



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 07:58 pm GMT

PDB ID : 6TAX  
EMDB ID : EMD-10429  
Title : Mouse RNF213 wild type protein  
Authors : Ahel, J.; Meinhart, A.; Haselbach, D.; Clausen, T.  
Deposited on : 2019-10-31  
Resolution : 3.20 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](mailto: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>.

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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 : 1.8.4, 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)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

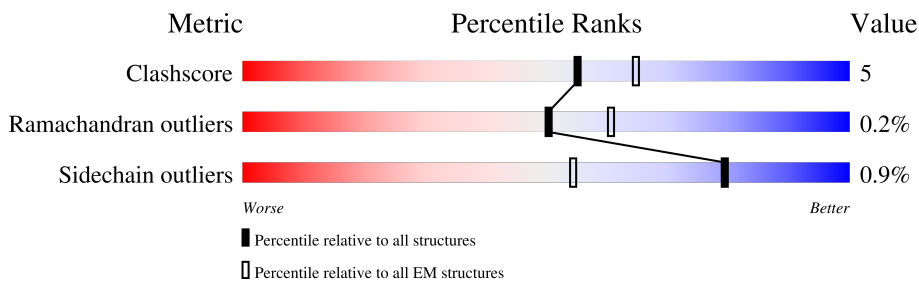
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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  $\geq 3$ , 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	4638	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35235 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 RNF213,E3 ubiquitin-protein ligase RNF213,E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4416	35201	22426	6055	6513	207	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	?	-	ASN	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

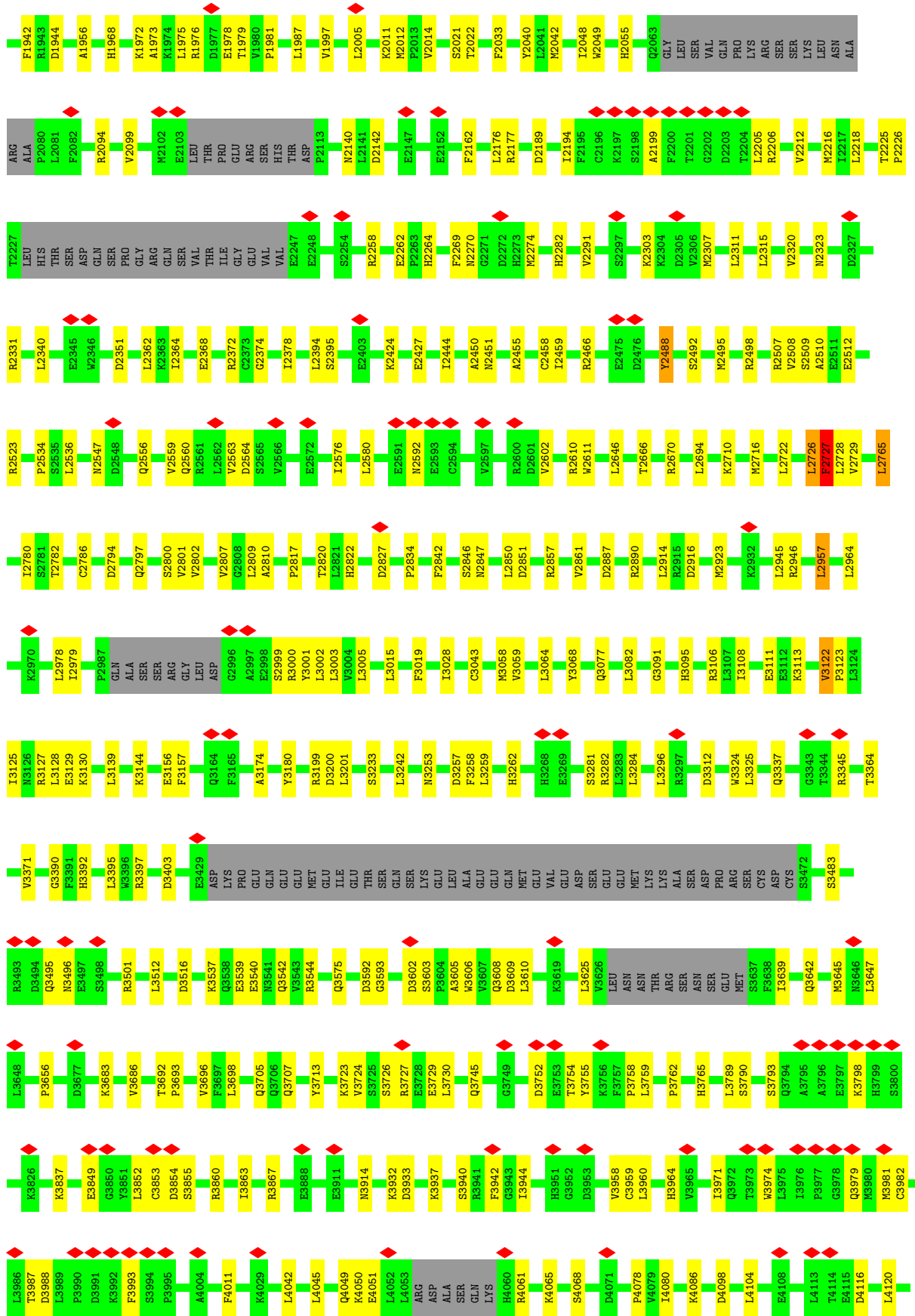
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

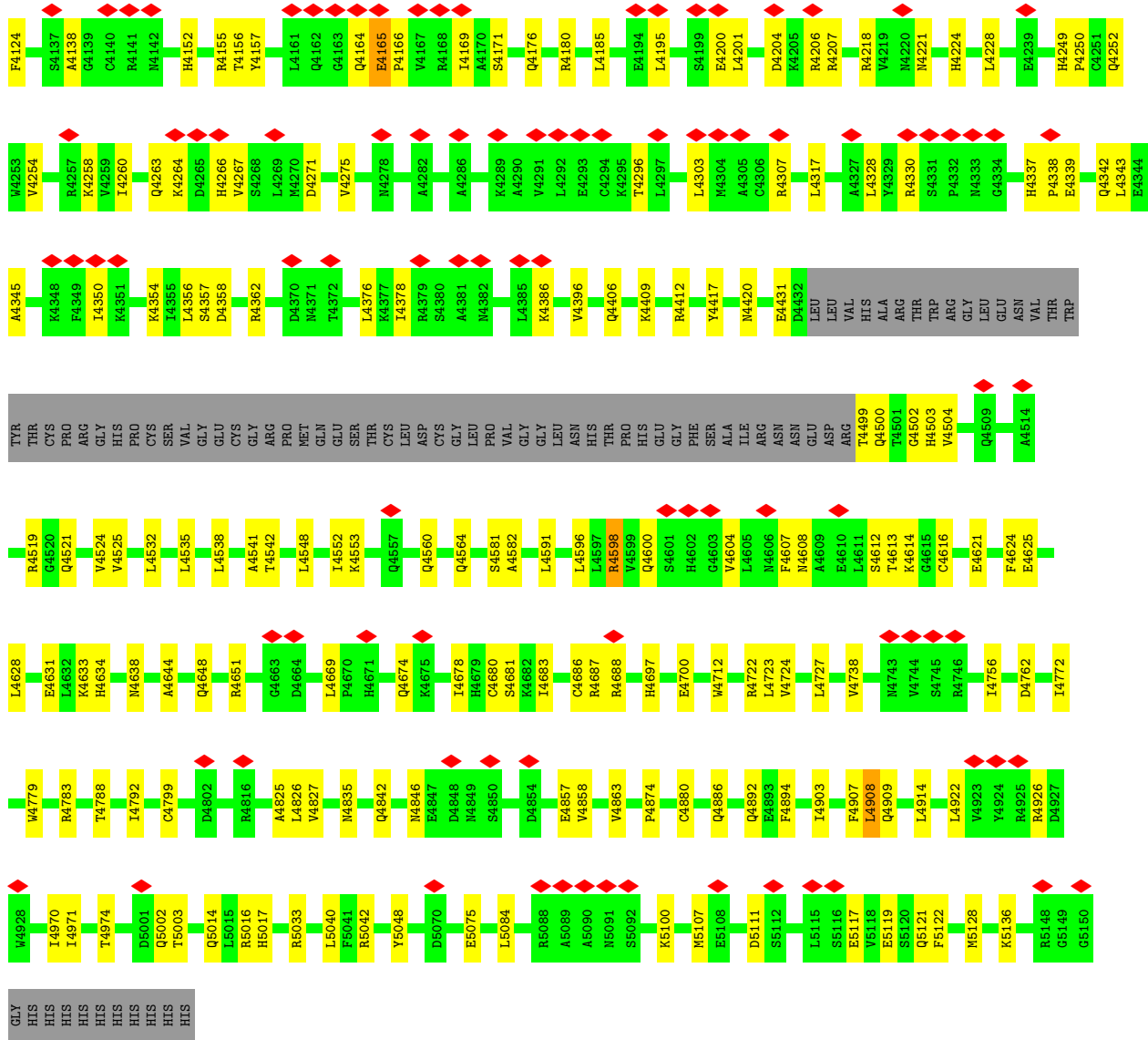
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	374683	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size ( $\text{\AA}$ )	366.08, 366.08, 366.08	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	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: ATP, ZN, MG

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	0.44	0/35588	0.63	11/48145 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1975	LEU	CA-CB-CG	8.76	135.44	115.30
1	A	3602	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	894	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	3933	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	3395	LEU	CA-CB-CG	6.69	130.68	115.30
1	A	878	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	4596	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	2765	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	3512	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	2727	PHE	CB-CG-CD1	5.20	124.44	120.80
1	A	2726	LEU	CB-CG-CD2	-5.16	102.23	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	GLU	Peptide
1	A	1170	GLU	Peptide
1	A	1373	ILE	Peptide
1	A	1494	LEU	Peptide
1	A	1845	THR	Peptide
1	A	2225	THR	Peptide
1	A	2262	GLU	Peptide
1	A	3122	VAL	Peptide
1	A	4165	GLU	Peptide
1	A	659	GLU	Peptide
1	A	688	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35201	0	35074	373	0
2	A	31	0	12	0	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
All	All	35235	0	35086	373	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 5.

