



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 01:09 PM EST

PDB ID : 6CHS
EMDB ID : EMD-7476
Title : Cdc48-Npl4 complex in the presence of ATP-gamma-S
Authors : Kim, K.H.; Bodnar, N.O.; Walz, T.; Rapoport, T.A.
Deposited on : 2018-02-22
Resolution : 4.30 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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

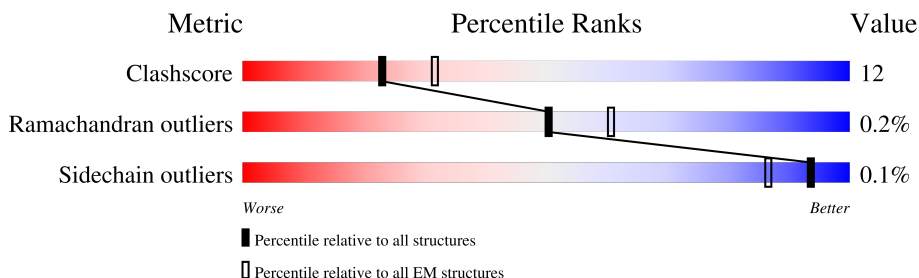
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	659	
2	D	819	
2	E	819	
2	F	819	
2	H	819	
2	I	819	
2	J	819	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29502 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 Npl4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3658	2326	626	684	22		

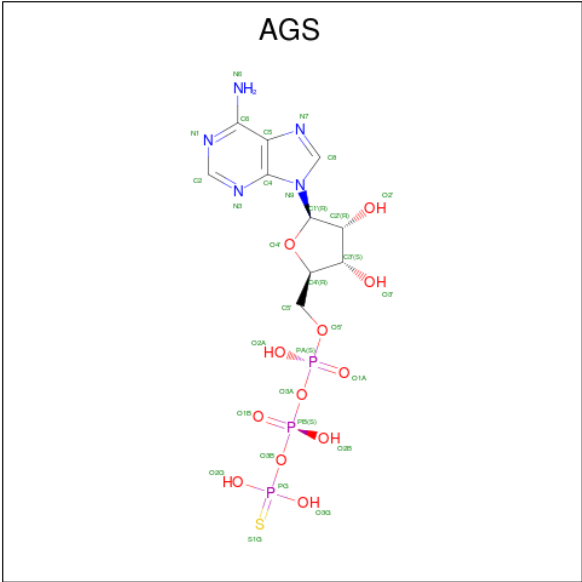
- Molecule 2 is a protein called Putative cell division control protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	550	Total	C	N	O	S	0	0
			4243	2662	746	813	22		
2	I	550	Total	C	N	O	S	0	0
			4243	2662	746	813	22		
2	J	550	Total	C	N	O	S	0	0
			4243	2662	746	813	22		
2	D	550	Total	C	N	O	S	0	0
			4243	2662	746	813	22		
2	E	550	Total	C	N	O	S	0	0
			4243	2662	746	813	22		
2	F	550	Total	C	N	O	S	0	0
			4243	2662	746	813	22		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
4	H	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	H	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	I	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	I	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	J	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	J	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

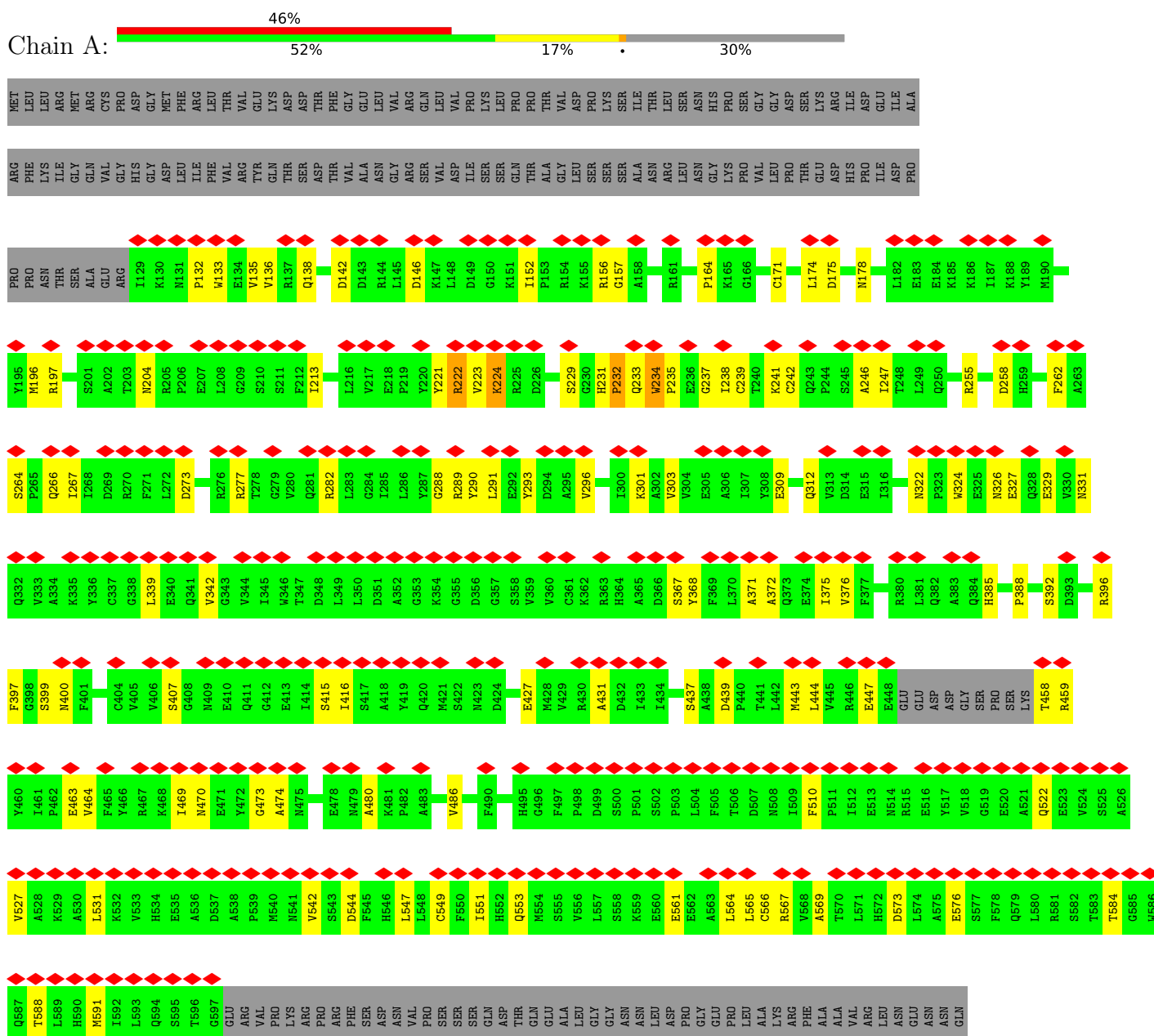
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	H	2	Total 2	Mg 2	0
5	I	2	Total 2	Mg 2	0
5	J	2	Total 2	Mg 2	0
5	D	2	Total 2	Mg 2	0
5	E	2	Total 2	Mg 2	0
5	F	2	Total 2	Mg 2	0

3 Residue-property plots

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

• Molecule 1: Npl4



SER
SER
PRO
LYS
PRO
PRO
TYR
ALA
PRO
SER
SER
TRP
ASN
LEU

• Molecule 2: Putative cell division control protein



MET
ALA
PRO
GLU
LEU
SER
LYS
GLN
ASP
HIS
LYS
LYS
LYS
LYS
VAL
ASN
LEU
THR
ASP
PRO
GLY
SER
LYS
GLY
ALA
GLU
HIS
THR
ARG
VAL
GLU
GLU
ASN
ASP
LEU
THR
ALA
ALA
THR
ASP
ALA
TLE
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LEU
ALA
ASP
TLE
ASN
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ALA
R303
R304
A305
F306
E307
E308
A309
E310
I319
D323
A326
F327
K328
R329
E330
K331
T332
R333
E334
E335
V336
E337
S248
I249
Q250

CYS
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ASP
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ALA
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A305
F306
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A309
E310
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R329
E330
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T332
R333
E334
E335
V336
E337
S248
I249
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VAL
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N215
D220
D221
I222
Q223
Q224
A230
R233
E237
L238
P239
L240
R241
Q244
L245
F246
K247
S248
I249
Q250

G256
V257
P262
K267
R272
A273
V274
A275
G276
F283
L284
I285
N291
S292
K293
M294
A295
Q296
E299
L302
R303
K304
A305
F306
E307
E308
A309
E310
I319
D323
A326
F327
K328
R329
E330
K331
T332
R333
E334
E335
V336
E337
S248
I249
Q250

L345
D349
K352
A353
S355
R356
T363
R364
R365
F366
N367
S368
I369
D370
R378
F379
M294
A295
Q296
E299
L302
R303
K304
A305
F306
E307
E308
A309
E310
I319
D323
A326
F327
K328
R329
E330
K331
T332
R333
E334
E335
V336
E337
S248
I249
Q250

D447
L448
D449
E450
D451
T452
L453
D454
A455
L458
D459
T464
M467
Y470
A471
L472
G473
V474
S475
N476
P477
S478
A479
L480
R481
E482
V485
V488
P489
R492
W493
D495
L496
L499
E500
Q501
Q504
K507
Q511
Y512
F520
L521
F522
G524
L525

S528
R529
G530
V531
L532
P536
T539
G540
K541
T542
M543
L544
K546
A547
V548
A549
N550
E551
M555
K560
G561
P562
E563
S566
M567
W568
F569
G570
E571
S572
E573
S574
N575
L576
R577
D578
I579
F580
D581
K582
A583
R584
A585
A586
V590
D594
E595
L596
D597
S598
I599
A600

K601
A602
R603
G604
G605
S606
T607
G608
D609
A610
G611
G612
A613
S614
N619
E624
M625
D626
T629
S630
K631
K632
F635
G638
A639
T640
N641
R642
L646
D647
P648
A649
L650
C651
R652
D653
P654
R655
L656
D657
Q658
E667
R670
L671
L674
R679
K680
T681
P682
V683

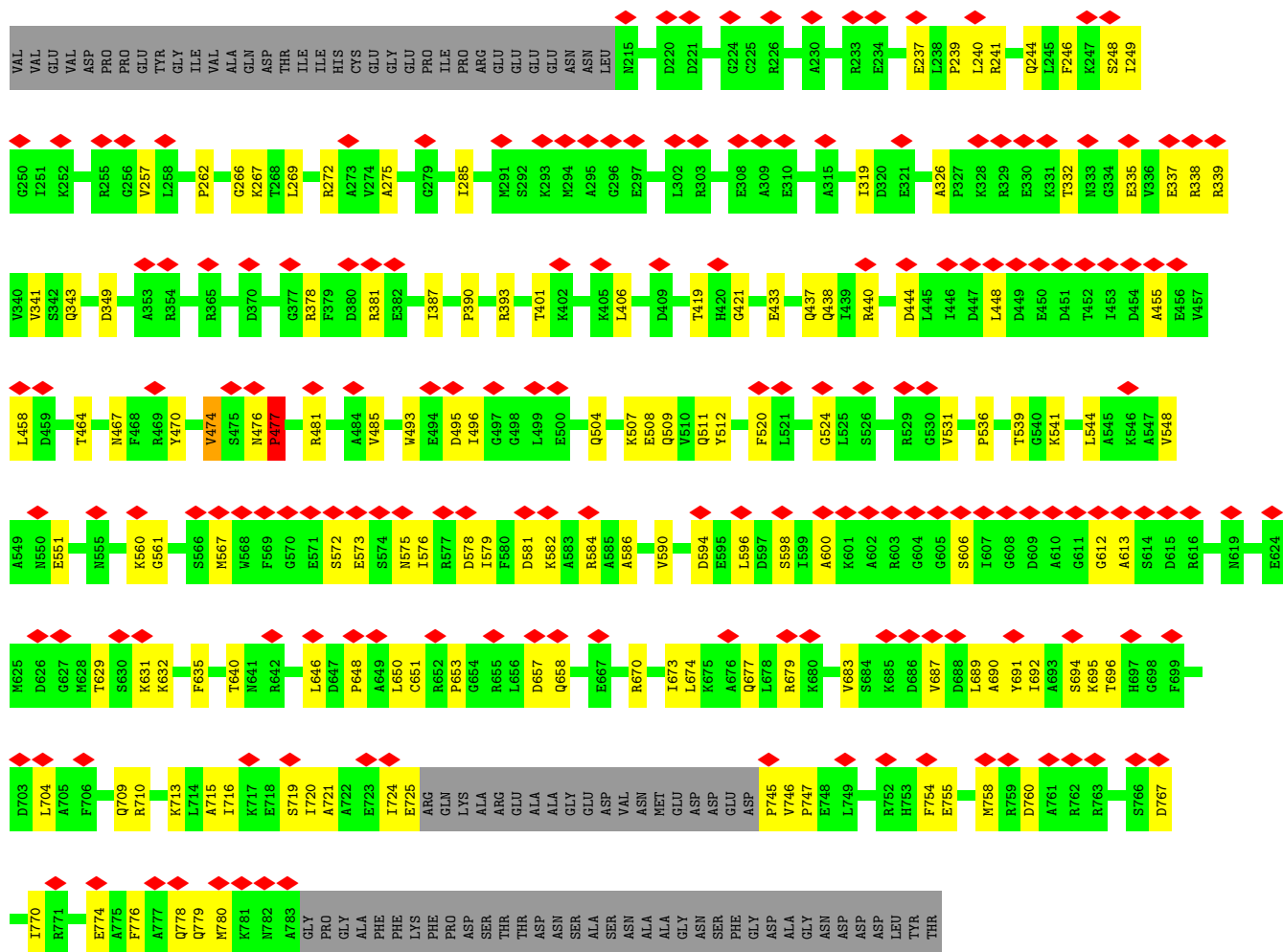
S684
K685
D686
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D689
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Y691
L692
A693
S694
K695
T696
H697
G701
A702
D703
L704
Q709
R710
A715
I716
K717
E718
S719
E723
I724
E725
ARG
GLN
LYS
LYS
ALA
ARG
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V746
P747
E748
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R752
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E755
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M758
R759
D760
A761
R762
R763
S764
V765
S766
D767
I770
R771
E774
A775
A777
Q778
Q779
M780
K781
M782
A783
GLY
PRO
GLY
ALA
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ASP
SER
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THR
ASP
ASN
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ALA
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ASN
ASP
ASP

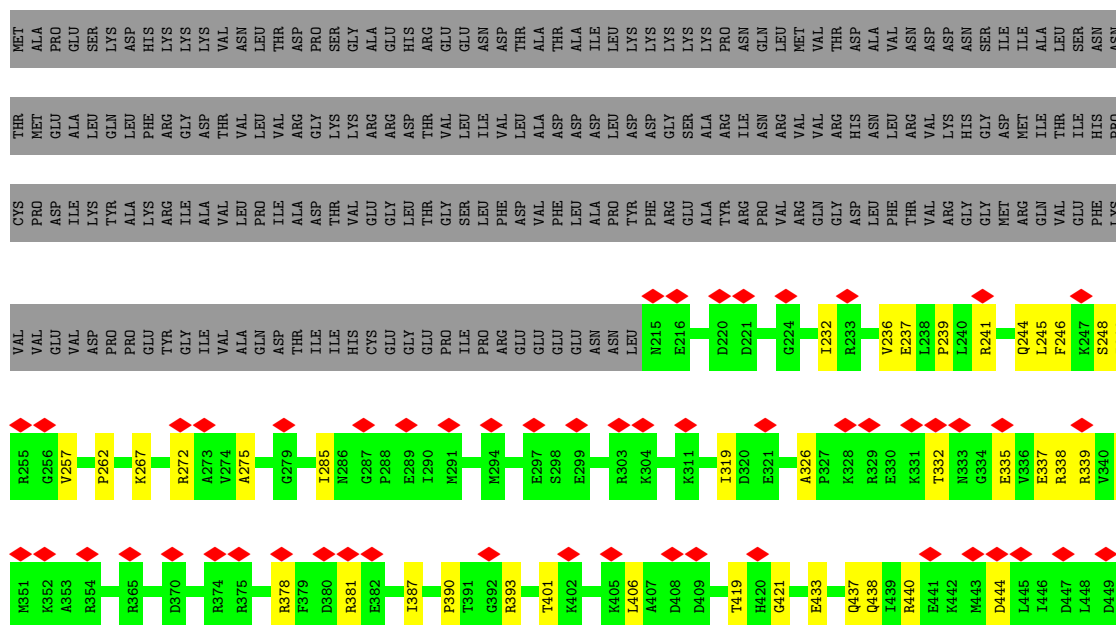
LEU
TYR
THR

• Molecule 2: Putative cell division control protein





• Molecule 2: Putative cell division control protein









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91883	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 ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/3752	0.57	0/5100
2	D	0.39	0/4311	0.52	0/5819
2	E	0.38	0/4311	0.51	0/5819
2	F	0.39	0/4311	0.52	0/5819
2	H	0.39	0/4311	0.51	0/5819
2	I	0.39	0/4311	0.52	0/5819
2	J	0.39	0/4311	0.52	0/5819
All	All	0.39	0/29618	0.53	0/40014

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3658	0	3576	115	0
2	D	4243	0	4280	96	0
2	E	4243	0	4279	131	0
2	F	4243	0	4278	86	0
2	H	4243	0	4279	104	0
2	I	4243	0	4279	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	4243	0	4279	105	0
3	A	2	0	0	0	0
4	D	62	0	24	1	0
4	E	62	0	24	6	0
4	F	62	0	24	3	0
4	H	62	0	24	1	0
4	I	62	0	24	5	0
4	J	62	0	24	5	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	H	2	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0
All	All	29502	0	29394	731	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 12.

