Full wwPDB EM Validation Report ⓘ

Aug 28, 2024 – 07:58 am BST

PDB ID	:	8P4O
EMDB ID	:	EMD-17421
Title	:	CryoEM structure of a GroEL7-GroES7 cage with encapsulated ordered substrate MetK in the presence of ADP-BeFx
Authors	:	Wagner, J.; Beck, F.; Bracher, A.; Caravajal, A.I.; Wan, W.; Bohn, S.; Koerner, R.; Baumeister, W.; Fernandez-Busnadiego, R.; Hartl, F.U.
Deposited on	:	2023-05-23
Resolution	:	3.04 Å(reported)
Based on initial models	:	5OPX, 1SX3

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:

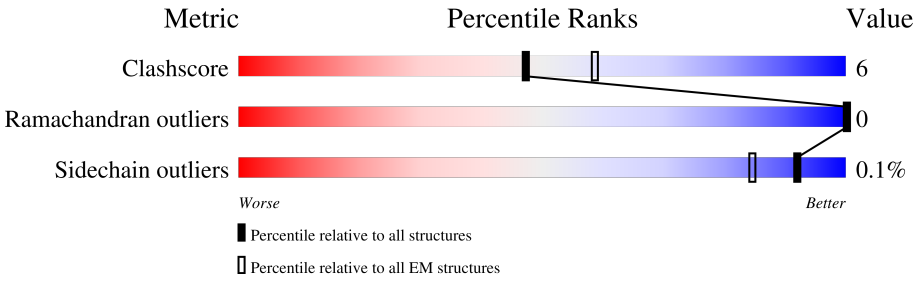
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 3.04 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	547	9% 80% 16% ·
1	B	547	8% 83% 13% ·
1	C	547	10% 83% 13% ·
1	D	547	11% 83% 13% ·
1	E	547	6% 82% 14% ·
1	F	547	6% 83% 12% ·
1	G	547	7% 82% 14% ·
2	O	97	25% 79% 19% ·

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Mol	Chain	Length	Quality of chain
2	P	97	20% 78% 20%
2	Q	97	20% 84% 14%
2	R	97	23% 86% 12%
2	S	97	22% 88% 9%
2	T	97	20% 87% 11%
2	U	97	23% 90% 8%
3	1	384	76% 81% 18%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 34605 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 Chaperonin GroEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	B	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	C	524	Total	C	N	O	S	0	0
			3847	2393	665	769	20		
1	D	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	E	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	F	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	G	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		

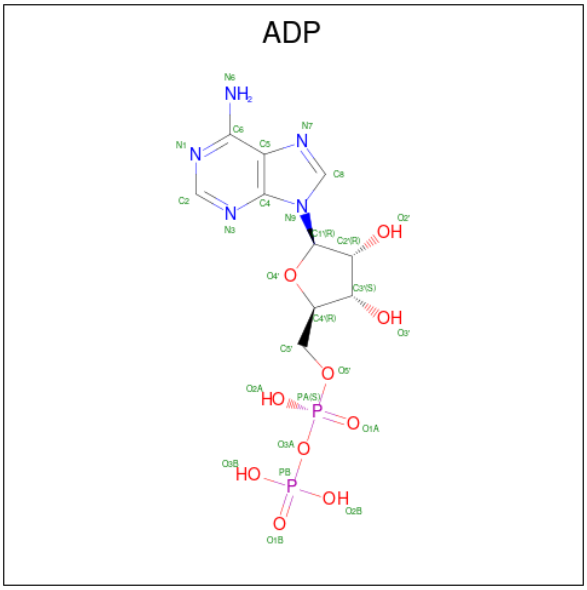
- Molecule 2 is a protein called Co-chaperonin GroES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	95	Total	C	N	O	S	0	0
			644	404	117	122	1		
2	P	95	Total	C	N	O	S	0	0
			644	404	117	122	1		
2	Q	95	Total	C	N	O	S	0	0
			644	404	117	122	1		
2	R	95	Total	C	N	O	S	0	0
			644	404	117	122	1		
2	S	95	Total	C	N	O	S	0	0
			644	404	117	122	1		
2	T	95	Total	C	N	O	S	0	0
			644	404	117	122	1		
2	U	95	Total	C	N	O	S	0	0
			644	404	117	122	1		

- Molecule 3 is a protein called S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	379	Total	C	N	O	S	0	0
			2892	1825	492	562	13		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

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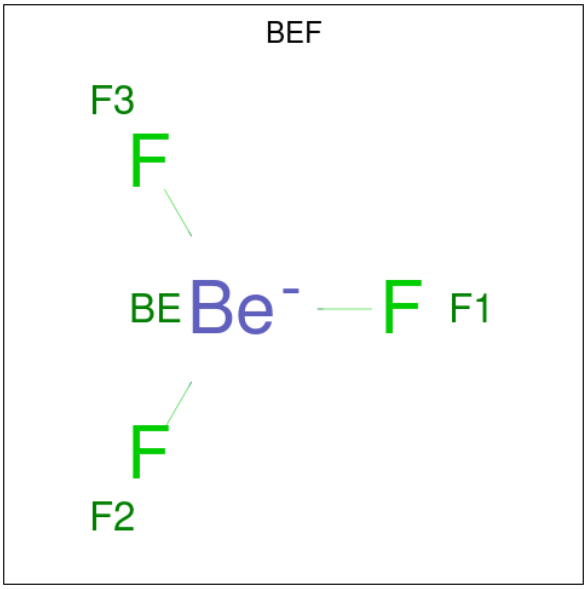
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Mg 1 1	0
5	C	1	Total Mg 1 1	0
5	D	1	Total Mg 1 1	0
5	E	1	Total Mg 1 1	0
5	F	1	Total Mg 1 1	0
5	G	1	Total Mg 1 1	0

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Be F 4 1 3	0
6	B	1	Total Be F 4 1 3	0
6	C	1	Total Be F 4 1 3	0
6	D	1	Total Be F 4 1 3	0
6	E	1	Total Be F 4 1 3	0

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Mol	Chain	Residues	Atoms	AltConf
6	F	1	Total Be F 4 1 3	0
6	G	1	Total Be F 4 1 3	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total K 1 1	0
7	B	1	Total K 1 1	0
7	C	1	Total K 1 1	0
7	D	1	Total K 1 1	0
7	E	1	Total K 1 1	0
7	F	1	Total K 1 1	0
7	G	1	Total K 1 1	0

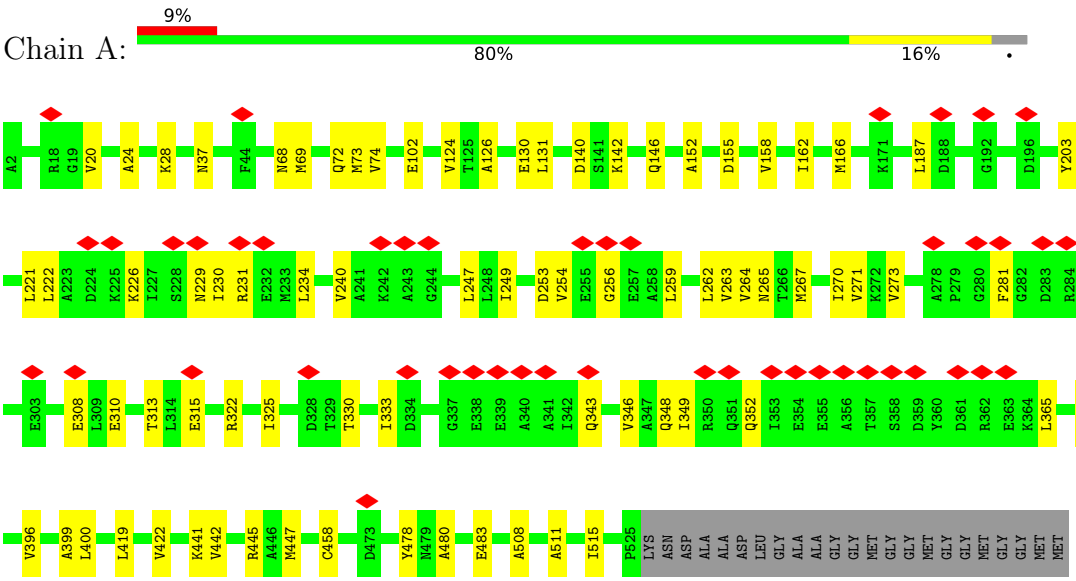
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	AltConf
8	A	3	Total O 3 3	0
8	B	3	Total O 3 3	0
8	C	3	Total O 3 3	0
8	D	3	Total O 3 3	0
8	E	3	Total O 3 3	0
8	F	3	Total O 3 3	0
8	G	3	Total O 3 3	0

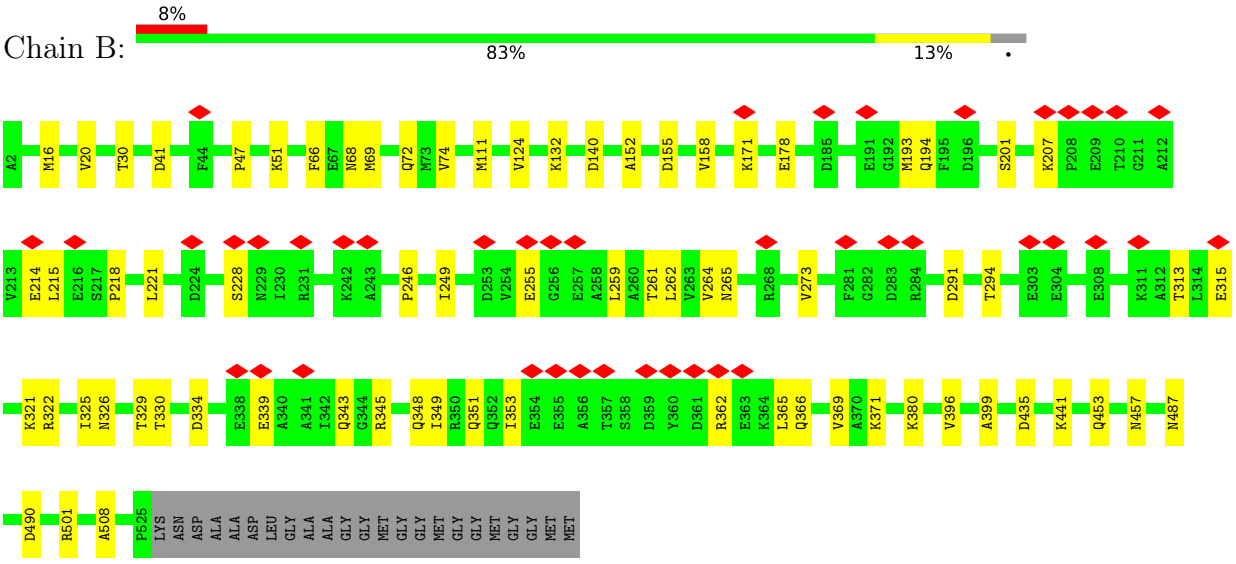
3 Residue-property plots (i)