All (373) 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:611:LYS:O	1:A:614:LEU:HB2	1.88	0.73
1:A:3122:VAL:HG22	1:A:3125:ILE:HD12	1.74	0.70
1:A:2847:ASN:HD22	1:A:3123:PRO:HG3	1.58	0.69
1:A:4200:GLU:HA	1:A:4206:ARG:HH21	1.60	0.67
1:A:3713:TYR:HH	1:A:3765:HIS:HE2	1.40	0.66
1:A:5014:GLN:H	1:A:5017:HIS:HD2	1.44	0.65
1:A:4907:PHE:HB2	1:A:4908:LEU:HD23	1.79	0.65
1:A:2005:LEU:HB3	1:A:2011:LYS:HZ1	1.63	0.64
1:A:3501:ARG:HH12	1:A:3593:GLY:HA2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:VAL:HG11	1:A:1378:GLN:HG3	1.81	0.63
1:A:4783:ARG:HB2	1:A:4799:CYS:HB2	1.80	0.62
1:A:4221:ASN:O	1:A:4224:HIS:ND1	2.33	0.62
1:A:788:GLU:HG3	1:A:840:LEU:HD11	1.82	0.62
1:A:2226:PRO:HA	1:A:2258:ARG:HH12	1.65	0.62
1:A:2307:MET:HG3	1:A:2311:LEU:HD23	1.82	0.61
1:A:3091:GLY:HA2	1:A:3095:HIS:O	2.00	0.61
1:A:4275:VAL:HG11	1:A:4591:LEU:HA	1.82	0.61
1:A:1495:SER:HG	1:A:1498:SER:H	1.49	0.61
1:A:2507:ARG:NH2	1:A:2809:LEU:O	2.34	0.60
1:A:1329:LEU:HD21	1:A:1442:MET:HG3	1.83	0.60
1:A:2374:GLY:O	1:A:2466:ARG:NH2	2.35	0.60
1:A:1829:PRO:HD3	1:A:1861:GLN:HB3	1.84	0.59
1:A:5040:LEU:HD21	1:A:5136:LYS:HE2	1.85	0.59
1:A:802:GLN:HB3	1:A:804:ARG:H	1.66	0.59
1:A:2523:ARG:HG3	1:A:2851:ASP:HB3	1.84	0.59
1:A:4078:PRO:HD2	1:A:4886:GLN:HE21	1.67	0.59
1:A:4328:LEU:HD13	1:A:4337:HIS:HB3	1.85	0.59
1:A:4521:GLN:NE2	1:A:4621:GLU:OE1	2.32	0.59
1:A:725:ARG:NH2	1:A:756:ASP:OD2	2.36	0.58
1:A:3645:MET:HB2	1:A:3647:LEU:HD23	1.85	0.58
1:A:4086:LYS:NZ	1:A:4880:CYS:SG	2.76	0.58
1:A:4842:GLN:HA	1:A:4846:ASN:HB2	1.84	0.58
1:A:3068:TYR:OH	1:A:3127:ARG:NH2	2.36	0.58
1:A:3258:PHE:O	1:A:3262:HIS:HB2	2.04	0.58
1:A:987:LEU:HA	1:A:990:LEU:HD13	1.85	0.58
1:A:4378:ILE:HG12	1:A:4564:GLN:HE21	1.67	0.58
1:A:2042:MET:HG3	1:A:2048:ILE:HG12	1.85	0.58
1:A:4644:ALA:O	1:A:4648:GLN:NE2	2.37	0.57
1:A:895:SER:O	1:A:902:ARG:NH1	2.37	0.57
1:A:4525:VAL:HG11	1:A:4625:GLU:HG3	1.85	0.57
1:A:3015:LEU:HD23	1:A:3019:PHE:HD2	1.70	0.57
1:A:626:GLY:HA2	1:A:631:LEU:HD23	1.86	0.57
1:A:1028:LEU:HD21	1:A:1062:ALA:HB1	1.87	0.57
1:A:5117:GLU:O	1:A:5121:GLN:HB2	2.05	0.57
1:A:687:GLN:NE2	1:A:690:ASP:OD1	2.30	0.57
1:A:4330:ARG:HH12	1:A:4376:LEU:HD23	1.70	0.57
1:A:2887:ASP:OD1	1:A:2890:ARG:NH1	2.38	0.57
1:A:3605:ALA:O	1:A:3609:ASP:HB2	2.05	0.57
1:A:3139:LEU:O	1:A:3144:LYS:NZ	2.37	0.56
1:A:4396:VAL:HG11	1:A:4535:LEU:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3000:ARG:O	1:A:3077:GLN:NE2	2.39	0.56
1:A:3539:GLU:HA	1:A:3542:GLN:HG2	1.86	0.56
1:A:4065:LYS:NZ	1:A:4068:SER:O	2.38	0.56
1:A:887:SER:O	1:A:890:LYS:NZ	2.33	0.56
1:A:1434:GLY:HA3	1:A:1468:LEU:HD11	1.88	0.56
1:A:2827:ASP:HB2	1:A:2834:PRO:HB3	1.88	0.56
1:A:3603:SER:HB2	1:A:3608:GLN:HE22	1.69	0.56
1:A:2395:SER:HB2	1:A:2444:ILE:HD11	1.88	0.56
1:A:4185:LEU:HD22	1:A:4228:LEU:HD12	1.87	0.56
1:A:4252:GLN:HE21	1:A:4260:ILE:HG21	1.71	0.56
1:A:2807:VAL:HG23	1:A:2846:SER:HB2	1.89	0.55
1:A:3693:PRO:HA	1:A:3696:VAL:HG22	1.88	0.55
1:A:2040:TYR:HA	1:A:2049:TRP:O	2.06	0.55
1:A:1156:GLU:HG2	1:A:1157:ILE:HG12	1.89	0.55
1:A:1781:ARG:NH2	1:A:1817:PRO:O	2.37	0.55
1:A:1931:VAL:HG13	1:A:1935:LEU:HD23	1.89	0.55
1:A:2946:ARG:NH2	1:A:2999:SER:OG	2.40	0.55
1:A:3959:CYS:HA	1:A:3964:HIS:O	2.07	0.55
1:A:3259:LEU:HD13	1:A:3296:LEU:HD11	1.89	0.54
1:A:704:ARG:NH2	1:A:736:SER:O	2.37	0.54
1:A:1556:MET:HG3	1:A:3043:CYS:HB3	1.90	0.54
1:A:1377:ARG:NH2	1:A:1463:ASP:OD1	2.40	0.54
1:A:956:ARG:NH1	1:A:957:ASP:OD2	2.41	0.54
1:A:2282:HIS:ND1	1:A:2323:ASN:OD1	2.37	0.54
1:A:2611:TRP:HB2	1:A:2722:LEU:HD21	1.89	0.54
1:A:3960:LEU:HB2	1:A:3964:HIS:HB2	1.89	0.54
1:A:2822:HIS:O	1:A:2857:ARG:NH1	2.40	0.54
1:A:3974:TRP:O	1:A:3979:GLN:NE2	2.40	0.54
1:A:4164:GLN:HG3	1:A:4169:ILE:HG22	1.89	0.54
1:A:4338:PRO:O	1:A:4343:LEU:N	2.41	0.54
1:A:4204:ASP:OD1	1:A:4207:ARG:NH2	2.41	0.54
1:A:1595:ASN:HD21	1:A:1645:PHE:HE2	1.56	0.53
1:A:3284:LEU:HB2	1:A:3337:GLN:HE22	1.73	0.53
1:A:836:GLU:OE1	1:A:914:ARG:NH1	2.41	0.53
1:A:2556:GLN:O	1:A:2560:GLN:NE2	2.42	0.53
1:A:3981:MET:HA	1:A:3988:ASP:HA	1.91	0.53
1:A:695:LEU:HD22	1:A:698:ILE:HD12	1.89	0.53
1:A:4263:GLN:HE21	1:A:4267:VAL:HG11	1.74	0.53
1:A:1216:THR:HG21	1:A:1245:CYS:HB2	1.90	0.53
1:A:1420:ILE:HG23	1:A:3082:LEU:HD22	1.90	0.53
1:A:3058:MET:HG2	1:A:3106:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4634:HIS:O	1:A:4638:ASN:ND2	2.42	0.53
1:A:4542:THR:HA	1:A:4560:GLN:HE21	1.72	0.52
1:A:4598:ARG:NH2	1:A:4631:GLU:OE2	2.41	0.52
1:A:4678:ILE:HD12	1:A:4683:ILE:HD13	1.91	0.52
1:A:599:LEU:HD21	1:A:652:LEU:HD22	1.90	0.52
1:A:685:LYS:HE2	1:A:3540:GLU:HB3	1.91	0.52
1:A:2666:THR:O	1:A:2670:ARG:NH1	2.43	0.52
1:A:2492:SER:HB2	1:A:2592:ASN:HD21	1.75	0.52
1:A:4165:GLU:OE2	1:A:4674:GLN:NE2	2.40	0.52
1:A:1316:VAL:HA	1:A:1341:LEU:HD21	1.90	0.52
1:A:4971:ILE:HA	1:A:4974:THR:HG22	1.90	0.52
1:A:2794:ASP:OD2	1:A:2797:GLN:NE2	2.43	0.52
1:A:4378:ILE:HD11	1:A:4538:LEU:HD21	1.92	0.52
1:A:1820:THR:OG1	1:A:1822:ASP:OD1	2.23	0.52
1:A:3726:SER:OG	1:A:3727:ARG:N	2.43	0.52
1:A:4525:VAL:HG13	1:A:4628:LEU:HD12	1.91	0.52
1:A:1363:PHE:O	1:A:1367:LYS:N	2.38	0.52
1:A:892:ARG:NH2	1:A:941:GLU:OE1	2.42	0.51
1:A:1021:VAL:HG12	1:A:1065:VAL:HG22	1.90	0.51
1:A:1120:ARG:O	1:A:1167:LYS:NZ	2.43	0.51
1:A:4176:GLN:HE22	1:A:4180:ARG:HE	1.58	0.51
1:A:1368:GLN:HA	1:A:1371:GLN:HG2	1.92	0.51
1:A:4271:ASP:HB3	1:A:4651:ARG:HH22	1.75	0.51
1:A:2199:ALA:HB2	1:A:2205:LEU:HD22	1.91	0.51
1:A:3790:SER:O	1:A:3793:SER:HB2	2.10	0.51
1:A:831:ASN:O	1:A:832:HIS:ND1	2.44	0.51
1:A:4339:GLU:HA	1:A:4343:LEU:HD22	1.93	0.51
1:A:5033:ARG:HH12	1:A:5042:ARG:HH21	1.57	0.51
1:A:3281:SER:HB2	1:A:3403:ASP:HA	1.93	0.51
1:A:2576:ILE:HG12	1:A:2646:LEU:HD13	1.93	0.51
1:A:4608:ASN:ND2	1:A:4612:SER:OG	2.43	0.51
1:A:477:UNK:O	1:A:481:UNK:N	2.43	0.50
1:A:4499:THR:OG1	1:A:4500:GLN:N	2.44	0.50
1:A:3003:LEU:HB2	1:A:3128:LEU:HB3	1.93	0.50
1:A:4502:GLY:HA3	1:A:4553:LYS:HE2	1.93	0.50
