Full wwPDB EM Validation Report (i)

Mar 8, 2026 – 05:42 PM UTC

PDB ID	:	9M3Z / pdb_00009m3z
EMDB ID	:	EMD-63612
Title	:	Arabidopsis thaliana CDC48A-NPL4-UFD1B (AtCNU) complex
Authors	:	Huntington, B.; Arold, S.T.
Deposited on	:	2025-03-03
Resolution	:	3.90 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 (i) 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 (i)) were used in the production of this report:

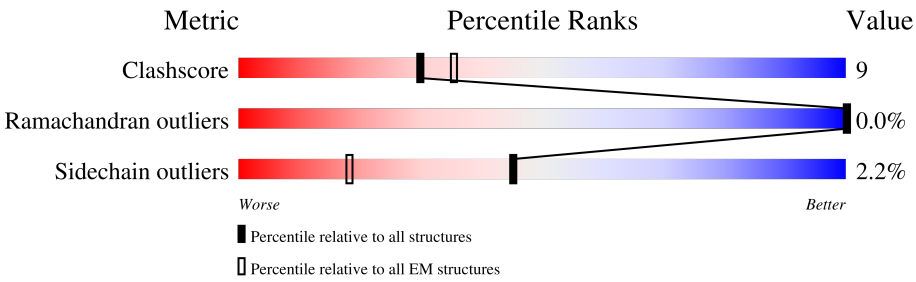
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

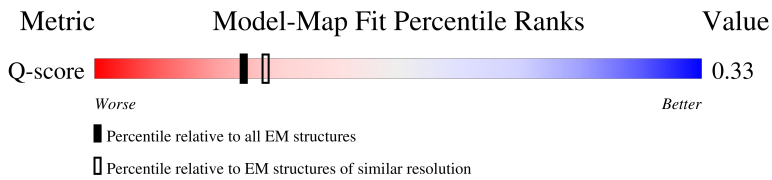
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	814	6% 74% 19% • 7%
1	B	814	• 72% 20% • 7%
1	C	814	7% 69% 24% • 7%
1	D	814	11% 71% 21% • 7%

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Mol	Chain	Length	Quality of chain
1	E	814	17% 72% 21% 7%
1	F	814	13% 72% 22% 7%
2	G	418	69% 76% 22%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39218 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 Cell division control protein 48 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	761	5938	3719	1044	1146	29	0	0
1	B	761	5938	3719	1044	1146	29	0	0
1	C	761	5938	3719	1044	1146	29	0	0
1	D	761	5938	3719	1044	1146	29	0	0
1	E	761	5938	3719	1044	1146	29	0	0
1	F	761	5938	3719	1044	1146	29	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P54609
A	-3	PRO	-	expression tag	UNP P54609
A	-2	LEU	-	expression tag	UNP P54609
A	-1	GLY	-	expression tag	UNP P54609
A	0	SER	-	expression tag	UNP P54609
B	-4	GLY	-	expression tag	UNP P54609
B	-3	PRO	-	expression tag	UNP P54609
B	-2	LEU	-	expression tag	UNP P54609
B	-1	GLY	-	expression tag	UNP P54609
B	0	SER	-	expression tag	UNP P54609
C	-4	GLY	-	expression tag	UNP P54609
C	-3	PRO	-	expression tag	UNP P54609
C	-2	LEU	-	expression tag	UNP P54609
C	-1	GLY	-	expression tag	UNP P54609
C	0	SER	-	expression tag	UNP P54609
D	-4	GLY	-	expression tag	UNP P54609
D	-3	PRO	-	expression tag	UNP P54609
D	-2	LEU	-	expression tag	UNP P54609

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P54609
D	0	SER	-	expression tag	UNP P54609
E	-4	GLY	-	expression tag	UNP P54609
E	-3	PRO	-	expression tag	UNP P54609
E	-2	LEU	-	expression tag	UNP P54609
E	-1	GLY	-	expression tag	UNP P54609
E	0	SER	-	expression tag	UNP P54609
F	-4	GLY	-	expression tag	UNP P54609
F	-3	PRO	-	expression tag	UNP P54609
F	-2	LEU	-	expression tag	UNP P54609
F	-1	GLY	-	expression tag	UNP P54609
F	0	SER	-	expression tag	UNP P54609

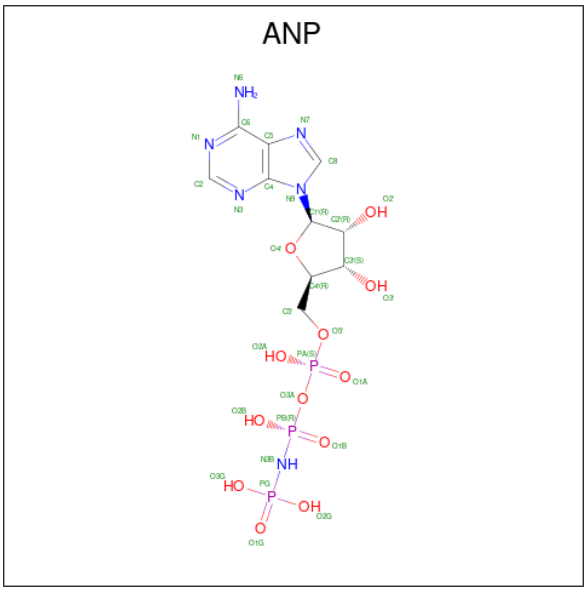
- Molecule 2 is a protein called NPL4-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	413	3236	2039	553	623	21	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	GLY	-	expression tag	UNP O82264
G	-3	PRO	-	expression tag	UNP O82264
G	-2	LEU	-	expression tag	UNP O82264
G	-1	GLY	-	expression tag	UNP O82264
G	0	SER	-	expression tag	UNP O82264

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

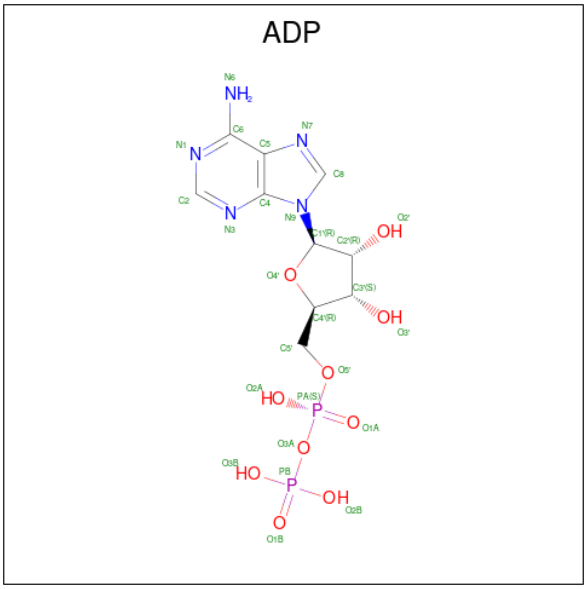


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	F	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



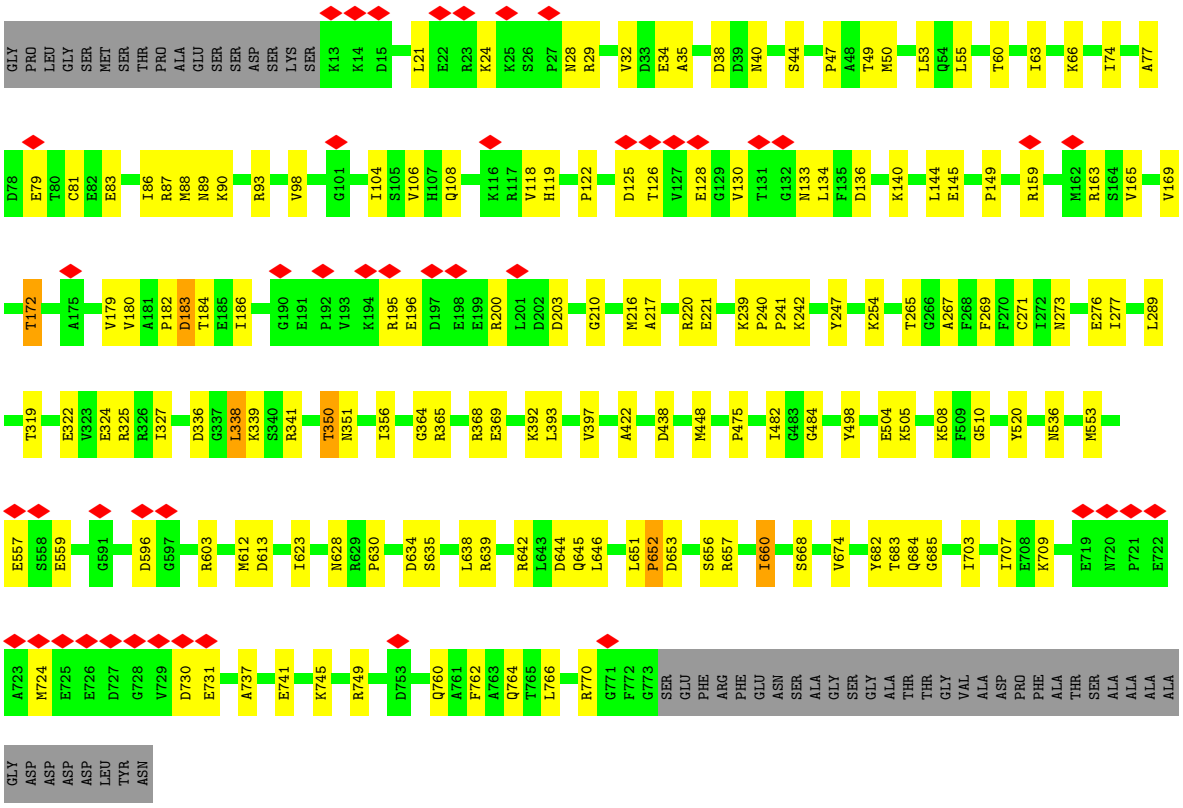
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

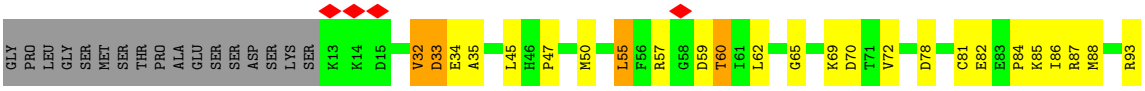
• Molecule 1: Cell division control protein 48 homolog A

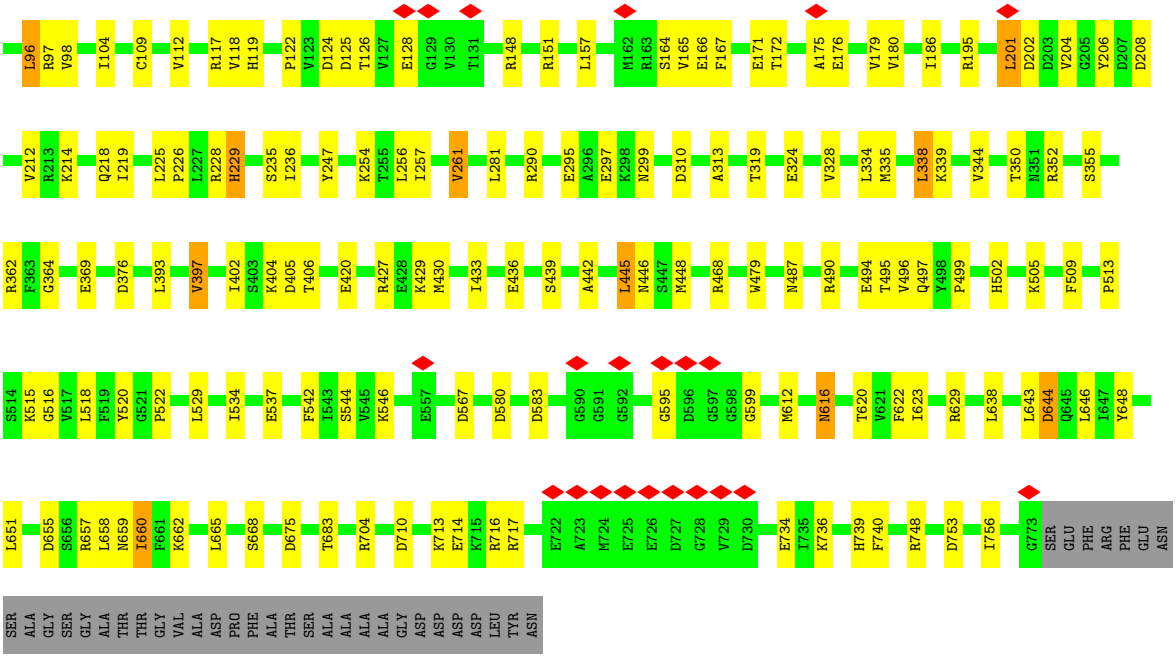
Chain A:



• Molecule 1: Cell division control protein 48 homolog A

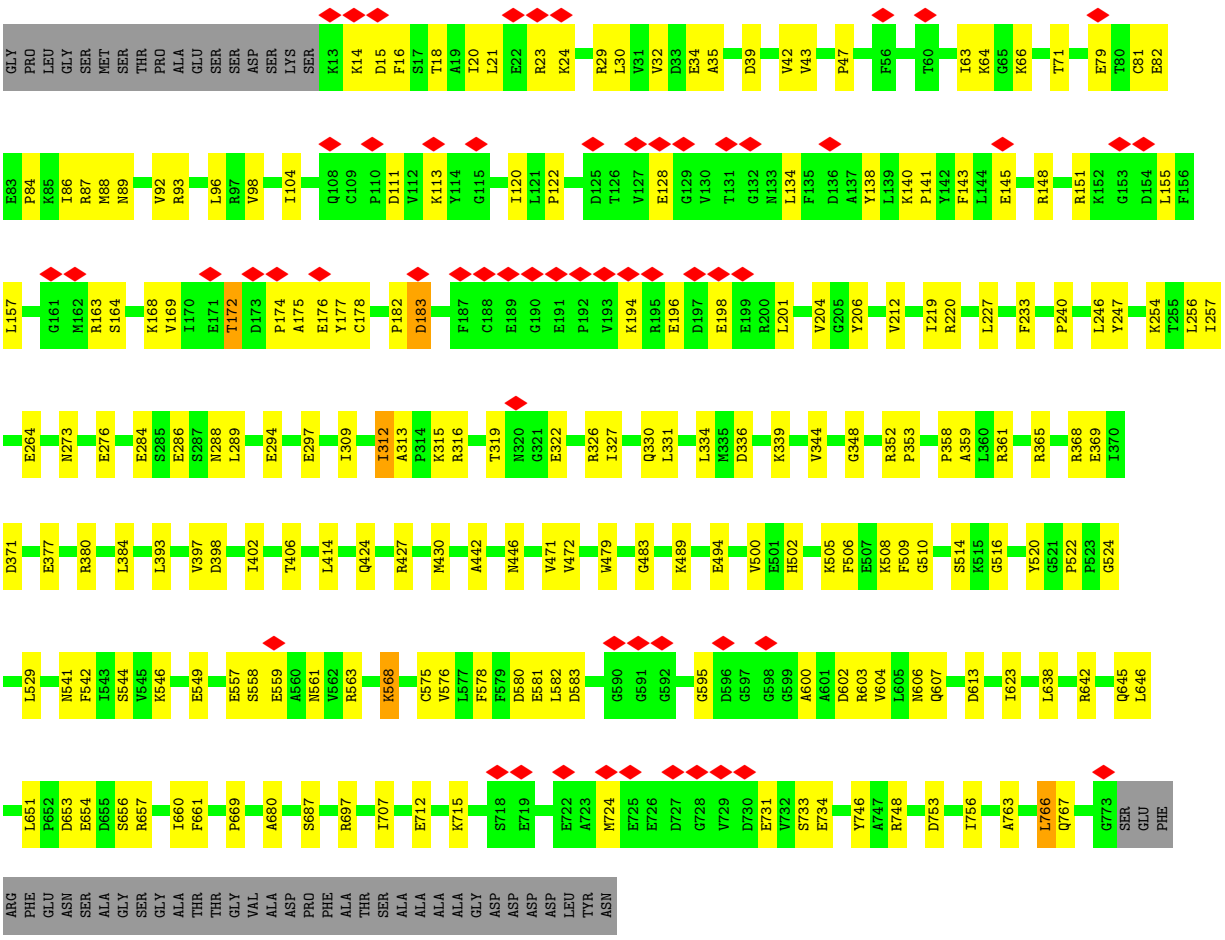
Chain B:





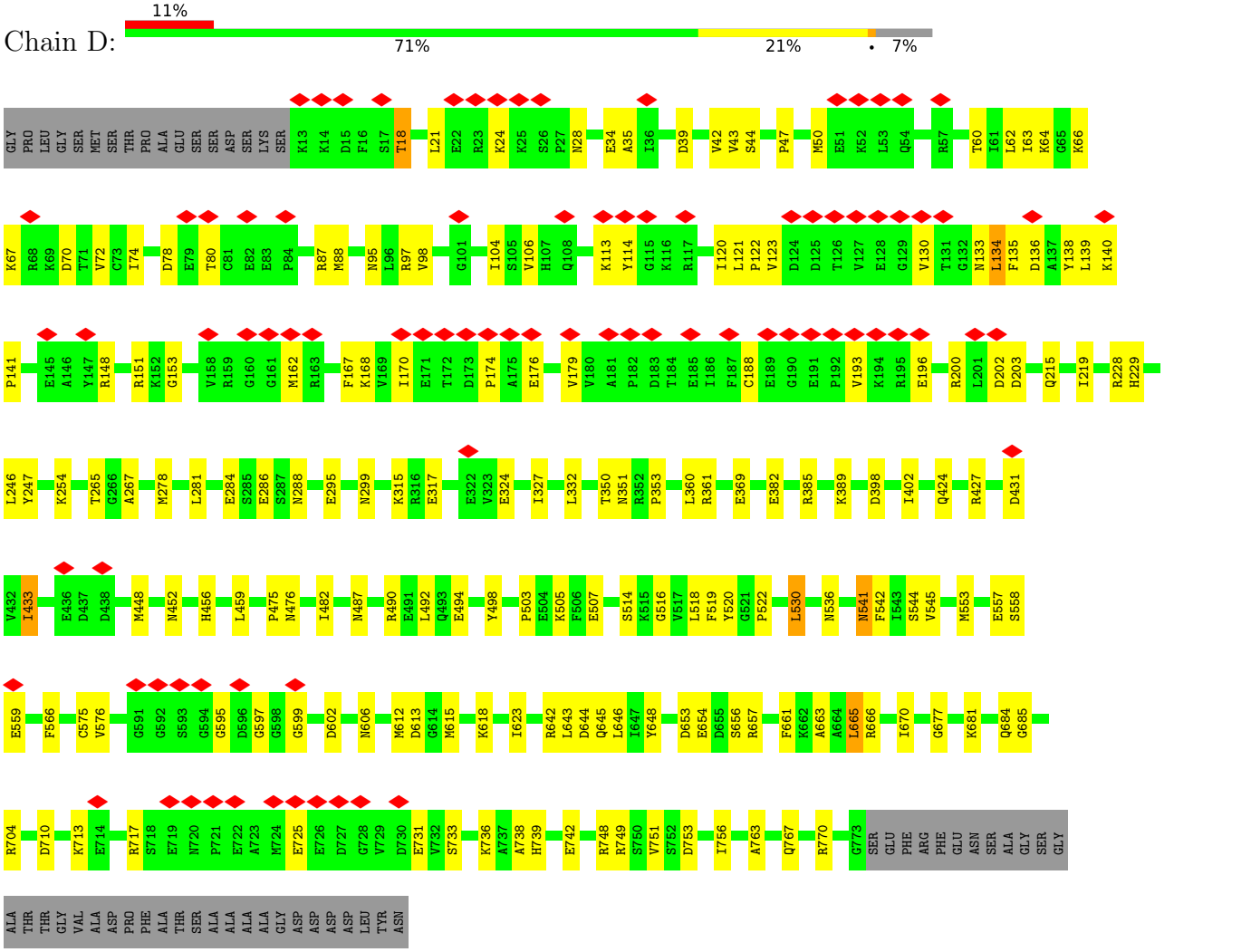
- Molecule 1: Cell division control protein 48 homolog A

Chain C:



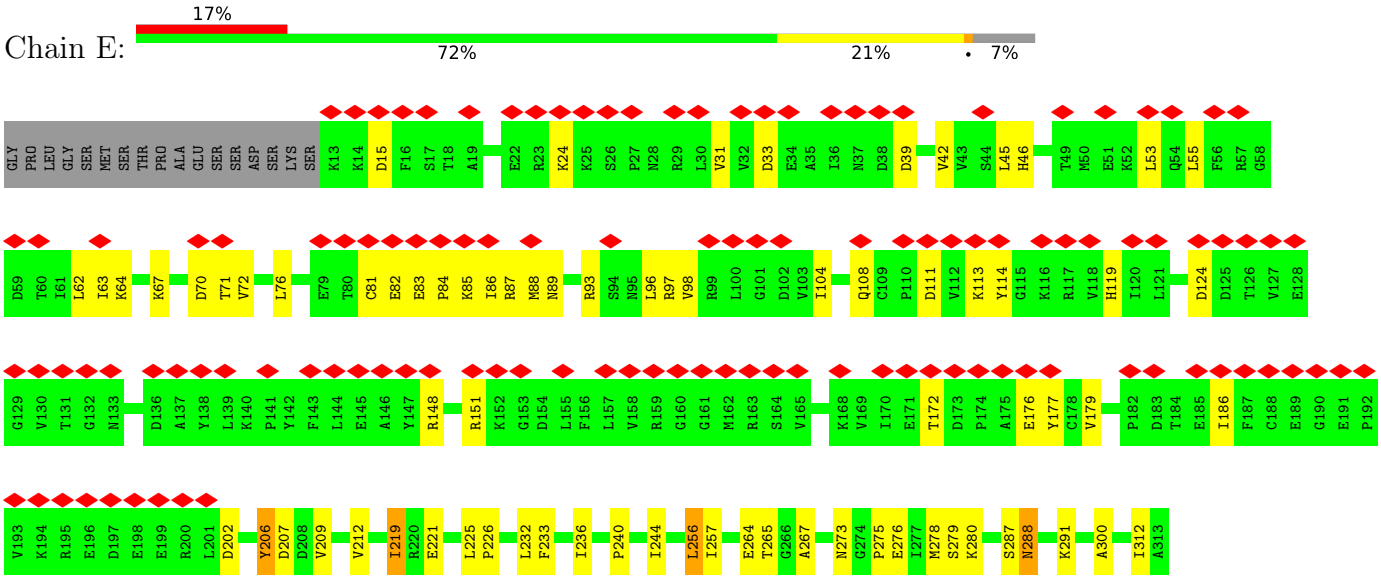
• Molecule 1: Cell division control protein 48 homolog A

