



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:24 PM UTC

PDB ID : 8DAT / pdb_00008dat
EMDB ID : EMD-27275
Title : Saccharomyces cerevisiae Ufd1/Npl4/Cdc48 complex bound to three ubiquitin moieties in presence of SUMO-ubiquitin(K48polyUb)-mEOS and ATP, state 1 (intB)
Authors : Lee, H.G.; Lima, C.D.
Deposited on : 2022-06-14
Resolution : 3.80 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

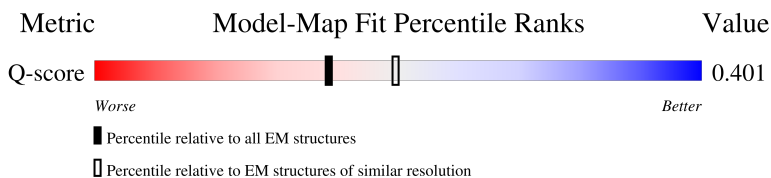
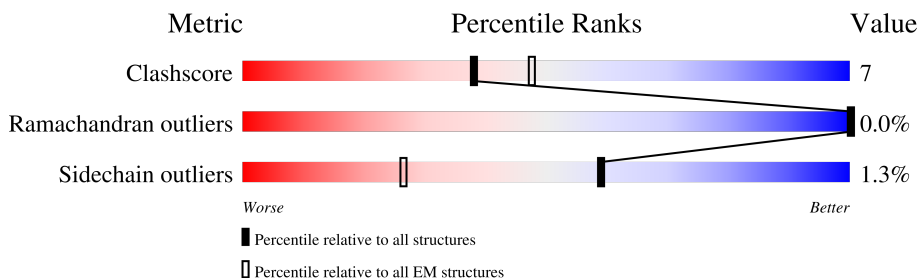
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	A	838	23% (red), 71% (green), 14% (yellow), 15% (grey)
1	B	838	6% (red), 57% (green), 9% (yellow), 33% (grey)
1	C	838	24% (red), 70% (green), 16% (yellow), 15% (grey)
1	D	838	7% (red), 56% (green), 11% (yellow), 33% (grey)

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Mol	Chain	Length	Quality of chain
1	E	838	<p>5% 54% 10% 36%</p>
1	F	838	<p>5% 55% 9% 35%</p>
2	G	583	<p>5% 65% 15% 19%</p>
3	H	363	<p>12% 84%</p>
4	J	76	<p>68% 26%</p>
4	K	76	<p>66% 32%</p>
4	L	76	<p>7% 67% 32%</p>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34635 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	712	5560	3497	966	1072	25	0	0
1	B	561	4361	2737	771	833	20	0	0
1	C	716	5590	3513	974	1078	25	0	0
1	D	561	4365	2734	769	842	20	0	0
1	E	539	4174	2623	725	806	20	0	0
1	F	541	4190	2632	730	808	20	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P25694
A	-1	SER	-	expression tag	UNP P25694
A	0	HIS	-	expression tag	UNP P25694
B	-2	GLY	-	expression tag	UNP P25694
B	-1	SER	-	expression tag	UNP P25694
B	0	HIS	-	expression tag	UNP P25694
C	-2	GLY	-	expression tag	UNP P25694
C	-1	SER	-	expression tag	UNP P25694
C	0	HIS	-	expression tag	UNP P25694
D	-2	GLY	-	expression tag	UNP P25694
D	-1	SER	-	expression tag	UNP P25694
D	0	HIS	-	expression tag	UNP P25694
E	-2	GLY	-	expression tag	UNP P25694
E	-1	SER	-	expression tag	UNP P25694
E	0	HIS	-	expression tag	UNP P25694
F	-2	GLY	-	expression tag	UNP P25694
F	-1	SER	-	expression tag	UNP P25694
F	0	HIS	-	expression tag	UNP P25694

- Molecule 2 is a protein called Nuclear protein localization protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	474	3815	2415	640	739	21	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP P33755
G	-1	SER	-	expression tag	UNP P33755
G	0	HIS	-	expression tag	UNP P33755

- Molecule 3 is a protein called Ubiquitin fusion degradation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	59	453	292	74	84	3	0	0

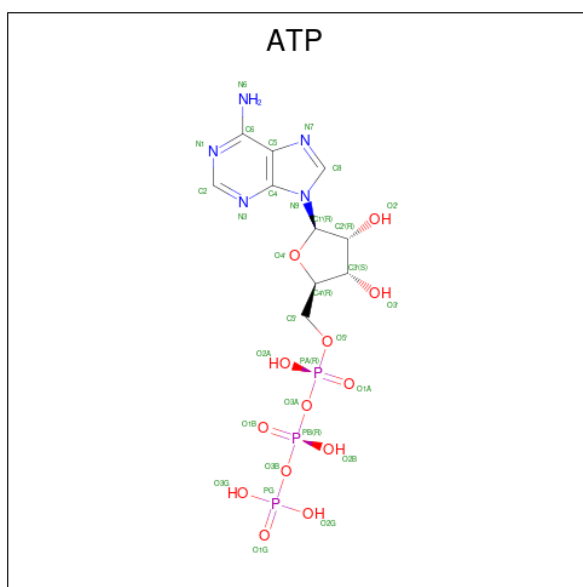
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P53044
H	0	SER	-	expression tag	UNP P53044

- Molecule 4 is a protein called Ubiquitin.

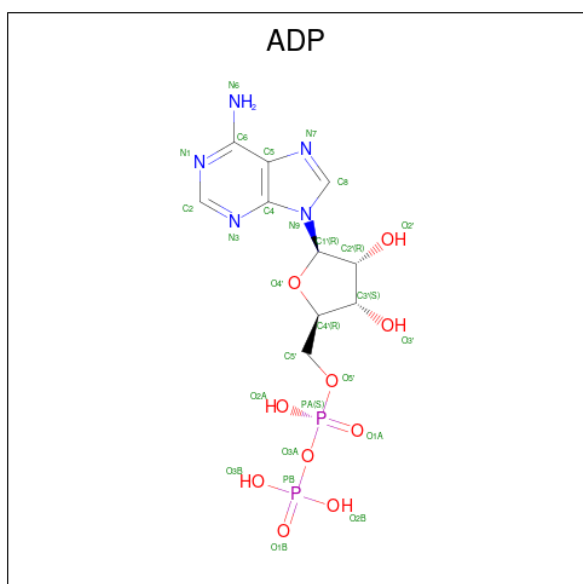
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	73	581	365	99	116	1	0	0
4	K	76	600	375	105	119	1	0	0
4	L	76	600	375	105	119	1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

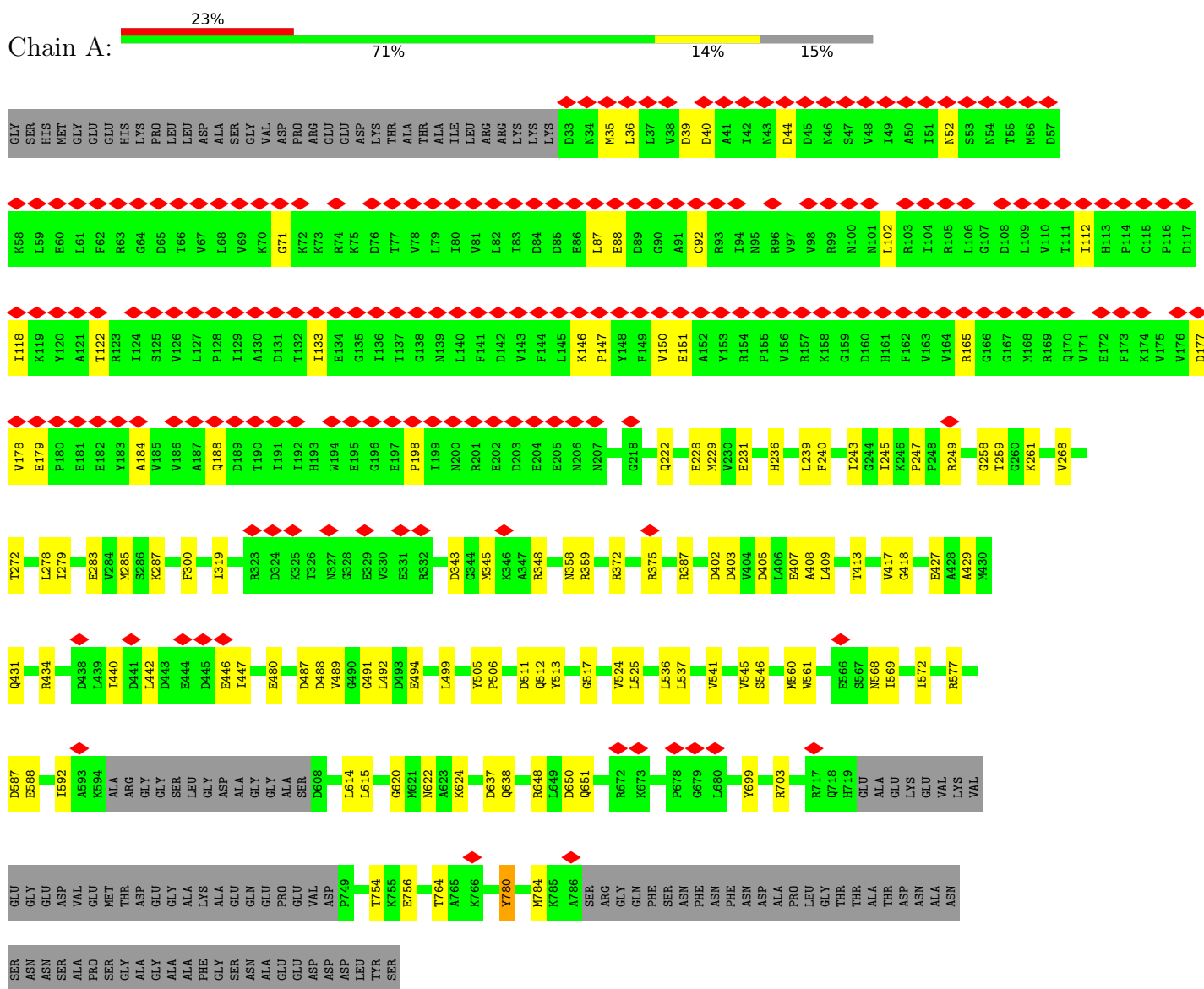
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	G	2	Total	Zn	0
			2	2	

3 Residue-property plots

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

- Molecule 1: Cell division control protein 48



PHE
GLN
GLY
GLN
GLY
ILE
SER
LEU
ARG
LYS
SER
ASN
LYS
ARG
LYS
THR
LYS
SER
SER
ASP
HIS
ASP
SER
SER
LYS
SER
LYS
ALA
PRO
LYS
SER
PRO
GLU
VAL
ILE
GLU
ILE
ASP

- Molecule 4: Ubiquitin

Chain J: 68% 26%

M101 K106 T107 K111 T112 I113 V117 E118 S128 Q131 D132 K133 E134 G135 I136 Q141 Q149 R154 T155 L156 S157 D158 Q162 V170 L171 R172 L173 ARG GLY GLY

- Molecule 4: Ubiquitin

Chain K: 66% 32%

M201 F204 V205 K206 G210 V217 E218 I223 Q231 G235 I236 D239 Q240 R241 R242 E251 D252 G253 R254 T255 L256 N260 I261 Q262 S265 T266 L267 V270 L271 G276

- Molecule 4: Ubiquitin

Chain L: 7% 67% 32%

K301 Q302 K306 T307 L308 T309 G310 V317 D321 T322 I323 Q331 G335 I336 D339 Q340 Q341 G347 K348 E351 D352 G353 R354 Y359 R360 T361 Q362 R363 E364 S365 T366 L367 R372 L373 G376

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.577	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.077	Depositor
Minimum map value	-22.853	Depositor
Average map value	-0.022	Depositor
Map value standard deviation	1.089	Depositor
Recommended contour level	9	Depositor
Map size (Å)	408.576, 408.576, 408.576	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	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, ATP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/5650	0.21	0/7645
1	B	0.13	0/4426	0.23	0/5973
1	C	0.10	0/5680	0.22	0/7684
1	D	0.11	0/4431	0.22	0/5980
1	E	0.09	0/4242	0.21	0/5734
1	F	0.10	0/4258	0.23	0/5754
2	G	0.14	0/3906	0.28	0/5275
3	H	0.12	0/462	0.26	0/617
4	J	0.11	0/586	0.24	0/788
4	K	0.12	0/605	0.28	0/812
4	L	0.11	0/605	0.26	0/812
All	All	0.11	0/34851	0.23	0/47074

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	5560	0	5587	85	0
1	B	4361	0	4415	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5590	0	5616	88	0
1	D	4365	0	4392	64	0
1	E	4174	0	4197	63	0
1	F	4190	0	4215	59	0
2	G	3815	0	3688	62	0
3	H	453	0	458	13	0
4	J	581	0	600	15	0
4	K	600	0	620	20	0
4	L	600	0	622	15	0
5	A	31	0	12	2	0
5	B	31	0	12	1	0
5	D	31	0	12	1	0
5	E	31	0	12	1	0
5	F	31	0	12	1	0
6	A	27	0	12	1	0
6	B	27	0	12	0	0
6	C	54	0	24	0	0
6	D	27	0	12	1	0
6	E	27	0	12	2	0
6	F	27	0	12	1	0
7	G	2	0	0	0	0
All	All	34635	0	34554	510	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 7.

