



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:24 PM UTC

PDB ID : 7OTV / pdb_00007otv
EMDB ID : EMD-13067
Title : DNA-PKcs in complex with wortmannin
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 3.24 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.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

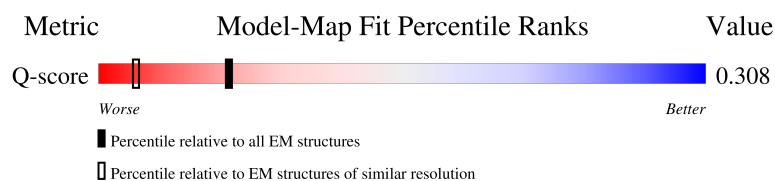
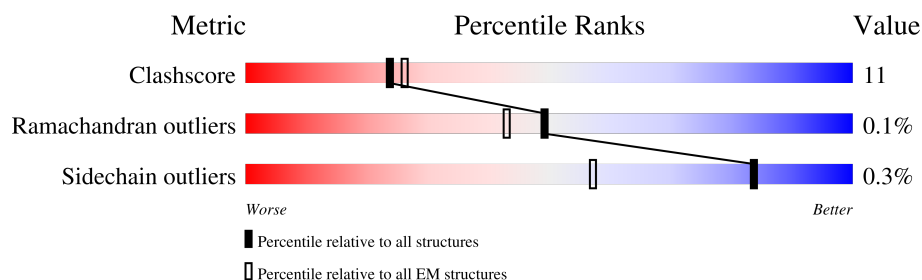
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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	14594 (2.74 - 3.74)

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	4148	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KWT	A	6101	-	-	X	-

2 Entry composition [i](#)

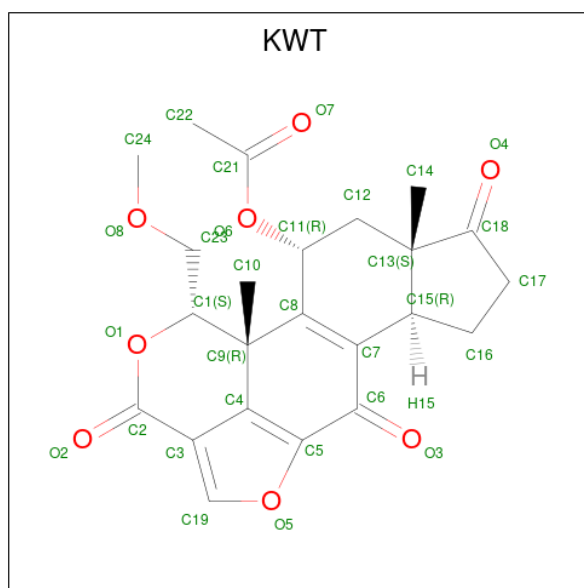
There are 2 unique types of molecules in this entry. The entry contains 29041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3656	29010	18609	4903	5307	191	0	0

- Molecule 2 is (1S,6BR,9AS,11R,11BR)-9A,11B-DIMETHYL-1-[(METHYLOXY)METHYL]-3,6,9-TRIOXO-1,6,6B,7,8,9,9A,10,11,11B-DECAHYDRO-3H-FURO[4, 3,2-DE]INDENO[4,5-H][2]BENZOPYRAN-11-YL ACETATE (CCD ID: KWT) (formula: $C_{23}H_{24}O_8$) (labeled as "Ligand of Interest" by depositor).



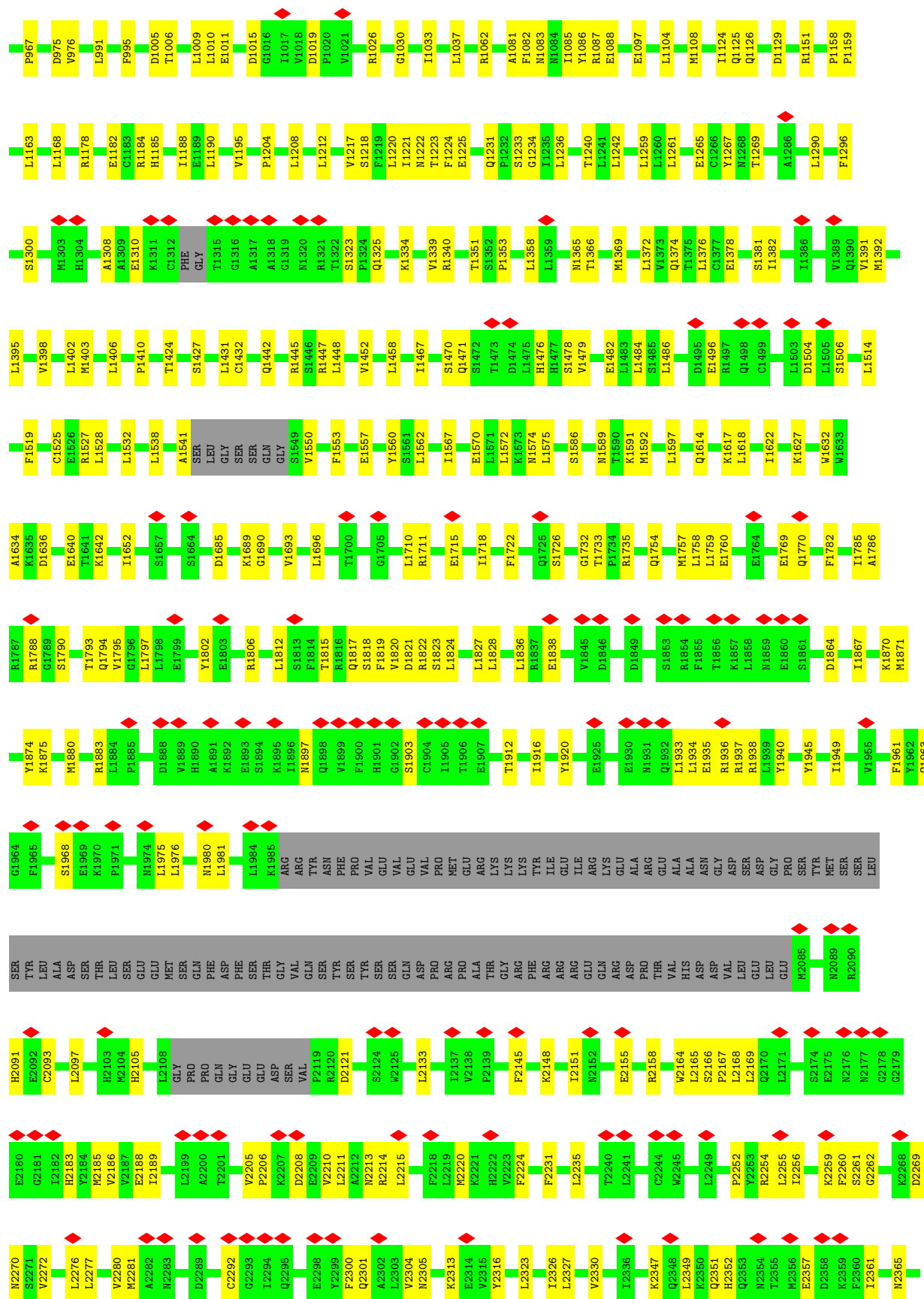
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	31	23	8	0

3 Residue-property plots

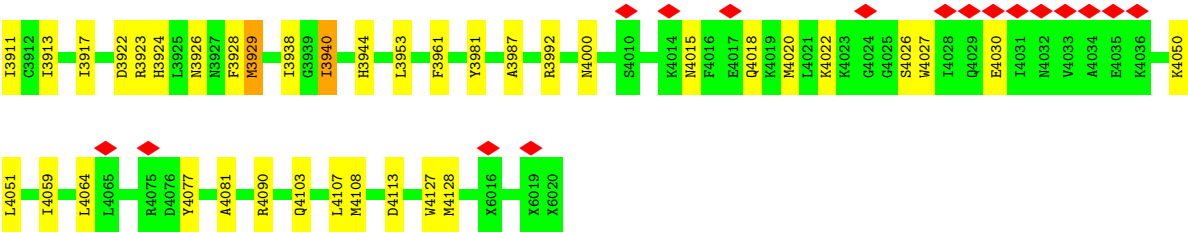
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs





V3752	G3648	T3558	ASP	ASN	I3065	P2902	LYS	ASP	T2368
K3753	S3649	K3558	SER	SER	I3066	ALA	ARG	THR	K2369
G3754	K3650	K3561	ALA	MET	K3067	GLU	LEU	GLN	P2372
G3755	L3651	L3575	GLU	ASN	L3077	LEU	PRO	THR	P2373
E3756	L3652	L3576	ASP	VAL	L3078	PRO	ALA	GLN	L2374
S3779	R3653	N3580	L3439	GLN	L3089	LYS	ARG	THR	K2375
A3780	R3654	P3581	ASP	ASP	L3090	VAL	VAL	ALA	D2376
R3789	K3655	L3446	GLY	GLY	Q3093	ARG	LYS	ASP	L2385
L3790	E3582	V3447	ASP	ASP	D3094	VAL	ASN	GLY	N2474
L3656	E3448	E3447	PRO	PRO	D3095	ARG	LYS	ASP	L2476
S3657	K3449	K3450	SER	SER	V3096	GLY	VAL	SER	P2389
D3658	M3450	L3456	ASP	ARG	L3097	ALA	VAL	PHE	V2392
D3661	L3456	R3467	MET	MET	R3098	ARG	LYS	ASP	L2396
K3796	R3468	L3468	GLU	GLU	A3099	GLY	ALA	TRP	C2397
L3802	N3664	L3471	VAL	GLN	K3100	P2917	ALA	LEU	L2400
L3803	M3665	E3477	GLN	GLN	I3103	P2918	ALA	THR	R2404
E3804	L3666	E3478	ASP	GLU	Q3104	D2919	ALA	GLY	V2405
W3805	L3667	E3479	ASP	GLU	I3108	V2920	ARG	THR	E2406
L3806	L3668	E3480	ASP	GLU	Q3109	R2922	ARG	PRO	M2493
T3809	K3669	S3481	ASP	GLU	I3111	E2925	ARG	PHE	E2497
V3810	M3670	L3482	ASP	GLU	M3111	Y2930	ARG	VAL	K2408
N3671	K3672	K3483	ASP	GLU	S3116	Y2933	ARG	THR	L2411
K3672	N3672	T3484	ASP	GLU	L3121	R2940	ARG	GLN	V2412
P3676	K3676	F3495	ASP	GLU	E3137	S2945	ARG	ALA	F2413
L3880	L3680	L3496	ASP	GLU	I3138	E2946	ARG	THR	V2414
K3681	K3681	M3502	ASP	GLU	Q3139	L2957	ARG	GLY	L2415
E3882	C3683	L3506	ASP	GLU	I3142	L2959	ARG	THR	F2420
S3684	S3684	D3507	ASP	GLU	I3145	A3006	ARG	THR	K2424
P3685	P3685	A3513	ASP	GLU	L3151	K3009	ARG	THR	R2425
W3686	W3686	V3514	ASP	GLU	S3152	L3010	ARG	THR	H2426
M3687	M3687	Q3515	ASP	GLU	Q3154	E3012	ARG	THR	K2427
F3694	F3694	L3616	ASP	GLU	R3167	Y3013	ARG	THR	E2430
E3700	E3700	G3618	ASP	GLU	M3176	C3014	ARG	THR	R2431
K3710	K3710	A3622	ASP	GLU	R3186	S3015	ARG	THR	Q2432
P3711	P3711	L3625	ASP	GLU	C3187	T3016	ARG	THR	K2433
E3714	E3714	G3626	ASP	GLU	K3192	K3029	ARG	THR	V2434
R3718	R3718	A3627	ASP	GLU	K3196	E3033	ARG	THR	I2439
F3628	F3628	F3628	ASP	GLU	L3197	F3034	ARG	THR	T2440
R3629	R3629	L3633	ASP	GLU	THR	F3035	ARG	THR	K2441
L3633	L3633	F3636	ASP	GLU	PRO	S3047	ARG	THR	L2442
F3636	F3636	E3639	ASP	GLU	LEU	L3053	ARG	THR	N2443
F3640	F3640	N3430	ASP	GLU	PRO	L3062	ARG	THR	P2444
H3643	H3643	ALA	ASP	GLU	ASP	L3062	ARG	THR	K2445
F3644	F3644	SER	ASP	GLU	ASP	L3062	ARG	THR	L2455
G3645	G3645	VAL	ASP	GLU	ASP	L3062	ARG	THR	M2456
G3647	G3647	ILE	ASP	GLU	ASP	L3062	ARG	THR	F2457



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.589	Depositor
Minimum map value	-1.600	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	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: KWT

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	0.26	0/29502	0.40	1/39893 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	3483	MET	N-CA-C	8.43	121.23	111.11

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	29010	0	29193	603	0
2	A	31	0	23	23	0
All	All	29041	0	29216	603	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 11.

