



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:56 PM UTC

PDB ID : 7OTM / pdb_00007otm
EMDB ID : EMD-13062
Title : Cryo-EM structure of DNA-PKcs in complex with NU7441
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 3.33 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

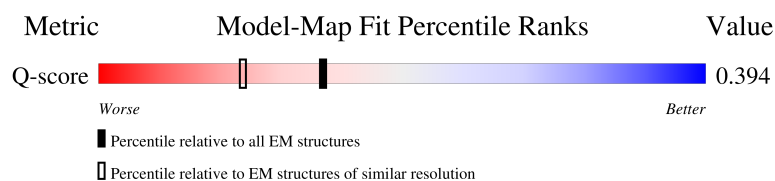
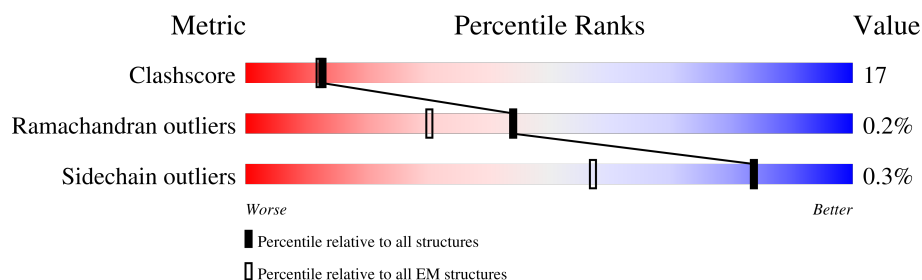
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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	14484 (2.83 - 3.83)

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	

2 Entry composition [i](#)

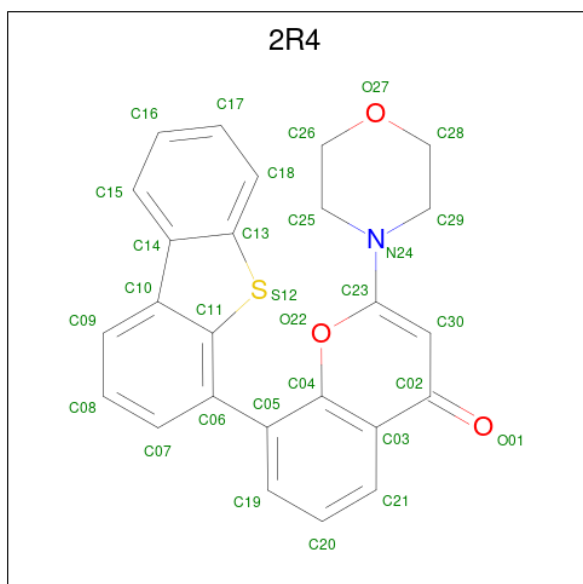
There are 2 unique types of molecules in this entry. The entry contains 29040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-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 8-(dibenzo[b,d]thiophen-4-yl)-2-(morpholin-4-yl)-4H-chromen-4-one (CCD ID: 2R4) (formula: C₂₅H₁₉NO₃S) (labeled as "Ligand of Interest" by depositor).

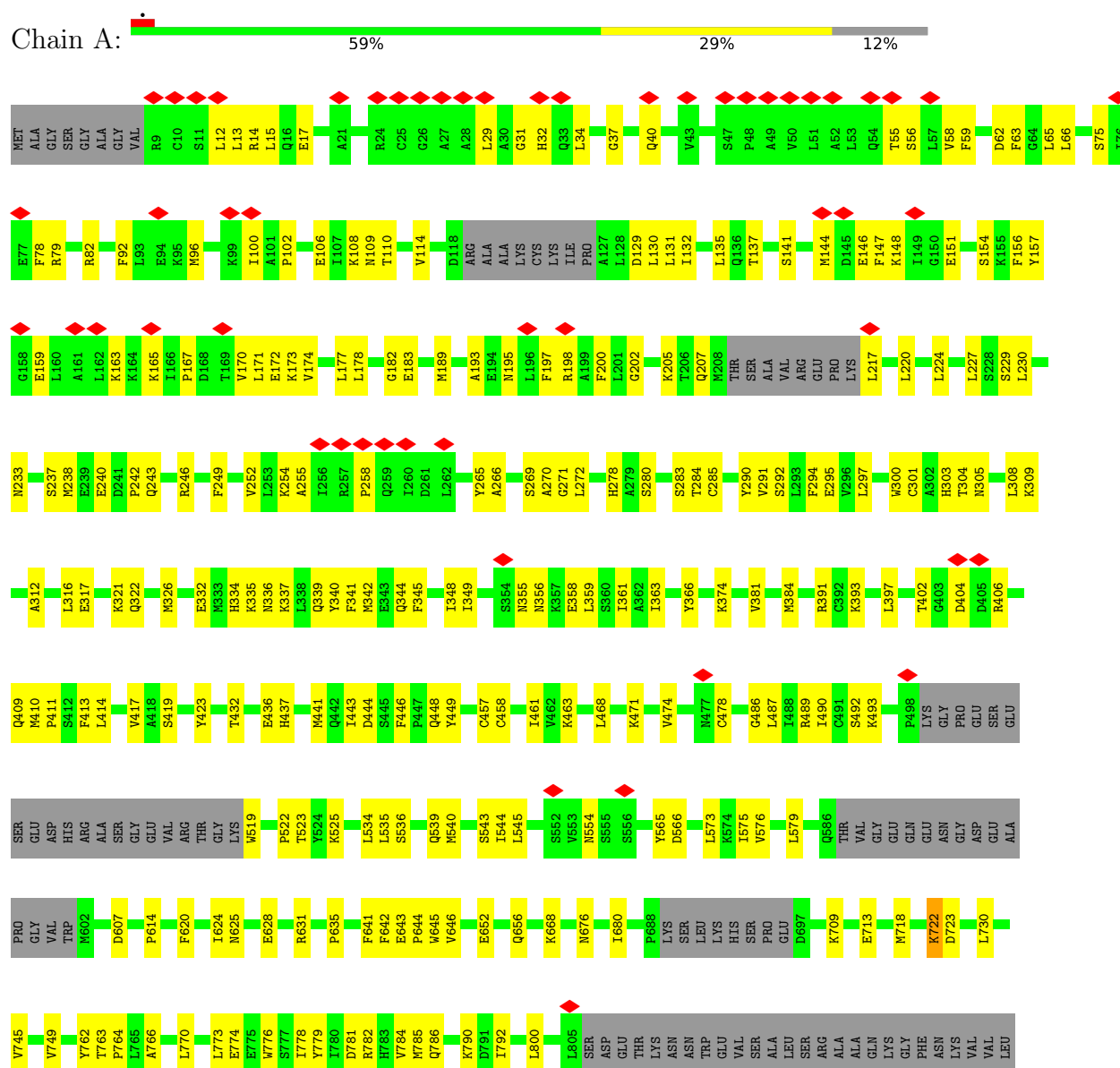


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	30	25	1	3	1	0

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-PKCs



[illegible]



W4038 Y4039 P4040 R4041 Q4042 K4043 L4044 C4045	V3937 L3938 G3939 T3940 F3946 P3954 V3955 P3956 K3959 R3965 L3968 L3972 P3973 K3974 L3979 K3984 R3992 L3997 L3998 K4002 D4003 V4004 R4005 V4006 K4007 P4009 S4010 F4011 D4012 V4013 K4014 Q4018 K4023 G4024 D4025 W4027 L4028 Q4029 E4030 L4031 K4032 V4033 K4034	E3807 N3808 T3809 L3816 K3825 L3829 S3830 D3831 A3834 K3840 L3843 T3844 K3845 R3846 H3850 M3858 Y3859 F3871 R3872 K3873 S3874 E3875 P3876 S3876 D3881 L3882 L3883 F3887 P4008 S4011 D4012 V4013 K4014 Q4018	S3731 L3732 R3733 P3734 T3735 K3736 L3737 L3738 L3739 L3740 H3743 D3744 P3749 F3750 L3751 V3752 K3753 E3756 L3757 R3758 T3759 P3760 D3761 K3681 C3682 V3764 E3765 P3766 L3767 M3771 D3778 S3779 A3780 C3781 L3695 L3699 E3700 P3702 G3703 Q3704 P3711 L3712 H3716 V3717 R3718 G3801 L3802 T3803 E3804 V3905 L3806	S3649 K3650 K3654 D3661 L3662 T3663 K3664 K3665 L3666 L3667 L3668 K3669 K3670 N3671 K3672 K3673 S3674 P3677 L3680 K3681 C3682 V3694 P3695 K3696 K3687 F3690 K3691 V3692 S3693 F3694 L3695 L3699 E3700 P3702 G3703 Q3704 P3711 L3712 H3716 V3717 R3718 G3801 L3802 T3803 E3804 V3905 L3806	V3555 L3558 L3562 S3563 Q3564 G3565 V3567 D3570 A3574 L3575 L3578 D3587 V3588 S3589 V3592 C3593 K3596 K3597 K3598 T3599 P3600 V3601 K3604 K3605 L3606 M3609 K3616 L3617 G3618 A3622 P3623 G3624 L3625 G3626 A3627 F3628 K3629 R3630 L3633 Q3634 L3635 F3636 F3640 K3646	K3449 L3451 L3454 L3463 K3466 L3468 L3469 R3474 L3475 L3483 T3484 L3487 V3490 P3491 C3492 K3493 K3498 V3503 K3504 L3505 V3506 D3509 V3512 A3513 G3514 K3515 L3516 S3517 V3518 T3522 V3525 L3529 V3530 T3531 P3532 F3533 L3534 L3535 F3542 K3543 K3551 K3646
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115505	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 ($e^-/\text{\AA}^2$)	47.3	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	2.057	Depositor
Minimum map value	-0.958	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2R4

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	0.36	0/29502	0.52	8/39893 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3735	PRO	CB-CA-C	9.78	123.75	111.23
1	A	2337	LEU	N-CA-C	6.71	120.82	112.03
1	A	3735	PRO	N-CA-C	-6.38	101.07	111.21
1	A	4024	GLY	N-CA-C	-5.47	106.16	112.50
1	A	1386	ILE	N-CA-C	-5.44	107.55	112.12
1	A	3753	LYS	N-CA-C	-5.32	101.80	110.20
1	A	722	LYS	N-CA-C	5.07	116.01	108.60
1	A	3804	GLU	N-CA-C	5.04	121.53	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29010	0	29195	921	0
2	A	30	0	19	8	0
All	All	29040	0	29214	921	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 17.