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

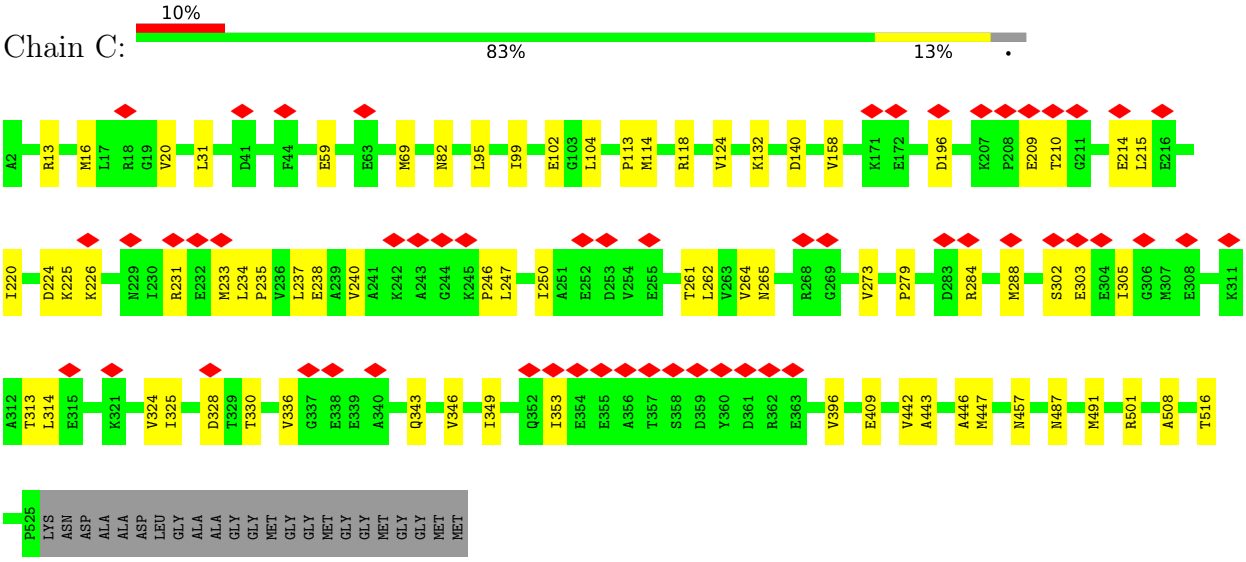
• Molecule 1: Chaperonin GroEL



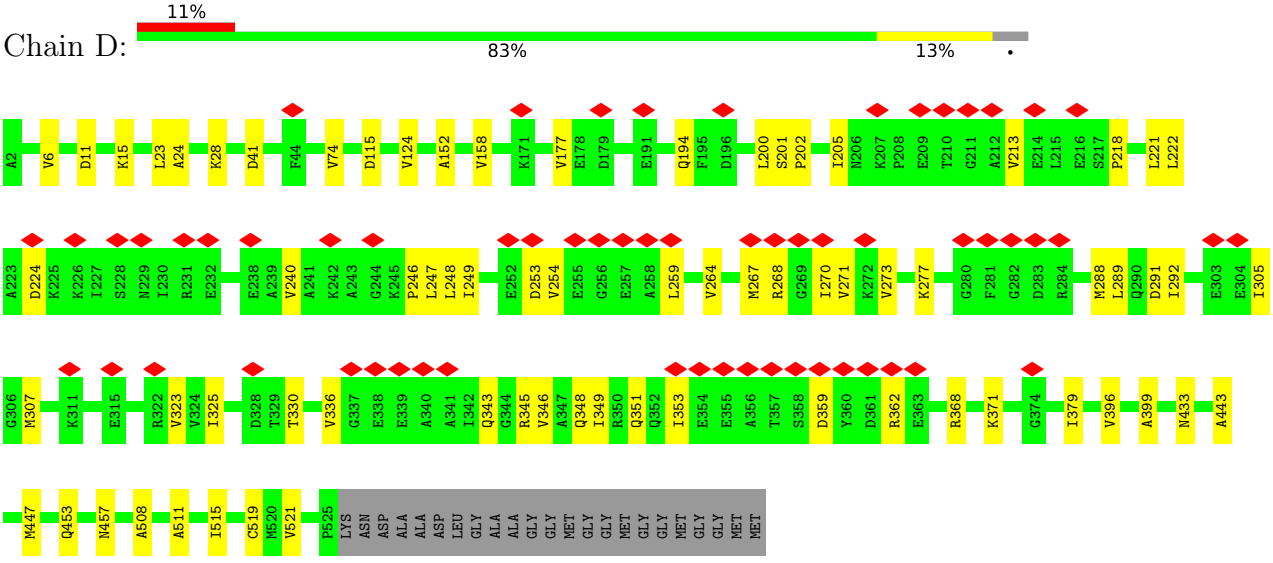
• Molecule 1: Chaperonin GroEL



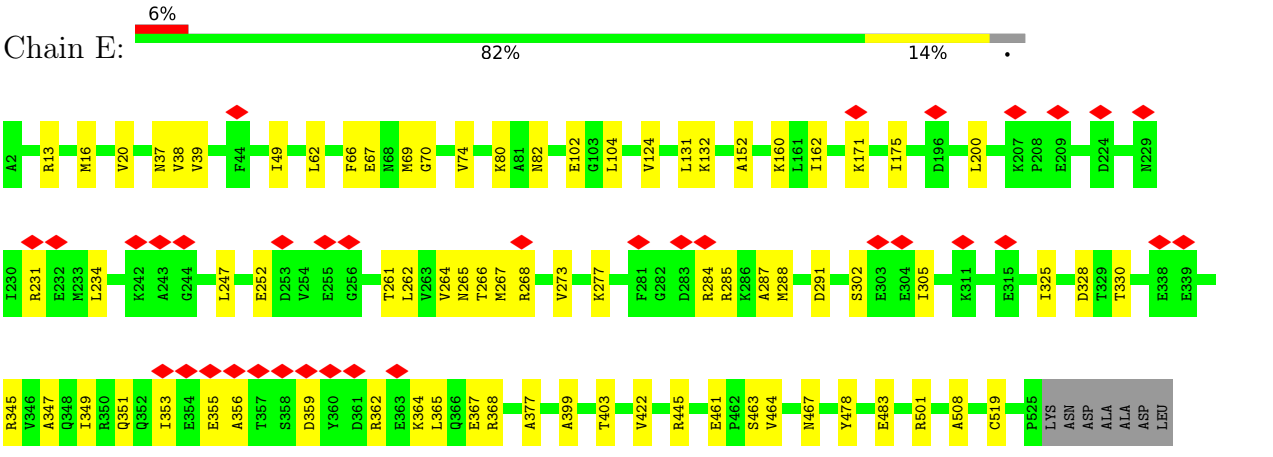
• Molecule 1: Chaperonin GroEL

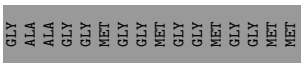


• Molecule 1: Chaperonin GroEL

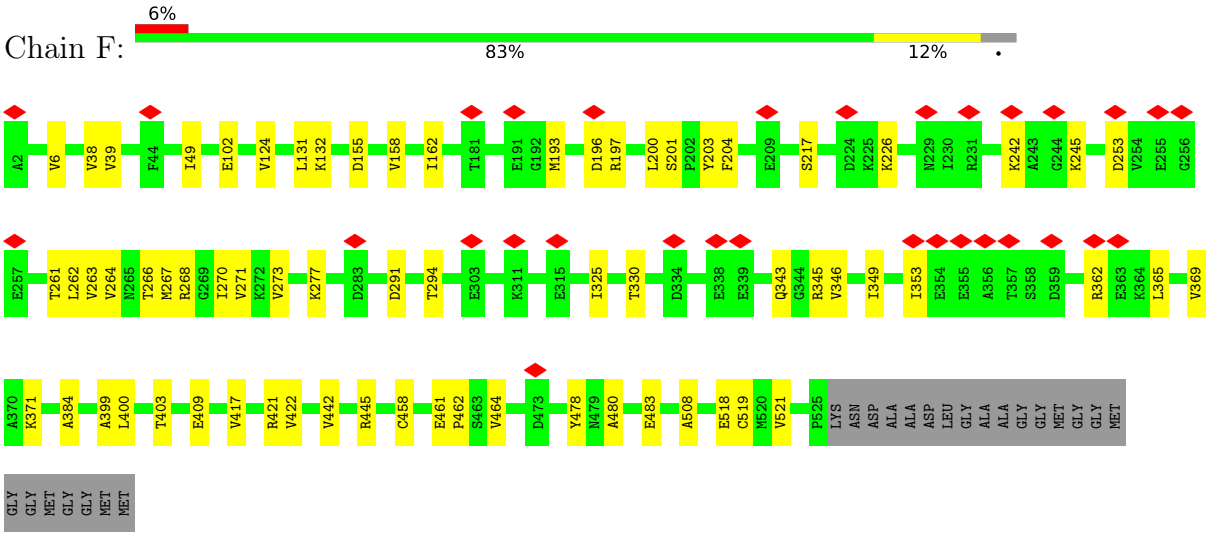


• Molecule 1: Chaperonin GroEL

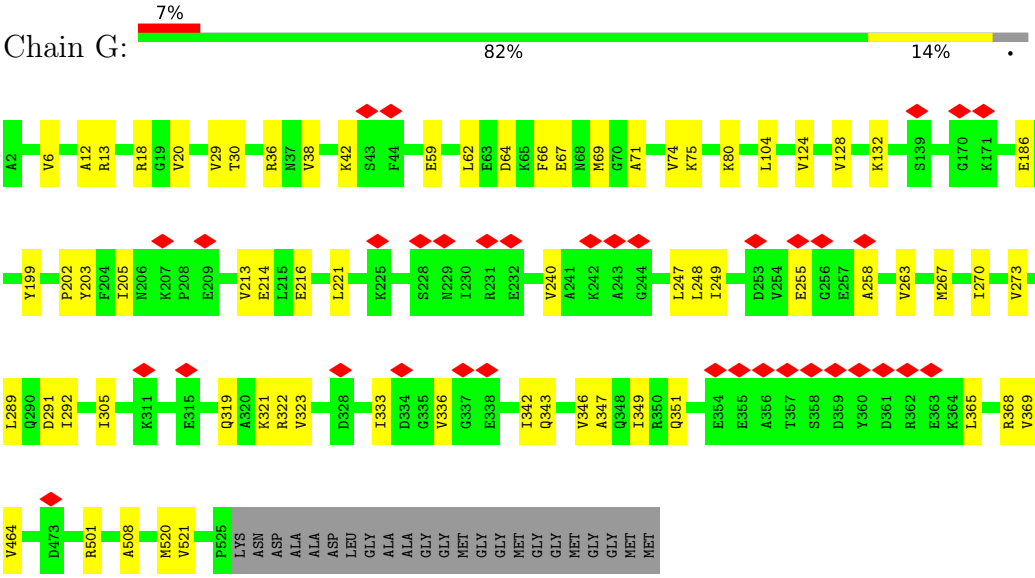




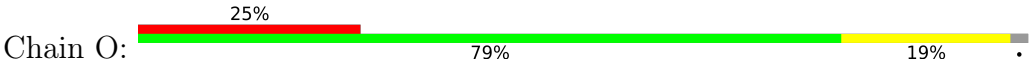
• Molecule 1: Chaperonin GroEL

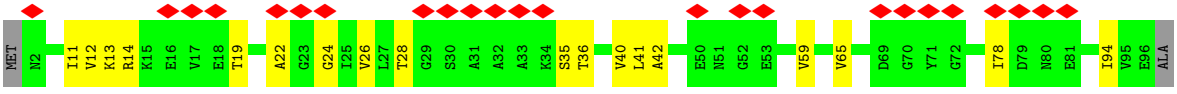


• Molecule 1: Chaperonin GroEL

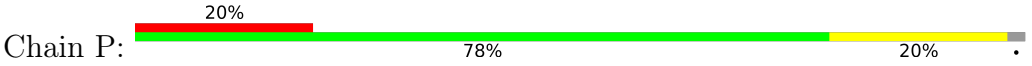


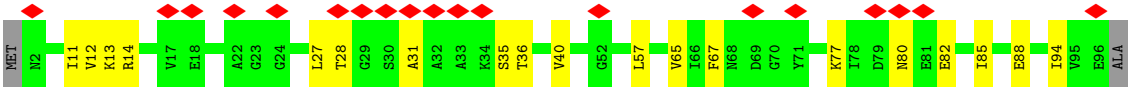
• Molecule 2: Co-chaperonin GroES



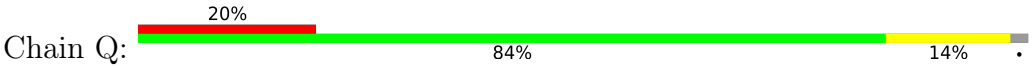


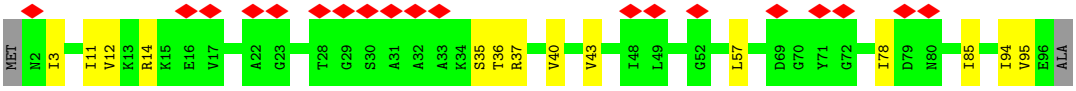
• Molecule 2: Co-chaperonin GroES



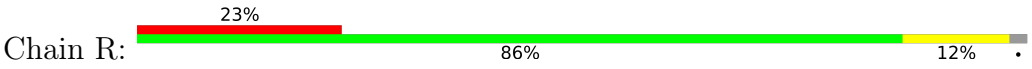


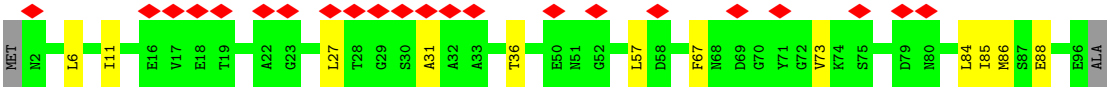
• Molecule 2: Co-chaperonin GroES



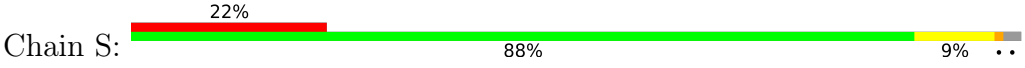


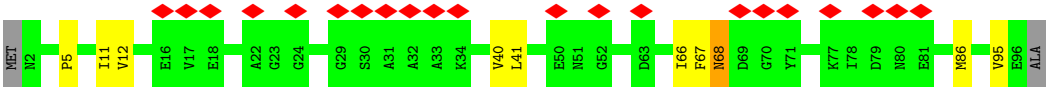
• Molecule 2: Co-chaperonin GroES



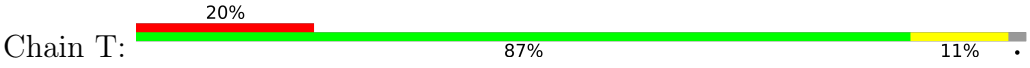


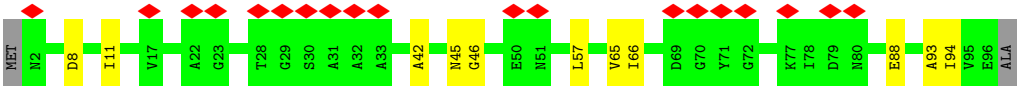
• Molecule 2: Co-chaperonin GroES



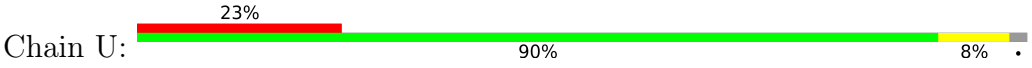


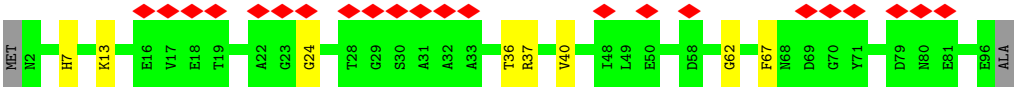
• Molecule 2: Co-chaperonin GroES



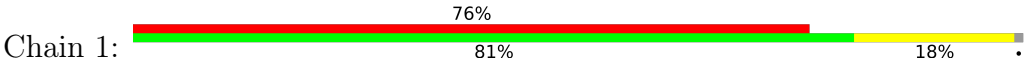


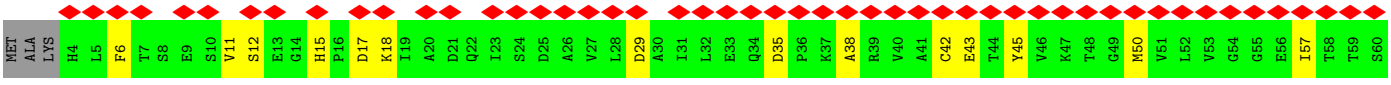
• Molecule 2: Co-chaperonin GroES

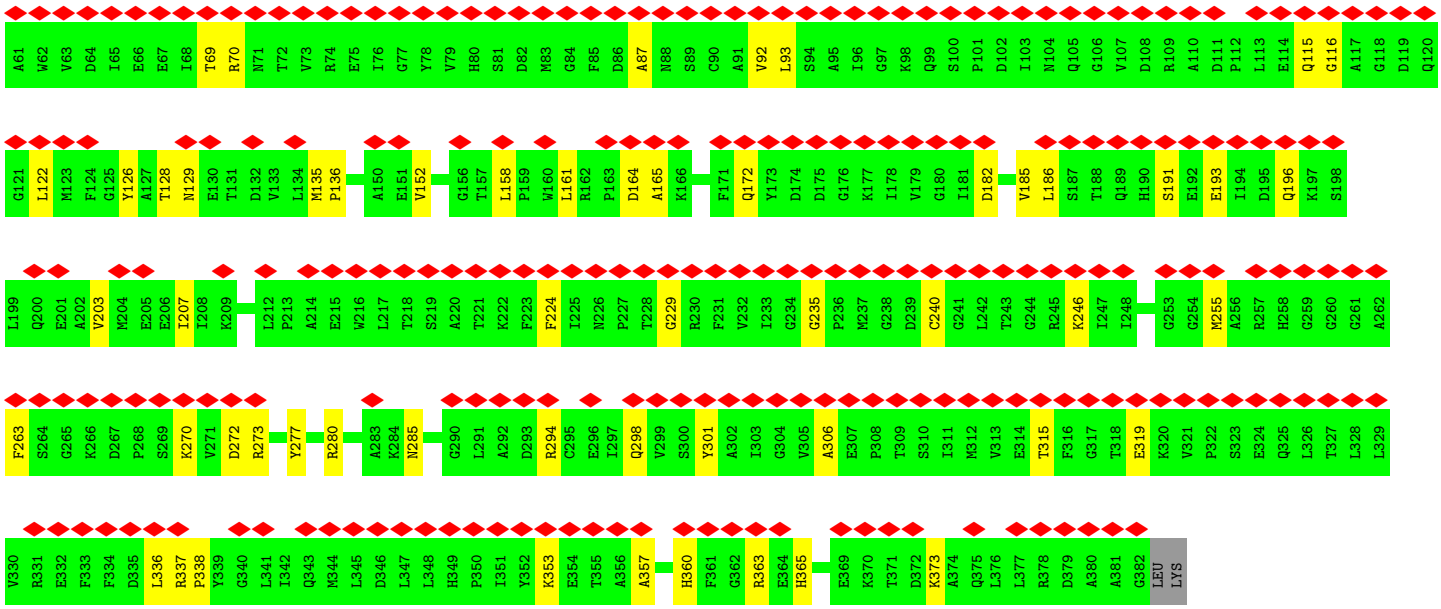




• Molecule 3: S-adenosylmethionine synthase






A61 W62 V63 D64 I65 E66 E67 I68 T69 R70 N71 T72 V73 R74 E75 I76 G77 Y78 V79 H80 S81 D82 M83 G84 F85 D86 A87 N88 S89 C90 A91 V92 L93 S94 A95 I96 G97 K98 Q99 S100 P101 D102 I103 N104 Q105 G106 V107 D108 R109 A110 D111 P112 L113 E114 Q115 G116 A117 G118 D119 Q120
G121 L122 M123 F124 G125 Y126 A127 T128 N129 E130 T131 D132 V133 L134 M135 P136 A150 E151 V152 G156 T157 L158 P159 W160 L161 R162 P163 D164 A165 K166 F171 Q172 Y173 D174 D175 G176 K177 I178 V179 G180 I181 D182 V185 L186 S187 T188 Q189 H190 S191 E192 E193 I194 D195 Q196 K197 S198
L199 Q200 E201 A202 V203 M204 E205 E206 I207 I208 K209 L212 P213 A214 E215 W216 L217 T218 S219 A220 T221 K222 F223 F224 I225 N226 P227 T228 G229 R230 F231 V232 I233 G234 G235 P236 M237 G238 D239 C240 G241 L242 T243 G244 R245 K246 I247 I248 G253 G254 M255 A256 R257 H258 G259 G260 G261 A262
F263 S264 G265 K266 D267 P268 S269 K270 V271 D272 R273 Y277 R280 A283 K284 N285 G290 L291 A292 D293 R294 C295 E296 I297 Q298 V299 S300 Y301 A302 I303 G304 V305 A306 E307 P308 T309 S310 I311 M312 V313 E314 T315 F316 G317 T318 E319 K320 V321 P322 S323 E324 Q325 L326 T327 L328 L329
V330 R331 E332 F333 F334 D335 L336 R337 P338 Y339 G340 L341 I342 Q343 M344 L345 D346 L347 L348 H349 P350 I351 Y352 K353 E354 T355 A356 A357 H360 F361 G362 R363 E364 H365 E369 K370 T371 D372 K373 A374 Q375 L376 L377 R378 D379 A380 A381 G382 LEU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	454545	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.948	Depositor
Minimum map value	-2.696	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	0.671	Depositor
Map size (Å)	279.04, 279.04, 279.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, BEF, ADP

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	0.25	0/3879	0.48	0/5238
1	B	0.25	0/3879	0.47	0/5238
1	C	0.24	0/3875	0.49	0/5233
1	D	0.25	0/3879	0.48	0/5238
1	E	0.25	0/3879	0.47	0/5238
1	F	0.25	0/3879	0.48	0/5238
1	G	0.24	0/3879	0.47	0/5238
2	O	0.24	0/647	0.51	0/882
2	P	0.24	0/647	0.49	0/882
2	Q	0.24	0/647	0.50	0/882
2	R	0.24	0/647	0.50	0/882
2	S	0.24	0/647	0.50	0/882
2	T	0.24	0/647	0.50	0/882
2	U	0.24	0/647	0.51	0/882
3	1	0.24	0/2951	0.48	0/4007
All	All	0.24	0/34629	0.48	0/46842