All (603) 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:3809:THR:CB	1:A:3929:MET:CE	2.16	1.22
1:A:3809:THR:CB	1:A:3929:MET:HE3	1.72	1.14
1:A:3809:THR:HB	1:A:3929:MET:HE3	1.14	1.14
1:A:3751:LEU:HD13	2:A:6101:KWT:H143	1.15	1.09
1:A:3809:THR:CG2	1:A:3929:MET:HE1	1.87	1.04
1:A:3809:THR:HB	1:A:3929:MET:CE	1.82	1.03
1:A:3809:THR:HG21	1:A:3929:MET:HE1	1.37	1.03
1:A:3809:THR:CB	1:A:3929:MET:HE1	1.86	1.01
1:A:3809:THR:OG1	1:A:3929:MET:CE	2.09	1.01
1:A:3811:THR:HG21	2:A:6101:KWT:H223	1.42	1.00
1:A:3751:LEU:CD1	2:A:6101:KWT:H143	1.90	1.00
1:A:3444:ALA:HA	1:A:3482:LEU:CD2	1.99	0.93
1:A:3805:TRP:CE3	2:A:6101:KWT:H141	2.04	0.92
1:A:3811:THR:CG2	2:A:6101:KWT:H223	2.00	0.91
1:A:3803:ILE:CD1	2:A:6101:KWT:C6	2.51	0.88
1:A:3751:LEU:HD13	2:A:6101:KWT:C14	2.04	0.85
1:A:3728:VAL:HG22	1:A:3736:LYS:CD	2.07	0.83
1:A:3803:ILE:HD12	2:A:6101:KWT:O3	1.78	0.83
1:A:3728:VAL:HG22	1:A:3736:LYS:HD2	1.60	0.82
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.46	0.79
1:A:403:GLY:H	1:A:406:ARG:HH12	1.29	0.78
1:A:3444:ALA:O	1:A:3482:LEU:HD21	1.83	0.78
1:A:3751:LEU:HD12	1:A:3805:TRP:CE3	2.18	0.78
1:A:899:ARG:HE	1:A:2568:MET:HB2	1.48	0.78
1:A:3751:LEU:HD21	2:A:6101:KWT:H101	1.67	0.75
1:A:1212:LEU:HD11	1:A:1217:VAL:HA	1.69	0.74
1:A:2796:ALA:O	1:A:2800:ARG:NH1	2.21	0.74
1:A:3298:LEU:HD12	1:A:3333:THR:HG23	1.69	0.73
1:A:3751:LEU:HD12	1:A:3805:TRP:HE3	1.51	0.73
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.20	0.72
1:A:3444:ALA:CA	1:A:3482:LEU:CD2	2.67	0.72
1:A:4050:LYS:HE3	1:A:4059:ILE:HG21	1.71	0.72
1:A:1933:LEU:HD13	1:A:1936:ARG:HB3	1.72	0.71
1:A:3803:ILE:HD12	2:A:6101:KWT:C6	2.19	0.71
1:A:356:ASN:ND2	1:A:404:ASP:O	2.24	0.70
1:A:3444:ALA:HB1	1:A:3482:LEU:HD22	1.73	0.70
1:A:3809:THR:OG1	1:A:3929:MET:HE1	1.81	0.70
1:A:3444:ALA:CB	1:A:3482:LEU:HD22	2.21	0.70
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.56	0.70
1:A:1484:LEU:HD11	1:A:1527:ARG:HH12	1.56	0.70
1:A:2151:ILE:HG21	1:A:2188:GLU:HG2	1.73	0.70
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.63	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3520:GLU:OE2	1:A:3524:ASN:ND2	2.25	0.69
1:A:1097:GLU:OE2	1:A:1151:ARG:NH2	2.25	0.69
1:A:3580:ASN:ND2	1:A:3734:ARG:HB2	2.08	0.69
1:A:899:ARG:NH2	1:A:2568:MET:SD	2.65	0.69
1:A:3186:ARG:HD3	1:A:3238:MET:HE1	1.74	0.69
1:A:3803:ILE:CD1	2:A:6101:KWT:O3	2.40	0.69
1:A:3281:CYS:HB2	1:A:3329:LEU:HD23	1.75	0.68
1:A:75:SER:H	1:A:78:PHE:HB3	1.59	0.68
1:A:709:LYS:NZ	1:A:713:GLU:OE2	2.27	0.68
1:A:767:GLU:HG2	1:A:851:ILE:HD11	1.75	0.68
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.26	0.68
1:A:3145:ILE:HD11	1:A:3196:LYS:HD2	1.74	0.68
1:A:1185:HIS:NE2	1:A:1265:GLU:OE2	2.26	0.67
1:A:1225:GLU:HB3	1:A:1236:LEU:HB2	1.76	0.67
1:A:3811:THR:HG21	2:A:6101:KWT:C22	2.23	0.67
1:A:16:GLN:NE2	1:A:17:GLU:OE2	2.27	0.67
1:A:38:LEU:O	1:A:41:GLU:HB3	1.95	0.67
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.76	0.67
1:A:1334:LYS:NZ	1:A:1382:ILE:O	2.28	0.66
1:A:1369:MET:HE1	1:A:1406:LEU:HD11	1.77	0.66
1:A:3495:PHE:HB3	1:A:3502:MET:HE1	1.75	0.66
1:A:4064:LEU:HD13	1:A:4077:TYR:HB3	1.78	0.66
1:A:3751:LEU:CD2	2:A:6101:KWT:H101	2.26	0.65
1:A:774:GLU:HG2	1:A:858:MET:HE3	1.79	0.64
1:A:2365:ASN:HD22	1:A:2396:LEU:HD13	1.63	0.64
1:A:3911:ILE:HD12	1:A:3928:PHE:HE1	1.62	0.64
1:A:90:CYS:O	1:A:93:LEU:HB3	1.98	0.64
1:A:2169:LEU:HD11	1:A:2215:LEU:HD22	1.80	0.64
1:A:1897:ASN:HB3	1:A:1903:SER:HB2	1.81	0.63
1:A:3448:GLU:HB3	1:A:3482:LEU:HD11	1.81	0.63
1:A:3924:HIS:ND1	1:A:3926:ASN:OD1	2.29	0.63
1:A:463:LYS:HD3	1:A:545:LEU:HD22	1.80	0.63
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.31	0.63
1:A:3009:LYS:O	1:A:3013:TYR:HB3	1.98	0.63
1:A:2563:LEU:HD13	1:A:2812:LEU:HD11	1.80	0.63
1:A:1432:CYS:HB3	1:A:1486:LEU:HD11	1.79	0.62
1:A:3809:THR:CG2	1:A:3929:MET:CE	2.62	0.62
1:A:3580:ASN:HD21	1:A:3734:ARG:HB2	1.63	0.62
1:A:3809:THR:HG21	1:A:3929:MET:CE	2.19	0.62
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.33	0.62
1:A:173:LYS:HA	1:A:176:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3580:ASN:HD21	1:A:3734:ARG:CB	2.11	0.62
1:A:374:LYS:HD2	1:A:423:TYR:HB3	1.82	0.62
1:A:1754:GLN:HA	1:A:1785:ILE:HD11	1.81	0.62
1:A:2439:ILE:O	1:A:2443:MET:HG3	2.00	0.61
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.34	0.61
1:A:3477:GLU:HA	1:A:3477:GLU:OE1	2.01	0.61
1:A:93:LEU:O	1:A:97:GLY:N	2.25	0.61
1:A:2155:GLU:OE2	1:A:2158:ARG:NH2	2.34	0.60
1:A:3666:LEU:O	1:A:3670:MET:HG3	2.01	0.60
1:A:3444:ALA:HA	1:A:3482:LEU:HD21	1.82	0.60
1:A:2406:GLU:OE1	1:A:2441:LYS:NZ	2.34	0.60
1:A:186:PRO:HA	1:A:189:MET:HE1	1.83	0.60
1:A:1358:LEU:HD11	1:A:1410:PRO:HG2	1.84	0.60
1:A:3425:ARG:NH1	1:A:4000:ASN:OD1	2.35	0.60
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.35	0.60
1:A:3864:ARG:NH1	1:A:3868:VAL:HG21	2.17	0.60
1:A:3284:SER:HB3	1:A:3301:LEU:HD12	1.84	0.59
1:A:3295:GLU:OE2	1:A:3295:GLU:N	2.33	0.59
1:A:3444:ALA:CA	1:A:3482:LEU:HD21	2.32	0.59
1:A:3728:VAL:HG22	1:A:3736:LYS:HD3	1.83	0.59
1:A:108:LYS:HZ2	1:A:156:PHE:HZ	1.51	0.59
1:A:203:GLU:O	1:A:206:THR:OG1	2.20	0.59
1:A:2091:HIS:CE1	1:A:2093:CYS:SG	2.96	0.58
1:A:3154:GLN:OE1	1:A:3226:ASP:N	2.36	0.58
1:A:3444:ALA:HB2	1:A:3478:GLU:HG2	1.85	0.58
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.67	0.58
1:A:1819:PHE:O	1:A:1823:SER:OG	2.22	0.58
1:A:1267:TYR:CD2	1:A:1290:LEU:HD22	2.39	0.58
1:A:2357:GLU:HB3	1:A:2385:LEU:HD21	1.85	0.58
1:A:4081:ALA:O	1:A:4090:ARG:NH1	2.36	0.58
1:A:1871:MET:HG2	1:A:1940:TYR:HA	1.84	0.58
1:A:3646:LYS:H	1:A:3650:LYS:HB3	1.68	0.58
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.85	0.58
1:A:1104:LEU:HD23	1:A:1168:LEU:HD21	1.86	0.58
1:A:718:MET:HE3	1:A:726:LEU:HD11	1.86	0.58
1:A:628:GLU:OE2	1:A:631:ARG:NH2	2.37	0.57
1:A:3929:MET:HG3	1:A:3940:ILE:CD1	2.34	0.57
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.37	0.57
1:A:205:LYS:HG2	1:A:249:PHE:HZ	1.70	0.57
1:A:2361:ILE:HD12	1:A:2389:PHE:HE2	1.67	0.57
1:A:3244:ASP:OD1	1:A:3247:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:PHE:HB2	1:A:2272:VAL:HG11	1.87	0.57
1:A:2347:LYS:O	1:A:2351:GLN:NE2	2.37	0.57
1:A:606:SER:OG	1:A:1026:ARG:NH2	2.37	0.57
1:A:3751:LEU:CD1	2:A:6101:KWT:C14	2.73	0.57
1:A:1376:LEU:HD22	1:A:1403:MET:HE1	1.86	0.57
1:A:1541:ALA:HB2	1:A:1550:VAL:HG12	1.87	0.57
1:A:1769:GLU:O	1:A:1822:ARG:NH2	2.24	0.57
1:A:1975:LEU:HD12	1:A:1976:LEU:HD12	1.86	0.57
1:A:1125:GLN:NE2	1:A:1129:ASP:OD2	2.37	0.56
1:A:3961:PHE:HE2	1:A:4107:LEU:HD13	1.70	0.56
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.78	0.56
1:A:1011:GLU:O	1:A:1015:ASP:N	2.38	0.56
1:A:2443:MET:SD	1:A:2476:ILE:HG23	2.46	0.56
1:A:131:LEU:HD22	1:A:173:LYS:HD2	1.85	0.56
1:A:1867:ILE:O	1:A:1871:MET:HG3	2.06	0.56
1:A:3596:LEU:HD12	1:A:3601:VAL:HA	1.88	0.56
1:A:2254:ARG:NH1	1:A:2292:CYS:O	2.39	0.56
1:A:2260:PHE:O	1:A:2270:ASN:ND2	2.38	0.56
1:A:229:SER:HA	1:A:274:LEU:HD13	1.88	0.56
1:A:1754:GLN:HG3	1:A:1785:ILE:HG13	1.88	0.56
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.38	0.56
1:A:3751:LEU:HD11	2:A:6101:KWT:H101	1.86	0.56
1:A:3803:ILE:HD11	2:A:6101:KWT:C6	2.34	0.56
1:A:3575:LEU:HD12	1:A:3796:MET:HE1	1.88	0.55
1:A:1224:PHE:HD2	1:A:1267:TYR:HE1	1.54	0.55
1:A:3796:MET:HE2	1:A:3802:LEU:HG	1.87	0.55
1:A:3406:ALA:O	1:A:3409:VAL:HG12	2.06	0.55
1:A:205:LYS:HG2	1:A:249:PHE:CZ	2.41	0.55
1:A:771:ASN:OD1	1:A:854:ARG:NH2	2.40	0.55
1:A:56:SER:HA	1:A:59:PHE:CD2	2.42	0.55
1:A:1874:TYR:HE2	1:A:1940:TYR:HE1	1.54	0.55
1:A:3710:LYS:HB2	1:A:3711:PRO:HD2	1.88	0.55
1:A:3639:GLU:O	1:A:3643:HIS:N	2.28	0.55
1:A:3680:LEU:HD23	1:A:3682:GLU:H	1.71	0.55
1:A:3751:LEU:HD22	1:A:3803:ILE:HD11	1.88	0.55
1:A:3097:ASP:OD1	1:A:3098:ARG:N	2.37	0.55
1:A:1828:LEU:HD22	1:A:1880:MET:HE3	1.89	0.55
1:A:2168:LEU:HD22	1:A:2189:ILE:HD11	1.89	0.55
1:A:3523:ASP:OD1	1:A:3561:LYS:NZ	2.31	0.55
1:A:13:LEU:HD23	1:A:14:ARG:HE	1.70	0.55
1:A:1812:LEU:O	1:A:1815:THR:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:GLN:HG3	1:A:1445:ARG:HH12	1.71	0.54
1:A:1920:TYR:HE1	1:A:1963:GLN:CB	2.20	0.54
1:A:1961:PHE:O	1:A:1961:PHE:CD1	2.59	0.54
1:A:3735:PRO:HG3	2:A:6101:KWT:H102	1.89	0.54
1:A:4027:TRP:HE3	1:A:4030:GLU:HB3	1.72	0.54
1:A:1267:TYR:HD2	1:A:1290:LEU:HD22	1.72	0.54
1:A:1815:THR:O	1:A:1818:SER:OG	2.25	0.54
1:A:3137:GLU:OE1	1:A:3186:ARG:NH2	2.35	0.54
1:A:3661:ASP:HA	1:A:3664:ASN:HD21	1.72	0.54
1:A:849:GLU:OE1	1:A:3108:GLN:NE2	2.38	0.54
1:A:3605:ASN:OD1	1:A:3606:ILE:N	2.40	0.54
1:A:3608:LYS:O	1:A:3611:GLU:HG3	2.07	0.54
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.90	0.54
1:A:901:MET:SD	1:A:2535:THR:OG1	2.64	0.54
1:A:1920:TYR:CE1	1:A:1963:GLN:CB	2.91	0.54
1:A:1759:LEU:HD12	1:A:1785:ILE:HD13	1.88	0.54
1:A:3495:PHE:HB3	1:A:3502:MET:CE	2.38	0.54
1:A:56:SER:HA	1:A:59:PHE:HD2	1.73	0.53
1:A:59:PHE:HA	1:A:62:ASP:HB2	1.91	0.53
1:A:2999:LEU:HD21	1:A:3015:SER:O	2.09	0.53
1:A:2474:TYR:HD2	1:A:2517:LEU:HD12	1.74	0.53
1:A:2918:PRO:HB2	1:A:2922:ARG:HH22	1.73	0.53
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.29	0.53
1:A:79:ARG:HA	1:A:82:ARG:HB2	1.90	0.53
1:A:2411:LEU:HD11	1:A:2415:LEU:HD23	1.90	0.53
1:A:2091:HIS:HE1	1:A:2093:CYS:SG	2.32	0.53
1:A:3444:ALA:C	1:A:3482:LEU:HD21	2.33	0.53
1:A:355:ASN:HB3	1:A:358:GLU:HG2	1.90	0.53
1:A:1528:LEU:HD21	1:A:1567:ILE:HG23	1.90	0.53
1:A:131:LEU:O	1:A:135:LEU:HG	2.08	0.53
1:A:251:PHE:HA	1:A:254:LYS:HZ2	1.74	0.53
1:A:301:CYS:O	1:A:309:LYS:NZ	2.38	0.53
1:A:3661:ASP:HA	1:A:3664:ASN:ND2	2.24	0.53
1:A:129:ASP:OD1	1:A:129:ASP:N	2.40	0.53
1:A:796:LEU:HD23	1:A:855:VAL:HG13	1.90	0.52
1:A:1108:MET:HE1	1:A:1190:LEU:HD22	1.91	0.52
1:A:3033:GLU:HG3	1:A:3034:PRO:HD3	1.91	0.52
