



Full wwPDB EM Validation Report ⓘ

Sep 22, 2022 – 08:32 am BST

PDB ID : 7Z37
EMDB ID : EMD-14472
Title : Structure of the RAF1-HSP90-CDC37 complex (RHC-II)
Authors : Mesa, P.; Garcia-Alonso, S.; Barbacid, M.; Montoya, G.
Deposited on : 2022-03-01
Resolution : 3.67 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.dev8
Mogul : 1.8.4, 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)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.30

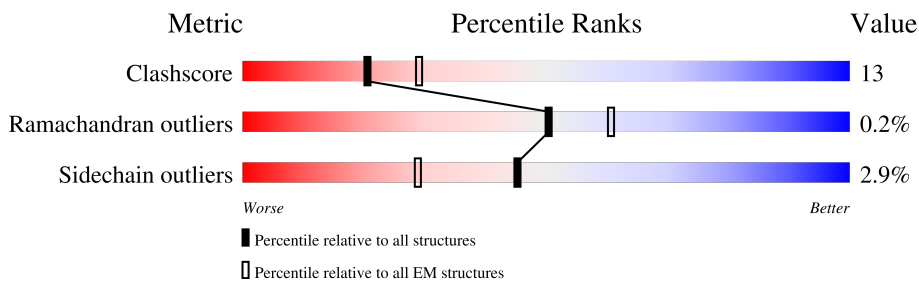
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.67 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	AP1	732	
1	BP1	732	
2	CP1	659	
3	DP1	394	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14256 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 Heat shock protein HSP 90-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AP1	636	5158	3270	868	997	23	0	0
1	BP1	638	5173	3280	870	1000	23	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP1	-7	MET	-	initiating methionine	UNP P08238
AP1	-6	TYR	-	expression tag	UNP P08238
AP1	-5	PRO	-	expression tag	UNP P08238
AP1	-4	TYR	-	expression tag	UNP P08238
AP1	-3	ASP	-	expression tag	UNP P08238
AP1	-2	VAL	-	expression tag	UNP P08238
AP1	-1	PRO	-	expression tag	UNP P08238
AP1	0	ASP	-	expression tag	UNP P08238
AP1	1	TYR	-	expression tag	UNP P08238
AP1	2	ALA	-	expression tag	UNP P08238
BP1	-7	MET	-	initiating methionine	UNP P08238
BP1	-6	TYR	-	expression tag	UNP P08238
BP1	-5	PRO	-	expression tag	UNP P08238
BP1	-4	TYR	-	expression tag	UNP P08238
BP1	-3	ASP	-	expression tag	UNP P08238
BP1	-2	VAL	-	expression tag	UNP P08238
BP1	-1	PRO	-	expression tag	UNP P08238
BP1	0	ASP	-	expression tag	UNP P08238
BP1	1	TYR	-	expression tag	UNP P08238
BP1	2	ALA	-	expression tag	UNP P08238

- Molecule 2 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CP1	193	1564	1008	264	279	13	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CP1	419	VAL	ILE	conflict	UNP P04049
CP1	420	ILE	VAL	conflict	UNP P04049
CP1	649	GLY	-	expression tag	UNP P04049
CP1	650	SER	-	expression tag	UNP P04049
CP1	651	ALA	-	expression tag	UNP P04049
CP1	652	TRP	-	expression tag	UNP P04049
CP1	653	SER	-	expression tag	UNP P04049
CP1	654	HIS	-	expression tag	UNP P04049
CP1	655	PRO	-	expression tag	UNP P04049
CP1	656	GLN	-	expression tag	UNP P04049
CP1	657	PHE	-	expression tag	UNP P04049
CP1	658	GLU	-	expression tag	UNP P04049
CP1	659	LYS	-	expression tag	UNP P04049

- Molecule 3 is a protein called Hsp90 co-chaperone Cdc37.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
3	DP1	273	2299	1429	411	443	1	15	0	0

There are 16 discrepancies between the modelled and reference sequences:

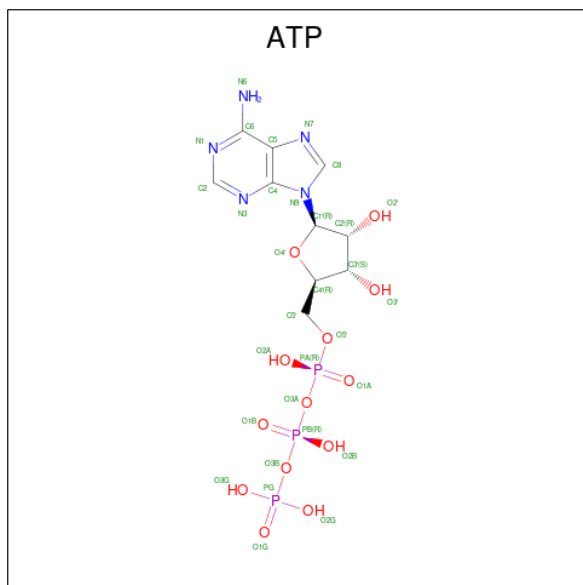
Chain	Residue	Modelled	Actual	Comment	Reference
DP1	379	THR	-	expression tag	UNP Q16543
DP1	380	ARG	-	expression tag	UNP Q16543
DP1	381	THR	-	expression tag	UNP Q16543
DP1	382	ARG	-	expression tag	UNP Q16543
DP1	383	PRO	-	expression tag	UNP Q16543
DP1	384	LEU	-	expression tag	UNP Q16543
DP1	385	GLU	-	expression tag	UNP Q16543
DP1	386	GLN	-	expression tag	UNP Q16543
DP1	387	LYS	-	expression tag	UNP Q16543
DP1	388	LEU	-	expression tag	UNP Q16543
DP1	389	ILE	-	expression tag	UNP Q16543
DP1	390	SER	-	expression tag	UNP Q16543
DP1	391	GLU	-	expression tag	UNP Q16543
DP1	392	GLU	-	expression tag	UNP Q16543

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Chain	Residue	Modelled	Actual	Comment	Reference
DP1	393	ASP	-	expression tag	UNP Q16543
DP1	394	LEU	-	expression tag	UNP Q16543

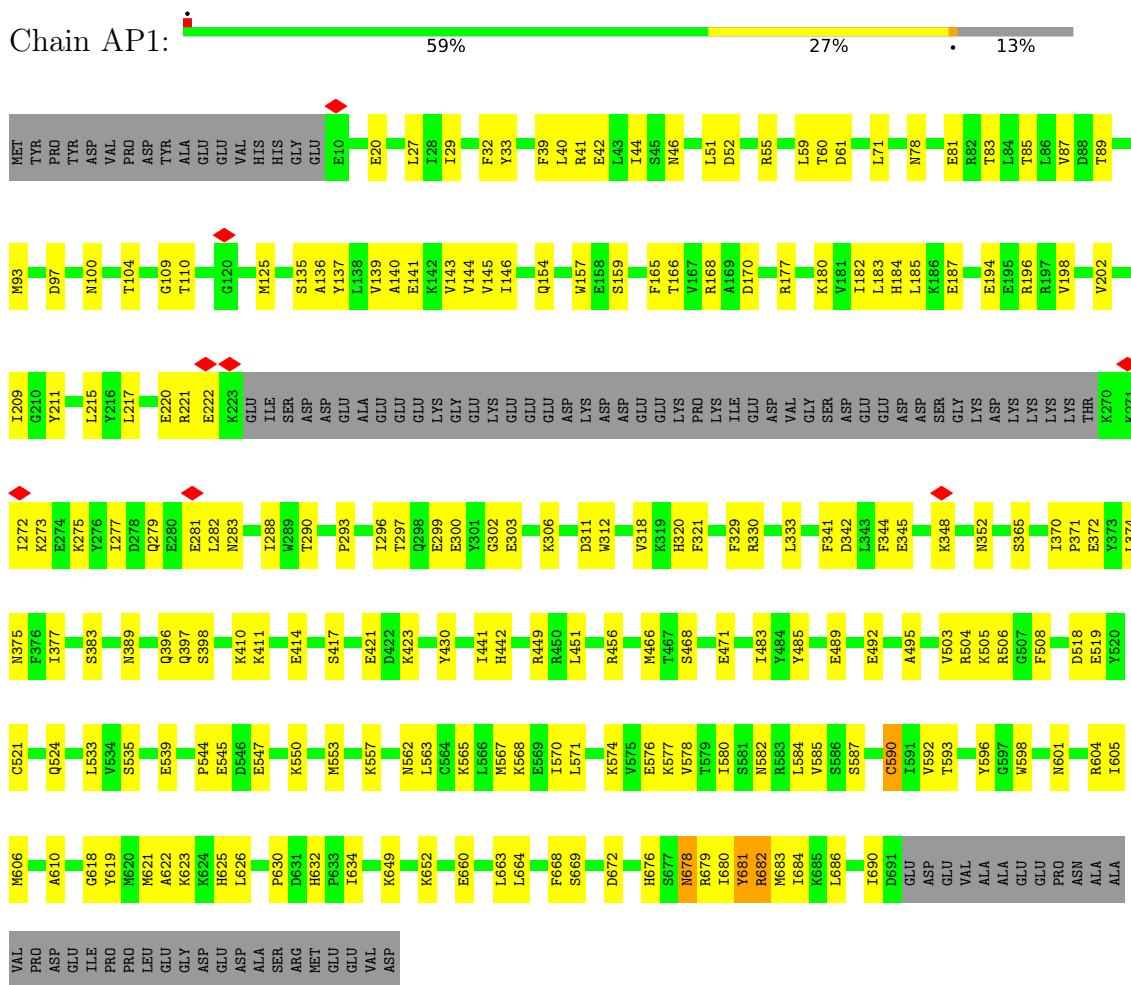
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



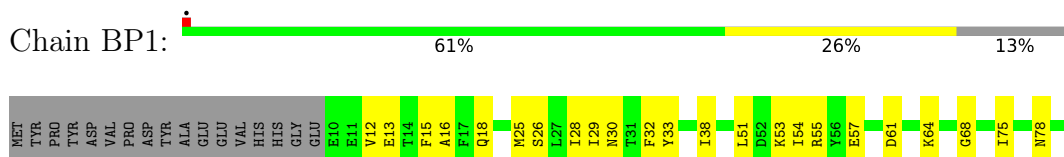
3 Residue-property plots

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: Heat shock protein HSP 90-beta



- Molecule 1: Heat shock protein HSP 90-beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46000	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: SEP, ATP

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	AP1	0.28	0/5242	0.51	0/7042
1	BP1	0.28	0/5257	0.52	0/7062
2	CP1	0.59	2/1599 (0.1%)	0.98	6/2155 (0.3%)
3	DP1	0.26	0/2326	0.54	0/3108
All	All	0.33	2/14424 (0.0%)	0.59	6/19367 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CP1	524	PRO	CB-CG	16.01	2.30	1.50
2	CP1	524	PRO	CG-CD	-12.38	1.09	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CP1	524	PRO	CA-N-CD	-21.38	81.57	111.50
2	CP1	524	PRO	CB-CG-CD	-20.88	25.07	106.50
2	CP1	524	PRO	N-CD-CG	12.83	122.45	103.20
2	CP1	547	PRO	CA-N-CD	-9.74	97.87	111.50
2	CP1	523	ASN	C-N-CD	9.07	147.46	128.40
2	CP1	524	PRO	N-CA-CB	-8.09	93.60	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AP1	5158	0	5206	135	0
1	BP1	5173	0	5224	129	0
2	CP1	1564	0	1576	63	0
3	DP1	2299	0	2258	80	0
4	AP1	31	0	12	2	0
4	BP1	31	0	12	1	0
All	All	14256	0	14288	385	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 13.