1:A:2694:LEU:HD22	1:A:2710:LYS:HG2	1.92	0.50
1:A:4532:LEU:HD22	1:A:4624:PHE:HZ	1.76	0.50
1:A:2716:MET:HA	1:A:2726:LEU:HD21	1.94	0.50
1:A:4835:ASN:OD1	1:A:4914:LEU:N	2.43	0.50
1:A:1917:PRO:HD2	1:A:1920:ASN:HD22	1.75	0.50
1:A:3958:VAL:HG21	1:A:3993:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2802:VAL:HG23	1:A:2842:PHE:HD1	1.77	0.50
1:A:1021:VAL:HG11	1:A:1068:LYS:HD3	1.94	0.50
1:A:2291:VAL:HB	1:A:2307:MET:HB3	1.93	0.50
1:A:3005:LEU:HD23	1:A:3113:LYS:HA	1.94	0.50
1:A:3122:VAL:HG13	1:A:3125:ILE:HB	1.93	0.50
1:A:4296:THR:HB	1:A:4345:ALA:HB1	1.94	0.49
1:A:4688:ARG:NH2	1:A:4892:GLN:OE1	2.45	0.49
1:A:689:GLU:OE1	1:A:704:ARG:NH2	2.42	0.49
1:A:2450:ALA:HB1	1:A:2459:ILE:HD13	1.93	0.49
1:A:2455:ALA:O	1:A:2458:CYS:HB2	2.12	0.49
1:A:3683:LYS:HG2	1:A:3754:THR:HG21	1.93	0.49
1:A:2580:LEU:HD13	1:A:2602:VAL:HG13	1.94	0.49
1:A:3156:GLU:HB2	1:A:3233:SER:HB2	1.93	0.49
1:A:682:LYS:HE3	1:A:816:THR:HB	1.94	0.49
1:A:1678:LEU:HD22	1:A:1703:LEU:HD21	1.94	0.49
1:A:2509:SER:HB3	1:A:2512:GLU:HG3	1.94	0.49
1:A:4524:VAL:HG21	1:A:4697:HIS:HD2	1.77	0.49
1:A:4604:VAL:HG12	1:A:4607:PHE:HE1	1.76	0.49
1:A:2189:ASP:HB3	1:A:2269:PHE:HB2	1.94	0.49
1:A:3005:LEU:HA	1:A:3111:GLU:O	2.12	0.49
1:A:3324:TRP:HH2	1:A:3371:VAL:HG13	1.76	0.49
1:A:3495:GLN:HE22	1:A:3642:GLN:HA	1.78	0.49
1:A:4970:ILE:HD11	1:A:5002:GLN:HG3	1.94	0.49
1:A:3483:SER:OG	1:A:3575:GLN:NE2	2.45	0.49
1:A:3610:LEU:HD23	1:A:3656:PRO:HD2	1.95	0.49
1:A:706:LYS:NZ	1:A:707:ALA:O	2.41	0.49
1:A:1541:ARG:NH1	1:A:1542:THR:O	2.46	0.49
1:A:4045:LEU:O	1:A:4065:LYS:NZ	2.38	0.49
1:A:5002:GLN:HG2	1:A:5003:THR:H	1.78	0.49
1:A:896:ILE:HD11	1:A:899:ALA:HA	1.95	0.49
1:A:3281:SER:OG	1:A:3282:ARG:N	2.45	0.48
1:A:3752:ASP:HA	1:A:3755:TYR:HB2	1.95	0.48
1:A:4762:ASP:N	1:A:4762:ASP:OD1	2.42	0.48
1:A:4138:ALA:HB2	1:A:4874:PRO:HG3	1.94	0.48
1:A:2364:ILE:HG23	1:A:2394:LEU:HD13	1.94	0.48
1:A:3849:GLU:OE2	1:A:3867:ARG:NH2	2.45	0.48
1:A:2780:ILE:HD11	1:A:2820:THR:HG21	1.94	0.48
1:A:4303:LEU:HD11	1:A:4317:LEU:HD13	1.96	0.48
1:A:1383:GLU:OE2	1:A:1386:ARG:NH2	2.47	0.48
1:A:2916:ASP:OD1	1:A:3000:ARG:NH1	2.39	0.48
1:A:714:LEU:HD22	1:A:742:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:GLN:NE2	1:A:1374:SER:O	2.47	0.48
1:A:3157:PHE:HE1	1:A:3242:LEU:HD13	1.79	0.48
1:A:3723:LYS:N	1:A:4857:GLU:OE1	2.41	0.48
1:A:3837:LYS:HE2	1:A:4909:GLN:HE22	1.78	0.48
1:A:4700:GLU:OE2	1:A:4712:TRP:NE1	2.41	0.48
1:A:1212:PHE:HA	1:A:1215:GLU:HG2	1.96	0.47
1:A:3253:ASN:ND2	1:A:3257:ASP:OD2	2.48	0.47
1:A:1083:LEU:HD12	1:A:1086:ILE:HD11	1.96	0.47
1:A:1139:ARG:HH21	1:A:2964:LEU:HD12	1.79	0.47
1:A:1324:GLN:HG3	1:A:1385:ALA:HB1	1.97	0.47
1:A:803:HIS:HB3	1:A:851:LEU:HB3	1.95	0.47
1:A:3312:ASP:OD1	1:A:3312:ASP:N	2.47	0.47
1:A:1013:HIS:HB3	1:A:1017:PRO:HG2	1.97	0.47
1:A:1826:LEU:HD11	1:A:2033:PHE:HD2	1.80	0.47
1:A:2140:ASN:ND2	1:A:2142:ASP:OD2	2.47	0.47
1:A:3707:GLN:HG2	1:A:3759:LEU:HD22	1.97	0.47
1:A:4500:GLN:HG3	1:A:4504:VAL:HG21	1.97	0.47
1:A:4249:HIS:HD2	1:A:4250:PRO:HD2	1.80	0.47
1:A:4338:PRO:HA	1:A:4342:GLN:HB2	1.95	0.47
1:A:1041:CYS:HB2	1:A:1048:ILE:HD13	1.96	0.47
1:A:3686:VAL:HG22	1:A:3762:PRO:HG2	1.96	0.47
1:A:3516:ASP:N	1:A:3516:ASP:OD1	2.48	0.47
1:A:3610:LEU:HB3	1:A:3656:PRO:HG2	1.96	0.47
1:A:2315:LEU:HD23	1:A:2320:VAL:HG11	1.98	0.46
1:A:2765:LEU:HB3	1:A:2801:VAL:HG13	1.96	0.46
1:A:3724:VAL:HG21	1:A:3730:LEU:HD13	1.98	0.46
1:A:3932:LYS:HA	1:A:4011:PHE:HE2	1.80	0.46
1:A:4185:LEU:HD11	1:A:4224:HIS:HB2	1.96	0.46
1:A:4417:TYR:HB3	1:A:4420:ASN:HD22	1.80	0.46
1:A:1513:ALA:HB2	1:A:1587:PHE:HZ	1.80	0.46
1:A:1809:ILE:HD13	1:A:1889:VAL:HG11	1.97	0.46
1:A:2162:PHE:HB3	1:A:2176:LEU:HD22	1.97	0.46
1:A:4228:LEU:HD22	1:A:4254:VAL:HB	1.96	0.46
1:A:3855:SER:O	1:A:3860:ARG:NH1	2.48	0.46
1:A:1956:ALA:HB3	1:A:2534:PRO:HB2	1.98	0.46
1:A:3789:LEU:O	1:A:3793:SER:N	2.47	0.46
1:A:1590:LEU:HD13	1:A:1598:PHE:HD2	1.81	0.46
1:A:2270:ASN:ND2	1:A:2340:LEU:O	2.48	0.46
1:A:998:PHE:HZ	1:A:1040:LEU:HD13	1.81	0.46
1:A:2729:VAL:HG22	1:A:2846:SER:HB3	1.97	0.46
1:A:4358:ASP:O	1:A:4362:ARG:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2005:LEU:HD22	1:A:2011:LYS:HD3	1.97	0.46
1:A:4098:ASP:N	1:A:4098:ASP:OD1	2.48	0.46
1:A:4613:THR:OG1	1:A:4616:CYS:SG	2.72	0.46
1:A:762:LEU:HB2	1:A:814:TYR:CZ	2.51	0.46
1:A:1262:THR:HG23	1:A:1265:GLU:H	1.81	0.46
1:A:3982:CYS:HB3	1:A:3987:THR:H	1.81	0.45
1:A:4258:LYS:HE3	1:A:4669:LEU:HD23	1.98	0.45
1:A:4378:ILE:HG22	1:A:4386:LYS:HE2	1.97	0.45
1:A:4738:VAL:HA	1:A:4922:LEU:HD21	1.97	0.45
1:A:2564:ASP:HB3	1:A:2610:ARG:HH12	1.81	0.45
1:A:2728:LEU:HD23	1:A:2861:VAL:HB	1.97	0.45
1:A:4157:TYR:O	1:A:4218:ARG:NH2	2.49	0.45
1:A:1530:LEU:HD12	1:A:1543:TYR:HE2	1.82	0.45
1:A:4503:HIS:HB3	1:A:4552:ILE:HA	1.99	0.45
1:A:731:PHE:HB3	1:A:760:ARG:HH21	1.80	0.45
1:A:612:LYS:O	1:A:615:ASP:HB2	2.16	0.45
1:A:2979:ILE:HG23	1:A:3002:LEU:HD11	1.98	0.45
1:A:4104:LEU:HB2	1:A:4124:PHE:HE2	1.81	0.45
1:A:784:LYS:HG3	1:A:837:ILE:HD11	1.99	0.45
1:A:983:GLN:HG2	1:A:3201:LEU:HD23	1.99	0.45
1:A:1729:GLN:OE1	1:A:1746:GLN:NE2	2.50	0.45
1:A:1981:PRO:HB2	1:A:2014:VAL:HG13	1.98	0.45
1:A:3639:ILE:HA	1:A:4926:ARG:HH11	1.82	0.45
1:A:4406:GLN:HA	1:A:4409:LYS:HE2	1.99	0.45
1:A:4779:TRP:HE3	1:A:4826:LEU:HD22	1.81	0.45
1:A:669:PRO:HB3	1:A:726:VAL:HG21	1.99	0.45
1:A:3605:ALA:O	1:A:3609:ASP:CB	2.65	0.45
1:A:2424:LYS:HA	1:A:2427:GLU:HG2	1.97	0.45
1:A:4050:LYS:HD2	1:A:4061:ARG:HH11	1.81	0.45
1:A:3592:ASP:OD1	1:A:3592:ASP:N	2.50	0.44
1:A:3852:LEU:HD22	1:A:3863:ILE:HG13	1.99	0.44
1:A:4680:CYS:SG	1:A:4681:SER:N	2.90	0.44
1:A:2847:ASN:ND2	1:A:3123:PRO:HG3	2.30	0.44
1:A:1978:GLU:HG2	1:A:1979:THR:H	1.83	0.44
1:A:2946:ARG:HG3	1:A:2978:LEU:HD22	1.98	0.44
1:A:3745:GLN:NE2	1:A:3758:PRO:O	2.42	0.44
1:A:669:PRO:HG3	1:A:730:LEU:HD22	1.99	0.44
1:A:982:SER:HA	1:A:3201:LEU:HD21	1.98	0.44
1:A:1704:VAL:HA	1:A:1707:THR:HG22	1.98	0.44