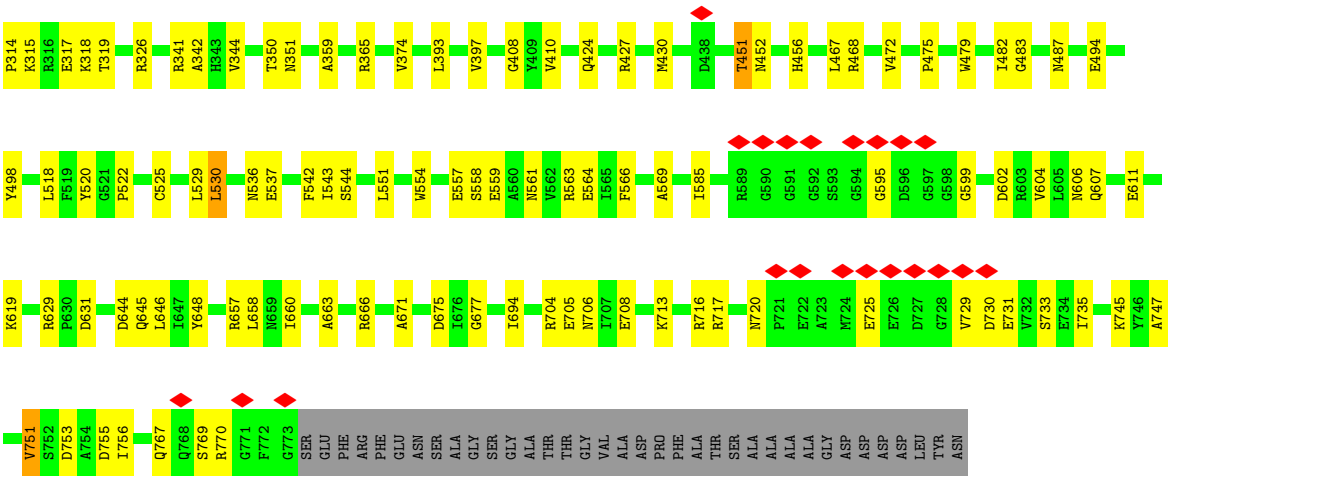
Chain D:



• Molecule 1: Cell division control protein 48 homolog A

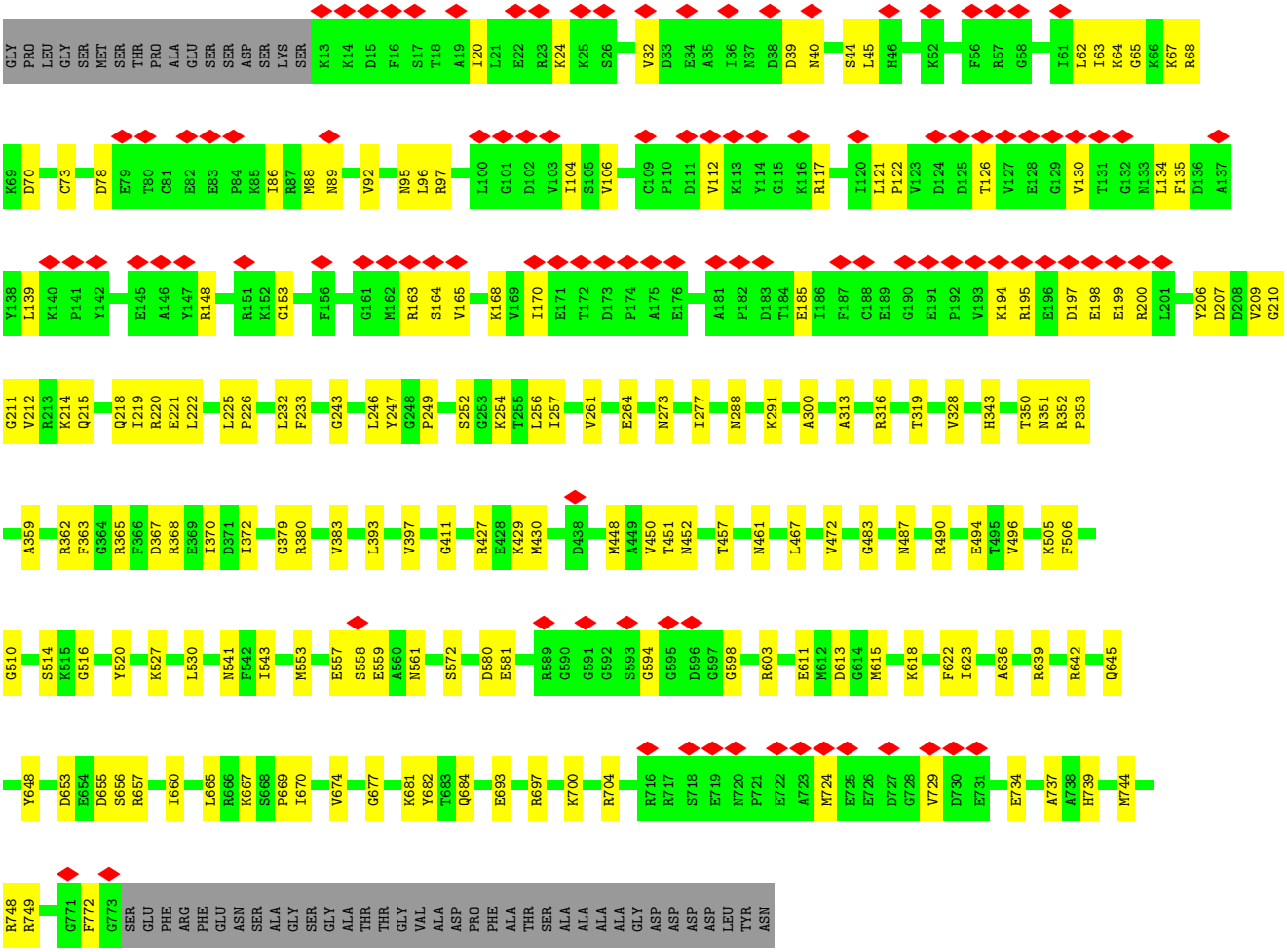
Chain E:





• Molecule 1: Cell division control protein 48 homolog A

Chain F:



• Molecule 2: NPL4-like protein 2

Chain G:

GLY PRO LEU GLY SER M1 M2 M3 L4 R5 I6 R9 D10 G11 L12 E13 R14 V15 T16 A17 E18 H21 I22 T23 V24 S25 Q26 L27 I31 A32 D33 Q34 L35 Q36 I37 H40 K41 Q42 T43 L44 S45 L50 L51 L52 A53 K54 T55 P56 A57 D58 L59 F62 T63 D64

L65 T66 D67 P68 N69 L70 P71 L72 S73 S74 L75 N76 L77 G78 L83 D88 G89 E90 R91 S92 I93 P94 G95 A96 P97 P98 V99 T100 P101 A102 G103 T110 I115 A116 R117 R120 V121 T122 R123 Q124 E125 T126 S127 H128 C129 D130 S131 V132 S133 F134 D135 R136 D137 A138 A139

N140 A141 F142 Q143 H144 Y145 V146 N147 E148 S149 L150 A151 F152 A153 V154 K155 R156 G157 G158 F159 M160 Y161 G162 T163 V164 T165 E166 E167 G168 Q169 V170 E171 V172 D173 F174 P178 G182 T183 E184 A185 N186 L187 I188 L189 M190 R191 D192 A193 D194 E195 E196 K197 R198 V199 D200 A201 I202 A203

M204 G205 L206 G207 M208 R209 R210 V211 G212 F213 I214 F215 N216 Q217 T218 V219 V220 Q221 D222 K223 T224 E225 Y226 T227 L228 S229 N230 A231 E232 V233 L234 Q235 A236 A237 E238 L239 H240 A241 E242 S243 E244 L245 K246 E247 W248 A251 V252 V253 K254 L255 E256 V257 N258 E259 D260 G261 G262 A263 D264

V265 H266 F267 E268 A269 F270 Q271 M272 S273 D274 I277 E282 E283 W284 F285 E286 T287 E288 I289 M290 P291 D292 D293 D294 P295 K296 L297 S298 K299 M300 K301 K302 E303 V304 V305 V306 G307 V308 K309 D310 L311 K312 E313 V314 D315 N316 D317 F318 F319 L320 V321 L322 V323 R324 I325 L326 D327 H328

Q329 G330 P331 L332 S333 S334 T335 F336 P337 I338 E339 N340 R341 S342 S343 R344 A345 T346 M347 R348 A349 L350 K351 T352 H353 L354 D355 R356 A357 K358 S359 L360 P361 L362 V363 K364 K365 M366 S367 D368 F369 H370 L371 L372 L373 F374 V375 A376 Q377 F378 L379 D380 V381 S382 S383 D384 V385 P386 A387 L388

A389 E390 C391 V392 R393 L394 Q395 S396 P397 V398 P399 E400 G401 Y402 A403 L404 L405 I406 E407 S408 M409 A410 N411 T412 C413

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	199000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	422.39877, 422.39877, 422.39877	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.17333, 1.17333, 1.17333	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.12	0/6034	0.29	0/8137
1	B	0.12	0/6034	0.29	0/8137
1	C	0.12	0/6034	0.28	0/8137
1	D	0.12	0/6034	0.27	0/8137
1	E	0.10	0/6034	0.25	0/8137
1	F	0.11	0/6034	0.27	0/8137
2	G	0.09	0/3293	0.26	0/4456
All	All	0.11	0/39497	0.28	0/53278

