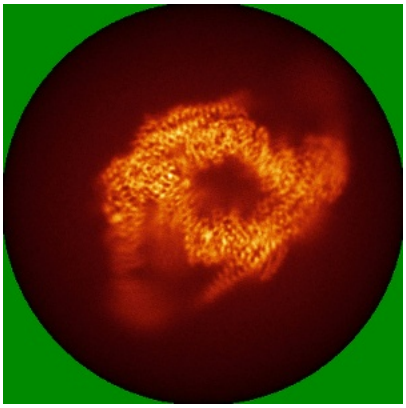

X

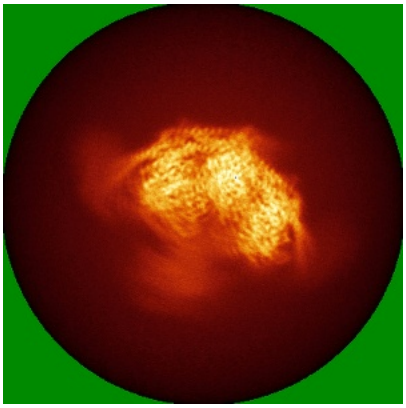

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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

X Y Z

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

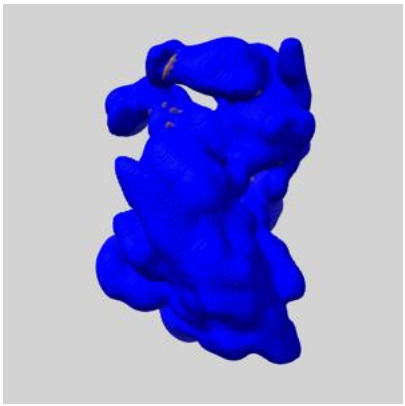
6.6 Mask visualisation (i)

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

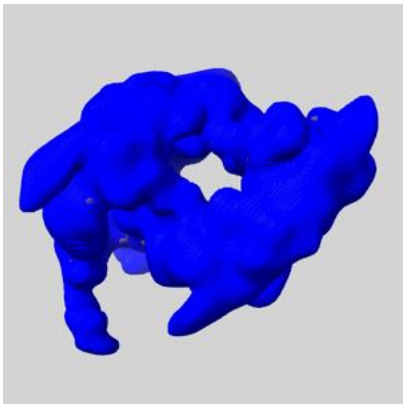
A mask typically either:

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

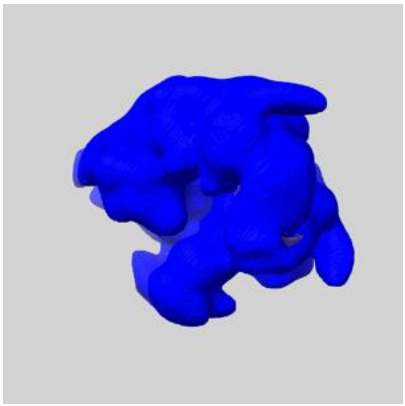
6.6.1 emd_17980_msk_1.map (i)