All (510) 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:C:36:LEU:HD11	1:C:55:THR:HG21	1.43	0.97
2:G:259:ARG:NH2	2:G:286:GLU:OE1	2.05	0.89
1:E:262:THR:OG1	5:E:901:ATP:O3G	1.96	0.83
4:L:306:LYS:NZ	4:L:310:GLY:O	2.11	0.83
2:G:167:ILE:O	2:G:171:SER:OG	1.96	0.82
2:G:351:SER:OG	2:G:354:GLU:OE2	1.98	0.81
1:C:163:VAL:O	1:C:165:ARG:NH1	2.13	0.80
1:F:327:ASN:O	1:F:332:ARG:NH2	2.16	0.79
1:F:458:THR:OG1	1:F:460:ASP:OD1	1.99	0.79
1:B:262:THR:OG1	5:B:901:ATP:O3G	1.98	0.79
1:D:715:ALA:O	1:D:719:HIS:ND1	2.15	0.79
1:A:699:TYR:OH	1:A:703:ARG:NH2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:GLN:N	1:B:690:GLN:OE1	2.14	0.79
1:A:703:ARG:NH1	1:A:764:THR:O	2.16	0.79
1:A:44:ASP:OD2	1:A:165:ARG:NH1	2.17	0.78
1:B:480:GLU:N	1:B:480:GLU:OE1	2.16	0.78
1:D:634:ASN:O	1:D:777:TYR:OH	2.02	0.78
1:B:660:GLU:OE1	1:B:663:ARG:NH2	2.17	0.78
1:C:494:GLU:N	1:C:494:GLU:OE1	2.17	0.77
4:J:149:GLN:OE1	4:J:149:GLN:N	2.18	0.77
1:A:247:PRO:O	1:A:249:ARG:NH1	2.18	0.77
4:J:107:THR:HG21	4:J:113:ILE:HD12	1.68	0.76
1:C:94:ILE:O	1:C:99:ARG:NH1	2.20	0.75
1:D:207:ASN:OD1	1:D:209:ASN:ND2	2.19	0.75
1:E:608:ASP:N	1:E:608:ASP:OD1	2.19	0.75
3:H:252:ARG:NH2	3:H:284:THR:O	2.19	0.75
4:L:336:ILE:O	4:L:341:GLN:NE2	2.20	0.75
1:A:409:LEU:O	1:A:413:THR:HG22	1.87	0.75
1:F:331:GLU:N	1:F:331:GLU:OE1	2.20	0.74
4:K:262:GLN:O	4:K:265:SER:OG	2.03	0.74
1:D:470:ASN:OD1	1:E:625:LYS:NZ	2.20	0.74
4:L:351:GLU:N	4:L:351:GLU:OE1	2.20	0.74
2:G:497:GLN:OE1	2:G:497:GLN:N	2.21	0.74
4:J:101:MET:N	4:J:117:VAL:O	2.21	0.74
1:A:431:GLN:OE1	1:A:434:ARG:NH1	2.21	0.74
1:C:84:ASP:OD2	1:C:93:ARG:NH2	2.21	0.74
1:D:635:ARG:NE	1:D:638:GLN:OE1	2.21	0.73
2:G:558:GLU:OE1	2:G:559:SER:N	2.21	0.73
2:G:417:SER:OG	2:G:422:MET:O	2.07	0.73
1:A:146:LYS:O	1:A:150:VAL:HG23	1.88	0.73
1:C:86:GLU:OE1	1:C:86:GLU:N	2.22	0.73
1:B:767:ARG:O	1:C:788:ARG:NH2	2.22	0.73
2:G:412:ASP:OD2	2:G:432:ARG:NH1	2.21	0.73
1:E:513:TYR:O	1:E:517:GLY:N	2.21	0.72
1:F:784:MET:O	1:F:787:SER:OG	2.06	0.72
2:G:115:GLU:N	2:G:115:GLU:OE1	2.22	0.72
1:D:407:GLU:OE1	1:D:407:GLU:N	2.22	0.72
1:A:287:LYS:O	1:B:333:ARG:NH1	2.21	0.72
1:E:480:GLU:N	1:E:480:GLU:OE1	2.22	0.72
1:E:294:SER:OG	1:E:298:LYS:NZ	2.22	0.71
1:F:302:GLU:N	1:F:302:GLU:OE1	2.22	0.71
1:C:123:ARG:NH2	1:C:179:GLU:OE2	2.22	0.71
2:G:562:LYS:O	2:G:565:SER:OG	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:494:GLU:N	1:F:494:GLU:OE1	2.22	0.71
1:B:24:THR:HG22	1:B:224:ALA:CB	2.21	0.70
1:E:303:ALA:CB	1:E:311:ILE:HD11	2.20	0.70
1:A:222:GLN:N	1:A:222:GLN:OE1	2.25	0.70
1:D:494:GLU:N	1:D:494:GLU:OE1	2.23	0.70
1:B:249:ARG:NH2	1:B:347:ALA:O	2.25	0.70
1:D:331:GLU:OE1	1:D:331:GLU:N	2.23	0.70
1:F:409:LEU:O	1:F:413:THR:HG22	1.90	0.70
2:G:243:GLU:OE1	2:G:243:GLU:N	2.24	0.70
1:F:554:GLY:N	1:F:588:GLU:OE2	2.23	0.70
1:A:261:LYS:N	5:A:901:ATP:O2B	2.25	0.70
1:A:480:GLU:N	1:A:480:GLU:OE1	2.26	0.69
4:K:236:ILE:O	4:K:241:GLN:NE2	2.23	0.69
2:G:374:GLN:N	2:G:374:GLN:OE1	2.25	0.69
2:G:251:ALA:O	2:G:255:THR:HG22	1.92	0.69
1:C:331:GLU:N	1:C:331:GLU:OE1	2.25	0.69
1:E:231:GLU:HG2	1:E:272:THR:HG22	1.73	0.69
4:J:136:ILE:O	4:J:141:GLN:NE2	2.25	0.69
1:B:359:ARG:NH2	1:B:566:GLU:OE1	2.25	0.69
1:A:231:GLU:HG2	1:A:272:THR:HG22	1.74	0.68
4:K:223:ILE:HG22	4:K:254:ARG:O	1.93	0.68
1:B:280:ASN:ND2	1:B:283:GLU:OE1	2.25	0.68
1:F:407:GLU:N	1:F:407:GLU:OE1	2.27	0.68
1:D:434:ARG:NH1	1:E:228:GLU:OE2	2.27	0.68
1:C:667:LEU:CD2	1:C:697:LEU:HD13	2.24	0.68
2:G:451:GLU:N	2:G:451:GLU:OE1	2.27	0.68
1:B:283:GLU:OE1	2:G:217:SER:OG	2.12	0.67
1:C:560:MET:HE1	1:C:572:ILE:HD11	1.76	0.67
1:D:531:GLY:N	6:D:902:ADP:O1B	2.21	0.67
4:K:218:GLU:N	4:K:218:GLU:OE1	2.28	0.67
1:A:536:LEU:HD12	1:A:537:LEU:N	2.10	0.66
1:B:444:GLU:OE1	1:B:444:GLU:N	2.28	0.66
1:F:693:SER:N	1:F:696:ASP:OD2	2.29	0.66
1:C:122:THR:N	1:C:179:GLU:O	2.29	0.65
1:E:238:GLN:N	1:E:238:GLN:OE1	2.28	0.65
1:E:409:LEU:O	1:E:413:THR:HG22	1.97	0.65
1:D:222:GLN:N	1:D:222:GLN:OE1	2.28	0.65
2:G:391:GLU:N	2:G:391:GLU:OE1	2.30	0.65
1:A:88:GLU:N	1:A:88:GLU:OE1	2.30	0.65
1:C:74:ARG:O	1:C:74:ARG:HG2	1.96	0.65
4:L:323:ILE:HG22	4:L:354:ARG:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:663:ARG:NH2	1:E:690:GLN:OE1	2.30	0.64
1:F:531:GLY:N	6:F:902:ADP:O1B	2.22	0.64
1:B:222:GLN:N	1:B:222:GLN:OE1	2.29	0.64
1:A:407:GLU:N	1:A:407:GLU:OE1	2.29	0.63
1:C:398:MET:HE1	1:D:245:ILE:HG22	1.80	0.63
4:J:101:MET:HA	4:J:101:MET:HE2	1.79	0.63
4:J:154:ARG:NE	4:J:158:ASP:OD2	2.30	0.62
1:B:391:LEU:O	1:B:395:THR:OG1	2.12	0.62
4:J:162:GLN:N	4:J:162:GLN:OE1	2.32	0.62
1:D:203:ASP:OD1	1:D:204:GLU:N	2.32	0.62
1:E:676:LEU:HD11	1:E:680:LEU:HD23	1.81	0.62
1:A:52:ASN:ND2	1:A:87:LEU:O	2.31	0.62
1:A:229:MET:HE1	1:A:375:ARG:HD2	1.80	0.62
2:G:260:PHE:HE2	2:G:324:LEU:HD12	1.64	0.62
2:G:296:LEU:HD11	3:H:299:LEU:HD23	1.81	0.62
4:J:131:GLN:O	4:J:135:GLY:N	2.33	0.62
1:C:39:ASP:OD1	1:C:40:ASP:N	2.33	0.62
2:G:229:GLN:NE2	2:G:231:PHE:O	2.32	0.62
2:G:316:GLU:N	2:G:316:GLU:OE1	2.32	0.62
2:G:260:PHE:CE2	2:G:324:LEU:HD12	2.35	0.61
1:B:317:ASP:OD1	1:B:318:SER:N	2.33	0.61
1:C:200:ASN:OD1	1:C:202:GLU:N	2.28	0.61
1:C:681:GLU:N	1:C:681:GLU:OE1	2.34	0.61
1:D:387:ARG:NE	1:D:413:THR:O	2.34	0.61
1:F:387:ARG:NE	1:F:413:THR:O	2.32	0.61
4:K:251:GLU:N	4:K:251:GLU:OE1	2.34	0.61
1:B:387:ARG:NE	1:B:413:THR:O	2.32	0.61
4:K:239:ASP:O	4:K:242:ARG:NH1	2.33	0.61
1:E:222:GLN:OE1	1:E:222:GLN:N	2.34	0.61
1:E:568:ASN:OD1	1:E:569:ILE:N	2.34	0.61
1:F:681:GLU:OE1	1:F:683:THR:N	2.34	0.61
1:E:304:GLU:OE2	1:E:349:SER:OG	2.11	0.61
2:G:230:GLU:OE1	2:G:230:GLU:N	2.34	0.60
4:K:239:ASP:OD1	4:K:240:GLN:N	2.32	0.60
1:D:618:MET:HE1	1:D:649:LEU:HD21	1.82	0.60
1:A:268:VAL:O	1:A:272:THR:HG23	2.02	0.60
1:A:39:ASP:OD1	1:A:40:ASP:N	2.34	0.60
1:B:503:VAL:HG21	1:B:541:VAL:HG13	1.84	0.60
1:C:703:ARG:NH2	1:C:707:TYR:OH	2.35	0.60
1:E:494:GLU:OE1	1:E:494:GLU:N	2.31	0.60
1:A:780:TYR:CD1	1:A:784:MET:HE3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:331:GLN:O	4:L:335:GLY:N	2.32	0.60
4:L:351:GLU:OE1	4:L:359:TYR:OH	2.20	0.60
1:A:560:MET:HE1	1:A:572:ILE:HD11	1.84	0.59
1:B:331:GLU:OE1	1:B:331:GLU:N	2.35	0.59
1:D:499:LEU:HD13	1:D:537:LEU:HD21	1.83	0.59
2:G:373:GLU:OE1	2:G:373:GLU:N	2.34	0.59
3:H:249:ASN:ND2	3:H:281:MET:SD	2.75	0.59
4:K:201:MET:N	4:K:217:VAL:O	2.36	0.59
1:C:222:GLN:N	1:C:222:GLN:OE1	2.35	0.59
2:G:434:VAL:HG23	2:G:434:VAL:O	2.03	0.59
1:D:202:GLU:OE1	1:D:202:GLU:N	2.34	0.58
1:A:405:ASP:O	1:A:408:ALA:N	2.36	0.58
2:G:263:MET:HE2	2:G:281:VAL:HG11	1.85	0.58
1:B:294:SER:OG	2:G:436:GLU:OE1	2.11	0.58
1:A:231:GLU:CG	1:A:272:THR:HG22	2.33	0.58
1:F:211:VAL:HG23	1:F:211:VAL:O	2.04	0.57
1:C:203:ASP:OD1	1:C:204:GLU:N	2.37	0.57
1:B:511:ASP:OD1	1:B:512:GLN:N	2.37	0.57
1:C:391:LEU:O	1:C:395:THR:OG1	2.14	0.57
1:D:499:LEU:CD1	1:D:537:LEU:HD21	2.34	0.57
1:E:285:MET:HE2	1:E:285:MET:HA	1.85	0.57
2:G:495:MET:SD	2:G:495:MET:N	2.77	0.57
4:J:106:LYS:NZ	4:J:112:THR:OG1	2.35	0.57
1:C:238:GLN:OE1	1:C:238:GLN:N	2.35	0.56
1:E:429:ALA:CB	1:F:245:ILE:HG21	2.36	0.56
2:G:418:THR:HG22	3:H:290:ALA:H	1.69	0.56
1:C:499:LEU:HD23	1:C:541:VAL:CG2	2.36	0.56
1:E:303:ALA:HB3	1:E:311:ILE:HD11	1.86	0.56
1:F:499:LEU:O	1:F:503:VAL:HG22	2.05	0.56
1:C:240:PHE:O	1:C:244:GLY:N	2.39	0.56
1:F:525:LEU:HD23	1:F:526:PHE:N	2.21	0.56
1:E:405:ASP:O	1:E:408:ALA:N	2.39	0.56
1:F:222:GLN:OE1	1:F:222:GLN:N	2.38	0.56
1:C:358:ASN:OD1	1:C:359:ARG:N	2.38	0.55
1:C:405:ASP:O	1:C:408:ALA:N	2.39	0.55
1:C:52:ASN:ND2	1:C:87:LEU:O	2.40	0.55
1:E:766:LYS:NZ	1:F:786:ALA:O	2.27	0.55
1:F:209:ASN:OD1	1:F:266:ARG:NH2	2.39	0.55
1:C:218:GLY:N	1:C:389:GLU:OE1	2.39	0.55
1:C:387:ARG:NE	1:C:413:THR:O	2.39	0.55
1:E:358:ASN:OD1	1:E:359:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD23	1:A:279:ILE:N	2.22	0.55
2:G:290:HIS:NE2	2:G:292:GLU:OE2	2.37	0.55
1:D:329:GLU:OE2	1:D:333:ARG:NH2	2.39	0.55
1:E:489:VAL:HA	6:E:902:ADP:HN61	1.72	0.55
2:G:500:ASP:OD1	2:G:500:ASP:N	2.39	0.55
1:A:491:GLY:C	1:A:492:LEU:HD23	2.31	0.55
1:D:705:ALA:HB1	1:E:518:LEU:HD11	1.87	0.55
1:C:140:LEU:HD21	1:C:173:PHE:CE2	2.42	0.55
1:C:231:GLU:HG2	1:C:272:THR:HG22	1.89	0.55
1:E:229:MET:HE3	1:E:375:ARG:CD	2.37	0.55
1:C:46:ASN:OD1	1:C:148:TYR:OH	2.24	0.55
1:A:402:ASP:OD1	1:A:403:ASP:N	2.39	0.54
4:K:201:MET:HE2	4:K:256:LEU:HD13	1.88	0.54
2:G:255:THR:HG23	2:G:257:MET:H	1.73	0.54
1:F:587:ASP:OD1	1:F:588:GLU:N	2.41	0.54
1:E:387:ARG:NE	1:E:413:THR:O	2.41	0.54
1:E:766:LYS:O	1:F:788:ARG:NH2	2.41	0.54
1:D:648:ARG:O	1:D:650:ASP:N	2.41	0.54
3:H:310:GLU:N	3:H:310:GLU:OE1	2.41	0.54
1:C:300:PHE:CD1	1:C:341:LEU:HD13	2.42	0.54
1:D:279:ILE:HD11	1:D:299:ALA:HB1	1.89	0.54
2:G:356:ILE:HD11	2:G:414:ILE:CG2	2.38	0.53
1:F:413:THR:O	1:F:413:THR:HG23	2.08	0.53
1:E:709:ILE:HD11	1:F:512:GLN:HB3	1.91	0.53
1:F:477:THR:O	1:F:575:LYS:NZ	2.42	0.53
1:F:637:ASP:OD1	1:F:638:GLN:N	2.42	0.53
1:B:374:ASP:OD1	1:B:375:ARG:N	2.36	0.53
1:F:513:TYR:O	1:F:517:GLY:N	2.41	0.53
1:A:754:THR:OG1	1:A:756:GLU:OE2	2.27	0.53
2:G:324:LEU:HD23	2:G:324:LEU:H	1.74	0.53
2:G:472:ASN:O	2:G:475:THR:HG22	2.09	0.53
1:D:288:MET:HE1	1:E:333:ARG:NH1	2.24	0.52
4:L:340:GLN:O	4:L:372:ARG:N	2.38	0.52
1:A:494:GLU:OE1	1:A:494:GLU:N	2.36	0.52
1:A:577:ARG:NH2	1:A:620:GLY:O	2.43	0.52
1:E:617:GLU:N	1:E:617:GLU:OE1	2.42	0.52
1:D:303:ALA:HB3	1:D:311:ILE:HD11	1.92	0.52
1:F:528:GLY:O	1:F:634:ASN:ND2	2.40	0.52
1:A:780:TYR:HD1	1:A:784:MET:HE3	1.75	0.52
4:K:201:MET:HE1	4:K:261:ILE:O	2.09	0.52
1:A:133:ILE:HD11	1:A:198:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ALA:CB	1:C:311:ILE:HD11	2.40	0.51
1:A:622:ASN:OD1	1:A:624:LYS:N	2.43	0.51
1:A:358:ASN:OD1	1:A:359:ARG:N	2.44	0.51
1:A:427:GLU:OE2	1:B:375:ARG:NH1	2.44	0.51
1:C:407:GLU:OE1	1:C:407:GLU:N	2.39	0.51
1:C:671:LEU:HD21	1:C:701:VAL:HG13	1.93	0.51
1:D:263:LEU:HD23	1:D:263:LEU:C	2.35	0.51
1:F:405:ASP:O	1:F:408:ALA:N	2.43	0.51
1:F:681:GLU:OE1	1:F:683:THR:OG1	2.20	0.51
1:A:489:VAL:HA	6:A:902:ADP:HN61	1.75	0.51
1:B:256:PRO:HG3	1:B:478:VAL:HG12	1.91	0.51
1:E:528:GLY:O	1:E:634:ASN:ND2	2.41	0.51
1:E:637:ASP:OD1	1:E:638:GLN:N	2.43	0.51
4:J:101:MET:HE3	4:J:118:GLU:HA	1.91	0.51
1:B:398:MET:HE2	1:C:245:ILE:HG22	1.91	0.51
1:D:249:ARG:NH1	1:D:349:SER:O	2.42	0.51
1:F:360:PRO:O	1:F:368:ARG:NH1	2.44	0.51
1:A:413:THR:O	1:A:413:THR:HG23	2.11	0.51
1:A:650:ASP:OD1	1:A:651:GLN:N	2.44	0.51
1:C:718:GLN:OE1	1:C:718:GLN:N	2.44	0.51
1:A:177:ASP:OD1	1:A:178:VAL:N	2.44	0.51
1:C:587:ASP:OD1	1:C:588:GLU:N	2.44	0.50
1:D:279:ILE:HD11	1:D:299:ALA:CB	2.40	0.50
4:K:267:LEU:N	4:K:267:LEU:HD22	2.26	0.50
1:D:211:VAL:HG23	1:D:211:VAL:O	2.11	0.50
1:A:447:ILE:HD11	1:B:236:HIS:ND1	2.26	0.50
1:A:637:ASP:OD1	1:A:638:GLN:N	2.44	0.50
4:J:107:THR:CG2	4:J:113:ILE:HD12	2.39	0.50
4:L:352:ASP:N	4:L:352:ASP:OD1	2.43	0.50
1:A:283:GLU:HA	1:B:340:THR:HG21	1.93	0.50
2:G:557:GLU:O	2:G:561:LEU:HD13	2.12	0.50
1:B:499:LEU:O	1:B:503:VAL:HG22	2.11	0.50
1:C:667:LEU:HD22	1:C:697:LEU:HD13	1.93	0.50
1:D:441:ASP:OD1	1:D:443:ASP:N	2.44	0.50
4:K:256:LEU:O	4:K:260:ASN:N	2.44	0.50
1:D:399:LYS:NZ	1:D:453:ASP:O	2.44	0.50
1:D:587:ASP:OD1	1:D:588:GLU:N	2.45	0.50
1:E:413:THR:O	1:E:413:THR:HG23	2.11	0.50
2:G:256:GLY:C	2:G:257:MET:HE2	2.37	0.50
1:D:331:GLU:O	1:D:335:VAL:HG23	2.11	0.49
2:G:524:ILE:O	2:G:524:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:LEU:HD23	1:C:541:VAL:HG21	1.94	0.49
1:C:376:GLU:N	1:C:376:GLU:OE1	2.45	0.49
1:C:398:MET:CE	1:D:245:ILE:HG22	2.42	0.49
1:A:387:ARG:NE	1:A:413:THR:O	2.45	0.49
1:C:659:ASP:OD1	1:C:660:GLU:N	2.41	0.49