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 (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	5938	0	5961	103	0
1	B	5938	0	5961	117	0
1	C	5938	0	5961	135	0
1	D	5938	0	5961	114	0
1	E	5938	0	5960	116	0
1	F	5938	0	5960	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3236	0	3232	61	0
3	A	31	0	13	4	0
3	B	31	0	13	2	0
3	C	31	0	13	1	0
3	D	31	0	13	1	0
3	E	31	0	13	0	0
3	F	31	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	27	0	12	1	0
5	B	27	0	12	1	0
5	C	27	0	12	2	0
5	D	27	0	12	1	0
5	E	27	0	12	3	0
5	F	27	0	12	3	0
All	All	39218	0	39146	709	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (709) 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)
1:F:352:ARG:HD3	1:F:353:PRO:HD2	1.56	0.86
1:C:516:GLY:HA2	1:C:623:ILE:O	1.78	0.83
2:G:206:LEU:HB3	2:G:208:MET:HE3	1.68	0.76
1:A:484:GLY:HA3	1:A:656:SER:HB3	1.65	0.76
1:F:665:LEU:HB3	1:F:670:ILE:HD11	1.68	0.75
1:C:35:ALA:HA	1:C:87:ARG:HB3	1.68	0.75
1:D:122:PRO:HG3	1:D:134:LEU:HD13	1.69	0.74
1:E:557:GLU:HB3	1:E:561:ASN:HB2	1.70	0.74
1:B:82:GLU:H	1:B:85:LYS:HE2	1.52	0.73
1:C:113:LYS:HD2	1:C:174:PRO:HG2	1.71	0.72
1:C:309:ILE:HD11	1:C:348:GLY:HA3	1.70	0.72
1:B:82:GLU:HG2	1:B:84:PRO:HD2	1.70	0.71
1:B:50:MET:HG3	1:B:55:LEU:HB3	1.73	0.71
1:C:483:GLY:H	5:C:903:ADP:HN62	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:MET:O	1:F:24:LYS:NZ	2.23	0.70
1:C:669:PRO:HB2	1:C:734:GLU:HG2	1.73	0.69
1:B:704:ARG:HH21	1:C:494:GLU:HB3	1.58	0.69
1:D:153:GLY:HA2	1:D:168:LYS:HE2	1.75	0.69
2:G:134:PHE:HA	2:G:172:VAL:HB	1.74	0.69
1:B:118:VAL:HG23	1:B:172:THR:HG22	1.74	0.68
2:G:245:LEU:HG	2:G:247:GLU:H	1.58	0.68
1:A:653:ASP:N	1:A:656:SER:OG	2.27	0.68
1:D:516:GLY:HA2	1:D:623:ILE:O	1.94	0.68
1:B:57:ARG:O	2:G:5:ARG:NH1	2.23	0.67
1:B:98:VAL:HG11	1:B:104:ILE:HD11	1.77	0.67
1:A:265:THR:HG23	1:A:267:ALA:H	1.58	0.67
2:G:293:ASP:HB3	2:G:299:LYS:HE3	1.76	0.66
1:D:44:SER:HB2	1:D:87:ARG:HB2	1.77	0.66
1:E:424:GLN:OE1	1:E:427:ARG:NH1	2.28	0.66
2:G:226:TYR:HD2	2:G:296:LYS:HD3	1.61	0.66
1:D:487:ASN:OD1	1:D:490:ARG:NH2	2.28	0.66
1:A:133:ASN:ND2	1:A:136:ASP:OD2	2.29	0.65
1:A:498:TYR:OH	1:F:704:ARG:NH1	2.30	0.65
1:C:284:GLU:O	1:C:288:ASN:ND2	2.29	0.65
1:D:595:GLY:HA3	1:E:595:GLY:H	1.60	0.65
1:A:559:GLU:HB2	1:A:603:ARG:HH21	1.62	0.65
1:B:97:ARG:HH22	1:B:201:LEU:HG	1.62	0.65
1:C:505:LYS:O	1:C:508:LYS:HB3	1.96	0.65
1:B:612:MET:O	1:B:616:ASN:ND2	2.27	0.64
1:A:66:LYS:HG2	1:A:98:VAL:HG12	1.80	0.64
1:B:228:ARG:O	1:B:229:HIS:ND1	2.31	0.64
5:E:903:ADP:O2B	1:F:639:ARG:NH1	2.30	0.64
1:A:145:GLU:HG2	1:A:182:PRO:HG3	1.79	0.64
1:C:43:VAL:HG21	1:C:63:ILE:HD11	1.80	0.64
1:C:359:ALA:O	1:C:365:ARG:NH1	2.30	0.64
1:C:514:SER:OG	1:C:645:GLN:NE2	2.30	0.64
1:D:113:LYS:HD2	1:D:174:PRO:HG2	1.80	0.64
1:D:281:LEU:HA	1:E:326:ARG:HH21	1.63	0.64
1:D:612:MET:HE1	1:D:643:LEU:HG	1.80	0.64
1:C:284:GLU:HG3	1:C:288:ASN:HD21	1.63	0.64
1:A:136:ASP:HA	1:A:140:LYS:HG3	1.78	0.64
1:E:731:GLU:HG2	1:E:733:SER:H	1.63	0.64
1:B:502:HIS:HB3	1:B:505:LYS:HD3	1.80	0.63
1:E:602:ASP:O	1:E:606:ASN:ND2	2.30	0.63
1:A:53:LEU:O	1:A:108:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:HG2	1:C:98:VAL:HG12	1.81	0.63
1:C:502:HIS:HB3	1:C:505:LYS:HD3	1.81	0.63
1:E:86:ILE:HG21	1:E:104:ILE:HD11	1.80	0.63
1:D:553:MET:HE3	1:D:557:GLU:HB2	1.81	0.63
1:D:767:GLN:O	1:D:770:ARG:NH1	2.32	0.63
1:E:265:THR:HG23	1:E:267:ALA:H	1.64	0.63
1:F:214:LYS:NZ	1:F:218:GLN:OE1	2.32	0.63
1:D:685:GLY:HA3	1:D:749:ARG:HH21	1.63	0.62
1:D:736:LYS:HG3	1:D:738:ALA:H	1.64	0.62
1:F:557:GLU:HB3	1:F:561:ASN:HD21	1.64	0.62
1:A:639:ARG:NH1	5:F:903:ADP:O3B	2.33	0.62
1:B:117:ARG:HH12	1:B:186:ILE:HD13	1.64	0.62
1:C:169:VAL:HG11	1:C:172:THR:HG23	1.81	0.62
1:C:424:GLN:OE1	1:C:427:ARG:NH2	2.33	0.62
1:F:153:GLY:HA2	1:F:168:LYS:HE2	1.81	0.62
1:D:284:GLU:HG3	1:D:288:ASN:HD21	1.65	0.62
1:A:216:MET:HE3	1:A:220:ARG:HE	1.65	0.62
1:C:559:GLU:OE2	1:C:603:ARG:NH1	2.33	0.62
1:F:126:THR:HB	1:F:165:VAL:HA	1.82	0.61
2:G:173:ASP:HB3	2:G:332:LEU:HD12	1.82	0.61
1:E:694:ILE:HD11	1:E:747:ALA:HB2	1.80	0.61
1:B:93:ARG:HG3	1:B:98:VAL:HG23	1.82	0.61
1:B:515:LYS:HD3	1:B:620:THR:HA	1.81	0.61
1:A:200:ARG:NH1	1:A:203:ASP:OD2	2.34	0.61
1:E:278:MET:HG2	1:E:312:ILE:HG22	1.82	0.61
1:B:125:ASP:OD2	1:B:195:ARG:NH1	2.33	0.61
1:A:47:PRO:HG3	1:A:77:ALA:HB1	1.81	0.61
1:D:254:LYS:NZ	3:D:901:ANP:O3G	2.28	0.61
1:A:50:MET:HG3	1:A:55:LEU:HB3	1.83	0.61
1:A:90:LYS:HE2	1:A:93:ARG:HH21	1.66	0.61
1:D:748:ARG:HD3	1:E:769:SER:HB2	1.83	0.61
2:G:189:LEU:HB2	2:G:191:ARG:HH21	1.66	0.61
1:A:35:ALA:HA	1:A:87:ARG:HB3	1.82	0.60
1:A:741:GLU:OE2	1:A:745:LYS:NZ	2.32	0.60
1:B:529:LEU:HD11	5:B:903:ADP:H2'	1.82	0.60
1:A:24:LYS:NZ	1:F:430:MET:O	2.32	0.60
1:E:767:GLN:O	1:E:770:ARG:NH1	2.35	0.60
1:F:40:ASN:OD1	1:F:148:ARG:NH1	2.35	0.60
1:D:424:GLN:OE1	1:D:427:ARG:NH2	2.35	0.60
1:F:615:MET:HG2	1:F:618:LYS:HE2	1.83	0.59
1:B:644:ASP:N	1:B:644:ASP:OD1	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:GLU:O	1:D:299:ASN:ND2	2.35	0.59
2:G:123:ARG:NH1	2:G:317:ASP:O	2.34	0.59
3:A:901:ANP:HNB1	1:B:362:ARG:HD2	1.67	0.59
1:F:39:ASP:O	1:F:89:ASN:ND2	2.36	0.59
1:A:438:ASP:HA	1:B:229:HIS:HE1	1.66	0.59
1:E:287:SER:OG	1:E:291:LYS:NZ	2.35	0.59
1:D:284:GLU:O	1:D:288:ASN:ND2	2.36	0.59
1:A:707:ILE:HB	1:B:505:LYS:HZ1	1.67	0.59
1:C:86:ILE:HG21	1:C:104:ILE:HD11	1.84	0.59
1:E:212:VAL:HG21	1:E:257:ILE:HD11	1.85	0.59
2:G:25:SER:HB3	2:G:68:PRO:HB2	1.85	0.59
1:A:86:ILE:HG21	1:A:104:ILE:HD11	1.84	0.59
1:A:128:GLU:HB3	1:A:163:ARG:HG2	1.84	0.59
1:E:63:ILE:HD13	1:E:88:MET:HE1	1.85	0.59
1:E:751:VAL:HG23	1:E:755:ASP:HB2	1.85	0.59
1:B:658:LEU:HG	1:B:662:LYS:HZ2	1.67	0.58
1:E:219:ILE:HD11	1:E:244:ILE:HG21	1.85	0.58
1:A:122:PRO:HG3	1:A:134:LEU:HD13	1.84	0.58
1:C:442:ALA:O	1:C:446:ASN:ND2	2.33	0.58
2:G:228:LEU:O	2:G:316:ASN:ND2	2.36	0.58
1:A:760:GLN:NE2	1:A:764:GLN:OE1	2.37	0.58
1:C:613:ASP:OD1	1:C:642:ARG:NE	2.36	0.58
1:A:40:ASN:OD1	1:A:89:ASN:ND2	2.36	0.58
1:A:336:ASP:OD1	1:A:365:ARG:NH1	2.34	0.58
1:C:128:GLU:O	1:C:163:ARG:NH1	2.35	0.58
1:C:559:GLU:O	1:C:607:GLN:NE2	2.36	0.58
1:D:42:VAL:HG22	1:D:74:ILE:HB	1.84	0.58
2:G:217:GLN:NE2	2:G:227:THR:O	2.35	0.58
1:C:557:GLU:HB2	1:C:561:ASN:HB2	1.86	0.58
1:B:256:LEU:HD22	3:B:901:ANP:H2'	1.83	0.58
1:F:247:TYR:HB3	1:F:350:THR:HG23	1.86	0.58
1:C:151:ARG:NH1	1:C:176:GLU:O	2.37	0.58
1:D:95:ASN:O	1:D:97:ARG:NH1	2.36	0.58
1:D:385:ARG:O	1:D:389:LYS:NZ	2.33	0.58
1:A:510:GLY:HA3	1:F:667:LYS:HD2	1.86	0.58
1:B:546:LYS:HG2	1:B:580:ASP:HB3	1.85	0.57
1:C:157:LEU:HD11	1:C:164:SER:HB3	1.85	0.57
1:B:659:ASN:HA	1:B:662:LYS:HZ3	1.68	0.57
1:D:704:ARG:HH11	1:E:494:GLU:HB3	1.66	0.57
1:B:88:MET:O	1:B:93:ARG:NH1	2.32	0.57
1:C:86:ILE:HG23	1:C:88:MET:HE1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASP:OD2	1:A:642:ARG:NH1	2.38	0.57
1:C:212:VAL:HG21	1:C:257:ILE:HD11	1.87	0.57
1:C:247:TYR:CZ	1:C:371:ASP:HB3	2.40	0.57
1:D:704:ARG:HD2	1:E:498:TYR:HE2	1.68	0.57
1:E:559:GLU:OE1	1:E:607:GLN:NE2	2.38	0.57
1:A:88:MET:O	1:A:93:ARG:NH1	2.37	0.57
1:D:613:ASP:OD2	1:D:642:ARG:NH2	2.36	0.57
1:E:563:ARG:NE	1:E:611:GLU:OE2	2.38	0.57
1:C:336:ASP:OD2	1:C:365:ARG:NH2	2.35	0.56
1:E:314:PRO:HG2	1:E:319:THR:HB	1.87	0.56
1:A:118:VAL:HG13	1:A:172:THR:HA	1.86	0.56
1:A:520:TYR:HE2	1:A:646:LEU:HB3	1.71	0.56
1:B:310:ASP:OD2	1:B:352:ARG:NH2	2.39	0.56
1:F:64:LYS:HG2	1:F:70:ASP:HB3	1.87	0.56
2:G:27:LEU:HB2	2:G:72:LEU:HD11	1.87	0.56
1:A:44:SER:HB2	1:A:87:ARG:HB2	1.87	0.56
1:D:88:MET:HE1	1:D:104:ILE:HD11	1.87	0.56
1:D:575:CYS:SG	1:D:576:VAL:N	2.78	0.56
1:C:580:ASP:OD1	1:C:581:GLU:N	2.37	0.56
1:D:748:ARG:HE	1:E:767:GLN:HA	1.70	0.56
1:F:527:LYS:NZ	5:F:903:ADP:O1B	2.37	0.56
1:F:541:ASN:ND2	1:F:572:SER:O	2.39	0.56
1:C:194:LYS:NZ	1:C:196:GLU:OE1	2.37	0.56
1:D:64:LYS:HD2	1:D:70:ASP:HB3	1.86	0.56
1:A:144:LEU:HG	1:A:145:GLU:HG3	1.88	0.56
1:D:278:MET:HE1	1:D:327:ILE:HG21	1.88	0.56
1:A:764:GLN:HE21	1:A:770:ARG:HD3	1.70	0.56
1:C:254:LYS:NZ	3:C:901:ANP:O3G	2.24	0.56
1:B:59:ASP:OD2	2:G:14:ARG:NH2	2.39	0.55
1:C:34:GLU:OE1	1:C:93:ARG:NH1	2.37	0.55
1:C:522:PRO:HG2	1:C:651:LEU:HG	1.87	0.55
1:D:653:ASP:N	1:D:656:SER:OG	2.39	0.55
1:C:377:GLU:OE2	1:C:380:ARG:NH2	2.39	0.55
1:D:265:THR:HG23	1:D:267:ALA:H	1.71	0.55
1:C:273:ASN:HB3	1:C:276:GLU:HB3	1.88	0.55
1:D:130:VAL:HG21	1:D:134:LEU:HD21	1.89	0.55
1:B:32:VAL:HA	1:B:86:ILE:HG22	1.89	0.55
1:D:475:PRO:O	1:D:536:ASN:ND2	2.33	0.55
1:A:210:GLY:H	3:A:901:ANP:HN62	1.54	0.55
1:A:393:LEU:HD12	1:A:397:VAL:HG11	1.87	0.55
1:F:195:ARG:NH1	1:F:198:GLU:OE2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:GLY:HA3	1:E:467:LEU:HD23	1.88	0.55
1:A:247:TYR:HB3	1:A:350:THR:HG23	1.88	0.55
1:A:508:LYS:O	1:F:667:LYS:NZ	2.40	0.55
2:G:9:ARG:HG3	2:G:51:LEU:HD12	1.89	0.55
2:G:221:GLN:O	2:G:224:THR:OG1	2.23	0.55
1:A:221:GLU:OE1	1:F:427:ARG:NE	2.40	0.54
1:C:21:LEU:HD23	1:C:220:ARG:HD2	1.89	0.54
1:E:359:ALA:O	1:E:365:ARG:NH1	2.39	0.54
1:B:33:ASP:OD1	1:B:33:ASP:N	2.38	0.54
1:D:70:ASP:N	1:D:70:ASP:OD1	2.39	0.54
1:D:684:GLN:O	1:D:749:ARG:NH2	2.40	0.54
1:A:668:SER:OG	1:B:509:PHE:O	2.25	0.54
1:B:429:LYS:NZ	1:B:448:MET:SD	2.77	0.54
1:C:654:GLU:HG3	1:C:657:ARG:HH22	1.72	0.54
1:D:602:ASP:O	1:D:606:ASN:ND2	2.41	0.54
1:E:716:ARG:HH12	1:E:720:ASN:HB3	1.73	0.54
1:C:430:MET:O	1:D:24:LYS:NZ	2.34	0.54
1:B:65:GLY:HA3	1:B:96:LEU:HD12	1.90	0.54
1:B:126:THR:HB	1:B:165:VAL:HA	1.90	0.54
1:D:663:ALA:O	1:D:666:ARG:NE	2.40	0.54
1:B:214:LYS:NZ	1:B:218:GLN:OE1	2.41	0.54
1:E:93:ARG:HD3	1:E:98:VAL:HG23	1.89	0.54
2:G:24:VAL:HB	2:G:68:PRO:HA	1.89	0.54
2:G:31:ILE:HG23	2:G:35:LEU:HD12	1.89	0.54
1:D:492:LEU:HD11	1:D:519:PHE:HZ	1.72	0.54
1:D:597:GLY:HA3	1:E:599:GLY:HA3	1.89	0.54
1:D:612:MET:HE2	1:D:642:ARG:HA	1.90	0.54
1:B:542:PHE:HE1	1:B:544:SER:HB2	1.73	0.53
1:B:59:ASP:OD1	2:G:5:ARG:NH1	2.35	0.53
1:B:295:GLU:OE2	1:B:299:ASN:ND2	2.41	0.53
1:C:638:LEU:HD12	1:C:646:LEU:HD11	1.89	0.53
1:E:468:ARG:NH2	1:F:611:GLU:OE2	2.41	0.53
1:F:20:ILE:HG12	1:F:220:ARG:HH12	1.73	0.53
1:F:135:PHE:HA	1:F:139:LEU:HB2	1.91	0.53
1:F:514:SER:HB3	1:F:645:GLN:HE21	1.73	0.53
1:F:121:LEU:HD12	1:F:170:ILE:HG13	1.90	0.53
1:F:693:GLU:OE2	1:F:697:ARG:NH2	2.42	0.53
1:C:712:GLU:HA	1:C:715:LYS:HE2	1.91	0.53
1:A:74:ILE:HG13	1:A:149:PRO:HG3	1.91	0.53
2:G:3:MET:HE3	2:G:14:ARG:HB3	1.90	0.53
1:B:427:ARG:HD3	1:C:20:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:MET:HE2	1:C:20:ILE:HG23	1.91	0.52
1:C:529:LEU:HD11	5:C:903:ADP:H2'	1.91	0.52
1:A:596:ASP:HB2	1:B:599:GLY:HA3	1.91	0.52
1:B:393:LEU:HD22	1:B:397:VAL:HG11	1.91	0.52
1:D:63:ILE:HG12	1:D:106:VAL:HG12	1.91	0.52
1:D:18:THR:HG22	1:D:21:LEU:HB2	1.91	0.52
1:F:288:ASN:HA	1:F:291:LYS:HE3	1.91	0.52
1:A:242:LYS:HD3	1:A:338:LEU:HD11	1.92	0.52
1:D:34:GLU:O	1:D:87:ARG:NH1	2.38	0.52
1:D:494:GLU:HA	1:D:498:TYR:CD1	2.45	0.52
1:B:638:LEU:HD22	1:B:646:LEU:HD21	1.91	0.52
1:C:393:LEU:HD21	1:C:397:VAL:HG21	1.91	0.52
2:G:115:ILE:HG12	2:G:120:ARG:HH21	1.75	0.52
1:A:657:ARG:HA	1:A:660:ILE:HG22	1.90	0.52
1:A:350:THR:OG1	1:A:351:ASN:N	2.42	0.52
2:G:225:GLU:H	2:G:296:LYS:HE3	1.75	0.52
1:E:518:LEU:HD22	1:E:646:LEU:HD22	1.92	0.52
2:G:3:MET:SD	2:G:16:THR:OG1	2.64	0.52
1:A:47:PRO:HG2	1:A:79:GLU:HG3	1.91	0.51
1:B:45:LEU:HD11	1:B:86:ILE:HG13	1.93	0.51
1:B:516:GLY:HA2	1:B:623:ILE:O	2.09	0.51
1:C:219:ILE:HD11	1:C:246:LEU:HD21	1.92	0.51
1:A:81:CYS:HB2	1:A:87:ARG:HE	1.76	0.51
1:C:731:GLU:HG2	1:C:733:SER:H	1.74	0.51
1:E:595:GLY:HA3	1:F:594:GLY:HA2	1.93	0.51
2:G:45:SER:HB3	2:G:50:LEU:HD22	1.91	0.51
1:B:713:LYS:HG3	1:B:716:ARG:HH21	1.75	0.51
1:C:657:ARG:HA	1:C:660:ILE:HG22	1.92	0.51
1:E:472:VAL:HG22	1:E:543:ILE:HG12	1.93	0.51
1:F:39:ASP:OD1	1:F:148:ARG:NH1	2.33	0.51
1:C:151:ARG:HG2	1:C:177:TYR:HB3	1.92	0.51
1:F:451:THR:OG1	1:F:452:ASN:N	2.38	0.51
1:F:506:PHE:O	1:F:510:GLY:N	2.42	0.51
1:C:24:LYS:O	1:C:29:ARG:NH1	2.44	0.51
1:A:651:LEU:O	1:A:657:ARG:NH2	2.43	0.51
1:B:520:TYR:CZ	1:B:648:TYR:HB2	2.46	0.51
1:C:183:ASP:OD1	1:C:183:ASP:N	2.42	0.51
1:E:53:LEU:O	1:E:108:GLN:NE2	2.44	0.51
1:F:300:ALA:HB1	1:F:343:HIS:HB2	1.92	0.51
1:A:392:LYS:NZ	1:B:235:SER:O	2.40	0.50
1:B:442:ALA:O	1:B:446:ASN:ND2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:ASP:O	1:C:606:ASN:ND2	2.44	0.50
1:C:657:ARG:NH2	1:C:680:ALA:O	2.35	0.50
1:F:62:LEU:HD11	1:F:70:ASP:HB2	1.93	0.50
1:D:39:ASP:HB3	1:D:42:VAL:HB	1.93	0.50
1:F:122:PRO:HG3	1:F:134:LEU:HD22	1.93	0.50
1:B:212:VAL:HG21	1:B:257:ILE:HD11	1.94	0.50
1:F:254:LYS:NZ	3:F:901:ANP:O1B	2.43	0.50
1:B:668:SER:OG	1:C:509:PHE:O	2.21	0.50
1:C:613:ASP:OD2	1:C:642:ARG:NH2	2.44	0.50
1:C:653:ASP:H	1:C:656:SER:HB2	1.77	0.50
1:E:706:ASN:ND2	1:E:733:SER:OG	2.44	0.50
1:F:95:ASN:O	1:F:97:ARG:NH1	2.45	0.50
1:B:595:GLY:HA3	1:C:595:GLY:HA2	1.94	0.50
1:D:28:ASN:ND2	1:D:106:VAL:O	2.37	0.50
1:F:210:GLY:O	3:F:901:ANP:N6	2.37	0.50
1:B:310:ASP:OD2	1:B:355:SER:OG	2.28	0.50
1:B:479:TRP:CE2	1:B:537:GLU:HG3	2.47	0.50
1:C:289:LEU:HD12	1:C:327:ILE:HD11	1.93	0.50
1:D:123:VAL:HG13	1:D:193:VAL:HG12	1.94	0.50
1:E:111:ASP:OD1	1:E:111:ASP:N	2.44	0.50
1:F:457:THR:O	1:F:461:ASN:ND2	2.36	0.50
1:C:707:ILE:HD13	1:D:505:LYS:HE2	1.94	0.50
1:C:763:ALA:O	1:C:767:GLN:HG2	2.12	0.50
1:C:138:TYR:C	1:C:141:PRO:HD2	2.37	0.49
1:E:151:ARG:NH2	1:E:176:GLU:OE1	2.45	0.49
2:G:72:LEU:HA	2:G:75:LEU:HD12	1.93	0.49
1:A:322:GLU:OE2	1:A:325:ARG:NH2	2.44	0.49
1:A:612:MET:HE2	1:A:623:ILE:HG21	1.95	0.49
1:C:322:GLU:OE1	1:C:326:ARG:NE	2.44	0.49
1:D:433:ILE:O	1:E:24:LYS:NZ	2.45	0.49
1:E:427:ARG:NE	1:F:221:GLU:OE1	2.38	0.49
1:E:39:ASP:HB3	1:E:42:VAL:HB	1.95	0.49
1:E:704:ARG:NH1	1:F:494:GLU:OE1	2.41	0.49
1:F:63:ILE:HG12	1:F:106:VAL:HG22	1.93	0.49
1:B:119:HIS:N	1:B:171:GLU:O	2.44	0.49
1:B:281:LEU:H	1:B:281:LEU:HD23	1.77	0.49
1:F:88:MET:SD	1:F:92:VAL:HB	2.52	0.49
1:F:483:GLY:O	5:F:903:ADP:N6	2.43	0.49
1:F:669:PRO:HB2	1:F:734:GLU:HG2	1.93	0.49
1:B:112:VAL:HB	2:G:11:GLY:HA2	1.93	0.49
1:B:518:LEU:HD13	1:B:643:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:LYS:NZ	1:E:288:ASN:OD1	2.45	0.49
1:E:393:LEU:HD12	1:E:397:VAL:HG11	1.94	0.49
1:A:180:VAL:HA	1:A:184:THR:HG21	1.95	0.49
1:A:504:GLU:O	1:A:508:LYS:HG2	2.12	0.49
1:C:402:ILE:O	1:C:406:THR:HG22	2.12	0.49
1:E:71:THR:HG22	1:E:96:LEU:HD21	1.94	0.49
1:E:644:ASP:OD1	1:E:645:GLN:N	2.44	0.49
1:A:652:PRO:HB2	1:A:657:ARG:HH21	1.77	0.49
1:D:60:THR:HG22	1:D:72:VAL:HG12	1.95	0.49
1:D:219:ILE:HD11	1:D:246:LEU:HD21	1.94	0.49
1:C:284:GLU:HG3	1:C:288:ASN:ND2	2.27	0.49
1:D:121:LEU:HD12	1:D:170:ILE:HG13	1.95	0.49
1:E:675:ASP:OD1	1:E:675:ASP:N	2.45	0.49
2:G:159:PHE:HE2	2:G:178:PRO:HG3	1.78	0.49
1:B:436:GLU:OE2	1:C:23:ARG:NH1	2.43	0.49
1:C:316:ARG:HG3	1:C:319:THR:HG22	1.95	0.49
1:E:585:ILE:HD12	1:E:604:VAL:HG21	1.95	0.49
1:A:140:LYS:HD2	1:A:144:LEU:HD22	1.94	0.48
1:A:766:LEU:HB3	1:F:748:ARG:HG3	1.94	0.48
1:C:88:MET:SD	1:C:88:MET:N	2.86	0.48
1:D:43:VAL:N	1:D:74:ILE:O	2.38	0.48
1:D:196:GLU:OE2	1:E:341:ARG:NH2	2.46	0.48
1:D:514:SER:O	1:D:645:GLN:NE2	2.46	0.48
1:E:273:ASN:HB3	1:E:276:GLU:HB3	1.95	0.48
1:F:380:ARG:HA	1:F:383:VAL:HG12	1.95	0.48
2:G:290:MET:HE3	2:G:291:PRO:HD2	1.94	0.48
2:G:306:VAL:HG22	2:G:314:VAL:HG22	1.95	0.48
1:E:119:HIS:HA	1:E:186:ILE:HD13	1.95	0.48
2:G:24:VAL:HG13	2:G:44:LEU:HD12	1.96	0.48
1:A:34:GLU:HA	1:A:93:ARG:HH12	1.77	0.48
1:B:748:ARG:HD2	1:C:766:LEU:HD12	1.95	0.48
1:C:30:LEU:HD22	1:C:84:PRO:HA	1.93	0.48
1:F:636:ALA:O	1:F:642:ARG:NH1	2.38	0.48
1:C:563:ARG:NH1	1:C:607:GLN:HE21	2.12	0.48
1:A:657:ARG:NH1	1:A:684:GLN:O	2.42	0.48
1:B:60:THR:HG22	1:B:72:VAL:HG12	1.95	0.48
1:D:350:THR:OG1	1:D:351:ASN:N	2.47	0.48
1:F:219:ILE:HG22	1:F:261:VAL:HG21	1.95	0.48
1:F:359:ALA:O	1:F:365:ARG:NH1	2.47	0.48
1:C:64:LYS:HZ3	1:C:64:LYS:HB3	1.78	0.48
1:D:492:LEU:HD12	1:D:530:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:ARG:O	1:D:644:ASP:N	2.47	0.48
1:B:78:ASP:OD1	1:B:81:CYS:N	2.47	0.48
1:C:71:THR:HG22	1:C:96:LEU:HD21	1.95	0.48
1:D:654:GLU:OE2	1:D:657:ARG:NH2	2.47	0.48
1:F:246:LEU:HD23	1:F:370:ILE:HB	1.96	0.48
1:A:448:MET:HG2	1:B:236:ILE:HD11	1.96	0.48
1:D:677:GLY:O	1:D:681:LYS:HG2	2.13	0.48
1:E:81:CYS:HA	1:E:87:ARG:HH21	1.78	0.48
1:E:427:ARG:NH2	1:F:221:GLU:OE2	2.32	0.48
1:F:226:PRO:HG3	1:F:233:PHE:HE2	1.78	0.48
1:F:674:VAL:HG22	1:F:737:ALA:HA	1.95	0.48
1:B:35:ALA:HB2	1:B:87:ARG:HB3	1.95	0.47
1:B:157:LEU:HD11	1:B:164:SER:HB3	1.96	0.47
1:C:479:TRP:CZ3	1:C:489:LYS:HG2	2.49	0.47
1:E:209:VAL:HG22	1:E:256:LEU:HD12	1.96	0.47
1:E:482:ILE:HD12	1:E:530:LEU:HD22	1.95	0.47
1:E:705:GLU:O	1:E:708:GLU:HG3	2.13	0.47
1:F:350:THR:OG1	1:F:351:ASN:N	2.46	0.47
1:D:665:LEU:HD13	1:D:670:ILE:HD13	1.96	0.47
1:F:487:ASN:OD1	1:F:490:ARG:NH2	2.47	0.47
1:B:290:ARG:HA	1:B:334:LEU:HD11	1.96	0.47
1:C:297:GLU:HG2	1:C:344:VAL:HG21	1.96	0.47
1:F:677:GLY:O	1:F:681:LYS:HG2	2.14	0.47
1:A:28:ASN:ND2	1:A:106:VAL:O	2.39	0.47
1:B:497:GLN:HG3	1:B:534:ILE:HD11	1.97	0.47
1:C:39:ASP:HB3	1:C:42:VAL:HB	1.96	0.47
1:D:286:GLU:OE1	1:D:286:GLU:N	2.43	0.47
2:G:45:SER:HA	2:G:65:LEU:HB2	1.96	0.47
2:G:191:ARG:HH22	2:G:235:GLN:HE22	1.62	0.47
1:B:62:LEU:HB2	1:B:109:CYS:SG	2.55	0.47
1:B:714:GLU:CD	1:B:717:ARG:HH12	2.21	0.47
1:C:81:CYS:HB2	1:C:87:ARG:HE	1.79	0.47
1:C:353:PRO:O	1:C:361:ARG:NH2	2.47	0.47
2:G:234:LEU:HD21	2:G:285:PHE:HB3	1.96	0.47
1:B:339:LYS:NZ	1:B:364:GLY:O	2.48	0.47
1:B:499:PRO:HB3	1:B:513:PRO:HG2	1.97	0.47
1:D:62:LEU:HD11	1:D:70:ASP:HB2	1.96	0.47
1:D:518:LEU:HB3	1:D:646:LEU:HD22	1.96	0.47
1:E:97:ARG:NE	1:E:202:ASP:OD2	2.47	0.47
1:E:225:LEU:HB3	1:E:226:PRO:HD3	1.96	0.47
1:B:151:ARG:NH2	2:G:100:THR:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:PRO:HG2	1:B:651:LEU:HG	1.96	0.47
1:A:247:TYR:CE2	1:A:369:GLU:HB3	2.50	0.47
1:B:402:ILE:O	1:B:406:THR:HG22	2.15	0.47
1:C:546:LYS:NZ	1:C:549:GLU:OE2	2.33	0.47
1:D:558:SER:OG	1:D:559:GLU:N	2.45	0.47
1:E:483:GLY:H	5:E:903:ADP:HN62	1.62	0.47
1:B:204:VAL:HG13	1:B:208:ASP:HB2	1.96	0.47
1:E:55:LEU:HD21	1:E:108:GLN:HG2	1.97	0.47
1:B:254:LYS:NZ	3:B:901:ANP:O3G	2.37	0.46
1:D:215:GLN:OE1	1:D:215:GLN:N	2.47	0.46
1:A:38:ASP:OD2	1:A:159:ARG:NH1	2.40	0.46
1:C:336:ASP:OD1	1:C:365:ARG:NE	2.45	0.46
1:C:506:PHE:O	1:C:510:GLY:N	2.46	0.46
1:D:448:MET:HE3	1:E:232:LEU:HD11	1.96	0.46
1:E:67:LYS:NZ	1:E:202:ASP:OD1	2.41	0.46
1:F:472:VAL:HG22	1:F:543:ILE:HG12	1.98	0.46
1:E:64:LYS:HD2	1:E:70:ASP:HB3	1.97	0.46
1:B:219:ILE:HG22	1:B:261:VAL:HG21	1.97	0.46
1:C:81:CYS:SG	1:C:82:GLU:N	2.89	0.46
1:C:315:LYS:HG3	1:C:358:PRO:HD3	1.97	0.46
1:D:710:ASP:HA	1:D:713:LYS:HG2	1.98	0.46
1:E:479:TRP:HE1	1:E:537:GLU:CD	2.23	0.46
1:B:32:VAL:HG23	1:B:88:MET:HB3	1.97	0.46
1:C:339:LYS:HZ1	1:C:365:ARG:H	1.62	0.46
1:C:472:VAL:HG13	1:C:541:ASN:HB3	1.97	0.46
1:C:753:ASP:HA	1:C:756:ILE:HD12	1.97	0.46
1:F:215:GLN:HG2	1:F:372:ILE:HD13	1.97	0.46
1:A:646:LEU:HD12	1:A:766:LEU:HD11	1.98	0.46
1:B:583:ASP:OD2	1:B:629:ARG:NE	2.45	0.46
1:E:31:VAL:N	1:E:84:PRO:O	2.37	0.46
1:F:222:LEU:HD21	1:F:368:ARG:HG3	1.97	0.46
1:F:653:ASP:H	1:F:656:SER:HB2	1.80	0.46
1:A:32:VAL:HG13	1:A:88:MET:SD	2.56	0.46
1:C:120:ILE:HG12	1:C:169:VAL:HG22	1.97	0.46
1:D:753:ASP:HA	1:D:756:ILE:HG12	1.98	0.46
1:E:551:LEU:HD12	1:E:551:LEU:HA	1.79	0.46
1:A:24:LYS:O	1:A:29:ARG:NH1	2.49	0.46
1:A:195:ARG:HH21	1:A:196:GLU:HA	1.81	0.46
2:G:212:GLY:HA2	2:G:248:TRP:CD2	2.52	0.46
1:B:657:ARG:HA	1:B:660:ILE:HG22	1.98	0.45
1:C:14:LYS:HB3	1:C:16:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:558:SER:OG	1:E:559:GLU:N	2.49	0.45
1:E:629:ARG:NH2	1:E:631:ASP:OD2	2.49	0.45
2:G:55:THR:HG22	2:G:57:ALA:H	1.80	0.45
1:B:225:LEU:HB3	1:B:226:PRO:HD3	1.97	0.45
1:B:714:GLU:OE1	1:B:717:ARG:NH1	2.46	0.45
1:E:522:PRO:HG2	1:E:525:CYS:SG	2.56	0.45
1:A:269:PHE:CE2	1:A:271:CYS:HB2	2.52	0.45
1:F:367:ASP:OD1	1:F:368:ARG:N	2.47	0.45
1:F:496:VAL:HG22	1:F:622:PHE:CZ	2.52	0.45
1:C:724:MET:SD	1:C:724:MET:N	2.89	0.45
1:D:39:ASP:OD2	1:D:148:ARG:NH1	2.50	0.45
1:C:82:GLU:HB3	1:C:84:PRO:HD2	1.98	0.45
1:D:151:ARG:NH1	1:D:176:GLU:O	2.49	0.45
1:E:89:ASN:O	1:E:93:ARG:N	2.43	0.45
1:A:339:LYS:NZ	1:A:364:GLY:O	2.40	0.45
1:D:78:ASP:OD1	1:D:80:THR:OG1	2.31	0.45
1:E:658:LEU:HD21	1:E:677:GLY:HA2	1.98	0.45
2:G:5:ARG:HG2	2:G:14:ARG:HG2	1.98	0.45
1:B:33:ASP:O	1:B:88:MET:N	2.50	0.45
1:C:653:ASP:N	1:C:656:SER:HB2	2.31	0.45
1:F:163:ARG:HE	1:F:164:SER:N	2.14	0.45
1:B:583:ASP:CG	1:B:629:ARG:HE	2.23	0.45
1:C:32:VAL:HG13	1:C:88:MET:SD	2.57	0.45
1:C:206:TYR:CG	1:C:264:GLU:HG3	2.52	0.45
2:G:336:PHE:HE1	2:G:350:LEU:HA	1.80	0.45
1:A:504:GLU:OE2	1:A:505:LYS:NZ	2.50	0.45
1:C:155:LEU:HD23	1:C:168:LYS:HB2	1.98	0.45
1:E:451:THR:OG1	1:E:452:ASN:N	2.50	0.45
1:E:554:TRP:NE1	1:E:559:GLU:OE2	2.50	0.45
1:E:566:PHE:O	1:E:569:ALA:HB3	2.17	0.45
1:F:65:GLY:HA2	1:F:104:ILE:HG22	1.99	0.45
1:F:557:GLU:OE1	1:F:561:ASN:ND2	2.49	0.45
1:A:683:THR:O	1:A:685:GLY:N	2.48	0.45
1:B:487:ASN:N	1:B:487:ASN:OD1	2.48	0.45
1:E:33:ASP:O	1:E:93:ARG:NH2	2.50	0.45
1:F:219:ILE:HD11	1:F:370:ILE:HG13	1.98	0.45
1:F:243:GLY:HA3	1:F:365:ARG:O	2.17	0.45
1:B:429:LYS:HB3	1:B:429:LYS:HE2	1.78	0.44
1:F:32:VAL:HG22	1:F:104:ILE:HD13	2.00	0.44
1:F:655:ASP:N	1:F:655:ASP:OD1	2.49	0.44
1:B:420:GLU:OE1	1:C:368:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:GLY:O	1:D:599:GLY:N	2.51	0.44
1:E:70:ASP:OD1	1:E:70:ASP:N	2.50	0.44
1:E:671:ALA:HB2	1:E:735:ILE:HB	2.00	0.44
1:F:45:LEU:HD23	1:F:86:ILE:HA	1.99	0.44
1:F:63:ILE:HG21	1:F:104:ILE:HD12	1.98	0.44
1:F:194:LYS:NZ	1:F:197:ASP:OD1	2.43	0.44
1:F:558:SER:OG	1:F:559:GLU:N	2.46	0.44
1:F:429:LYS:HE2	1:F:448:MET:HG2	1.99	0.44
2:G:40:HIS:ND1	2:G:41:LYS:HG3	2.32	0.44
2:G:205:GLY:HA3	2:G:389:ALA:HB3	2.00	0.44
1:C:198:GLU:HA	1:C:201:LEU:HG	2.00	0.44
1:C:361:ARG:NH1	1:C:369:GLU:OE2	2.39	0.44
1:D:228:ARG:HG2	1:D:229:HIS:ND1	2.32	0.44
1:E:46:HIS:ND1	1:E:83:GLU:OE2	2.51	0.44
1:E:315:LYS:NZ	1:E:317:GLU:OE2	2.42	0.44
1:F:249:PRO:HG2	1:F:252:SER:HB3	1.99	0.44
1:F:700:LYS:HE3	1:F:700:LYS:HB2	1.81	0.44
1:A:63:ILE:HG23	1:A:104:ILE:HD13	1.98	0.44
1:B:313:ALA:HA	1:B:328:VAL:HG22	2.00	0.44
1:A:169:VAL:HG11	1:A:172:THR:HG23	2.00	0.44
1:A:644:ASP:OD1	1:A:645:GLN:HG3	2.17	0.44
1:C:520:TYR:HE2	1:C:646:LEU:HB3	1.83	0.44
1:D:542:PHE:HE1	1:D:544:SER:HB2	1.83	0.44
1:C:145:GLU:HA	1:C:182:PRO:HG3	2.00	0.44
1:E:233:PHE:CE2	1:E:240:PRO:HB3	2.53	0.44
1:F:44:SER:HB3	1:F:78:ASP:OD2	2.17	0.44
1:F:362:ARG:HG2	1:F:363:PHE:H	1.82	0.44
1:B:657:ARG:NH2	1:B:683:THR:O	2.50	0.44
1:D:120:ILE:HG22	1:D:167:PHE:HB3	2.00	0.44
1:E:81:CYS:SG	1:E:82:GLU:N	2.90	0.44
1:F:516:GLY:HA2	1:F:623:ILE:O	2.17	0.44
2:G:156:ARG:NH2	2:G:340:ASN:O	2.48	0.44
1:A:241:PRO:HG3	1:A:368:ARG:HE	1.83	0.43
1:A:482:ILE:HG22	5:A:903:ADP:N1	2.33	0.43
1:B:97:ARG:HH21	1:B:202:ASP:HB2	1.83	0.43
1:E:663:ALA:HA	1:E:666:ARG:HD3	2.00	0.43
1:B:176:GLU:H	1:B:176:GLU:HG2	1.66	0.43
1:B:704:ARG:NE	1:C:494:GLU:OE1	2.46	0.43
1:C:143:PHE:HA	1:C:148:ARG:HD2	2.00	0.43
1:E:233:PHE:HA	1:E:236:ILE:HG22	2.00	0.43
1:F:67:LYS:O	1:F:68:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HD2	1:A:240:PRO:HD2	1.98	0.43
1:A:724:MET:SD	1:A:724:MET:N	2.77	0.43
1:B:47:PRO:HA	1:B:50:MET:HE2	2.01	0.43
1:C:111:ASP:OD1	1:C:111:ASP:N	2.43	0.43
1:C:384:LEU:HD21	1:C:414:LEU:HD22	1.99	0.43
1:C:524:GLY:O	1:C:687:SER:HB3	2.17	0.43
1:F:653:ASP:N	1:F:656:SER:HB2	2.33	0.43
1:A:553:MET:HE3	1:A:557:GLU:HG2	2.00	0.43
1:A:657:ARG:HD2	1:A:682:TYR:HB2	1.99	0.43
1:D:402:ILE:HG23	1:D:459:LEU:HD12	2.00	0.43
1:E:88:MET:HB3	1:E:93:ARG:HE	1.84	0.43
1:E:151:ARG:HG2	1:E:177:TYR:HB3	1.99	0.43
1:A:119:HIS:HA	1:A:186:ILE:HG12	2.00	0.43
1:A:273:ASN:HB2	1:A:276:GLU:HB3	2.00	0.43
1:B:148:ARG:O	1:B:180:VAL:HG22	2.18	0.43
1:C:575:CYS:SG	1:C:576:VAL:N	2.91	0.43
1:A:289:LEU:HD12	1:A:327:ILE:HD11	2.01	0.43
1:C:32:VAL:HG21	1:C:98:VAL:HG21	2.01	0.43
1:C:39:ASP:O	1:C:89:ASN:ND2	2.51	0.43
1:D:114:TYR:HD1	1:D:179:VAL:HB	1.83	0.43
1:D:717:ARG:NH2	1:D:725:GLU:OE1	2.51	0.43
1:E:72:VAL:HG21	1:E:177:TYR:CD2	2.54	0.43
2:G:6:ILE:HD13	2:G:83:LEU:HB2	2.00	0.43
1:C:398:ASP:OD1	1:C:398:ASP:N	2.51	0.43
1:C:653:ASP:O	1:C:657:ARG:N	2.31	0.43
1:D:67:LYS:HE2	1:D:203:ASP:N	2.34	0.43
1:E:430:MET:HE3	1:F:225:LEU:HD22	1.99	0.43
1:E:475:PRO:O	1:E:536:ASN:ND2	2.34	0.43
1:A:422:ALA:HB1	1:B:236:ILE:HG21	2.00	0.43
1:B:335:MET:HA	1:B:338:LEU:HD23	2.01	0.43
1:D:162:MET:SD	1:D:162:MET:N	2.86	0.43
1:F:724:MET:H	1:F:724:MET:HG3	1.70	0.43
1:D:200:ARG:HD2	1:D:200:ARG:HA	1.89	0.43
1:F:553:MET:HB3	1:F:561:ASN:ND2	2.34	0.43
1:F:657:ARG:HA	1:F:660:ILE:HG22	2.00	0.43
2:G:379:LEU:HD23	2:G:379:LEU:HA	1.89	0.43
1:A:49:THR:OG1	1:A:83:GLU:OE2	2.34	0.43
1:A:674:VAL:HG22	1:A:737:ALA:HB2	1.99	0.43
1:A:709:LYS:NZ	1:A:731:GLU:OE2	2.34	0.43
1:B:433:ILE:O	1:C:24:LYS:NZ	2.52	0.43
1:B:439:SER:HA	1:B:445:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:PRO:HG2	1:C:79:GLU:HG3	2.01	0.43
1:D:541:ASN:OD1	1:D:541:ASN:N	2.52	0.43
1:D:566:PHE:HD1	1:D:615:MET:HE3	1.83	0.43
1:E:275:PRO:O	1:E:279:SER:N	2.52	0.43
1:E:561:ASN:O	1:E:564:GLU:HB2	2.19	0.43
1:B:665:LEU:HD11	1:B:740:PHE:HZ	1.84	0.42
1:D:135:PHE:HA	1:D:139:LEU:HB2	2.01	0.42
1:F:117:ARG:NE	1:F:185:GLU:O	2.46	0.42
1:B:195:ARG:HE	1:B:195:ARG:HA	1.84	0.42
1:B:495:THR:HG22	1:B:622:PHE:HZ	1.84	0.42
1:B:753:ASP:HA	1:B:756:ILE:HG22	2.01	0.42
1:D:136:ASP:HA	1:D:140:LYS:HD3	2.00	0.42
1:D:398:ASP:OD1	1:D:398:ASP:N	2.48	0.42
1:E:111:ASP:OD2	1:E:113:LYS:NZ	2.51	0.42
1:E:631:ASP:OD1	1:E:631:ASP:N	2.52	0.42
2:G:206:LEU:O	2:G:393:ARG:HD3	2.19	0.42
1:A:324:GLU:O	1:A:327:ILE:HG22	2.19	0.42
1:A:657:ARG:HD2	1:A:682:TYR:CG	2.54	0.42
1:B:34:GLU:OE1	1:B:93:ARG:NH2	2.44	0.42
1:B:172:THR:OG1	1:B:175:ALA:O	2.37	0.42
1:B:247:TYR:HB3	1:B:350:THR:HG23	2.00	0.42
1:C:339:LYS:NZ	1:C:365:ARG:H	2.17	0.42
1:D:138:TYR:C	1:D:141:PRO:HD2	2.44	0.42
1:E:114:TYR:HD1	1:E:179:VAL:HB	1.84	0.42
1:E:487:ASN:N	1:E:487:ASN:OD1	2.52	0.42
1:E:520:TYR:CZ	1:E:648:TYR:HB2	2.55	0.42
1:F:411:GLY:HA3	3:F:901:ANP:C8	2.50	0.42
2:G:115:ILE:HG12	2:G:120:ARG:NH2	2.33	0.42
1:C:312:ILE:HD11	1:C:331:LEU:HD22	2.01	0.42
1:C:600:ALA:O	1:C:604:VAL:HG22	2.19	0.42
1:E:39:ASP:CG	1:E:148:ARG:HH12	2.27	0.42
1:E:300:ALA:HB2	1:E:342:ALA:HB1	2.01	0.42
1:B:710:ASP:O	1:B:714:GLU:HG2	2.19	0.42
1:C:233:PHE:CE2	1:C:240:PRO:HB3	2.54	0.42
1:D:522:PRO:HB3	1:D:751:VAL:HG11	2.00	0.42
1:E:619:LYS:HE2	1:E:619:LYS:HB2	1.91	0.42
1:F:215:GLN:OE1	1:F:215:GLN:N	2.52	0.42
1:C:88:MET:HB2	1:C:92:VAL:HB	2.02	0.42
1:C:172:THR:OG1	1:C:175:ALA:O	2.37	0.42
1:D:739:HIS:HA	1:D:742:GLU:HG2	2.00	0.42
1:E:717:ARG:NE	1:E:725:GLU:OE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:23:THR:OG1	2:G:26:GLN:OE1	2.23	0.42
1:D:67:LYS:NZ	1:D:202:ASP:OD1	2.36	0.42
1:D:324:GLU:O	1:D:327:ILE:HG22	2.20	0.42
1:E:33:ASP:OD2	1:E:85:LYS:HD3	2.20	0.42
1:F:130:VAL:HG11	1:F:134:LEU:HG	2.01	0.42
1:F:207:ASP:OD1	1:F:207:ASP:N	2.42	0.42
1:F:520:TYR:CZ	1:F:648:TYR:HB2	2.55	0.42
1:F:598:GLY:O	1:F:603:ARG:NH1	2.47	0.42
1:F:748:ARG:HG2	1:F:749:ARG:H	1.84	0.42
1:D:431:ASP:OD1	1:D:431:ASP:N	2.50	0.42
1:E:730:ASP:OD2	1:F:505:LYS:NZ	2.44	0.42
1:A:638:LEU:HD11	1:A:646:LEU:HD11	2.01	0.42
1:A:685:GLY:HA3	1:A:749:ARG:CZ	2.50	0.42
1:D:520:TYR:CZ	1:D:648:TYR:HB2	2.55	0.42
1:D:665:LEU:HD22	1:D:670:ILE:HG21	2.02	0.42
2:G:24:VAL:HG23	2:G:70:LEU:O	2.20	0.42
2:G:206:LEU:HD13	2:G:332:LEU:HD11	2.01	0.42
2:G:277:ILE:HD12	2:G:277:ILE:HA	1.88	0.42
1:A:183:ASP:OD1	1:A:183:ASP:N	2.51	0.41
1:D:315:LYS:HG2	1:D:317:GLU:HG3	2.02	0.41
1:D:763:ALA:O	1:D:767:GLN:N	2.50	0.41
1:F:247:TYR:CD2	1:F:353:PRO:HD3	2.55	0.41
1:C:286:GLU:OE1	1:C:286:GLU:N	2.47	0.41
1:D:35:ALA:HA	1:D:87:ARG:HB3	2.02	0.41
1:D:47:PRO:HA	1:D:50:MET:HE3	2.03	0.41
1:F:393:LEU:HD12	1:F:397:VAL:HG11	2.01	0.41
1:F:580:ASP:OD1	1:F:581:GLU:N	2.53	0.41
1:F:653:ASP:O	1:F:657:ARG:N	2.43	0.41
2:G:22:ILE:HG13	2:G:72:LEU:HD12	2.00	0.41
2:G:225:GLU:N	2:G:296:LYS:HE3	2.36	0.41
2:G:270:PHE:HD1	2:G:322:LEU:HA	1.85	0.41
1:C:578:PHE:HE2	1:C:580:ASP:HB2	1.86	0.41
1:D:361:ARG:HD3	1:D:369:GLU:OE2	2.20	0.41
1:E:15:ASP:OD1	1:E:15:ASP:N	2.46	0.41
1:F:211:GLY:HA2	1:F:379:GLY:HA2	2.02	0.41
2:G:155:LYS:HE2	2:G:232:GLU:HG2	2.01	0.41
1:C:542:PHE:CE1	1:C:544:SER:HB2	2.56	0.41
1:F:212:VAL:HG21	1:F:257:ILE:HD11	2.03	0.41
2:G:363:VAL:HG21	2:G:395:GLN:HA	2.02	0.41
3:A:901:ANP:N3B	1:B:362:ARG:HD2	2.35	0.41
1:B:655:ASP:OD1	1:B:655:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:LYS:HE2	1:C:568:LYS:HB2	1.93	0.41
1:D:140:LYS:HG2	1:D:141:PRO:HD3	2.02	0.41
1:D:503:PRO:O	1:D:507:GLU:HG2	2.20	0.41
1:E:207:ASP:OD1	1:E:207:ASP:N	2.50	0.41
1:E:350:THR:OG1	1:E:351:ASN:N	2.53	0.41
1:E:542:PHE:CE2	1:E:544:SER:HB2	2.55	0.41
1:A:21:LEU:HD11	1:A:217:ALA:HB2	2.03	0.41
1:B:124:ASP:O	1:B:128:GLU:HG3	2.20	0.41
1:D:482:ILE:O	5:D:903:ADP:N6	2.45	0.41
2:G:5:ARG:HB3	2:G:12:LEU:HD11	2.01	0.41
1:C:174:PRO:HD2	1:C:178:CYS:HB3	2.01	0.41
1:F:73:CYS:SG	1:F:92:VAL:HG11	2.61	0.41
1:F:657:ARG:NH1	1:F:684:GLN:HA	2.36	0.41
2:G:248:TRP:CD1	2:G:272:MET:HE3	2.56	0.41
1:A:277:ILE:HD13	1:A:277:ILE:HA	1.88	0.41
1:A:730:ASP:N	1:A:730:ASP:OD1	2.50	0.41
1:E:273:ASN:OD1	1:E:275:PRO:HD2	2.21	0.41
1:F:206:TYR:CZ	1:F:264:GLU:HG2	2.56	0.41
1:A:356:ILE:HD12	1:A:356:ILE:HA	1.80	0.41
1:A:475:PRO:HG2	1:A:536:ASN:HB2	2.02	0.41
1:A:630:PRO:HB2	1:A:762:PHE:CE2	2.56	0.41
1:B:122:PRO:HA	1:B:167:PHE:HA	2.03	0.41
1:B:247:TYR:HE2	1:B:369:GLU:HB3	1.85	0.41
1:C:15:ASP:OD1	1:C:15:ASP:N	2.53	0.41
1:C:122:PRO:HG3	1:C:134:LEU:HD12	2.03	0.41
1:C:140:LYS:CG	1:C:141:PRO:HD3	2.51	0.41
1:C:204:VAL:HG11	1:C:256:LEU:HD11	2.03	0.41
1:C:339:LYS:HA	1:C:339:LYS:HD3	1.85	0.41
1:D:284:GLU:HG3	1:D:288:ASN:ND2	2.31	0.41
1:E:529:LEU:HD23	5:E:903:ADP:H5'2	2.02	0.41
1:A:122:PRO:HB3	1:A:134:LEU:HD22	2.02	0.41
1:A:221:GLU:OE2	1:F:427:ARG:NH2	2.53	0.41
1:B:487:ASN:O	1:B:490:ARG:HG2	2.21	0.41
1:A:254:LYS:NZ	3:A:901:ANP:O3G	2.38	0.40
1:B:736:LYS:HG2	1:B:739:HIS:CE1	2.56	0.40
1:C:558:SER:OG	1:C:559:GLU:N	2.54	0.40
1:D:64:LYS:HE3	1:D:64:LYS:HB3	1.97	0.40
1:E:45:LEU:N	1:E:76:LEU:O	2.47	0.40
1:F:88:MET:HE3	1:F:88:MET:HB3	1.85	0.40
1:F:163:ARG:HE	1:F:164:SER:H	1.68	0.40
1:F:313:ALA:HA	1:F:328:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLU:HG2	1:B:344:VAL:HG21	2.03	0.40
1:C:81:CYS:HA	1:C:87:ARG:HH21	1.86	0.40
1:C:330:GLN:HE21	1:C:334:LEU:HG	1.85	0.40
1:C:582:LEU:HD23	1:C:582:LEU:HA	1.93	0.40
1:D:133:ASN:HD21	1:D:188:CYS:H	1.69	0.40
1:D:731:GLU:HG2	1:D:733:SER:H	1.85	0.40
1:E:374:VAL:HG22	1:E:410:VAL:HG12	2.03	0.40
1:F:199:GLU:HG2	1:F:200:ARG:HE	1.86	0.40
1:A:126:THR:O	1:A:165:VAL:HG13	2.21	0.40
1:A:634:ASP:OD1	1:A:635:SER:N	2.55	0.40
1:B:496:VAL:HG22	1:B:622:PHE:CE2	2.56	0.40
1:C:748:ARG:HH12	1:D:646:LEU:HD12	1.87	0.40
1:E:62:LEU:HD12	1:E:71:THR:O	2.22	0.40
1:E:318:LYS:HG3	1:F:316:ARG:NH1	2.36	0.40
1:E:753:ASP:HA	1:E:756:ILE:HG22	2.04	0.40
1:F:209:VAL:HG22	1:F:256:LEU:HG	2.04	0.40
1:F:225:LEU:HB3	1:F:226:PRO:HD3	2.04	0.40
1:F:277:ILE:HD13	1:F:277:ILE:HA	1.90	0.40
2:G:234:LEU:HD12	2:G:289:ILE:HD11	2.03	0.40
1:B:126:THR:HG21	1:B:166:GLU:H	1.87	0.40
1:D:66:LYS:HG2	1:D:98:VAL:HG12	2.04	0.40
1:D:332:LEU:HD21	1:D:360:LEU:HG	2.02	0.40
1:E:206:TYR:CG	1:E:264:GLU:HG3	2.57	0.40
1:F:92:VAL:O	1:F:96:LEU:N	2.46	0.40
2:G:23:THR:HA	2:G:71:PRO:HA	2.04	0.40
2:G:138:ALA:HA	2:G:334:SER:HB2	2.03	0.40
1:B:69:LYS:HE2	1:B:69:LYS:HB2	1.93	0.40
1:B:376:ASP:OD1	1:B:376:ASP:N	2.34	0.40
1:C:145:GLU:HG2	1:C:182:PRO:HG3	2.02	0.40
1:C:309:ILE:HG22	1:C:313:ALA:HB3	2.03	0.40
1:C:697:ARG:NH1	1:C:746:TYR:HB2	2.36	0.40
1:D:247:TYR:CE2	1:D:353:PRO:HB3	2.57	0.40
1:D:618:LYS:HE2	1:D:618:LYS:HB2	1.98	0.40
1:E:124:ASP:OD1	1:E:124:ASP:N	2.54	0.40
1:E:657:ARG:HA	1:E:660:ILE:HG22	2.03	0.40
1:E:658:LEU:HD23	1:E:658:LEU:HA	1.94	0.40
1:E:745:LYS:NZ	1:F:772:PHE:O	2.52	0.40
2:G:37:ILE:O	2:G:42:GLN:NE2	2.53	0.40
2:G:156:ARG:HD2	2:G:156:ARG:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	759/814 (93%)	718 (95%)	40 (5%)	1 (0%)	48	80
1	B	759/814 (93%)	709 (93%)	50 (7%)	0	100	100
1	C	759/814 (93%)	721 (95%)	38 (5%)	0	100	100
1	D	759/814 (93%)	720 (95%)	39 (5%)	0	100	100
1	E	759/814 (93%)	728 (96%)	31 (4%)	0	100	100
1	F	759/814 (93%)	725 (96%)	34 (4%)	0	100	100
2	G	411/418 (98%)	409 (100%)	2 (0%)	0	100	100
All	All	4965/5302 (94%)	4730 (95%)	234 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	PRO

