



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 04:57 AM UTC

PDB ID : 9E10 / pdb_00009e10
EMDB ID : EMD-47379
Title : Dimeric motor domains from phi dynein-1 under Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 2.71 Å(reported)

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

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

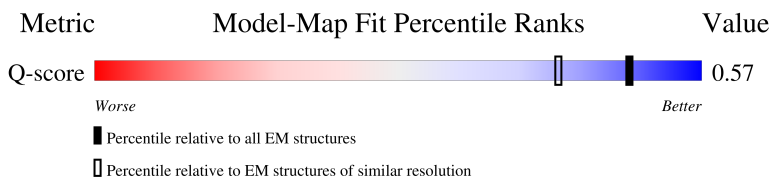
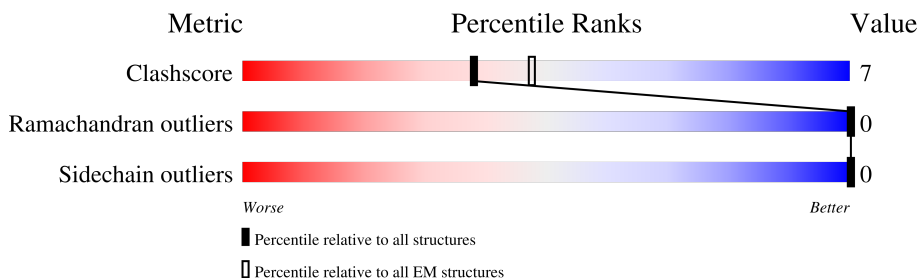
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.71 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10297 (2.21 - 3.21)

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	4646	
1	B	4646	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47414 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2937	Total	C	N	O	S	0	0
			23593	15028	4070	4378	117		
1	B	2937	Total	C	N	O	S	0	0
			23593	15028	4070	4378	117		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



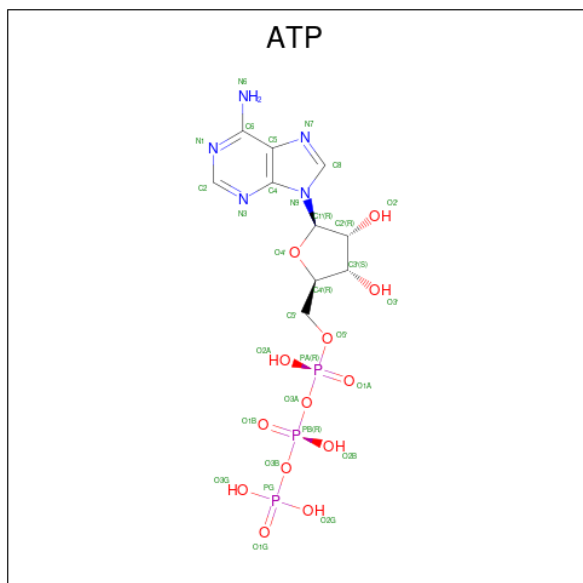
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



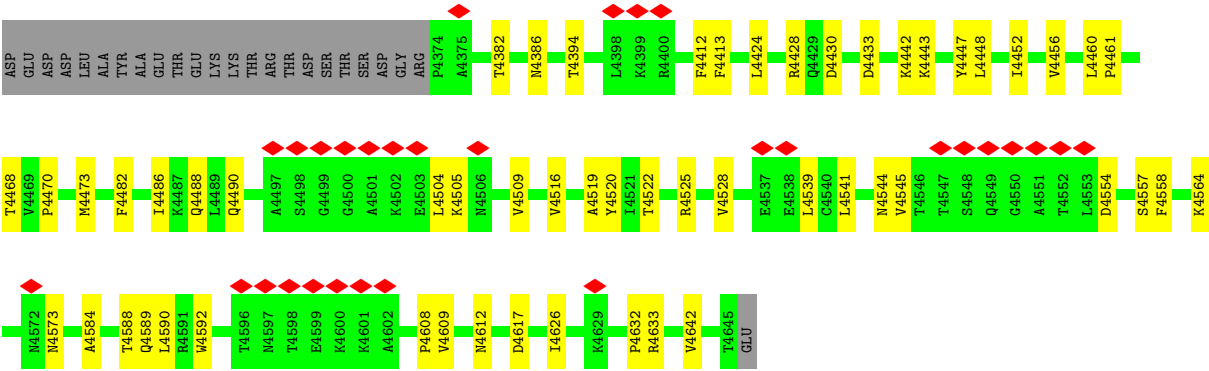
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

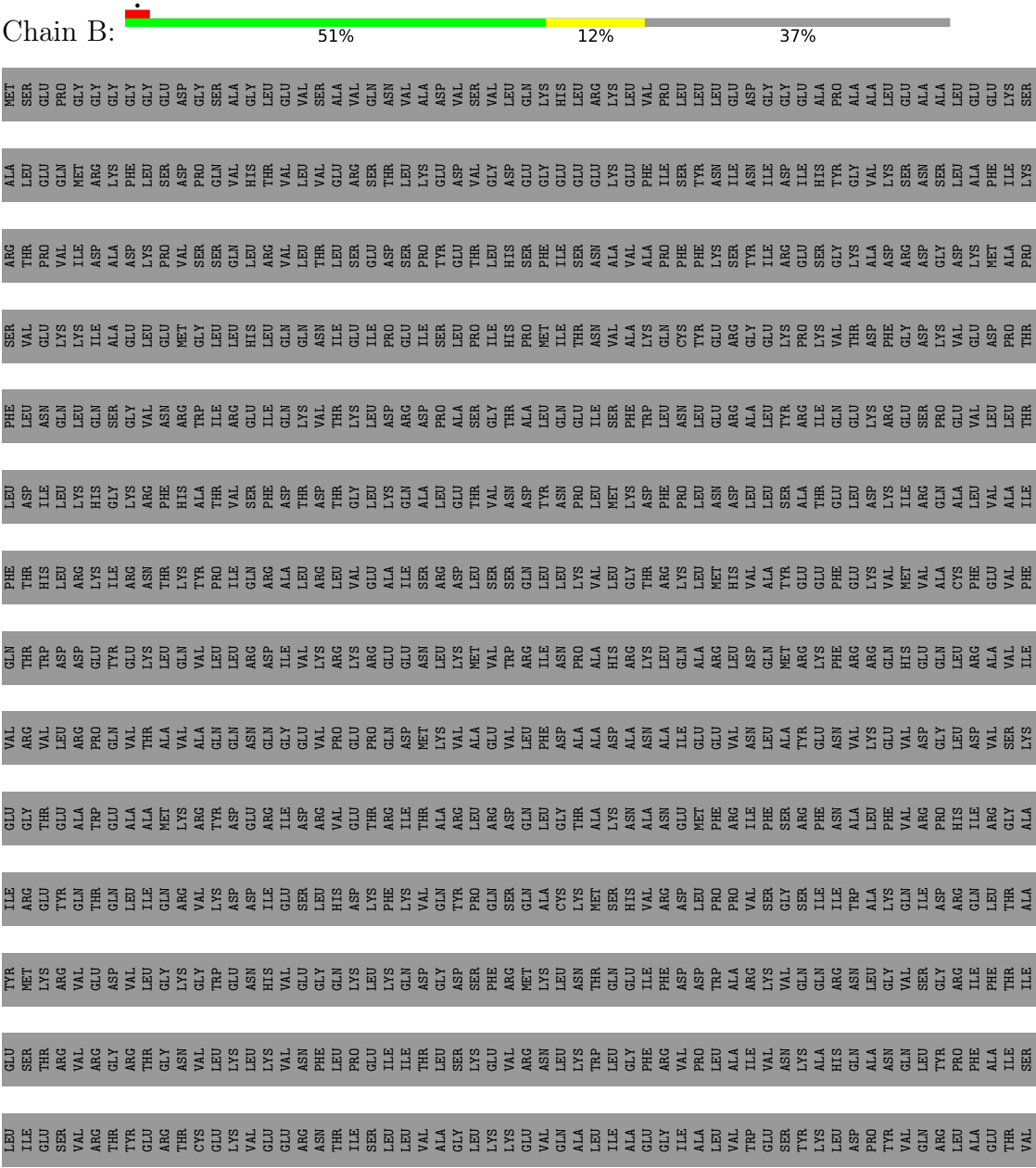
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	

PHE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	
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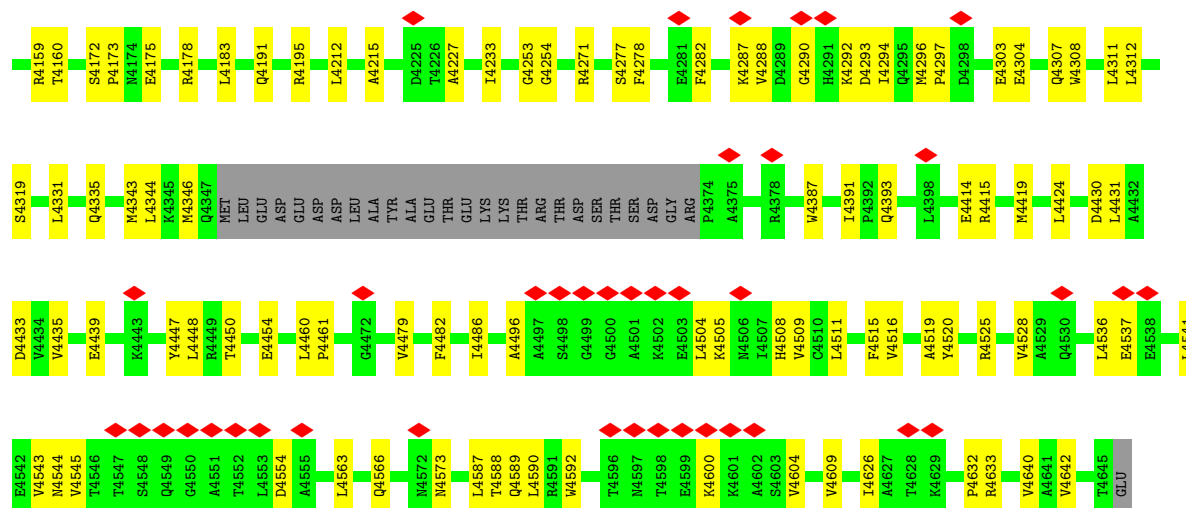


● Molecule 1: Cytoplasmic dynein 1 heavy chain 1





A3986	D3902	D3762	R3569	S3456	ALA	GLN	ASP	T3099	G2937	N2752	P2525	ASP
I3987	L3909	D3763	Q3563	E3457	ILE	ILE	SER	E3100	K2943	M2755	A2529	GLY
H3988		D3764	Q3563	A3458	ALA	ARG	LYS	Q3104	A2951	T2770	P2530	GLY
R3989			Q3563	A3459	LEU	SER	ASP	T3110	L2956	F2784	N2531	GLY
L3990			Q3563	A3460	ASN	ILE	ASP	S3111	L2956		D2536	ALA
F3996			Q3563	A3461	TYR	ILE	LEU	S3112	L2956		D2536	ALA
M4004			Q3563	A3462	ALA	ASP	ASP	M3113	L2956		D2536	ALA
M4007			Q3563	A3463	ASP	ASP	ASP	M3114	L2956		D2536	ALA
T4011			Q3563	A3464	LEU	LEU	ASP	M3115	L2956		D2536	ALA
M4012			Q3563	A3465	LEU	LEU	ASP	M3116	L2956		D2536	ALA
L4013			Q3563	A3466	LEU	LEU	ASP	M3117	L2956		D2536	ALA
F4017			Q3563	A3467	LEU	LEU	ASP	M3118	L2956		D2536	ALA
M4018			Q3563	A3468	LEU	LEU	ASP	M3119	L2956		D2536	ALA
S4019			Q3563	A3469	LEU	LEU	ASP	M3120	L2956		D2536	ALA
L4020			Q3563	A3470	LEU	LEU	ASP	M3121	L2956		D2536	ALA
M4021			Q3563	A3471	LEU	LEU	ASP	M3122	L2956		D2536	ALA
P4037			Q3563	A3472	LEU	LEU	ASP	M3123	L2956		D2536	ALA
Y4049			Q3563	A3473	LEU	LEU	ASP	M3124	L2956		D2536	ALA
Q4065			Q3563	A3474	LEU	LEU	ASP	M3125	L2956		D2536	ALA
K4082			Q3563	A3475	LEU	LEU	ASP	M3126	L2956		D2536	ALA
T4086			Q3563	A3476	LEU	LEU	ASP	M3127	L2956		D2536	ALA
A4087			Q3563	A3477	LEU	LEU	ASP	M3128	L2956		D2536	ALA
V4088			Q3563	A3478	LEU	LEU	ASP	M3129	L2956		D2536	ALA
R4092			Q3563	A3479	LEU	LEU	ASP	M3130	L2956		D2536	ALA
M4095			Q3563	A3480	LEU	LEU	ASP	M3131	L2956		D2536	ALA
L4096			Q3563	A3481	LEU	LEU	ASP	M3132	L2956		D2536	ALA
K4097			Q3563	A3482	LEU	LEU	ASP	M3133	L2956		D2536	ALA
W4105			Q3563	A3483	LEU	LEU	ASP	M3134	L2956		D2536	ALA
M4107			Q3563	A3484	LEU	LEU	ASP	M3135	L2956		D2536	ALA
L4116			Q3563	A3485	LEU	LEU	ASP	M3136	L2956		D2536	ALA
Q4117			Q3563	A3486	LEU	LEU	ASP	M3137	L2956		D2536	ALA
P4118			Q3563	A3487	LEU	LEU	ASP	M3138	L2956		D2536	ALA
N4131			Q3563	A3488	LEU	LEU	ASP	M3139	L2956		D2536	ALA
P4132			Q3563	A3489	LEU	LEU	ASP	M3140	L2956		D2536	ALA
K4133			Q3563	A3490	LEU	LEU	ASP	M3141	L2956		D2536	ALA
V4135			Q3563	A3491	LEU	LEU	ASP	M3142	L2956		D2536	ALA
N4137			Q3563	A3492	LEU	LEU	ASP	M3143	L2956		D2536	ALA
L4138			Q3563	A3493	LEU	LEU	ASP	M3144	L2956		D2536	ALA
P4150			Q3563	A3494	LEU	LEU	ASP	M3145	L2956		D2536	ALA
N4156			Q3563	A3495	LEU	LEU	ASP	M3146	L2956		D2536	ALA
			Q3563	A3496	LEU	LEU	ASP	M3147	L2956		D2536	ALA
			Q3563	A3497	LEU	LEU	ASP	M3148	L2956		D2536	ALA
			Q3563	A3498	LEU	LEU	ASP	M3149	L2956		D2536	ALA
			Q3563	A3499	LEU	LEU	ASP	M3150	L2956		D2536	ALA
			Q3563	A3500	LEU	LEU	ASP	M3151	L2956		D2536	ALA
			Q3563	A3501	LEU	LEU	ASP	M3152	L2956		D2536	ALA
			Q3563	A3502	LEU	LEU	ASP	M3153	L2956		D2536	ALA
			Q3563	A3503	LEU	LEU	ASP	M3154	L2956		D2536	ALA
			Q3563	A3504	LEU	LEU	ASP	M3155	L2956		D2536	ALA
			Q3563	A3505	LEU	LEU	ASP	M3156	L2956		D2536	ALA
			Q3563	A3506	LEU	LEU	ASP	M3157	L2956		D2536	ALA
			Q3563	A3507	LEU	LEU	ASP	M3158	L2956		D2536	ALA
			Q3563	A3508	LEU	LEU	ASP	M3159	L2956		D2536	ALA
			Q3563	A3509	LEU	LEU	ASP	M3160	L2956		D2536	ALA
			Q3563	A3510	LEU	LEU	ASP	M3161	L2956		D2536	ALA
			Q3563	A3511	LEU	LEU	ASP	M3162	L2956		D2536	ALA
			Q3563	A3512	LEU	LEU	ASP	M3163	L2956		D2536	ALA
			Q3563	A3513	LEU	LEU	ASP	M3164	L2956		D2536	ALA
			Q3563	A3514	LEU	LEU	ASP	M3165	L2956		D2536	ALA
			Q3563	A3515	LEU	LEU	ASP	M3166	L2956		D2536	ALA
			Q3563	A3516	LEU	LEU	ASP	M3167	L2956		D2536	ALA
			Q3563	A3517	LEU	LEU	ASP	M3168	L2956		D2536	ALA
			Q3563	A3518	LEU	LEU	ASP	M3169	L2956		D2536	ALA
			Q3563	A3519	LEU	LEU	ASP	M3170	L2956		D2536	ALA
			Q3563	A3520	LEU	LEU	ASP	M3171	L2956		D2536	ALA
			Q3563	A3521	LEU	LEU	ASP	M3172	L2956		D2536	ALA
			Q3563	A3522	LEU	LEU	ASP	M3173	L2956		D2536	ALA
			Q3563	A3523	LEU	LEU	ASP	M3174	L2956		D2536	ALA
			Q3563	A3524	LEU	LEU	ASP	M3175	L2956		D2536	ALA
			Q3563	A3525	LEU	LEU	ASP	M3176	L2956		D2536	ALA
			Q3563	A3526	LEU	LEU	ASP	M3177	L2956		D2536	ALA
			Q3563	A3527	LEU	LEU	ASP	M3178	L2956		D2536	ALA
			Q3563	A3528	LEU	LEU	ASP	M3179	L2956		D2536	ALA
			Q3563	A3529	LEU	LEU	ASP	M3180	L2956		D2536	ALA
			Q3563	A3530	LEU	LEU	ASP	M3181	L2956		D2536	ALA
			Q3563	A3531	LEU	LEU	ASP	M3182	L2956		D2536	ALA
			Q3563	A3532	LEU	LEU	ASP	M3183	L2956		D2536	ALA
			Q3563	A3533	LEU	LEU	ASP	M3184	L2956		D2536	ALA
			Q3563	A3534	LEU	LEU	ASP	M3185	L2956		D2536	ALA
			Q3563	A3535	LEU	LEU	ASP	M3186	L2956		D2536	ALA
			Q3563	A3536	LEU	LEU	ASP	M3187	L2956		D2536	ALA
			Q3563	A3537	LEU	LEU	ASP	M3188	L2956		D2536	ALA
			Q3563	A3538	LEU	LEU	ASP	M3189	L2956		D2536	ALA
			Q3563	A3539	LEU	LEU	ASP	M3190	L2956		D2536	ALA
			Q3563	A3540	LEU	LEU	ASP	M3191	L2956		D2536	ALA
			Q3563	A3541	LEU	LEU	ASP	M3192	L2956		D2536	ALA
			Q3563	A3542	LEU	LEU	ASP	M3193	L2956		D2536	ALA
			Q3563	A3543	LEU	LEU	ASP	M3194	L2956		D2536	ALA
			Q3563	A3544	LEU	LEU	ASP	M3195	L2956		D2536	ALA
			Q3563	A3545	LEU	LEU	ASP	M3196	L2956		D2536	ALA
			Q3563	A3546	LEU	LEU	ASP	M3197	L2956		D2536	ALA
			Q3563	A3547	LEU	LEU	ASP	M3198	L2956		D2536	ALA
			Q3563	A3548	LEU	LEU	ASP	M3199	L2956		D2536	ALA
			Q3563	A3549	LEU	LEU	ASP	M3200	L2956		D2536	ALA
			Q3563	A3550	LEU	LEU	ASP	M3201	L2956		D2536	ALA
			Q3563	A3551	LEU	LEU	ASP	M3202	L2956		D2536	ALA
			Q3563	A3552	LEU	LEU	ASP	M3203	L2956		D2536	ALA
			Q3563	A3553	LEU	LEU	ASP	M3204	L2956		D2536	ALA
			Q3563	A3554	LEU	LEU	ASP	M3205	L2956		D2536	ALA
			Q3563	A3555	LEU	LEU	ASP	M3206	L2956		D2536	ALA
			Q3563	A3556	LEU	LEU	ASP	M3207	L2956		D2536	ALA
			Q3563	A3557	LEU	LEU	ASP	M3208	L2956		D2536	ALA
			Q3563	A3558	LEU	LEU	ASP	M3209	L2956		D2536	ALA
			Q3563	A3559	LEU	LEU	ASP	M3210	L2956		D2536	ALA
			Q3563	A3560	LEU	LEU	ASP	M3211	L2956		D2536	ALA
			Q3563	A3561	LEU	LEU	ASP	M3212	L2956		D2536	ALA
			Q3563	A3562	LEU	LEU	ASP	M3213	L2956		D2536	ALA
			Q3563	A3563	LEU	LEU	ASP	M3214	L2956		D2536	ALA
			Q3563	A3564	LEU	LEU	ASP	M3215	L2956		D2536	ALA
			Q3563	A3565	LEU	LEU	ASP	M3216	L2956		D2536	ALA
			Q3563	A3566	LEU	LEU	ASP	M3217	L2956		D2536	ALA
			Q3563	A3567	LEU	LEU	ASP	M3218	L2956		D2536	ALA
			Q3563	A3568	LEU	LEU	ASP	M3219	L2956		D2536	ALA
			Q3563	A3569	LEU	LEU	ASP	M3220	L2956		D2536	ALA
			Q3563	A3570	LEU	LEU	ASP	M3221	L2956		D2536	ALA
			Q3563	A3571	LEU	LEU	ASP	M3222	L2956		D2536	ALA
			Q3563	A3572	LEU	LEU	ASP	M3223	L2956		D2536	ALA
			Q3563	A3573	LEU	LEU	ASP	M3224	L2956		D2536	ALA
			Q3563	A3574	LEU	LEU	ASP	M3225	L2956		D2536	ALA
			Q3563	A3575	LEU	LEU	ASP	M3226	L2956		D2536	ALA
			Q3563	A3576	LEU	LEU	ASP	M3227	L2956		D2536	ALA
			Q3563	A3577	LEU	LEU	ASP	M3228	L2956		D2536	ALA
			Q3563	A3578	LEU	LEU	ASP	M3229	L2956		D2536	ALA
			Q3563	A3579	LEU	LEU	ASP	M3230	L2956		D2536	ALA
			Q3563	A3580	LEU	LEU	ASP	M3231	L2956		D2536	ALA
			Q3563	A3581	LEU	LEU	ASP	M3232	L2956		D2536	ALA
			Q3563	A3582	LEU	LEU	ASP	M3233	L2956		D2536	ALA
			Q3563	A3583	LEU	LEU	ASP	M3234				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.763	Depositor
Minimum map value	-1.378	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	A	0.13	0/24093	0.29	0/32651
1	B	0.13	0/24093	0.30	0/32651
All	All	0.13	0/48186	0.29	0/65302