X



Y

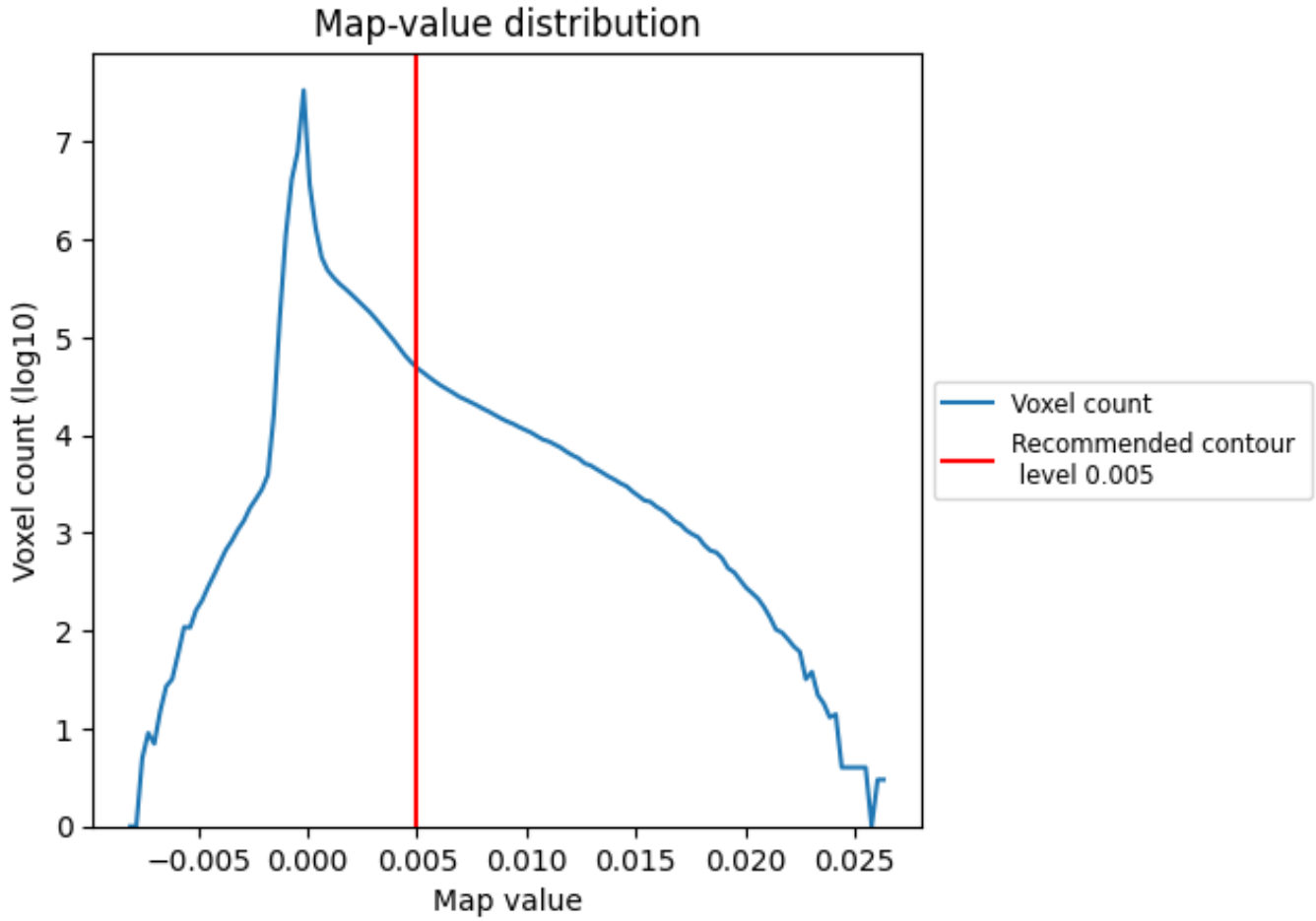


Z

7 Map analysis