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	645/683 (94%)	632 (98%)	13 (2%)	48	65
1	B	645/683 (94%)	619 (96%)	26 (4%)	28	51
1	C	645/683 (94%)	632 (98%)	13 (2%)	48	65
1	D	645/683 (94%)	633 (98%)	12 (2%)	50	66
1	E	645/683 (94%)	632 (98%)	13 (2%)	48	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	645/683 (94%)	633 (98%)	12 (2%)	50	66
2	G	358/361 (99%)	353 (99%)	5 (1%)	59	71
All	All	4228/4459 (95%)	4134 (98%)	94 (2%)	45	64

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	125	ASP
1	A	130	VAL
1	A	172	THR
1	A	179	VAL
1	A	183	ASP
1	A	319	THR
1	A	338	LEU
1	A	341	ARG
1	A	350	THR
1	A	628	ASN
1	A	660	ILE
1	A	703	ILE
1	B	32	VAL
1	B	33	ASP
1	B	55	LEU
1	B	60	THR
1	B	70	ASP
1	B	96	LEU
1	B	179	VAL
1	B	201	LEU
1	B	206	TYR
1	B	229	HIS
1	B	261	VAL
1	B	319	THR
1	B	324	GLU
1	B	338	LEU
1	B	397	VAL
1	B	404	LYS
1	B	405	ASP
1	B	445	LEU
1	B	468	ARG
1	B	494	GLU
1	B	567	ASP

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Mol	Chain	Res	Type
1	B	616	ASN
1	B	644	ASP
1	B	660	ILE
1	B	675	ASP
1	B	734	GLU
1	C	18	THR
1	C	172	THR
1	C	183	ASP
1	C	227	LEU
1	C	294	GLU
1	C	312	ILE
1	C	352	ARG
1	C	471	VAL
1	C	500	VAL
1	C	568	LYS
1	C	583	ASP
1	C	661	PHE
1	C	766	LEU
1	D	18	THR
1	D	134	LEU
1	D	382	GLU
1	D	433	ILE
1	D	452	ASN
1	D	456	HIS
1	D	476	ASN
1	D	530	LEU
1	D	541	ASN
1	D	545	VAL
1	D	661	PHE
1	D	665	LEU
1	E	172	THR
1	E	206	TYR
1	E	219	ILE
1	E	221	GLU
1	E	256	LEU
1	E	288	ASN
1	E	344	VAL
1	E	451	THR
1	E	456	HIS
1	E	530	LEU
1	E	713	LYS
1	E	729	VAL