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	3851	0	3972	52	0
1	B	3851	0	3972	43	0
1	C	3847	0	3967	41	0
1	D	3851	0	3972	43	0
1	E	3851	0	3972	49	0
1	F	3851	0	3972	43	0
1	G	3851	0	3972	47	0
2	O	644	0	633	12	0
2	P	644	0	633	11	0
2	Q	644	0	633	8	0
2	R	644	0	633	7	0
2	S	644	0	633	7	0
2	T	644	0	633	7	0
2	U	644	0	633	6	0
3	1	2892	0	2831	42	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	1	0
4	G	27	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	A	4	0	0	1	0
6	B	4	0	0	1	0
6	C	4	0	0	1	0
6	D	4	0	0	1	0
6	E	4	0	0	1	0
6	F	4	0	0	1	0
6	G	4	0	0	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	3	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
8	G	3	0	0	0	0
All	All	34605	0	35145	407	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 (407) 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)
2:Q:11:ILE:HG22	2:Q:85:ILE:HG12	1.72	0.72
1:B:193:MET:HG3	1:B:371:LYS:HG2	1.71	0.71
2:P:11:ILE:HG22	2:P:85:ILE:HG12	1.72	0.71
1:G:284:ARG:HH22	1:G:368:ARG:HD2	1.57	0.69
1:D:23:LEU:HD23	1:D:74:VAL:HG13	1.74	0.69
3:1:306:ALA:HB1	3:1:337:ARG:HH22	1.58	0.68
1:F:132:LYS:NZ	1:F:409:GLU:OE2	2.27	0.68
1:A:226:LYS:HE3	1:A:253:ASP:HB3	1.76	0.67
1:D:177:VAL:HG12	1:D:379:ILE:HB	1.76	0.67
1:C:262:LEU:HD22	1:C:273:VAL:HG21	1.76	0.66
3:1:42:CYS:HB2	3:1:57:ILE:HD11	1.78	0.66
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.78	0.65
1:B:362:ARG:HG2	1:B:366:GLN:HE22	1.62	0.65
1:G:66:PHE:HA	1:G:69:MET:HG3	1.77	0.65
3:1:122:LEU:HD21	3:1:298:GLN:HB3	1.79	0.65
1:B:313:THR:HG23	1:B:315:GLU:H	1.62	0.64
1:C:233:MET:HB3	1:C:237:LEU:HD13	1.79	0.64
1:F:291:ASP:OD1	1:F:345:ARG:NH2	2.28	0.64
1:D:359:ASP:O	1:D:362:ARG:N	2.31	0.64
2:P:65:VAL:HG12	2:P:94:ILE:HG22	1.79	0.63
1:E:519:CYS:HB3	1:F:38:VAL:HG22	1.81	0.63
1:F:226:LYS:HG3	1:F:253:ASP:HB3	1.80	0.62
4:G:1600:ADP:PB	6:G:1602:BEF:F1	2.47	0.62
1:E:261:THR:O	1:E:265:ASN:ND2	2.33	0.62
1:F:270:ILE:HG23	1:F:271:VAL:HG22	1.81	0.62
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:11:ILE:HG22	2:R:85:ILE:HG12	1.82	0.62
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.82	0.61
3:1:70:ARG:NH1	3:1:87:ALA:O	2.32	0.61
1:B:291:ASP:OD1	1:B:345:ARG:NH2	2.30	0.61
1:G:132:LYS:NZ	1:G:409:GLU:OE2	2.31	0.61
2:T:45:ASN:OD1	2:T:46:GLY:N	2.33	0.60
1:A:348:GLN:HE21	1:A:352:GLN:HE22	1.49	0.60
2:S:68:ASN:ND2	2:S:68:ASN:O	2.33	0.60
3:1:6:PHE:HE2	3:1:255:MET:HG2	1.67	0.60
1:A:231:ARG:HA	1:A:234:LEU:HD23	1.84	0.60
1:C:240:VAL:HG11	1:C:247:LEU:HD12	1.84	0.59
3:1:17:ASP:OD2	3:1:246:LYS:NZ	2.34	0.59
1:B:207:LYS:HD2	1:B:214:GLU:HG3	1.83	0.59
1:B:178:GLU:OE1	1:B:380:LYS:NZ	2.31	0.59
1:G:240:VAL:HG21	1:G:247:LEU:HD12	1.84	0.59
1:G:18:ARG:NH1	1:G:67:GLU:OE2	2.35	0.59
1:F:162:ILE:HD12	1:F:400:LEU:HD13	1.84	0.59
4:F:1600:ADP:PB	6:F:1602:BEF:F1	2.50	0.59
2:O:78:ILE:HG22	2:U:37:ARG:HH22	1.68	0.59
4:E:1600:ADP:PB	6:E:1602:BEF:F1	2.51	0.58
1:A:240:VAL:HG11	1:A:247:LEU:HD12	1.85	0.58
4:D:1600:ADP:PB	6:D:1602:BEF:F1	2.51	0.58
1:E:80:LYS:NZ	1:F:384:ALA:O	2.36	0.58
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.86	0.58
1:D:248:LEU:HD22	1:D:323:VAL:HG11	1.84	0.58
1:D:253:ASP:OD1	1:D:254:VAL:N	2.35	0.58
1:E:252:GLU:OE2	1:E:285:ARG:NH1	2.37	0.58
1:F:217:SER:OG	1:F:245:LYS:NZ	2.36	0.58
1:A:102:GLU:HG2	1:A:445:ARG:HH12	1.69	0.58
1:G:186:GLU:HB3	1:G:380:LYS:HB2	1.85	0.58
1:C:214:GLU:HG3	1:C:324:VAL:HG22	1.85	0.58
1:A:221:LEU:HD23	1:A:249:ILE:HG12	1.85	0.57
1:B:261:THR:O	1:B:265:ASN:ND2	2.37	0.57
1:G:6:VAL:HG22	1:G:521:VAL:HG12	1.87	0.57
1:B:155:ASP:HB3	1:B:158:VAL:HG12	1.86	0.57
1:D:222:LEU:HD22	1:D:289:LEU:HD11	1.86	0.57
2:R:73:VAL:HG13	2:R:86:MET:HB3	1.87	0.57
1:A:20:VAL:HG13	1:A:74:VAL:HG21	1.87	0.57
3:1:196:GLN:NE2	3:1:229:GLY:O	2.38	0.57
4:A:1600:ADP:PB	6:A:1602:BEF:F1	2.52	0.56
1:B:214:GLU:OE1	1:B:322:ARG:NH1	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:CYS:HB3	1:E:38:VAL:HG22	1.86	0.56
1:B:294:THR:HG21	1:B:345:ARG:HG3	1.86	0.56
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.86	0.56
1:F:262:LEU:HD22	1:F:273:VAL:HG11	1.88	0.56
4:B:1600:ADP:PB	6:B:1602:BEF:F1	2.48	0.56
1:G:193:MET:HG3	1:G:371:LYS:HG2	1.88	0.56
2:P:12:VAL:HG12	2:P:40:VAL:HG12	1.88	0.56
3:1:35:ASP:HB3	3:1:38:ALA:HB2	1.88	0.56
1:G:214:GLU:OE2	1:G:322:ARG:NH1	2.39	0.55
2:O:14:ARG:NH1	2:O:35:SER:O	2.38	0.55
1:A:37:ASN:ND2	1:A:391:GLU:OE2	2.39	0.55
3:1:11:VAL:HB	3:1:15:HIS:CD2	2.41	0.55
1:E:264:VAL:HG22	1:E:268:ARG:HH12	1.71	0.55
1:F:200:LEU:HD21	1:F:277:LYS:HE3	1.89	0.55
1:E:132:LYS:HZ3	1:E:501:ARG:HE	1.55	0.54
1:F:346:VAL:HA	1:F:349:ILE:HG22	1.89	0.54
1:G:349:ILE:HD11	1:G:365:LEU:HD22	1.89	0.54
3:1:301:TYR:OH	3:1:336:LEU:O	2.26	0.54
1:A:162:ILE:HD12	1:A:400:LEU:HD13	1.90	0.54
1:E:364:LYS:O	1:E:367:GLU:HG3	2.08	0.54
3:1:135:MET:SD	3:1:136:PRO:HD2	2.48	0.54
1:A:187:LEU:HD11	1:A:377:ALA:HB1	1.89	0.53
1:B:218:PRO:HB3	1:B:246:PRO:HB2	1.89	0.53
1:G:132:LYS:HZ3	1:G:501:ARG:HE	1.55	0.53
1:F:365:LEU:O	1:F:369:VAL:HG23	2.07	0.53
1:G:12:ALA:HB1	1:G:520:MET:HG3	1.90	0.53
1:D:453:GLN:NE2	1:D:457:ASN:OD1	2.40	0.53
1:D:24:ALA:O	1:D:28:LYS:HB2	2.09	0.53
1:A:262:LEU:HD22	1:A:273:VAL:HG21	1.89	0.53
3:1:185:VAL:HG22	3:1:224:PHE:HB2	1.91	0.53
2:U:40:VAL:HG23	2:U:62:GLY:H	1.73	0.53
3:1:158:LEU:HB3	3:1:161:LEU:HG	1.90	0.53
1:E:359:ASP:HA	1:E:362:ARG:HB2	1.89	0.53
1:A:384:ALA:O	1:G:80:LYS:NZ	2.41	0.53
1:G:461:GLU:HB2	1:G:464:VAL:HG12	1.89	0.53
2:O:59:VAL:HG12	2:O:94:ILE:HD11	1.91	0.52
2:Q:12:VAL:HG12	2:Q:40:VAL:HA	1.91	0.52
1:D:221:LEU:HD23	1:D:249:ILE:HG12	1.90	0.52
1:E:478:TYR:OH	1:E:483:GLU:OE1	2.23	0.52
1:G:365:LEU:O	1:G:369:VAL:HG23	2.08	0.52
1:A:69:MET:O	1:A:73:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:116:GLY:HA2	3:1:306:ALA:HA	1.91	0.52
3:1:357:ALA:O	3:1:363:ARG:NH2	2.38	0.52
1:C:261:THR:O	1:C:265:ASN:ND2	2.42	0.52
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.91	0.52
1:B:201:SER:HB2	1:B:259:LEU:HD23	1.92	0.52
1:G:343:GLN:HA	1:G:346:VAL:HG22	1.92	0.52
1:A:349:ILE:HD11	1:A:365:LEU:HG	1.92	0.52
1:A:24:ALA:O	1:A:28:LYS:HB2	2.10	0.52
1:F:461:GLU:HG3	1:F:464:VAL:HG12	1.92	0.52
1:C:132:LYS:NZ	1:C:501:ARG:HE	2.09	0.51
3:1:273:ARG:NH1	3:1:277:TYR:OH	2.43	0.51
3:1:191:SER:OG	3:1:193:GLU:OE1	2.20	0.51
1:E:356:ALA:O	1:E:362:ARG:NE	2.44	0.51
1:D:291:ASP:OD2	1:D:368:ARG:NH1	2.41	0.51
1:F:478:TYR:OH	1:F:483:GLU:OE1	2.20	0.51
1:E:305:ILE:O	1:E:305:ILE:HG13	2.11	0.51
1:B:264:VAL:HG21	2:P:28:THR:HG21	1.93	0.51
1:E:461:GLU:HB2	1:E:464:VAL:HG12	1.91	0.51
1:G:347:ALA:O	1:G:351:GLN:HG2	2.10	0.51
1:B:326:ASN:HB2	1:B:329:THR:HG22	1.93	0.51
1:C:284:ARG:HG2	1:C:288:MET:HE2	1.93	0.50
1:D:270:ILE:HG22	1:D:271:VAL:HG13	1.92	0.50
1:A:131:LEU:HG	1:A:422:VAL:HG21	1.93	0.50
1:B:111:MET:HG3	1:B:435:ASP:OD1	2.10	0.50
2:P:77:LYS:HA	2:P:82:GLU:HA	1.93	0.50
1:F:518:GLU:HG2	1:G:29:VAL:HG21	1.92	0.50
3:1:337:ARG:NE	3:1:338:PRO:HD2	2.26	0.50
1:F:294:THR:HG21	1:F:345:ARG:HG3	1.93	0.50
3:1:203:VAL:HG23	3:1:207:ILE:HD12	1.93	0.50
1:C:158:VAL:HG21	1:C:396:VAL:HG22	1.92	0.50
1:C:196:ASP:OD2	1:C:196:ASP:N	2.44	0.50
1:D:194:GLN:O	1:D:371:LYS:NZ	2.39	0.50
1:A:478:TYR:OH	1:A:483:GLU:OE1	2.27	0.50
1:C:225:LYS:HE3	1:C:303:GLU:HB2	1.94	0.50
3:1:29:ASP:OD2	3:1:353:LYS:N	2.45	0.50
1:G:221:LEU:HD23	1:G:249:ILE:HG12	1.94	0.49
2:S:68:ASN:HD22	2:S:68:ASN:C	2.14	0.49
2:R:57:LEU:HD22	2:R:88:GLU:HG3	1.95	0.49
1:B:16:MET:O	1:B:20:VAL:HG23	2.13	0.49
1:D:115:ASP:OD2	1:D:433:ASN:ND2	2.35	0.49
1:D:325:ILE:HG12	1:D:330:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HB3	1:A:447:MET:HG3	1.93	0.49
1:C:487:ASN:O	1:C:491:MET:HG3	2.11	0.49
1:G:291:ASP:OD2	1:G:368:ARG:NE	2.43	0.49
2:O:19:THR:HB	2:O:26:VAL:HG13	1.94	0.49
2:Q:37:ARG:HE	2:Q:95:VAL:HG21	1.77	0.49
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.94	0.49
1:A:253:ASP:OD1	1:A:254:VAL:N	2.46	0.49
1:D:305:ILE:HG23	1:D:307:MET:HG2	1.95	0.49
2:O:36:THR:O	2:O:36:THR:HG22	2.13	0.49
1:A:285:ARG:HH21	1:A:286:LYS:NZ	2.10	0.49
1:D:152:ALA:HB2	1:D:399:ALA:HB2	1.94	0.48
1:G:199:TYR:CE2	1:G:202:PRO:HA	2.48	0.48
1:E:132:LYS:NZ	1:E:501:ARG:HE	2.11	0.48
1:E:463:SER:O	1:E:467:ASN:ND2	2.34	0.48
1:C:113:PRO:HB2	1:C:516:THR:HG23	1.96	0.48
1:F:262:LEU:O	1:F:266:THR:HG23	2.12	0.48
1:C:102:GLU:HB2	1:C:442:VAL:HG13	1.95	0.48
3:1:315:THR:HG21	3:1:319:GLU:HB3	1.94	0.48
1:D:11:ASP:O	1:D:15:LYS:HG2	2.14	0.48
1:A:346:VAL:HA	1:A:349:ILE:HG22	1.94	0.48
1:D:247:LEU:HB3	1:D:273:VAL:HG12	1.95	0.48
1:E:284:ARG:O	1:E:288:MET:HG3	2.14	0.48
3:1:126:TYR:O	3:1:280:ARG:NH1	2.43	0.48
1:C:220:ILE:HG23	1:C:250:ILE:HD13	1.96	0.48
2:Q:94:ILE:HG12	2:R:6:LEU:HD21	1.96	0.48
1:A:289:LEU:HA	1:A:292:ILE:HD12	1.95	0.47
1:B:339:GLU:O	1:B:343:GLN:HG2	2.14	0.47
2:O:11:ILE:HD11	2:O:42:ALA:HB3	1.97	0.47
2:T:88:GLU:OE2	2:U:7:HIS:NE2	2.45	0.47
1:C:443:ALA:O	1:C:447:MET:HG3	2.15	0.47
1:G:248:LEU:HD22	1:G:323:VAL:HG11	1.96	0.47
1:G:322:ARG:HB3	1:G:333:ILE:HD11	1.96	0.47
2:S:12:VAL:HG12	2:S:40:VAL:HG12	1.96	0.47
2:S:67:PHE:HB2	2:S:86:MET:HE1	1.96	0.47
1:B:487:ASN:HB3	1:B:490:ASP:HB2	1.96	0.47
1:D:240:VAL:HG11	1:D:247:LEU:HD12	1.96	0.47
1:D:240:VAL:HG21	1:D:247:LEU:HD13	1.97	0.47
1:F:349:ILE:HD11	1:F:365:LEU:HG	1.96	0.47
1:A:68:ASN:O	1:A:72:GLN:HG2	2.14	0.47
1:A:142:LYS:O	1:A:146:GLN:HG3	2.14	0.47
1:A:263:VAL:O	1:A:267:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LEU:HD21	1:D:277:LYS:HE2	1.97	0.47
1:D:288:MET:O	1:D:292:ILE:HG13	2.15	0.47
3:1:172:GLN:HB3	3:1:182:ASP:OD2	2.14	0.47
1:C:140:ASP:N	1:C:140:ASP:OD1	2.46	0.47
1:E:247:LEU:HB3	1:E:273:VAL:HG12	1.97	0.47
1:G:216:GLU:OE1	1:G:216:GLU:N	2.47	0.47
1:G:319:GLN:HB2	1:G:336:VAL:HG11	1.97	0.47
1:E:16:MET:O	1:E:20:VAL:HG23	2.15	0.47
1:D:264:VAL:HA	1:D:267:MET:HG2	1.96	0.46
1:E:160:LYS:HB2	1:E:160:LYS:HE2	1.70	0.46
1:B:66:PHE:HA	1:B:69:MET:HE3	1.96	0.46
1:B:194:GLN:OE1	1:B:329:THR:OG1	2.23	0.46
1:A:229:ASN:OD1	1:A:230:ILE:N	2.48	0.46
1:B:140:ASP:OD1	1:B:140:ASP:N	2.46	0.46
1:G:20:VAL:HG13	1:G:74:VAL:HG21	1.96	0.46
2:R:73:VAL:HG11	2:R:84:LEU:HD23	1.97	0.46
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.56	0.46
2:U:36:THR:OG1	2:U:67:PHE:O	2.33	0.46
2:Q:14:ARG:NH1	2:Q:35:SER:O	2.48	0.46
3:1:263:PHE:HB3	3:1:360:HIS:CE1	2.50	0.46
1:B:30:THR:HB	1:B:51:LYS:HG2	1.97	0.46
1:C:409:GLU:OE2	1:C:501:ARG:NH2	2.49	0.46
1:D:336:VAL:HG12	1:D:336:VAL:O	2.16	0.46