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	23593	0	23658	333	0
1	B	23593	0	23657	368	0
2	A	81	0	36	3	0
2	B	81	0	36	2	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	47414	0	47411	700	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (700) 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:2320:ASP:OD1	1:A:2321:ASP:N	2.12	0.83
1:B:2320:ASP:OD1	1:B:2321:ASP:N	2.13	0.80
1:B:3970:VAL:HB	1:B:3989:ARG:HD3	1.65	0.78
1:B:2452:LEU:HD13	1:B:2729:ARG:HH21	1.52	0.73
1:B:2492:ARG:HE	1:B:2525:PRO:HG2	1.54	0.73
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.70	0.72
1:A:4544:ASN:HA	1:A:4573:ASN:HD21	1.55	0.71
1:A:2452:LEU:HD13	1:A:2729:ARG:HH21	1.54	0.71
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.72	0.71
1:B:2600:GLY:HA3	1:B:2603:MET:HE2	1.72	0.70
1:A:4488:GLN:HE22	1:A:4509:VAL:HG23	1.56	0.70
1:B:2221:MET:HG2	1:B:2343:PHE:HB2	1.74	0.70
1:B:4541:LEU:HD11	1:B:4590:LEU:HB3	1.72	0.69
1:B:3114:ASP:O	1:B:3140:ARG:NH2	2.26	0.69
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.75	0.69
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.74	0.68
1:B:1478:VAL:HG12	1:B:1488:ARG:HH21	1.58	0.68
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.76	0.68
1:A:1959:GLU:HB3	1:A:1962:ARG:HD3	1.74	0.67
1:B:3485:GLU:N	1:B:3485:GLU:OE1	2.27	0.67
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.76	0.67
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.28	0.67
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.27	0.67
1:B:4037:PRO:HB2	1:B:4118:PRO:HG2	1.77	0.67
1:B:2481:MET:HE2	1:B:2486:LEU:HA	1.77	0.66
1:B:2921:ARG:HH11	1:B:3092:ASN:HD21	1.41	0.66
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.29	0.66
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.77	0.66
1:B:1623:ARG:NH2	1:B:1634:ASP:OD1	2.28	0.66
1:B:4150:PRO:O	1:B:4195:ARG:NH2	2.26	0.66
1:B:2623:SER:OG	1:B:3081:THR:O	2.14	0.65
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.77	0.65
1:A:2934:LEU:HD11	1:A:3068:MET:HE3	1.77	0.65
1:B:4544:ASN:HA	1:B:4573:ASN:HD21	1.61	0.65
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.77	0.65
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	1.79	0.65
1:A:2091:ARG:NH2	2:A:4701:ADP:O2A	2.29	0.65
1:B:3502:THR:HG22	1:B:3542:GLN:HB3	1.78	0.65
1:B:3981:THR:HG23	1:B:3984:GLY:H	1.61	0.65
1:B:2481:MET:HE3	1:B:2485:GLN:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.78	0.65
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	1.78	0.65
1:B:3580:LEU:HD13	1:B:3600:ILE:HD11	1.77	0.65
1:B:1962:ARG:NH2	1:B:2314:ASN:OD1	2.30	0.64
1:B:2974:GLU:OE1	1:B:2977:ARG:NH1	2.30	0.64
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.79	0.64
1:B:3745:LEU:HD11	1:B:3776:GLU:HG2	1.78	0.64
1:B:4020:ILE:HG23	1:B:4021:MET:HE2	1.78	0.64
1:B:3839:VAL:HG21	1:B:3863:LEU:HA	1.80	0.64
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.80	0.64
1:A:1567:ARG:O	1:A:1571:ILE:HG13	1.97	0.64
1:B:3638:VAL:HG12	1:B:3681:THR:HB	1.80	0.64
1:B:2969:GLY:HA2	1:B:3004:PHE:HE1	1.63	0.64
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	1.79	0.63
1:B:4271:ARG:HG3	1:B:4633:ARG:HH21	1.63	0.63
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.64	0.63
1:A:2115:LYS:NZ	1:A:2126:GLU:OE2	2.32	0.63
1:B:3983:ILE:O	1:B:3987:ILE:HD12	1.99	0.62
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.81	0.62
1:B:1810:HIS:NE2	1:B:1876:GLN:O	2.32	0.62
1:B:1959:GLU:HB3	1:B:1962:ARG:HD3	1.81	0.62
1:B:2816:LEU:HD11	1:B:2820:GLY:HA3	1.81	0.62
1:A:3983:ILE:O	1:A:3987:ILE:HD12	1.99	0.62
1:B:4304:GLU:OE1	1:B:4304:GLU:N	2.29	0.62
1:B:1721:VAL:HA	1:B:1724:VAL:HG12	1.82	0.62
1:B:3017:VAL:HB	1:B:3020:LEU:HB2	1.81	0.62
1:A:2188:GLU:OE2	1:A:2243:ARG:NH2	2.32	0.61
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.32	0.61
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.33	0.61
1:A:3985:GLN:OE1	1:A:3989:ARG:NH1	2.32	0.61
1:B:1756:ILE:O	1:B:1760:GLU:HG2	2.00	0.61
1:B:2956:LEU:HD23	1:B:2989:LYS:HB3	1.83	0.61
1:B:2149:LEU:HD11	1:B:2157:LEU:HD22	1.83	0.61
1:A:3984:GLY:O	1:A:3988:HIS:ND1	2.34	0.61
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.83	0.61
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.34	0.61
1:B:4393:GLN:N	1:B:4393:GLN:OE1	2.34	0.61
1:A:1478:VAL:HG21	1:A:1488:ARG:HE	1.65	0.61
1:B:2138:ILE:HD12	1:B:2161:LEU:HD22	1.83	0.61
1:B:4287:LYS:HD2	1:B:4290:GLY:HA2	1.82	0.61
1:A:1515:VAL:HG13	1:A:1516:PHE:HD1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.19	0.60
1:B:4391:ILE:HD11	1:B:4479:VAL:HG13	1.83	0.60
1:B:4419:MET:HE2	1:B:4515:PHE:HD2	1.65	0.60
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.34	0.60
1:A:1751:VAL:HG11	1:A:1878:LYS:HE3	1.83	0.60
1:A:2179:ARG:NH2	1:A:2205:GLU:OE2	2.34	0.60
1:B:3985:GLN:OE1	1:B:3989:ARG:NH2	2.35	0.60
1:B:4065:GLN:HB3	1:B:4092:ARG:HD2	1.83	0.60
1:A:4433:ASP:HB3	1:A:4448:LEU:HD21	1.83	0.60
1:B:3974:TRP:NE1	1:B:3976:GLU:OE2	2.32	0.59
1:B:2837:LEU:HD13	1:B:2842:GLU:HB3	1.84	0.59
1:A:1567:ARG:HH12	1:B:3043:MET:HB2	1.67	0.59
1:A:1962:ARG:NH2	1:A:2314:ASN:OD1	2.35	0.59
1:B:4505:LYS:NZ	1:B:4554:ASP:O	2.35	0.59
1:B:2492:ARG:NH1	1:B:2543:GLY:O	2.36	0.59
1:A:4031:VAL:HG21	1:A:4058:LEU:HD21	1.84	0.58
1:B:3239:LYS:HG2	1:B:3451:TYR:CZ	2.38	0.58
1:B:4430:ASP:OD2	1:B:4447:TYR:OH	2.21	0.58
1:A:3451:TYR:HA	1:A:3454:LEU:HG	1.85	0.58
1:B:2590:PRO:HA	1:B:2708:PHE:O	2.02	0.58
1:A:2590:PRO:HA	1:A:2708:PHE:O	2.04	0.58
1:A:4296:MET:HE3	1:A:4297:PRO:HD2	1.85	0.58
1:B:2290:SER:HB2	1:B:2295:LEU:HG	1.85	0.58
1:B:4096:LEU:HD13	1:B:4105:TRP:HH2	1.68	0.58
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.86	0.58
1:A:1570:SER:O	1:A:1574:GLU:HG3	2.04	0.58
1:A:3985:GLN:O	1:A:3989:ARG:HG3	2.04	0.58
1:B:4227:ALA:HB2	1:B:4233:ILE:HD12	1.85	0.58
1:A:3880:HIS:HD2	1:A:4021:MET:HG3	1.68	0.58
1:B:2562:VAL:HG11	1:B:2755:MET:HB3	1.86	0.58
1:B:3191:ARG:HG2	1:B:3503:ILE:HD13	1.85	0.58
1:B:2784:PHE:HB2	1:B:2794:TYR:HE2	1.68	0.57
1:A:4382:THR:O	1:A:4386:ASN:ND2	2.31	0.57
1:B:4508:HIS:CE1	1:B:4587:LEU:HD11	2.40	0.57
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.69	0.57
1:A:3031:THR:O	1:A:3035:GLU:HG3	2.04	0.57
1:A:4505:LYS:NZ	1:A:4557:SER:O	2.31	0.57
1:B:3451:TYR:HA	1:B:3454:LEU:HG	1.87	0.57
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	1.85	0.57
1:A:1515:VAL:HG13	1:A:1516:PHE:CD1	2.40	0.57
1:A:2000:GLU:OE1	1:A:2005:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.87	0.56
1:A:1577:ALA:O	1:A:1581:LYS:HG3	2.05	0.56
1:A:3191:ARG:HG2	1:A:3503:ILE:HD13	1.87	0.56
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.70	0.56
1:B:4292:LYS:HD2	1:B:4293:ASP:H	1.71	0.56
1:B:1623:ARG:NH1	1:B:1632:VAL:O	2.38	0.56
1:B:2967:TYR:OH	1:B:2975:ASP:OD2	2.20	0.56
1:B:2848:GLU:O	1:B:2852:THR:HG23	2.05	0.56
1:B:1959:GLU:OE1	1:B:2025:ARG:NH1	2.38	0.56
1:B:4150:PRO:HG3	1:B:4159:ARG:NH1	2.20	0.56
1:A:3194:LEU:HD23	1:A:3500:MET:HG2	1.86	0.56
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.38	0.56
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.03	0.56
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	1.87	0.56
1:B:1850:GLN:HB3	1:B:1856:GLN:HG2	1.88	0.56
1:B:3723:ASP:OD1	1:B:3724:VAL:N	2.39	0.56
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.88	0.56
1:B:3215:VAL:HG21	1:B:3479:LEU:HD11	1.88	0.56
1:B:4387:TRP:O	1:B:4391:ILE:HG12	2.06	0.56
1:A:2837:LEU:O	1:A:2843:ARG:NH2	2.39	0.55
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.36	0.55
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	1.88	0.55
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.39	0.55
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.87	0.55
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.27	0.55
1:B:3929:VAL:O	1:B:3933:GLU:HG3	2.07	0.55
1:A:3239:LYS:HG2	1:A:3451:TYR:CZ	2.42	0.55
1:A:4021:MET:HE3	1:A:4021:MET:HA	1.88	0.55
1:A:4049:TYR:OH	1:A:4191:GLN:NE2	2.40	0.55
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.40	0.55
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.88	0.55
1:A:4412:PHE:HE1	1:A:4516:VAL:HG23	1.72	0.55
1:A:4413:PHE:HD2	1:A:4504:LEU:HD11	1.71	0.55
1:B:2437:LEU:HD21	1:B:2451:ARG:HG3	1.88	0.55
1:B:3935:VAL:HG13	1:B:3947:LEU:HD23	1.89	0.55
1:B:4137:ASN:OD1	1:B:4138:LEU:N	2.40	0.55
1:B:2581:LEU:HD11	1:B:2593:LEU:HD21	1.89	0.54
1:A:2949:PHE:CZ	1:A:2953:MET:HE3	2.41	0.54
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.42	0.54
1:A:3225:LYS:HD2	1:A:3461:ILE:HG13	1.89	0.54
1:B:1873:LEU:O	1:B:1876:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3872:ALA:HB1	1:A:3880:HIS:CD2	2.42	0.54
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.89	0.54
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.40	0.54
1:B:2000:GLU:OE1	1:B:2005:GLN:NE2	2.41	0.54
1:A:1965:GLU:HG2	1:A:2026:SER:HB3	1.88	0.54
1:A:2848:GLU:O	1:A:2852:THR:HG23	2.08	0.54
1:B:2844:ARG:O	1:B:2848:GLU:HG3	2.08	0.54
1:B:3487:GLU:O	1:B:3491:LYS:HG3	2.07	0.54
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.90	0.54
1:B:3984:GLY:O	1:B:3988:HIS:ND1	2.38	0.54
1:A:1817:HIS:CE1	1:A:1881:GLN:HG2	2.43	0.54
1:B:2752:ASN:ND2	1:B:2755:MET:HE2	2.22	0.54
1:A:1959:GLU:OE1	1:A:2025:ARG:NH1	2.41	0.53
1:B:2603:MET:HE1	2:B:4703:ADP:N7	2.22	0.53
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.90	0.53
1:B:3110:THR:O	1:B:3140:ARG:NH1	2.41	0.53
1:A:1810:HIS:CD2	1:A:1878:LYS:HB2	2.42	0.53
1:A:3790:VAL:O	1:A:3793:GLU:HG3	2.08	0.53
1:B:3892:LEU:HD13	1:B:3983:ILE:HG21	1.91	0.53
1:A:1463:LEU:CD2	1:A:1507:MET:HE1	2.39	0.53
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.89	0.53
1:B:3559:ARG:O	1:B:3563:GLN:HG3	2.08	0.53
1:A:1459:LEU:HD22	1:A:1507:MET:HE3	1.89	0.53
1:A:3654:ARG:HG2	1:A:3656:THR:HG23	1.90	0.53
1:B:2134:GLN:O	1:B:2138:ILE:HG12	2.09	0.53
1:B:3127:PRO:HG3	1:B:3538:GLN:HB3	1.91	0.53
1:A:4276:ARG:HH21	1:A:4279:ASP:HB3	1.74	0.53
1:B:1570:SER:O	1:B:1574:GLU:HG3	2.09	0.53
1:B:1914:GLU:HG3	2:B:4701:ADP:H2'	1.91	0.53
1:B:2304:ASP:OD1	1:B:2726:ARG:NH2	2.41	0.53
1:A:1476:ASP:OD2	1:A:1488:ARG:NH1	2.42	0.53
1:B:2231:SER:OG	3:B:4702:ATP:O1A	2.26	0.53
1:A:2457:SER:O	1:A:2461:MET:HG2	2.10	0.52
1:B:1946:VAL:HG22	1:B:2006:VAL:HG21	1.90	0.52
1:B:3546:ASP:OD1	1:B:3547:ILE:N	2.43	0.52
1:A:2112:LYS:O	1:A:2116:GLU:HG2	2.09	0.52
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.40	0.52
1:A:4002:LEU:HD11	1:A:4335:GLN:HB3	1.91	0.52
1:B:2047:GLN:OE1	1:B:2067:ASN:ND2	2.42	0.52
1:A:3131:ASP:N	1:A:3131:ASP:OD1	2.41	0.52
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4277:SER:HA	1:B:4282:PHE:CD2	2.44	0.52
1:A:1564:GLU:OE1	1:A:1564:GLU:N	2.34	0.52
1:A:4394:THR:O	1:A:4490:GLN:NE2	2.36	0.52
1:B:3924:ILE:HD12	1:B:3948:ILE:HG23	1.92	0.52
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.92	0.52
1:B:1934:GLU:OE2	1:B:2261:LYS:NZ	2.36	0.52
1:B:3933:GLU:O	1:B:3937:ARG:HG3	2.09	0.52
1:B:3584:ASN:O	1:B:3651:ARG:NH2	2.43	0.51
1:B:4095:MET:HE3	1:B:4097:LYS:HE2	1.92	0.51
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.92	0.51
1:B:3935:VAL:HG22	1:B:3996:PHE:HE2	1.75	0.51
1:A:1806:ARG:O	1:A:1810:HIS:ND1	2.26	0.51
1:B:2231:SER:HA	1:B:2234:TRP:CD1	2.46	0.51
1:B:2752:ASN:HD22	1:B:2755:MET:HE2	1.76	0.51
1:A:1769:MET:HE1	1:A:1778:LEU:HG	1.93	0.51
1:A:2412:MET:O	1:A:2416:GLN:HG3	2.11	0.51
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.44	0.51
1:B:3454:LEU:HA	1:B:3457:GLU:HG2	1.93	0.51
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.93	0.51
1:B:2066:ALA:HA	1:B:2069:ILE:HG22	1.93	0.51
1:B:2788:THR:HG22	1:B:2789:GLN:HG2	1.93	0.51
1:B:3691:ASP:O	1:B:3695:ARG:HG3	2.10	0.51
1:B:3154:LEU:HG	1:B:3516:TYR:CD1	2.46	0.51
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.93	0.51
1:A:2917:ASP:O	1:A:2921:ARG:HG3	2.11	0.51
1:A:3877:HIS:HA	1:A:3880:HIS:ND1	2.25	0.51
1:A:3928:THR:HG22	1:A:3931:GLN:HG3	1.92	0.51
1:B:1619:LEU:HD21	1:B:1638:LEU:HD23	1.92	0.51
1:B:3161:LEU:HD21	1:B:3524:MET:HE3	1.92	0.51
1:A:1840:SER:HA	1:A:1862:ALA:HB2	1.93	0.51
1:A:2819:GLU:HG3	1:A:2866:ALA:HB2	1.93	0.51
1:A:3225:LYS:HG3	1:A:3465:LEU:HD12	1.92	0.51
1:B:4545:VAL:HG22	1:B:4588:THR:HG22	1.93	0.51
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.44	0.50
1:A:3514:ILE:HD11	1:A:3553:LEU:HD22	1.93	0.50
1:A:4626:ILE:HD13	1:A:4632:PRO:HD3	1.93	0.50
1:B:2665:GLU:HB3	1:B:2668:LEU:HD12	1.91	0.50
1:B:4609:VAL:HG22	1:B:4642:VAL:HB	1.93	0.50
1:A:1873:LEU:O	1:A:1876:GLN:NE2	2.43	0.50
1:B:1478:VAL:O	1:B:1485:ARG:HA	2.11	0.50
1:B:1567:ARG:O	1:B:1571:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3851:ASP:HB3	1:B:3854:GLN:HG2	1.94	0.50
1:B:4307:GLN:O	1:B:4311:LEU:HG	2.10	0.50
1:B:4626:ILE:HD13	1:B:4632:PRO:HD3	1.93	0.50
1:A:1619:LEU:HD21	1:A:1638:LEU:HD23	1.93	0.50
1:A:3161:LEU:HD21	1:A:3524:MET:HE3	1.93	0.50
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.44	0.50
1:B:1574:GLU:OE1	1:B:1603:ARG:NH2	2.27	0.50
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.92	0.50
1:A:3588:LEU:HD21	1:A:3638:VAL:HG11	1.93	0.50
1:A:4271:ARG:HD3	1:A:4633:ARG:NH1	2.26	0.50
1:B:1785:VAL:HG13	1:B:1815:LEU:HD12	1.93	0.50
1:B:3481:SER:O	1:B:3774:LYS:NZ	2.45	0.50
1:B:3514:ILE:HD11	1:B:3553:LEU:HD22	1.94	0.50
1:B:3591:ASP:O	1:B:3682:ARG:HA	2.12	0.50
1:B:4566:GLN:O	1:B:4640:VAL:HA	2.12	0.50
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.94	0.50
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.93	0.50
1:A:3900:THR:OG1	1:A:3902:ASP:OD2	2.19	0.50
1:A:4541:LEU:HB2	1:A:4592:TRP:CZ3	2.47	0.50
1:B:1760:GLU:O	1:B:1764:THR:HG23	2.11	0.50
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.94	0.49
1:B:3731:LEU:O	1:B:3735:GLN:HG3	2.13	0.49
1:B:3825:TYR:OH	1:B:3879:ASP:OD2	2.26	0.49
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.93	0.49
1:B:3135:GLN:O	1:B:3137:PRO:HD3	2.11	0.49
1:B:3208:ILE:HG21	1:B:3486:ARG:HD3	1.94	0.49
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.45	0.49
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	1.95	0.49
1:B:4544:ASN:HD22	1:B:4589:GLN:HE21	1.60	0.49
1:A:1556:ASP:OD2	1:A:1556:ASP:N	2.44	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.94	0.49
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.25	0.49
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.13	0.49
1:B:1839:LEU:O	1:B:1843:ARG:NH1	2.46	0.49
1:B:2104:LYS:HA	1:B:2136:ILE:HD13	1.94	0.49
1:B:2412:MET:O	1:B:2416:GLN:HG3	2.13	0.49
1:B:2433:VAL:HG22	1:B:2498:ILE:HD11	1.95	0.49
1:A:1843:ARG:HH12	1:A:1862:ALA:H	1.61	0.49
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.94	0.49
1:B:3946:ASP:OD1	1:B:3950:LYS:NZ	2.45	0.49
1:A:1494:PHE:O	1:A:1498:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2540:SER:OG	1:A:2544:GLU:O	2.28	0.49
1:A:1934:GLU:OE2	1:A:2261:LYS:NZ	2.37	0.49
1:B:1721:VAL:O	1:B:1725:GLU:HG2	2.12	0.49
1:A:2156:LEU:O	1:A:2160:LEU:HG	2.12	0.49
1:A:4190:ILE:HG13	1:A:4191:GLN:N	2.28	0.49
1:B:2538:GLU:OE2	1:B:2551:LYS:NZ	2.35	0.49
1:B:3654:ARG:NH2	1:B:3668:ASP:OD1	2.45	0.49
1:A:4413:PHE:CD2	1:A:4504:LEU:HD11	2.48	0.49
1:B:2590:PRO:HB2	1:B:2731:VAL:HG12	1.95	0.49
1:B:3143:ILE:HD13	1:B:3541:ILE:HD13	1.95	0.49
1:B:2125:GLY:O	1:B:2128:ALA:N	2.45	0.49
1:A:2103:VAL:HA	1:A:2106:GLU:HG2	1.95	0.48
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.13	0.48
1:B:1706:GLU:O	1:B:1709:MET:HG2	2.13	0.48
1:B:3475:SER:O	1:B:3479:LEU:HG	2.13	0.48
1:A:2592:VAL:HB	1:A:2733:VAL:HG22	1.95	0.48
1:A:2949:PHE:CE2	1:A:2953:MET:HE3	2.48	0.48
1:B:3933:GLU:HA	1:B:3936:VAL:HG22	1.93	0.48
1:B:4082:LYS:O	1:B:4086:THR:HG23	2.14	0.48
1:B:1462:PHE:O	1:B:1465:GLN:HG2	2.14	0.48
1:B:3099:THR:HG23	1:B:3148:VAL:HG11	1.95	0.48
1:B:3451:TYR:CD1	1:B:3454:LEU:HD21	2.48	0.48
1:A:1914:GLU:HG2	2:A:4701:ADP:O1A	2.14	0.48
1:A:2851:ASP:HA	1:A:2867:MET:HE1	1.96	0.48
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.94	0.48
1:B:1661:VAL:HG22	1:B:1676:ILE:HD12	1.94	0.48
1:B:1965:GLU:HG2	1:B:2026:SER:HB3	1.94	0.48
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.48	0.48
1:B:1774:ASP:OD1	1:B:1775:ALA:N	2.43	0.48
1:B:1810:HIS:CD2	1:B:1878:LYS:HB2	2.49	0.48
1:B:1836:PHE:HA	1:B:1839:LEU:HB2	1.95	0.48
1:B:2210:LEU:O	1:B:2214:THR:HG23	2.14	0.48
1:B:2422:ILE:HD13	1:B:2487:GLU:HA	1.95	0.48
1:B:3654:ARG:HG2	1:B:3656:THR:HG23	1.96	0.48
1:A:1752:LEU:O	1:A:1756:ILE:HG13	2.14	0.48
1:A:3621:LYS:HA	1:A:3624:GLU:HG2	1.96	0.48
1:B:2075:LEU:O	1:B:2079:GLN:HB2	2.14	0.48
1:B:2752:ASN:OD1	1:B:2770:THR:OG1	2.17	0.48
1:A:3817:SER:OG	1:A:4346:MET:HB2	2.14	0.48
1:A:4452:ILE:O	1:A:4456:VAL:HG13	2.14	0.48
1:B:4175:GLU:N	1:B:4175:GLU:OE1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1782:LEU:HD13	1:B:1822:THR:HB	1.96	0.47
1:A:1497:VAL:O	1:A:1501:ILE:HG13	2.13	0.47
1:A:4082:LYS:O	1:A:4086:THR:HG23	2.14	0.47
1:B:1497:VAL:O	1:B:1501:ILE:HG13	2.14	0.47
1:B:3683:ASP:HB3	1:B:3686:VAL:HG13	1.96	0.47
1:B:3770:LEU:O	1:B:3774:LYS:HG2	2.14	0.47
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.96	0.47
1:A:2925:ILE:HD12	1:A:3090:VAL:HG21	1.96	0.47
1:A:3206:ARG:HG2	1:A:3206:ARG:HH11	1.78	0.47
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.96	0.47
1:B:3491:LYS:HE3	1:B:3491:LYS:HB3	1.68	0.47
1:A:2478:ASP:OD1	1:A:2479:PHE:N	2.47	0.47
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.47	0.47
1:B:1476:ASP:OD1	1:B:1488:ARG:HD2	2.13	0.47
1:B:2905:LEU:HD11	1:B:3652:GLU:HB3	1.96	0.47
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.15	0.47
1:A:3787:THR:HA	1:A:3790:VAL:HG12	1.97	0.47
1:A:4172:SER:OG	1:A:4173:PRO:HD3	2.15	0.47
1:A:4308:TRP:CH2	1:A:4312:LEU:HD21	2.50	0.47
1:B:2359:CYS:HB2	1:B:2361:MET:HE2	1.96	0.47
1:A:2053:MET:HE1	1:A:2094:LYS:HG3	1.96	0.47
1:A:4065:GLN:HB3	1:A:4092:ARG:HD2	1.95	0.47
1:B:1978:ILE:HD11	1:B:2001:LEU:HD11	1.96	0.47
1:B:2854:ALA:HB3	1:B:2867:MET:HE1	1.96	0.47
1:B:2917:ASP:O	1:B:2921:ARG:HG3	2.15	0.47