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Mol	Chain	Res	Type
1	E	751	VAL
1	F	112	VAL
1	F	232	LEU
1	F	273	ASN
1	F	319	THR
1	F	450	VAL
1	F	467	LEU
1	F	530	LEU
1	F	613	ASP
1	F	682	TYR
1	F	729	VAL
1	F	739	HIS
1	F	744	MET
2	G	99	VAL
2	G	110	THR
2	G	132	VAL
2	G	252	VAL
2	G	315	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	288	ASN
1	A	354	ASN
1	A	588	GLN
1	A	645	GLN
1	A	696	GLN
1	A	739	HIS
1	A	760	GLN
1	B	354	ASN
1	B	452	ASN
1	B	456	HIS
1	B	497	GLN
1	B	536	ASN
1	B	588	GLN
1	B	659	ASN
1	B	767	GLN
1	C	28	ASN
1	C	299	ASN
1	C	330	GLN
1	C	493	GLN

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Mol	Chain	Res	Type
1	C	561	ASN
1	C	588	GLN
1	C	607	GLN
1	C	645	GLN
1	C	696	GLN
1	D	218	GLN
1	D	288	ASN
1	D	351	ASN
1	D	407	HIS
1	D	452	ASN
1	D	539	GLN
1	D	616	ASN
1	D	696	GLN
1	D	739	HIS
1	E	89	ASN
1	E	493	GLN
1	E	588	GLN
1	E	607	GLN
1	E	764	GLN
1	E	767	GLN
1	F	119	HIS
1	F	561	ASN
1	F	571	GLN
1	F	588	GLN
1	F	645	GLN
1	F	720	ASN
2	G	76	ASN
2	G	143	GLN
2	G	329	GLN
2	G	370	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	ANP	E	901	4	33,33,33	2.25	5 (15%)	45,52,52	1.17	3 (6%)
5	ADP	A	903	-	28,29,29	1.42	5 (17%)	43,45,45	1.83	8 (18%)
3	ANP	D	901	4	33,33,33	2.26	5 (15%)	45,52,52	1.17	3 (6%)
5	ADP	D	903	-	28,29,29	1.42	4 (14%)	43,45,45	1.94	8 (18%)
3	ANP	C	901	4	33,33,33	2.24	5 (15%)	45,52,52	1.16	3 (6%)
3	ANP	B	901	4	33,33,33	2.24	5 (15%)	45,52,52	1.15	3 (6%)
5	ADP	C	903	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
5	ADP	E	903	-	28,29,29	1.41	4 (14%)	43,45,45	1.91	8 (18%)
5	ADP	F	903	-	28,29,29	1.40	4 (14%)	43,45,45	1.90	8 (18%)
3	ANP	F	901	4	33,33,33	2.33	5 (15%)	45,52,52	1.19	3 (6%)
5	ADP	B	903	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
3	ANP	A	901	4	33,33,33	2.29	5 (15%)	45,52,52	1.19	3 (6%)

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
3	ANP	E	901	4	-	8/18/38/38	0/3/3/3
5	ADP	A	903	-	-	2/16/32/32	0/3/3/3
3	ANP	D	901	4	-	7/18/38/38	0/3/3/3
5	ADP	D	903	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	C	901	4	-	5/18/38/38	0/3/3/3
3	ANP	B	901	4	-	8/18/38/38	0/3/3/3
5	ADP	C	903	-	-	3/16/32/32	0/3/3/3
5	ADP	E	903	-	-	4/16/32/32	0/3/3/3
5	ADP	F	903	-	-	3/16/32/32	0/3/3/3
3	ANP	F	901	4	-	8/18/38/38	0/3/3/3
5	ADP	B	903	-	-	1/16/32/32	0/3/3/3
3	ANP	A	901	4	-	5/18/38/38	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	ANP	PB-O3A	9.00	1.70	1.59
3	A	901	ANP	PB-O3A	8.73	1.69	1.59
3	D	901	ANP	PB-O3A	8.60	1.69	1.59
3	E	901	ANP	PB-O3A	8.55	1.69	1.59
3	C	901	ANP	PB-O3A	8.44	1.69	1.59
3	B	901	ANP	PB-O3A	8.42	1.69	1.59
3	F	901	ANP	PG-N3B	6.33	1.79	1.63
3	A	901	ANP	PG-N3B	6.25	1.79	1.63
3	B	901	ANP	PG-N3B	6.18	1.79	1.63
3	E	901	ANP	PG-N3B	6.14	1.79	1.63
3	C	901	ANP	PG-N3B	6.14	1.79	1.63
3	D	901	ANP	PG-N3B	6.11	1.79	1.63
5	D	903	ADP	C5-C4	4.84	1.47	1.39
5	E	903	ADP	C5-C4	4.76	1.47	1.39
5	F	903	ADP	C5-C4	4.71	1.47	1.39
3	A	901	ANP	PG-O1G	4.70	1.53	1.46
3	F	901	ANP	PG-O1G	4.70	1.53	1.46
5	C	903	ADP	C5-C4	4.69	1.47	1.39
5	A	903	ADP	C5-C4	4.68	1.47	1.39
5	B	903	ADP	C5-C4	4.68	1.47	1.39
3	E	901	ANP	PG-O1G	4.65	1.53	1.46
3	D	901	ANP	PG-O1G	4.65	1.53	1.46
3	C	901	ANP	PG-O1G	4.64	1.53	1.46
3	B	901	ANP	PG-O1G	4.57	1.53	1.46
5	D	903	ADP	C5-C6	2.73	1.48	1.41
5	E	903	ADP	C5-C6	2.71	1.48	1.41
5	B	903	ADP	C5-C6	2.68	1.48	1.41
3	E	901	ANP	PB-O1B	2.68	1.50	1.46
5	F	903	ADP	C5-C6	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ANP	PB-O1B	2.64	1.50	1.46
5	C	903	ADP	C5-C6	2.64	1.48	1.41
3	F	901	ANP	PB-O1B	2.62	1.50	1.46
3	A	901	ANP	PB-O1B	2.62	1.50	1.46
3	D	901	ANP	PB-O1B	2.62	1.50	1.46
5	A	903	ADP	C5-C6	2.56	1.48	1.41
3	B	901	ANP	PB-O1B	2.55	1.50	1.46
5	E	903	ADP	C5-N7	-2.48	1.34	1.39
5	F	903	ADP	C5-N7	-2.48	1.34	1.39
5	A	903	ADP	C5-N7	-2.44	1.34	1.39
5	C	903	ADP	C5-N7	-2.43	1.34	1.39
5	D	903	ADP	C5-N7	-2.39	1.34	1.39
5	B	903	ADP	C5-N7	-2.37	1.34	1.39
3	C	901	ANP	PB-O2B	-2.35	1.50	1.56
3	A	901	ANP	PB-O2B	-2.34	1.50	1.56
3	B	901	ANP	PB-O2B	-2.34	1.50	1.56
3	E	901	ANP	PB-O2B	-2.27	1.50	1.56
5	A	903	ADP	C8-N7	2.27	1.36	1.31
5	B	903	ADP	C8-N7	2.27	1.36	1.31
3	F	901	ANP	PB-O2B	-2.27	1.50	1.56
3	D	901	ANP	PB-O2B	-2.26	1.50	1.56
5	D	903	ADP	C8-N7	2.21	1.35	1.31
5	C	903	ADP	C8-N7	2.20	1.35	1.31
5	E	903	ADP	C8-N7	2.19	1.35	1.31
5	F	903	ADP	C8-N7	2.19	1.35	1.31
5	A	903	ADP	PA-O3A	2.03	1.61	1.59

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	903	ADP	C5-C4-N3	-6.64	117.58	126.72
5	E	903	ADP	C5-C4-N3	-6.53	117.73	126.72
5	F	903	ADP	C5-C4-N3	-6.32	118.02	126.72
5	C	903	ADP	C5-C4-N3	-6.20	118.18	126.72
5	A	903	ADP	C5-C4-N3	-6.09	118.33	126.72
5	B	903	ADP	C5-C4-N3	-6.04	118.40	126.72
5	D	903	ADP	N3-C4-N9	5.30	136.18	127.17
5	E	903	ADP	N3-C4-N9	5.15	135.93	127.17
5	F	903	ADP	N3-C4-N9	5.13	135.89	127.17
5	C	903	ADP	N3-C4-N9	4.90	135.51	127.17
3	E	901	ANP	O2B-PB-O1B	4.88	120.34	109.87
3	B	901	ANP	O2B-PB-O1B	4.81	120.18	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	ANP	O2B-PB-O1B	4.81	120.17	109.87
5	A	903	ADP	N3-C4-N9	4.78	135.30	127.17
3	D	901	ANP	O2B-PB-O1B	4.77	120.11	109.87
5	B	903	ADP	N3-C4-N9	4.77	135.28	127.17
3	C	901	ANP	O2B-PB-O1B	4.74	120.04	109.87
3	F	901	ANP	O2B-PB-O1B	4.70	119.96	109.87
5	D	903	ADP	C2-N3-C4	4.09	121.83	111.83
3	D	901	ANP	O1G-PG-N3B	-3.93	105.98	111.77
5	E	903	ADP	C2-N3-C4	3.92	121.39	111.83
3	A	901	ANP	O1G-PG-N3B	-3.91	106.01	111.77
5	F	903	ADP	C2-N3-C4	3.88	121.30	111.83
5	C	903	ADP	C2-N3-C4	3.78	121.07	111.83
5	B	903	ADP	C2-N3-C4	3.76	121.00	111.83
3	B	901	ANP	O1G-PG-N3B	-3.75	106.24	111.77
5	A	903	ADP	C2-N3-C4	3.75	120.98	111.83
3	C	901	ANP	O1G-PG-N3B	-3.73	106.28	111.77
3	E	901	ANP	O1G-PG-N3B	-3.63	106.42	111.77
3	F	901	ANP	O1G-PG-N3B	-3.59	106.48	111.77
5	B	903	ADP	C4-C5-N7	-3.51	106.57	110.58
5	C	903	ADP	C4-C5-N7	-3.44	106.65	110.58
5	E	903	ADP	C4-C5-N7	-3.43	106.66	110.58
5	A	903	ADP	C4-C5-N7	-3.40	106.69	110.58
5	D	903	ADP	N3-C2-N1	-3.36	123.49	128.58
5	D	903	ADP	C4-C5-N7	-3.33	106.77	110.58
5	F	903	ADP	C4-C5-N7	-3.23	106.88	110.58
5	F	903	ADP	N3-C2-N1	-3.22	123.71	128.58
5	A	903	ADP	N3-C2-N1	-3.21	123.73	128.58
5	B	903	ADP	N3-C2-N1	-3.20	123.74	128.58
5	C	903	ADP	N3-C2-N1	-3.16	123.79	128.58
5	E	903	ADP	N3-C2-N1	-3.06	123.94	128.58
3	B	901	ANP	O2G-PG-O3G	2.73	114.92	107.59
5	F	903	ADP	C3'-C2'-C1'	2.71	106.58	101.46
3	A	901	ANP	O2G-PG-O3G	2.66	114.74	107.59
3	D	901	ANP	O2G-PG-O3G	2.64	114.70	107.59
3	E	901	ANP	O2G-PG-O3G	2.61	114.61	107.59
5	D	903	ADP	C3'-C2'-C1'	2.60	106.38	101.46
5	B	903	ADP	C3'-C2'-C1'	2.60	106.38	101.46
3	C	901	ANP	O2G-PG-O3G	2.59	114.55	107.59
5	B	903	ADP	C5-N7-C8	2.55	107.46	103.45
5	B	903	ADP	C4-N9-C8	2.55	108.41	105.74
5	E	903	ADP	C3'-C2'-C1'	2.54	106.27	101.46
5	E	903	ADP	C5-N7-C8	2.50	107.38	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	903	ADP	C5-N7-C8	2.46	107.32	103.45
5	D	903	ADP	C5-N7-C8	2.45	107.30	103.45
5	C	903	ADP	C3'-C2'-C1'	2.44	106.08	101.46
3	F	901	ANP	O2G-PG-O3G	2.44	114.14	107.59
5	A	903	ADP	C3'-C2'-C1'	2.42	106.04	101.46
5	A	903	ADP	C5-N7-C8	2.42	107.25	103.45
5	F	903	ADP	C5-N7-C8	2.41	107.24	103.45
5	F	903	ADP	C4-N9-C8	2.36	108.22	105.74
5	C	903	ADP	C4-N9-C8	2.33	108.19	105.74
5	A	903	ADP	C4-N9-C8	2.32	108.17	105.74
5	D	903	ADP	C4-N9-C8	2.13	107.97	105.74
5	E	903	ADP	C4-N9-C8	2.10	107.95	105.74

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ANP	PB-N3B-PG-O1G
3	A	901	ANP	PG-N3B-PB-O1B
3	A	901	ANP	PG-N3B-PB-O3A
3	A	901	ANP	PA-O3A-PB-O2B
3	A	901	ANP	C5'-O5'-PA-O2A
3	B	901	ANP	PB-N3B-PG-O1G
3	B	901	ANP	PG-N3B-PB-O1B
3	B	901	ANP	PG-N3B-PB-O3A
3	B	901	ANP	C5'-O5'-PA-O1A
3	B	901	ANP	C5'-O5'-PA-O2A
3	B	901	ANP	C5'-O5'-PA-O3A
3	B	901	ANP	O4'-C4'-C5'-O5'
3	C	901	ANP	PB-N3B-PG-O1G
3	C	901	ANP	PG-N3B-PB-O1B
3	C	901	ANP	PG-N3B-PB-O3A
3	C	901	ANP	C5'-O5'-PA-O2A
3	D	901	ANP	PB-N3B-PG-O1G
3	D	901	ANP	PG-N3B-PB-O1B
3	D	901	ANP	PG-N3B-PB-O3A
3	D	901	ANP	PA-O3A-PB-O2B
3	D	901	ANP	C5'-O5'-PA-O1A
3	D	901	ANP	C5'-O5'-PA-O2A
3	D	901	ANP	C5'-O5'-PA-O3A
3	E	901	ANP	PB-N3B-PG-O1G
3	E	901	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	E	901	ANP	PG-N3B-PB-O3A
3	E	901	ANP	C5'-O5'-PA-O1A
3	E	901	ANP	C5'-O5'-PA-O3A
3	E	901	ANP	O4'-C4'-C5'-O5'
3	F	901	ANP	PG-N3B-PB-O1B
3	F	901	ANP	PG-N3B-PB-O3A
3	F	901	ANP	PA-O3A-PB-O2B
3	F	901	ANP	C5'-O5'-PA-O1A
3	F	901	ANP	C5'-O5'-PA-O2A
3	F	901	ANP	C5'-O5'-PA-O3A
5	A	903	ADP	O4'-C4'-C5'-O5'
5	A	903	ADP	C3'-C4'-C5'-O5'
5	C	903	ADP	C5'-O5'-PA-O1A
5	D	903	ADP	C5'-O5'-PA-O1A
5	D	903	ADP	C5'-O5'-PA-O3A
5	E	903	ADP	C5'-O5'-PA-O1A
5	E	903	ADP	C5'-O5'-PA-O3A
5	F	903	ADP	C5'-O5'-PA-O3A
3	B	901	ANP	C3'-C4'-C5'-O5'
3	E	901	ANP	C3'-C4'-C5'-O5'
3	E	901	ANP	C4'-C5'-O5'-PA
5	D	903	ADP	C2'-C1'-N9-C4
5	D	903	ADP	C2'-C1'-N9-C8
5	F	903	ADP	C5'-O5'-PA-O1A
5	E	903	ADP	C2'-C1'-N9-C8
5	E	903	ADP	C2'-C1'-N9-C4
3	F	901	ANP	C4'-C5'-O5'-PA
5	B	903	ADP	O4'-C4'-C5'-O5'
3	C	901	ANP	PB-O3A-PA-O2A
5	C	903	ADP	PB-O3A-PA-O1A
3	F	901	ANP	PA-O3A-PB-O1B
5	F	903	ADP	C2'-C1'-N9-C8
5	C	903	ADP	PB-O3A-PA-O2A

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	903	ADP	1	0
3	D	901	ANP	1	0
5	D	903	ADP	1	0
3	C	901	ANP	1	0

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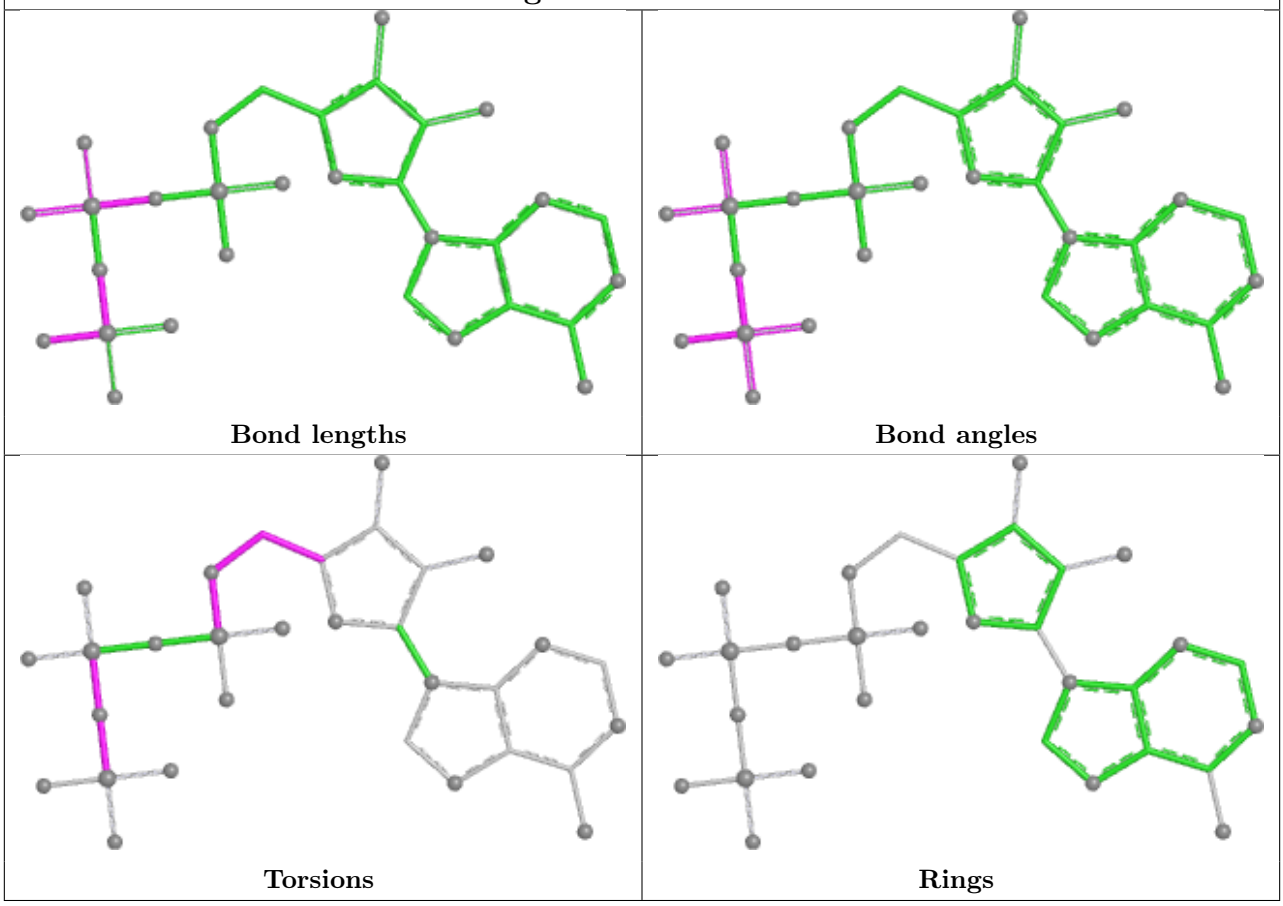
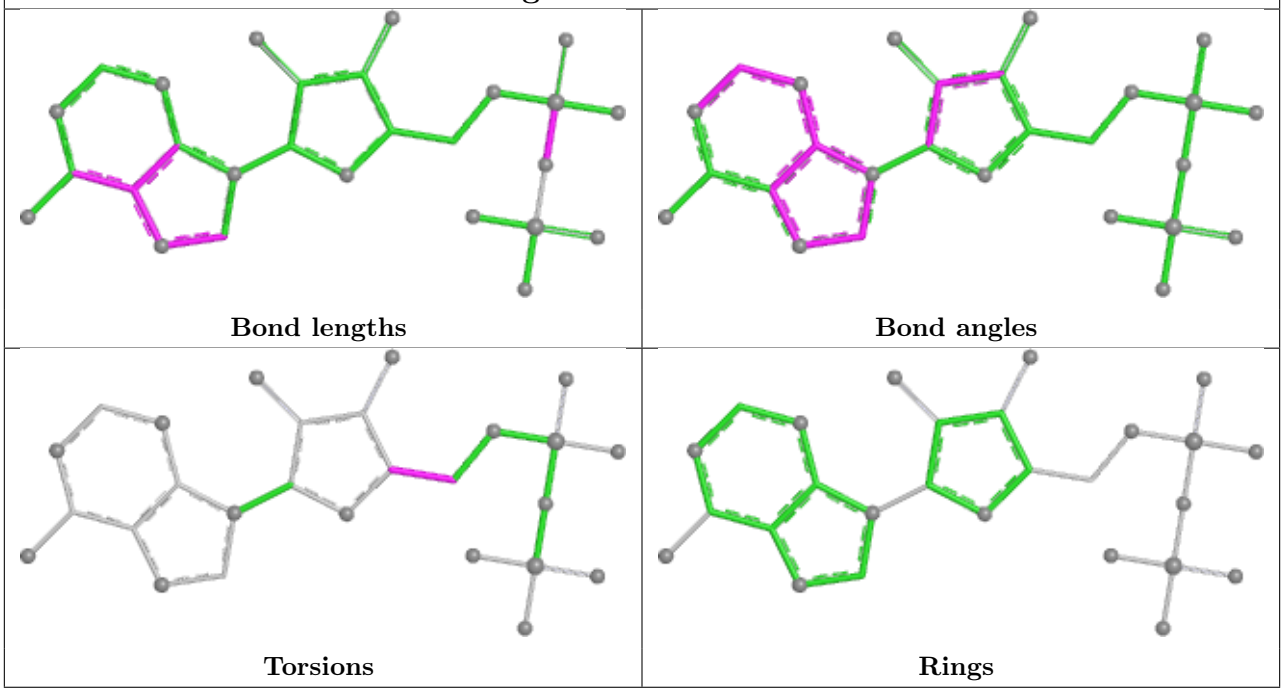
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ANP	2	0
5	C	903	ADP	2	0
5	E	903	ADP	3	0
5	F	903	ADP	3	0
3	F	901	ANP	3	0
5	B	903	ADP	1	0
3	A	901	ANP	4	0

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.

