



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:45 AM UTC

PDB ID : 7OTW / pdb_00007otw
EMDB ID : EMD-13068
Title : DNA-PKcs in complex with AZD7648
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 2.99 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

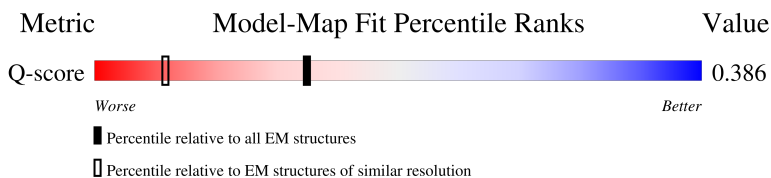
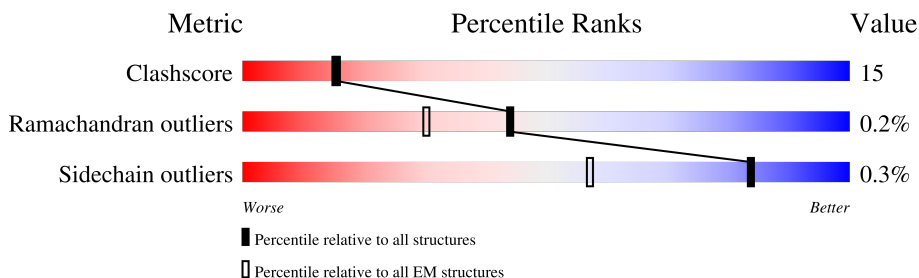
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 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	13287 (2.49 - 3.49)

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](#)

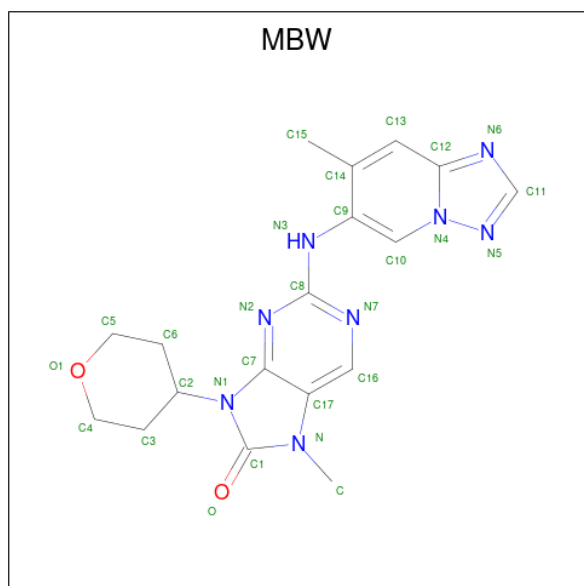
There are 2 unique types of molecules in this entry. The entry contains 29038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 7-methyl-2-[(7-methyl-[1,2,4]triazolo[1,5-a]pyridin-6-yl)amino]-9-(oxan-4-yl)purin-8-one (CCD ID: MBW) (formula: C₁₈H₂₀N₈O₂) (labeled as "Ligand of Interest" by depositor).

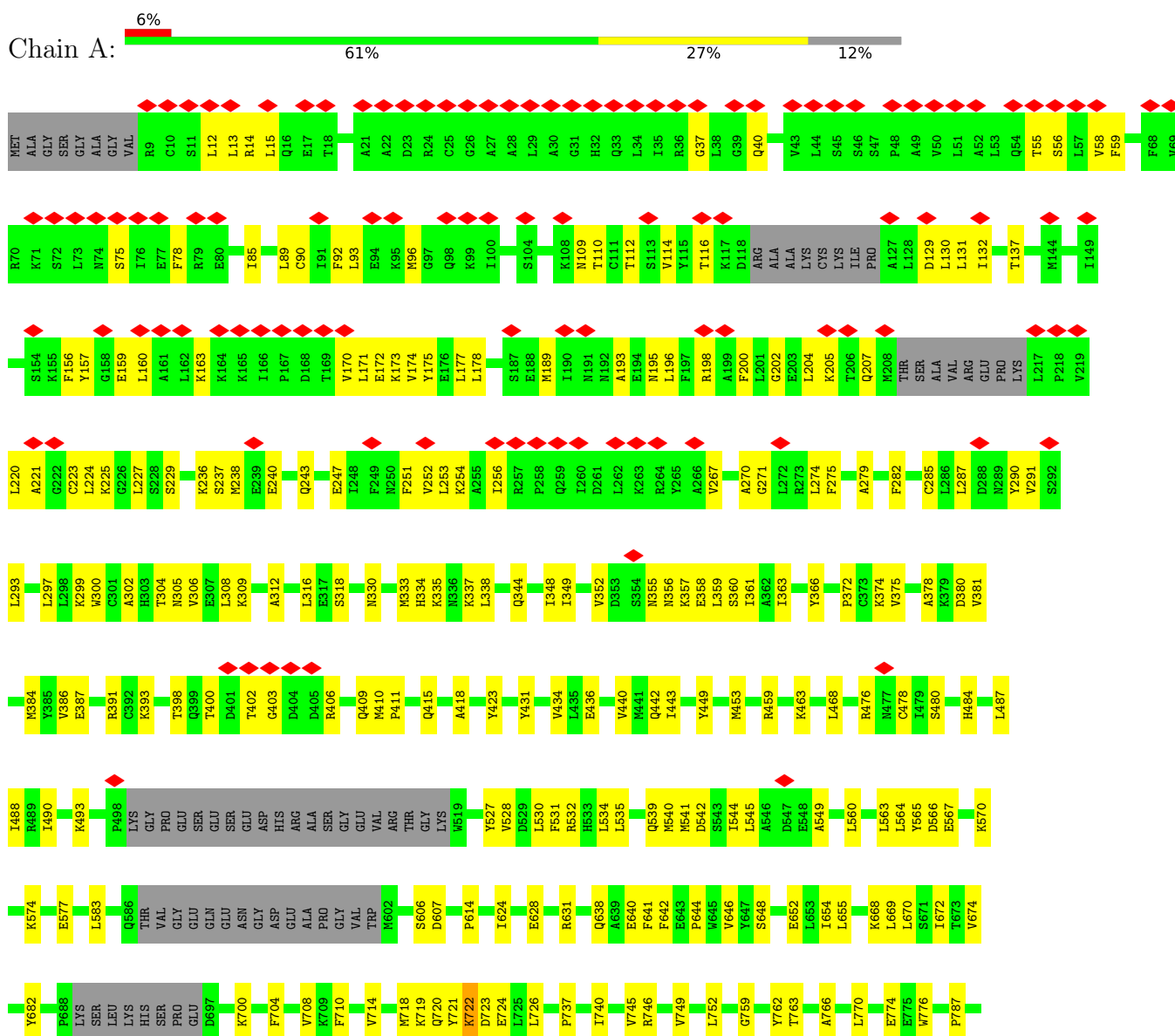


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	28	18	8	2	0

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







R4082	Q3966	F3636	A3730	S3731	Y3442
G4083	F3967	F3640	R3734	S3731	I3535
S4084	I3968	K3646	P3735	R3734	I3540
H4087	N3969	K3650	K3736	P3735	S3541
R4090	M3971	K3655	R3741	K3736	E3448
E4095	L3972	L3656	G3742	L3655	F3542
	P3973	H3743	H3743	D3658	K3543
	L3979	P3749	P3749	L3666	D3544
	S3982	E3875	K3763	K3667	G3548
I3983	S3876	D3881	L3758	L3666	K3552
M3984	M3984	L3882	R3759	L3666	F3554
	A3987	L3883	R3763	K3667	V3555
	P3995	K3884	N3772	K3667	K3561
	T3999	R3885	A3780	K3667	Q3564
	M4000	A3886	R3784	K3667	V3567
	M4002	E3895	L3788	K3667	I3568
	V4006	S3907	R3789	K3667	A3574
	K4007	H3908	V3794	K3667	L3575
	E4008	A3909	P3795	K3667	T3484
	F4011	L3910	M3796	K3667	K3485
	G4024	C3912	T3797	K3667	E3486
	G4025	L3913	S3798	K3667	I3487
	I4028	D3922	L3699	K3667	P3491
		L3925	E3700	K3667	C3492
		N3926	G3701	K3667	W3493
		N3927	P3702	K3667	F3495
		F3928	G3703	K3667	I3496
		M3929	Q3704	K3667	S3497
		Q3930	Y3705	K3667	V3498
		A3931	D3706	K3667	I3499
		M3932	G3707	K3667	S3500
		T3938	K3710	K3667	K3502
		G3939	P3711	K3667	L3505
		I3940	L3712	K3667	L3506
		D3941	P3713	K3667	D3507
		F3946	E3714	K3667	V3518
		V3955	Y3715	K3667	E3519
		K3959	H3716	K3667	F3520
		T4060	V3717	K3667	I3521
		C4061	R3718	K3667	D3523
		D4062	F3722	K3667	P3526
		D4076	V3726	K3667	Q3527
		V4080	T3727	K3667	F3528
		A4081	M3729	K3667	I3529
				K3667	V3530
				K3667	Y3531

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	164192	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 ($e^-/\text{\AA}^2$)	46.8	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	1.623	Depositor
Minimum map value	-0.529	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.042	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/29502	0.54	7/39893 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3455	LYS	N-CA-C	-7.25	103.46	111.36
1	A	4028	ILE	N-CA-C	-7.17	106.90	113.71
1	A	3231	ILE	N-CA-C	-5.82	107.14	112.96
1	A	3753	LYS	N-CA-C	-5.67	101.66	110.10
1	A	1085	ILE	CA-C-N	-5.11	111.84	121.66
1	A	1085	ILE	C-N-CA	-5.11	111.84	121.66
1	A	3693	GLU	N-CA-C	5.05	121.55	110.80

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	29194	812	0
2	A	28	0	0	0	0
All	All	29038	0	29194	812	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 15.