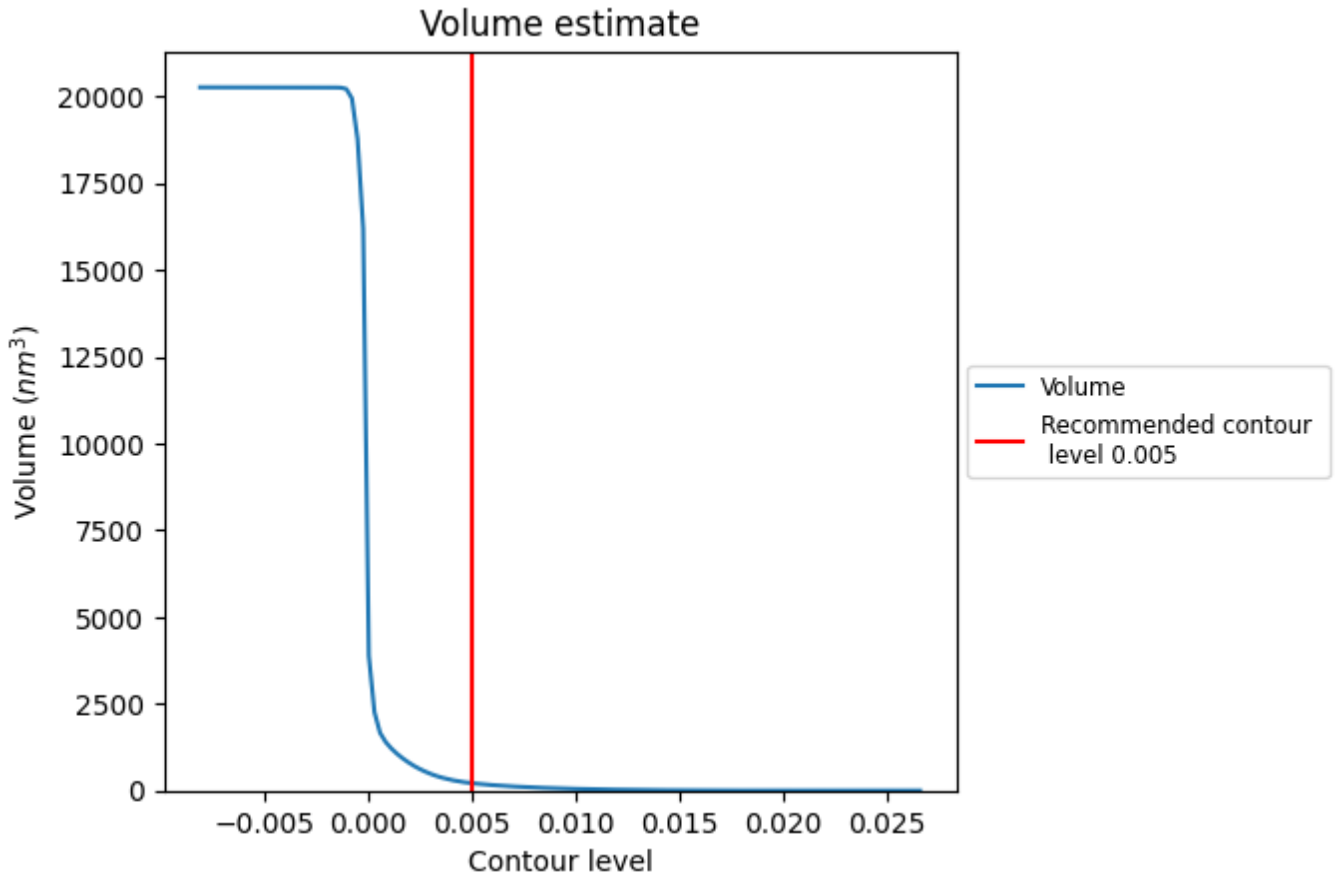
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

