



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:18 AM UTC

PDB ID : 7OTY / pdb_00007oty
EMDB ID : EMD-13069
Title : DNA-PKcs in complex with M3814
Authors : Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on : 2021-06-10
Resolution : 2.96 Å(reported)

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

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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

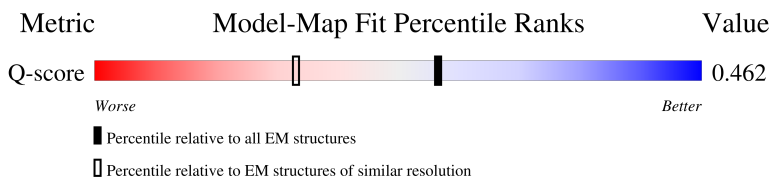
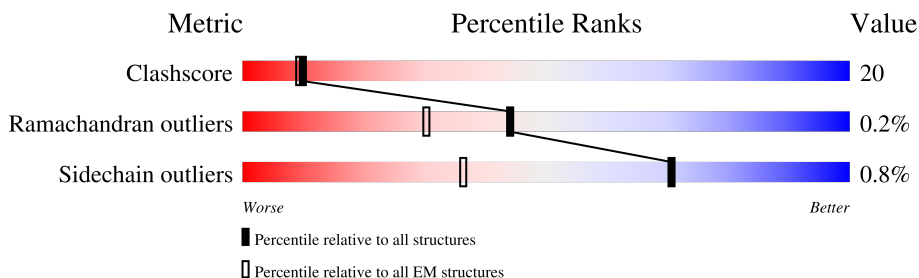
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	13155 (2.46 - 3.46)

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](#)

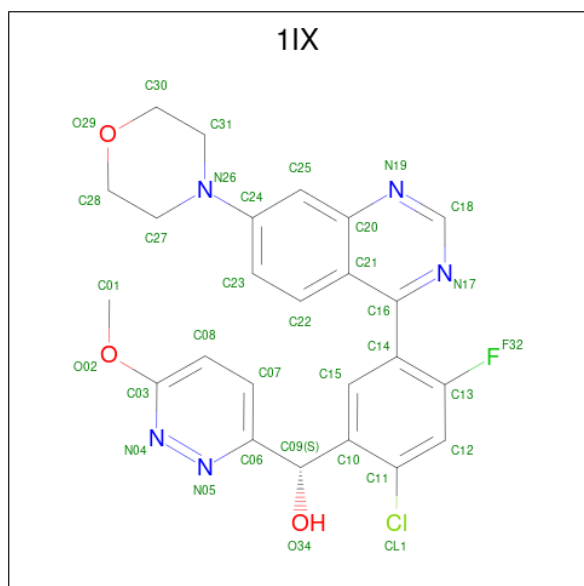
There are 2 unique types of molecules in this entry. The entry contains 29034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	3656	Total	C	N	O	S	0	0
			29000	18604	4900	5305	191		

- Molecule 2 is ({S})-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl]-(6-methoxypyridazin-3-yl)methanol (CCD ID: 1IX) (formula: C₂₄H₂₁ClFN₅O₃) (labeled as "Ligand of Interest" by depositor).



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





L3135	L3136	F3144	I3145	Q3154	L3157	F3169	K3172	I3182	I3183	C3187	F3188	F3189	I3193	E3194	E3195	K3196	L3197	THR	PRO	PRO	PRO	GLU	GLU	ASP	ASN	SER	SER	MET	ASN	VAL	ASP	GLN	ASP	ASP	GLY	ASP	PRO	ASP	GLU	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	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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	209036	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.272	Depositor
Minimum map value	-2.388	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.29	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: IIX

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	0.52	0/29492	0.61	8/39881 (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	3494	GLN	N-CA-C	-7.43	102.87	110.97
1	A	3492	CYS	N-CA-C	6.71	119.81	107.73
1	A	3753	LYS	N-CA-C	-6.64	100.00	109.96
1	A	1884	LEU	CA-C-N	-6.37	113.97	120.85
1	A	1884	LEU	C-N-CA	-6.37	113.97	120.85
1	A	3972	LEU	N-CA-C	5.25	119.39	112.35
1	A	1690	GLY	CA-C-N	-5.23	113.56	122.56
1	A	1690	GLY	C-N-CA	-5.23	113.56	122.56

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	29000	0	29178	1076	0
2	A	34	0	0	1	0
All	All	29034	0	29178	1076	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 20.

All (1076) 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:1019:ASP:H	1:A:1020:PRO:CD	1.54	1.21
1:A:3575:LEU:CD1	1:A:3802:LEU:HD11	1.71	1.19
1:A:3752:VAL:HG22	1:A:3802:LEU:CD2	1.75	1.17
1:A:3075:LYS:O	1:A:3079:GLU:HG2	1.49	1.13
1:A:1019:ASP:H	1:A:1020:PRO:HD2	1.10	1.08
1:A:2097:LEU:HD11	1:A:2149:LEU:HD22	1.35	1.07
1:A:2436:LEU:HD11	1:A:2461:PHE:CZ	1.91	1.06
1:A:3925:LEU:HG	1:A:3962:ARG:NH2	1.69	1.05
1:A:3752:VAL:HG22	1:A:3802:LEU:HD21	1.05	1.05
1:A:2093:CYS:O	1:A:2096:PRO:HG2	1.57	1.05
1:A:3575:LEU:HD11	1:A:3802:LEU:HD11	1.35	1.04
1:A:662:LEU:HD23	1:A:721:TYR:OH	1.64	0.98
1:A:3493:TRP:CZ3	1:A:3711:PRO:HB3	1.98	0.97
1:A:2555:LEU:CD1	1:A:2806:LYS:HA	1.96	0.94
1:A:2097:LEU:CD1	1:A:2149:LEU:HD22	1.97	0.94
1:A:3575:LEU:HD13	1:A:3802:LEU:HD11	1.46	0.93
1:A:3194:GLU:HB3	1:A:3231:ILE:HD11	1.51	0.92
1:A:1933:LEU:H	1:A:1937:ARG:HH11	1.16	0.92
1:A:3588:TRP:HE1	1:A:3609:MET:HB2	1.36	0.91
1:A:1019:ASP:N	1:A:1020:PRO:CD	2.33	0.90
1:A:3493:TRP:CE3	1:A:3711:PRO:HB3	2.07	0.89
1:A:4020:MET:HE2	1:A:4023:LYS:HE3	1.54	0.89
1:A:3031:TRP:HH2	1:A:3040:TYR:HB2	1.37	0.87
1:A:2436:LEU:HD11	1:A:2461:PHE:CE1	2.09	0.87
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	1.56	0.87
1:A:1482:GLU:O	1:A:1486:LEU:HB2	1.74	0.86
1:A:2546:TYR:HB2	1:A:2554:PHE:CE1	2.11	0.86
1:A:662:LEU:HD23	1:A:721:TYR:CZ	2.09	0.86
1:A:172:GLU:HB3	1:A:220:LEU:HD12	1.58	0.85
1:A:1626:TRP:HE1	1:A:1674:THR:HG21	1.39	0.85
1:A:3791:TYR:CE2	1:A:3803:ILE:CD1	2.59	0.85
1:A:2365:ASN:HD22	1:A:2396:LEU:HD12	1.42	0.84
1:A:3288:SER:O	1:A:3289:ARG:NH1	2.11	0.84
1:A:3462:ARG:HD3	1:A:3494:GLN:HB3	1.61	0.83
1:A:240:GLU:HB2	1:A:243:GLN:HE22	1.43	0.82
1:A:3187:CYS:SG	1:A:3239:LYS:NZ	2.52	0.82
1:A:3267:LYS:HA	1:A:3273:LEU:HD12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3750:PHE:CD2	1:A:3804:GLU:HA	2.14	0.82
1:A:1420:ARG:NH2	1:A:1466:ASN:O	2.13	0.81
1:A:3791:TYR:HE2	1:A:3803:ILE:HD12	1.43	0.81
1:A:3750:PHE:CE2	1:A:3804:GLU:HB2	2.16	0.81
1:A:2095:ALA:N	1:A:2096:PRO:HD2	1.96	0.81
1:A:3750:PHE:HE2	1:A:3804:GLU:HB2	1.46	0.80
1:A:917:LEU:O	1:A:921:ALA:HB2	1.80	0.80
1:A:2555:LEU:HD11	1:A:2806:LYS:HA	1.60	0.80
1:A:3596:LEU:HB2	1:A:3601:VAL:HG22	1.62	0.80
1:A:1980:ASN:ND2	1:A:2141:ASN:OD1	2.15	0.79
1:A:3575:LEU:HD11	1:A:3802:LEU:CD1	2.12	0.79
1:A:2395:THR:HA	1:A:2398:LEU:HD12	1.63	0.79
1:A:221:ALA:O	1:A:225:LYS:NZ	2.16	0.79
1:A:3753:LYS:CD	1:A:3756:GLU:OE1	2.31	0.79
1:A:3145:ILE:HD11	1:A:3196:LYS:HD2	1.63	0.78
1:A:2457:PRO:HA	1:A:2460:GLU:OE1	1.84	0.78
1:A:1976:LEU:HD13	1:A:2091:HIS:NE2	1.98	0.78
1:A:3011:LEU:HD23	1:A:3047:SER:HB3	1.65	0.78
