



Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 06:29 PM EDT

PDB ID : 9E0Z / pdb_00009e0z
EMDB ID : EMD-47378
Title : Dimeric motor domains from phi-like dynein-1 bound to a Lis1 dimer under Nde1-Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

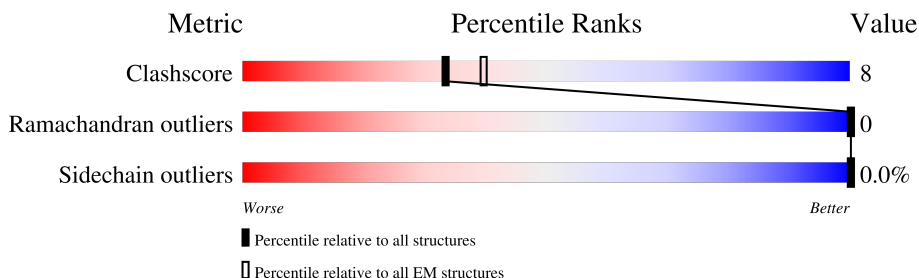
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	410	
2	D	410	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 52502 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.

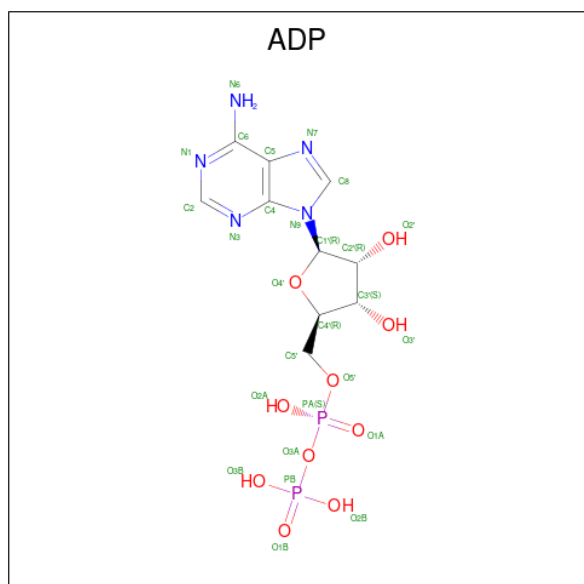
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

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 a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

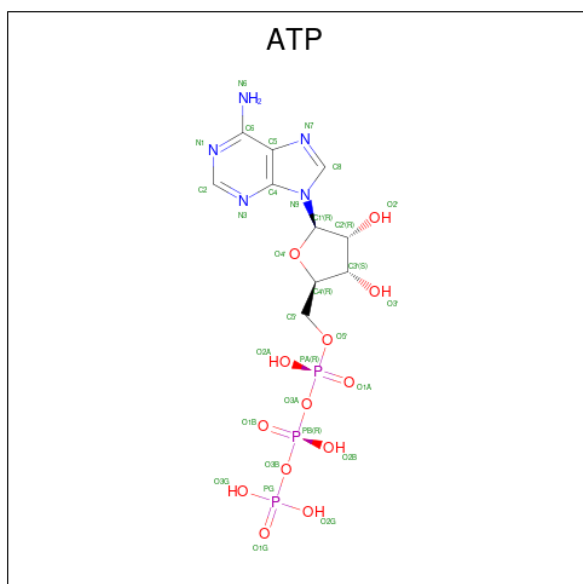
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
2	D	319	Total	C	N	O	S	0	0
			2531	1593	446	472	20		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 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
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	B	2	2	2	0



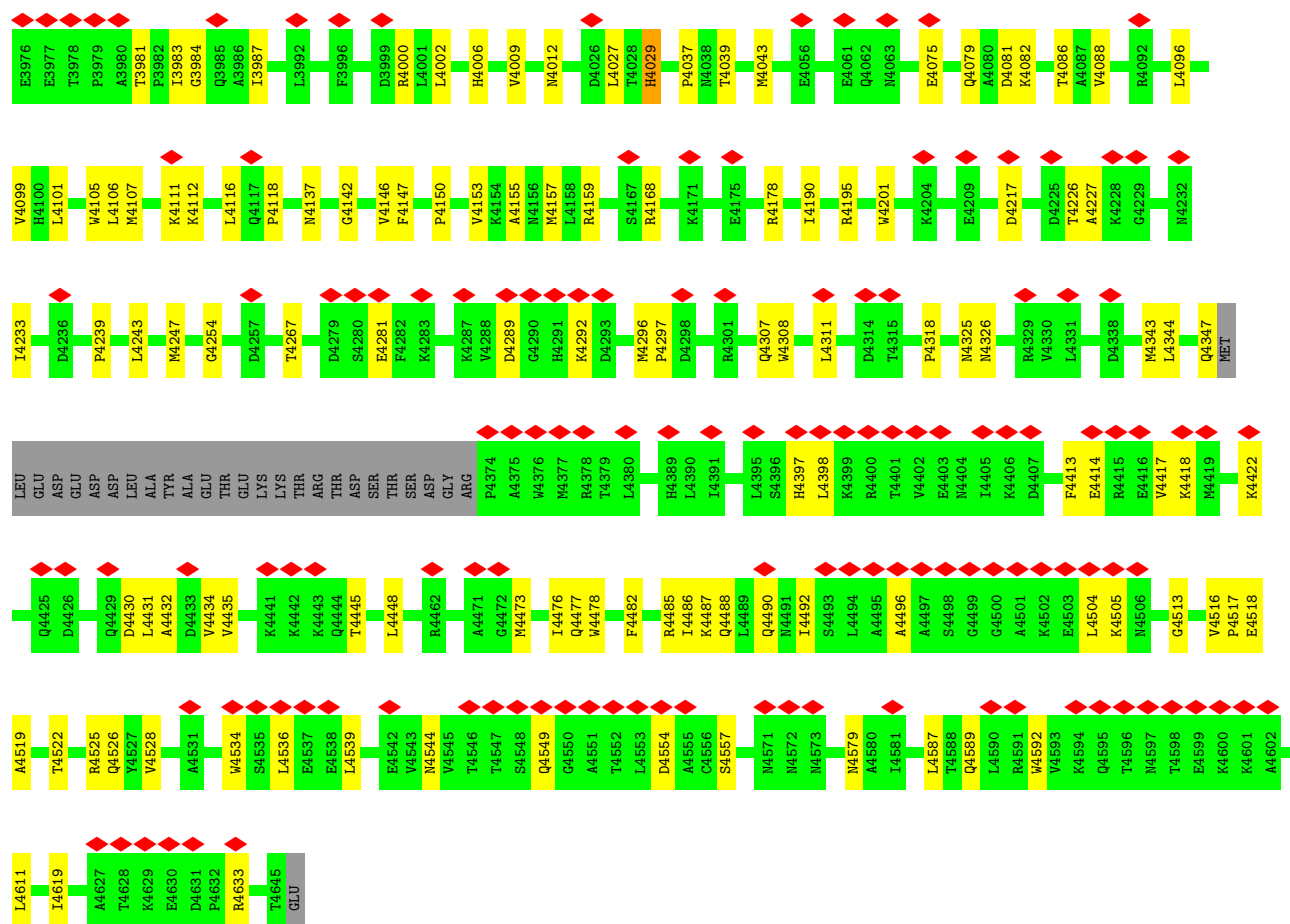


THR	THR	THR	ASP	TRP	LYS	GLN	ILE	ARG	SER	ILE	ILE	MET	ARG	GLU	ASN	PHE	ILE	PRO	THR	VAL	ASN	PHE	SER	ALA	GLU	GLY	ILE	ASP	ALA	ILE	GLY	ASN	LYS	LYS	ASN	TYR	MET	SER	ASN	ARG	ASP	TYR	GLY	ILE	VAL	ASN	ILE	ARG	ALA	SER	LEU	ALA	CYS	GLY	PRO
A4432	D4433	Q4436	W4437	Q4438	Q4439	Q4440	K4441	K4442	K4443	K4447	L4460	P4461	K4462	S4463	S4464	S4465	W4466	W4467	T4468	W4469	P4470	A4471	G4472	I4486	K4487	Q4488	L4489	Q4490	N4491	I4492	S4493	L4494	A4495	A4496	A4497	S4498	Q4499	G4500	A4501	K4502	E4503	L4504	R4415	W4416	W4417	K4418	L4423	E4518	A4519	I4520	T4521	T4522	R4525		
L4541	E4542	Y4545	T4546	T4547	S4548	Q4549	G4550	A4551	T4552	G4472	I4486	K4487	Q4488	L4489	Q4490	N4491	I4492	S4493	L4494	A4495	A4496	A4497	S4498	Q4499	G4500	A4501	K4502	E4503	L4504	R4415	W4416	W4417	K4418	L4423	E4518	A4519	I4520	T4521	T4522	R4525															
Q4526	Y4527	Y4528	A4529	Q4530	A4531	N4532	S4533	W4534	S4535	W4536	E4537	E4538	L4541	E4542	Y4545	T4546	T4547	S4548	Q4549	G4550	A4551	T4552	L4553	D4554	A4555	K4564	N4571	N4572	N4573	K4574	N4579	A4584	T4588	Q4589	L4590	R4591	N4592	W4593	K4594	Q4595	T4596	N4597	T4598	E4599	K4600	K4601	A4602	S4603	W4604	W4605	P4608				
A3980	T3981	P3982	G3911	G3984	E3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	R3923	L3924	Q3925	G3926	L3927	E3930	A3934	S3939	C3940	L3941	F3944	K3945	D3946	L3947	I3948	A3949	K3950	V3951	Q3952	A3953	D3954	E3955	Q3956	G3958	I3959	W3960	L3961	D3962	P3966	E3967	Q3968	T3969	Y3972	E3976	E3977	T3978	P3979				
V3780	T3781	R3782	K3783	V3784	E3785	E3786	T3787	D3788	T3789	V3790	M3791	Q3792	E3793	V3794	T3796	Q3799	L3804	S3809	L3824	V3839	N3845	L3846	K3847	G3848	Q3854	T3860	K3861	D3862	L3863	F3868	A3872	M3875	L3876	A3884	A3888	K3891	L3892	T3895	V3896	G3897	E3898	D3902													
S3674	T3681	P3684	D3691	S3694	L3708	Q3709	D3723	V3724	D3725	F3582	N3584	R3585	S3589	L3734	Q3595	A3596	T3597	D3606	R3607	R3611	T3612	S3613	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	P3643	N3650	R3651	E3652	V3653	R3654	R3655	T3656	G3657	R3658	R3659	D3666	Q3667	D3668												
A3452	V3453	L3454	T3455	S3456	E3457	A3458	Q3459	T3461	K3462	A3463	A3466	A3467	V3468	E3469	A3470	K3471	L3734	Q3595	A3596	T3597	D3606	R3607	R3611	T3612	S3613	E3624	R3628	L3634	V3635	Q3636	D3637	V3638	P3643	N3650	R3651	E3652	V3653	R3654	R3655	T3656	G3657	R3658	R3659	D3666	Q3667	D3668									
E3449	E3450	Y3451	E3494	T3495	F3496	K3497	T3502	S3510	Y3516	A3517	D3521	R3525	V3532	Q3542	F3543	R3544																																							

[illegible]

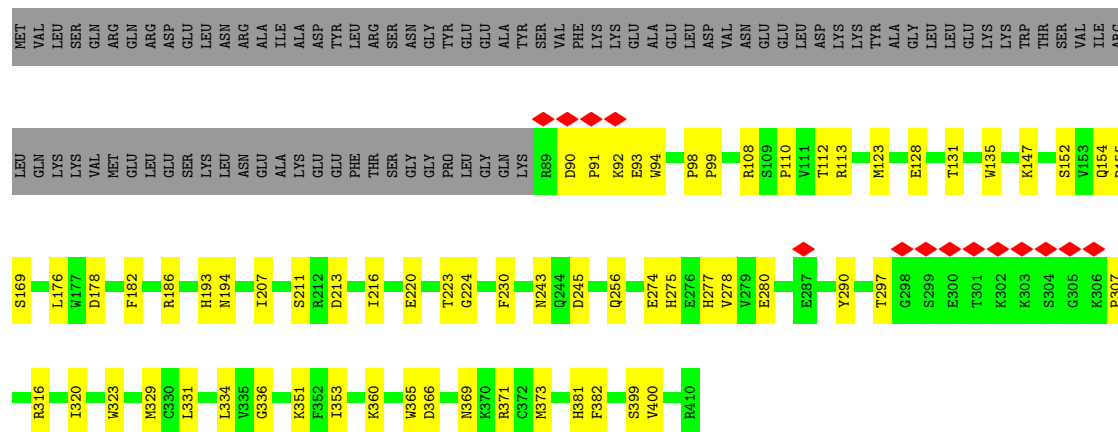






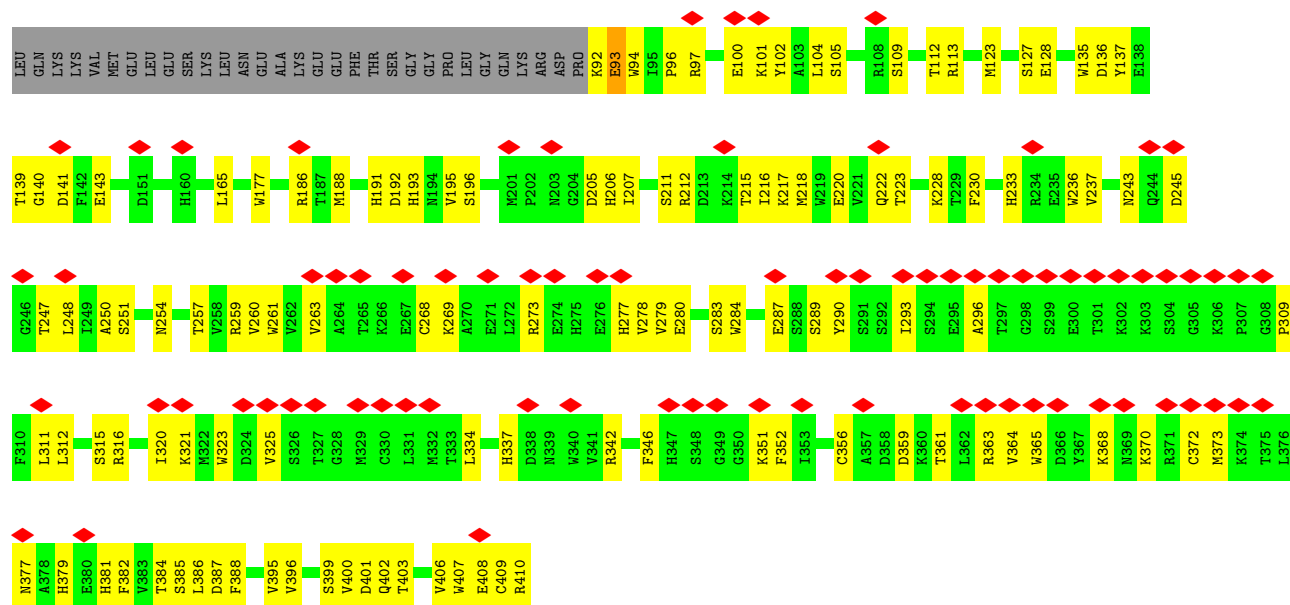
• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain C: 62% 16% 21%



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain D: 20% 48% 29% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215049	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	1.498	Depositor
Minimum map value	-0.699	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	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 [i](#)

5.1 Standard geometry [i](#)

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	0.12	0/24093	0.29	0/32651
1	B	0.12	0/24093	0.29	0/32651
2	C	0.12	0/2624	0.32	0/3555
2	D	0.16	0/2597	0.38	1/3518 (0.0%)
All	All	0.12	0/53407	0.30	1/72375 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	93	GLU	N-CA-C	-5.10	106.90	112.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23593	0	23658	377	0
1	B	23593	0	23658	351	0
2	C	2557	0	2487	42	0
2	D	2531	0	2463	87	0
3	A	81	0	36	2	0
3	B	81	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	12	1	0
4	B	31	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	52502	0	52362	854	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 8.