All (921) 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:3911:ILE:HD11	1:A:3928:PHE:CE2	1.57	1.37
1:A:2576:MET:HE2	1:A:2787:HIS:CE1	1.63	1.31
1:A:3911:ILE:CD1	1:A:3928:PHE:CE2	2.31	1.13
1:A:3753:LYS:HD3	1:A:3803:ILE:HD11	1.32	1.10
1:A:3804:GLU:HG3	1:A:3804:GLU:O	1.53	1.03
1:A:3911:ILE:CD1	1:A:3928:PHE:HE2	1.71	0.99
1:A:3911:ILE:HD11	1:A:3928:PHE:HE2	0.84	0.98
1:A:3809:THR:HB	1:A:3929:MET:HE3	1.42	0.97
1:A:3804:GLU:O	1:A:3804:GLU:CG	2.10	0.97
1:A:3729:MET:HE3	1:A:3731:SER:HB2	1.47	0.95
1:A:3929:MET:HB2	1:A:3938:ILE:HB	1.50	0.94
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.42	0.92
1:A:2576:MET:HE2	1:A:2787:HIS:HE1	1.27	0.92
1:A:3753:LYS:CD	1:A:3803:ILE:HD11	2.00	0.91
1:A:147:PHE:O	1:A:151:GLU:HB2	1.72	0.89
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	1.58	0.86
1:A:3753:LYS:HG2	1:A:3803:ILE:CD1	2.06	0.85
1:A:999:LYS:HG3	1:A:1000:LYS:HG2	1.58	0.84
1:A:3806:LEU:HD12	1:A:3938:ILE:HD13	1.58	0.84
1:A:3809:THR:HB	1:A:3929:MET:CE	2.08	0.84
1:A:3793:VAL:HG22	1:A:3803:ILE:HG22	1.61	0.83
1:A:3506:LEU:HD11	1:A:3518:VAL:HG21	1.62	0.81
1:A:3578:LEU:O	1:A:3736:LYS:NZ	2.13	0.81
1:A:3670:MET:O	1:A:3674:SER:HB3	1.82	0.79
1:A:536:SER:O	1:A:539:GLN:NE2	2.15	0.79
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.55	0.79
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.16	0.79
1:A:1407:LYS:HB2	1:A:1463:LEU:HD21	1.65	0.78
1:A:3844:THR:HG22	1:A:3850:HIS:HB3	1.65	0.78
1:A:1175:HIS:HB3	1:A:1178:ARG:HE	1.48	0.78
1:A:3503:VAL:HA	1:A:3506:LEU:HD13	1.66	0.77
1:A:272:LEU:HD11	1:A:312:ALA:HA	1.68	0.76
1:A:131:LEU:HD13	1:A:173:LYS:HB2	1.68	0.76
1:A:1684:LEU:HB2	1:A:1689:LYS:HE3	1.68	0.75
1:A:4081:ALA:O	1:A:4090:ARG:NH1	2.19	0.75
1:A:2482:ASP:OD1	1:A:2485:ARG:NH2	2.19	0.75
1:A:1298:LEU:O	1:A:1370:ARG:NH2	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2576:MET:CE	1:A:2787:HIS:CE1	2.59	0.75
1:A:1097:GLU:OE2	1:A:1151:ARG:NH2	2.18	0.74
1:A:3753:LYS:HG2	1:A:3803:ILE:HD13	1.68	0.74
1:A:356:ASN:ND2	1:A:404:ASP:O	2.22	0.73
1:A:3998:LEU:HG	1:A:4002:MET:HE3	1.69	0.73
1:A:774:GLU:HG2	1:A:858:MET:HE1	1.70	0.73
1:A:917:LEU:O	1:A:921:ALA:HB2	1.89	0.73
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.20	0.72
1:A:2171:LEU:O	1:A:2177:ASN:ND2	2.22	0.72
1:A:2493:ASN:HA	1:A:2496:GLN:HE22	1.54	0.72
1:A:1727:ARG:NH2	1:A:1771:GLN:O	2.23	0.71
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.22	0.71
1:A:147:PHE:O	1:A:151:GLU:CB	2.39	0.71
1:A:3469:LEU:HD12	1:A:3505:LEU:HD21	1.73	0.71
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.71	0.71
1:A:280:SER:O	1:A:283:SER:OG	2.07	0.71
1:A:2260:PHE:HA	1:A:2270:ASN:HA	1.71	0.71
1:A:463:LYS:HD3	1:A:545:LEU:HD22	1.73	0.71
1:A:2575:PRO:HB2	1:A:2784:GLN:HB3	1.73	0.71
1:A:3763:ARG:HH12	1:A:4008:GLU:HG2	1.56	0.71
1:A:3587:ASP:OD2	1:A:3733:ARG:NH2	2.22	0.70
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.25	0.70
1:A:631:ARG:HH22	1:A:668:LYS:HD2	1.56	0.70
1:A:2518:GLN:HE22	1:A:2522:ARG:HD3	1.57	0.70
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.73	0.70
1:A:1828:LEU:O	1:A:1883:ARG:NH2	2.25	0.70
1:A:446:PHE:HD1	1:A:457:CYS:HG	1.40	0.70
1:A:2133:LEU:HB2	1:A:2146:LEU:HD23	1.73	0.70
1:A:2347:LYS:O	1:A:2351:GLN:NE2	2.24	0.70
1:A:3646:LYS:H	1:A:3650:LYS:HB3	1.57	0.70
1:A:3859:TYR:HE1	1:A:4119:ARG:HB2	1.55	0.70
1:A:3729:MET:HB3	2:A:6101:2R4:C18	2.22	0.69
1:A:2330:VAL:HG11	1:A:2337:LEU:HD11	1.74	0.69
1:A:2432:GLN:OE1	1:A:2464:HIS:NE2	2.25	0.69
1:A:2786:LYS:O	1:A:2789:SER:N	2.24	0.69
1:A:1758:LEU:HD23	1:A:1761:LEU:HD12	1.75	0.69
1:A:2330:VAL:CG1	1:A:2337:LEU:HD11	2.23	0.68
1:A:3846:MET:SD	1:A:3858:MET:HG2	2.34	0.68
1:A:2223:VAL:HG11	1:A:2238:ILE:HD11	1.75	0.67
1:A:3809:THR:CB	1:A:3929:MET:CE	2.72	0.67
1:A:3361:GLU:O	1:A:3367:SER:OG	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3911:ILE:HD12	1:A:3928:PHE:CE2	2.29	0.67
1:A:356:ASN:HD22	1:A:404:ASP:HB3	1.60	0.67
1:A:2347:LYS:HG2	1:A:2351:GLN:HE22	1.58	0.67
1:A:2839:ASP:OD1	1:A:2842:ARG:NH2	2.28	0.67
1:A:4050:LYS:HE3	1:A:4059:ILE:HG21	1.75	0.67
1:A:461:ILE:HG23	1:A:534:LEU:HD21	1.77	0.67
1:A:2123:PRO:HD2	1:A:2126:MET:HE2	1.76	0.67
1:A:2216:LEU:HD22	1:A:2249:LEU:HD23	1.75	0.67
1:A:3626:GLY:O	1:A:3630:ARG:HB2	1.95	0.67
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.61	0.66
1:A:3134:ALA:HB2	1:A:3182:ILE:HG22	1.77	0.66
1:A:917:LEU:O	1:A:921:ALA:CB	2.42	0.66
1:A:3341:LEU:HD11	1:A:3360:LEU:HD21	1.78	0.66
1:A:3791:TYR:HB2	1:A:3804:GLU:HG2	1.78	0.66
1:A:3012:GLU:HG3	1:A:3013:TYR:N	2.11	0.66
1:A:1657:SER:HB3	1:A:1659:VAL:HG13	1.78	0.65
1:A:2796:ALA:O	1:A:2800:ARG:NH1	2.30	0.65
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.78	0.65
1:A:1257:LEU:HD12	1:A:1337:VAL:HG21	1.77	0.65
1:A:1817:GLN:OE1	1:A:1875:LYS:NZ	2.29	0.65
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	1.78	0.65
1:A:154:SER:HA	1:A:157:TYR:HD2	1.62	0.64
1:A:355:ASN:HB3	1:A:358:GLU:HG2	1.80	0.64
1:A:2424:MET:HE1	1:A:2439:ILE:HD11	1.79	0.64
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.30	0.64
1:A:3757:ASP:OD2	1:A:3759:ARG:NH1	2.29	0.64
1:A:1977:ILE:HG13	1:A:1979:GLU:H	1.61	0.64
1:A:1268:ASN:ND2	1:A:1343:GLU:OE2	2.30	0.64
1:A:1075:ARG:NH1	1:A:1117:ASP:OD2	2.22	0.64
1:A:1185:HIS:NE2	1:A:1265:GLU:OE2	2.28	0.64
1:A:1920:TYR:O	1:A:1924:THR:CB	2.46	0.64
1:A:2540:LEU:HD11	1:A:2832:ILE:HG23	1.79	0.64
1:A:2576:MET:O	1:A:2576:MET:HG3	1.98	0.64
1:A:709:LYS:O	1:A:713:GLU:HG2	1.98	0.64
1:A:2304:VAL:HG22	1:A:2323:LEU:HD21	1.79	0.64
1:A:2522:ARG:NH1	1:A:2564:GLU:OE1	2.31	0.64
1:A:566:ASP:OD1	1:A:645:TRP:NE1	2.23	0.63
1:A:3685:PRO:HG2	1:A:3687:MET:HB2	1.81	0.63
1:A:1751:GLU:O	1:A:1788:ARG:NH1	2.31	0.63
1:A:2349:LEU:HA	1:A:2352:HIS:CE1	2.34	0.63
1:A:2185:MET:O	1:A:2189:ILE:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1479:VAL:HG21	1:A:1524:LEU:HD11	1.80	0.62
1:A:3316:LEU:HD12	1:A:3323:PHE:HD1	1.65	0.62
1:A:1397:ASP:OD1	1:A:1460:ARG:NH2	2.32	0.62
1:A:3281:CYS:HB2	1:A:3329:LEU:HD23	1.82	0.62
1:A:1568:ASN:ND2	1:A:1603:GLN:OE1	2.31	0.62
1:A:1949:ILE:HD12	1:A:2100:LEU:HD22	1.80	0.62
1:A:2168:LEU:HD23	1:A:2193:ILE:HD11	1.82	0.62
1:A:4014:LYS:O	1:A:4018:GLN:NE2	2.32	0.62
1:A:2398:LEU:HD12	1:A:2431:ARG:HG3	1.80	0.62
1:A:3791:TYR:CB	1:A:3804:GLU:HG2	2.30	0.62
1:A:1365:ASN:HA	1:A:1368:LEU:HB2	1.80	0.62
1:A:2279:ILE:O	1:A:2283:ASN:ND2	2.31	0.62
1:A:2452:ARG:O	1:A:2452:ARG:NH1	2.33	0.62
1:A:3058:ASP:O	1:A:3059:GLN:NE2	2.33	0.62
1:A:3145:ILE:HD11	1:A:3196:LYS:HD2	1.80	0.62
1:A:3753:LYS:CG	1:A:3803:ILE:CD1	2.76	0.62
1:A:2239:LYS:HB3	1:A:2279:ILE:HD12	1.81	0.62
1:A:2519:LEU:O	1:A:2523:ASN:ND2	2.33	0.62
1:A:3506:LEU:HD21	1:A:3518:VAL:HG11	1.82	0.62
1:A:3685:PRO:HB2	1:A:3687:MET:H	1.65	0.62
1:A:3831:ASP:HB3	1:A:3834:ALA:HB2	1.82	0.61
1:A:1432:CYS:HB2	1:A:1486:LEU:HD11	1.81	0.61
1:A:444:ASP:OD2	1:A:489:ARG:NE	2.29	0.61
1:A:1975:LEU:HD12	1:A:1976:LEU:HG	1.81	0.61
1:A:1202:ARG:CZ	1:A:1207:TRP:HA	2.31	0.61
1:A:3366:SER:OG	1:A:3368:GLU:OE2	2.18	0.61
1:A:305:ASN:HB3	1:A:308:LEU:HB3	1.82	0.61
1:A:3416:LEU:HD23	1:A:3449:LYS:HG3	1.83	0.61
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.73	0.61
1:A:3622:ALA:HB1	1:A:3623:PRO:HD2	1.83	0.61
1:A:3670:MET:O	1:A:3674:SER:CB	2.48	0.61
1:A:943:GLY:HA3	1:A:2577:PHE:CE1	2.34	0.61
1:A:1251:GLN:HB3	1:A:1254:LEU:HD12	1.82	0.60
1:A:1810:PRO:HA	1:A:1816:ARG:HH12	1.65	0.60
1:A:2330:VAL:HG11	1:A:2337:LEU:CD1	2.31	0.60
1:A:1118:GLU:HG3	1:A:1120:SER:H	1.66	0.60
1:A:1134:LEU:O	1:A:1138:ILE:HD12	2.01	0.60
1:A:1175:HIS:HB3	1:A:1178:ARG:NE	2.16	0.60
1:A:6012:UNK:O	1:A:6016:UNK:N	2.34	0.60
1:A:1079:SER:HA	1:A:1107:TYR:HE1	1.67	0.60
1:A:1770:GLN:HB3	1:A:1814:PHE:HZ	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1755:SER:OG	1:A:1758:LEU:HB2	2.01	0.60
1:A:3493:TRP:CG	1:A:3711:PRO:HB3	2.37	0.60
1:A:1603:GLN:HG3	1:A:1606:ARG:NH2	2.17	0.60
1:A:2328:ARG:HH21	1:A:2371:PHE:HD1	1.50	0.60
1:A:2365:ASN:ND2	1:A:2396:LEU:O	2.35	0.60
1:A:3530:VAL:O	1:A:3534:ILE:HG13	2.02	0.59
1:A:3797:THR:HG22	1:A:3798:SER:H	1.66	0.59
1:A:1011:GLU:OE1	1:A:1032:CYS:HB3	2.02	0.59
1:A:1066:LEU:HB2	1:A:1078:ALA:HB2	1.83	0.59
1:A:165:LYS:HB2	1:A:167:PRO:HD2	1.83	0.59
1:A:3737:ARG:HG3	1:A:3750:PHE:O	2.02	0.59
1:A:1867:ILE:HA	1:A:1870:LYS:HE3	1.85	0.59
1:A:3378:TYR:OH	1:A:3426:LYS:NZ	2.36	0.59
1:A:355:ASN:OD1	1:A:356:ASN:N	2.34	0.59
1:A:1224:PHE:HD2	1:A:1267:TYR:HE1	1.51	0.59
1:A:614:PRO:HB3	1:A:620:PHE:CD1	2.37	0.59
1:A:1702:LEU:O	1:A:1707:LEU:HB2	2.03	0.59
1:A:1820:VAL:O	1:A:1825:LEU:HD23	2.03	0.59
1:A:1868:THR:HA	1:A:1871:MET:HE2	1.84	0.59
1:A:2298:GLU:OE1	1:A:2301:GLN:NE2	2.33	0.59
1:A:2389:PHE:CD2	1:A:2393:LEU:HB2	2.38	0.59
1:A:3686:TRP:HZ3	1:A:3690:PHE:HD1	1.50	0.59
1:A:1786:ALA:HB2	1:A:1827:LEU:HD23	1.85	0.58
1:A:2474:TYR:O	1:A:2478:MET:HG3	2.03	0.58
1:A:3450:MET:HE2	1:A:3468:LEU:HD11	1.85	0.58
1:A:3751:LEU:HB3	1:A:3803:ILE:HG12	1.85	0.58
1:A:3825:LYS:O	1:A:3829:LEU:HG	2.04	0.58
1:A:301:CYS:O	1:A:309:LYS:NZ	2.34	0.58
1:A:1372:LEU:HD11	1:A:1402:LEU:HD11	1.84	0.58
1:A:3758:LEU:HD12	1:A:3801:GLY:HA3	1.84	0.58
1:A:1080:LEU:O	1:A:1084:ASN:ND2	2.35	0.58
1:A:2786:LYS:NZ	1:A:2788:SER:OG	2.36	0.58
1:A:3805:TRP:HZ3	2:A:6101:2R4:C09	2.16	0.58
1:A:652:GLU:O	1:A:656:GLN:HG2	2.04	0.58
1:A:1811:ARG:HH11	1:A:1816:ARG:HH11	1.51	0.58
1:A:554:ASN:HB2	1:A:1549:SER:HB3	1.85	0.58
1:A:2843:PHE:O	1:A:2847:THR:OG1	2.13	0.58
1:A:159:GLU:O	1:A:163:LYS:HG2	2.03	0.58
1:A:2183:HIS:CE1	1:A:2185:MET:HB2	2.38	0.58
1:A:2274:ILE:HG23	1:A:2322:VAL:HG21	1.85	0.57
1:A:2425:ARG:HE	1:A:2457:PRO:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:VAL:HG13	1:A:2473:MET:HE1	1.85	0.57
1:A:3313:SER:HA	1:A:3316:LEU:HB2	1.84	0.57
1:A:2817:LEU:HD13	1:A:2820:MET:HE3	1.86	0.57
1:A:3295:GLU:OE2	1:A:3295:GLU:N	2.31	0.57
1:A:4012:ASP:OD1	1:A:4013:TRP:N	2.37	0.57
1:A:1102:GLU:OE2	1:A:1152:ARG:NE	2.38	0.57
1:A:2318:ALA:O	1:A:2322:VAL:HG23	2.04	0.57
1:A:3806:LEU:CD1	1:A:3938:ILE:HD13	2.33	0.57
1:A:322:GLN:O	1:A:326:MET:HG2	2.04	0.57
1:A:2412:TYR:HA	1:A:2415:LEU:HB2	1.87	0.57
1:A:3522:THR:OG1	1:A:3558:ILE:HD11	2.05	0.57
1:A:2478:MET:HE3	1:A:2524:PHE:CD1	2.39	0.57
1:A:2088:LEU:HA	1:A:2094:MET:HG2	1.86	0.57
1:A:2124:SER:HA	1:A:2127:LYS:HB2	1.85	0.57
1:A:2828:GLU:O	1:A:2832:ILE:HG12	2.05	0.57
1:A:4027:TRP:HE3	1:A:4030:GLU:HB3	1.69	0.57
1:A:1733:THR:O	1:A:1737:ASN:ND2	2.38	0.57
1:A:2973:ASP:O	1:A:2977:ASN:ND2	2.38	0.56
1:A:3771:MET:HE1	1:A:3914:SER:HB3	1.86	0.56
1:A:109:ASN:OD1	1:A:110:THR:N	2.37	0.56
1:A:1365:ASN:O	1:A:1369:MET:HG2	2.04	0.56
1:A:79:ARG:HA	1:A:82:ARG:HB2	1.87	0.56
1:A:1424:THR:HG23	1:A:1427:SER:H	1.70	0.56
1:A:1762:MET:HA	1:A:1762:MET:HE2	1.87	0.56
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.39	0.56
1:A:2477:LEU:HD23	1:A:2480:ILE:HD12	1.87	0.56
1:A:3575:LEU:HD12	1:A:3796:MET:HE1	1.86	0.56
1:A:3722:PHE:CD1	1:A:3740:ILE:HG12	2.41	0.56
1:A:3763:ARG:HG3	1:A:4011:PHE:HZ	1.70	0.56
1:A:3923:ARG:HD3	1:A:3928:PHE:HE1	1.69	0.56
1:A:238:MET:HE1	1:A:284:THR:H	1.70	0.56
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.06	0.56
1:A:776:TRP:HE3	1:A:785:MET:HE1	1.71	0.56
1:A:2470:ARG:NH1	1:A:2513:GLU:OE2	2.39	0.56
1:A:3622:ALA:HB3	1:A:3625:LEU:HD11	1.87	0.56
1:A:1652:ILE:O	1:A:1655:ILE:HG22	2.06	0.56
1:A:535:LEU:HD11	1:A:565:TYR:HD1	1.71	0.56
1:A:898:PHE:HB2	1:A:901:MET:O	2.06	0.56
1:A:2327:LEU:HA	1:A:2330:VAL:HG22	1.86	0.56
1:A:2576:MET:CE	1:A:2787:HIS:HE1	2.11	0.56
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3484:THR:HG22	1:A:3513:ALA:HB2	1.88	0.55
1:A:56:SER:HA	1:A:59:PHE:CD2	2.40	0.55
1:A:1173:LEU:HA	1:A:1176:CYS:SG	2.46	0.55
1:A:1370:ARG:HD2	1:A:1371:VAL:N	2.21	0.55
1:A:1864:ASP:O	1:A:1868:THR:OG1	2.18	0.55
1:A:1871:MET:HA	1:A:1874:TYR:HD2	1.70	0.55
1:A:2257:PHE:CE1	1:A:2261:SER:HB2	2.41	0.55
1:A:3027:LEU:HA	1:A:3030:ILE:HG22	1.88	0.55
1:A:3285:HIS:HD2	1:A:3298:LEU:HD11	1.71	0.55
1:A:3753:LYS:CG	1:A:3803:ILE:HD11	2.36	0.55
1:A:3574:ALA:HB1	1:A:3687:MET:HG3	1.86	0.55
1:A:290:TYR:CE2	1:A:291:VAL:HG13	2.41	0.55
1:A:291:VAL:HG12	1:A:340:TYR:CE2	2.41	0.55
1:A:358:GLU:HA	1:A:361:ILE:HD12	1.89	0.55
1:A:1224:PHE:HD2	1:A:1267:TYR:CE1	2.25	0.55
1:A:2129:LEU:HB3	1:A:2146:LEU:HD21	1.88	0.55
1:A:3646:LYS:N	1:A:3650:LYS:HB3	2.22	0.55
1:A:1342:MET:O	1:A:1345:THR:OG1	2.21	0.55
1:A:3353:GLU:O	1:A:3356:ALA:N	2.27	0.55
1:A:2194:LEU:HD11	1:A:2241:LEU:HA	1.89	0.55
1:A:781:ASP:HB3	1:A:784:VAL:HG23	1.88	0.55
1:A:3843:LEU:HD22	1:A:3858:MET:HG3	1.89	0.55
1:A:2785:ILE:O	1:A:2789:SER:HB2	2.07	0.55
1:A:339:GLN:HA	1:A:342:MET:HG3	1.89	0.54
1:A:2129:LEU:HD12	1:A:2146:LEU:HD13	1.87	0.54
1:A:2486:ASP:HB3	1:A:2489:SER:HB2	1.88	0.54
1:A:59:PHE:HA	1:A:62:ASP:HB2	1.88	0.54
1:A:3681:LYS:NZ	1:A:3723:ASP:O	2.37	0.54
1:A:3722:PHE:HD1	1:A:3740:ILE:HG12	1.71	0.54
1:A:254:LYS:HZ2	1:A:271:GLY:HA3	1.72	0.54
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.90	0.54
1:A:1825:LEU:HD12	1:A:1879:VAL:HG21	1.89	0.54
1:A:2471:GLU:HA	1:A:2517:LEU:HD11	1.89	0.54
1:A:2824:LYS:HB3	1:A:2828:GLU:HG3	1.90	0.54
1:A:3451:LEU:HD12	1:A:3454:LEU:HD12	1.90	0.54
1:A:1014:LEU:HD13	1:A:1025:LEU:HD21	1.90	0.54
1:A:1596:VAL:HG12	1:A:1600:MET:HE2	1.90	0.54
1:A:1795:VAL:HA	1:A:1798:LEU:HD12	1.90	0.54
1:A:2446:LEU:HD21	1:A:2454:LEU:HD12	1.89	0.54
1:A:3293:CYS:O	1:A:3297:VAL:HG23	2.06	0.54
1:A:3929:MET:O	1:A:3937:VAL:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:O	1:A:96:MET:HG3	2.08	0.54
1:A:238:MET:HE1	1:A:285:CYS:H	1.72	0.54
1:A:2542:LEU:HD21	1:A:2558:ALA:HA	1.90	0.54
1:A:3269:ARG:C	1:A:3271:ASP:H	2.16	0.54
1:A:3792:SER:N	1:A:3804:GLU:HB3	2.22	0.54
1:A:3805:TRP:CZ3	2:A:6101:2R4:C09	2.91	0.54
1:A:943:GLY:HA3	1:A:2577:PHE:CZ	2.43	0.54
1:A:1848:ILE:HG21	1:A:1911:LEU:HD11	1.88	0.54
1:A:3033:GLU:HG3	1:A:3034:PRO:HD3	1.90	0.54
1:A:3281:CYS:SG	1:A:3301:LEU:HD11	2.48	0.54
1:A:63:PHE:HD1	1:A:66:LEU:HD12	1.73	0.53
1:A:2232:ARG:HA	1:A:2235:LEU:HD12	1.90	0.53
1:A:2349:LEU:HA	1:A:2352:HIS:HE1	1.71	0.53
1:A:195:ASN:O	1:A:198:ARG:HG3	2.08	0.53
1:A:2104:MET:HA	1:A:2107:SER:HB3	1.90	0.53
1:A:4060:THR:O	1:A:4064:LEU:HD23	2.08	0.53
1:A:410:MET:HB3	1:A:411:PRO:HD3	1.90	0.53
1:A:1611:GLN:HB3	1:A:1614:GLN:HB3	1.91	0.53
1:A:3344:GLU:OE2	1:A:3348:LEU:HD23	2.07	0.53
1:A:3687:MET:HE3	1:A:3722:PHE:CG	2.44	0.53