All (812) 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:3810:VAL:CG2	1:A:3932:MET:SD	2.45	1.05
1:A:3810:VAL:HG21	1:A:3932:MET:SD	2.02	1.00
1:A:3812:LEU:HB3	1:A:3925:LEU:O	1.73	0.88
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.06	0.87
1:A:3451:LEU:HD23	1:A:3454:LEU:HD12	1.56	0.87
1:A:3469:LEU:HD12	1:A:3505:LEU:HD21	1.57	0.86
1:A:3810:VAL:HG22	1:A:3932:MET:CG	2.06	0.84
1:A:721:TYR:HD2	1:A:726:LEU:HA	1.41	0.83
1:A:2102:LYS:HA	1:A:2105:HIS:HD2	1.44	0.82
1:A:1412:LYS:HA	1:A:1415:LEU:HD12	1.62	0.82
1:A:2216:LEU:HG	1:A:2220:MET:HE1	1.59	0.82
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.53	0.81
1:A:3810:VAL:HG22	1:A:3932:MET:HG2	1.62	0.81
1:A:2365:ASN:HD21	1:A:2399:GLU:HB2	1.47	0.80
1:A:240:GLU:HB2	1:A:243:GLN:HE22	1.47	0.79
1:A:3810:VAL:HG22	1:A:3932:MET:SD	2.20	0.79
1:A:1251:GLN:HB3	1:A:1254:LEU:HD12	1.63	0.79
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.56	0.78
1:A:1202:ARG:HH12	1:A:1210:ASP:HB2	1.47	0.78
1:A:3491:PRO:HB3	1:A:3493:TRP:NE1	1.99	0.78
1:A:3809:THR:HG22	1:A:3931:ALA:HA	1.68	0.76
1:A:1104:LEU:HD23	1:A:1168:LEU:HD11	1.67	0.75
1:A:1754:GLN:HA	1:A:1785:ILE:HD11	1.68	0.74
1:A:1980:ASN:HB2	1:A:1982:ILE:HG12	1.69	0.74
1:A:4081:ALA:O	1:A:4090:ARG:NH1	2.21	0.73
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.52	0.73
1:A:2091:HIS:NE2	1:A:2093:CYS:SG	2.62	0.73
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	1.70	0.73
1:A:721:TYR:CD2	1:A:726:LEU:HA	2.24	0.72
1:A:2575:PRO:HA	1:A:2786:LYS:H	1.55	0.72
1:A:3527:GLN:HA	1:A:3530:VAL:HG12	1.70	0.72
1:A:3666:LEU:HB3	1:A:3670:MET:HE3	1.72	0.72
1:A:2455:LEU:HD22	1:A:2498:ILE:HG23	1.71	0.72
1:A:13:LEU:HD23	1:A:14:ARG:HE	1.56	0.71
1:A:3711:PRO:O	1:A:3713:PRO:HD3	1.91	0.71
1:A:2254:ARG:NH1	1:A:2292:CYS:O	2.24	0.70
1:A:3622:ALA:HB3	1:A:3625:LEU:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4090:ARG:NH2	1:A:4113:ASP:OD2	2.25	0.70
1:A:358:GLU:HA	1:A:361:ILE:HD12	1.72	0.70
1:A:1357:LYS:HA	1:A:1361:LYS:HD3	1.71	0.70
1:A:3169:PRO:HD3	1:A:3182:ILE:HD11	1.74	0.70
1:A:3734:ARG:O	1:A:3736:LYS:NZ	2.25	0.70
1:A:3406:ALA:O	1:A:3409:VAL:HG12	1.92	0.69
1:A:1151:ARG:HB2	1:A:1163:LEU:HB2	1.74	0.69
1:A:2887:PRO:HG2	1:A:3895:GLU:HG3	1.72	0.69
1:A:1267:TYR:CE2	1:A:1290:LEU:HD13	2.28	0.69
1:A:415:GLN:O	1:A:463:LYS:NZ	2.25	0.69
1:A:1795:VAL:HG21	1:A:1838:GLU:HG3	1.75	0.69
1:A:1406:LEU:HB3	1:A:1415:LEU:HD11	1.74	0.68
1:A:2257:PHE:O	1:A:2261:SER:HB3	1.92	0.68
1:A:3666:LEU:O	1:A:3670:MET:HG3	1.93	0.68
1:A:403:GLY:H	1:A:406:ARG:HH12	1.41	0.68
1:A:1248:PHE:HB2	1:A:1309:ALA:HA	1.76	0.68
1:A:3491:PRO:HB3	1:A:3493:TRP:HE1	1.58	0.68
1:A:721:TYR:HB3	1:A:726:LEU:HB2	1.75	0.68
1:A:1242:LEU:HG	1:A:1310:GLU:HB2	1.74	0.68
1:A:1444:ASP:HA	1:A:1447:ARG:HG2	1.76	0.68
1:A:402:THR:HA	1:A:406:ARG:HH22	1.59	0.68
1:A:2563:LEU:HD13	1:A:2812:LEU:HD11	1.76	0.67
1:A:2365:ASN:ND2	1:A:2399:GLU:OE1	2.27	0.67
1:A:2379:MET:HE1	1:A:2404:ARG:HB2	1.75	0.67
1:A:1975:LEU:HD12	1:A:1976:LEU:HD12	1.76	0.67
1:A:3481:SER:O	1:A:3485:LYS:N	2.22	0.67
1:A:1355:GLY:HA2	1:A:1358:LEU:HD12	1.77	0.67
1:A:2373:PRO:HA	1:A:2404:ARG:HD2	1.77	0.67
1:A:3685:PRO:HB2	1:A:3687:MET:H	1.57	0.67
1:A:1554:SER:HB3	1:A:1557:GLU:OE1	1.94	0.67
1:A:12:LEU:HA	1:A:15:LEU:HB3	1.77	0.67
1:A:4058:VAL:HG22	1:A:4082:ARG:HH22	1.59	0.67
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.27	0.66
1:A:2102:LYS:HA	1:A:2105:HIS:CD2	2.29	0.66
1:A:542:ASP:HA	1:A:545:LEU:HD12	1.77	0.66
1:A:1801:VAL:HG13	1:A:1804:MET:HE2	1.76	0.66
1:A:787:PRO:O	1:A:790:LYS:NZ	2.29	0.66
1:A:1605:PHE:O	1:A:1608:ARG:NH2	2.25	0.66
1:A:355:ASN:OD1	1:A:356:ASN:N	2.29	0.66
1:A:3256:MET:HG2	1:A:3260:LYS:HE2	1.77	0.66
1:A:1938:ARG:NH1	1:A:2092:GLU:OE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1642:LYS:NZ	1:A:1681:ASP:OD2	2.29	0.65
1:A:221:ALA:O	1:A:225:LYS:NZ	2.27	0.65
1:A:2884:LEU:HD12	1:A:3116:SER:HB2	1.77	0.65
1:A:1407:LYS:NZ	1:A:1461:ALA:O	2.20	0.65
1:A:4039:TYR:HD2	1:A:4042:GLN:HG2	1.60	0.65
1:A:3012:GLU:HA	1:A:3016:THR:HG22	1.78	0.65
1:A:189:MET:HG3	1:A:193:ALA:HB2	1.77	0.65
1:A:1185:HIS:NE2	1:A:1265:GLU:OE2	2.29	0.65
1:A:3137:GLU:OE1	1:A:3186:ARG:NH2	2.18	0.65
1:A:3497:SER:HB3	1:A:3707:GLY:HA3	1.77	0.65
1:A:75:SER:H	1:A:78:PHE:HB3	1.61	0.65
1:A:1290:LEU:H	1:A:1290:LEU:HD23	1.62	0.64
1:A:3315:TYR:CZ	1:A:3318:LYS:HE2	2.33	0.64
1:A:1445:ARG:HG3	1:A:1510:LEU:HD13	1.79	0.64
1:A:2281:MET:SD	1:A:2287:PRO:HG3	2.38	0.64
1:A:1448:LEU:HB3	1:A:1510:LEU:HD11	1.80	0.64
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.79	0.64
1:A:1637:SER:HB3	1:A:1642:LYS:HE2	1.80	0.64
1:A:3878:VAL:O	1:A:3965:ARG:NH2	2.31	0.64
1:A:1420:ARG:HE	1:A:1467:ILE:HA	1.62	0.64
1:A:3531:TYR:O	1:A:3535:ILE:HG13	1.98	0.64
1:A:3012:GLU:HB3	1:A:3047:SER:OG	1.98	0.64
1:A:1782:PHE:HA	1:A:1785:ILE:HG22	1.79	0.63
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.79	0.63
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.31	0.63
1:A:3702:PRO:HB2	1:A:3794:VAL:HG11	1.78	0.63
1:A:2395:THR:O	1:A:2399:GLU:HG3	1.98	0.63
1:A:3191:SER:OG	1:A:3235:LYS:NZ	2.27	0.63
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.80	0.63
1:A:737:PRO:HD2	1:A:740:ILE:HD12	1.80	0.63
1:A:1224:PHE:HD2	1:A:1267:TYR:HE1	1.46	0.63
1:A:1476:HIS:HB3	1:A:1479:VAL:HG22	1.79	0.62
1:A:1759:LEU:HG	1:A:1782:PHE:HE1	1.64	0.62
1:A:3494:GLN:C	1:A:3496:ILE:H	2.07	0.62
1:A:195:ASN:OD1	1:A:196:LEU:N	2.32	0.62
1:A:539:GLN:HE22	1:A:541:MET:HE3	1.65	0.62
1:A:917:LEU:O	1:A:921:ALA:HB2	1.99	0.62
1:A:3284:SER:HB3	1:A:3301:LEU:HD12	1.80	0.62
1:A:875:SER:HA	1:A:878:GLU:HB2	1.81	0.61
1:A:2239:LYS:HB2	1:A:2279:ILE:HD12	1.80	0.61
1:A:4060:THR:HG21	1:A:4110:GLN:HE22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2406:GLU:OE1	1:A:2406:GLU:N	2.29	0.61
1:A:3281:CYS:HB2	1:A:3329:LEU:HD23	1.82	0.61
1:A:1358:LEU:HD21	1:A:1410:PRO:HB2	1.82	0.61
1:A:3763:ARG:HG3	1:A:4011:PHE:HZ	1.64	0.61
1:A:2517:LEU:HA	1:A:2520:ILE:HD12	1.83	0.61
1:A:1290:LEU:HG	1:A:1291:LEU:HD22	1.82	0.61
1:A:1298:LEU:O	1:A:1367:HIS:NE2	2.25	0.61
1:A:2347:LYS:O	1:A:2351:GLN:NE2	2.33	0.61
1:A:3006:ALA:HB3	1:A:3257:LYS:HE2	1.82	0.61
1:A:566:ASP:O	1:A:570:LYS:HG2	2.01	0.60
1:A:3960:PRO:HD3	1:A:4110:GLN:HG2	1.83	0.60
1:A:403:GLY:O	1:A:406:ARG:NH1	2.34	0.60
1:A:1729:PHE:HB3	1:A:1736:PHE:HB2	1.84	0.60
1:A:1227:GLY:N	1:A:1233:SER:O	2.35	0.60
1:A:1241:LEU:H	1:A:1296:PHE:HE2	1.48	0.60
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.83	0.60
1:A:1324:PRO:O	1:A:1327:GLY:N	2.35	0.60
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.36	0.60
1:A:989:MET:SD	1:A:1035:GLU:HG3	2.41	0.60
1:A:3678:GLY:HA3	1:A:3728:VAL:HG21	1.82	0.60
1:A:3416:LEU:HD21	1:A:3445:LEU:HD21	1.83	0.60
1:A:2376:ASP:OD1	1:A:2404:ARG:NE	2.35	0.59
1:A:360:SER:OG	1:A:409:GLN:OE1	2.19	0.59
1:A:2540:LEU:HD21	1:A:2832:ILE:HG23	1.84	0.59
1:A:1056:THR:HG21	1:A:1095:LEU:HD21	1.85	0.59
1:A:3194:GLU:HB2	1:A:3231:ILE:HD11	1.84	0.59
1:A:3646:LYS:H	1:A:3650:LYS:HB2	1.67	0.59
1:A:3844:THR:HB	1:A:3850:HIS:HB3	1.85	0.59
1:A:1709:GLU:HA	1:A:1712:ARG:HE	1.68	0.59
1:A:2869:LEU:HB2	1:A:2900:LEU:HD13	1.83	0.59
1:A:3244:ASP:OD1	1:A:3247:ARG:NH1	2.33	0.59
1:A:1184:ARG:NH1	1:A:1265:GLU:OE1	2.35	0.59
1:A:1452:VAL:HG23	1:A:1517:LEU:HD22	1.84	0.59
1:A:3027:LEU:HA	1:A:3030:ILE:HG22	1.85	0.59
1:A:3726:VAL:HG13	1:A:3736:LYS:HB3	1.85	0.59
1:A:796:LEU:HD23	1:A:855:VAL:HG13	1.85	0.59
1:A:2371:PHE:CD2	1:A:2374:LEU:HB2	2.38	0.59
1:A:528:VAL:HG12	1:A:532:ARG:HE	1.68	0.59
1:A:923:ASP:OD2	1:A:2800:ARG:NH2	2.36	0.59
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.38	0.59
1:A:2410:GLU:O	1:A:2414:GLN:NE2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3009:LYS:O	1:A:3013:TYR:HB3	2.02	0.59
1:A:606:SER:OG	1:A:1026:ARG:NH2	2.36	0.59
1:A:3523:ASP:OD1	1:A:3561:LYS:NZ	2.20	0.59
1:A:3450:MET:SD	1:A:3468:LEU:HD21	2.42	0.58
1:A:1684:LEU:HB3	1:A:1688:LEU:HD22	1.84	0.58
1:A:1739:TYR:OH	1:A:1772:HIS:NE2	2.29	0.58
1:A:3875:GLU:HG2	1:A:3965:ARG:HD3	1.85	0.58
1:A:238:MET:HE3	1:A:282:PHE:HA	1.86	0.58
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.84	0.58
1:A:1224:PHE:CD2	1:A:1267:TYR:HE1	2.20	0.58
1:A:1611:GLN:HB3	1:A:1614:GLN:HG2	1.83	0.58
1:A:1933:LEU:HD13	1:A:1936:ARG:HB2	1.85	0.58
1:A:1153:LEU:HD13	1:A:1163:LEU:HD21	1.84	0.58
1:A:3965:ARG:O	1:A:3969:ASN:HB2	2.03	0.58
1:A:1078:ALA:O	1:A:1107:TYR:OH	2.16	0.58
1:A:1763:THR:HG21	1:A:1804:MET:HE1	1.84	0.58
1:A:3031:TRP:HE1	1:A:3041:LEU:HB2	1.68	0.58
1:A:200:PHE:HE1	1:A:224:LEU:HD22	1.69	0.57
1:A:995:PHE:HD2	1:A:1005:ASP:HA	1.69	0.57
1:A:1607:GLU:OE2	1:A:1614:GLN:NE2	2.36	0.57
1:A:1812:LEU:HG	1:A:1814:PHE:HB3	1.86	0.57
1:A:3033:GLU:CD	1:A:3034:PRO:HD3	2.29	0.57
1:A:3589:SER:OG	1:A:3593:ARG:NH2	2.37	0.57
1:A:2190:VAL:HG11	1:A:2237:ILE:HG23	1.87	0.57
1:A:2183:HIS:CE1	1:A:2185:MET:HE2	2.39	0.57
1:A:2408:MET:HE1	1:A:2411:LEU:HD13	1.87	0.57
1:A:3580:ASN:HB2	1:A:3583:LEU:HD12	1.87	0.57
1:A:172:GLU:HB3	1:A:220:LEU:HD12	1.85	0.57
1:A:2371:PHE:HD2	1:A:2374:LEU:HB2	1.68	0.57
1:A:3646:LYS:N	1:A:3650:LYS:HB2	2.20	0.57
1:A:2999:LEU:HD21	1:A:3015:SER:O	2.05	0.57
1:A:1444:ASP:OD1	1:A:1444:ASP:N	2.37	0.57
1:A:3812:LEU:HD22	1:A:3928:PHE:HB2	1.86	0.57
1:A:648:SER:O	1:A:652:GLU:HG2	2.05	0.56
1:A:1265:GLU:HG3	1:A:1340:ARG:HH21	1.70	0.56
1:A:1589:ASN:OD1	1:A:1592:MET:N	2.36	0.56
1:A:2937:ASP:OD1	1:A:3982:SER:OG	2.21	0.56
1:A:539:GLN:HG2	1:A:540:MET:N	2.21	0.56
1:A:642:PHE:CE2	1:A:646:VAL:HG22	2.40	0.56