1:A:1558:LYS:HD3	1:A:1565:THR:HG21	1.97	0.47
1:A:1860:GLN:HA	1:A:1864:ALA:O	2.15	0.47
1:A:2982:ARG:HA	1:A:2986:LYS:HE2	1.96	0.47
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.97	0.47
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.96	0.47
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.49	0.47
1:B:3031:THR:O	1:B:3035:GLU:HG3	2.14	0.47
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.96	0.47
1:B:4296:MET:HE3	1:B:4297:PRO:HD2	1.97	0.47
1:B:4331:LEU:O	1:B:4335:GLN:HG3	2.14	0.47
1:B:4435:VAL:O	1:B:4439:GLU:HG3	2.14	0.47
1:A:4424:LEU:HD12	1:A:4428:ARG:HG3	1.97	0.47
1:B:1840:SER:HA	1:B:1862:ALA:HB2	1.97	0.47
1:B:1987:ASN:OD1	1:B:1990:TYR:HB3	2.15	0.47
1:B:2039:LEU:HD12	1:B:4254:GLY:HA2	1.97	0.47
1:B:2538:GLU:HB3	1:B:2548:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2075:LEU:O	1:A:2079:GLN:HB2	2.14	0.47
1:A:3606:ASP:OD1	1:A:3606:ASP:N	2.47	0.47
1:B:3835:ILE:HD13	1:B:3867:ALA:HA	1.97	0.47
1:B:4528:VAL:HG11	1:B:4592:TRP:HB2	1.96	0.47
1:B:4178:ARG:NH2	1:B:4297:PRO:O	2.48	0.47
1:B:2132:PRO:HB2	1:B:2135:GLU:HB2	1.96	0.46
1:A:3475:SER:O	1:A:3479:LEU:HG	2.14	0.46
1:A:4039:THR:HG23	1:A:4142:GLY:HA2	1.98	0.46
1:B:4007:MET:O	1:B:4011:THR:HG23	2.14	0.46
1:B:4433:ASP:HB3	1:B:4448:LEU:HD21	1.97	0.46
1:A:2176:THR:O	1:A:2180:GLU:HG2	2.15	0.46
1:A:2620:LEU:HD21	1:A:2634:THR:OG1	2.15	0.46
1:A:3451:TYR:CD1	1:A:3454:LEU:HD21	2.50	0.46
1:B:3237:ASN:O	1:B:3241:LYS:HG2	2.14	0.46
1:A:1987:ASN:OD1	1:A:1990:TYR:HB3	2.14	0.46
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	1.97	0.46
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.97	0.46
1:B:2103:VAL:HA	1:B:2106:GLU:HG2	1.96	0.46
1:B:4013:LEU:HD13	1:B:4017:PHE:CE2	2.51	0.46
1:A:4095:MET:HE3	1:A:4097:LYS:HE2	1.97	0.46
1:B:3154:LEU:HD21	1:B:3532:TRP:HZ2	1.81	0.46
1:A:1598:GLN:O	1:A:1602:GLU:HG3	2.15	0.46
1:B:2410:SER:HB3	1:B:2413:LEU:HB2	1.98	0.46
1:B:2446:ILE:HG12	1:B:2505:ASP:O	2.16	0.46
1:B:3133:LEU:HD11	1:B:3141:GLU:HB3	1.98	0.46
1:B:3954:ASP:OD1	1:B:3957:PHE:N	2.49	0.46
1:B:1860:GLN:HA	1:B:1864:ALA:O	2.15	0.46
1:B:2138:ILE:HD11	1:B:2165:PHE:CG	2.51	0.46
1:A:3880:HIS:CD2	1:A:4021:MET:HG3	2.48	0.46
1:B:1989:ASN:OD1	1:B:1990:TYR:N	2.48	0.46
1:A:2138:ILE:HG22	1:A:2170:TYR:HB2	1.98	0.46
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.97	0.46
1:B:1469:VAL:O	1:B:1473:TYR:HB2	2.15	0.46
1:B:2820:GLY:O	1:B:2824:ILE:HG13	2.16	0.46
1:B:3763:ASP:OD1	1:B:3763:ASP:N	2.49	0.46
1:B:4509:VAL:HG11	1:B:4520:TYR:CZ	2.51	0.46
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.17	0.45
1:A:3967:GLU:OE2	1:A:3968:GLN:NE2	2.49	0.45
1:B:1843:ARG:HH12	1:B:1862:ALA:H	1.64	0.45
1:B:2104:LYS:O	1:B:2108:ILE:HG12	2.16	0.45
1:B:2895:ALA:O	1:B:2898:LYS:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.98	0.45
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.98	0.45
1:A:4564:LYS:HD3	1:A:4584:ALA:HA	1.98	0.45
1:B:1572:SER:O	1:B:1576:LEU:HG	2.16	0.45
1:B:2374:ILE:HD13	1:B:2452:LEU:HD21	1.97	0.45
1:B:3113:MET:SD	1:B:3184:ALA:HA	2.57	0.45
1:A:1850:GLN:HG3	1:A:1852:ASP:H	1.82	0.45
1:A:2065:LEU:HD22	1:A:2137:LEU:HD12	1.97	0.45
1:A:2995:ASP:OD2	1:A:3067:THR:OG1	2.34	0.45
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.17	0.45
1:B:3608:LYS:HE3	1:B:3608:LYS:HB2	1.69	0.45
1:A:3030:MET:HE2	1:A:3030:MET:HA	1.98	0.45
1:B:1565:THR:O	1:B:1569:GLN:HG2	2.16	0.45
1:B:1798:MET:HE2	1:B:1798:MET:HB3	1.86	0.45
1:B:2308:ASP:O	1:B:2312:VAL:HG12	2.17	0.45
1:B:2572:LEU:O	1:B:2576:ARG:HG3	2.16	0.45
1:B:3691:ASP:OD1	1:B:3692:LEU:N	2.48	0.45
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.98	0.45
1:A:1863:ASN:HD22	1:A:1897:GLU:HG2	1.81	0.45
1:B:2297:LYS:O	1:B:2338:ASN:ND2	2.46	0.45
1:A:1477:LEU:HA	1:A:1486:LEU:O	2.17	0.45
1:A:2065:LEU:HB3	1:A:2137:LEU:HD11	1.99	0.45
1:A:2572:LEU:O	1:A:2576:ARG:HG3	2.16	0.45
1:B:4450:THR:O	1:B:4454:GLU:HG3	2.16	0.45
1:A:1580:LYS:O	1:A:1584:LYS:HG2	2.17	0.45
1:B:1663:SER:HG	1:B:1677:SER:HG	1.60	0.45
1:B:4516:VAL:HG12	1:B:4519:ALA:H	1.82	0.45
1:A:3452:ALA:HA	1:A:3455:ILE:HG22	1.99	0.45
1:B:2073:PHE:HZ	1:B:2096:VAL:HG21	1.81	0.45
1:B:3786:GLU:O	1:B:3789:ILE:HG12	2.17	0.45
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.32	0.45
1:B:1478:VAL:HG12	1:B:1488:ARG:NH2	2.28	0.45
1:B:1752:LEU:O	1:B:1756:ILE:HG13	2.16	0.45
1:B:2224:GLY:O	1:B:2346:GLN:HA	2.17	0.45
1:B:4107:MET:HE2	1:B:4135:PRO:HG3	1.99	0.45
1:A:1802:PRO:O	1:A:1806:ARG:HG3	2.17	0.45
1:A:2760:PRO:HA	1:A:2763:ARG:HG3	1.99	0.45
1:B:1537:TRP:CH2	1:B:1582:VAL:HG21	2.52	0.45
1:B:2894:LYS:HE3	1:B:2894:LYS:HB2	1.79	0.45
1:B:3868:PHE:CZ	1:B:4018:MET:HG2	2.51	0.45
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1945:PHE:HB3	1:A:1978:ILE:HD11	1.98	0.44
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.23	0.44
1:A:3492:THR:HA	1:A:3495:THR:HG22	1.99	0.44
1:A:4007:MET:O	1:A:4011:THR:HG23	2.17	0.44
1:B:2943:LYS:HG2	1:B:3094:PHE:CD2	2.52	0.44
1:B:3206:ARG:HH22	1:B:3207:LYS:HE3	1.82	0.44
1:B:3909:LEU:HB3	1:B:4344:LEU:HD21	1.99	0.44
1:B:4156:ASN:C	1:B:4156:ASN:HD22	2.25	0.44
1:A:1949:CYS:SG	1:A:2012:MET:HE3	2.57	0.44
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	2.00	0.44
1:A:2820:GLY:O	1:A:2824:ILE:HG13	2.17	0.44
1:A:2894:LYS:HE3	1:A:2894:LYS:HB2	1.81	0.44
1:B:1458:ALA:HA	1:B:1461:GLU:HG2	1.98	0.44
1:B:4288:VAL:HG11	1:B:4294:ILE:HG13	2.00	0.44
1:A:3028:THR:O	1:A:3032:GLN:HG3	2.17	0.44
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	2.00	0.44
1:B:3100:GLU:O	1:B:3104:GLN:HG3	2.17	0.44
1:B:4172:SER:OG	1:B:4173:PRO:HD3	2.16	0.44
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.83	0.44
1:B:3606:ASP:OD1	1:B:3606:ASP:N	2.49	0.44
1:B:3817:SER:O	1:B:4346:MET:HG2	2.16	0.44
1:A:1760:GLU:O	1:A:1764:THR:HG23	2.17	0.44
1:A:3608:LYS:HE3	1:A:3608:LYS:HB2	1.81	0.44
1:A:4173:PRO:HG2	1:A:4176:ARG:HH21	1.82	0.44
1:B:1724:VAL:HG23	1:B:1727:PHE:HD2	1.82	0.44
1:B:3588:LEU:HD21	1:B:3638:VAL:HG11	2.00	0.44
1:B:3780:VAL:O	1:B:3784:VAL:HG23	2.18	0.44
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.43	0.44
1:A:2061:THR:OG1	1:A:2133:GLU:OE1	2.32	0.44
1:B:2356:VAL:HG13	1:B:2361:MET:HE3	2.00	0.44
1:B:2592:VAL:HB	1:B:2733:VAL:HG22	2.00	0.44
1:B:2641:TYR:CZ	1:B:2650:LEU:HD13	2.53	0.44
1:A:2279:LEU:HA	1:A:2698:GLN:HG2	2.00	0.43
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.18	0.43
1:A:2956:LEU:HD13	1:A:2991:ALA:HB2	2.00	0.43
1:A:4065:GLN:OE1	1:A:4092:ARG:NH1	2.49	0.43
1:B:2154:ILE:HB	1:B:2155:PRO:HD3	2.00	0.43
1:B:3781:THR:O	1:B:3785:GLU:OE1	2.36	0.43
1:B:3931:GLN:O	1:B:3935:VAL:HG23	2.17	0.43
1:A:2593:LEU:HD11	1:A:2605:LEU:HB2	1.99	0.43
1:A:4302:ARG:HG2	1:A:4302:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2411:PRO:O	1:B:2415:ILE:HG13	2.19	0.43
1:B:3190:LYS:HB3	1:B:3503:ILE:HD11	2.00	0.43
1:A:4443:LYS:HB3	1:A:4443:LYS:HE3	1.71	0.43
1:A:4519:ALA:HA	1:A:4522:THR:HG22	2.00	0.43
1:B:2206:LYS:HD3	1:B:2206:LYS:HA	1.76	0.43
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.54	0.43
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.45	0.43
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.54	0.43
1:B:2423:MET:HE3	1:B:2423:MET:HB2	1.86	0.43
1:B:4131:ASN:OD1	1:B:4133:LYS:HG2	2.18	0.43
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	2.01	0.43
1:B:1537:TRP:HH2	1:B:1582:VAL:HG21	1.84	0.43
1:B:1618:TYR:HD1	1:B:1621:ARG:NH2	2.16	0.43
1:B:2937:GLY:C	1:B:3070:PRO:HD3	2.43	0.43
1:B:3781:THR:O	1:B:3784:VAL:HB	2.18	0.43
1:B:4288:VAL:O	1:B:4319:SER:OG	2.29	0.43
1:B:4343:MET:HE2	1:B:4343:MET:HB3	1.88	0.43
1:B:4424:LEU:HA	1:B:4482:PHE:HZ	1.84	0.43
1:B:4508:HIS:ND1	1:B:4587:LEU:HD11	2.34	0.43
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.84	0.43
1:B:1697:LYS:HB2	1:B:1700:GLU:OE2	2.18	0.43
1:B:2802:TRP:CZ2	1:B:2829:ALA:HB2	2.54	0.43
1:B:3591:ASP:O	1:B:3591:ASP:OD1	2.37	0.43
1:B:4600:LYS:HD3	1:B:4604:VAL:HB	2.00	0.43
1:A:4131:ASN:OD1	1:A:4133:LYS:HG2	2.19	0.43
1:B:4511:LEU:HD12	1:B:4563:LEU:HD21	2.00	0.43
1:A:3908:PHE:CZ	1:A:4340:ILE:HD11	2.54	0.43
1:B:2517:TYR:CE2	1:B:2521:ILE:HD13	2.54	0.43
1:B:3452:ALA:HA	1:B:3455:ILE:HG22	2.01	0.43
1:B:3520:PHE:HB3	1:B:3524:MET:HB3	2.01	0.43
1:A:1797:LEU:HD23	1:A:1797:LEU:HA	1.89	0.43
1:A:3100:GLU:O	1:A:3104:GLN:HG3	2.19	0.43
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.19	0.43
1:B:2865:LYS:HA	1:B:2865:LYS:HD2	1.91	0.43
1:B:3158:ASN:ND2	1:B:3169:MET:O	2.48	0.43
1:B:3497:LYS:HA	1:B:3497:LYS:HD3	1.66	0.43
1:B:3924:ILE:HG23	1:B:3927:LEU:HB2	2.01	0.43
1:A:2104:LYS:O	1:A:2108:ILE:HG12	2.19	0.42
1:A:3209:LYS:O	1:A:3212:VAL:HG12	2.19	0.42
1:B:1467:ARG:HG2	1:B:1523:TRP:HZ2	1.84	0.42
1:B:1985:HIS:CD2	1:B:1997:ILE:HG13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3808:CYS:HB3	1:B:3832:PHE:HZ	1.85	0.42
1:B:4297:PRO:HG3	1:B:4308:TRP:CD2	2.54	0.42
1:B:4297:PRO:HG3	1:B:4308:TRP:CG	2.54	0.42
1:A:1711:VAL:HG13	1:A:1853:VAL:HG21	2.01	0.42
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.19	0.42
1:A:2877:LEU:HD13	1:A:2888:GLU:HG2	2.01	0.42
1:A:4545:VAL:HG22	1:A:4588:THR:HG22	2.01	0.42
1:B:2446:ILE:HD13	1:B:2735:TYR:CD1	2.54	0.42
1:A:2517:TYR:CE2	1:A:2521:ILE:HD13	2.55	0.42
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.55	0.42
1:A:4247:MET:HG2	1:A:4251:ILE:HD12	2.01	0.42
1:B:3207:LYS:HA	1:B:3207:LYS:HD3	1.84	0.42
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.59	0.42
1:A:3212:VAL:O	1:A:3215:VAL:HG12	2.20	0.42
1:B:2418:ASP:O	1:B:2422:ILE:HG13	2.19	0.42
1:B:2499:LEU:HD23	1:B:2499:LEU:HA	1.91	0.42
1:B:2816:LEU:HD12	1:B:2817:PRO:HD2	2.01	0.42
1:B:3176:TYR:O	1:B:3180:ILE:HG12	2.18	0.42
1:B:4106:LEU:HD23	1:B:4106:LEU:HA	1.92	0.42
1:B:4460:LEU:HD12	1:B:4461:PRO:HD2	2.01	0.42
1:A:1931:ASN:HD21	1:A:2316:ASN:HB2	1.84	0.42
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.19	0.42
1:A:3763:ASP:OD1	1:A:3763:ASP:N	2.50	0.42
1:A:3908:PHE:CZ	1:A:3990:LEU:HD21	2.54	0.42
1:A:4302:ARG:NH1	1:A:4306:VAL:HG21	2.35	0.42
1:B:1478:VAL:HG12	1:B:1488:ARG:HE	1.84	0.42
1:B:2839:GLU:HB2	1:B:2842:GLU:OE1	2.19	0.42
1:B:3174:ARG:NH1	1:B:3650:ASN:OD1	2.53	0.42
1:B:4107:MET:HG2	1:B:4137:ASN:HD21	1.83	0.42
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.54	0.42
1:A:4509:VAL:HG11	1:A:4520:TYR:CZ	2.54	0.42
1:A:4525:ARG:NH2	1:A:4539:LEU:O	2.36	0.42
1:B:1623:ARG:HD3	1:B:1630:TYR:HA	2.00	0.42
1:B:3229:LEU:HD12	1:B:3461:ILE:HG23	2.02	0.42
1:B:4088:VAL:HG11	1:B:4116:LEU:HD21	2.00	0.42
1:B:4303:GLU:OE1	1:B:4303:GLU:N	2.50	0.42
1:A:2641:TYR:CZ	1:A:2650:LEU:HD13	2.55	0.42
1:A:2844:ARG:O	1:A:2848:GLU:HG2	2.20	0.42
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.32	0.42
1:B:3873:ARG:HD3	1:B:3873:ARG:HA	1.82	0.42
1:B:4082:LYS:HB2	1:B:4082:LYS:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4308:TRP:CH2	1:B:4312:LEU:HD21	2.55	0.42
1:A:1576:LEU:O	1:A:1580:LYS:HG3	2.20	0.42
1:B:2590:PRO:O	1:B:2732:PRO:HD2	2.19	0.42
1:B:3650:ASN:HD21	1:B:3695:ARG:HH11	1.68	0.42
1:B:4183:LEU:HD11	1:B:4215:ALA:HB1	2.01	0.42
1:B:4525:ARG:HD3	1:B:4536:LEU:HB3	2.01	0.42
1:A:1769:MET:SD	1:A:1777:PRO:HD2	2.59	0.42
1:A:2667:ASN:ND2	1:A:2712:CYS:HB2	2.34	0.42
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.19	0.42
1:A:4468:THR:HG21	1:A:4617:ASP:OD2	2.20	0.42
1:B:1493:LEU:O	1:B:1497:VAL:HG23	2.19	0.42
1:B:2925:ILE:HD12	1:B:3090:VAL:HG21	2.02	0.42
1:B:3175:HIS:HB3	1:B:3516:TYR:CE1	2.55	0.42
1:B:4160:THR:HG23	1:B:4212:LEU:HD21	2.02	0.42
1:B:1667:ASN:ND2	1:B:1672:VAL:HB	2.35	0.42
1:B:3033:CYS:SG	1:B:3054:PHE:HB2	2.60	0.42
1:B:3150:VAL:O	1:B:3154:LEU:HD23	2.18	0.42
1:B:3782:ARG:HA	1:B:3785:GLU:CD	2.45	0.42
1:B:4525:ARG:NH1	1:B:4536:LEU:O	2.53	0.42
1:A:2018:MET:HE2	1:A:2018:MET:HB3	1.90	0.41
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	2.02	0.41
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	2.01	0.41
1:A:4558:PHE:O	1:A:4589:GLN:HA	2.20	0.41
1:B:1619:LEU:HD11	1:B:1638:LEU:HG	2.01	0.41
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.49	0.41
1:A:3172:THR:HG21	1:A:3694:SER:HB3	2.02	0.41
1:B:1652:LYS:HB2	1:B:1652:LYS:HE2	1.83	0.41
1:B:1673:VAL:N	1:B:1690:VAL:O	2.44	0.41
1:B:2956:LEU:CD2	1:B:2989:LYS:HB3	2.49	0.41
1:B:3068:MET:HE1	1:B:3078:ARG:HG3	2.02	0.41
1:B:3976:GLU:HB3	1:B:3978:THR:O	2.20	0.41
1:B:2529:ALA:HA	1:B:2530:PRO:HD3	1.94	0.41
1:B:2667:ASN:ND2	1:B:2712:CYS:HB2	2.35	0.41
1:B:3844:PRO:HA	1:B:3847:LYS:HE3	2.02	0.41
1:A:3520:PHE:CD1	1:A:3524:MET:HG2	2.56	0.41
1:B:3891:LYS:HD2	1:B:4013:LEU:HD23	2.03	0.41
1:A:1766:LEU:HD23	1:A:1766:LEU:HA	1.93	0.41
1:A:3033:CYS:SG	1:A:3054:PHE:HB2	2.60	0.41
1:A:4020:ILE:HD12	1:A:4020:ILE:H	1.85	0.41
1:A:4157:MET:HE2	1:A:4157:MET:HB3	1.96	0.41
1:B:1467:ARG:HG2	1:B:1523:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3227:GLN:HA	1:B:3230:GLU:HG2	2.03	0.41
1:B:3495:THR:O	1:B:3499:GLN:HG3	2.20	0.41
1:B:4431:LEU:HD23	1:B:4431:LEU:HA	1.92	0.41
1:A:4105:TRP:CH2	1:A:4109:LEU:HD22	2.56	0.41
1:A:4196:TYR:HE1	1:A:4328:GLU:HB3	1.85	0.41
1:A:4442:LYS:HE3	1:A:4442:LYS:HB2	1.81	0.41
1:B:3126:MET:HA	1:B:3127:PRO:HD3	1.96	0.41
1:B:3211:THR:O	1:B:3215:VAL:HG23	2.20	0.41
1:B:4175:GLU:HG3	1:B:4278:PHE:CE2	2.55	0.41
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.21	0.41
1:A:1589:MET:HE3	1:A:1589:MET:HA	2.03	0.41
1:A:3046:SER:HB3	1:A:3049:GLU:HG2	2.02	0.41
1:B:2973:ASP:O	1:B:2977:ARG:HG3	2.21	0.41
1:B:2976:LEU:HB3	1:B:3020:LEU:HD21	2.02	0.41
1:A:3683:ASP:HB3	1:A:3686:VAL:HG13	2.01	0.41
1:B:3931:GLN:HE22	1:B:3961:LEU:HD11	1.86	0.41
1:B:3982:PRO:HA	1:B:3985:GLN:HE21	1.84	0.41
1:B:3990:LEU:HA	1:B:4004:MET:HG2	2.02	0.41
1:B:4496:ALA:HB2	1:B:4504:LEU:HD12	2.02	0.41
1:B:4543:VAL:HG12	1:B:4590:LEU:HD22	2.01	0.41
1:A:2142:CYS:HA	1:A:2146:VAL:HG23	2.02	0.41
1:A:2411:PRO:O	1:A:2415:ILE:HG13	2.21	0.41
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.21	0.41
1:A:3214:GLN:O	1:A:3217:GLU:HG3	2.20	0.41
1:A:3239:LYS:HG2	1:A:3451:TYR:OH	2.21	0.41
1:A:3546:ASP:OD1	1:A:3547:ILE:N	2.54	0.41
1:A:3781:THR:O	1:A:3785:GLU:OE1	2.38	0.41
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	2.02	0.41
1:A:4412:PHE:CE2	1:A:4520:TYR:HB2	2.56	0.41
1:B:1984:GLU:OE1	1:B:1997:ILE:HG23	2.20	0.41
1:B:2560:HIS:CE1	1:B:2561:LYS:HG3	2.56	0.41
1:B:2951:ALA:HB1	1:B:2956:LEU:HB2	2.02	0.41
1:B:3520:PHE:CD1	1:B:3524:MET:HG2	2.56	0.41
1:B:3885:MET:HE1	1:B:3990:LEU:HD21	2.03	0.41
1:A:2231:SER:O	1:A:2235:ARG:HG3	2.21	0.41
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.41
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.80	0.41
1:A:4188:ALA:O	1:A:4192:GLU:HG2	2.21	0.41
1:B:1911:GLY:O	1:B:1915:SER:OG	2.32	0.41
1:B:3214:GLN:O	1:B:3217:GLU:HG3	2.21	0.41
1:B:3837:HIS:ND1	1:B:3837:HIS:C	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3982:PRO:HA	1:B:3985:GLN:HG2	2.03	0.41
1:A:1774:ASP:OD1	1:A:1775:ALA:N	2.47	0.40
1:A:3229:LEU:HD11	1:A:3462:LYS:HB2	2.03	0.40
1:A:3591:ASP:OD2	1:A:3595:GLN:N	2.54	0.40
1:B:1751:VAL:O	1:B:1755:GLN:HG3	2.21	0.40
1:B:2054:LEU:HD23	1:B:2054:LEU:HA	1.94	0.40
1:B:2172:ARG:HE	1:B:2175:MET:HE1	1.87	0.40
1:B:2457:SER:O	1:B:2461:MET:HG3	2.21	0.40
1:B:3716:VAL:HB	1:B:3836:TYR:OH	2.21	0.40
1:B:4414:GLU:HG3	1:B:4415:ARG:N	2.35	0.40
1:A:2007:LYS:HE3	1:A:2007:LYS:HB3	1.94	0.40
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	2.03	0.40
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.56	0.40
1:B:1887:ARG:NH2	1:B:4253:GLY:O	2.54	0.40
1:A:1493:LEU:O	1:A:1497:VAL:HG23	2.21	0.40
1:A:1570:SER:O	1:A:1573:THR:OG1	2.32	0.40
1:A:1784:ASN:O	1:A:1787:VAL:HG22	2.20	0.40
1:A:4470:PRO:HD2	1:A:4473:MET:HE3	2.03	0.40
1:B:1478:VAL:CG1	1:B:1488:ARG:HE	2.34	0.40
1:B:1941:MET:HE2	1:B:1960:PHE:HE1	1.85	0.40
1:B:2458:LEU:O	1:B:2462:LEU:HG	2.22	0.40
1:B:2499:LEU:HD21	1:B:2515:GLY:HA2	2.02	0.40
1:B:2536:ASP:OD1	1:B:2572:LEU:HD21	2.22	0.40
1:B:4482:PHE:O	1:B:4486:ILE:HG12	2.21	0.40
1:A:1911:GLY:O	1:A:1915:SER:OG	2.28	0.40
1:A:2268:LEU:HD12	1:A:2268:LEU:HA	1.96	0.40
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	2.03	0.40
1:A:3167:ARG:NH1	1:A:3685:THR:HA	2.37	0.40
1:A:3746:GLU:OE2	1:A:3750:LEU:HG	2.21	0.40
1:A:3776:GLU:O	1:A:3780:VAL:HG22	2.21	0.40
1:A:4159:ARG:HE	1:A:4159:ARG:HB2	1.79	0.40
1:B:2067:ASN:ND2	1:B:4537:GLU:OE1	2.51	0.40
1:B:2075:LEU:HD21	1:B:4536:LEU:HD21	2.03	0.40
1:B:2265:TYR:OH	1:B:2311:TRP:O	2.28	0.40
1:B:2441:PHE:CD1	1:B:2449:LEU:HD23	2.56	0.40
1:B:3553:LEU:HB2	1:B:3578:ILE:HD13	2.03	0.40
1:A:2574:THR:O	1:A:2578:GLU:HG3	2.21	0.40
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.21	0.40
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.21	0.40
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.55	0.40
1:B:2028:LEU:HG	1:B:2032:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2814:GLU:OE1	1:B:2814:GLU:HA	2.22	0.40
1:B:2956:LEU:HD13	1:B:2991:ALA:HB2	2.02	0.40
1:B:3114:ASP:O	1:B:3116:GLU:HG2	2.22	0.40
1:B:4049:TYR:OH	1:B:4191:GLN:OE1	2.36	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	2929/4646 (63%)	2881 (98%)	48 (2%)	0	100	100
1	B	2929/4646 (63%)	2889 (99%)	40 (1%)	0	100	100
All	All	5858/9292 (63%)	5770 (98%)	88 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2605/4125 (63%)	2605 (100%)	0	100	100
1	B	2605/4125 (63%)	2605 (100%)	0	100	100
All	All	5210/8250 (63%)	5210 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1817	HIS
1	A	2130	ASN
1	A	2215	GLN
1	A	2217	ASN
1	A	2476	HIS
1	A	2485	GLN
1	A	2588	HIS
1	A	2689	HIS
1	A	2730	HIS
1	A	3032	GLN
1	A	3522	GLN
1	A	3912	ASN
1	A	4114	HIS
1	A	4191	GLN
1	A	4335	GLN
1	A	4347	GLN
1	A	4429	GLN
1	A	4488	GLN
1	A	4544	ASN
1	A	4566	GLN
1	A	4571	ASN
1	B	1779	HIS
1	B	1939	GLN
1	B	2067	ASN
1	B	2109	GLN
1	B	2130	ASN
1	B	2215	GLN
1	B	2217	ASN
1	B	2430	ASN
1	B	2464	GLN
1	B	2689	HIS
1	B	2752	ASN
1	B	2834	GLN
1	B	3063	HIS
1	B	3092	ASN
1	B	3499	GLN
1	B	3522	GLN
1	B	3535	HIS
1	B	3985	GLN