All (731) 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:A:234:TRP:CZ3	1:A:238:ILE:HD12	1.67	1.28
2:E:285:ILE:HD11	2:E:290:ILE:HD11	1.28	1.15
2:F:476:ASN:HB2	2:F:477:PRO:HD3	1.28	1.13
2:E:285:ILE:CG2	2:E:319:ILE:HG12	1.78	1.13
2:I:433:GLU:HB2	2:I:476:ASN:HD21	1.12	1.09
2:D:476:ASN:HB2	2:D:477:PRO:HD3	1.28	1.09
1:A:372:ALA:O	1:A:375:ILE:HG13	1.54	1.05
2:I:474:VAL:O	2:I:477:PRO:HD2	1.58	1.03
1:A:234:TRP:CH2	1:A:238:ILE:HD12	1.95	1.02
2:E:474:VAL:O	2:E:477:PRO:HD2	1.61	1.00
2:E:474:VAL:HG22	2:E:475:SER:H	1.26	1.00
1:A:223:VAL:HG11	1:A:234:TRP:HB2	1.41	1.00
2:H:474:VAL:O	2:H:477:PRO:HD2	1.63	0.98
2:I:433:GLU:CB	2:I:476:ASN:HD21	1.77	0.98
1:A:234:TRP:HB3	1:A:235:PRO:HD3	1.45	0.97
2:D:476:ASN:HB2	2:D:477:PRO:CD	1.94	0.97
2:I:474:VAL:HG12	2:I:475:SER:H	1.30	0.97
2:I:474:VAL:HG12	2:I:475:SER:N	1.80	0.96
2:F:476:ASN:HB2	2:F:477:PRO:CD	1.94	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TRP:HZ3	1:A:238:ILE:HB	1.34	0.93
2:E:471:ALA:O	2:E:474:VAL:HG12	1.68	0.92
2:E:474:VAL:HG13	2:E:477:PRO:HD3	1.53	0.91
1:A:234:TRP:CZ3	1:A:238:ILE:CD1	2.53	0.89
2:H:474:VAL:HG12	2:H:475:SER:N	1.87	0.88
2:E:474:VAL:HG22	2:E:475:SER:N	1.90	0.88
1:A:223:VAL:HG11	1:A:234:TRP:CB	2.05	0.87
2:J:476:ASN:HB2	2:J:477:PRO:HD3	1.56	0.86
2:I:474:VAL:CG1	2:I:475:SER:H	1.89	0.85
2:I:433:GLU:HB2	2:I:476:ASN:ND2	1.92	0.85
1:A:234:TRP:CZ3	1:A:238:ILE:HB	2.12	0.84
2:I:433:GLU:CB	2:I:476:ASN:ND2	2.40	0.84
2:J:721:ALA:O	2:J:724:ILE:HG12	1.77	0.84
2:E:285:ILE:HD11	2:E:290:ILE:CD1	2.07	0.84
2:E:285:ILE:HG21	2:E:319:ILE:HG12	1.60	0.84
1:A:223:VAL:CG1	1:A:234:TRP:HB2	2.08	0.83
1:A:234:TRP:HZ3	1:A:238:ILE:HD12	1.37	0.82
2:H:474:VAL:HG12	2:H:475:SER:H	1.43	0.81
2:E:476:ASN:N	2:E:477:PRO:CD	2.43	0.81
2:E:476:ASN:H	2:E:477:PRO:CD	1.94	0.81
2:E:474:VAL:O	2:E:477:PRO:CD	2.28	0.80
2:E:721:ALA:O	2:E:724:ILE:HG12	1.83	0.79
2:J:476:ASN:HB2	2:J:477:PRO:CD	2.13	0.78
1:A:372:ALA:O	1:A:375:ILE:CG1	2.31	0.77
2:H:474:VAL:CG1	2:H:475:SER:H	1.98	0.77
2:I:472:LEU:O	2:I:477:PRO:HG3	1.85	0.76
1:A:234:TRP:HZ3	1:A:238:ILE:CB	1.99	0.76
2:E:474:VAL:CG2	2:E:475:SER:H	1.99	0.75
1:A:234:TRP:HZ3	1:A:238:ILE:CD1	1.96	0.75
2:I:474:VAL:O	2:I:477:PRO:CD	2.33	0.74
1:A:233:GLN:HA	1:A:233:GLN:NE2	2.02	0.74
1:A:255:ARG:HE	1:A:258:ASP:HA	1.52	0.73
1:A:223:VAL:HG11	1:A:234:TRP:CG	2.24	0.72
1:A:282:ARG:NH2	1:A:309:GLU:OE1	2.22	0.72
1:A:372:ALA:HA	1:A:375:ILE:HG12	1.72	0.72
1:A:234:TRP:CB	1:A:235:PRO:HD3	2.20	0.72
2:H:474:VAL:CG1	2:H:475:SER:N	2.52	0.72
2:J:721:ALA:HA	2:J:724:ILE:CD1	2.20	0.71
2:E:474:VAL:CG1	2:E:477:PRO:HD3	2.20	0.71
2:J:745:PRO:C	2:J:747:PRO:HD3	2.10	0.71
1:A:231:HIS:HE1	1:A:242:CYS:SG	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:721:ALA:O	2:E:725:GLU:HG3	1.92	0.69
2:E:426:ASP:OD2	2:E:479:ALA:HB1	1.93	0.69
2:I:474:VAL:C	2:I:477:PRO:HD2	2.14	0.67
2:E:275:ALA:HB1	2:E:282:PHE:CD2	2.29	0.67
1:A:224:LYS:HB2	1:A:242:CYS:O	1.94	0.67
2:H:474:VAL:O	2:H:477:PRO:CD	2.39	0.67
2:E:476:ASN:N	2:E:477:PRO:HD2	2.09	0.67
2:H:283:PHE:CE2	2:H:305:ALA:CB	2.78	0.66
2:E:426:ASP:OD2	2:E:479:ALA:CB	2.44	0.65
1:A:375:ILE:CD1	1:A:376:VAL:HG23	2.27	0.65
1:A:204:ASN:HD21	1:A:213:ILE:HB	1.62	0.65
2:H:493:TRP:HE1	2:H:551:GLU:HB2	1.62	0.65
2:E:476:ASN:H	2:E:477:PRO:HD3	1.60	0.65
2:J:493:TRP:HE1	2:J:551:GLU:HB2	1.62	0.65
2:I:493:TRP:HE1	2:I:551:GLU:HB2	1.62	0.65
2:D:493:TRP:HE1	2:D:551:GLU:HB2	1.62	0.65
2:E:493:TRP:HE1	2:E:551:GLU:HB2	1.62	0.64
2:I:511:GLN:HE21	2:I:548:VAL:HG23	1.62	0.64
1:A:324:TRP:NE1	1:A:326:ASN:OD1	2.30	0.64
2:H:476:ASN:HB2	2:H:477:PRO:HD3	1.78	0.64
2:E:474:VAL:HG13	2:E:476:ASN:H	1.62	0.64
2:E:511:GLN:HE21	2:E:548:VAL:HG23	1.62	0.64
2:F:493:TRP:HE1	2:F:551:GLU:HB2	1.62	0.64
1:A:327:GLU:O	1:A:331:ASN:ND2	2.30	0.64
2:F:476:ASN:CB	2:F:477:PRO:HD3	2.18	0.64
2:H:511:GLN:HE21	2:H:548:VAL:HG23	1.62	0.64
2:F:511:GLN:HE21	2:F:548:VAL:HG23	1.62	0.64
2:E:285:ILE:HG22	2:E:319:ILE:HG12	1.77	0.64
2:I:567:MET:HB3	2:I:572:SER:HB2	1.80	0.64
2:J:511:GLN:HE21	2:J:548:VAL:HG23	1.62	0.64
2:H:567:MET:HB3	2:H:572:SER:HB2	1.80	0.64
2:F:393:ARG:NH1	2:F:419:THR:O	2.31	0.63
2:E:596:LEU:HB2	2:E:640:THR:HB	1.81	0.63
2:F:596:LEU:HB2	2:F:640:THR:HB	1.81	0.63
1:A:152:ILE:HB	1:A:174:LEU:HB2	1.79	0.63
1:A:234:TRP:HZ3	1:A:238:ILE:CG1	2.11	0.63
2:D:596:LEU:HB2	2:D:640:THR:HB	1.81	0.63
2:E:393:ARG:NH1	2:E:419:THR:O	2.31	0.63
2:J:393:ARG:NH1	2:J:419:THR:O	2.31	0.63
2:D:567:MET:HB3	2:D:572:SER:HB2	1.80	0.63
2:D:511:GLN:HE21	2:D:548:VAL:HG23	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:567:MET:HB3	2:F:572:SER:HB2	1.80	0.63
2:H:393:ARG:NH1	2:H:419:THR:O	2.31	0.62
2:J:474:VAL:HG23	2:J:477:PRO:HD2	1.81	0.62
2:J:567:MET:HB3	2:J:572:SER:HB2	1.80	0.62
2:D:393:ARG:NH1	2:D:419:THR:O	2.31	0.62
2:I:393:ARG:NH1	2:I:419:THR:O	2.31	0.62
2:I:745:PRO:HG2	2:I:747:PRO:HD3	1.81	0.62
2:E:472:LEU:HD23	2:E:472:LEU:O	1.99	0.62
1:A:222:ARG:O	1:A:223:VAL:HG23	1.99	0.62
2:E:567:MET:HB3	2:E:572:SER:HB2	1.80	0.62
2:J:721:ALA:O	2:J:724:ILE:CG1	2.46	0.62
2:J:596:LEU:HB2	2:J:640:THR:HB	1.81	0.62
2:J:746:VAL:HG23	2:J:746:VAL:O	2.00	0.62
2:D:745:PRO:HG2	2:D:747:PRO:HD3	1.82	0.62
2:H:596:LEU:HB2	2:H:640:THR:HB	1.81	0.61
2:I:596:LEU:HB2	2:I:640:THR:HB	1.81	0.61
2:I:746:VAL:HG23	2:I:746:VAL:O	2.01	0.61
2:E:745:PRO:HG2	2:E:747:PRO:HD3	1.82	0.61
1:A:157:GLY:H	1:A:171:CYS:HB3	1.65	0.61
2:H:476:ASN:N	2:H:477:PRO:HD2	2.15	0.61
2:H:283:PHE:CE2	2:H:305:ALA:HB1	2.36	0.61
2:F:745:PRO:HG2	2:F:747:PRO:HD3	1.82	0.60
2:I:262:PRO:O	2:I:267:LYS:NZ	2.33	0.60
2:J:721:ALA:O	2:J:725:GLU:HG3	2.01	0.60
1:A:221:TYR:CE2	1:A:247:ILE:HG12	2.36	0.60
2:E:283:PHE:CG	2:E:284:LEU:N	2.70	0.60
2:H:339:ARG:NH1	2:I:294:MET:SD	2.74	0.60
2:H:746:VAL:HG23	2:H:746:VAL:O	2.01	0.60
2:E:237:GLU:OE1	2:E:241:ARG:NH1	2.35	0.60
1:A:289:ARG:HE	1:A:291:LEU:HD11	1.65	0.60
4:J:901:AGS:O1A	4:J:901:AGS:O1B	2.20	0.60
2:H:237:GLU:OE1	2:H:241:ARG:NH1	2.35	0.59
2:J:237:GLU:OE1	2:J:241:ARG:NH1	2.35	0.59
2:I:390:PRO:HA	2:I:393:ARG:HG2	1.84	0.59
2:H:390:PRO:HA	2:H:393:ARG:HG2	1.85	0.59
2:H:285:ILE:O	2:H:319:ILE:HA	2.03	0.59
2:J:390:PRO:HA	2:J:393:ARG:HG2	1.84	0.59
2:D:476:ASN:CB	2:D:477:PRO:HD3	2.18	0.59
1:A:565:LEU:O	1:A:569:ALA:N	2.34	0.59
1:A:231:HIS:O	1:A:232:PRO:O	2.21	0.59
1:A:234:TRP:N	1:A:235:PRO:CD	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:HB2	1:A:237:GLY:N	2.18	0.59
2:D:476:ASN:CB	2:D:477:PRO:CD	2.68	0.59
2:H:472:LEU:O	2:H:477:PRO:HG3	2.03	0.58
2:I:237:GLU:OE1	2:I:241:ARG:NH1	2.35	0.58
2:D:511:GLN:NE2	2:D:551:GLU:OE1	2.37	0.58
2:F:237:GLU:OE1	2:F:241:ARG:NH1	2.35	0.58
2:H:285:ILE:HG22	2:H:319:ILE:HG23	1.86	0.58
2:F:390:PRO:HA	2:F:393:ARG:HG2	1.84	0.58
2:D:237:GLU:OE1	2:D:241:ARG:NH1	2.35	0.58
2:D:390:PRO:HA	2:D:393:ARG:HG2	1.85	0.58
1:A:156:ARG:HD2	1:A:164:PRO:HA	1.85	0.58
2:F:262:PRO:O	2:F:267:LYS:NZ	2.33	0.58
2:H:285:ILE:O	2:H:285:ILE:HG22	2.04	0.58
2:F:511:GLN:NE2	2:F:551:GLU:OE1	2.36	0.58
2:I:511:GLN:NE2	2:I:551:GLU:OE1	2.37	0.57
2:D:495:ASP:OD1	2:D:679:ARG:NH1	2.37	0.57
2:E:495:ASP:OD1	2:E:679:ARG:NH1	2.37	0.57
2:J:495:ASP:OD1	2:J:679:ARG:NH1	2.37	0.57
2:J:511:GLN:NE2	2:J:551:GLU:OE1	2.37	0.57
2:E:390:PRO:HA	2:E:393:ARG:HG2	1.85	0.57
1:A:375:ILE:HD11	1:A:376:VAL:HG23	1.85	0.57
2:I:495:ASP:OD1	2:I:679:ARG:NH1	2.37	0.57
2:E:285:ILE:HG23	2:E:319:ILE:HG12	1.78	0.57
2:E:438:GLN:OE1	2:E:467:ASN:ND2	2.38	0.57
2:H:262:PRO:O	2:H:267:LYS:NZ	2.33	0.57
2:I:470:TYR:O	2:I:474:VAL:HG23	2.05	0.57
2:E:511:GLN:NE2	2:E:551:GLU:OE1	2.36	0.57
2:F:495:ASP:OD1	2:F:679:ARG:NH1	2.37	0.57
2:I:476:ASN:N	2:I:477:PRO:HD2	2.20	0.57
2:D:438:GLN:OE1	2:D:467:ASN:ND2	2.38	0.57
2:H:283:PHE:CZ	2:H:305:ALA:HA	2.40	0.57
2:H:511:GLN:NE2	2:H:551:GLU:OE1	2.36	0.57
2:H:682:PRO:HB2	2:H:747:PRO:O	2.05	0.57
1:A:233:GLN:HB3	1:A:235:PRO:HD2	1.87	0.56
1:A:231:HIS:CD2	1:A:239:CYS:SG	2.97	0.56
2:H:495:ASP:OD1	2:H:679:ARG:NH1	2.37	0.56
2:J:476:ASN:CB	2:J:477:PRO:CD	2.80	0.56
1:A:222:ARG:O	1:A:223:VAL:CG2	2.53	0.56
2:E:283:PHE:CD2	2:E:284:LEU:N	2.73	0.56
1:A:229:SER:HB2	1:A:241:LYS:HD2	1.88	0.56
2:E:262:PRO:O	2:E:267:LYS:NZ	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:ALA:CB	2:E:282:PHE:CD2	2.88	0.56
2:F:269:LEU:HD22	4:F:901:AGS:H2'	1.88	0.56
1:A:224:LYS:HB2	1:A:242:CYS:HA	1.88	0.56
2:H:474:VAL:C	2:H:477:PRO:HD2	2.26	0.56
2:H:584:ARG:HG3	2:H:632:LYS:HE2	1.88	0.56
2:F:438:GLN:OE1	2:F:467:ASN:ND2	2.38	0.56
2:D:476:ASN:N	2:D:477:PRO:HD2	2.21	0.55
2:D:710:ARG:NH1	2:D:760:ASP:O	2.40	0.55
4:E:901:AGS:O2B	4:E:901:AGS:O1A	2.23	0.55
2:J:721:ALA:HA	2:J:724:ILE:HD11	1.88	0.55
2:E:285:ILE:CD1	2:E:290:ILE:HD11	2.19	0.55
2:I:332:THR:HG23	2:I:338:ARG:HE	1.72	0.55
2:I:536:PRO:O	2:I:541:LYS:NZ	2.40	0.55
2:I:710:ARG:NH1	2:I:760:ASP:O	2.40	0.55
2:J:536:PRO:O	2:J:541:LYS:NZ	2.40	0.55
2:H:332:THR:HG23	2:H:338:ARG:HE	1.72	0.55
2:H:536:PRO:O	2:H:541:LYS:NZ	2.40	0.55
4:I:901:AGS:O1B	4:I:901:AGS:O2A	2.24	0.55
2:D:332:THR:HG23	2:D:338:ARG:HE	1.71	0.55
1:A:233:GLN:O	1:A:237:GLY:O	2.24	0.55
2:I:584:ARG:HG3	2:I:632:LYS:HE2	1.88	0.55
2:I:629:THR:HB	2:I:632:LYS:HG2	1.89	0.55
2:J:332:THR:HG23	2:J:338:ARG:HE	1.71	0.55
2:J:584:ARG:HG3	2:J:632:LYS:HE2	1.88	0.55
2:F:710:ARG:NH1	2:F:760:ASP:O	2.40	0.55
2:J:629:THR:HG22	2:J:631:LYS:H	1.72	0.55
2:E:464:THR:H	2:E:467:ASN:HD22	1.55	0.55
2:E:471:ALA:O	2:E:474:VAL:CG1	2.49	0.55
2:E:629:THR:HB	2:E:632:LYS:HG2	1.89	0.55
2:I:520:PHE:O	2:I:524:GLY:N	2.40	0.55
2:J:746:VAL:N	2:J:747:PRO:CD	2.70	0.55
2:D:464:THR:H	2:D:467:ASN:HD22	1.55	0.55
2:E:332:THR:HG23	2:E:338:ARG:HE	1.72	0.55
2:F:476:ASN:N	2:F:477:PRO:HD2	2.21	0.55
2:H:629:THR:HB	2:H:632:LYS:HG2	1.89	0.55
2:H:629:THR:HG22	2:H:631:LYS:H	1.72	0.55
2:J:721:ALA:HA	2:J:724:ILE:HG12	1.87	0.55
1:A:234:TRP:HB3	1:A:235:PRO:CD	2.30	0.54
2:H:470:TYR:O	2:H:474:VAL:HG23	2.07	0.54
2:I:629:THR:HG22	2:I:631:LYS:H	1.72	0.54
2:D:629:THR:HB	2:D:632:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:536:PRO:O	2:D:541:LYS:NZ	2.40	0.54
2:F:332:THR:HG23	2:F:338:ARG:HE	1.71	0.54
1:A:527:VAL:HG13	1:A:531:LEU:HD13	1.90	0.54
2:H:520:PHE:O	2:H:524:GLY:N	2.40	0.54
2:H:710:ARG:NH1	2:H:760:ASP:O	2.40	0.54
2:H:709:GLN:HG2	2:F:525:LEU:HD21	1.90	0.54
2:J:438:GLN:OE1	2:J:467:ASN:ND2	2.38	0.54
4:F:901:AGS:O2A	4:F:901:AGS:O2B	2.26	0.54
2:H:464:THR:H	2:H:467:ASN:HD22	1.55	0.54
2:H:512:TYR:CD1	2:I:720:ILE:HD11	2.43	0.54
2:D:584:ARG:HG3	2:D:632:LYS:HE2	1.88	0.54
2:D:629:THR:HG22	2:D:631:LYS:H	1.72	0.54
2:E:641:ASN:ND2	4:E:902:AGS:O3G	2.40	0.54
2:E:710:ARG:NH1	2:E:760:ASP:O	2.40	0.54
1:A:133:TRP:HA	1:A:136:VAL:HG22	1.90	0.54
1:A:470:ASN:OD1	1:A:474:ALA:N	2.40	0.54
2:J:710:ARG:NH1	2:J:760:ASP:O	2.40	0.54
4:I:902:AGS:O1A	4:I:902:AGS:O2B	2.25	0.54
2:F:584:ARG:HG3	2:F:632:LYS:HE2	1.88	0.54
2:F:629:THR:HB	2:F:632:LYS:HG2	1.89	0.54
2:H:438:GLN:OE1	2:H:467:ASN:ND2	2.38	0.54
2:D:520:PHE:O	2:D:524:GLY:N	2.40	0.54
2:E:520:PHE:O	2:E:524:GLY:N	2.40	0.54
2:F:520:PHE:O	2:F:524:GLY:N	2.40	0.54
2:I:575:ASN:HA	2:I:578:ASP:HB2	1.90	0.54
2:D:262:PRO:O	2:D:267:LYS:NZ	2.33	0.54
2:E:480:LEU:N	2:E:480:LEU:HD12	2.23	0.54
2:E:575:ASN:HA	2:E:578:ASP:HB2	1.90	0.54
2:F:629:THR:HG22	2:F:631:LYS:H	1.72	0.54
1:A:146:ASP:HA	1:A:197:ARG:HH21	1.73	0.53
2:H:285:ILE:CG2	2:H:319:ILE:HG12	2.37	0.53
2:I:244:GLN:O	2:I:248:SER:N	2.39	0.53
2:J:746:VAL:N	2:J:747:PRO:HD3	2.23	0.53
2:J:520:PHE:O	2:J:524:GLY:N	2.40	0.53
2:J:629:THR:HB	2:J:632:LYS:HG2	1.89	0.53
2:E:536:PRO:O	2:E:541:LYS:NZ	2.40	0.53
2:E:584:ARG:HG3	2:E:632:LYS:HE2	1.88	0.53
2:E:629:THR:HG22	2:E:631:LYS:H	1.72	0.53
2:F:332:THR:OG1	2:F:337:GLU:OE1	2.26	0.53
2:F:575:ASN:HA	2:F:578:ASP:HB2	1.90	0.53
2:H:590:VAL:HG12	2:H:635:PHE:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:474:VAL:CG1	2:I:475:SER:N	2.47	0.53
2:J:721:ALA:C	2:J:724:ILE:HG12	2.29	0.53
1:A:469:ILE:HG23	1:A:473:GLY:HA2	1.91	0.53
2:J:575:ASN:HA	2:J:578:ASP:HB2	1.90	0.53
2:D:332:THR:OG1	2:D:337:GLU:OE1	2.26	0.53
2:E:590:VAL:HG12	2:E:635:PHE:HB3	1.91	0.53
1:A:312:GLN:HA	1:A:322:ASN:H	1.74	0.53
2:I:474:VAL:O	2:I:477:PRO:HG2	2.09	0.53
2:I:590:VAL:HG12	2:I:635:PHE:HB3	1.91	0.53
2:E:285:ILE:HG23	2:E:285:ILE:O	2.08	0.53
1:A:224:LYS:CB	1:A:242:CYS:HA	2.38	0.53
2:J:464:THR:H	2:J:467:ASN:HD22	1.55	0.53
2:F:536:PRO:O	2:F:541:LYS:NZ	2.40	0.53
2:J:590:VAL:HG12	2:J:635:PHE:HB3	1.91	0.53
2:F:464:THR:H	2:F:467:ASN:HD22	1.55	0.53
2:F:754:PHE:O	2:F:758:MET:N	2.37	0.53
2:J:600:ALA:HA	2:J:613:ALA:HA	1.91	0.52
2:J:332:THR:OG1	2:J:337:GLU:OE1	2.26	0.52
2:J:754:PHE:O	2:J:758:MET:N	2.37	0.52
2:D:590:VAL:HG12	2:D:635:PHE:HB3	1.91	0.52
1:A:573:ASP:HB3	1:A:576:GLU:HB2	1.90	0.52
2:E:332:THR:OG1	2:E:337:GLU:OE1	2.26	0.52
2:E:474:VAL:C	2:E:477:PRO:HD2	2.29	0.52
2:I:241:ARG:HH21	2:J:448:LEU:HB3	1.73	0.52
2:D:575:ASN:HA	2:D:578:ASP:HB2	1.90	0.52
1:A:293:TYR:HB2	1:A:301:LYS:HB3	1.90	0.52
4:H:901:AGS:O2A	4:H:901:AGS:O1B	2.27	0.52
2:D:600:ALA:HA	2:D:613:ALA:HA	1.91	0.52
2:H:575:ASN:HA	2:H:578:ASP:HB2	1.90	0.52
2:I:600:ALA:HA	2:I:613:ALA:HA	1.91	0.52
2:E:720:ILE:O	2:E:724:ILE:HG23	2.09	0.52
2:E:600:ALA:HA	2:E:613:ALA:HA	1.91	0.51
1:A:549:CYS:O	1:A:553:GLN:N	2.39	0.51
2:I:474:VAL:O	2:I:477:PRO:CG	2.58	0.51
2:D:584:ARG:HD3	2:E:478:SER:HB3	1.92	0.51
1:A:196:MET:SD	1:A:197:ARG:NH1	2.83	0.51
1:A:264:SER:HB3	1:A:267:ILE:HG13	1.93	0.51
2:D:433:GLU:HB2	2:D:476:ASN:ND2	2.26	0.51
1:A:443:MET:HB2	1:A:486:VAL:HG12	1.93	0.51
2:D:433:GLU:HG2	2:D:474:VAL:HG21	1.93	0.51
2:D:754:PHE:O	2:D:758:MET:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:600:ALA:HA	2:H:613:ALA:HA	1.91	0.51
2:I:332:THR:OG1	2:I:337:GLU:OE1	2.26	0.51
2:F:433:GLU:HG2	2:F:474:VAL:HG21	1.93	0.51
2:F:590:VAL:HG12	2:F:635:PHE:HB3	1.91	0.51
1:A:326:ASN:HB2	1:A:329:GLU:HB2	1.92	0.51
2:H:754:PHE:O	2:H:758:MET:N	2.37	0.51
2:F:600:ALA:HA	2:F:613:ALA:HA	1.91	0.51
1:A:288:GLY:HA2	1:A:339:LEU:HD22	1.92	0.50
2:E:244:GLN:O	2:E:248:SER:N	2.39	0.50
2:E:496:ILE:HD13	2:E:544:LEU:HD23	1.94	0.50
2:H:244:GLN:O	2:H:248:SER:N	2.39	0.50
2:I:509:GLN:NE2	2:I:658:GLN:OE1	2.45	0.50
1:A:463:GLU:OE2	2:F:303:ARG:NH2	2.45	0.50
2:J:509:GLN:NE2	2:J:658:GLN:OE1	2.45	0.50
2:D:509:GLN:NE2	2:D:658:GLN:OE1	2.45	0.50
2:J:262:PRO:O	2:J:267:LYS:NZ	2.33	0.50
2:E:285:ILE:HD11	2:E:290:ILE:CG1	2.41	0.50
2:D:244:GLN:O	2:D:248:SER:N	2.39	0.50
2:E:720:ILE:HA	2:E:723:GLU:HB3	1.93	0.50
2:H:496:ILE:HD13	2:H:544:LEU:HD23	1.94	0.50
2:F:509:GLN:NE2	2:F:658:GLN:OE1	2.45	0.50
2:I:724:ILE:HG22	2:I:724:ILE:O	2.11	0.50
2:H:476:ASN:HB2	2:H:477:PRO:CD	2.42	0.50
2:E:721:ALA:HA	2:E:724:ILE:CD1	2.42	0.49
2:F:496:ILE:HD13	2:F:544:LEU:HD23	1.94	0.49
1:A:588:THR:HA	1:A:591:MET:HG2	1.93	0.49
2:I:496:ILE:HD13	2:I:544:LEU:HD23	1.94	0.49
2:I:690:ALA:O	2:I:694:SER:N	2.44	0.49
2:E:509:GLN:NE2	2:E:658:GLN:OE1	2.45	0.49
2:F:536:PRO:HG2	2:F:539:THR:HG21	1.95	0.49
2:J:244:GLN:O	2:J:248:SER:N	2.39	0.49
2:D:683:VAL:HG22	2:D:687:VAL:HG21	1.95	0.49
2:E:648:PRO:HA	2:E:651:CYS:HB2	1.94	0.49
2:F:433:GLU:HB2	2:F:476:ASN:ND2	2.27	0.49
2:D:536:PRO:HG2	2:D:539:THR:HG21	1.95	0.49
2:F:720:ILE:HA	2:F:723:GLU:HB3	1.95	0.49
2:I:536:PRO:HG2	2:I:539:THR:HG21	1.95	0.49
2:J:339:ARG:O	2:J:343:GLN:N	2.43	0.49
2:J:683:VAL:HG22	2:J:687:VAL:HG21	1.95	0.49
2:E:683:VAL:HG22	2:E:687:VAL:HG21	1.95	0.49
2:H:648:PRO:HA	2:H:651:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:582:LYS:O	2:D:586:ALA:N	2.43	0.49
2:E:285:ILE:HG23	2:E:319:ILE:HG23	1.95	0.49
1:A:224:LYS:HD3	1:A:241:LYS:O	2.12	0.49
2:H:401:THR:HB	2:H:406:LEU:HD11	1.95	0.49
2:J:648:PRO:HA	2:J:651:CYS:HB2	1.94	0.49
2:J:721:ALA:HA	2:J:724:ILE:CG1	2.41	0.49
2:E:401:THR:HB	2:E:406:LEU:HD11	1.95	0.49
2:F:401:THR:HB	2:F:406:LEU:HD11	1.95	0.49
2:I:433:GLU:CG	2:I:476:ASN:ND2	2.75	0.49
2:I:476:ASN:HB2	2:I:477:PRO:HD3	1.94	0.49
2:E:715:ALA:O	2:E:719:SER:N	2.46	0.49
2:F:648:PRO:HA	2:F:651:CYS:HB2	1.94	0.49
1:A:234:TRP:CB	1:A:235:PRO:CD	2.88	0.49
2:H:573:GLU:HA	2:H:576:ILE:HG12	1.95	0.49
2:J:690:ALA:O	2:J:694:SER:N	2.44	0.49
2:E:433:GLU:HG2	2:E:474:VAL:HG21	1.94	0.49
2:F:683:VAL:HG22	2:F:687:VAL:HG21	1.95	0.49
2:H:332:THR:OG1	2:H:337:GLU:OE1	2.26	0.48
2:H:536:PRO:HG2	2:H:539:THR:HG21	1.95	0.48
2:I:582:LYS:O	2:I:586:ALA:N	2.43	0.48
2:J:582:LYS:O	2:J:586:ALA:N	2.43	0.48
1:A:221:TYR:HB2	1:A:427:GLU:HG3	1.95	0.48
2:H:715:ALA:O	2:H:719:SER:N	2.46	0.48
2:D:496:ILE:HD13	2:D:544:LEU:HD23	1.94	0.48
2:D:648:PRO:HA	2:D:651:CYS:HB2	1.94	0.48
2:E:573:GLU:HA	2:E:576:ILE:HG12	1.95	0.48
1:A:234:TRP:O	1:A:237:GLY:O	2.30	0.48
1:A:566:CYS:HA	1:A:569:ALA:HB3	1.96	0.48
2:I:401:THR:HB	2:I:406:LEU:HD11	1.95	0.48
2:I:715:ALA:O	2:I:719:SER:N	2.46	0.48
2:J:496:ILE:HD13	2:J:544:LEU:HD23	1.94	0.48
2:D:541:LYS:N	4:D:902:AGS:O2A	2.46	0.48
2:D:573:GLU:HA	2:D:576:ILE:HG12	1.95	0.48
1:A:132:PRO:HD3	2:E:311:LYS:HZ1	1.78	0.48
1:A:262:PHE:HE2	1:A:416:ILE:HD13	1.79	0.48
1:A:447:GLU:O	1:A:459:ARG:NH2	2.47	0.48
2:F:690:ALA:O	2:F:694:SER:N	2.44	0.48
1:A:367:SER:OG	1:A:368:TYR:N	2.47	0.48
2:I:573:GLU:HA	2:I:576:ILE:HG12	1.95	0.48
2:I:648:PRO:HA	2:I:651:CYS:HB2	1.94	0.48
2:E:754:PHE:O	2:E:758:MET:N	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:SER:OG	1:A:439:ASP:O	2.30	0.48
2:H:567:MET:O	2:H:572:SER:N	2.40	0.48
2:J:715:ALA:O	2:J:719:SER:N	2.46	0.48
2:E:536:PRO:HG2	2:E:539:THR:HG21	1.95	0.48
2:J:536:PRO:HG2	2:J:539:THR:HG21	1.95	0.48
2:F:573:GLU:HA	2:F:576:ILE:HG12	1.95	0.48
2:H:683:VAL:HG22	2:H:687:VAL:HG21	1.95	0.48
2:I:433:GLU:HG2	2:I:476:ASN:ND2	2.29	0.48
2:I:653:PRO:HA	2:I:657:ASP:HB3	1.96	0.48
2:I:683:VAL:HG22	2:I:687:VAL:HG21	1.95	0.48
2:D:715:ALA:O	2:D:719:SER:N	2.46	0.48
2:E:531:VAL:HA	2:E:658:GLN:HB2	1.96	0.48
1:A:427:GLU:O	1:A:431:ALA:N	2.39	0.48
2:J:401:THR:HB	2:J:406:LEU:HD11	1.95	0.48
2:E:582:LYS:O	2:E:586:ALA:N	2.43	0.48
1:A:222:ARG:C	1:A:223:VAL:HG23	2.33	0.47
1:A:264:SER:OG	1:A:266:GLN:OE1	2.31	0.47
2:H:653:PRO:HA	2:H:657:ASP:HB3	1.96	0.47
2:J:539:THR:N	4:J:902:AGS:O1B	2.39	0.47
2:J:573:GLU:HA	2:J:576:ILE:HG12	1.95	0.47
2:J:653:PRO:HA	2:J:657:ASP:HB3	1.96	0.47
2:D:401:THR:HB	2:D:406:LEU:HD11	1.95	0.47
2:F:653:PRO:HA	2:F:657:ASP:HB3	1.96	0.47
2:F:715:ALA:O	2:F:719:SER:N	2.46	0.47
1:A:234:TRP:CZ3	1:A:238:ILE:CG1	2.94	0.47
1:A:584:THR:O	1:A:588:THR:N	2.41	0.47
2:H:531:VAL:HA	2:H:658:GLN:HB2	1.96	0.47
2:J:721:ALA:CA	2:J:724:ILE:HG12	2.45	0.47
2:F:444:ASP:OD1	2:F:444:ASP:N	2.48	0.47
2:I:754:PHE:O	2:I:758:MET:N	2.37	0.47
2:D:421:GLY:HA3	2:D:481:ARG:HD3	1.97	0.47
2:D:653:PRO:HA	2:D:657:ASP:HB3	1.96	0.47
2:D:444:ASP:OD1	2:D:444:ASP:N	2.48	0.47
2:I:246:PHE:HA	2:I:249:ILE:HG22	1.97	0.47
2:J:246:PHE:HA	2:J:249:ILE:HG22	1.97	0.47
2:F:421:GLY:HA3	2:F:481:ARG:HD3	1.97	0.47
2:F:674:LEU:HD21	2:F:704:LEU:HB3	1.96	0.47
1:A:224:LYS:HB2	1:A:242:CYS:C	2.34	0.47
2:H:246:PHE:HA	2:H:249:ILE:HG22	1.97	0.47
2:I:646:LEU:HD21	2:I:650:LEU:HD23	1.97	0.47
2:J:421:GLY:HA3	2:J:481:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:437:GLN:HA	2:J:440:ARG:HD2	1.97	0.47
2:J:444:ASP:N	2:J:444:ASP:OD1	2.48	0.47
2:J:476:ASN:CB	2:J:477:PRO:HD3	2.34	0.47
2:D:241:ARG:HH21	2:E:448:LEU:HB3	1.80	0.47
2:D:246:PHE:HA	2:D:249:ILE:HG22	1.96	0.47
2:D:531:VAL:HA	2:D:658:GLN:HB2	1.96	0.47
2:E:541:LYS:NZ	4:E:902:AGS:O2B	2.47	0.47
2:F:246:PHE:HA	2:F:249:ILE:HG22	1.96	0.47
2:F:437:GLN:HA	2:F:440:ARG:HD2	1.97	0.47
2:F:531:VAL:HA	2:F:658:GLN:HB2	1.96	0.47
2:F:646:LEU:HD21	2:F:650:LEU:HD23	1.97	0.47
1:A:531:LEU:HD11	1:A:551:ILE:HD11	1.96	0.47
2:H:437:GLN:HA	2:H:440:ARG:HD2	1.97	0.47
2:J:531:VAL:HA	2:J:658:GLN:HB2	1.96	0.47
2:D:567:MET:O	2:D:572:SER:N	2.40	0.47
2:E:674:LEU:HD21	2:E:704:LEU:HB3	1.96	0.47
2:H:582:LYS:O	2:H:586:ALA:N	2.43	0.47
2:J:674:LEU:HD21	2:J:704:LEU:HB3	1.96	0.47
2:D:674:LEU:HD21	2:D:704:LEU:HB3	1.96	0.47
1:A:375:ILE:CD1	1:A:376:VAL:CG2	2.93	0.47
1:A:542:VAL:HG21	1:A:565:LEU:HD11	1.96	0.47
2:H:474:VAL:O	2:H:477:PRO:HG2	2.15	0.47
2:H:674:LEU:HD21	2:H:704:LEU:HB3	1.96	0.47
2:I:670:ARG:NE	2:I:696:THR:O	2.48	0.47
2:J:646:LEU:HD21	2:J:650:LEU:HD23	1.97	0.47
2:D:437:GLN:HA	2:D:440:ARG:HD2	1.97	0.47
2:F:244:GLN:O	2:F:248:SER:N	2.39	0.47
2:H:444:ASP:N	2:H:444:ASP:OD1	2.48	0.46
2:D:433:GLU:HB2	2:D:476:ASN:HD21	1.80	0.46
2:F:576:ILE:HA	2:F:579:ILE:HD12	1.97	0.46
2:F:670:ARG:NE	2:F:696:THR:O	2.48	0.46
2:H:476:ASN:N	2:H:477:PRO:CD	2.77	0.46
2:H:576:ILE:HA	2:H:579:ILE:HD12	1.98	0.46
2:I:421:GLY:HA3	2:I:481:ARG:HD3	1.97	0.46
2:D:584:ARG:CD	2:E:478:SER:HB3	2.45	0.46
2:D:646:LEU:HD21	2:D:650:LEU:HD23	1.97	0.46
2:E:472:LEU:O	2:E:477:PRO:HG3	2.15	0.46
2:E:653:PRO:HA	2:E:657:ASP:HB3	1.96	0.46
4:E:902:AGS:O2A	4:E:902:AGS:O1B	2.28	0.46
2:F:266:GLY:N	4:F:901:AGS:O2B	2.47	0.46
2:H:670:ARG:NE	2:H:696:THR:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:567:MET:O	2:I:572:SER:N	2.40	0.46
2:E:444:ASP:N	2:E:444:ASP:OD1	2.48	0.46
2:H:646:LEU:HD21	2:H:650:LEU:HD23	1.97	0.46
2:I:674:LEU:HD21	2:I:704:LEU:HB3	1.96	0.46
2:J:266:GLY:N	4:J:901:AGS:O1A	2.43	0.46
2:D:670:ARG:NE	2:D:696:THR:O	2.48	0.46
2:E:646:LEU:HD21	2:E:650:LEU:HD23	1.97	0.46
1:A:138:GLN:HB3	1:A:142:ASP:HB2	1.97	0.46
2:H:339:ARG:O	2:H:343:GLN:N	2.43	0.46
2:H:421:GLY:HA3	2:H:481:ARG:HD3	1.97	0.46
2:I:531:VAL:HA	2:I:658:GLN:HB2	1.96	0.46
2:J:470:TYR:O	2:J:474:VAL:HG13	2.16	0.46
4:J:902:AGS:O2A	4:J:902:AGS:O2B	2.28	0.46
2:E:437:GLN:HA	2:E:440:ARG:HD2	1.97	0.46
2:I:746:VAL:O	2:I:748:GLU:N	2.39	0.46
2:J:670:ARG:NE	2:J:696:THR:O	2.48	0.46
2:D:720:ILE:HA	2:D:723:GLU:HB3	1.98	0.46
2:I:444:ASP:OD1	2:I:444:ASP:N	2.48	0.46
2:D:576:ILE:HA	2:D:579:ILE:HD12	1.98	0.46
2:I:476:ASN:N	2:I:477:PRO:CD	2.78	0.46
2:I:576:ILE:HA	2:I:579:ILE:HD12	1.98	0.46
2:D:339:ARG:O	2:D:343:GLN:N	2.43	0.46
2:D:560:LYS:HG2	2:D:594:ASP:HB3	1.98	0.46
2:E:246:PHE:HA	2:E:249:ILE:HG22	1.97	0.46
2:F:722:ALA:HA	2:F:725:GLU:HB2	1.98	0.46
2:H:523:PHE:HE1	2:I:747:PRO:HA	1.81	0.46
2:I:285:ILE:HB	2:I:319:ILE:HG12	1.98	0.46
2:J:269:LEU:HD22	4:J:901:AGS:H2'	1.96	0.46
2:H:283:PHE:HE2	2:H:305:ALA:CB	2.26	0.45
2:I:560:LYS:HG2	2:I:594:ASP:HB3	1.98	0.45
2:J:745:PRO:CB	2:J:747:PRO:HD3	2.46	0.45
2:J:755:GLU:HA	2:J:758:MET:HB2	1.98	0.45
2:H:285:ILE:HD11	2:H:305:ALA:CB	2.46	0.45
2:I:437:GLN:HA	2:I:440:ARG:HD2	1.97	0.45
2:E:560:LYS:HG2	2:E:594:ASP:HB3	1.98	0.45
2:E:723:GLU:O	2:E:723:GLU:HG2	2.17	0.45
2:E:755:GLU:HA	2:E:758:MET:HB2	1.98	0.45
2:F:767:ASP:HA	2:F:770:ILE:HD12	1.99	0.45
1:A:224:LYS:HB2	1:A:242:CYS:CA	2.45	0.45
2:H:767:ASP:HA	2:H:770:ILE:HD12	1.99	0.45
2:E:690:ALA:O	2:E:694:SER:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:285:ILE:HB	2:F:319:ILE:HG12	1.98	0.45
1:A:437:SER:HB3	1:A:444:LEU:HG	1.98	0.45
2:J:433:GLU:HG2	2:J:474:VAL:HG21	1.99	0.45
2:F:339:ARG:O	2:F:343:GLN:N	2.43	0.45
1:A:273:ASP:HB3	1:A:277:ARG:HH22	1.82	0.45
2:H:755:GLU:HA	2:H:758:MET:HB2	1.98	0.45
2:J:745:PRO:HG2	2:J:747:PRO:HD3	1.98	0.45
2:D:285:ILE:HB	2:D:319:ILE:HG12	1.98	0.45
2:E:767:ASP:HA	2:E:770:ILE:HD12	1.99	0.45
1:A:146:ASP:HA	1:A:197:ARG:NH2	2.31	0.45
1:A:324:TRP:CH2	1:A:327:GLU:HA	2.52	0.45
1:A:385:HIS:O	1:A:399:SER:OG	2.25	0.45
2:J:433:GLU:HB2	2:J:476:ASN:OD1	2.17	0.45
2:D:690:ALA:O	2:D:694:SER:N	2.44	0.45
2:D:767:ASP:HA	2:D:770:ILE:HD12	1.99	0.45
2:E:670:ARG:NE	2:E:696:THR:O	2.48	0.45
2:F:755:GLU:HA	2:F:758:MET:HB2	1.98	0.45
1:A:175:ASP:HB2	1:A:178:ASN:HB2	1.98	0.45
2:J:285:ILE:HB	2:J:319:ILE:HG12	1.98	0.45
2:J:576:ILE:HA	2:J:579:ILE:HD12	1.98	0.45
2:D:476:ASN:N	2:D:477:PRO:CD	2.79	0.45
2:H:690:ALA:O	2:H:694:SER:N	2.44	0.45
2:F:560:LYS:HG2	2:F:594:ASP:HB3	1.98	0.45
1:A:290:TYR:OH	1:A:342:VAL:O	2.35	0.45
2:I:339:ARG:O	2:I:343:GLN:N	2.43	0.45
2:J:720:ILE:O	2:J:724:ILE:HG23	2.16	0.45
2:D:755:GLU:HA	2:D:758:MET:HB2	1.98	0.45
1:A:234:TRP:O	1:A:234:TRP:CE3	2.70	0.44
2:I:755:GLU:HA	2:I:758:MET:HB2	1.98	0.44
2:J:387:ILE:HD13	2:J:485:VAL:HG23	1.99	0.44
2:J:560:LYS:HG2	2:J:594:ASP:HB3	1.98	0.44
1:A:464:VAL:HB	1:A:480:ALA:HB3	1.99	0.44
2:I:767:ASP:HA	2:I:770:ILE:HD12	1.99	0.44
2:E:426:ASP:OD2	2:E:479:ALA:HB2	2.18	0.44
2:E:576:ILE:HA	2:E:579:ILE:HD12	1.98	0.44
2:F:476:ASN:N	2:F:477:PRO:CD	2.79	0.44
1:A:234:TRP:N	1:A:235:PRO:HD2	2.31	0.44
1:A:510:PHE:HZ	1:A:522:GLN:HG2	1.81	0.44
2:H:474:VAL:O	2:H:477:PRO:CG	2.64	0.44
2:I:541:LYS:NZ	4:I:902:AGS:O1B	2.49	0.44
2:F:582:LYS:O	2:F:586:ALA:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:689:LEU:HD23	2:H:692:ILE:HD12	2.00	0.44
2:J:578:ASP:HA	2:J:581:ASP:HB2	2.00	0.44
2:D:616:ARG:HG2	2:E:569:PHE:CE1	2.52	0.44
2:E:282:PHE:CD1	2:E:282:PHE:O	2.70	0.44
2:E:540:GLY:H	4:E:902:AGS:H5'1	1.82	0.44
2:F:433:GLU:HB2	2:F:476:ASN:HD21	1.81	0.44
1:A:561:GLU:O	1:A:565:LEU:N	2.48	0.44
2:I:387:ILE:HD13	2:I:485:VAL:HG23	1.99	0.44
2:I:508:GLU:HB3	2:J:713:LYS:HD2	1.98	0.44
2:D:387:ILE:HD13	2:D:485:VAL:HG23	1.99	0.44
2:E:721:ALA:O	2:E:724:ILE:CG1	2.59	0.44
2:F:567:MET:O	2:F:572:SER:N	2.40	0.44
2:I:266:GLY:N	4:I:901:AGS:O2A	2.41	0.44
2:J:567:MET:O	2:J:572:SER:N	2.40	0.44
2:E:266:GLY:N	4:E:901:AGS:O1A	2.42	0.44
2:E:339:ARG:O	2:E:343:GLN:N	2.43	0.44
1:A:564:LEU:HD12	1:A:567:ARG:HD3	1.99	0.44
1:A:234:TRP:NE1	1:A:458:THR:O	2.51	0.44
1:A:246:ALA:HB3	2:F:297:GLU:HG2	2.00	0.44
2:J:512:TYR:CD1	2:D:720:ILE:HD11	2.53	0.44
2:J:779:GLN:HB2	2:D:762:ARG:HH21	1.82	0.44
2:H:387:ILE:HD13	2:H:485:VAL:HG23	1.99	0.43
2:H:560:LYS:HG2	2:H:594:ASP:HB3	1.98	0.43
1:A:289:ARG:NE	1:A:291:LEU:HD11	2.31	0.43
2:H:578:ASP:HA	2:H:581:ASP:HB2	2.00	0.43
2:E:474:VAL:C	2:E:477:PRO:CD	2.86	0.43
2:F:387:ILE:HD13	2:F:485:VAL:HG23	1.99	0.43
2:F:578:ASP:HA	2:F:581:ASP:HB2	2.00	0.43
2:F:689:LEU:HD23	2:F:692:ILE:HD12	2.00	0.43
1:A:443:MET:HE2	1:A:486:VAL:HG12	2.01	0.43
2:J:767:ASP:HA	2:J:770:ILE:HD12	1.99	0.43
2:E:421:GLY:HA3	2:E:481:ARG:HD3	2.00	0.43
2:F:774:GLU:O	2:F:778:GLN:N	2.47	0.43
1:A:293:TYR:HD2	1:A:296:VAL:HG22	1.83	0.43
2:I:257:VAL:HA	2:I:381:ARG:HB2	2.01	0.43
2:J:257:VAL:HA	2:J:381:ARG:HB2	2.01	0.43
2:J:689:LEU:HD23	2:J:692:ILE:HD12	2.00	0.43
2:E:720:ILE:HG22	2:E:723:GLU:OE1	2.19	0.43
2:D:257:VAL:HA	2:D:381:ARG:HB2	2.01	0.43
2:H:433:GLU:HB2	2:H:476:ASN:HD21	1.82	0.43
1:A:232:PRO:HB2	1:A:237:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:691:TYR:CZ	2:H:695:LYS:HD2	2.54	0.43
2:I:578:ASP:HA	2:I:581:ASP:HB2	2.00	0.43
2:E:387:ILE:HD13	2:E:485:VAL:HG23	1.99	0.43
2:E:689:LEU:HD23	2:E:692:ILE:HD12	2.00	0.43
2:I:239:PRO:HG3	2:I:246:PHE:HE2	1.84	0.43
2:I:543:MET:HE3	2:I:543:MET:HB2	1.88	0.43
2:D:691:TYR:CZ	2:D:695:LYS:HD2	2.54	0.43
2:F:239:PRO:HG3	2:F:246:PHE:HE2	1.84	0.43
2:F:606:SER:HA	2:F:612:GLY:HA2	2.01	0.43
1:A:291:LEU:HD12	1:A:303:VAL:HG21	2.01	0.43
1:A:392:SER:HB2	1:A:397:PHE:HB2	2.00	0.43
1:A:290:TYR:OH	1:A:400:ASN:O	2.24	0.42
1:A:407:SER:O	1:A:415:SER:N	2.51	0.42
2:H:239:PRO:HG3	2:H:246:PHE:HE2	1.84	0.42
2:H:285:ILE:HD11	2:H:305:ALA:HB2	2.02	0.42
2:J:691:TYR:CZ	2:J:695:LYS:HD2	2.54	0.42
2:D:239:PRO:HG3	2:D:246:PHE:HE2	1.84	0.42
2:E:239:PRO:HG3	2:E:246:PHE:HE2	1.84	0.42
2:F:464:THR:H	2:F:467:ASN:ND2	2.17	0.42
2:I:526:SER:HA	2:I:527:PRO:HD3	1.90	0.42
2:I:689:LEU:HD23	2:I:692:ILE:HD12	2.00	0.42
2:E:691:TYR:CZ	2:E:695:LYS:HD2	2.54	0.42
2:E:326:ALA:HA	2:E:341:VAL:HG22	2.02	0.42
2:I:272:ARG:HA	2:I:275:ALA:HB3	2.02	0.42
2:I:326:ALA:HA	2:I:341:VAL:HG22	2.01	0.42
2:D:335:GLU:OE2	2:D:338:ARG:NH1	2.53	0.42
2:D:512:TYR:CD1	2:E:720:ILE:HD11	2.55	0.42
2:D:559:VAL:O	2:D:594:ASP:N	2.49	0.42
2:D:606:SER:HA	2:D:612:GLY:HA2	2.01	0.42
2:F:272:ARG:HA	2:F:275:ALA:HB3	2.02	0.42
2:F:335:GLU:OE2	2:F:338:ARG:NH1	2.53	0.42
2:H:257:VAL:HA	2:H:381:ARG:HB2	2.01	0.42
2:H:349:ASP:OD2	2:H:378:ARG:NH2	2.53	0.42
2:H:543:MET:HE3	2:H:543:MET:HB2	1.90	0.42
2:I:691:TYR:CZ	2:I:695:LYS:HD2	2.54	0.42
2:E:606:SER:HA	2:E:612:GLY:HA2	2.01	0.42
2:H:606:SER:HA	2:H:612:GLY:HA2	2.01	0.42
2:I:606:SER:HA	2:I:612:GLY:HA2	2.01	0.42
2:J:326:ALA:HA	2:J:341:VAL:HG22	2.01	0.42
2:J:508:GLU:HB3	2:D:713:LYS:HD2	2.01	0.42
2:D:349:ASP:OD2	2:D:378:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:578:ASP:HA	2:D:581:ASP:HB2	2.00	0.42
2:D:689:LEU:HD23	2:D:692:ILE:HD12	2.00	0.42
2:F:691:TYR:CZ	2:F:695:LYS:HD2	2.54	0.42
1:A:232:PRO:HB2	1:A:237:GLY:CA	2.49	0.42
1:A:388:PRO:HA	1:A:396:ARG:HA	2.02	0.42
2:J:673:ILE:O	2:J:677:GLN:N	2.45	0.42
2:D:464:THR:H	2:D:467:ASN:ND2	2.17	0.42
2:E:349:ASP:OD2	2:E:378:ARG:NH2	2.53	0.42
2:F:326:ALA:HA	2:F:341:VAL:HG22	2.01	0.42
2:F:488:VAL:HA	2:F:489:PRO:HD3	1.90	0.42
2:I:349:ASP:OD2	2:I:378:ARG:NH2	2.53	0.42
2:I:525:LEU:HD21	2:J:709:GLN:HG2	2.02	0.42
2:J:239:PRO:HG3	2:J:246:PHE:HE2	1.84	0.42
2:E:567:MET:O	2:E:572:SER:N	2.40	0.42
2:E:578:ASP:HA	2:E:581:ASP:HB2	2.00	0.42
2:H:776:PHE:HD1	2:H:780:MET:HG3	1.85	0.42
2:J:464:THR:H	2:J:467:ASN:ND2	2.17	0.42
2:D:326:ALA:HA	2:D:341:VAL:HG22	2.01	0.42
2:F:257:VAL:HA	2:F:381:ARG:HB2	2.01	0.42
2:H:326:ALA:HA	2:H:341:VAL:HG22	2.01	0.41
2:J:745:PRO:HB2	2:J:747:PRO:HD3	2.02	0.41
2:E:257:VAL:HA	2:E:381:ARG:HB2	2.01	0.41
2:H:464:THR:H	2:H:467:ASN:ND2	2.17	0.41
2:I:335:GLU:OE2	2:I:338:ARG:NH1	2.53	0.41
2:H:241:ARG:HH21	2:I:448:LEU:HB3	1.85	0.41
2:I:488:VAL:HA	2:I:489:PRO:HD3	1.90	0.41
2:J:774:GLU:O	2:J:778:GLN:N	2.47	0.41
2:D:720:ILE:HG22	2:D:723:GLU:OE1	2.20	0.41
2:E:433:GLU:HB2	2:E:476:ASN:ND2	2.35	0.41
2:F:776:PHE:HD1	2:F:780:MET:HG3	1.85	0.41
2:I:774:GLU:O	2:I:778:GLN:N	2.47	0.41
2:J:716:ILE:HA	2:J:719:SER:HB2	2.03	0.41
1:A:234:TRP:HE1	1:A:458:THR:C	2.23	0.41
1:A:544:ASP:HB3	1:A:547:LEU:HB3	2.01	0.41
2:H:488:VAL:HA	2:H:489:PRO:HD3	1.89	0.41
2:H:575:ASN:O	2:H:579:ILE:N	2.53	0.41
2:I:363:THR:HG21	2:I:369:ILE:HD11	2.03	0.41
2:I:472:LEU:O	2:I:477:PRO:CG	2.64	0.41
2:D:575:ASN:O	2:D:579:ILE:N	2.53	0.41
2:E:464:THR:H	2:E:467:ASN:ND2	2.17	0.41
2:E:474:VAL:O	2:E:477:PRO:CG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:335:GLU:OE2	2:J:338:ARG:NH1	2.53	0.41
2:E:716:ILE:HA	2:E:719:SER:HB2	2.03	0.41
2:H:272:ARG:HA	2:H:275:ALA:HB3	2.02	0.41
2:D:272:ARG:HA	2:D:275:ALA:HB3	2.02	0.41
2:E:272:ARG:HA	2:E:275:ALA:HB3	2.02	0.41
2:E:335:GLU:OE2	2:E:338:ARG:NH1	2.53	0.41
2:E:666:ASP:OD1	2:E:669:GLY:N	2.45	0.41
2:H:335:GLU:OE2	2:H:338:ARG:NH1	2.53	0.41
2:I:455:ALA:HA	2:I:458:LEU:HD12	2.03	0.41
2:J:240:LEU:HD23	2:J:240:LEU:HA	1.95	0.41
2:J:272:ARG:HA	2:J:275:ALA:HB3	2.02	0.41
2:D:716:ILE:HA	2:D:719:SER:HB2	2.03	0.41
1:A:132:PRO:HA	1:A:135:VAL:HG22	2.03	0.41
2:H:455:ALA:HA	2:H:458:LEU:HD12	2.03	0.41
2:H:597:ASP:O	2:H:601:LYS:N	2.53	0.41
2:I:575:ASN:O	2:I:579:ILE:N	2.53	0.41
2:J:349:ASP:OD2	2:J:378:ARG:NH2	2.53	0.41
2:J:606:SER:HA	2:J:612:GLY:HA2	2.01	0.41
2:D:245:LEU:HD21	2:E:453:ILE:HG21	2.03	0.41
2:D:488:VAL:HA	2:D:489:PRO:HD3	1.90	0.41
2:D:774:GLU:O	2:D:778:GLN:N	2.47	0.41
2:E:455:ALA:HA	2:E:458:LEU:HD12	2.03	0.41
2:E:474:VAL:CG2	2:E:475:SER:N	2.60	0.41
2:F:597:ASP:O	2:F:601:LYS:N	2.53	0.41
1:A:372:ALA:HA	1:A:375:ILE:CG1	2.46	0.41
1:A:375:ILE:HD11	1:A:376:VAL:CG2	2.51	0.41
2:I:504:GLN:HA	2:I:507:LYS:HD2	2.03	0.41
2:I:776:PHE:HD1	2:I:780:MET:HG3	1.85	0.41
2:J:455:ALA:HA	2:J:458:LEU:HD12	2.03	0.41
2:E:363:THR:HG21	2:E:369:ILE:HD11	2.03	0.41
2:D:232:ILE:O	2:D:236:VAL:N	2.51	0.40
2:D:455:ALA:HA	2:D:458:LEU:HD12	2.03	0.40
2:F:349:ASP:OD2	2:F:378:ARG:NH2	2.53	0.40
2:I:433:GLU:CG	2:I:476:ASN:HD21	2.28	0.40
2:I:561:GLY:HA3	2:I:598:SER:HB2	2.03	0.40
2:J:504:GLN:HA	2:J:507:LYS:HD2	2.03	0.40
2:D:339:ARG:NH1	2:E:294:MET:HG2	2.36	0.40
2:D:504:GLN:HA	2:D:507:LYS:HD2	2.03	0.40
2:D:776:PHE:HD1	2:D:780:MET:HG3	1.85	0.40
2:H:363:THR:HG21	2:H:369:ILE:HD11	2.03	0.40
2:H:504:GLN:HA	2:H:507:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:561:GLY:HA3	2:H:598:SER:HB2	2.03	0.40
2:J:776:PHE:HD1	2:J:780:MET:HG3	1.85	0.40
1:A:375:ILE:HD12	1:A:376:VAL:N	2.37	0.40
2:H:716:ILE:HA	2:H:719:SER:HB2	2.03	0.40
2:E:474:VAL:O	2:E:477:PRO:HG2	2.22	0.40
2:F:455:ALA:HA	2:F:458:LEU:HD12	2.03	0.40
2:F:561:GLY:HA3	2:F:598:SER:HB2	2.03	0.40
2:F:716:ILE:HA	2:F:719:SER:HB2	2.03	0.40
1:A:371:ALA:O	1:A:375:ILE:HG23	2.22	0.40
2:I:269:LEU:HD22	4:I:901:AGS:H2'	2.02	0.40
2:I:716:ILE:HA	2:I:719:SER:HB2	2.03	0.40
2:J:561:GLY:HA3	2:J:598:SER:HB2	2.03	0.40
2:D:593:LEU:HD23	2:D:593:LEU:HA	1.94	0.40
2:E:249:ILE:HG23	2:E:251:ILE:HG23	2.04	0.40
2:E:776:PHE:HD1	2:E:780:MET:HG3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	456/659 (69%)	412 (90%)	41 (9%)	3 (1%)	22	62
2	D	546/819 (67%)	519 (95%)	27 (5%)	0	100	100
2	E	546/819 (67%)	517 (95%)	28 (5%)	1 (0%)	47	81
2	F	546/819 (67%)	519 (95%)	26 (5%)	1 (0%)	47	81
2	H	546/819 (67%)	520 (95%)	25 (5%)	1 (0%)	47	81
2	I	546/819 (67%)	518 (95%)	28 (5%)	0	100	100
2	J	546/819 (67%)	519 (95%)	25 (5%)	2 (0%)	34	72
All	All	3732/5573 (67%)	3524 (94%)	200 (5%)	8 (0%)	50	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	PRO
2	H	478	SER
2	J	474	VAL
2	E	478	SER
1	A	224	LYS
2	J	477	PRO
1	A	222	ARG
2	F	477	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/576 (70%)	400 (100%)	1 (0%)	93	96
2	D	455/683 (67%)	454 (100%)	1 (0%)	93	96
2	E	455/683 (67%)	455 (100%)	0	100	100
2	F	455/683 (67%)	454 (100%)	1 (0%)	93	96
2	H	455/683 (67%)	455 (100%)	0	100	100
2	I	455/683 (67%)	455 (100%)	0	100	100
2	J	455/683 (67%)	454 (100%)	1 (0%)	93	96
All	All	3131/4674 (67%)	3127 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	TRP
2	J	477	PRO
2	D	477	PRO
2	F	477	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	476	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 14 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$
4	AGS	I	902	5	26,33,33	0.85	1 (3%)	26,52,52	1.34	2 (7%)
4	AGS	J	902	5	26,33,33	0.78	0	26,52,52	1.35	2 (7%)
4	AGS	E	902	5	26,33,33	0.73	0	26,52,52	1.22	2 (7%)
4	AGS	I	901	5	26,33,33	0.85	1 (3%)	26,52,52	1.28	2 (7%)
4	AGS	D	902	5	26,33,33	0.76	0	26,52,52	1.35	2 (7%)
4	AGS	H	902	5	26,33,33	0.84	1 (3%)	26,52,52	1.37	2 (7%)
4	AGS	D	901	5	26,33,33	0.78	1 (3%)	26,52,52	1.59	2 (7%)
4	AGS	F	901	5	26,33,33	0.72	0	26,52,52	1.38	2 (7%)
4	AGS	E	901	5	26,33,33	0.83	2 (7%)	26,52,52	1.30	2 (7%)
4	AGS	H	901	5	26,33,33	0.83	1 (3%)	26,52,52	1.09	2 (7%)
4	AGS	J	901	5	26,33,33	0.87	1 (3%)	26,52,52	1.32	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AGS	F	902	5	26,33,33	0.81	0	26,52,52	1.26	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	I	902	5	-	6/17/38/38	0/3/3/3
4	AGS	J	902	5	-	6/17/38/38	0/3/3/3
4	AGS	E	902	5	-	5/17/38/38	0/3/3/3
4	AGS	I	901	5	-	6/17/38/38	0/3/3/3
4	AGS	D	902	5	-	5/17/38/38	0/3/3/3
4	AGS	H	902	5	-	1/17/38/38	0/3/3/3
4	AGS	D	901	5	-	3/17/38/38	0/3/3/3
4	AGS	F	901	5	-	8/17/38/38	0/3/3/3
4	AGS	E	901	5	-	6/17/38/38	0/3/3/3
4	AGS	H	901	5	-	6/17/38/38	0/3/3/3
4	AGS	J	901	5	-	8/17/38/38	0/3/3/3
4	AGS	F	902	5	-	5/17/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	AGS	PG-S1G	2.16	1.95	1.90
4	J	901	AGS	PA-O2A	-2.09	1.45	1.55
4	H	901	AGS	PG-S1G	2.08	1.95	1.90
4	I	902	AGS	PG-S1G	2.07	1.95	1.90
4	H	902	AGS	PG-S1G	2.03	1.95	1.90
4	I	901	AGS	PG-S1G	2.03	1.95	1.90
4	E	901	AGS	PA-O2A	-2.01	1.45	1.55
4	E	901	AGS	PG-S1G	2.01	1.95	1.90