All (854) 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:2686:MET:HE2	1:A:2703:LEU:HD11	1.65	0.79
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.64	0.79
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	1.64	0.79
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.65	0.78
1:A:2644:THR:HG22	1:A:2646:ASN:H	1.49	0.78
2:D:94:TRP:HB3	2:D:409:CYS:HB3	1.67	0.77
2:D:311:LEU:HB3	2:D:323:TRP:HB2	1.68	0.75
1:B:3229:LEU:O	1:B:3233:ASN:ND2	2.18	0.75
1:B:2163:ASP:OD2	1:B:4526:GLN:NE2	2.19	0.75
2:C:381:HIS:HD2	2:C:400:VAL:HB	1.51	0.74
2:D:259:ARG:HE	2:D:261:TRP:HE1	1.36	0.73
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.70	0.72
1:A:1529:ARG:HE	1:A:1592:LEU:HD11	1.56	0.71
1:A:2481:MET:HE2	1:A:2486:LEU:HA	1.72	0.71
1:A:1558:LYS:HG3	1:A:1565:THR:HG21	1.72	0.70
1:B:2538:GLU:OE2	1:B:2551:LYS:NZ	2.24	0.70
2:C:92:LYS:HE2	2:C:351:LYS:HE3	1.74	0.70
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.73	0.69
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.74	0.69
1:A:3628:ARG:HH22	1:B:3628:ARG:HH22	1.40	0.69
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.56	0.69
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.75	0.69
1:B:4326:ASN:ND2	1:B:4579:ASN:O	2.25	0.68
2:D:243:ASN:ND2	2:D:245:ASP:OD1	2.27	0.68
1:A:2578:GLU:OE2	1:A:2607:SER:OG	2.11	0.68
1:B:2616:GLU:OE1	1:B:2654:GLN:NE2	2.26	0.68
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.74	0.68
1:B:2562:VAL:O	1:B:2804:ARG:NH1	2.27	0.68
2:D:243:ASN:HB3	2:D:284:TRP:HZ3	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2152:GLU:OE1	1:A:4418:LYS:NZ	2.27	0.67
1:B:2452:LEU:HD13	1:B:2729:ARG:HH21	1.59	0.67
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.28	0.67
2:C:280:GLU:OE2	2:C:316:ARG:NE	2.28	0.67
1:A:2970:GLU:N	1:A:2970:GLU:OE1	2.26	0.66
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.28	0.66
1:B:4178:ARG:HH21	1:B:4296:MET:HG3	1.57	0.66
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.29	0.66
1:A:2091:ARG:HD2	1:A:2357:SER:HB2	1.78	0.66
1:B:2181:GLU:HG3	1:B:2244:LEU:HB2	1.78	0.65
1:A:1673:VAL:HG23	1:A:1692:ILE:HD11	1.78	0.65
1:A:3239:LYS:HG2	1:A:3451:TYR:HE1	1.59	0.65
1:A:2828:GLU:OE1	1:A:2924:ARG:NH2	2.26	0.65
1:B:3638:VAL:HG12	1:B:3681:THR:HB	1.79	0.65
1:B:4525:ARG:NH1	1:B:4536:LEU:O	2.30	0.65
1:B:4505:LYS:NZ	1:B:4554:ASP:O	2.28	0.65
1:B:1958:ASP:HA	1:B:2017:THR:HB	1.79	0.65
1:B:1477:LEU:HB3	1:B:1485:ARG:HG3	1.79	0.65
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.79	0.65
1:A:2682:PHE:O	1:A:2686:MET:HG3	1.97	0.64
1:A:1582:VAL:HG13	1:A:1591:VAL:HG11	1.79	0.64
1:A:4043:MET:HE1	1:A:4055:VAL:HG21	1.79	0.64
1:B:2139:GLN:NE2	1:B:2143:GLU:OE2	2.28	0.64
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.63	0.64
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.80	0.64
1:B:2581:LEU:HD11	1:B:2593:LEU:HD21	1.79	0.64
1:A:2091:ARG:NH1	1:A:2320:ASP:OD1	2.31	0.64
1:B:2091:ARG:NH1	1:B:2320:ASP:OD1	2.29	0.64
1:A:4230:ARG:HH21	1:A:4233:ILE:HG13	1.63	0.64
1:B:2138:ILE:HD12	1:B:2161:LEU:HD22	1.80	0.64
1:B:2671:MET:HG2	1:B:2677:GLN:HG3	1.80	0.64
1:B:1526:LYS:HG2	1:B:1529:ARG:HH21	1.63	0.63
1:A:3624:GLU:OE2	1:A:3667:GLN:NE2	2.32	0.63
1:B:1933:ASP:HB2	1:B:1962:ARG:HH21	1.61	0.63
1:A:1643:ASN:HD22	1:A:1649:LYS:HD2	1.64	0.63
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.79	0.63
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.31	0.63
1:B:3557:ASP:OD1	1:B:3743:ARG:NH1	2.31	0.63
1:B:4281:GLU:N	1:B:4281:GLU:OE2	2.30	0.63
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.79	0.63
1:B:3129:VAL:HG21	1:B:3149:PHE:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4096:LEU:HD13	1:B:4105:TRP:HH2	1.64	0.63
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.31	0.63
1:A:1463:LEU:HD21	1:A:1507:MET:HE1	1.81	0.62
1:A:1814:GLU:OE2	1:A:1818:GLN:NE2	2.32	0.62
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.32	0.62
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.32	0.62
1:B:1914:GLU:HG3	3:B:4701:ADP:H2'	1.82	0.62
1:A:2647:GLY:HA3	1:A:2702:LYS:HZ1	1.64	0.62
1:B:3239:LYS:HB3	1:B:3451:TYR:HE1	1.64	0.62
2:C:297:THR:HG21	2:C:331:LEU:HD13	1.81	0.62
1:A:2452:LEU:HD13	1:A:2729:ARG:HH21	1.65	0.62
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	1.81	0.62
1:B:3731:LEU:HD23	1:B:3787:THR:HG23	1.80	0.62
1:B:2302:VAL:HA	1:B:2342:MET:HB2	1.82	0.62
1:B:1606:ASP:O	1:B:1610:LYS:HG2	2.00	0.62
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.32	0.61
1:A:3208:ILE:HG21	1:A:3486:ARG:HD3	1.82	0.61
1:A:2060:ARG:HE	1:A:2061:THR:HG23	1.65	0.61
2:C:90:ASP:HB3	2:C:93:GLU:HB3	1.81	0.61
1:A:3946:ASP:OD2	1:A:3950:LYS:NZ	2.33	0.61
1:B:1959:GLU:OE1	1:B:2025:ARG:NH1	2.33	0.61
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.83	0.61
1:A:3584:ASN:O	1:A:3651:ARG:NH1	2.29	0.61
1:A:3872:ALA:HA	1:A:3875:MET:HB3	1.83	0.61
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.34	0.61
2:D:359:ASP:OD2	2:D:363:ARG:NH2	2.34	0.61
1:B:3239:LYS:HE3	1:B:3239:LYS:HA	1.83	0.60
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.83	0.60
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.82	0.60
1:B:3167:ARG:HH12	1:B:3685:THR:HA	1.67	0.60
2:D:243:ASN:ND2	2:D:247:THR:OG1	2.34	0.60
1:A:2103:VAL:HG23	1:A:2136:ILE:HG23	1.83	0.60
1:A:3845:ASN:ND2	1:A:3862:ASP:OD2	2.34	0.60
1:B:1965:GLU:HG2	1:B:2026:SER:HB3	1.83	0.60
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.83	0.60
1:B:4178:ARG:NH2	1:B:4297:PRO:O	2.34	0.60
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.83	0.60
1:B:3178:ASP:OD2	1:B:3585:ARG:NE	2.35	0.60
2:D:105:SER:HB3	2:D:403:THR:HG22	1.84	0.60
2:D:396:VAL:HG12	2:D:406:VAL:HG22	1.83	0.60
1:A:4107:MET:HG3	1:A:4137:ASN:HD21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:THR:HG22	2:D:273:ARG:HB3	1.84	0.60
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.82	0.60
1:B:3520:PHE:HB3	1:B:3524:MET:HB3	1.84	0.60
2:C:360:LYS:HE3	2:C:381:HIS:HA	1.84	0.60
1:A:2088:PHE:HE1	1:A:2148:LYS:HZ1	1.50	0.59
1:A:4266:ASN:O	1:A:4270:GLU:HG2	2.03	0.59
1:A:3469:GLU:OE2	1:A:3473:ASN:ND2	2.35	0.59
1:B:2995:ASP:OD1	1:B:2996:GLU:N	2.35	0.59
1:B:2905:LEU:HD11	1:B:3652:GLU:HB3	1.84	0.59
1:B:4398:LEU:HG	1:B:4417:VAL:HG11	1.83	0.59
1:A:2839:GLU:OE2	1:A:2839:GLU:N	2.36	0.59
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.67	0.59
1:B:3597:THR:O	1:B:3601:MET:HG2	2.03	0.59
1:A:2447:MET:HE1	1:A:2723:LEU:HD12	1.84	0.58
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.83	0.58
2:C:278:VAL:HB	2:C:316:ARG:HD2	1.85	0.58
1:B:3839:VAL:HG21	1:B:3863:LEU:HA	1.84	0.58
1:B:4430:ASP:O	1:B:4434:VAL:HG23	2.03	0.58
1:A:2620:LEU:HD11	1:A:2661:LEU:HD22	1.85	0.58
1:B:2488:ARG:O	1:B:2492:ARG:HG2	2.04	0.58
1:B:3619:PHE:HZ	1:B:3645:LEU:HD21	1.67	0.58
1:A:1777:PRO:O	1:A:1780:SER:OG	2.19	0.58
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	1.85	0.58
2:C:320:ILE:HB	2:C:334:LEU:HB2	1.85	0.58
1:B:1839:LEU:O	1:B:1843:ARG:NH1	2.36	0.58
1:B:2788:THR:HG22	1:B:2789:GLN:HG2	1.86	0.58
1:B:2457:SER:HB3	1:B:2732:PRO:HB3	1.86	0.58
1:B:2944:THR:O	1:B:2948:ARG:HG3	2.04	0.58
1:B:1491:ASP:OD1	1:B:1492:ASP:N	2.36	0.58
1:B:2221:MET:HG2	1:B:2343:PHE:HB2	1.85	0.58
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.85	0.57
1:B:3983:ILE:O	1:B:3987:ILE:HD12	2.04	0.57
2:D:188:MET:HE1	2:D:207:ILE:HD12	1.86	0.57
1:B:1569:GLN:O	1:B:1573:THR:HG23	2.05	0.57
1:B:4075:GLU:O	1:B:4079:GLN:HG2	2.03	0.57
1:B:1607:LEU:O	1:B:1611:ILE:HG12	2.03	0.57
1:B:2449:LEU:HA	1:B:2453:ARG:HH21	1.68	0.57
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.69	0.57
1:B:2047:GLN:HE22	1:B:2067:ASN:HA	1.69	0.57
1:B:4029:HIS:HD1	1:B:4029:HIS:C	2.13	0.57
1:A:2242:GLU:OE1	1:A:2248:GLU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2185:VAL:HA	1:B:2188:GLU:HG2	1.86	0.57
1:A:2427:PHE:HE1	1:A:2433:VAL:HG21	1.69	0.57
1:B:1708:GLU:HA	1:B:1711:VAL:HG22	1.87	0.57
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.87	0.57
1:B:3459:GLN:HA	1:B:3462:LYS:HD2	1.87	0.57
1:A:1508:LYS:HD3	1:A:1513:TYR:CZ	2.40	0.56
1:A:4260:PHE:HE2	1:A:4618:LEU:HD21	1.70	0.56
1:B:1537:TRP:CE3	1:B:1601:LEU:HD11	2.40	0.56
1:A:4409:LEU:HD21	1:A:4504:LEU:HB3	1.87	0.56
1:B:2499:LEU:HD23	1:B:2514:LEU:HD23	1.88	0.56
1:B:2775:GLU:HG2	1:B:2779:MET:HE2	1.86	0.56
1:B:4082:LYS:O	1:B:4086:THR:HG23	2.05	0.56
2:C:216:ILE:HB	2:C:230:PHE:HB2	1.86	0.56
2:D:216:ILE:HD11	2:D:237:VAL:HG11	1.86	0.56
1:A:3487:GLU:HA	1:A:3490:GLU:HG2	1.87	0.56
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.70	0.56
1:B:1467:ARG:HD2	1:B:1523:TRP:HZ2	1.71	0.56
1:B:2433:VAL:HG22	1:B:2498:ILE:HD11	1.88	0.56
1:B:4002:LEU:O	1:B:4006:HIS:ND1	2.32	0.56
2:D:279:VAL:HA	2:D:315:SER:HA	1.88	0.56
1:B:1474:GLU:N	1:B:1474:GLU:OE2	2.38	0.56
1:A:2427:PHE:CE1	1:A:2433:VAL:HG21	2.41	0.56
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.88	0.56
2:C:243:ASN:ND2	2:C:245:ASP:OD1	2.39	0.56
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.88	0.56
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	1.87	0.56
1:B:4081:ASP:OD1	1:B:4112:LYS:NZ	2.36	0.56
2:D:233:HIS:NE2	2:D:251:SER:OG	2.32	0.56
2:D:277:HIS:CG	2:D:278:VAL:H	2.23	0.56
1:A:2905:LEU:HD11	1:A:3652:GLU:HG2	1.88	0.55
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.40	0.55
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.06	0.55
1:B:1533:LEU:HD11	1:B:1597:VAL:HG22	1.87	0.55
1:B:1623:ARG:NH2	1:B:1634:ASP:OD1	2.39	0.55
1:B:2446:ILE:HD11	1:B:2714:PRO:HB3	1.89	0.55
1:A:4492:ILE:HG22	1:A:4507:ILE:HD13	1.89	0.55
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.87	0.55
1:B:3230:GLU:HA	1:B:3233:ASN:HD21	1.71	0.55
1:B:3468:VAL:O	1:B:3472:VAL:HG23	2.06	0.55
2:C:98:PRO:HG2	2:C:99:PRO:HD3	1.88	0.55
1:A:2148:LYS:HB2	1:A:2361:MET:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4081:ASP:OD1	1:A:4112:LYS:NZ	2.36	0.55
2:D:254:ASN:HD22	2:D:278:VAL:HG11	1.72	0.55
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.39	0.55
1:A:2820:GLY:O	1:A:2824:ILE:HD12	2.06	0.55
1:B:1494:PHE:O	1:B:1498:LYS:HG2	2.06	0.55
1:B:3607:ARG:NH2	1:B:3674:SER:O	2.39	0.55
1:B:2684:ARG:NH1	1:B:2688:GLU:OE1	2.39	0.54
2:C:131:THR:HG22	2:C:147:LYS:HG2	1.88	0.54
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.40	0.54
1:B:2265:TYR:OH	1:B:2311:TRP:O	2.24	0.54
1:B:2760:PRO:HB3	1:B:2763:ARG:HH21	1.72	0.54
1:B:3219:ARG:NH2	1:B:3472:VAL:HG13	2.22	0.54
1:B:3239:LYS:HB3	1:B:3451:TYR:CE1	2.42	0.54
1:B:3942:PRO:O	1:B:3945:LYS:NZ	2.34	0.54
1:A:2302:VAL:HA	1:A:2342:MET:HB2	1.89	0.54
1:A:2464:GLN:HA	1:A:2467:ARG:HG3	1.89	0.54
1:B:1627:PRO:HB3	1:B:1950:GLN:HB3	1.90	0.54
2:D:236:TRP:HB3	2:D:254:ASN:OD1	2.07	0.54
1:A:3211:THR:HG22	1:A:3479:LEU:HD11	1.89	0.54
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	1.89	0.54
2:C:112:THR:HG21	2:C:154:GLN:HA	1.90	0.54
1:A:2996:GLU:HG3	1:A:3078:ARG:HH12	1.73	0.54
1:B:2091:ARG:NH2	3:B:4701:ADP:O3A	2.41	0.54
2:C:186:ARG:HD3	2:C:224:GLY:HA3	1.89	0.54
2:C:381:HIS:CD2	2:C:382:PHE:H	2.26	0.54
1:B:2863:ARG:HG3	1:B:2863:ARG:HH11	1.73	0.54
1:B:3172:THR:HG21	1:B:3694:SER:HB3	1.90	0.54
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.90	0.54
1:B:2590:PRO:HB2	1:B:2731:VAL:HG12	1.90	0.54
1:A:1619:LEU:HD21	1:A:1638:LEU:HG	1.90	0.53
1:A:2584:TRP:HE3	1:A:2591:LEU:HD22	1.72	0.53
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.90	0.53
1:A:2619:GLY:O	1:A:3014:ASN:ND2	2.35	0.53
1:B:2465:ALA:HB2	1:B:2493:TYR:CD1	2.43	0.53
1:B:3005:LEU:HD22	1:B:3082:SER:HB2	1.89	0.53
1:B:4037:PRO:HB2	1:B:4118:PRO:HG2	1.89	0.53
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.90	0.53
1:B:3017:VAL:HB	1:B:3020:LEU:HB2	1.90	0.53
2:C:312:LEU:HD21	2:C:353:ILE:HD13	1.90	0.53
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.91	0.53
1:A:4292:LYS:HD2	1:A:4293:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1897:GLU:O	1:B:1899:ARG:NH1	2.42	0.53
1:B:2183:LYS:O	1:B:2187:GLN:HG2	2.08	0.53
2:D:370:LYS:NZ	2:D:373:MET:SD	2.82	0.53
1:A:1769:MET:SD	1:A:1777:PRO:HD2	2.49	0.53
1:A:2581:LEU:HD22	1:A:2604:THR:HG22	1.90	0.53
1:B:3735:GLN:HG3	1:B:3787:THR:HG21	1.91	0.53
1:B:3875:MET:HE1	1:B:3883:PHE:HB2	1.91	0.53
2:C:274:GLU:HB2	2:C:323:TRP:HH2	1.74	0.53
2:D:196:SER:OG	2:D:236:TRP:NE1	2.40	0.53
1:A:1554:SER:O	1:A:1558:LYS:NZ	2.39	0.53
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.44	0.53
1:A:4247:MET:HG2	1:A:4251:ILE:HD12	1.90	0.53
1:B:3167:ARG:NH1	1:B:3685:THR:HA	2.23	0.53
1:B:3584:ASN:O	1:B:3651:ARG:NH2	2.41	0.53
1:B:4549:GLN:HG3	1:B:4587:LEU:HB2	1.91	0.53
2:C:277:HIS:ND1	2:C:316:ARG:HB2	2.24	0.53
1:B:1959:GLU:HB3	1:B:1962:ARG:HD3	1.91	0.53
1:A:3124:ASP:OD1	1:A:3125:TYR:N	2.42	0.52
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.52
1:B:3981:THR:HG23	1:B:3984:GLY:H	1.72	0.52
2:D:191:HIS:HD2	2:D:195:VAL:HG22	1.74	0.52
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.42	0.52
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.90	0.52
1:B:3782:ARG:NH1	1:B:3786:GLU:OE2	2.43	0.52
1:B:3888:ALA:HB1	1:B:4012:ASN:HD22	1.74	0.52
2:D:372:CYS:O	2:D:373:MET:HE2	2.09	0.52
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.91	0.52
2:D:356:CYS:SG	2:D:386:LEU:HD22	2.50	0.52
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	1.92	0.52
1:B:3479:LEU:O	1:B:3486:ARG:NH2	2.42	0.52
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.25	0.52
1:A:2304:ASP:OD1	1:A:2726:ARG:NH1	2.36	0.52
2:D:212:ARG:HD3	2:D:236:TRP:CG	2.43	0.52
1:A:4039:THR:HG23	1:A:4142:GLY:HA2	1.91	0.52
1:A:2574:THR:O	1:A:2578:GLU:HG2	2.10	0.51
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	1.92	0.51
2:D:92:LYS:HG3	2:D:93:GLU:H	1.74	0.51
2:D:191:HIS:HB2	2:D:217:LYS:HD2	1.91	0.51
1:A:4408:PRO:HB3	1:A:4411:ARG:HH21	1.76	0.51
1:B:1623:ARG:NH1	1:B:1629:PHE:O	2.43	0.51
1:B:3107:LYS:HD2	1:B:3144:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4155:ALA:O	1:B:4159:ARG:HG3	2.10	0.51
2:D:381:HIS:CE1	2:D:382:PHE:HD2	2.28	0.51
1:B:3458:ALA:O	1:B:3462:LYS:HG3	2.10	0.51
2:D:269:LYS:NZ	2:D:325:VAL:O	2.43	0.51
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.46	0.51
1:B:1508:LYS:HG2	1:B:1513:TYR:CZ	2.46	0.51
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	1.92	0.51
1:B:2257:LYS:NZ	1:B:2308:ASP:OD2	2.33	0.51
1:A:2108:ILE:HD11	1:A:2131:LEU:HD22	1.93	0.51
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.11	0.51
1:B:2175:MET:HE2	1:B:2208:LEU:HD22	1.93	0.51
1:B:4190:ILE:HD12	1:B:4201:TRP:HZ2	1.76	0.51
1:A:2107:ARG:O	1:A:2110:LYS:HG3	2.11	0.51
1:A:2964:HIS:HA	1:A:3643:PRO:HD2	1.92	0.51
1:B:4473:MET:HE2	1:B:4478:TRP:HB2	1.93	0.51
1:A:1479:ASN:HA	1:A:1485:ARG:HD2	1.93	0.50
1:B:3791:MET:O	1:B:3795:GLU:HG3	2.11	0.50
2:C:275:HIS:NE2	2:C:313:SER:OG	2.43	0.50
1:A:1480:TYR:HB2	1:A:1486:LEU:HD23	1.93	0.50
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.93	0.50
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	1.92	0.50
1:A:1897:GLU:O	1:A:1899:ARG:NH1	2.44	0.50
1:A:3458:ALA:O	1:A:3461:ILE:HG22	2.11	0.50
1:B:1460:GLU:O	1:B:1464:LYS:HG3	2.11	0.50
1:B:1515:VAL:HG13	1:B:1516:PHE:CD2	2.47	0.50
1:B:3158:ASN:ND2	1:B:3169:MET:O	2.44	0.50
1:A:2175:MET:SD	1:A:2175:MET:N	2.84	0.50
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.76	0.50
1:B:1699:ASN:OD1	1:B:1700:GLU:N	2.45	0.50
2:C:381:HIS:CG	2:C:382:PHE:H	2.30	0.50
2:D:351:LYS:HG3	2:D:352:PHE:CD2	2.47	0.50
1:A:1507:MET:O	1:A:1510:SER:OG	2.24	0.50
1:B:2176:THR:O	1:B:2180:GLU:HG2	2.12	0.50
1:A:1543:ARG:O	1:A:1547:LEU:HD23	2.12	0.50
1:B:3477:ALA:HA	1:B:3480:LYS:HE3	1.94	0.50
2:D:334:LEU:HD23	2:D:365:TRP:HE3	1.77	0.50
1:B:1561:LEU:HB3	1:B:1564:GLU:HB2	1.93	0.50
2:C:353:ILE:HB	2:C:365:TRP:HB2	1.93	0.50
1:A:2110:LYS:HA	1:A:2113:ARG:HE	1.77	0.50
1:A:2446:ILE:HG23	1:A:2447:MET:HG3	1.94	0.49
1:B:1943:ARG:HG2	1:B:1943:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2518:ILE:O	1:B:2522:THR:HG22	2.11	0.49
2:D:109:SER:N	2:D:402:GLN:OE1	2.45	0.49
1:A:1965:GLU:HG3	1:A:2026:SER:HB3	1.94	0.49
1:B:1804:ARG:O	1:B:1808:LEU:HG	2.13	0.49
1:B:2423:MET:HE1	1:B:2462:LEU:HD22	1.93	0.49
1:A:1480:TYR:OH	1:A:1548:GLU:OE2	2.22	0.49
1:A:2078:GLU:OE1	1:A:4522:THR:OG1	2.24	0.49
1:A:2635:PHE:CE2	1:A:2686:MET:HE1	2.47	0.49
1:A:3048:GLU:N	1:A:3048:GLU:OE1	2.45	0.49
1:B:4243:LEU:O	1:B:4247:MET:HG3	2.12	0.49
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.95	0.49
1:A:2588:HIS:HD2	1:A:2707:GLN:HE21	1.60	0.49
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.45	0.49
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.95	0.49
1:B:2784:PHE:HB2	1:B:2794:TYR:HE2	1.78	0.49
1:B:3154:LEU:HG	1:B:3516:TYR:CD1	2.47	0.49
1:A:1533:LEU:HD11	1:A:1597:VAL:HG22	1.95	0.49
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.94	0.49
1:A:2994:MET:HE2	1:A:2999:VAL:HG22	1.95	0.49
1:A:3741:ARG:NH2	1:A:3776:GLU:OE1	2.46	0.49
1:B:1469:VAL:O	1:B:1473:TYR:HB2	2.12	0.49
1:B:2538:GLU:HB3	1:B:2548:TRP:CE2	2.47	0.49
1:B:3551:GLU:HA	1:B:3559:ARG:HH12	1.77	0.49
1:B:3728:ARG:HH11	1:B:3728:ARG:HG2	1.78	0.49
1:A:2562:VAL:HG21	1:A:2755:MET:HB2	1.95	0.49
1:A:3960:TRP:HD1	1:A:3969:THR:HG23	1.78	0.49
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.48	0.49
1:A:4541:LEU:HB2	1:A:4592:TRP:CZ3	2.47	0.49
1:B:1617:GLU:O	1:B:1621:ARG:HG3	2.11	0.49
1:B:2623:SER:OG	1:B:3006:GLU:OE1	2.31	0.49
1:B:3099:THR:HG23	1:B:3148:VAL:HG11	1.94	0.49
2:D:104:LEU:HD23	2:D:135:TRP:CE3	2.47	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.95	0.49
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	1.95	0.49
1:A:3239:LYS:HG2	1:A:3451:TYR:CE1	2.45	0.49
2:D:395:VAL:HG23	2:D:407:TRP:HD1	1.77	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.13	0.49
1:B:2290:SER:HB2	1:B:2295:LEU:HG	1.94	0.49
1:B:3131:ASP:OD1	1:B:3132:LYS:N	2.45	0.49
1:B:3483:SER:O	1:B:3486:ARG:HG2	2.13	0.49
1:B:3751:GLN:O	1:B:3754:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4153:VAL:O	1:B:4157:MET:HG3	2.13	0.49
2:C:211:SER:OG	2:C:213:ASP:OD1	2.31	0.49
2:C:220:GLU:OE2	2:C:223:THR:OG1	2.26	0.49
2:D:287:GLU:HA	2:D:290:TYR:CD1	2.47	0.48
2:D:379:HIS:HB3	2:D:401:ASP:OD2	2.12	0.48
1:B:4043:MET:HE2	1:B:4147:PHE:CE2	2.48	0.48
1:B:4088:VAL:HG11	1:B:4116:LEU:HD23	1.95	0.48
1:B:4150:PRO:O	1:B:4195:ARG:NH2	2.44	0.48
2:D:192:ASP:OD1	2:D:193:HIS:N	2.46	0.48
1:A:1497:VAL:O	1:A:1501:ILE:HG12	2.13	0.48
1:A:1933:ASP:OD2	1:A:2314:ASN:ND2	2.43	0.48
1:A:3034:LYS:NZ	1:A:3044:LEU:O	2.45	0.48
1:A:3597:THR:HG21	1:A:3611:ARG:HH12	1.78	0.48
1:B:2231:SER:HA	1:B:2234:TRP:CD1	2.49	0.48
1:B:3177:LEU:HD23	1:B:3180:ILE:HD11	1.95	0.48
2:D:205:ASP:O	2:D:206:HIS:ND1	2.44	0.48
2:D:165:LEU:HB3	2:D:177:TRP:HB2	1.95	0.48
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.95	0.48
1:A:1637:LEU:O	1:A:1641:ILE:HG12	2.14	0.48
1:A:1946:VAL:HG13	1:A:2006:VAL:HG21	1.95	0.48
1:A:3030:MET:HE3	1:A:3047:HIS:HB3	1.95	0.48
1:B:1728:GLY:C	1:B:1729:LYS:HG2	2.38	0.48
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	1.94	0.48
1:B:3031:THR:O	1:B:3035:GLU:HG3	2.14	0.48
2:D:206:HIS:CD2	2:D:218:MET:HE3	2.48	0.48
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.94	0.48
1:B:2437:LEU:HD21	1:B:2451:ARG:HG3	1.95	0.48
1:B:4487:LYS:O	1:B:4490:GLN:HG2	2.13	0.48
2:C:110:PRO:HB3	2:C:400:VAL:HA	1.94	0.48
2:D:109:SER:O	2:D:127:SER:OG	2.31	0.48
1:A:2102:ASN:O	1:A:2106:GLU:HG2	2.12	0.48
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.48	0.48
1:B:2304:ASP:OD1	1:B:2684:ARG:NH2	2.46	0.48
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.95	0.48
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.95	0.48
1:A:4545:VAL:O	1:A:4573:ASN:ND2	2.47	0.48
1:B:3723:ASP:OD1	1:B:3724:VAL:N	2.47	0.48
1:B:3885:MET:HE3	1:B:4343:MET:HE1	1.95	0.48
1:A:1527:LEU:HA	1:A:1530:ILE:HG12	1.96	0.47
1:B:3114:ASP:O	1:B:3140:ARG:NH2	2.47	0.47
1:B:3220:ARG:HA	1:B:3223:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4496:ALA:HB2	1:B:4504:LEU:HD21	1.96	0.47
1:B:3790:VAL:O	1:B:3793:GLU:HG3	2.14	0.47
2:D:109:SER:HA	2:D:402:GLN:HE22	1.79	0.47
1:A:1913:THR:OG1	1:A:1958:ASP:OD1	2.32	0.47
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	1.96	0.47
1:A:2472:TYR:HD2	1:A:2481:MET:HB2	1.79	0.47
1:A:3459:GLN:HA	1:A:3462:LYS:HG2	1.96	0.47
1:A:1537:TRP:CE3	1:A:1601:LEU:HD11	2.50	0.47
1:A:2786:GLN:HG3	1:A:2790:PRO:HA	1.96	0.47
1:A:4303:GLU:O	1:A:4307:GLN:HG3	2.15	0.47
1:B:2802:TRP:CZ2	1:B:2829:ALA:HB2	2.49	0.47
1:A:1513:TYR:CE2	1:A:1517:GLU:HG3	2.50	0.47
1:A:2088:PHE:HE1	1:A:2148:LYS:NZ	2.12	0.47
1:B:1616:GLY:O	1:B:1620:GLU:HG2	2.15	0.47
1:A:4043:MET:HE2	1:A:4125:PHE:HB3	1.96	0.47
1:B:3457:GLU:O	1:B:3461:ILE:HG12	2.15	0.47
2:D:228:LYS:NZ	2:D:263:VAL:O	2.48	0.47
1:A:1623:ARG:NH1	1:A:1629:PHE:O	2.48	0.47
1:A:1842:MET:HA	1:A:1861:MET:HB2	1.97	0.47
1:A:2190:TYR:CE2	1:A:2385:ILE:HD11	2.50	0.47
1:A:2641:TYR:CE2	1:A:2694:ARG:HD3	2.49	0.47
1:A:2837:LEU:HD13	1:A:2842:GLU:HB3	1.97	0.47
1:A:3772:ASN:OD1	1:A:3775:ARG:NH1	2.47	0.47
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.50	0.47
1:B:2481:MET:HG2	1:B:2486:LEU:HD13	1.97	0.47
1:B:3884:ALA:HB1	1:B:4009:VAL:HG11	1.97	0.47
1:B:4227:ALA:HB2	1:B:4233:ILE:HD12	1.96	0.47
1:B:4267:THR:HG23	1:B:4633:ARG:HG2	1.97	0.47
2:D:215:THR:OG1	2:D:230:PHE:O	2.19	0.47
1:A:1619:LEU:O	1:A:1623:ARG:HG3	2.15	0.47
1:A:2423:MET:HG2	1:A:2494:LEU:HD12	1.97	0.47
1:B:2635:PHE:HE1	1:B:2661:LEU:HD11	1.80	0.47
1:B:3479:LEU:HD12	1:B:3486:ARG:HH22	1.80	0.47
1:A:1860:GLN:HG2	1:A:1865:LYS:HG3	1.97	0.47
1:A:2324:LEU:HD23	1:A:2334:SER:HA	1.97	0.47
1:A:3804:LEU:HD13	1:A:3860:THR:HG22	1.96	0.47
1:A:4171:LYS:HE2	1:A:4171:LYS:HA	1.97	0.47
1:B:1698:ILE:HD12	1:B:1701:TRP:NE1	2.29	0.47
1:B:2091:ARG:HD2	1:B:2357:SER:HB2	1.97	0.47
1:A:1609:GLY:O	1:A:1613:LYS:HG3	2.15	0.47
1:A:2384:SER:HB2	1:A:2385:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3191:ARG:HG3	1:B:3500:MET:HE1	1.96	0.47
2:C:91:PRO:HA	2:C:94:TRP:HZ3	1.80	0.47
2:D:296:ALA:HB2	2:D:368:LYS:HG3	1.96	0.47
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.97	0.46
1:A:4219:VAL:HA	1:A:4243:LEU:HD21	1.97	0.46
1:B:2307:VAL:HG23	1:B:2345:VAL:HG11	1.96	0.46
1:B:2943:LYS:HG2	1:B:3094:PHE:HD2	1.81	0.46
1:B:3135:GLN:O	1:B:3137:PRO:HD3	2.14	0.46
2:D:363:ARG:HD2	2:D:365:TRP:HE1	1.80	0.46
1:A:2635:PHE:CE1	1:A:2661:LEU:HD11	2.51	0.46
1:A:3008:MET:O	1:A:3012:LEU:HG	2.15	0.46
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.47	0.46
1:B:2467:ARG:HG3	1:B:2467:ARG:HH11	1.81	0.46
1:B:2792:TYR:OH	1:B:2842:GLU:OE1	2.25	0.46
2:C:108:ARG:HH12	2:D:143:GLU:CD	2.23	0.46
2:D:92:LYS:N	2:D:94:TRP:CD1	2.84	0.46
2:D:254:ASN:ND2	2:D:278:VAL:HG11	2.29	0.46
1:A:1478:VAL:HG23	1:A:1488:ARG:CZ	2.45	0.46
1:A:2369:LEU:HD11	4:A:4702:ATP:C5	2.51	0.46
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.98	0.46
1:B:3229:LEU:HD21	1:B:3462:LYS:HG2	1.96	0.46
2:D:139:THR:OG1	2:D:141:ASP:OD2	2.23	0.46
1:A:1529:ARG:HH21	1:A:1592:LEU:HD21	1.81	0.46
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.49	0.46
1:B:2603:MET:HE1	3:B:4703:ADP:C5	2.51	0.46
1:B:3483:SER:O	1:B:3487:GLU:HG2	2.15	0.46
2:D:277:HIS:CE1	2:D:316:ARG:HD2	2.49	0.46
1:A:1888:CYS:HA	1:A:2039:LEU:HD22	1.97	0.46
1:A:1941:MET:HG3	1:A:1971:VAL:HG21	1.97	0.46
1:A:2588:HIS:CD2	1:A:2707:GLN:HE21	2.33	0.46
1:A:4605:VAL:HG13	1:A:4626:ILE:HD11	1.98	0.46
1:B:4488:GLN:O	1:B:4492:ILE:HD12	2.15	0.46
2:D:399:SER:OG	2:D:400:VAL:N	2.49	0.46
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.97	0.46
1:B:4413:PHE:CE2	1:B:4492:ILE:HG21	2.51	0.46
1:A:1539:ASP:O	1:A:1543:ARG:HG2	2.16	0.46
1:A:2094:LYS:NZ	3:A:4701:ADP:O2'	2.41	0.46
1:A:2581:LEU:HD23	1:A:2605:LEU:HA	1.97	0.46
1:A:3482:LEU:HD11	1:A:3770:LEU:HD23	1.98	0.46
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.97	0.46
1:B:2964:HIS:H	1:B:2967:TYR:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4544:ASN:OD1	1:B:4589:GLN:HB2	2.16	0.46
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.50	0.46
1:B:2039:LEU:HD12	1:B:4254:GLY:HA2	1.98	0.46
1:B:2514:LEU:O	1:B:2518:ILE:HG12	2.16	0.46
1:B:3130:TYR:CZ	1:B:3132:LYS:HB2	2.50	0.46
1:A:1618:TYR:O	1:A:1622:GLU:HG2	2.16	0.46
1:A:2175:MET:O	1:A:2179:ARG:HG3	2.16	0.46
1:A:2588:HIS:HA	1:A:2707:GLN:NE2	2.30	0.46
2:C:123:MET:HE2	2:C:135:TRP:HB2	1.98	0.46
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.15	0.46
1:A:2378:PHE:HE2	1:A:2427:PHE:HE2	1.64	0.46
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.98	0.46
1:B:2987:ASN:OD1	1:B:3060:ARG:NH2	2.49	0.46
2:D:211:SER:OG	2:D:212:ARG:N	2.49	0.46
1:A:1703:THR:HG22	1:A:1707:LYS:HE2	1.98	0.45
1:B:2134:GLN:O	1:B:2138:ILE:HG12	2.16	0.45
1:B:3174:ARG:NH1	1:B:3650:ASN:OD1	2.50	0.45
1:B:4029:HIS:C	1:B:4029:HIS:ND1	2.73	0.45
1:A:1737:THR:HA	1:A:1740:THR:HG22	1.98	0.45
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.45	0.45
2:C:274:GLU:HB2	2:C:323:TRP:CH2	2.51	0.45
1:A:3751:GLN:OE1	1:A:3755:GLU:HB2	2.16	0.45
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	1.99	0.45
1:A:4487:LYS:O	1:A:4490:GLN:HG2	2.16	0.45
1:B:1543:ARG:HA	1:B:1546:TYR:CE1	2.51	0.45
1:B:1547:LEU:HD12	1:B:1608:LEU:HD22	1.97	0.45
1:B:3967:GLU:OE2	1:B:4000:ARG:NH2	2.40	0.45
1:A:1959:GLU:HB3	1:A:1962:ARG:HD3	1.98	0.45
1:B:1461:GLU:HA	1:B:1464:LYS:HD2	1.98	0.45
1:B:1477:LEU:C	1:B:1485:ARG:HE	2.24	0.45
1:B:2430:ASN:O	1:B:2435:LYS:NZ	2.50	0.45
1:B:3175:HIS:HB3	1:B:3516:TYR:CE1	2.51	0.45
1:B:3478:LEU:HD11	1:B:3770:LEU:HB3	1.99	0.45
2:D:259:ARG:HB2	2:D:268:CYS:SG	2.56	0.45
1:A:1709:MET:O	1:A:1713:LEU:HD23	2.17	0.45
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.16	0.45
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	1.98	0.45
1:B:1619:LEU:HD21	1:B:1638:LEU:HD23	1.98	0.45
1:B:2065:LEU:HD21	1:B:2134:GLN:HG2	1.99	0.45
1:B:2066:ALA:HA	1:B:2069:ILE:HG22	1.99	0.45
1:B:4307:GLN:O	1:B:4311:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:ASP:OD1	2:D:388:PHE:N	2.49	0.45
1:A:1529:ARG:NE	1:A:1592:LEU:HD11	2.30	0.45
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.31	0.45
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.98	0.45
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.47	0.45
1:B:4112:LYS:O	1:B:4116:LEU:HD13	2.16	0.45
1:B:4318:PRO:HG2	1:B:4325:ASN:HA	1.99	0.45
2:D:206:HIS:CE1	2:D:220:GLU:HG2	2.51	0.45
1:A:1462:PHE:O	1:A:1466:ILE:HG13	2.17	0.45
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.31	0.45
1:A:4381:HIS:HD2	1:A:4438:CYS:HB2	1.82	0.45
1:B:2665:GLU:HB3	1:B:2668:LEU:HD12	1.99	0.45
1:B:3876:LEU:HD23	1:B:4146:VAL:HG11	1.99	0.45
1:A:1476:ASP:HB3	1:A:1488:ARG:NH1	2.32	0.45
1:A:1802:PRO:O	1:A:1806:ARG:HG2	2.16	0.45
1:A:3451:TYR:O	1:A:3455:ILE:HG23	2.17	0.45
1:A:2110:LYS:HA	1:A:2113:ARG:HH21	1.80	0.45
1:A:2934:LEU:HD13	1:A:3085:LEU:HD11	1.99	0.45
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.99	0.45
1:A:4525:ARG:HD2	1:A:4592:TRP:CH2	2.51	0.45
1:B:2969:GLY:HA2	1:B:3004:PHE:HE1	1.82	0.45
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.82	0.45
1:A:4381:HIS:NE2	1:A:4439:GLU:OE1	2.50	0.45
1:B:2943:LYS:HG2	1:B:3094:PHE:CD2	2.52	0.45
2:C:128:GLU:HA	2:C:152:SER:HB2	1.99	0.45
1:A:1599:ARG:HD2	1:A:1599:ARG:N	2.32	0.44
1:A:1600:SER:HA	1:A:1603:ARG:HG2	1.99	0.44
1:A:2484:GLU:O	1:A:2487:GLU:HG3	2.17	0.44
1:A:2755:MET:HG3	1:A:2807:PHE:HB2	1.99	0.44
1:A:2872:LEU:HD22	1:A:2920:LEU:HD12	1.99	0.44
1:A:4377:MET:SD	1:A:4438:CYS:HA	2.56	0.44
1:A:4463:SER:HG	1:A:4464:TRP:CD1	2.35	0.44
1:B:2138:ILE:HD11	1:B:2165:PHE:CG	2.52	0.44
2:D:361:THR:HG22	2:D:377:ASN:HA	2.00	0.44
1:B:3212:VAL:HG12	1:B:3479:LEU:HD11	1.99	0.44
2:C:152:SER:C	2:C:169:SER:HG	2.24	0.44
2:D:259:ARG:HH21	2:D:268:CYS:HB2	1.82	0.44
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.81	0.44
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.99	0.44
1:B:2094:LYS:HD2	3:B:4701:ADP:H1'	2.00	0.44
1:B:3117:LYS:HE2	1:B:3117:LYS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3551:GLU:HA	1:B:3559:ARG:NH1	2.31	0.44
1:B:4431:LEU:HD23	1:B:4431:LEU:HA	1.87	0.44
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.97	0.44
1:B:1991:ASP:O	1:B:1994:SER:OG	2.32	0.44
1:B:2603:MET:HE1	3:B:4703:ADP:N7	2.33	0.44
2:D:283:SER:O	2:D:312:LEU:HB3	2.17	0.44
1:A:1819:ARG:HD2	1:A:1823:ARG:NH2	2.32	0.44
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.99	0.44
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.57	0.44
1:B:3664:LEU:HB3	1:B:3669:ILE:HD12	1.98	0.44
1:B:3776:GLU:HA	1:B:3779:GLU:HG2	1.99	0.44
2:C:369:ASN:HB2	2:C:371:ARG:HG2	1.99	0.44
2:D:112:THR:HA	2:D:384:THR:HG21	2.00	0.44
1:A:2762:LEU:HD13	1:A:2765:TYR:HD2	1.82	0.44
1:A:3214:GLN:NE2	1:A:3761:LEU:HB2	2.32	0.44
1:A:3459:GLN:OE1	1:A:3462:LYS:HD3	2.17	0.44
1:B:2190:TYR:CE2	1:B:2385:ILE:HD11	2.52	0.44
1:B:2319:LEU:HD13	1:B:2359:CYS:SG	2.57	0.44
1:B:3096:ASP:OD1	1:B:3097:TRP:N	2.50	0.44
1:B:3211:THR:O	1:B:3215:VAL:HG23	2.18	0.44
1:B:3615:LEU:HD11	1:B:4111:LYS:HD3	2.00	0.44
2:D:97:ARG:HE	2:D:410:ARG:HB2	1.82	0.44
2:D:312:LEU:HD22	2:D:346:PHE:CE1	2.53	0.44
1:A:1571:ILE:HD13	1:A:1607:LEU:HB3	1.98	0.44
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.83	0.44
1:B:1698:ILE:HD12	1:B:1701:TRP:HE1	1.83	0.44
1:B:3846:LEU:HD22	1:B:3855:ARG:HD2	1.98	0.44
1:B:4445:THR:H	1:B:4448:LEU:HB2	1.83	0.44
2:D:220:GLU:OE1	2:D:223:THR:OG1	2.27	0.44
2:D:230:PHE:HB3	2:D:261:TRP:CZ3	2.52	0.44
1:A:3824:LEU:HD11	1:A:4044:CYS:SG	2.58	0.44
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.00	0.44
1:B:1470:TRP:NE1	1:B:1527:LEU:HD21	2.33	0.44
1:B:1882:THR:HA	1:B:2048:LEU:HD23	1.98	0.44
2:D:123:MET:HE2	2:D:137:TYR:HB3	1.99	0.44
1:A:2176:THR:O	1:A:2179:ARG:N	2.50	0.44
1:A:2983:SER:HB2	1:A:2990:ILE:HD12	2.00	0.44
1:B:1701:TRP:O	1:B:1705:VAL:HG23	2.18	0.44
1:B:1939:GLN:HB2	1:B:2273:ARG:NH2	2.33	0.44
1:B:2488:ARG:HG2	1:B:2492:ARG:HH12	1.83	0.44
1:B:2590:PRO:O	1:B:2732:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3644:VAL:HG22	1:B:3664:LEU:HD11	1.98	0.44
1:B:4297:PRO:HG3	1:B:4308:TRP:CD2	2.53	0.44
1:B:4432:ALA:HA	1:B:4435:VAL:HG22	1.99	0.44
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.53	0.43
1:B:2967:TYR:OH	1:B:2975:ASP:OD2	2.36	0.43
1:A:2087:ASP:O	1:A:2088:PHE:HD1	2.01	0.43
1:A:2584:TRP:CE3	1:A:2591:LEU:HD22	2.52	0.43
1:A:2641:TYR:CZ	1:A:2650:LEU:HD12	2.52	0.43
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.40	0.43
1:A:3775:ARG:O	1:A:3779:GLU:OE1	2.35	0.43
1:B:3135:GLN:HB2	1:B:3136:PRO:HD3	2.00	0.43
1:A:1803:LEU:HD11	1:A:1875:VAL:HG21	1.99	0.43
1:A:2110:LYS:CB	1:A:2113:ARG:HH21	2.31	0.43
1:A:2649:VAL:HG22	1:A:2702:LYS:HB2	2.00	0.43
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.82	0.43
1:B:1459:LEU:HD21	1:B:1510:SER:OG	2.18	0.43
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.19	0.43
1:A:3790:VAL:O	1:A:3793:GLU:HG2	2.19	0.43
1:B:2221:MET:HE1	1:B:2355:THR:HG22	1.99	0.43
1:B:2372:ASP:OD2	1:B:2429:SER:OG	2.31	0.43
1:B:3013:ALA:HA	1:B:3088:ARG:HG3	2.00	0.43
1:B:3071:SER:OG	1:B:3073:GLU:OE1	2.36	0.43
1:B:4414:GLU:HA	1:B:4417:VAL:HG12	2.01	0.43
1:B:4534:TRP:HE3	1:B:4539:LEU:HD21	1.83	0.43
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.51	0.43
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.51	0.43
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.00	0.43
1:B:2073:PHE:HZ	1:B:2096:VAL:HG21	1.83	0.43
1:B:2808:GLU:OE2	1:B:2811:ARG:NH2	2.35	0.43
1:B:4413:PHE:CD2	1:B:4492:ILE:HG21	2.54	0.43
2:D:280:GLU:OE1	2:D:316:ARG:NH2	2.51	0.43
1:A:1620:GLU:HA	1:A:1623:ARG:HD2	1.99	0.43
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.83	0.43
1:A:2980:LEU:HD21	1:A:3011:LEU:HD11	1.99	0.43
1:A:3607:ARG:NH2	1:A:3674:SER:O	2.34	0.43
1:A:3948:ILE:HA	1:A:3951:VAL:HG12	2.01	0.43
1:B:2270:PRO:HA	1:B:2273:ARG:HH11	1.83	0.43
1:B:2879:LYS:HE2	2:C:336:GLY:HA2	1.99	0.43
2:C:366:ASP:HB2	2:C:373:MET:SD	2.58	0.43
2:D:216:ILE:HB	2:D:230:PHE:HB2	2.00	0.43
1:A:4292:LYS:HD2	1:A:4293:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1860:GLN:HG2	1:B:1865:LYS:HG2	2.01	0.43
1:B:2324:LEU:HD22	1:B:2332:ARG:HB3	2.01	0.43
1:B:3224:ILE:O	1:B:3227:GLN:HG3	2.18	0.43
1:B:3786:GLU:O	1:B:3789:ILE:HG22	2.19	0.43
1:B:4482:PHE:O	1:B:4486:ILE:HG12	2.19	0.43
2:C:329:MET:HE3	2:C:329:MET:HB3	1.81	0.43
1:A:2472:TYR:CD2	1:A:2481:MET:HB2	2.53	0.43
1:A:3731:LEU:O	1:A:3735:GLN:HG3	2.19	0.43
1:A:4414:GLU:OE2	1:A:4418:LYS:HD2	2.19	0.43
1:B:1508:LYS:HA	1:B:1513:TYR:CD1	2.54	0.43
1:B:3772:ASN:HA	1:B:3775:ARG:NH1	2.33	0.43
2:D:321:LYS:HD2	2:D:323:TRP:CZ2	2.54	0.43
1:B:1666:LEU:HD23	1:B:1673:VAL:HA	2.01	0.43
1:A:2900:PHE:CE1	1:A:2904:GLU:HB2	2.53	0.43
1:A:3220:ARG:O	1:A:3224:ILE:HG12	2.19	0.43
1:A:3868:PHE:CZ	1:A:4018:MET:HG2	2.54	0.43
1:B:1558:LYS:HD3	1:B:1558:LYS:N	2.34	0.43
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	2.00	0.43
1:B:4476:ILE:HG13	1:B:4477:GLN:N	2.34	0.43
2:D:250:ALA:HB2	2:D:260:VAL:HG22	2.00	0.43
1:B:1500:HIS:O	1:B:1504:VAL:HG23	2.18	0.42
1:B:1657:MET:HE3	1:B:1657:MET:HB2	1.89	0.42
1:B:2461:MET:HG2	1:B:2583:THR:HG21	2.00	0.42
1:B:3825:TYR:CZ	1:B:3875:MET:HG3	2.54	0.42
2:C:290:TYR:HD2	2:C:307:PRO:HD2	1.84	0.42
1:A:2869:ARG:O	1:A:2869:ARG:HD3	2.19	0.42
1:B:1479:ASN:HD21	1:B:1482:ASN:H	1.67	0.42
1:B:3194:LEU:HD23	1:B:3500:MET:SD	2.59	0.42
1:B:3562:TRP:HB3	1:B:3567:LEU:HD22	2.00	0.42
1:A:2378:PHE:HE1	1:A:2463:HIS:NE2	2.18	0.42
1:A:2449:LEU:HA	1:A:2453:ARG:NH2	2.33	0.42
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	2.01	0.42
1:B:1673:VAL:N	1:B:1690:VAL:O	2.41	0.42
1:B:3623:LEU:O	1:B:3627:LEU:HG	2.20	0.42
1:B:4226:THR:HG21	1:B:4239:PRO:HD3	2.02	0.42
2:D:243:ASN:ND2	2:D:248:LEU:H	2.18	0.42
1:A:1966:ARG:HA	1:A:4101:LEU:HD13	2.02	0.42
1:B:2818:VAL:O	1:B:2822:ILE:HG12	2.20	0.42
2:C:216:ILE:O	2:C:230:PHE:N	2.46	0.42
1:A:1643:ASN:HD22	1:A:1649:LYS:CD	2.31	0.42
1:A:2104:LYS:O	1:A:2108:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3167:ARG:NE	1:B:3687:GLU:OE2	2.53	0.42
2:D:96:PRO:HA	2:D:408:GLU:O	2.20	0.42
1:A:2073:PHE:HZ	1:A:2096:VAL:HG21	1.84	0.42
1:A:2221:MET:HE1	1:A:2355:THR:HG22	2.02	0.42
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	2.02	0.42
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.45	0.42
1:B:2629:GLU:OE2	1:B:2633:LYS:HD3	2.19	0.42
1:B:2896:ARG:HA	1:B:2896:ARG:HD3	1.80	0.42
1:B:3716:VAL:HB	1:B:3836:TYR:OH	2.20	0.42
1:B:4039:THR:HG23	1:B:4142:GLY:HA2	2.02	0.42
2:D:243:ASN:HD21	2:D:247:THR:H	1.68	0.42
2:D:364:VAL:C	2:D:365:TRP:HD1	2.27	0.42
1:A:2118:ARG:O	1:A:2118:ARG:NH1	2.53	0.42
1:A:2691:GLY:HA3	1:A:2701:VAL:O	2.20	0.42
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.54	0.42
1:B:1817:HIS:CD2	1:B:1881:GLN:HG2	2.55	0.42
1:B:2149:LEU:HD11	1:B:2157:LEU:HD22	2.01	0.42
1:B:3659:ARG:H	1:B:3659:ARG:CZ	2.32	0.42
1:B:3792:GLN:HA	1:B:3792:GLN:OE1	2.20	0.42
1:B:1581:LYS:HA	1:B:1584:LYS:HE3	2.01	0.42
1:B:1755:GLN:HG2	1:B:1814:GLU:OE1	2.19	0.42
1:B:2498:ILE:HG23	1:B:2502:LEU:HD22	2.01	0.42
1:B:2511:ARG:HD3	1:B:2535:ILE:HD13	2.01	0.42
2:C:113:ARG:HD2	2:C:155:ASP:HA	2.00	0.42
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.20	0.42
1:B:4107:MET:HE1	1:B:4137:ASN:HB2	2.02	0.42
1:B:4517:PRO:HG2	1:B:4619:ILE:HD12	2.02	0.42
1:B:4554:ASP:OD2	1:B:4557:SER:OG	2.30	0.42
2:D:113:ARG:HA	2:D:385:SER:HB3	2.02	0.42
2:D:136:ASP:O	2:D:140:GLY:N	2.50	0.42
1:A:1708:GLU:HA	1:A:1711:VAL:HG22	2.01	0.42
1:A:3030:MET:HE1	1:A:3051:TYR:HB2	2.01	0.42
1:A:3607:ARG:HE	1:A:3607:ARG:HB3	1.70	0.42
1:A:3709:GLN:HG3	1:A:3809:SER:HB3	2.02	0.42
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.93	0.42
1:B:4422:LYS:HD3	1:B:4422:LYS:O	2.20	0.42
1:B:3214:GLN:NE2	1:B:3761:LEU:HB2	2.34	0.41
1:B:4344:LEU:O	1:B:4347:GLN:HG3	2.20	0.41
2:D:101:LYS:HB2	2:D:408:GLU:OE2	2.20	0.41
2:D:186:ARG:NH2	2:D:222:GLN:O	2.53	0.41
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	2.01	0.41
1:A:3738:PHE:CE2	1:A:3783:LYS:HB3	2.55	0.41
1:B:1558:LYS:HD2	1:B:1565:THR:HG21	2.03	0.41
1:B:2413:LEU:O	1:B:2417:ARG:HG3	2.20	0.41
1:B:3219:ARG:NH2	1:B:3472:VAL:HG22	2.35	0.41
1:B:3521:ASP:N	1:B:3521:ASP:OD1	2.51	0.41
2:D:101:LYS:HG2	2:D:102:TYR:CD2	2.55	0.41
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	2.02	0.41
1:A:1769:MET:SD	1:A:1769:MET:N	2.93	0.41
1:A:2214:THR:HA	1:A:2220:LEU:HD21	2.02	0.41
1:A:2499:LEU:HD12	1:A:2514:LEU:HD23	2.02	0.41
1:A:3913:GLU:OE1	1:A:3913:GLU:N	2.53	0.41
1:B:3893:LYS:HB3	1:B:3893:LYS:HE2	1.92	0.41
1:A:1477:LEU:C	1:A:1485:ARG:HH21	2.26	0.41
1:A:1697:LYS:HB2	1:A:1700:GLU:OE2	2.20	0.41
1:A:4343:MET:HE2	1:A:4343:MET:HB3	1.89	0.41
1:B:3488:ARG:HG3	1:B:3489:TRP:CD1	2.55	0.41
1:A:3044:LEU:HD22	1:A:3049:GLU:HG3	2.02	0.41
1:A:3593:SER:OG	1:A:3595:GLN:HG3	2.21	0.41
1:B:1859:ILE:HD11	1:B:1868:TYR:HD1	1.86	0.41
1:B:1943:ARG:HG2	1:B:1943:ARG:NH1	2.35	0.41
1:B:2273:ARG:HA	1:B:2273:ARG:HD2	1.78	0.41
1:B:2467:ARG:HG3	1:B:2467:ARG:NH1	2.36	0.41
1:B:3888:ALA:HB1	1:B:4012:ASN:ND2	2.35	0.41
1:B:4528:VAL:HG11	1:B:4592:TRP:HB2	2.02	0.41
2:D:277:HIS:CG	2:D:278:VAL:N	2.88	0.41
1:A:1466:ILE:HG12	1:A:1500:HIS:ND1	2.34	0.41
1:A:2076:CYS:HB3	1:A:2088:PHE:CE2	2.55	0.41
1:A:4431:LEU:HD23	1:A:4431:LEU:HA	1.87	0.41
1:A:2591:LEU:HA	1:A:2731:VAL:HG13	2.02	0.41
1:A:3684:PRO:HD2	1:A:4140:ARG:NH2	2.35	0.41
1:B:2078:GLU:OE1	1:B:4518:GLU:HG3	2.20	0.41
1:B:2457:SER:OG	1:B:2501:SER:HB3	2.20	0.41
1:B:2544:GLU:N	1:B:2544:GLU:OE2	2.53	0.41
1:B:3452:ALA:HA	1:B:3455:ILE:HG22	2.03	0.41
1:B:4519:ALA:HA	1:B:4522:THR:HG22	2.03	0.41
2:D:243:ASN:HB3	2:D:284:TRP:CZ3	2.47	0.41
2:D:311:LEU:O	2:D:323:TRP:N	2.31	0.41
2:D:342:ARG:NH2	2:D:384:THR:HG23	2.36	0.41
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.41
1:A:3154:LEU:HD11	1:A:3516:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4075:GLU:C	1:A:4079:GLN:HE21	2.28	0.41
1:A:4463:SER:O	1:A:4466:HIS:NE2	2.54	0.41
1:A:4564:LYS:HD3	1:A:4584:ALA:HA	2.02	0.41
1:B:2054:LEU:HD23	1:B:2054:LEU:HA	1.90	0.41
1:B:2063:GLU:O	1:B:2067:ASN:ND2	2.54	0.41
1:B:3154:LEU:HD11	1:B:3516:TYR:HB3	2.03	0.41
1:B:3495:THR:O	1:B:3499:GLN:HG3	2.21	0.41
1:B:3835:ILE:HG23	1:B:3866:VAL:HG12	2.03	0.41
1:B:4516:VAL:HG12	1:B:4519:ALA:H	1.85	0.41
2:C:176:LEU:HD13	2:C:207:ILE:HD11	2.03	0.41
2:D:309:PRO:HB2	2:D:325:VAL:HB	2.02	0.41
1:A:1580:LYS:HA	1:A:1580:LYS:HD3	1.81	0.41
1:A:1604:LEU:HD23	1:A:1604:LEU:HA	1.85	0.41
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.54	0.41
1:A:1735:PRO:O	1:A:1739:ILE:HG12	2.21	0.41
1:A:2108:ILE:O	1:A:2112:LYS:HG2	2.21	0.41
1:A:2386:PRO:HA	1:A:2416:GLN:OE1	2.21	0.41
1:A:2471:GLN:O	1:A:2475:ASN:ND2	2.54	0.41
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.56	0.41
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.54	0.41
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.56	0.41
1:A:3215:VAL:HG12	1:A:3219:ARG:NH2	2.35	0.41
1:A:4098:ASN:N	1:A:4127:THR:O	2.53	0.41
1:B:1547:LEU:HD23	1:B:1547:LEU:HA	1.92	0.41
1:B:1882:THR:HG22	1:B:2048:LEU:HD23	2.03	0.41
1:B:2419:ALA:O	1:B:2423:MET:HG2	2.20	0.41
1:B:2449:LEU:HA	1:B:2453:ARG:NH2	2.36	0.41
1:B:2863:ARG:HG3	1:B:2863:ARG:NH1	2.33	0.41
1:B:2968:THR:HG23	1:B:2970:GLU:HG2	2.03	0.41
1:B:3026:TYR:CZ	1:B:3030:MET:HE3	2.56	0.41
1:B:3030:MET:HE1	1:B:3051:TYR:HB2	2.03	0.41
1:B:3200:HIS:HD2	1:B:3754:ASN:OD1	2.04	0.41
2:D:243:ASN:CG	2:D:248:LEU:H	2.28	0.41
1:A:3783:LYS:O	1:A:3786:GLU:HG2	2.21	0.41
1:A:3839:VAL:HG11	1:A:3863:LEU:HD13	2.03	0.41
1:B:4289:ASP:OD1	1:B:4292:LYS:HG2	2.21	0.41
2:C:256:GLN:HG2	2:C:277:HIS:C	2.46	0.41
2:C:382:PHE:O	2:C:399:SER:OG	2.34	0.41
1:A:1476:ASP:O	1:A:1487:ILE:HA	2.20	0.40
1:A:2792:TYR:OH	1:A:2842:GLU:OE1	2.33	0.40
1:A:3612:THR:OG1	1:A:3613:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4110:GLU:HG3	1:A:4138:LEU:HA	2.03	0.40
1:B:3628:ARG:HG2	1:B:3628:ARG:HH11	1.85	0.40
2:C:193:HIS:CG	2:C:194:ASN:H	2.39	0.40
1:A:2091:ARG:NH1	3:A:4701:ADP:H5'2	2.36	0.40
1:A:2635:PHE:HE1	1:A:2661:LEU:HD11	1.86	0.40
1:B:2996:GLU:HB2	1:B:3078:ARG:HH12	1.85	0.40
1:B:3559:ARG:O	1:B:3563:GLN:HG2	2.21	0.40
2:D:289:SER:O	2:D:293:ILE:HG12	2.21	0.40
1:A:1572:SER:O	1:A:1576:LEU:HG	2.21	0.40
1:A:2268:LEU:HD12	1:A:2268:LEU:HA	1.90	0.40
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.21	0.40
1:A:2822:ILE:HD11	1:A:2858:PHE:CD1	2.57	0.40
1:A:3033:CYS:SG	1:A:3054:PHE:HB2	2.61	0.40
1:A:3484:ALA:O	1:A:3487:GLU:HG3	2.20	0.40
1:A:3966:PRO:HG3	1:A:3997:ARG:NH1	2.35	0.40
1:A:4285:ALA:O	1:A:4293:ASP:HB2	2.22	0.40
1:B:1467:ARG:NH2	1:B:1471:ASN:HB3	2.35	0.40
1:B:1966:ARG:HA	1:B:4101:LEU:HD13	2.03	0.40
1:B:2060:ARG:HB2	1:B:2060:ARG:NH1	2.36	0.40
1:B:2231:SER:HA	1:B:2234:TRP:NE1	2.36	0.40
1:B:2668:LEU:N	1:B:2669:PRO:HD2	2.37	0.40
1:B:4168:ARG:NH2	1:B:4217:ASP:OD1	2.55	0.40
1:B:4296:MET:HE2	1:B:4296:MET:HA	2.03	0.40
1:B:4397:HIS:NE2	1:B:4418:LYS:HA	2.37	0.40
2:C:178:ASP:O	2:C:182:PHE:N	2.54	0.40
2:D:100:GLU:HB3	2:D:407:TRP:CZ3	2.56	0.40
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.22	0.40
1:A:3786:GLU:O	1:A:3789:ILE:HG22	2.21	0.40
1:B:1547:LEU:HA	1:B:1550:ILE:HG22	2.04	0.40
1:B:4027:LEU:HD11	1:B:4043:MET:HE1	2.03	0.40
1:B:4297:PRO:HG3	1:B:4308:TRP:CG	2.56	0.40
2:D:127:SER:OG	2:D:128:GLU:N	2.54	0.40
2:D:212:ARG:HD3	2:D:236:TRP:HB2	2.04	0.40
2:D:320:ILE:HD11	2:D:337:HIS:CD2	2.57	0.40
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.38	0.40
1:A:3730:ASP:O	1:A:3734:LEU:HG	2.21	0.40
1:A:3767:ILE:HD12	1:A:3767:ILE:H	1.87	0.40
1:A:4156:ASN:C	1:A:4156:ASN:HD22	2.27	0.40
1:B:1478:VAL:C	1:B:1485:ARG:HD2	2.47	0.40
1:B:1511:PRO:HG2	1:B:1512:TYR:CD1	2.56	0.40
1:B:1703:THR:HA	1:B:1706:GLU:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2691:GLY:HA2	1:B:2703:LEU:HG	2.03	0.40
1:B:3016:GLU:OE1	1:B:3051:TYR:OH	2.24	0.40
1:B:3478:LEU:HD13	1:B:3771:GLU:HG3	2.02	0.40
1:B:3624:GLU:OE2	1:B:3628:ARG:HD3	2.21	0.40
1:B:4485:ARG:HG2	1:B:4513:GLY:HA2	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	2929/4646 (63%)	2885 (98%)	44 (2%)	0	100	100
1	B	2929/4646 (63%)	2872 (98%)	57 (2%)	0	100	100
2	C	320/410 (78%)	306 (96%)	14 (4%)	0	100	100
2	D	317/410 (77%)	300 (95%)	17 (5%)	0	100	100
All	All	6495/10112 (64%)	6363 (98%)	132 (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%)	2604 (100%)	1 (0%)	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	2605/4125 (63%)	2604 (100%)	1 (0%)	100	100
2	C	287/364 (79%)	287 (100%)	0	100	100
2	D	284/364 (78%)	284 (100%)	0	100	100
All	All	5781/8978 (64%)	5779 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4397	HIS
1	B	4029	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1850	GLN
1	A	1856	GLN
1	A	1950	GLN
1	A	2067	ASN
1	A	2102	ASN
1	A	2171	HIS
1	A	2212	GLN
1	A	2263	HIS
1	A	2549	GLN
1	A	2588	HIS
1	A	2677	GLN
1	A	2707	GLN
1	A	2781	GLN
1	A	2827	HIS
1	A	2928	GLN
1	A	3152	GLN
1	A	3523	GLN
1	A	3526	GLN
1	A	3535	HIS
1	A	3538	GLN
1	A	3820	GLN
1	A	3826	GLN
1	A	3877	HIS
1	A	3985	GLN
1	A	4012	ASN
1	A	4062	GLN