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Mol	Chain	Res	Type
1	B	4029	HIS
1	B	4114	HIS
1	B	4232	ASN
1	B	4249	GLN
1	B	4335	GLN
1	B	4506	ASN
1	B	4589	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	ADP	B	4701	4	28,29,29	1.40	4 (14%)	43,45,45	1.82	9 (20%)
2	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	9 (20%)
3	ATP	A	4702	4	32,33,33	0.34	0	48,52,52	0.28	0
3	ATP	B	4702	4	32,33,33	0.34	0	48,52,52	0.28	0
2	ADP	B	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
2	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4701	4	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
2	ADP	B	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	9 (20%)

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	ADP	B	4701	4	-	4/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	4/22/38/38	0/3/3/3
3	ATP	B	4702	4	-	4/22/38/38	0/3/3/3
2	ADP	B	4704	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4701	4	-	3/16/32/32	0/3/3/3
2	ADP	B	4703	-	-	1/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4703	ADP	C5-C4	4.74	1.47	1.39
2	A	4704	ADP	C5-C4	4.66	1.47	1.39
2	A	4703	ADP	C5-C4	4.66	1.47	1.39
2	B	4704	ADP	C5-C4	4.63	1.47	1.39
2	A	4701	ADP	C5-C4	4.60	1.47	1.39
2	B	4701	ADP	C5-C4	4.56	1.47	1.39
2	B	4701	ADP	C5-C6	2.67	1.48	1.41
2	B	4704	ADP	C5-C6	2.67	1.48	1.41
2	A	4703	ADP	C5-C6	2.67	1.48	1.41
2	A	4701	ADP	C5-C6	2.67	1.48	1.41
2	A	4704	ADP	C5-C6	2.66	1.48	1.41
2	B	4703	ADP	C5-C6	2.66	1.48	1.41
2	A	4704	ADP	C5-N7	-2.38	1.34	1.39
2	A	4701	ADP	C5-N7	-2.34	1.34	1.39
2	B	4701	ADP	C5-N7	-2.33	1.34	1.39
2	B	4704	ADP	C5-N7	-2.33	1.34	1.39
2	A	4703	ADP	C5-N7	-2.30	1.34	1.39
2	B	4703	ADP	C8-N7	2.30	1.36	1.31
2	B	4704	ADP	C8-N7	2.28	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C8-N7	2.27	1.36	1.31
2	A	4703	ADP	C8-N7	2.26	1.36	1.31
2	B	4703	ADP	C5-N7	-2.24	1.35	1.39
2	A	4701	ADP	C8-N7	2.23	1.36	1.31
2	B	4701	ADP	C8-N7	2.23	1.36	1.31