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	AGS	PA-O3A-PB	-6.95	108.99	132.83
4	F	901	AGS	PA-O3A-PB	-5.85	112.77	132.83
4	D	902	AGS	PA-O3A-PB	-5.49	113.99	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	901	AGS	PA-O3A-PB	-5.48	114.03	132.83
4	I	902	AGS	PA-O3A-PB	-5.43	114.18	132.83
4	E	901	AGS	PA-O3A-PB	-5.39	114.33	132.83
4	J	902	AGS	PA-O3A-PB	-5.32	114.56	132.83
4	H	902	AGS	PA-O3A-PB	-5.28	114.69	132.83
4	I	901	AGS	PA-O3A-PB	-5.18	115.06	132.83
4	F	902	AGS	PA-O3A-PB	-4.87	116.10	132.83
4	E	902	AGS	PA-O3A-PB	-4.64	116.90	132.83
4	H	901	AGS	PA-O3A-PB	-4.01	119.08	132.83
4	H	901	AGS	C5-C6-N6	2.24	123.76	120.35
4	F	902	AGS	C5-C6-N6	2.24	123.76	120.35
4	F	901	AGS	C5-C6-N6	2.24	123.75	120.35
4	E	901	AGS	C5-C6-N6	2.23	123.75	120.35
4	J	901	AGS	C5-C6-N6	2.21	123.72	120.35
4	I	901	AGS	C5-C6-N6	2.21	123.71	120.35
4	D	901	AGS	C5-C6-N6	2.19	123.68	120.35
4	H	902	AGS	C5-C6-N6	2.18	123.67	120.35
4	E	902	AGS	C5-C6-N6	2.17	123.65	120.35
4	I	902	AGS	C5-C6-N6	2.16	123.63	120.35
4	J	902	AGS	C5-C6-N6	2.12	123.58	120.35
4	D	902	AGS	C5-C6-N6	2.11	123.56	120.35