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Mol	Chain	Res	Type
1	A	4079	GLN
1	A	4114	HIS
1	A	4389	HIS
1	A	4429	GLN
1	A	4436	GLN
1	A	4466	HIS
1	A	4490	GLN
1	A	4506	ASN
1	A	4566	GLN
1	A	4589	GLN
1	B	1541	GLN
1	B	1643	ASN
1	B	1670	ASN
1	B	1755	GLN
1	B	1841	GLN
1	B	1950	GLN
1	B	1979	GLN
1	B	2047	GLN
1	B	2263	HIS
1	B	2464	GLN
1	B	2485	GLN
1	B	2752	ASN
1	B	2827	HIS
1	B	3063	HIS
1	B	3214	GLN
1	B	3233	ASN
1	B	3535	HIS
1	B	3744	GLN
1	B	3820	GLN
1	B	3877	HIS
1	B	4012	ASN
1	B	4098	ASN
1	B	4156	ASN
1	B	4191	GLN
1	B	4249	GLN
1	B	4258	ASN
1	B	4566	GLN
2	C	369	ASN
2	C	377	ASN
2	C	381	HIS
2	D	189	HIS
2	D	377	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
3	ADP	A	4701	5	24,29,29	0.89	0	29,45,45	1.22	2 (6%)
3	ADP	B	4704	-	24,29,29	0.86	0	29,45,45	1.19	2 (6%)
3	ADP	B	4701	5	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
3	ADP	A	4703	-	24,29,29	0.89	0	29,45,45	1.23	2 (6%)
3	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.20	2 (6%)
4	ATP	A	4702	5	28,33,33	0.66	0	34,52,52	0.58	1 (2%)
4	ATP	B	4702	5	28,33,33	0.67	0	34,52,52	0.59	1 (2%)
3	ADP	B	4703	-	24,29,29	0.88	0	29,45,45	1.23	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	4701	5	-	0/12/32/32	0/3/3/3
3	ADP	B	4704	-	-	1/12/32/32	0/3/3/3
3	ADP	B	4701	5	-	3/12/32/32	0/3/3/3
3	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
3	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
4	ATP	A	4702	5	-	5/18/38/38	0/3/3/3
4	ATP	B	4702	5	-	4/18/38/38	0/3/3/3
3	ADP	B	4703	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4703	ADP	N3-C2-N1	-3.73	123.61	128.67
3	A	4701	ADP	N3-C2-N1	-3.72	123.62	128.67
3	A	4703	ADP	N3-C2-N1	-3.69	123.66	128.67
3	B	4704	ADP	N3-C2-N1	-3.68	123.67	128.67
3	A	4704	ADP	N3-C2-N1	-3.68	123.67	128.67
3	B	4701	ADP	N3-C2-N1	-3.66	123.70	128.67
3	A	4701	ADP	C4-C5-N7	-2.57	106.62	109.34
3	B	4704	ADP	C4-C5-N7	-2.56	106.63	109.34
3	B	4703	ADP	C4-C5-N7	-2.55	106.64	109.34
3	A	4703	ADP	C4-C5-N7	-2.52	106.67	109.34
3	B	4701	ADP	C4-C5-N7	-2.52	106.67	109.34
3	A	4704	ADP	C4-C5-N7	-2.51	106.69	109.34
4	B	4702	ATP	C5-C6-N6	2.33	123.86	120.31
4	A	4702	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4703	ADP	C5'-O5'-PA-O1A
3	A	4703	ADP	C5'-O5'-PA-O3A
3	B	4701	ADP	C5'-O5'-PA-O1A
3	B	4701	ADP	C5'-O5'-PA-O2A
3	B	4701	ADP	C5'-O5'-PA-O3A
3	B	4703	ADP	C5'-O5'-PA-O1A
3	B	4703	ADP	C5'-O5'-PA-O3A
4	B	4702	ATP	O4'-C4'-C5'-O5'
4	A	4702	ATP	O4'-C4'-C5'-O5'