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4703	ADP	C5-C4-N3	-6.07	118.36	126.72
2	A	4703	ADP	C5-C4-N3	-5.92	118.56	126.72
2	B	4704	ADP	C5-C4-N3	-5.88	118.62	126.72
2	A	4704	ADP	C5-C4-N3	-5.83	118.69	126.72
2	A	4701	ADP	C5-C4-N3	-5.71	118.85	126.72
2	B	4701	ADP	C5-C4-N3	-5.68	118.89	126.72
2	B	4703	ADP	N3-C4-N9	4.86	135.44	127.17
2	A	4703	ADP	N3-C4-N9	4.76	135.26	127.17
2	B	4704	ADP	N3-C4-N9	4.66	135.09	127.17
2	A	4704	ADP	N3-C4-N9	4.61	135.02	127.17
2	A	4701	ADP	N3-C4-N9	4.57	134.94	127.17
2	B	4701	ADP	N3-C4-N9	4.54	134.89	127.17
2	B	4703	ADP	C2-N3-C4	3.84	121.22	111.83
2	A	4703	ADP	C2-N3-C4	3.78	121.06	111.83
2	B	4704	ADP	C2-N3-C4	3.69	120.84	111.83
2	A	4701	ADP	C2-N3-C4	3.68	120.83	111.83
2	A	4704	ADP	C2-N3-C4	3.67	120.80	111.83
2	B	4701	ADP	C2-N3-C4	3.66	120.76	111.83
2	A	4704	ADP	C4-C5-N7	-3.46	106.62	110.58
2	B	4704	ADP	C4-C5-N7	-3.44	106.65	110.58
2	B	4703	ADP	C4-C5-N7	-3.42	106.67	110.58
2	A	4701	ADP	C4-C5-N7	-3.40	106.70	110.58
2	B	4701	ADP	C4-C5-N7	-3.40	106.70	110.58
2	A	4703	ADP	C4-C5-N7	-3.39	106.71	110.58
2	B	4703	ADP	N3-C2-N1	-3.34	123.52	128.58
2	A	4703	ADP	N3-C2-N1	-3.33	123.54	128.58
2	A	4701	ADP	N3-C2-N1	-3.31	123.57	128.58
2	B	4701	ADP	N3-C2-N1	-3.30	123.59	128.58
2	A	4704	ADP	N3-C2-N1	-3.21	123.72	128.58
2	B	4704	ADP	N3-C2-N1	-3.20	123.74	128.58
2	B	4701	ADP	C4-N9-C8	2.70	108.58	105.74
2	A	4701	ADP	C4-N9-C8	2.67	108.55	105.74
2	A	4703	ADP	C4-N9-C8	2.67	108.54	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4703	ADP	C4-N9-C8	2.58	108.44	105.74
2	A	4704	ADP	C4-N9-C8	2.57	108.44	105.74
2	B	4704	ADP	C4-N9-C8	2.57	108.44	105.74
2	B	4704	ADP	C3'-C2'-C1'	2.57	106.32	101.46
2	A	4704	ADP	C3'-C2'-C1'	2.57	106.32	101.46
2	A	4703	ADP	C5-N7-C8	2.54	107.44	103.45
2	A	4704	ADP	C5-N7-C8	2.53	107.42	103.45
2	B	4703	ADP	C5-N7-C8	2.51	107.40	103.45
2	A	4703	ADP	C3'-C2'-C1'	2.50	106.19	101.46
2	B	4701	ADP	C5-N7-C8	2.49	107.36	103.45
2	B	4704	ADP	C5-N7-C8	2.47	107.34	103.45
2	A	4701	ADP	C5-N7-C8	2.46	107.32	103.45
2	B	4703	ADP	C3'-C2'-C1'	2.45	106.09	101.46
2	B	4701	ADP	C3'-C2'-C1'	2.09	105.43	101.46
2	A	4701	ADP	C6-C5-N7	2.08	136.10	132.09
2	B	4701	ADP	C6-C5-N7	2.08	136.10	132.09
2	A	4701	ADP	C3'-C2'-C1'	2.08	105.39	101.46
2	A	4703	ADP	C6-C5-N7	2.07	136.07	132.09
2	A	4704	ADP	C6-C5-N7	2.04	136.02	132.09
2	B	4703	ADP	C6-C5-N7	2.02	135.99	132.09
2	B	4704	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	B	4701	ADP	C5'-O5'-PA-O1A
2	B	4701	ADP	C5'-O5'-PA-O2A
2	B	4701	ADP	C5'-O5'-PA-O3A
2	B	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	B	4702	ATP	O4'-C4'-C5'-O5'
2	B	4704	ADP	O4'-C4'-C5'-O5'
2	B	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	B	4701	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O2B

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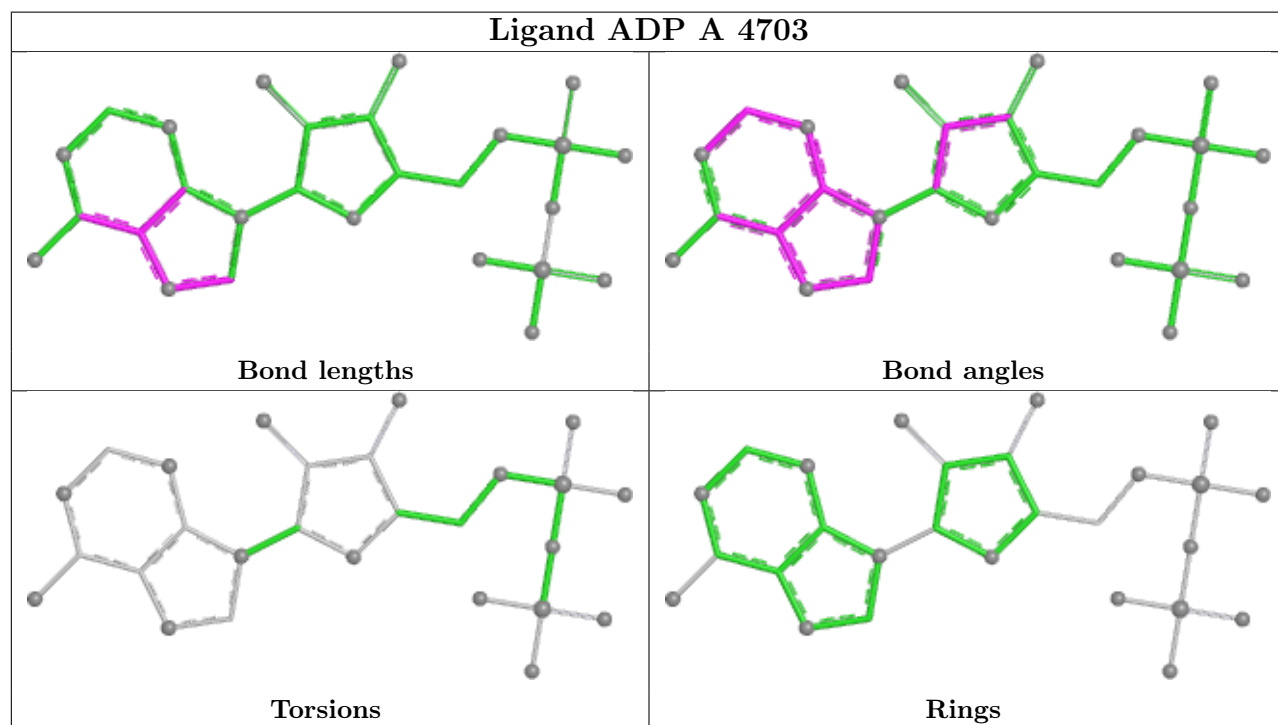
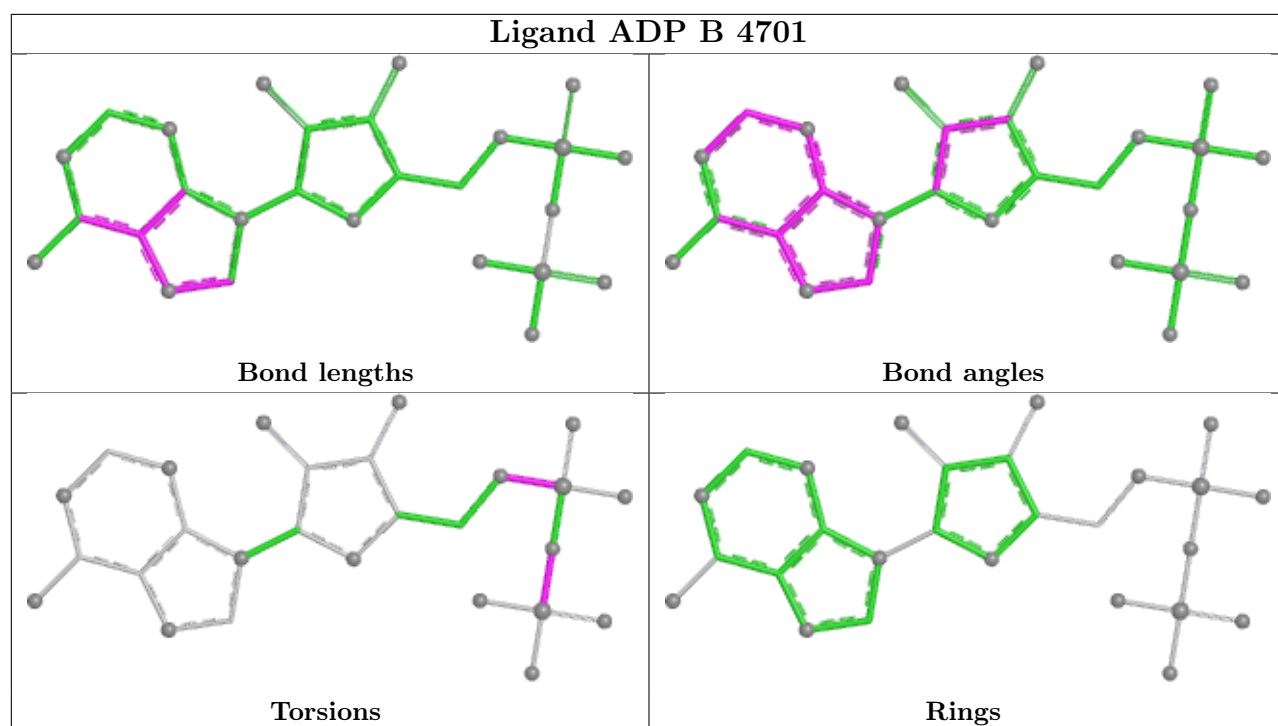
Mol	Chain	Res	Type	Atoms
3	B	4702	ATP	PA-O3A-PB-O2B
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	B	4702	ATP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O1B
3	B	4702	ATP	PA-O3A-PB-O1B
2	B	4703	ADP	O4'-C4'-C5'-O5'

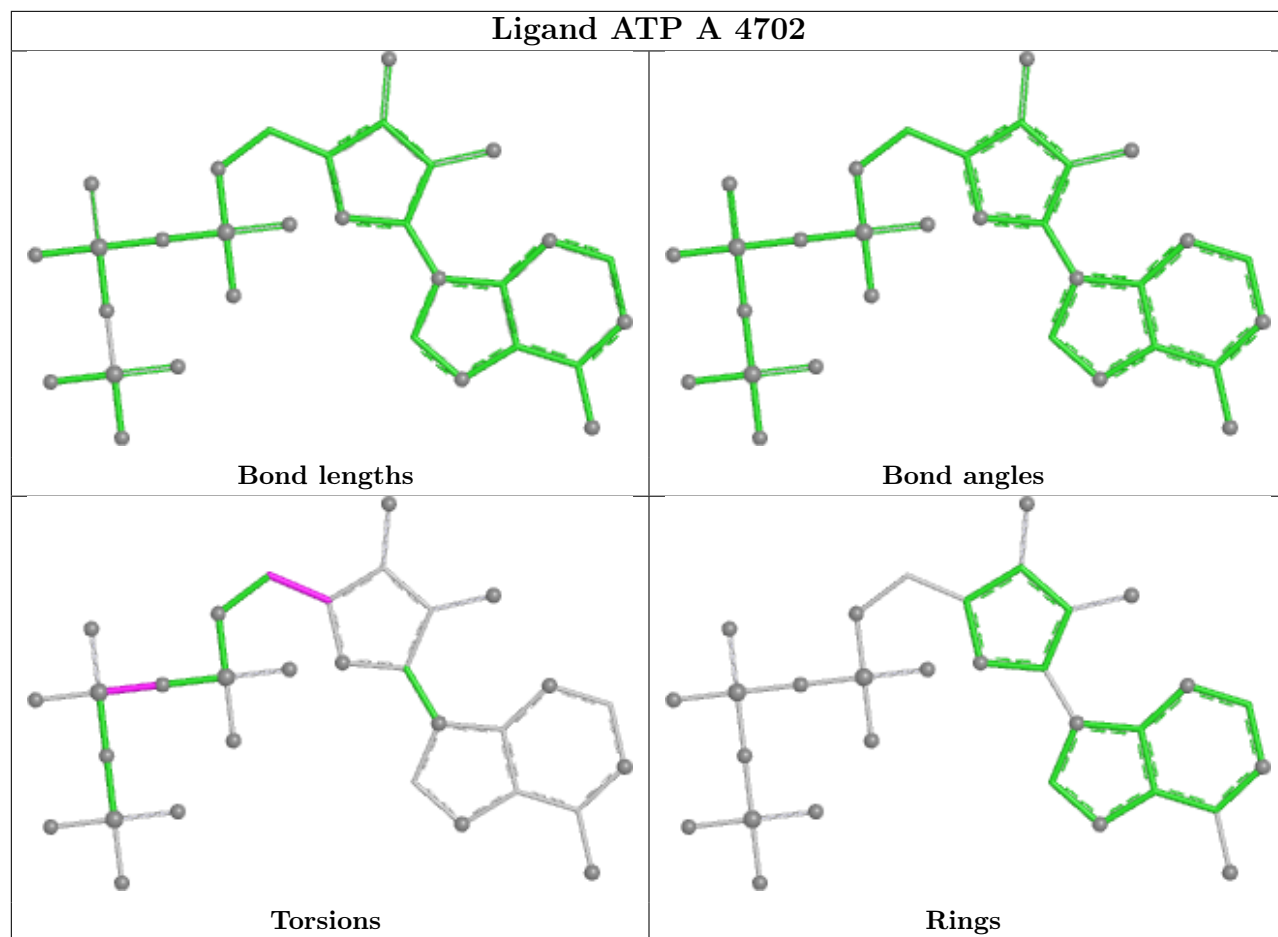
There are no ring outliers.