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	901	AGS	C5'-O5'-PA-O1A
4	H	901	AGS	C5'-O5'-PA-O2A
4	H	901	AGS	O4'-C4'-C5'-O5'
4	I	901	AGS	C5'-O5'-PA-O2A
4	I	902	AGS	C5'-O5'-PA-O1A
4	I	902	AGS	C5'-O5'-PA-O2A
4	I	902	AGS	C5'-O5'-PA-O3A
4	I	902	AGS	O4'-C4'-C5'-O5'
4	J	901	AGS	PB-O3B-PG-O2G
4	J	901	AGS	PB-O3B-PG-O3G
4	J	901	AGS	C5'-O5'-PA-O1A
4	J	902	AGS	C5'-O5'-PA-O3A
4	D	901	AGS	PB-O3B-PG-O2G
4	D	901	AGS	PB-O3B-PG-O3G
4	D	902	AGS	C5'-O5'-PA-O2A
4	D	902	AGS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	D	902	AGS	O4'-C4'-C5'-O5'
4	E	901	AGS	C5'-O5'-PA-O1A
4	E	902	AGS	C5'-O5'-PA-O2A
4	E	902	AGS	C5'-O5'-PA-O3A
4	F	901	AGS	PB-O3B-PG-O2G
4	F	901	AGS	PB-O3B-PG-O3G
4	F	901	AGS	C5'-O5'-PA-O1A
4	F	901	AGS	C5'-O5'-PA-O2A
4	I	901	AGS	O4'-C4'-C5'-O5'
4	J	901	AGS	O4'-C4'-C5'-O5'
4	E	901	AGS	O4'-C4'-C5'-O5'
4	E	902	AGS	O4'-C4'-C5'-O5'
4	F	901	AGS	O4'-C4'-C5'-O5'
4	F	901	AGS	C3'-C4'-C5'-O5'
4	I	902	AGS	C3'-C4'-C5'-O5'
4	J	902	AGS	O4'-C4'-C5'-O5'
4	J	902	AGS	C3'-C4'-C5'-O5'
4	D	902	AGS	C3'-C4'-C5'-O5'
4	E	902	AGS	C3'-C4'-C5'-O5'
4	H	901	AGS	C5'-O5'-PA-O3A
4	I	901	AGS	C5'-O5'-PA-O3A
4	J	901	AGS	C5'-O5'-PA-O3A
4	E	901	AGS	C5'-O5'-PA-O3A
4	F	901	AGS	C5'-O5'-PA-O3A
4	F	902	AGS	C5'-O5'-PA-O3A
4	E	901	AGS	C3'-C4'-C5'-O5'
4	J	902	AGS	PA-O3A-PB-O2B
4	I	901	AGS	C5'-O5'-PA-O1A
4	J	901	AGS	C5'-O5'-PA-O2A
4	J	902	AGS	C5'-O5'-PA-O1A
4	J	902	AGS	C5'-O5'-PA-O2A
4	D	902	AGS	C5'-O5'-PA-O1A
4	E	901	AGS	C5'-O5'-PA-O2A
4	E	902	AGS	C5'-O5'-PA-O1A
4	I	901	AGS	C3'-C4'-C5'-O5'
4	J	901	AGS	C3'-C4'-C5'-O5'
4	H	902	AGS	PA-O3A-PB-O2B
4	I	902	AGS	PA-O3A-PB-O2B
4	E	901	AGS	PA-O3A-PB-O2B
4	F	902	AGS	PA-O3A-PB-O2B
4	F	901	AGS	C4'-C5'-O5'-PA
4	H	901	AGS	C3'-C4'-C5'-O5'