1:A:3575:LEU:CD1	1:A:3802:LEU:CD1	2.59	0.78
1:A:243:GLN:HG3	1:A:246:ARG:HH21	1.46	0.78
1:A:3132:VAL:O	1:A:3136:THR:HG23	1.85	0.77
1:A:3341:LEU:HD11	1:A:3360:LEU:HD21	1.67	0.77
1:A:1019:ASP:N	1:A:1020:PRO:HD2	1.93	0.77
1:A:1871:MET:SD	1:A:1936:ARG:NH2	2.58	0.77
1:A:3960:PRO:HD3	1:A:4110:GLN:HG2	1.66	0.77
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.18	0.76
1:A:803:SER:O	1:A:852:ARG:NH1	2.18	0.76
1:A:721:TYR:O	1:A:726:LEU:HD22	1.86	0.76
1:A:3791:TYR:HE2	1:A:3803:ILE:CD1	1.99	0.76
1:A:2519:LEU:O	1:A:2523:ASN:ND2	2.19	0.75
1:A:917:LEU:O	1:A:921:ALA:CB	2.34	0.75
1:A:3710:LYS:HB2	1:A:3711:PRO:HD2	1.69	0.75
1:A:2254:ARG:NH1	1:A:2292:CYS:O	2.20	0.75
1:A:2486:ASP:HB3	1:A:2489:SER:HB2	1.67	0.75
1:A:1240:THR:HG22	1:A:1242:LEU:H	1.52	0.75
1:A:3154:GLN:OE1	1:A:3226:ASP:N	2.20	0.74
1:A:356:ASN:HD22	1:A:404:ASP:HB3	1.52	0.74
1:A:2898:LEU:HD21	1:A:3972:LEU:HB3	1.70	0.73
1:A:1150:LYS:NZ	1:A:1161:ALA:O	2.19	0.73
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.21	0.73
1:A:131:LEU:HD13	1:A:173:LYS:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1274:ARG:HH12	1:A:1351:THR:HG23	1.54	0.72
1:A:2093:CYS:C	1:A:2096:PRO:HG2	2.15	0.72
1:A:3386:SER:O	1:A:3390:GLN:NE2	2.23	0.72
1:A:3791:TYR:CE2	1:A:3803:ILE:HD11	2.24	0.72
1:A:1661:PHE:HE2	1:A:1671:VAL:HG11	1.55	0.72
1:A:1945:TYR:O	1:A:1949:ILE:HD12	1.90	0.72
1:A:4020:MET:CE	1:A:4023:LYS:HE3	2.20	0.72
1:A:2464:HIS:O	1:A:2470:ARG:NH1	2.24	0.71
1:A:3588:TRP:NE1	1:A:3609:MET:HB2	2.06	0.71
1:A:967:PRO:HD3	1:A:1010:LEU:HD12	1.72	0.71
1:A:2458:VAL:O	1:A:2461:PHE:CD2	2.44	0.71
1:A:3753:LYS:HD2	1:A:3756:GLU:OE1	1.91	0.71
1:A:3963:LEU:HG	1:A:4112:THR:CG2	2.20	0.71
1:A:1078:ALA:O	1:A:1107:TYR:OH	2.08	0.70
1:A:3285:HIS:HD2	1:A:3298:LEU:HD11	1.56	0.70
1:A:175:TYR:HB3	1:A:227:LEU:HD22	1.73	0.70
1:A:1825:LEU:HD22	1:A:1879:VAL:HG21	1.73	0.70
1:A:1931:ASN:HA	1:A:1934:LEU:HD21	1.74	0.69
1:A:931:CYS:O	1:A:984:TYR:OH	2.10	0.69
1:A:860:GLY:HA3	1:A:3136:THR:HG21	1.75	0.69
1:A:1976:LEU:CD1	1:A:2091:HIS:NE2	2.56	0.69
1:A:3996:GLY:O	1:A:4000:ASN:ND2	2.26	0.69
1:A:273:ARG:NH2	1:A:307:GLU:OE2	2.26	0.69
1:A:1643:MET:HG3	1:A:1688:LEU:HD11	1.75	0.69
1:A:1557:GLU:HA	1:A:1592:MET:HE1	1.75	0.69
1:A:2093:CYS:O	1:A:2096:PRO:CG	2.39	0.69
1:A:2555:LEU:CD1	1:A:2806:LYS:CA	2.71	0.68
1:A:1942:CYS:O	1:A:1946:ASN:ND2	2.25	0.68
1:A:671:SER:O	1:A:675:ARG:HG3	1.94	0.68
1:A:2094:MET:O	1:A:2097:LEU:HD23	1.94	0.68
1:A:3878:VAL:O	1:A:3965:ARG:NH2	2.27	0.68
1:A:1083:ASN:ND2	1:A:1126:GLN:OE1	2.27	0.68
1:A:1975:LEU:HD12	1:A:1976:LEU:HD22	1.75	0.68
1:A:1023:SER:HB3	1:A:1026:ARG:HH11	1.59	0.67
1:A:1372:LEU:HD13	1:A:1402:LEU:HD23	1.76	0.67
1:A:3867:THR:OG1	1:A:4119:ARG:NH1	2.26	0.67
1:A:3964:THR:OG1	1:A:3967:PHE:HD2	1.76	0.67
1:A:662:LEU:CD2	1:A:721:TYR:OH	2.40	0.67
1:A:3232:ARG:HH21	1:A:3269:ARG:HH21	1.40	0.67
1:A:1710:LEU:HG	1:A:1757:MET:HE1	1.77	0.67
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3469:LEU:HD22	1:A:3505:LEU:HD21	1.76	0.67
1:A:2301:GLN:OE1	1:A:2305:ASN:ND2	2.27	0.67
1:A:3498:TRP:HE3	1:A:3501:HIS:CD2	2.12	0.67
1:A:463:LYS:HD3	1:A:545:LEU:HD22	1.76	0.67
1:A:1661:PHE:CE2	1:A:1671:VAL:HG11	2.29	0.67
1:A:3685:PRO:HB2	1:A:3687:MET:H	1.60	0.67
1:A:41:GLU:OE2	1:A:45:SER:OG	2.11	0.67
1:A:2556:SER:OG	1:A:2799:GLN:HA	1.95	0.66
1:A:2094:MET:HA	1:A:2097:LEU:CD2	2.25	0.66
1:A:3076:ALA:O	1:A:3080:LEU:HD23	1.95	0.66
1:A:471:LYS:HA	1:A:1551:ILE:HD12	1.76	0.66
1:A:1234:GLY:HA2	1:A:1259:LEU:HD12	1.76	0.66
1:A:2410:GLU:O	1:A:2414:GLN:NE2	2.27	0.66
1:A:2093:CYS:HA	1:A:2096:PRO:HG3	1.77	0.66
1:A:3752:VAL:CG2	1:A:3802:LEU:CD2	2.66	0.66
1:A:2094:MET:HA	1:A:2097:LEU:HD23	1.78	0.66
1:A:1633:TRP:CE2	1:A:1674:THR:HG22	2.31	0.66
1:A:1210:ASP:O	1:A:1213:LYS:HG3	1.95	0.66
1:A:1897:ASN:HB3	1:A:1903:SER:HB2	1.78	0.66
1:A:3522:THR:HG21	1:A:3558:ILE:HG23	1.76	0.66
1:A:3964:THR:OG1	1:A:3967:PHE:CD2	2.49	0.65
1:A:3281:CYS:SG	1:A:3301:LEU:HD11	2.36	0.65
1:A:3943:GLY:HA3	1:A:4023:LYS:HZ3	1.60	0.65
1:A:3963:LEU:HG	1:A:4112:THR:HG22	1.79	0.65
1:A:2426:HIS:O	1:A:2432:GLN:NE2	2.28	0.65
1:A:3169:PRO:HD3	1:A:3182:ILE:HD11	1.77	0.65
1:A:3418:ASP:OD1	1:A:3419:PHE:N	2.30	0.65
1:A:287:LEU:HD22	1:A:337:LYS:HE2	1.77	0.65
1:A:1437:TYR:HD2	1:A:1507:CYS:HB3	1.62	0.65
1:A:3428:GLU:OE2	1:A:3474:ARG:NH1	2.30	0.65
1:A:3925:LEU:HG	1:A:3962:ARG:HH22	1.58	0.65
1:A:2474:TYR:O	1:A:2478:MET:HG3	1.96	0.65
1:A:3079:GLU:O	1:A:3083:SER:OG	2.14	0.65
1:A:3278:GLN:HB2	1:A:3329:LEU:HD12	1.80	0.64
1:A:3308:ASP:HA	1:A:3311:ASN:HB3	1.80	0.64
1:A:533:HIS:HB3	1:A:541:MET:HE1	1.79	0.64
1:A:2408:MET:HE2	1:A:2411:LEU:HD13	1.79	0.64
1:A:225:LYS:HE2	1:A:253:LEU:HD13	1.79	0.64
1:A:888:ARG:O	1:A:3889:ARG:NH2	2.23	0.64
1:A:2898:LEU:HG	1:A:3973:PRO:HG3	1.79	0.64
1:A:3714:GLU:N	1:A:3714:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1840:PHE:HA	1:A:1843:ILE:HG12	1.78	0.64
1:A:2806:LYS:HG3	1:A:2857:CYS:HB2	1.79	0.64
1:A:989:MET:O	1:A:993:HIS:ND1	2.31	0.64
1:A:3058:ASP:O	1:A:3059:GLN:NE2	2.25	0.64
1:A:2458:VAL:O	1:A:2461:PHE:HD2	1.80	0.64