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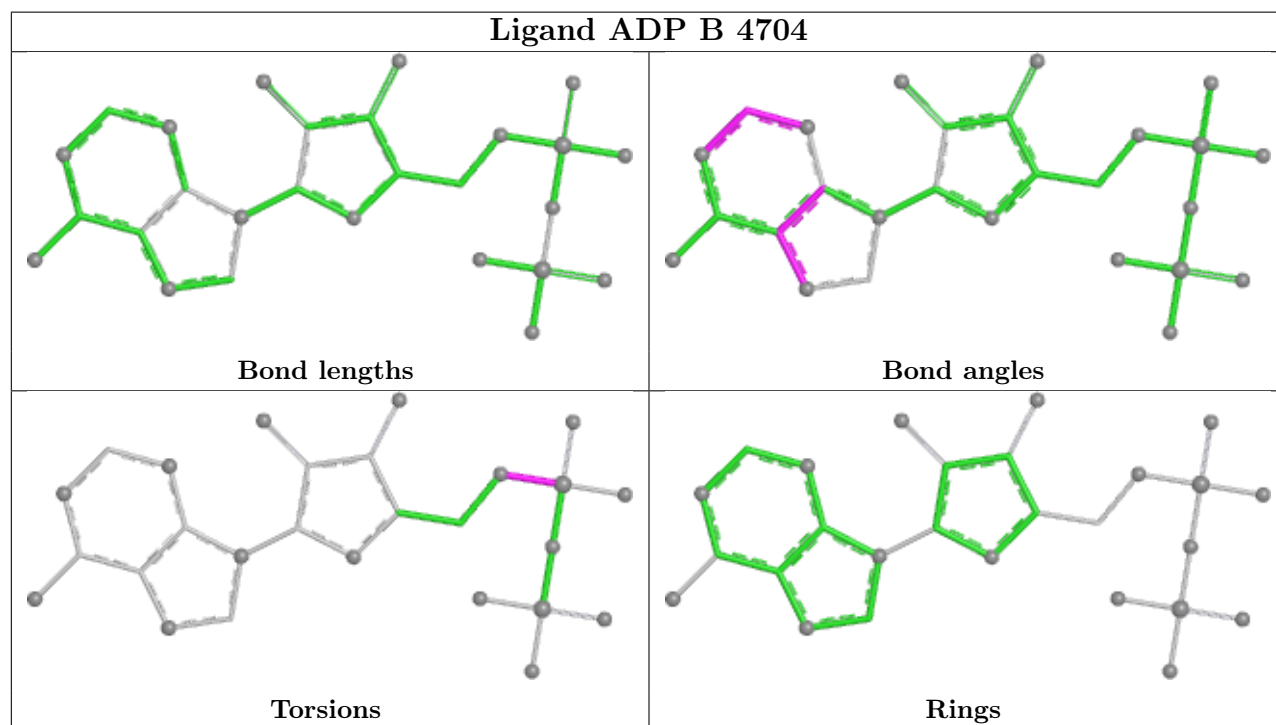
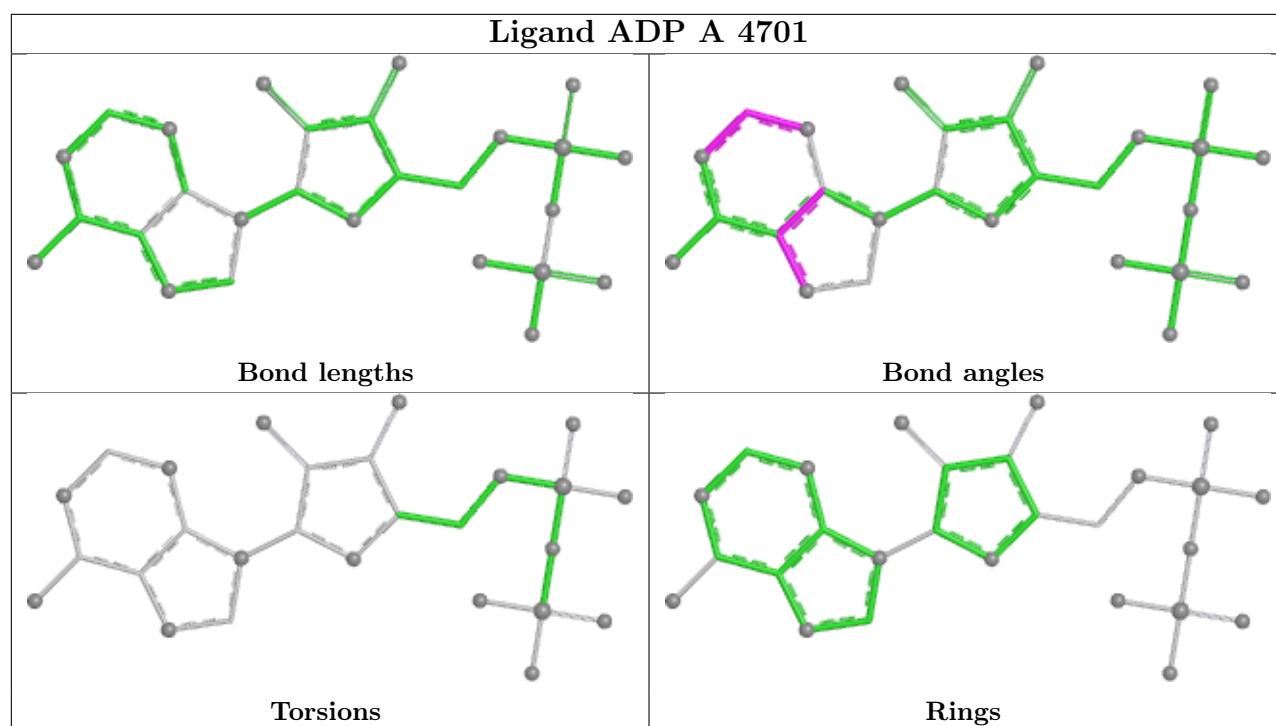
Mol	Chain	Res	Type	Atoms
4	B	4702	ATP	C3'-C4'-C5'-O5'
3	B	4703	ADP	O4'-C4'-C5'-O5'
3	B	4703	ADP	C3'-C4'-C5'-O5'
3	A	4703	ADP	O4'-C4'-C5'-O5'
4	A	4702	ATP	C3'-C4'-C5'-O5'
3	A	4703	ADP	C3'-C4'-C5'-O5'
4	B	4702	ATP	PA-O3A-PB-O2B
3	A	4703	ADP	C5'-O5'-PA-O2A
3	A	4704	ADP	C5'-O5'-PA-O1A
3	B	4703	ADP	C5'-O5'-PA-O2A
3	B	4704	ADP	C5'-O5'-PA-O1A
4	A	4702	ATP	PA-O3A-PB-O1B
4	A	4702	ATP	PA-O3A-PB-O2B
4	A	4702	ATP	PB-O3B-PG-O3G
4	B	4702	ATP	PA-O3A-PB-O1B