1:A:3687:MET:HE3	1:A:3722:PHE:CD1	2.44	0.53
1:A:1863:PHE:HA	1:A:1866:GLN:OE1	2.08	0.53
1:A:2577:PHE:HD2	1:A:2784:GLN:HA	1.72	0.53
1:A:3137:GLU:OE1	1:A:3186:ARG:NH2	2.33	0.53
1:A:437:HIS:O	1:A:441:MET:HG3	2.08	0.53
1:A:1078:ALA:O	1:A:1107:TYR:OH	2.22	0.53
1:A:1538:LEU:HD21	1:A:1555:HIS:CG	2.43	0.53
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.40	0.53
1:A:292:SER:HA	1:A:295:GLU:OE2	2.08	0.53
1:A:718:MET:HE1	1:A:730:LEU:HD21	1.91	0.53
1:A:4074:PHE:HA	1:A:4077:TYR:CD2	2.44	0.53
1:A:1241:LEU:HD11	1:A:1253:THR:HA	1.91	0.53
1:A:3029:LYS:C	1:A:3031:TRP:H	2.16	0.53
1:A:3493:TRP:CZ2	1:A:3711:PRO:HD3	2.43	0.53
1:A:1399:CYS:O	1:A:1402:LEU:HG	2.08	0.53
1:A:1585:SER:OG	1:A:1588:ASP:OD1	2.25	0.53
1:A:2443:MET:HE3	1:A:2476:ILE:HG23	1.91	0.53
1:A:3923:ARG:HD3	1:A:3928:PHE:CE1	2.43	0.53
1:A:1104:LEU:HD23	1:A:1168:LEU:HD21	1.91	0.52
1:A:243:GLN:HG3	1:A:246:ARG:HH12	1.74	0.52
1:A:864:GLY:O	1:A:868:LYS:NZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:PRO:HA	1:A:1049:GLN:HB2	1.91	0.52
1:A:1452:VAL:HG23	1:A:1517:LEU:HD22	1.91	0.52
1:A:2559:THR:O	1:A:2563:LEU:HB2	2.09	0.52
1:A:2987:THR:HG23	1:A:2990:GLU:H	1.75	0.52
1:A:3729:MET:O	1:A:3729:MET:HG3	2.06	0.52
1:A:2461:PHE:HB2	1:A:2473:MET:SD	2.49	0.52
1:A:3327:ASN:HB3	1:A:3388:ALA:HB2	1.90	0.52
1:A:3466:PRO:HA	1:A:3469:LEU:HD23	1.92	0.52
1:A:1686:LEU:HD23	1:A:1738:ASN:HB3	1.91	0.52
1:A:1714:LEU:HD12	1:A:1757:MET:HE1	1.91	0.52
1:A:2233:HIS:O	1:A:2237:ILE:HG12	2.09	0.52
1:A:1741:ASP:OD1	1:A:1742:CYS:N	2.43	0.52
1:A:3998:LEU:O	1:A:4002:MET:HG3	2.10	0.52
1:A:3542:PHE:HZ	1:A:3555:VAL:HG21	1.74	0.52
1:A:2802:PRO:HG2	1:A:2803:ILE:HD12	1.92	0.52
1:A:131:LEU:HD12	1:A:132:ILE:N	2.25	0.52
1:A:304:THR:HA	1:A:309:LYS:HE2	1.92	0.52
1:A:1484:LEU:O	1:A:1489:LYS:HG2	2.09	0.52
1:A:2548:PRO:HB2	1:A:2848:PHE:HD1	1.74	0.52
1:A:3753:LYS:CD	1:A:3803:ILE:CD1	2.81	0.52
1:A:356:ASN:ND2	1:A:404:ASP:HB3	2.24	0.52
1:A:913:ARG:HH11	1:A:2803:ILE:HD13	1.74	0.52
1:A:1367:HIS:O	1:A:1370:ARG:HG3	2.09	0.52
1:A:1802:TYR:CZ	1:A:1806:ARG:HD3	2.45	0.52
1:A:1935:GLU:CD	1:A:1938:ARG:HE	2.16	0.51
1:A:2540:LEU:HD11	1:A:2832:ILE:HD12	1.91	0.51
1:A:406:ARG:HB2	1:A:409:GLN:HE22	1.75	0.51
1:A:3416:LEU:HD21	1:A:3445:LEU:HD21	1.91	0.51
1:A:1445:ARG:HG3	1:A:1510:LEU:HD13	1.93	0.51
1:A:2211:LEU:HA	1:A:2214:ARG:HG2	1.92	0.51
1:A:2421:VAL:HG13	1:A:2457:PRO:HG3	1.93	0.51
1:A:1668:PHE:CD1	1:A:1669:PRO:HD3	2.46	0.51
1:A:1983:ASP:HA	1:A:2184:TYR:OH	2.09	0.51
1:A:2577:PHE:HB2	1:A:2784:GLN:HG2	1.93	0.51
1:A:773:LEU:HD13	1:A:792:ILE:HG21	1.91	0.51
1:A:1424:THR:O	1:A:1428:ILE:HG13	2.10	0.51
1:A:2439:ILE:HA	1:A:2442:MET:HE2	1.93	0.51
1:A:3605:ASN:OD1	1:A:3606:ILE:N	2.43	0.51
1:A:4027:TRP:CE3	1:A:4030:GLU:HB3	2.44	0.51
1:A:13:LEU:O	1:A:14:ARG:NE	2.42	0.51
1:A:1195:VAL:HA	1:A:1198:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:PRO:HA	1:A:676:ASN:HD22	1.75	0.51
1:A:1764:GLU:OE1	1:A:1768:ARG:NH2	2.38	0.51
1:A:1358:LEU:HD11	1:A:1410:PRO:HB2	1.92	0.51
1:A:200:PHE:CZ	1:A:227:LEU:HD23	2.46	0.50
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.11	0.50
1:A:374:LYS:HD3	1:A:423:TYR:HB3	1.93	0.50
1:A:2085:MET:HE3	1:A:2089:ASN:HB2	1.93	0.50
1:A:2298:GLU:HA	1:A:2301:GLN:NE2	2.26	0.50
1:A:3570:ASP:HB3	1:A:3686:TRP:CZ2	2.45	0.50
1:A:3077:ILE:HA	1:A:3080:LEU:HG	1.92	0.50
1:A:924:ARG:O	1:A:924:ARG:HG2	2.11	0.50
1:A:1105:VAL:O	1:A:1109:GLU:HG2	2.11	0.50
1:A:303:HIS:CE1	1:A:305:ASN:HB2	2.46	0.50
1:A:631:ARG:HH21	1:A:668:LYS:HB3	1.75	0.50
1:A:1402:LEU:HD12	1:A:1403:MET:N	2.27	0.50
1:A:1657:SER:OG	1:A:1658:SER:N	2.45	0.50
1:A:1716:GLN:HA	1:A:1719:VAL:HG22	1.92	0.50
1:A:2439:ILE:HG22	1:A:2443:MET:HE1	1.92	0.50
1:A:240:GLU:HB3	1:A:242:PRO:HD2	1.94	0.50
1:A:255:ALA:HB2	1:A:300:TRP:HZ2	1.77	0.50
1:A:1436:LEU:HD23	1:A:1436:LEU:H	1.76	0.50
1:A:1802:TYR:CE1	1:A:1806:ARG:HD3	2.47	0.50
1:A:1864:ASP:OD1	1:A:1865:THR:N	2.45	0.50
1:A:2443:MET:O	1:A:2445:LYS:N	2.42	0.50
1:A:3704:GLN:OE1	1:A:3716:HIS:HB3	2.12	0.50
1:A:3796:MET:O	1:A:3797:THR:OG1	2.25	0.50
1:A:3858:MET:HE1	1:A:4119:ARG:CB	2.41	0.50
1:A:3451:LEU:HD11	1:A:3490:VAL:HG21	1.94	0.50
1:A:3466:PRO:HG3	1:A:3498:TRP:CZ3	2.47	0.50
1:A:3718:ARG:H	1:A:3743:HIS:CE1	2.30	0.50
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.93	0.50
1:A:489:ARG:O	1:A:492:SER:OG	2.26	0.50
1:A:1242:LEU:HG	1:A:1310:GLU:HB2	1.93	0.50
1:A:1980:ASN:ND2	1:A:2141:ASN:OD1	2.45	0.50
1:A:2091:HIS:NE2	1:A:2093:CYS:SG	2.83	0.50
1:A:2281:MET:HG2	1:A:2287:PRO:HG3	1.93	0.50
1:A:37:GLY:O	1:A:40:GLN:HG2	2.11	0.49
1:A:849:GLU:HG2	1:A:850:GLU:N	2.26	0.49
1:A:3564:GLN:HG2	1:A:3565:GLY:N	2.27	0.49
1:A:3928:PHE:HD2	1:A:3937:VAL:HG11	1.77	0.49
1:A:381:VAL:HA	1:A:384:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:PRO:HD3	1:A:449:TYR:OH	2.12	0.49
1:A:986:PRO:C	1:A:990:GLN:HE21	2.20	0.49
1:A:2245:TRP:O	1:A:2249:LEU:HD13	2.11	0.49
1:A:2252:PRO:C	1:A:2254:ARG:H	2.19	0.49
1:A:2365:ASN:OD1	1:A:2396:LEU:HB3	2.12	0.49
1:A:2466:SER:C	1:A:2468:THR:H	2.19	0.49
1:A:1104:LEU:HA	1:A:1134:LEU:HD13	1.95	0.49
1:A:2148:LYS:HG2	1:A:2185:MET:HE1	1.95	0.49
1:A:2245:TRP:HB3	1:A:2249:LEU:HD13	1.94	0.49
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.45	0.49
1:A:3809:THR:OG1	1:A:3929:MET:CE	2.59	0.49
1:A:938:VAL:HG21	1:A:969:LEU:HD11	1.93	0.49
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.13	0.49
1:A:3509:ASP:OD1	1:A:3509:ASP:N	2.45	0.49
1:A:131:LEU:O	1:A:135:LEU:HG	2.13	0.49
1:A:931:CYS:O	1:A:984:TYR:OH	2.28	0.49
1:A:4008:GLU:HG3	1:A:4010:SER:HB3	1.94	0.49
1:A:800:LEU:O	1:A:3115:SER:OG	2.27	0.49
1:A:3319:ASN:OD1	1:A:3320:ILE:N	2.45	0.49
1:A:3859:TYR:CE1	1:A:4119:ARG:HD3	2.48	0.49
1:A:3723:ASP:HB3	1:A:3739:ILE:HB	1.95	0.49
1:A:984:TYR:O	1:A:988:VAL:HG22	2.13	0.49
1:A:1016:GLY:O	1:A:1018:VAL:N	2.46	0.49
1:A:1414:ILE:O	1:A:1417:THR:OG1	2.25	0.49
1:A:3529:ILE:HG23	1:A:3562:LEU:HD11	1.94	0.49
1:A:258:PRO:HG3	1:A:300:TRP:HH2	1.77	0.48
1:A:1136:ARG:HA	1:A:1139:GLU:HG2	1.93	0.48
1:A:1148:ALA:HB2	1:A:1164:CYS:HB2	1.95	0.48
1:A:1052:SER:OG	1:A:1054:VAL:HG12	2.13	0.48
1:A:3531:TYR:O	1:A:3535:ILE:HG13	2.13	0.48
1:A:3797:THR:HG22	1:A:3798:SER:N	2.28	0.48
1:A:2898:LEU:HD21	1:A:3972:LEU:HB3	1.93	0.48
1:A:3425:ARG:O	1:A:3428:GLU:N	2.46	0.48
1:A:1476:HIS:CE1	1:A:1478:SER:HB3	2.48	0.48
1:A:1766:LEU:HB2	1:A:1778:PHE:CD2	2.48	0.48
1:A:1850:VAL:HG21	1:A:1873:TYR:CE2	2.48	0.48
1:A:2917:PRO:HB2	1:A:2919:ASP:OD1	2.12	0.48
1:A:448:GLN:OE1	1:A:519:TRP:N	2.47	0.48
1:A:1532:LEU:HD11	1:A:1567:ILE:HG21	1.94	0.48
1:A:2548:PRO:HB2	1:A:2848:PHE:CD1	2.48	0.48
1:A:2999:LEU:HD21	1:A:3015:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3940:ILE:HG22	2:A:6101:2R4:H291	1.96	0.48
1:A:237:SER:O	1:A:243:GLN:NE2	2.47	0.48
1:A:860:GLY:HA3	1:A:3136:THR:HG21	1.94	0.48
1:A:1154:PRO:HD2	1:A:1157:PHE:CD2	2.49	0.48
1:A:1202:ARG:HH12	1:A:1210:ASP:HB2	1.78	0.48
1:A:763:THR:HG23	1:A:851:ILE:CD1	2.43	0.48
1:A:1087:ARG:HG2	1:A:1090:ARG:NH1	2.28	0.48
1:A:2494:ASP:HA	1:A:2497:GLU:HG3	1.95	0.48
1:A:3348:LEU:HA	1:A:3351:ILE:HG12	1.96	0.48
1:A:3761:ASP:O	1:A:3765:GLU:HG2	2.14	0.48
1:A:1690:GLY:O	1:A:1693:VAL:HG12	2.14	0.48
1:A:2151:ILE:HD13	1:A:2192:THR:OG1	2.14	0.48
1:A:2428:ASP:HB3	1:A:2431:ARG:HB3	1.95	0.48
1:A:62:ASP:O	1:A:65:LEU:HG	2.13	0.48
1:A:458:CYS:HA	1:A:461:ILE:HG22	1.95	0.48
1:A:642:PHE:CE2	1:A:646:VAL:HG22	2.48	0.48
1:A:1195:VAL:HG13	1:A:1198:LEU:HD12	1.95	0.48
1:A:1205:ASN:HB2	1:A:1275:THR:HA	1.94	0.48
1:A:1389:VAL:HG13	1:A:1390:GLN:N	2.29	0.48
1:A:2127:LYS:HA	1:A:2130:HIS:HB3	1.96	0.48
1:A:2129:LEU:HB3	1:A:2146:LEU:CD2	2.44	0.48
1:A:2379:MET:HA	1:A:2382:VAL:HG12	1.96	0.48
1:A:2457:PRO:HA	1:A:2460:GLU:OE1	2.13	0.48
1:A:3324:ARG:O	1:A:3328:ILE:HG12	2.14	0.48
1:A:3627:ALA:HB3	1:A:3683:CYS:HB2	1.95	0.48
1:A:3924:HIS:ND1	1:A:3926:ASN:OD1	2.45	0.48
1:A:1672:PHE:CE2	1:A:1702:LEU:HD13	2.49	0.48
1:A:2298:GLU:HA	1:A:2301:GLN:CD	2.39	0.48
1:A:2817:LEU:HD13	1:A:2820:MET:CE	2.44	0.47
1:A:3923:ARG:HB3	1:A:3928:PHE:HE1	1.78	0.47
1:A:901:MET:SD	1:A:2535:THR:OG1	2.67	0.47
1:A:1186:LYS:O	1:A:1190:LEU:HG	2.14	0.47
1:A:3686:TRP:CZ3	1:A:3690:PHE:HD1	2.32	0.47
1:A:344:GLN:O	1:A:348:ILE:HG12	2.15	0.47
1:A:1202:ARG:HH22	1:A:1210:ASP:HB3	1.79	0.47
1:A:1212:LEU:HD21	1:A:1217:VAL:HG22	1.97	0.47
1:A:3088:LEU:O	1:A:3092:LEU:HD12	2.15	0.47
1:A:31:GLY:HA2	1:A:34:LEU:HB2	1.96	0.47
1:A:1476:HIS:HB3	1:A:1479:VAL:HG22	1.96	0.47
1:A:3662:ILE:O	1:A:3666:LEU:HD13	2.13	0.47
1:A:2092:GLU:N	1:A:2092:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2473:MET:HA	1:A:2476:ILE:HD12	1.97	0.47
1:A:2930:TYR:HA	1:A:2933:ILE:HG22	1.95	0.47
1:A:3535:ILE:HD11	1:A:3795:PRO:O	2.15	0.47
1:A:406:ARG:HB2	1:A:409:GLN:NE2	2.29	0.47
1:A:766:ALA:HB3	1:A:851:ILE:HD13	1.96	0.47
1:A:1158:PRO:N	1:A:1159:PRO:HD2	2.28	0.47
1:A:1271:ILE:HD12	1:A:1344:PHE:HE1	1.80	0.47
1:A:1378:GLU:HG2	1:A:1378:GLU:O	2.14	0.47
1:A:1477:HIS:O	1:A:1481:THR:HG22	2.14	0.47
1:A:1580:LEU:O	1:A:1584:GLN:HG3	2.15	0.47
1:A:2329:TYR:O	1:A:2332:GLU:HG3	2.15	0.47
1:A:55:THR:O	1:A:58:VAL:HG12	2.14	0.47
1:A:75:SER:H	1:A:78:PHE:HB3	1.78	0.47
1:A:540:MET:HA	1:A:543:SER:OG	2.15	0.47
1:A:607:ASP:HB3	1:A:1023:SER:OG	2.14	0.47
1:A:763:THR:HG23	1:A:851:ILE:HD11	1.97	0.47
1:A:856:VAL:HG21	1:A:3111:MET:HG2	1.97	0.47
1:A:1633:TRP:CD1	1:A:1645:VAL:HG11	2.50	0.47
1:A:1726:SER:O	1:A:1726:SER:OG	2.26	0.47
1:A:2227:LYS:HB2	1:A:2230:VAL:HG22	1.95	0.47
1:A:2443:MET:HG3	1:A:2479:TRP:CZ3	2.49	0.47
1:A:12:LEU:HA	1:A:15:LEU:HB3	1.97	0.47
1:A:419:SER:OG	1:A:463:LYS:NZ	2.44	0.47
1:A:2097:LEU:O	1:A:2101:VAL:HG22	2.15	0.47
1:A:4008:GLU:HG3	1:A:4010:SER:H	1.78	0.47
1:A:1373:VAL:HG21	1:A:1418:HIS:HB3	1.97	0.47
1:A:1980:ASN:OD1	1:A:1981:LEU:N	2.45	0.47
1:A:2233:HIS:HA	1:A:2236:GLU:HG2	1.97	0.47
1:A:3729:MET:O	1:A:3731:SER:N	2.43	0.47
1:A:1221:ILE:CD1	1:A:1288:SER:HA	2.45	0.47
1:A:1235:ILE:HG22	1:A:1256:TRP:NE1	2.30	0.47
1:A:493:LYS:HD2	1:A:522:PRO:HG2	1.96	0.46
1:A:1718:ILE:O	1:A:1722:PHE:HB2	2.14	0.46
1:A:3194:GLU:HG3	1:A:3231:ILE:HD11	1.97	0.46
1:A:3564:GLN:HG2	1:A:3565:GLY:H	1.79	0.46
1:A:3681:LYS:O	1:A:3685:PRO:HD2	2.14	0.46
1:A:363:ILE:HG13	1:A:413:PHE:CE2	2.51	0.46
1:A:1402:LEU:HD12	1:A:1402:LEU:C	2.40	0.46
1:A:3744:ASP:OD1	1:A:3744:ASP:N	2.48	0.46
1:A:933:LEU:HG	1:A:937:MET:HE2	1.97	0.46
1:A:1376:LEU:HD13	1:A:1399:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3661:ASP:HA	1:A:3664:ASN:ND2	2.31	0.46
1:A:3664:ASN:OD1	1:A:3665:MET:N	2.47	0.46
1:A:3954:PRO:HD2	1:A:4027:TRP:HB3	1.96	0.46
1:A:100:ILE:HB	1:A:102:PRO:HD3	1.97	0.46
1:A:349:ILE:HD13	1:A:366:TYR:HE2	1.79	0.46
1:A:745:VAL:O	1:A:749:VAL:HG23	2.15	0.46
1:A:762:TYR:CE2	1:A:764:PRO:HB2	2.50	0.46
1:A:2577:PHE:CD2	1:A:2784:GLN:HA	2.49	0.46
1:A:334:HIS:HB3	1:A:337:LYS:HD2	1.97	0.46
1:A:1723:PRO:HG3	1:A:1729:PHE:CZ	2.50	0.46
1:A:2371:PHE:CD2	1:A:2374:LEU:HB2	2.50	0.46
1:A:4002:MET:O	1:A:4006:VAL:HG12	2.15	0.46
1:A:2123:PRO:HB2	1:A:2125:TRP:CD1	2.50	0.46
1:A:3661:ASP:HA	1:A:3664:ASN:HD21	1.80	0.46
1:A:1045:THR:OG1	1:A:1047:GLN:OE1	2.30	0.46
1:A:2575:PRO:CB	1:A:2784:GLN:HB3	2.44	0.46
1:A:172:GLU:HB3	1:A:220:LEU:HD13	1.97	0.46
1:A:1767:CYS:O	1:A:1815:THR:HG23	2.16	0.46
1:A:2817:LEU:HA	1:A:2820:MET:HE3	1.98	0.46
1:A:3630:ARG:O	1:A:3634:GLN:HG2	2.15	0.46
1:A:317:GLU:O	1:A:321:LYS:HG2	2.16	0.46
1:A:943:GLY:C	1:A:2577:PHE:CE1	2.94	0.46
1:A:1605:PHE:CD1	1:A:1608:ARG:HD3	2.51	0.46
1:A:3493:TRP:CD1	1:A:3711:PRO:HB3	2.50	0.46
1:A:3786:LEU:HD22	1:A:3910:LEU:HD22	1.97	0.46
1:A:402:THR:HA	1:A:406:ARG:HH12	1.81	0.46
1:A:575:ILE:O	1:A:579:LEU:HD13	2.15	0.46
1:A:3012:GLU:HG3	1:A:3013:TYR:H	1.81	0.46
1:A:3072:GLU:C	1:A:3074:GLN:H	2.23	0.46
1:A:3913:ILE:HB	1:A:3984:MET:HG2	1.97	0.46
1:A:471:LYS:HB2	1:A:474:VAL:HB	1.97	0.45
1:A:1115:HIS:ND1	1:A:1180:GLN:HA	2.31	0.45
1:A:2261:SER:OG	1:A:2262:GLY:N	2.49	0.45
1:A:2339:GLU:H	1:A:2339:GLU:CD	2.24	0.45
1:A:3729:MET:CB	2:A:6101:2R4:C18	2.93	0.45
1:A:3858:MET:HE1	1:A:4119:ARG:HB3	1.98	0.45
1:A:540:MET:O	1:A:544:ILE:HG12	2.16	0.45
1:A:1811:ARG:NH2	1:A:1819:PHE:HE2	2.14	0.45
1:A:2533:SER:O	1:A:2565:MET:HE2	2.15	0.45
1:A:2877:SER:OG	1:A:2925:GLU:HB3	2.17	0.45
1:A:2891:ARG:O	1:A:2895:GLU:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2953:THR:HB	1:A:2994:TRP:HE1	1.81	0.45
1:A:3483:MET:HG3	1:A:3513:ALA:HB1	1.98	0.45
1:A:3840:LYS:O	1:A:3844:THR:HG23	2.16	0.45
1:A:607:ASP:OD1	1:A:607:ASP:N	2.44	0.45
1:A:1871:MET:HA	1:A:1874:TYR:CD2	2.51	0.45
1:A:2352:HIS:NE2	1:A:2360:PHE:HA	2.31	0.45
1:A:2430:GLU:H	1:A:2430:GLU:CD	2.24	0.45
1:A:265:TYR:O	1:A:269:SER:OG	2.20	0.45
1:A:446:PHE:HD1	1:A:457:CYS:SG	2.38	0.45
1:A:493:LYS:O	1:A:625:ASN:ND2	2.50	0.45
1:A:2454:LEU:C	1:A:2457:PRO:HD2	2.42	0.45
1:A:3271:ASP:HB2	1:A:3315:TYR:CE2	2.51	0.45
1:A:1640:GLU:OE1	1:A:1640:GLU:N	2.46	0.45
1:A:1863:PHE:HZ	1:A:1932:GLN:HB3	1.82	0.45
1:A:2527:HIS:HB3	1:A:2530:ARG:NH1	2.32	0.45
1:A:2863:CYS:SG	1:A:2895:GLU:HG3	2.56	0.45
1:A:2255:LEU:O	1:A:2259:LYS:HG2	2.17	0.45
1:A:3360:LEU:HD11	1:A:3377:LEU:HD11	1.98	0.45
1:A:3442:TYR:O	1:A:3446:VAL:HG23	2.17	0.45
1:A:359:LEU:HD21	1:A:391:ARG:HH11	1.82	0.45
1:A:2183:HIS:ND1	1:A:2185:MET:HB2	2.32	0.45
1:A:3805:TRP:HZ3	2:A:6101:2R4:C08	2.30	0.45
1:A:985:GLU:HB3	1:A:986:PRO:HD3	1.99	0.45
1:A:1092:GLU:HG2	1:A:1095:LEU:HG	1.99	0.45
1:A:1202:ARG:HH22	1:A:1210:ASP:CB	2.30	0.45
1:A:1388:ASP:HA	1:A:1392:MET:CE	2.46	0.45
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	1.98	0.45
1:A:1872:GLY:O	1:A:1876:ILE:HG13	2.17	0.45
1:A:2554:PHE:C	1:A:2556:SER:H	2.24	0.45
1:A:3622:ALA:HB3	1:A:3625:LEU:CD1	2.47	0.45
1:A:3723:ASP:OD1	1:A:3724:GLU:N	2.50	0.45
1:A:3858:MET:HB3	1:A:3858:MET:HE3	1.64	0.45
1:A:1454:ALA:O	1:A:1458:LEU:HD23	2.16	0.45
1:A:1492:ALA:HB2	1:A:1538:LEU:HD13	1.98	0.45
1:A:2236:GLU:HA	1:A:2239:LYS:HG2	1.99	0.45
1:A:1222:ASN:HA	1:A:1236:LEU:HD13	1.99	0.45
1:A:2157:PHE:HA	1:A:2160:TYR:HD2	1.80	0.45
1:A:3100:LYS:HA	1:A:3103:ILE:HG22	1.98	0.45
1:A:3484:THR:O	1:A:3487:ILE:HG22	2.17	0.45
1:A:182:GLY:O	1:A:233:ASN:ND2	2.50	0.44
1:A:341:PHE:HA	1:A:344:GLN:HE21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:TRP:HB3	1:A:785:MET:HE2	1.99	0.44
1:A:782:ARG:O	1:A:786:GLN:HB2	2.17	0.44
1:A:1799:GLU:HA	1:A:1802:TYR:HB3	1.97	0.44