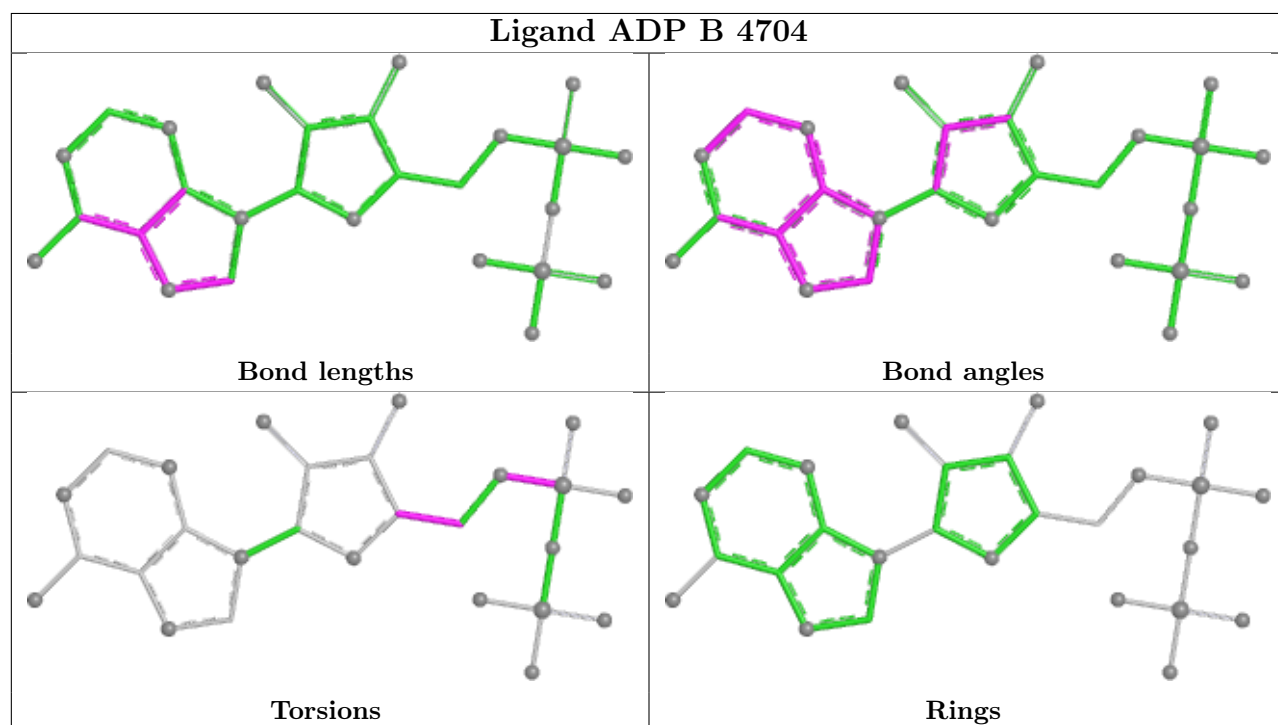
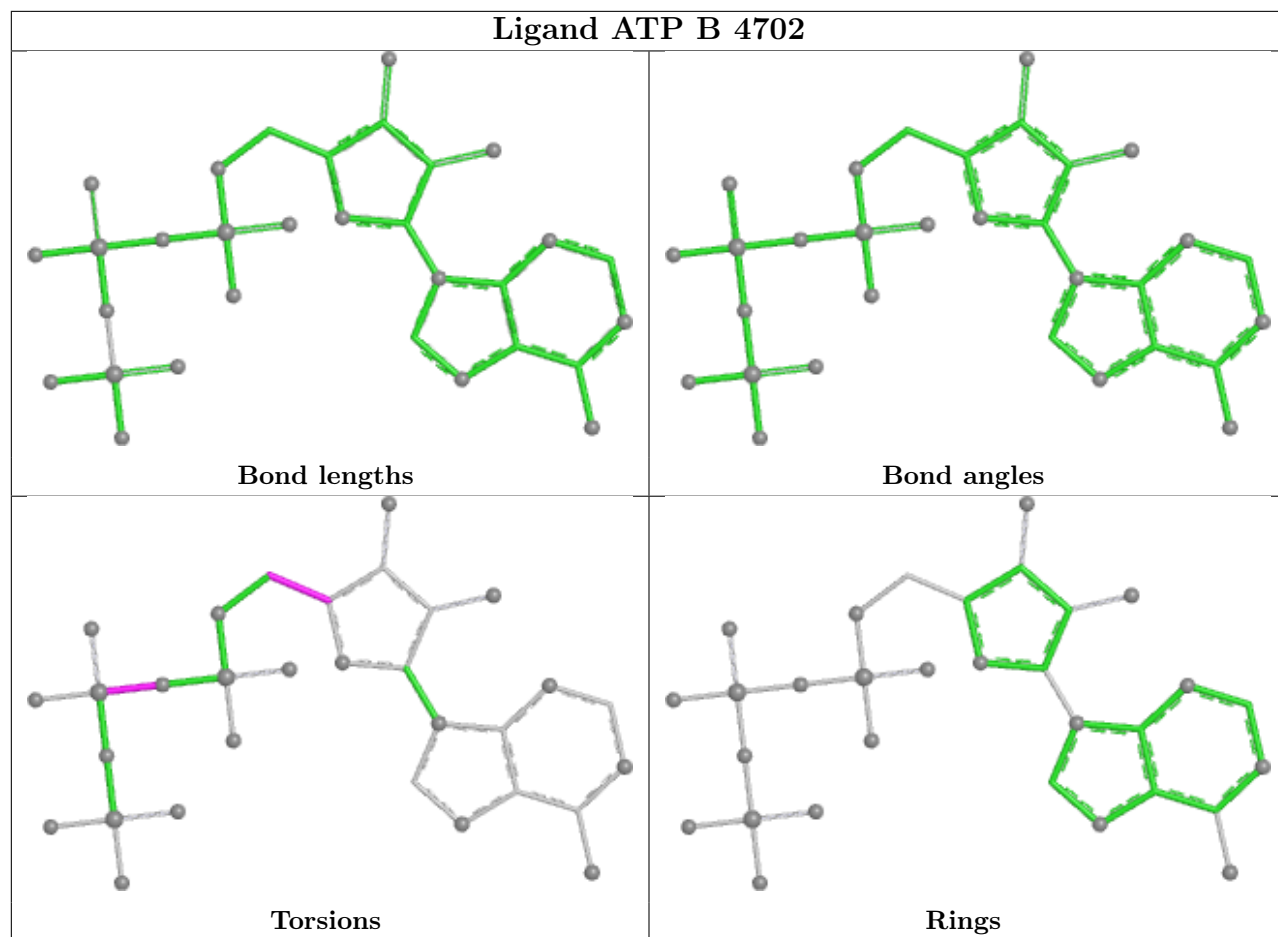
4 monomers are involved in 6 short contacts:

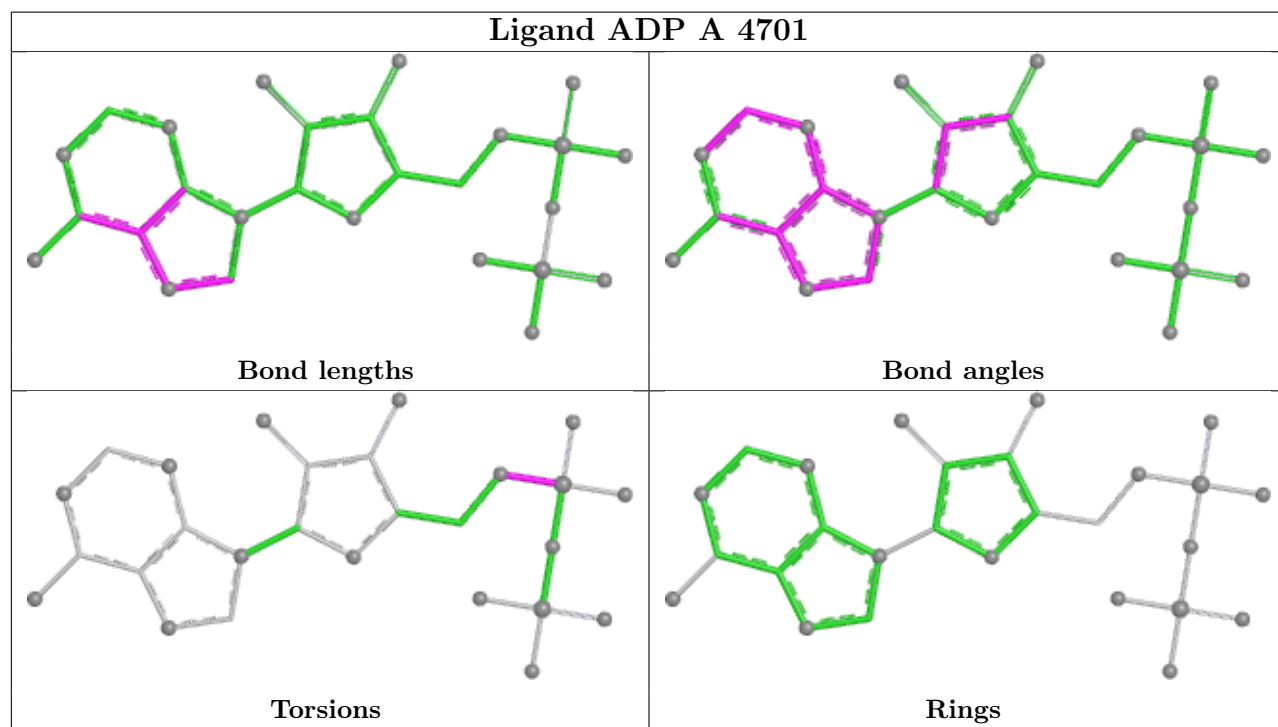
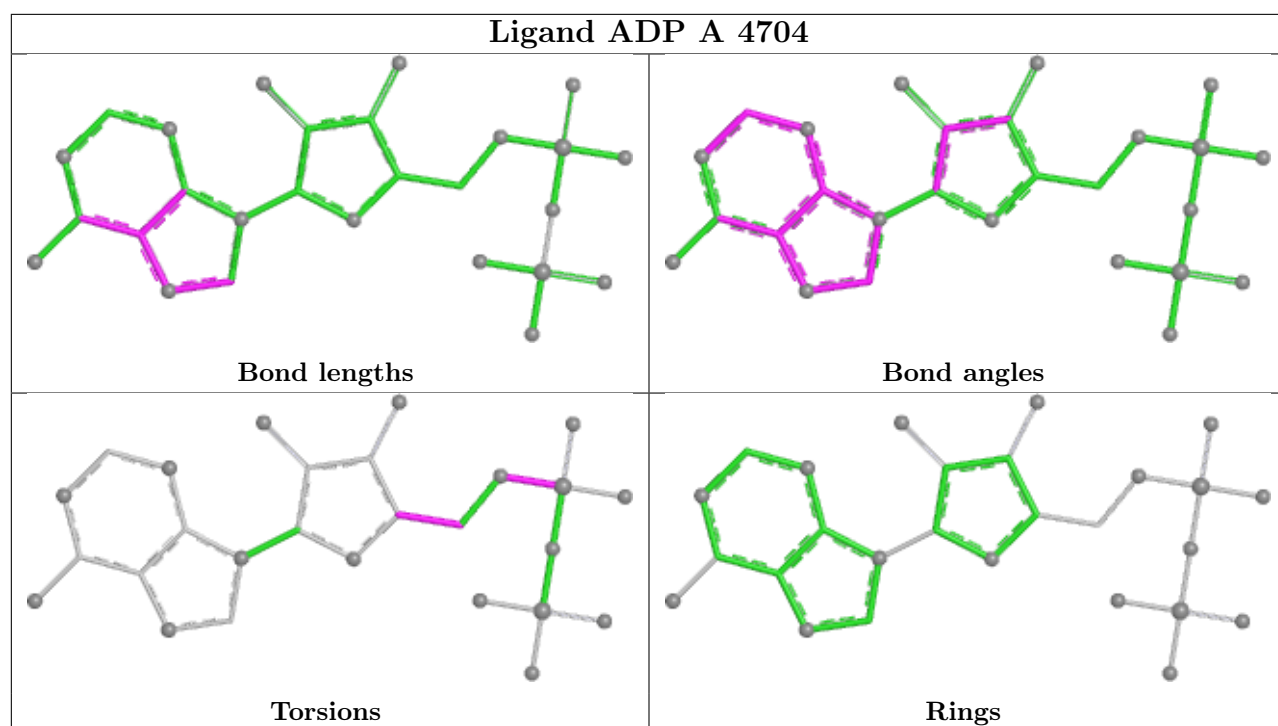
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4701	ADP	1	0
3	B	4702	ATP	1	0
2	A	4701	ADP	3	0
2	B	4703	ADP	1	0

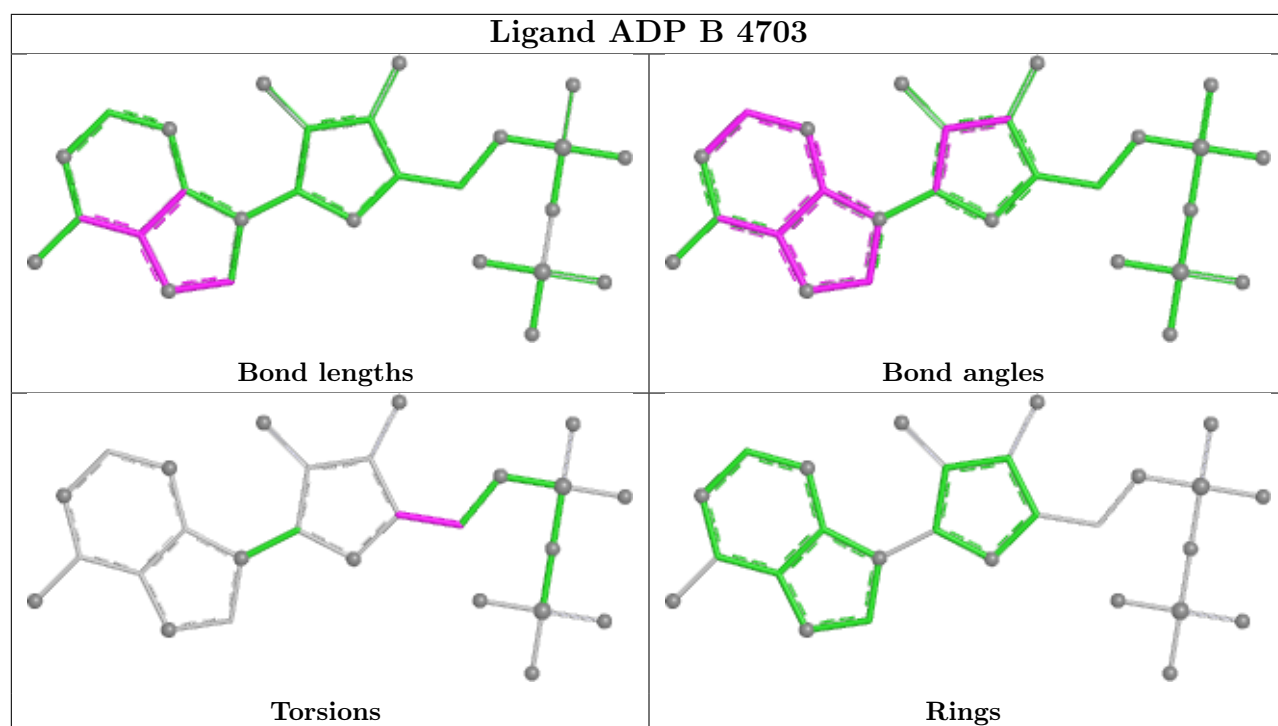
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

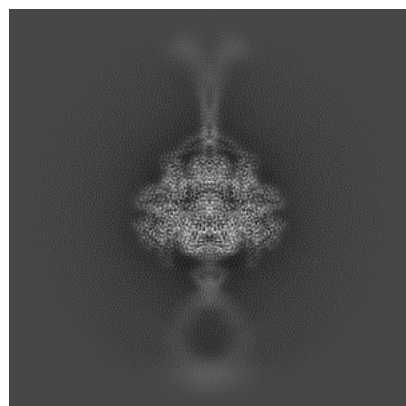
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47379. These allow visual inspection of the internal detail of the map and identification of artifacts.