1:A:917:LEU:O	1:A:921:ALA:CB	2.52	0.56
1:A:3618:GLY:H	1:A:3633:ILE:HG12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HA	1:A:59:PHE:CD2	2.41	0.56
1:A:3176:MET:HE3	1:A:3246:ALA:HA	1.88	0.56
1:A:3685:PRO:HG2	1:A:3687:MET:HB2	1.88	0.56
1:A:359:LEU:O	1:A:363:ILE:HG12	2.06	0.56
1:A:1639:LEU:O	1:A:1643:MET:HG2	2.05	0.56
1:A:2286:PRO:HG2	1:A:2289:ASP:HB2	1.87	0.56
1:A:423:TYR:OH	1:A:549:ALA:O	2.18	0.56
1:A:1805:PHE:O	1:A:1816:ARG:NH2	2.31	0.56
1:A:2220:MET:HG3	1:A:2276:LEU:HD13	1.88	0.56
1:A:1260:LEU:O	1:A:1264:LEU:HG	2.06	0.56
1:A:3394:GLU:OE1	1:A:3394:GLU:N	2.39	0.56
1:A:853:ILE:HG12	1:A:3111:MET:HE1	1.88	0.55
1:A:3496:ILE:HB	1:A:3707:GLY:HA2	1.88	0.55
1:A:1447:ARG:O	1:A:1451:VAL:HG23	2.06	0.55
1:A:3564:GLN:HE21	1:A:3567:VAL:HG12	1.72	0.55
1:A:3418:ASP:O	1:A:3422:GLN:HG2	2.06	0.55
1:A:3491:PRO:CB	1:A:3493:TRP:NE1	2.70	0.55
1:A:131:LEU:HD22	1:A:173:LYS:HD2	1.87	0.55
1:A:1443:VAL:O	1:A:1446:SER:OG	2.23	0.55
1:A:4084:SER:OG	1:A:4087:HIS:ND1	2.32	0.55
1:A:1921:ASP:OD1	1:A:1922:ALA:N	2.40	0.55
1:A:2270:ASN:O	1:A:2274:ILE:HG12	2.06	0.55
1:A:2464:HIS:CE1	1:A:2466:SER:HB2	2.41	0.55
1:A:3451:LEU:O	1:A:3454:LEU:HB2	2.07	0.55
1:A:3451:LEU:CD2	1:A:3454:LEU:HD12	2.34	0.55
1:A:3496:ILE:HA	1:A:3499:ILE:HD11	1.88	0.55
1:A:2890:ILE:O	1:A:2894:GLU:HG3	2.06	0.55
1:A:3478:GLU:OE1	1:A:3478:GLU:N	2.39	0.55
1:A:156:PHE:HB3	1:A:178:LEU:HB2	1.89	0.55
1:A:891:ARG:N	1:A:908:ASP:OD2	2.26	0.55
1:A:1563:PHE:O	1:A:1567:ILE:HG12	2.07	0.55
1:A:1975:LEU:HD13	1:A:2093:CYS:SG	2.46	0.55
1:A:2382:VAL:HG11	1:A:2400:VAL:HG11	1.88	0.54
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.89	0.54
1:A:349:ILE:HD11	1:A:391:ARG:HG3	1.90	0.54
1:A:2415:LEU:HD12	1:A:2420:PHE:CG	2.42	0.54
1:A:1335:CYS:HB2	1:A:1384:PHE:CE2	2.42	0.54
1:A:3278:GLN:HB2	1:A:3329:LEU:HD22	1.88	0.54
1:A:2257:PHE:O	1:A:2261:SER:CB	2.55	0.54
1:A:1714:LEU:O	1:A:1718:ILE:HG23	2.08	0.54
1:A:3176:MET:HE3	1:A:3246:ALA:CA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:HIS:CD2	1:A:1180:GLN:HA	2.42	0.54
1:A:2571:ASP:OD1	1:A:2574:ASN:ND2	2.41	0.54
1:A:3134:ALA:HB2	1:A:3182:ILE:HG22	1.89	0.54
1:A:3500:SER:OG	1:A:3763:ARG:NH2	2.41	0.54
1:A:3542:PHE:HZ	1:A:3555:VAL:HG21	1.72	0.54
1:A:3749:PRO:HB2	1:A:3805:TRP:HB3	1.90	0.54
1:A:1851:LEU:HD23	1:A:1870:LYS:HG2	1.89	0.54
1:A:2785:ILE:O	1:A:2789:SER:OG	2.20	0.54
1:A:3356:ALA:O	1:A:3359:ILE:HG22	2.07	0.54
1:A:3507:ASP:HB3	1:A:3540:TYR:CD1	2.43	0.54
1:A:157:TYR:OH	1:A:189:MET:SD	2.59	0.54
1:A:1976:LEU:HD22	1:A:2142:ILE:HG13	1.89	0.54
1:A:1298:LEU:HB3	1:A:1367:HIS:HD2	1.72	0.53
1:A:901:MET:HB3	1:A:2823:PHE:CE2	2.43	0.53
1:A:2091:HIS:HD2	1:A:2094:MET:H	1.57	0.53
1:A:2235:LEU:HD12	1:A:2279:ILE:HG13	1.90	0.53
1:A:4039:TYR:CE2	1:A:4041:ARG:HB3	2.43	0.53
1:A:229:SER:HB3	1:A:274:LEU:HB2	1.90	0.53
1:A:800:LEU:O	1:A:852:ARG:NH2	2.39	0.53
1:A:3527:GLN:HA	1:A:3530:VAL:CG1	2.37	0.53
1:A:1868:THR:HG23	1:A:1871:MET:HE2	1.90	0.53
1:A:3003:ASN:OD1	1:A:3046:ARG:NH1	2.41	0.53
1:A:2478:MET:HG2	1:A:2524:PHE:CE1	2.43	0.53
1:A:3518:VAL:O	1:A:3521:ILE:HG22	2.08	0.53
1:A:3842:TRP:NE1	1:A:3846:MET:HE3	2.23	0.53
1:A:967:PRO:O	1:A:971:ARG:HG3	2.09	0.53
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.31	0.53
1:A:3627:ALA:N	1:A:3683:CYS:O	2.41	0.53
1:A:6017:UNK:O	1:A:6019:UNK:N	2.42	0.53
1:A:393:LYS:HB2	1:A:434:VAL:HG11	1.91	0.53
1:A:535:LEU:HD13	1:A:565:TYR:HD1	1.73	0.53
1:A:2277:LEU:O	1:A:2281:MET:HG2	2.09	0.53
1:A:305:ASN:HB3	1:A:308:LEU:HB3	1.89	0.53
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.44	0.53
1:A:719:LYS:HB2	1:A:720:GLN:NE2	2.23	0.52
1:A:3259:LEU:HD21	1:A:3280:TYR:HA	1.90	0.52
1:A:1431:LEU:HD12	1:A:1447:ARG:HD2	1.91	0.52
1:A:1641:THR:O	1:A:1645:VAL:HG23	2.10	0.52
1:A:2255:LEU:O	1:A:2259:LYS:HG2	2.09	0.52
1:A:3711:PRO:O	1:A:3713:PRO:CD	2.58	0.52
1:A:3876:SER:HA	1:A:3965:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD22	1:A:178:LEU:HD11	1.92	0.52
1:A:4120:THR:HB	1:A:4126:PRO:HG3	1.91	0.52
1:A:1568:ASN:HA	1:A:1571:LEU:HD12	1.90	0.52
1:A:252:VAL:O	1:A:256:ILE:HB	2.09	0.52
1:A:873:VAL:HA	1:A:876:SER:HB2	1.92	0.52
1:A:1775:GLU:O	1:A:1779:GLN:HG2	2.08	0.52
1:A:3925:LEU:HG	1:A:3962:ARG:NH2	2.24	0.52
1:A:436:GLU:O	1:A:440:VAL:HG23	2.10	0.52
1:A:1442:GLN:HG3	1:A:1445:ARG:NH1	2.25	0.52
1:A:372:PRO:HA	1:A:375:VAL:HG22	1.92	0.52
1:A:985:GLU:HG2	1:A:986:PRO:HD3	1.91	0.52
1:A:1208:LEU:HA	1:A:1211:VAL:HG12	1.90	0.52
1:A:1515:LEU:HD21	1:A:1567:ILE:HD11	1.92	0.52
1:A:1826:THR:O	1:A:1830:HIS:ND1	2.37	0.52
1:A:352:VAL:HB	1:A:1735:ARG:HD2	1.92	0.51
1:A:718:MET:HE2	1:A:726:LEU:HD11	1.91	0.51
1:A:3129:LEU:O	1:A:3132:VAL:HG12	2.11	0.51
1:A:3335:ARG:HH12	1:A:3422:GLN:HG3	1.75	0.51
1:A:251:PHE:HA	1:A:254:LYS:HZ2	1.75	0.51
1:A:418:ALA:HB3	1:A:463:LYS:HZ3	1.75	0.51
1:A:745:VAL:O	1:A:749:VAL:HG23	2.10	0.51
1:A:3702:PRO:CB	1:A:3794:VAL:HG11	2.40	0.51
1:A:2842:ARG:O	1:A:2846:THR:OG1	2.27	0.51
1:A:3542:PHE:HE2	1:A:3552:LYS:HA	1.75	0.51
1:A:3806:LEU:N	1:A:3806:LEU:HD23	2.25	0.51
1:A:484:HIS:NE2	1:A:488:ILE:HD11	2.26	0.51
1:A:1897:ASN:HB3	1:A:1903:SER:HB2	1.93	0.51
1:A:2542:LEU:HD21	1:A:2558:ALA:HA	1.91	0.51
1:A:3834:ALA:HB1	1:A:3836:PRO:HD2	1.92	0.51
1:A:112:THR:O	1:A:116:THR:HG23	2.10	0.51
1:A:1333:SER:O	1:A:1337:VAL:HG23	2.10	0.51
1:A:2415:LEU:HB3	1:A:2420:PHE:HB2	1.93	0.51
1:A:2449:VAL:O	1:A:2453:GLU:HG2	2.11	0.51
1:A:3763:ARG:HG3	1:A:4011:PHE:CZ	2.44	0.51
1:A:3574:ALA:HB1	1:A:3687:MET:HG3	1.92	0.51
1:A:2183:HIS:CE1	1:A:2185:MET:HB2	2.46	0.51
1:A:2559:THR:O	1:A:2563:LEU:HB2	2.09	0.51
1:A:3872:ARG:HH21	1:A:4114:PRO:HB3	1.76	0.51
1:A:4076:ASP:O	1:A:4080:VAL:HG12	2.10	0.51
1:A:624:ILE:O	1:A:628:GLU:HG2	2.11	0.51
1:A:3029:LYS:C	1:A:3031:TRP:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3498:TRP:O	1:A:3502:MET:HG3	2.11	0.51
1:A:3797:THR:HG22	1:A:3798:SER:N	2.26	0.51
1:A:172:GLU:H	1:A:172:GLU:CD	2.19	0.51
1:A:1384:PHE:CD2	1:A:1395:LEU:HD11	2.46	0.51
1:A:1972:GLU:HA	1:A:1975:LEU:HG	1.93	0.51
1:A:2101:VAL:HG21	1:A:2153:THR:HG21	1.93	0.51
1:A:236:LYS:HG2	1:A:243:GLN:NE2	2.26	0.51
1:A:721:TYR:CB	1:A:726:LEU:HB2	2.40	0.51
1:A:2287:PRO:HG2	1:A:2326:ILE:HG23	1.93	0.51
1:A:3353:GLU:HG2	1:A:3355:LYS:HG3	1.93	0.51
1:A:913:ARG:NH1	1:A:2801:ASP:OD1	2.44	0.50
1:A:1557:GLU:HG3	1:A:1592:MET:SD	2.51	0.50
1:A:1983:ASP:O	1:A:2185:MET:HE1	2.11	0.50
1:A:3069:MET:HE3	1:A:3078:LEU:HD23	1.92	0.50
1:A:1592:MET:HE3	1:A:1596:VAL:HG23	1.92	0.50
1:A:2950:LYS:HD2	1:A:2981:TRP:CZ3	2.46	0.50
1:A:2094:MET:HB3	1:A:2145:PHE:CE1	2.46	0.50
1:A:2567:SER:HA	1:A:2572:TYR:CG	2.45	0.50
1:A:3153:SER:OG	1:A:3154:GLN:N	2.44	0.50
1:A:92:PHE:O	1:A:96:MET:HG2	2.12	0.50
1:A:93:LEU:HD22	1:A:137:THR:HG22	1.92	0.50
1:A:2133:LEU:HD13	1:A:2146:LEU:HB2	1.94	0.50
1:A:2536:LEU:HD21	1:A:2820:MET:HE2	1.94	0.50
1:A:3542:PHE:CE2	1:A:3552:LYS:HA	2.45	0.50
1:A:3544:ASP:HB3	1:A:3548:GLY:H	1.77	0.50
1:A:2383:PHE:CD2	1:A:2414:GLN:HG2	2.47	0.50
1:A:3859:TYR:HE1	1:A:4080:VAL:HG11	1.76	0.50
1:A:237:SER:O	1:A:243:GLN:NE2	2.44	0.50
1:A:290:TYR:CE1	1:A:337:LYS:HE3	2.47	0.50
1:A:3072:GLU:C	1:A:3074:GLN:H	2.19	0.50
1:A:189:MET:HE3	1:A:193:ALA:N	2.27	0.50
1:A:443:ILE:HG23	1:A:530:LEU:HD21	1.93	0.50
1:A:2371:PHE:CD1	1:A:2373:PRO:HD2	2.46	0.50
1:A:998:ASN:OD1	1:A:999:LYS:N	2.45	0.50
1:A:2223:VAL:HG21	1:A:2276:LEU:HD11	1.93	0.50
1:A:3995:PRO:O	1:A:3999:THR:OG1	2.21	0.50
1:A:1296:PHE:O	1:A:1299:GLU:HG3	2.10	0.50
1:A:4002:MET:O	1:A:4006:VAL:HG13	2.12	0.50
1:A:1468:LEU:O	1:A:1476:HIS:NE2	2.42	0.49
1:A:2252:PRO:O	1:A:2254:ARG:HD2	2.12	0.49
1:A:3574:ALA:HB2	1:A:3686:TRP:NE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3575:LEU:HD12	1:A:3796:MET:HE1	1.94	0.49
1:A:37:GLY:O	1:A:40:GLN:HG2	2.11	0.49
1:A:476:ARG:O	1:A:480:SER:OG	2.31	0.49
1:A:1244:LEU:H	1:A:1244:LEU:HD23	1.76	0.49
1:A:2365:ASN:ND2	1:A:2399:GLU:HB2	2.22	0.49
1:A:3542:PHE:CZ	1:A:3555:VAL:HG21	2.48	0.49
1:A:1500:LEU:HD13	1:A:1540:THR:HG21	1.94	0.49
1:A:2813:PHE:CE1	1:A:2817:LEU:HD11	2.47	0.49
1:A:2877:SER:OG	1:A:2925:GLU:HB3	2.11	0.49
1:A:3626:GLY:HA3	1:A:3684:SER:O	2.13	0.49
1:A:1406:LEU:HD13	1:A:1415:LEU:HD21	1.94	0.49
1:A:1575:LEU:HD11	1:A:1617:LYS:HB3	1.95	0.49
1:A:3929:MET:SD	1:A:3940:ILE:HG21	2.52	0.49
1:A:468:LEU:HD13	1:A:478:CYS:HB3	1.94	0.49
1:A:1702:LEU:HG	1:A:1706:SER:HB3	1.94	0.49
1:A:1867:ILE:HA	1:A:1870:LYS:HE3	1.94	0.49
1:A:287:LEU:HD13	1:A:334:HIS:NE2	2.28	0.49
1:A:670:LEU:O	1:A:674:VAL:HG23	2.13	0.49
1:A:1632:TRP:HE3	1:A:1645:VAL:HG22	1.77	0.49
1:A:2231:PHE:CE1	1:A:2272:VAL:HG12	2.47	0.49
1:A:2510:LEU:O	1:A:2518:GLN:NE2	2.24	0.49
1:A:3439:LEU:HD12	1:A:3439:LEU:O	2.12	0.49
1:A:3464:LYS:HE2	1:A:4000:ASN:HD22	1.78	0.49
1:A:3726:VAL:CG1	1:A:3736:LYS:HB3	2.41	0.49
1:A:3446:VAL:O	1:A:3450:MET:HG2	2.12	0.49
1:A:563:LEU:O	1:A:567:GLU:HG2	2.13	0.48
1:A:1172:LEU:HD22	1:A:1187:SER:HA	1.95	0.48
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.95	0.48
1:A:3492:CYS:HB3	1:A:3520:GLU:OE1	2.13	0.48
1:A:3964:THR:H	1:A:3967:PHE:HD2	1.60	0.48
1:A:1568:ASN:HD21	1:A:1603:GLN:HG3	1.77	0.48
1:A:3269:ARG:C	1:A:3271:ASP:H	2.21	0.48
1:A:381:VAL:HA	1:A:384:MET:HE3	1.95	0.48
1:A:1365:ASN:HA	1:A:1368:LEU:HB3	1.94	0.48
1:A:3494:GLN:C	1:A:3496:ILE:N	2.69	0.48
1:A:90:CYS:SG	1:A:132:ILE:HG12	2.53	0.48
1:A:752:LEU:HD22	1:A:776:TRP:CZ3	2.48	0.48
1:A:1124:ILE:HG23	1:A:1182:GLU:HG2	1.96	0.48
1:A:1268:ASN:HD22	1:A:1340:ARG:NH2	2.11	0.48
1:A:1426:GLN:O	1:A:1430:GLU:HG3	2.13	0.48