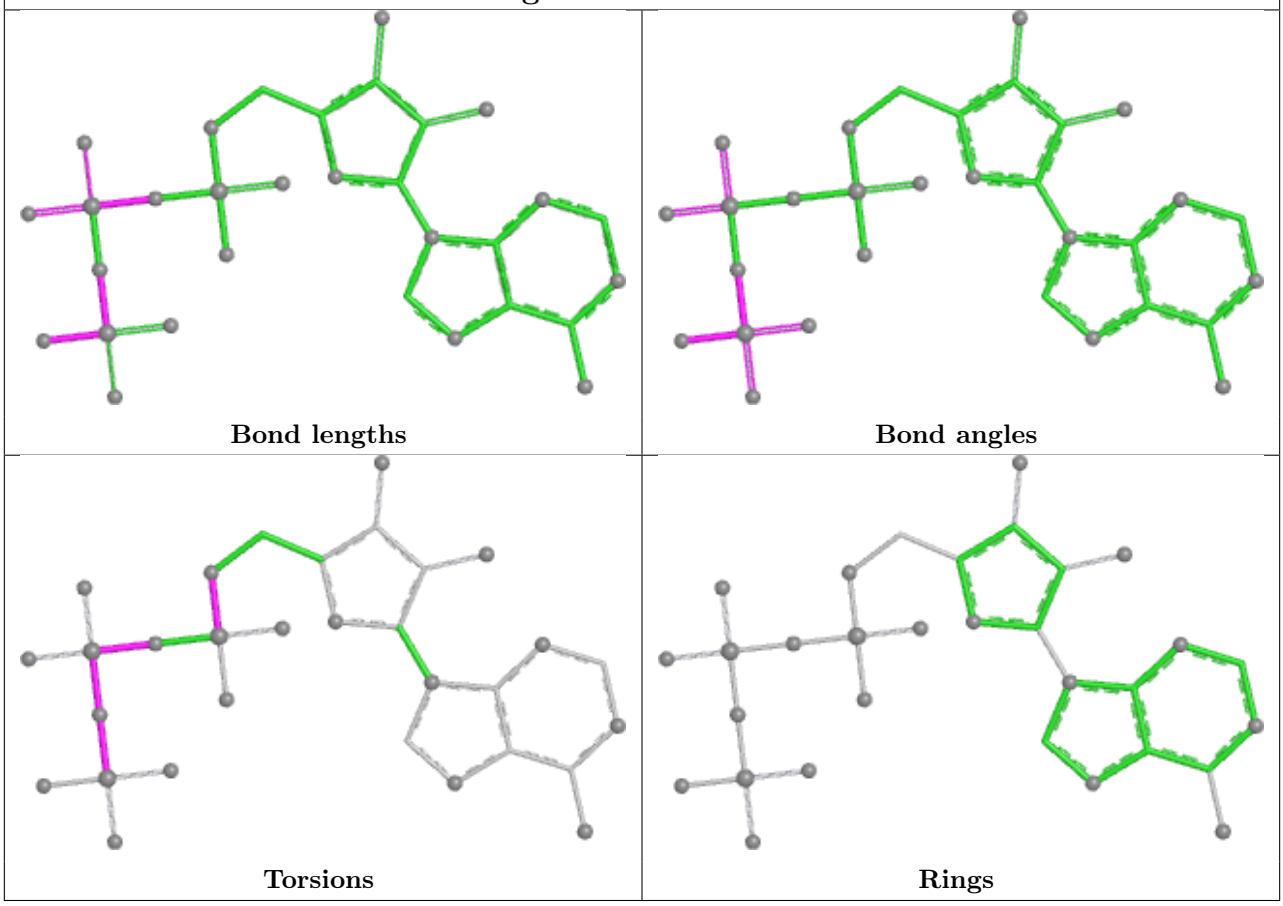
Ligand ANP E 901



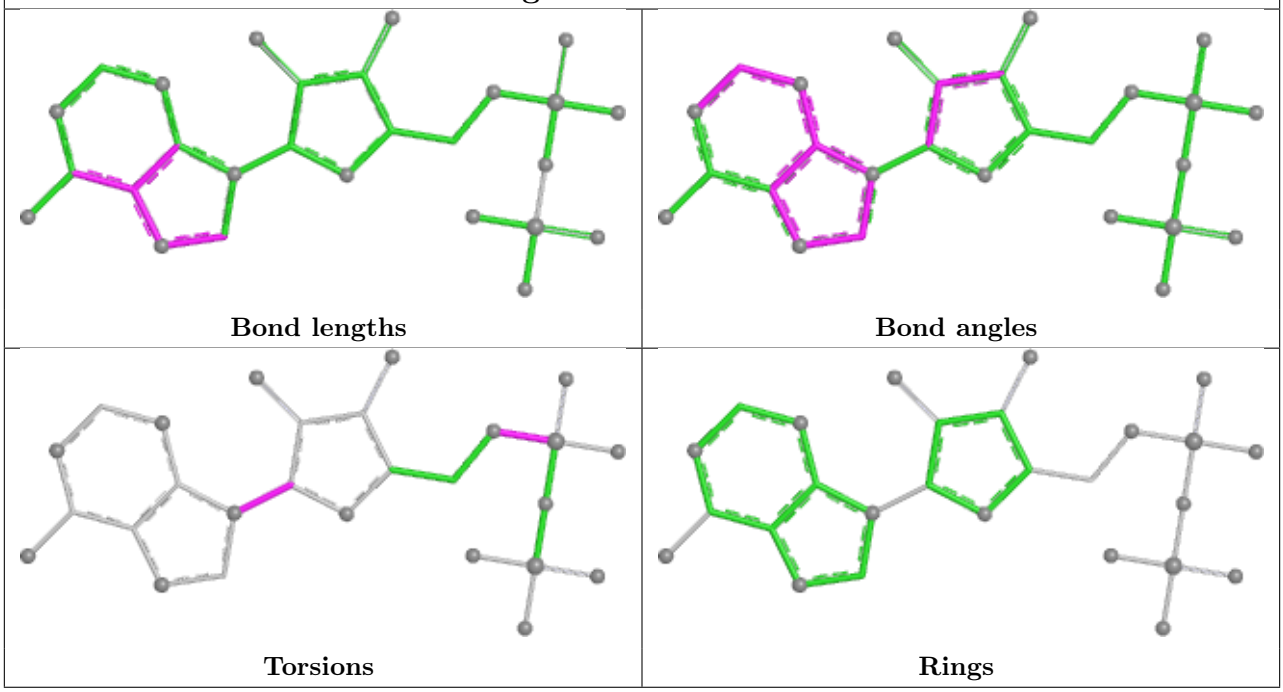
Ligand ADP A 903



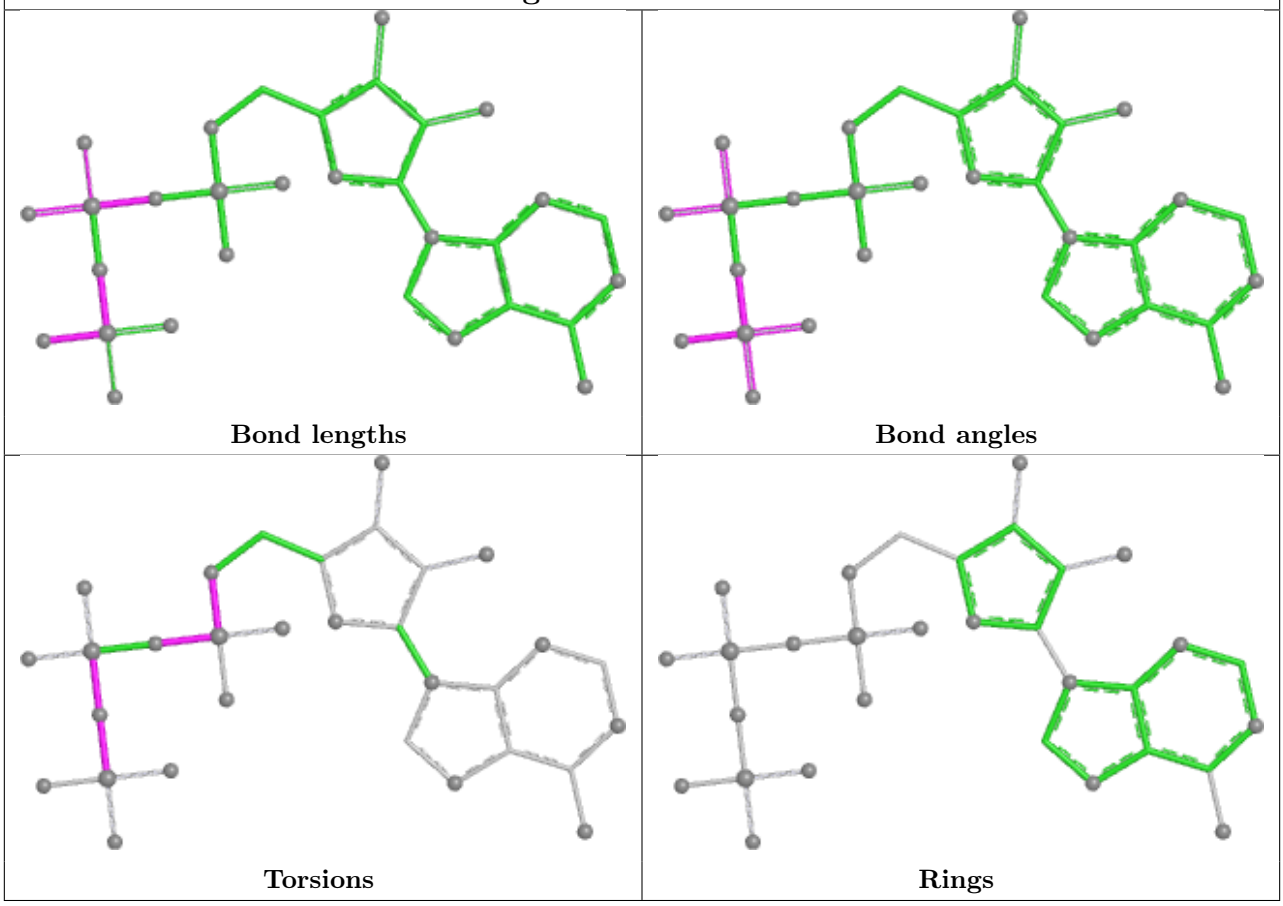
Ligand ANP D 901



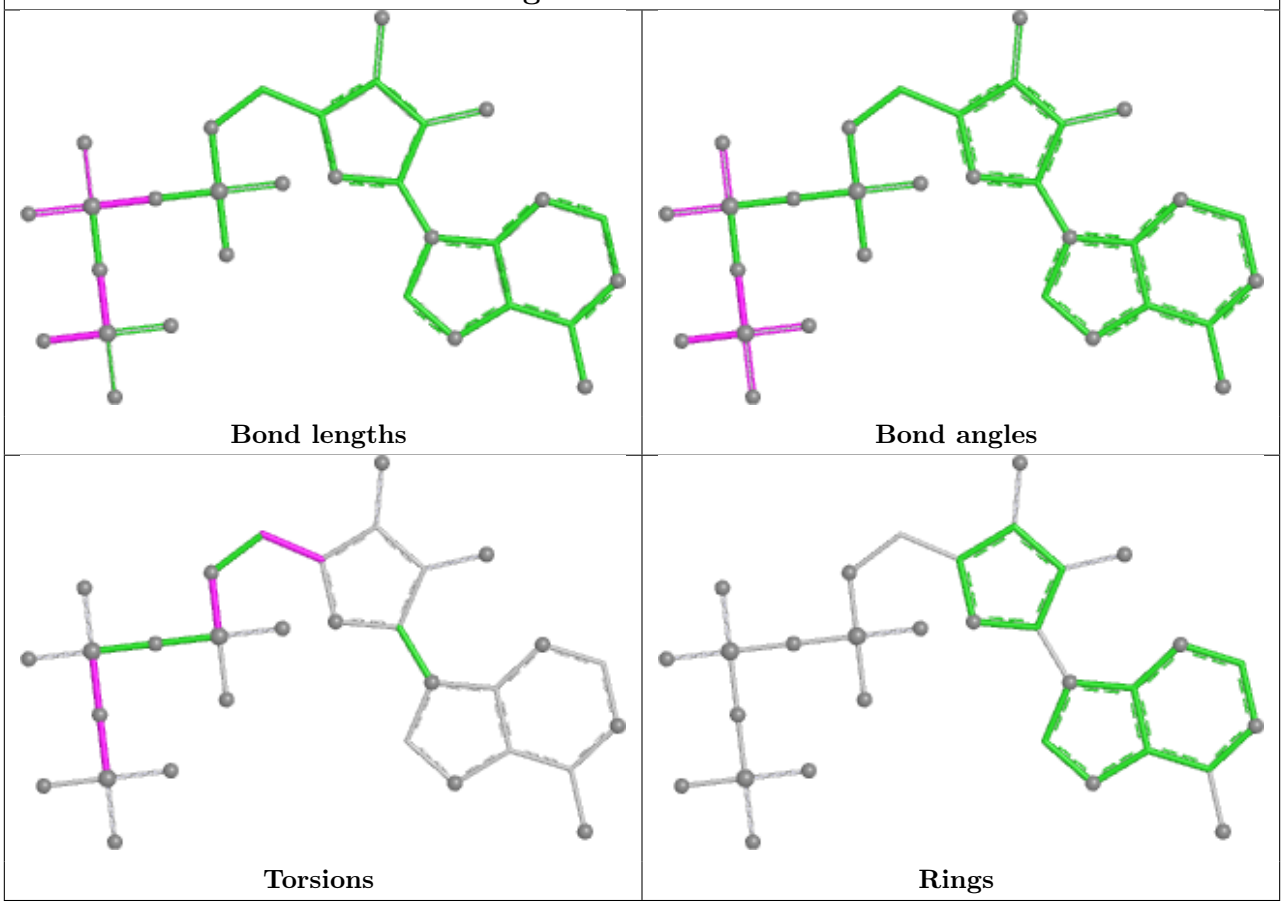
Ligand ADP D 903



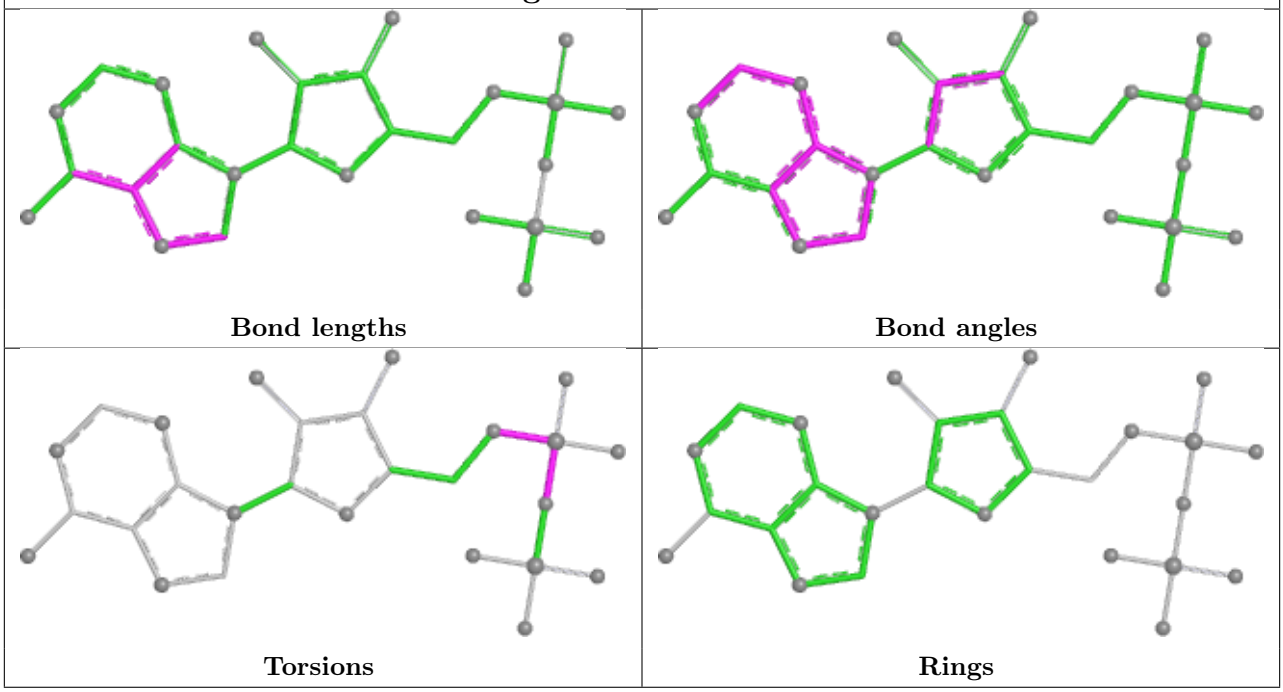
Ligand ANP C 901

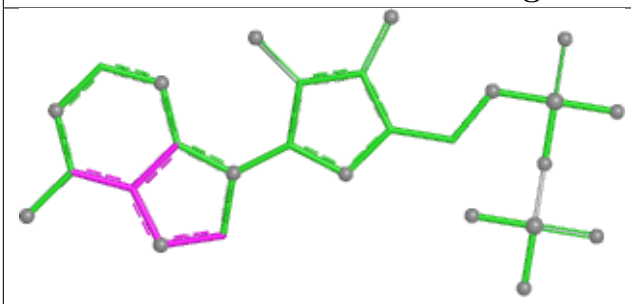
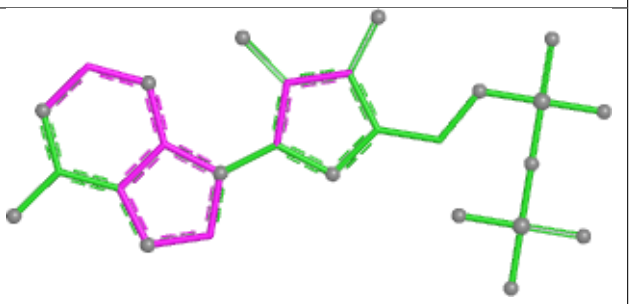
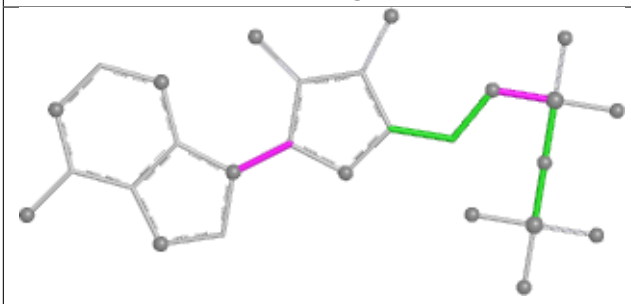
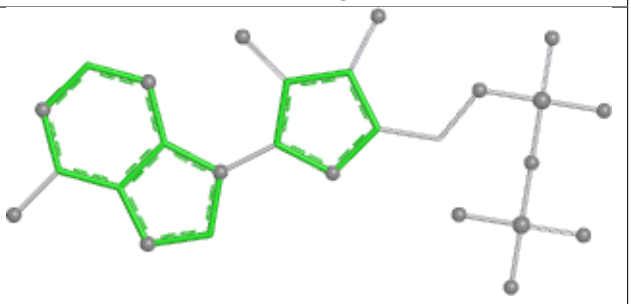


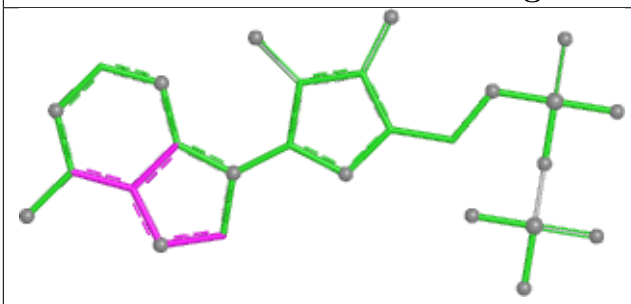
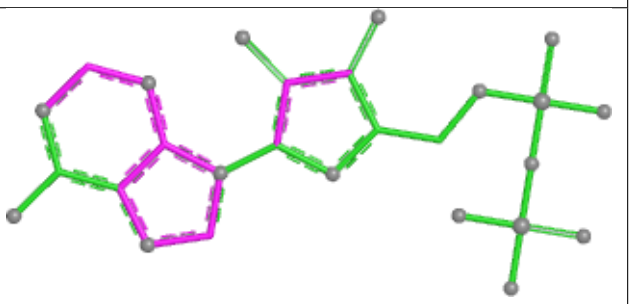
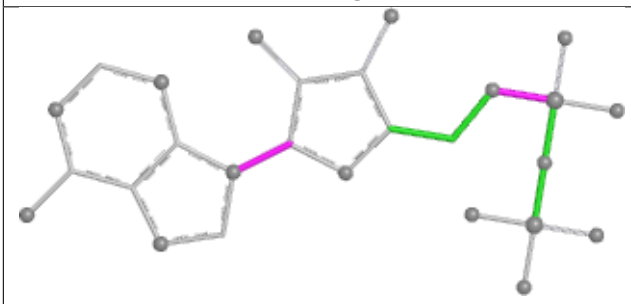
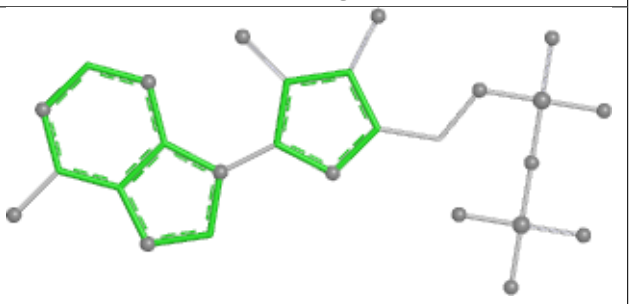
Ligand ANP B 901