1:A:2140:LEU:O	1:A:2144:LEU:HG	1.97	0.63
1:A:1118:GLU:HG3	1:A:1120:SER:H	1.63	0.63
1:A:2420:PHE:O	1:A:2423:VAL:HG12	1.98	0.63
1:A:3463:LEU:HD23	1:A:3997:LEU:HD11	1.79	0.63
1:A:1016:GLY:O	1:A:1018:VAL:N	2.31	0.63
1:A:1770:GLN:HB3	1:A:1814:PHE:HZ	1.62	0.63
1:A:1811:ARG:HH21	1:A:1819:PHE:HE2	1.44	0.63
1:A:1863:PHE:HA	1:A:1866:GLN:CD	2.24	0.63
1:A:1169:VAL:HG21	1:A:1198:LEU:HD21	1.81	0.63
1:A:2556:SER:OG	1:A:2799:GLN:CB	2.47	0.63
1:A:3753:LYS:CE	1:A:3756:GLU:OE1	2.47	0.63
1:A:2884:LEU:HD12	1:A:3116:SER:HB2	1.81	0.63
1:A:2093:CYS:HA	1:A:2096:PRO:CG	2.30	0.62
1:A:19:LEU:HD11	1:A:38:LEU:HD22	1.79	0.62
1:A:20:SER:O	1:A:24:ARG:HB2	1.99	0.62
1:A:2446:LEU:HD21	1:A:2454:LEU:HD12	1.80	0.62
1:A:1640:GLU:HA	1:A:1643:MET:HE2	1.80	0.62
1:A:1770:GLN:HB3	1:A:1814:PHE:CZ	2.34	0.62
1:A:2843:PHE:O	1:A:2847:THR:OG1	2.12	0.62
1:A:3344:GLU:OE2	1:A:3348:LEU:HD23	1.99	0.62
1:A:174:VAL:HA	1:A:177:LEU:HD23	1.82	0.62
1:A:2213:ASN:OD1	1:A:2214:ARG:N	2.33	0.62
1:A:722:LYS:HA	1:A:726:LEU:HB2	1.81	0.62
1:A:1802:TYR:CE2	1:A:1843:ILE:HG22	2.35	0.62
1:A:3698:GLU:OE2	1:A:3718:ARG:NH2	2.31	0.61
1:A:1482:GLU:HG3	1:A:1486:LEU:HD22	1.82	0.61
1:A:2095:ALA:N	1:A:2096:PRO:CD	2.64	0.61
1:A:2428:ASP:H	1:A:2432:GLN:NE2	1.97	0.61
1:A:4104:VAL:O	1:A:4108:MET:HG2	2.01	0.61
1:A:1437:TYR:CD2	1:A:1507:CYS:HB3	2.34	0.61
1:A:2093:CYS:C	1:A:2096:PRO:CG	2.74	0.61
1:A:2183:HIS:CE1	1:A:2186:VAL:HG23	2.36	0.61
1:A:3995:PRO:O	1:A:3999:THR:OG1	2.13	0.61
1:A:905:ILE:HD12	1:A:2811:SER:HB3	1.81	0.61
1:A:1751:GLU:HA	1:A:1785:ILE:HG22	1.82	0.61
1:A:3493:TRP:CE3	1:A:3711:PRO:CB	2.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3495:PHE:HB3	1:A:3502:MET:HE1	1.83	0.61
1:A:3587:ASP:OD2	1:A:3733:ARG:NH2	2.26	0.61
1:A:1389:VAL:HG13	1:A:1390:GLN:H	1.65	0.61
1:A:3421:ASP:OD2	1:A:3425:ARG:NH1	2.33	0.61
1:A:2188:GLU:O	1:A:2192:THR:HG23	2.01	0.61
1:A:3701:ILE:O	1:A:3704:GLN:HG3	2.01	0.61
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.73	0.61
1:A:181:LEU:HA	1:A:184:VAL:HB	1.83	0.60
1:A:1459:HIS:HB2	1:A:1464:LEU:HD22	1.83	0.60
1:A:1671:VAL:O	1:A:1674:THR:OG1	2.16	0.60
1:A:2461:PHE:HE1	1:A:2469:CYS:HB3	1.66	0.60
1:A:2428:ASP:H	1:A:2432:GLN:HE21	1.48	0.60
1:A:2481:HIS:CD2	1:A:2485:ARG:HH22	2.19	0.60
1:A:3791:TYR:CE2	1:A:3803:ILE:HD12	2.27	0.60
1:A:1709:GLU:OE1	1:A:1709:GLU:N	2.34	0.60
1:A:1729:PHE:HB3	1:A:1736:PHE:HB2	1.82	0.60
1:A:2289:ASP:HB3	1:A:2290:PRO:HD3	1.82	0.60
1:A:3976:GLU:OE1	1:A:4108:MET:HE3	2.02	0.60
1:A:1212:LEU:HD11	1:A:1217:VAL:HA	1.84	0.60
1:A:2461:PHE:HB2	1:A:2473:MET:SD	2.42	0.60
1:A:4013:TRP:NE1	1:A:4017:GLU:OE1	2.35	0.60
1:A:2158:ARG:HH21	1:A:2199:LEU:HD11	1.66	0.60
1:A:2368:THR:HG23	1:A:2372:PRO:HA	1.84	0.60
1:A:722:LYS:HA	1:A:726:LEU:CD2	2.32	0.59
1:A:634:LEU:HD12	1:A:672:ILE:HD11	1.84	0.59
1:A:1018:VAL:HG13	1:A:1026:ARG:HG3	1.84	0.59
1:A:1241:LEU:HD11	1:A:1253:THR:HA	1.82	0.59
1:A:2120:ARG:HB3	1:A:2160:TYR:HE1	1.67	0.59
1:A:3288:SER:C	1:A:3289:ARG:HH11	2.07	0.59
1:A:4081:ALA:O	1:A:4090:ARG:NH1	2.35	0.59
1:A:1797:LEU:O	1:A:1800:SER:OG	2.18	0.59
1:A:3538:GLU:OE2	1:A:3798:SER:N	2.31	0.59
1:A:1839:PHE:O	1:A:1843:ILE:HG23	2.02	0.59
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	1.84	0.59
1:A:16:GLN:NE2	1:A:17:GLU:OE2	2.36	0.59
1:A:2254:ARG:HH12	1:A:2292:CYS:N	1.99	0.59
1:A:3462:ARG:O	1:A:3498:TRP:NE1	2.36	0.59
1:A:3751:LEU:HG	1:A:3803:ILE:HG23	1.84	0.59
1:A:1101:PHE:HD2	1:A:1163:LEU:HD21	1.67	0.59
1:A:3642:LYS:HA	1:A:3646:LYS:HA	1.84	0.59
1:A:4012:ASP:OD1	1:A:4013:TRP:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3588:TRP:HE1	1:A:3609:MET:CB	2.14	0.58
1:A:2468:THR:HA	1:A:2471:GLU:HG2	1.84	0.58
1:A:3066:ASP:O	1:A:3070:HIS:ND1	2.37	0.58
1:A:3462:ARG:HD3	1:A:3494:GLN:HA	1.84	0.58
1:A:3711:PRO:O	1:A:3713:PRO:HD3	2.03	0.58
1:A:722:LYS:HA	1:A:726:LEU:CB	2.33	0.58
1:A:1019:ASP:H	1:A:1020:PRO:HD3	1.60	0.58
1:A:3031:TRP:CH2	1:A:3040:TYR:HB2	2.28	0.58
1:A:1424:THR:HG23	1:A:1427:SER:H	1.67	0.58
1:A:523:THR:HG23	1:A:525:LYS:H	1.67	0.58
1:A:606:SER:OG	1:A:1023:SER:HB2	2.02	0.58
1:A:2377:ARG:HG3	1:A:2378:PHE:CD1	2.39	0.58
1:A:848:LEU:O	1:A:852:ARG:HG3	2.03	0.58
1:A:1976:LEU:HD21	1:A:2145:PHE:CD2	2.39	0.58
1:A:3751:LEU:HD21	1:A:3803:ILE:HD13	1.85	0.58
1:A:108:LYS:HZ3	1:A:152:LEU:H	1.50	0.58
1:A:1554:SER:HB3	1:A:1557:GLU:HB3	1.86	0.58
1:A:3495:PHE:CD1	1:A:3502:MET:HE1	2.38	0.58
1:A:3962:ARG:HG2	1:A:3967:PHE:CE2	2.39	0.58
1:A:64:GLY:HA2	1:A:67:VAL:HG12	1.85	0.58
1:A:2094:MET:HE2	1:A:2152:ASN:HD22	1.69	0.58
1:A:240:GLU:HB2	1:A:243:GLN:NE2	2.18	0.58
1:A:2477:LEU:HD23	1:A:2480:ILE:HD12	1.85	0.58
1:A:2538:ARG:O	1:A:2542:LEU:HD23	2.04	0.58
1:A:1358:LEU:HD11	1:A:1410:PRO:HG2	1.86	0.57
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.04	0.57
1:A:3692:VAL:HG22	1:A:3692:VAL:O	2.03	0.57
1:A:905:ILE:HG23	1:A:2811:SER:HB3	1.85	0.57
1:A:2202:PRO:HG2	1:A:2245:TRP:CD2	2.39	0.57
1:A:2274:ILE:HD12	1:A:2318:ALA:HB3	1.86	0.57
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	1.86	0.57
1:A:3751:LEU:HG	1:A:3751:LEU:O	2.03	0.57