All (385) 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)
3:DP1:48:GLU:HB3	3:DP1:52:ARG:HH12	1.43	0.82
2:CP1:598:LEU:HG	2:CP1:600:PRO:HD2	1.61	0.81
1:BP1:61:ASP:HB3	1:BP1:64:LYS:HZ1	1.45	0.80
1:AP1:649:LYS:HA	1:AP1:652:LYS:HZ3	1.50	0.76
2:CP1:599:PHE:HA	2:CP1:602:ILE:HB	1.68	0.76
3:DP1:158:GLN:HB3	3:DP1:181:LEU:HD11	1.70	0.74
1:BP1:449:ARG:O	1:BP1:449:ARG:NH1	2.21	0.72
2:CP1:450:ARG:HG2	2:CP1:606:ILE:HD12	1.71	0.71
1:BP1:33:TYR:HB3	1:BP1:38:ILE:HD11	1.70	0.71
1:BP1:156:ALA:HB3	1:BP1:168:ARG:HB3	1.72	0.71
1:BP1:218:GLU:N	1:BP1:218:GLU:OE2	2.22	0.71
1:BP1:145:VAL:HB	1:BP1:157:TRP:HB3	1.73	0.71
1:BP1:281:GLU:OE1	1:BP1:284:LYS:NZ	2.23	0.71
1:AP1:311:ASP:OD2	3:DP1:231:ARG:NH1	2.24	0.70
1:BP1:319:LYS:HB2	1:BP1:415:LEU:HD22	1.73	0.70
3:DP1:50:LEU:HD21	3:DP1:102:LEU:HA	1.74	0.69
3:DP1:105:MET:HE1	3:DP1:106:ARG:HH21	1.57	0.69
1:AP1:456:ARG:HB3	1:AP1:466:MET:HB3	1.75	0.69
2:CP1:411:TYR:HE1	3:DP1:251:GLY:HA3	1.56	0.69
1:AP1:136:ALA:HB1	1:AP1:183:LEU:HD21	1.73	0.69
1:BP1:340:PRO:HD2	1:BP1:343:LEU:HD12	1.73	0.69
1:AP1:222:GLU:HB3	1:AP1:272:ILE:HB	1.76	0.68
1:BP1:389:ASN:ND2	1:BP1:396:GLN:OE1	2.26	0.68
1:AP1:680:ILE:HG21	1:BP1:661:THR:HG21	1.75	0.67
1:AP1:577:LYS:HB3	1:AP1:625:HIS:HD1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:557:LYS:HD3	1:BP1:580:ILE:HD11	1.76	0.67
1:AP1:679:ARG:HA	1:AP1:682:ARG:HE	1.61	0.66
1:BP1:580:ILE:HG22	1:BP1:628:ILE:HB	1.77	0.66
3:DP1:238:PHE:HA	3:DP1:241:ILE:HG22	1.77	0.66
1:AP1:570:ILE:HG23	1:AP1:571:LEU:HG	1.76	0.66
1:BP1:350:LYS:NZ	1:BP1:352:ASN:OD1	2.28	0.66
3:DP1:172:GLN:HB2	3:DP1:238:PHE:HD2	1.61	0.66
1:AP1:423:LYS:HE3	1:AP1:423:LYS:HA	1.79	0.65
1:AP1:632:HIS:HD2	1:AP1:634:ILE:HG12	1.61	0.65
1:BP1:637:THR:O	1:BP1:640:GLN:NE2	2.29	0.65
2:CP1:430:TYR:HD1	2:CP1:431:LYS:H	1.43	0.65
3:DP1:90:GLN:NE2	3:DP1:94:GLU:OE2	2.31	0.64
1:AP1:442:HIS:CE1	1:AP1:524:GLN:HE22	2.16	0.63
1:BP1:549:GLU:O	1:BP1:553:MET:HG2	1.99	0.63
3:DP1:174:TYR:O	3:DP1:178:ASN:ND2	2.33	0.62
1:AP1:333:LEU:HB3	1:AP1:377:ILE:HD11	1.82	0.62
1:AP1:220:GLU:HG3	1:AP1:277:ILE:HG12	1.81	0.61
1:AP1:664:LEU:HD11	1:BP1:664:LEU:HD11	1.82	0.61
1:BP1:535:SER:HB3	1:BP1:538:LYS:HG3	1.81	0.61
1:AP1:584:LEU:HD21	1:AP1:590:CYS:HB3	1.82	0.61
1:BP1:649:LYS:HE3	1:BP1:649:LYS:HA	1.81	0.61
2:CP1:538:LEU:HD13	2:CP1:541:LEU:HD21	1.82	0.61
1:AP1:632:HIS:CD2	1:AP1:634:ILE:HG12	2.35	0.61
1:BP1:346:ASN:HB2	2:CP1:422:GLN:HB2	1.83	0.61
1:BP1:16:ALA:O	1:BP1:18:GLN:NE2	2.32	0.61
3:DP1:162:PHE:CE1	3:DP1:175:LEU:HG	2.35	0.61
3:DP1:190:LEU:HD13	3:DP1:193:TRP:HZ3	1.64	0.61
1:AP1:83:THR:HG22	1:AP1:184:HIS:HA	1.82	0.60
1:AP1:372:GLU:O	1:AP1:375:ASN:ND2	2.31	0.60
1:BP1:352:ASN:HD21	1:BP1:370:ILE:HG21	1.65	0.60
2:CP1:533:SER:O	2:CP1:537:VAL:HG23	2.01	0.60
2:CP1:582:LYS:HB2	2:CP1:583:ARG:HH11	1.67	0.60
1:AP1:389:ASN:ND2	1:AP1:396:GLN:OE1	2.32	0.60
2:CP1:579:LYS:O	2:CP1:583:ARG:NH1	2.33	0.60
1:BP1:68:GLY:O	1:BP1:177:ARG:NH2	2.34	0.59
2:CP1:587:ASP:HA	2:CP1:590:LYS:HD3	1.83	0.59
1:BP1:289:TRP:HA	1:BP1:320:HIS:CE1	2.38	0.59
3:DP1:190:LEU:HB3	3:DP1:213:THR:HG23	1.86	0.58
1:AP1:545:GLU:OE2	1:AP1:550:LYS:NZ	2.34	0.58
2:CP1:579:LYS:HB3	2:CP1:583:ARG:HH12	1.69	0.58
1:AP1:168:ARG:HH21	1:BP1:12:VAL:HB	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:85:THR:HG23	1:AP1:182:ILE:HG13	1.86	0.58
1:AP1:187:GLU:OE1	1:AP1:187:GLU:N	2.37	0.58
1:BP1:288:ILE:HG22	1:BP1:291:ARG:HH21	1.69	0.57
3:DP1:237:PHE:HA	3:DP1:240:LYS:HG3	1.86	0.57
2:CP1:485:GLY:HA2	3:DP1:31:TRP:HH2	1.70	0.57
1:AP1:649:LYS:HA	1:AP1:652:LYS:NZ	2.19	0.57
1:BP1:148:LYS:HB2	1:BP1:154:GLN:HB3	1.86	0.57
3:DP1:183:CYS:SG	3:DP1:186:THR:OG1	2.56	0.57
1:BP1:495:ALA:O	1:BP1:504:ARG:NH2	2.37	0.57
1:AP1:505:LYS:HD3	1:AP1:585:VAL:HG21	1.87	0.57
1:BP1:636:GLU:HB2	1:BP1:639:ARG:HH21	1.70	0.56
2:CP1:433:LEU:O	2:CP1:437:GLU:N	2.37	0.56
1:AP1:547:GLU:H	1:AP1:547:GLU:CD	2.07	0.56
1:BP1:302:GLY:O	1:BP1:306:LYS:HG2	2.05	0.56
3:DP1:95:GLU:O	3:DP1:99:GLU:HG2	2.06	0.56
1:BP1:472:TYR:HE2	1:BP1:483:ILE:HG12	1.71	0.56
2:CP1:508:SER:OG	2:CP1:509:VAL:N	2.37	0.56
2:CP1:511:TRP:HZ3	2:CP1:536:ILE:HG13	1.70	0.56
1:AP1:61:ASP:OD1	1:AP1:61:ASP:N	2.39	0.56
1:BP1:424:GLU:HG3	1:BP1:428:LYS:HZ2	1.70	0.56
3:DP1:51:ASP:HB3	3:DP1:55:ARG:HH22	1.70	0.56
1:AP1:468:SER:N	1:AP1:471:GLU:OE1	2.37	0.56
1:AP1:562:ASN:HA	1:AP1:565:LYS:HE3	1.88	0.56
1:BP1:551:LYS:O	1:BP1:555:GLU:HG2	2.06	0.55
1:BP1:628:ILE:HG23	1:BP1:635:VAL:HG11	1.87	0.55
2:CP1:546:LEU:O	2:CP1:549:SER:OG	2.24	0.55
3:DP1:254:ASP:OD1	3:DP1:255:GLU:N	2.40	0.55
2:CP1:433:LEU:HA	2:CP1:436:GLN:HB3	1.87	0.55
1:AP1:87:VAL:HG22	1:AP1:180:LYS:HG2	1.89	0.55
1:BP1:369:LEU:HD13	1:BP1:401:LEU:HD22	1.87	0.55
3:DP1:53:GLY:HA3	3:DP1:98:TRP:CZ3	2.40	0.55
1:BP1:591:ILE:HG12	1:BP1:626:LEU:HD13	1.87	0.55
1:AP1:495:ALA:O	1:AP1:504:ARG:NH1	2.39	0.55
1:BP1:211:TYR:O	1:BP1:283:ASN:ND2	2.40	0.55
1:AP1:145:VAL:HB	1:AP1:157:TRP:HB3	1.89	0.55
1:AP1:539:GLU:N	1:AP1:593:THR:O	2.36	0.55
3:DP1:85:GLN:HA	3:DP1:85:GLN:NE2	2.22	0.55
1:BP1:51:LEU:HD23	1:BP1:90:GLY:HA2	1.88	0.54
2:CP1:599:PHE:O	2:CP1:603:LEU:HD22	2.07	0.54
1:BP1:57:GLU:O	1:BP1:64:LYS:NZ	2.41	0.54
1:BP1:25:MET:HE2	1:BP1:105:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CP1:441:GLN:N	2:CP1:441:GLN:OE1	2.38	0.54
1:AP1:220:GLU:HB3	1:AP1:275:LYS:HE3	1.89	0.54
1:AP1:396:GLN:NE2	1:BP1:30:ASN:O	2.39	0.53
1:AP1:109:GLY:N	4:AP1:801:ATP:O3'	2.41	0.53
1:BP1:316:LEU:HD21	1:BP1:429:PHE:HB2	1.88	0.53
1:BP1:26:SER:OG	3:DP1:2:VAL:O	2.26	0.53
1:BP1:502:ARG:HH11	1:BP1:582:ASN:HB3	1.71	0.53
2:CP1:430:TYR:OH	2:CP1:490:ALA:O	2.26	0.53
1:BP1:553:MET:O	1:BP1:557:LYS:HG2	2.09	0.53
3:DP1:166:ARG:HH12	3:DP1:208:GLN:HA	1.73	0.53
1:BP1:583:ARG:NH2	1:BP1:627:GLU:OE1	2.41	0.53
1:BP1:335:ILE:HD11	1:BP1:415:LEU:HD21	1.91	0.53
1:AP1:51:LEU:HD22	1:AP1:71:LEU:HB3	1.91	0.53
1:AP1:604:ARG:HH21	1:AP1:605:ILE:HD11	1.74	0.53
1:AP1:553:MET:O	1:AP1:557:LYS:HG3	2.10	0.52
1:AP1:489:GLU:HB2	1:AP1:604:ARG:HH12	1.73	0.52
1:AP1:610:ALA:HB3	2:CP1:421:THR:HG21	1.90	0.52
1:AP1:660:GLU:OE1	1:AP1:676:HIS:ND1	2.31	0.52
3:DP1:50:LEU:HA	3:DP1:98:TRP:HZ3	1.73	0.52
1:AP1:678:ASN:HA	1:AP1:681:TYR:CD2	2.45	0.52
1:AP1:277:ILE:HG22	1:AP1:279:GLN:HB2	1.91	0.52
1:BP1:282:LEU:H	1:BP1:282:LEU:HD23	1.74	0.52
1:AP1:352:ASN:H	1:AP1:365:SER:HB2	1.74	0.52