1:A:1652:ILE:O	1:A:1655:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2220:MET:HA	1:A:2223:VAL:HG23	1.96	0.48
1:A:2316:TYR:OH	1:A:2359:LYS:HD2	2.13	0.48
1:A:2894:GLU:HB3	1:A:3973:PRO:HG2	1.94	0.48
1:A:1087:ARG:HG2	1:A:1090:ARG:NH1	2.29	0.48
1:A:1442:GLN:HG3	1:A:1445:ARG:HH12	1.79	0.48
1:A:1471:GLN:N	1:A:1471:GLN:OE1	2.47	0.48
1:A:3705:TYR:CE1	1:A:3716:HIS:NE2	2.78	0.48
1:A:535:LEU:HD13	1:A:565:TYR:CD1	2.48	0.48
1:A:759:GLY:HA2	1:A:762:TYR:O	2.13	0.48
1:A:1748:ASP:HA	1:A:1751:GLU:OE1	2.14	0.48
1:A:2251:ILE:HB	1:A:2253:TYR:CE2	2.49	0.48
1:A:1158:PRO:N	1:A:1159:PRO:HD2	2.28	0.48
1:A:1323:SER:O	1:A:1325:GLN:N	2.46	0.48
1:A:1479:VAL:HG12	1:A:1518:ALA:HA	1.96	0.48
1:A:3332:THR:O	1:A:3336:ILE:HG13	2.14	0.48
1:A:3466:PRO:HG3	1:A:3498:TRP:CH2	2.49	0.48
1:A:3487:ILE:HD11	1:A:3495:PHE:CZ	2.48	0.48
1:A:3578:LEU:O	1:A:3736:LYS:HE2	2.14	0.48
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	1.95	0.48
1:A:2133:LEU:HD23	1:A:2164:TRP:HZ3	1.77	0.48
1:A:2461:PHE:HB2	1:A:2473:MET:HG3	1.94	0.48
1:A:3361:GLU:HB3	1:A:3367:SER:OG	2.14	0.48
1:A:851:ILE:O	1:A:855:VAL:HG23	2.14	0.48
1:A:1488:TYR:O	1:A:1491:ILE:HG12	2.14	0.48
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.47	0.48
1:A:3800:LEU:HG	1:A:3801:GLY:N	2.29	0.48
1:A:1290:LEU:O	1:A:1294:VAL:HG23	2.14	0.47
1:A:2168:LEU:HB3	1:A:2189:ILE:HD11	1.96	0.47
1:A:3729:MET:HE3	1:A:3805:TRP:CH2	2.49	0.47
1:A:721:TYR:HB2	1:A:726:LEU:HD13	1.96	0.47
1:A:774:GLU:CD	1:A:854:ARG:HH21	2.20	0.47
1:A:1208:LEU:HD22	1:A:1275:THR:HG22	1.94	0.47
1:A:2094:MET:HB3	1:A:2145:PHE:HE1	1.79	0.47
1:A:2361:ILE:HB	1:A:2393:LEU:HD12	1.96	0.47
1:A:2475:ASN:HA	1:A:2478:MET:HE3	1.96	0.47
1:A:304:THR:HA	1:A:309:LYS:HE2	1.96	0.47
1:A:344:GLN:O	1:A:348:ILE:HG12	2.14	0.47
1:A:770:LEU:O	1:A:774:GLU:HG3	2.13	0.47
1:A:1375:THR:O	1:A:1379:PRO:HG3	2.13	0.47
1:A:2443:MET:HE2	1:A:2443:MET:HB3	1.73	0.47
1:A:3797:THR:HG22	1:A:3798:SER:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1770:GLN:HA	1:A:1822:ARG:NH2	2.29	0.47
1:A:3282:ARG:HE	1:A:3329:LEU:HD11	1.80	0.47
1:A:3806:LEU:N	1:A:3806:LEU:CD2	2.76	0.47
1:A:531:PHE:CD1	1:A:534:LEU:HD12	2.50	0.47
1:A:1016:GLY:O	1:A:1018:VAL:N	2.48	0.47
1:A:1324:PRO:C	1:A:1327:GLY:H	2.23	0.47
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.95	0.47
1:A:2178:GLY:O	1:A:2183:HIS:NE2	2.47	0.47
1:A:3753:LYS:HA	1:A:3753:LYS:HD3	1.56	0.47
1:A:387:GLU:O	1:A:391:ARG:HG2	2.14	0.47
1:A:631:ARG:HH22	1:A:668:LYS:HD2	1.78	0.47
1:A:898:PHE:HB2	1:A:901:MET:O	2.15	0.47
1:A:1267:TYR:HB3	1:A:1344:PHE:CZ	2.50	0.47
1:A:2554:PHE:C	1:A:2556:SER:H	2.22	0.47
1:A:3103:ILE:O	1:A:3107:ILE:HG12	2.14	0.47
1:A:3354:ASP:OD1	1:A:3355:LYS:N	2.47	0.47
1:A:3636:PHE:CE2	1:A:3670:MET:HG2	2.50	0.47
1:A:3940:ILE:HD12	1:A:3941:ASP:HB2	1.96	0.47
1:A:172:GLU:CD	1:A:220:LEU:HA	2.40	0.47
1:A:1384:PHE:HB3	1:A:1392:MET:HE1	1.97	0.47
1:A:3753:LYS:HG3	1:A:3758:LEU:HD21	1.96	0.47
1:A:330:ASN:HB2	1:A:333:MET:SD	2.55	0.47
1:A:2446:LEU:HG	1:A:2450:GLU:HB2	1.97	0.47
1:A:202:GLY:HA2	1:A:205:LYS:HE3	1.96	0.47
1:A:1475:LEU:HD13	1:A:1527:ARG:HD2	1.97	0.47
1:A:3499:ILE:HD12	1:A:3499:ILE:H	1.78	0.47
1:A:3704:GLN:HE22	1:A:3717:VAL:HB	1.79	0.47
1:A:225:LYS:HE2	1:A:270:ALA:HB3	1.96	0.46
1:A:2894:GLU:OE2	1:A:2930:TYR:OH	2.32	0.46
1:A:2931:ARG:HB2	1:A:2939:LEU:HD22	1.97	0.46
1:A:3484:THR:O	1:A:3487:ILE:HG22	2.15	0.46
1:A:1335:CYS:HB2	1:A:1384:PHE:CZ	2.50	0.46
1:A:2164:TRP:O	1:A:2167:PRO:HD2	2.14	0.46
1:A:3700:GLU:OE1	1:A:3716:HIS:HB2	2.16	0.46
1:A:225:LYS:HD3	1:A:253:LEU:HD21	1.97	0.46
1:A:1249:SER:OG	1:A:1250:LEU:N	2.49	0.46
1:A:1570:GLU:O	1:A:1573:LYS:HB3	2.15	0.46
1:A:3907:SER:O	1:A:3911:ILE:HG23	2.14	0.46
1:A:899:ARG:NH2	1:A:2568:MET:SD	2.88	0.46
1:A:1632:TRP:CE3	1:A:1645:VAL:HG22	2.50	0.46
1:A:1802:TYR:HB2	1:A:1839:PHE:HZ	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2227:LYS:HB2	1:A:2230:VAL:HG12	1.96	0.46
1:A:3294:SER:O	1:A:3298:LEU:HD23	2.16	0.46
1:A:1241:LEU:O	1:A:1244:LEU:HB3	2.16	0.46
1:A:1290:LEU:HG	1:A:1291:LEU:N	2.30	0.46
1:A:3519:GLU:HB2	1:A:3554:PHE:CE1	2.50	0.46
1:A:1265:GLU:HG3	1:A:1340:ARG:NH2	2.31	0.46
1:A:3300:VAL:O	1:A:3303:THR:HG22	2.16	0.46
1:A:366:TYR:CD1	1:A:384:MET:HB2	2.50	0.46
1:A:793:LEU:HD12	1:A:869:ASN:HB2	1.98	0.46
1:A:3731:SER:O	1:A:3734:ARG:NH2	2.48	0.46
1:A:4044:ILE:HD12	1:A:4047:ALA:HB3	1.98	0.46
1:A:978:GLN:OE1	1:A:981:ARG:NH2	2.41	0.46
1:A:1240:THR:HG22	1:A:1242:LEU:N	2.27	0.46
1:A:2231:PHE:HE1	1:A:2272:VAL:HG12	1.80	0.46
1:A:400:THR:HG21	1:A:1741:ASP:HA	1.97	0.46
1:A:1222:ASN:HA	1:A:1236:LEU:HD13	1.98	0.46
1:A:2523:ASN:HA	1:A:2526:SER:OG	2.15	0.46
1:A:300:TRP:HB3	1:A:312:ALA:HB2	1.98	0.46
1:A:2466:SER:C	1:A:2468:THR:H	2.24	0.46
1:A:2365:ASN:HD21	1:A:2399:GLU:CB	2.24	0.45
1:A:2464:HIS:ND1	1:A:2466:SER:HB2	2.31	0.45
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.49	0.45
1:A:3699:LEU:HD12	1:A:3699:LEU:HA	1.78	0.45
1:A:275:PHE:CZ	1:A:293:LEU:HD21	2.51	0.45
1:A:1031:ARG:HE	1:A:1031:ARG:HB3	1.50	0.45
1:A:1755:SER:HB3	1:A:1758:LEU:HB2	1.98	0.45
1:A:1920:TYR:HA	1:A:1923:PHE:CE2	2.50	0.45
1:A:2371:PHE:CE1	1:A:2373:PRO:HD2	2.51	0.45
1:A:3449:LYS:HA	1:A:3449:LYS:HD3	1.78	0.45
1:A:560:LEU:HG	1:A:564:LEU:HD23	1.98	0.45
1:A:1424:THR:HG23	1:A:1427:SER:H	1.82	0.45
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.16	0.45
1:A:1470:SER:HB2	1:A:1476:HIS:HA	1.97	0.45
1:A:1980:ASN:ND2	1:A:2141:ASN:OD1	2.50	0.45
1:A:2289:ASP:HB3	1:A:2290:PRO:HD3	1.98	0.45
1:A:3496:ILE:HD11	1:A:3521:ILE:HD11	1.98	0.45
1:A:763:THR:O	1:A:766:ALA:N	2.49	0.45
1:A:3344:GLU:OE1	1:A:3348:LEU:HD22	2.17	0.45
1:A:129:ASP:OD1	1:A:129:ASP:N	2.50	0.45
1:A:1335:CYS:HA	1:A:1338:VAL:HG22	1.98	0.45
1:A:2254:ARG:HH12	1:A:2292:CYS:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2917:PRO:HB2	1:A:2919:ASP:OD1	2.16	0.45
1:A:1335:CYS:O	1:A:1339:VAL:HG12	2.16	0.45
1:A:1802:TYR:O	1:A:1806:ARG:HG2	2.17	0.45
1:A:2288:TYR:CZ	1:A:2299:TYR:HB3	2.51	0.45
1:A:3256:MET:HE1	1:A:3287:ARG:NH1	2.31	0.45
1:A:3413:TYR:CD1	1:A:3449:LYS:HD2	2.52	0.45
1:A:1142:HIS:O	1:A:1146:ASN:ND2	2.49	0.45
1:A:1522:GLY:O	1:A:1524:LEU:N	2.50	0.45
1:A:1525:CYS:SG	1:A:1577:LEU:HD22	2.57	0.45
1:A:2506:LEU:HD13	1:A:2524:PHE:HE2	1.81	0.45
1:A:225:LYS:HD3	1:A:253:LEU:CD2	2.46	0.44
1:A:1105:VAL:HG21	1:A:1154:PRO:HB3	1.99	0.44
1:A:1630:ASP:HA	1:A:1633:TRP:NE1	2.31	0.44
1:A:1684:LEU:HB2	1:A:1689:LYS:HE3	1.99	0.44
1:A:1718:ILE:O	1:A:1722:PHE:HB2	2.18	0.44
1:A:3285:HIS:CE1	1:A:3332:THR:HB	2.52	0.44
1:A:3705:TYR:CZ	1:A:3716:HIS:CD2	3.05	0.44
1:A:279:ALA:HB3	1:A:318:SER:HB3	1.99	0.44
1:A:1583:MET:HE2	1:A:1628:LYS:HB2	1.98	0.44
1:A:3138:ILE:O	1:A:3142:ILE:HG12	2.18	0.44
1:A:3182:ILE:HG21	1:A:3182:ILE:HD13	1.80	0.44
1:A:3699:LEU:O	1:A:3718:ARG:HB3	2.17	0.44
1:A:2104:MET:HE2	1:A:2125:TRP:CZ2	2.52	0.44
1:A:2412:TYR:CE2	1:A:2450:GLU:HG2	2.52	0.44
1:A:3161:LEU:HD21	1:A:3231:ILE:HG22	1.98	0.44
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	2.00	0.44
1:A:1271:ILE:HD12	1:A:1344:PHE:CZ	2.53	0.44
1:A:1604:SER:O	1:A:1608:ARG:N	2.51	0.44
1:A:1772:HIS:HE1	1:A:1774:MET:HE2	1.82	0.44
1:A:2522:ARG:NH2	1:A:2564:GLU:OE1	2.50	0.44
1:A:3448:GLU:HB2	1:A:3482:LEU:HD11	1.99	0.44
1:A:459:ARG:HD3	1:A:544:ILE:HD11	2.00	0.44
1:A:531:PHE:HD1	1:A:534:LEU:HD12	1.81	0.44
1:A:934:LEU:O	1:A:938:VAL:HG23	2.18	0.44
1:A:1075:ARG:NH1	1:A:1123:THR:HG21	2.33	0.44
1:A:1203:SER:OG	1:A:1206:LEU:HD13	2.17	0.44
1:A:403:GLY:H	1:A:406:ARG:NH1	2.13	0.44
1:A:710:PHE:O	1:A:714:VAL:HG12	2.17	0.44
1:A:195:ASN:O	1:A:198:ARG:HG3	2.18	0.44
1:A:355:ASN:OD1	1:A:357:LYS:N	2.32	0.44
1:A:386:VAL:HG22	1:A:431:TYR:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LYS:HD2	1:A:722:LYS:HA	1.33	0.44
1:A:1030:GLY:O	1:A:1033:ILE:HG22	2.17	0.44
1:A:1080:LEU:O	1:A:1084:ASN:ND2	2.46	0.44
1:A:1449:ALA:HA	1:A:1452:VAL:HG12	1.99	0.44
1:A:1726:SER:OG	1:A:1726:SER:O	2.27	0.44
1:A:411:PRO:HD3	1:A:449:TYR:OH	2.18	0.44
1:A:2339:GLU:HG2	1:A:2340:SER:N	2.33	0.44
1:A:2528:GLU:HG2	1:A:2533:SER:HB3	2.00	0.44
1:A:2976:LEU:HD11	1:A:2995:GLU:HA	1.99	0.44
1:A:3285:HIS:HE2	1:A:3333:THR:HG1	1.63	0.44
1:A:3301:LEU:C	1:A:3301:LEU:HD23	2.43	0.44
1:A:3540:TYR:HD1	1:A:3542:PHE:CE1	2.36	0.44
1:A:1298:LEU:HB3	1:A:1367:HIS:CD2	2.51	0.44
1:A:3710:LYS:HB2	1:A:3711:PRO:HD3	1.99	0.44
1:A:3859:TYR:CE1	1:A:4119:ARG:HD3	2.53	0.44
1:A:4058:VAL:HG21	1:A:4095:GLU:HB2	2.00	0.44
1:A:410:MET:HE3	1:A:442:GLN:CD	2.42	0.43
1:A:1104:LEU:HA	1:A:1134:LEU:HD13	2.00	0.43
1:A:2269:ASP:O	1:A:2272:VAL:HG22	2.17	0.43
1:A:2492:ASP:C	1:A:2494:ASP:H	2.27	0.43
1:A:3065:ILE:HD13	1:A:3065:ILE:HA	1.83	0.43
1:A:3718:ARG:HG3	1:A:3743:HIS:CE1	2.53	0.43
1:A:170:VAL:O	1:A:171:LEU:HD22	2.18	0.43
1:A:923:ASP:C	1:A:925:GLN:H	2.25	0.43
1:A:1361:LYS:N	1:A:1361:LYS:HD2	2.33	0.43
1:A:1538:LEU:HD21	1:A:1555:HIS:ND1	2.33	0.43
1:A:2419:ASP:OD2	1:A:2422:GLN:HB3	2.18	0.43
1:A:3335:ARG:NH1	1:A:3422:GLN:HG3	2.34	0.43
1:A:3867:THR:OG1	1:A:4119:ARG:NH1	2.39	0.43
1:A:175:TYR:HB3	1:A:227:LEU:HD22	2.00	0.43
1:A:1463:LEU:O	1:A:1467:ILE:HG12	2.18	0.43
1:A:1678:LEU:HD22	1:A:1684:LEU:HD11	2.01	0.43
1:A:2261:SER:OG	1:A:2262:GLY:N	2.50	0.43
1:A:2301:GLN:HA	1:A:2304:VAL:HG22	2.01	0.43
1:A:2386:LEU:HB3	1:A:2387:PRO:HD3	2.00	0.43
1:A:2843:PHE:O	1:A:2847:THR:OG1	2.26	0.43
1:A:240:GLU:HB2	1:A:243:GLN:NE2	2.26	0.43
1:A:1289:SER:O	1:A:1289:SER:OG	2.36	0.43
1:A:3466:PRO:HA	1:A:3469:LEU:HD23	2.00	0.43
1:A:3535:ILE:HD11	1:A:3795:PRO:O	2.19	0.43