1:D:537:LEU:C	1:D:537:LEU:HD23	2.36	0.49
1:B:568:ASN:OD1	1:B:569:ILE:N	2.45	0.49
3:H:232:VAL:HG23	3:H:233:LEU:HD12	1.94	0.49
1:C:445:ASP:OD2	1:D:235:ARG:NH2	2.45	0.49
1:D:314:ASP:OD1	1:D:315:GLU:N	2.45	0.49
1:F:372:ARG:O	1:F:374:ASP:N	2.44	0.49
2:G:532:TYR:O	2:G:535:SER:OG	2.22	0.49
1:C:36:LEU:CD1	1:C:55:THR:HG21	2.30	0.49
1:B:26:ILE:HD11	1:B:227:ARG:HB2	1.95	0.49
2:G:357:MET:HE1	3:H:299:LEU:HD21	1.95	0.49
1:C:560:MET:CE	1:C:572:ILE:HD11	2.42	0.48
1:F:374:ASP:OD1	1:F:375:ARG:N	2.42	0.48
1:C:69:VAL:HG21	1:C:79:LEU:HD12	1.95	0.48
1:C:348:ARG:O	1:C:348:ARG:NE	2.46	0.48
1:F:503:VAL:HG21	1:F:541:VAL:HG13	1.95	0.48
1:F:511:ASP:OD1	1:F:512:GLN:N	2.47	0.48
1:F:591:SER:OG	1:F:592:ILE:HD12	2.13	0.48
4:L:302:GLN:O	4:L:364:GLU:N	2.37	0.48
1:C:177:ASP:OD1	1:C:178:VAL:N	2.46	0.48
1:E:560:MET:HE1	1:E:572:ILE:HD11	1.95	0.48
1:E:771:ASP:OD1	1:E:775:ARG:NH1	2.46	0.48
2:G:357:MET:CE	3:H:299:LEU:HD21	2.44	0.48
1:D:460:ASP:OD1	1:D:460:ASP:N	2.44	0.48
3:H:233:LEU:CD2	3:H:305:MET:HE3	2.43	0.48
1:A:446:GLU:N	1:A:446:GLU:OE1	2.46	0.48
1:A:568:ASN:OD1	1:A:569:ILE:N	2.46	0.48
1:A:240:PHE:HA	1:A:243:ILE:HG22	1.95	0.48
1:A:343:ASP:OD2	1:A:372:ARG:NH2	2.47	0.48
1:C:518:LEU:HD23	1:C:519:SER:N	2.29	0.48
1:A:447:ILE:HD12	1:A:447:ILE:N	2.29	0.48
1:D:261:LYS:N	5:D:901:ATP:O2B	2.47	0.48
1:E:412:GLU:OE1	1:E:463:ARG:NH1	2.47	0.48
1:F:293:GLU:OE1	1:F:293:GLU:N	2.44	0.47
3:H:281:MET:HA	3:H:281:MET:HE2	1.95	0.47
1:F:460:ASP:OD1	1:F:460:ASP:N	2.45	0.47
1:D:445:ASP:OD1	1:D:446:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASP:OD1	1:A:512:GLN:N	2.46	0.47
2:G:547:LEU:C	2:G:547:LEU:HD23	2.40	0.47
1:E:229:MET:HE3	1:E:375:ARG:HD3	1.96	0.47
2:G:395:ASP:OD1	2:G:396:ILE:N	2.48	0.47
1:A:285:MET:HG2	1:A:319:ILE:HG22	1.96	0.47
1:B:405:ASP:O	1:B:408:ALA:N	2.47	0.47
1:D:231:GLU:HG2	1:D:272:THR:HG22	1.97	0.47
1:C:395:THR:HB	1:C:400:LEU:HD11	1.97	0.47
1:E:293:GLU:OE2	1:E:333:ARG:NH1	2.46	0.47
1:E:433:ILE:HD13	1:E:455:LEU:HD11	1.97	0.47
2:G:548:ILE:O	2:G:552:VAL:HG12	2.14	0.47
3:H:233:LEU:HD23	3:H:305:MET:HE3	1.97	0.47
1:D:249:ARG:NH2	1:D:349:SER:O	2.45	0.47
4:L:366:THR:O	4:L:366:THR:HG23	2.15	0.47
1:A:36:LEU:HD12	1:A:112:ILE:HD12	1.97	0.47
1:A:499:LEU:HD23	1:A:541:VAL:CG2	2.45	0.47
1:B:503:VAL:HG23	1:B:504:GLU:N	2.30	0.47
1:E:211:VAL:HG23	1:E:211:VAL:O	2.14	0.47
4:L:362:GLN:O	4:L:365:SER:OG	2.23	0.47
1:C:650:ASP:OD1	1:C:651:GLN:N	2.48	0.47
1:A:151:GLU:N	1:A:188:GLN:OE1	2.47	0.46
1:A:228:GLU:OE2	1:F:434:ARG:NH2	2.49	0.46
1:A:615:LEU:HD11	1:A:648:ARG:HD3	1.97	0.46
1:A:429:ALA:CB	1:B:245:ILE:HD13	2.46	0.46
1:C:148:TYR:O	1:C:154:ARG:NE	2.37	0.46
1:F:492:LEU:N	1:F:492:LEU:HD12	2.31	0.46
1:A:446:GLU:C	1:A:447:ILE:HD12	2.41	0.46
2:G:257:MET:HE2	2:G:257:MET:HA	1.98	0.46
1:C:648:ARG:O	1:C:650:ASP:N	2.48	0.46
1:D:320:ALA:HA	1:D:335:VAL:HG22	1.97	0.46
1:E:619:ASP:OD2	1:E:648:ARG:NH2	2.47	0.46
4:L:367:LEU:N	4:L:367:LEU:HD22	2.31	0.46
1:A:229:MET:HE1	1:A:375:ARG:CD	2.44	0.46
1:C:207:ASN:O	1:C:209:ASN:N	2.47	0.46
1:C:529:PRO:HG2	1:C:657:LEU:HD21	1.98	0.46
2:G:461:TYR:C	2:G:462:LEU:HD12	2.40	0.46
1:A:245:ILE:HD13	1:F:429:ALA:CB	2.45	0.46
1:B:525:LEU:HD23	1:B:525:LEU:C	2.41	0.46
1:E:536:LEU:CD1	6:E:902:ADP:C8	2.99	0.46
2:G:511:VAL:HG11	2:G:523:LYS:HD2	1.98	0.46
1:A:587:ASP:OD1	1:A:588:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:204:PHE:N	4:K:265:SER:O	2.47	0.46
1:A:429:ALA:HB1	1:B:245:ILE:HD13	1.97	0.46
1:B:285:MET:HE2	1:B:285:MET:HA	1.98	0.46
1:C:698:LEU:HD23	1:C:698:LEU:C	2.40	0.46
1:A:487:ASP:OD1	1:A:488:ASP:N	2.49	0.45
1:D:447:ILE:HD13	1:D:452:LEU:HD21	1.97	0.45
1:F:231:GLU:O	1:F:235:ARG:N	2.38	0.45
1:C:669:ALA:O	1:C:672:ARG:NH1	2.48	0.45
1:F:261:LYS:N	5:F:901:ATP:O2B	2.49	0.45
1:A:245:ILE:HD13	1:F:429:ALA:HB1	1.97	0.45
1:E:511:ASP:OD1	1:E:512:GLN:N	2.49	0.45
4:K:206:LYS:NZ	4:K:210:GLY:O	2.48	0.45
1:A:71:GLY:N	1:A:102:LEU:HD12	2.32	0.45
1:D:518:LEU:HD23	1:D:519:SER:N	2.32	0.45
1:E:424:LEU:HD12	1:E:465:ALA:HB1	1.97	0.45
1:A:259:THR:HG22	1:A:417:VAL:HG13	1.99	0.45
1:E:433:ILE:HD13	1:E:455:LEU:CD1	2.47	0.45
2:G:356:ILE:HD11	2:G:414:ILE:HG22	1.98	0.45
4:J:128:SER:O	4:J:131:GLN:HG3	2.17	0.45
1:B:249:ARG:NH2	1:B:349:SER:O	2.49	0.45
1:C:359:ARG:NE	1:C:566:GLU:O	2.50	0.45
1:B:372:ARG:O	1:B:374:ASP:N	2.50	0.45
1:D:614:LEU:C	1:D:614:LEU:HD23	2.42	0.45
1:A:118:ILE:HD11	1:A:184:ALA:O	2.17	0.45
1:C:663:ARG:O	1:C:667:LEU:HD23	2.17	0.45
1:F:381:ILE:HG23	1:F:478:VAL:HG11	1.99	0.45
1:A:648:ARG:O	1:A:650:ASP:N	2.50	0.45
1:E:429:ALA:HB1	1:F:245:ILE:HD13	1.99	0.45
1:F:557:LEU:HB2	1:F:592:ILE:HD11	1.99	0.44
4:L:339:ASP:OD1	4:L:340:GLN:N	2.50	0.44
1:B:398:MET:HE1	1:B:425:CYS:HB3	1.99	0.44
1:C:325:LYS:O	1:C:326:THR:C	2.60	0.44
1:D:614:LEU:HD23	1:D:614:LEU:O	2.16	0.44
1:A:703:ARG:NH1	1:A:764:THR:OG1	2.50	0.44
1:D:288:MET:HE2	1:D:288:MET:HA	1.98	0.44
1:E:368:ARG:NH2	1:E:376:GLU:OE2	2.46	0.44
1:F:503:VAL:HG23	1:F:504:GLU:N	2.32	0.44
2:G:332:ALA:N	2:G:338:SER:O	2.42	0.44
1:B:211:VAL:O	1:B:211:VAL:HG23	2.18	0.44
1:D:303:ALA:CB	1:D:311:ILE:HD11	2.48	0.44
2:G:285:TYR:HD2	2:G:307:MET:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:231:GLN:O	4:K:235:GLY:N	2.44	0.44
1:C:74:ARG:O	1:C:74:ARG:CG	2.62	0.44
4:J:170:VAL:HG22	4:J:171:LEU:N	2.32	0.44
1:B:767:ARG:NH2	1:B:769:VAL:O	2.51	0.44
1:E:310:ILE:O	1:E:311:ILE:C	2.60	0.44
1:B:27:LEU:HD11	1:B:224:ALA:HB2	2.00	0.44
1:E:279:ILE:O	1:E:280:ASN:C	2.61	0.44
1:E:677:GLU:OE1	1:E:755:LYS:N	2.50	0.44
1:A:300:PHE:CE1	1:A:345:MET:HE3	2.53	0.44
1:A:513:TYR:O	1:A:517:GLY:N	2.51	0.43
1:B:229:MET:SD	1:B:251:VAL:HG22	2.58	0.43
1:D:326:THR:HG22	1:E:332:ARG:NH2	2.34	0.43
4:K:223:ILE:HG21	4:K:251:GLU:O	2.18	0.43
1:B:525:LEU:HD21	1:B:633:THR:CG2	2.49	0.43
1:C:381:ILE:HG23	1:C:478:VAL:HG11	2.00	0.43
1:D:324:ASP:OD1	1:D:325:LYS:N	2.52	0.43
4:J:155:THR:OG1	4:J:156:LEU:N	2.50	0.43
1:C:222:GLN:HG2	1:C:379:ILE:HD13	1.99	0.43
1:C:505:TYR:HB2	1:C:506:PRO:HD3	1.99	0.43
1:C:614:LEU:HD23	1:C:614:LEU:C	2.44	0.43
1:C:630:ILE:HD12	1:C:630:ILE:N	2.33	0.43
1:C:698:LEU:HD23	1:C:698:LEU:O	2.17	0.43
1:E:232:LEU:HB2	1:E:233:PRO:HD3	1.99	0.43
1:A:489:VAL:HG12	1:A:536:LEU:HD13	1.99	0.43
1:F:317:ASP:OD1	1:F:317:ASP:N	2.50	0.43
1:D:232:LEU:HB2	1:D:233:PRO:HD3	2.01	0.43
2:G:262:TYR:CD1	2:G:307:MET:HE3	2.54	0.43
2:G:296:LEU:HD12	2:G:296:LEU:C	2.43	0.43
4:L:321:ASP:OD1	4:L:322:THR:N	2.52	0.43
1:A:545:VAL:O	1:A:546:SER:OG	2.25	0.43
1:D:618:MET:HE1	1:D:649:LEU:CD2	2.47	0.43
1:E:268:VAL:O	1:E:272:THR:HG23	2.18	0.43
1:B:417:VAL:HG12	1:B:418:GLY:N	2.33	0.43
1:B:477:THR:O	1:B:575:LYS:NZ	2.52	0.43
4:K:252:ASP:OD1	4:K:252:ASP:N	2.49	0.43
1:E:317:ASP:OD1	1:E:318:SER:N	2.52	0.43
1:E:626:ASN:OD1	1:E:626:ASN:N	2.50	0.43
2:G:257:MET:HE1	2:G:293:GLN:HG2	2.01	0.43
1:E:667:LEU:CD2	1:E:697:LEU:HD13	2.48	0.43
2:G:490:SER:OG	2:G:491:ASN:N	2.52	0.43
1:A:236:HIS:HB3	1:A:239:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ARG:O	1:D:374:ASP:N	2.52	0.42
1:E:263:LEU:C	1:E:263:LEU:HD23	2.44	0.42
1:A:146:LYS:HB3	1:A:147:PRO:HD3	2.00	0.42
1:D:650:ASP:OD1	1:D:651:GLN:N	2.51	0.42
1:F:263:LEU:C	1:F:263:LEU:HD23	2.44	0.42
2:G:187:SER:OG	2:G:188:SER:N	2.51	0.42
2:G:327:THR:HG22	2:G:386:ILE:HD12	2.01	0.42
1:A:417:VAL:HG12	1:A:418:GLY:H	1.85	0.42
1:E:307:ALA:HB3	1:E:308:PRO:HD3	2.01	0.42
1:B:336:SER:O	1:B:340:THR:HG23	2.20	0.42
1:C:232:LEU:HB2	1:C:233:PRO:HD3	2.00	0.42
1:E:429:ALA:CB	1:F:245:ILE:HD13	2.49	0.42
4:K:270:VAL:HG22	4:K:271:LEU:N	2.34	0.42
1:B:100:ASN:O	1:B:103:ARG:NH1	2.51	0.42
1:B:637:ASP:OD1	1:B:638:GLN:N	2.52	0.42
1:C:35:MET:SD	1:C:35:MET:N	2.93	0.42
2:G:296:LEU:HD12	2:G:296:LEU:O	2.19	0.42
2:G:547:LEU:HD23	2:G:547:LEU:O	2.20	0.42
1:D:505:TYR:HB2	1:D:506:PRO:HD3	2.02	0.42
1:F:232:LEU:HB2	1:F:233:PRO:HD3	2.01	0.42
1:A:258:GLY:N	5:A:901:ATP:O1B	2.52	0.42
1:A:780:TYR:CE1	1:A:784:MET:HE3	2.55	0.42
1:B:263:LEU:HD23	1:B:263:LEU:O	2.20	0.42
1:B:622:ASN:OD1	1:B:623:ALA:N	2.52	0.42
1:C:122:THR:OG1	1:C:179:GLU:O	2.35	0.42
1:C:372:ARG:O	1:C:374:ASP:N	2.52	0.42
1:B:240:PHE:O	1:B:244:GLY:N	2.47	0.42
1:C:440:ILE:HD11	1:C:451:VAL:HG11	2.01	0.42
1:D:378:ASP:OD1	1:D:379:ILE:N	2.53	0.42
1:D:440:ILE:HD13	1:D:447:ILE:HD11	2.02	0.42
1:F:590:ASP:OD1	1:F:591:SER:N	2.52	0.42
3:H:242:ILE:O	3:H:244:TYR:N	2.52	0.42
1:B:24:THR:HG22	1:B:224:ALA:HB2	2.00	0.42
1:C:146:LYS:HB3	1:C:147:PRO:HD3	2.02	0.42
1:F:452:LEU:HD23	1:F:452:LEU:C	2.44	0.42
1:F:690:GLN:O	1:F:767:ARG:NH2	2.48	0.42
1:A:442:LEU:N	1:A:442:LEU:HD12	2.35	0.41
1:B:417:VAL:HG12	1:B:418:GLY:H	1.84	0.41
1:D:405:ASP:O	1:D:408:ALA:N	2.52	0.41
1:E:650:ASP:OD1	1:E:651:GLN:N	2.52	0.41
4:K:266:THR:O	4:K:266:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:N	1:A:92:CYS:O	2.53	0.41
1:A:505:TYR:HB2	1:A:506:PRO:HD3	2.02	0.41
1:D:706:LYS:HA	1:D:709:ILE:HG22	2.02	0.41
2:G:516:ASP:N	2:G:516:ASP:OD1	2.52	0.41
2:G:546:LEU:HD12	2:G:547:LEU:N	2.34	0.41
1:C:615:LEU:HD21	1:C:643:ILE:HD13	2.03	0.41
1:C:784:MET:O	1:C:787:SER:OG	2.34	0.41
1:A:561:TRP:CE3	1:A:592:ILE:HG23	2.55	0.41
1:D:637:ASP:OD1	1:D:637:ASP:N	2.53	0.41
1:E:409:LEU:CD2	1:E:459:MET:HE1	2.50	0.41
1:F:323:ARG:O	1:F:326:THR:OG1	2.34	0.41
2:G:429:THR:HG22	2:G:432:ARG:HE	1.86	0.41
1:B:316:ILE:HG23	1:B:363:ILE:HD12	2.01	0.41
1:C:124:ILE:HD13	1:C:186:VAL:HG22	2.02	0.41
1:C:149:PHE:CD1	1:C:186:VAL:HG11	2.55	0.41
4:K:270:VAL:HG22	4:K:271:LEU:H	1.85	0.41
1:B:590:ASP:OD1	1:B:591:SER:N	2.53	0.41
1:C:263:LEU:O	1:C:263:LEU:HD23	2.20	0.41
1:C:124:ILE:HD11	1:C:192:ILE:HG12	2.03	0.41
1:D:524:VAL:HG21	1:D:653:ILE:HD12	2.02	0.41
1:B:499:LEU:HD23	1:B:541:VAL:CG2	2.50	0.41
1:F:586:LEU:HB3	1:F:589:LEU:HD21	2.03	0.41
4:J:171:LEU:C	4:J:171:LEU:HD23	2.45	0.41
1:A:35:MET:SD	1:A:35:MET:N	2.94	0.41
1:C:136:ILE:HD11	1:C:169:ARG:HD3	2.03	0.41
1:F:505:TYR:HB2	1:F:506:PRO:HD3	2.03	0.41
2:G:209:GLU:HB2	2:G:210:PRO:HD2	2.03	0.41
2:G:529:LEU:HD23	2:G:529:LEU:C	2.46	0.41
1:A:614:LEU:O	1:A:614:LEU:HD23	2.20	0.40
1:C:49:ILE:HB	1:C:79:LEU:HD13	2.02	0.40
3:H:292:LEU:C	3:H:292:LEU:HD23	2.46	0.40
1:A:122:THR:HG22	1:A:179:GLU:O	2.22	0.40
1:A:434:ARG:NE	1:B:228:GLU:OE2	2.54	0.40
1:A:524:VAL:HG12	1:A:525:LEU:N	2.36	0.40
1:C:525:LEU:HD11	1:C:633:THR:HG22	2.02	0.40
1:D:568:ASN:OD1	1:D:569:ILE:N	2.52	0.40
4:L:301:MET:N	4:L:317:VAL:O	2.55	0.40
1:B:342:MET:HE1	1:B:373:PHE:CZ	2.56	0.40
1:D:254:TYR:OH	1:D:376:GLU:OE1	2.24	0.40
1:F:424:LEU:HD12	1:F:465:ALA:HB1	2.03	0.40
2:G:168:SER:O	2:G:170:HIS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:VAL:O	1:C:272:THR:HG23	2.22	0.40
1:C:277:PHE:O	1:C:278:LEU:C	2.65	0.40
1:C:405:ASP:O	1:C:406:LEU:C	2.64	0.40
1:C:424:LEU:HD12	1:C:465:ALA:HB1	2.03	0.40
1:D:513:TYR:O	1:D:517:GLY:N	2.53	0.40
1:E:405:ASP:O	1:E:406:LEU:C	2.64	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	706/838 (84%)	683 (97%)	23 (3%)	0	100	100
1	B	549/838 (66%)	521 (95%)	28 (5%)	0	100	100
1	C	710/838 (85%)	686 (97%)	24 (3%)	0	100	100
1	D	551/838 (66%)	526 (96%)	25 (4%)	0	100	100
1	E	533/838 (64%)	508 (95%)	25 (5%)	0	100	100
1	F	535/838 (64%)	514 (96%)	21 (4%)	0	100	100
2	G	472/583 (81%)	422 (89%)	49 (10%)	1 (0%)	43	73
3	H	55/363 (15%)	47 (86%)	8 (14%)	0	100	100
4	J	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
4	K	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
4	L	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	4330/6202 (70%)	4114 (95%)	215 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	189	TYR