2:R:36:THR:OG1	2:R:67:PHE:O	2.34	0.46
3:1:12:SER:HB3	3:1:165:ALA:HB3	1.98	0.46
1:D:443:ALA:O	1:D:447:MET:HG2	2.16	0.45
1:F:196:ASP:OD1	1:F:196:ASP:N	2.49	0.45
2:T:11:ILE:HD12	2:T:42:ALA:HB3	1.97	0.45
1:B:228:SER:HA	1:B:255:GLU:HG2	1.97	0.45
1:D:264:VAL:O	1:D:268:ARG:HG3	2.16	0.45
1:E:62:LEU:HD22	1:E:67:GLU:HB3	1.98	0.45
2:P:36:THR:OG1	2:P:67:PHE:O	2.34	0.45
1:D:305:ILE:HD11	1:E:267:MET:SD	2.56	0.45
1:G:263:VAL:O	1:G:267:MET:HG3	2.16	0.45
1:A:256:GLY:HA2	1:A:259:LEU:HD12	1.97	0.45
1:F:201:SER:HB3	1:F:204:PHE:CE2	2.51	0.45
2:O:65:VAL:HG12	2:O:94:ILE:HG12	1.98	0.45
2:S:5:PRO:HG3	2:S:11:ILE:HG23	1.97	0.45
1:A:247:LEU:HD21	1:A:249:ILE:HG13	1.98	0.45
1:E:124:VAL:HG21	1:E:508:ALA:HB2	1.99	0.45
3:1:128:THR:HG22	3:1:294:ARG:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:OE1	1:A:343:GLN:HA	2.17	0.45
1:C:16:MET:O	1:C:20:VAL:HG23	2.17	0.45
1:C:261:THR:HA	1:C:264:VAL:HG12	1.99	0.45
1:E:305:ILE:HD11	1:F:267:MET:SD	2.56	0.45
1:E:131:LEU:HG	1:E:422:VAL:HG21	1.99	0.45
2:P:57:LEU:HD22	2:P:88:GLU:HG3	1.99	0.45
1:A:281:PHE:HA	1:A:285:ARG:NH1	2.32	0.45
1:E:262:LEU:HD22	1:E:273:VAL:HG21	1.98	0.45
1:E:347:ALA:O	1:E:351:GLN:HG3	2.17	0.45
1:F:203:TYR:HB2	1:F:263:VAL:HG21	1.98	0.45
1:F:242:LYS:N	1:F:242:LYS:HD2	2.32	0.45
2:T:8:ASP:HA	2:T:57:LEU:HD11	1.99	0.45
4:C:1600:ADP:PB	6:C:1602:BEF:F1	2.55	0.45
1:E:302:SER:HB3	1:E:305:ILE:HG22	1.99	0.45
1:F:155:ASP:HB3	1:F:158:VAL:HG12	1.99	0.45
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.48	0.44
1:B:345:ARG:O	1:B:349:ILE:HG13	2.17	0.44
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.99	0.44
2:T:65:VAL:HG12	2:T:94:ILE:HG12	1.99	0.44
1:A:155:ASP:HB3	1:A:158:VAL:HG12	1.99	0.44
1:E:287:ALA:HB1	1:E:368:ARG:NH2	2.33	0.44
1:E:102:GLU:HG2	1:E:445:ARG:HH12	1.82	0.44
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.48	0.44
2:P:13:LYS:HE2	2:P:13:LYS:HB3	1.70	0.44
3:1:45:TYR:OH	3:1:240:CYS:SG	2.62	0.44
1:G:289:LEU:HD23	1:G:292:ILE:HD12	1.99	0.44
2:Q:36:THR:O	2:Q:36:THR:HG22	2.17	0.44
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.99	0.44
1:C:336:VAL:HG12	1:C:336:VAL:O	2.17	0.44
1:E:70:GLY:O	1:E:74:VAL:HG23	2.16	0.44
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.98	0.44
1:G:128:VAL:O	1:G:132:LYS:HG2	2.17	0.44
1:C:302:SER:HB3	1:C:305:ILE:HG22	2.00	0.44
1:C:114:MET:O	1:C:118:ARG:HG3	2.17	0.44
1:D:6:VAL:HG22	1:D:521:VAL:HG12	1.99	0.44
1:D:348:GLN:O	1:D:351:GLN:HG3	2.18	0.44
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.48	0.44
2:R:27:LEU:HD23	2:R:31:ALA:HB1	1.99	0.44
3:1:270:LYS:HA	3:1:270:LYS:HD3	1.80	0.44
1:E:349:ILE:HG23	1:E:365:LEU:HD12	2.00	0.44
2:P:14:ARG:NH1	2:P:35:SER:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:OD1	1:A:140:ASP:N	2.51	0.43
1:A:349:ILE:HG23	1:A:369:VAL:HG22	2.00	0.43
1:B:453:GLN:NE2	1:B:457:ASN:OD1	2.47	0.43
2:T:8:ASP:OD1	2:T:8:ASP:N	2.50	0.43
1:A:270:ILE:HD13	2:O:24:GLY:O	2.18	0.43
1:A:322:ARG:HB2	1:A:333:ILE:HD11	2.01	0.43
1:B:221:LEU:HD23	1:B:249:ILE:HG12	2.01	0.43
1:C:59:GLU:O	1:C:59:GLU:HG3	2.18	0.43
1:G:62:LEU:HD22	1:G:67:GLU:HB3	1.99	0.43
1:B:152:ALA:HB2	1:B:399:ALA:HB2	1.99	0.43
1:G:203:TYR:CD1	1:G:267:MET:HE1	2.53	0.43
3:1:17:ASP:OD1	3:1:18:LYS:N	2.52	0.43
3:1:136:PRO:HB3	3:1:255:MET:SD	2.59	0.43
1:C:313:THR:OG1	1:C:314:LEU:N	2.52	0.43
1:D:205:ILE:HA	1:D:213:VAL:HB	2.01	0.43
1:A:162:ILE:O	1:A:166:MET:HG3	2.19	0.43
1:A:511:ALA:O	1:A:515:ILE:HG23	2.18	0.43
1:F:343:GLN:HA	1:F:346:VAL:HG22	2.01	0.43
1:G:346:VAL:HA	1:G:349:ILE:HG22	2.00	0.43
1:E:171:LYS:HA	1:E:171:LYS:HD2	1.85	0.43
1:F:6:VAL:HG22	1:F:521:VAL:HG23	2.00	0.43
2:O:12:VAL:HG12	2:O:40:VAL:HG12	2.01	0.43
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.43
1:B:365:LEU:O	1:B:369:VAL:HG23	2.19	0.43
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.49	0.43
1:A:265:ASN:HB3	1:A:271:VAL:HG22	2.01	0.42
1:D:343:GLN:HA	1:D:346:VAL:HG12	2.01	0.42
1:E:20:VAL:HG22	1:E:74:VAL:HG21	2.00	0.42
1:A:222:LEU:HD22	1:A:293:ALA:HB2	2.02	0.42
1:E:328:ASP:OD1	1:E:328:ASP:N	2.51	0.42
1:F:197:ARG:HD2	1:F:277:LYS:HB2	1.99	0.42
1:G:30:THR:HG22	1:G:36:ARG:O	2.18	0.42
1:G:342:ILE:O	1:G:346:VAL:HG13	2.18	0.42
2:T:66:ILE:HD11	2:T:93:ALA:HB3	2.00	0.42
1:A:203:TYR:CZ	1:G:305:ILE:HD12	2.54	0.42
2:O:22:ALA:HB2	2:P:80:ASN:HD21	1.84	0.42
3:1:115:GLN:O	3:1:337:ARG:NH2	2.52	0.42
1:A:264:VAL:HG21	2:O:28:THR:HG21	2.01	0.42
3:1:50:MET:HE1	3:1:93:LEU:HD23	2.00	0.42
1:G:255:GLU:OE2	1:G:258:ALA:N	2.52	0.42
2:Q:3:ILE:HD11	2:Q:78:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:VAL:HG21	1:D:396:VAL:HG22	2.00	0.42
1:F:102:GLU:HB2	1:F:442:VAL:HG13	2.01	0.42
1:F:193:MET:HG3	1:F:371:LYS:HG2	2.01	0.42
1:F:261:THR:HA	1:F:264:VAL:HG12	2.01	0.42
1:G:71:ALA:O	1:G:75:LYS:HG3	2.19	0.42
1:D:201:SER:HB2	1:D:259:LEU:HD23	2.02	0.42
1:E:291:ASP:OD1	1:E:345:ARG:NE	2.42	0.42
3:1:186:LEU:HD22	3:1:203:VAL:HG21	2.02	0.42
1:A:152:ALA:HB2	1:A:399:ALA:HB2	2.01	0.42
1:A:158:VAL:HG21	1:A:396:VAL:HG22	2.01	0.42
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.49	0.42
1:B:41:ASP:HA	1:B:47:PRO:HB3	2.02	0.42
1:B:215:LEU:HD22	1:B:246:PRO:HB3	2.02	0.42
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.50	0.42
1:C:209:GLU:HG2	1:C:210:THR:N	2.34	0.42
1:D:202:PRO:O	1:D:205:ILE:HG12	2.20	0.42
1:F:39:VAL:HB	1:F:49:ILE:HD13	2.01	0.42
2:S:66:ILE:HD11	2:S:95:VAL:HG23	2.02	0.42
1:C:343:GLN:HA	1:C:346:VAL:HG22	2.00	0.42
2:P:27:LEU:HD22	2:P:31:ALA:HB1	2.02	0.42
1:F:461:GLU:HA	1:F:462:PRO:HD3	1.94	0.41
1:G:205:ILE:HA	1:G:213:VAL:HG22	2.01	0.41
3:1:164:ASP:OD2	3:1:235:GLY:N	2.53	0.41
3:1:270:LYS:HG3	3:1:272:ASP:H	1.85	0.41
1:B:158:VAL:HG21	1:B:396:VAL:HG22	2.01	0.41
1:B:348:GLN:O	1:B:351:GLN:HG3	2.20	0.41
1:B:441:LYS:HD3	1:B:441:LYS:HA	1.81	0.41
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.49	0.41
1:D:511:ALA:O	1:D:515:ILE:HG23	2.20	0.41
1:A:308:GLU:HG3	1:A:310:GLU:HG2	2.02	0.41
1:C:99:ILE:HD13	1:C:446:ALA:HB3	2.03	0.41
1:C:349:ILE:O	1:C:353:ILE:HG13	2.20	0.41
1:E:13:ARG:HD2	1:E:104:LEU:HD22	2.02	0.41
1:F:417:VAL:O	1:F:421:ARG:HG2	2.19	0.41
1:G:64:ASP:HB3	1:G:67:GLU:HG3	2.02	0.41
2:O:13:LYS:HD3	2:O:41:LEU:HD21	2.02	0.41
1:E:39:VAL:HG22	1:E:49:ILE:HG12	2.01	0.41
1:G:270:ILE:HD13	2:U:24:GLY:O	2.20	0.41
2:U:13:LYS:HB3	2:U:13:LYS:HE2	1.83	0.41
1:A:313:THR:HG23	1:A:315:GLU:H	1.85	0.41
1:E:66:PHE:HA	1:E:69:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LEU:HG	1:F:422:VAL:HG21	2.02	0.41
3:1:193:GLU:OE1	3:1:193:GLU:N	2.46	0.41
3:1:285:ASN:ND2	3:1:373:LYS:HB2	2.35	0.41
1:C:31:LEU:O	1:C:457:ASN:ND2	2.53	0.41
1:C:231:ARG:NE	1:C:231:ARG:HA	2.35	0.41
1:D:218:PRO:HB3	1:D:246:PRO:HB2	2.02	0.41
1:E:175:ILE:HG12	1:E:377:ALA:HB3	2.02	0.41
1:G:247:LEU:HB3	1:G:273:VAL:HG12	2.01	0.41
1:G:321:LYS:HA	1:G:321:LYS:HD2	1.68	0.41
1:A:124:VAL:HG21	1:A:508:ALA:HB2	2.03	0.41
1:C:224:ASP:OD1	1:C:224:ASP:N	2.53	0.41
1:C:231:ARG:HA	1:C:234:LEU:HD23	2.02	0.41
1:C:235:PRO:O	1:C:238:GLU:HG2	2.20	0.41
2:S:11:ILE:HG13	2:S:41:LEU:HB2	2.03	0.41
3:1:6:PHE:CE2	3:1:255:MET:HG2	2.52	0.41
1:F:102:GLU:HG2	1:F:445:ARG:HE	1.85	0.41
1:B:262:LEU:HD22	1:B:273:VAL:HG21	2.02	0.41
1:C:95:LEU:O	1:C:99:ILE:HG12	2.20	0.41
1:C:279:PRO:HG2	1:C:288:MET:SD	2.61	0.41
1:E:231:ARG:HA	1:E:234:LEU:HD23	2.02	0.41
1:E:262:LEU:O	1:E:266:THR:HG23	2.21	0.41
1:F:353:ILE:HG23	1:F:362:ARG:HD2	2.03	0.41
1:B:68:ASN:O	1:B:72:GLN:HG2	2.21	0.41
1:C:69:MET:HE2	1:D:41:ASP:HB2	2.02	0.41
1:C:215:LEU:HD23	1:C:246:PRO:HB2	2.03	0.41
1:E:152:ALA:HB2	1:E:399:ALA:HB2	2.02	0.41
1:E:349:ILE:O	1:E:353:ILE:HG13	2.21	0.41
1:B:20:VAL:HG22	1:B:74:VAL:HG21	2.03	0.40
2:Q:43:VAL:HG22	2:Q:57:LEU:HD12	2.03	0.40
3:1:152:VAL:HG12	3:1:158:LEU:HB2	2.03	0.40
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.61	0.40
1:B:132:LYS:NZ	1:B:501:ARG:HE	2.19	0.40
1:B:349:ILE:O	1:B:353:ILE:HG13	2.21	0.40
1:E:37:ASN:HD22	1:E:49:ILE:HG22	1.87	0.40
1:E:162:ILE:HG21	1:E:403:THR:HG21	2.03	0.40
1:E:355:GLU:N	1:E:355:GLU:OE1	2.55	0.40
1:F:264:VAL:O	1:F:268:ARG:HG2	2.22	0.40
3:1:363:ARG:HB3	3:1:365:HIS:CE1	2.55	0.40
1:A:126:ALA:O	1:A:130:GLU:HG2	2.21	0.40
1:B:321:LYS:HB2	1:B:334:ASP:HB3	2.04	0.40
1:C:328:ASP:OD1	1:C:328:ASP:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:VAL:HG21	1:F:508:ALA:HB2	2.03	0.40
1:F:399:ALA:O	1:F:403:THR:HG23	2.22	0.40
1:G:42:LYS:NZ	1:G:59:GLU:OE2	2.55	0.40
1:D:224:ASP:OD1	1:D:289:LEU:HD23	2.22	0.40
1:D:349:ILE:O	1:D:353:ILE:HG13	2.21	0.40
3:1:69:THR:HG21	3:1:92:VAL:HG21	2.03	0.40
1:A:325:ILE:HG12	1:A:330:THR:HG23	2.03	0.40
1:A:441:LYS:HD3	1:A:441:LYS:HA	1.77	0.40
1:B:171:LYS:HA	1:B:171:LYS:HD2	1.86	0.40
1:D:305:ILE:CG2	1:D:307:MET:HG2	2.51	0.40
1:D:345:ARG:O	1:D:349:ILE:HG13	2.21	0.40
3:1:42:CYS:SG	3:1:43:GLU:N	2.94	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	522/547 (95%)	519 (99%)	3 (1%)	0	100	100
1	B	522/547 (95%)	517 (99%)	5 (1%)	0	100	100
1	C	522/547 (95%)	517 (99%)	5 (1%)	0	100	100
1	D	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	E	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	F	522/547 (95%)	518 (99%)	4 (1%)	0	100	100
1	G	522/547 (95%)	520 (100%)	2 (0%)	0	100	100
2	O	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
2	P	93/97 (96%)	91 (98%)	2 (2%)	0	100	100
2	Q	93/97 (96%)	92 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
2	S	93/97 (96%)	91 (98%)	2 (2%)	0	100	100
2	T	93/97 (96%)	91 (98%)	2 (2%)	0	100	100
2	U	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
3	1	377/384 (98%)	369 (98%)	8 (2%)	0	100	100
All	All	4682/4892 (96%)	4633 (99%)	49 (1%)	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	403/414 (97%)	403 (100%)	0	100	100
1	B	403/414 (97%)	403 (100%)	0	100	100
1	C	402/414 (97%)	400 (100%)	2 (0%)	86	93
1	D	403/414 (97%)	403 (100%)	0	100	100
1	E	403/414 (97%)	402 (100%)	1 (0%)	92	96
1	F	403/414 (97%)	403 (100%)	0	100	100
1	G	403/414 (97%)	403 (100%)	0	100	100
2	O	62/80 (78%)	62 (100%)	0	100	100
2	P	62/80 (78%)	62 (100%)	0	100	100
2	Q	62/80 (78%)	62 (100%)	0	100	100
2	R	62/80 (78%)	62 (100%)	0	100	100
2	S	62/80 (78%)	61 (98%)	1 (2%)	58	79
2	T	62/80 (78%)	62 (100%)	0	100	100
2	U	62/80 (78%)	62 (100%)	0	100	100
3	1	304/312 (97%)	303 (100%)	1 (0%)	91	95
All	All	3558/3770 (94%)	3553 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	82	ASN
1	C	226	LYS
1	E	82	ASN
2	S	68	ASN
3	1	129	ASN