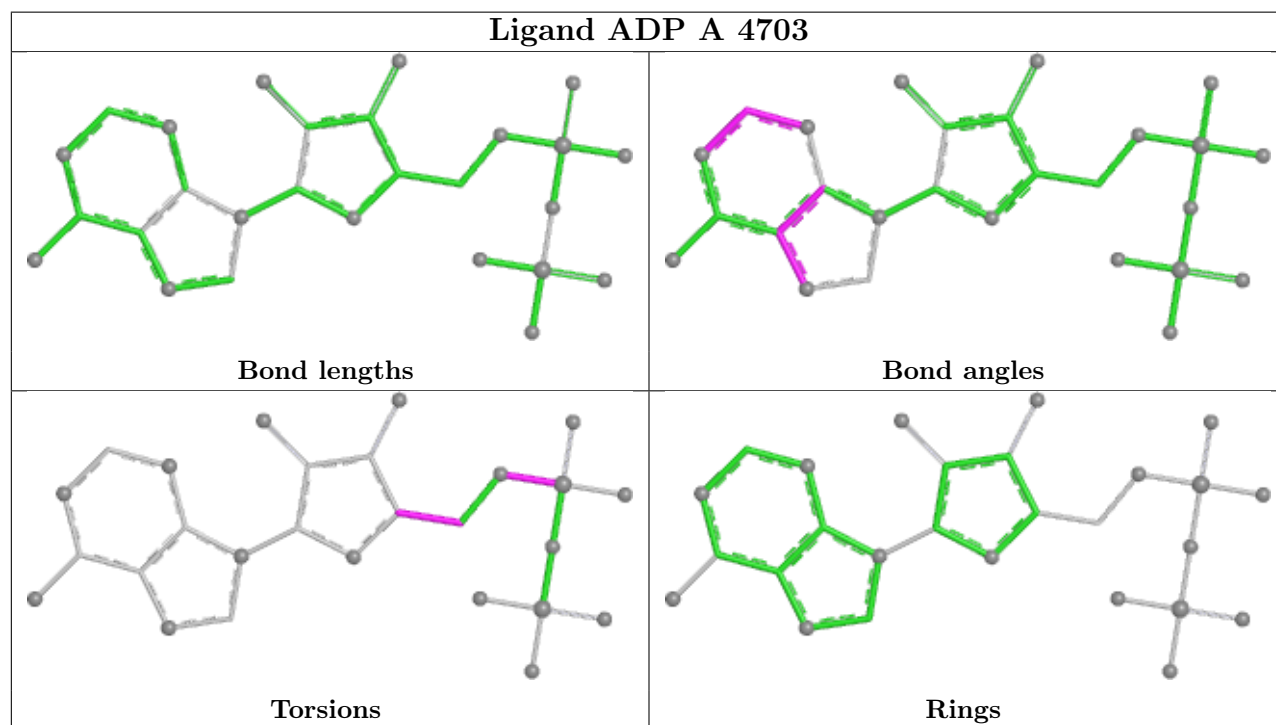
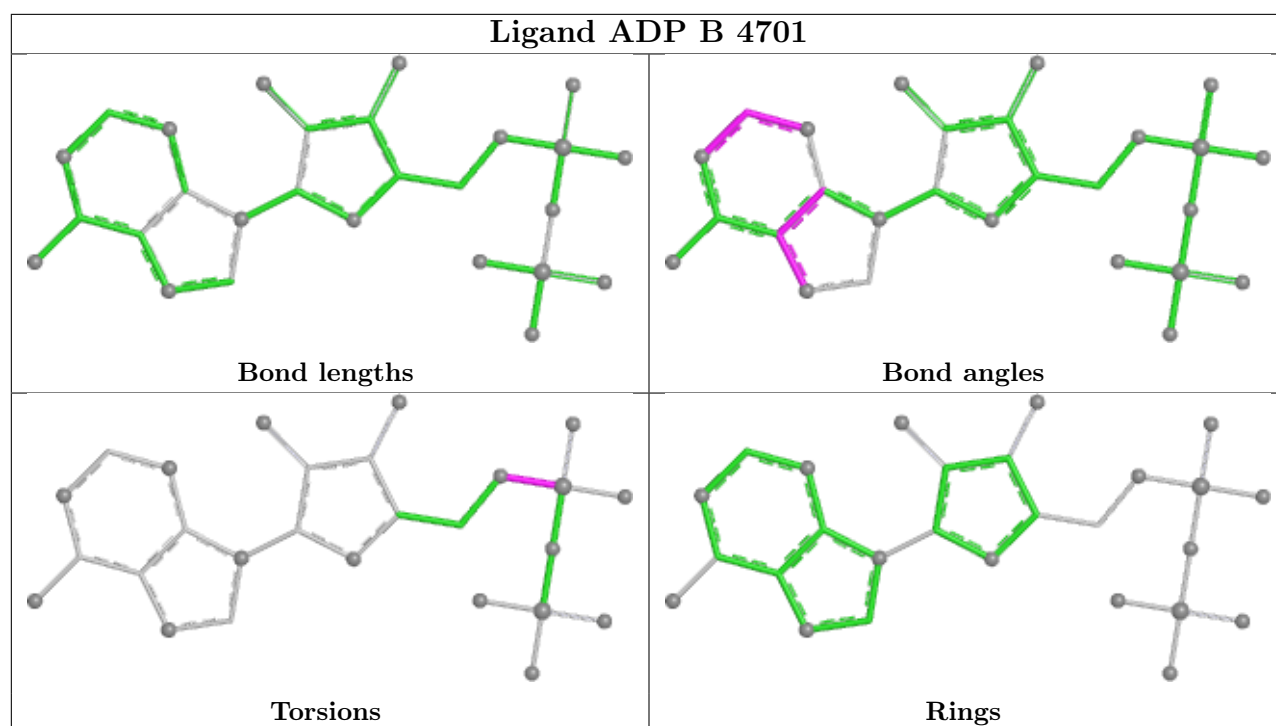
There are no ring outliers.