1:A:3232:ARG:HH21	1:A:3269:ARG:NH2	2.02	0.57
1:A:3462:ARG:HD3	1:A:3494:GLN:CB	2.33	0.57
1:A:2555:LEU:HD13	1:A:2806:LYS:HA	1.86	0.57
1:A:631:ARG:HH22	1:A:668:LYS:HD2	1.69	0.57
1:A:1358:LEU:HD21	1:A:1410:PRO:HB2	1.86	0.57
1:A:2451:LEU:HD22	1:A:2498:ILE:HD13	1.85	0.57
1:A:1335:CYS:HB3	1:A:1384:PHE:CE1	2.39	0.57
1:A:2093:CYS:C	1:A:2096:PRO:HD2	2.30	0.57
1:A:3859:TYR:CD2	1:A:4077:TYR:HE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2239:LYS:HB3	1:A:2279:ILE:HD12	1.87	0.57
1:A:12:LEU:HA	1:A:15:LEU:HB3	1.86	0.57
1:A:195:ASN:OD1	1:A:196:LEU:N	2.37	0.57
1:A:3011:LEU:O	1:A:3016:THR:HG22	2.05	0.57
1:A:3319:ASN:OD1	1:A:3391:ALA:HB1	2.05	0.57
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	1.85	0.57
1:A:3493:TRP:CZ3	1:A:3711:PRO:CB	2.81	0.57
1:A:12:LEU:O	1:A:16:GLN:HG2	2.05	0.56
1:A:2279:ILE:O	1:A:2283:ASN:ND2	2.37	0.56
1:A:3813:LYS:NZ	1:A:4125:GLU:OE2	2.36	0.56
1:A:50:VAL:HA	1:A:53:LEU:HB2	1.86	0.56
1:A:1097:GLU:OE2	1:A:1151:ARG:NH2	2.29	0.56
1:A:2318:ALA:HA	1:A:2321:GLU:CD	2.30	0.56
1:A:3072:GLU:C	1:A:3074:GLN:H	2.13	0.56
1:A:3943:GLY:HA3	1:A:4023:LYS:NZ	2.20	0.56
1:A:1657:SER:HB3	1:A:1659:VAL:HG13	1.88	0.56
1:A:1873:TYR:O	1:A:1877:LEU:HD23	2.04	0.56
1:A:1892:LYS:HA	1:A:1908:GLY:HA2	1.87	0.56
1:A:2094:MET:C	1:A:2096:PRO:HD2	2.31	0.56
1:A:56:SER:HA	1:A:59:PHE:CD2	2.40	0.56
1:A:65:LEU:HA	1:A:68:PHE:CD2	2.41	0.56
1:A:1853:SER:O	1:A:1855:PHE:N	2.34	0.56
1:A:3062:LEU:HD13	1:A:3093:GLN:NE2	2.21	0.56
1:A:356:ASN:ND2	1:A:404:ASP:HB3	2.21	0.56
1:A:722:LYS:CA	1:A:726:LEU:HB2	2.36	0.56
1:A:796:LEU:HD23	1:A:855:VAL:HG13	1.87	0.56
1:A:1804:MET:O	1:A:1811:ARG:NH2	2.35	0.56
1:A:2365:ASN:O	1:A:2369:LYS:HG2	2.05	0.56
1:A:3144:PHE:HZ	1:A:3157:LEU:HD22	1.70	0.56
1:A:4013:TRP:HE1	1:A:4034:ALA:HB1	1.70	0.56
1:A:403:GLY:O	1:A:406:ARG:NH1	2.38	0.55
1:A:1729:PHE:CE1	1:A:1735:ARG:HG2	2.41	0.55
1:A:131:LEU:HD12	1:A:132:ILE:N	2.21	0.55
1:A:2482:ASP:HA	1:A:2485:ARG:NH2	2.22	0.55
1:A:3394:GLU:OE1	1:A:3394:GLU:N	2.39	0.55
1:A:3493:TRP:HA	1:A:3496:ILE:HG12	1.87	0.55
1:A:2349:LEU:HA	1:A:2352:HIS:CE1	2.41	0.55
1:A:129:ASP:OD1	1:A:129:ASP:N	2.40	0.55
1:A:3288:SER:O	1:A:3289:ARG:HD3	2.07	0.55
1:A:3493:TRP:CH2	1:A:3711:PRO:HB3	2.41	0.55
1:A:1101:PHE:CZ	1:A:1145:LEU:HD22	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1463:LEU:O	1:A:1467:ILE:HG12	2.06	0.55
1:A:1142:HIS:O	1:A:1146:ASN:ND2	2.39	0.55
1:A:1828:LEU:HD21	1:A:1876:ILE:HG23	1.89	0.55
1:A:3992:ARG:NH1	1:A:4103:GLN:OE1	2.39	0.55
1:A:3518:VAL:O	1:A:3521:ILE:HG22	2.07	0.55
1:A:3596:LEU:HD12	1:A:3601:VAL:HA	1.88	0.55
1:A:540:MET:O	1:A:544:ILE:HG12	2.06	0.55
1:A:1871:MET:HG2	1:A:1875:LYS:HZ2	1.72	0.55
1:A:2220:MET:HE1	1:A:2252:PRO:HG2	1.88	0.55
1:A:2786:LYS:O	1:A:2789:SER:N	2.30	0.55
1:A:738:HIS:O	1:A:742:GLU:HB2	2.07	0.55
1:A:1046:PRO:HA	1:A:1049:GLN:HB2	1.89	0.55
1:A:2183:HIS:CE1	1:A:2185:MET:HB3	2.42	0.55
1:A:2330:VAL:HG22	1:A:2334:LYS:HA	1.88	0.55
1:A:1239:PRO:HB3	1:A:1289:SER:OG	2.07	0.54
1:A:2120:ARG:HB3	1:A:2160:TYR:CE1	2.43	0.54
1:A:2551:GLU:OE1	1:A:2847:THR:HG23	2.07	0.54
1:A:3527:GLN:HE21	1:A:3568:ILE:HD11	1.72	0.54
1:A:1820:VAL:O	1:A:1825:LEU:HG	2.07	0.54
1:A:294:PHE:CE1	1:A:316:LEU:HD11	2.43	0.54
1:A:971:ARG:HH22	1:A:1014:LEU:HD22	1.72	0.54
1:A:3820:MET:HG2	1:A:3882:LEU:HD21	1.90	0.54
1:A:59:PHE:HA	1:A:62:ASP:HB2	1.88	0.54
1:A:225:LYS:HE2	1:A:267:VAL:HG13	1.89	0.54
1:A:1375:THR:HG22	1:A:1395:LEU:HD21	1.90	0.54
1:A:356:ASN:ND2	1:A:404:ASP:O	2.40	0.54
1:A:892:LEU:HD21	1:A:941:MET:HG2	1.89	0.54
1:A:1261:LEU:HD11	1:A:1340:ARG:HG3	1.90	0.54
1:A:1781:SER:O	1:A:1785:ILE:HG23	2.08	0.54
1:A:1369:MET:HE1	1:A:1406:LEU:HD22	1.88	0.54
1:A:1802:TYR:O	1:A:1805:PHE:HB3	2.07	0.54
1:A:1920:TYR:O	1:A:1924:THR:CB	2.55	0.54
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.42	0.54
1:A:3749:PRO:HG3	1:A:3807:GLU:OE2	2.07	0.54
1:A:536:SER:O	1:A:539:GLN:HG2	2.08	0.54
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.81	0.54
1:A:580:ASP:HB3	1:A:616:LYS:HD2	1.88	0.54
1:A:2362:VAL:HA	1:A:2396:LEU:HD21	1.90	0.54
1:A:2563:LEU:HD13	1:A:2812:LEU:HD11	1.90	0.54
1:A:2898:LEU:CD2	1:A:3972:LEU:HG	2.38	0.54
1:A:1224:PHE:HD1	1:A:1266:CYS:HG	1.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:ASN:CG	1:A:1437:TYR:H	2.15	0.54
1:A:2396:LEU:HA	1:A:2399:GLU:OE1	2.08	0.54
1:A:3666:LEU:O	1:A:3670:MET:HG3	2.08	0.54
1:A:3796:MET:O	1:A:3797:THR:OG1	2.21	0.54
1:A:1375:THR:HG23	1:A:1379:PRO:HB3	1.90	0.53
1:A:1750:LEU:HD11	1:A:1759:LEU:HA	1.90	0.53
1:A:1949:ILE:HG23	1:A:2100:LEU:HD13	1.89	0.53
1:A:2967:GLU:O	1:A:2971:GLN:HG3	2.08	0.53
1:A:919:LEU:HD11	1:A:968:VAL:HG13	1.89	0.53
1:A:3406:ALA:O	1:A:3409:VAL:HG12	2.09	0.53
1:A:3750:PHE:CD2	1:A:3804:GLU:CA	2.90	0.53
1:A:1633:TRP:NE1	1:A:1674:THR:HG22	2.24	0.53
1:A:989:MET:SD	1:A:1035:GLU:HG3	2.49	0.53
1:A:3587:ASP:OD1	1:A:3733:ARG:NH1	2.37	0.53
1:A:683:PHE:O	1:A:686:VAL:HG12	2.09	0.53
1:A:773:LEU:HD13	1:A:792:ILE:HG21	1.90	0.53
1:A:3026:ASP:O	1:A:3030:ILE:HG22	2.08	0.53
1:A:1119:LYS:NZ	1:A:1182:GLU:OE2	2.42	0.53