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	348	GLN
1	F	453	GLN
2	S	68	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 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	$\#\|Z\|>2$
4	ADP	D	1600	7,5	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
6	BEF	F	1602	-	0,3,3	-	-	-		
6	BEF	C	1602	4	0,3,3	-	-	-		
6	BEF	D	1602	-	0,3,3	-	-	-		
4	ADP	G	1600	7,6,5	24,29,29	0.92	1 (4%)	29,45,45	1.40	4 (13%)
6	BEF	B	1602	4	0,3,3	-	-	-		
6	BEF	A	1602	4	0,3,3	-	-	-		
6	BEF	E	1602	4	0,3,3	-	-	-		
4	ADP	A	1600	7,6,5	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
6	BEF	G	1602	4	0,3,3	-	-	-		
4	ADP	B	1600	7,6,5	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
4	ADP	E	1600	7,6,5	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
4	ADP	F	1600	7,5	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
4	ADP	C	1600	7,6,5	24,29,29	0.92	1 (4%)	29,45,45	1.41	4 (13%)

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
4	ADP	D	1600	7,5	-	5/12/32/32	0/3/3/3
4	ADP	G	1600	7,6,5	-	5/12/32/32	0/3/3/3
4	ADP	A	1600	7,6,5	-	4/12/32/32	0/3/3/3
4	ADP	B	1600	7,6,5	-	5/12/32/32	0/3/3/3
4	ADP	E	1600	7,6,5	-	4/12/32/32	0/3/3/3
4	ADP	F	1600	7,5	-	5/12/32/32	0/3/3/3
4	ADP	C	1600	7,6,5	-	5/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1600	ADP	C5-C4	2.45	1.47	1.40
4	B	1600	ADP	C5-C4	2.44	1.47	1.40
4	F	1600	ADP	C5-C4	2.43	1.47	1.40
4	C	1600	ADP	C5-C4	2.42	1.47	1.40
4	G	1600	ADP	C5-C4	2.41	1.47	1.40
4	D	1600	ADP	C5-C4	2.41	1.47	1.40
4	A	1600	ADP	C5-C4	2.39	1.47	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1600	ADP	C3'-C2'-C1'	3.31	105.96	100.98
4	C	1600	ADP	N3-C2-N1	-3.27	123.57	128.68
4	E	1600	ADP	N3-C2-N1	-3.25	123.59	128.68
4	E	1600	ADP	C3'-C2'-C1'	3.25	105.87	100.98
4	B	1600	ADP	N3-C2-N1	-3.25	123.60	128.68
4	A	1600	ADP	N3-C2-N1	-3.24	123.61	128.68
4	D	1600	ADP	N3-C2-N1	-3.24	123.62	128.68
4	B	1600	ADP	C3'-C2'-C1'	3.23	105.84	100.98
4	C	1600	ADP	C3'-C2'-C1'	3.23	105.84	100.98
4	F	1600	ADP	N3-C2-N1	-3.22	123.64	128.68
4	D	1600	ADP	C3'-C2'-C1'	3.20	105.80	100.98
4	G	1600	ADP	N3-C2-N1	-3.20	123.67	128.68
4	A	1600	ADP	C3'-C2'-C1'	3.20	105.80	100.98
4	G	1600	ADP	C3'-C2'-C1'	3.14	105.71	100.98
4	A	1600	ADP	PA-O3A-PB	-2.89	122.91	132.83
4	F	1600	ADP	PA-O3A-PB	-2.80	123.23	132.83
4	D	1600	ADP	PA-O3A-PB	-2.74	123.41	132.83
4	G	1600	ADP	C4-C5-N7	-2.73	106.56	109.40
4	B	1600	ADP	PA-O3A-PB	-2.69	123.59	132.83
4	E	1600	ADP	C4-C5-N7	-2.69	106.60	109.40
4	D	1600	ADP	C4-C5-N7	-2.68	106.61	109.40
4	A	1600	ADP	C4-C5-N7	-2.66	106.63	109.40
4	F	1600	ADP	C4-C5-N7	-2.66	106.63	109.40
4	B	1600	ADP	C4-C5-N7	-2.63	106.65	109.40
4	C	1600	ADP	C4-C5-N7	-2.63	106.65	109.40
4	E	1600	ADP	PA-O3A-PB	-2.55	124.08	132.83
4	G	1600	ADP	PA-O3A-PB	-2.48	124.30	132.83
4	C	1600	ADP	PA-O3A-PB	-2.47	124.34	132.83

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1600	ADP	PA-O3A-PB-O2B
4	B	1600	ADP	PA-O3A-PB-O3B
4	C	1600	ADP	PA-O3A-PB-O2B
4	C	1600	ADP	O4'-C4'-C5'-O5'
4	D	1600	ADP	O4'-C4'-C5'-O5'
4	E	1600	ADP	PA-O3A-PB-O2B
4	E	1600	ADP	PA-O3A-PB-O3B
4	F	1600	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	G	1600	ADP	PA-O3A-PB-O2B
4	G	1600	ADP	PA-O3A-PB-O3B
4	G	1600	ADP	O4'-C4'-C5'-O5'
4	A	1600	ADP	O4'-C4'-C5'-O5'
4	A	1600	ADP	C3'-C4'-C5'-O5'
4	B	1600	ADP	O4'-C4'-C5'-O5'
4	B	1600	ADP	C3'-C4'-C5'-O5'
4	E	1600	ADP	O4'-C4'-C5'-O5'
4	F	1600	ADP	O4'-C4'-C5'-O5'
4	F	1600	ADP	C3'-C4'-C5'-O5'
4	C	1600	ADP	C3'-C4'-C5'-O5'
4	D	1600	ADP	C3'-C4'-C5'-O5'
4	G	1600	ADP	C3'-C4'-C5'-O5'
4	E	1600	ADP	C3'-C4'-C5'-O5'
4	D	1600	ADP	PA-O3A-PB-O2B
4	D	1600	ADP	PA-O3A-PB-O3B
4	G	1600	ADP	PA-O3A-PB-O1B
4	A	1600	ADP	PA-O3A-PB-O3B
4	C	1600	ADP	PA-O3A-PB-O3B
4	F	1600	ADP	PA-O3A-PB-O2B
4	F	1600	ADP	PA-O3A-PB-O3B
4	A	1600	ADP	C5'-O5'-PA-O1A
4	B	1600	ADP	C5'-O5'-PA-O1A
4	C	1600	ADP	C5'-O5'-PA-O1A
4	D	1600	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

14 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1600	ADP	1	0
6	F	1602	BEF	1	0
6	C	1602	BEF	1	0
6	D	1602	BEF	1	0
4	G	1600	ADP	1	0
6	B	1602	BEF	1	0
6	A	1602	BEF	1	0
6	E	1602	BEF	1	0
4	A	1600	ADP	1	0
6	G	1602	BEF	1	0
4	B	1600	ADP	1	0
4	E	1600	ADP	1	0

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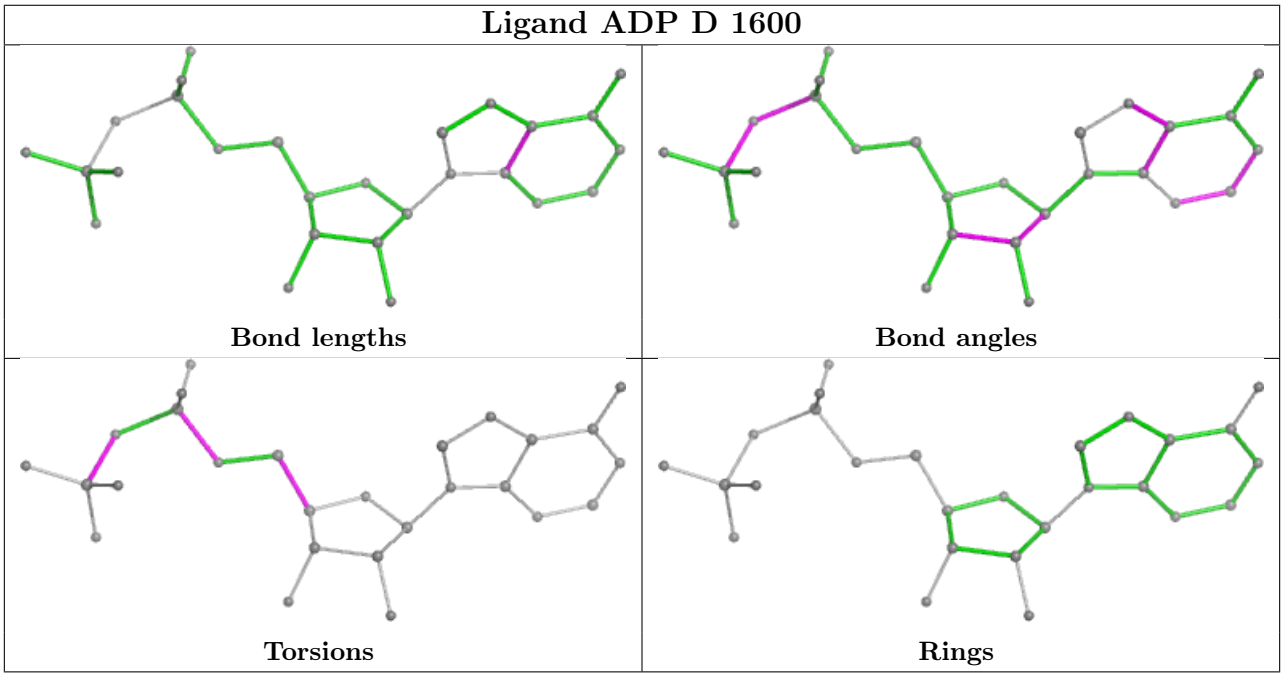
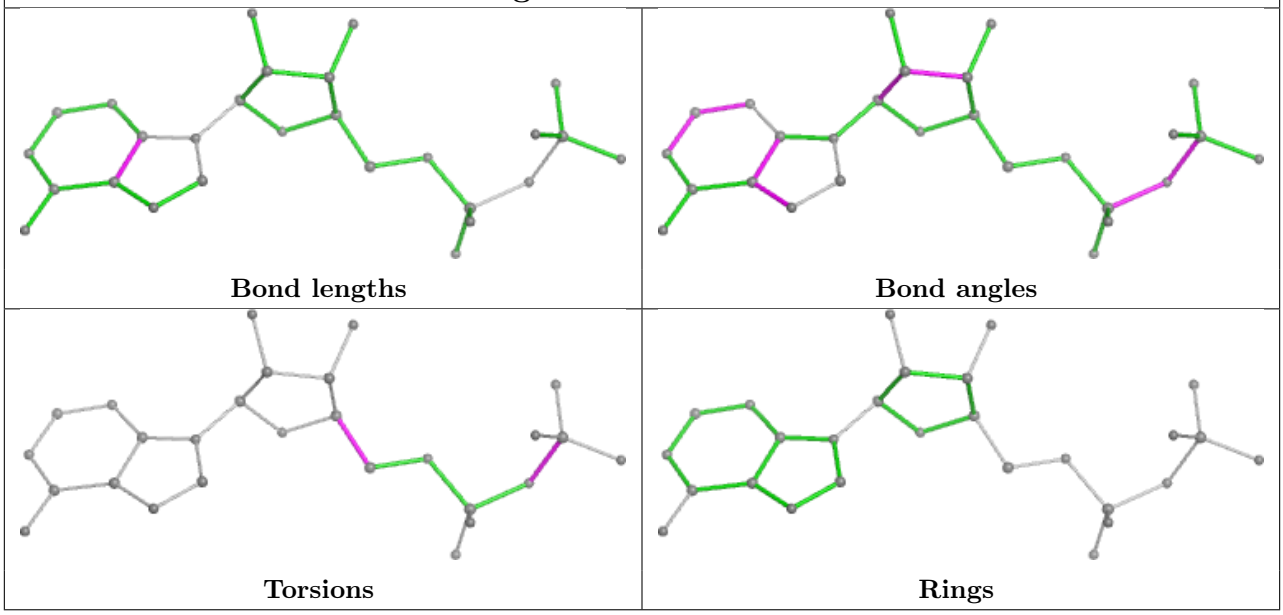
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1600	ADP	1	0
4	C	1600	ADP	1	0

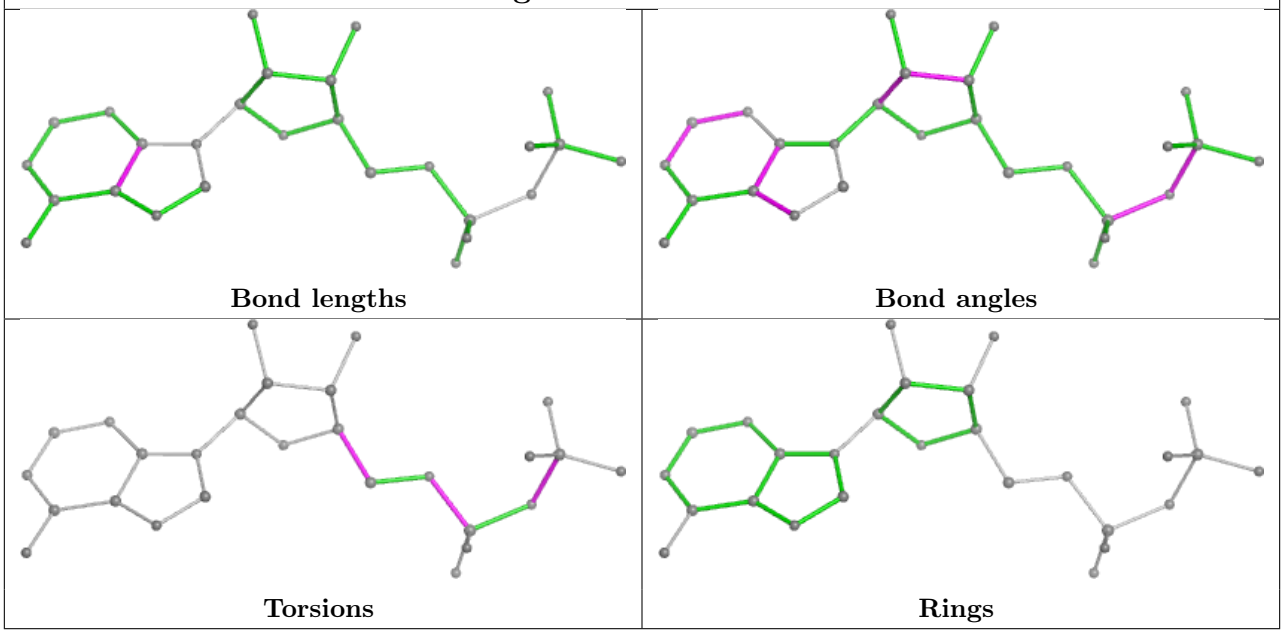
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