1:A:299:LYS:HD3	1:A:302:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:TYR:HB3	1:A:453:MET:HB2	2.01	0.43
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	2.00	0.43
1:A:1568:ASN:ND2	1:A:1603:GLN:HG3	2.33	0.43
1:A:2375:ALA:HB3	1:A:2404:ARG:HD3	1.99	0.43
1:A:2812:LEU:HD23	1:A:2812:LEU:HA	1.86	0.43
1:A:3029:LYS:C	1:A:3031:TRP:N	2.77	0.43
1:A:3858:MET:HE2	1:A:3858:MET:HB3	1.90	0.43
1:A:109:ASN:OD1	1:A:110:THR:N	2.52	0.43
1:A:975:ASP:OD1	1:A:976:VAL:N	2.50	0.43
1:A:2364:LEU:HD13	1:A:2400:VAL:HG21	2.00	0.43
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	2.00	0.43
1:A:3636:PHE:O	1:A:3640:PHE:HB2	2.17	0.43
1:A:1235:ILE:O	1:A:1289:SER:OG	2.34	0.43
1:A:1713:VAL:O	1:A:1716:GLN:HG2	2.18	0.43
1:A:1778:PHE:O	1:A:1782:PHE:HD2	2.01	0.43
1:A:2877:SER:HG	1:A:2925:GLU:HB3	1.83	0.43
1:A:3568:ILE:HD13	1:A:3699:LEU:HD11	2.01	0.43
1:A:3692:VAL:HG13	1:A:3692:VAL:O	2.18	0.43
1:A:3959:MET:HE1	1:A:4120:THR:HG23	2.01	0.43
1:A:1607:GLU:O	1:A:1611:GLN:HB2	2.17	0.43
1:A:1801:VAL:O	1:A:1804:MET:HG2	2.18	0.43
1:A:2506:LEU:HD13	1:A:2524:PHE:CE2	2.53	0.43
1:A:3526:PRO:O	1:A:3527:GLN:HB2	2.18	0.43
1:A:3759:ARG:O	1:A:3763:ARG:HG2	2.18	0.43
1:A:3909:ALA:HB1	1:A:3984:MET:HG3	2.01	0.43
1:A:923:ASP:O	1:A:925:GLN:N	2.52	0.43
1:A:1525:CYS:SG	1:A:1526:GLU:N	2.92	0.43
1:A:1864:ASP:OD1	1:A:1864:ASP:N	2.52	0.43
1:A:1922:ALA:O	1:A:1941:HIS:ND1	2.52	0.43
1:A:2898:LEU:HG	1:A:3973:PRO:HG3	2.01	0.43
1:A:3266:SER:O	1:A:3267:LYS:HB2	2.18	0.43
1:A:3722:PHE:O	1:A:3741:ARG:NE	2.52	0.43
1:A:1093:GLU:OE2	1:A:1093:GLU:N	2.49	0.42
1:A:290:TYR:CD2	1:A:291:VAL:HG13	2.54	0.42
1:A:1373:VAL:HG21	1:A:1418:HIS:HB3	2.01	0.42
1:A:2380:ASN:OD1	1:A:2381:ALA:N	2.52	0.42
1:A:2393:LEU:HD13	1:A:2396:LEU:HG	2.02	0.42
1:A:2917:PRO:O	1:A:2920:VAL:HG12	2.19	0.42
1:A:159:GLU:O	1:A:163:LYS:HG2	2.19	0.42
1:A:300:TRP:CE3	1:A:308:LEU:HD11	2.54	0.42
1:A:493:LYS:HE3	1:A:527:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:GLN:HB3	1:A:1232:PRO:HD3	2.01	0.42
1:A:1570:GLU:HG2	1:A:1573:LYS:HE3	2.01	0.42
1:A:2837:LEU:HD13	1:A:2868:LEU:HA	2.00	0.42
1:A:3578:LEU:HB3	1:A:3736:LYS:HG3	2.01	0.42
1:A:297:LEU:HD13	1:A:316:LEU:HB2	2.01	0.42
1:A:1097:GLU:OE2	1:A:1151:ARG:NE	2.49	0.42
1:A:1202:ARG:HD2	1:A:1206:LEU:HB3	2.00	0.42
1:A:1504:ASP:C	1:A:1506:SER:H	2.27	0.42
1:A:3020:ASP:HB2	1:A:3030:ILE:HD13	2.00	0.42
1:A:3345:PRO:C	1:A:3347:CYS:H	2.28	0.42
1:A:3616:ALA:O	1:A:3629:ARG:HD3	2.19	0.42
1:A:3881:ASP:HB2	1:A:3884:LYS:HB3	2.01	0.42
1:A:378:ALA:O	1:A:380:ASP:N	2.48	0.42
1:A:1257:LEU:HD11	1:A:1330:TYR:CE1	2.54	0.42
1:A:670:LEU:HD13	1:A:710:PHE:HE2	1.84	0.42
1:A:1239:PRO:HB3	1:A:1289:SER:OG	2.19	0.42
1:A:1240:THR:CG2	1:A:1242:LEU:HB2	2.50	0.42
1:A:1270:PHE:O	1:A:1275:THR:HB	2.19	0.42
1:A:1271:ILE:HD12	1:A:1344:PHE:CE1	2.54	0.42
1:A:174:VAL:O	1:A:177:LEU:HG	2.20	0.42
1:A:669:LEU:HD12	1:A:672:ILE:HD12	2.02	0.42
1:A:999:LYS:HG3	1:A:1000:LYS:HG2	2.01	0.42
1:A:1436:LEU:HD23	1:A:1436:LEU:H	1.83	0.42
1:A:1739:TYR:HE1	1:A:1774:MET:HE1	1.85	0.42
1:A:1980:ASN:OD1	1:A:1981:LEU:N	2.50	0.42
1:A:3487:ILE:HD12	1:A:3487:ILE:HA	1.87	0.42
1:A:3772:ASN:OD1	1:A:3788:LEU:HB2	2.20	0.42
1:A:3979:LEU:O	1:A:3983:ILE:HG12	2.19	0.42
1:A:1045:THR:OG1	1:A:1046:PRO:HD2	2.20	0.42
1:A:1102:GLU:OE1	1:A:1154:PRO:HA	2.19	0.42
1:A:1414:ILE:HD11	1:A:1418:HIS:CE1	2.55	0.42
1:A:1779:GLN:O	1:A:1783:ARG:HG3	2.19	0.42
1:A:3256:MET:HB2	1:A:3283:LEU:HD21	2.02	0.42
1:A:3451:LEU:HD23	1:A:3451:LEU:HA	1.90	0.42
1:A:3913:ILE:HG21	1:A:3987:ALA:HB3	2.01	0.42
1:A:1793:THR:O	1:A:1797:LEU:HG	2.20	0.42
1:A:3278:GLN:O	1:A:3282:ARG:HD3	2.20	0.42
1:A:3585:PHE:CD2	1:A:3670:MET:HE1	2.55	0.42
1:A:3712:LEU:HA	1:A:3713:PRO:HD2	1.84	0.42
1:A:3763:ARG:HE	1:A:4008:GLU:CD	2.28	0.42
1:A:2194:LEU:O	1:A:2197:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3065:ILE:HD12	1:A:3078:LEU:HD21	2.02	0.42
1:A:487:LEU:HD12	1:A:490:ILE:HD11	2.00	0.41
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	2.01	0.41
1:A:995:PHE:HB3	1:A:1005:ASP:OD1	2.20	0.41
1:A:1290:LEU:CG	1:A:1291:LEU:HD22	2.48	0.41
1:A:1802:TYR:CZ	1:A:1806:ARG:HD2	2.55	0.41
1:A:3728:VAL:HG22	1:A:3736:LYS:HD3	2.01	0.41
1:A:129:ASP:O	1:A:132:ILE:HG22	2.20	0.41
1:A:335:LYS:HA	1:A:338:LEU:HG	2.00	0.41
1:A:638:GLN:HB2	1:A:640:GLU:OE1	2.20	0.41
1:A:971:ARG:HH22	1:A:1014:LEU:HD22	1.84	0.41
1:A:1402:LEU:HD23	1:A:1406:LEU:HD12	2.02	0.41
1:A:1525:CYS:CB	1:A:1574:ASN:HD21	2.33	0.41
1:A:3308:ASP:HB3	1:A:3312:VAL:HA	2.02	0.41
1:A:3681:LYS:HG3	1:A:3688:SER:HB2	2.01	0.41
1:A:1108:MET:HE3	1:A:1172:LEU:HD21	2.02	0.41
1:A:1254:LEU:HD13	1:A:1329:ARG:NE	2.36	0.41
1:A:1493:PRO:HG3	1:A:1499:CYS:HB3	2.02	0.41
1:A:1533:LEU:HD11	1:A:1582:LEU:HD23	2.03	0.41
1:A:1583:MET:HA	1:A:1586:SER:HB2	2.02	0.41
1:A:2183:HIS:ND1	1:A:2185:MET:HE2	2.36	0.41
1:A:2786:LYS:O	1:A:2788:SER:N	2.52	0.41
1:A:55:THR:O	1:A:58:VAL:HG12	2.19	0.41
1:A:1069:HIS:NE2	1:A:3741:ARG:HD2	2.36	0.41
1:A:1832:SER:HA	1:A:1836:LEU:HD11	2.01	0.41
1:A:3100:LYS:HB2	1:A:3100:LYS:HE3	1.85	0.41
1:A:3846:MET:SD	1:A:3862:ALA:HB2	2.60	0.41
1:A:3881:ASP:O	1:A:3885:ARG:HG3	2.20	0.41
1:A:3946:PHE:HE1	1:A:4002:MET:HE2	1.85	0.41
1:A:204:LEU:O	1:A:207:GLN:HB3	2.20	0.41
1:A:641:PHE:O	1:A:644:PRO:HD2	2.21	0.41
1:A:1276:VAL:HG12	1:A:1277:GLY:O	2.21	0.41
1:A:2256:ILE:HD12	1:A:2256:ILE:H	1.86	0.41
1:A:225:LYS:HD2	1:A:271:GLY:CA	2.51	0.41
1:A:306:VAL:C	1:A:308:LEU:H	2.29	0.41
1:A:1818:SER:HB2	1:A:1822:ARG:HE	1.86	0.41
1:A:1863:PHE:HA	1:A:1866:GLN:OE1	2.20	0.41
1:A:1912:THR:O	1:A:1916:ILE:HG12	2.21	0.41
1:A:2269:ASP:N	1:A:2269:ASP:OD1	2.52	0.41
1:A:3758:LEU:HD12	1:A:3801:GLY:HA3	2.03	0.41
1:A:583:LEU:HD23	1:A:614:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ASP:HB3	1:A:1023:SER:OG	2.21	0.41
1:A:682:TYR:O	1:A:700:LYS:HD3	2.21	0.41
1:A:1475:LEU:HD22	1:A:1524:LEU:HD12	2.01	0.41
1:A:1767:CYS:HB3	1:A:1818:SER:OG	2.21	0.41
1:A:2574:ASN:O	1:A:2786:LYS:HA	2.20	0.41
1:A:3655:LYS:HB3	1:A:3658:ASP:H	1.86	0.41
1:A:3743:HIS:CD2	1:A:3743:HIS:C	2.98	0.41
1:A:3855:TYR:HB2	1:A:3955:VAL:HG22	2.02	0.41
1:A:655:LEU:HA	1:A:655:LEU:HD12	1.74	0.41
1:A:1685:ASP:OD1	1:A:1685:ASP:N	2.53	0.41
1:A:2205:VAL:O	1:A:2208:ASP:N	2.53	0.41
1:A:2575:PRO:HB2	1:A:2784:GLN:HB3	2.03	0.41
1:A:3506:LEU:HD11	1:A:3518:VAL:HG21	2.03	0.41
1:A:746:ARG:HD3	1:A:746:ARG:O	2.20	0.41
1:A:995:PHE:O	1:A:1000:LYS:HB2	2.21	0.41
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.41
1:A:1348:LEU:HD23	1:A:1348:LEU:HA	1.89	0.41
1:A:1478:SER:O	1:A:1482:GLU:HG3	2.21	0.41
1:A:1754:GLN:HG3	1:A:1785:ILE:HG13	2.02	0.41
1:A:1767:CYS:HB2	1:A:1819:PHE:CE1	2.56	0.41
1:A:1868:THR:HA	1:A:1871:MET:HE2	2.03	0.41
1:A:2347:LYS:HA	1:A:2350:LYS:HE3	2.02	0.41
1:A:2443:MET:HE3	1:A:2479:TRP:CD2	2.55	0.41
1:A:3082:TYR:O	1:A:3086:LEU:HG	2.21	0.41
1:A:3442:TYR:O	1:A:3446:VAL:HG23	2.21	0.41
1:A:4120:THR:HG22	1:A:4121:TRP:N	2.35	0.41
1:A:225:LYS:HE3	1:A:267:VAL:HA	2.03	0.41
1:A:539:GLN:NE2	1:A:541:MET:HE3	2.34	0.41
1:A:1221:ILE:HD13	1:A:1287:GLN:O	2.21	0.41
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.21	0.41
1:A:2400:VAL:HA	1:A:2403:CYS:SG	2.60	0.41
1:A:3169:PRO:CD	1:A:3182:ILE:HD11	2.48	0.41
1:A:3780:ALA:O	1:A:3784:ARG:HD3	2.20	0.41
1:A:3969:ASN:O	1:A:3972:LEU:HB2	2.21	0.41
1:A:1011:GLU:O	1:A:1015:ASP:N	2.47	0.40
1:A:1603:GLN:OE1	1:A:1606:ARG:NE	2.23	0.40
1:A:2194:LEU:HD23	1:A:2194:LEU:HA	1.88	0.40
1:A:2411:LEU:HG	1:A:2412:TYR:H	1.87	0.40
1:A:2438:ILE:O	1:A:2442:MET:HG3	2.21	0.40
1:A:3065:ILE:O	1:A:3069:MET:HG2	2.21	0.40
1:A:4055:ASN:HB2	1:A:4095:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:O	1:A:89:LEU:HG	2.21	0.40
1:A:398:THR:HG22	1:A:398:THR:O	2.21	0.40
1:A:1173:LEU:HA	1:A:1176:CYS:SG	2.61	0.40
1:A:3427:GLU:HG3	1:A:3439:LEU:HD11	2.03	0.40
1:A:3499:ILE:HG21	1:A:3529:ILE:HG13	2.04	0.40
1:A:3655:LYS:C	1:A:3657:SER:H	2.30	0.40
1:A:172:GLU:CG	1:A:223:CYS:HB2	2.51	0.40
1:A:574:LYS:O	1:A:577:GLU:HG3	2.22	0.40
1:A:905:ILE:HD13	1:A:905:ILE:HG21	1.84	0.40
1:A:941:MET:HB3	1:A:958:MET:HE1	2.03	0.40
1:A:1328:GLU:HA	1:A:1331:ASN:HB2	2.02	0.40
1:A:1605:PHE:HA	1:A:1608:ARG:HD3	2.03	0.40
1:A:1632:TRP:O	1:A:1637:SER:OG	2.33	0.40
1:A:1636:ASP:N	1:A:1636:ASP:OD1	2.52	0.40
1:A:2443:MET:C	1:A:2445:LYS:H	2.30	0.40
1:A:2879:GLY:O	1:A:2883:SER:OG	2.30	0.40
1:A:3078:LEU:HA	1:A:3078:LEU:HD12	1.77	0.40
1:A:3493:TRP:CD1	1:A:3493:TRP:H	2.38	0.40
1:A:290:TYR:CE2	1:A:291:VAL:HG13	2.56	0.40
1:A:374:LYS:HD3	1:A:381:VAL:HG11	2.02	0.40
1:A:410:MET:HE3	1:A:442:GLN:HA	2.03	0.40
1:A:654:ILE:HG13	1:A:670:LEU:HD21	2.03	0.40
1:A:704:PHE:O	1:A:708:VAL:HG23	2.21	0.40
1:A:970:LEU:HD22	1:A:1014:LEU:HD12	2.03	0.40
1:A:975:ASP:O	1:A:981:ARG:NH1	2.55	0.40
1:A:1102:GLU:O	1:A:1106:ILE:HG12	2.22	0.40
1:A:1272:GLY:O	1:A:1274:ARG:NH1	2.52	0.40
1:A:2207:LYS:O	1:A:2211:LEU:HG	2.22	0.40
1:A:2553:HIS:O	1:A:2557:LEU:HG	2.21	0.40
1:A:2575:PRO:HA	1:A:2786:LYS:N	2.28	0.40
1:A:2987:THR:HG22	1:A:2989:ALA:H	1.87	0.40
1:A:3266:SER:C	1:A:3268:THR:H	2.28	0.40
1:A:3710:LYS:HB2	1:A:3711:PRO:CD	2.52	0.40
1:A:3883:LEU:HG	1:A:3970:LEU:HD22	2.03	0.40
1:A:1240:THR:HG22	1:A:1242:LEU:HB2	2.03	0.40
1:A:1585:SER:O	1:A:1585:SER:OG	2.32	0.40
1:A:2304:VAL:HG12	1:A:2323:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3602/4148 (87%)	3237 (90%)	359 (10%)	6 (0%)	43	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3693	GLU
1	A	3695	LEU
1	A	2787	HIS
1	A	3495	PHE
1	A	723	ASP
1	A	3685	PRO