1:A:2092:GLU:N	1:A:2092:GLU:OE1	2.42	0.53
1:A:2254:ARG:O	1:A:2257:PHE:N	2.42	0.53
1:A:2327:LEU:HD11	1:A:2345:VAL:HG21	1.89	0.53
1:A:2365:ASN:ND2	1:A:2396:LEU:HD12	2.19	0.53
1:A:108:LYS:HZ3	1:A:152:LEU:N	2.06	0.52
1:A:294:PHE:HE1	1:A:316:LEU:HD11	1.74	0.52
1:A:1933:LEU:H	1:A:1937:ARG:NH1	1.97	0.52
1:A:170:VAL:O	1:A:171:LEU:HD22	2.09	0.52
1:A:1851:LEU:HD21	1:A:1873:TYR:HB2	1.90	0.52
1:A:3786:LEU:HD22	1:A:3910:LEU:HD22	1.91	0.52
1:A:168:ASP:HB3	1:A:171:LEU:HD23	1.90	0.52
1:A:1231:GLN:O	1:A:1233:SER:N	2.34	0.52
1:A:1684:LEU:HD11	1:A:1688:LEU:HG	1.90	0.52
1:A:2466:SER:HG	1:A:2469:CYS:H	1.54	0.52
1:A:3569:GLN:NE2	1:A:3573:ASN:OD1	2.36	0.52
1:A:1568:ASN:OD1	1:A:1603:GLN:HG3	2.08	0.52
1:A:3134:ALA:HB2	1:A:3182:ILE:HG22	1.91	0.52
1:A:1670:GLU:O	1:A:1674:THR:HG23	2.09	0.52
1:A:3998:LEU:O	1:A:4002:MET:HG3	2.10	0.52
1:A:2338:GLU:HG2	1:A:2339:GLU:N	2.25	0.52
1:A:3925:LEU:CG	1:A:3962:ARG:NH2	2.59	0.52
1:A:391:ARG:O	1:A:395:MET:HG2	2.10	0.52
1:A:1611:GLN:HB3	1:A:1614:GLN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3730:ALA:O	2:A:6101:1IX:CL1	2.65	0.52
1:A:80:GLU:O	1:A:83:GLU:N	2.42	0.52
1:A:756:PHE:HE1	1:A:770:LEU:HD22	1.74	0.52
1:A:1014:LEU:O	1:A:1018:VAL:HG11	2.10	0.52
1:A:1675:TYR:HE1	1:A:1695:LEU:HB2	1.75	0.52
1:A:2522:ARG:NH2	1:A:2564:GLU:HG3	2.25	0.52
1:A:2919:ASP:OD1	1:A:2920:VAL:N	2.42	0.52
1:A:2987:THR:HG23	1:A:2990:GLU:H	1.74	0.52
1:A:3750:PHE:CE2	1:A:3804:GLU:CB	2.90	0.52
1:A:3791:TYR:CD2	1:A:3803:ILE:HG13	2.44	0.52
1:A:108:LYS:HE3	1:A:156:PHE:HZ	1.74	0.52
1:A:332:GLU:HG2	1:A:333:MET:H	1.75	0.52
1:A:399:GLN:NE2	1:A:405:ASP:O	2.43	0.52
1:A:1267:TYR:CD2	1:A:1290:LEU:HD22	2.45	0.52
1:A:2232:ARG:HA	1:A:2235:LEU:HD12	1.90	0.52
1:A:3864:ARG:HE	1:A:3868:VAL:HG21	1.74	0.52
1:A:959:TYR:OH	1:A:963:LYS:HE2	2.10	0.51
1:A:2231:PHE:CE2	1:A:2235:LEU:HD11	2.46	0.51
1:A:3685:PRO:CB	1:A:3687:MET:HG3	2.41	0.51
1:A:1328:GLU:HA	1:A:1331:ASN:HB2	1.92	0.51
1:A:1613:HIS:HA	1:A:1616:LEU:HD12	1.91	0.51
1:A:1799:GLU:HA	1:A:1802:TYR:HB3	1.92	0.51
1:A:573:LEU:HA	1:A:576:VAL:HG12	1.91	0.51
1:A:1389:VAL:HG22	1:A:1390:GLN:HG3	1.91	0.51
1:A:2190:VAL:HA	1:A:2193:ILE:HG12	1.92	0.51
1:A:355:ASN:OD1	1:A:356:ASN:N	2.44	0.51
1:A:1612:LYS:O	1:A:1616:LEU:HG	2.10	0.51
1:A:1652:ILE:O	1:A:1655:ILE:HG22	2.10	0.51
1:A:2497:GLU:HA	1:A:2500:LYS:HD3	1.90	0.51
1:A:2828:GLU:O	1:A:2832:ILE:HG12	2.09	0.51
1:A:131:LEU:HB2	1:A:173:LYS:HD2	1.93	0.51
1:A:3526:PRO:O	1:A:3527:GLN:HB2	2.10	0.51
1:A:923:ASP:O	1:A:925:GLN:N	2.44	0.51
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	1.92	0.51
1:A:305:ASN:HD21	1:A:308:LEU:HD22	1.76	0.51
1:A:1560:TYR:O	1:A:1564:SER:HB3	2.11	0.51
1:A:3379:GLN:O	1:A:3383:GLN:HG2	2.11	0.51
1:A:411:PRO:HG3	1:A:442:GLN:HE22	1.75	0.51
1:A:670:LEU:O	1:A:674:VAL:HG23	2.11	0.51
1:A:959:TYR:CZ	1:A:963:LYS:HE2	2.46	0.51
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:VAL:HG21	1:A:1154:PRO:HB3	1.93	0.51
1:A:2239:LYS:HA	1:A:2242:VAL:HG12	1.91	0.51
1:A:2277:LEU:O	1:A:2280:VAL:HG12	2.11	0.51
1:A:1820:VAL:HG23	1:A:1824:LEU:HD23	1.93	0.51
1:A:1871:MET:HG2	1:A:1875:LYS:NZ	2.26	0.51
1:A:2101:VAL:CG2	1:A:2153:THR:HG21	2.40	0.51
1:A:2371:PHE:HD2	1:A:2374:LEU:HB2	1.76	0.51
1:A:2548:PRO:HB2	1:A:2848:PHE:CD2	2.46	0.51
1:A:3065:ILE:HD12	1:A:3078:LEU:HD21	1.93	0.51
1:A:3194:GLU:HB3	1:A:3231:ILE:CD1	2.31	0.51
1:A:3390:GLN:HA	1:A:3393:GLU:HG2	1.92	0.51
1:A:3506:LEU:HD11	1:A:3518:VAL:HG11	1.93	0.51
1:A:907:LEU:HB3	1:A:937:MET:HE3	1.93	0.50
1:A:1708:GLU:OE1	1:A:1712:ARG:NH2	2.44	0.50
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.76	0.50
1:A:3332:THR:HA	1:A:3335:ARG:HG2	1.94	0.50
1:A:1068:LEU:HD11	1:A:1106:ILE:HG23	1.93	0.50
1:A:3512:VAL:HG22	1:A:3513:ALA:H	1.77	0.50
1:A:923:ASP:C	1:A:925:GLN:H	2.20	0.50
1:A:2094:MET:HE1	1:A:2149:LEU:HA	1.93	0.50
1:A:2236:GLU:HA	1:A:2239:LYS:HG2	1.92	0.50
1:A:2953:THR:HB	1:A:2994:TRP:HE1	1.75	0.50
1:A:254:LYS:HB3	1:A:300:TRP:CH2	2.47	0.50
1:A:1860:GLU:C	1:A:1862:THR:H	2.18	0.50
1:A:3033:GLU:CD	1:A:3034:PRO:HD3	2.37	0.50
1:A:3685:PRO:HB2	1:A:3687:MET:HG3	1.93	0.50
1:A:332:GLU:HG2	1:A:333:MET:N	2.27	0.50
1:A:3691:LYS:O	1:A:3693:GLU:N	2.45	0.50
1:A:3867:THR:HG21	1:A:4119:ARG:HE	1.76	0.50
1:A:3752:VAL:HA	1:A:3802:LEU:HD23	1.93	0.50
1:A:1723:PRO:HD3	1:A:1729:PHE:HE2	1.76	0.50
1:A:2133:LEU:HG	1:A:2167:PRO:HB2	1.93	0.50
1:A:3062:LEU:HD23	1:A:3062:LEU:H	1.76	0.50
1:A:3497:SER:HB3	1:A:3707:GLY:HA3	1.92	0.50
1:A:229:SER:HB3	1:A:274:LEU:HD13	1.94	0.50
1:A:435:LEU:O	1:A:439:VAL:HG23	2.12	0.50
1:A:1632:TRP:O	1:A:1637:SER:OG	2.21	0.50
1:A:3247:ARG:HD2	1:A:3283:LEU:HA	1.94	0.50
1:A:3335:ARG:O	1:A:3339:ASN:ND2	2.45	0.50
1:A:3463:LEU:HB3	1:A:3997:LEU:HD11	1.92	0.50
1:A:333:MET:HG2	1:A:334:HIS:CD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2555:LEU:HD13	1:A:2805:ALA:C	2.37	0.49
1:A:3298:LEU:HG	1:A:3336:ILE:HG21	1.94	0.49
1:A:3454:LEU:HD21	1:A:3462:ARG:HA	1.93	0.49
1:A:3792:SER:O	1:A:3803:ILE:HA	2.12	0.49
1:A:2190:VAL:O	1:A:2194:LEU:HG	2.12	0.49
1:A:3424:LEU:O	1:A:3428:GLU:HG2	2.12	0.49