1:A:5100:LYS:NZ	1:A:5119:GLU:O	2.34	0.44
1:A:1973:ALA:HA	1:A:1976:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2923:MET:HE1	1:A:2946:ARG:HD3	2.00	0.44
1:A:2945:LEU:HD13	1:A:2957:LEU:HD23	1.99	0.44
1:A:1189:LEU:HB2	1:A:1193:ILE:HD12	1.99	0.44
1:A:1557:LEU:HD12	1:A:3095:HIS:HD2	1.83	0.44
1:A:1855:SER:HA	1:A:1889:VAL:O	2.18	0.44
1:A:2005:LEU:HD11	1:A:2055:HIS:CD2	2.52	0.44
1:A:4880:CYS:HB3	1:A:4894:PHE:HE1	1.83	0.44
1:A:1390:LEU:HD13	1:A:1476:ALA:HA	2.00	0.44
1:A:2559:VAL:HG22	1:A:2563:VAL:HG23	1.99	0.44
1:A:1351:PHE:HD2	1:A:1353:ASN:H	1.66	0.44
1:A:1537:PRO:HB2	1:A:1538:GLU:H	1.66	0.44
1:A:4756:ILE:HD11	1:A:4772:ILE:HG21	2.00	0.44
1:A:865:SER:O	1:A:869:LEU:HB2	2.18	0.43
1:A:1721:GLU:HG2	1:A:1724:LYS:HE3	2.00	0.43
1:A:2810:ALA:HB1	1:A:2817:PRO:HG2	2.00	0.43
1:A:1987:LEU:HD11	1:A:1997:VAL:HG22	2.00	0.43
1:A:2094:ARG:HB2	1:A:2099:VAL:HG13	2.00	0.43
1:A:2378:ILE:HD11	1:A:2536:LEU:HD22	2.00	0.43
1:A:808:GLU:HG2	1:A:810:LEU:HD23	2.00	0.43
1:A:3610:LEU:HD13	1:A:3698:LEU:HD21	2.00	0.43
1:A:1207:HIS:NE2	1:A:2887:ASP:OD2	2.50	0.43
1:A:2786:CYS:HB2	1:A:2800:SER:HB3	2.00	0.43
1:A:3174:ALA:HA	1:A:3180:TYR:HB3	2.01	0.43
1:A:4164:GLN:HG2	1:A:4171:SER:H	1.82	0.43
1:A:608:THR:HA	1:A:655:ARG:HH21	1.83	0.43
1:A:690:ASP:HB2	1:A:696:GLU:H	1.83	0.43
1:A:5075:GLU:HG2	1:A:5107:MET:HG3	2.01	0.43
1:A:1701:GLN:HA	1:A:1704:VAL:HG12	2.00	0.43
1:A:3940:SER:HB3	1:A:3944:ILE:HG12	2.00	0.43
1:A:1383:GLU:HB3	1:A:1472:LEU:HD23	2.00	0.43
1:A:2822:HIS:CE1	1:A:2857:ARG:HD3	2.53	0.43
1:A:4581:SER:OG	1:A:4582:ALA:N	2.51	0.43
1:A:1365:LYS:O	1:A:1368:GLN:HB2	2.19	0.43
1:A:3325:LEU:HD13	1:A:3364:THR:HB	2.01	0.43
1:A:1384:LEU:HD13	1:A:1438:LEU:HD22	2.00	0.43
1:A:4431:GLU:O	1:A:4788:THR:OG1	2.37	0.43
1:A:1314:GLN:HE22	1:A:1373:ILE:HG23	1.84	0.43
1:A:1526:LEU:HB2	1:A:1584:VAL:HG21	2.01	0.43
1:A:2194:ILE:HG12	1:A:2274:MET:HB3	2.01	0.43
1:A:2331:ARG:NH2	1:A:2351:ASP:O	2.47	0.43
1:A:3200:ASP:N	1:A:3200:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4080:ILE:HD13	1:A:4120:LEU:HD13	2.01	0.43
1:A:1317:SER:HB3	1:A:1378:GLN:HE22	1.84	0.42
1:A:1746:GLN:HA	1:A:1749:VAL:HG22	2.01	0.42
1:A:1710:CYS:SG	1:A:1711:GLU:N	2.92	0.42
1:A:4354:LYS:HA	1:A:4357:SER:HB3	2.01	0.42
1:A:2507:ARG:HE	1:A:2508:VAL:HG13	1.83	0.42
1:A:4116:ASP:N	1:A:4116:ASP:OD1	2.53	0.42
1:A:4499:THR:HA	1:A:4614:LYS:HD2	2.01	0.42
1:A:2495:MET:HA	1:A:2498:ARG:HG2	2.00	0.42
1:A:3002:LEU:HD12	1:A:3108:ILE:HG12	2.02	0.42
1:A:4727:LEU:HD11	1:A:4827:VAL:HG13	2.01	0.42
1:A:1810:TYR:OH	1:A:1823:GLU:O	2.36	0.42
1:A:3958:VAL:HG11	1:A:3971:ILE:HG21	2.01	0.42
1:A:4409:LYS:HG2	1:A:4412:ARG:HH22	1.83	0.42
1:A:1144:VAL:HG22	1:A:1147:LEU:HB2	2.02	0.42
1:A:2509:SER:OG	1:A:2510:ALA:N	2.52	0.42
1:A:1256:LEU:HD11	1:A:1270:PHE:HZ	1.84	0.42
1:A:3064:LEU:O	1:A:3068:TYR:N	2.53	0.42
1:A:3853:CYS:SG	1:A:3854:ASP:N	2.93	0.42
1:A:4042:LEU:HD23	1:A:4045:LEU:HD21	2.02	0.42
1:A:3726:SER:HB3	1:A:3729:GLU:HB3	2.01	0.42
1:A:2212:VAL:O	1:A:2216:MET:HG2	2.20	0.42
1:A:2727:PHE:HD2	1:A:2850:LEU:HD13	1.85	0.42
1:A:3028:ILE:HD12	1:A:3059:VAL:HG13	2.02	0.42
1:A:3852:LEU:HD21	1:A:3860:ARG:HG2	2.02	0.42
1:A:849:LEU:HG	1:A:870:VAL:HG23	2.01	0.42
1:A:1450:ASP:HA	1:A:1453:ASN:HD22	1.84	0.42
1:A:4724:VAL:HG12	1:A:4863:VAL:HB	2.01	0.42
1:A:658:ASP:O	1:A:660:ARG:N	2.49	0.41
1:A:823:GLU:O	1:A:827:ASN:ND2	2.53	0.41
1:A:1520:ILE:HG13	1:A:1591:HIS:NE2	2.34	0.41
1:A:4541:ALA:HB2	1:A:4548:LEU:HG	2.02	0.41
1:A:4722:ARG:HB2	1:A:4723:LEU:HD12	2.01	0.41
1:A:4792:ILE:HD12	1:A:4825:ALA:HA	2.02	0.41
1:A:5048:TYR:CZ	1:A:5084:LEU:HD22	2.55	0.41
1:A:2782:THR:HG22	1:A:2802:VAL:HG12	2.01	0.41
1:A:4350:ILE:HG12	1:A:4356:LEU:HD11	2.02	0.41
1:A:1334:ASP:N	1:A:1334:ASP:OD1	2.53	0.41
1:A:2177:ARG:HH22	1:A:2466:ARG:NH1	2.18	0.41
1:A:908:GLU:OE2	1:A:937:ARG:NE	2.53	0.41
1:A:1981:PRO:HD2	1:A:2014:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2368:GLU:O	1:A:2372:ARG:HB2	2.20	0.41
1:A:2851:ASP:OD1	1:A:2851:ASP:N	2.54	0.41
1:A:1013:HIS:H	1:A:1017:PRO:HD2	1.84	0.41
1:A:3390:GLY:O	1:A:3392:HIS:N	2.54	0.41
1:A:1630:ASP:OD1	1:A:1630:ASP:N	2.51	0.41
1:A:3259:LEU:HD23	1:A:3259:LEU:HA	1.85	0.41
1:A:3537:LYS:HE3	1:A:3625:LEU:HD22	2.02	0.41
1:A:4195:LEU:HA	1:A:4201:LEU:HD11	2.02	0.41
1:A:3606:TRP:HD1	1:A:3705:GLN:HG3	1.85	0.41
1:A:688:PRO:HA	1:A:770:TYR:HE1	1.85	0.41
1:A:1408:VAL:HG21	1:A:1429:HIS:HD2	1.85	0.41
1:A:1554:LYS:HG2	1:A:3095:HIS:CE1	2.55	0.41
1:A:4264:LYS:HG3	1:A:4266:HIS:H	1.85	0.41
1:A:4686:CYS:SG	1:A:4687:ARG:N	2.94	0.41
1:A:641:ILE:HB	1:A:645:TRP:HZ3	1.87	0.40
1:A:1005:VAL:O	1:A:1009:SER:HB3	2.21	0.40
1:A:1437:SER:HA	1:A:1441:LYS:HD2	2.02	0.40
1:A:2021:SER:OG	1:A:2022:THR:N	2.54	0.40
1:A:2218:LEU:HD11	1:A:2303:LYS:HG3	2.03	0.40
1:A:2914:LEU:HD23	1:A:2914:LEU:HA	1.94	0.40
1:A:3937:LYS:HG2	1:A:3942:PHE:HA	2.03	0.40
1:A:4152:HIS:O	1:A:4156:THR:OG1	2.28	0.40
1:A:5100:LYS:HB2	1:A:5122:PHE:HD2	1.86	0.40
1:A:617:LEU:O	1:A:620:LEU:HB2	2.22	0.40
1:A:667:ILE:HA	1:A:670:LEU:HD13	2.03	0.40
1:A:3001:TYR:O	1:A:3129:GLU:HB3	2.21	0.40
1:A:1783:LEU:HD23	1:A:1783:LEU:HA	1.93	0.40
1:A:1942:PHE:O	1:A:1944:ASP:N	2.54	0.40
1:A:1968:HIS:NE2	1:A:1972:LYS:HE3	2.37	0.40
1:A:2264:HIS:HB2	1:A:2362:LEU:HD13	2.04	0.40
1:A:2451:ASN:HD21	1:A:2488:TYR:HE1	1.69	0.40
1:A:4051:GLU:O	1:A:4061:ARG:NE	2.54	0.40
1:A:5107:MET:HG2	1:A:5111:ASP:HB2	2.04	0.40
1:A:965:SER:O	1:A:969:GLU:HG2	2.22	0.40
1:A:3125:ILE:HG23	1:A:3130:LYS:HD2	2.04	0.40
1:A:4903:ILE:HG22	1:A:4908:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	4319/4638 (93%)	3901 (90%)	410 (10%)	8 (0%)	47 79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4600	GLN
1	A	1374	SER
1	A	5128	MET
1	A	2547	ASN
1	A	4049	GLN
1	A	3496	ASN
1	A	4166	PRO
1	A	1373	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3900/4107 (95%)	3866 (99%)	34 (1%)	78 91