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	91

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

Mol	Chain	Res	Type
1	A	722	LYS
1	A	724	GLU
1	A	3693	GLU
1	A	3695	LEU
1	A	3696	ARG

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Mol	Chain	Res	Type
1	A	3714	GLU
1	A	3753	LYS
1	A	3806	LEU
1	A	3810	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	A	533	HIS
1	A	1083	ASN
1	A	1146	ASN
1	A	1418	HIS
1	A	1426	GLN
1	A	1574	ASN
1	A	1610	ASN
1	A	1771	GLN
1	A	2103	HIS
1	A	2105	HIS
1	A	2170	GLN
1	A	2270	ASN
1	A	2305	ASN
1	A	2365	ASN
1	A	2784	GLN
1	A	2831	ASN
1	A	2885	GLN
1	A	3084	GLN
1	A	3122	HIS
1	A	3250	ASN
1	A	3430	ASN
1	A	3564	GLN
1	A	3569	GLN
1	A	3573	ASN
1	A	3969	ASN
1	A	4110	GLN
1	A	4115	ASN

5.3.3 RNA ⓘ

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	MBW	A	6101	-	31,32,32	0.34	0	32,47,47	1.11	1 (3%)

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	MBW	A	6101	-	-	5/8/16/16	1/5/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	MBW	C17-C7-N2	-5.38	122.71	126.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

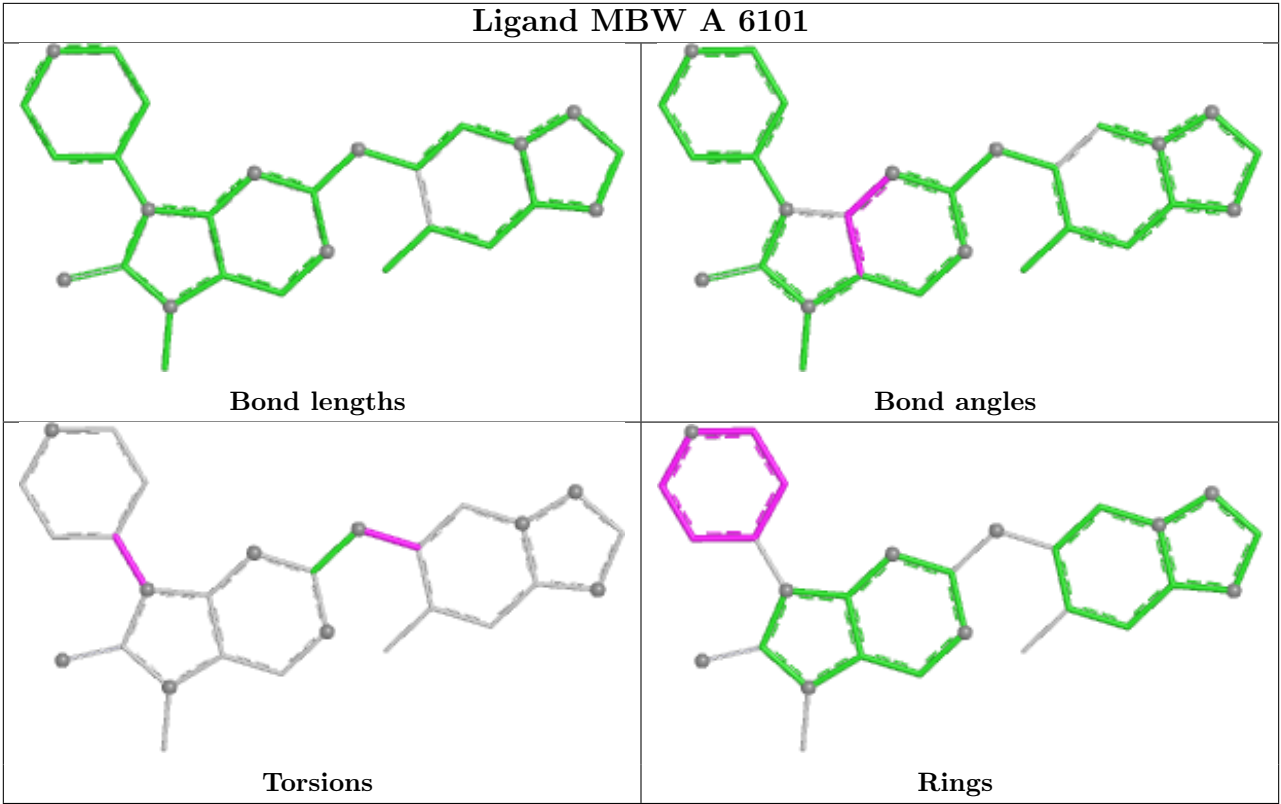
Mol	Chain	Res	Type	Atoms
2	A	6101	MBW	C3-C2-N1-C7
2	A	6101	MBW	C10-C9-N3-C8
2	A	6101	MBW	C3-C2-N1-C1
2	A	6101	MBW	C14-C9-N3-C8
2	A	6101	MBW	C6-C2-N1-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6101	MBW	C2-C3-C4-C5-C6-O1

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

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	82.11

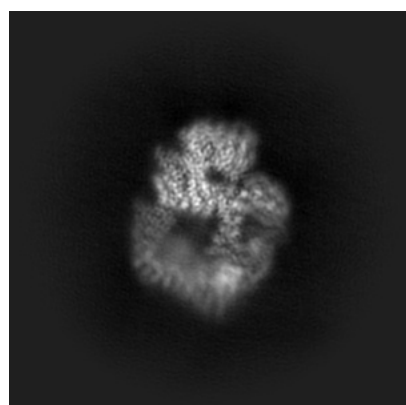
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13068. These allow visual inspection of the internal detail of the map and identification of artifacts.