3:DP1:59:ARG:HD2	3:DP1:60:LYS:N	2.25	0.52
1:AP1:306:LYS:HE3	1:AP1:312:TRP:HA	1.91	0.52
1:BP1:28:ILE:HG12	1:BP1:32:PHE:HE2	1.74	0.52
1:AP1:40:LEU:O	1:AP1:44:ILE:HG12	2.10	0.51
1:AP1:299:GLU:O	1:AP1:303:GLU:HG2	2.10	0.51
1:BP1:485:TYR:CZ	1:BP1:535:SER:HB2	2.46	0.51
2:CP1:551:ILE:HD12	2:CP1:556:GLN:HE22	1.75	0.51
1:AP1:52:ASP:OD1	1:AP1:55:ARG:NH2	2.43	0.51
1:AP1:370:ILE:HD12	1:AP1:371:PRO:HD2	1.93	0.51
1:AP1:563:LEU:O	1:AP1:567:MET:HG2	2.10	0.51
1:BP1:536:VAL:HG12	1:BP1:541:LEU:HD11	1.93	0.51
3:DP1:48:GLU:O	3:DP1:52:ARG:HG2	2.11	0.51
3:DP1:186:THR:O	3:DP1:190:LEU:HD23	2.11	0.51
1:AP1:29:ILE:HD12	1:AP1:137:TYR:HB2	1.93	0.51
2:CP1:527:PHE:O	2:CP1:531:VAL:HG23	2.11	0.51
3:DP1:190:LEU:HD13	3:DP1:193:TRP:CZ3	2.46	0.51
1:AP1:297:THR:OG1	1:AP1:300:GLU:OE2	2.29	0.51
1:BP1:75:ILE:HD11	1:BP1:213:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CP1:411:TYR:CE1	3:DP1:251:GLY:HA3	2.42	0.50
1:AP1:290:THR:O	1:AP1:330:ARG:NH1	2.44	0.50
1:AP1:618:GLY:HA2	1:AP1:621:MET:SD	2.52	0.50
3:DP1:172:GLN:HB2	3:DP1:238:PHE:CD2	2.44	0.50
1:AP1:209:ILE:O	1:AP1:283:ASN:ND2	2.37	0.50
1:BP1:343:LEU:HD11	1:BP1:376:PHE:HB3	1.94	0.50
1:BP1:356:TYR:O	1:BP1:382:ASP:HA	2.11	0.50
2:CP1:560:MET:HE1	2:CP1:565:TYR:H	1.77	0.50
3:DP1:51:ASP:HB3	3:DP1:55:ARG:NH2	2.26	0.50
1:BP1:29:ILE:HG12	1:BP1:137:TYR:HB2	1.94	0.50
1:BP1:152:ASP:OD1	1:BP1:153:GLU:N	2.44	0.50
1:BP1:584:LEU:HB2	1:BP1:629:ASN:HB2	1.93	0.50
1:AP1:410:LYS:O	1:AP1:414:GLU:HG2	2.12	0.50
1:AP1:442:HIS:CG	2:CP1:423:TRP:HZ2	2.30	0.50
1:BP1:500:VAL:HG13	1:BP1:504:ARG:HH12	1.77	0.50
3:DP1:48:GLU:HB3	3:DP1:52:ARG:NH1	2.20	0.50
1:AP1:519:GLU:OE2	1:AP1:601:ASN:HB3	2.13	0.49
1:BP1:594:SER:HB2	1:BP1:623:LYS:HB2	1.94	0.49
1:BP1:402:LYS:O	1:BP1:406:LYS:HG2	2.12	0.49
3:DP1:179:VAL:HG11	3:DP1:235:ARG:HH21	1.76	0.49
1:BP1:220:GLU:HB3	1:BP1:275:LYS:HB3	1.95	0.49
1:BP1:519:GLU:HA	1:BP1:522:VAL:HG22	1.95	0.49
1:BP1:641:LYS:HE2	1:BP1:651:VAL:HG12	1.95	0.49
1:AP1:154:GLN:HB3	1:AP1:170:ASP:HB3	1.94	0.49
1:AP1:421:GLU:OE1	1:AP1:421:GLU:N	2.46	0.49
1:BP1:28:ILE:HA	1:BP1:32:PHE:CD2	2.47	0.49
1:BP1:550:LYS:O	1:BP1:554:GLU:HG3	2.13	0.49
2:CP1:582:LYS:HB2	2:CP1:583:ARG:NH1	2.27	0.49
1:AP1:221:ARG:NH2	1:AP1:273:LYS:HB2	2.28	0.48
1:AP1:140:ALA:HB2	1:AP1:185:LEU:HD23	1.95	0.48
2:CP1:590:LYS:NZ	2:CP1:595:GLU:HB2	2.27	0.48
3:DP1:106:ARG:HA	3:DP1:106:ARG:NE	2.28	0.48
1:AP1:596:TYR:O	1:AP1:623:LYS:NZ	2.46	0.48
1:BP1:563:LEU:HD21	1:BP1:639:ARG:HG3	1.94	0.48
3:DP1:132:LYS:HG2	3:DP1:133:PRO:HD2	1.95	0.48
1:AP1:584:LEU:HD23	1:AP1:587:SER:HB2	1.95	0.48
2:CP1:607:GLU:O	2:CP1:610:GLN:HG2	2.14	0.48
1:AP1:32:PHE:HD2	1:AP1:33:TYR:CE1	2.32	0.48
1:AP1:100:ASN:O	1:AP1:104:THR:OG1	2.16	0.48
1:BP1:321:PHE:CE2	1:BP1:411:LYS:HG3	2.49	0.48
1:BP1:593:THR:HG22	1:BP1:622:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CP1:607:GLU:HG3	2:CP1:611:HIS:NE2	2.28	0.48
3:DP1:13:SEP:O3P	3:DP1:36:ARG:NH1	2.46	0.48
2:CP1:451:GLN:HE22	2:CP1:481:THR:HA	1.78	0.48
3:DP1:195:ILE:HD13	3:DP1:263:VAL:HG13	1.95	0.48
3:DP1:265:GLY:O	3:DP1:269:LEU:HG	2.14	0.48
1:AP1:492:GLU:OE1	1:AP1:492:GLU:N	2.45	0.48
1:BP1:579:THR:HG22	1:BP1:580:ILE:H	1.78	0.48
1:AP1:582:ASN:OD1	1:AP1:582:ASN:N	2.47	0.47
1:AP1:672:ASP:OD1	1:AP1:672:ASP:N	2.43	0.47
1:BP1:144:VAL:HG22	1:BP1:158:GLU:HG2	1.95	0.47
3:DP1:57:CYS:HA	3:DP1:60:LYS:HD3	1.95	0.47
1:BP1:519:GLU:O	1:BP1:523:GLN:HG3	2.14	0.47
1:BP1:603:GLU:O	1:BP1:607:LYS:HG2	2.14	0.47
2:CP1:511:TRP:CZ3	2:CP1:536:ILE:HG13	2.48	0.47
2:CP1:451:GLN:O	2:CP1:454:GLN:HG2	2.14	0.47
1:AP1:441:ILE:HG13	1:AP1:451:LEU:HB3	1.97	0.47
1:BP1:13:GLU:HG3	1:BP1:15:PHE:CE2	2.50	0.47
3:DP1:61:VAL:HB	3:DP1:92:ARG:NH1	2.28	0.47
1:BP1:224:GLU:HG2	1:BP1:270:LYS:HG3	1.96	0.47
3:DP1:114:TRP:HB3	3:DP1:119:LEU:HG	1.97	0.47
3:DP1:162:PHE:HD1	3:DP1:174:TYR:CE1	2.32	0.47
2:CP1:512:MET:SD	2:CP1:512:MET:N	2.87	0.47
1:AP1:318:VAL:HG13	3:DP1:128:MET:HB2	1.97	0.47
2:CP1:579:LYS:HB3	2:CP1:583:ARG:NH1	2.29	0.47
1:BP1:339:ALA:HB1	1:BP1:343:LEU:HD13	1.96	0.47
1:AP1:41:ARG:NH2	1:AP1:42:GLU:OE2	2.47	0.47
1:BP1:572:ASP:HB2	1:BP1:573:LYS:HD2	1.96	0.47
1:BP1:222:GLU:HB2	1:BP1:272:ILE:HB	1.97	0.46
1:BP1:317:ALA:HB3	1:BP1:335:ILE:HD13	1.97	0.46
2:CP1:475:PHE:O	2:CP1:483:LYS:N	2.44	0.46
1:BP1:578:VAL:HG22	1:BP1:626:LEU:HB3	1.97	0.46
1:AP1:159:SER:HB2	1:AP1:165:PHE:HB3	1.98	0.46
1:AP1:580:ILE:HG23	1:AP1:630:PRO:HD3	1.97	0.46
1:BP1:312:TRP:CD1	1:BP1:312:TRP:C	2.89	0.46
1:AP1:342:ASP:HB2	1:AP1:345:GLU:HB2	1.98	0.46
1:BP1:213:ILE:HG22	1:BP1:283:ASN:ND2	2.30	0.46
3:DP1:246:ARG:O	3:DP1:250:GLU:HG2	2.16	0.46
2:CP1:445:LEU:HD12	2:CP1:446:ILE:HG13	1.98	0.46
1:BP1:221:ARG:HB2	1:BP1:273:LYS:NZ	2.31	0.46
1:BP1:424:GLU:HG3	1:BP1:428:LYS:NZ	2.31	0.46
1:AP1:302:GLY:O	1:AP1:306:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DP1:65:GLN:OE1	3:DP1:92:ARG:NH1	2.49	0.45
1:AP1:592:VAL:HG23	1:AP1:625:HIS:HB2	1.98	0.45
1:AP1:681:TYR:HA	1:AP1:684:ILE:HG22	1.99	0.45
3:DP1:166:ARG:HH22	3:DP1:208:GLN:HA	1.81	0.45
3:DP1:212:GLN:O	3:DP1:215:VAL:HB	2.16	0.45
1:AP1:141:GLU:OE1	1:AP1:141:GLU:N	2.41	0.45
1:AP1:293:PRO:HD2	3:DP1:124:PHE:HE1	1.81	0.45
3:DP1:18:GLU:OE1	3:DP1:32:ARG:NH1	2.49	0.45
3:DP1:163:GLY:HA3	3:DP1:193:TRP:HH2	1.80	0.45
1:BP1:617:MET:SD	1:BP1:618:GLY:N	2.90	0.45
1:AP1:209:ILE:HG23	1:AP1:211:TYR:H	1.81	0.45
1:AP1:449:ARG:HA	1:AP1:449:ARG:NE	2.32	0.45
1:AP1:598:TRP:CH2	1:AP1:606:MET:HG3	2.52	0.45
1:BP1:101:ASN:HB3	4:BP1:801:ATP:H4'	1.99	0.45
1:AP1:78:ASN:OD1	1:AP1:81:GLU:N	2.50	0.45
2:CP1:572:LYS:HB2	2:CP1:572:LYS:HE2	1.71	0.45
1:AP1:20:GLU:HG3	1:BP1:107:LYS:HE2	1.99	0.45
1:AP1:293:PRO:HG3	1:AP1:320:HIS:ND1	2.32	0.45
1:BP1:437:LEU:HD22	1:BP1:451:LEU:HD11	1.99	0.45
1:AP1:196:ARG:CZ	1:AP1:196:ARG:HB3	2.48	0.44
3:DP1:216:MET:SD	3:DP1:216:MET:N	2.85	0.44
1:AP1:568:LYS:HE2	1:AP1:576:GLU:HA	1.98	0.44
1:AP1:143:VAL:HG12	1:AP1:183:LEU:HD23	1.98	0.44
1:BP1:422:ASP:OD1	1:BP1:422:ASP:N	2.51	0.44
1:BP1:599:THR:OG1	1:BP1:600:ALA:N	2.51	0.44
1:AP1:27:LEU:O	1:AP1:32:PHE:HB2	2.18	0.44
1:BP1:581:SER:HB3	1:BP1:627:GLU:OE2	2.16	0.44
2:CP1:439:LYS:NZ	2:CP1:544:GLY:HA3	2.33	0.44
3:DP1:236:GLN:H	3:DP1:236:GLN:NE2	2.16	0.44
1:AP1:577:LYS:HB3	1:AP1:625:HIS:ND1	2.30	0.44
1:BP1:221:ARG:NH1	1:BP1:222:GLU:O	2.50	0.44