1:A:3755:GLY:O	1:A:4022:LYS:HE3	2.12	0.49
1:A:109:ASN:OD1	1:A:110:THR:N	2.45	0.49
1:A:1675:TYR:CE1	1:A:1695:LEU:HB2	2.47	0.49
1:A:2877:SER:OG	1:A:2925:GLU:HB3	2.12	0.49
1:A:3490:VAL:HG12	1:A:3491:PRO:O	2.12	0.49
1:A:3575:LEU:HD13	1:A:3802:LEU:CD1	2.32	0.49
1:A:172:GLU:HG2	1:A:223:CYS:HB2	1.94	0.49
1:A:316:LEU:HD23	1:A:361:ILE:HD12	1.94	0.49
1:A:1255:CYS:CB	1:A:3694:PHE:CZ	2.61	0.49
1:A:2183:HIS:ND1	1:A:2185:MET:HB3	2.27	0.49
1:A:2357:GLU:HB3	1:A:2385:LEU:HD11	1.93	0.49
1:A:2786:LYS:O	1:A:2788:SER:N	2.45	0.49
1:A:3478:GLU:C	1:A:3480:LEU:H	2.20	0.49
1:A:970:LEU:HD23	1:A:1014:LEU:HD12	1.94	0.49
1:A:63:PHE:HA	1:A:66:LEU:HG	1.95	0.49
1:A:1212:LEU:HD13	1:A:1220:LEU:HD23	1.95	0.49
1:A:2255:LEU:O	1:A:2259:LYS:HG2	2.12	0.49
1:A:2286:PRO:HG2	1:A:2289:ASP:HB2	1.95	0.49
1:A:3418:ASP:O	1:A:3421:ASP:N	2.46	0.49
1:A:195:ASN:O	1:A:198:ARG:HG3	2.12	0.49
1:A:718:MET:HE1	1:A:751:ALA:HB2	1.94	0.49
1:A:1522:GLY:O	1:A:1524:LEU:N	2.46	0.49
1:A:1673:THR:O	1:A:1677:SER:OG	2.22	0.49
1:A:1714:LEU:O	1:A:1717:LEU:HB3	2.13	0.49
1:A:2353:GLN:HB2	1:A:2360:PHE:CD1	2.48	0.49
1:A:3519:GLU:HB2	1:A:3554:PHE:CZ	2.48	0.49
1:A:3800:LEU:HG	1:A:3801:GLY:H	1.77	0.49
1:A:14:ARG:CZ	1:A:17:GLU:HG3	2.43	0.49
1:A:354:SER:HA	1:A:1733:THR:HG21	1.94	0.49
1:A:1389:VAL:HG13	1:A:1390:GLN:N	2.27	0.49
1:A:2556:SER:OG	1:A:2799:GLN:CA	2.60	0.49
1:A:2566:THR:O	1:A:2569:SER:OG	2.14	0.49
1:A:3527:GLN:H	1:A:3530:VAL:HG23	1.77	0.49
1:A:656:GLN:OE1	1:A:659:ARG:NH2	2.44	0.49
1:A:1820:VAL:HA	1:A:1824:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1932:GLN:H	1:A:1937:ARG:HH12	1.60	0.49
1:A:1933:LEU:O	1:A:1937:ARG:NE	2.37	0.49
1:A:3026:ASP:N	1:A:3026:ASP:OD1	2.43	0.49
1:A:3228:SER:O	1:A:3228:SER:OG	2.28	0.49
1:A:3608:LYS:O	1:A:3611:GLU:HG3	2.12	0.49
1:A:3929:MET:SD	1:A:3940:ILE:HD13	2.53	0.49
1:A:404:ASP:H	1:A:1732:GLY:HA2	1.78	0.49
1:A:1416:GLU:HG2	1:A:1420:ARG:HE	1.77	0.49
1:A:2456:ASN:O	1:A:2460:GLU:OE1	2.30	0.49
1:A:1388:ASP:HA	1:A:1392:MET:HE2	1.95	0.48
1:A:1407:LYS:HG3	1:A:1412:LYS:HD3	1.93	0.48
1:A:1479:VAL:HG11	1:A:1521:PHE:CD1	2.47	0.48
1:A:2871:LEU:HD23	1:A:2876:VAL:HG22	1.95	0.48
1:A:3157:LEU:HD11	1:A:3193:ILE:HG21	1.95	0.48
1:A:3266:SER:OG	1:A:3267:LYS:N	2.45	0.48
1:A:3793:VAL:HG22	1:A:3803:ILE:HB	1.95	0.48
1:A:1211:VAL:HA	1:A:1214:GLU:CD	2.38	0.48
1:A:1709:GLU:HA	1:A:1712:ARG:HG2	1.95	0.48
1:A:363:ILE:HG13	1:A:413:PHE:CE2	2.47	0.48
1:A:1565:GLU:OE1	1:A:1565:GLU:N	2.43	0.48
1:A:1766:LEU:HD11	1:A:1775:GLU:HG3	1.95	0.48
1:A:2376:ASP:OD1	1:A:2404:ARG:HG2	2.13	0.48
1:A:3006:ALA:HB3	1:A:3257:LYS:HZ1	1.77	0.48
1:A:363:ILE:HG13	1:A:413:PHE:CZ	2.49	0.48
1:A:571:SER:HA	1:A:574:LYS:HE3	1.96	0.48
1:A:915:THR:HB	1:A:968:VAL:HG11	1.96	0.48
1:A:1716:GLN:HA	1:A:1719:VAL:HG12	1.95	0.48
1:A:1851:LEU:HA	1:A:1870:LYS:HG2	1.96	0.48
1:A:3295:GLU:OE1	1:A:3348:LEU:HD22	2.14	0.48
1:A:3316:LEU:HD23	1:A:3322:ALA:HB1	1.95	0.48
1:A:173:LYS:HB2	1:A:176:GLU:HB2	1.95	0.48
1:A:346:TYR:HB3	1:A:350:ARG:NH1	2.28	0.48
1:A:1158:PRO:N	1:A:1159:PRO:HD2	2.29	0.48
1:A:1751:GLU:CD	1:A:1784:ARG:HE	2.21	0.48
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.45	0.48
1:A:299:LYS:HE2	1:A:299:LYS:HA	1.94	0.48
1:A:1045:THR:H	1:A:1048:GLN:NE2	2.12	0.48
1:A:3278:GLN:HB2	1:A:3329:LEU:CD1	2.43	0.48
1:A:3519:GLU:HB2	1:A:3554:PHE:HZ	1.78	0.48
1:A:3972:LEU:HD12	1:A:3972:LEU:O	2.12	0.48
1:A:355:ASN:HB3	1:A:358:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:PRO:HD3	1:A:1163:LEU:HD11	1.95	0.48
1:A:1650:ALA:HB1	1:A:1654:GLN:HE22	1.78	0.48
1:A:1874:TYR:CE2	1:A:1940:TYR:HE1	2.31	0.48
1:A:2506:LEU:HD13	1:A:2524:PHE:CE2	2.48	0.48
1:A:2894:GLU:HG2	1:A:3973:PRO:HG2	1.95	0.48
1:A:3014:CYS:C	1:A:3016:THR:H	2.22	0.48
1:A:3684:SER:HB2	1:A:3685:PRO:CD	2.44	0.48
1:A:2158:ARG:HB2	1:A:2159:PRO:HD3	1.96	0.48
1:A:2443:MET:C	1:A:2445:LYS:H	2.21	0.48
1:A:3529:ILE:HG23	1:A:3562:LEU:HD11	1.96	0.48
1:A:131:LEU:HD13	1:A:173:LYS:CD	2.43	0.48
1:A:449:TYR:HB3	1:A:453:MET:HB3	1.96	0.48
1:A:1075:ARG:NH1	1:A:1123:THR:HG21	2.29	0.48
1:A:2492:ASP:HB3	1:A:2495:SER:H	1.77	0.48
1:A:2573:PRO:HA	1:A:2786:LYS:NZ	2.28	0.48
1:A:165:LYS:HB2	1:A:167:PRO:HD2	1.95	0.48
1:A:254:LYS:HB3	1:A:300:TRP:HH2	1.79	0.48
1:A:721:TYR:CE2	1:A:725:LEU:HD21	2.48	0.48
1:A:935:HIS:O	1:A:939:MET:HG2	2.12	0.48
1:A:1157:PHE:HB3	1:A:1159:PRO:HG2	1.94	0.48
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.44	0.48
1:A:3946:PHE:HE2	1:A:4005:PHE:CE2	2.32	0.48
1:A:19:LEU:HG	1:A:34:LEU:HD23	1.95	0.47
1:A:79:ARG:O	1:A:82:ARG:HB3	2.14	0.47
1:A:1301:ILE:HA	1:A:1334:LYS:HD2	1.95	0.47
1:A:1436:LEU:HD23	1:A:1436:LEU:H	1.79	0.47
1:A:1563:PHE:O	1:A:1567:ILE:HG12	2.14	0.47
1:A:2257:PHE:O	1:A:2261:SER:CB	2.62	0.47
1:A:3749:PRO:CG	1:A:3807:GLU:OE2	2.62	0.47
1:A:1798:LEU:HD11	1:A:1831:CYS:SG	2.54	0.47
1:A:1803:GLU:HG3	1:A:1806:ARG:HE	1.79	0.47
1:A:1980:ASN:ND2	1:A:1982:ILE:HG12	2.28	0.47
1:A:2224:PHE:HA	1:A:2231:PHE:CD1	2.50	0.47
1:A:2425:ARG:NH1	1:A:2460:GLU:OE2	2.45	0.47
1:A:3036:TYR:C	1:A:3038:GLU:H	2.22	0.47
1:A:75:SER:H	1:A:78:PHE:HB3	1.77	0.47