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	603/697 (86%)	600 (100%)	3 (0%)	81	81
1	B	468/697 (67%)	462 (99%)	6 (1%)	61	71
1	C	606/697 (87%)	602 (99%)	4 (1%)	76	77
1	D	469/697 (67%)	463 (99%)	6 (1%)	61	71
1	E	448/697 (64%)	442 (99%)	6 (1%)	61	71
1	F	449/697 (64%)	446 (99%)	3 (1%)	76	77
2	G	425/518 (82%)	411 (97%)	14 (3%)	33	56
3	H	50/315 (16%)	48 (96%)	2 (4%)	28	52
4	J	68/69 (99%)	66 (97%)	2 (3%)	37	58
4	K	69/69 (100%)	67 (97%)	2 (3%)	37	58
4	L	69/69 (100%)	67 (97%)	2 (3%)	37	58
All	All	3724/5222 (71%)	3674 (99%)	50 (1%)	59	71

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	ARG
1	A	440	ILE
1	A	780	TYR
1	B	22	THR
1	B	26	ILE
1	B	280	ASN
1	B	346	LYS
1	B	635	ARG
1	B	638	GLN
1	C	346	LYS
1	C	624	LYS

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Mol	Chain	Res	Type
1	C	718	GLN
1	C	778	GLU
1	D	208	MET
1	D	249	ARG
1	D	285	MET
1	D	437	MET
1	D	460	ASP
1	D	624	LYS
1	E	228	GLU
1	E	346	LYS
1	E	608	ASP
1	E	617	GLU
1	E	626	ASN
1	E	782	GLN
1	F	302	GLU
1	F	346	LYS
1	F	788	ARG
2	G	107	ARG
2	G	141	ASP
2	G	142	ARG
2	G	148	CYS
2	G	162	ASN
2	G	175	LYS
2	G	215	ILE
2	G	316	GLU
2	G	354	GLU
2	G	367	ASN
2	G	545	LYS
2	G	549	GLU
2	G	558	GLU
2	G	572	LEU
3	H	281	MET
3	H	307	LEU
4	J	106	LYS
4	J	111	LYS
4	K	252	ASP
4	K	267	LEU
4	L	352	ASP
4	L	373	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	327	ASN
1	A	337	GLN
1	A	414	HIS
1	A	432	GLN
1	A	548	ASN
1	A	718	GLN
1	B	209	ASN
1	B	280	ASN
1	B	719	HIS
1	C	295	ASN
1	C	337	GLN
1	C	716	HIS
1	D	209	ASN
1	D	414	HIS
1	D	612	ASN
1	E	414	HIS
1	F	414	HIS
1	F	548	ASN
2	G	177	ASN
2	G	185	ASN
2	G	313	GLN
2	G	361	HIS
4	K	241	GLN
4	L	360	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 14 ligands modelled in this entry, 2 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
6	ADP	A	902	-	28,29,29	0.47	0	43,45,45	0.43	0
6	ADP	E	902	-	28,29,29	0.45	0	43,45,45	0.48	0
6	ADP	B	902	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
6	ADP	C	901	-	28,29,29	0.44	0	43,45,45	0.49	0
6	ADP	C	902	-	28,29,29	1.37	4 (14%)	43,45,45	1.84	10 (23%)
5	ATP	E	901	-	32,33,33	0.33	0	48,52,52	0.68	0
5	ATP	B	901	-	32,33,33	0.34	0	48,52,52	0.68	0
6	ADP	F	902	-	28,29,29	1.39	5 (17%)	43,45,45	1.84	11 (25%)
6	ADP	D	902	-	28,29,29	1.38	4 (14%)	43,45,45	1.86	11 (25%)
5	ATP	F	901	-	32,33,33	0.34	0	48,52,52	0.68	0
5	ATP	A	901	-	32,33,33	0.37	0	48,52,52	0.68	0
5	ATP	D	901	-	32,33,33	0.34	0	48,52,52	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	902	-	-	9/16/32/32	0/3/3/3
6	ADP	E	902	-	-	9/16/32/32	0/3/3/3
6	ADP	B	902	-	-	4/16/32/32	0/3/3/3
6	ADP	C	901	-	-	5/16/32/32	0/3/3/3
6	ADP	C	902	-	-	7/16/32/32	0/3/3/3
5	ATP	E	901	-	-	4/22/38/38	0/3/3/3
5	ATP	B	901	-	-	6/22/38/38	0/3/3/3
6	ADP	F	902	-	-	6/16/32/32	0/3/3/3
6	ADP	D	902	-	-	5/16/32/32	0/3/3/3
5	ATP	F	901	-	-	5/22/38/38	0/3/3/3
5	ATP	A	901	-	-	7/22/38/38	0/3/3/3
5	ATP	D	901	-	-	2/22/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	902	ADP	C5-C4	4.57	1.47	1.39
6	D	902	ADP	C5-C4	4.51	1.47	1.39
6	C	902	ADP	C5-C4	4.50	1.47	1.39
6	F	902	ADP	C5-C4	4.48	1.47	1.39
6	B	902	ADP	C5-C6	2.71	1.48	1.41
6	F	902	ADP	C5-C6	2.69	1.48	1.41
6	D	902	ADP	C5-C6	2.61	1.48	1.41
6	C	902	ADP	C5-C6	2.60	1.48	1.41
6	B	902	ADP	C8-N7	2.45	1.36	1.31
6	D	902	ADP	C8-N7	2.41	1.36	1.31
6	B	902	ADP	C5-N7	-2.40	1.34	1.39
6	F	902	ADP	C8-N7	2.39	1.36	1.31
6	C	902	ADP	C8-N7	2.39	1.36	1.31
6	F	902	ADP	C5-N7	-2.35	1.34	1.39
6	C	902	ADP	C5-N7	-2.34	1.34	1.39
6	D	902	ADP	C5-N7	-2.33	1.34	1.39
6	F	902	ADP	C4-N9	-2.05	1.33	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	ADP	C5-C4-N3	-5.87	118.64	126.72
6	D	902	ADP	C5-C4-N3	-5.73	118.83	126.72
6	F	902	ADP	C5-C4-N3	-5.65	118.94	126.72
6	C	902	ADP	C5-C4-N3	-5.63	118.96	126.72
6	C	902	ADP	N3-C4-N9	4.44	134.71	127.17
6	D	902	ADP	N3-C4-N9	4.44	134.71	127.17
6	F	902	ADP	N3-C4-N9	4.13	134.20	127.17
6	B	902	ADP	N3-C4-N9	4.10	134.15	127.17
6	B	902	ADP	C4-C5-N7	-3.93	106.09	110.58
6	F	902	ADP	C2-N3-C4	3.90	121.36	111.83
6	B	902	ADP	C2-N3-C4	3.89	121.33	111.83
6	D	902	ADP	C2-N3-C4	3.86	121.26	111.83
6	F	902	ADP	N3-C2-N1	-3.80	122.84	128.58
6	C	902	ADP	C2-N3-C4	3.78	121.07	111.83
6	F	902	ADP	C4-C5-N7	-3.73	106.32	110.58
6	D	902	ADP	N3-C2-N1	-3.72	122.94	128.58
6	C	902	ADP	N3-C2-N1	-3.68	123.01	128.58
6	B	902	ADP	N3-C2-N1	-3.54	123.22	128.58
6	D	902	ADP	C4-C5-N7	-3.51	106.57	110.58
6	C	902	ADP	C4-C5-N7	-3.47	106.62	110.58
6	C	902	ADP	C4-N9-C8	2.89	108.78	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	ADP	C5-N7-C8	2.79	107.84	103.45
6	D	902	ADP	C4-N9-C8	2.75	108.63	105.74
6	F	902	ADP	C5-N7-C8	2.70	107.69	103.45
6	D	902	ADP	C5-N7-C8	2.68	107.66	103.45
6	C	902	ADP	C5-N7-C8	2.67	107.65	103.45
6	F	902	ADP	C6-C5-N7	2.45	136.82	132.09
6	F	902	ADP	C4-N9-C8	2.41	108.27	105.74
6	B	902	ADP	C6-C5-N7	2.39	136.69	132.09
6	C	902	ADP	N9-C8-N7	-2.33	110.63	113.94
6	D	902	ADP	N9-C8-N7	-2.29	110.69	113.94
6	D	902	ADP	C6-C5-N7	2.24	136.41	132.09
6	D	902	ADP	C3'-C2'-C1'	2.21	105.65	101.46
6	C	902	ADP	C6-C5-N7	2.18	136.30	132.09
6	F	902	ADP	N9-C8-N7	-2.17	110.85	113.94
6	C	902	ADP	C2-N1-C6	2.11	122.20	118.73
6	F	902	ADP	C2-N1-C6	2.10	122.18	118.73
6	D	902	ADP	C2-N1-C6	2.08	122.14	118.73
6	B	902	ADP	N9-C8-N7	-2.05	111.03	113.94
6	F	902	ADP	C3'-C2'-C1'	2.05	105.33	101.46
6	B	902	ADP	C3'-C2'-C1'	2.02	105.28	101.46

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	ATP	O4'-C1'-N9-C8
5	A	901	ATP	O4'-C1'-N9-C4
5	B	901	ATP	O4'-C1'-N9-C8
5	B	901	ATP	O4'-C1'-N9-C4
5	D	901	ATP	O4'-C1'-N9-C8
5	D	901	ATP	O4'-C1'-N9-C4
5	E	901	ATP	PB-O3B-PG-O2G
5	E	901	ATP	O4'-C1'-N9-C8
5	E	901	ATP	O4'-C1'-N9-C4
5	F	901	ATP	PB-O3B-PG-O2G
5	F	901	ATP	O4'-C1'-N9-C8
5	F	901	ATP	O4'-C1'-N9-C4
6	A	902	ADP	C5'-O5'-PA-O1A
6	A	902	ADP	C5'-O5'-PA-O2A
6	A	902	ADP	C5'-O5'-PA-O3A
6	A	902	ADP	O4'-C1'-N9-C8
6	A	902	ADP	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
6	C	901	ADP	PA-O3A-PB-O2B
6	C	901	ADP	PA-O3A-PB-O3B
6	C	901	ADP	O4'-C1'-N9-C8
6	C	901	ADP	O4'-C1'-N9-C4
6	E	902	ADP	C5'-O5'-PA-O1A
6	E	902	ADP	C5'-O5'-PA-O2A
6	E	902	ADP	C5'-O5'-PA-O3A
6	E	902	ADP	C4'-C5'-O5'-PA
6	E	902	ADP	O4'-C4'-C5'-O5'
6	F	902	ADP	C5'-O5'-PA-O3A
6	E	902	ADP	C3'-C4'-C5'-O5'
6	C	902	ADP	O4'-C1'-N9-C4
6	D	902	ADP	O4'-C1'-N9-C4
6	E	902	ADP	O4'-C1'-N9-C4
6	B	902	ADP	C2'-C1'-N9-C8
6	C	902	ADP	O4'-C1'-N9-C8
6	B	902	ADP	C2'-C1'-N9-C4
6	D	902	ADP	O4'-C1'-N9-C8
6	F	902	ADP	C2'-C1'-N9-C8
5	F	901	ATP	PA-O3A-PB-O1B
6	D	902	ADP	PB-O3A-PA-O1A
5	A	901	ATP	PB-O3B-PG-O1G
6	E	902	ADP	O4'-C1'-N9-C8
6	C	902	ADP	O4'-C4'-C5'-O5'
6	A	902	ADP	PB-O3A-PA-O1A
6	C	902	ADP	PB-O3A-PA-O1A
6	C	901	ADP	C5'-O5'-PA-O1A
6	C	902	ADP	C5'-O5'-PA-O3A
6	F	902	ADP	C5'-O5'-PA-O1A
6	A	902	ADP	C4'-C5'-O5'-PA
5	A	901	ATP	PA-O3A-PB-O1B
6	D	902	ADP	PB-O3A-PA-O2A
6	F	902	ADP	C2'-C1'-N9-C4
6	B	902	ADP	C3'-C4'-C5'-O5'
6	E	902	ADP	C2'-C1'-N9-C8
6	F	902	ADP	C3'-C4'-C5'-O5'
5	B	901	ATP	PB-O3B-PG-O1G
6	B	902	ADP	O4'-C4'-C5'-O5'
6	C	902	ADP	PB-O3A-PA-O2A
5	A	901	ATP	PB-O3B-PG-O2G
5	A	901	ATP	PB-O3B-PG-O3G
5	B	901	ATP	PB-O3B-PG-O2G

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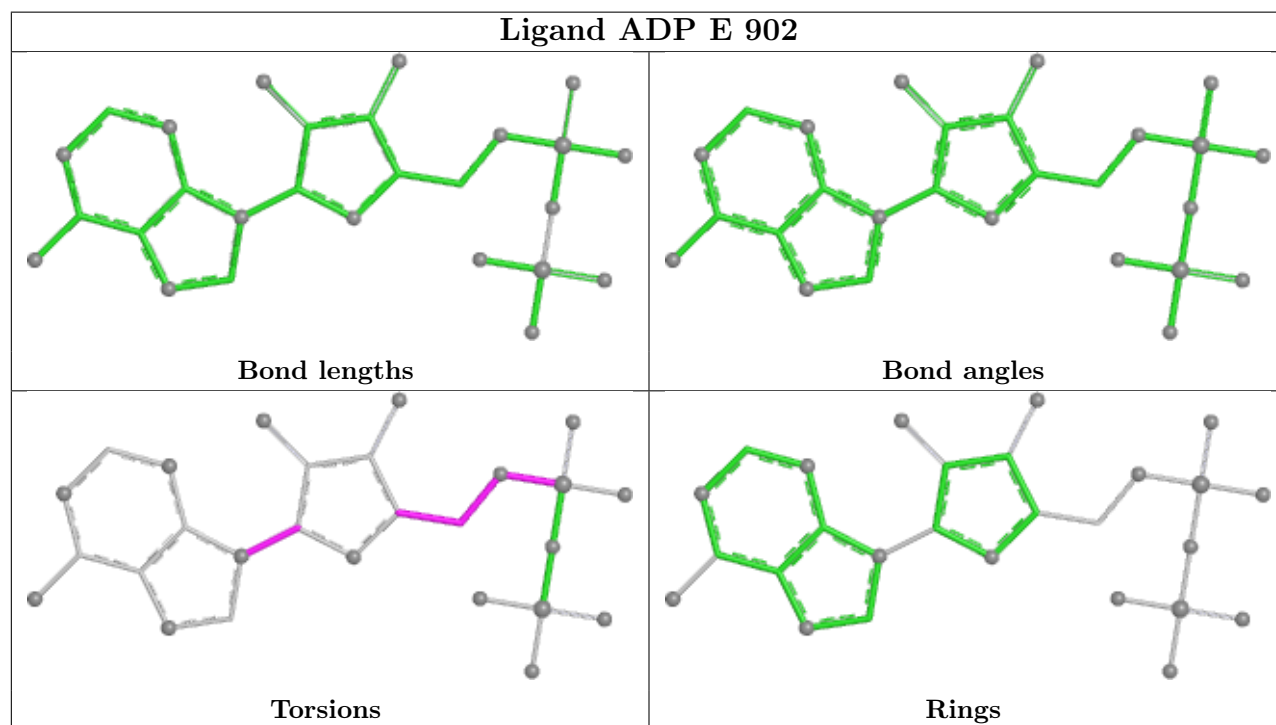
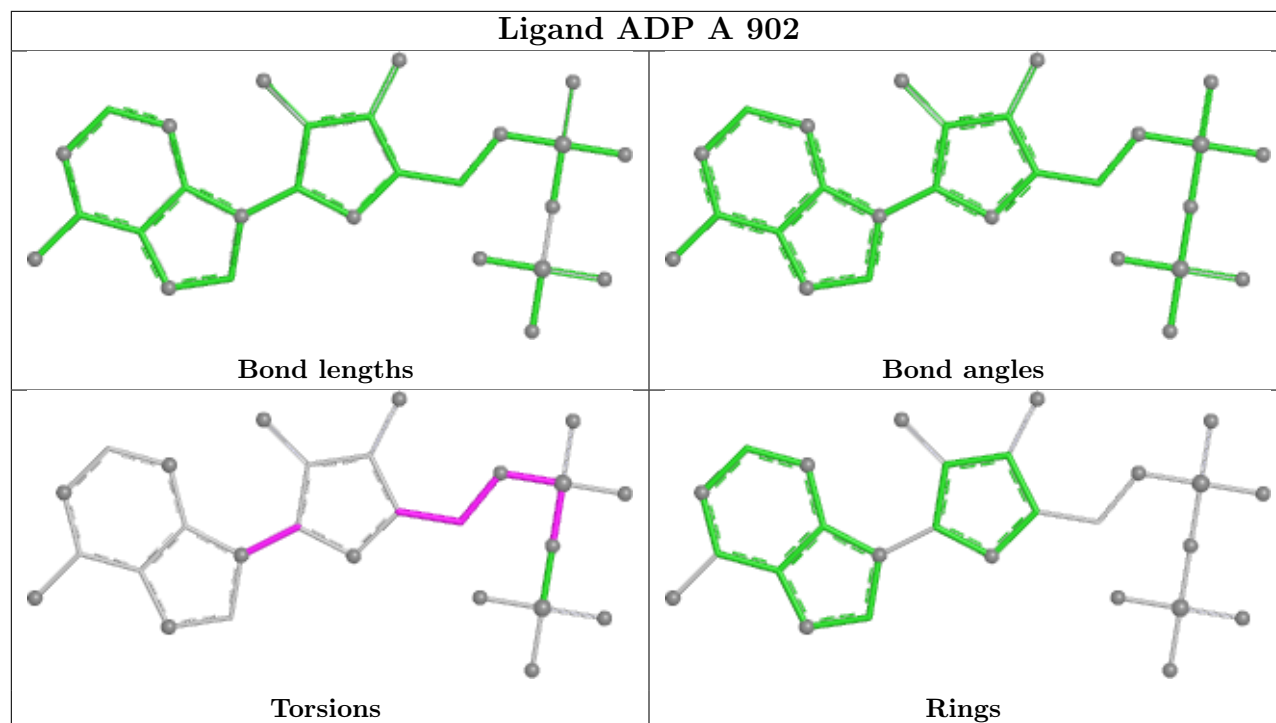
Mol	Chain	Res	Type	Atoms
5	B	901	ATP	PB-O3B-PG-O3G
6	A	902	ADP	O4'-C4'-C5'-O5'
6	D	902	ADP	C2'-C1'-N9-C8
5	F	901	ATP	O4'-C4'-C5'-O5'
6	C	902	ADP	C3'-C4'-C5'-O5'
6	F	902	ADP	O4'-C1'-N9-C8
6	A	902	ADP	PB-O3A-PA-O2A
5	B	901	ATP	O4'-C4'-C5'-O5'
5	E	901	ATP	O4'-C4'-C5'-O5'
5	A	901	ATP	PA-O3A-PB-O3B