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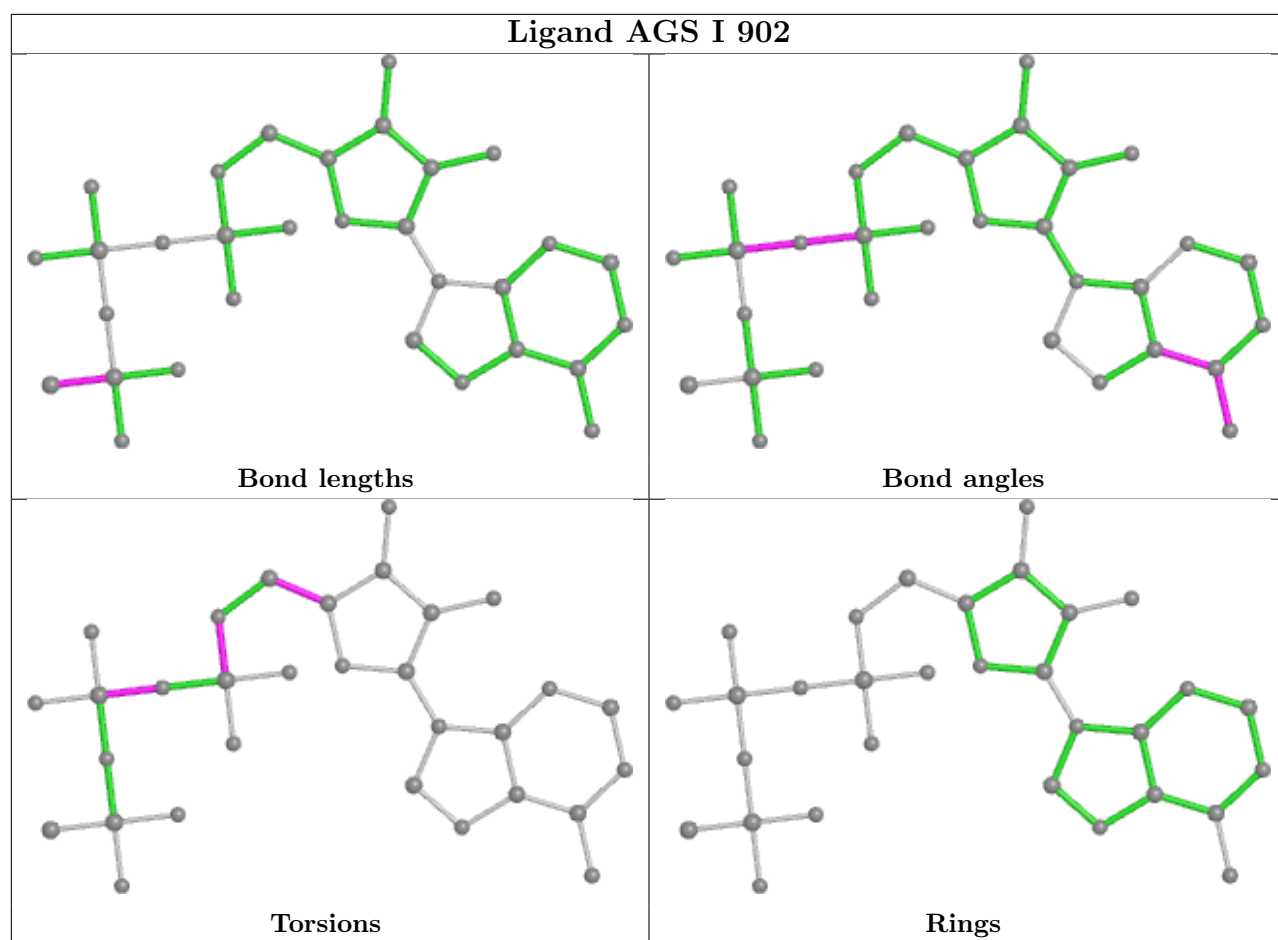
Mol	Chain	Res	Type	Atoms
4	H	901	AGS	PB-O3B-PG-O2G
4	I	901	AGS	PB-O3B-PG-O2G
4	F	902	AGS	PB-O3B-PG-O3G
4	F	902	AGS	PA-O3A-PB-O1B
4	J	901	AGS	PA-O3A-PB-O1B
4	F	902	AGS	C5'-O5'-PA-O1A
4	D	901	AGS	O4'-C4'-C5'-O5'

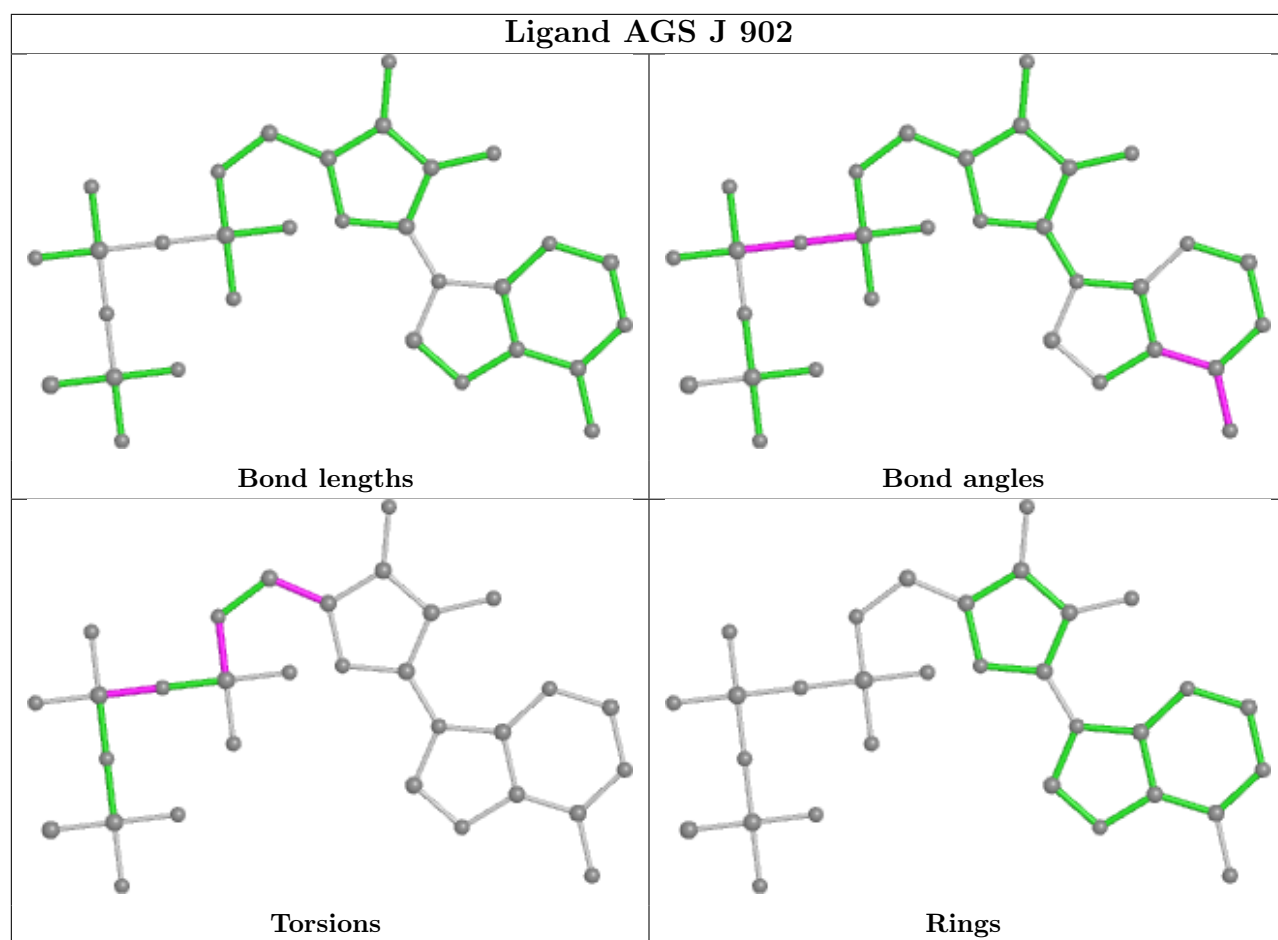
There are no ring outliers.

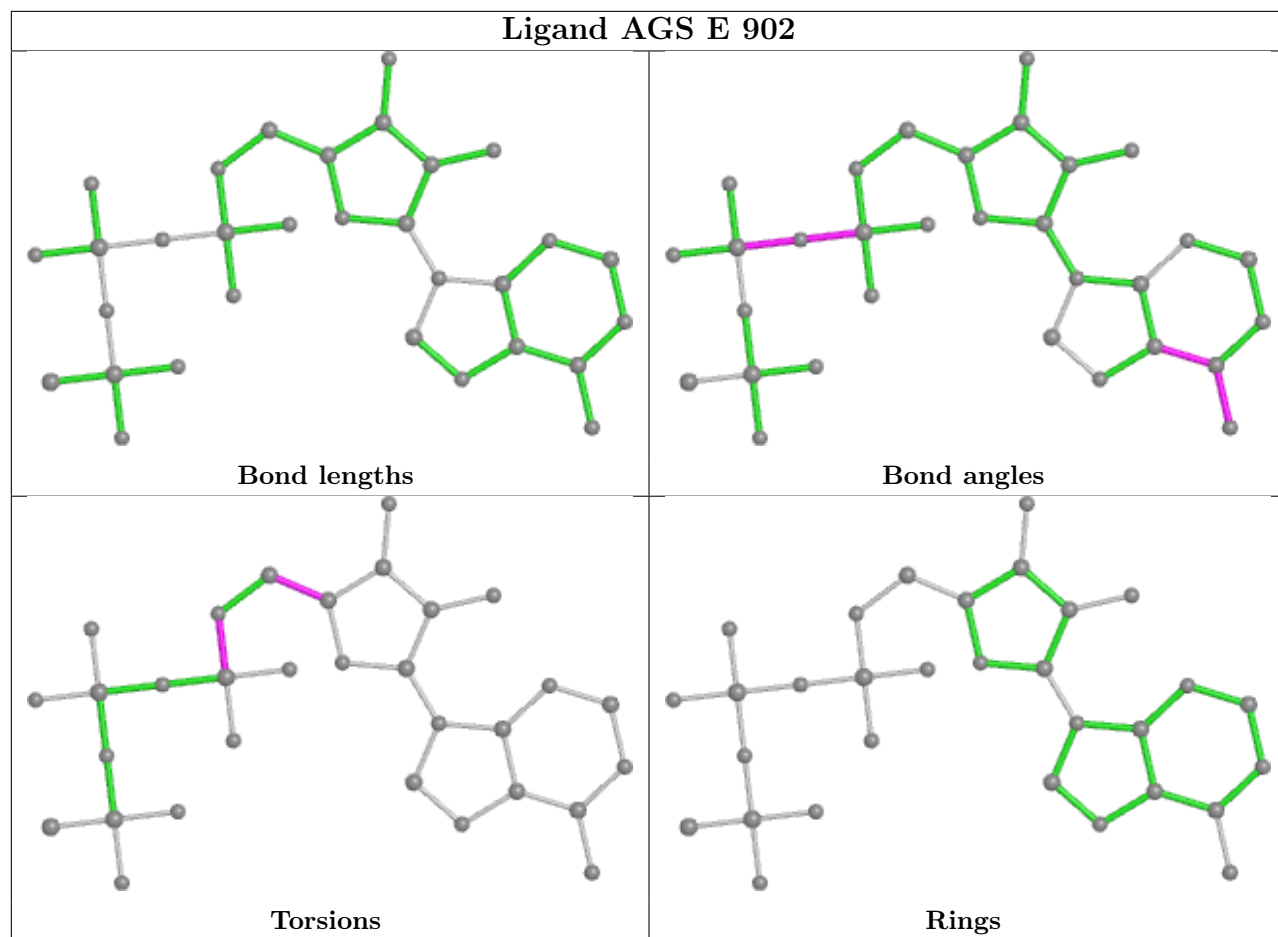
9 monomers are involved in 21 short contacts:

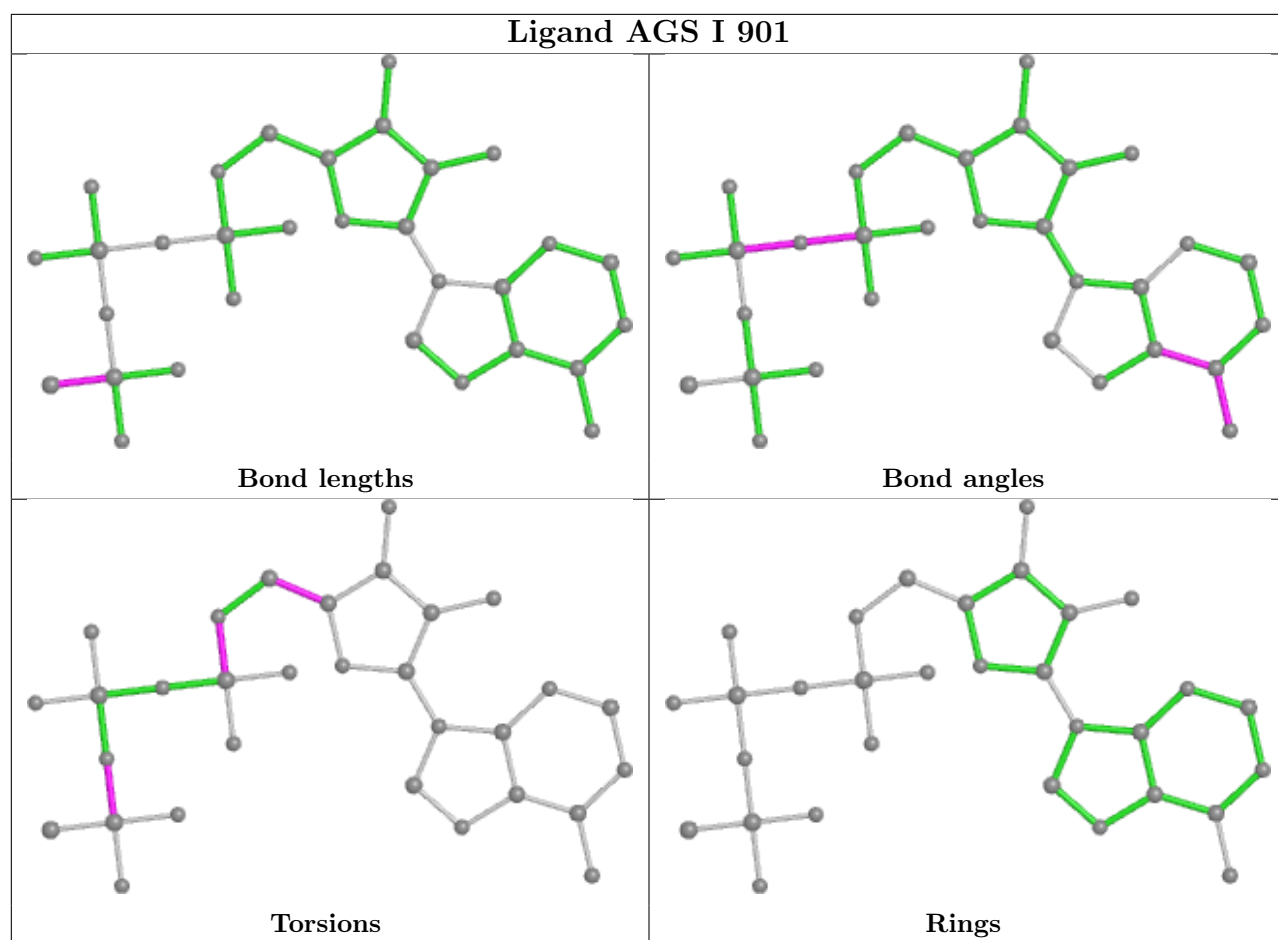
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	902	AGS	2	0
4	J	902	AGS	2	0
4	E	902	AGS	4	0
4	I	901	AGS	3	0
4	D	902	AGS	1	0
4	F	901	AGS	3	0
4	E	901	AGS	2	0
4	H	901	AGS	1	0
4	J	901	AGS	3	0