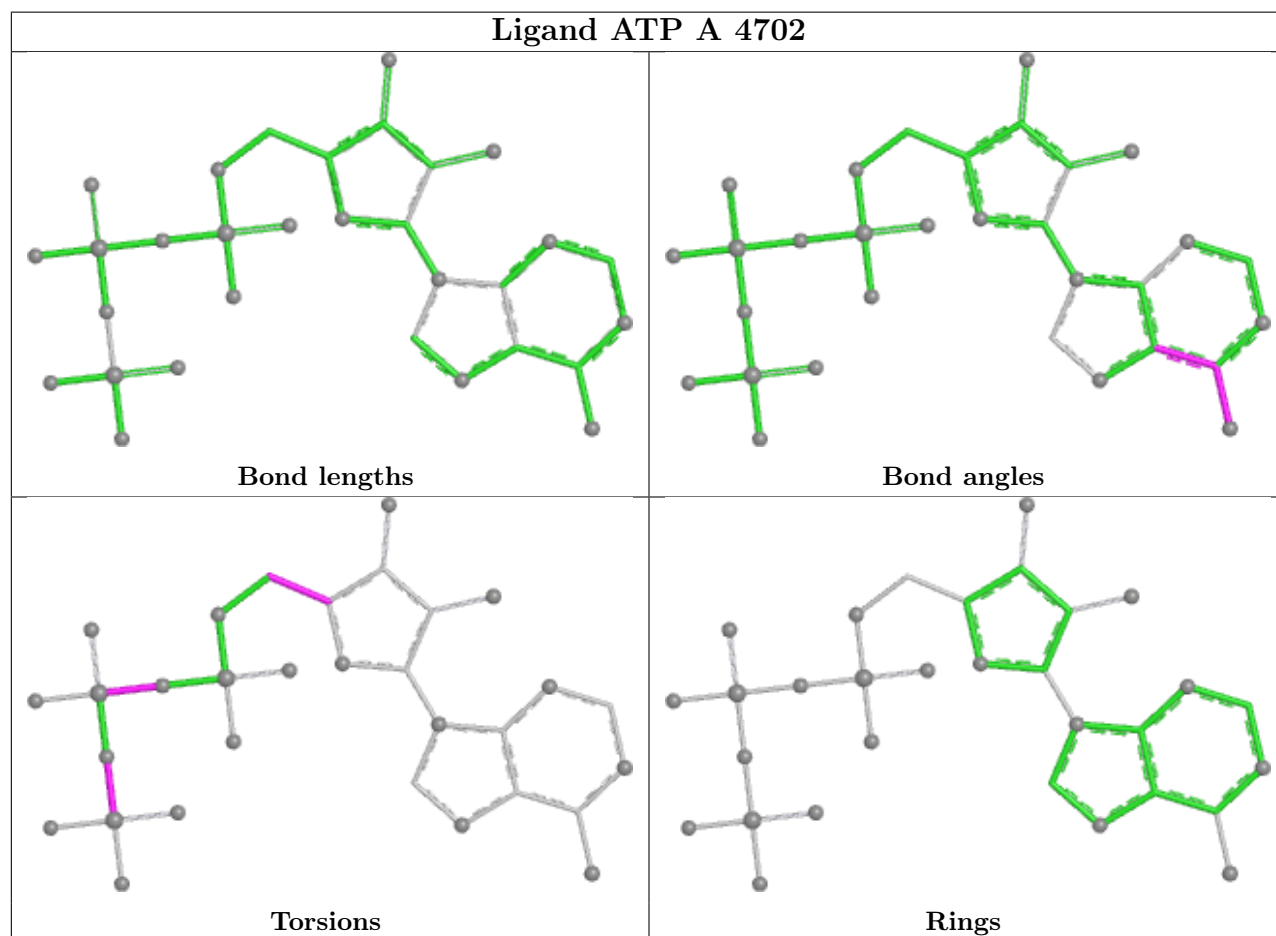
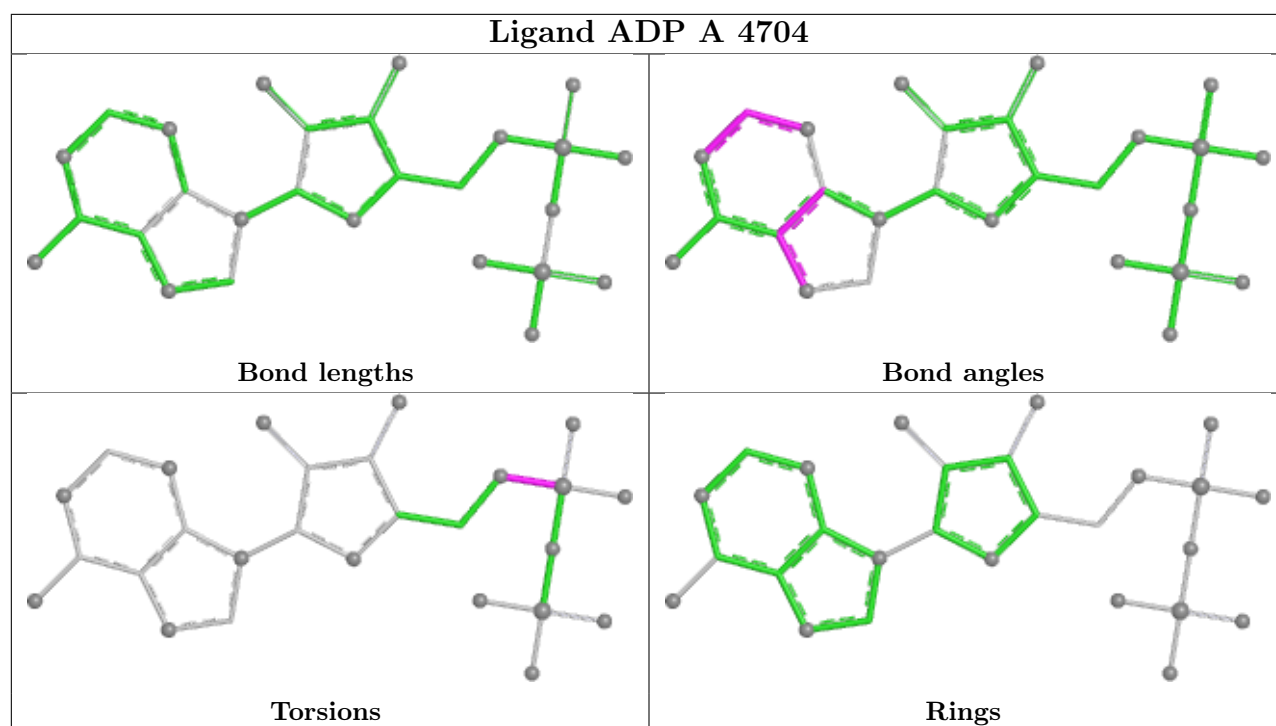
4 monomers are involved in 8 short contacts:

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

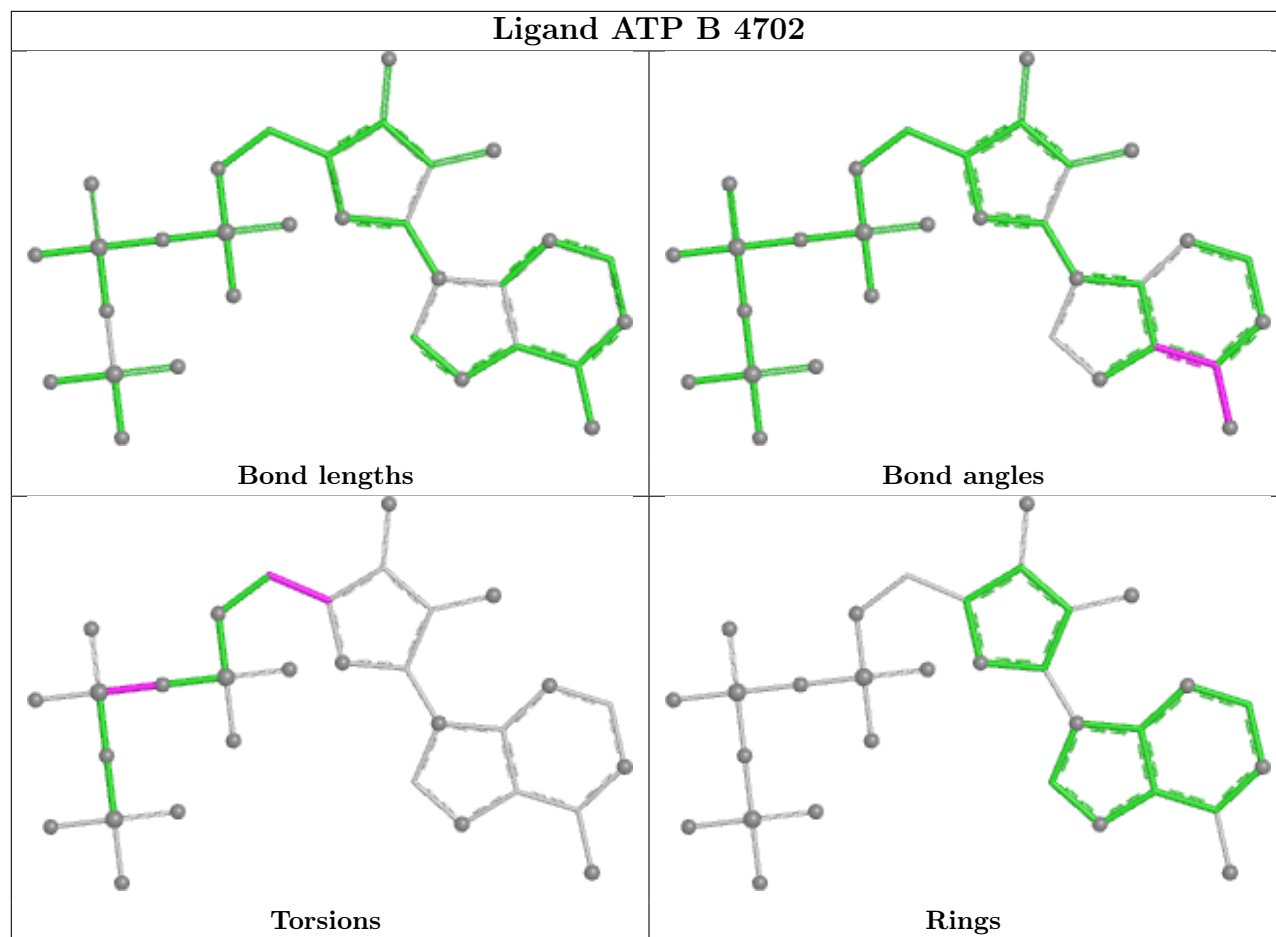
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



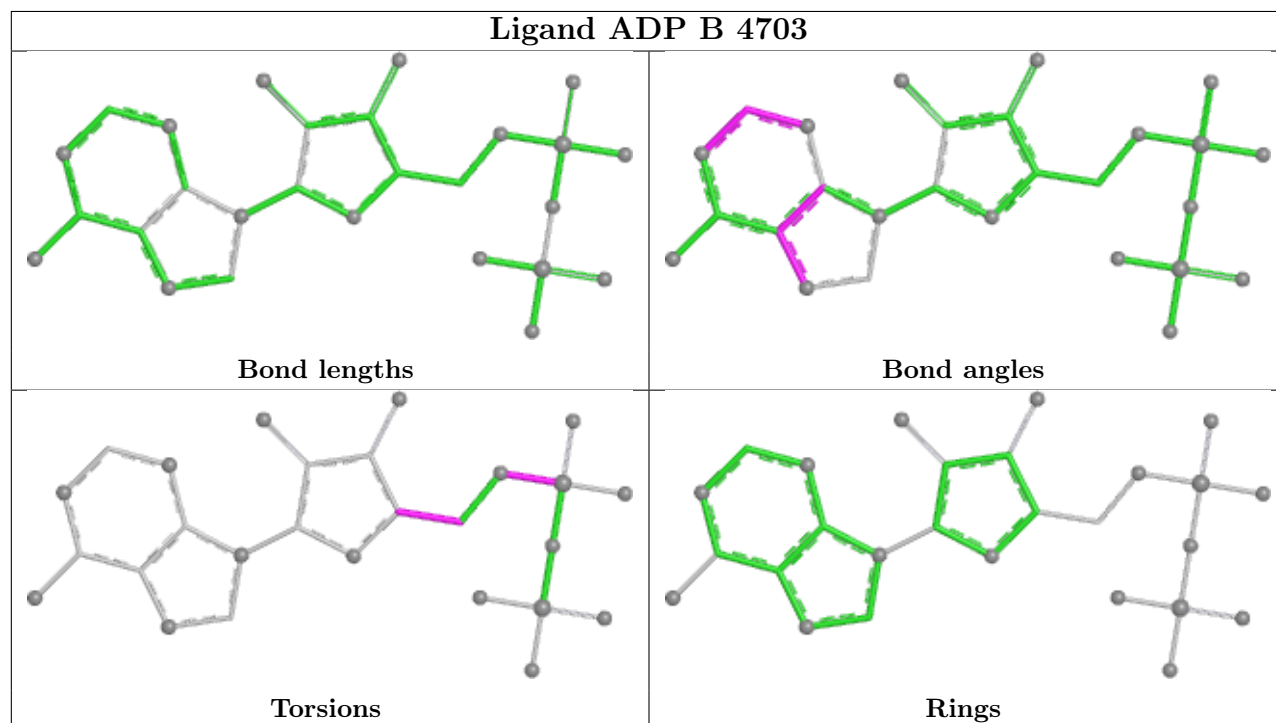




Ligand ATP B 4702



Ligand ADP B 4703



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.

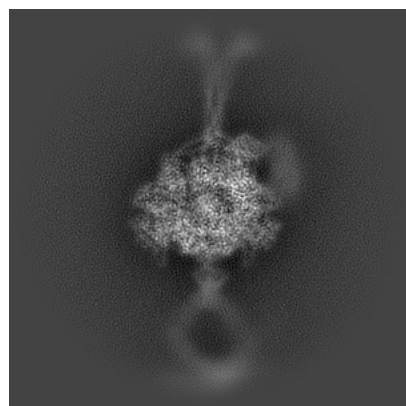
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47378. These allow visual inspection of the internal detail of the map and identification of artifacts.