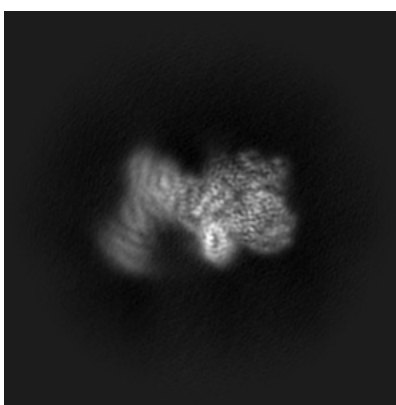
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

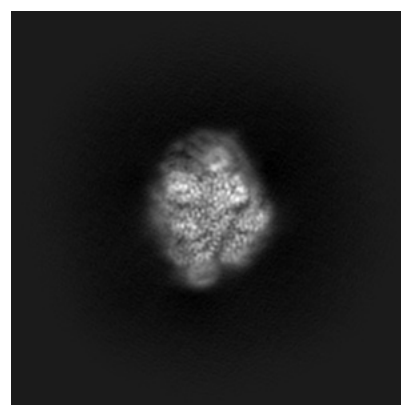
6.1.1 Primary map



X



Y

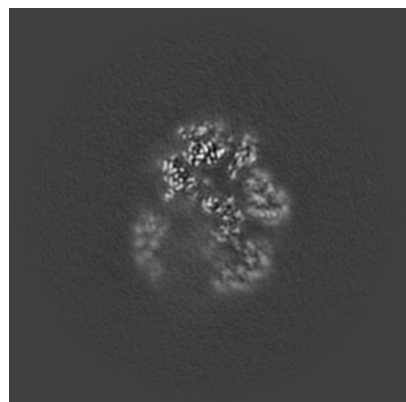


Z

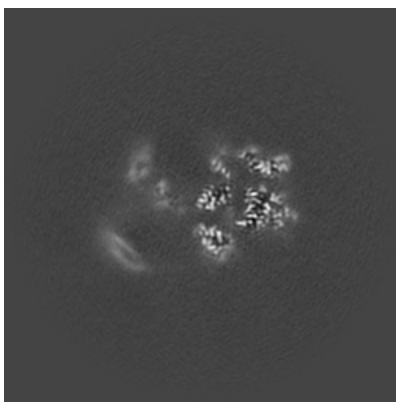
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

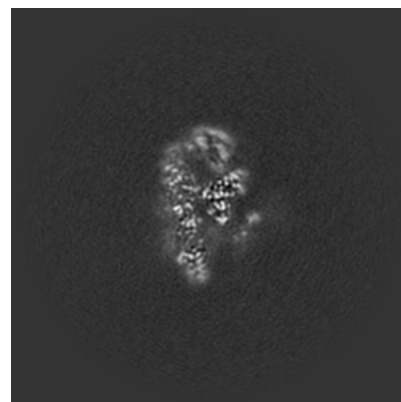
6.2.1 Primary map



X Index: 130



Y Index: 130

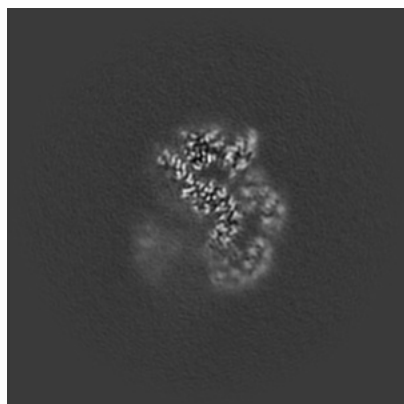


Z Index: 130

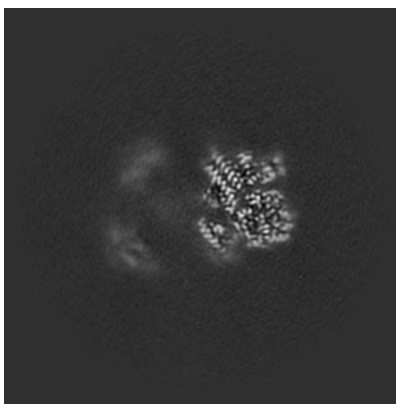
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

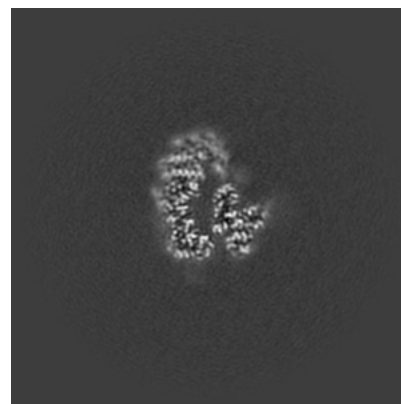
6.3.1 Primary map



X Index: 135



Y Index: 120

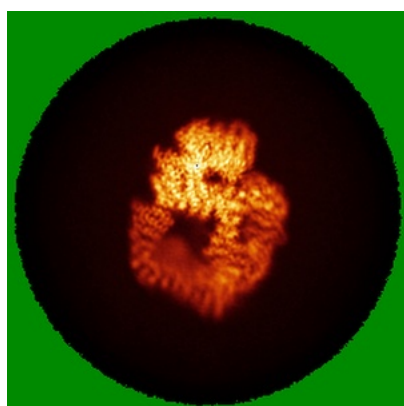


Z Index: 140

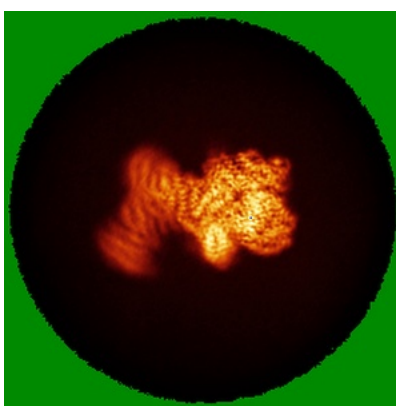
The images above show the largest variance slices of the map in three orthogonal directions.

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

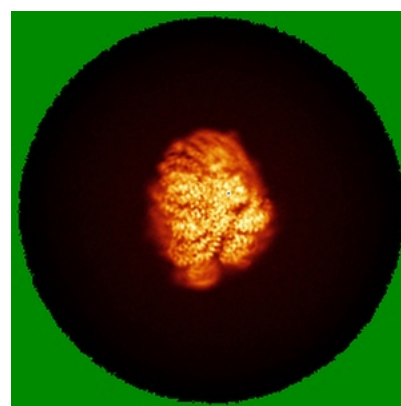
6.4.1 Primary map



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

This section was not generated.

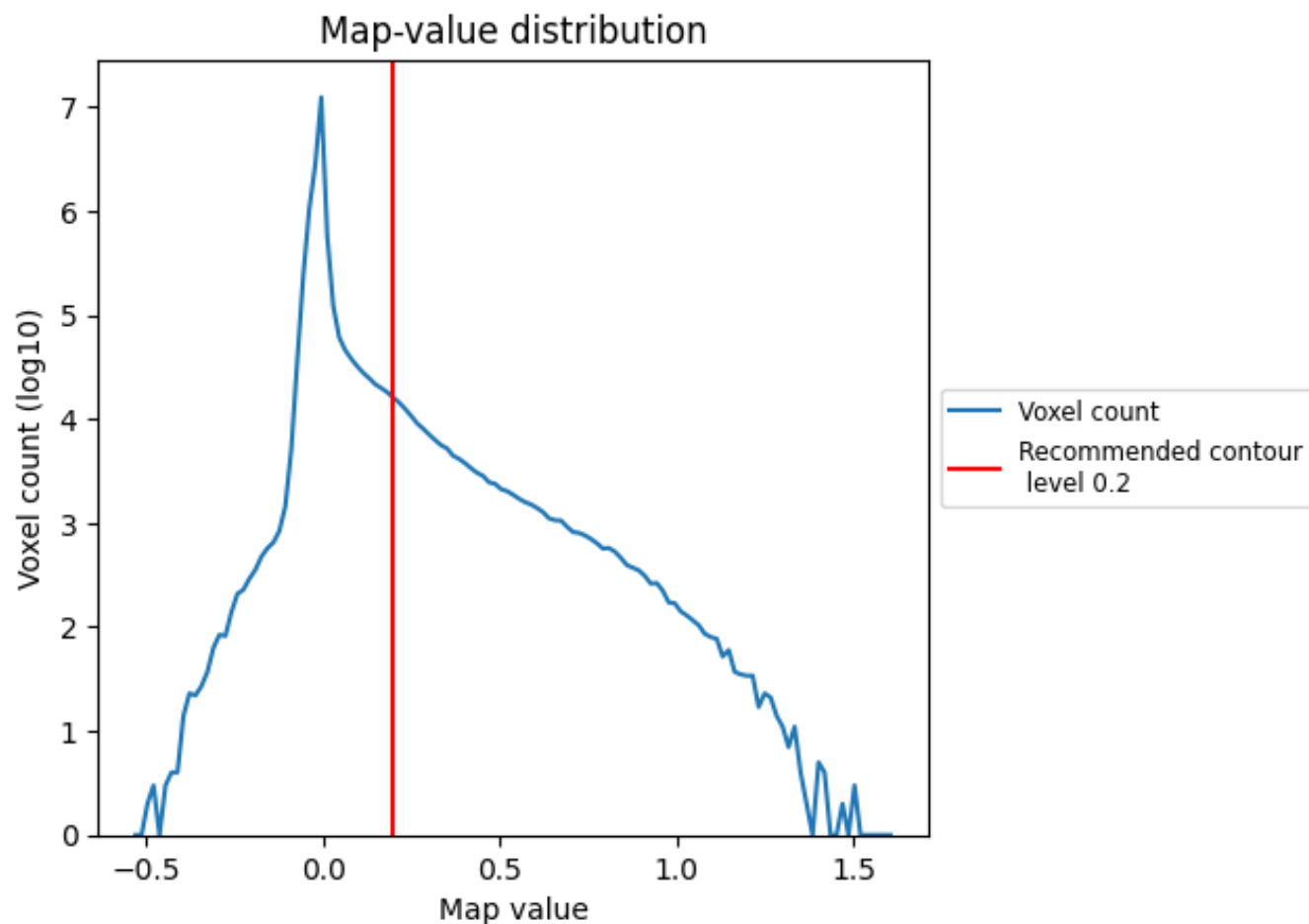
6.6 Mask visualisation

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

7 Map analysis [i](#)

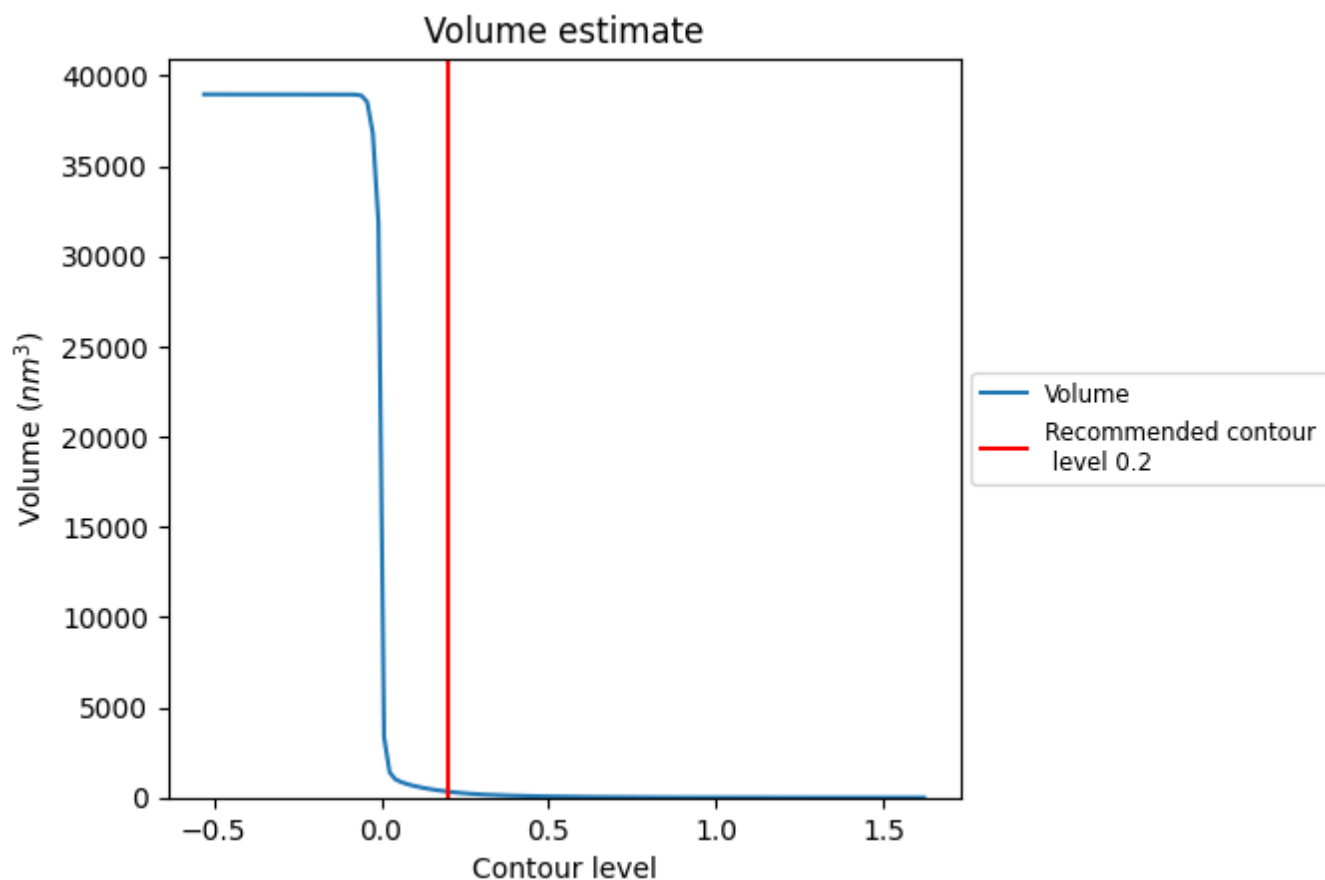
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