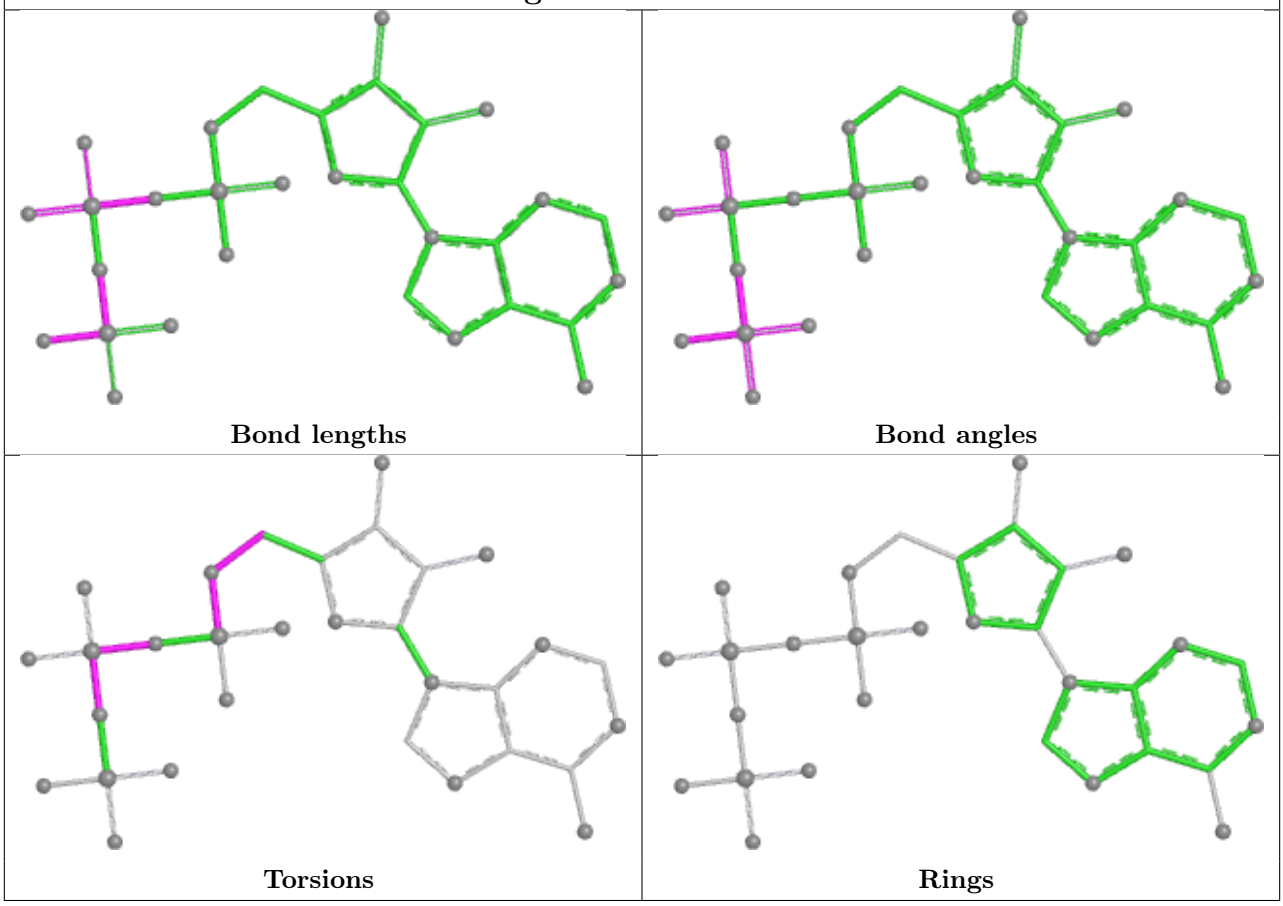
Ligand ADP C 903



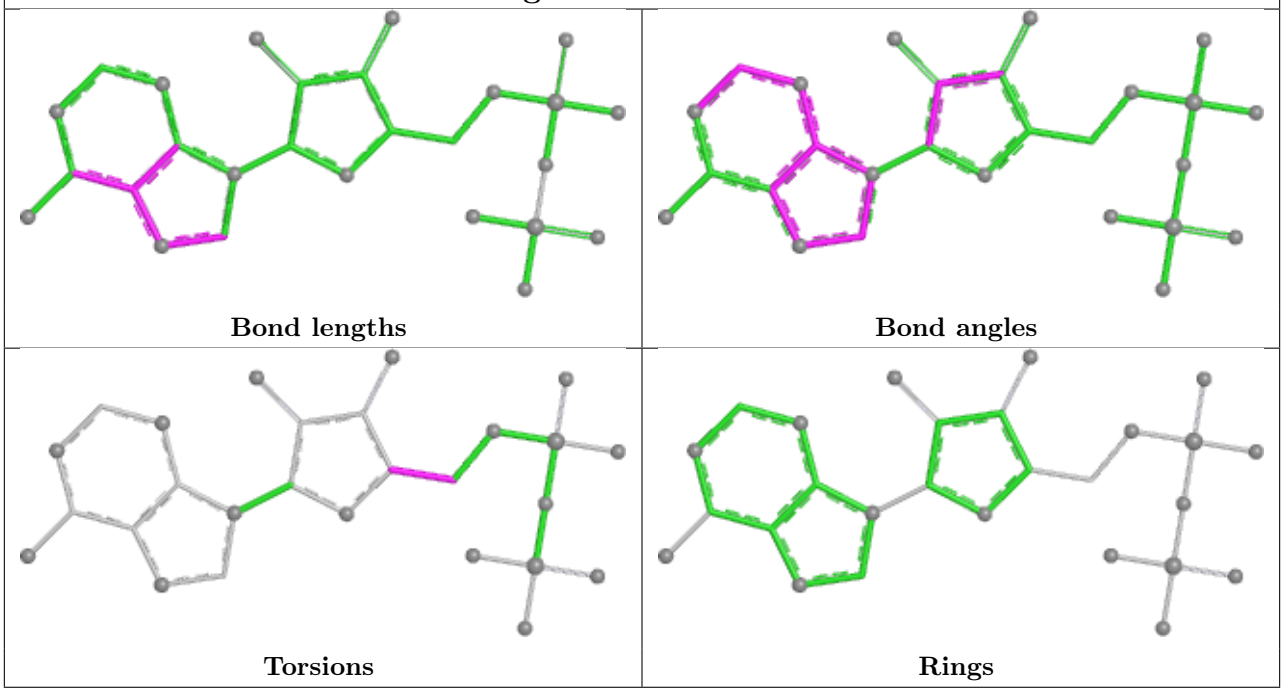
Ligand ADP E 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

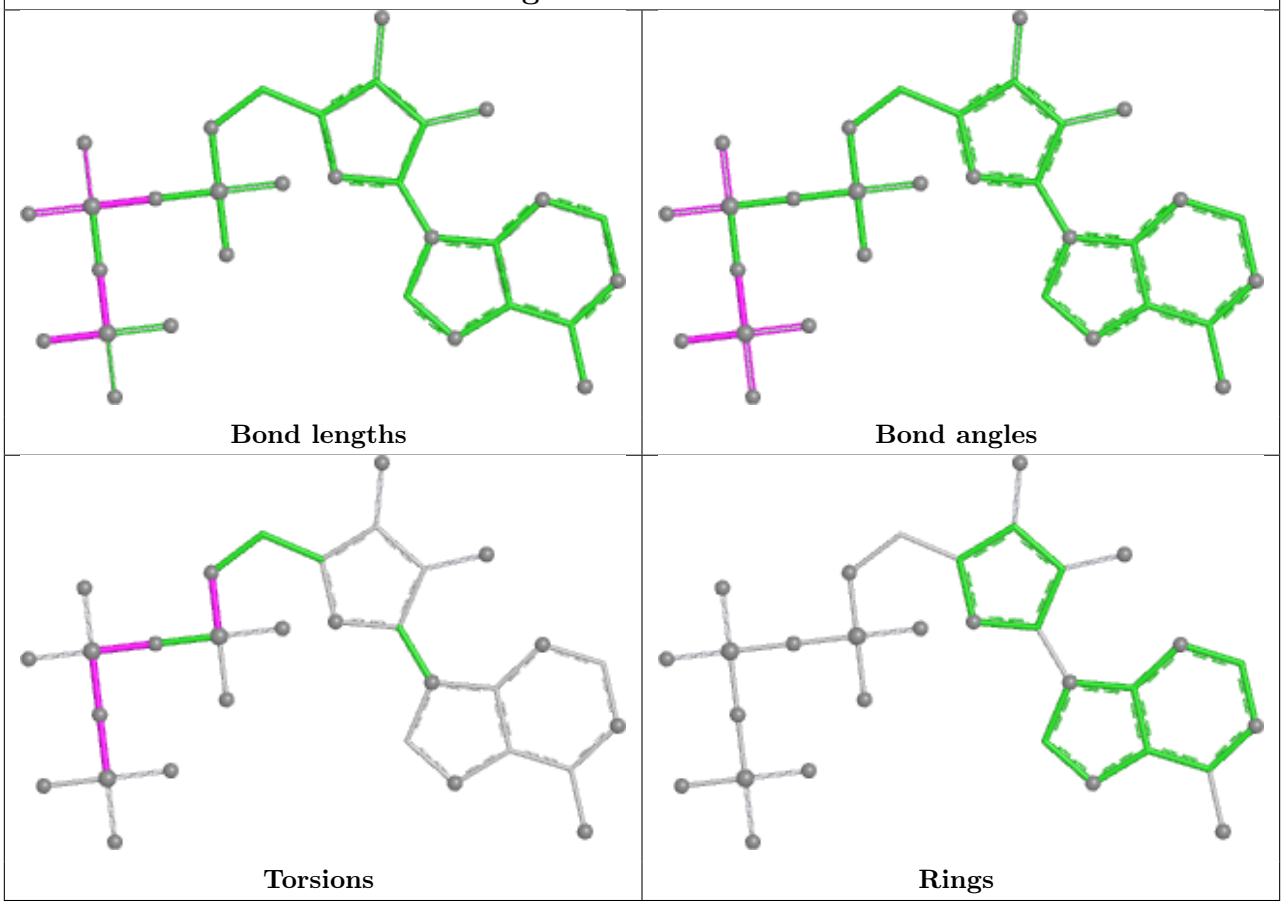
Ligand ANP F 901



Ligand ADP B 903



Ligand ANP A 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

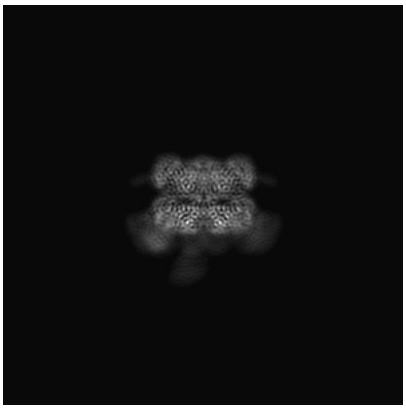
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-63612. These allow visual inspection of the internal detail of the map and identification of artifacts.

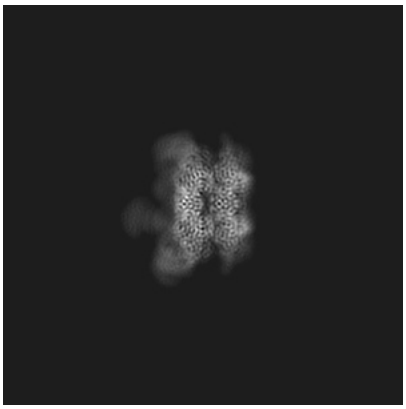
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

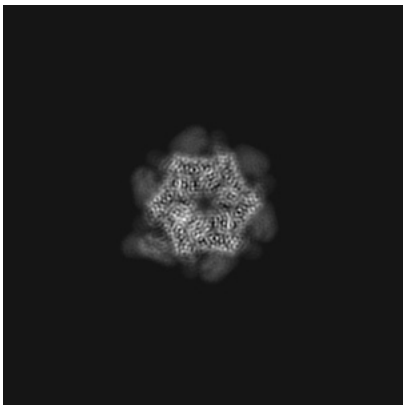
6.1.1 Primary map



X

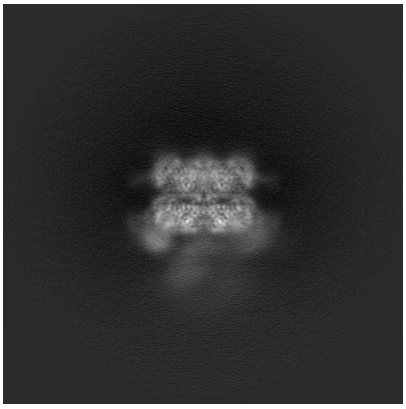


Y

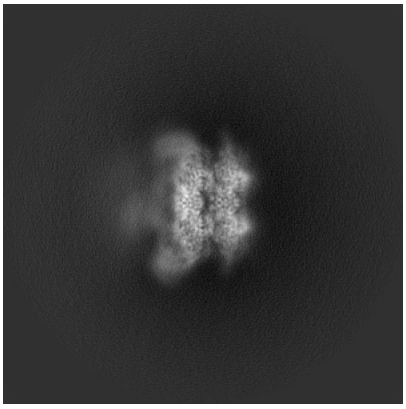


Z

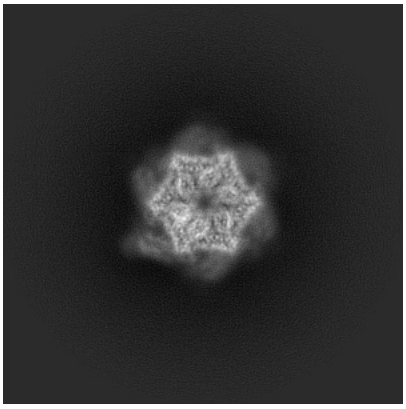
6.1.2 Raw map



X



Y



Z

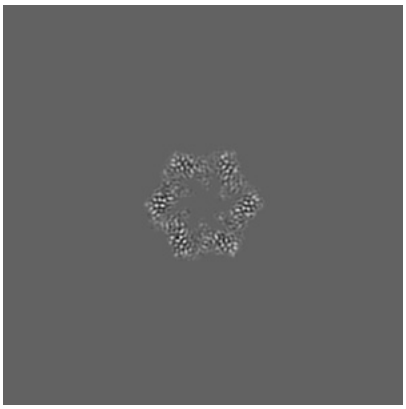
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

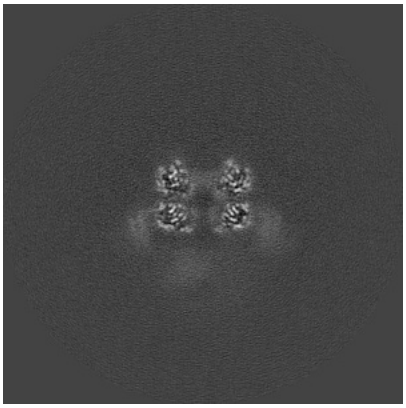
6.2.1 Primary map

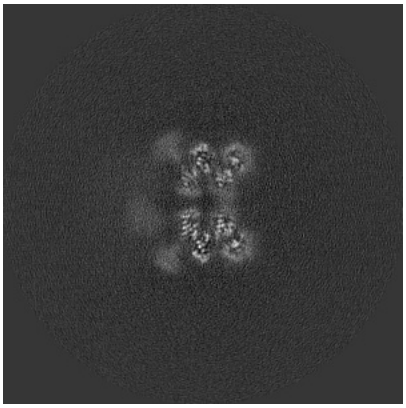
X Index: 180

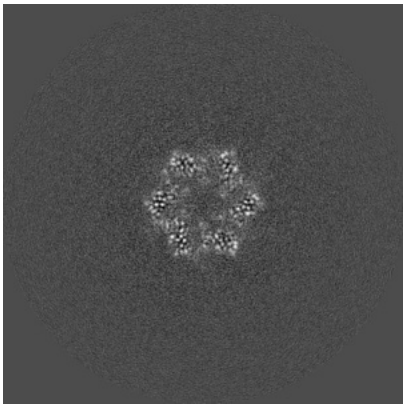
Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

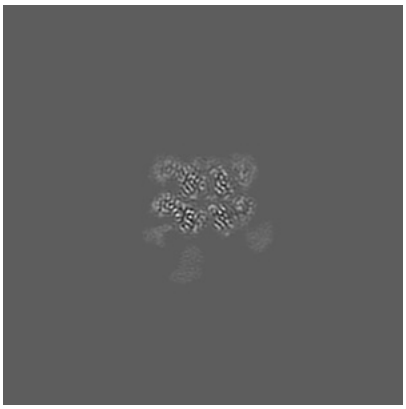

Y Index: 180

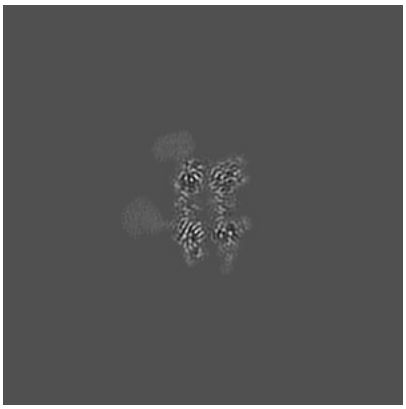

Z Index: 180

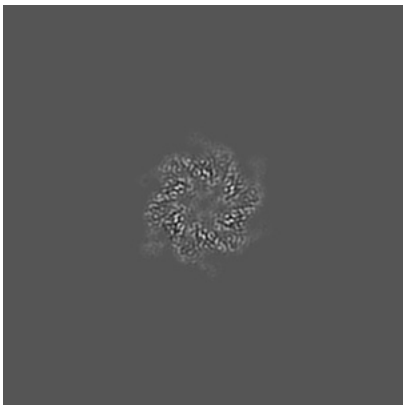
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

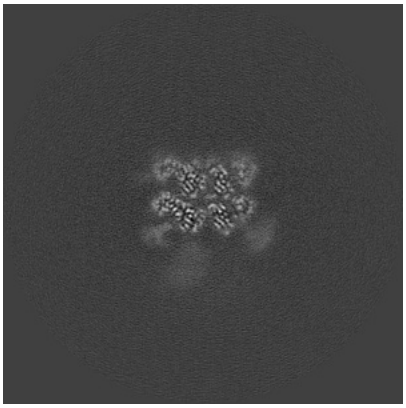
6.3.1 Primary map

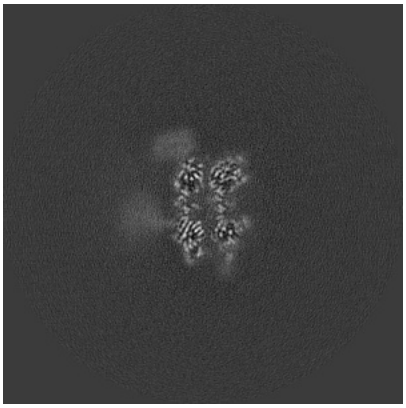

X Index: 156

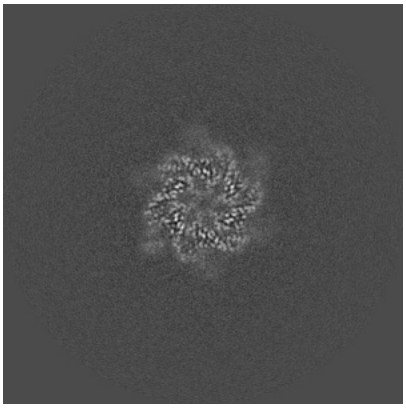

Y Index: 166


Z Index: 173

6.3.2 Raw map


X Index: 156

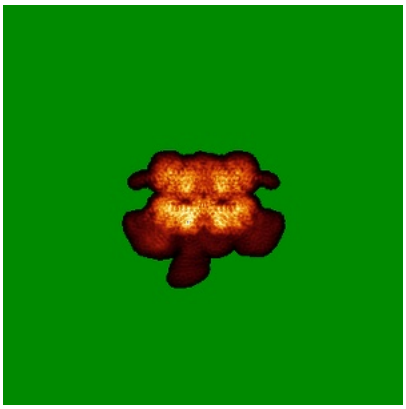

Y Index: 166

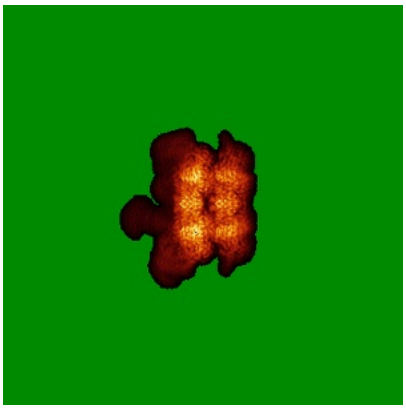

Z Index: 173

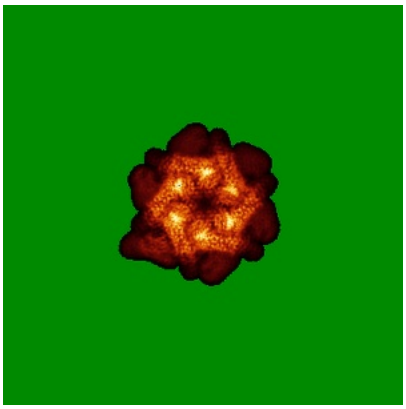
The images above show the largest variance slices of the map in three orthogonal directions.

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

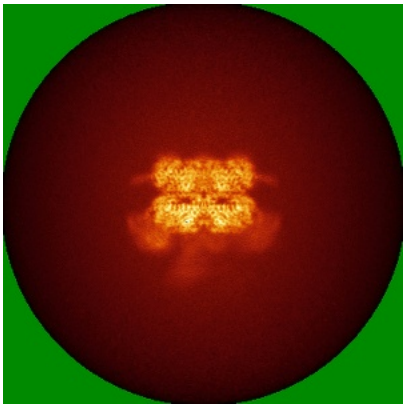
6.4.1 Primary map

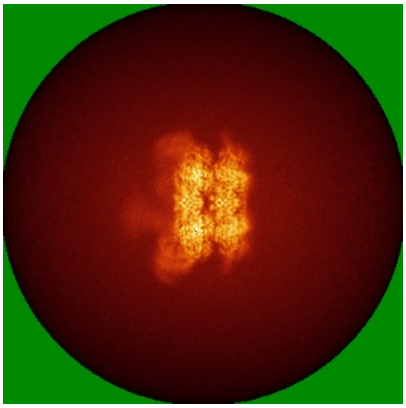

X

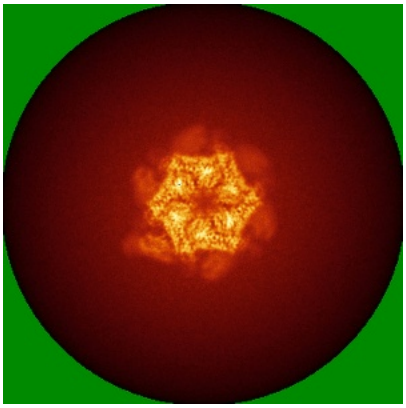

Y


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.

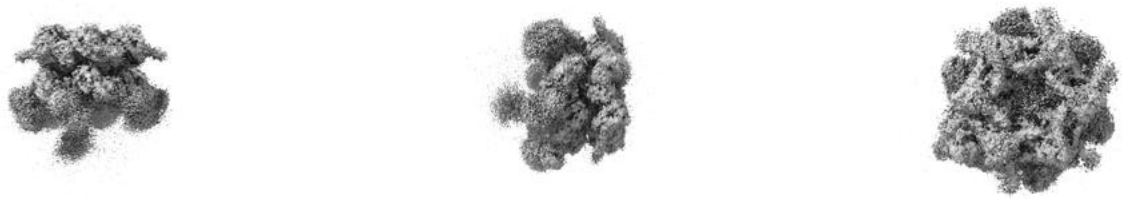
6.5 Orthogonal surface views (i)

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.