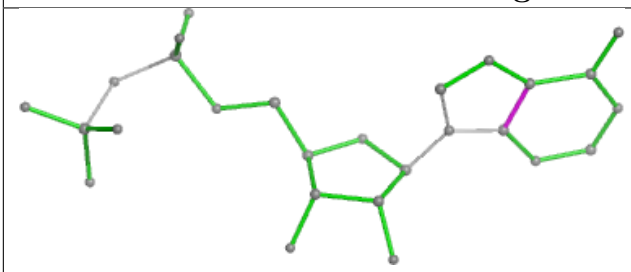
Ligand ADP G 1600



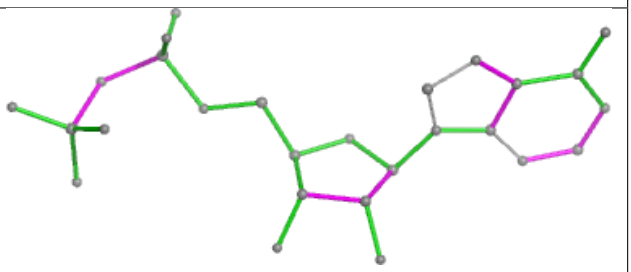
Ligand ADP A 1600



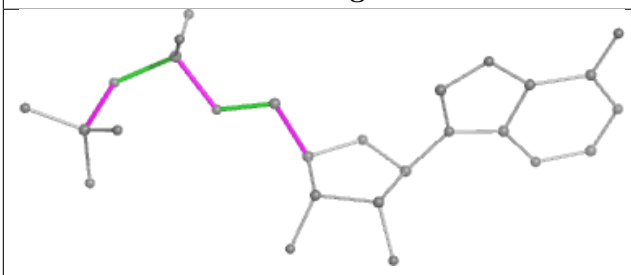
Ligand ADP B 1600



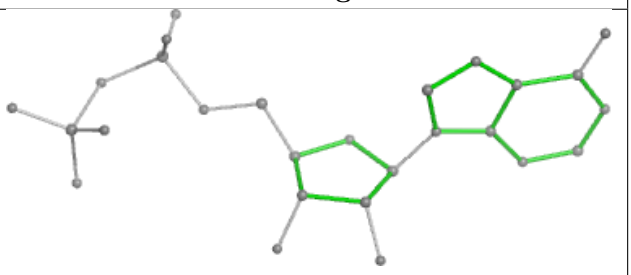
Bond lengths



Bond angles

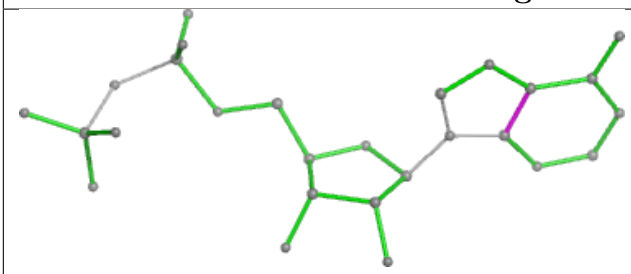


Torsions

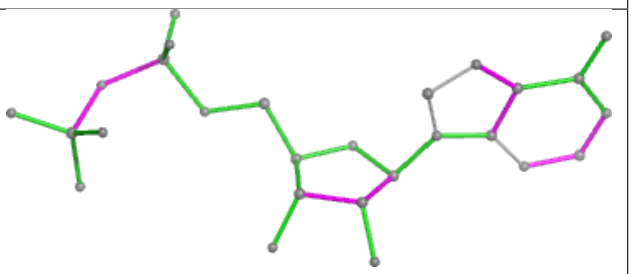


Rings

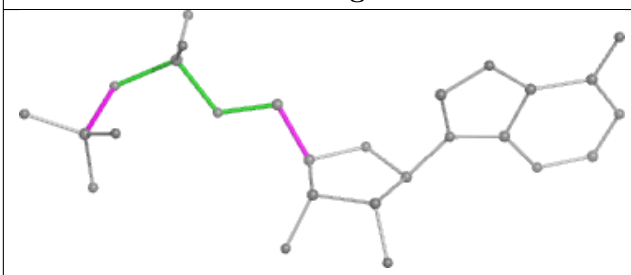
Ligand ADP E 1600



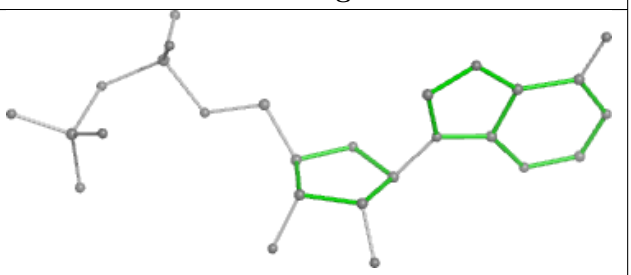
Bond lengths



Bond angles

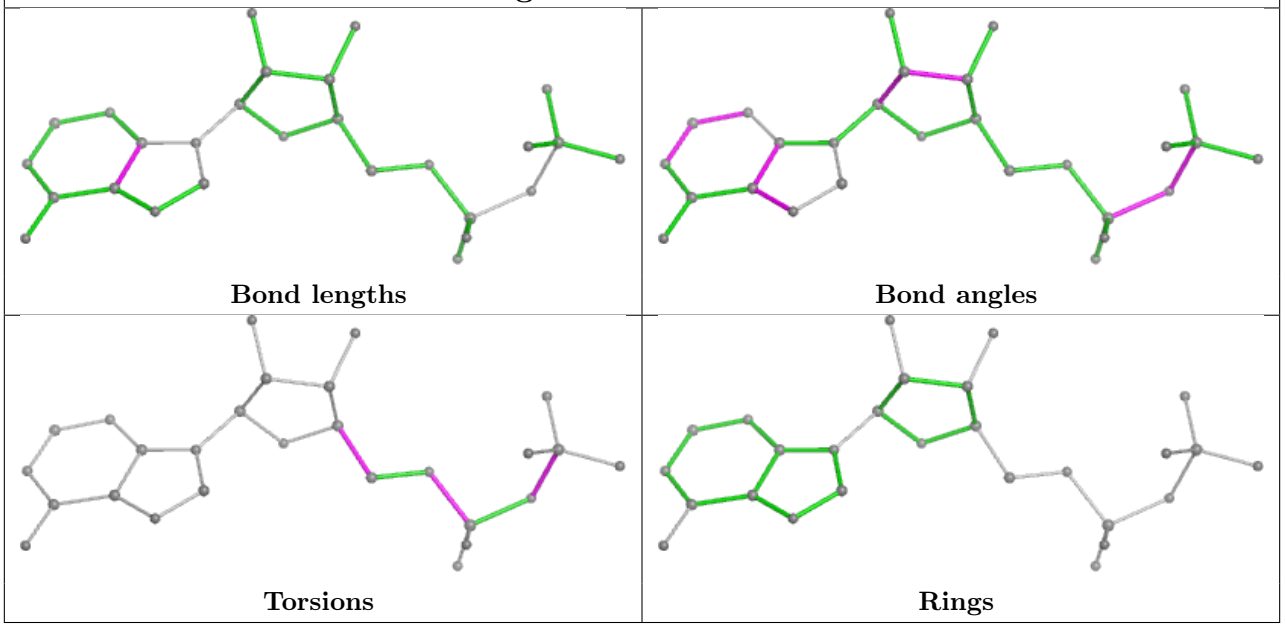


Torsions

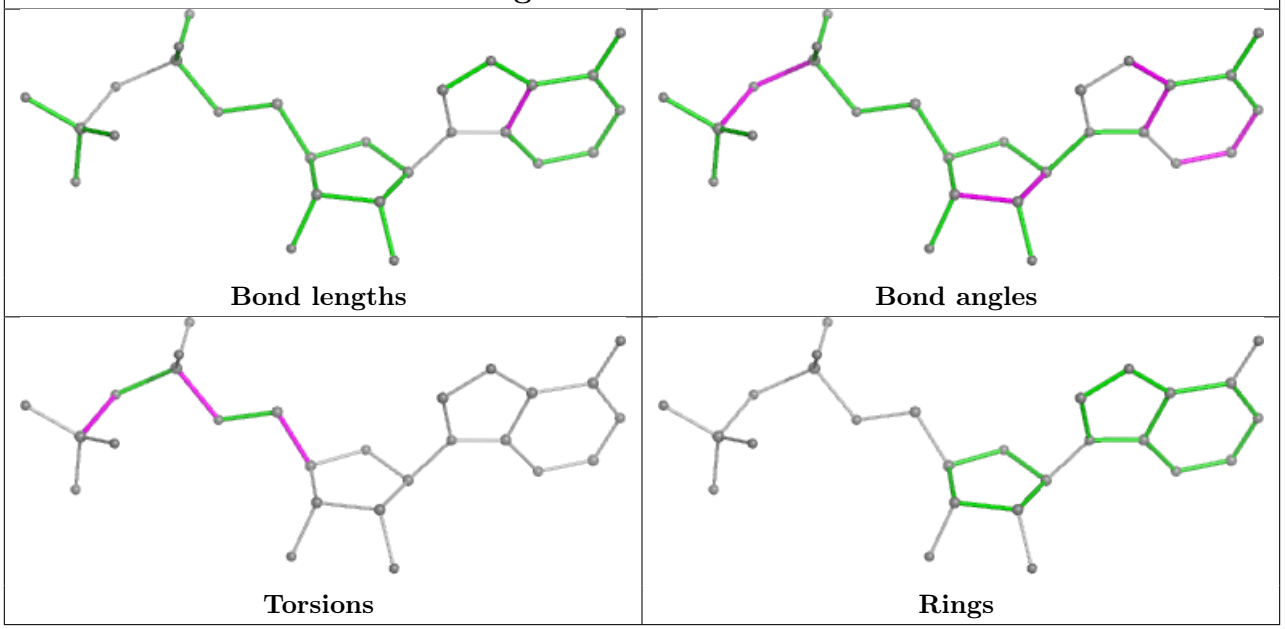


Rings

Ligand ADP F 1600



Ligand ADP C 1600



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.

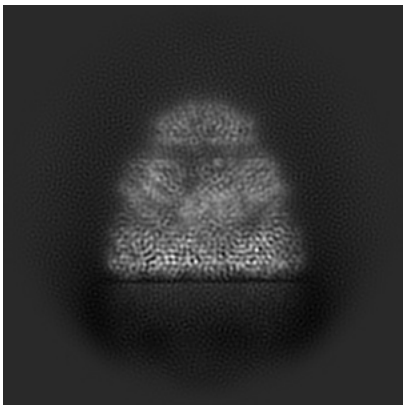
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17421. These allow visual inspection of the internal detail of the map and identification of artifacts.

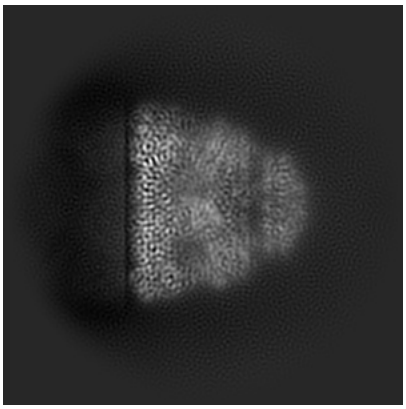
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

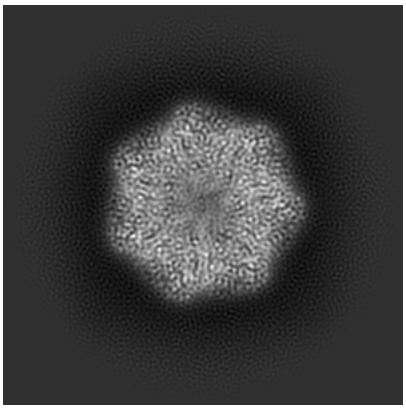
6.1.1 Primary map



X

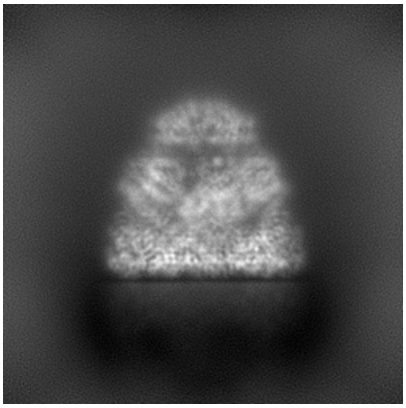


Y

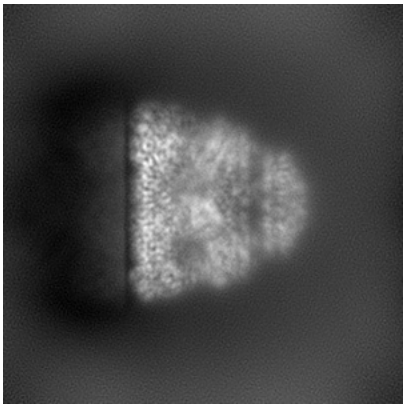


Z

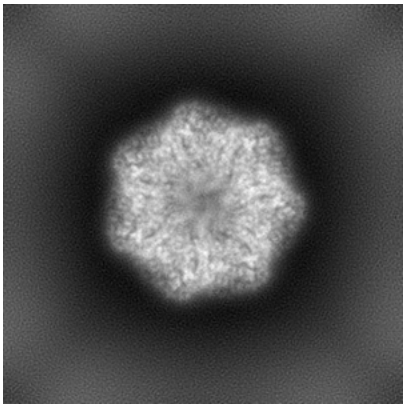
6.1.2 Raw map



X



Y

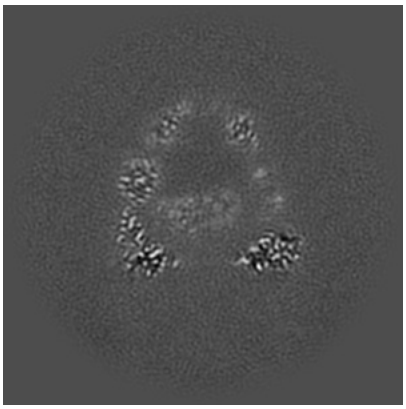


Z

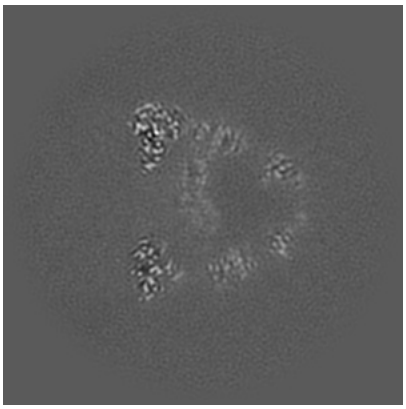
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