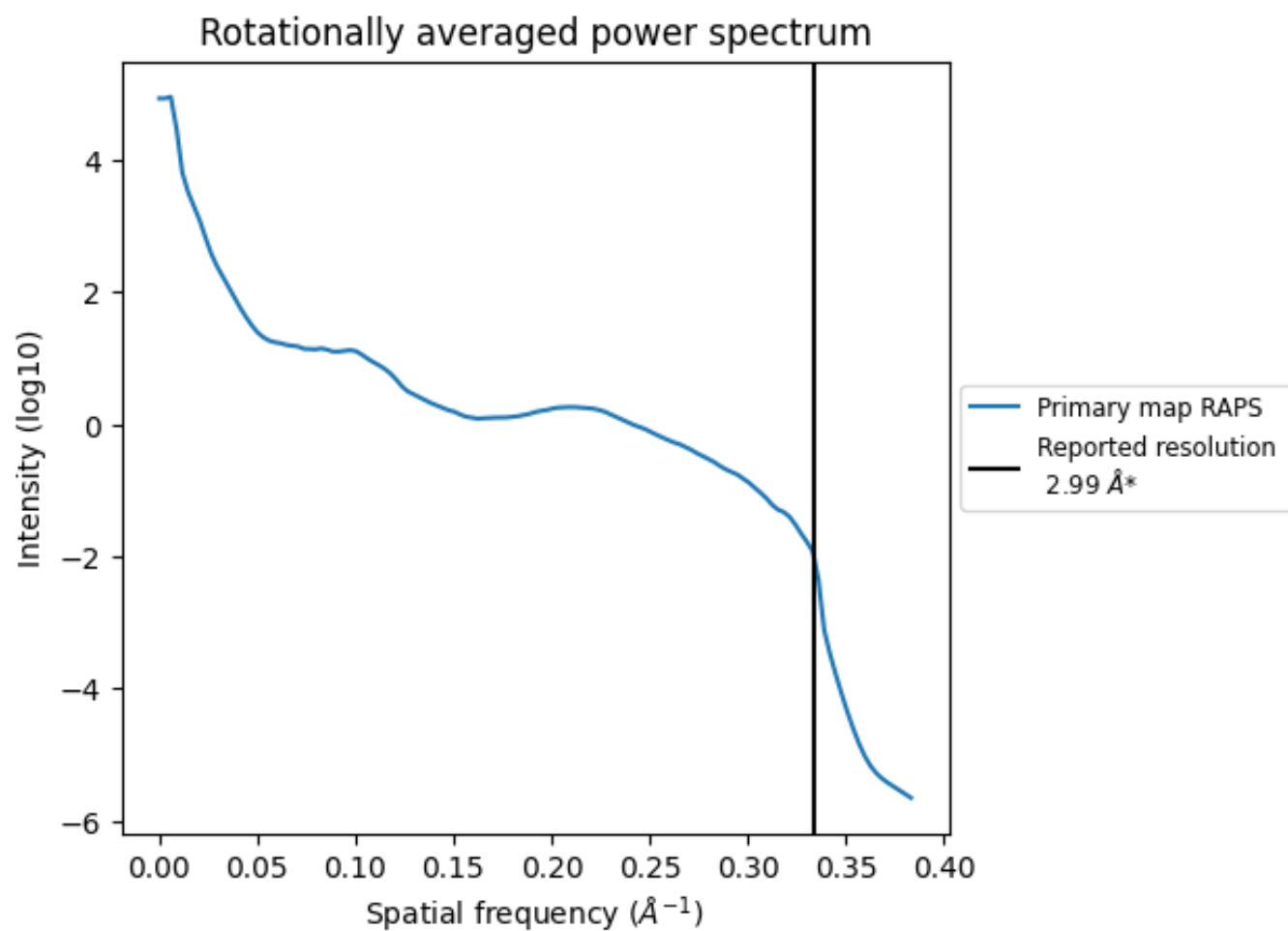
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 328 nm^3 ; this corresponds to an approximate mass of 296 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 0.334 Å⁻¹

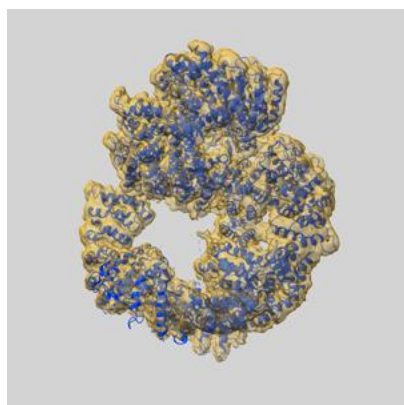
8 Fourier-Shell correlation

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

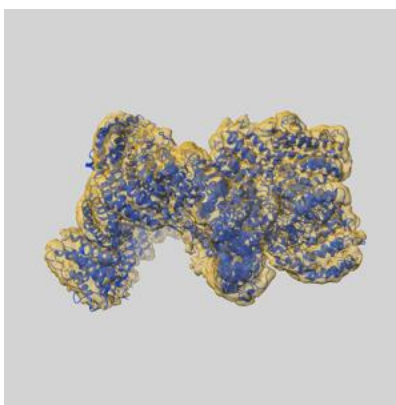
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13068 and PDB model 7OTW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

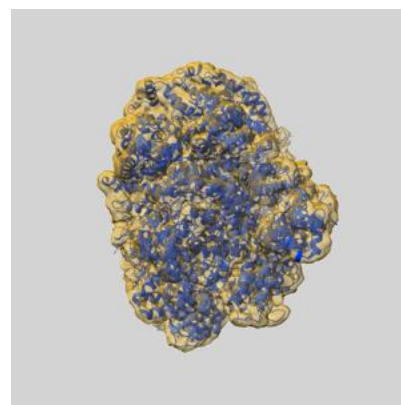
9.1 Map-model overlay [i](#)



X



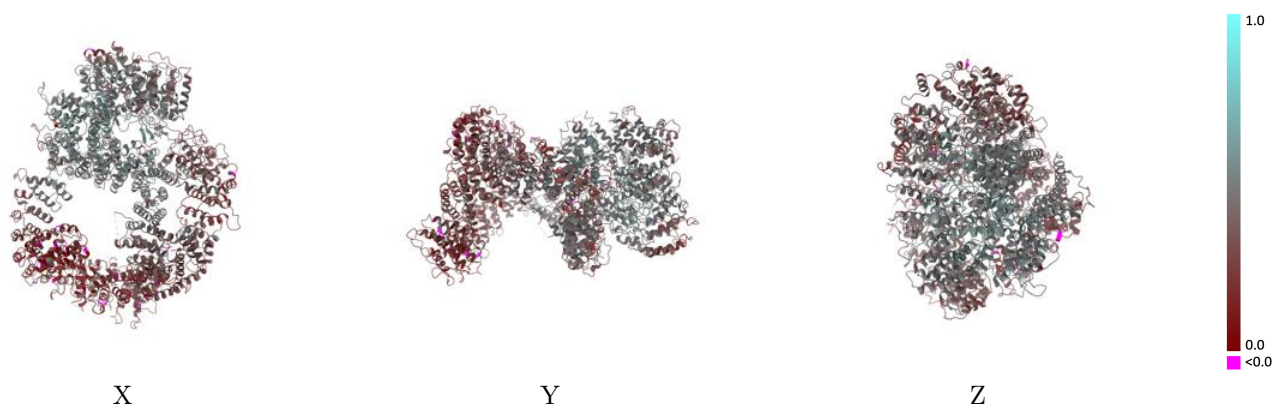
Y



Z

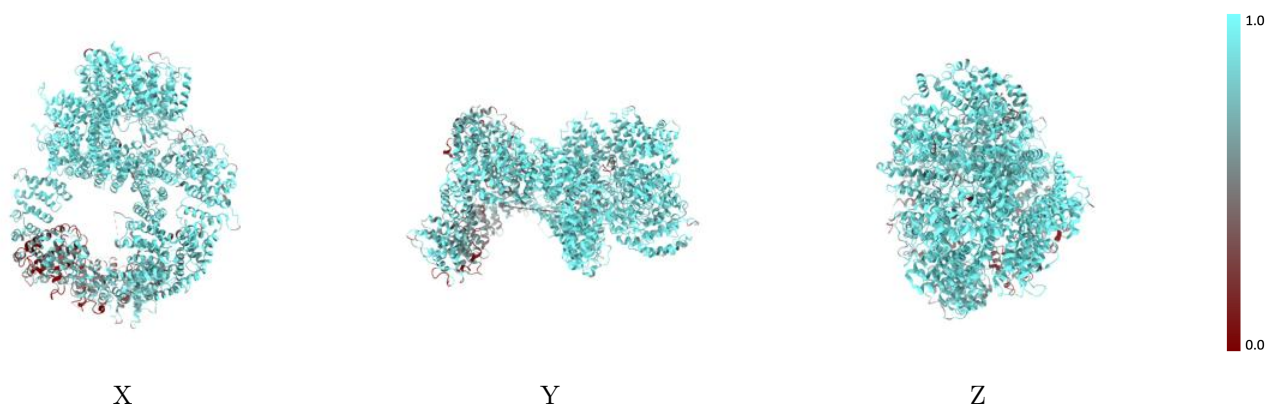
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



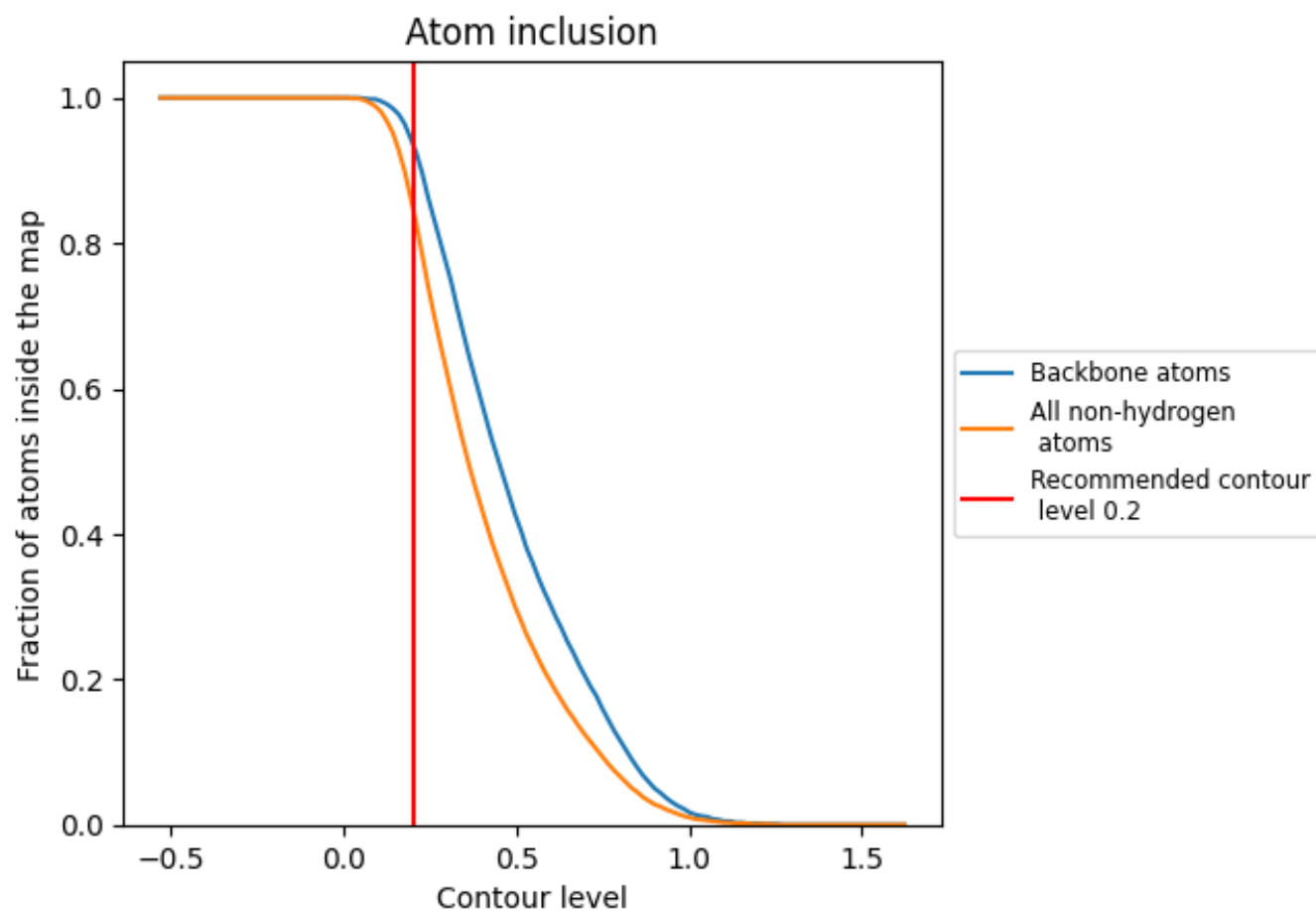
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 94% of all backbone atoms, 85% 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	0.8500	0.3860
A	0.8500	0.3860