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	612	LYS
1	A	655	ARG
1	A	687	GLN

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Mol	Chain	Res	Type
1	A	831	ASN
1	A	888	LEU
1	A	902	ARG
1	A	987	LEU
1	A	1018	VAL
1	A	1052	THR
1	A	1390	LEU
1	A	1460	ARG
1	A	1506	ARG
1	A	1724	LYS
1	A	1934	ARG
1	A	2012	MET
1	A	2206	ARG
1	A	2488	TYR
1	A	2727	PHE
1	A	2957	LEU
1	A	3199	ARG
1	A	3345	ARG
1	A	3397	ARG
1	A	3544	ARG
1	A	3692	THR
1	A	3798	LYS
1	A	3914	ASN
1	A	4155	ARG
1	A	4307	ARG
1	A	4519	ARG
1	A	4598	ARG
1	A	4633	LYS
1	A	4858	VAL
1	A	4908	LEU
1	A	5016	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	ASN
1	A	781	GLN
1	A	822	HIS
1	A	827	ASN
1	A	924	HIS
1	A	1186	HIS
1	A	1314	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1324	GLN
1	A	1378	GLN
1	A	1429	HIS
1	A	1453	ASN
1	A	1579	ASN
1	A	1595	ASN
1	A	1660	HIS
1	A	1791	GLN
1	A	1816	GLN
1	A	1920	ASN
1	A	1930	GLN
1	A	2139	GLN
1	A	2161	HIS
1	A	2451	ASN
1	A	2480	HIS
1	A	2797	GLN
1	A	3095	HIS
1	A	3131	HIS
1	A	3337	GLN
1	A	3542	GLN
1	A	3575	GLN
1	A	3608	GLN
1	A	3914	ASN
1	A	4008	HIS
1	A	4176	GLN
1	A	4196	GLN
1	A	4242	GLN
1	A	4249	HIS
1	A	4252	GLN
1	A	4420	ASN
1	A	4543	HIS
1	A	4560	GLN
1	A	4564	GLN
1	A	4608	ASN
1	A	4697	HIS
1	A	4701	GLN
1	A	4834	HIS
1	A	4846	ASN
1	A	4873	ASN
1	A	4886	GLN
1	A	4909	GLN
1	A	4932	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	5017	HIS
1	A	5028	HIS
1	A	5056	HIS
1	A	5146	GLN