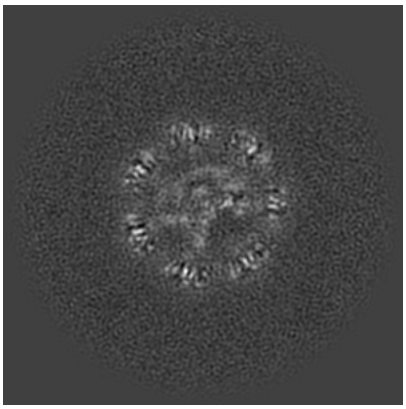
6.2.1 Primary map



X Index: 128

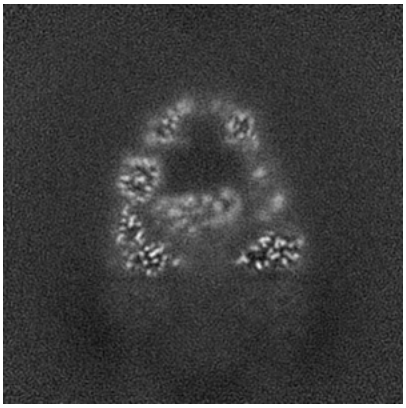


Y Index: 128

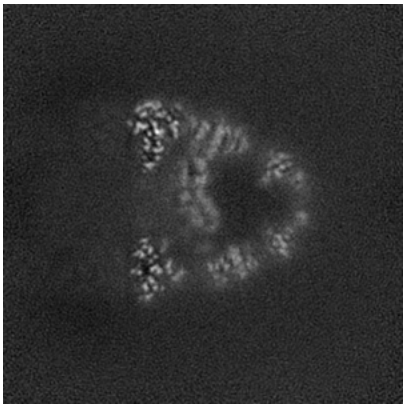


Z Index: 128

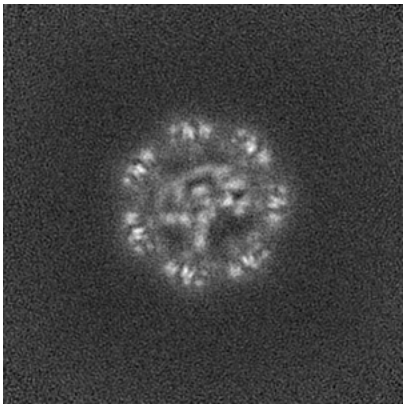
6.2.2 Raw map



X Index: 128



Y Index: 128

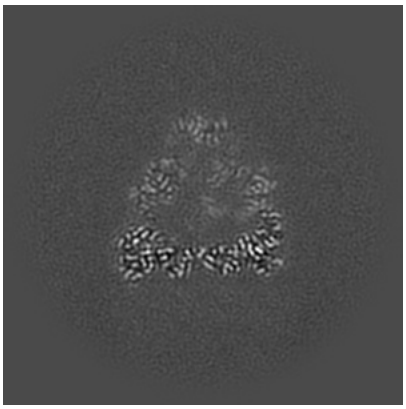


Z Index: 128

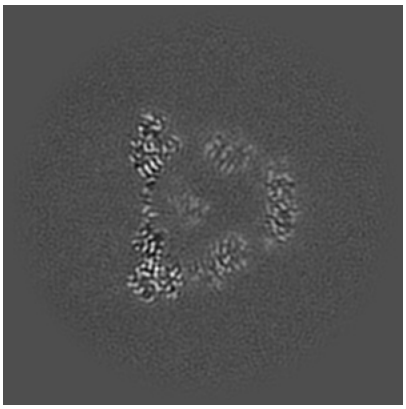
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

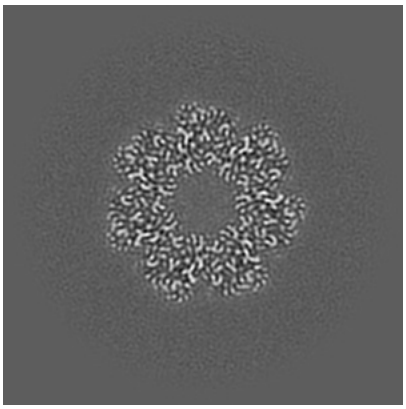
6.3.1 Primary map



X Index: 157

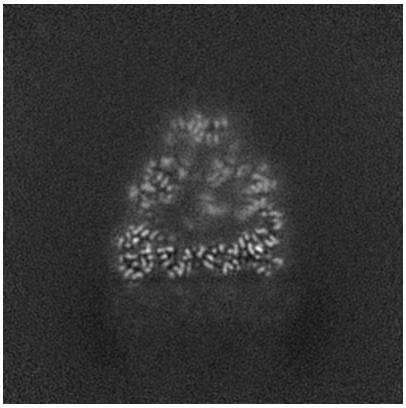


Y Index: 108

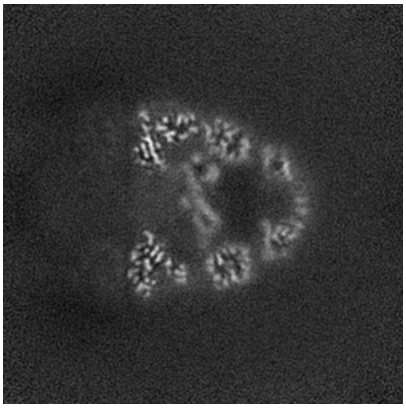


Z Index: 94

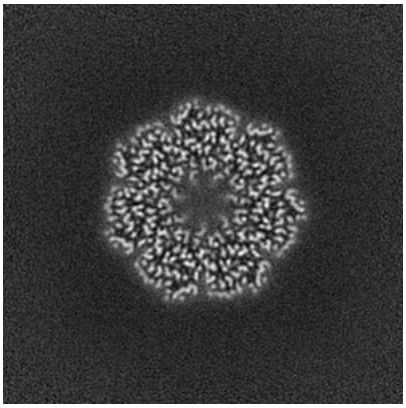
6.3.2 Raw map



X Index: 157



Y Index: 135

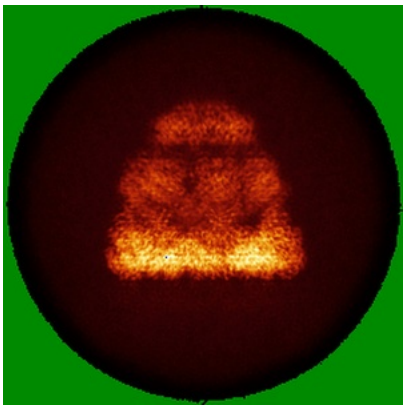


Z Index: 91

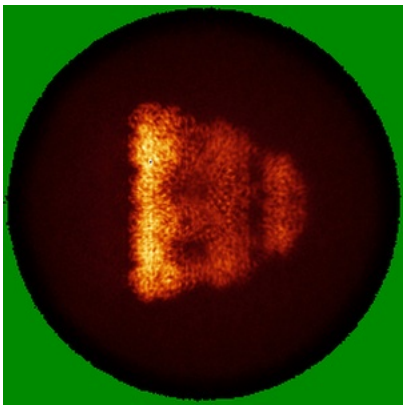
The images above show the largest variance slices of the map in three orthogonal directions.

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

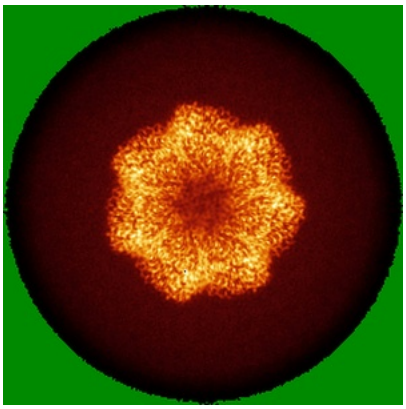
6.4.1 Primary map



X

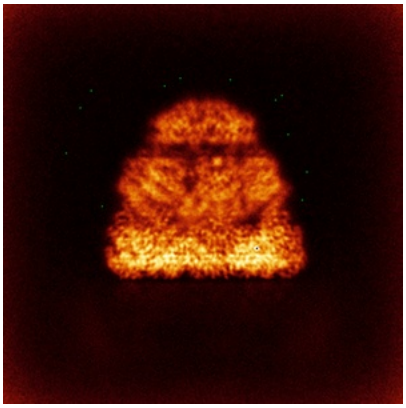


Y

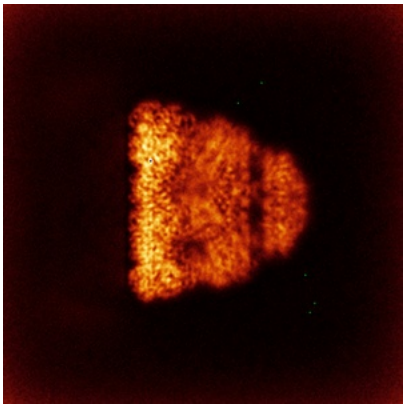


Z

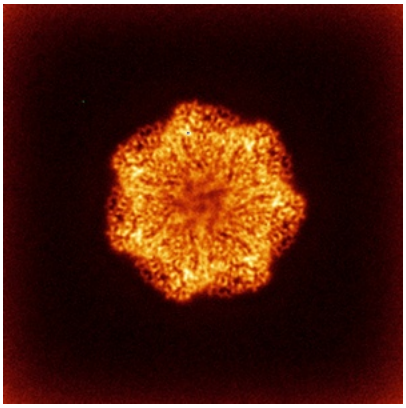
6.4.2 Raw map



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 0.671. 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.

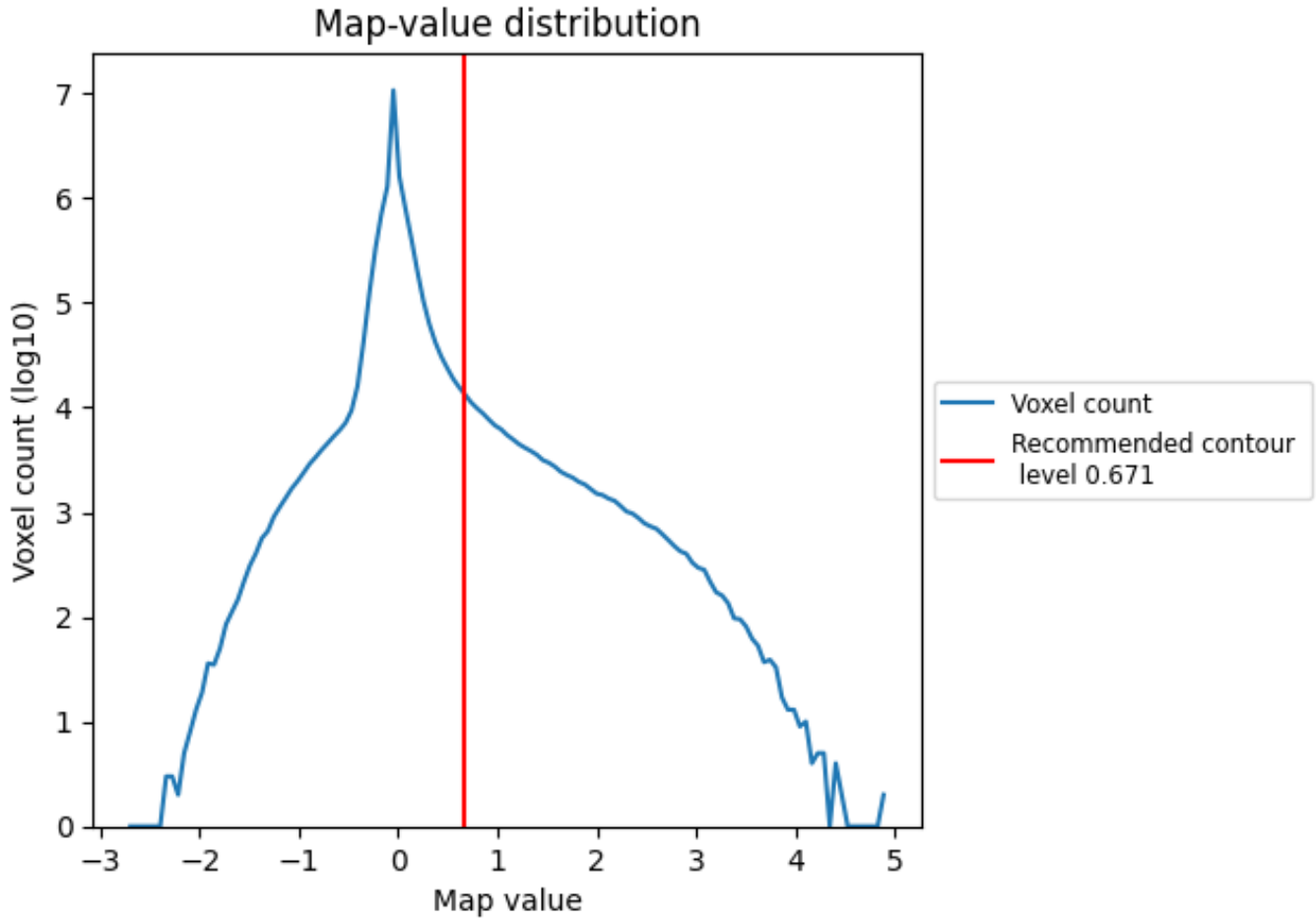
6.6 Mask visualisation (i)

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

7 Map analysis

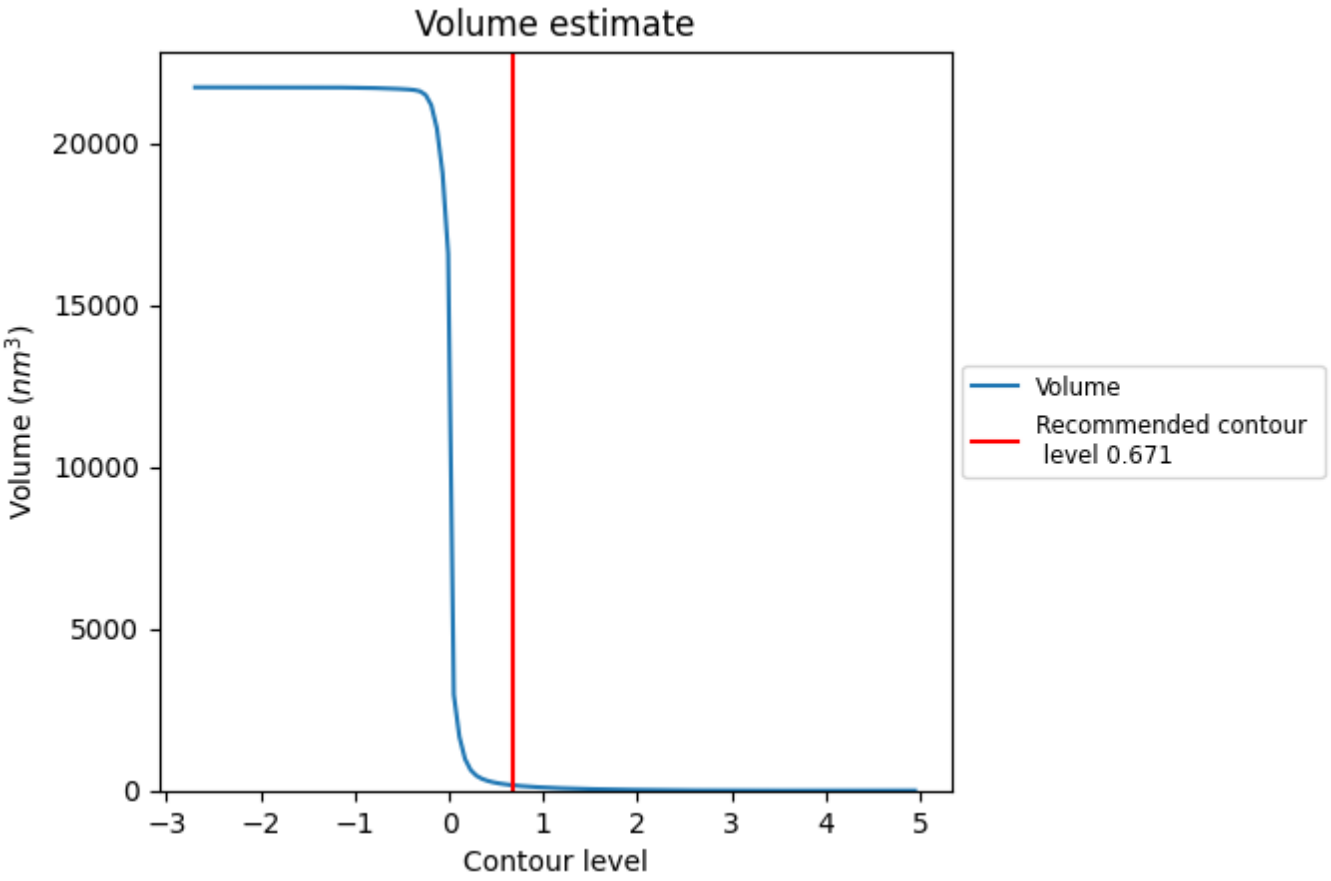
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