1:A:170:VAL:O	1:A:171:LEU:HD22	2.10	0.52
1:A:267:VAL:HG23	1:A:268:PRO:HD3	1.90	0.52
1:A:2148:LYS:HD3	1:A:2185:MET:HE1	1.90	0.52
1:A:1484:LEU:HD11	1:A:1527:ARG:NH1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1685:ASP:OD1	1:A:1685:ASP:N	2.42	0.52
1:A:2281:MET:HE1	1:A:2326:ILE:HA	1.91	0.52
1:A:1378:GLU:HG2	1:A:1378:GLU:O	2.10	0.52
1:A:3627:ALA:HB3	1:A:3683:CYS:HB2	1.91	0.52
1:A:3348:LEU:O	1:A:3352:GLU:HG2	2.09	0.52
1:A:3496:ILE:HD11	1:A:3521:ILE:HD11	1.92	0.52
1:A:3791:TYR:CE1	1:A:3940:ILE:HG22	2.45	0.52
1:A:13:LEU:O	1:A:14:ARG:NE	2.43	0.52
1:A:2933:ILE:HD11	1:A:3121:LEU:HD22	1.91	0.52
1:A:3733:ARG:HH21	1:A:3755:GLY:C	2.18	0.51
1:A:3751:LEU:HD11	2:A:6101:KWT:C10	2.39	0.51
1:A:2457:PRO:O	1:A:2460:GLU:HG2	2.10	0.51
1:A:3646:LYS:N	1:A:3650:LYS:HB3	2.25	0.51
1:A:1374:GLN:HE22	1:A:1381:SER:HB3	1.76	0.51
1:A:1575:LEU:H	1:A:1575:LEU:HD23	1.76	0.51
1:A:1710:LEU:HG	1:A:1757:MET:HE1	1.92	0.51
1:A:2205:VAL:HB	1:A:2208:ASP:HB2	1.92	0.51
1:A:2555:LEU:HD11	1:A:2854:PHE:HA	1.91	0.51
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.11	0.51
1:A:3137:GLU:CD	1:A:3186:ARG:HE	2.19	0.51
1:A:3507:ASP:HB3	1:A:3540:TYR:CD1	2.45	0.51
1:A:1519:PHE:CG	1:A:1570:GLU:HG3	2.45	0.51
1:A:2522:ARG:HG2	1:A:2561:PHE:HE1	1.76	0.51
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	1.93	0.51
1:A:3622:ALA:HB3	1:A:3625:LEU:HB2	1.92	0.51
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	1.93	0.51
1:A:36:ARG:HH21	1:A:39:GLY:HA3	1.76	0.51
1:A:708:VAL:HG22	1:A:740:ILE:HG23	1.92	0.51
1:A:2551:GLU:OE2	1:A:2849:SER:OG	2.28	0.51
1:A:3053:LEU:HD11	1:A:3088:LEU:HD13	1.92	0.51
1:A:1037:LEU:HD23	1:A:1085:ILE:HB	1.93	0.50
1:A:3414:MET:HE3	1:A:3414:MET:HA	1.92	0.50
1:A:3243:ILE:HD13	1:A:3259:LEU:HD13	1.92	0.50
1:A:3729:MET:HE2	1:A:3805:TRP:CH2	2.47	0.50
1:A:3944:HIS:NE2	1:A:4020:MET:SD	2.84	0.50
1:A:1224:PHE:HD2	1:A:1267:TYR:CE1	2.28	0.50
1:A:1557:GLU:HA	1:A:1592:MET:HE1	1.94	0.50
1:A:2256:ILE:HG22	1:A:2260:PHE:HE2	1.76	0.50
1:A:2424:MET:HE1	1:A:2439:ILE:HD11	1.92	0.50
1:A:242:PRO:O	1:A:245:SER:OG	2.24	0.50
1:A:2828:GLU:O	1:A:2832:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.11	0.50
1:A:1818:SER:HA	1:A:1821:ASP:HB3	1.94	0.50
1:A:3596:LEU:HB2	1:A:3601:VAL:HG22	1.94	0.50
1:A:403:GLY:O	1:A:406:ARG:NH1	2.45	0.49
1:A:1782:PHE:HA	1:A:1785:ILE:HG22	1.94	0.49
1:A:3809:THR:OG1	1:A:3929:MET:HE3	1.88	0.49
1:A:23:ASP:HA	1:A:30:ALA:HB1	1.93	0.49
1:A:1234:GLY:HA2	1:A:1259:LEU:HD22	1.93	0.49
1:A:2376:ASP:OD1	1:A:2404:ARG:NE	2.41	0.49
1:A:3751:LEU:CD1	2:A:6101:KWT:H101	2.42	0.49
1:A:3227:ILE:HD12	1:A:3227:ILE:H	1.78	0.49
1:A:3791:TYR:CZ	1:A:3940:ILE:HG22	2.47	0.49
1:A:2097:LEU:HD12	1:A:2145:PHE:HZ	1.77	0.49
1:A:1726:SER:O	1:A:1726:SER:OG	2.27	0.49
1:A:2365:ASN:ND2	1:A:2396:LEU:HD13	2.27	0.49
1:A:3911:ILE:CD1	1:A:3928:PHE:HE1	2.25	0.49
1:A:975:ASP:OD1	1:A:976:VAL:N	2.45	0.49
1:A:3929:MET:SD	2:A:6101:KWT:O4	2.70	0.49
1:A:1006:THR:HG22	1:A:1009:LEU:HB2	1.94	0.49
1:A:1339:VAL:HG23	1:A:1398:VAL:HG21	1.95	0.49
1:A:3805:TRP:CE3	2:A:6101:KWT:C14	2.88	0.49
1:A:1864:ASP:HA	1:A:1867:ILE:HG12	1.95	0.49
1:A:3062:LEU:HD13	1:A:3093:GLN:NE2	2.28	0.49
1:A:1208:LEU:HD21	1:A:1220:LEU:HD11	1.94	0.49
1:A:1871:MET:HE1	1:A:1936:ARG:HH21	1.77	0.49
1:A:1532:LEU:HD11	1:A:1560:TYR:HB2	1.94	0.49
1:A:1817:GLN:OE1	1:A:1936:ARG:NH2	2.41	0.49
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.46	0.49
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.48	0.49
1:A:2368:THR:HG23	1:A:2372:PRO:HA	1.93	0.49
1:A:2415:LEU:HD12	1:A:2420:PHE:CD1	2.48	0.49
1:A:3151:LEU:HD21	1:A:3197:LEU:HA	1.95	0.49
1:A:59:PHE:HB3	1:A:63:PHE:CE1	2.47	0.48
1:A:242:PRO:C	1:A:246:ARG:HE	2.20	0.48
1:A:3444:ALA:HA	1:A:3482:LEU:HD23	1.92	0.48
1:A:346:TYR:HB3	1:A:350:ARG:HH12	1.78	0.48
1:A:1586:SER:O	1:A:1632:TRP:NE1	2.43	0.48
1:A:1470:SER:HB3	1:A:1476:HIS:CD2	2.48	0.48
1:A:2940:ARG:HG2	1:A:2957:LEU:HD22	1.95	0.48
1:A:3104:GLN:OE1	1:A:3139:GLN:NE2	2.46	0.48
1:A:1933:LEU:HD12	1:A:1937:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.47	0.48
1:A:2259:LYS:HB3	1:A:2272:VAL:HG23	1.94	0.48
1:A:253:LEU:HD11	1:A:271:GLY:HA3	1.95	0.48
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.94	0.48
1:A:3587:ASP:CG	1:A:3733:ARG:HH12	2.21	0.48
1:A:923:ASP:C	1:A:925:GLN:H	2.21	0.48
1:A:2304:VAL:HG12	1:A:2323:LEU:HD11	1.96	0.48
1:A:2786:LYS:O	1:A:2788:SER:N	2.47	0.48
1:A:3587:ASP:OD2	1:A:3733:ARG:NH1	2.45	0.48
1:A:2261:SER:OG	1:A:2262:GLY:N	2.46	0.48
1:A:2301:GLN:OE1	1:A:2305:ASN:ND2	2.46	0.48
1:A:2877:SER:OG	1:A:2925:GLU:HB3	2.13	0.48
1:A:3446:VAL:O	1:A:3450:MET:HG2	2.13	0.48
1:A:3728:VAL:HG12	1:A:3734:ARG:HD3	1.96	0.48
1:A:1009:LEU:HD21	1:A:1062:ARG:NH1	2.29	0.47
1:A:225:LYS:HZ3	1:A:253:LEU:HD13	1.79	0.47
1:A:1086:TYR:C	1:A:1088:GLU:H	2.22	0.47
1:A:1471:GLN:N	1:A:1471:GLN:OE1	2.48	0.47
1:A:2542:LEU:HD21	1:A:2558:ALA:HA	1.95	0.47
1:A:1934:LEU:O	1:A:1938:ARG:N	2.43	0.47
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.14	0.47
1:A:2432:GLN:OE1	1:A:2464:HIS:NE2	2.45	0.47
1:A:3186:ARG:HD3	1:A:3238:MET:CE	2.44	0.47
1:A:1836:LEU:HA	1:A:1880:MET:HE1	1.97	0.47
1:A:3753:LYS:HD2	1:A:3753:LYS:HA	1.56	0.47
1:A:397:LEU:HD21	1:A:438:LEU:HD22	1.95	0.47
1:A:195:ASN:O	1:A:198:ARG:HG3	2.15	0.47
1:A:540:MET:SD	1:A:540:MET:N	2.88	0.47
1:A:1572:LEU:HD21	1:A:1618:LEU:HD22	1.96	0.47
1:A:1912:THR:O	1:A:1916:ILE:HG12	2.14	0.47
1:A:3444:ALA:HB2	1:A:3478:GLU:CG	2.44	0.47
1:A:439:VAL:O	1:A:442:GLN:HB3	2.15	0.47
1:A:3729:MET:SD	1:A:3729:MET:N	2.87	0.47
1:A:1323:SER:O	1:A:1325:GLN:N	2.48	0.47
1:A:3809:THR:OG1	1:A:3929:MET:SD	2.73	0.47
1:A:12:LEU:O	1:A:16:GLN:HG2	2.14	0.47
1:A:726:LEU:HD21	1:A:754:MET:SD	2.55	0.47
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.15	0.47
1:A:2121:ASP:OD1	1:A:2121:ASP:N	2.43	0.47
1:A:3344:GLU:OE2	1:A:3348:LEU:HD23	2.15	0.47
1:A:3803:ILE:CD1	2:A:6101:KWT:C5	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:O	1:A:66:LEU:HB2	2.15	0.46
1:A:180:LEU:HA	1:A:230:LEU:HD21	1.98	0.46
1:A:3789:ARG:NH2	1:A:3806:LEU:HD11	2.31	0.46
1:A:14:ARG:O	1:A:18:THR:HG23	2.15	0.46
1:A:1793:THR:O	1:A:1797:LEU:HG	2.15	0.46
1:A:2539:LEU:HD13	1:A:2562:LEU:HD11	1.97	0.46
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.48	0.46
1:A:1300:SER:O	1:A:1300:SER:OG	2.32	0.46
1:A:2785:ILE:O	1:A:2789:SER:HB2	2.16	0.46
1:A:2884:LEU:HD12	1:A:3116:SER:HB2	1.96	0.46
1:A:942:LEU:HD11	1:A:991:LEU:HD21	1.97	0.46
1:A:1711:ARG:NH2	1:A:1760:GLU:OE1	2.48	0.46
1:A:3410:ILE:HD11	1:A:3456:LEU:HB3	1.98	0.46
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.98	0.46
1:A:1586:SER:O	1:A:1586:SER:OG	2.34	0.46
1:A:2213:ASN:OD1	1:A:2214:ARG:N	2.48	0.46
1:A:586:GLN:HB2	1:A:613:HIS:CD2	2.51	0.46
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.98	0.46
1:A:3313:SER:HA	1:A:3316:LEU:HB2	1.96	0.46
1:A:1478:SER:O	1:A:1482:GLU:HG3	2.17	0.45
1:A:1572:LEU:HB3	1:A:1614:GLN:HE21	1.81	0.45
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.52	0.45
1:A:2252:PRO:C	1:A:2254:ARG:H	2.23	0.45
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.99	0.45
1:A:2408:MET:HE3	1:A:2411:LEU:HD22	1.98	0.45
1:A:2411:LEU:C	1:A:2413:PHE:H	2.24	0.45
1:A:3369:ASP:OD1	1:A:3369:ASP:N	2.49	0.45
1:A:3484:THR:HG23	1:A:3513:ALA:HA	1.97	0.45
1:A:1496:GLU:OE1	1:A:1496:GLU:N	2.42	0.45
1:A:3526:PRO:C	1:A:3528:ALA:H	2.23	0.45
1:A:2471:GLU:HA	1:A:2517:LEU:HD11	1.98	0.45
1:A:3636:PHE:CE2	1:A:3670:MET:HG2	2.52	0.45
1:A:189:MET:SD	1:A:189:MET:N	2.90	0.45
1:A:1484:LEU:HD21	1:A:1527:ARG:HH22	1.80	0.45
1:A:2164:TRP:C	1:A:2167:PRO:HD2	2.42	0.45
1:A:2576:MET:HB3	1:A:2787:HIS:CD2	2.52	0.45
1:A:861:SER:O	1:A:3167:ARG:NH1	2.46	0.45
1:A:1188:ILE:HD13	1:A:1269:THR:HG21	1.98	0.45
1:A:1538:LEU:HD12	1:A:1553:PHE:CE1	2.52	0.45
1:A:1935:GLU:OE2	1:A:1938:ARG:NE	2.34	0.45
1:A:4020:MET:HE2	1:A:4020:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4127:TRP:CD1	1:A:4128:MET:H	2.35	0.45
1:A:154:SER:HA	1:A:157:TYR:HD2	1.82	0.45
1:A:1221:ILE:HD12	1:A:1221:ILE:H	1.82	0.45
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.99	0.45
1:A:2930:TYR:HA	1:A:2933:ILE:HG22	1.98	0.45
1:A:100:ILE:HB	1:A:102:PRO:HD3	1.98	0.45
1:A:1158:PRO:N	1:A:1159:PRO:HD2	2.31	0.45
1:A:2361:ILE:HD12	1:A:2389:PHE:CE2	2.51	0.45
1:A:2863:CYS:SG	1:A:2895:GLU:HG3	2.57	0.45
1:A:487:LEU:HD12	1:A:490:ILE:HD11	1.99	0.45
1:A:2372:PRO:O	1:A:2374:LEU:N	2.50	0.45
1:A:3751:LEU:HD21	2:A:6101:KWT:C10	2.42	0.45
1:A:3603:LYS:HB3	1:A:3606:ILE:HG22	1.98	0.44
1:A:849:GLU:OE2	1:A:852:ARG:NH1	2.50	0.44
1:A:3467:ARG:O	1:A:3471:ILE:HG12	2.17	0.44
1:A:3779:SER:OG	1:A:3780:ALA:N	2.50	0.44
1:A:3878:VAL:HG21	1:A:4128:MET:HB3	1.98	0.44
1:A:396:PHE:HB3	1:A:441:MET:HE1	1.99	0.44
1:A:1786:ALA:HB2	1:A:1827:LEU:HD23	1.99	0.44
1:A:221:ALA:O	1:A:225:LYS:HE3	2.18	0.44
1:A:404:ASP:HB2	1:A:1732:GLY:O	2.17	0.44
1:A:1696:LEU:HA	1:A:1696:LEU:HD23	1.81	0.44
1:A:1864:ASP:N	1:A:1864:ASP:OD1	2.50	0.44
1:A:2522:ARG:HG2	1:A:2561:PHE:CE1	2.52	0.44
1:A:2559:THR:O	1:A:2563:LEU:HB2	2.16	0.44
1:A:3088:LEU:HD23	1:A:3088:LEU:HA	1.74	0.44
1:A:3383:GLN:O	1:A:3387:GLU:HG3	2.17	0.44
1:A:3478:GLU:CD	1:A:3478:GLU:N	2.75	0.44
1:A:2443:MET:C	1:A:2445:LYS:H	2.25	0.44
1:A:3604:LYS:HA	1:A:3607:GLU:HG2	2.00	0.44
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.99	0.44
1:A:151:GLU:HB3	1:A:153:PHE:CE1	2.53	0.44
1:A:493:LYS:O	1:A:625:ASN:ND2	2.51	0.44
1:A:2463:SER:O	1:A:2463:SER:OG	2.31	0.44
1:A:2575:PRO:HA	1:A:2786:LYS:H	1.83	0.44
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.52	0.44
1:A:1231:GLN:O	1:A:1233:SER:N	2.47	0.44