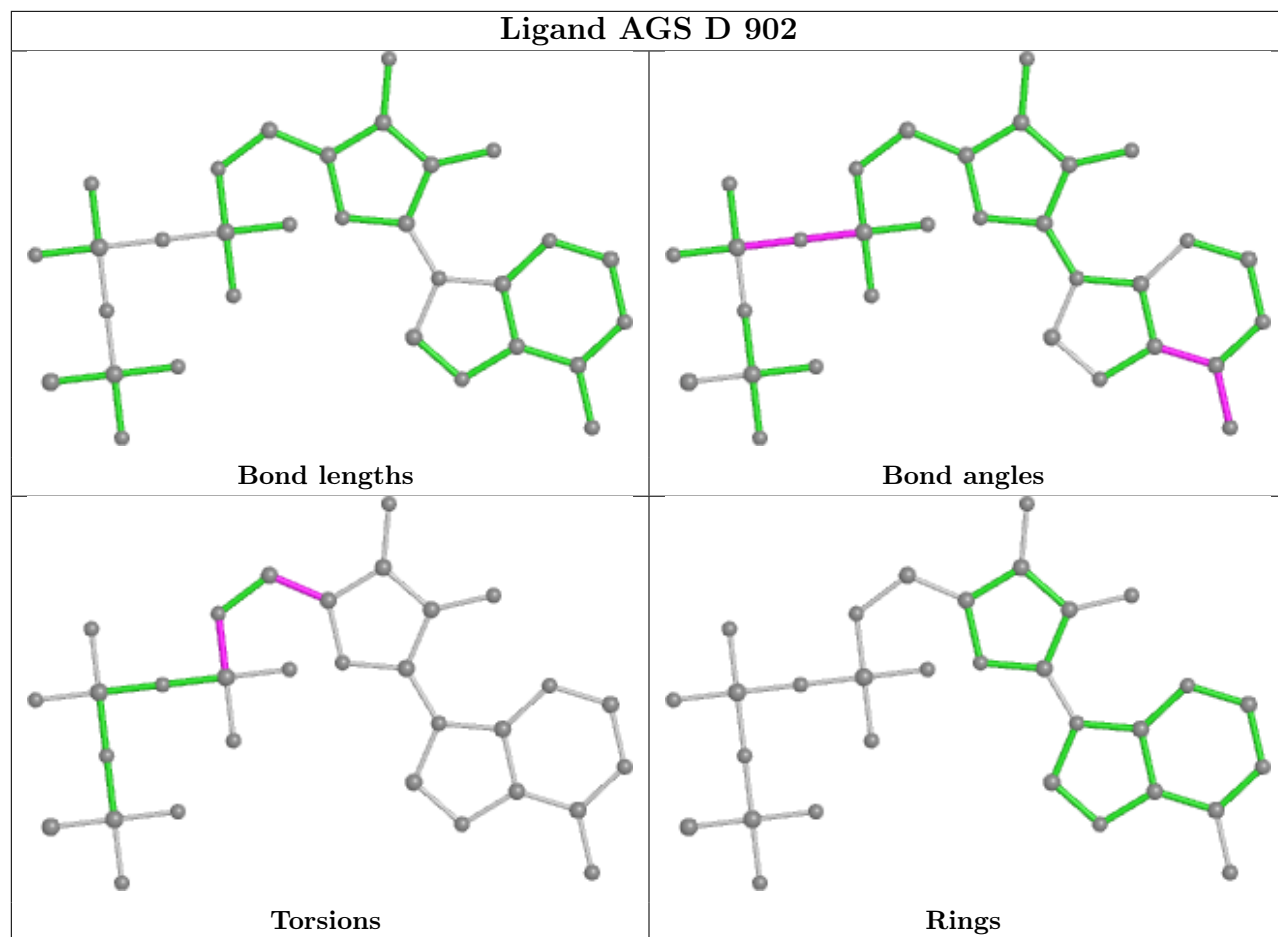
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