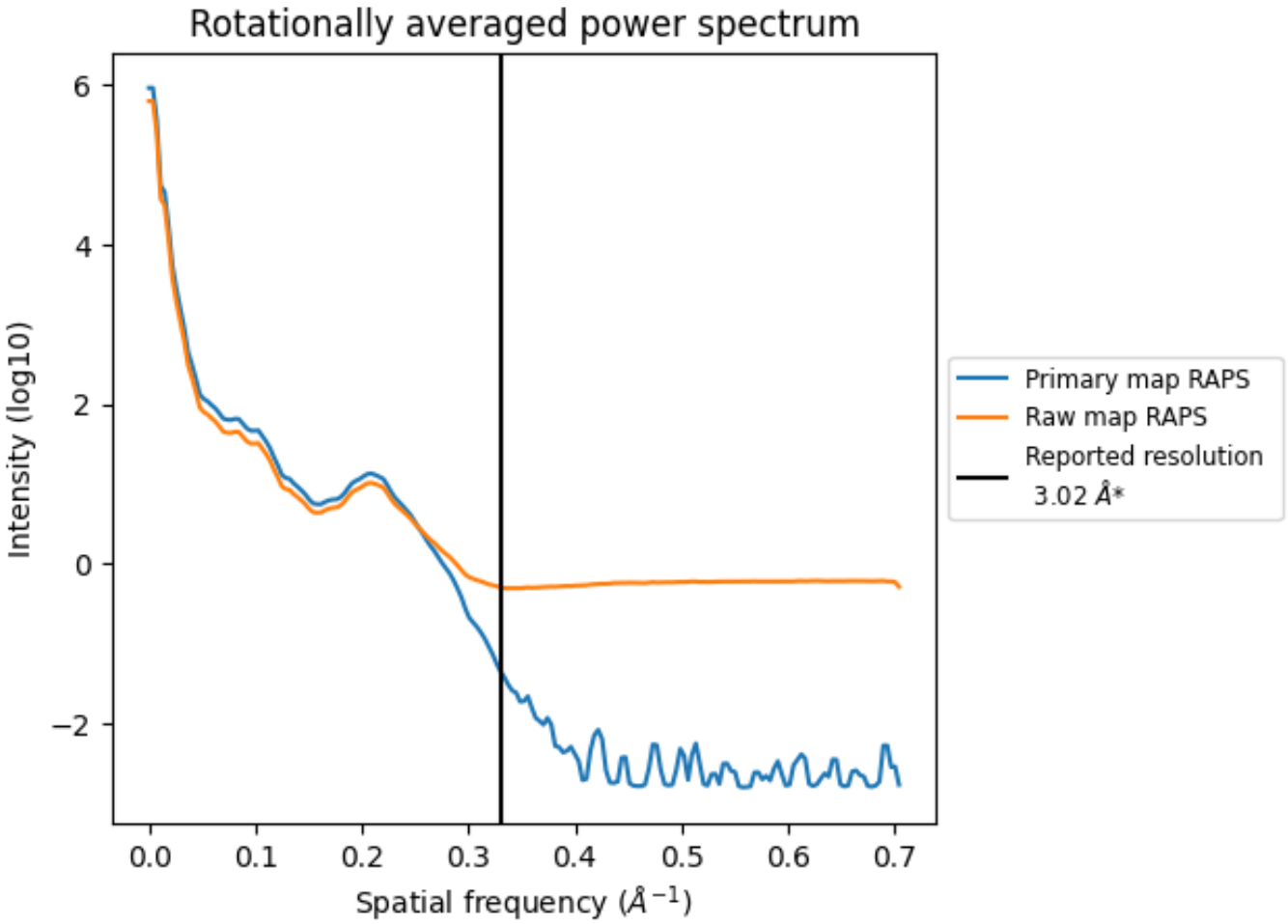
7.2 Volume estimate



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 193 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