1:AP1:59:LEU:HD12	1:AP1:60:THR:HG23	2.00	0.44
1:BP1:53:LYS:O	1:BP1:57:GLU:HG2	2.17	0.44
1:AP1:293:PRO:HD2	3:DP1:124:PHE:CE1	2.53	0.44
1:AP1:329:PHE:HB3	1:AP1:383:SER:HB2	2.00	0.44
1:AP1:421:GLU:O	1:AP1:423:LYS:HD2	2.18	0.44
3:DP1:28:LEU:HA	3:DP1:31:TRP:CE3	2.53	0.44
3:DP1:35:ALA:O	3:DP1:38:GLU:HG3	2.18	0.44
1:BP1:146:ILE:O	1:BP1:180:LYS:N	2.51	0.43
2:CP1:559:PHE:O	2:CP1:563:ARG:HG2	2.18	0.43
1:AP1:506:ARG:NH2	1:AP1:544:PRO:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CP1:457:ASP:OD1	2:CP1:603:LEU:HD21	2.18	0.43
1:AP1:483:ILE:HB	1:AP1:533:LEU:HG	2.00	0.43
1:BP1:117:LEU:HD12	1:BP1:120:GLY:H	1.83	0.43
1:AP1:110:THR:HG23	1:AP1:125:MET:HE2	2.00	0.43
1:AP1:683:MET:O	1:AP1:686:LEU:HG	2.17	0.43
1:BP1:437:LEU:HD23	1:BP1:437:LEU:HA	1.75	0.43
1:BP1:496:ASN:OD1	1:BP1:496:ASN:N	2.50	0.43
3:DP1:172:GLN:OE1	3:DP1:238:PHE:HB2	2.18	0.43
1:AP1:215:LEU:HD13	1:AP1:217:LEU:HD11	2.01	0.43
1:AP1:593:THR:HG23	1:AP1:622:ALA:HB1	1.99	0.43
2:CP1:602:ILE:O	2:CP1:606:ILE:HG12	2.19	0.43
1:AP1:681:TYR:O	1:AP1:684:ILE:HG22	2.19	0.43
1:AP1:684:ILE:HD11	1:BP1:654:LEU:HD11	2.00	0.43
1:BP1:25:MET:CE	1:BP1:105:ILE:HD11	2.48	0.43
1:BP1:78:ASN:O	1:BP1:82:ARG:N	2.50	0.43
1:BP1:98:LEU:HG	1:BP1:157:TRP:HD1	1.84	0.43
1:BP1:594:SER:OG	1:BP1:595:THR:N	2.50	0.43
3:DP1:241:ILE:HA	3:DP1:244:ALA:HB2	2.00	0.43
1:BP1:282:LEU:H	1:BP1:282:LEU:CD2	2.32	0.43
1:BP1:385:ASP:O	1:BP1:386:LEU:HD23	2.18	0.43
2:CP1:445:LEU:HD12	2:CP1:446:ILE:N	2.34	0.43
3:DP1:139:ASP:H	3:DP1:144:ARG:NE	2.16	0.43
1:BP1:640:GLN:H	1:BP1:640:GLN:HG3	1.67	0.43
2:CP1:517:ILE:HD13	2:CP1:517:ILE:HA	1.84	0.43
3:DP1:61:VAL:O	3:DP1:65:GLN:HG2	2.18	0.43
3:DP1:87:GLU:O	3:DP1:91:LEU:HG	2.19	0.43
1:AP1:89:THR:O	1:AP1:177:ARG:NH2	2.31	0.43
1:BP1:131:VAL:HG21	1:BP1:390:ILE:HD11	2.01	0.43
2:CP1:410:GLY:O	2:CP1:412:MET:N	2.51	0.43
1:AP1:144:VAL:HG22	1:AP1:182:ILE:HB	2.01	0.42
3:DP1:59:ARG:HD2	3:DP1:59:ARG:C	2.40	0.42
3:DP1:155:TYR:O	3:DP1:159:ILE:HG12	2.18	0.42
1:AP1:194:GLU:O	1:AP1:198:VAL:HG22	2.19	0.42
1:AP1:578:VAL:HG22	1:AP1:626:LEU:HB3	2.00	0.42
1:BP1:147:THR:HA	1:BP1:179:THR:HA	2.01	0.42
2:CP1:467:ARG:HD3	2:CP1:525:PHE:CE1	2.55	0.42
3:DP1:175:LEU:HD23	3:DP1:175:LEU:HA	1.88	0.42
1:BP1:194:GLU:O	1:BP1:198:VAL:HG22	2.20	0.42
1:BP1:405:ARG:HG3	1:BP1:406:LYS:HD3	2.01	0.42
1:BP1:580:ILE:CG2	1:BP1:628:ILE:HB	2.49	0.42
1:AP1:166:THR:HB	1:BP1:12:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:293:PRO:HA	1:AP1:296:ILE:HD12	2.01	0.42
1:BP1:367:ASP:OD1	1:BP1:367:ASP:N	2.51	0.42
1:BP1:583:ARG:CZ	1:BP1:592:VAL:HG11	2.50	0.42
1:BP1:593:THR:HG21	1:BP1:599:THR:HA	2.01	0.42
2:CP1:599:PHE:N	2:CP1:600:PRO:HD2	2.35	0.42
1:AP1:430:TYR:CE2	1:AP1:456:ARG:HB2	2.54	0.42
1:AP1:503:VAL:HG13	1:AP1:508:PHE:HB2	2.02	0.42
1:BP1:472:TYR:CE2	1:BP1:483:ILE:HG23	2.54	0.42
1:BP1:638:LEU:HA	1:BP1:641:LYS:HD3	2.02	0.42
2:CP1:412:MET:HB3	3:DP1:222:LEU:HD12	1.99	0.42
3:DP1:97:SER:O	3:DP1:101:LYS:HG3	2.19	0.42
1:BP1:86:LEU:HB3	1:BP1:181:VAL:HG22	2.02	0.42
1:AP1:146:ILE:HB	1:AP1:180:LYS:HB3	2.01	0.42
1:AP1:397:GLN:NE2	3:DP1:7:TRP:O	2.36	0.42
1:AP1:574:LYS:HB2	1:AP1:574:LYS:HE2	1.86	0.42
3:DP1:268:LYS:HA	3:DP1:268:LYS:HD3	1.82	0.42
1:AP1:348:LYS:HE3	1:AP1:348:LYS:HB3	1.83	0.42
1:BP1:55:ARG:NE	1:BP1:211:TYR:OH	2.45	0.42
1:BP1:98:LEU:HD21	1:BP1:157:TRP:HB2	2.02	0.42
2:CP1:514:PRO:HG2	2:CP1:591:LYS:HE2	2.02	0.42
1:BP1:438:LYS:HB3	1:BP1:521:CYS:HB2	2.00	0.41
1:BP1:601:ASN:OD1	1:BP1:604:ARG:NH2	2.46	0.41
2:CP1:411:TYR:O	2:CP1:413:THR:N	2.53	0.41
2:CP1:546:LEU:HD12	2:CP1:546:LEU:HA	1.87	0.41
3:DP1:53:GLY:O	3:DP1:56:GLU:HG2	2.19	0.41
3:DP1:179:VAL:HG11	3:DP1:235:ARG:NH2	2.35	0.41
1:AP1:321:PHE:CE2	1:AP1:411:LYS:HG3	2.55	0.41
1:BP1:111:LYS:O	1:BP1:115:GLU:HG2	2.20	0.41
2:CP1:579:LYS:HB3	2:CP1:583:ARG:HH22	1.85	0.41
1:AP1:288:ILE:HD13	1:AP1:288:ILE:HA	1.89	0.41
1:AP1:690:ILE:HD13	1:BP1:637:THR:HG21	2.02	0.41
1:BP1:607:LYS:NZ	1:BP1:617:MET:HG2	2.35	0.41
2:CP1:579:LYS:HD3	2:CP1:579:LYS:HA	1.71	0.41
3:DP1:22:ASN:OD1	3:DP1:22:ASN:C	2.59	0.41
3:DP1:235:ARG:HB2	3:DP1:236:GLN:HE21	1.85	0.41
1:AP1:279:GLN:NE2	1:AP1:281:GLU:HB2	2.36	0.41
1:AP1:344:PHE:CE2	1:BP1:611:LEU:HD12	2.55	0.41
1:BP1:114:MET:SD	1:BP1:125:MET:HB2	2.60	0.41
2:CP1:451:GLN:HA	2:CP1:454:GLN:OE1	2.19	0.41
2:CP1:605:SER:O	2:CP1:608:LEU:HG	2.19	0.41
3:DP1:134:GLU:OE1	3:DP1:134:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:39:PHE:CZ	1:AP1:139:VAL:HG21	2.56	0.41
1:AP1:217:LEU:O	1:AP1:277:ILE:N	2.34	0.41
1:AP1:684:ILE:HD12	1:AP1:684:ILE:HA	1.76	0.41
1:BP1:562:ASN:HA	1:BP1:565:LYS:HE3	2.03	0.41
2:CP1:441:GLN:NE2	2:CP1:444:GLN:HE21	2.19	0.41
3:DP1:38:GLU:O	3:DP1:42:GLN:HG2	2.20	0.41
1:AP1:485:TYR:CZ	1:AP1:535:SER:HB2	2.55	0.41
1:AP1:663:LEU:HG	1:AP1:668:PHE:HB2	2.02	0.41
2:CP1:514:PRO:HB3	2:CP1:561:VAL:O	2.20	0.41
3:DP1:83:ARG:HH21	3:DP1:84:LEU:HB2	1.85	0.41
1:AP1:46:ASN:ND2	4:AP1:801:ATP:O2A	2.52	0.41
1:AP1:93:MET:HB2	1:AP1:97:ASP:HB2	2.03	0.41
1:AP1:505:LYS:HE3	1:AP1:505:LYS:HB3	1.93	0.41
1:BP1:54:ILE:HD13	1:BP1:91:ILE:HG13	2.02	0.41
2:CP1:476:LEU:HD23	2:CP1:476:LEU:HA	1.88	0.41
2:CP1:580:ALA:O	2:CP1:584:LEU:HG	2.21	0.41
3:DP1:229:ASP:OD2	3:DP1:231:ARG:NH2	2.53	0.41
1:AP1:215:LEU:HB2	1:AP1:282:LEU:HD21	2.03	0.40
1:AP1:273:LYS:HE3	1:AP1:273:LYS:HB3	1.84	0.40
2:CP1:470:LYS:HG2	2:CP1:473:ASN:OD1	2.22	0.40
2:CP1:590:LYS:HZ1	2:CP1:595:GLU:HB2	1.86	0.40
3:DP1:45:LYS:HE3	3:DP1:45:LYS:HB3	1.91	0.40
3:DP1:88:ALA:O	3:DP1:92:ARG:HG2	2.20	0.40
3:DP1:166:ARG:HA	3:DP1:166:ARG:HD3	1.90	0.40
1:BP1:148:LYS:NZ	1:BP1:149:HIS:O	2.33	0.40
1:BP1:671:GLU:OE1	1:BP1:671:GLU:N	2.41	0.40
1:AP1:202:VAL:HG21	1:AP1:282:LEU:HD12	2.03	0.40
1:AP1:215:LEU:HD23	1:AP1:215:LEU:HA	1.90	0.40
2:CP1:453:ALA:HB2	2:CP1:534:TYR:OH	2.22	0.40
3:DP1:145:GLU:O	3:DP1:149:LYS:HG2	2.21	0.40
1:AP1:374:LEU:HD23	1:AP1:374:LEU:HA	1.83	0.40
3:DP1:60:LYS:HA	3:DP1:63:GLU:OE1	2.20	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	AP1	632/732 (86%)	606 (96%)	26 (4%)	0	100	100
1	BP1	634/732 (87%)	609 (96%)	25 (4%)	0	100	100
2	CP1	189/659 (29%)	168 (89%)	18 (10%)	3 (2%)	9	43
3	DP1	270/394 (68%)	258 (96%)	12 (4%)	0	100	100
All	All	1725/2517 (68%)	1641 (95%)	81 (5%)	3 (0%)	50	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CP1	429	LEU
2	CP1	411	TYR
2	CP1	412	MET