### 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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z  > 2$
2	ATP	A	5201	3	26,33,33	0.93	0	31,52,52	1.57	5 (16%)

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
2	ATP	A	5201	3	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5201	ATP	PB-O3B-PG	-3.41	121.13	132.83
2	A	5201	ATP	N3-C2-N1	-3.36	123.42	128.68
2	A	5201	ATP	PA-O3A-PB	-3.18	121.91	132.83
2	A	5201	ATP	C4-C5-N7	-2.93	106.34	109.40
2	A	5201	ATP	C3'-C2'-C1'	2.77	105.16	100.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

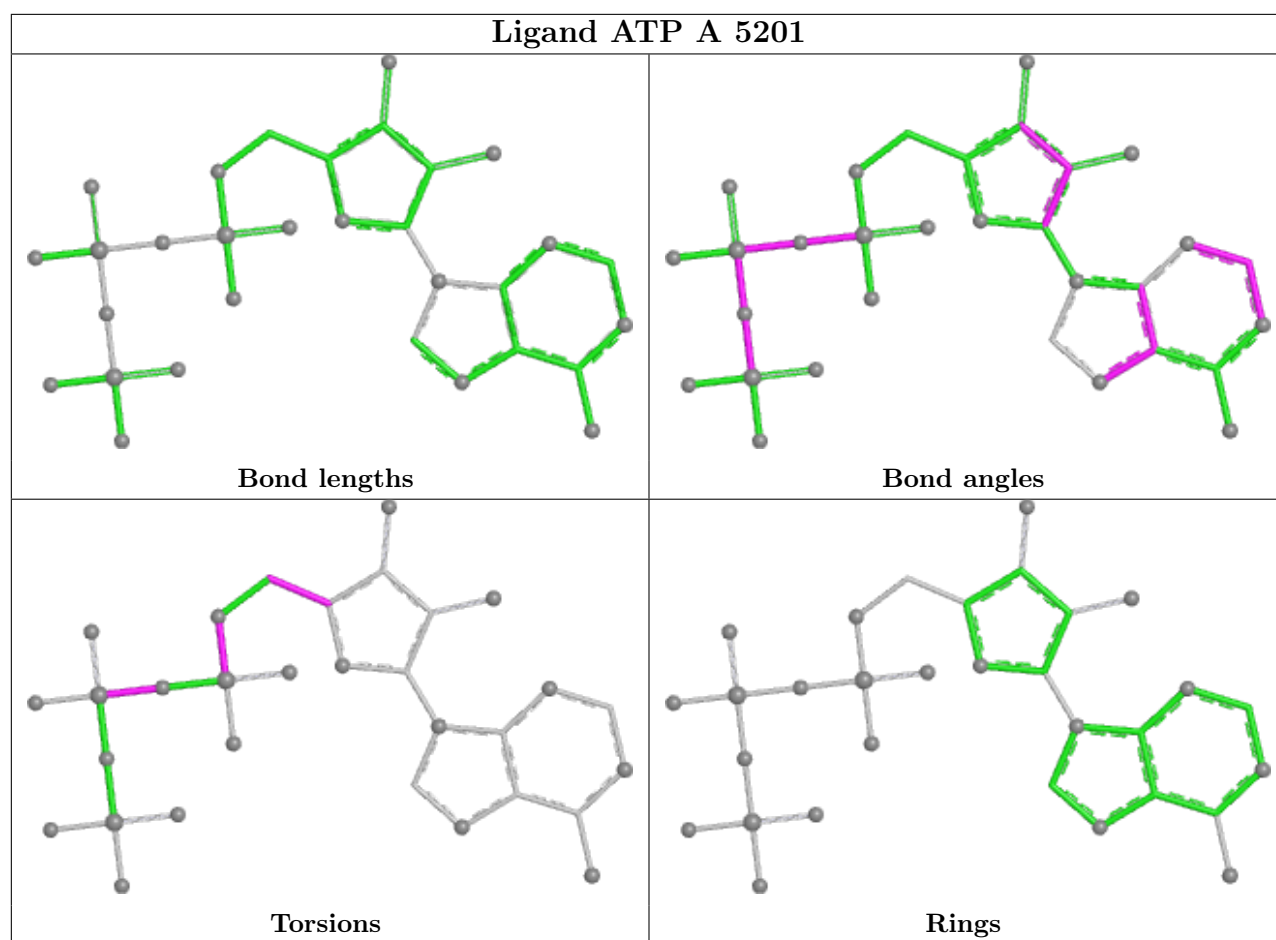
Mol	Chain	Res	Type	Atoms
2	A	5201	ATP	C5'-O5'-PA-O1A
2	A	5201	ATP	O4'-C4'-C5'-O5'
2	A	5201	ATP	C3'-C4'-C5'-O5'
2	A	5201	ATP	C5'-O5'-PA-O3A
2	A	5201	ATP	C5'-O5'-PA-O2A
2	A	5201	ATP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	541:UNK	C	591:LYS	N	13.40

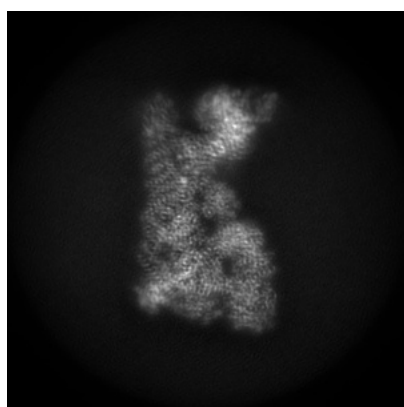
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10429. These allow visual inspection of the internal detail of the map and identification of artifacts.

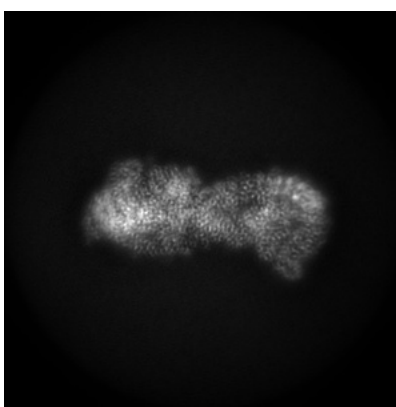
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

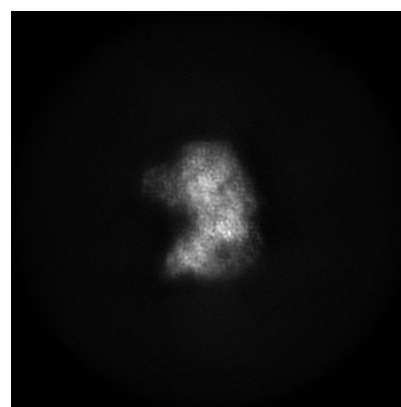
#### 6.1.1 Primary map



X



Y

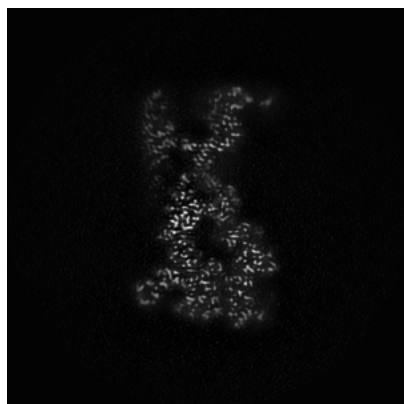


Z

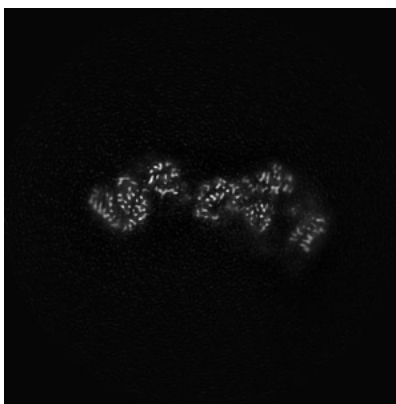
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

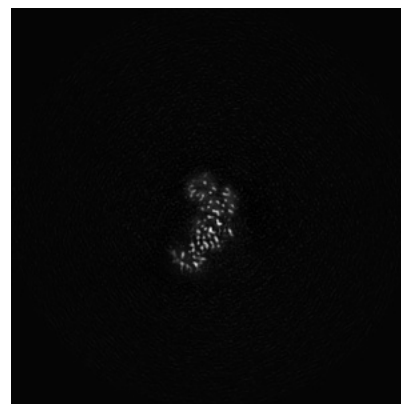
#### 6.2.1 Primary map



X Index: 176



Y Index: 176

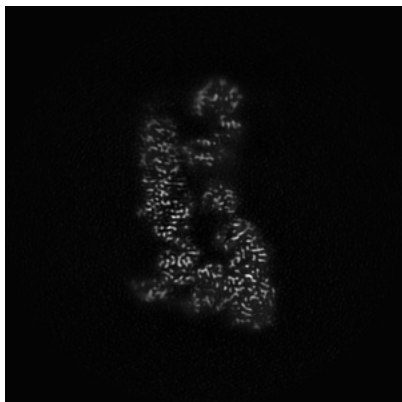


Z Index: 176

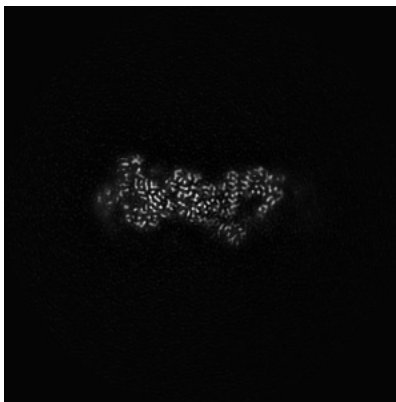
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

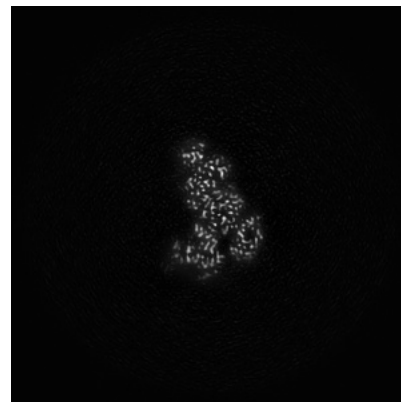
### 6.3.1 Primary map



X Index: 166



Y Index: 156

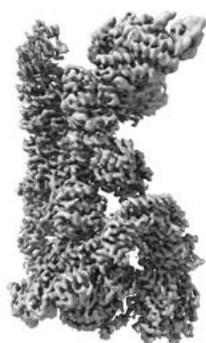


Z Index: 109

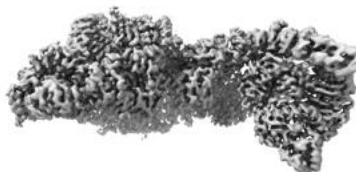
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