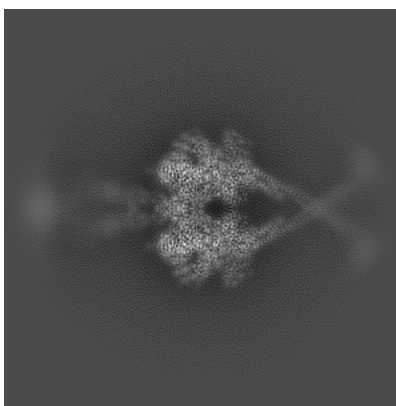
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

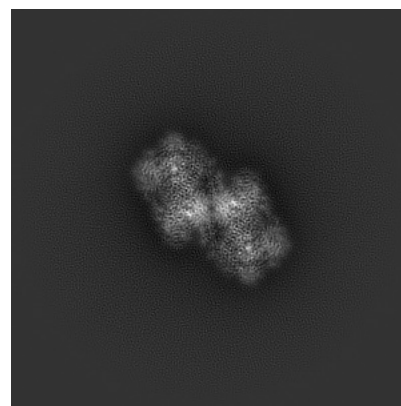
6.1.1 Primary map



X

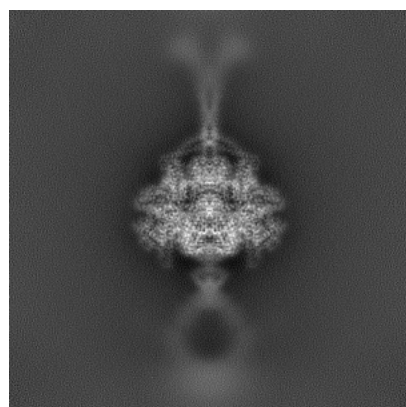


Y

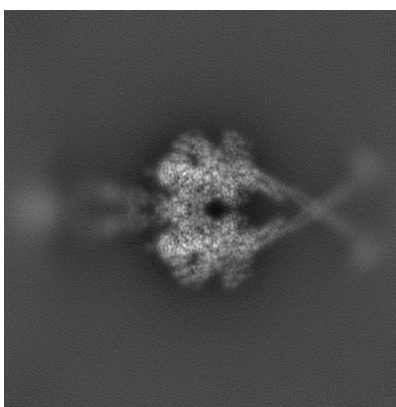


Z

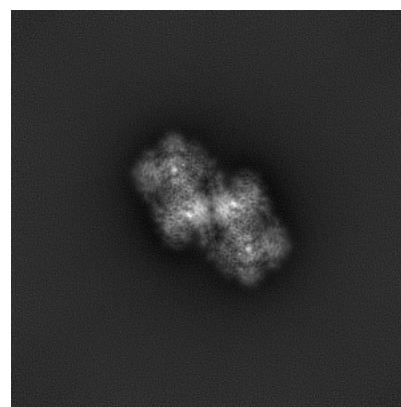
6.1.2 Raw map



X



Y

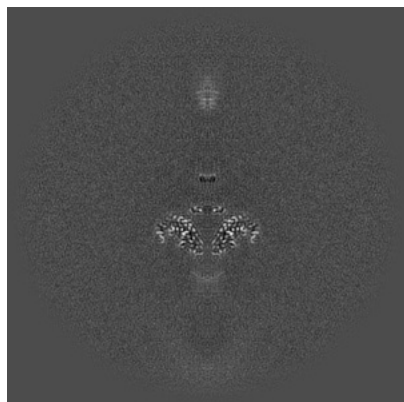


Z

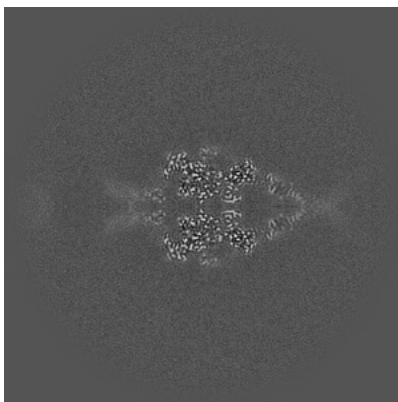
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

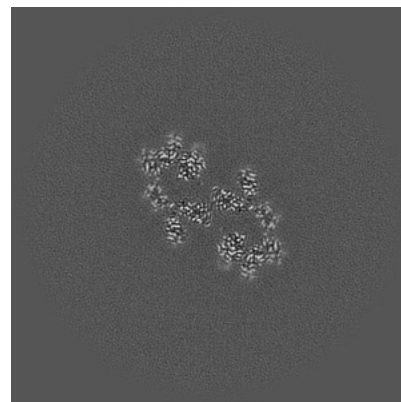
6.2.1 Primary map



X Index: 192

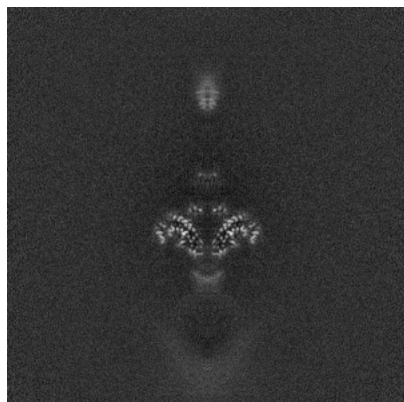


Y Index: 192

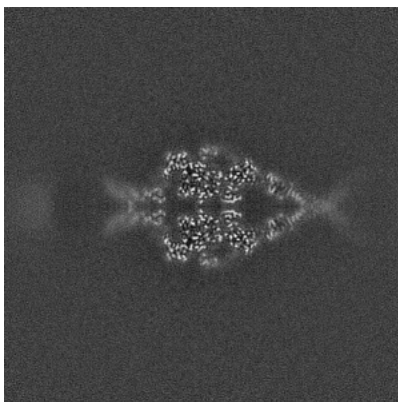


Z Index: 192

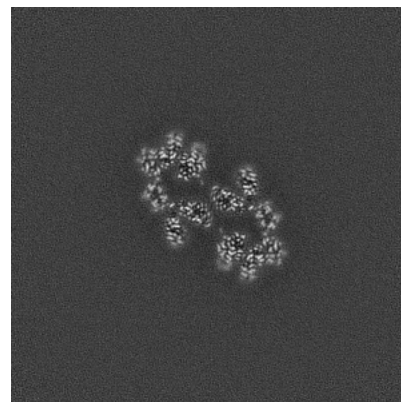
6.2.2 Raw map



X Index: 192



Y Index: 192

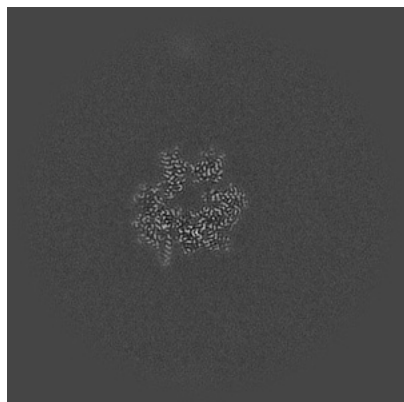


Z Index: 192

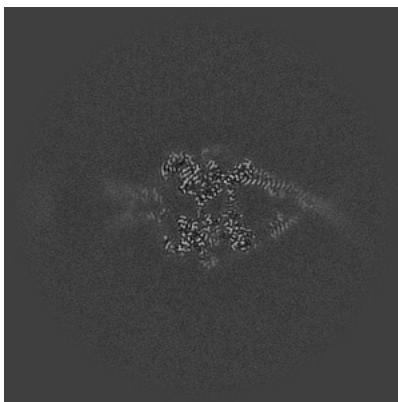
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

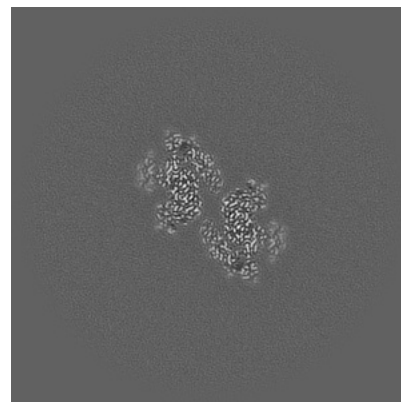
6.3.1 Primary map



X Index: 227

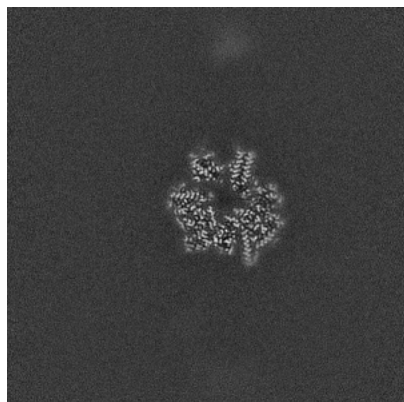


Y Index: 195

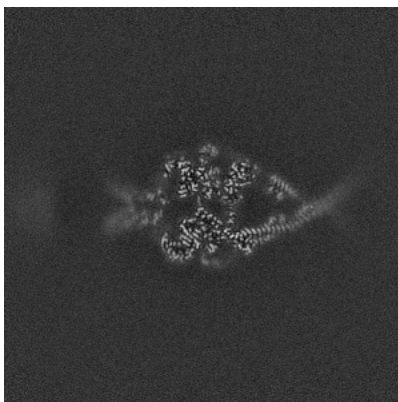


Z Index: 173

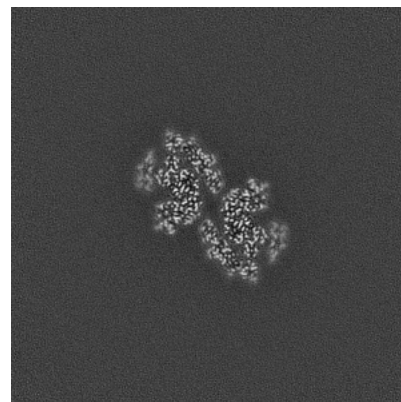
6.3.2 Raw map



X Index: 156



Y Index: 189

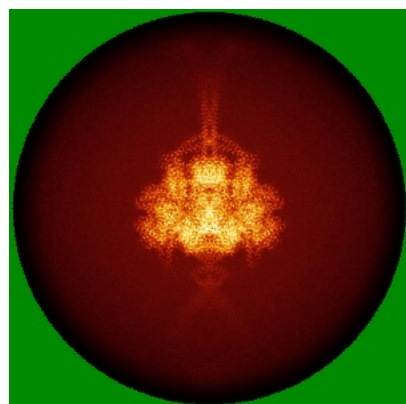


Z Index: 172

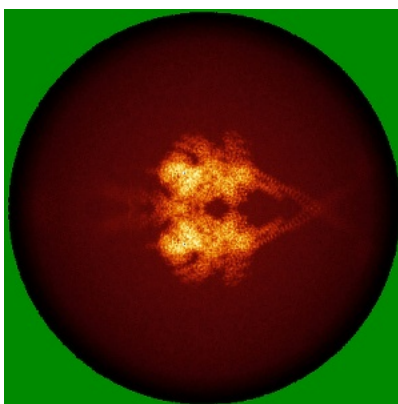
The images above show the largest variance slices of the map in three orthogonal directions.

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

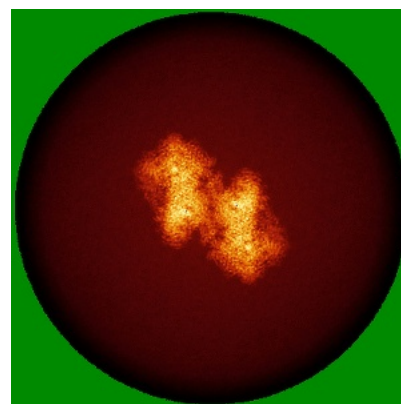
6.4.1 Primary map



X

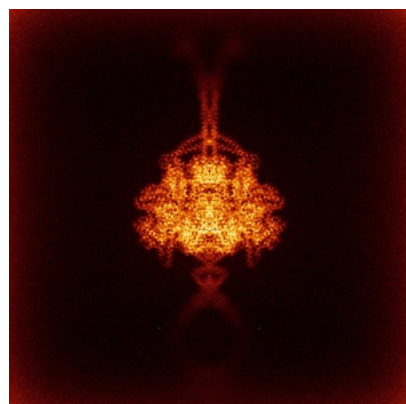


Y

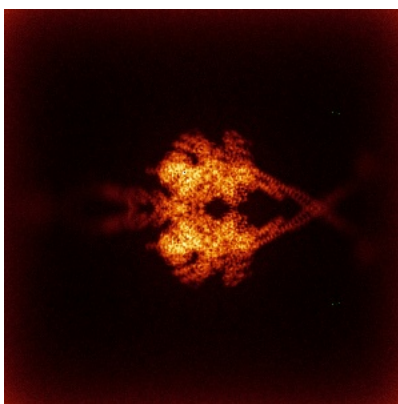


Z

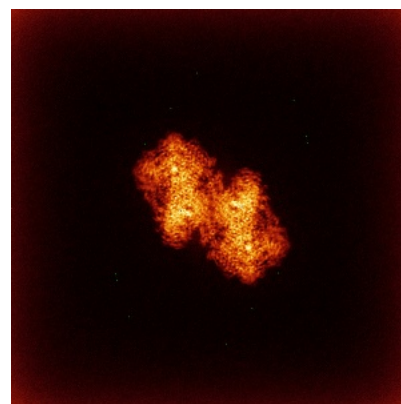
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

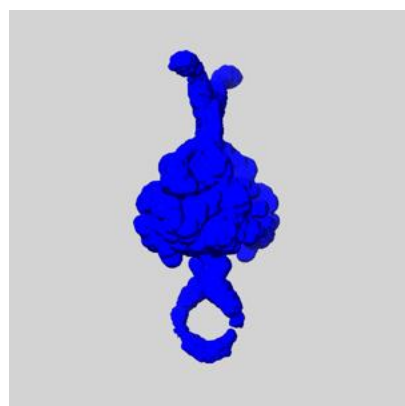
6.6 Mask visualisation [i](#)

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

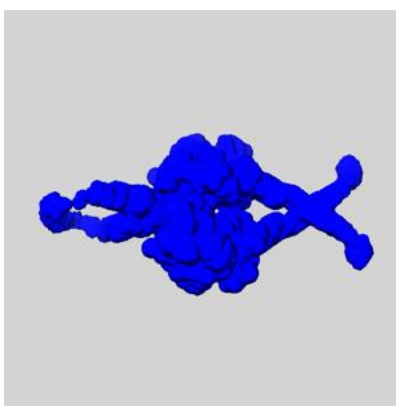
A mask typically either:

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

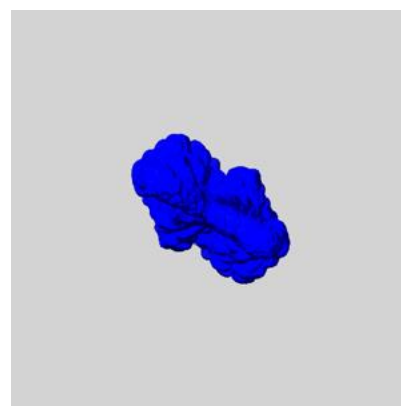
6.6.1 emd_47379_msk_1.map [i](#)



X



Y

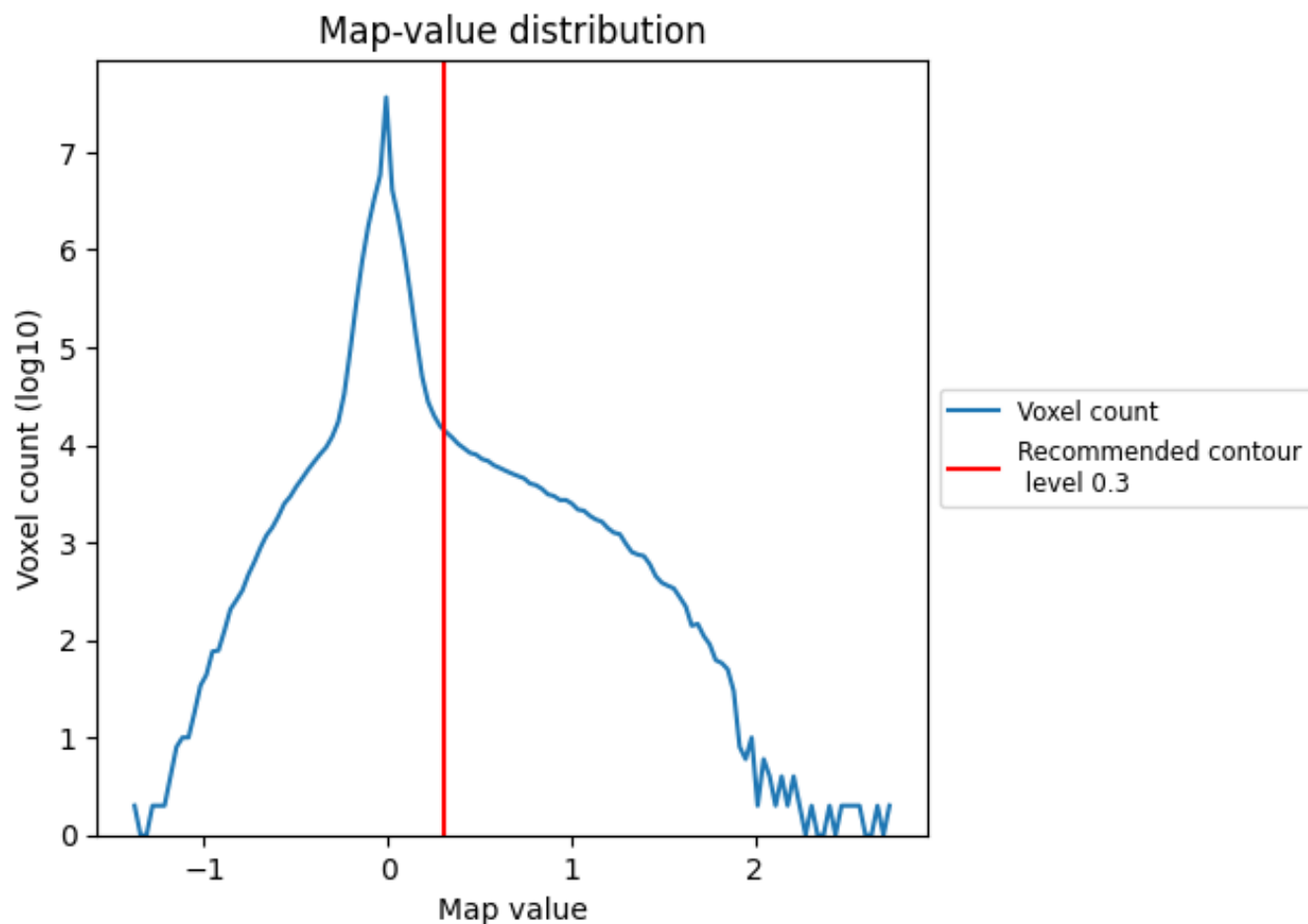


Z

7 Map analysis [i](#)

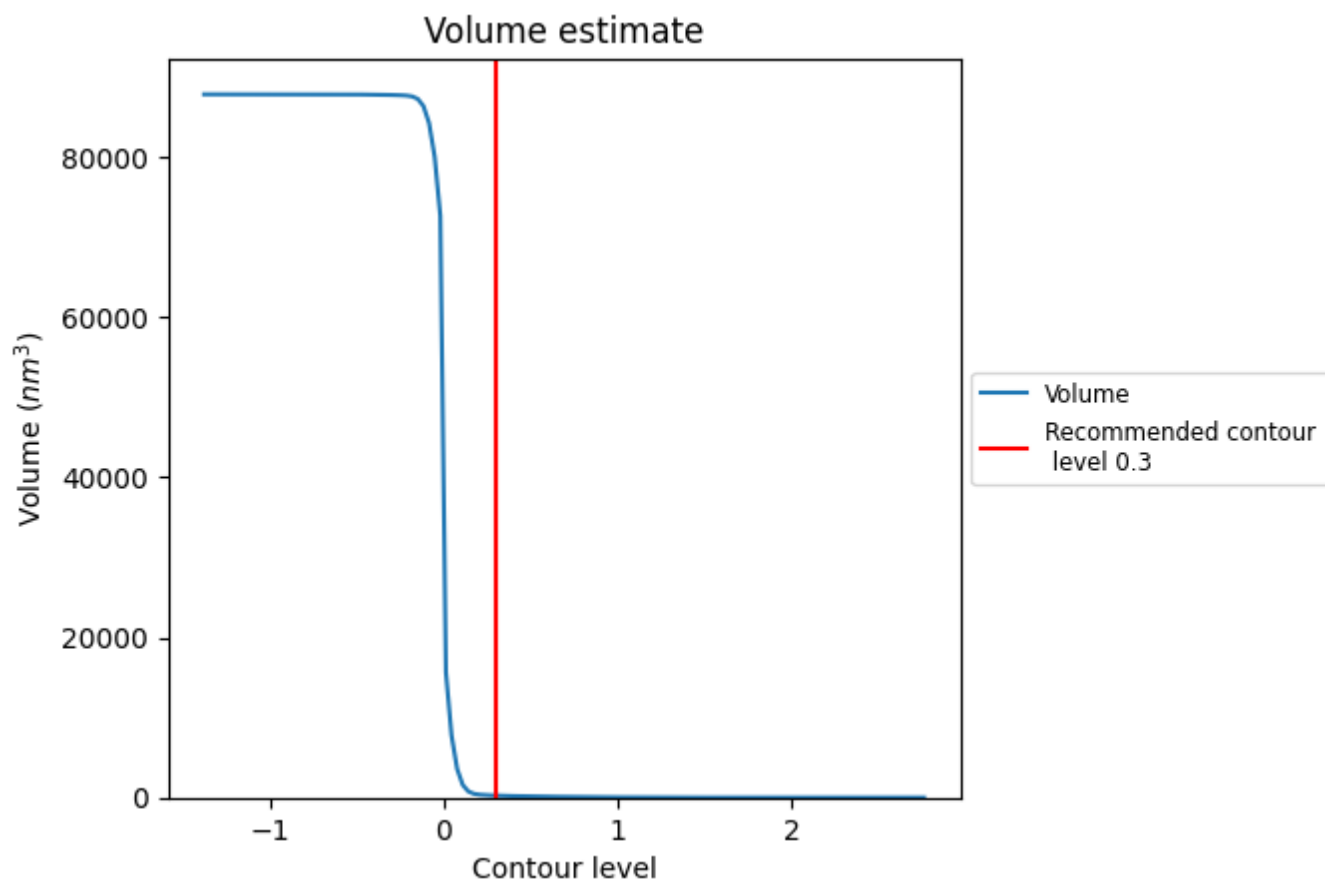
This section contains the results of statistical analysis of the map.