1:A:1427:SER:O	1:A:1431:LEU:HD23	2.18	0.44
1:A:1770:GLN:N	1:A:1770:GLN:OE1	2.51	0.44
1:A:1458:LEU:HD13	1:A:1467:ILE:HD11	2.00	0.44
1:A:3229:SER:OG	1:A:3232:ARG:NH1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:CZ	1:A:293:LEU:HD21	2.52	0.43
1:A:1019:ASP:HA	1:A:1026:ARG:HH11	1.82	0.43
1:A:225:LYS:HZ3	1:A:253:LEU:HD22	1.82	0.43
1:A:1124:ILE:HG23	1:A:1182:GLU:HG2	2.00	0.43
1:A:1690:GLY:HA2	1:A:1693:VAL:HG22	2.00	0.43
1:A:2506:LEU:HD23	1:A:2506:LEU:HA	1.83	0.43
1:A:3285:HIS:HD2	1:A:3298:LEU:HD11	1.83	0.43
1:A:3793:VAL:HG13	1:A:3803:ILE:HG22	1.99	0.43
1:A:671:SER:O	1:A:675:ARG:HG3	2.18	0.43
1:A:1365:ASN:OD1	1:A:1366:THR:N	2.51	0.43
1:A:1448:LEU:HD21	1:A:1514:LEU:HD11	1.99	0.43
1:A:2945:SER:HB2	1:A:2946:GLU:OE1	2.17	0.43
1:A:59:PHE:O	1:A:63:PHE:N	2.52	0.43
1:A:2415:LEU:HD12	1:A:2420:PHE:CG	2.53	0.43
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.52	0.43
1:A:1802:TYR:O	1:A:1806:ARG:HG2	2.19	0.43
1:A:3714:GLU:N	1:A:3714:GLU:OE1	2.51	0.43
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	2.01	0.43
1:A:1622:ILE:HG21	1:A:1652:ILE:HD11	2.00	0.43
1:A:1636:ASP:N	1:A:1636:ASP:OD1	2.50	0.43
1:A:3626:GLY:HA3	1:A:3684:SER:O	2.19	0.43
1:A:3655:LYS:C	1:A:3657:SER:H	2.26	0.43
1:A:958:MET:HE3	1:A:958:MET:HB2	1.86	0.43
1:A:355:ASN:OD1	1:A:356:ASN:N	2.52	0.43
1:A:770:LEU:HD12	1:A:770:LEU:HA	1.89	0.43
1:A:935:HIS:NE2	1:A:939:MET:HE2	2.34	0.43
1:A:1242:LEU:HA	1:A:1310:GLU:HB2	2.01	0.43
1:A:3449:LYS:HA	1:A:3449:LYS:HD3	1.72	0.43
1:A:12:LEU:HA	1:A:15:LEU:HB3	2.00	0.43
1:A:1640:GLU:OE1	1:A:1640:GLU:N	2.50	0.43
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.19	0.43
1:A:3077:ILE:HG13	1:A:3078:LEU:N	2.34	0.43
1:A:3176:MET:HE2	1:A:3246:ALA:HB2	2.00	0.43
1:A:3727:THR:HG22	1:A:3729:MET:SD	2.59	0.43
1:A:3843:LEU:HD21	1:A:3858:MET:HE2	2.00	0.43
1:A:579:LEU:HD23	1:A:579:LEU:HA	1.88	0.43
1:A:991:LEU:HD23	1:A:991:LEU:HA	1.85	0.43
1:A:2347:LYS:C	1:A:2351:GLN:HE22	2.27	0.43
1:A:3444:ALA:CA	1:A:3482:LEU:HD22	2.42	0.43
1:A:3981:TYR:HB2	1:A:4108:MET:HE1	2.00	0.43
1:A:79:ARG:O	1:A:82:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD12	1:A:132:ILE:N	2.33	0.42
1:A:253:LEU:HD12	1:A:254:LYS:N	2.34	0.42
1:A:737:PRO:HD2	1:A:740:ILE:HD12	2.01	0.42
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	2.00	0.42
1:A:1476:HIS:HB3	1:A:1479:VAL:HG22	2.01	0.42
1:A:1557:GLU:CA	1:A:1592:MET:HE1	2.49	0.42
1:A:2887:PRO:HB2	1:A:3895:GLU:HG3	2.00	0.42
1:A:3700:GLU:HA	1:A:3718:ARG:HA	2.00	0.42
1:A:3875:GLU:O	1:A:3878:VAL:HG12	2.19	0.42
1:A:192:ASN:OD1	1:A:192:ASN:N	2.52	0.42
1:A:1627:LYS:HD2	1:A:1627:LYS:HA	1.84	0.42
1:A:236:LYS:HD3	1:A:246:ARG:HH12	1.84	0.42
1:A:466:LEU:HB3	1:A:560:LEU:HD22	2.01	0.42
1:A:853:ILE:HA	1:A:3111:MET:HE1	2.00	0.42
1:A:1391:VAL:HG13	1:A:1392:MET:SD	2.59	0.42
1:A:2554:PHE:C	1:A:2556:SER:H	2.27	0.42
1:A:3681:LYS:O	1:A:3685:PRO:HD2	2.19	0.42
1:A:3816:LEU:HD21	1:A:3883:LEU:HD13	2.01	0.42
1:A:287:LEU:HG	1:A:326:MET:SD	2.59	0.42
1:A:563:LEU:O	1:A:567:GLU:HG2	2.19	0.42
1:A:1820:VAL:HG12	1:A:1824:LEU:HD23	2.00	0.42
1:A:3065:ILE:HD13	1:A:3065:ILE:HA	1.91	0.42
1:A:3260:LYS:HA	1:A:3260:LYS:HD2	1.83	0.42
1:A:3483:MET:O	1:A:3483:MET:HG3	2.16	0.42
1:A:1358:LEU:HD21	1:A:1410:PRO:HB2	2.01	0.42
1:A:2486:ASP:HB3	1:A:2489:SER:HB2	2.01	0.42
1:A:3011:LEU:O	1:A:3016:THR:OG1	2.21	0.42
1:A:3012:GLU:HB2	1:A:3047:SER:HB2	2.02	0.42
1:A:3913:ILE:HG21	1:A:3987:ALA:HB3	2.02	0.42
1:A:174:VAL:O	1:A:177:LEU:HG	2.18	0.42
1:A:195:ASN:OD1	1:A:196:LEU:N	2.52	0.42
1:A:1395:LEU:O	1:A:1398:VAL:HG22	2.20	0.42
1:A:3227:ILE:O	1:A:3228:SER:HB3	2.19	0.42
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	2.00	0.42
1:A:3879:PRO:HB2	1:A:3882:LEU:HG	2.01	0.42
1:A:60:SER:OG	1:A:61:ARG:N	2.53	0.42
1:A:1424:THR:HG23	1:A:1427:SER:H	1.85	0.42
1:A:2220:MET:HB3	1:A:2255:LEU:HD22	2.01	0.42
1:A:2576:MET:HB3	1:A:2787:HIS:NE2	2.34	0.42
1:A:3318:LYS:O	1:A:3322:ALA:HB3	2.19	0.42
1:A:3917:ILE:HD13	1:A:4051:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3922:ASP:O	1:A:3923:ARG:NE	2.49	0.42
1:A:29:LEU:HD13	1:A:32:HIS:HB3	2.02	0.42
1:A:202:GLY:HA2	1:A:205:LYS:HE2	2.02	0.42
1:A:275:PHE:HZ	1:A:293:LEU:HD21	1.84	0.42
1:A:469:ALA:HB2	1:A:479:ILE:HD11	2.02	0.42
1:A:1218:SER:O	1:A:1222:ASN:ND2	2.52	0.42
1:A:1718:ILE:O	1:A:1722:PHE:HB2	2.20	0.42
1:A:42:CYS:HA	1:A:88:PHE:CE1	2.55	0.42
1:A:3542:PHE:HZ	1:A:3555:VAL:HG11	1.84	0.42
1:A:3751:LEU:HD12	1:A:3805:TRP:CZ3	2.52	0.42
1:A:523:THR:HG23	1:A:525:LYS:H	1.85	0.42
1:A:1030:GLY:O	1:A:1033:ILE:HG22	2.20	0.42
1:A:1448:LEU:O	1:A:1452:VAL:HG13	2.20	0.42
1:A:2917:PRO:HB2	1:A:2919:ASP:OD1	2.20	0.42
1:A:3138:ILE:O	1:A:3142:ILE:HG12	2.20	0.42
1:A:3537:SER:HA	1:A:3540:TYR:CE2	2.55	0.42
1:A:4107:LEU:HD23	1:A:4107:LEU:HA	1.79	0.42
1:A:251:PHE:HA	1:A:254:LYS:NZ	2.35	0.41
1:A:1308:ALA:C	1:A:1310:GLU:H	2.28	0.41
1:A:2349:LEU:HA	1:A:2352:HIS:CE1	2.56	0.41
1:A:3100:LYS:O	1:A:3103:ILE:HG22	2.20	0.41
1:A:3506:LEU:HD23	1:A:3506:LEU:HA	1.81	0.41
1:A:31:GLY:HA2	1:A:34:LEU:HB2	2.03	0.41
1:A:35:ILE:HG21	1:A:80:GLU:HB3	2.02	0.41
1:A:438:LEU:O	1:A:442:GLN:N	2.49	0.41
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.72	0.41
1:A:995:PHE:HB3	1:A:1005:ASP:OD1	2.19	0.41
1:A:1178:ARG:O	1:A:1184:ARG:NH2	2.51	0.41
1:A:2411:LEU:HA	1:A:2411:LEU:HD12	1.87	0.41
1:A:2455:LEU:HD22	1:A:2498:ILE:HG23	2.01	0.41
1:A:109:ASN:OD1	1:A:110:THR:N	2.53	0.41
1:A:296:VAL:HG23	1:A:297:LEU:HD12	2.03	0.41
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.20	0.41
1:A:2397:CYS:O	1:A:2400:VAL:HG12	2.20	0.41
1:A:36:ARG:NE	1:A:36:ARG:HA	2.36	0.41
1:A:68:PHE:O	1:A:71:LYS:HB2	2.20	0.41
1:A:623:PHE:CE2	1:A:665:GLY:HA3	2.54	0.41
1:A:733:LEU:HD12	1:A:733:LEU:HA	1.85	0.41
1:A:2802:PRO:HG2	1:A:2803:ILE:HD12	2.02	0.41
1:A:3582:GLU:HG2	1:A:3583:LEU:N	2.34	0.41
1:A:3911:ILE:CD1	1:A:3928:PHE:CE1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:SER:HB3	1:A:852:ARG:HE	1.86	0.41
1:A:2097:LEU:HD23	1:A:2097:LEU:HA	1.81	0.41
1:A:2492:ASP:C	1:A:2494:ASP:H	2.28	0.41
1:A:3006:ALA:HB3	1:A:3257:LYS:HE2	2.01	0.41
1:A:3271:ASP:HB2	1:A:3315:TYR:CE2	2.55	0.41
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.50	0.41
1:A:220:LEU:O	1:A:224:LEU:HG	2.21	0.41
1:A:240:GLU:HB3	1:A:242:PRO:HD2	2.01	0.41
1:A:1758:LEU:HD23	1:A:1758:LEU:HA	1.84	0.41
1:A:3687:MET:HB3	1:A:3722:PHE:CD1	2.56	0.41
1:A:128:LEU:HD13	1:A:131:LEU:HD21	2.02	0.41
1:A:3953:LEU:HD22	1:A:4026:SER:HB3	2.02	0.41
1:A:363:ILE:HD13	1:A:363:ILE:HA	1.97	0.41
1:A:442:GLN:HG3	1:A:461:ILE:HD11	2.02	0.41
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.41
1:A:1220:LEU:O	1:A:1223:THR:OG1	2.27	0.41
1:A:1240:THR:HG23	1:A:1296:PHE:CG	2.56	0.41
1:A:1261:LEU:CD1	1:A:1340:ARG:HG3	2.51	0.41
1:A:1431:LEU:HD11	1:A:1447:ARG:NH2	2.35	0.41
1:A:1795:VAL:HG21	1:A:1838:GLU:HG3	2.03	0.41
1:A:1836:LEU:HD21	1:A:1883:ARG:HH21	1.85	0.41
1:A:2276:LEU:HD23	1:A:2276:LEU:HA	1.92	0.41
1:A:2277:LEU:O	1:A:2280:VAL:HG12	2.21	0.41
1:A:2425:ARG:HG2	1:A:2460:GLU:OE2	2.21	0.41
1:A:2578:GLU:H	1:A:2578:GLU:CD	2.29	0.41
1:A:2891:ARG:HD2	1:A:2891:ARG:HA	1.85	0.41
1:A:4015:ASN:O	1:A:4018:GLN:HG3	2.20	0.41
1:A:1589:ASN:C	1:A:1591:LYS:H	2.29	0.41
1:A:1754:GLN:HE22	1:A:1788:ARG:HD2	1.86	0.41
1:A:1871:MET:O	1:A:1875:LYS:HG3	2.20	0.41
1:A:2133:LEU:HD23	1:A:2164:TRP:CZ3	2.56	0.41
1:A:2392:VAL:O	1:A:2396:LEU:HD23	2.21	0.41
1:A:2433:LYS:NZ	1:A:2472:GLN:OE1	2.50	0.41
1:A:3728:VAL:CG1	1:A:3734:ARG:HD3	2.51	0.41
1:A:865:GLN:H	1:A:865:GLN:HG2	1.73	0.40
1:A:1374:GLN:HE22	1:A:1381:SER:CB	2.33	0.40
1:A:1504:ASP:C	1:A:1506:SER:H	2.30	0.40
1:A:1980:ASN:OD1	1:A:1981:LEU:N	2.49	0.40
1:A:2165:LEU:HD12	1:A:2165:LEU:HA	1.81	0.40
1:A:2211:LEU:HA	1:A:2214:ARG:HG2	2.02	0.40
1:A:2300:PHE:O	1:A:2304:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2466:SER:C	1:A:2468:THR:H	2.27	0.40
1:A:3192:LYS:HE2	1:A:3192:LYS:HB2	1.90	0.40
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.86	0.40
1:A:888:ARG:HB3	1:A:3889:ARG:HH21	1.85	0.40
1:A:1867:ILE:HA	1:A:1870:LYS:HE3	2.03	0.40
1:A:1945:TYR:O	1:A:1949:ILE:HG12	2.21	0.40
1:A:2392:VAL:HG12	1:A:2396:LEU:HD23	2.03	0.40
1:A:3227:ILE:HG22	1:A:3228:SER:N	2.36	0.40
1:A:3521:ILE:HD12	1:A:3521:ILE:HA	1.91	0.40
1:A:3558:ILE:HD13	1:A:3558:ILE:HA	1.96	0.40
1:A:249:PHE:O	1:A:252:VAL:HG12	2.21	0.40
1:A:346:TYR:HB3	1:A:350:ARG:NH1	2.36	0.40
1:A:3153:SER:OG	1:A:3154:GLN:N	2.55	0.40
1:A:165:LYS:HB2	1:A:167:PRO:HD2	2.03	0.40
1:A:1086:TYR:CE2	1:A:1087:ARG:HG3	2.56	0.40
1:A:1575:LEU:HD11	1:A:1617:LYS:HG3	2.03	0.40
1:A:1790:SER:O	1:A:1794:GLN:HG3	2.21	0.40
1:A:2231:PHE:O	1:A:2235:LEU:HD23	2.21	0.40
1:A:2430:GLU:O	1:A:2434:VAL:HG22	2.21	0.40
1:A:2785:ILE:HD12	1:A:2785:ILE:HA	1.96	0.40
1:A:3259:LEU:HD12	1:A:3259:LEU:HA	1.92	0.40
1:A:3756:GLU:HA	1:A:4022:LYS:NZ	2.37	0.40
1:A:3816:LEU:HA	1:A:3816:LEU:HD23	1.86	0.40
1:A:397:LEU:HD22	1:A:437:HIS:HB3	2.03	0.40
1:A:961:LEU:HD23	1:A:961:LEU:HA	1.94	0.40
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.85	0.40
1:A:1597:LEU:HD23	1:A:1597:LEU:HA	1.95	0.40
1:A:3929:MET:HB3	1:A:3929:MET:HE2	1.77	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	3602/4148 (87%)	3293 (91%)	305 (8%)	4 (0%)	48 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3481	SER
1	A	2787	HIS
1	A	3406	ALA
1	A	1968	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3196/3671 (87%)	3185 (100%)	11 (0%)	86 87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2105	HIS
1	A	3477	GLU
1	A	3478	GLU
1	A	3483	MET
1	A	3729	MET
1	A	3733	ARG
1	A	3752	VAL
1	A	3753	LYS
1	A	3806	LEU
1	A	3929	MET
1	A	3940	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN