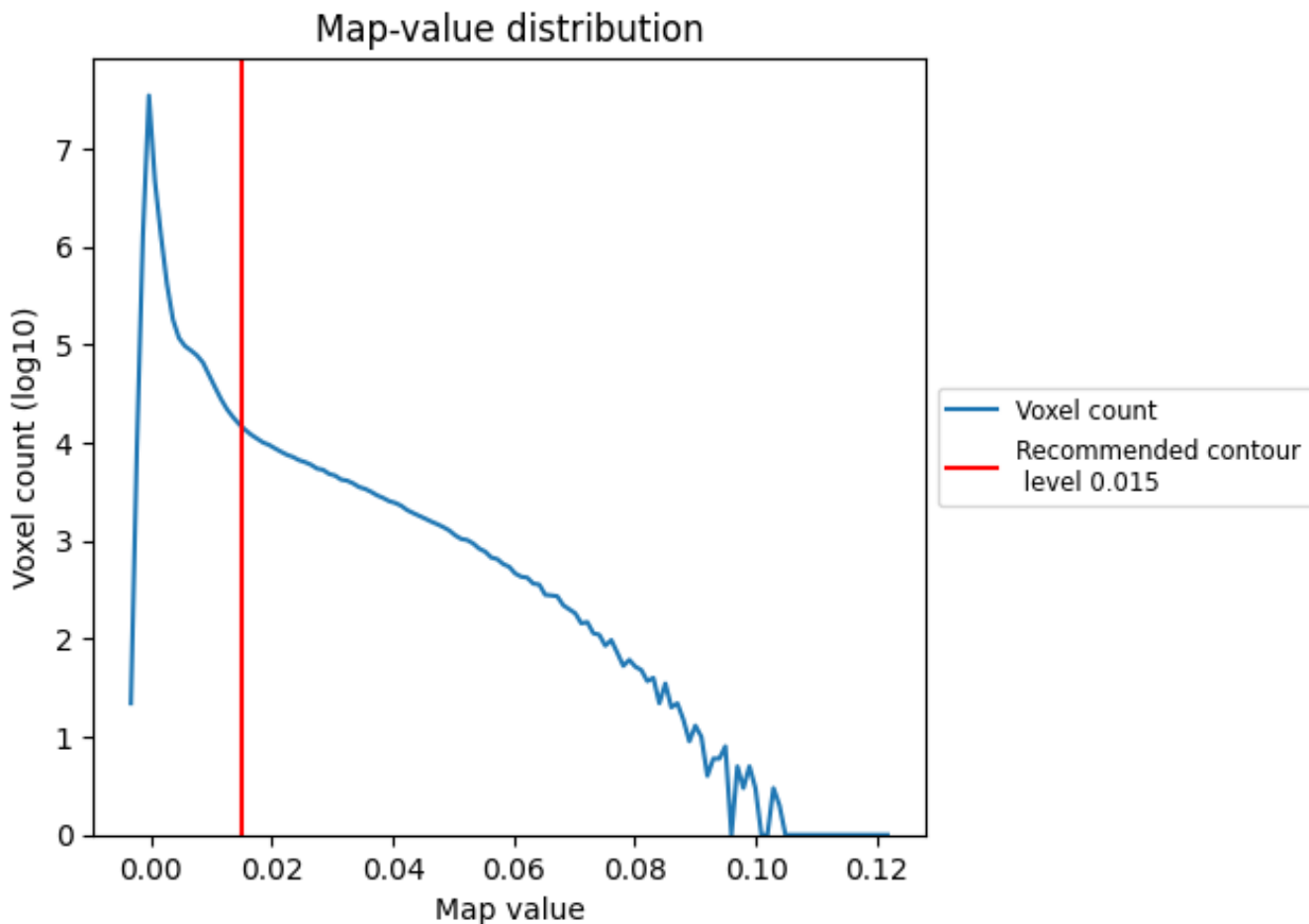
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

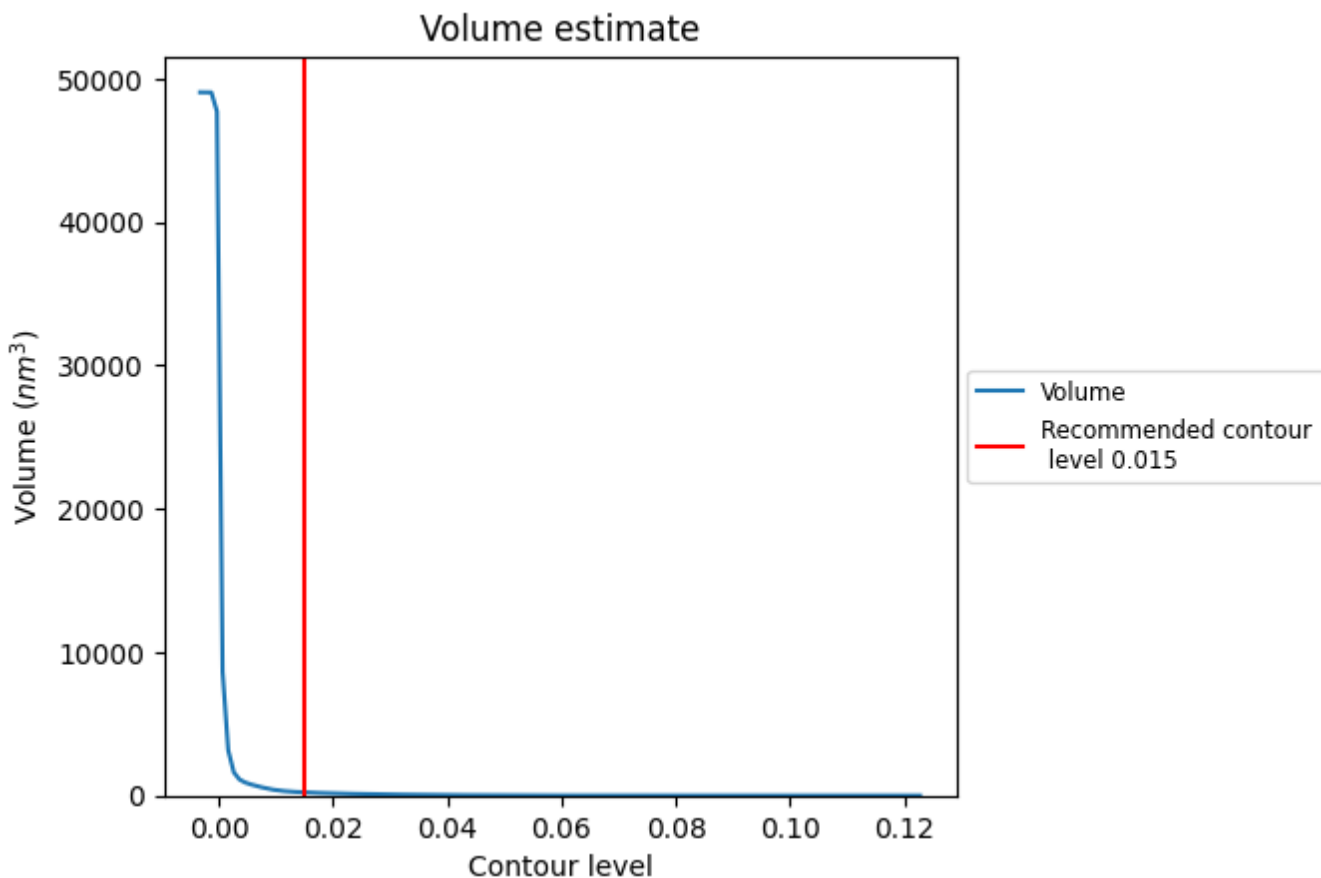
This section contains the results of statistical analysis of the map.

### 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.

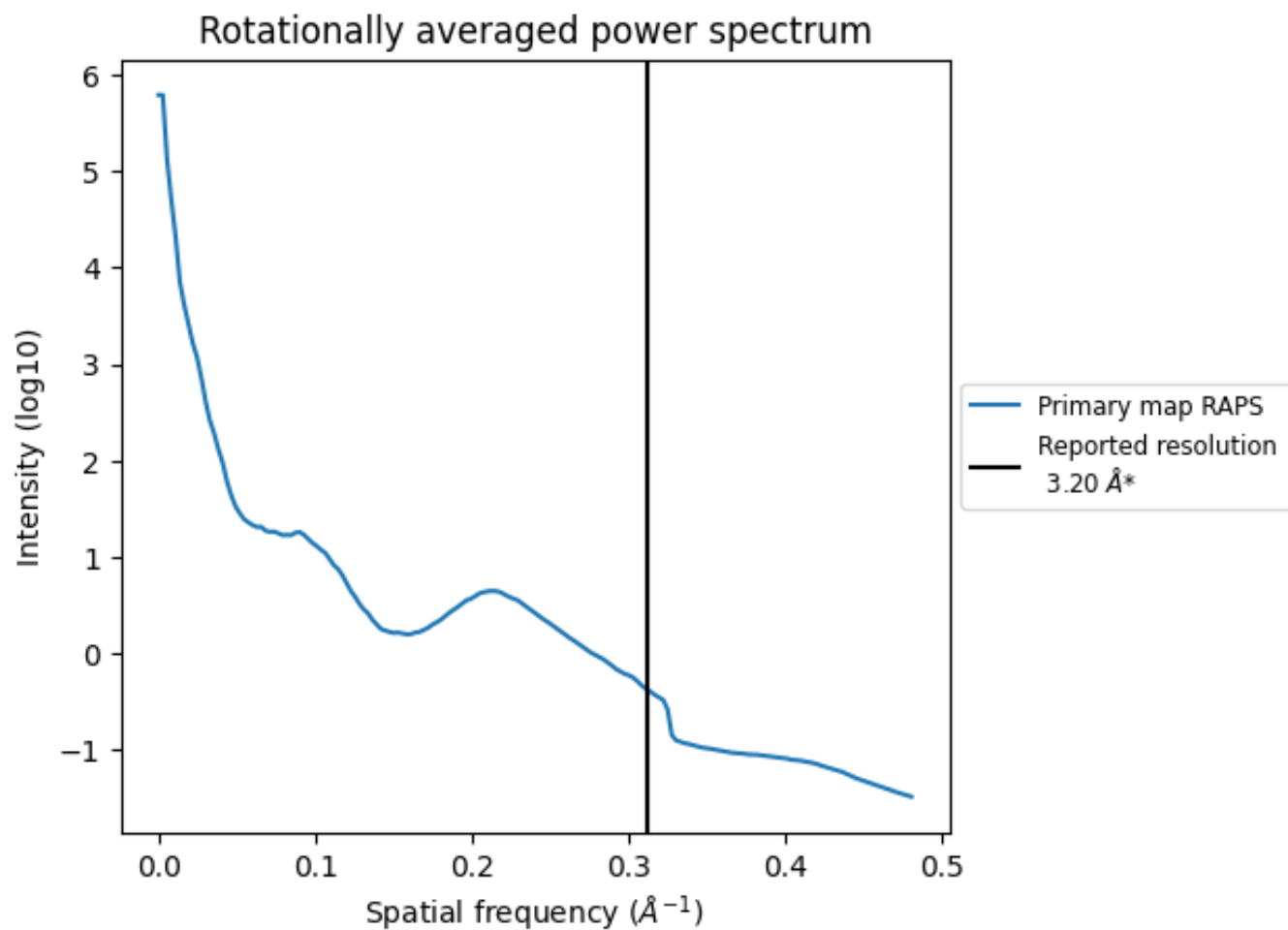
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm<sup>3</sup>; this corresponds to an approximate mass of 201 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 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