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.

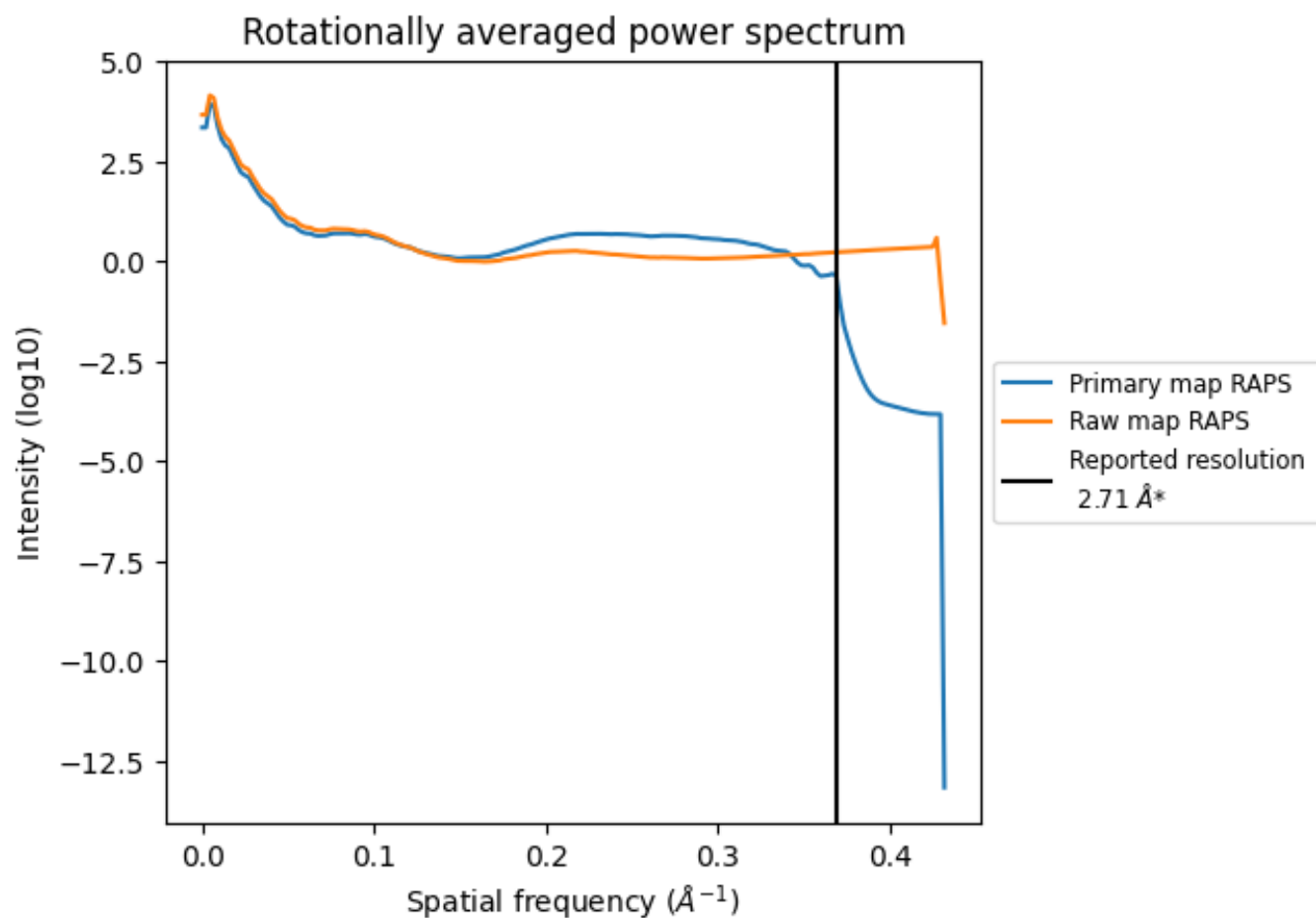
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm^3 ; this corresponds to an approximate mass of 225 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 ⓘ

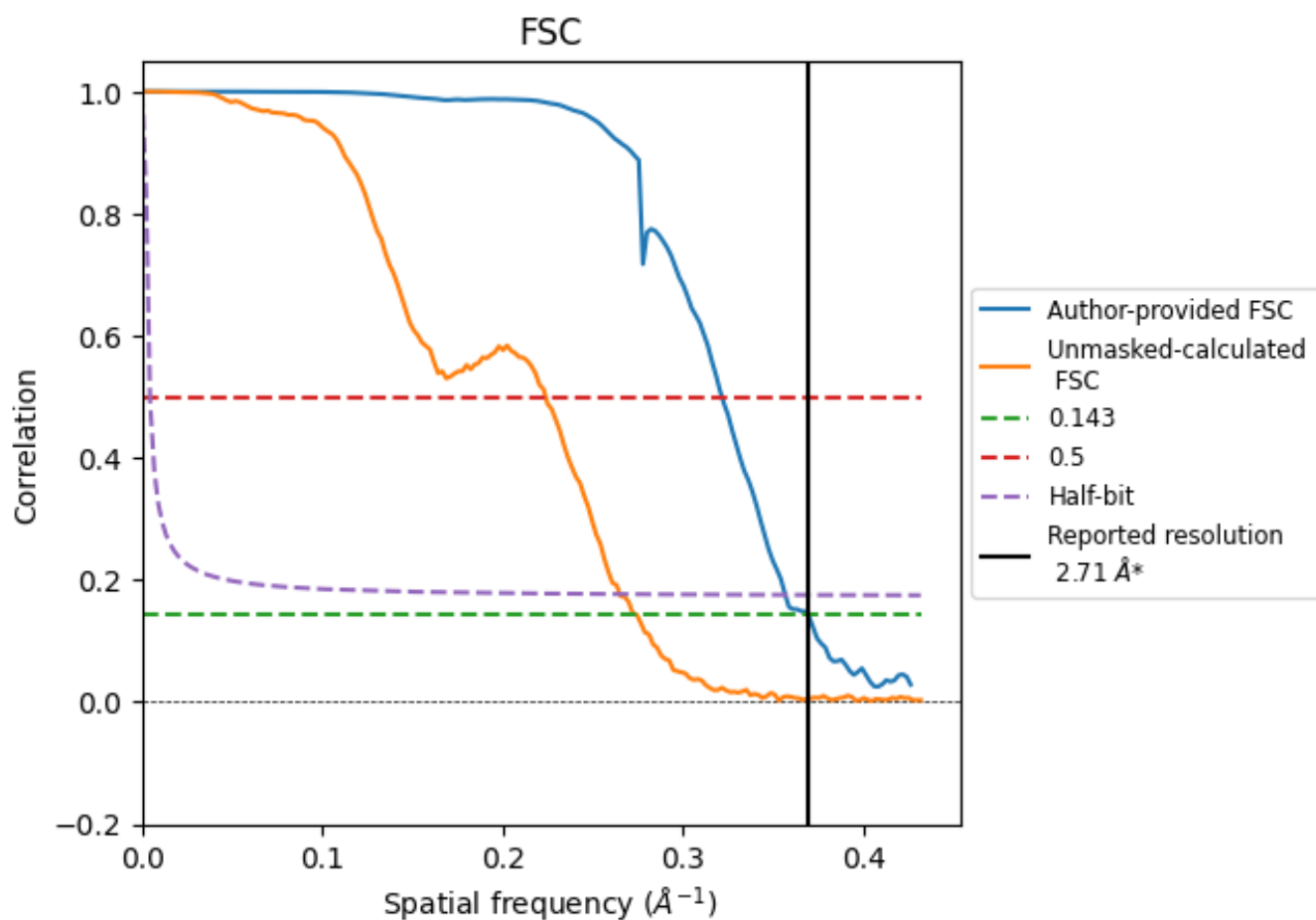


*Reported resolution corresponds to spatial frequency of 0.369 \AA^{-1}

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 0.369 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.71	3.11	2.80
Unmasked-calculated*	3.65	4.47	3.77

*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 3.65 differs from the reported value 2.71 by more than 10 %

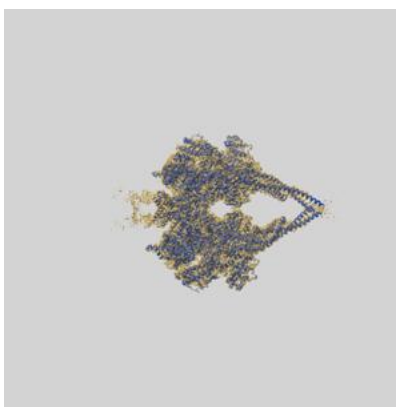
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47379 and PDB model 9E10. Per-residue inclusion information can be found in section [3](#) on page [5](#).

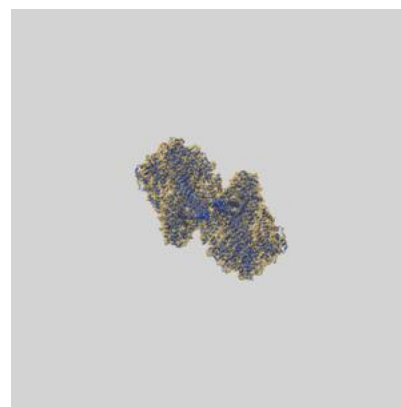
9.1 Map-model overlay [i](#)



X



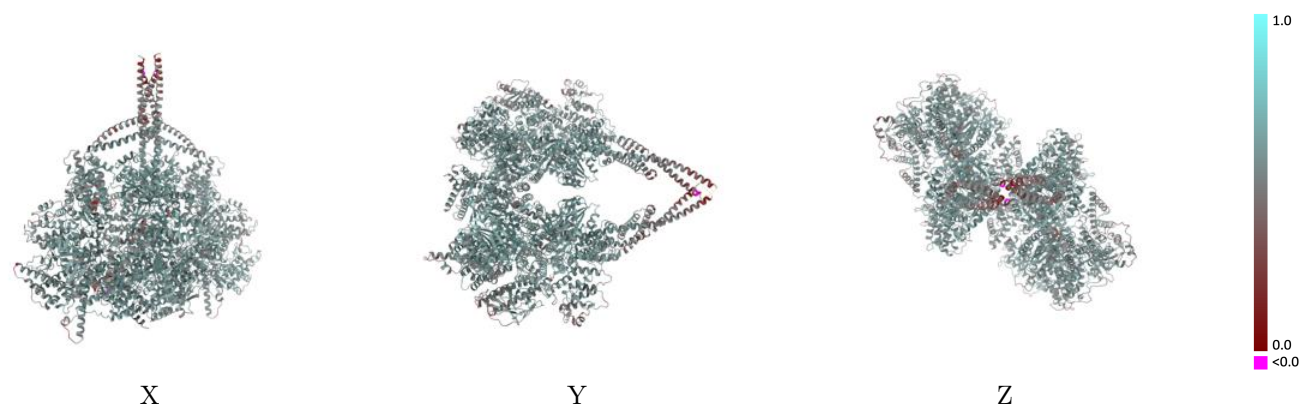
Y



Z

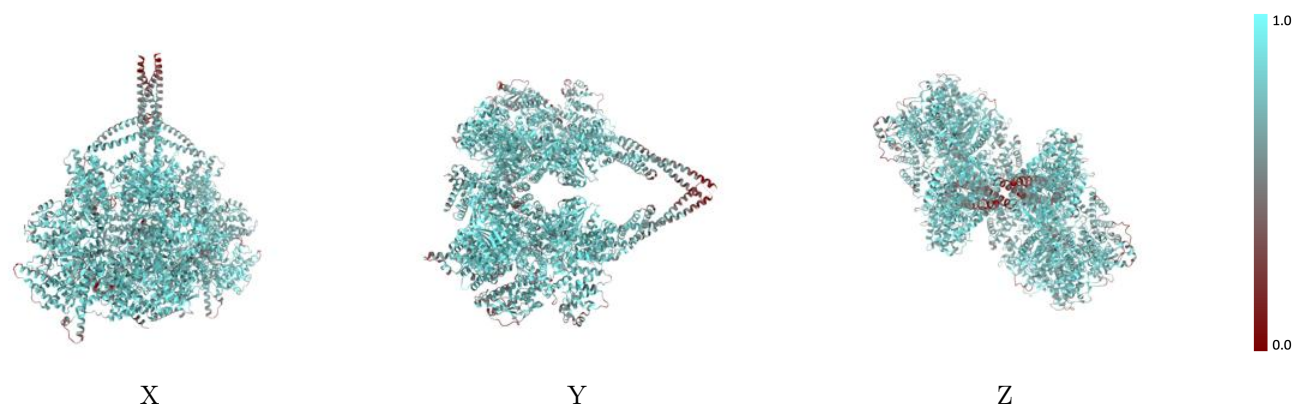
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



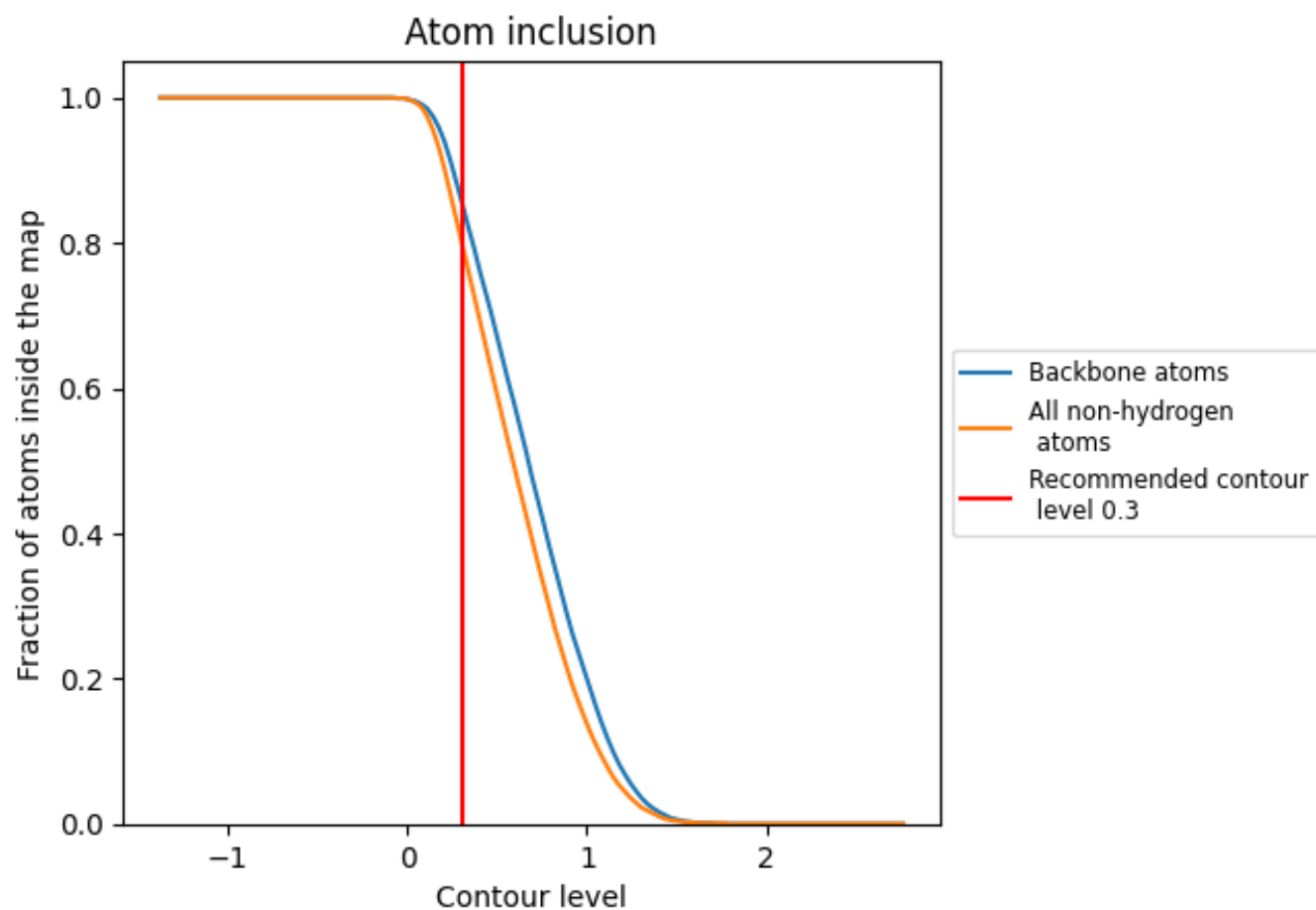
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8040	<div><div></div></div> 0.5700
A	<div><div></div></div> 0.8050	<div><div></div></div> 0.5710
B	<div><div></div></div> 0.8040	<div><div></div></div> 0.5700