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	AP1	575/659 (87%)	563 (98%)	12 (2%)	53	73
1	BP1	577/659 (88%)	570 (99%)	7 (1%)	71	84
2	CP1	174/588 (30%)	164 (94%)	10 (6%)	20	52
3	DP1	249/356 (70%)	232 (93%)	17 (7%)	16	47
All	All	1575/2262 (70%)	1529 (97%)	46 (3%)	45	66

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AP1	135	SER
1	AP1	341	PHE
1	AP1	398	SER

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Mol	Chain	Res	Type
1	AP1	417	SER
1	AP1	518	ASP
1	AP1	521	CYS
1	AP1	590	CYS
1	AP1	619	TYR
1	AP1	669	SER
1	AP1	678	ASN
1	AP1	681	TYR
1	AP1	682	ARG
1	BP1	312	TRP
1	BP1	338	ARG
1	BP1	464	ASP
1	BP1	508	PHE
1	BP1	521	CYS
1	BP1	542	GLU
1	BP1	596	TYR
2	CP1	447	ASP
2	CP1	458	TYR
2	CP1	459	LEU
2	CP1	466	HIS
2	CP1	471	SER
2	CP1	475	PHE
2	CP1	552	ASN
2	CP1	574	TYR
2	CP1	587	ASP
2	CP1	600	PRO
3	DP1	43	PHE
3	DP1	45	LYS
3	DP1	59	ARG
3	DP1	64	CYS
3	DP1	103	GLU
3	DP1	106	ARG
3	DP1	124	PHE
3	DP1	140	SER
3	DP1	162	PHE
3	DP1	174	TYR
3	DP1	193	TRP
3	DP1	216	MET
3	DP1	229	ASP
3	DP1	234	PHE
3	DP1	248	TYR
3	DP1	252	PHE

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Mol	Chain	Res	Type
3	DP1	259	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SEP	DP1	13	3	8,9,10	1.51	1 (12%)	8,12,14	1.77	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	DP1	13	3	-	4/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DP1	13	SEP	P-O1P	3.31	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DP1	13	SEP	P-OG-CB	-3.50	108.66	118.30
3	DP1	13	SEP	OG-CB-CA	3.02	111.09	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	DP1	13	SEP	CB-OG-P-O2P
3	DP1	13	SEP	CB-OG-P-O1P
3	DP1	13	SEP	CB-OG-P-O3P
3	DP1	13	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DP1	13	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	ATP	BP1	801	-	26,33,33	0.63	0	31,52,52	0.75	2 (6%)
4	ATP	AP1	801	-	26,33,33	0.64	0	31,52,52	0.78	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	BP1	801	-	-	11/18/38/38	0/3/3/3
4	ATP	AP1	801	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AP1	801	ATP	C5-C6-N6	2.31	123.86	120.35
4	BP1	801	ATP	C5-C6-N6	2.30	123.85	120.35
4	AP1	801	ATP	PB-O3B-PG	2.06	139.91	132.83
4	BP1	801	ATP	PB-O3B-PG	2.05	139.87	132.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AP1	801	ATP	C5'-O5'-PA-O1A
4	AP1	801	ATP	C5'-O5'-PA-O3A
4	BP1	801	ATP	C5'-O5'-PA-O2A
4	BP1	801	ATP	C5'-O5'-PA-O3A
4	BP1	801	ATP	O4'-C4'-C5'-O5'
4	BP1	801	ATP	C3'-C4'-C5'-O5'
4	BP1	801	ATP	PB-O3B-PG-O1G
4	AP1	801	ATP	PB-O3A-PA-O2A
4	AP1	801	ATP	C5'-O5'-PA-O2A
4	BP1	801	ATP	C5'-O5'-PA-O1A
4	BP1	801	ATP	PA-O3A-PB-O2B
4	BP1	801	ATP	PG-O3B-PB-O2B
4	BP1	801	ATP	PA-O3A-PB-O1B
4	AP1	801	ATP	O4'-C4'-C5'-O5'
4	AP1	801	ATP	PB-O3A-PA-O1A
4	BP1	801	ATP	PB-O3A-PA-O1A
4	BP1	801	ATP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

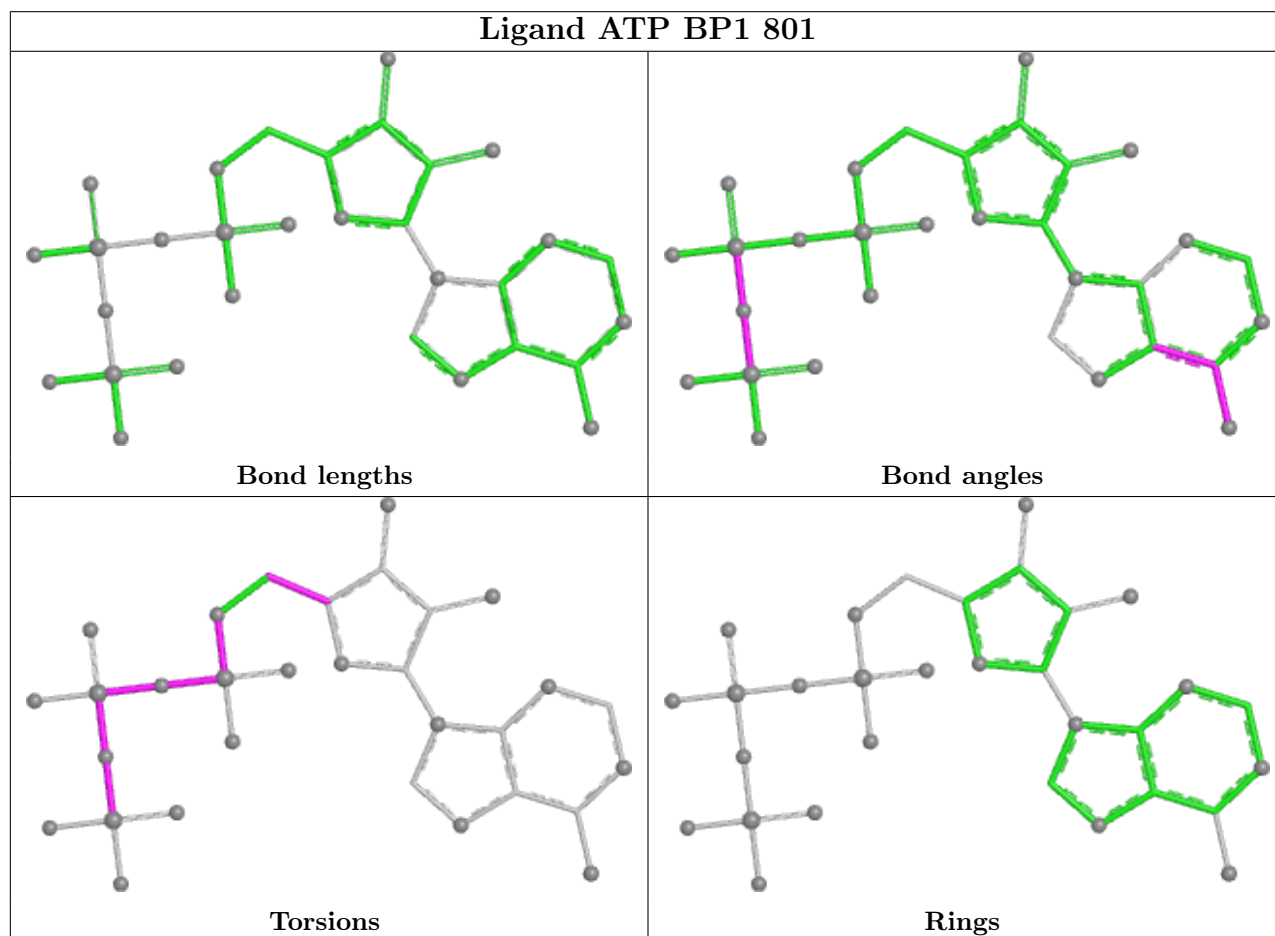
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BP1	801	ATP	1	0

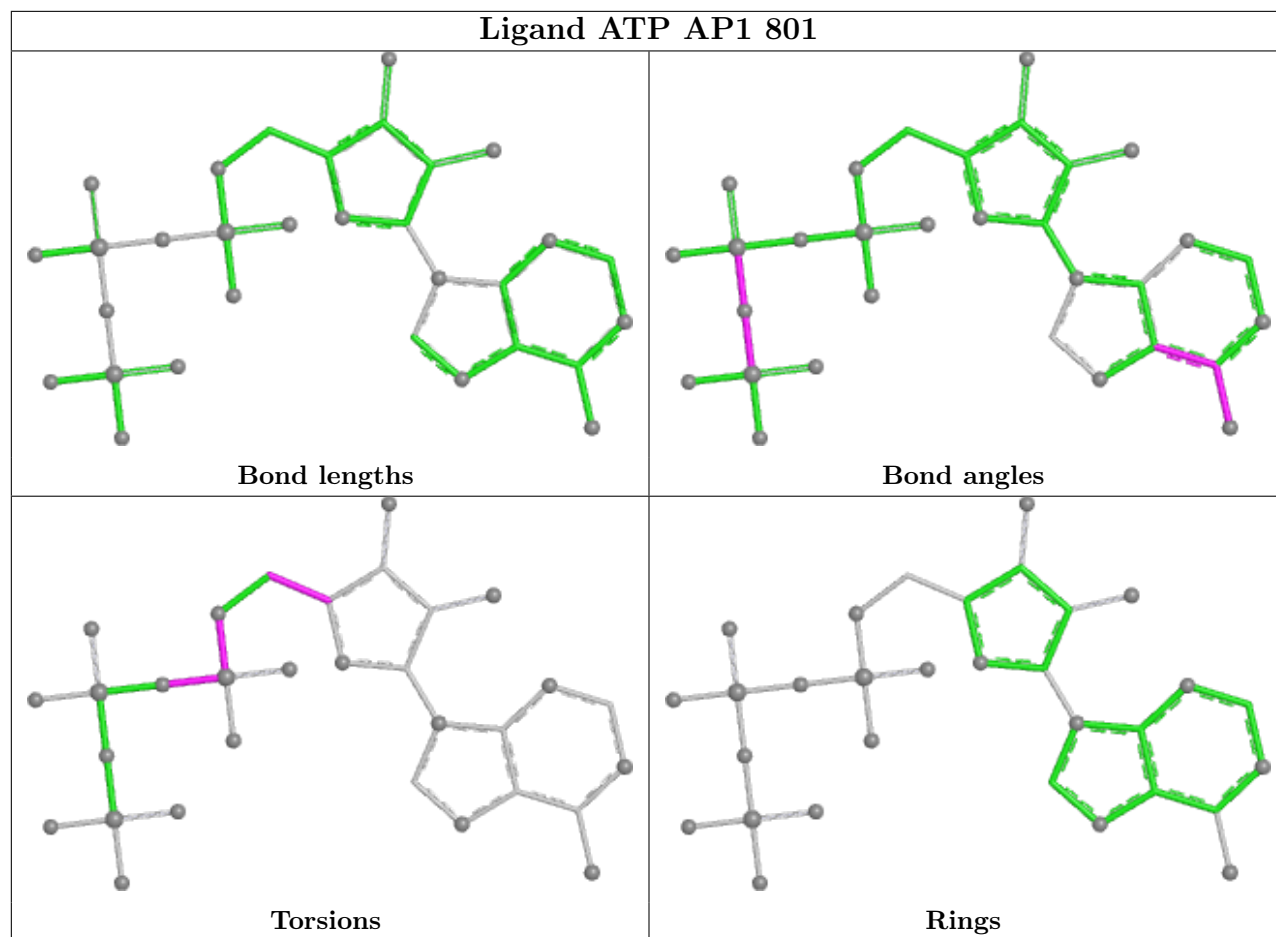
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AP1	801	ATP	2	0

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.

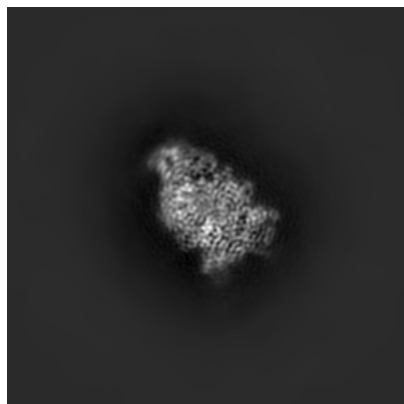
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14472. These allow visual inspection of the internal detail of the map and identification of artifacts.