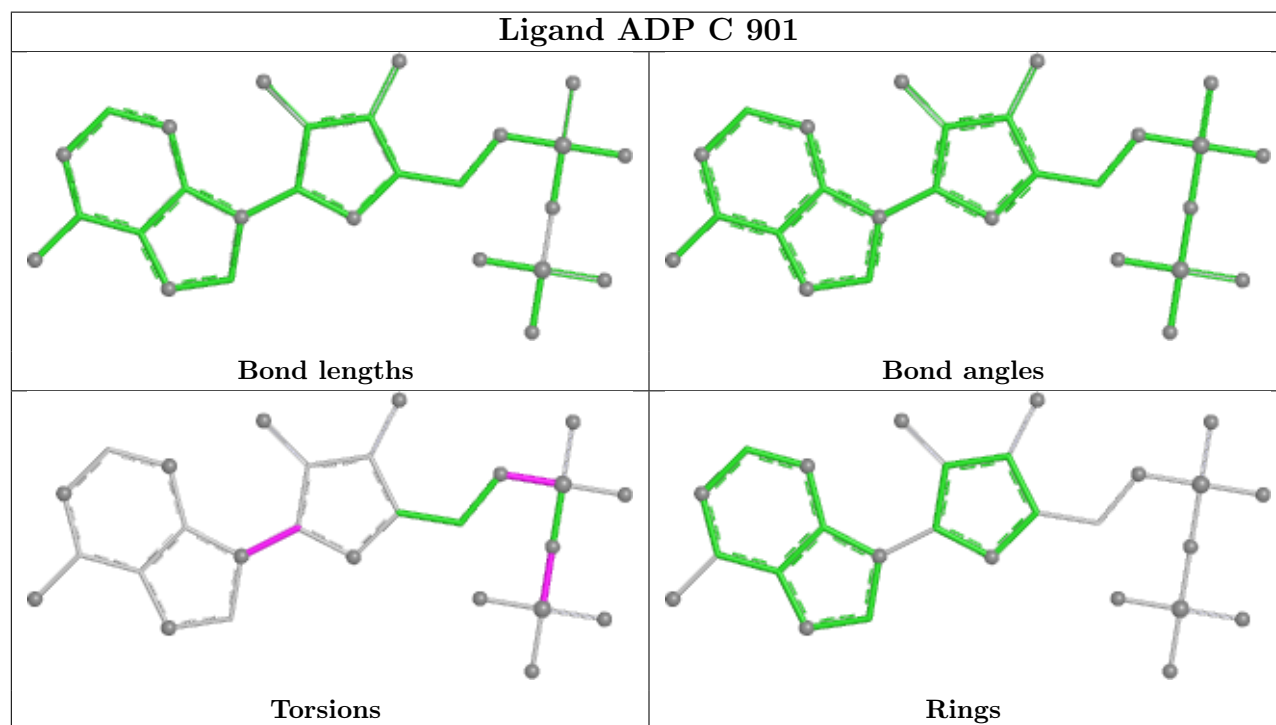
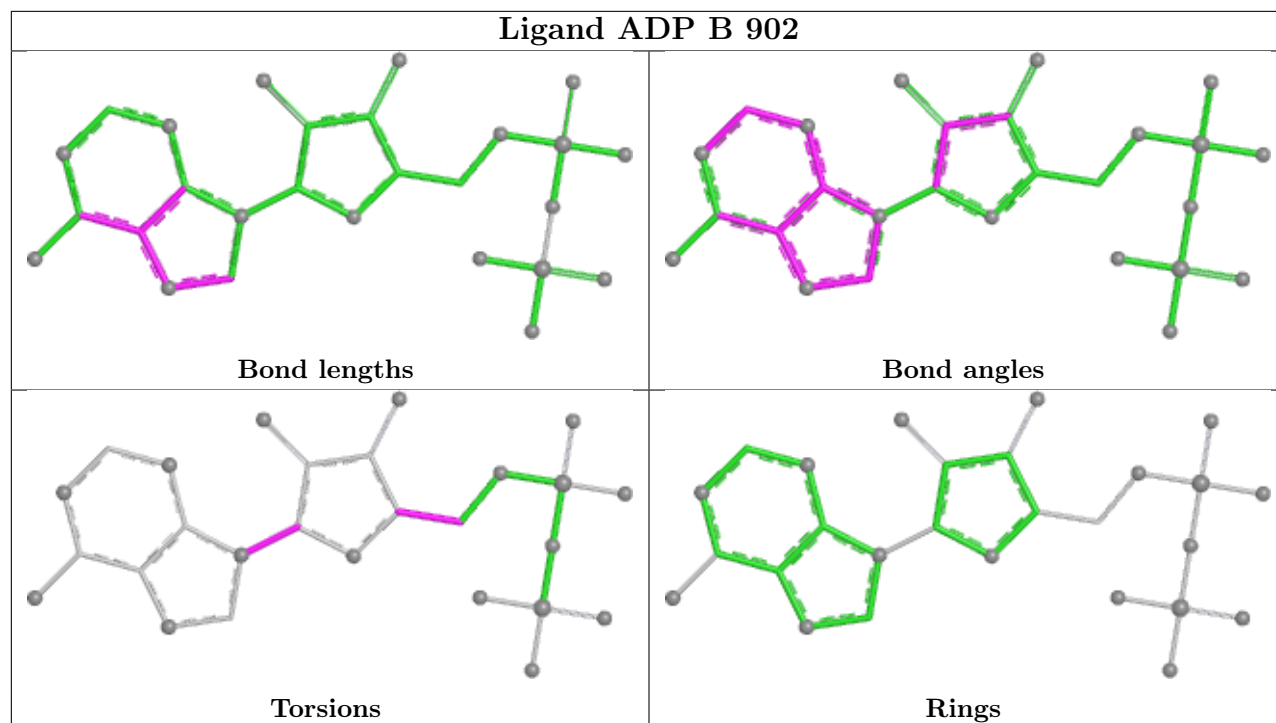
There are no ring outliers.

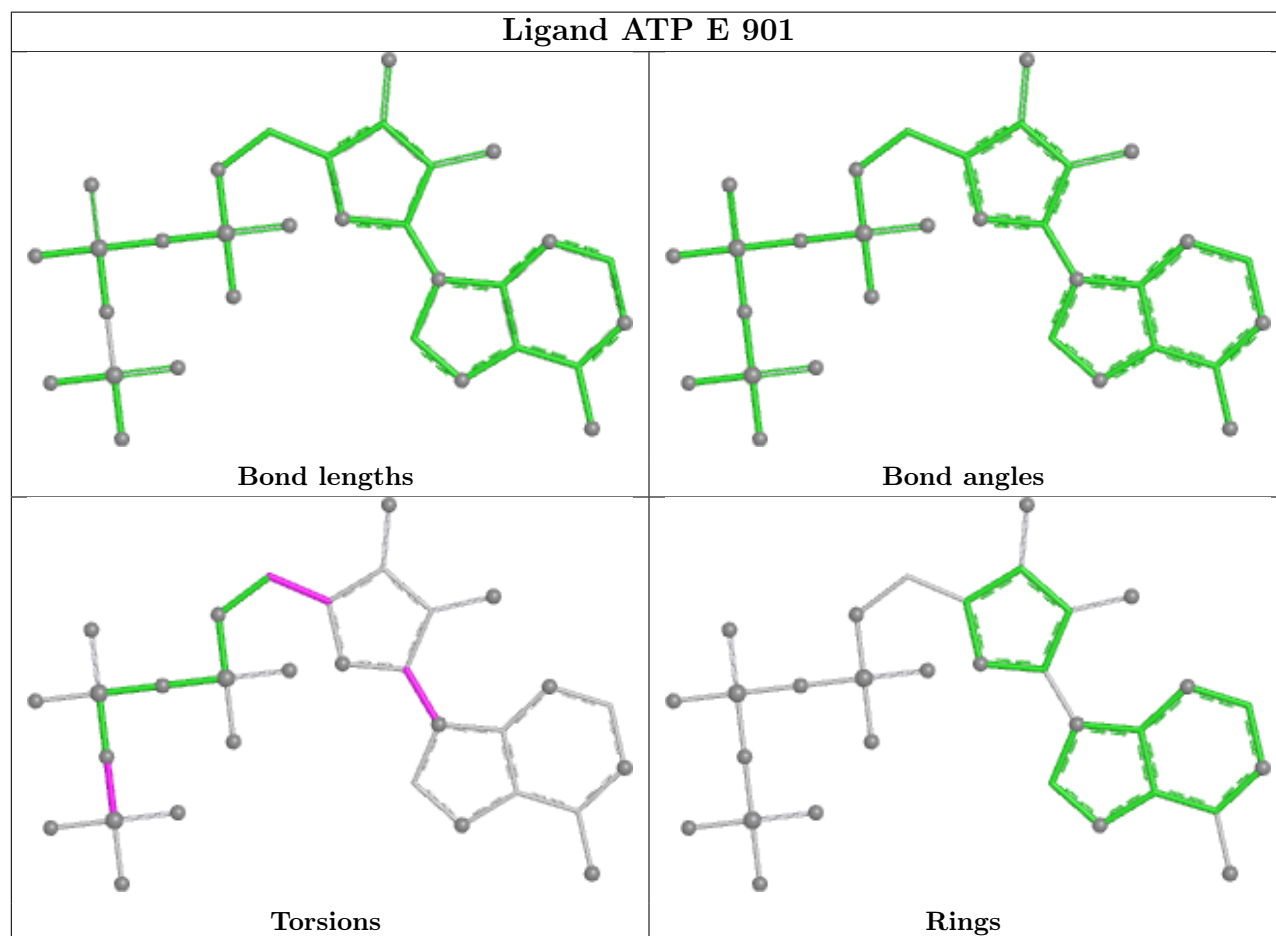
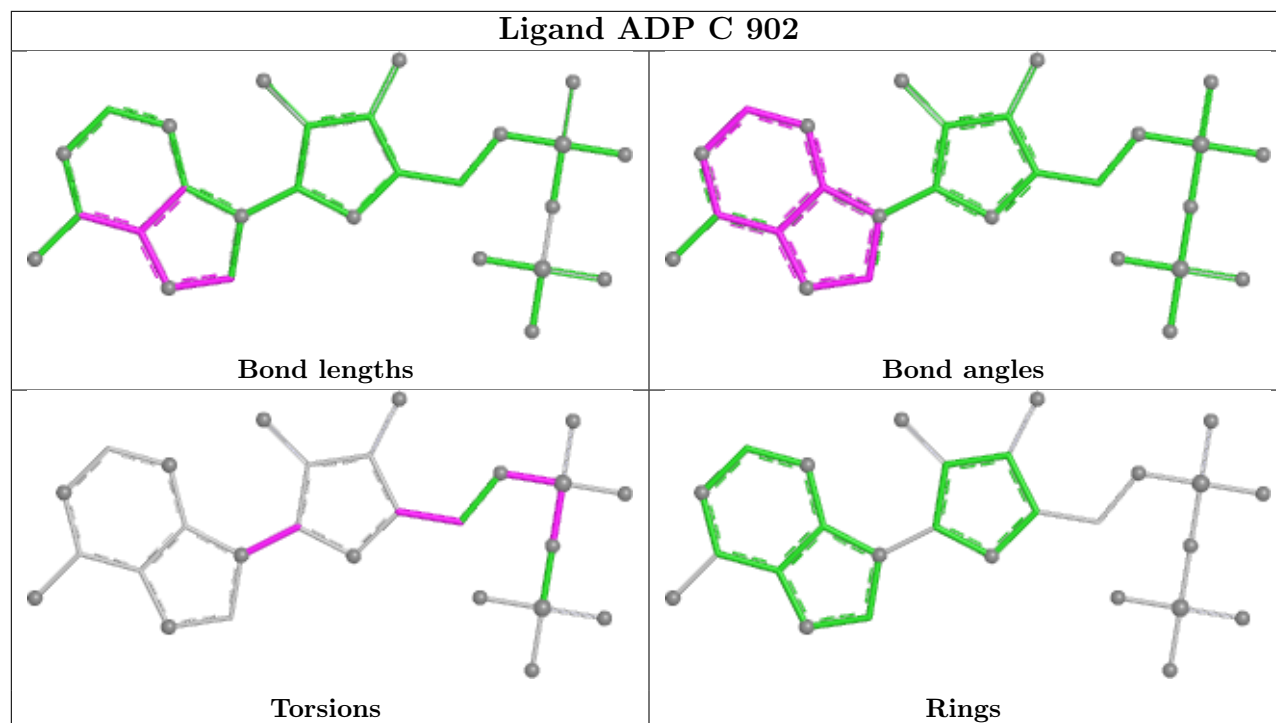
9 monomers are involved in 11 short contacts:

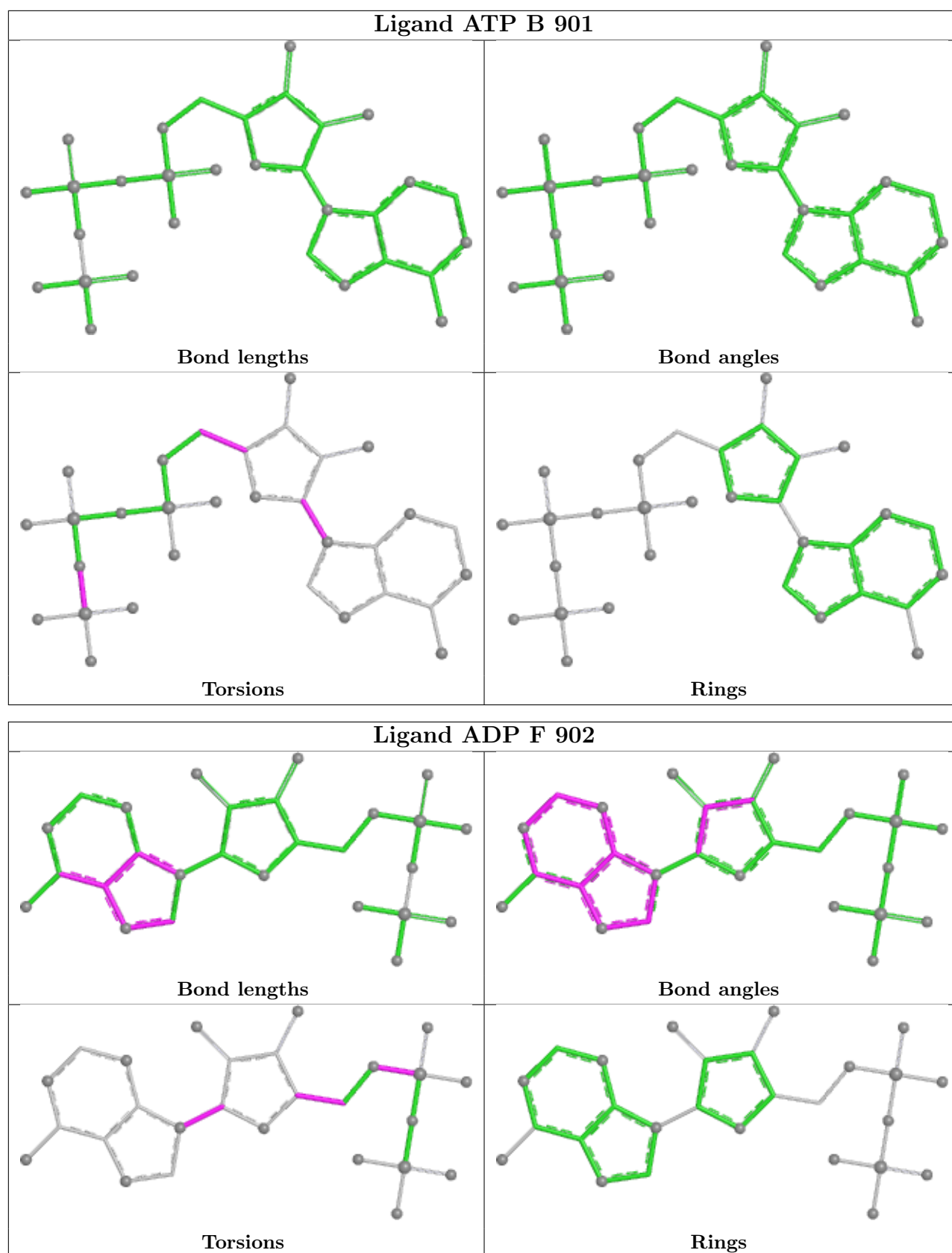
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	902	ADP	1	0
6	E	902	ADP	2	0
5	E	901	ATP	1	0
5	B	901	ATP	1	0
6	F	902	ADP	1	0
6	D	902	ADP	1	0
5	F	901	ATP	1	0
5	A	901	ATP	2	0
5	D	901	ATP	1	0