1:A:3011:LEU:HD23	1:A:3047:SER:HB2	1.99	0.44
1:A:3266:SER:C	1:A:3268:THR:H	2.25	0.44
1:A:3567:VAL:HG22	1:A:3699:LEU:HD22	1.99	0.44
1:A:4039:TYR:HB2	1:A:4042:GLN:HB2	2.00	0.44
1:A:238:MET:HE3	1:A:283:SER:H	1.82	0.44
1:A:2093:CYS:C	1:A:2096:PRO:HD2	2.43	0.44
1:A:996:THR:O	1:A:996:THR:HG22	2.17	0.44
1:A:1079:SER:HA	1:A:1107:TYR:CE1	2.50	0.44
1:A:1092:GLU:HB3	1:A:1095:LEU:HD12	1.99	0.44
1:A:1234:GLY:HA2	1:A:1259:LEU:HD22	1.99	0.44
1:A:1410:PRO:C	1:A:1412:LYS:H	2.26	0.44
1:A:1767:CYS:HB3	1:A:1818:SER:OG	2.17	0.44
1:A:2439:ILE:HG22	1:A:2443:MET:CE	2.48	0.44
1:A:266:ALA:O	1:A:270:ALA:HB2	2.18	0.44
1:A:393:LYS:HA	1:A:397:LEU:HD12	1.99	0.44
1:A:1037:LEU:HD22	1:A:1085:ILE:HD12	1.99	0.44
1:A:2317:ALA:HB1	1:A:2366:LYS:HE3	2.00	0.44
1:A:3702:PRO:HG2	1:A:3802:LEU:HD12	1.99	0.44
1:A:3786:LEU:O	1:A:3787:GLN:HG2	2.18	0.44
1:A:4076:ASP:O	1:A:4080:VAL:HG12	2.17	0.44
1:A:4121:TRP:CD1	1:A:4123:GLY:H	2.35	0.44
1:A:1324:PRO:O	1:A:1327:GLY:N	2.46	0.44
1:A:1365:ASN:HB2	1:A:1369:MET:HE2	1.99	0.44
1:A:1389:VAL:HG13	1:A:1390:GLN:H	1.83	0.44
1:A:1565:GLU:OE2	1:A:1565:GLU:N	2.41	0.44
1:A:1641:THR:O	1:A:1645:VAL:HG23	2.18	0.44
1:A:2443:MET:C	1:A:2445:LYS:H	2.24	0.44
1:A:2493:ASN:HA	1:A:2496:GLN:NE2	2.30	0.44
1:A:3763:ARG:HG3	1:A:4011:PHE:CZ	2.52	0.44
1:A:1099:PHE:CE1	1:A:1152:ARG:HD3	2.53	0.44
1:A:1441:ALA:HB1	1:A:1444:ASP:HB3	1.99	0.44
1:A:3767:LEU:HA	1:A:3767:LEU:HD23	1.81	0.44
1:A:4023:LYS:HB2	1:A:4023:LYS:HE2	1.93	0.44
1:A:4038:TRP:CH2	1:A:4043:LYS:HE3	2.53	0.44
1:A:4041:ARG:NH1	1:A:4045:CYS:SG	2.90	0.44
1:A:1202:ARG:NH2	1:A:1207:TRP:HA	2.32	0.44
1:A:1205:ASN:HA	1:A:1275:THR:HG23	2.00	0.44
1:A:1568:ASN:HA	1:A:1571:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1921:ASP:OD1	1:A:1922:ALA:N	2.50	0.44
1:A:2143:ARG:HB3	1:A:2171:LEU:HD13	1.99	0.44
1:A:3241:LYS:HE2	1:A:3241:LYS:HB2	1.80	0.44
1:A:3266:SER:OG	1:A:3267:LYS:N	2.47	0.44
1:A:4115:ASN:ND2	1:A:4115:ASN:O	2.51	0.44
1:A:129:ASP:OD1	1:A:129:ASP:N	2.51	0.44
1:A:523:THR:HG23	1:A:525:LYS:H	1.83	0.44
1:A:1358:LEU:HD23	1:A:1411:TYR:CZ	2.53	0.44
1:A:1593:VAL:O	1:A:1597:LEU:HD23	2.17	0.44
1:A:1751:GLU:HA	1:A:1785:ILE:CG2	2.47	0.44
1:A:1771:GLN:HA	1:A:1775:GLU:OE1	2.18	0.44
1:A:1818:SER:HB2	1:A:1822:ARG:HH22	1.82	0.44
1:A:2281:MET:HE1	1:A:2322:VAL:HG13	1.99	0.44
1:A:2496:GLN:HG2	1:A:2497:GLU:N	2.33	0.44
1:A:3589:SER:O	1:A:3593:ARG:HG3	2.18	0.44
1:A:3728:VAL:O	2:A:6101:2R4:H171	2.18	0.44
1:A:414:LEU:HA	1:A:417:VAL:HG12	1.98	0.43
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.51	0.43
1:A:1449:ALA:HB2	1:A:1510:LEU:HD12	2.00	0.43
1:A:1505:LEU:HD23	1:A:1505:LEU:O	2.17	0.43
1:A:1626:TRP:CD1	1:A:1670:GLU:HG3	2.53	0.43
1:A:2088:LEU:HD12	1:A:2094:MET:HG2	1.99	0.43
1:A:3680:LEU:HD23	1:A:3682:GLU:H	1.81	0.43
1:A:156:PHE:HA	1:A:159:GLU:HG2	2.00	0.43
1:A:189:MET:HE3	1:A:193:ALA:HB2	1.99	0.43
1:A:332:GLU:O	1:A:335:LYS:NZ	2.49	0.43
1:A:1093:GLU:HA	1:A:1096:VAL:HG12	2.01	0.43
1:A:1874:TYR:HE2	1:A:1940:TYR:HE1	1.65	0.43
1:A:1875:LYS:O	1:A:1878:ASP:HB3	2.18	0.43
1:A:3176:MET:SD	1:A:3179:TRP:HB2	2.59	0.43
1:A:3483:MET:HE3	1:A:3513:ALA:HB1	1.99	0.43
1:A:37:GLY:HA2	1:A:40:GLN:NE2	2.33	0.43
1:A:1367:HIS:O	1:A:1371:VAL:HG12	2.18	0.43
1:A:2330:VAL:HG12	1:A:2337:LEU:HD11	2.00	0.43
1:A:2379:MET:O	1:A:2382:VAL:HG12	2.18	0.43
1:A:2862:SER:OG	1:A:2868:LEU:O	2.37	0.43
1:A:468:LEU:HD21	1:A:478:CYS:HB3	2.01	0.43
1:A:1007:VAL:O	1:A:1011:GLU:HG3	2.18	0.43
1:A:1212:LEU:HD11	1:A:1217:VAL:HA	2.00	0.43
1:A:2455:LEU:HD12	1:A:2458:VAL:HB	2.01	0.43
1:A:631:ARG:NH2	1:A:668:LYS:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1480:GLY:O	1:A:1484:LEU:HD13	2.18	0.43
1:A:1592:MET:HE3	1:A:1592:MET:O	2.19	0.43
1:A:2208:ASP:HA	1:A:2211:LEU:HG	2.00	0.43
1:A:2398:LEU:HD23	1:A:2398:LEU:HA	1.73	0.43
1:A:2999:LEU:HD13	1:A:3043:TYR:CD2	2.53	0.43
1:A:3301:LEU:HD12	1:A:3301:LEU:HA	1.62	0.43
1:A:3405:PRO:C	1:A:3407:ALA:H	2.27	0.43
1:A:3792:SER:H	1:A:3804:GLU:HB3	1.82	0.43
1:A:3816:LEU:HD21	1:A:3883:LEU:HD13	2.01	0.43
1:A:297:LEU:HD13	1:A:316:LEU:HA	2.00	0.43
1:A:486:GLY:O	1:A:490:ILE:HG23	2.19	0.43
1:A:1101:PHE:CE1	1:A:1145:LEU:HD22	2.52	0.43
1:A:3450:MET:SD	1:A:3468:LEU:HD21	2.58	0.43
1:A:3531:TYR:HB2	1:A:3532:PRO:HD3	2.01	0.43
1:A:3596:LEU:HB2	1:A:3601:VAL:HG22	2.00	0.43
1:A:1108:MET:HG3	1:A:1178:ARG:HH12	1.83	0.43
1:A:1334:LYS:O	1:A:1338:VAL:HG23	2.19	0.43
1:A:1403:MET:HE1	1:A:1458:LEU:HD13	2.00	0.43
1:A:3483:MET:HG3	1:A:3513:ALA:CB	2.48	0.43
1:A:3704:GLN:HE22	1:A:3717:VAL:HB	1.83	0.43
1:A:207:GLN:HE22	1:A:217:LEU:HD12	1.83	0.43
1:A:624:ILE:O	1:A:628:GLU:HG2	2.19	0.43
1:A:998:ASN:HA	1:A:1001:PHE:CE1	2.54	0.43
1:A:1672:PHE:O	1:A:1676:ILE:HG12	2.18	0.43
1:A:1748:ASP:O	1:A:1751:GLU:HG2	2.19	0.43
1:A:2185:MET:HE3	1:A:2185:MET:HB3	1.82	0.43
1:A:2506:LEU:O	1:A:2525:TRP:NE1	2.34	0.43
1:A:3295:GLU:OE1	1:A:3348:LEU:HD22	2.19	0.43
1:A:3692:VAL:HG13	1:A:3692:VAL:O	2.19	0.43
1:A:249:PHE:HA	1:A:252:VAL:HG12	2.01	0.43
1:A:339:GLN:HA	1:A:342:MET:CG	2.49	0.43
1:A:359:LEU:HD12	1:A:359:LEU:HA	1.76	0.43
1:A:1525:CYS:SG	1:A:1526:GLU:N	2.92	0.43
1:A:2377:ARG:HG3	1:A:2378:PHE:HD1	1.83	0.43
1:A:3809:THR:HG22	1:A:3931:ALA:HA	2.00	0.43
1:A:144:MET:SD	1:A:144:MET:N	2.89	0.43
1:A:641:PHE:O	1:A:644:PRO:HD2	2.19	0.43
1:A:997:ASN:HB3	1:A:999:LYS:HG2	2.00	0.43
1:A:1235:ILE:HG22	1:A:1256:TRP:HE1	1.83	0.43
1:A:2347:LYS:C	1:A:2351:GLN:HE22	2.26	0.43
1:A:2411:LEU:O	1:A:2412:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2813:PHE:O	1:A:2817:LEU:HD23	2.18	0.43
1:A:943:GLY:CA	1:A:2577:PHE:CE1	3.02	0.42
1:A:1541:ALA:HA	1:A:1550:VAL:HA	2.01	0.42
1:A:1775:GLU:O	1:A:1779:GLN:HG2	2.19	0.42
1:A:2362:VAL:O	1:A:2366:LYS:HG2	2.19	0.42
1:A:2397:CYS:O	1:A:2400:VAL:HG12	2.18	0.42
1:A:3575:LEU:HD23	1:A:3687:MET:SD	2.59	0.42
1:A:3592:VAL:HG12	1:A:3609:MET:SD	2.59	0.42
1:A:3729:MET:HG3	1:A:3731:SER:H	1.83	0.42
1:A:3778:ASP:HB3	1:A:3781:CYS:HB2	1.99	0.42
1:A:183:GLU:HB2	1:A:230:LEU:HG	2.01	0.42
1:A:404:ASP:HB2	1:A:1732:GLY:O	2.19	0.42
1:A:1417:THR:HA	1:A:1420:ARG:HH21	1.83	0.42
1:A:1528:LEU:HD21	1:A:1567:ILE:HG23	2.01	0.42
1:A:1532:LEU:HD23	1:A:1532:LEU:HA	1.86	0.42
1:A:2555:LEU:HD22	1:A:2809:PHE:CD2	2.53	0.42
1:A:2577:PHE:CB	1:A:2784:GLN:HG2	2.49	0.42
1:A:3474:ARG:HG2	1:A:3475:TYR:H	1.84	0.42
1:A:170:VAL:O	1:A:171:LEU:HD22	2.19	0.42
1:A:1881:TYR:HB3	1:A:1954:CYS:SG	2.59	0.42
1:A:2270:ASN:O	1:A:2274:ILE:HG12	2.19	0.42
1:A:3006:ALA:HB3	1:A:3257:LYS:HE2	2.01	0.42
1:A:3873:LYS:O	1:A:3876:SER:OG	2.30	0.42
1:A:106:GLU:O	1:A:110:THR:OG1	2.23	0.42
1:A:432:THR:O	1:A:436:GLU:HG2	2.19	0.42
1:A:3751:LEU:CD2	1:A:3753:LYS:HD3	2.50	0.42
1:A:200:PHE:CE1	1:A:224:LEU:HD22	2.54	0.42
1:A:1149:LYS:HG2	1:A:1151:ARG:CZ	2.50	0.42
1:A:1403:MET:HE2	1:A:1463:LEU:HD12	2.01	0.42
1:A:1634:ALA:H	1:A:1637:SER:HB2	1.83	0.42
1:A:1759:LEU:HD13	1:A:1797:LEU:HD22	2.01	0.42
1:A:1933:LEU:HD13	1:A:1936:ARG:HG3	2.02	0.42
1:A:2213:ASN:O	1:A:2217:ASN:ND2	2.51	0.42
1:A:2350:LYS:HZ2	1:A:2353:GLN:HB3	1.85	0.42
1:A:3618:GLY:N	1:A:3633:ILE:HD12	2.33	0.42
1:A:29:LEU:HD13	1:A:32:HIS:HB3	2.01	0.42
1:A:2253:TYR:C	1:A:2254:ARG:HD2	2.45	0.42
1:A:3449:LYS:HA	1:A:3449:LYS:HD3	1.78	0.42
1:A:643:GLU:HG2	1:A:680:ILE:HD12	2.02	0.42
1:A:923:ASP:C	1:A:925:GLN:H	2.27	0.42
1:A:1496:GLU:HB2	1:A:1498:GLN:HE22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3759:ARG:O	1:A:3763:ARG:HG2	2.20	0.42
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.88	0.42
1:A:443:ILE:HG13	1:A:461:ILE:HD11	2.02	0.42
1:A:1226:GLY:HA2	1:A:1233:SER:O	2.20	0.42
1:A:2130:HIS:CD2	1:A:2167:PRO:HG2	2.54	0.42
1:A:3749:PRO:CG	1:A:3805:TRP:HD1	2.32	0.42
1:A:535:LEU:HD11	1:A:565:TYR:CD1	2.52	0.42
1:A:1256:TRP:CE3	1:A:1257:LEU:HD22	2.55	0.42
1:A:3107:ILE:O	1:A:3111:MET:HG3	2.19	0.42
1:A:3319:ASN:O	1:A:3323:PHE:HB3	2.20	0.42
1:A:3609:MET:HE2	1:A:3609:MET:HB3	1.98	0.42
1:A:3905:ALA:HB3	1:A:3979:LEU:HD23	2.01	0.42
1:A:3965:ARG:HA	1:A:3968:ILE:HG12	2.01	0.42
1:A:174:VAL:O	1:A:177:LEU:HG	2.20	0.42
1:A:1373:VAL:HG22	1:A:1419:LEU:HD23	2.01	0.42
1:A:1414:ILE:HG13	1:A:1418:HIS:CE1	2.55	0.42
1:A:1496:GLU:OE1	1:A:1496:GLU:N	2.50	0.42
1:A:1616:LEU:HD22	1:A:1659:VAL:HG21	2.02	0.42
1:A:2169:LEU:HB3	1:A:2211:LEU:HD13	2.01	0.42
1:A:2254:ARG:HH12	1:A:2292:CYS:C	2.27	0.42
1:A:2347:LYS:HG2	1:A:2351:GLN:NE2	2.30	0.42
1:A:2357:GLU:HA	1:A:2360:PHE:HB3	2.02	0.42
1:A:2790:LEU:C	1:A:2793:PRO:HD2	2.45	0.42
1:A:3483:MET:HE1	1:A:3487:ILE:HD12	2.01	0.42
1:A:3753:LYS:HG2	1:A:3803:ILE:HD11	1.93	0.42
1:A:3875:GLU:OE2	1:A:4127:TRP:HA	2.19	0.42
1:A:1794:GLN:O	1:A:1798:LEU:HG	2.19	0.41
1:A:1797:LEU:O	1:A:1800:SER:OG	2.30	0.41
1:A:2093:CYS:O	1:A:2097:LEU:HD23	2.20	0.41
1:A:2128:PHE:CD2	1:A:2129:LEU:HD22	2.55	0.41
1:A:2492:ASP:C	1:A:2494:ASP:H	2.27	0.41
1:A:3029:LYS:C	1:A:3031:TRP:N	2.77	0.41
1:A:3169:PRO:HD3	1:A:3182:ILE:HD11	2.01	0.41
1:A:393:LYS:HG3	1:A:397:LEU:HD12	2.02	0.41
1:A:573:LEU:HA	1:A:576:VAL:HG12	2.01	0.41
1:A:1491:ILE:HD12	1:A:1558:TYR:CD2	2.55	0.41
1:A:1782:PHE:HA	1:A:1785:ILE:HG12	2.02	0.41
1:A:2133:LEU:HD23	1:A:2164:TRP:HZ3	1.84	0.41
1:A:2259:LYS:HB3	1:A:2272:VAL:HG13	2.01	0.41
1:A:2272:VAL:O	1:A:2276:LEU:HG	2.19	0.41
1:A:3946:PHE:HB2	1:A:4043:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4039:TYR:CE2	1:A:4066:LEU:HD11	2.55	0.41
1:A:14:ARG:CZ	1:A:17:GLU:HG3	2.50	0.41
1:A:137:THR:O	1:A:141:SER:OG	2.22	0.41
1:A:790:LYS:HE3	1:A:790:LYS:HB3	1.91	0.41
1:A:1756:PRO:O	1:A:1760:GLU:HG2	2.20	0.41
1:A:2424:MET:SD	1:A:2457:PRO:HB2	2.60	0.41
1:A:2536:LEU:HD21	1:A:2820:MET:HE2	2.03	0.41
1:A:2851:PHE:CD2	1:A:2853:PRO:HD2	2.56	0.41
1:A:3243:ILE:HG21	1:A:3259:LEU:HD13	2.01	0.41
1:A:3959:MET:HE3	1:A:3959:MET:HB3	1.92	0.41
1:A:129:ASP:HA	1:A:132:ILE:HG22	2.02	0.41
1:A:1753:SER:OG	1:A:1755:SER:HB3	2.20	0.41
1:A:3406:ALA:O	1:A:3410:ILE:HG13	2.20	0.41
1:A:3463:LEU:HB3	1:A:3997:LEU:HD11	2.02	0.41
1:A:3791:TYR:CG	2:A:6101:2R4:H281	2.55	0.41
1:A:3974:MET:HE2	1:A:3974:MET:HB2	1.94	0.41
1:A:1335:CYS:HB3	1:A:1384:PHE:CE2	2.56	0.41
1:A:1811:ARG:NH1	1:A:1816:ARG:HH11	2.16	0.41
1:A:3051:LEU:HD23	1:A:3051:LEU:HA	1.86	0.41
1:A:3078:LEU:HA	1:A:3078:LEU:HD12	1.86	0.41
1:A:3293:CYS:HA	1:A:3296:GLN:CD	2.44	0.41
1:A:3911:ILE:HD11	1:A:3928:PHE:CD2	2.37	0.41
1:A:200:PHE:HZ	1:A:224:LEU:HA	1.84	0.41
1:A:1538:LEU:HD12	1:A:1553:PHE:CE2	2.55	0.41
1:A:2208:ASP:O	1:A:2211:LEU:HG	2.20	0.41
1:A:2254:ARG:NH2	1:A:2292:CYS:O	2.50	0.41
1:A:3525:TYR:OH	1:A:3712:LEU:N	2.54	0.41
1:A:132:ILE:HA	1:A:135:LEU:HD12	2.02	0.41
1:A:294:PHE:HE1	1:A:316:LEU:HD11	1.86	0.41
1:A:770:LEU:O	1:A:774:GLU:HG3	2.21	0.41
1:A:1685:ASP:OD1	1:A:1685:ASP:N	2.46	0.41
1:A:2236:GLU:O	1:A:2239:LYS:HG2	2.20	0.41
1:A:2334:LYS:C	1:A:2336:ILE:H	2.29	0.41
1:A:2535:THR:OG1	1:A:2536:LEU:N	2.53	0.41
1:A:3016:THR:HG21	1:A:3044:MET:HB2	2.03	0.41
1:A:3669:LYS:O	1:A:3672:LYS:HB2	2.20	0.41
1:A:3767:LEU:O	1:A:3771:MET:HG3	2.20	0.41
1:A:3925:LEU:HA	1:A:3925:LEU:HD23	1.82	0.41
1:A:202:GLY:HA2	1:A:205:LYS:HE2	2.02	0.41
1:A:1046:PRO:HG2	1:A:1047:GLN:HE22	1.86	0.41
1:A:2219:LEU:O	1:A:2223:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3077:ILE:HG13	1:A:3078:LEU:N	2.36	0.41
1:A:3439:LEU:HD12	1:A:3439:LEU:O	2.20	0.41
1:A:3626:GLY:HA3	1:A:3684:SER:O	2.21	0.41
1:A:159:GLU:HB2	1:A:163:LYS:NZ	2.36	0.41
1:A:1067:ALA:O	1:A:1075:ARG:HG2	2.20	0.41
1:A:1220:LEU:HD23	1:A:1220:LEU:HA	1.87	0.41
1:A:1620:THR:HG22	1:A:1624:GLN:HE22	1.86	0.41
1:A:2377:ARG:HG3	1:A:2378:PHE:CD1	2.56	0.41
1:A:2454:LEU:HD23	1:A:2454:LEU:HA	1.90	0.41
1:A:2454:LEU:O	1:A:2458:VAL:HG23	2.20	0.41
1:A:2854:PHE:O	1:A:2858:ILE:HG12	2.21	0.41
1:A:3176:MET:HE3	1:A:3246:ALA:HB2	2.02	0.41
1:A:3907:SER:O	1:A:3911:ILE:HG23	2.20	0.41
1:A:108:LYS:HZ3	1:A:151:GLU:HA	1.85	0.41
1:A:146:GLU:O	1:A:148:LYS:N	2.54	0.41
1:A:1339:VAL:HG23	1:A:1398:VAL:HG21	2.03	0.41
1:A:1711:ARG:NH2	1:A:1757:MET:HG2	2.35	0.41
1:A:2452:ARG:HD2	1:A:2452:ARG:HA	1.89	0.41
1:A:3992:ARG:HG2	1:A:4051:LEU:O	2.20	0.41
1:A:13:LEU:HD23	1:A:14:ARG:HE	1.86	0.40
1:A:229:SER:HB2	1:A:278:HIS:CD2	2.55	0.40
1:A:1211:VAL:O	1:A:1214:GLU:HB2	2.22	0.40
1:A:1271:ILE:HD12	1:A:1344:PHE:CE1	2.56	0.40
1:A:2269:ASP:O	1:A:2272:VAL:HG12	2.20	0.40
1:A:3492:CYS:SG	1:A:3517:SER:HA	2.61	0.40
1:A:3779:SER:O	1:A:3783:GLN:HG3	2.21	0.40
1:A:197:PHE:HA	1:A:200:PHE:HB3	2.04	0.40
1:A:441:MET:HA	1:A:444:ASP:HB2	2.02	0.40
1:A:718:MET:HE1	1:A:730:LEU:CD2	2.50	0.40
1:A:778:ILE:HG22	1:A:779:TYR:CD1	2.56	0.40
1:A:1977:ILE:HD12	1:A:1977:ILE:HA	1.96	0.40
1:A:2225:HIS:ND1	1:A:2230:VAL:HG21	2.35	0.40
1:A:2510:LEU:HA	1:A:2510:LEU:HD23	1.86	0.40
1:A:178:LEU:HD23	1:A:178:LEU:H	1.86	0.40
1:A:1033:ILE:HD11	1:A:1059:LEU:HD11	2.02	0.40
1:A:1504:ASP:C	1:A:1506:SER:H	2.29	0.40
1:A:2296:SER:O	1:A:2299:TYR:HB2	2.22	0.40
1:A:2547:SER:O	1:A:2549:LYS:N	2.54	0.40
1:A:2785:ILE:HD12	1:A:2785:ILE:HA	1.94	0.40
1:A:3088:LEU:HD23	1:A:3088:LEU:HA	1.89	0.40
1:A:3167:ARG:O	1:A:3167:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3512:VAL:HG12	1:A:3513:ALA:H	1.87	0.40
1:A:3636:PHE:CD2	1:A:3640:PHE:HD2	2.38	0.40
1:A:336:ASN:HA	1:A:339:GLN:OE1	2.22	0.40
1:A:782:ARG:H	1:A:782:ARG:HG3	1.63	0.40
1:A:890:LYS:HA	1:A:908:ASP:OD2	2.21	0.40
1:A:1850:VAL:HG21	1:A:1873:TYR:CD2	2.56	0.40
1:A:2169:LEU:HD11	1:A:2193:ILE:HG13	2.03	0.40
1:A:2240:THR:HA	1:A:2243:GLU:CD	2.46	0.40
1:A:2288:TYR:CD2	1:A:2296:SER:HB3	2.56	0.40
1:A:3090:TYR:HE2	1:A:3102:TYR:HE2	1.69	0.40
1:A:3956:PRO:HG2	1:A:4064:LEU:HD11	2.02	0.40
1:A:345:PHE:O	1:A:349:ILE:HG22	2.21	0.40
1:A:487:LEU:HD23	1:A:487:LEU:HA	1.85	0.40
1:A:1033:ILE:HD11	1:A:1059:LEU:HD21	2.04	0.40
1:A:1838:GLU:O	1:A:1842:THR:OG1	2.29	0.40
1:A:2260:PHE:O	1:A:2270:ASN:ND2	2.55	0.40
1:A:2289:ASP:HB3	1:A:2290:PRO:HD3	2.03	0.40
1:A:2825:THR:HG22	1:A:2828:GLU:HG2	2.04	0.40
1:A:2999:LEU:HA	1:A:2999:LEU:HD23	1.87	0.40
1:A:3314:SER:C	1:A:3316:LEU:H	2.30	0.40
1:A:3574:ALA:HB2	1:A:3686:TRP:NE1	2.37	0.40
1:A:3871:PHE:CD1	1:A:4118:GLY:HA2	2.57	0.40
1:A:3887:PHE:CD2	1:A:3900:LEU:HB3	2.56	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%)	3262 (91%)	332 (9%)	8 (0%)	43 71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	723	ASP
1	A	2336	ILE
1	A	3730	ALA
1	A	3406	ALA
1	A	3804	GLU
1	A	2787	HIS
1	A	4026	SER
1	A	1813	SER