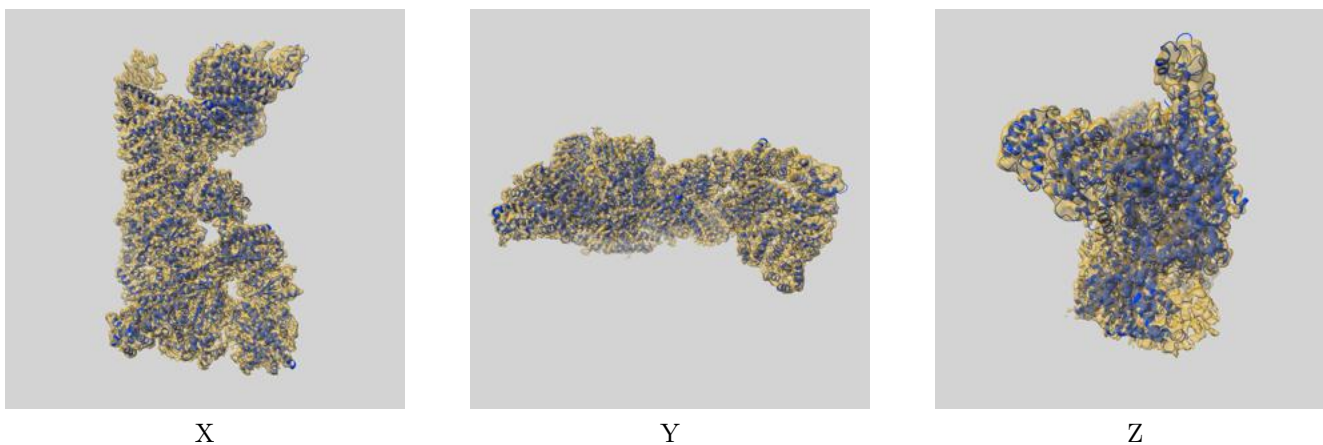
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

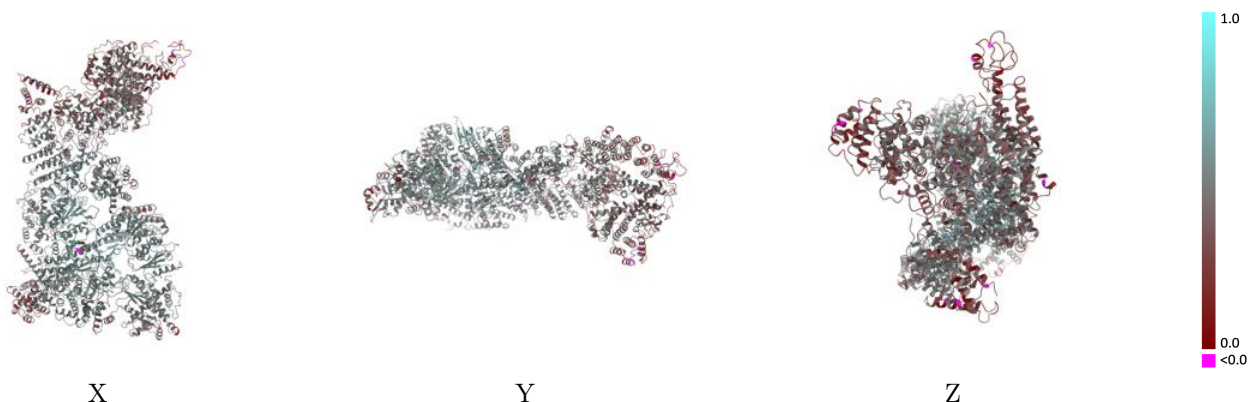
This section contains information regarding the fit between EMDB map EMD-10429 and PDB model 6TAX. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



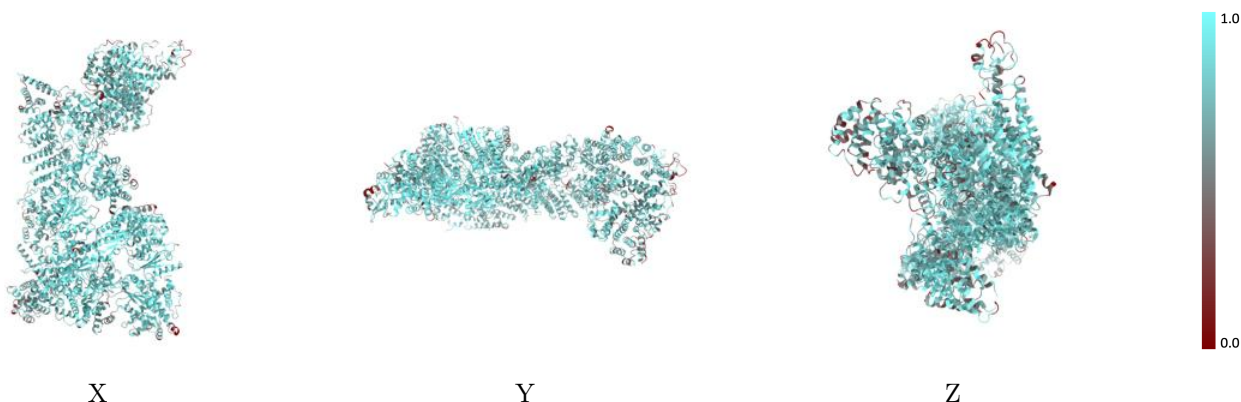
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



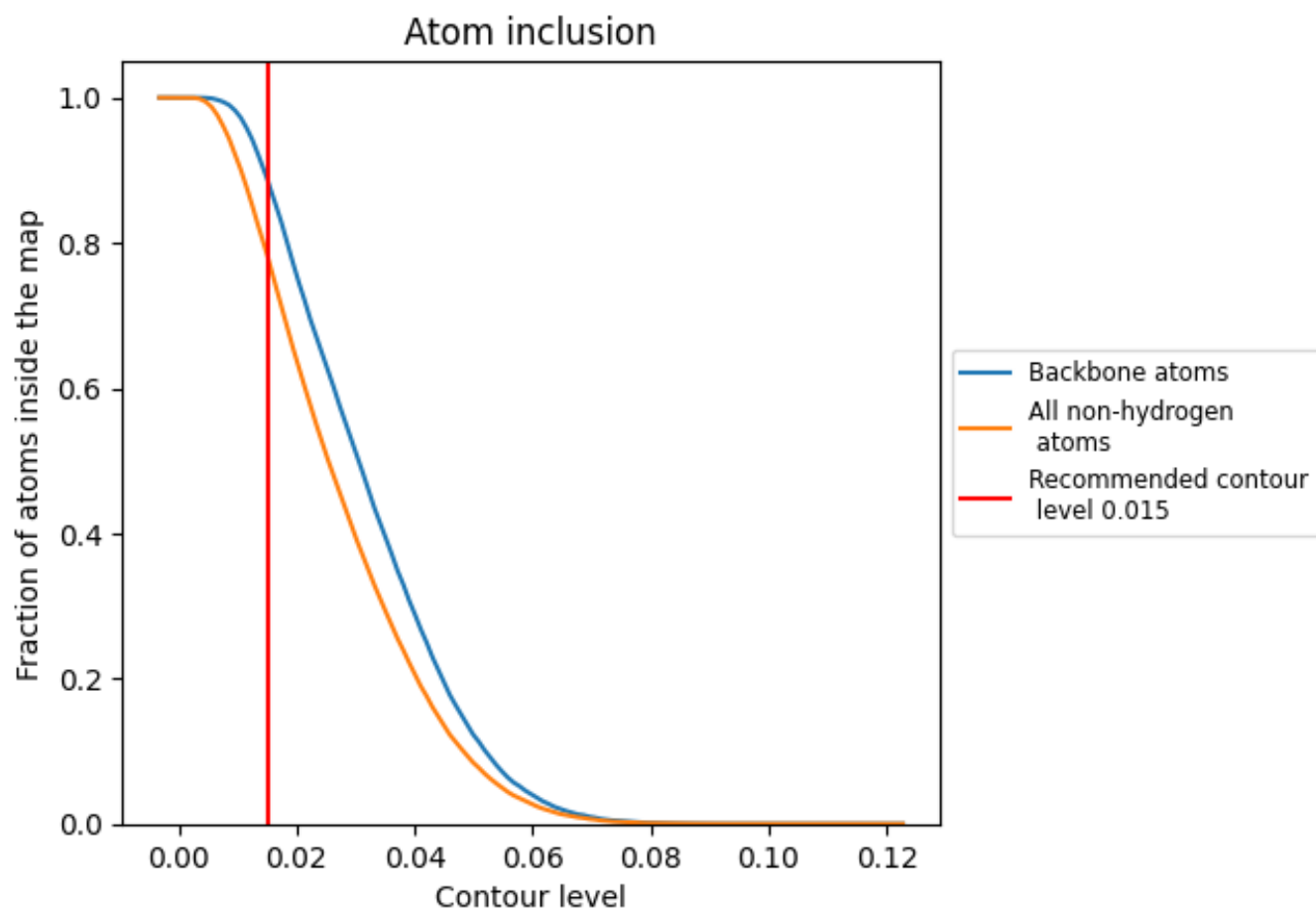
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).





## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7836	 0.4510
A	 0.7836	 0.4510