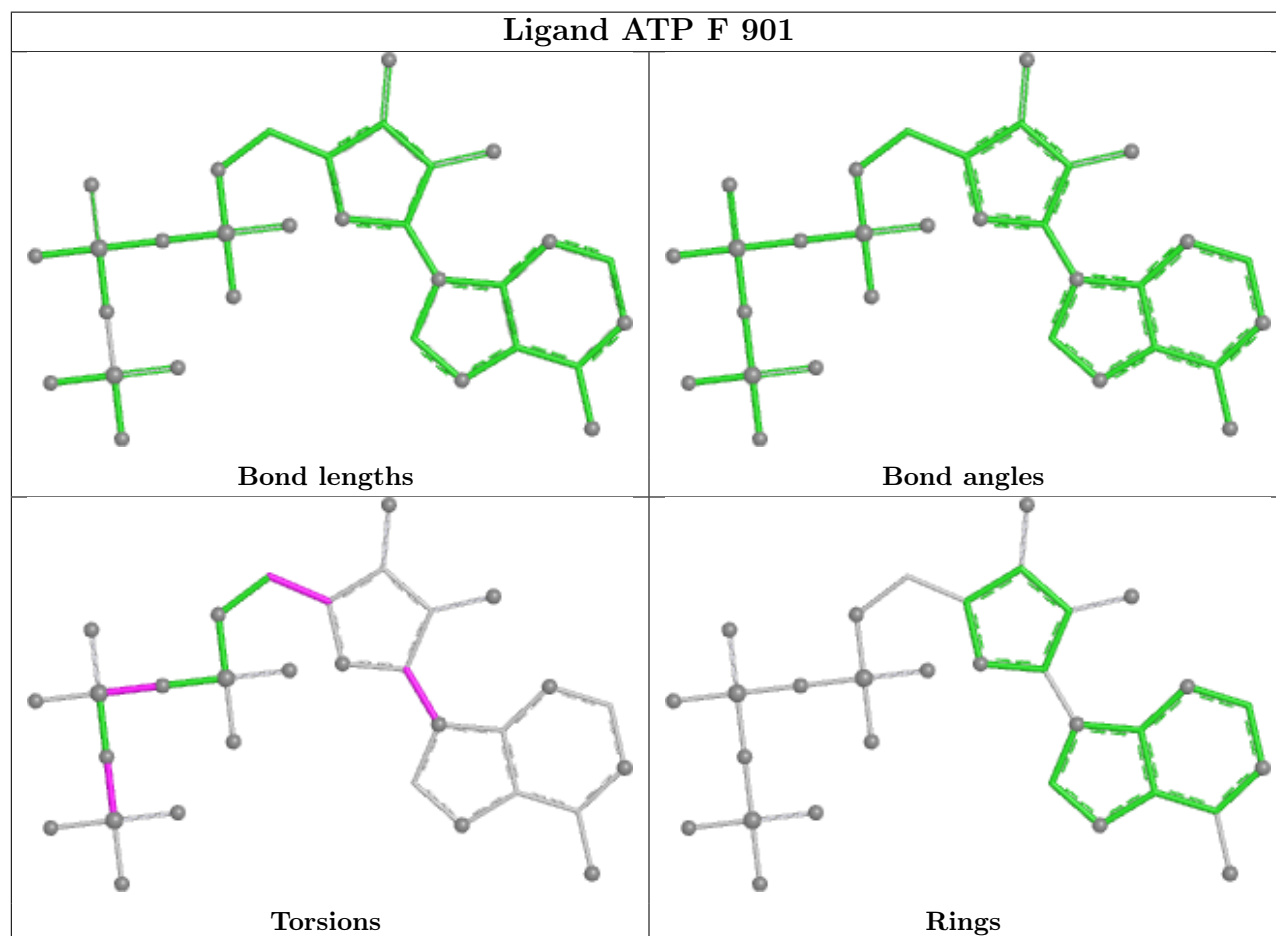
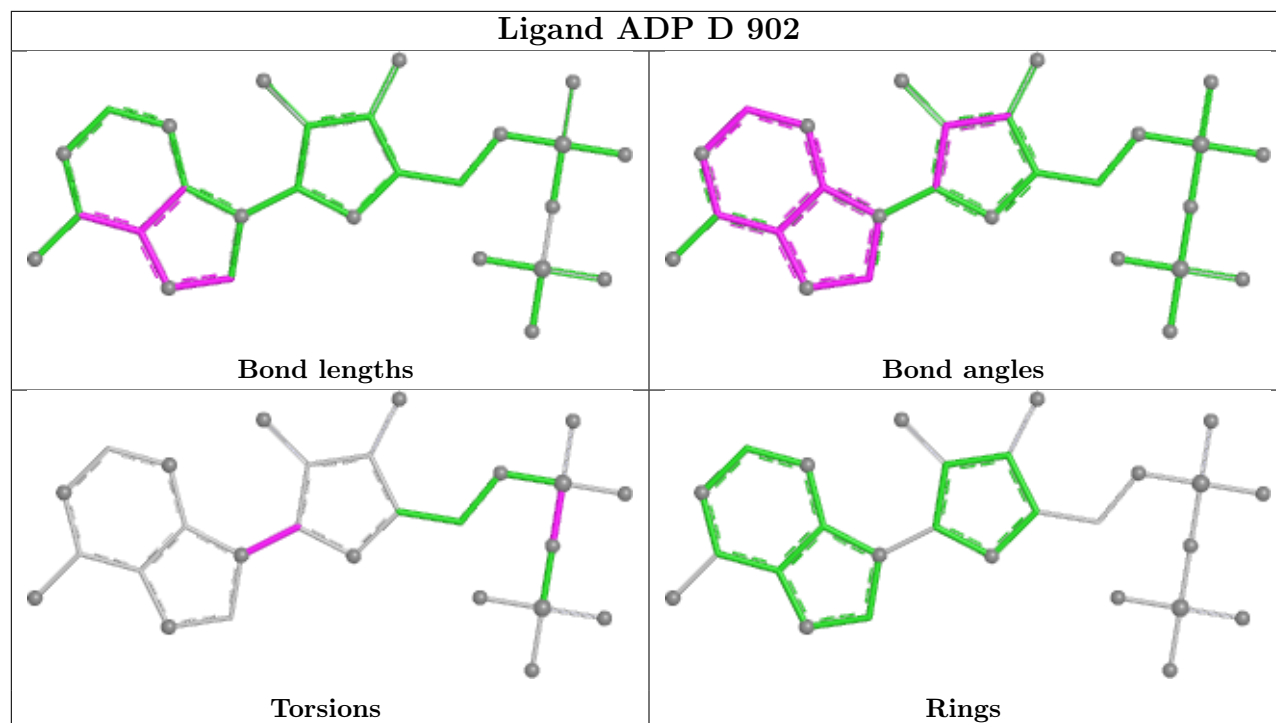
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

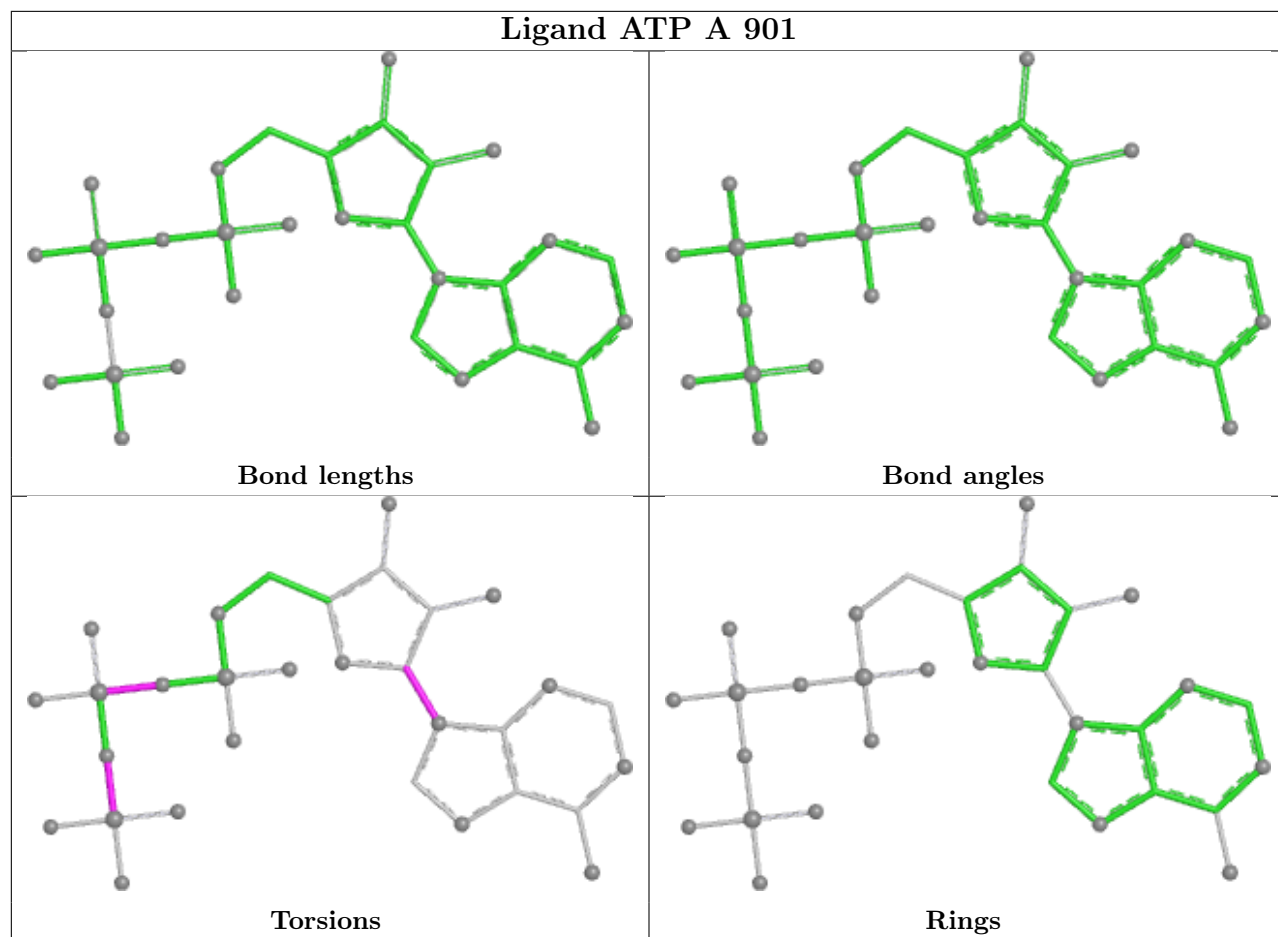


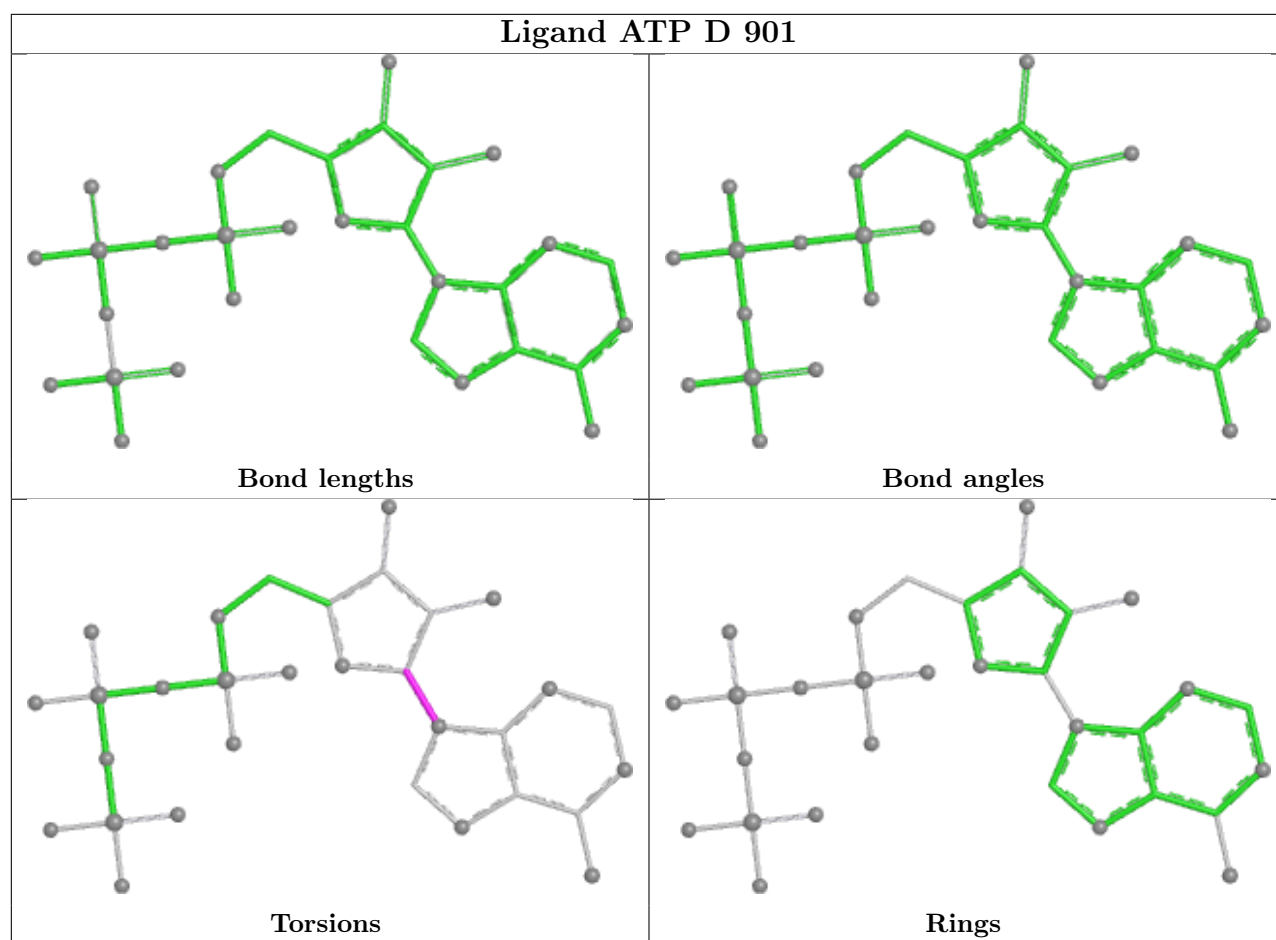












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

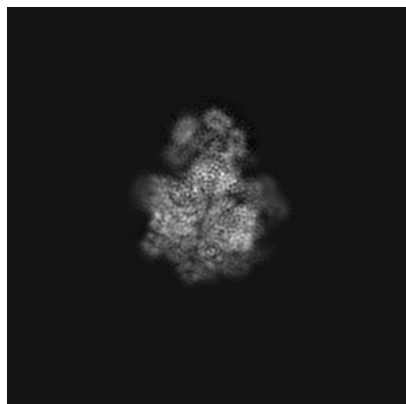
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27275. These allow visual inspection of the internal detail of the map and identification of artifacts.

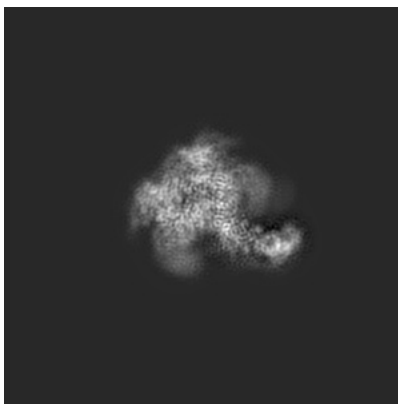
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

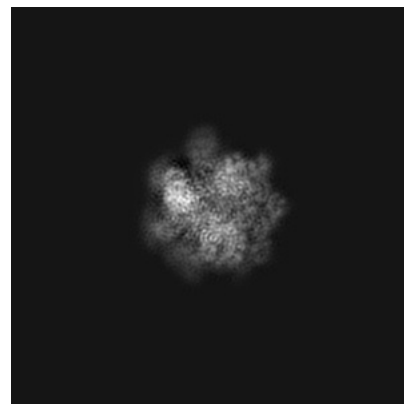
6.1.1 Primary map



X

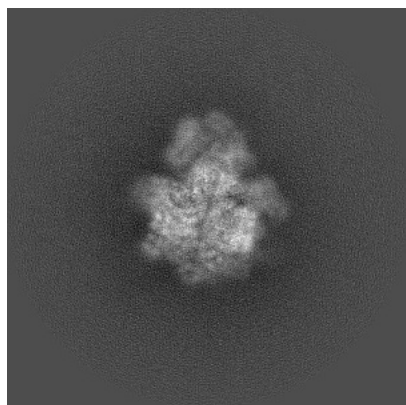


Y

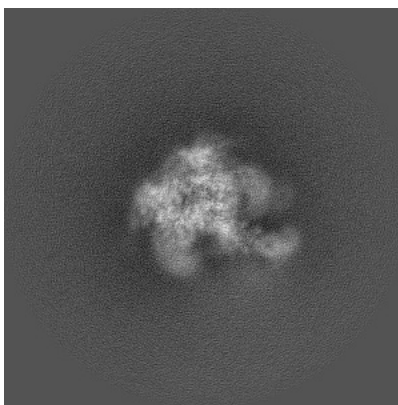


Z

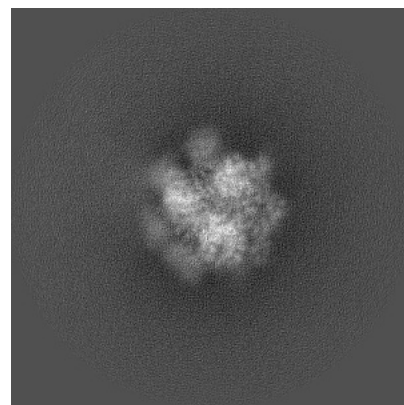
6.1.2 Raw map



X



Y

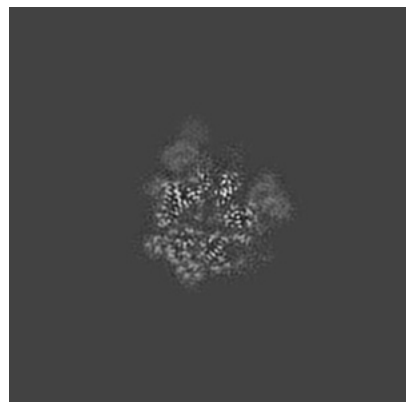


Z

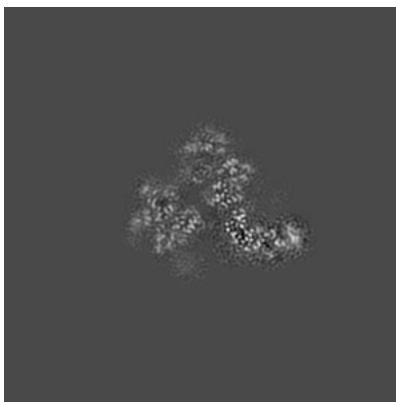
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