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	3196/3671 (87%)	3187 (100%)	9 (0%)	86 85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	722	LYS
1	A	2576	MET
1	A	3728	VAL
1	A	3729	MET
1	A	3753	LYS
1	A	3756	GLU
1	A	3803	ILE
1	A	3804	GLU
1	A	3807	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	GLN
1	A	356	ASN
1	A	638	GLN
1	A	990	GLN
1	A	1374	GLN

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Mol	Chain	Res	Type
1	A	1459	HIS
1	A	1574	ASN
1	A	1614	GLN
1	A	1691	GLN
1	A	1737	ASN
1	A	2163	HIS
1	A	2170	GLN
1	A	2225	HIS
1	A	2305	ASN
1	A	2351	GLN
1	A	2518	GLN
1	A	2553	HIS
1	A	2831	ASN
1	A	3327	ASN
1	A	3573	ASN
1	A	4110	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2R4	A	6101	-	33,35,35	1.33	3 (9%)	45,51,51	1.30	6 (13%)

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	2R4	A	6101	-	-	4/8/16/16	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	2R4	C03-C02	-3.48	1.42	1.48
2	A	6101	2R4	C06-C05	-3.30	1.43	1.49
2	A	6101	2R4	C30-C02	-2.18	1.40	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	2R4	O22-C04-C03	-3.59	117.31	121.25
2	A	6101	2R4	C10-C11-C06	2.64	123.35	121.63
2	A	6101	2R4	C07-C06-C11	-2.25	116.36	118.84
2	A	6101	2R4	C19-C05-C06	2.19	123.16	118.74
2	A	6101	2R4	O01-C02-C30	-2.14	118.46	121.88
2	A	6101	2R4	C13-S12-C11	2.07	92.82	91.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