1:A:1473:THR:OG1	1:A:1474:ASP:N	2.48	0.47
1:A:2540:LEU:HD11	1:A:2832:ILE:HG23	1.95	0.47
1:A:3518:VAL:O	1:A:3522:THR:HG23	2.15	0.47
1:A:3663:THR:HA	1:A:3666:LEU:HD13	1.97	0.47
1:A:1014:LEU:HB2	1:A:1029:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:LYS:HE3	1:A:1408:MET:HE3	1.96	0.47
1:A:1811:ARG:NH2	1:A:1819:PHE:HE2	2.11	0.47
1:A:2183:HIS:HD1	1:A:2185:MET:HB3	1.78	0.47
1:A:3301:LEU:HA	1:A:3301:LEU:HD12	1.59	0.47
1:A:3593:ARG:O	1:A:3597:ALA:HB2	2.15	0.47
1:A:3819:THR:HG21	1:A:3886:ALA:HB2	1.96	0.47
1:A:4015:ASN:HA	1:A:4018:GLN:HG2	1.95	0.47
1:A:1101:PHE:HD2	1:A:1163:LEU:CD2	2.26	0.47
1:A:1355:GLY:O	1:A:1358:LEU:HB2	2.14	0.47
1:A:1537:VAL:HG21	1:A:1552:HIS:HD2	1.78	0.47
1:A:2253:TYR:HB3	1:A:2288:TYR:HD1	1.79	0.47
1:A:2364:LEU:HG	1:A:2400:VAL:HG21	1.97	0.47
1:A:2849:SER:O	1:A:2849:SER:OG	2.29	0.47
1:A:3881:ASP:OD1	1:A:3881:ASP:N	2.45	0.47
1:A:4013:TRP:NE1	1:A:4034:ALA:HB1	2.30	0.47
1:A:23:ASP:HA	1:A:30:ALA:HB1	1.96	0.47
1:A:1066:LEU:HB3	1:A:1078:ALA:HB2	1.97	0.47
1:A:1186:LYS:O	1:A:1190:LEU:HG	2.13	0.47
1:A:1217:VAL:O	1:A:1221:ILE:HD12	2.14	0.47
1:A:1195:VAL:HA	1:A:1198:LEU:HD23	1.96	0.47
1:A:3062:LEU:HD13	1:A:3093:GLN:CD	2.39	0.47
1:A:3527:GLN:HA	1:A:3530:VAL:HG23	1.97	0.47
1:A:3567:VAL:HG22	1:A:3699:LEU:HD13	1.96	0.47
1:A:3999:THR:O	1:A:4003:ASP:HB2	2.14	0.47
1:A:3999:THR:HG21	1:A:4048:LYS:HG3	1.96	0.47
1:A:539:GLN:HG3	1:A:540:MET:N	2.29	0.47
1:A:1400:VAL:HA	1:A:1403:MET:HE3	1.97	0.47
1:A:2348:GLN:HA	1:A:2351:GLN:OE1	2.14	0.47
1:A:3418:ASP:O	1:A:3419:PHE:C	2.57	0.47
1:A:3791:TYR:HD2	1:A:3803:ILE:HG13	1.78	0.47
1:A:3964:THR:HG1	1:A:3967:PHE:HD2	1.53	0.47
1:A:64:GLY:O	1:A:67:VAL:HG12	2.15	0.47
1:A:243:GLN:HG3	1:A:246:ARG:NH2	2.25	0.47
1:A:546:ALA:HA	1:A:550:PHE:HE1	1.80	0.47
1:A:1662:ASN:OD1	1:A:1663:THR:N	2.42	0.47
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.97	0.47
1:A:3881:ASP:HB2	1:A:3884:LYS:HB3	1.97	0.47
1:A:182:GLY:O	1:A:233:ASN:ND2	2.48	0.47
1:A:624:ILE:O	1:A:628:GLU:HG2	2.15	0.47
1:A:1203:SER:OG	1:A:1206:LEU:HG	2.15	0.47
1:A:3075:LYS:O	1:A:3079:GLU:CG	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3172:LYS:HE2	1:A:3776:ALA:O	2.15	0.47
1:A:404:ASP:HB2	1:A:1732:GLY:O	2.16	0.46
1:A:1355:GLY:HA2	1:A:1358:LEU:HG	1.97	0.46
1:A:1391:VAL:HG23	1:A:1392:MET:SD	2.56	0.46
1:A:1427:SER:O	1:A:1431:LEU:HD23	2.16	0.46
1:A:3810:VAL:HG12	1:A:3932:MET:HE3	1.97	0.46
1:A:1154:PRO:HG2	1:A:1157:PHE:CZ	2.50	0.46
1:A:1687:HIS:O	1:A:1691:GLN:OE1	2.33	0.46
1:A:2412:TYR:HA	1:A:2415:LEU:HB2	1.96	0.46
1:A:3232:ARG:NH2	1:A:3269:ARG:HH21	2.12	0.46
1:A:59:PHE:HD1	1:A:62:ASP:HB2	1.81	0.46
1:A:911:LEU:O	1:A:915:THR:HG23	2.15	0.46
1:A:1135:CYS:HB2	1:A:1194:PHE:HZ	1.80	0.46
1:A:2254:ARG:O	1:A:2257:PHE:HB3	2.15	0.46
1:A:3462:ARG:CD	1:A:3494:GLN:HB3	2.37	0.46
1:A:1222:ASN:ND2	1:A:1231:GLN:OE1	2.33	0.46
1:A:2085:MET:SD	1:A:2088:LEU:HB3	2.55	0.46
1:A:2371:PHE:CD2	1:A:2374:LEU:HB2	2.51	0.46
1:A:2785:ILE:O	1:A:2789:SER:HB2	2.15	0.46
1:A:3639:GLU:O	1:A:3642:LYS:N	2.49	0.46
1:A:3760:GLN:OE1	1:A:4019:LYS:HE3	2.15	0.46
1:A:108:LYS:HE3	1:A:156:PHE:CZ	2.49	0.46
1:A:662:LEU:CD2	1:A:721:TYR:CZ	2.92	0.46
1:A:1785:ILE:HG13	1:A:1786:ALA:N	2.30	0.46
1:A:3494:GLN:H	1:A:3494:GLN:HG2	1.45	0.46
1:A:221:ALA:HA	1:A:224:LEU:HG	1.97	0.46
1:A:476:ARG:O	1:A:478:CYS:N	2.49	0.46
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.15	0.46
1:A:2097:LEU:HD12	1:A:2149:LEU:HD22	1.93	0.46
1:A:2356:MET:C	1:A:2358:ASP:H	2.23	0.46
1:A:2844:LEU:HD11	1:A:2871:LEU:HD21	1.97	0.46
1:A:3014:CYS:O	1:A:3016:THR:N	2.48	0.46
1:A:3254:LEU:O	1:A:3258:LEU:HG	2.16	0.46
1:A:3820:MET:HE2	1:A:3882:LEU:HD11	1.98	0.46
1:A:398:THR:HG22	1:A:398:THR:O	2.16	0.46
1:A:628:GLU:O	1:A:632:GLU:HG2	2.16	0.46
1:A:1801:VAL:HA	1:A:1804:MET:HE2	1.98	0.46
1:A:2414:GLN:H	1:A:2414:GLN:CD	2.23	0.46
1:A:2930:TYR:O	1:A:2933:ILE:HG22	2.15	0.46
1:A:434:VAL:O	1:A:438:LEU:HD23	2.15	0.46
1:A:2134:GLY:O	1:A:2136:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2425:ARG:NH1	1:A:2460:GLU:CD	2.73	0.46
1:A:3462:ARG:CD	1:A:3494:GLN:HA	2.45	0.46
1:A:4084:SER:OG	1:A:4086:ASP:OD1	2.30	0.46
1:A:250:ASN:O	1:A:253:LEU:HG	2.15	0.46
1:A:898:PHE:HB2	1:A:901:MET:O	2.16	0.46
1:A:1016:GLY:C	1:A:1018:VAL:H	2.23	0.46
1:A:1479:VAL:HA	1:A:1482:GLU:HB3	1.97	0.46
1:A:1765:VAL:HG22	1:A:1768:ARG:NH2	2.31	0.46
1:A:2218:PHE:CD2	1:A:2219:LEU:HD12	2.50	0.46
1:A:108:LYS:HZ3	1:A:151:GLU:HA	1.81	0.45
1:A:662:LEU:CD2	1:A:721:TYR:CE1	2.99	0.45
1:A:1045:THR:H	1:A:1048:GLN:HE21	1.62	0.45
1:A:1407:LYS:HG2	1:A:1408:MET:HE2	1.98	0.45
1:A:1823:SER:O	1:A:1827:LEU:HG	2.16	0.45
1:A:2411:LEU:C	1:A:2413:PHE:H	2.23	0.45
1:A:3031:TRP:HE1	1:A:3041:LEU:HD13	1.81	0.45
1:A:3325:ASP:HA	1:A:3328:ILE:HG12	1.97	0.45
1:A:1367:HIS:O	1:A:1370:ARG:HG2	2.15	0.45
1:A:2155:GLU:O	1:A:2158:ARG:HG2	2.17	0.45
1:A:2478:MET:HE3	1:A:2524:PHE:CD1	2.52	0.45
1:A:3232:ARG:HD3	1:A:3265:GLU:OE2	2.16	0.45
1:A:3751:LEU:CG	1:A:3803:ILE:HG23	2.45	0.45
1:A:782:ARG:O	1:A:786:GLN:HB2	2.17	0.45
1:A:1252:ALA:O	1:A:1255:CYS:HB3	2.16	0.45