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Mol	Chain	Res	Type
1	A	484	HIS
1	A	869	ASN
1	A	1083	ASN
1	A	1222	ASN
1	A	1426	GLN
1	A	1457	GLN
1	A	1574	ASN
1	A	1771	GLN
1	A	2091	HIS
1	A	2283	ASN
1	A	2305	ASN
1	A	2351	GLN
1	A	2365	ASN
1	A	2422	GLN
1	A	2514	ASN
1	A	2553	HIS
1	A	2784	GLN
1	A	2954	GLN
1	A	3093	GLN
1	A	3122	HIS
1	A	3139	GLN
1	A	3154	GLN
1	A	3422	GLN
1	A	3470	GLN
1	A	3515	GLN
1	A	3580	ASN
1	A	3787	GLN
1	A	3903	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	KWT	A	6101	-	32,35,35	16.94	12 (37%)	35,57,57	8.69	12 (34%)

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	KWT	A	6101	-	-	0/7/75/75	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	KWT	O5-C19	94.60	3.09	1.37
2	A	6101	KWT	C11-C8	9.40	1.61	1.51
2	A	6101	KWT	C15-C7	5.22	1.59	1.52
2	A	6101	KWT	C5-C4	4.80	1.42	1.34
2	A	6101	KWT	O1-C2	4.51	1.43	1.35
2	A	6101	KWT	C3-C2	4.10	1.58	1.47
2	A	6101	KWT	C8-C7	3.09	1.41	1.35
2	A	6101	KWT	O6-C21	2.77	1.41	1.35
2	A	6101	KWT	C7-C6	2.65	1.54	1.47
2	A	6101	KWT	C23-C1	2.50	1.56	1.50
2	A	6101	KWT	C12-C11	2.44	1.57	1.52
2	A	6101	KWT	C12-C13	2.22	1.57	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	KWT	O5-C19-C3	-37.69	72.73	111.19
2	A	6101	KWT	C19-O5-C5	-25.14	81.37	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	KWT	O5-C5-C4	21.52	123.27	110.22
2	A	6101	KWT	C9-C4-C5	-5.28	117.45	125.96
2	A	6101	KWT	C11-O6-C21	4.11	123.10	117.00
2	A	6101	KWT	C16-C17-C18	-3.60	102.23	105.70
2	A	6101	KWT	C10-C9-C8	-3.47	103.32	108.71
2	A	6101	KWT	C9-C4-C3	-3.10	117.70	124.61
2	A	6101	KWT	C14-C13-C15	2.82	117.25	112.05
2	A	6101	KWT	C14-C13-C18	2.54	109.86	105.18
2	A	6101	KWT	C1-O1-C2	2.49	125.86	119.56
2	A	6101	KWT	C17-C18-C13	2.36	110.91	108.56