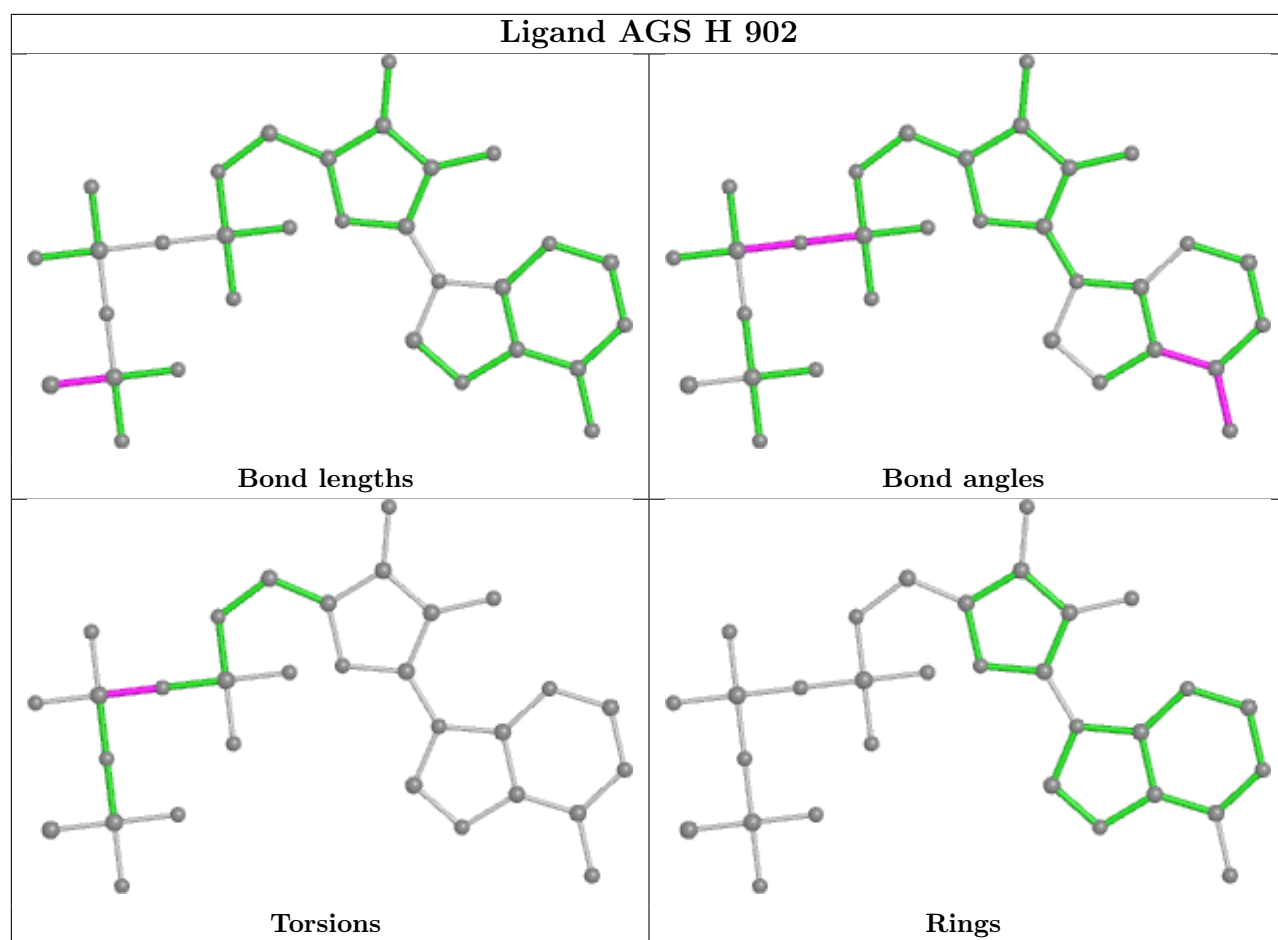


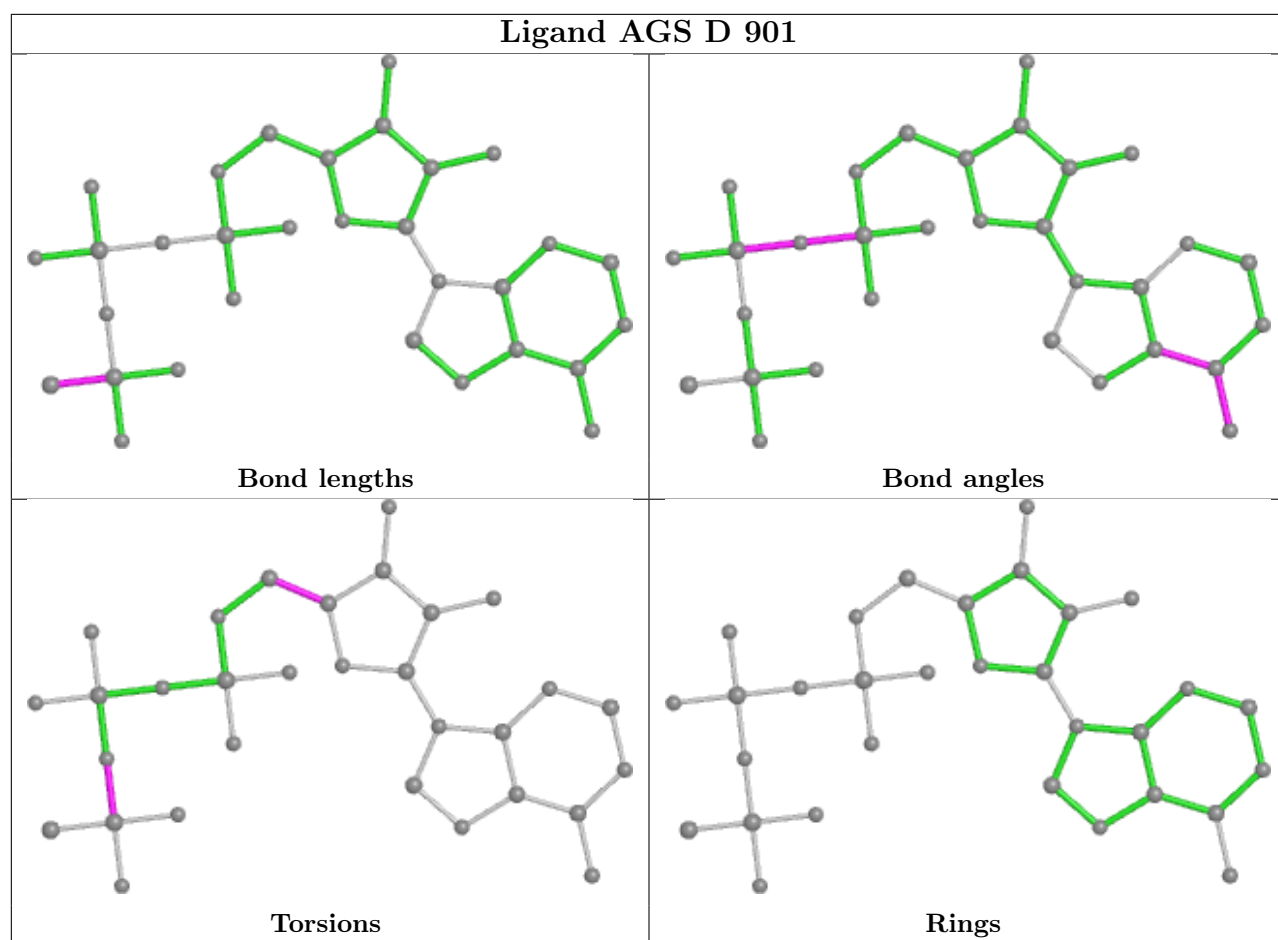


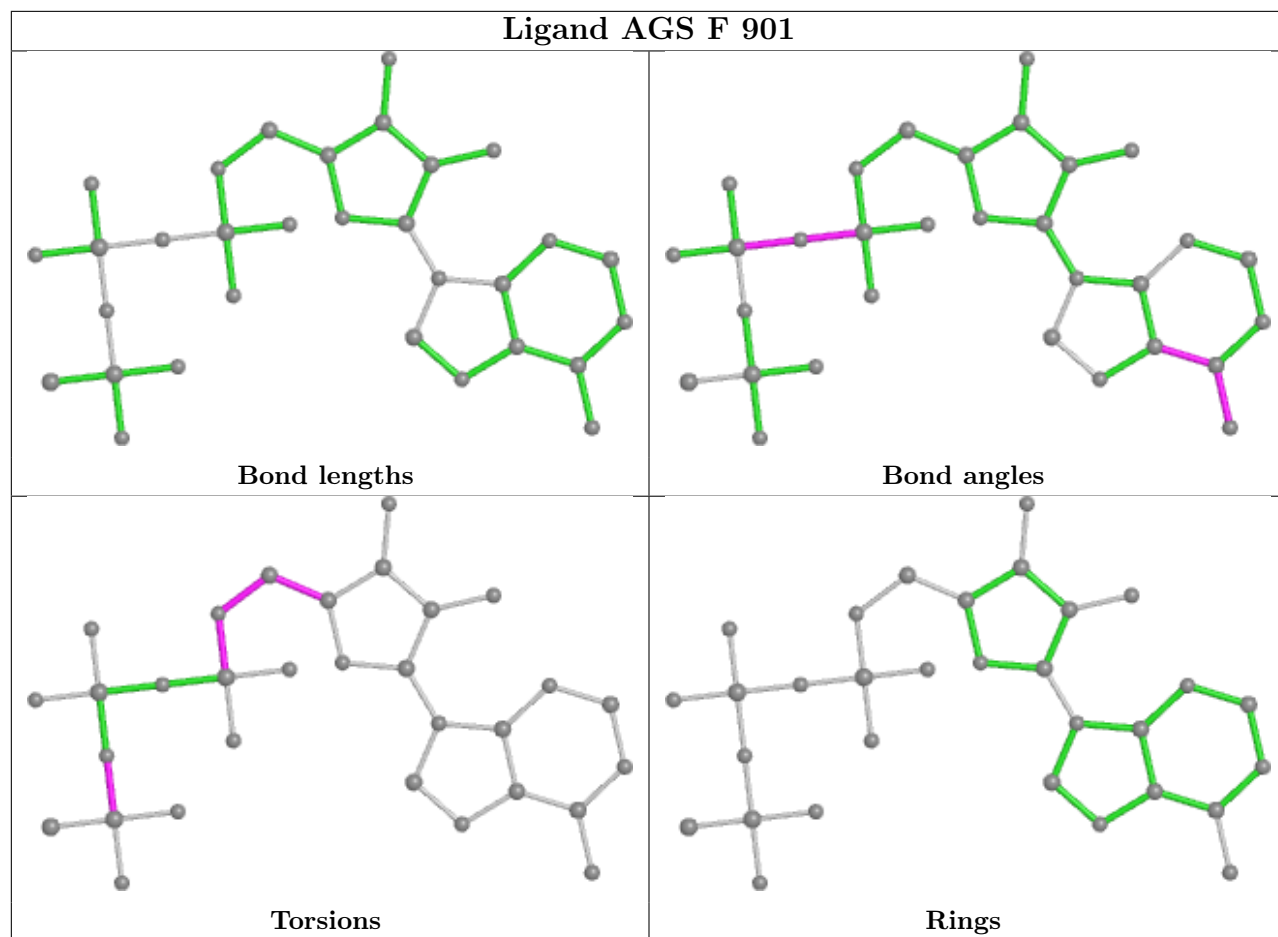


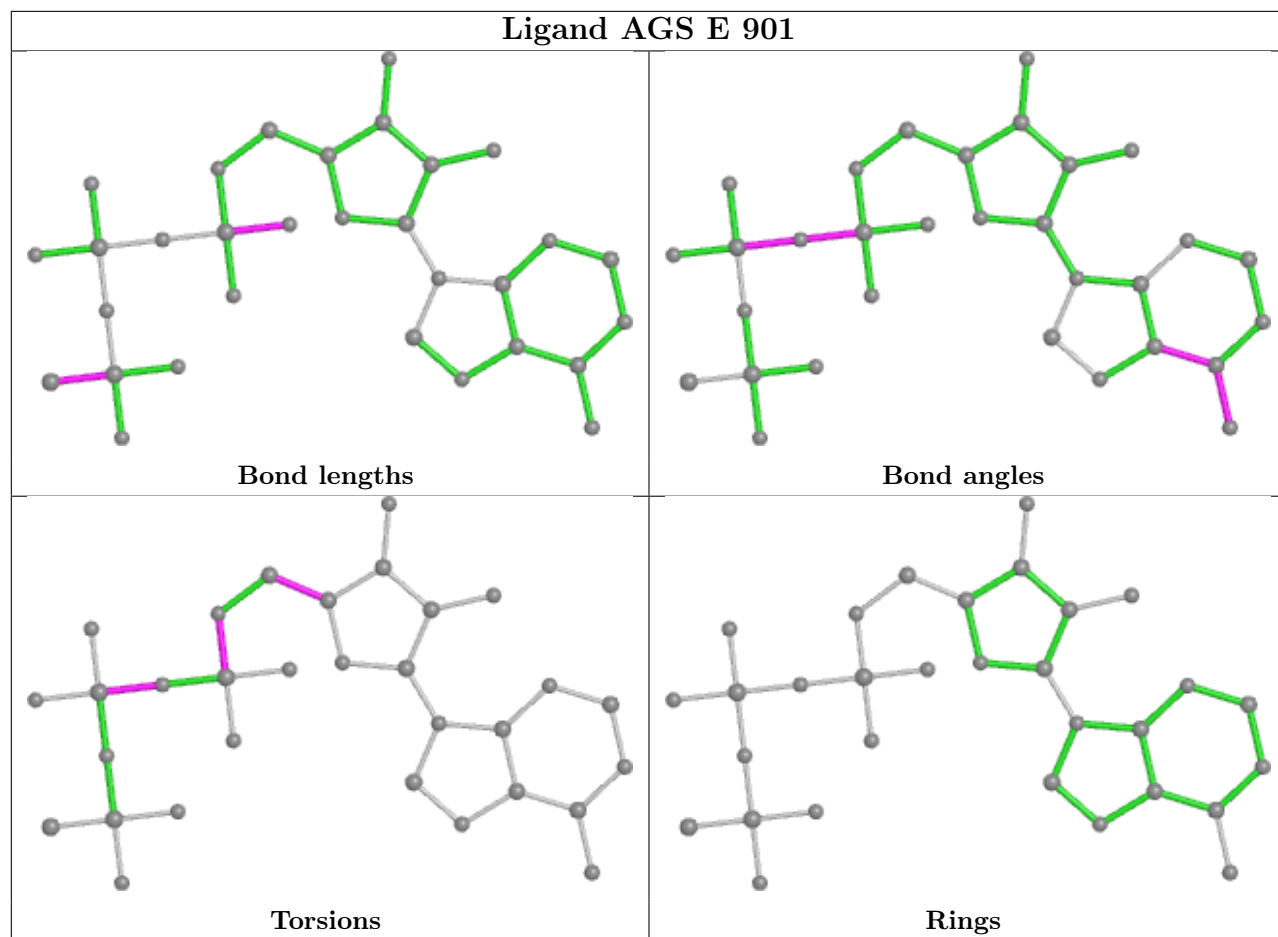


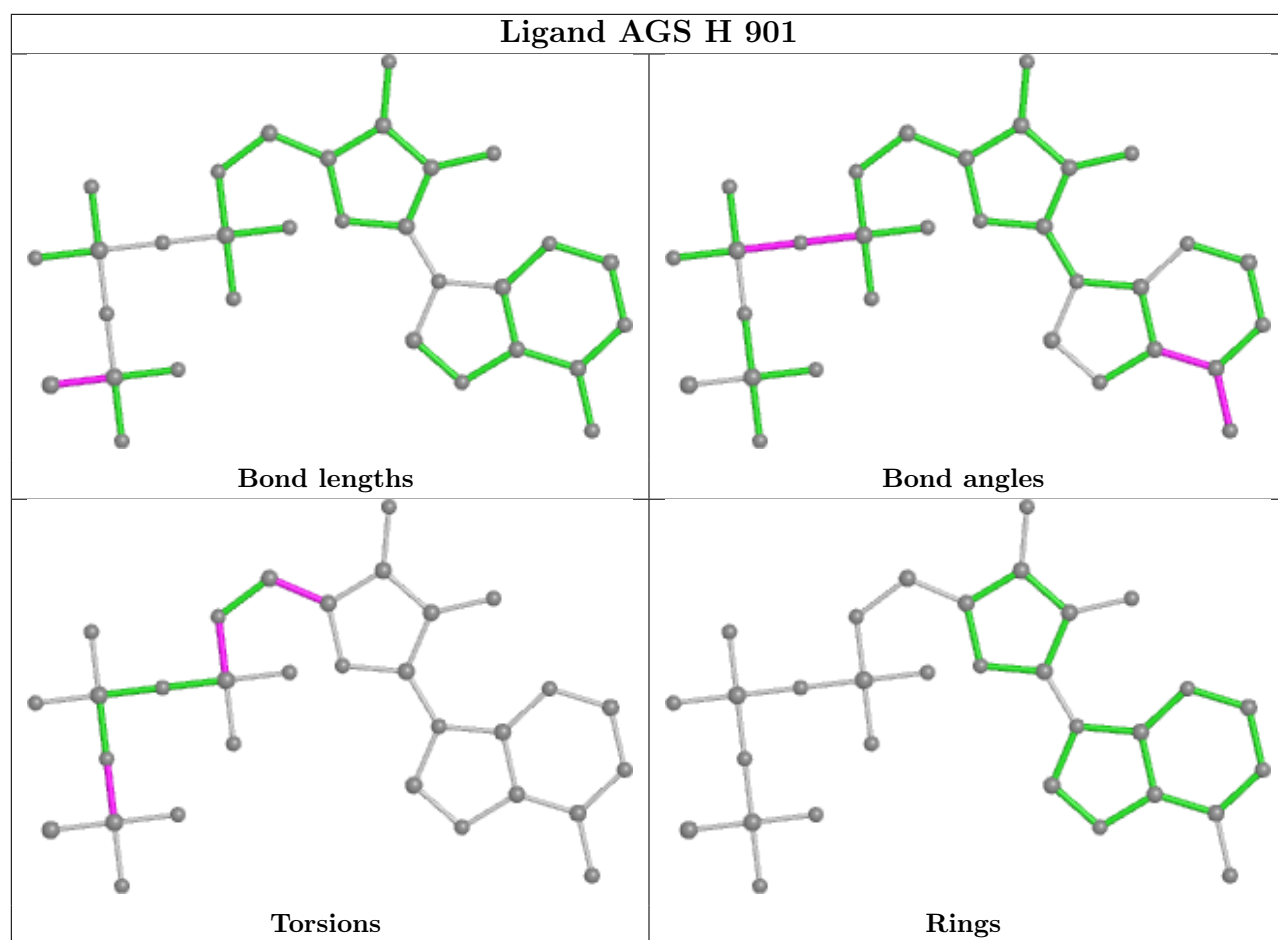




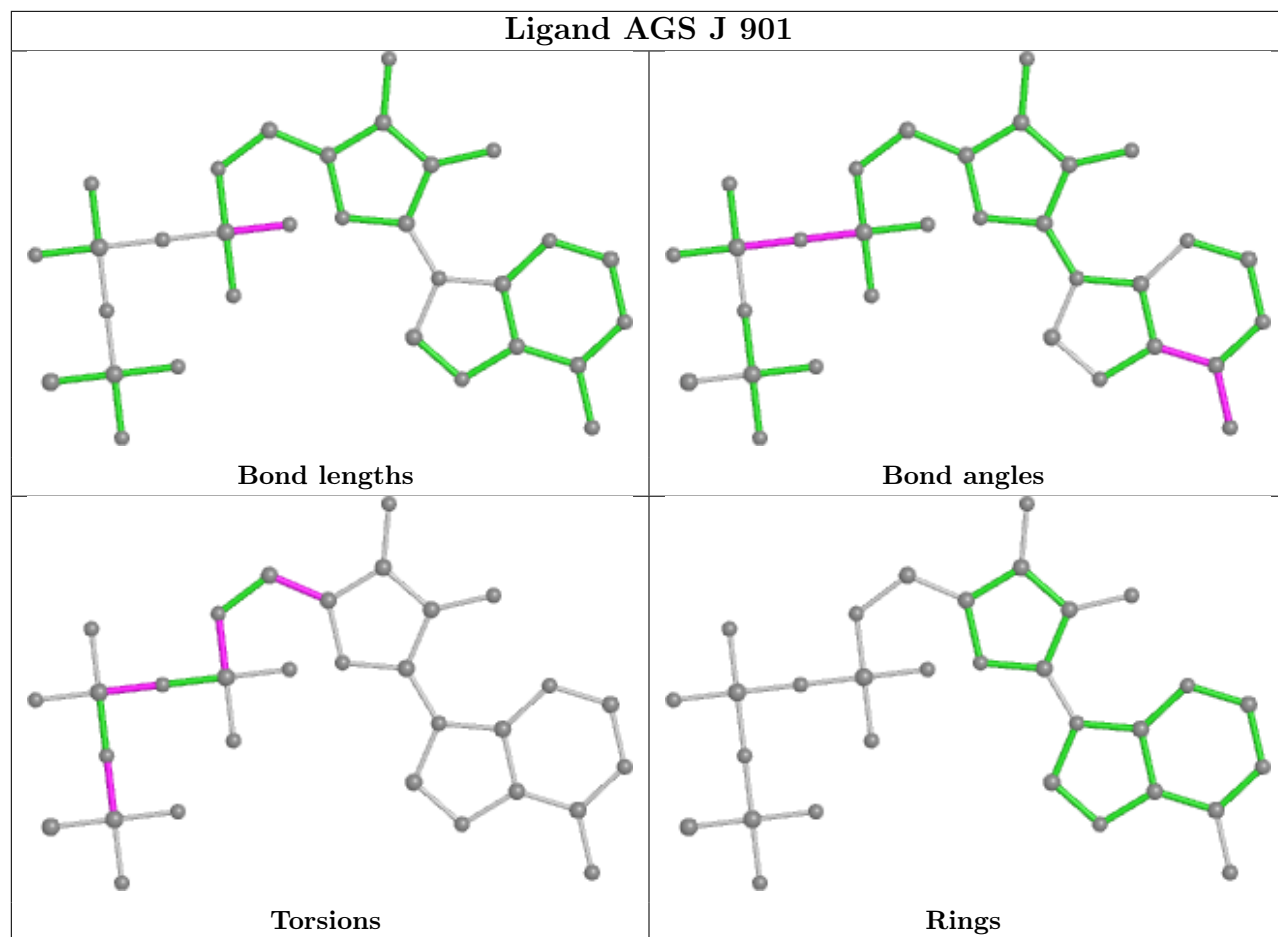


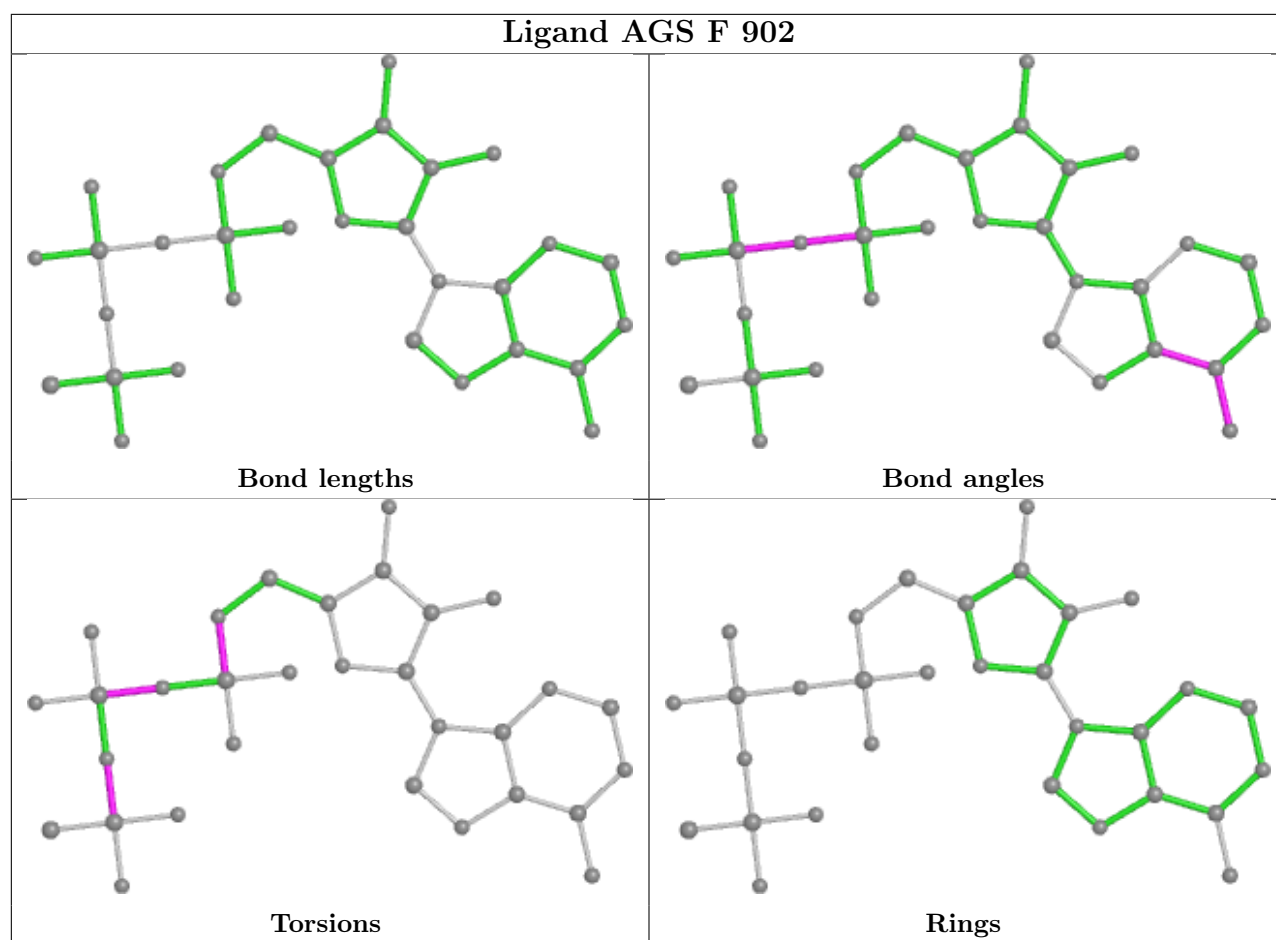






Ligand AGS J 901





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.

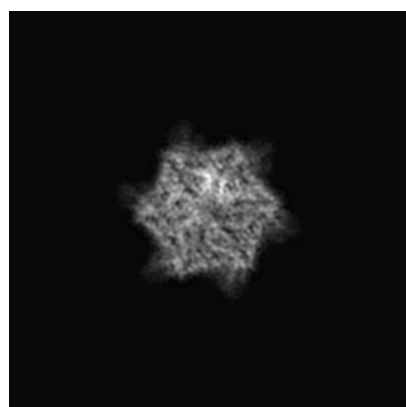
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7476. These allow visual inspection of the internal detail of the map and identification of artifacts.

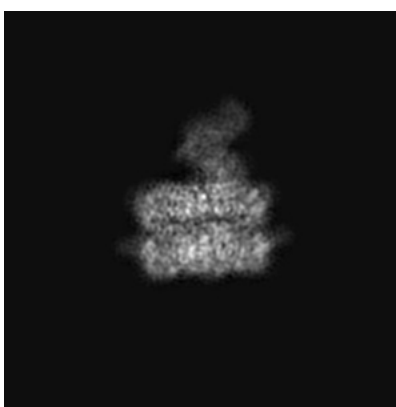
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

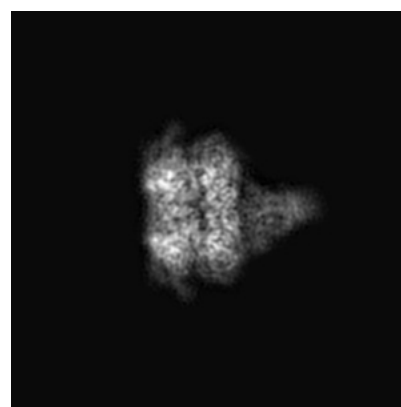
6.1.1 Primary map



X



Y

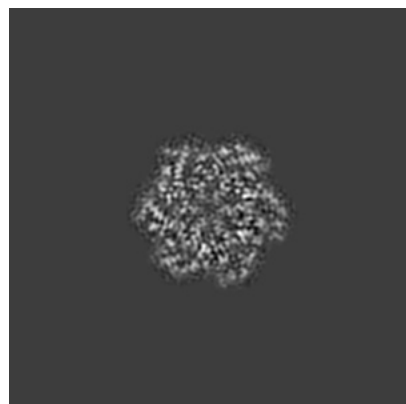


Z

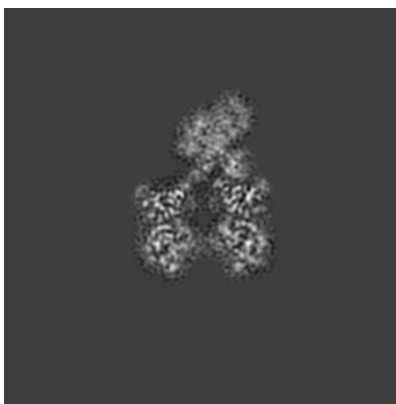
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

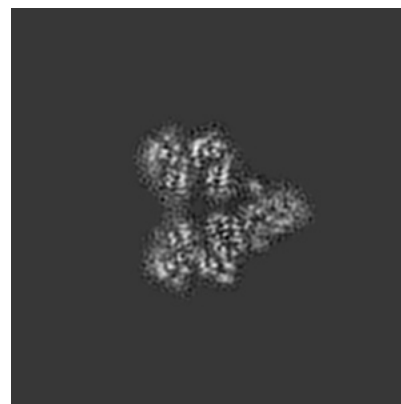
6.2.1 Primary map



X Index: 128



Y Index: 128

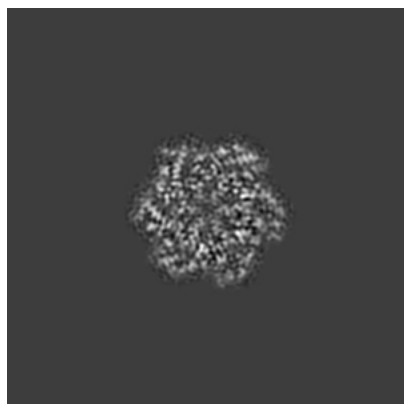


Z Index: 128

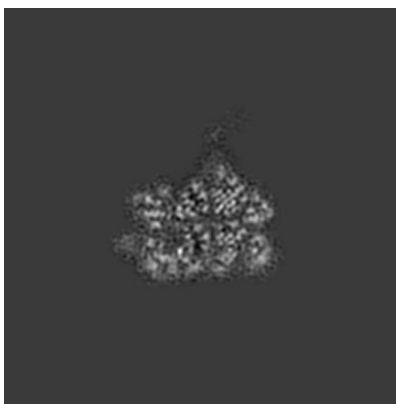
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

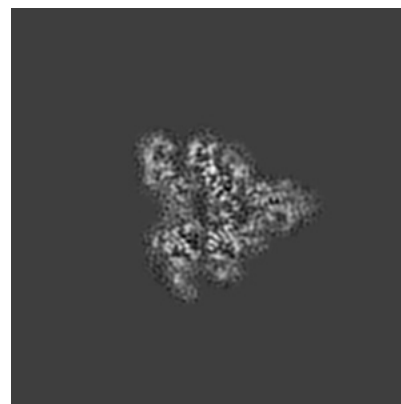
6.3.1 Primary map



X Index: 128



Y Index: 146

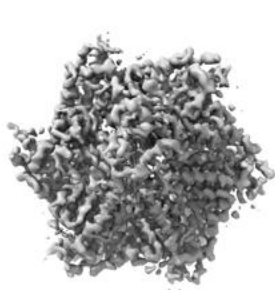


Z Index: 136

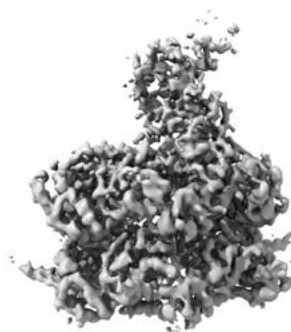
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