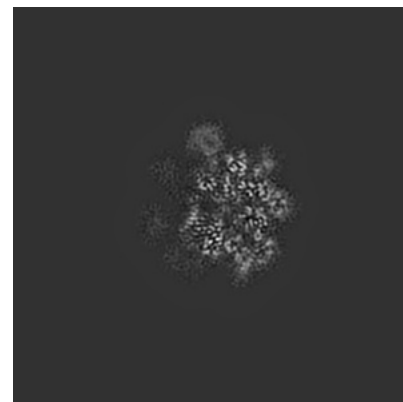
6.2.1 Primary map



X Index: 192

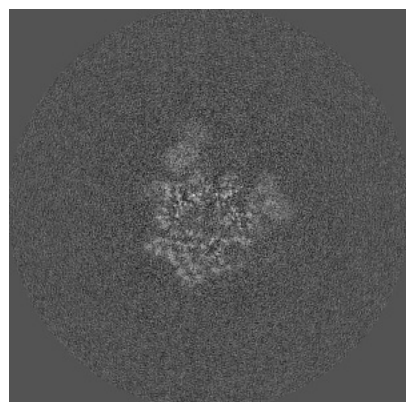


Y Index: 192

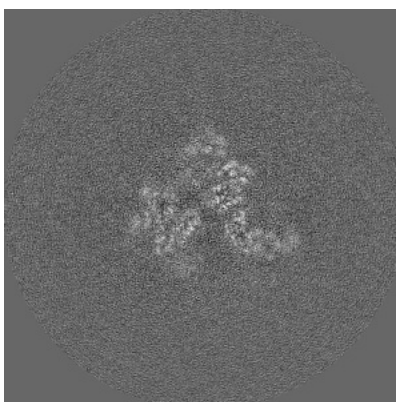


Z Index: 192

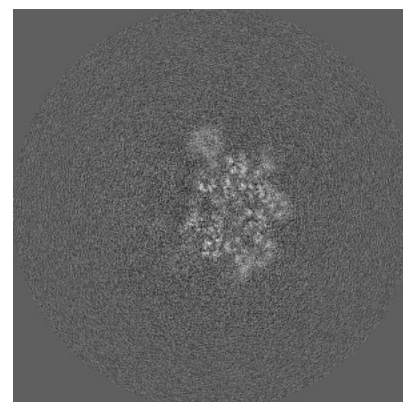
6.2.2 Raw map



X Index: 192



Y Index: 192

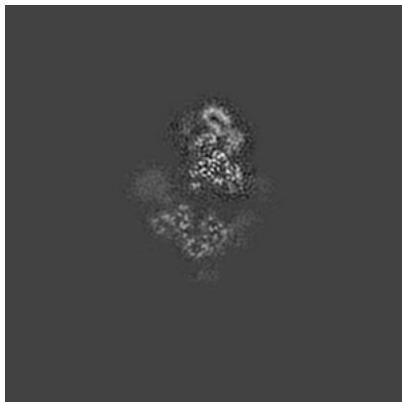


Z Index: 192

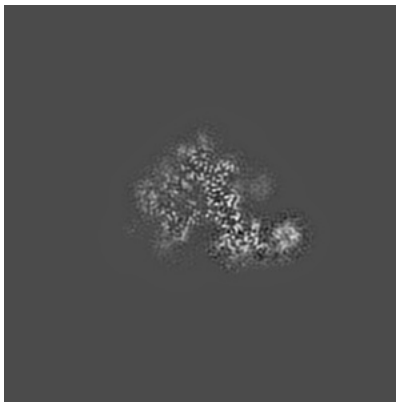
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

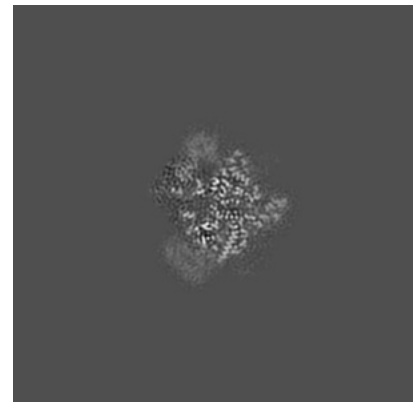
6.3.1 Primary map



X Index: 163

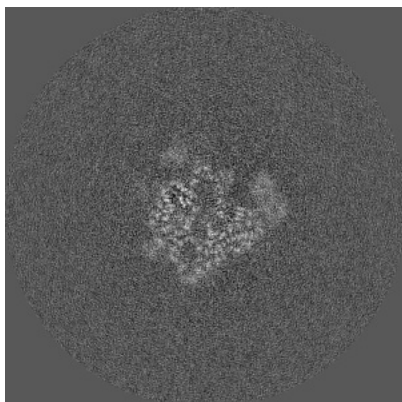


Y Index: 206

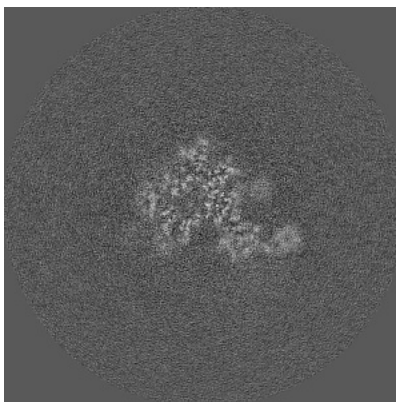


Z Index: 208

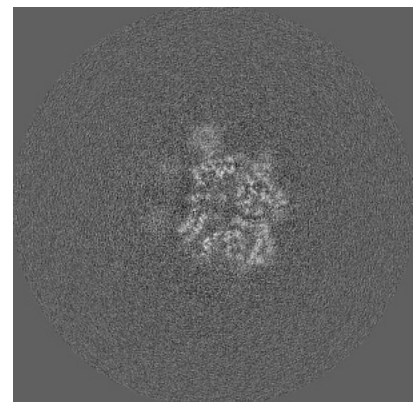
6.3.2 Raw map



X Index: 184



Y Index: 205

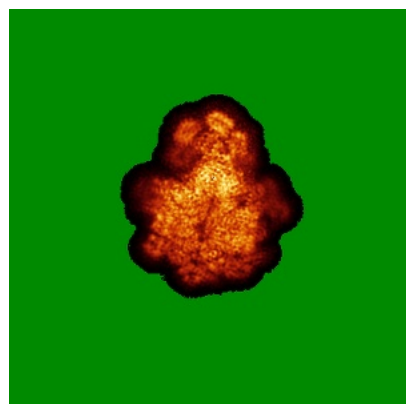


Z Index: 188

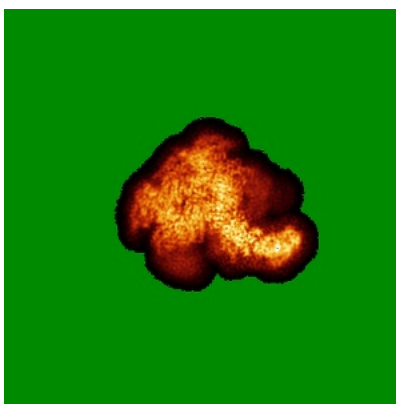
The images above show the largest variance slices of the map in three orthogonal directions.

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

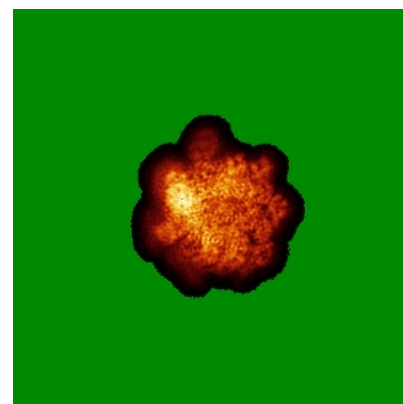
6.4.1 Primary map



X

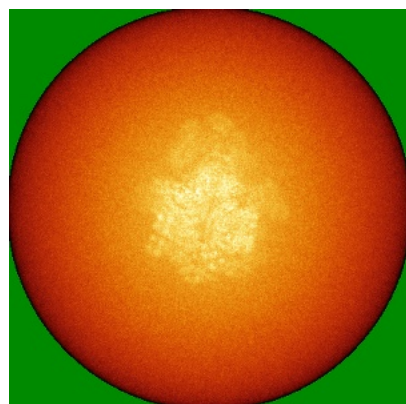


Y

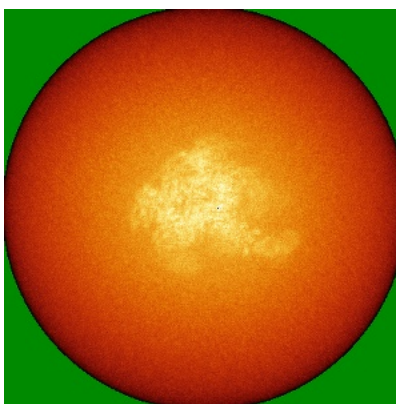


Z

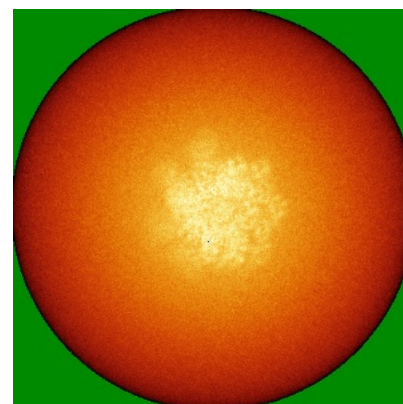
6.4.2 Raw map



X



Y



Z

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

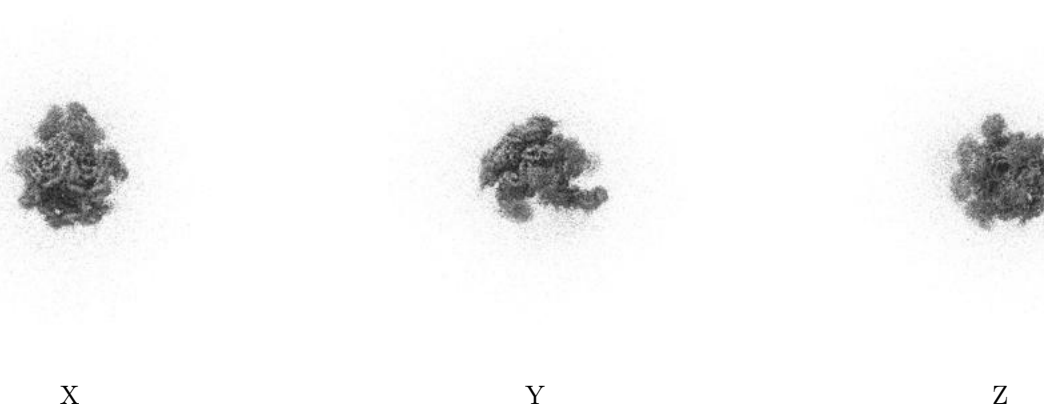
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

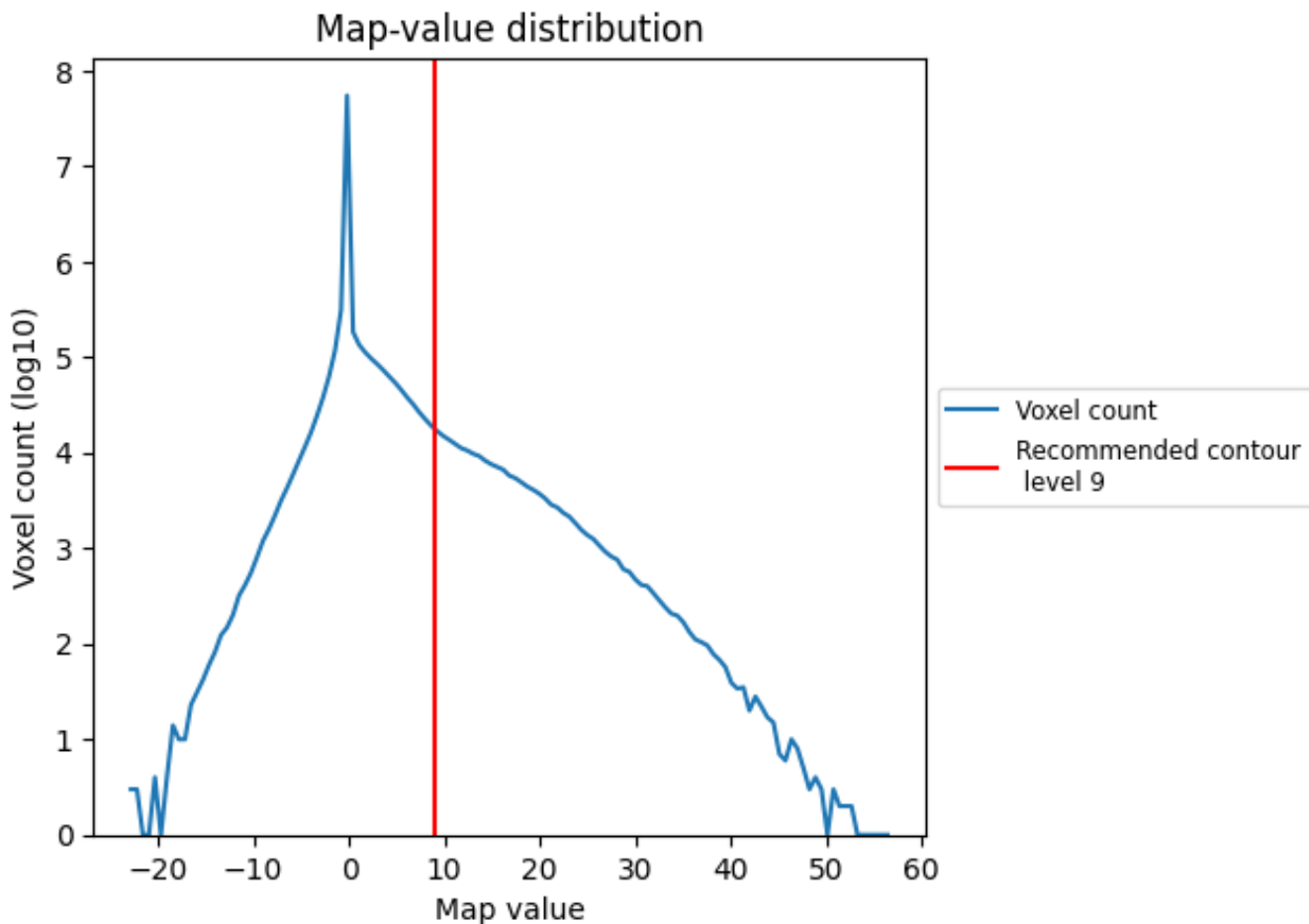
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

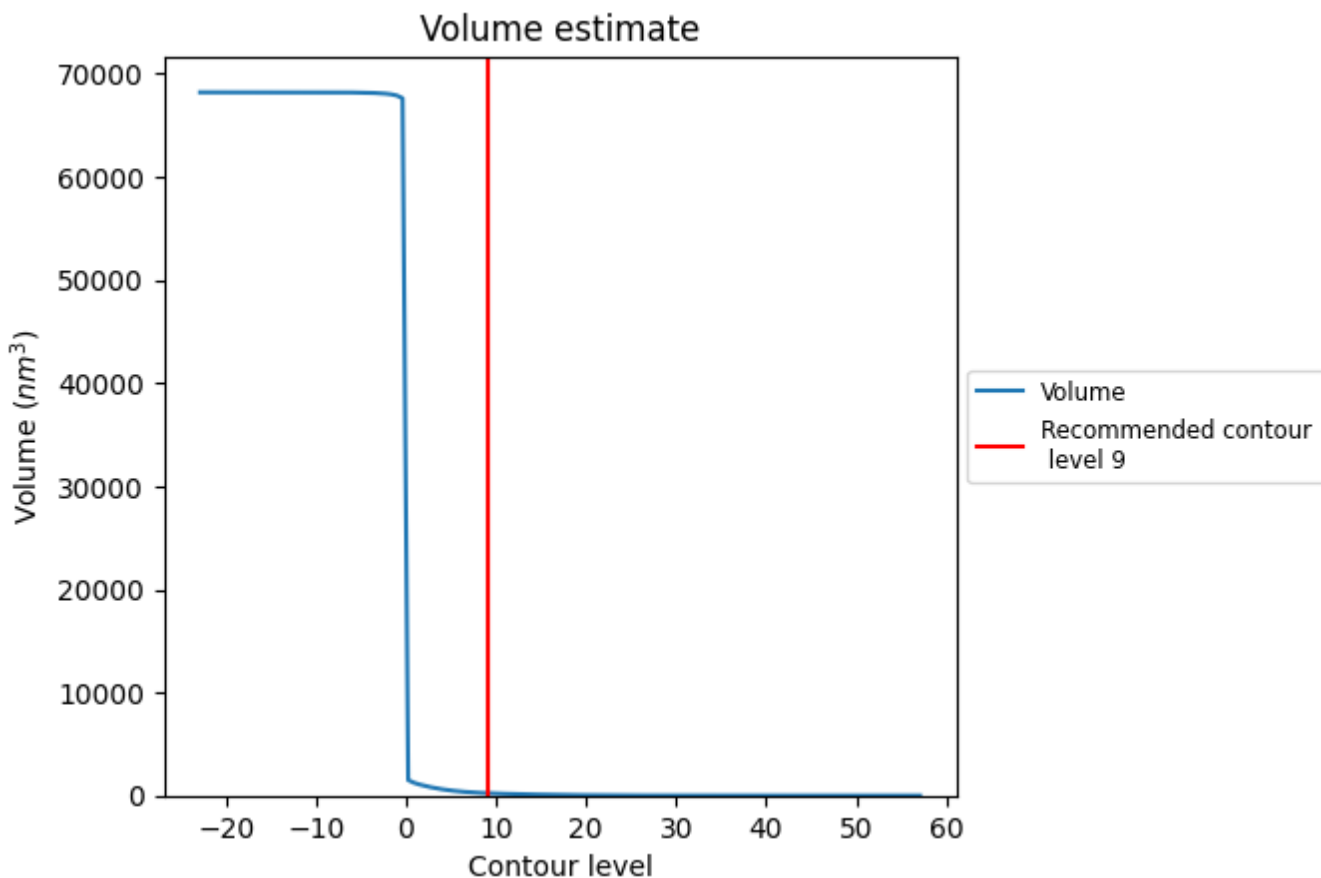
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