There are no chirality outliers.

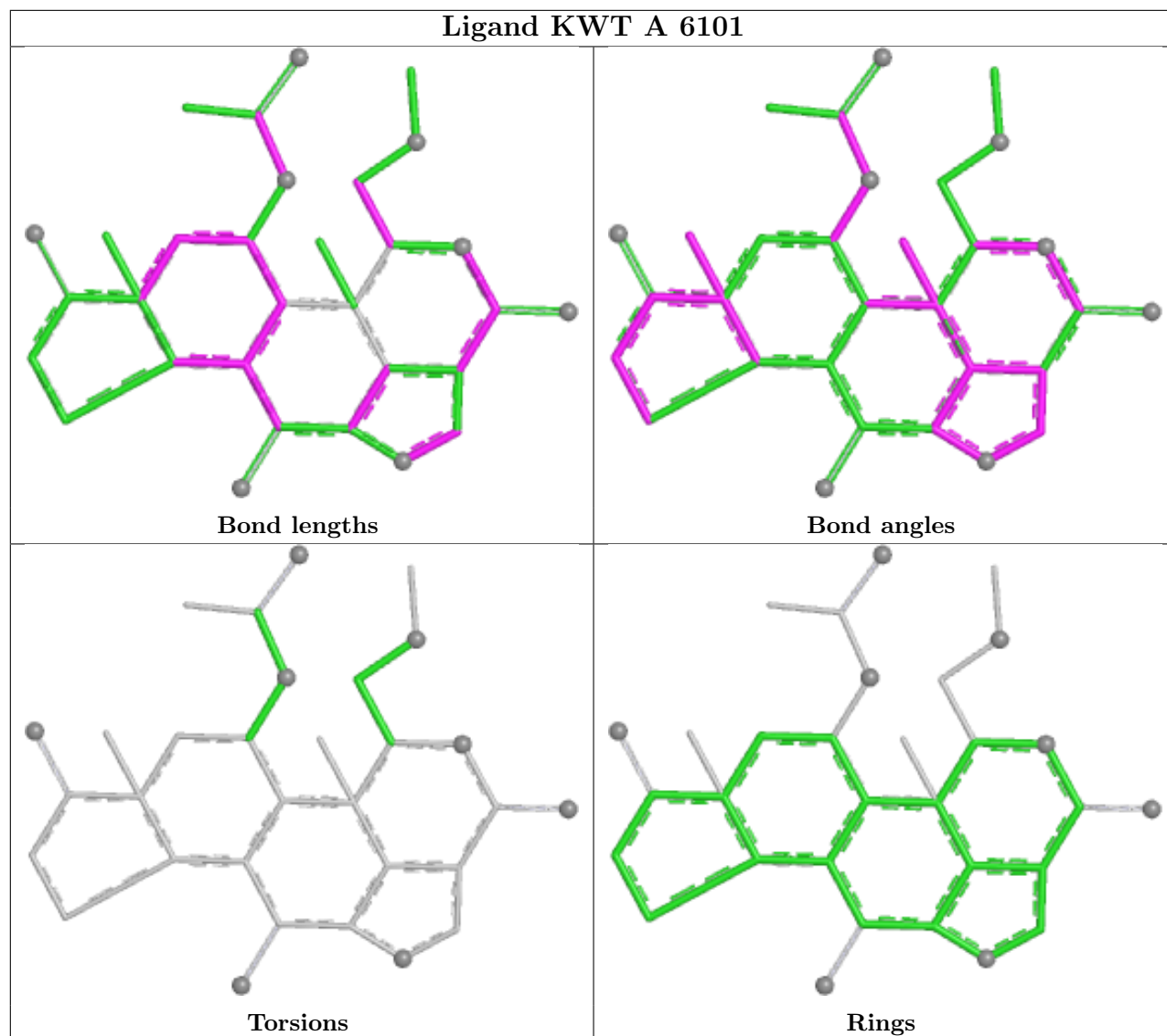
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	KWT	23	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	6001:UNK	N	84.17

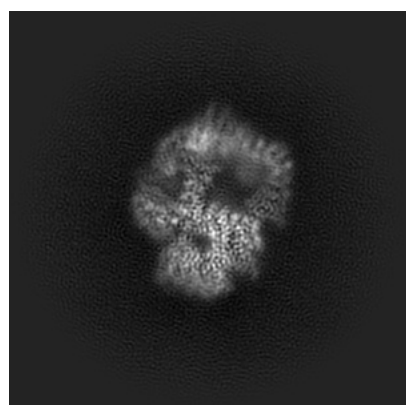
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13067. These allow visual inspection of the internal detail of the map and identification of artifacts.

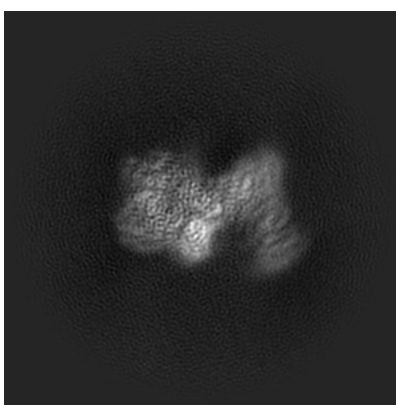
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

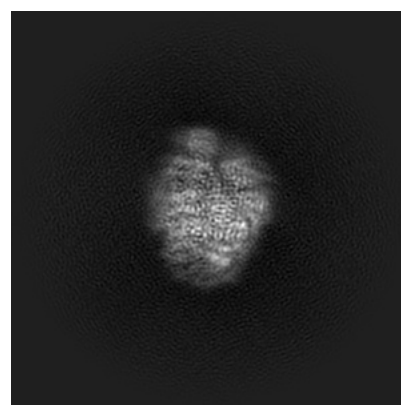
6.1.1 Primary map



X



Y

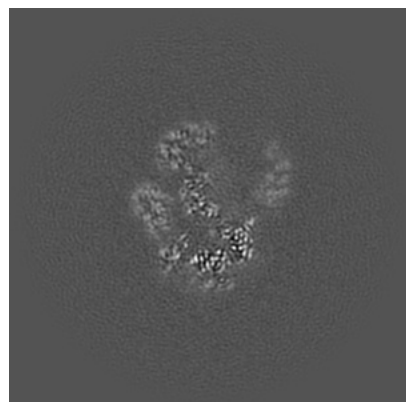


Z

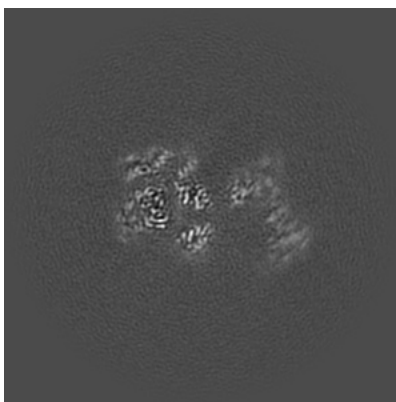
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