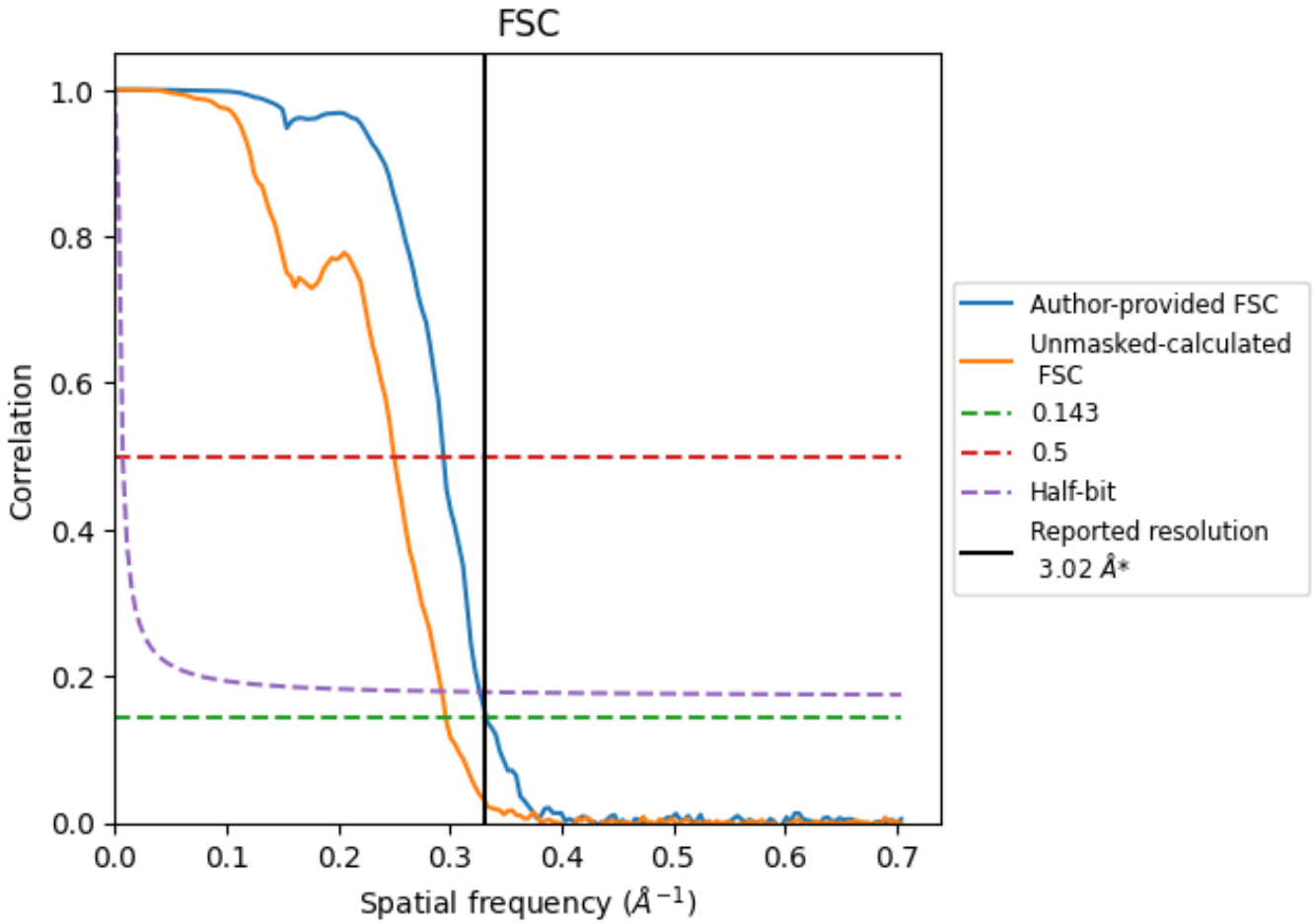


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8.2 Resolution estimates (i)

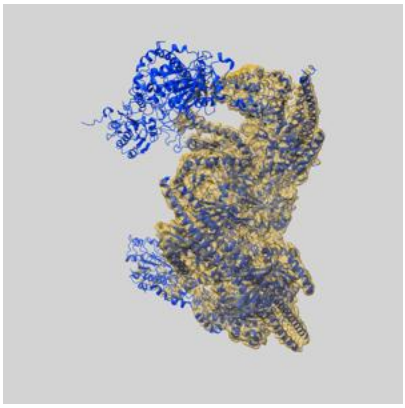
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.00	3.40	3.06
Unmasked-calculated*	3.37	4.00	3.42

*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 3.37 differs from the reported value 3.02 by more than 10 %

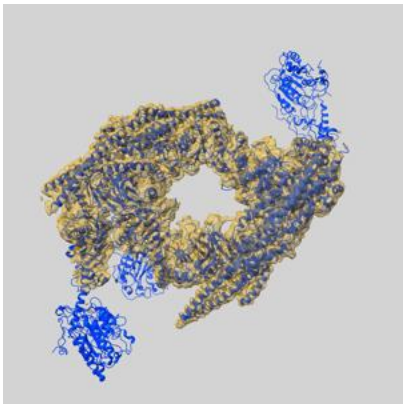
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17980 and PDB model 8PVY. Per-residue inclusion information can be found in section 3 on page 7.