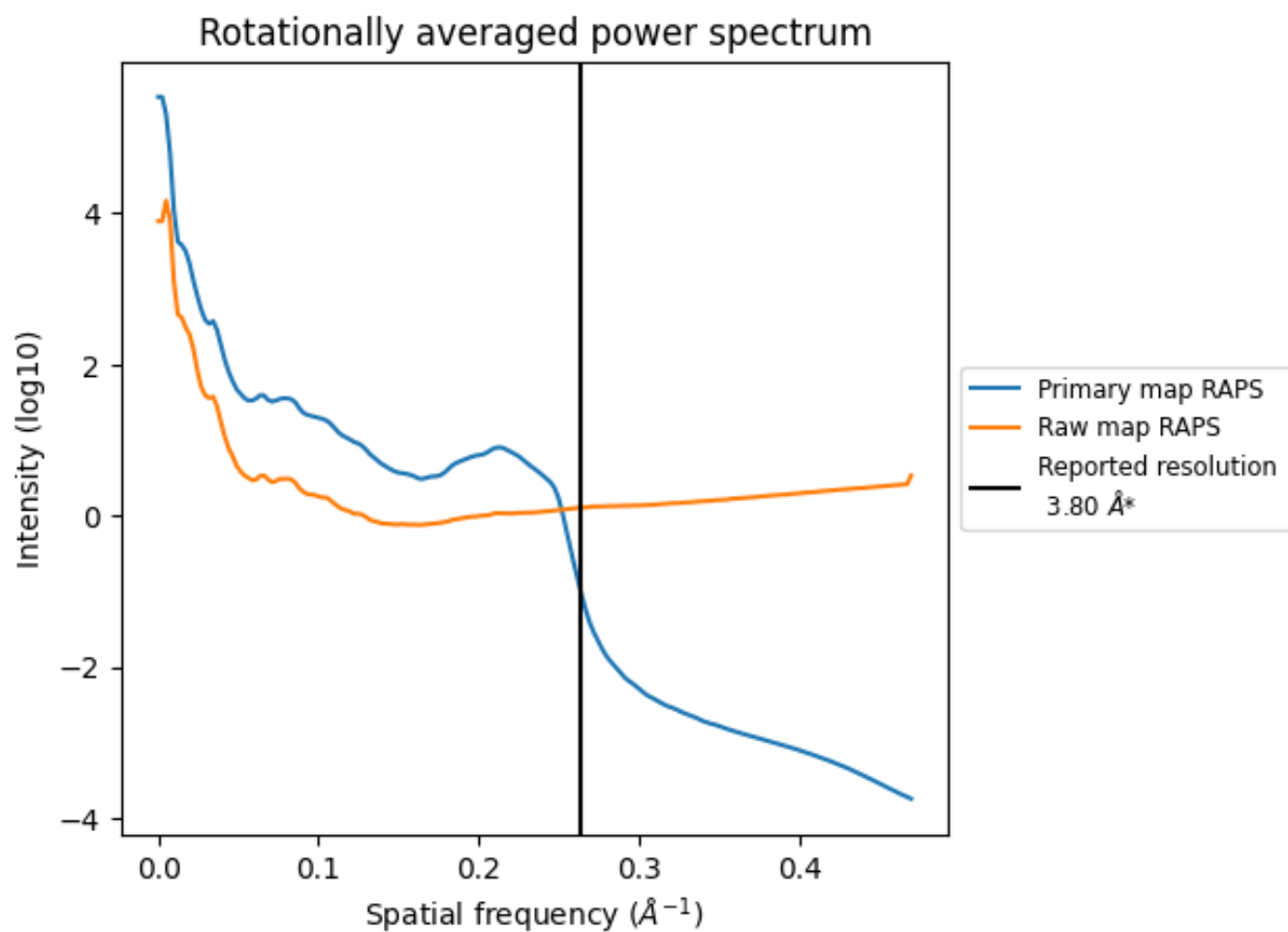
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 230 nm³; this corresponds to an approximate mass of 208 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

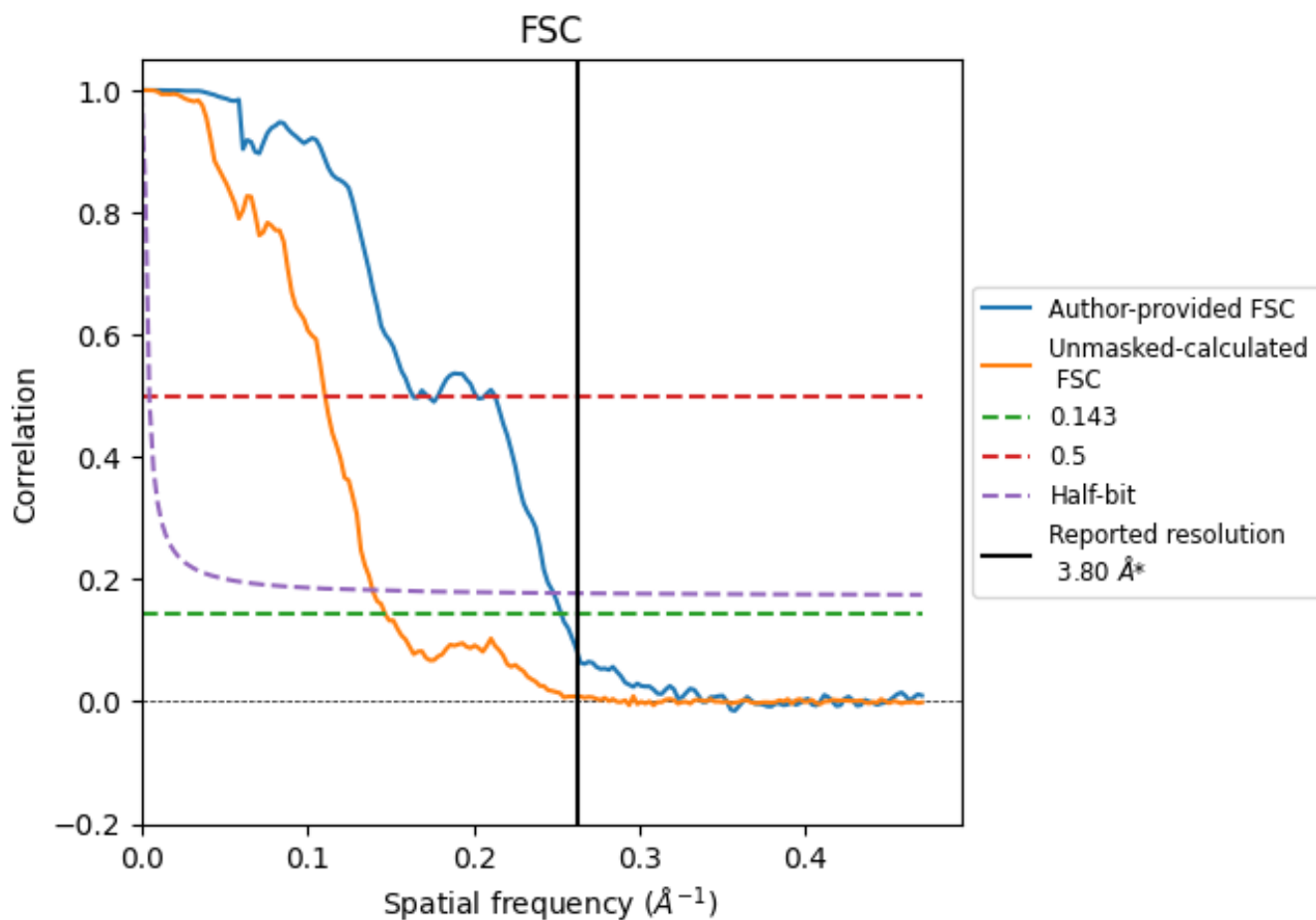


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

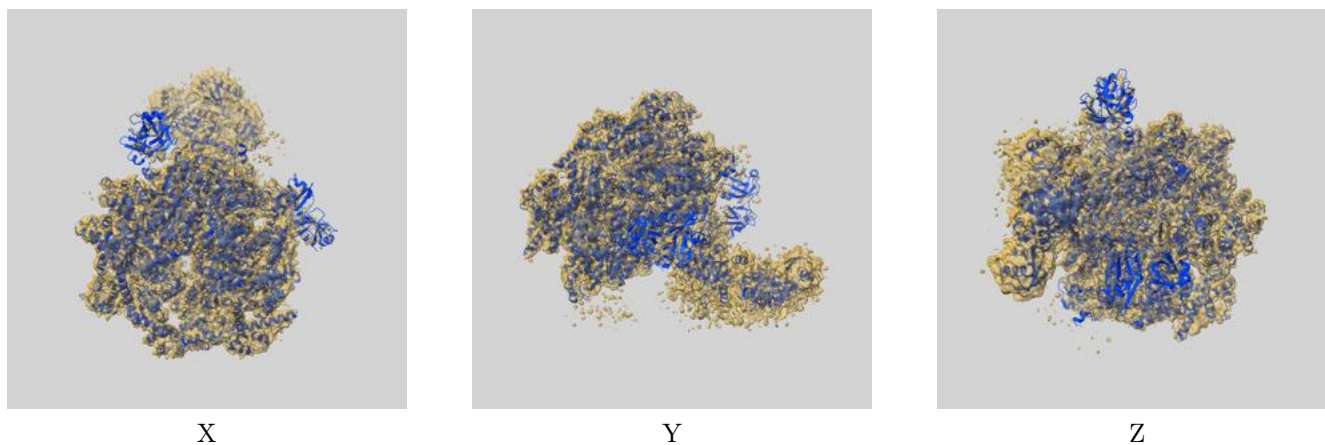
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.96	6.12	4.03
Unmasked-calculated*	6.82	9.04	7.18

*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 6.82 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

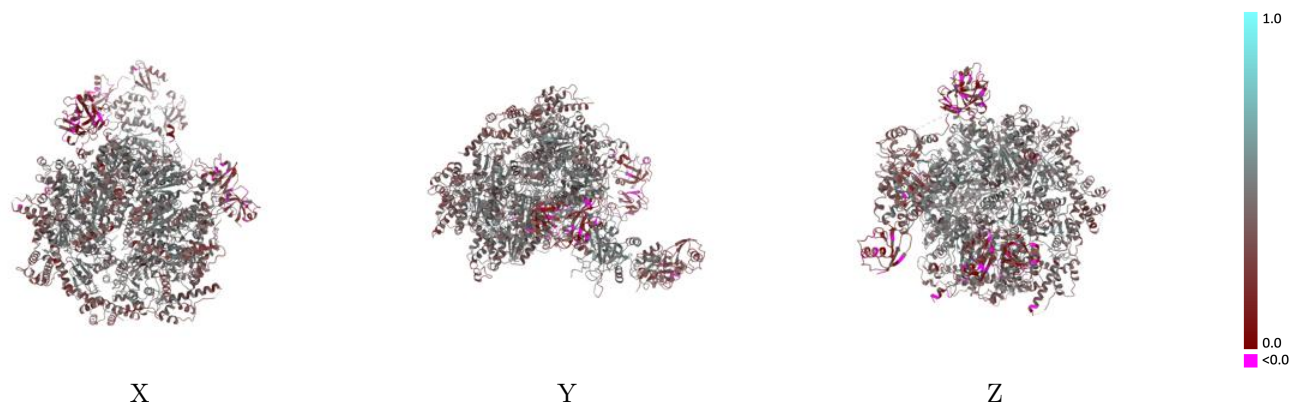
This section contains information regarding the fit between EMDB map EMD-27275 and PDB model 8DAT. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



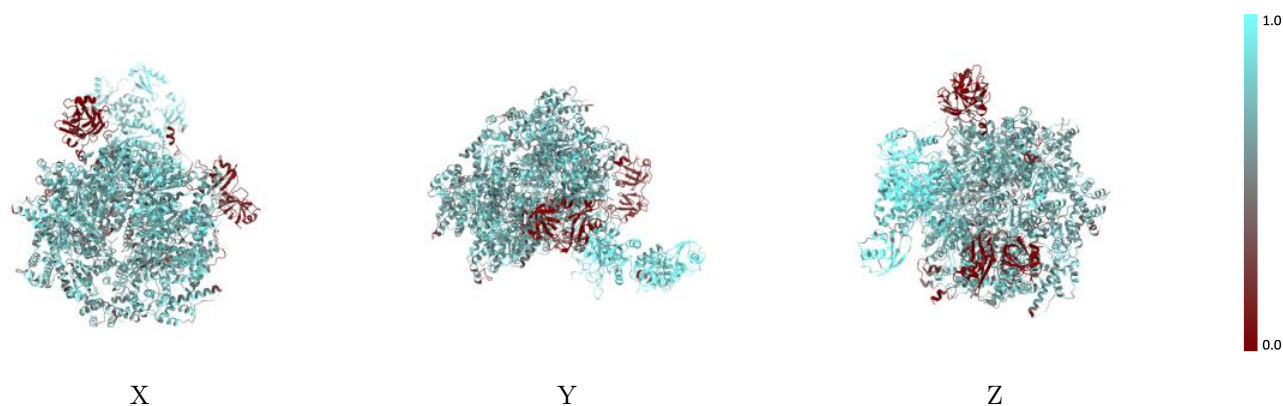
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



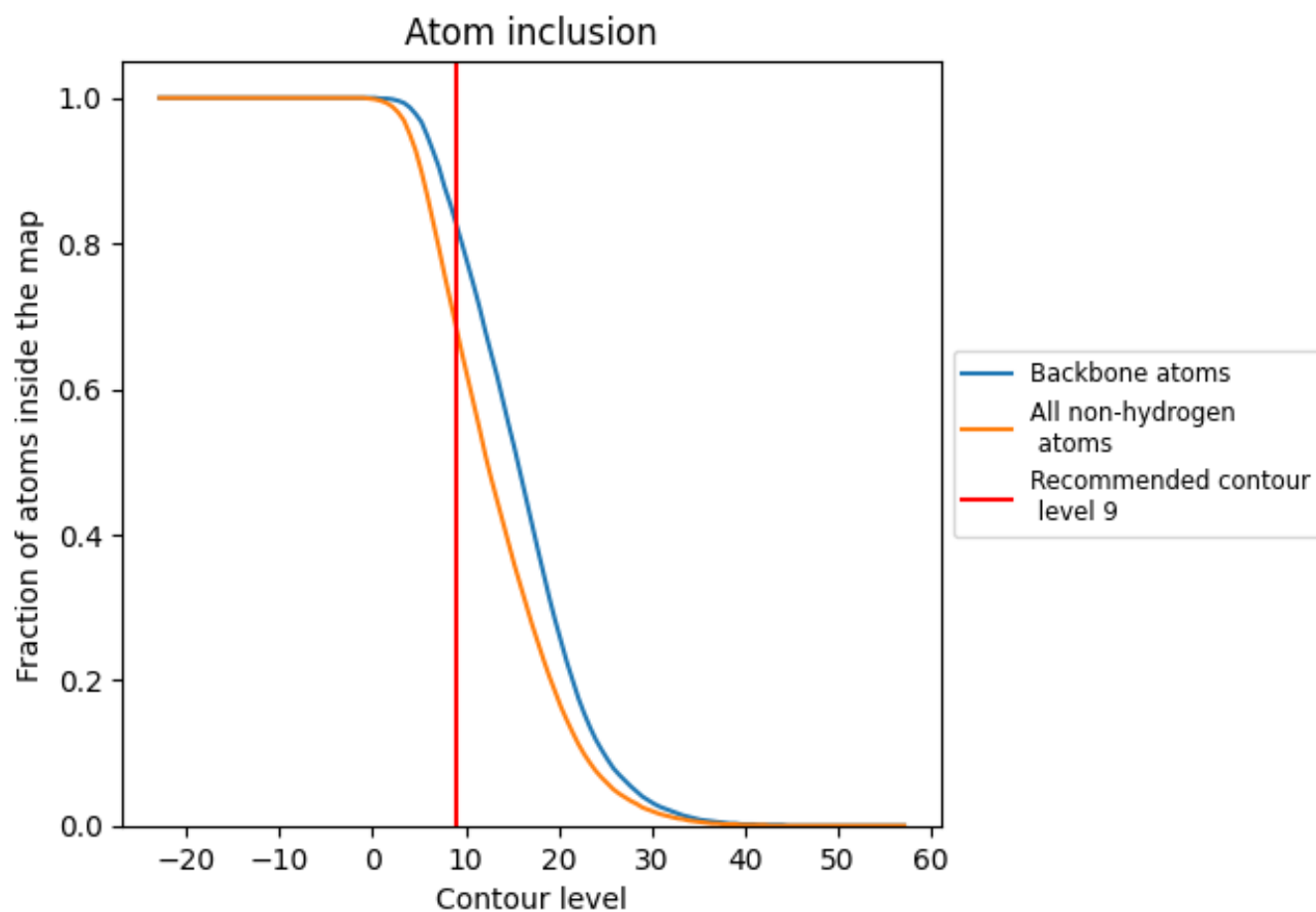
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (9).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 83% 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 (9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.4010
A	 0.5590	 0.3710
B	 0.7060	 0.4270
C	 0.5600	 0.3670
D	 0.6870	 0.4150
E	 0.7000	 0.4130
F	 0.7070	 0.4220
G	 0.8620	 0.4600
H	 0.8330	 0.4140
J	 0.8760	 0.3580
K	 0.9700	 0.3020
L	 0.8360	 0.2030