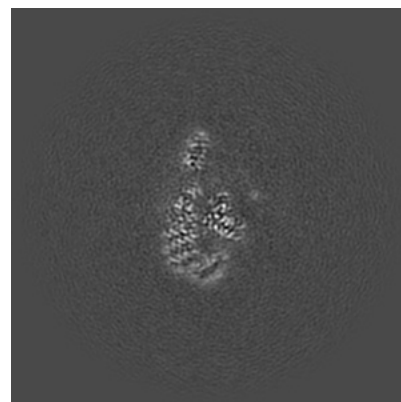
6.2.1 Primary map



X Index: 130



Y Index: 130

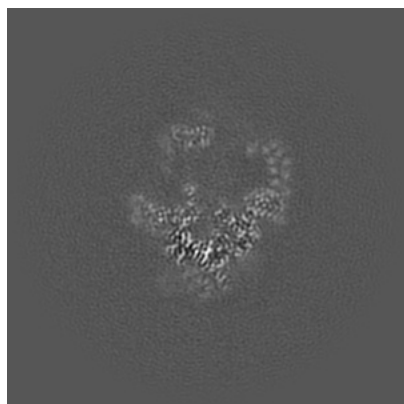


Z Index: 130

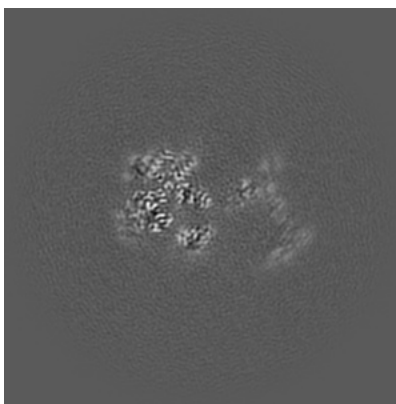
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

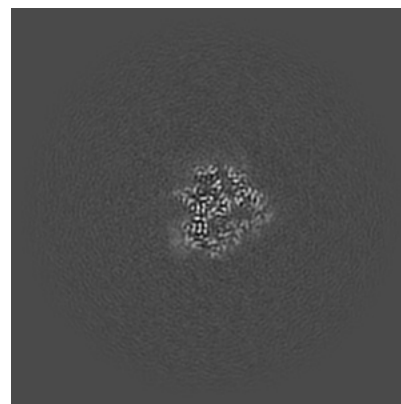
6.3.1 Primary map



X Index: 121



Y Index: 132

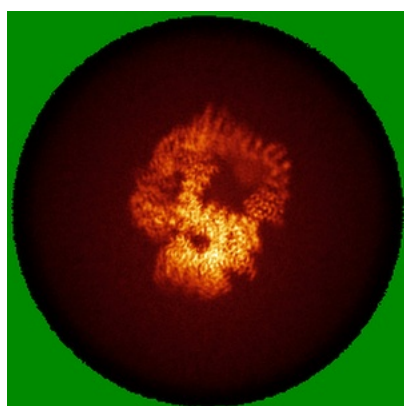


Z Index: 101

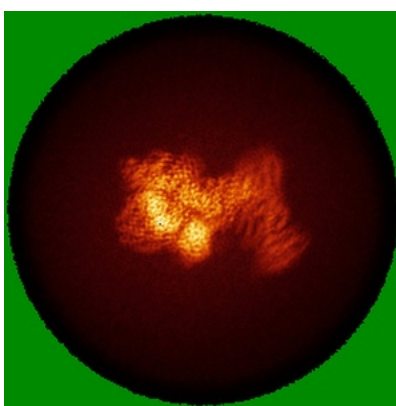
The images above show the largest variance slices of the map in three orthogonal directions.

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

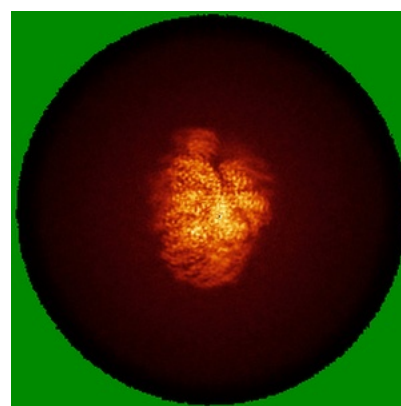
6.4.1 Primary map



X



Y



Z

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

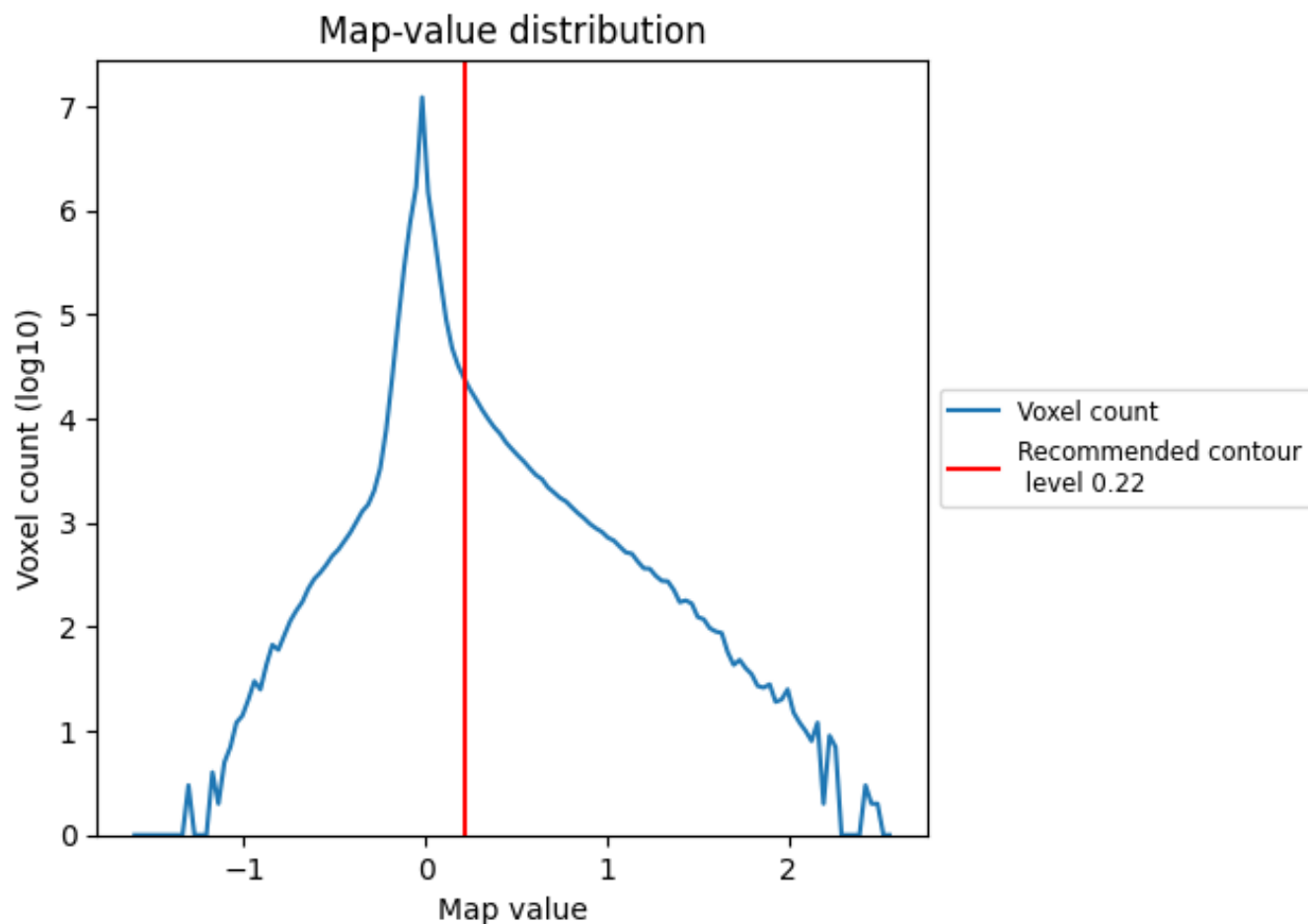
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

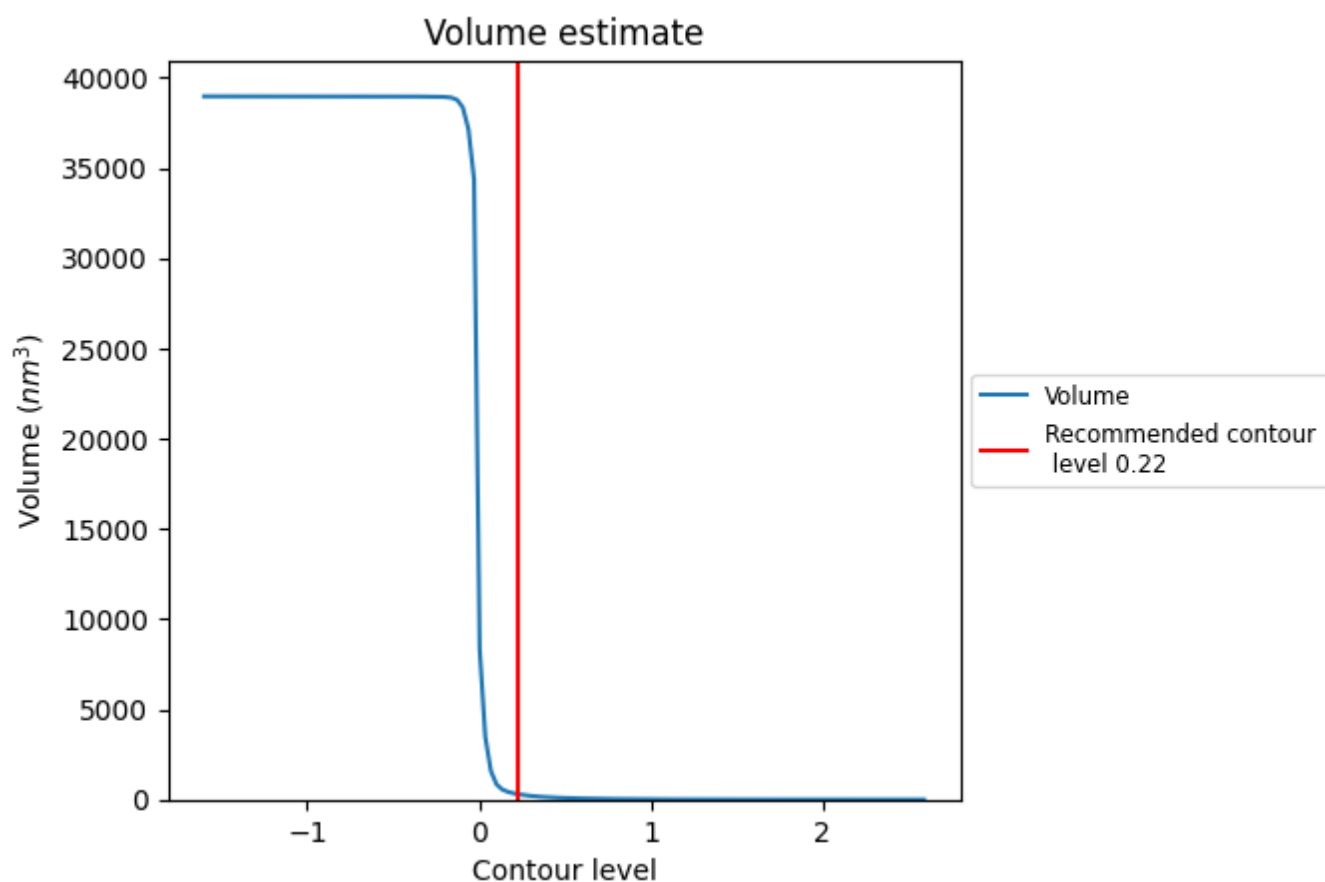
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