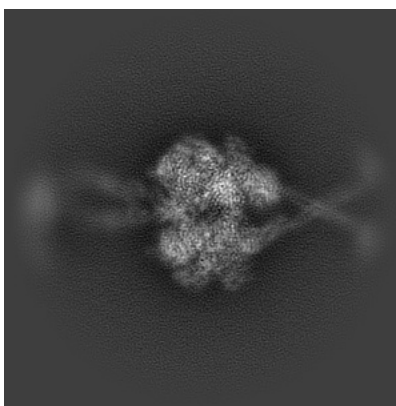
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

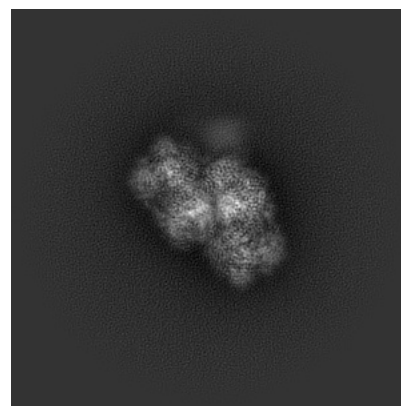
6.1.1 Primary map



X

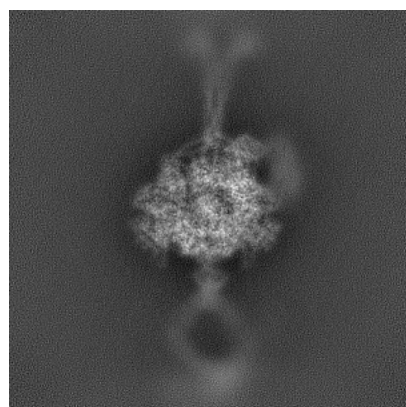


Y

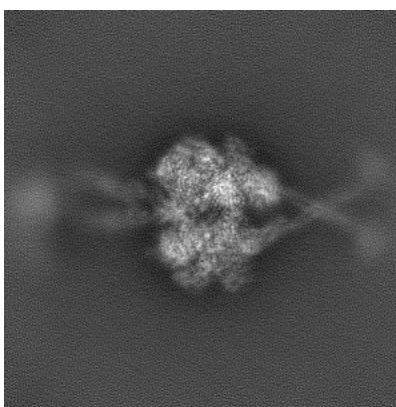


Z

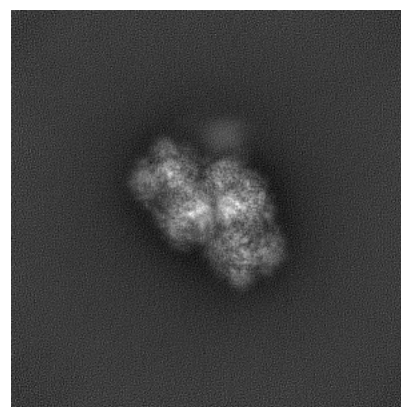
6.1.2 Raw map



X



Y

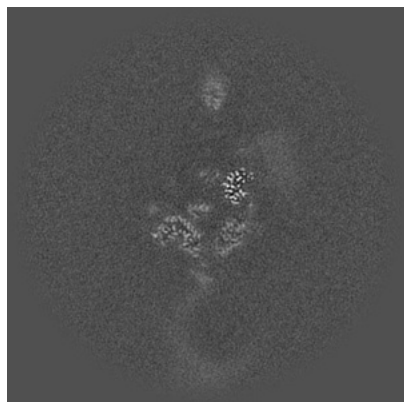


Z

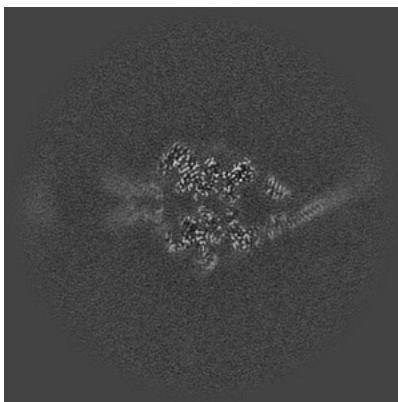
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

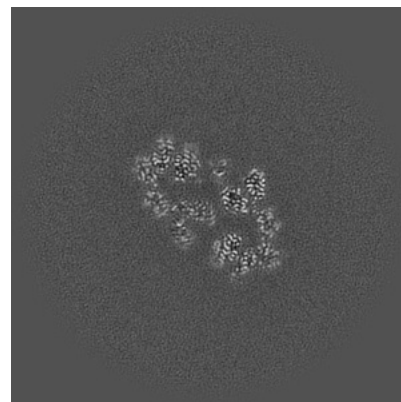
6.2.1 Primary map



X Index: 192

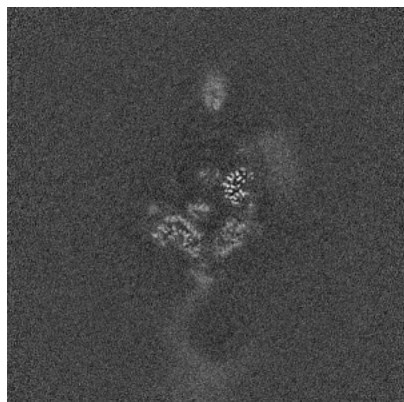


Y Index: 192

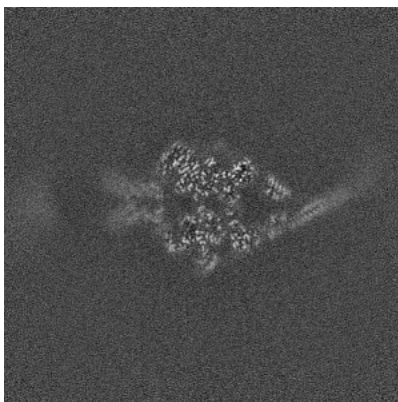


Z Index: 192

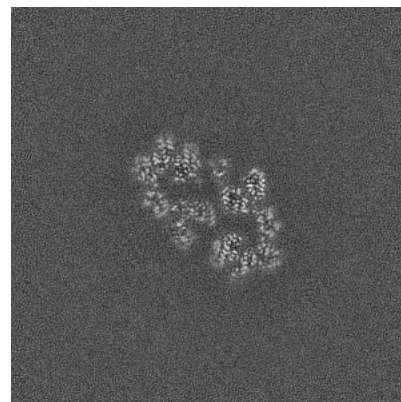
6.2.2 Raw map



X Index: 192



Y Index: 192

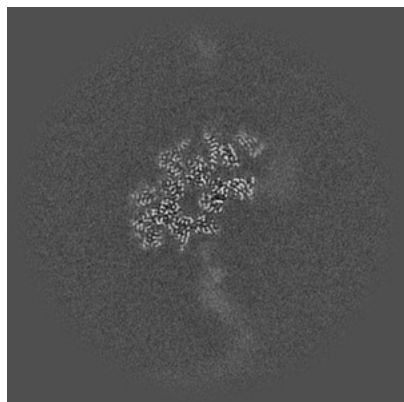


Z Index: 192

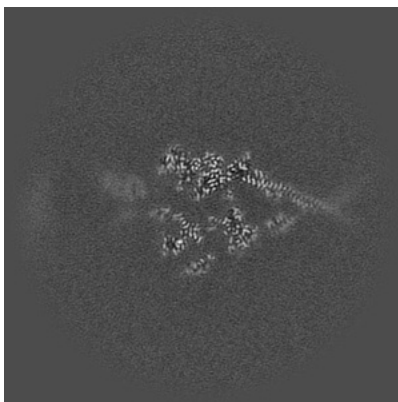
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

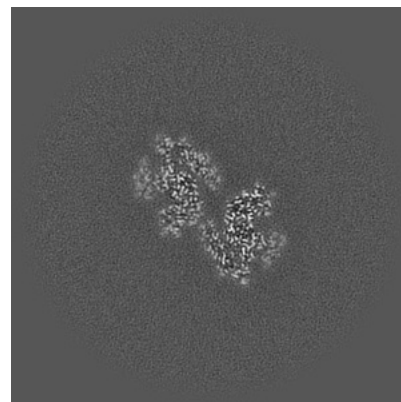
6.3.1 Primary map



X Index: 215

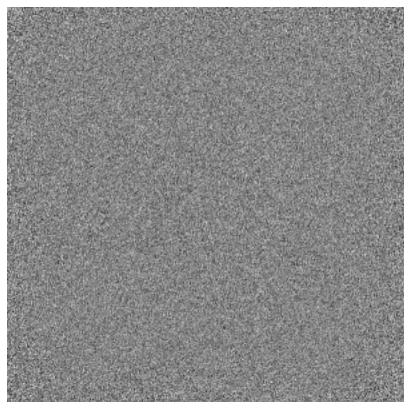


Y Index: 199

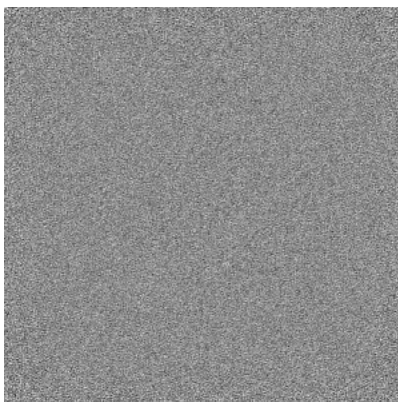


Z Index: 173

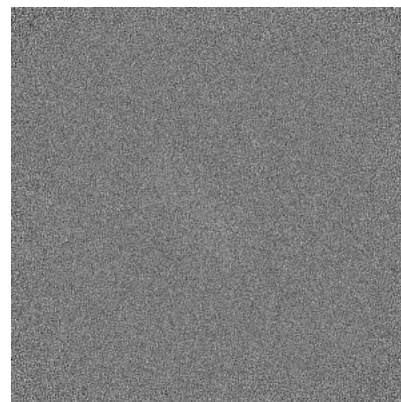
6.3.2 Raw map



X Index: 0



Y Index: 0

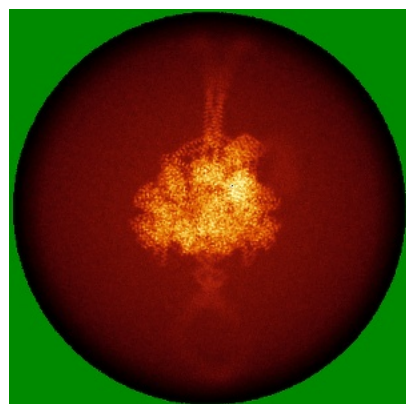


Z Index: 0

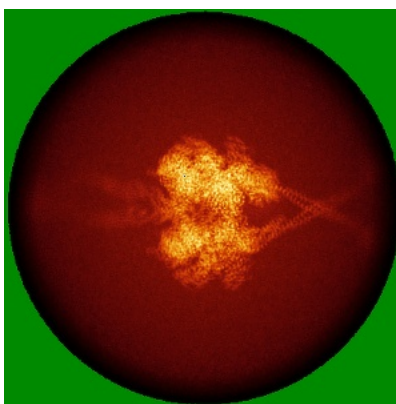
The images above show the largest variance slices of the map in three orthogonal directions.

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

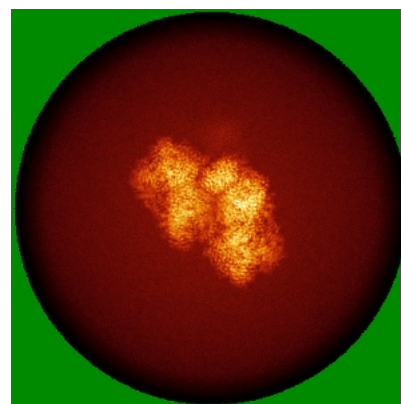
6.4.1 Primary map



X

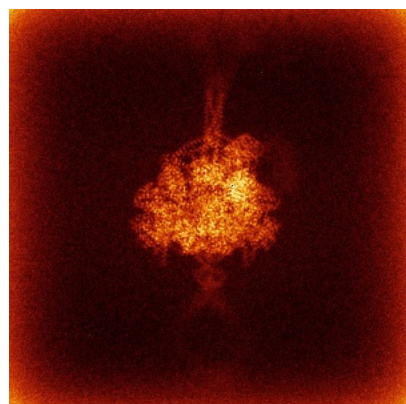


Y

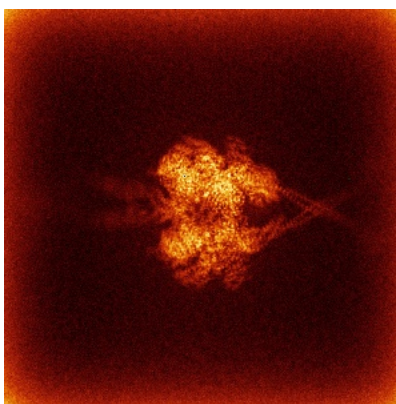


Z

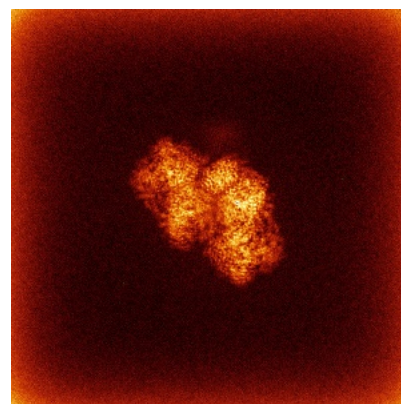
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 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



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.

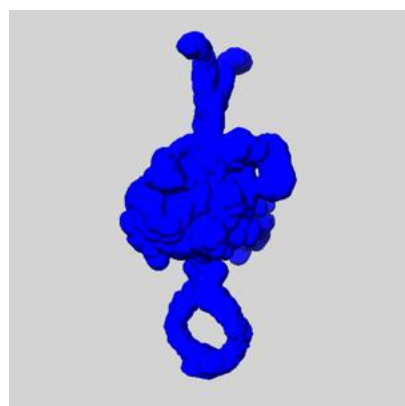
6.6 Mask visualisation [i](#)

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

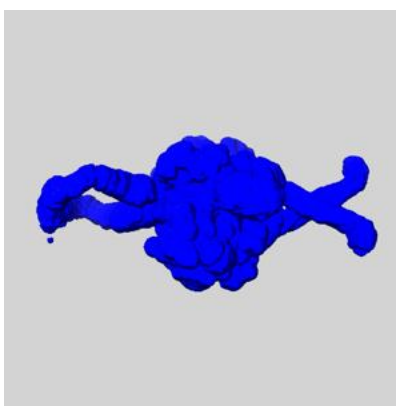
A mask typically either:

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

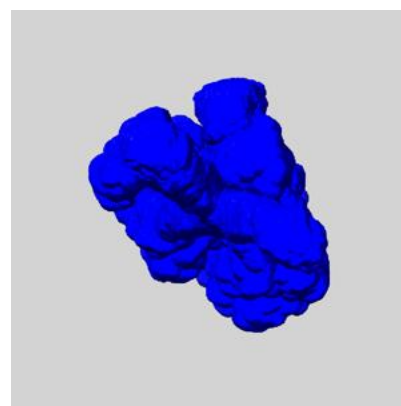
6.6.1 emd_47378_msk_1.map [i](#)



X



Y

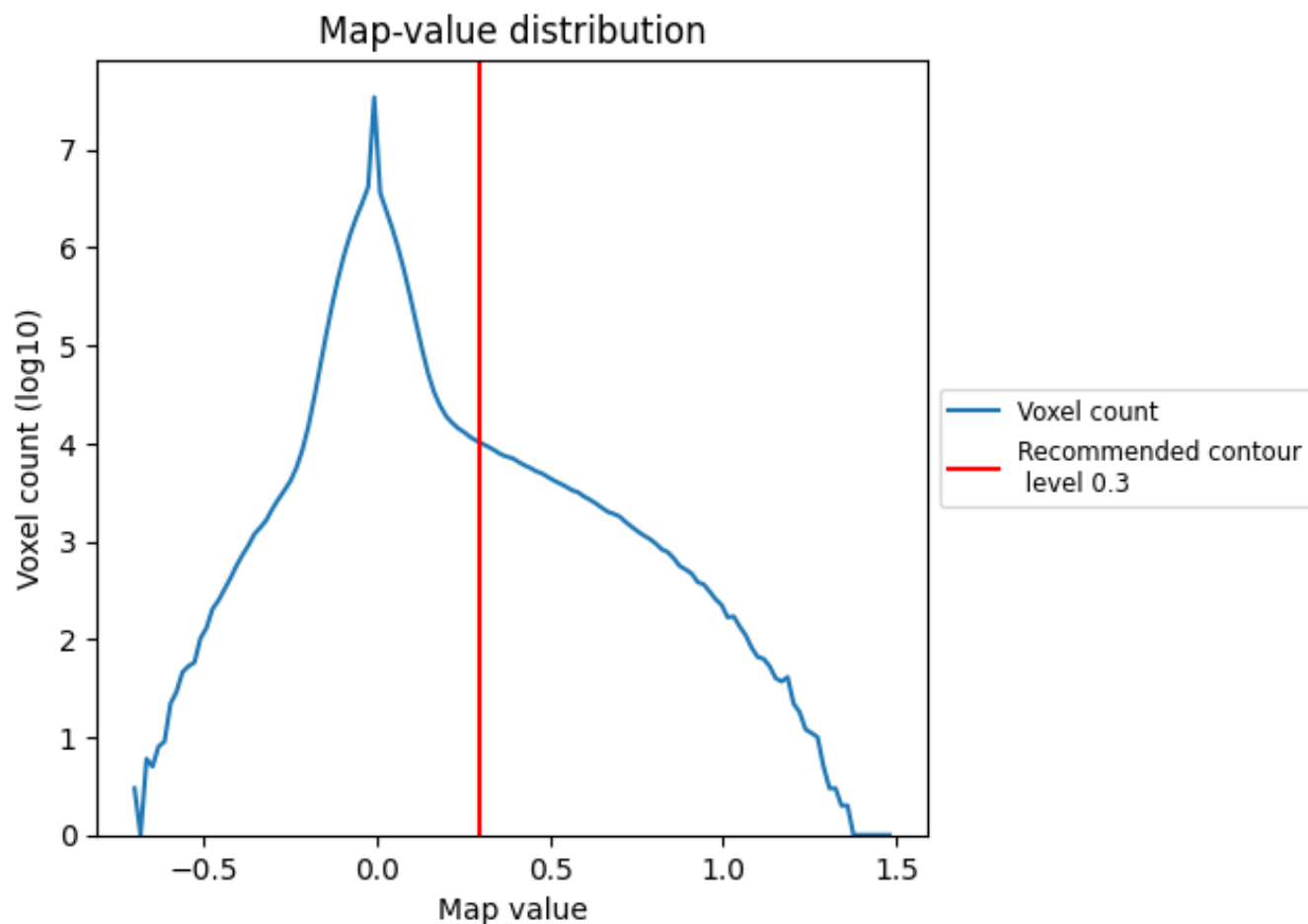


Z

7 Map analysis [i](#)

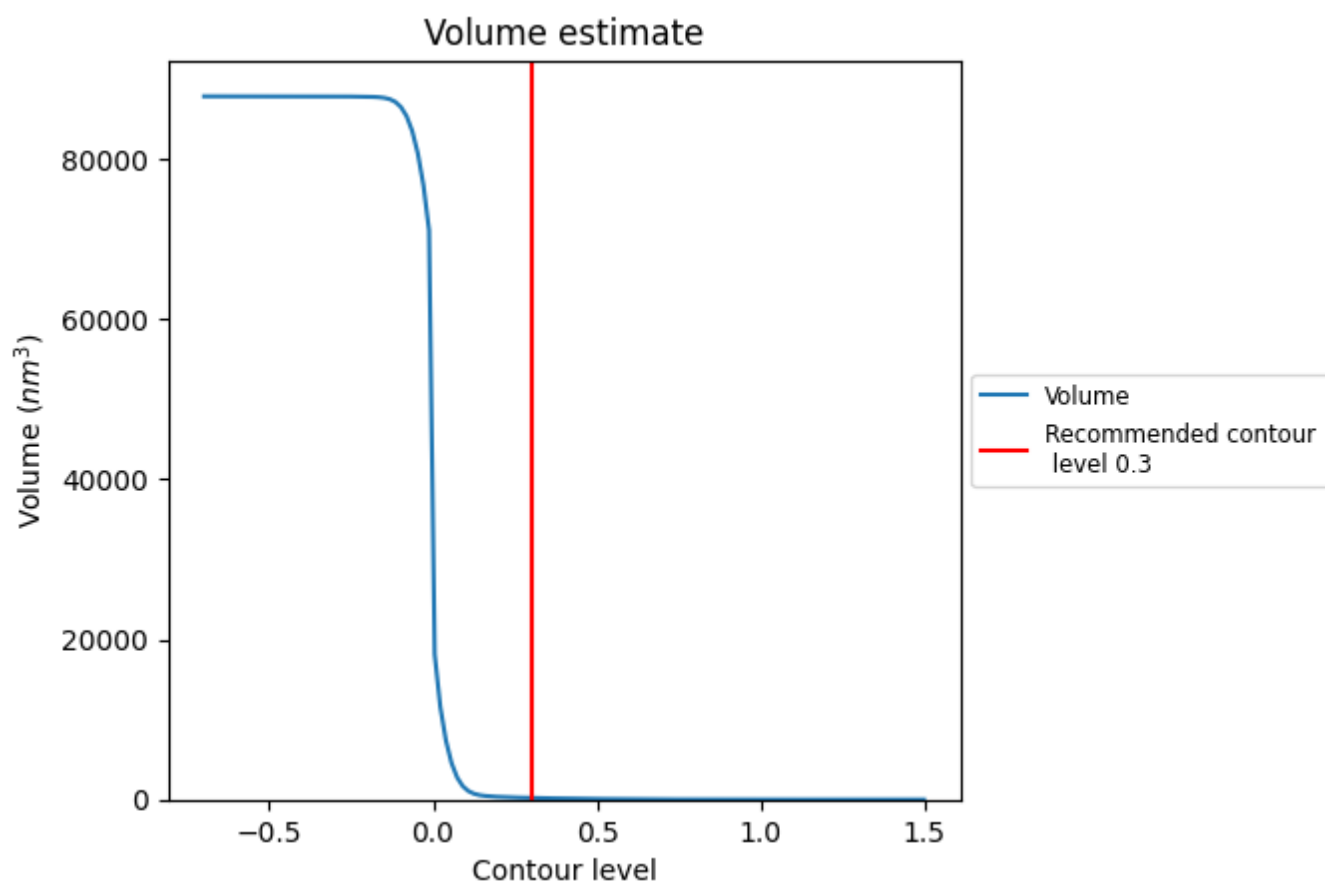
This section contains the results of statistical analysis of the map.