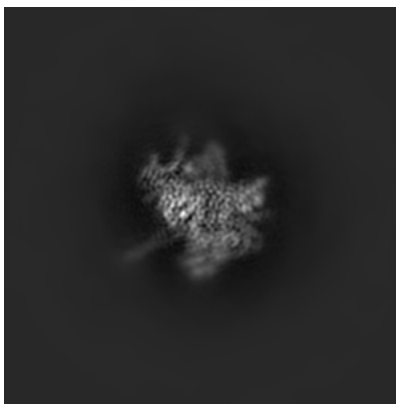
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

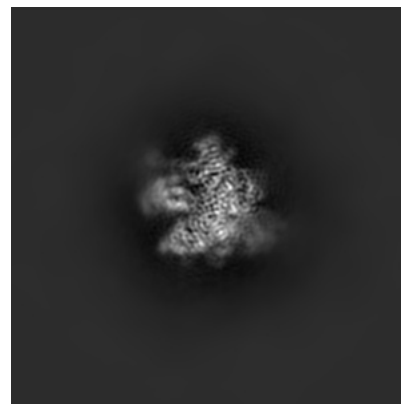
6.1.1 Primary map



X

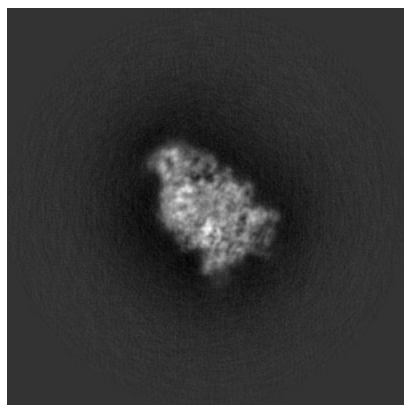


Y

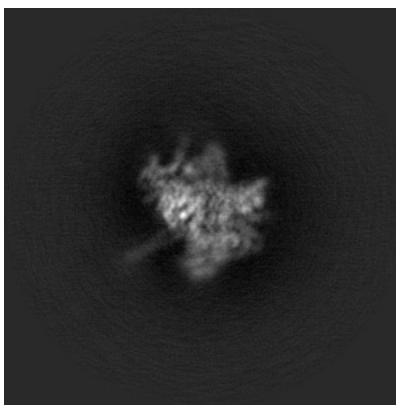


Z

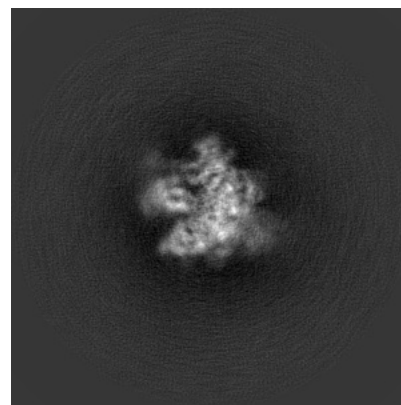
6.1.2 Raw map



X



Y

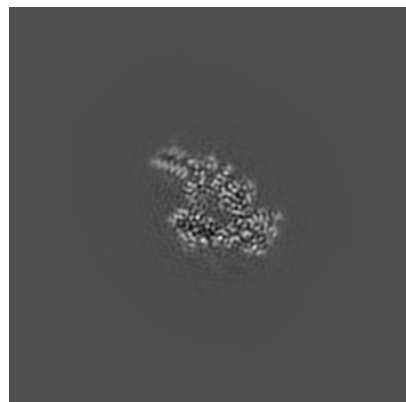


Z

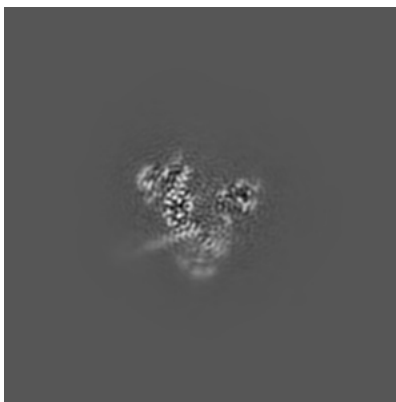
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

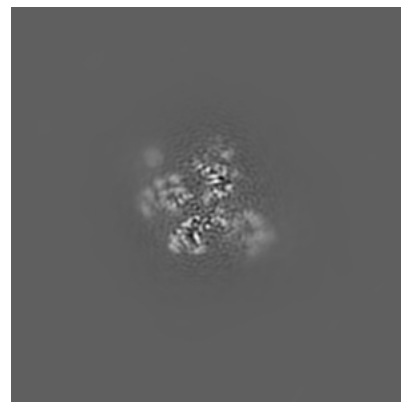
6.2.1 Primary map



X Index: 192

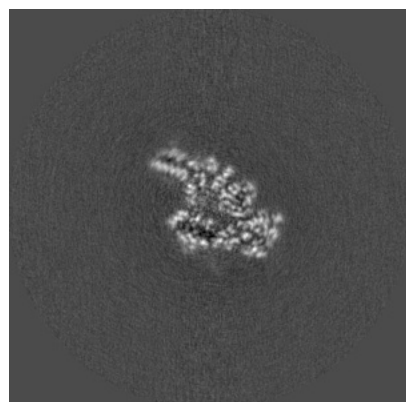


Y Index: 192

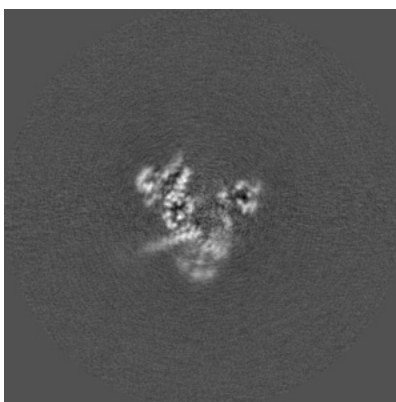


Z Index: 192

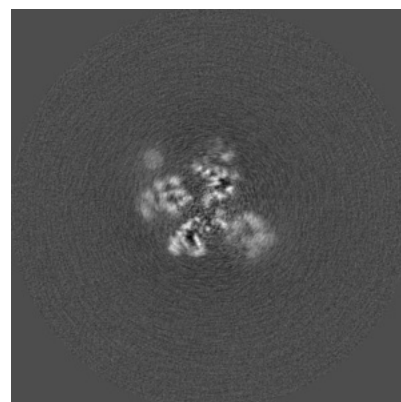
6.2.2 Raw map



X Index: 192



Y Index: 192

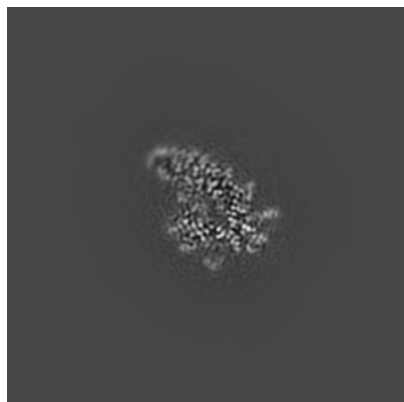


Z Index: 192

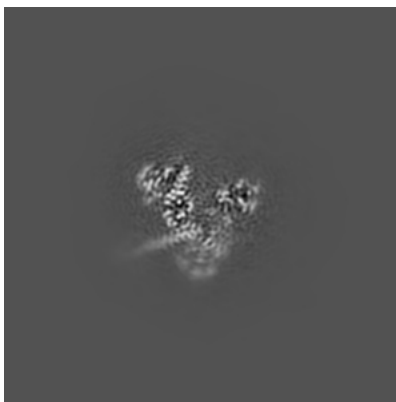
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

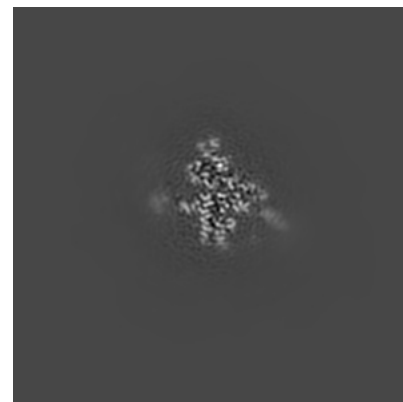
6.3.1 Primary map



X Index: 198

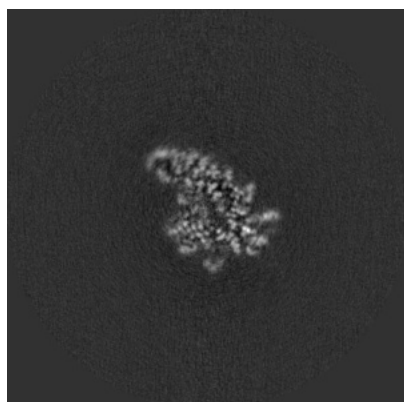


Y Index: 193

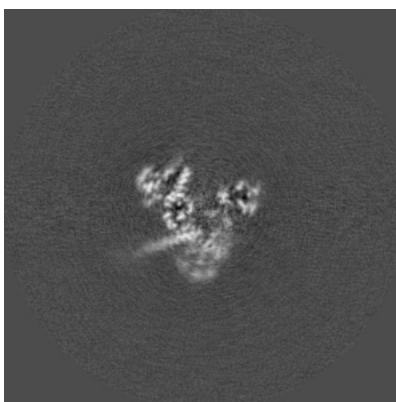


Z Index: 171

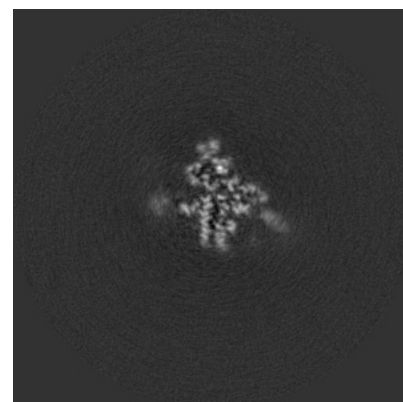
6.3.2 Raw map



X Index: 198



Y Index: 193

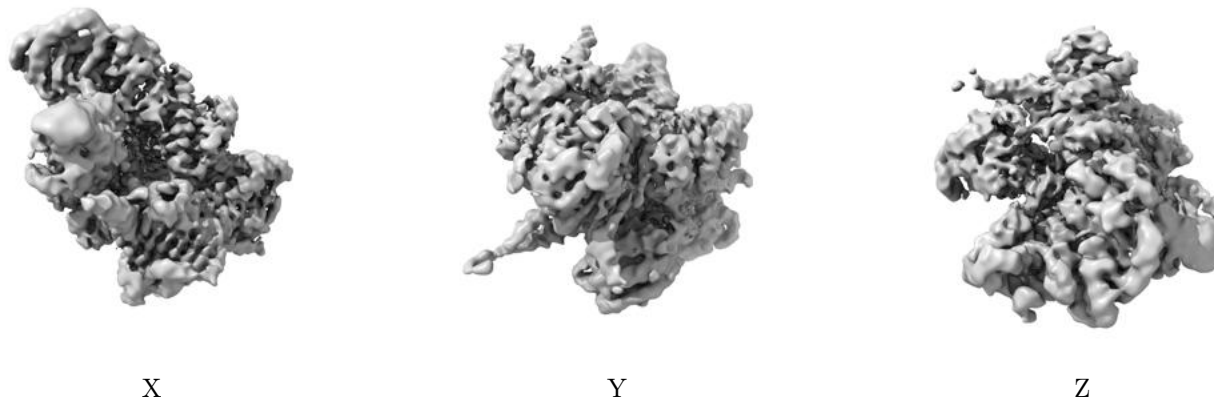


Z Index: 171

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

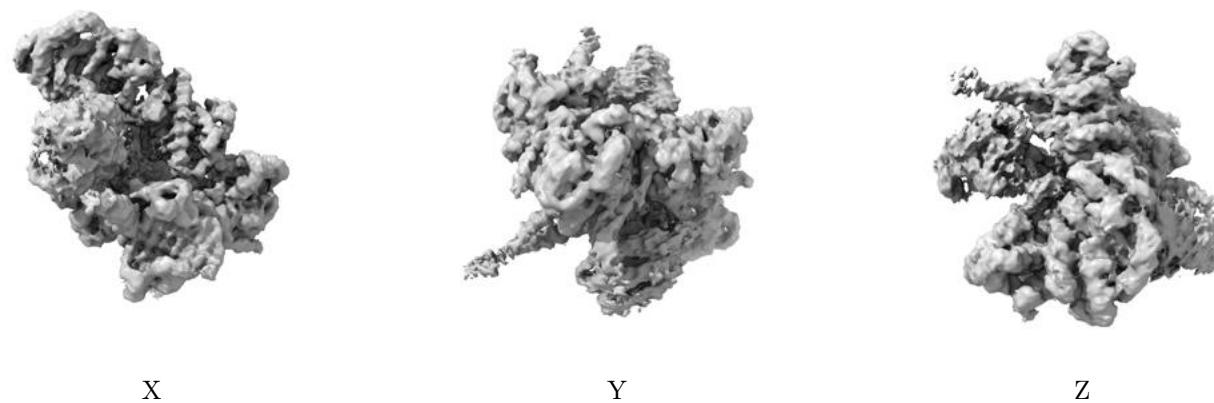
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