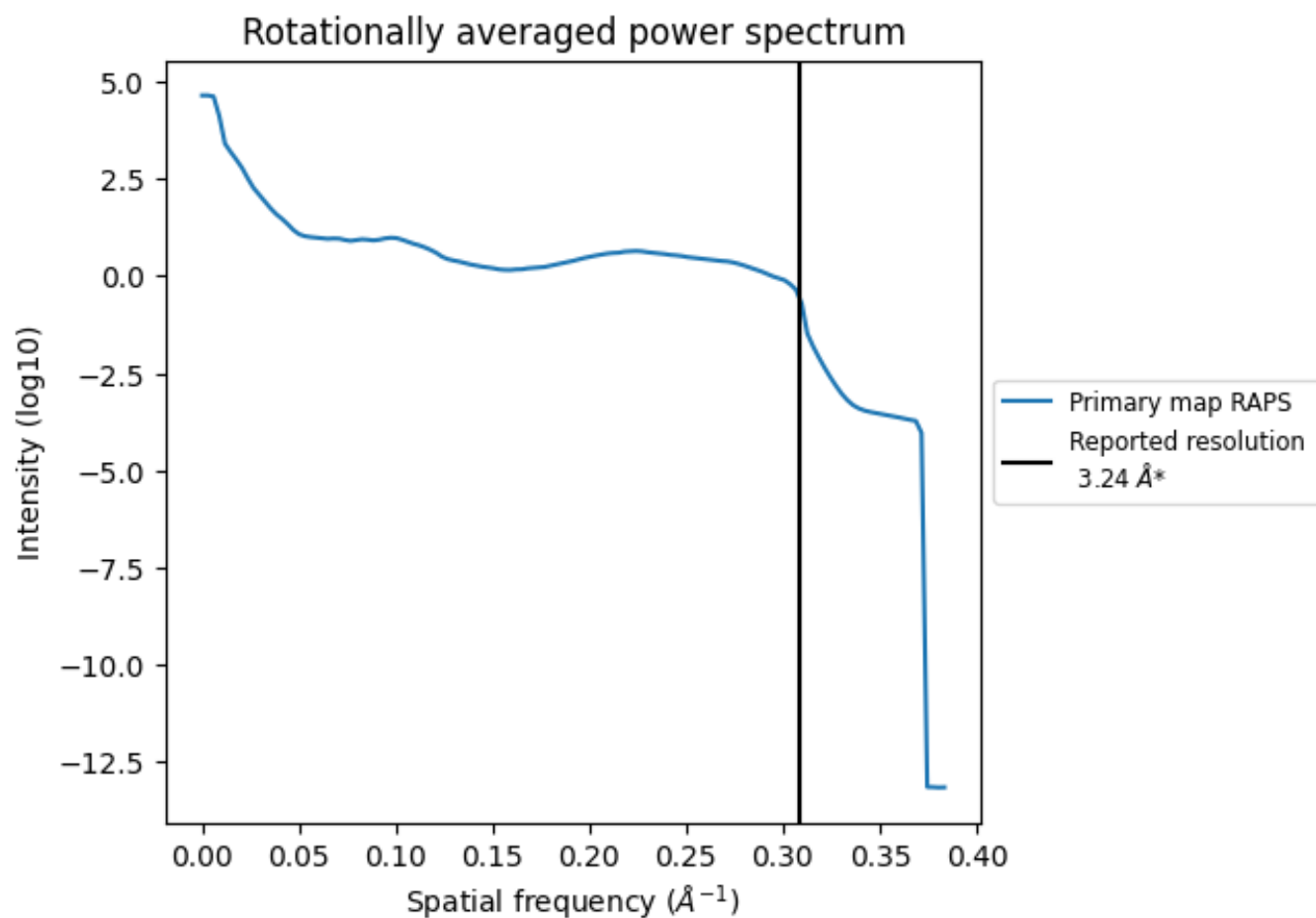
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm³; this corresponds to an approximate mass of 281 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 0.309 Å⁻¹

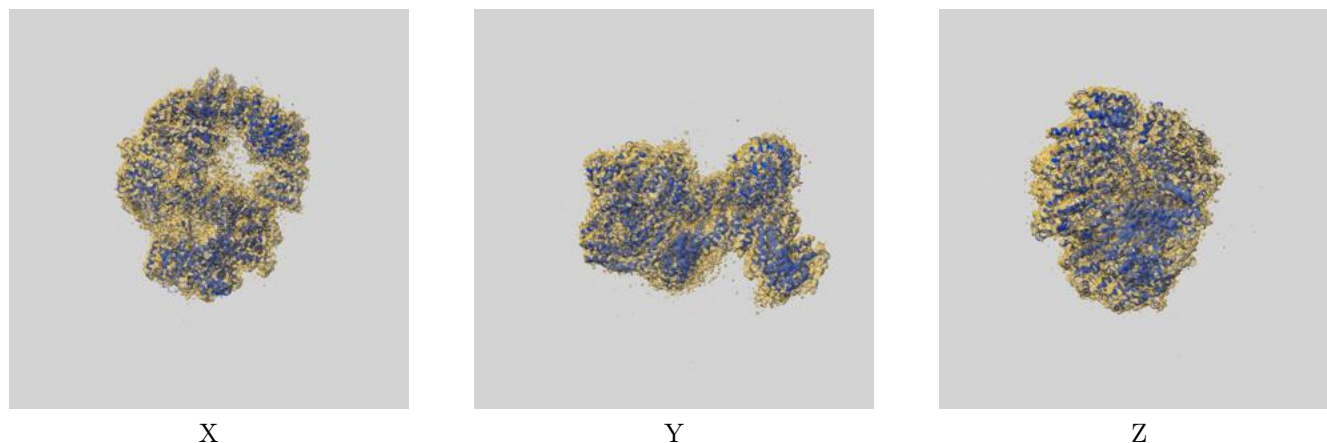
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

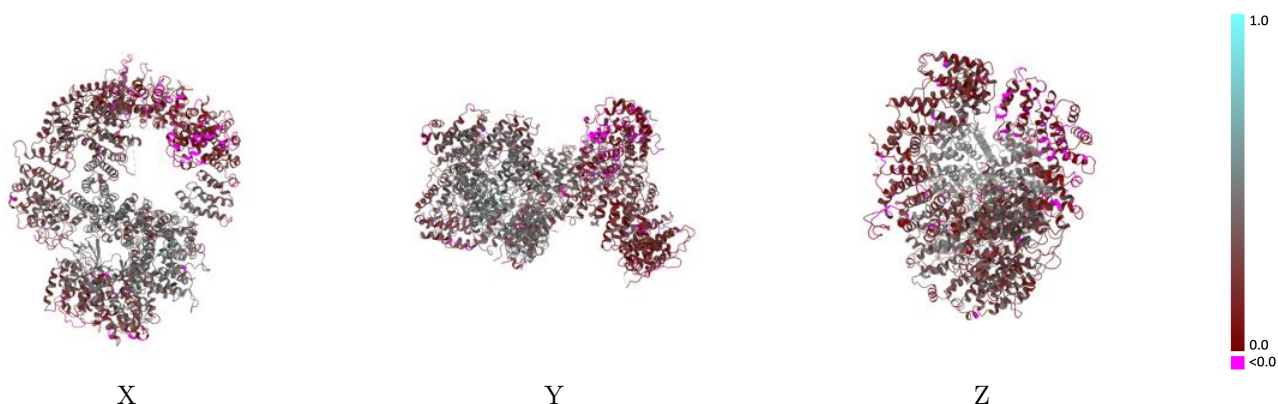
This section contains information regarding the fit between EMDB map EMD-13067 and PDB model 7OTV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



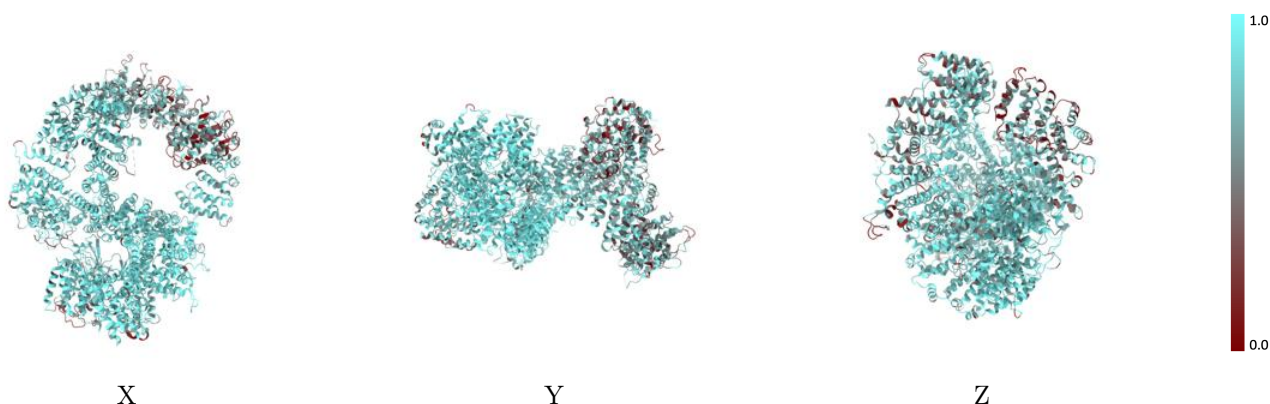
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



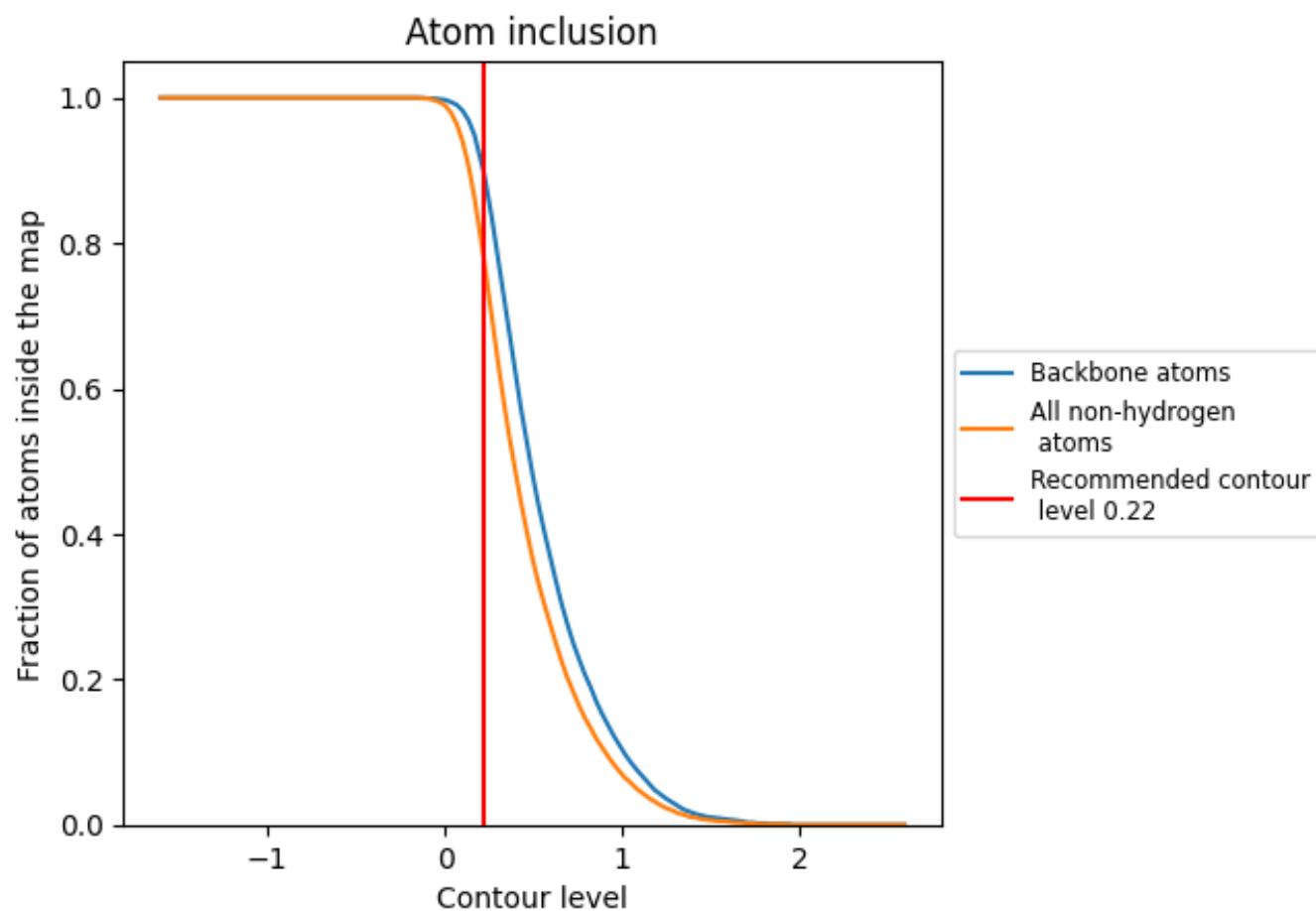
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.3080
A	0.7790	0.3080