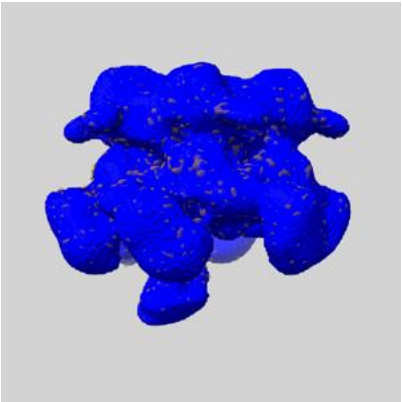
6.6 Mask visualisation (i)

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

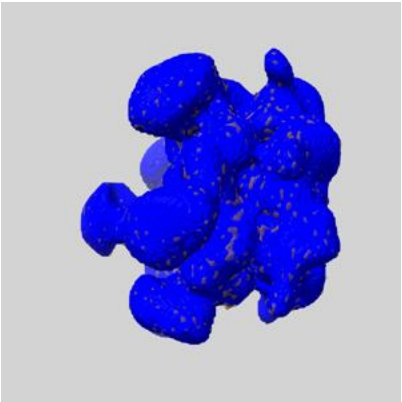
A mask typically either:

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

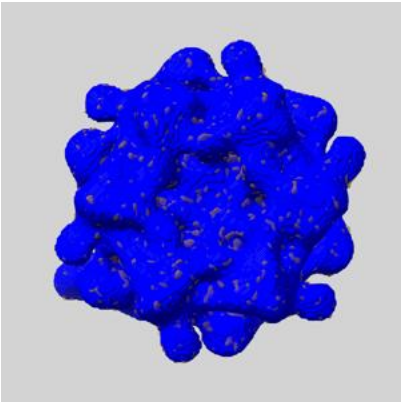
6.6.1 emd_63612_msk_1.map (i)



X



Y

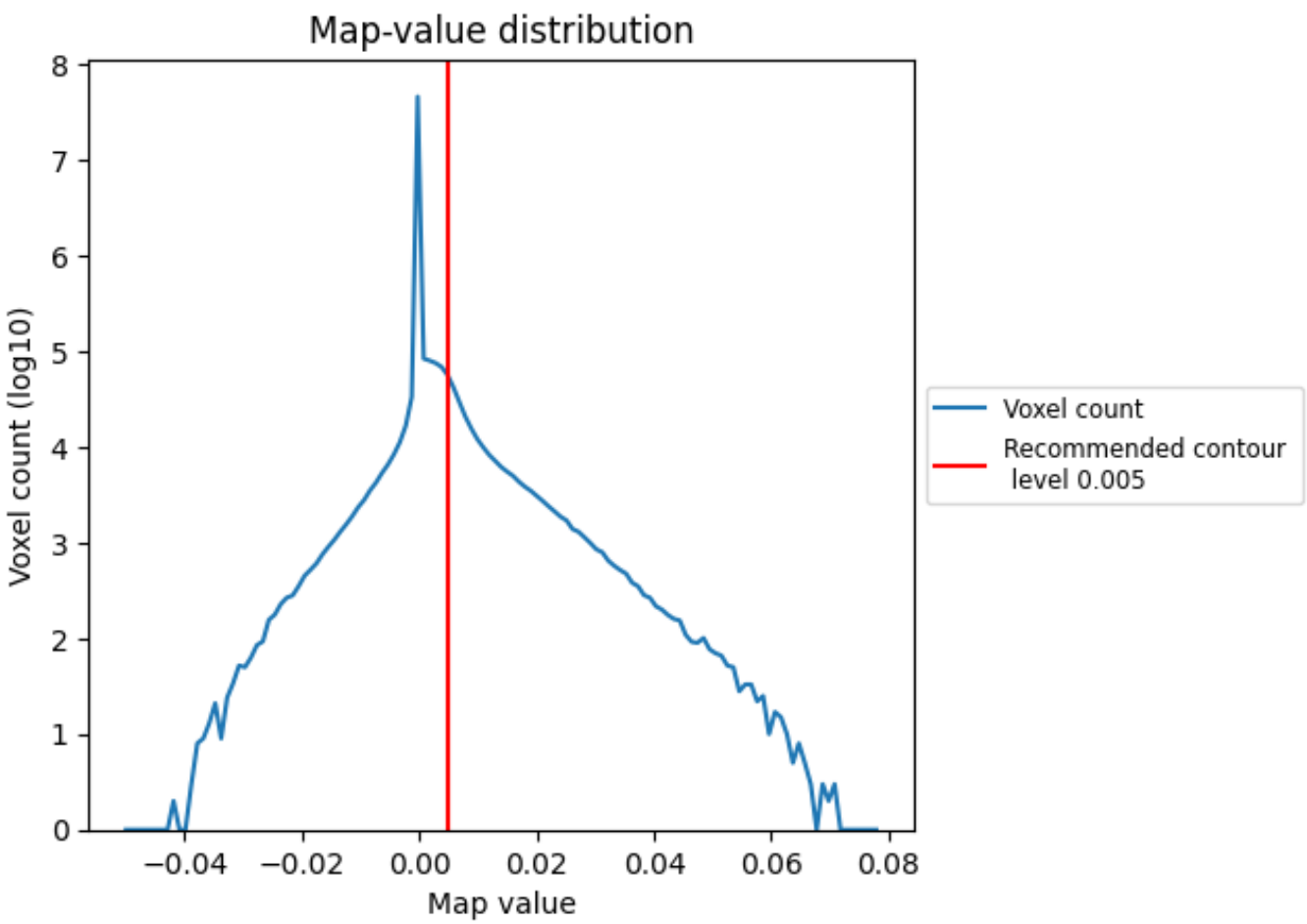


Z

7 Map analysis (i)

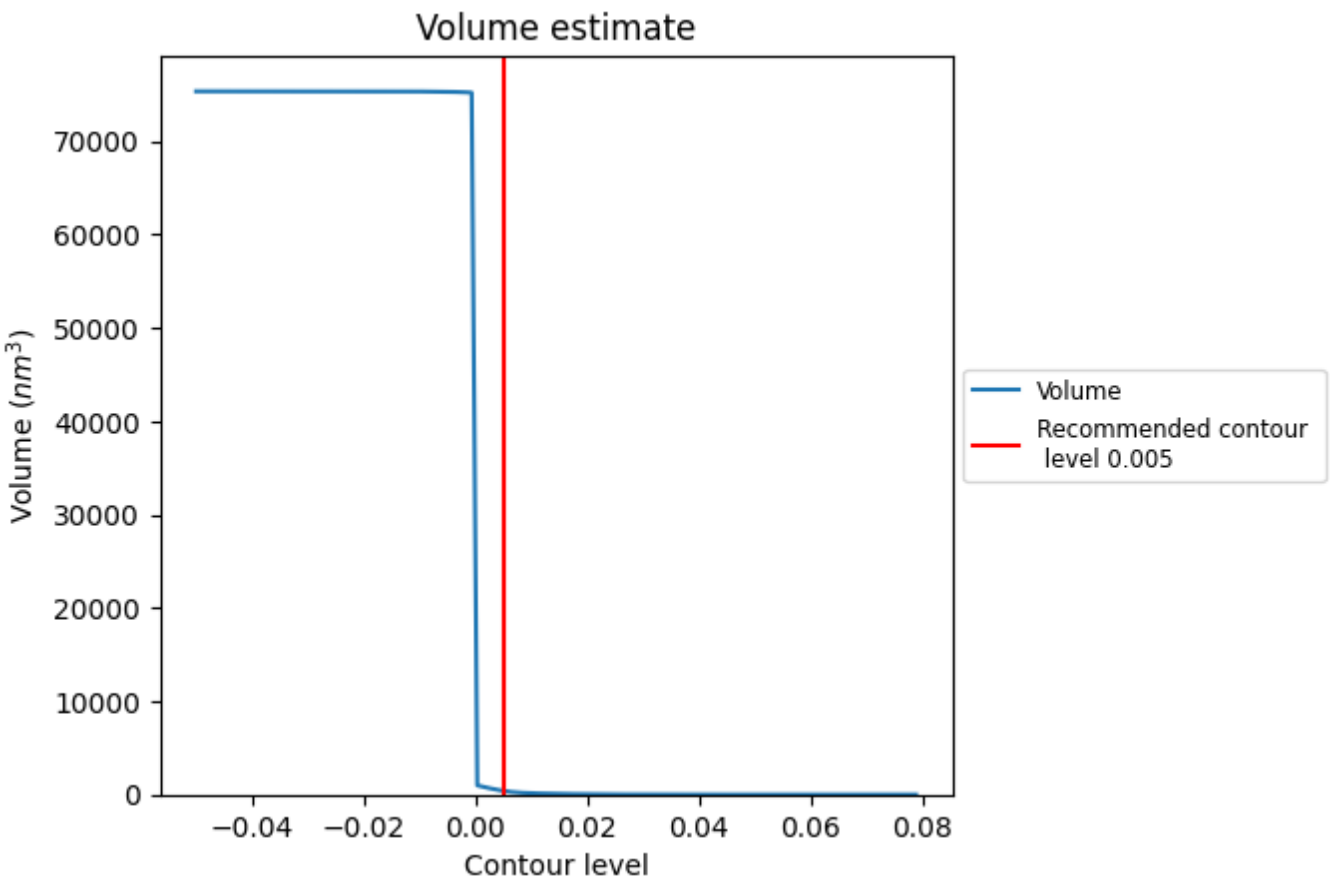
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

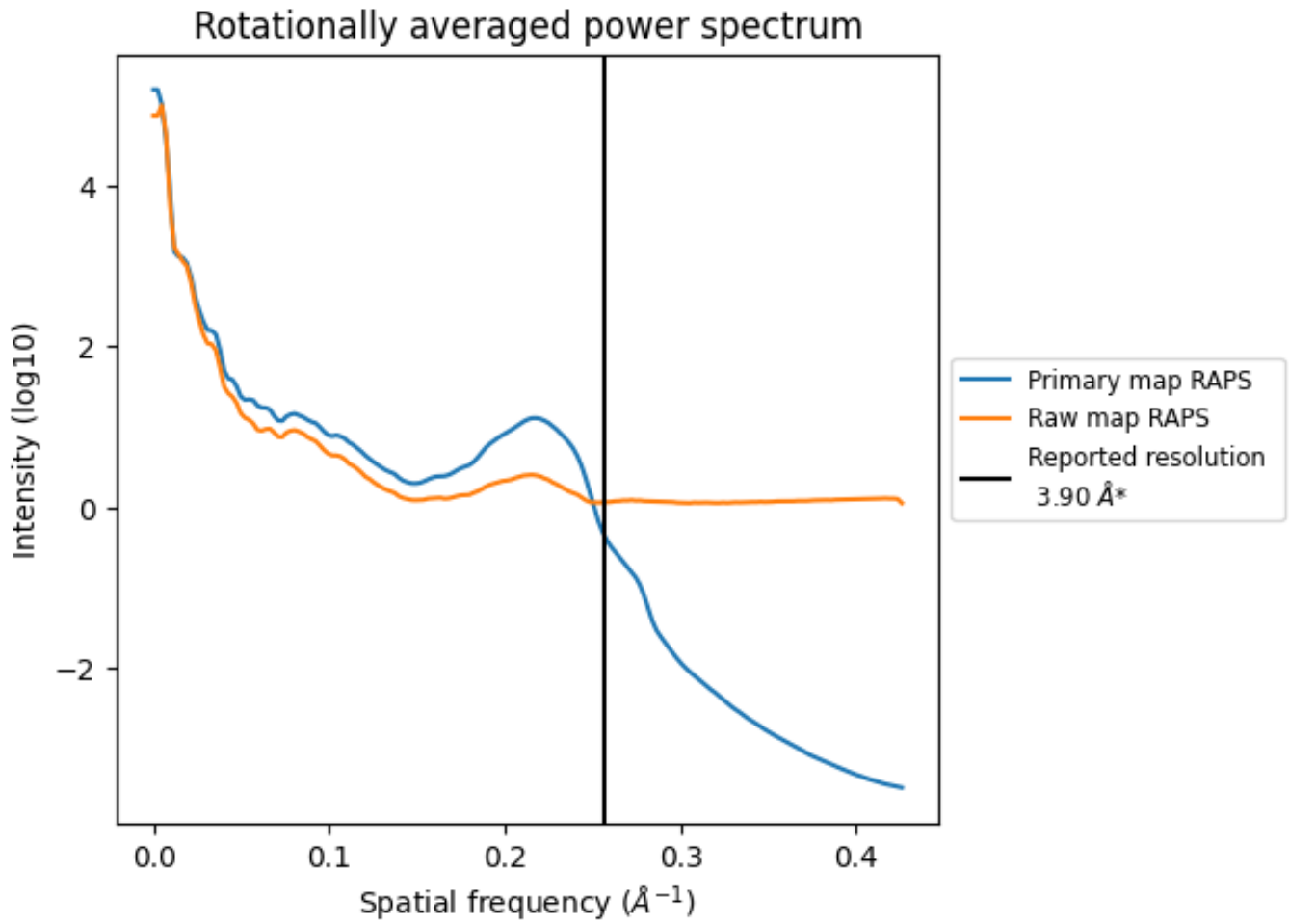
7.2 Volume estimate (i)



The volume at the recommended contour level is 398 nm^3; this corresponds to an approximate mass of 360 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)

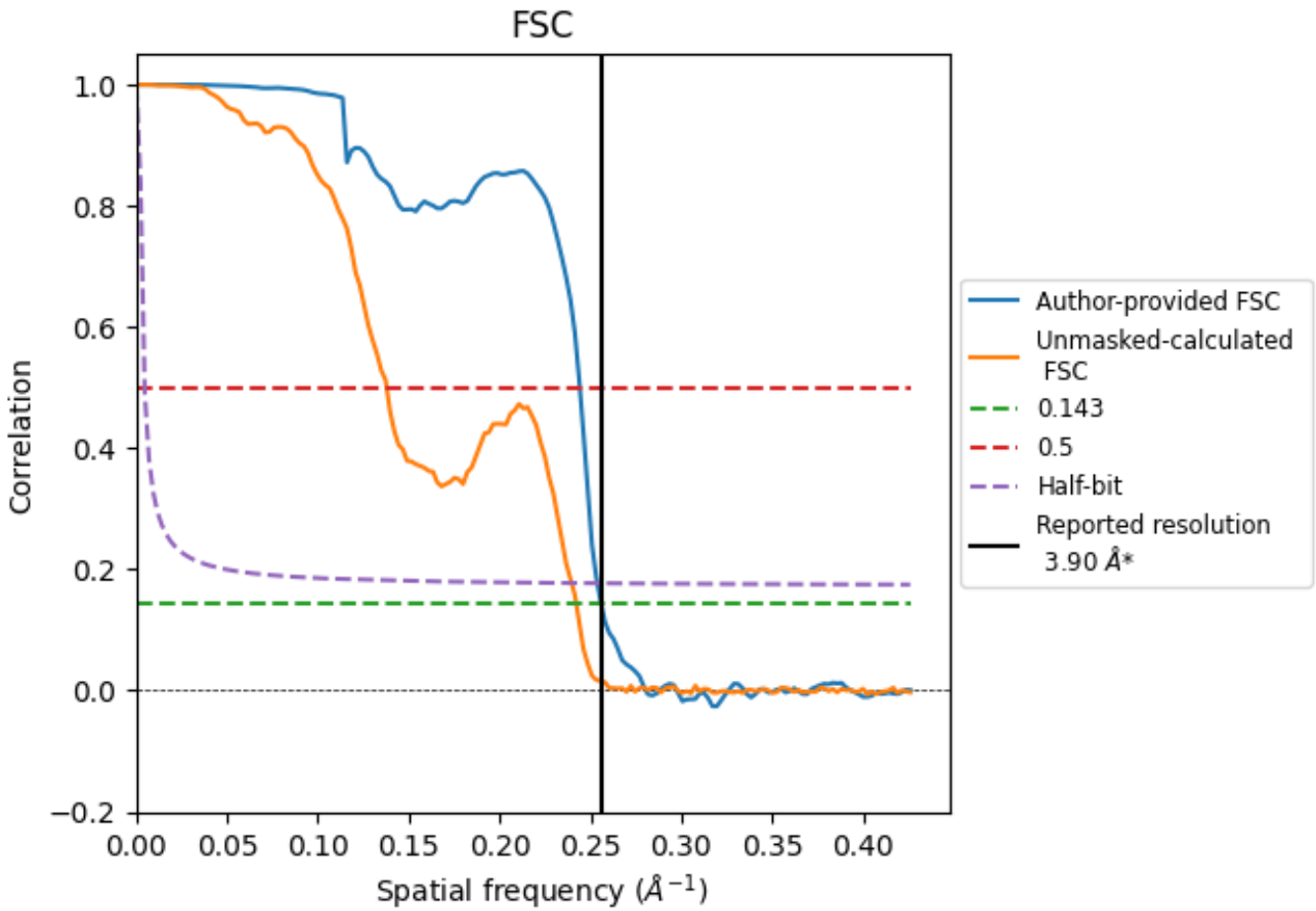


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

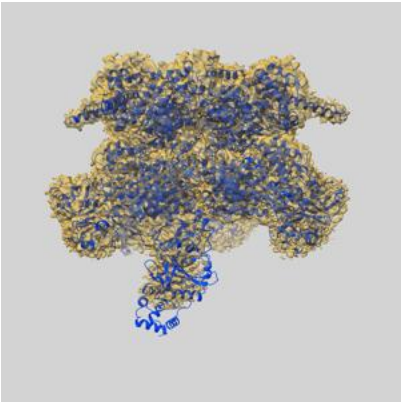
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.10	3.94
Unmasked-calculated*	4.13	7.25	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

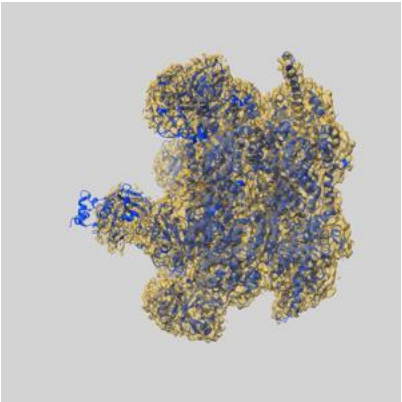
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-63612 and PDB model 9M3Z. Per-residue inclusion information can be found in section 3 on page 8.

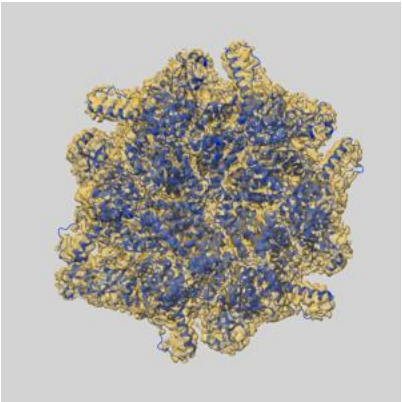
9.1 Map-model overlay (i)



X



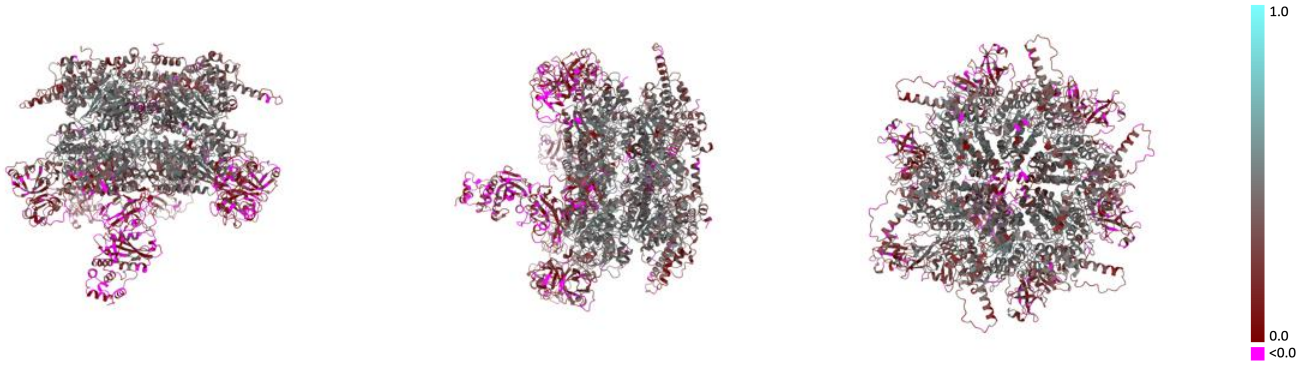
Y



Z

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

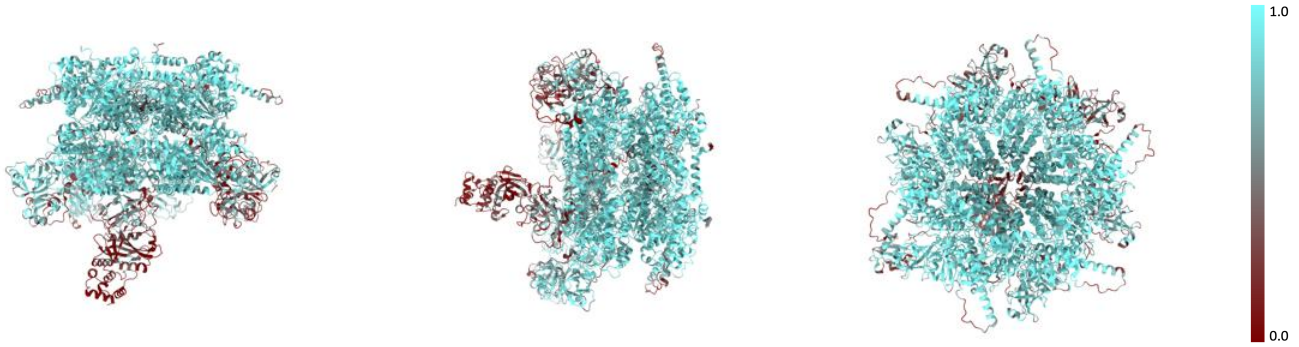
9.2 Q-score mapped to coordinate model (i)



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.

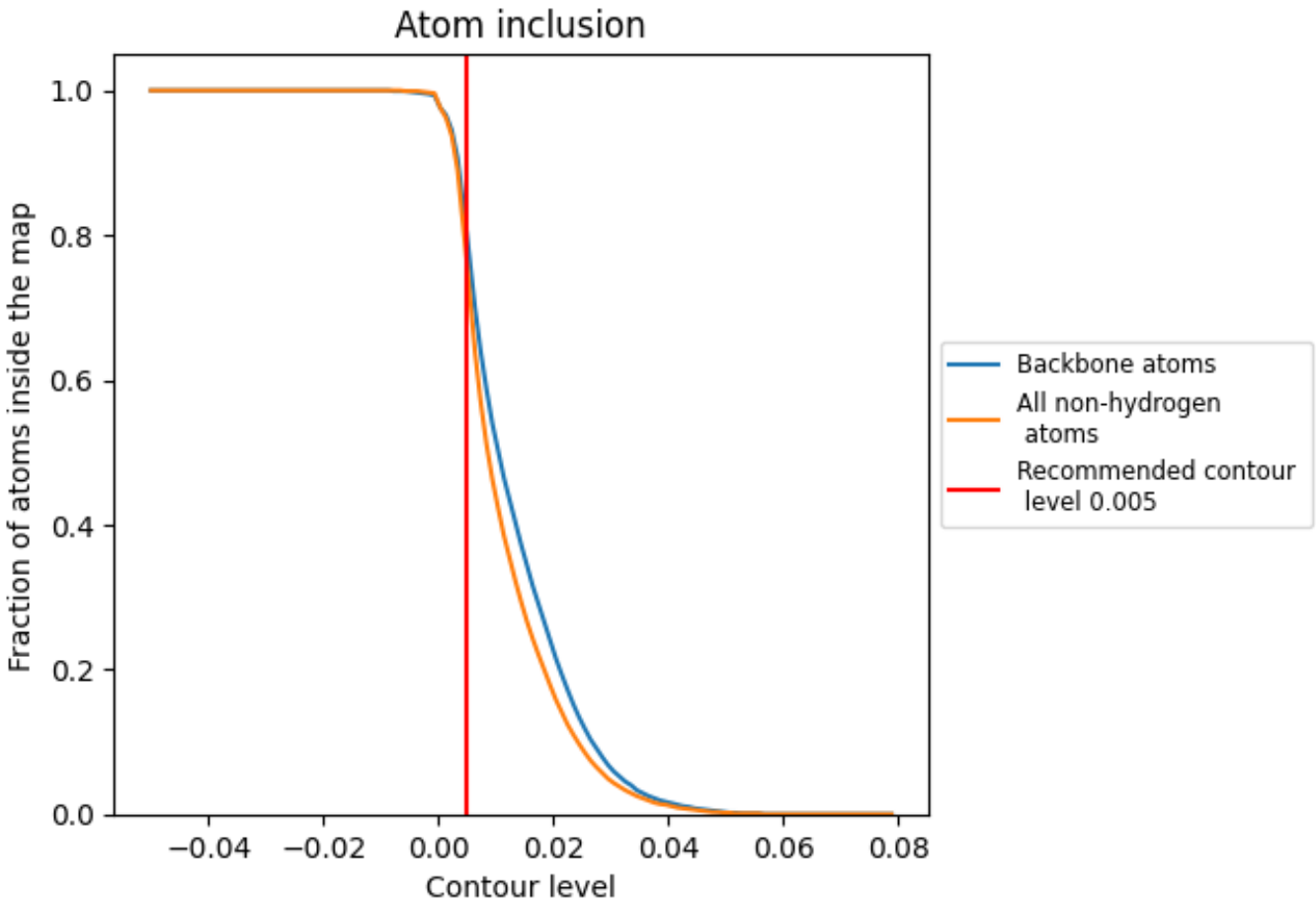
9.3 Atom inclusion mapped to coordinate model (i)



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, 80% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.7610	0.3300
A	0.8350	0.3610
B	0.8730	0.3850
C	0.8230	0.3650
D	0.7900	0.3370
E	0.7280	0.3110
F	0.7790	0.3470
G	0.2820	0.0960