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.

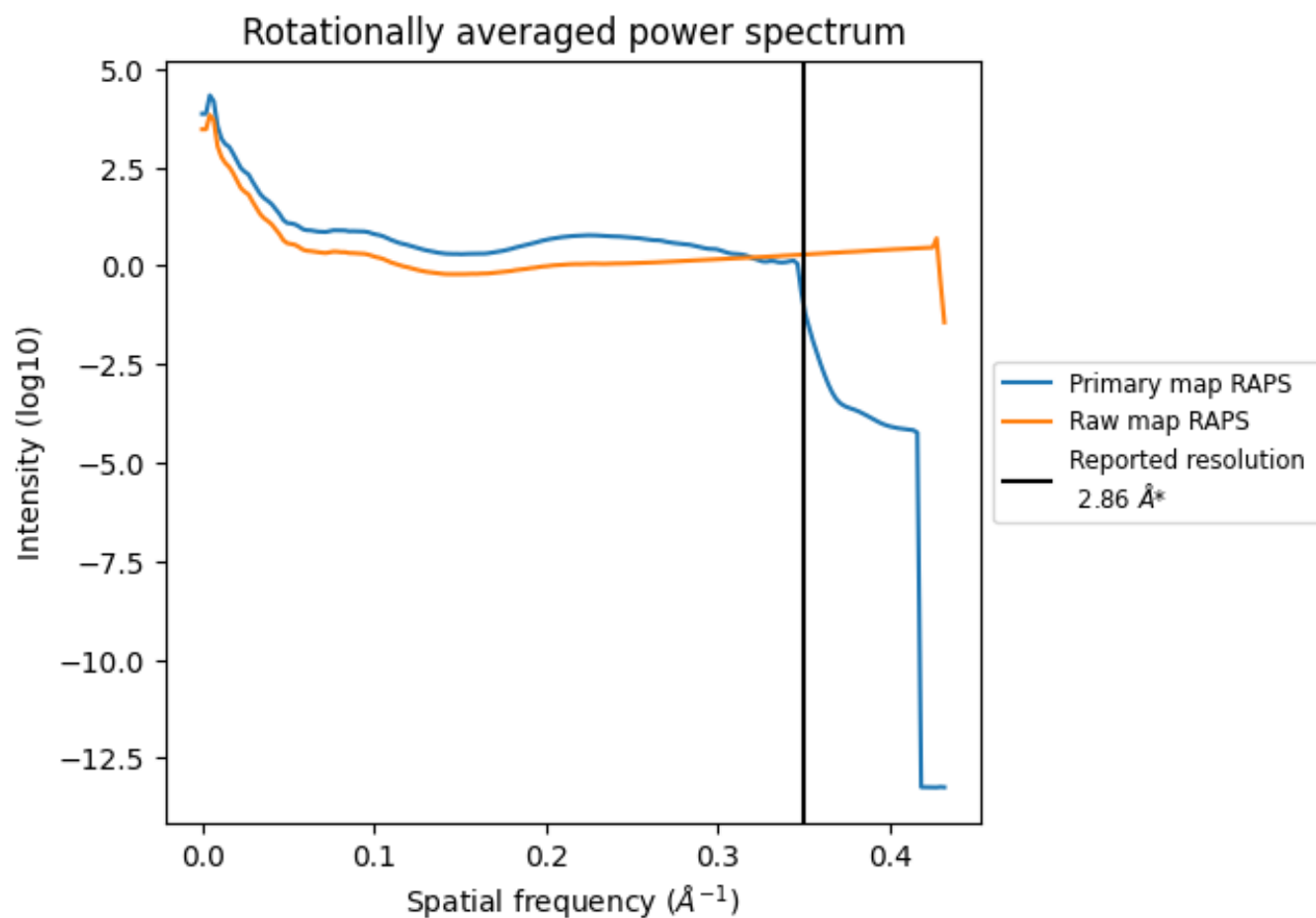
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm^3 ; this corresponds to an approximate mass of 187 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 ⓘ

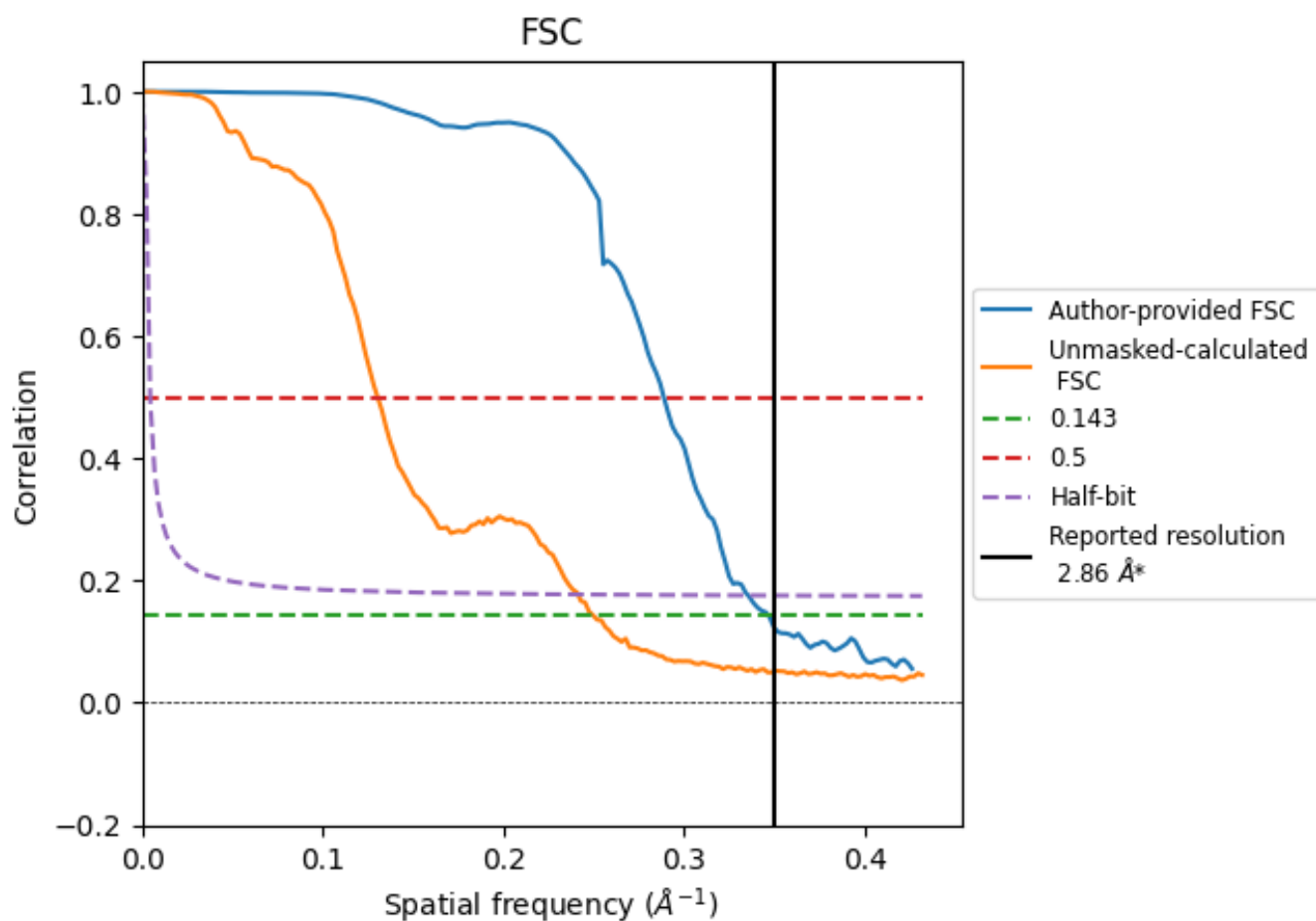


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 \AA^{-1}

8.2 Resolution estimates [i](#)

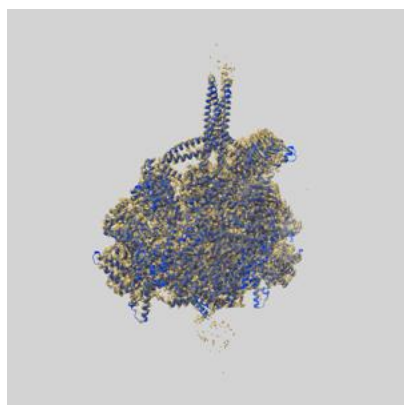
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.88	3.46	2.98
Unmasked-calculated*	4.00	7.67	4.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 2.86 by more than 10 %

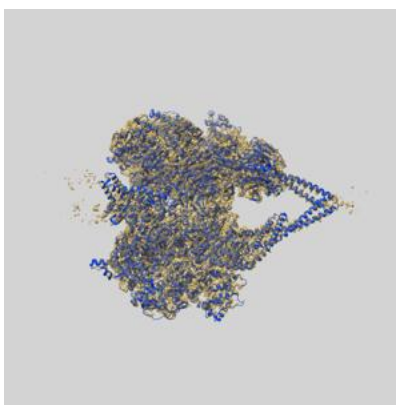
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47378 and PDB model 9E0Z. Per-residue inclusion information can be found in section [3](#) on page [6](#).

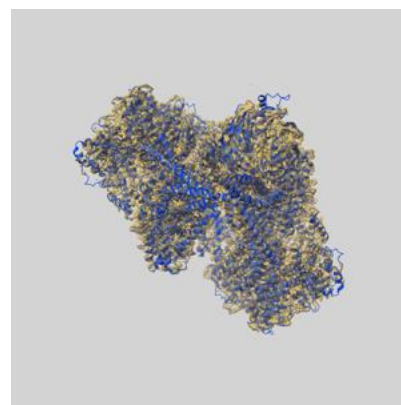
9.1 Map-model overlay [i](#)



X



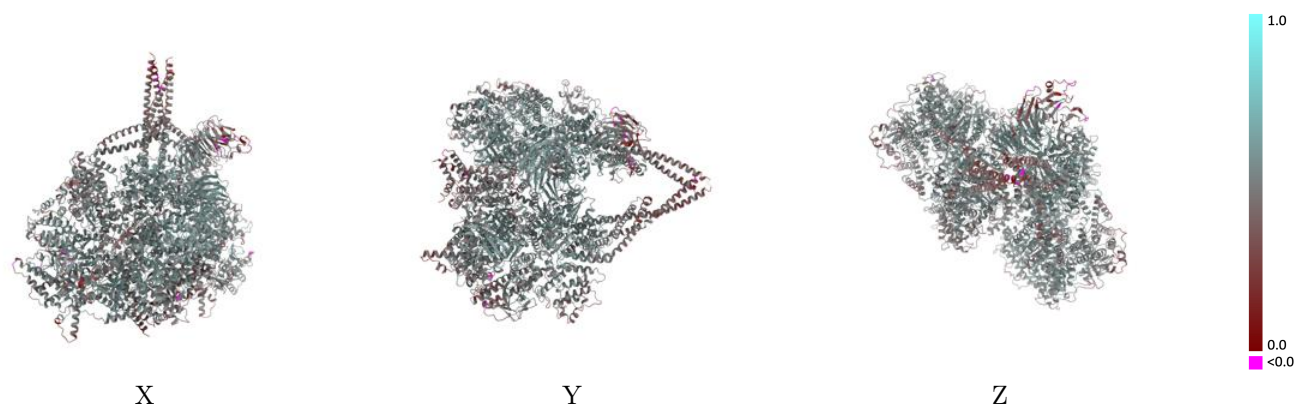
Y



Z

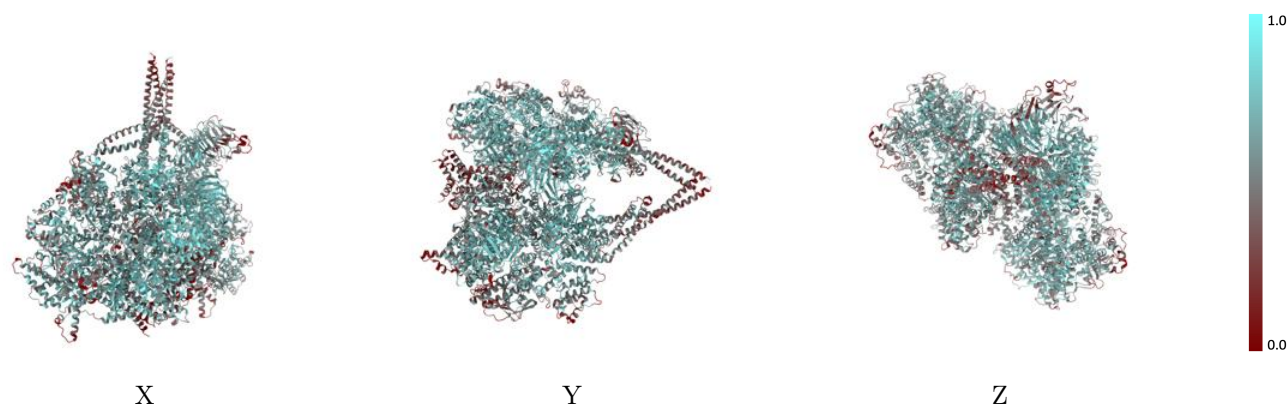
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



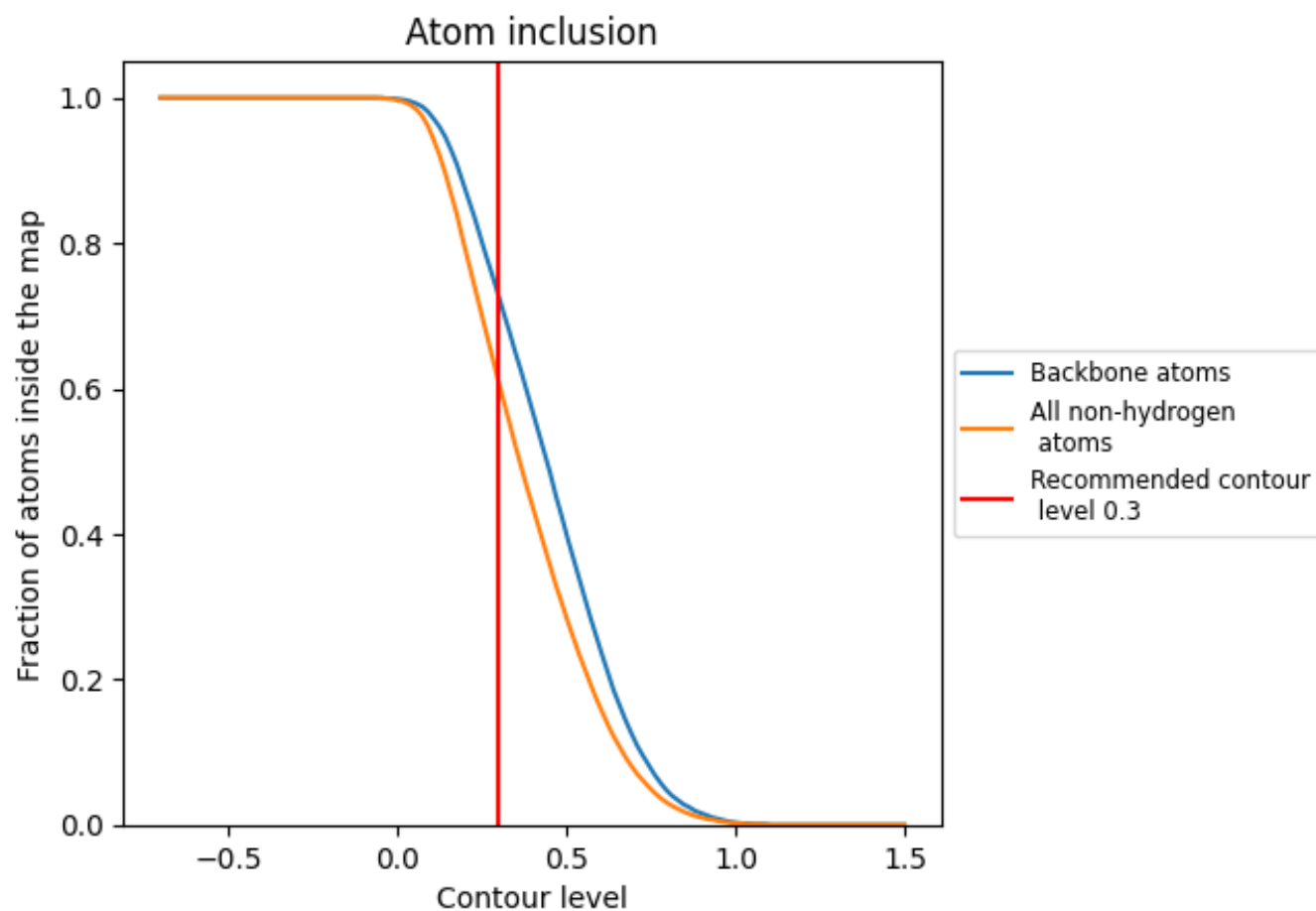
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 73% of all backbone atoms, 61% 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> 0.6080	<div></div> 0.5020
A	<div></div> 0.5740	<div></div> 0.4920
B	<div></div> 0.6360	<div></div> 0.5130
C	<div></div> 0.7400	<div></div> 0.5600
D	<div></div> 0.5350	<div></div> 0.4330