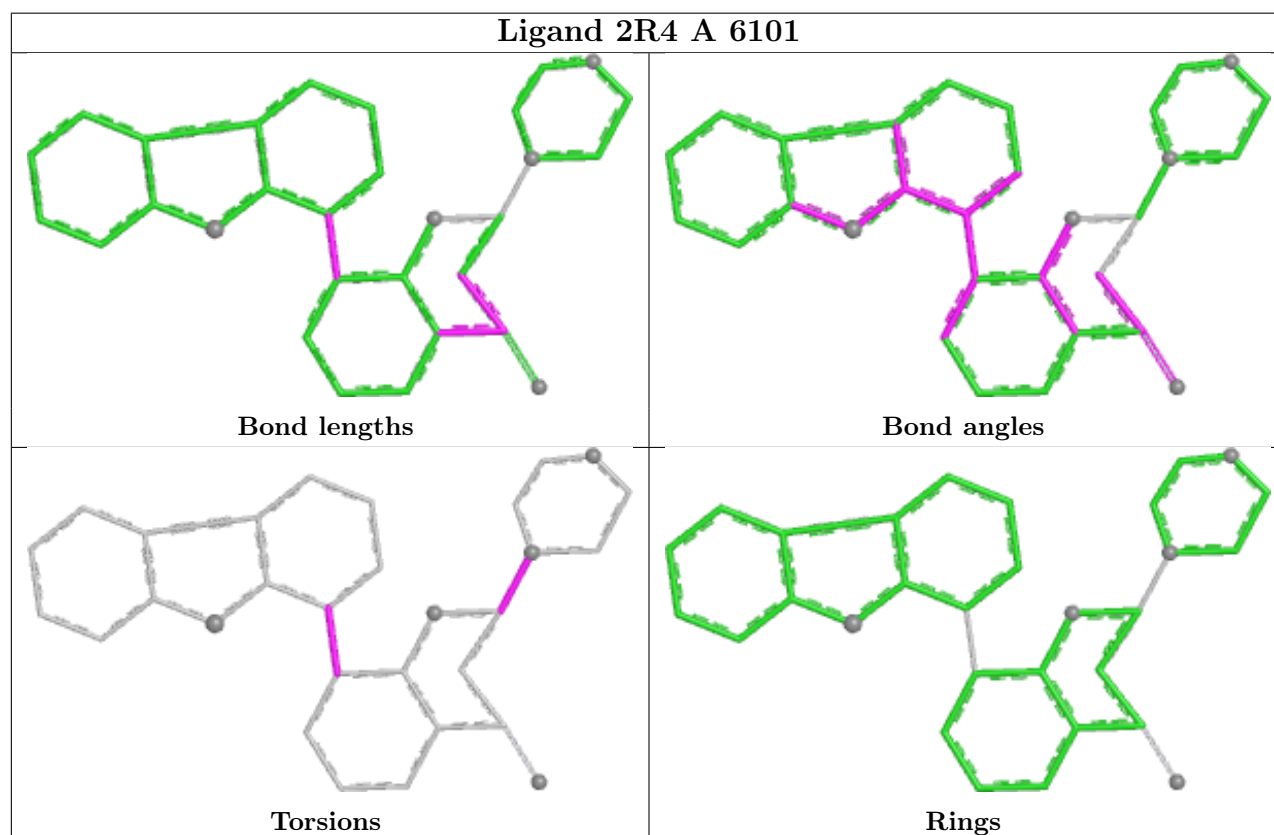
Mol	Chain	Res	Type	Atoms
2	A	6101	2R4	C19-C05-C06-C11
2	A	6101	2R4	C04-C05-C06-C11
2	A	6101	2R4	C30-C23-N24-C25
2	A	6101	2R4	C04-C05-C06-C07