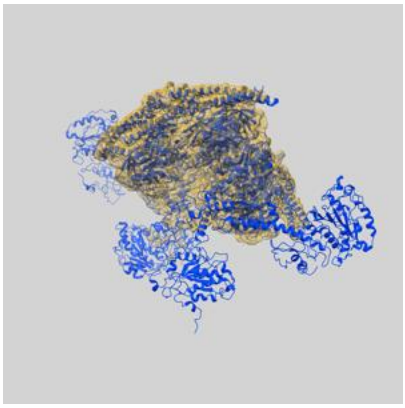
9.1 Map-model overlay



X



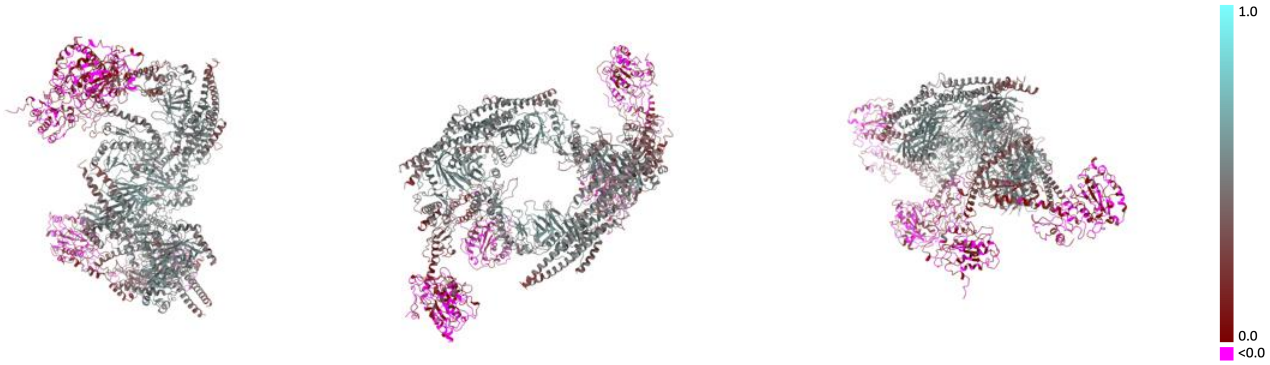
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

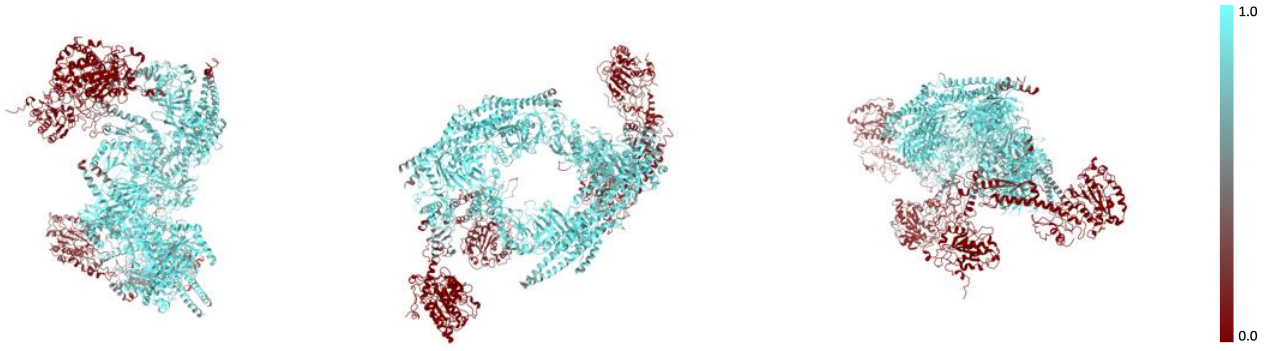
9.2 Q-score mapped to coordinate model (i)



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.