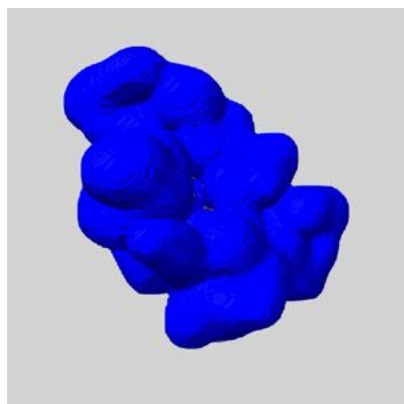
6.5 Mask visualisation [i](#)

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

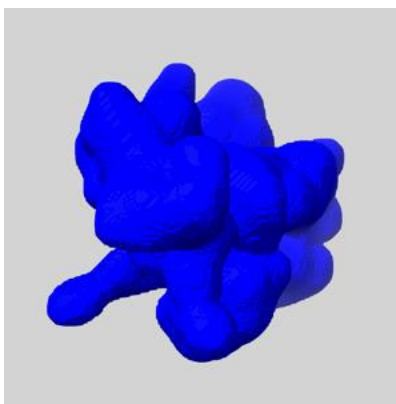
A mask typically either:

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

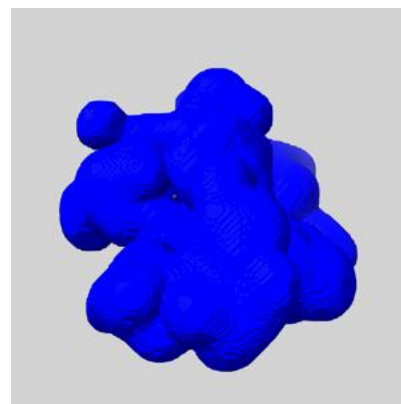
6.5.1 emd_14472_msk_1.map [i](#)



X



Y

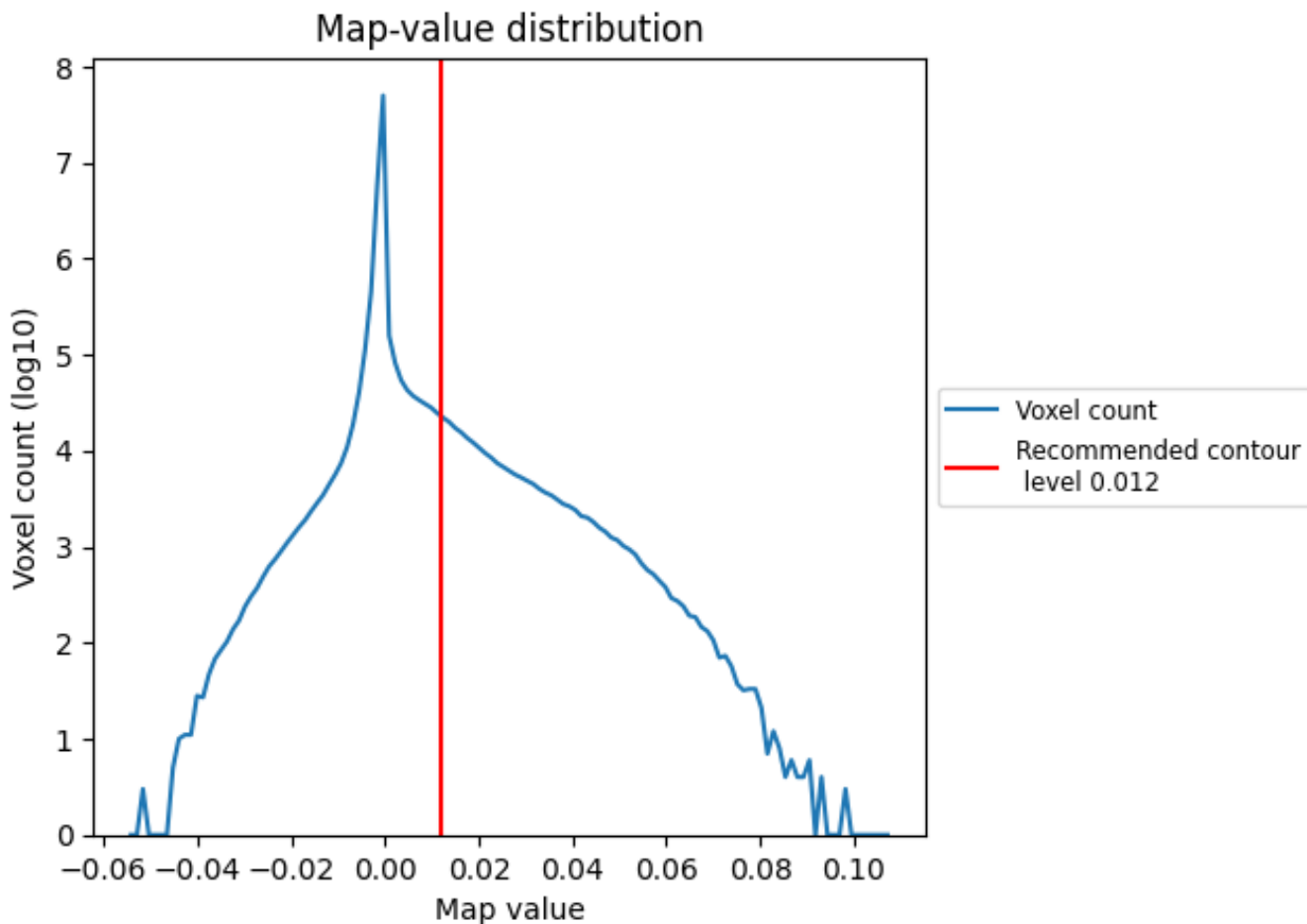


Z

7 Map analysis [i](#)

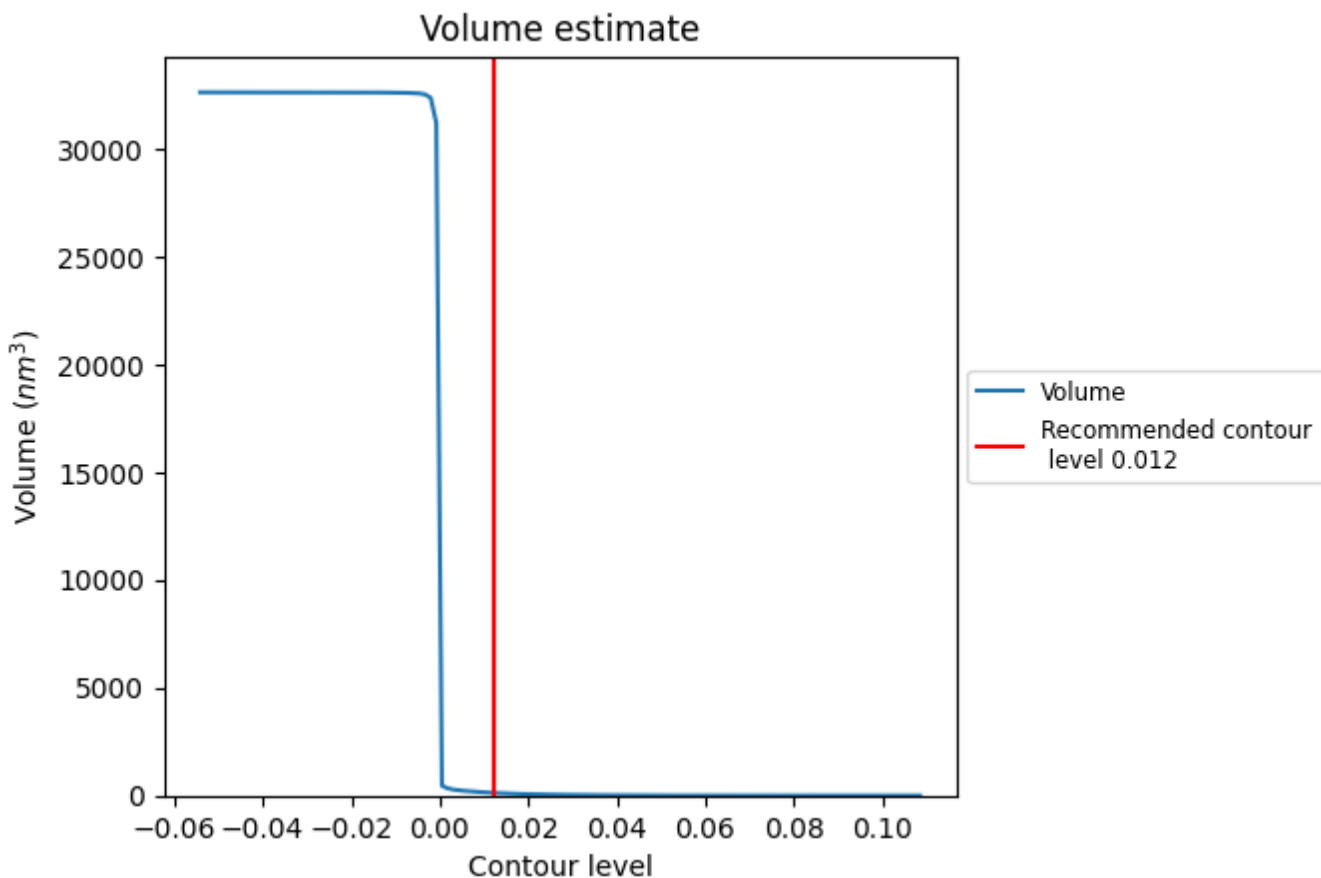
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