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	2R4	8	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

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	83.48

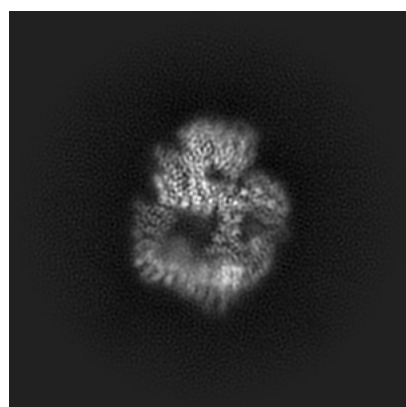
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13062. These allow visual inspection of the internal detail of the map and identification of artifacts.

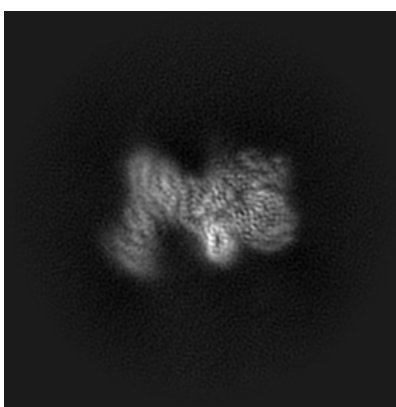
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

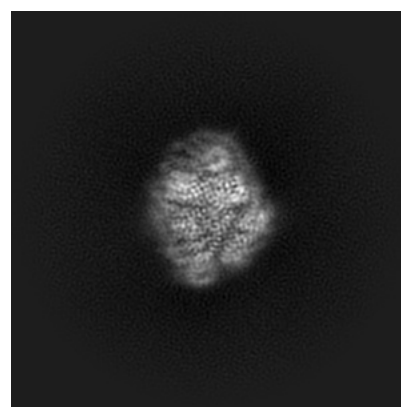
6.1.1 Primary map



X



Y

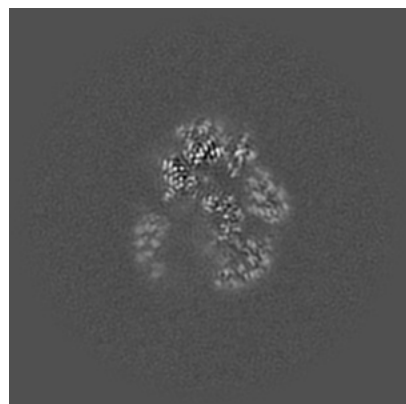


Z

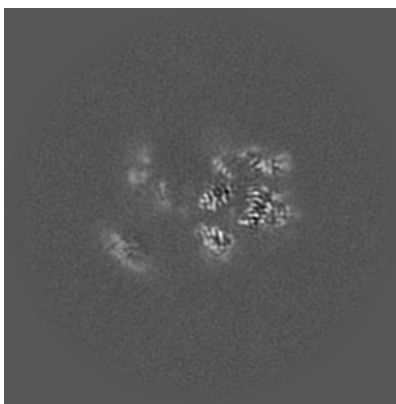
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

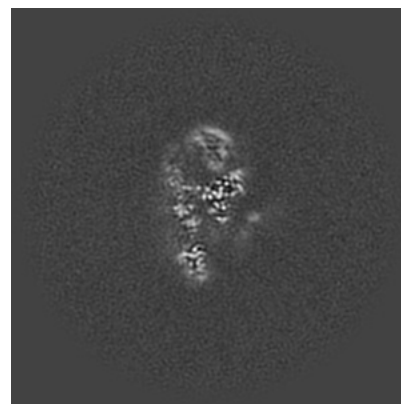
6.2.1 Primary map



X Index: 130



Y Index: 130

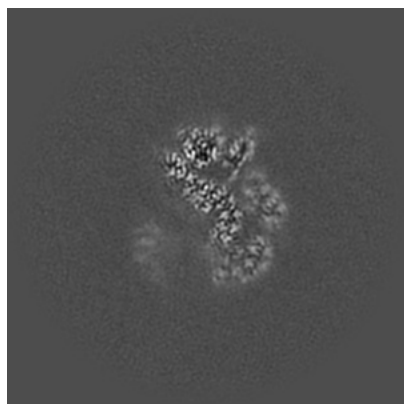


Z Index: 130

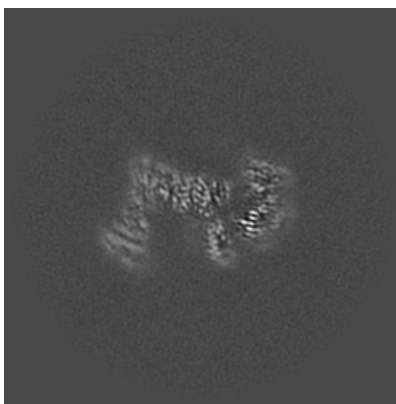
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

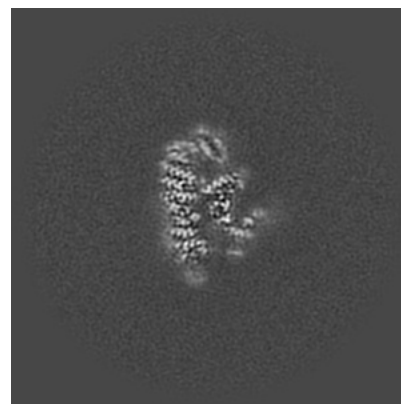
6.3.1 Primary map



X Index: 134



Y Index: 139

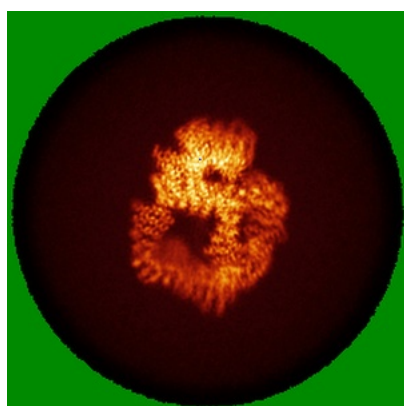


Z Index: 134

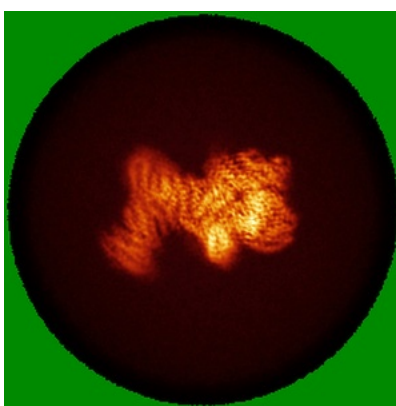
The images above show the largest variance slices of the map in three orthogonal directions.

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

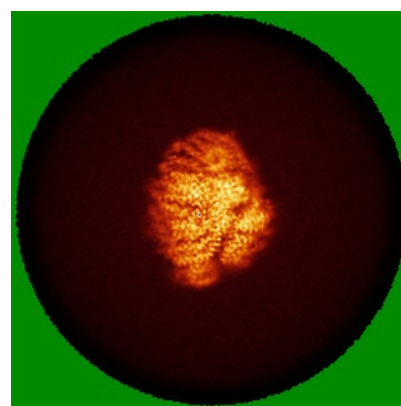
6.4.1 Primary map



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

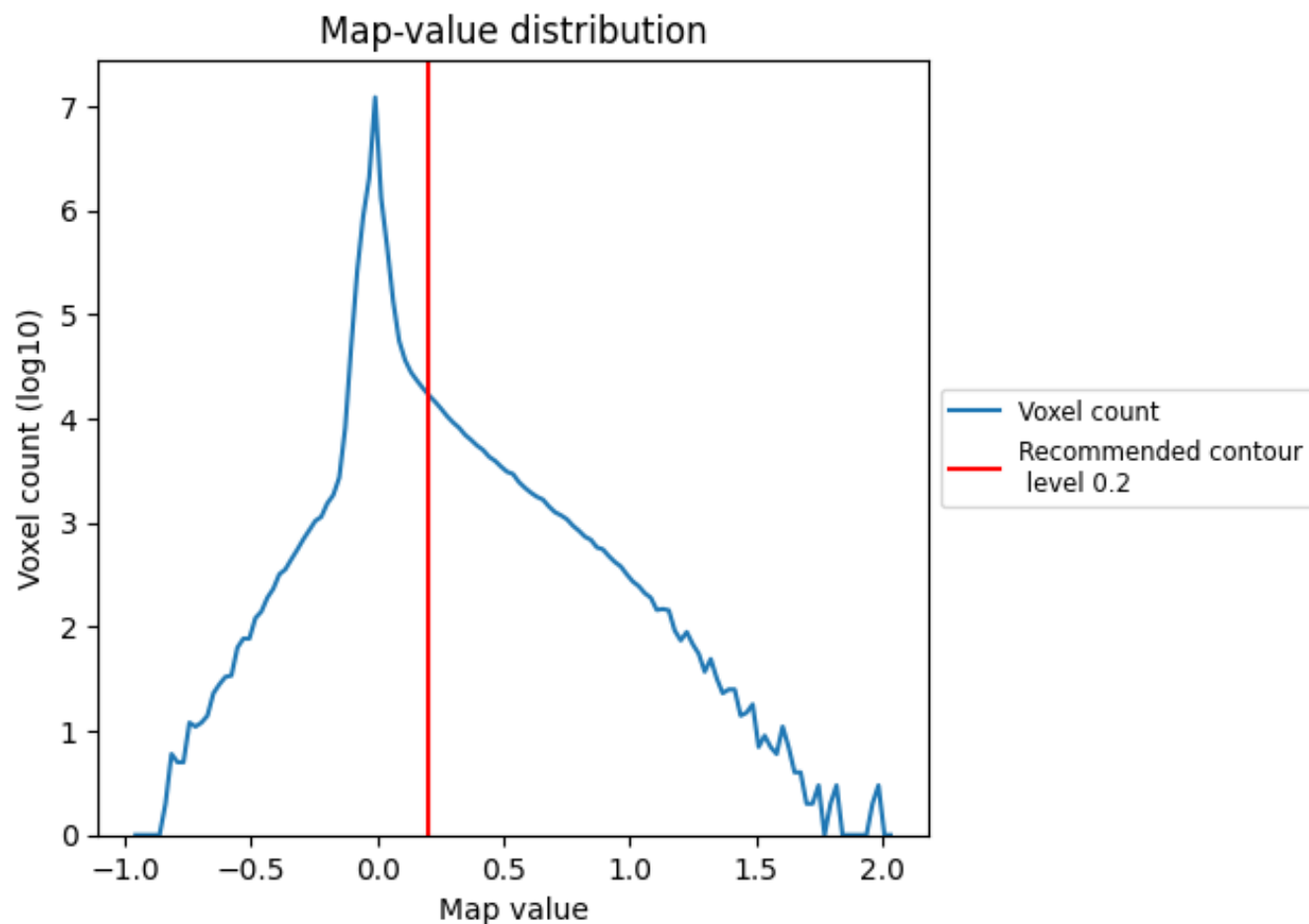
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