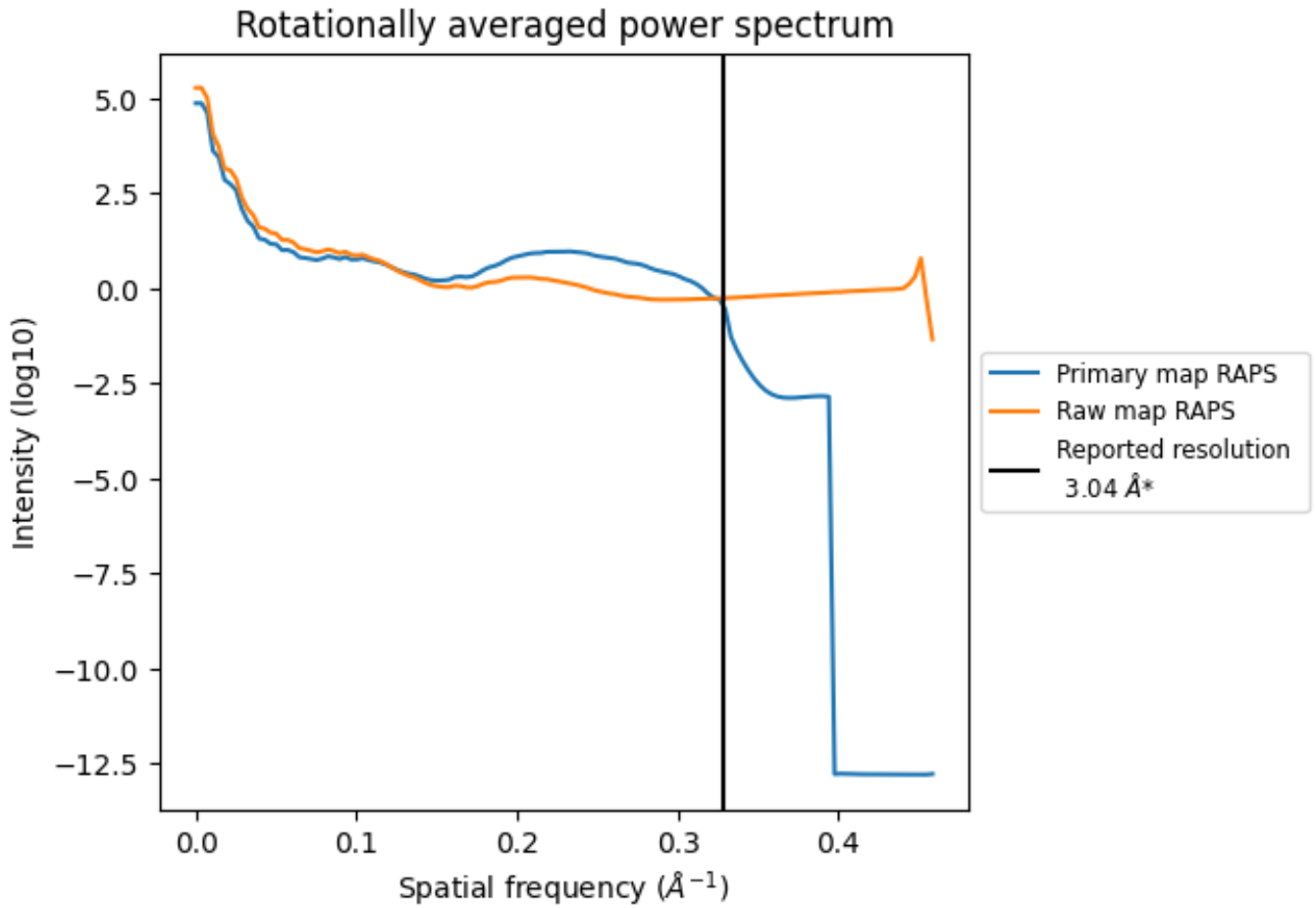
7.2 Volume estimate



The volume at the recommended contour level is 167 nm^3; this corresponds to an approximate mass of 151 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)

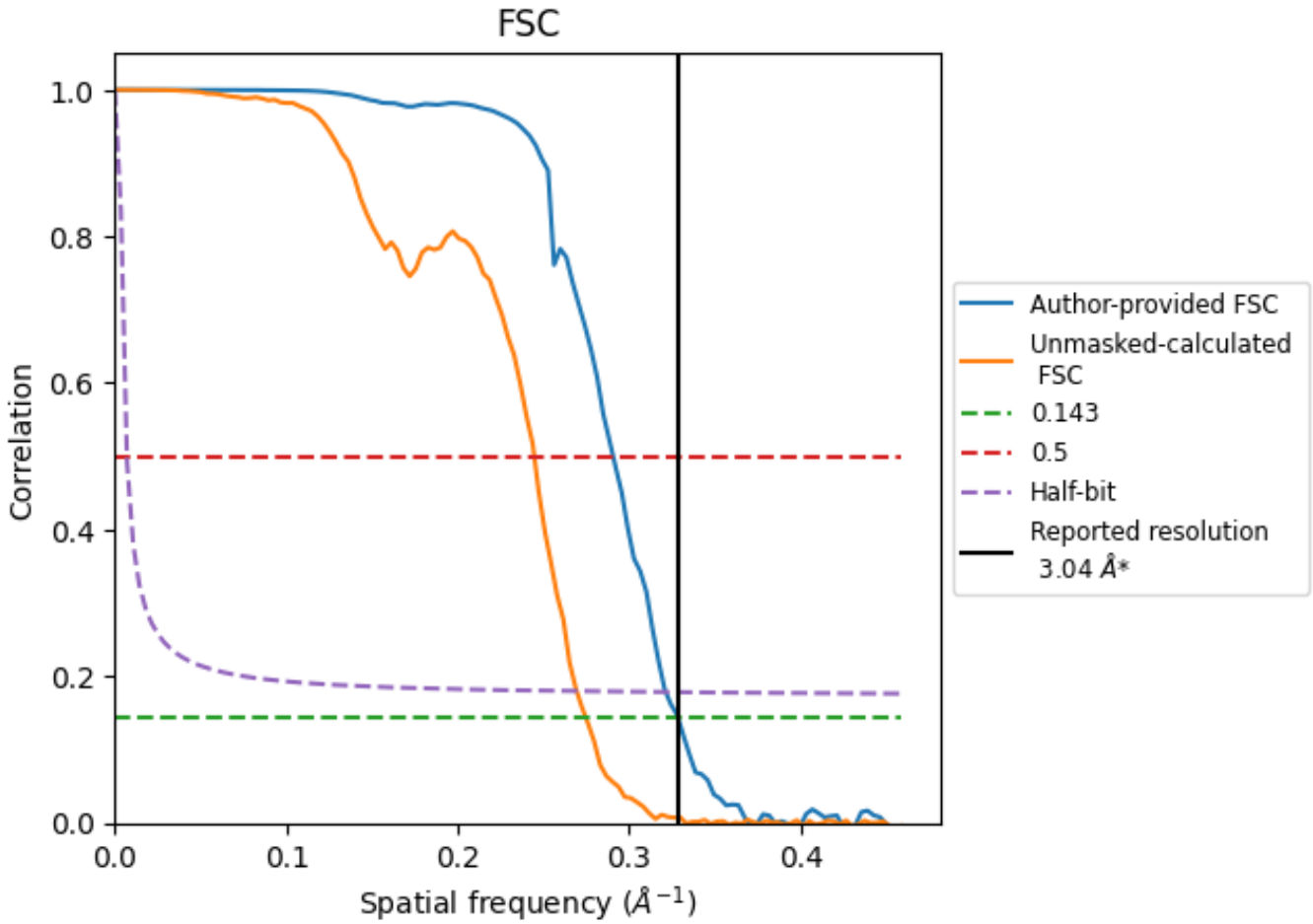


*Reported resolution corresponds to spatial frequency of 0.329 $Å^{-1}$

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 0.329 Å^{-1}

8.2 Resolution estimates (i)

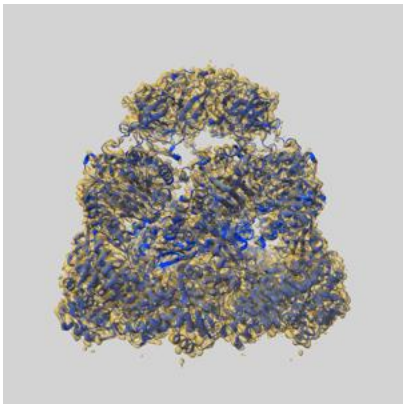
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.44	3.11
Unmasked-calculated*	3.64	4.09	3.71

*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 3.64 differs from the reported value 3.04 by more than 10 %

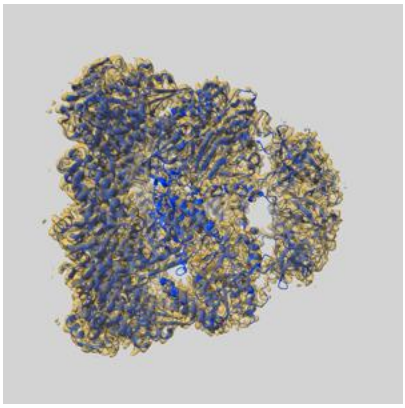
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17421 and PDB model 8P4O. Per-residue inclusion information can be found in section 3 on page 8.

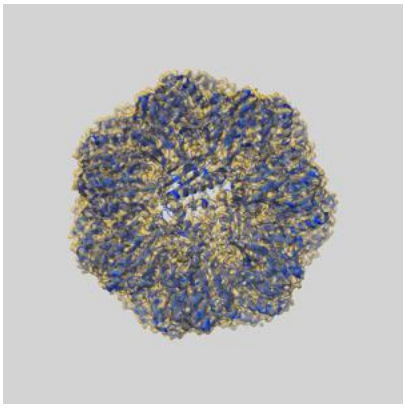
9.1 Map-model overlay



X



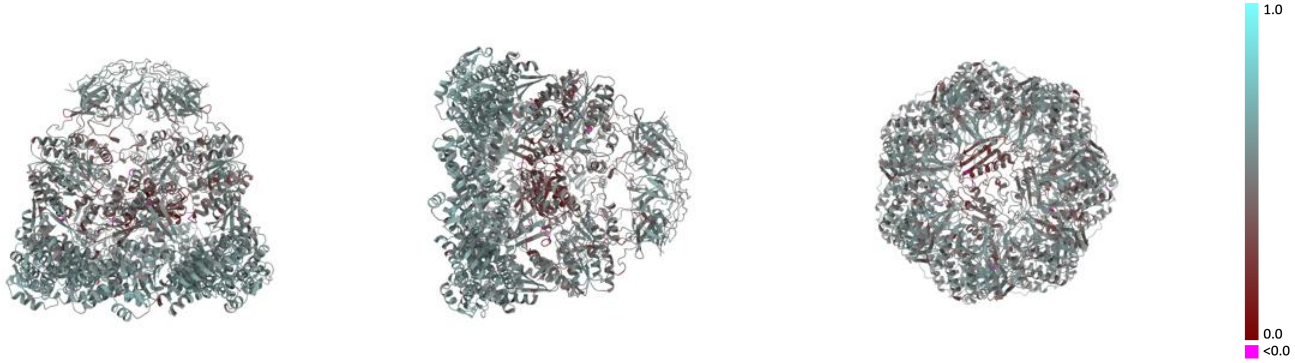
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.671 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.

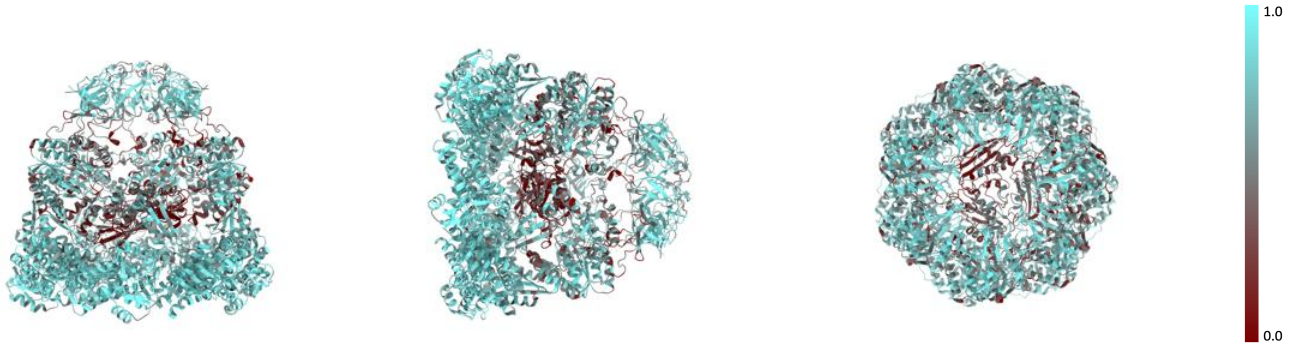
9.2 Q-score mapped to coordinate model (i)



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.

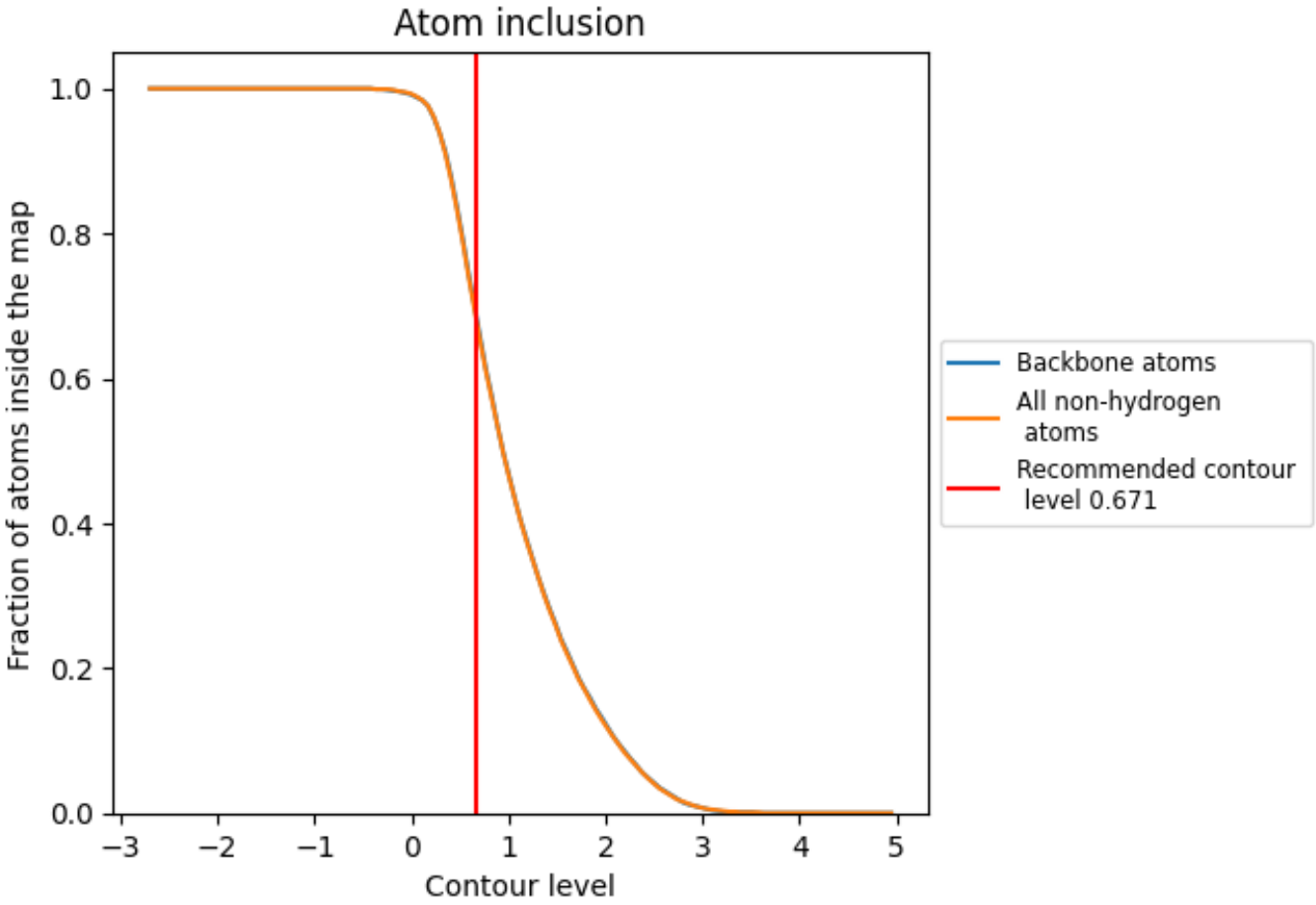
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.671).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.671) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6790	0.5030
1	0.2340	0.3270
A	0.7320	0.5170
B	0.7330	0.5230
C	0.7170	0.5140
D	0.7160	0.5150
E	0.7540	0.5310
F	0.7550	0.5290
G	0.7490	0.5280
O	0.6450	0.4930
P	0.6480	0.5040
Q	0.6480	0.4920
R	0.6370	0.5000
S	0.6510	0.5030
T	0.6680	0.5000
U	0.6480	0.4900