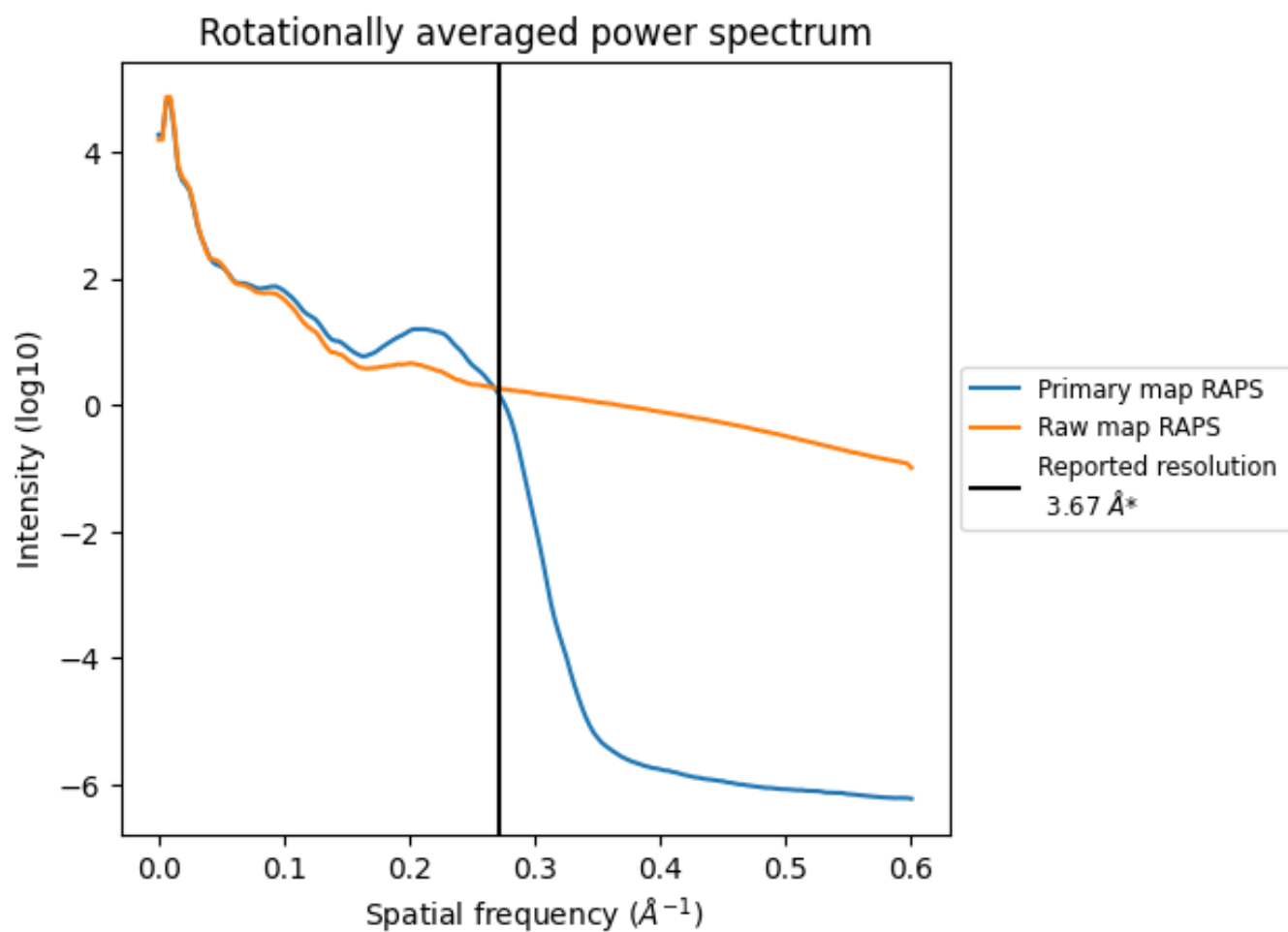
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 126 nm³; this corresponds to an approximate mass of 114 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

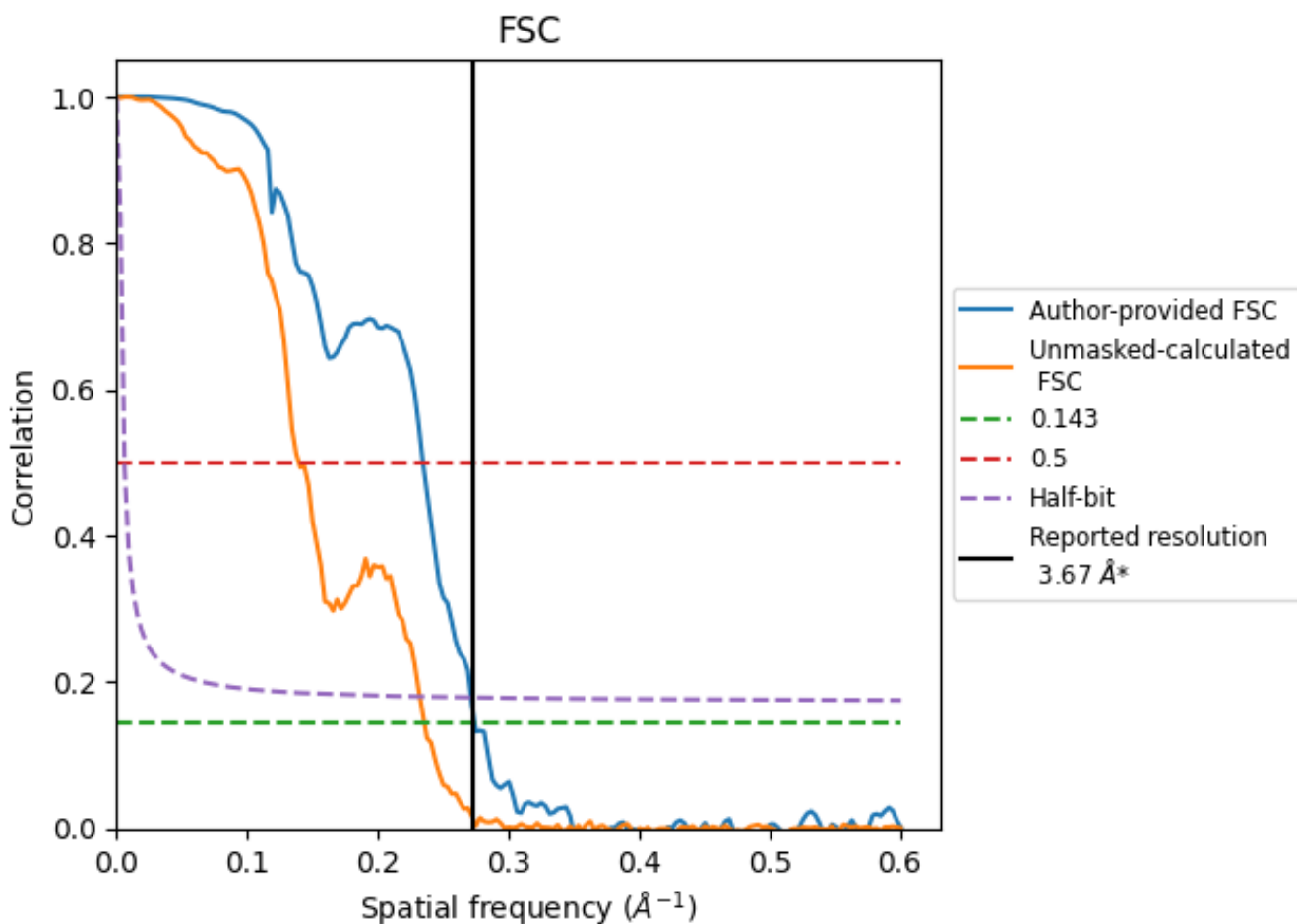


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 Å⁻¹

8.2 Resolution estimates [i](#)

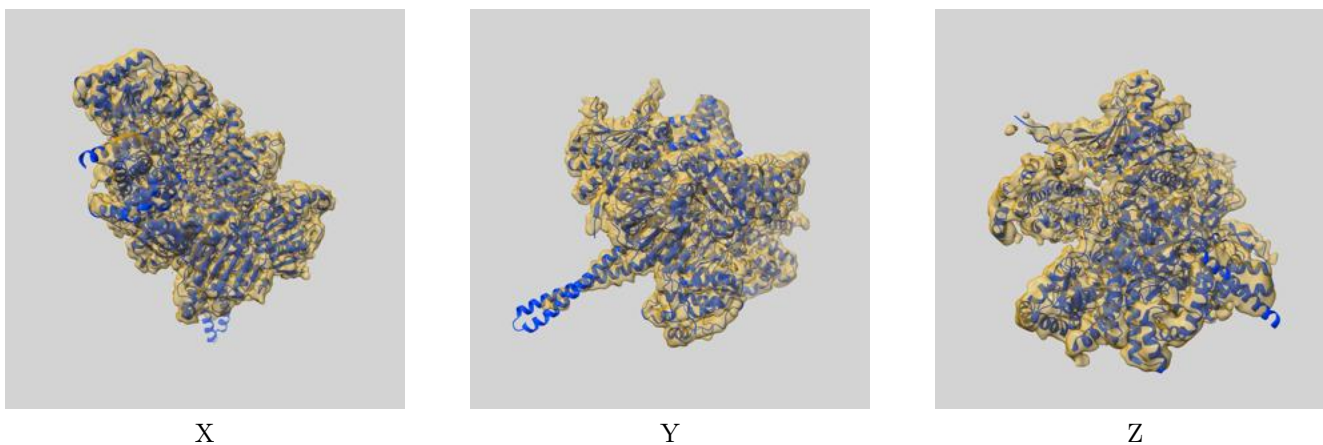
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.64	4.26	3.68
Unmasked-calculated*	4.24	7.16	4.30

*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 4.24 differs from the reported value 3.67 by more than 10 %

9 Map-model fit [i](#)

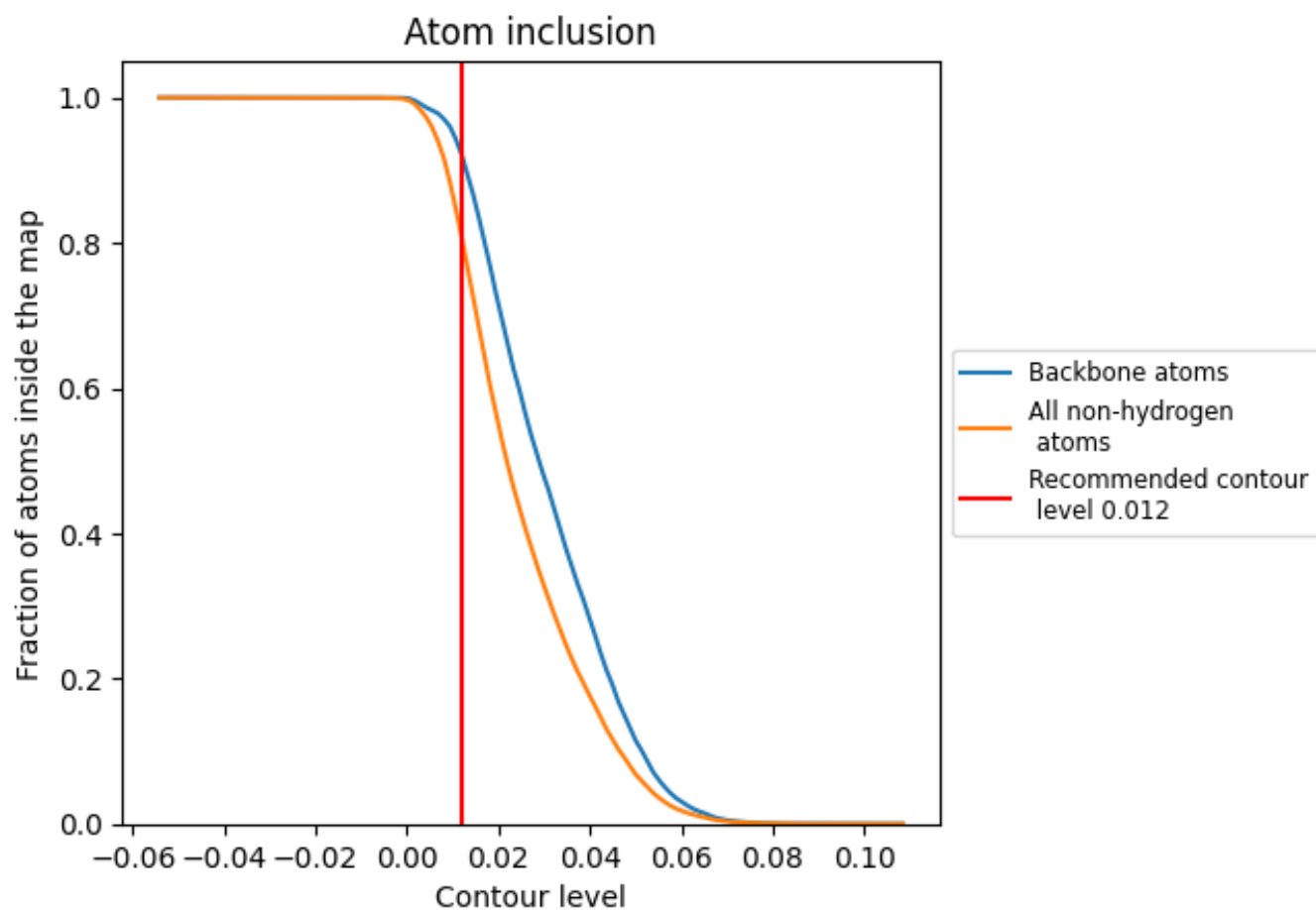
This section contains information regarding the fit between EMDB map EMD-14472 and PDB model 7Z37. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.012 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 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.