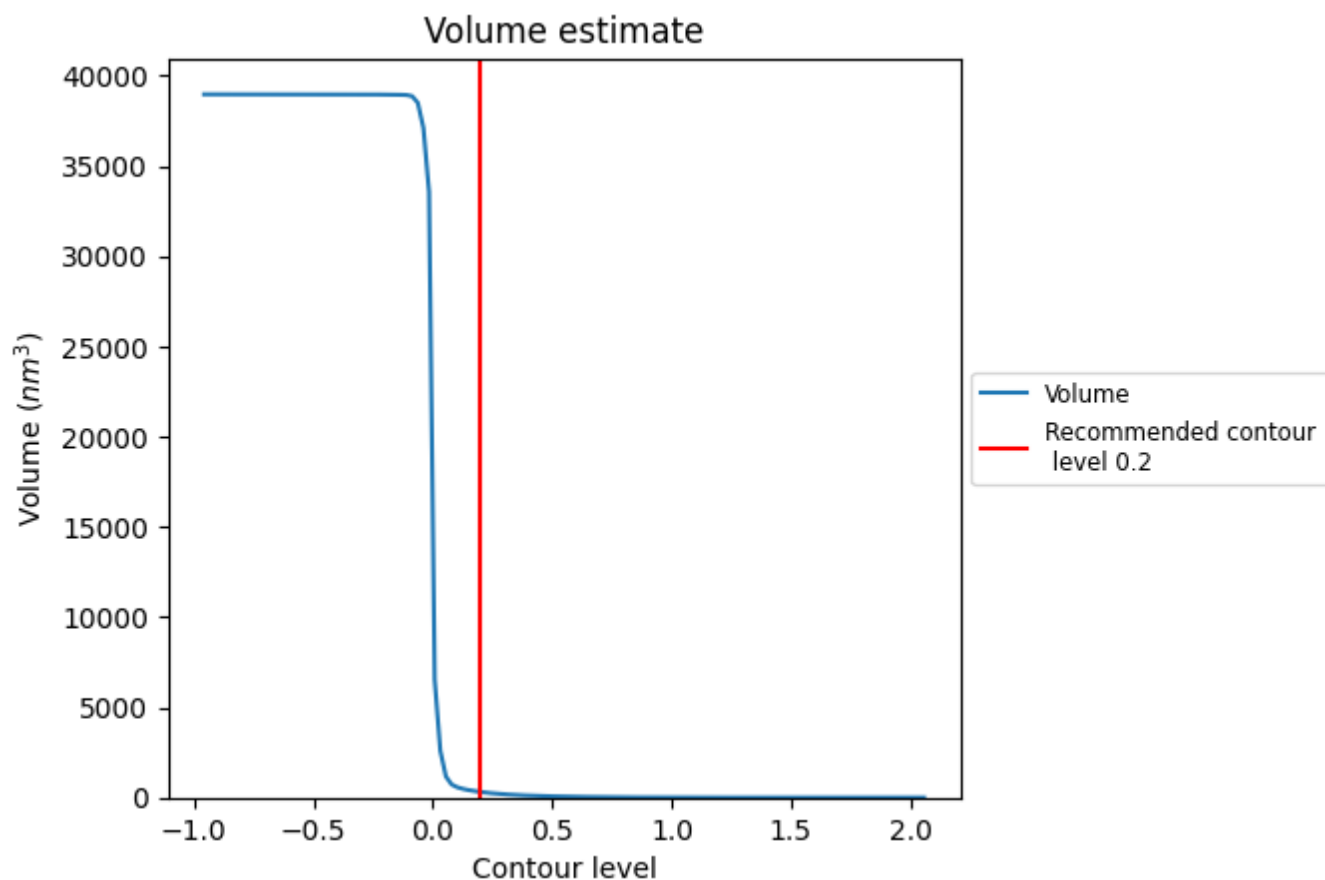
This section contains the results of statistical analysis of the map.

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.

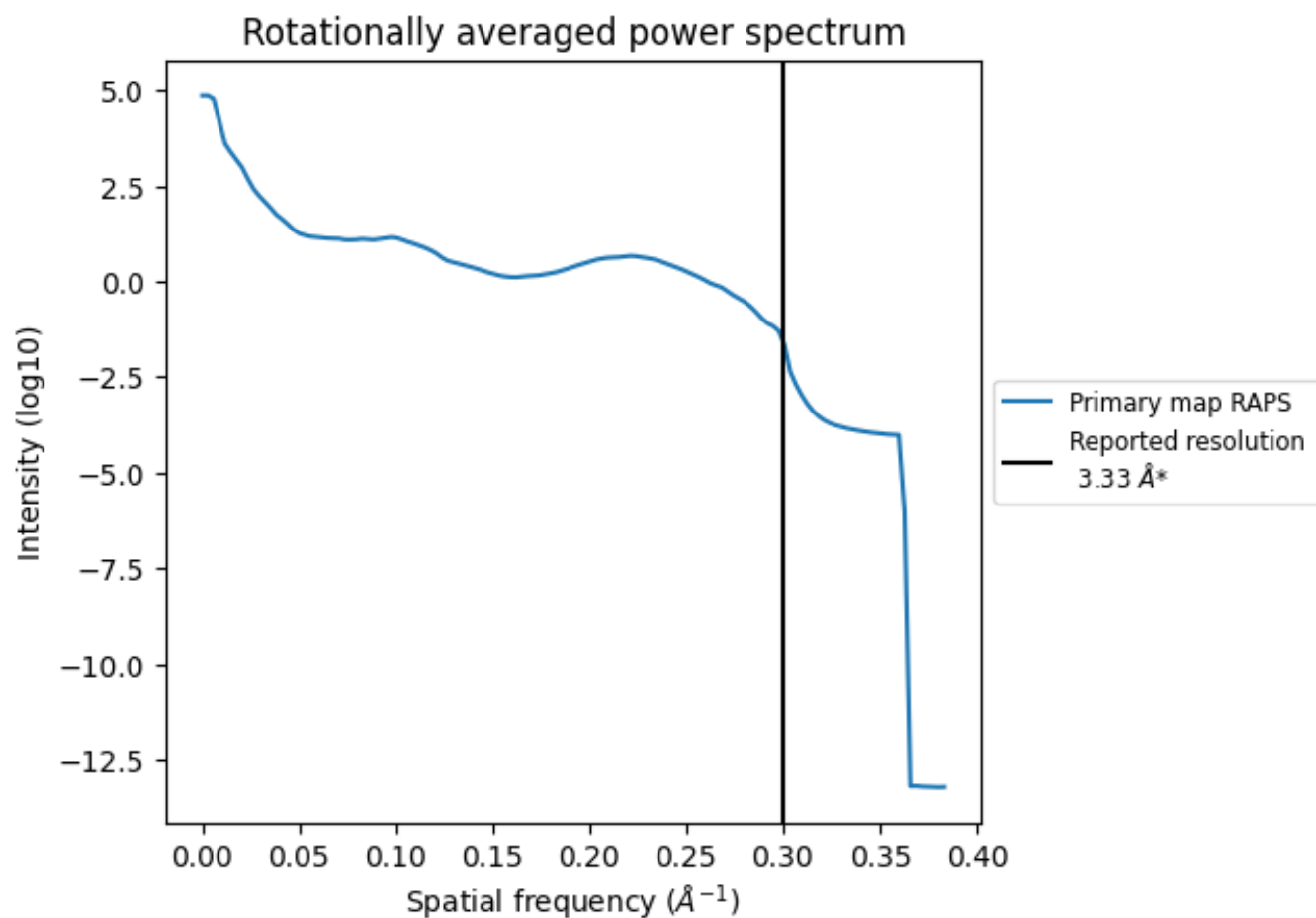
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 310 nm^3 ; this corresponds to an approximate mass of 280 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 0.300 Å⁻¹

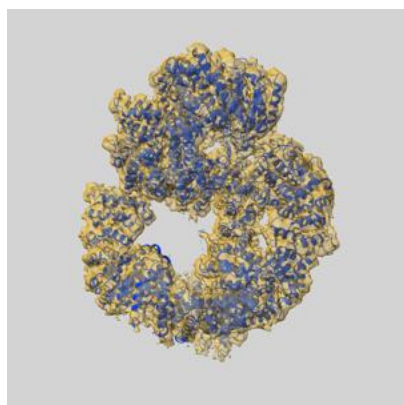
8 Fourier-Shell correlation

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

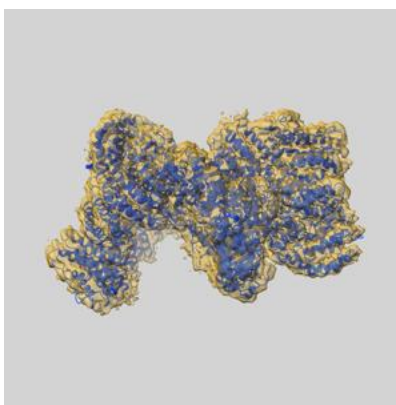
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13062 and PDB model 7OTM. Per-residue inclusion information can be found in section [3](#) on page [4](#).

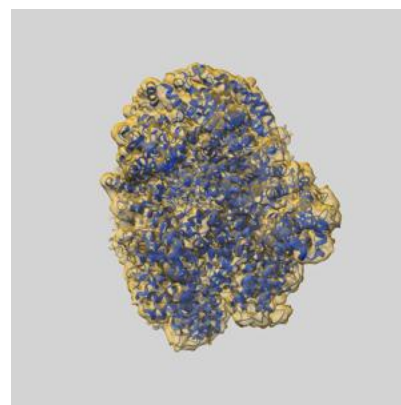
9.1 Map-model overlay [i](#)



X



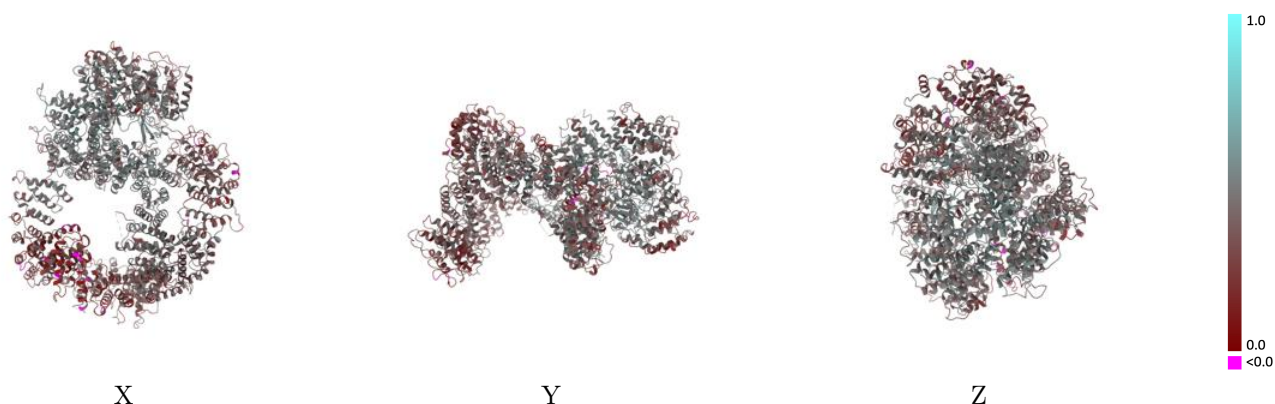
Y



Z

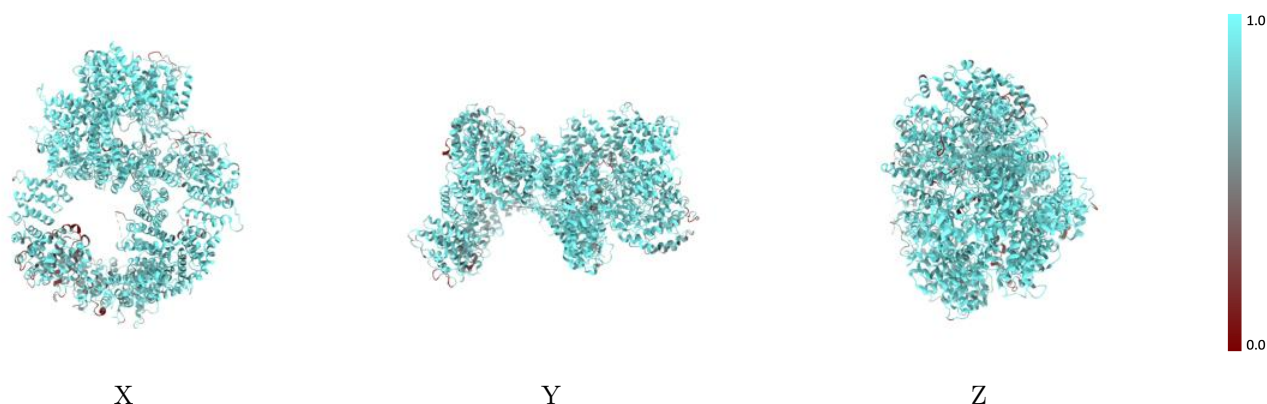
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



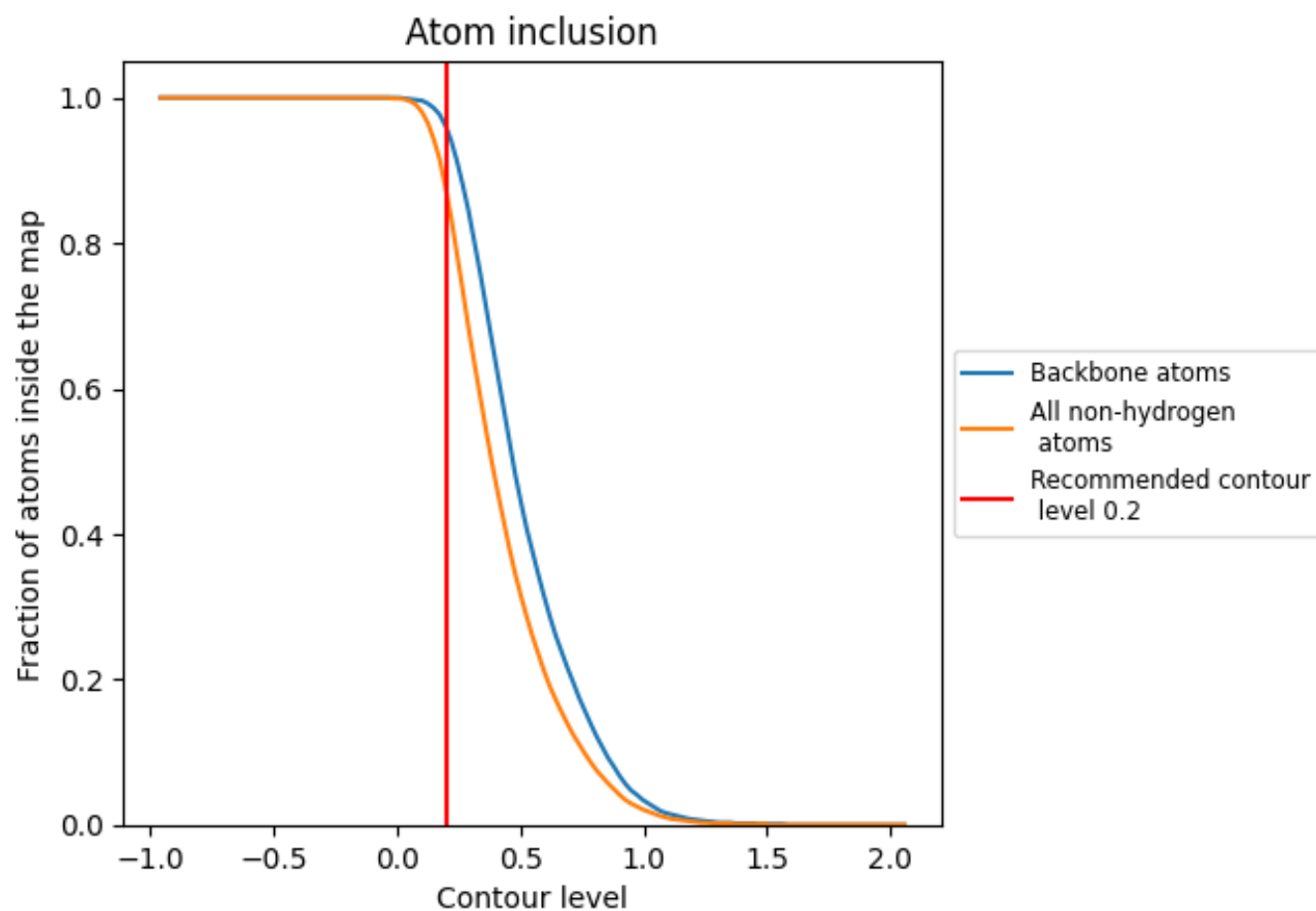
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.3940
A	0.8710	0.3940