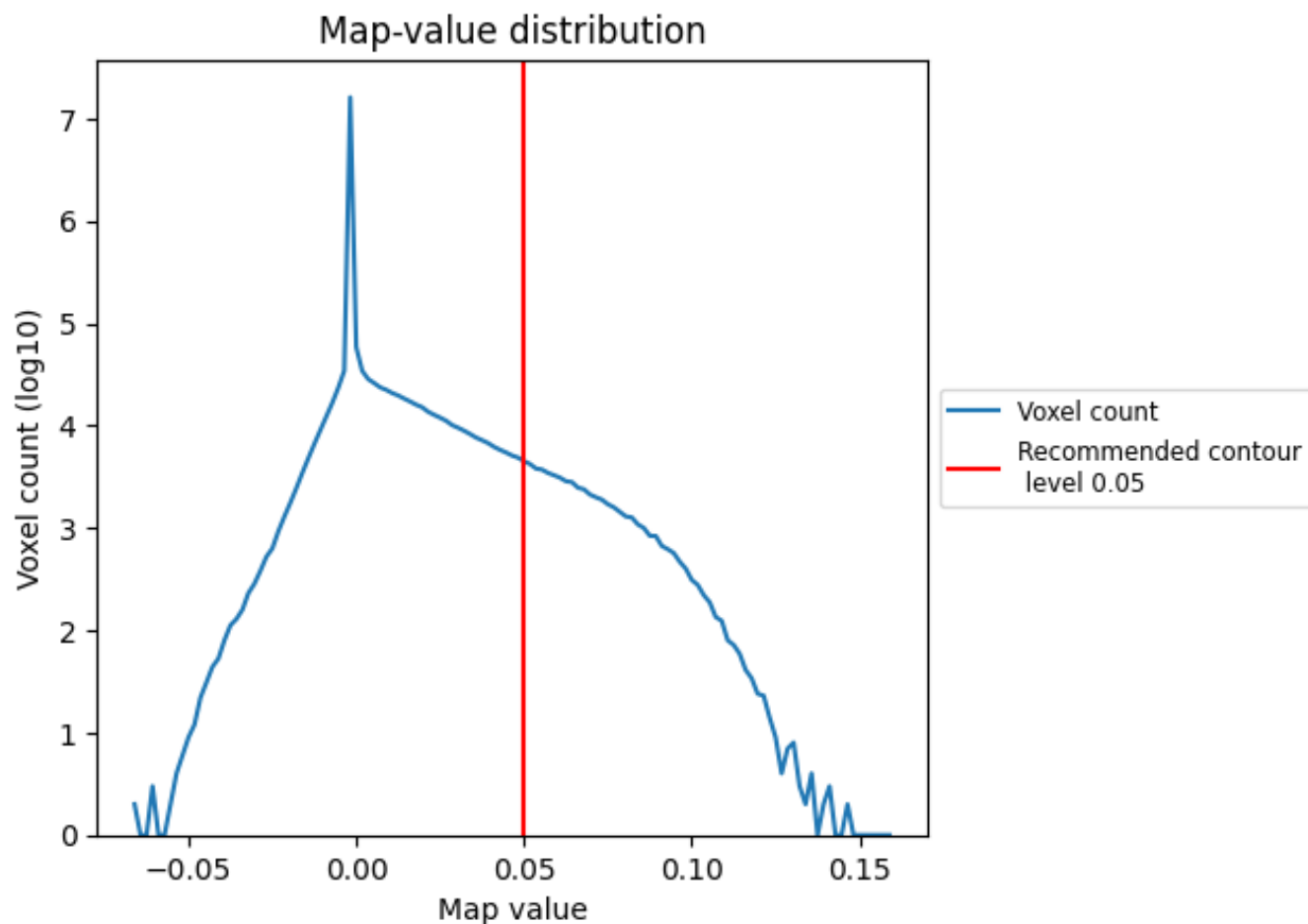
6.5 Mask visualisation

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

7 Map analysis [i](#)

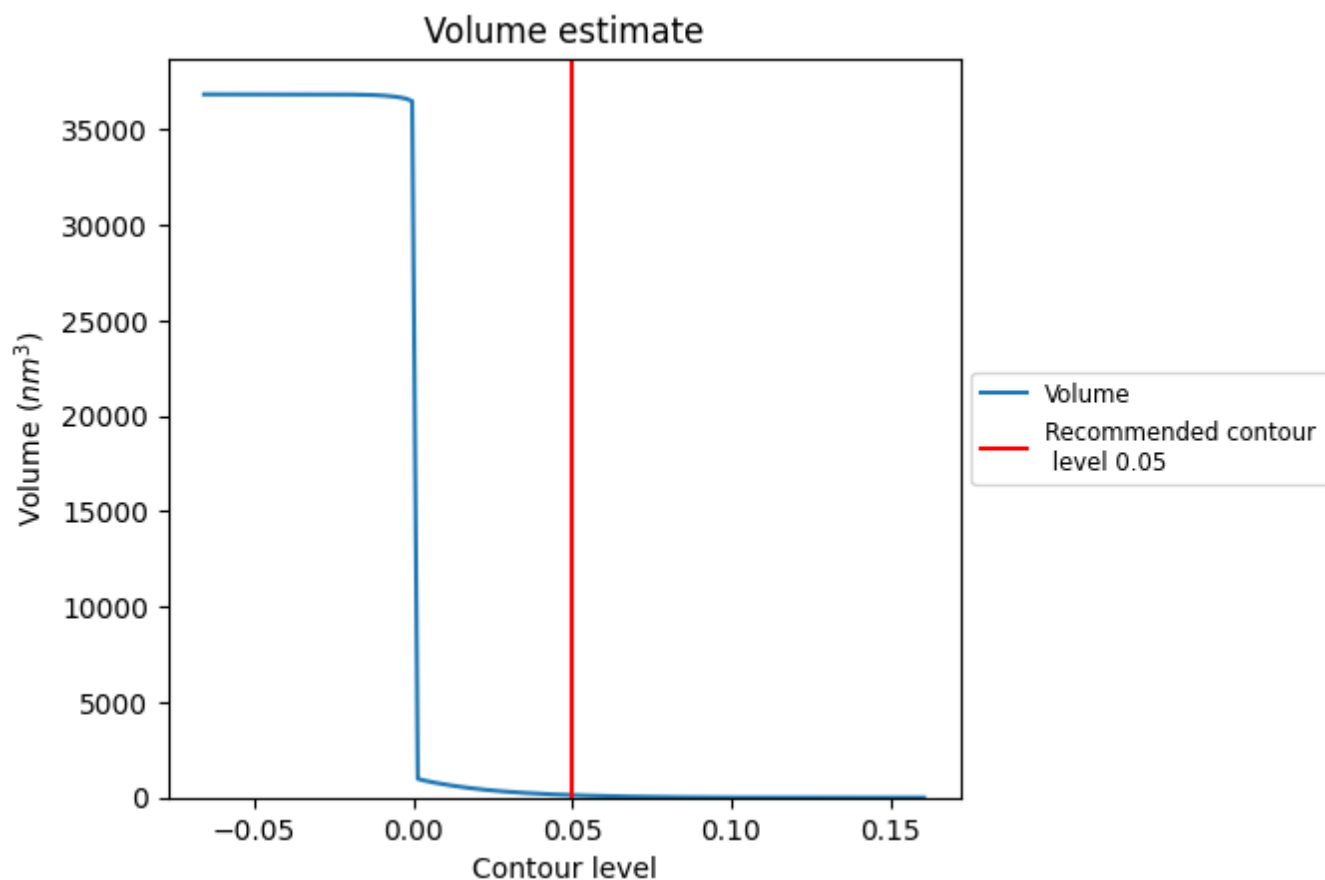
This section contains the results of statistical analysis of the map.

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.

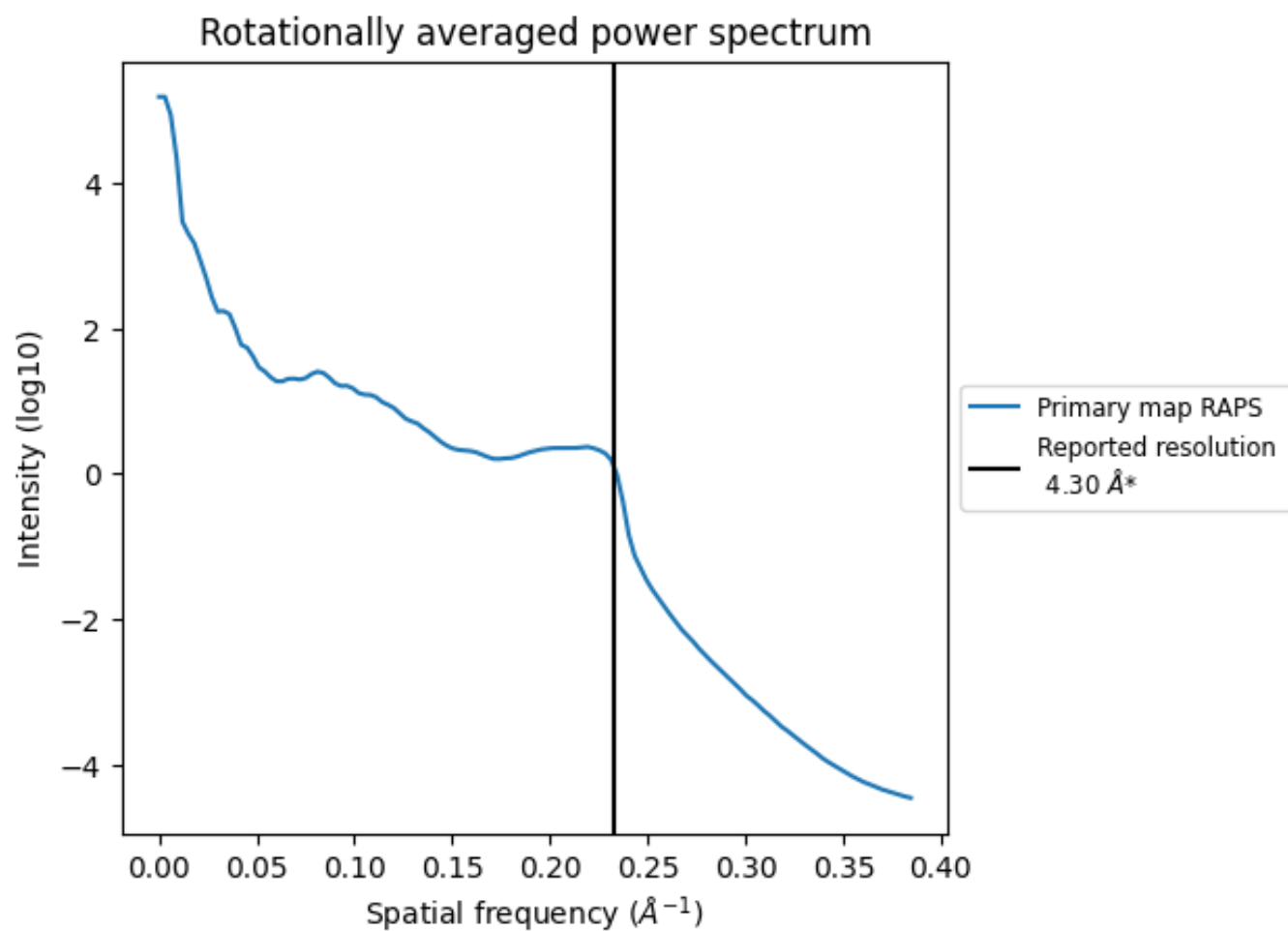
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm^3 ; this corresponds to an approximate mass of 116 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

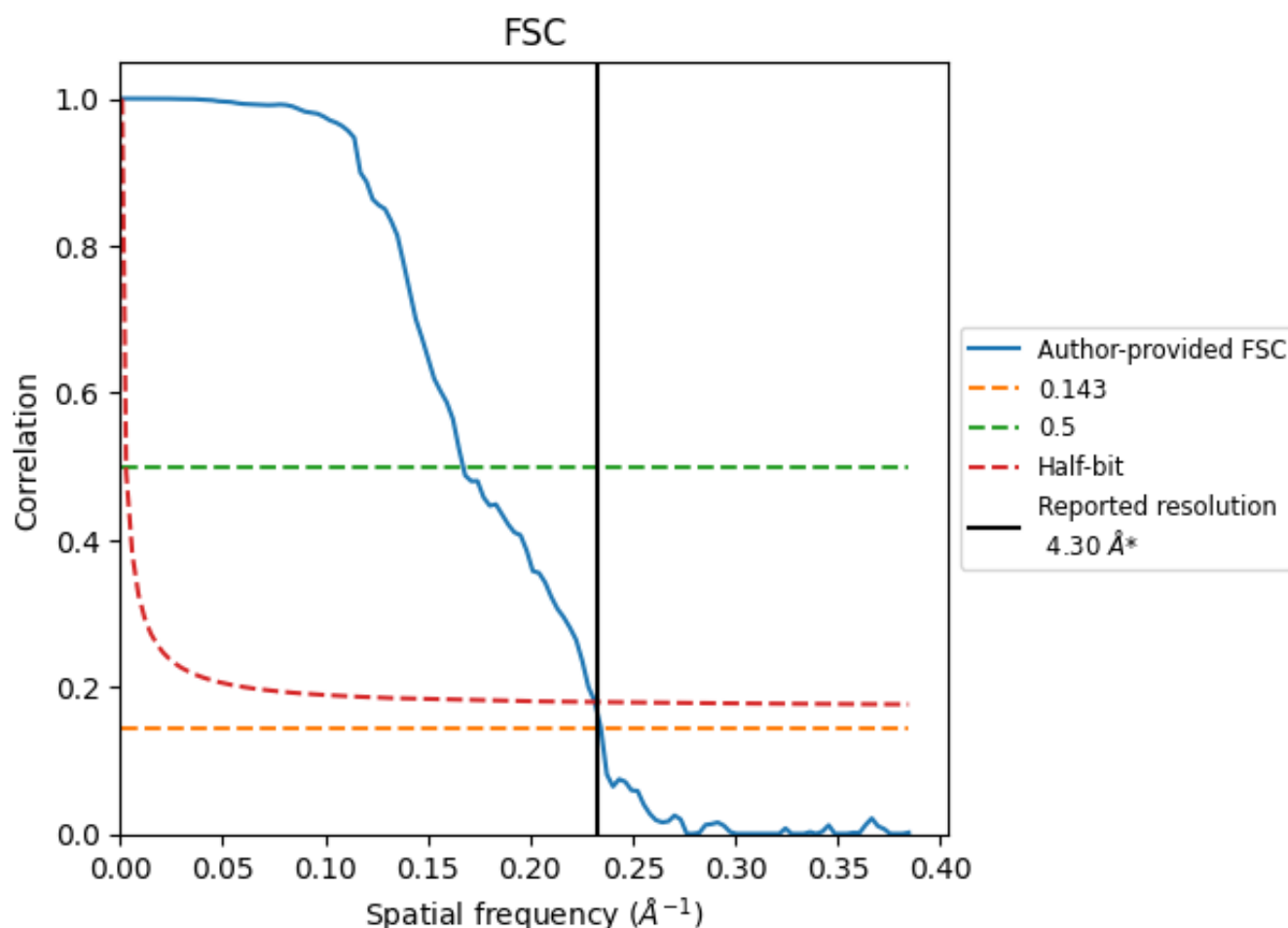


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

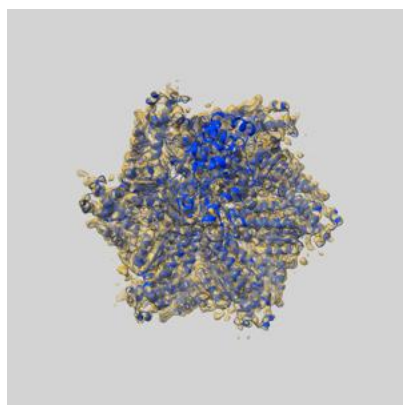
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	5.98	4.32
Unmasked-calculated*	-	-	-

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

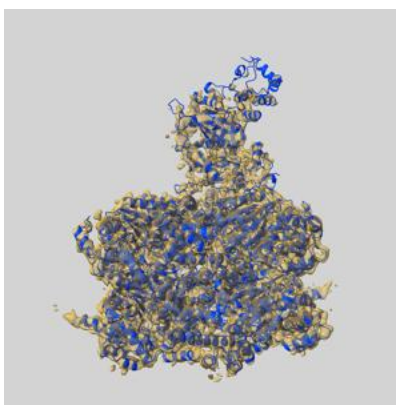
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7476 and PDB model 6CHS. Per-residue inclusion information can be found in section 3 on page 6.

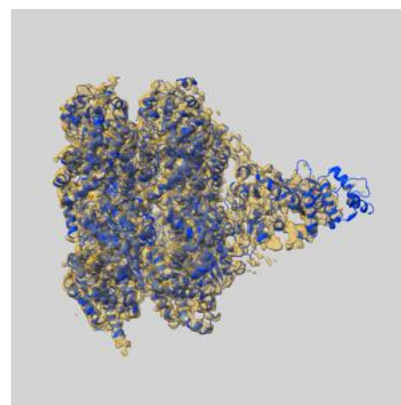
9.1 Map-model overlay [i](#)



X



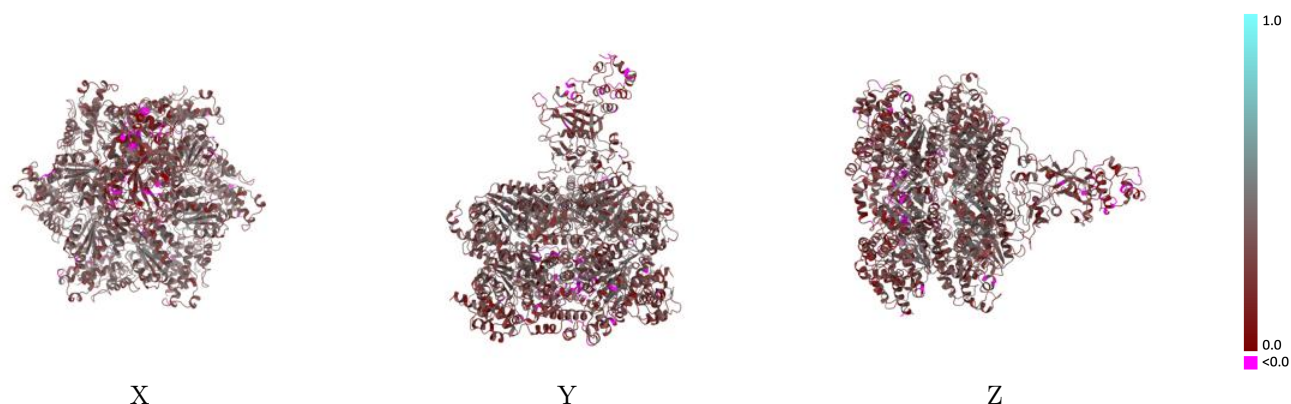
Y



Z

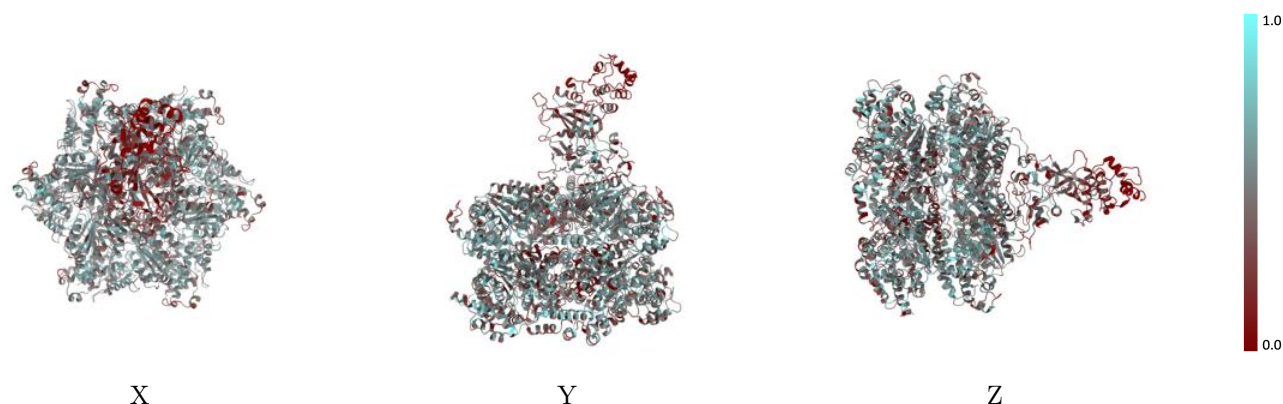
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



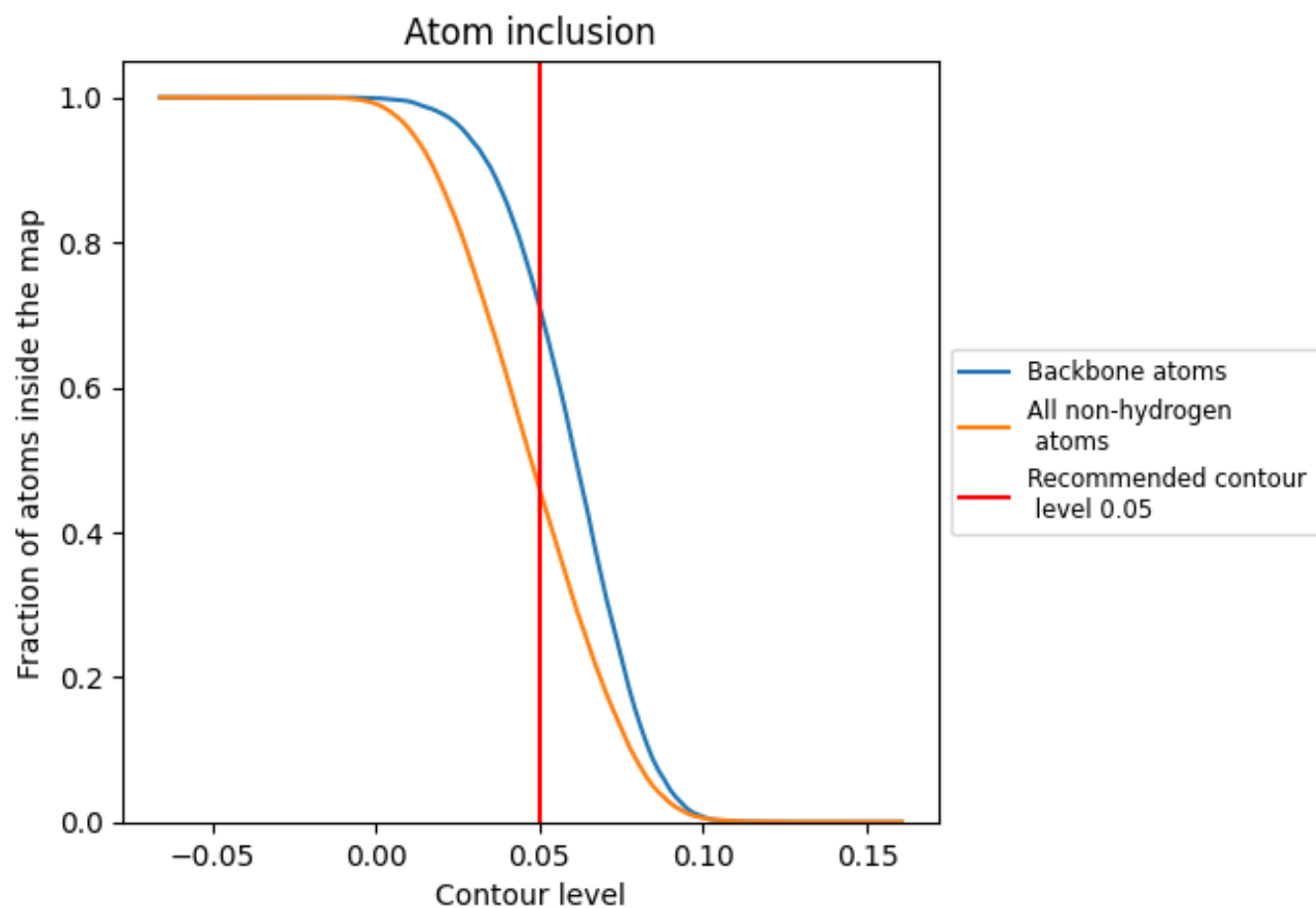
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.4596</div>	<div><div></div>0.2860</div>
A	<div><div></div>0.2940</div>	<div><div></div>0.2370</div>
D	<div><div></div>0.4784</div>	<div><div></div>0.2890</div>
E	<div><div></div>0.4742</div>	<div><div></div>0.2960</div>
F	<div><div></div>0.4865</div>	<div><div></div>0.2890</div>
H	<div><div></div>0.4860</div>	<div><div></div>0.3000</div>
I	<div><div></div>0.4872</div>	<div><div></div>0.2950</div>
J	<div><div></div>0.4856</div>	<div><div></div>0.2880</div>

1.0

0.0

<0.0