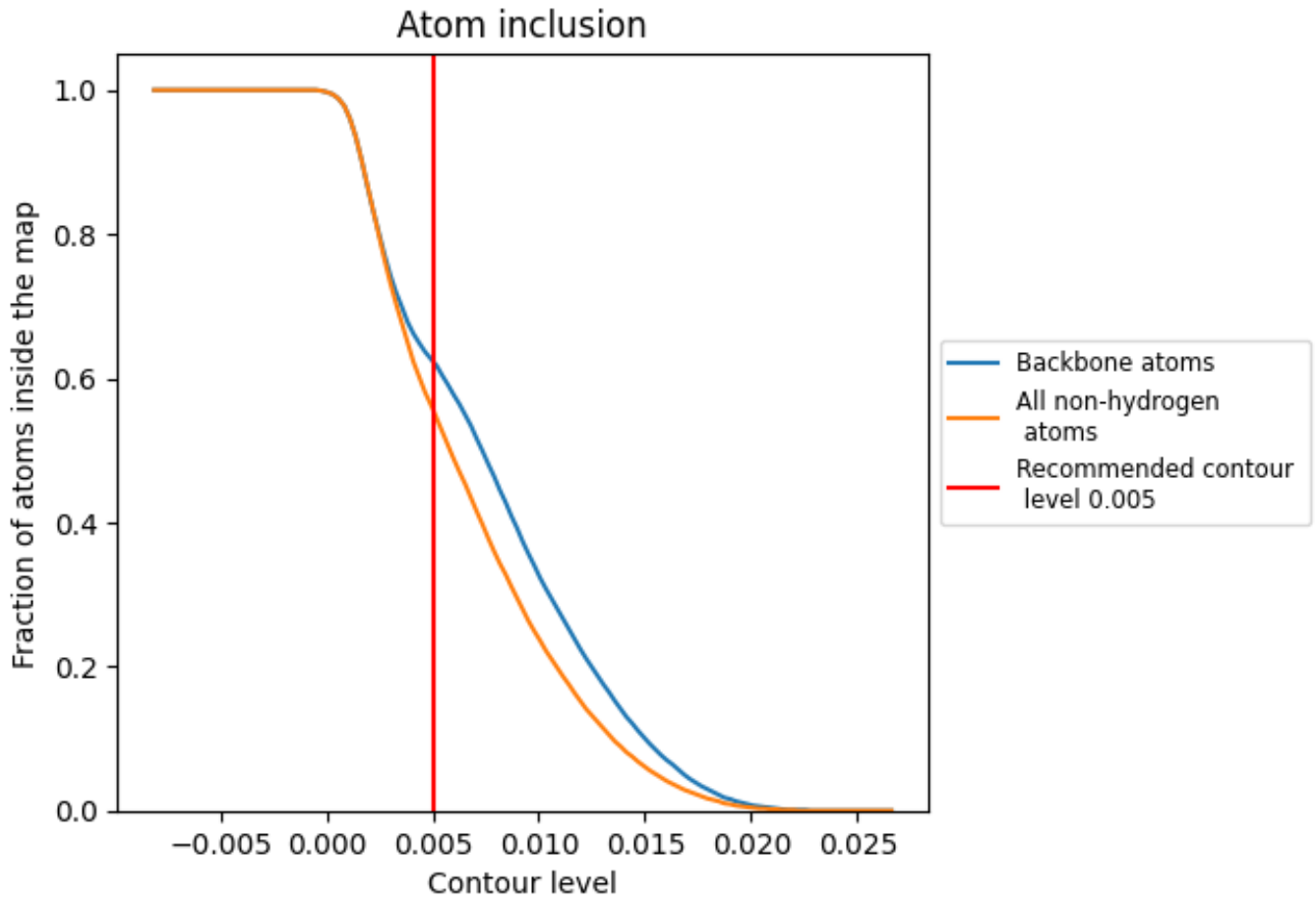
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 56% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5580	0.3320
A	0.8980	0.4890
B	0.8980	0.5130
C	0.9190	0.5040
D	0.9050	0.4980
E	0.4670	0.2780
F	0.5580	0.3500
G	0.9040	0.4830
H	0.8260	0.4730
I	0.8460	0.4740
J	0.8970	0.5000
K	0.6160	0.3690
L	0.2620	0.2230
M	0.0040	0.0210
N	0.0000	0.0530
O	0.0000	0.0350
P	0.0000	0.0340