1:A:1839:PHE:O	1:A:1842:THR:OG1	2.26	0.45
1:A:2330:VAL:O	1:A:2334:LYS:HB3	2.16	0.45
1:A:3354:ASP:OD1	1:A:3354:ASP:N	2.49	0.45
1:A:1367:HIS:HA	1:A:1370:ARG:HD2	1.98	0.45
1:A:1626:TRP:NE1	1:A:1674:THR:HG21	2.20	0.45
1:A:1821:ASP:OD1	1:A:1875:LYS:HE2	2.17	0.45
1:A:1527:ARG:HD2	1:A:1527:ARG:O	2.17	0.45
1:A:3278:GLN:HB3	1:A:3326:GLN:NE2	2.32	0.45
1:A:3622:ALA:HB1	1:A:3623:PRO:HD2	1.99	0.45
1:A:493:LYS:HD2	1:A:522:PRO:HG2	1.99	0.45
1:A:984:TYR:HD1	1:A:987:LEU:HD23	1.81	0.45
1:A:1976:LEU:HD13	1:A:1976:LEU:HA	1.76	0.45
1:A:2261:SER:OG	1:A:2262:GLY:N	2.50	0.45
1:A:2540:LEU:HD11	1:A:2832:ILE:HD12	1.98	0.45
1:A:938:VAL:O	1:A:942:LEU:HD13	2.17	0.45
1:A:1478:SER:O	1:A:1482:GLU:HB2	2.16	0.45
1:A:1068:LEU:CD1	1:A:1106:ILE:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1743:MET:SD	1:A:1762:MET:HE1	2.57	0.45
1:A:261:ASP:OD1	1:A:262:LEU:N	2.49	0.45
1:A:662:LEU:HD23	1:A:721:TYR:CE1	2.51	0.45
1:A:1333:SER:O	1:A:1337:VAL:HG23	2.16	0.45
1:A:1448:LEU:O	1:A:1452:VAL:HG13	2.17	0.45
1:A:1657:SER:OG	1:A:1658:SER:N	2.50	0.45
1:A:1750:LEU:HD23	1:A:1785:ILE:HG21	1.99	0.45
1:A:3243:ILE:HG12	1:A:3258:LEU:HB2	1.99	0.45
1:A:3462:ARG:HD3	1:A:3494:GLN:CA	2.45	0.45
1:A:878:GLU:O	1:A:3933:GLU:HB2	2.16	0.45
1:A:1348:LEU:HA	1:A:1348:LEU:HD23	1.77	0.45
1:A:1358:LEU:HD23	1:A:1411:TYR:CE1	2.51	0.45
1:A:1525:CYS:HB3	1:A:1570:GLU:OE2	2.17	0.45
1:A:1712:ARG:O	1:A:1716:GLN:HG3	2.17	0.45
1:A:2211:LEU:HA	1:A:2214:ARG:HG2	1.99	0.45
1:A:2395:THR:O	1:A:2399:GLU:OE1	2.35	0.45
1:A:2559:THR:O	1:A:2563:LEU:HB2	2.16	0.45
1:A:3016:THR:HG23	1:A:3017:ALA:N	2.32	0.45
1:A:3232:ARG:HD2	1:A:3232:ARG:O	2.17	0.45
1:A:3465:PHE:CZ	1:A:3502:MET:HE2	2.52	0.45
1:A:3750:PHE:CE2	1:A:3804:GLU:CA	3.00	0.45
1:A:399:GLN:HG2	1:A:405:ASP:OD2	2.17	0.44
1:A:607:ASP:HB3	1:A:1023:SER:OG	2.17	0.44
1:A:1108:MET:HE1	1:A:1186:LYS:HB3	1.99	0.44
1:A:319:PHE:CE1	1:A:323:VAL:HG21	2.52	0.44
1:A:446:PHE:HD1	1:A:457:CYS:SG	2.40	0.44
1:A:1075:ARG:HH12	1:A:1123:THR:HG21	1.82	0.44
1:A:1880:MET:HG2	1:A:1884:LEU:HD12	1.99	0.44
1:A:1980:ASN:HB2	1:A:1982:ILE:HG23	1.99	0.44
1:A:3329:LEU:HA	1:A:3329:LEU:HD23	1.73	0.44
1:A:3661:ASP:HA	1:A:3664:ASN:ND2	2.32	0.44
1:A:3684:SER:HB2	1:A:3685:PRO:HD3	1.98	0.44
1:A:204:LEU:O	1:A:207:GLN:HB3	2.18	0.44
1:A:225:LYS:HD2	1:A:270:ALA:HB3	1.99	0.44
1:A:1729:PHE:HE1	1:A:1735:ARG:NE	2.15	0.44
1:A:1932:GLN:H	1:A:1937:ARG:NH1	2.15	0.44
1:A:3009:LYS:O	1:A:3013:TYR:CB	2.66	0.44
1:A:3059:GLN:O	1:A:3063:THR:HG23	2.18	0.44
1:A:3327:ASN:CB	1:A:3388:ALA:HB2	2.46	0.44
1:A:975:ASP:OD1	1:A:976:VAL:N	2.50	0.44
1:A:1431:LEU:O	1:A:1434:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2093:CYS:C	1:A:2096:PRO:CD	2.91	0.44
1:A:193:ALA:O	1:A:197:PHE:HB2	2.17	0.44
1:A:585:ILE:HA	1:A:611:ASN:O	2.17	0.44
1:A:2205:VAL:HB	1:A:2208:ASP:HB3	1.98	0.44
1:A:2921:LEU:O	1:A:2925:GLU:HG2	2.17	0.44
1:A:3293:CYS:O	1:A:3297:VAL:HG23	2.17	0.44
1:A:1471:GLN:N	1:A:1471:GLN:OE1	2.51	0.44
1:A:1704:GLY:C	1:A:1706:SER:H	2.26	0.44
1:A:1851:LEU:HD23	1:A:1870:LYS:HG2	2.00	0.44
1:A:2211:LEU:HA	1:A:2214:ARG:NE	2.33	0.44
1:A:3499:ILE:HD11	1:A:3529:ILE:HD12	2.00	0.44
1:A:3646:LYS:N	1:A:3650:LYS:HB3	2.32	0.44
1:A:16:GLN:HE22	1:A:62:ASP:HB3	1.81	0.44
1:A:83:GLU:HA	1:A:129:ASP:OD2	2.18	0.44
1:A:267:VAL:HB	1:A:268:PRO:HD3	1.99	0.44
1:A:722:LYS:HA	1:A:726:LEU:HD23	1.99	0.44
1:A:1897:ASN:CB	1:A:1903:SER:HB2	2.47	0.44
1:A:1945:TYR:CE2	1:A:1949:ILE:HD11	2.52	0.44
1:A:2327:LEU:O	1:A:2330:VAL:HG12	2.18	0.44
1:A:1195:VAL:O	1:A:1198:LEU:HD23	2.17	0.44
1:A:1255:CYS:HB2	1:A:3694:PHE:CZ	2.27	0.44
1:A:1459:HIS:HA	1:A:1464:LEU:HB2	2.00	0.44
1:A:2447:LYS:N	1:A:2450:GLU:OE1	2.37	0.44
1:A:2869:LEU:HB2	1:A:2900:LEU:HD13	1.99	0.44
1:A:3450:MET:O	1:A:3453:ALA:HB3	2.18	0.44
1:A:3731:SER:H	1:A:3734:ARG:NH2	2.16	0.44
1:A:3752:VAL:HG22	1:A:3802:LEU:HD23	1.87	0.44
1:A:316:LEU:HD12	1:A:319:PHE:HD2	1.83	0.44
1:A:965:THR:O	1:A:968:VAL:N	2.48	0.44
1:A:1208:LEU:HD11	1:A:1220:LEU:HD21	1.99	0.44
1:A:1850:VAL:HG12	1:A:1870:LYS:HG3	2.00	0.44
1:A:1019:ASP:N	1:A:1020:PRO:HD3	2.25	0.43
1:A:1769:GLU:O	1:A:1822:ARG:NH2	2.44	0.43
1:A:3182:ILE:HG13	1:A:3183:ILE:N	2.33	0.43
1:A:3478:GLU:C	1:A:3480:LEU:N	2.76	0.43
1:A:3520:GLU:C	1:A:3520:GLU:CD	2.86	0.43
1:A:1838:GLU:N	1:A:1838:GLU:OE1	2.51	0.43
1:A:2201:THR:OG1	1:A:2203:THR:HG22	2.19	0.43
1:A:2220:MET:HE1	1:A:2252:PRO:CG	2.48	0.43
1:A:2454:LEU:HD23	1:A:2454:LEU:HA	1.78	0.43
1:A:3618:GLY:O	1:A:3633:ILE:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TYR:HB3	1:A:350:ARG:HH12	1.84	0.43
1:A:642:PHE:CE2	1:A:646:VAL:HG22	2.54	0.43
1:A:1414:ILE:O	1:A:1417:THR:OG1	2.31	0.43
1:A:1572:LEU:HD12	1:A:1600:MET:HE3	1.99	0.43
1:A:2206:PRO:O	1:A:2210:VAL:HG23	2.18	0.43
1:A:2443:MET:HE1	1:A:2476:ILE:HG23	1.99	0.43
1:A:3522:THR:HG21	1:A:3558:ILE:CG2	2.46	0.43
1:A:3551:ASN:O	1:A:3555:VAL:HG13	2.17	0.43
1:A:1274:ARG:NH1	1:A:1351:THR:HG23	2.29	0.43
1:A:1407:LYS:HB2	1:A:1463:LEU:HD21	2.00	0.43
1:A:1729:PHE:HE1	1:A:1735:ARG:HE	1.67	0.43
1:A:2093:CYS:CA	1:A:2096:PRO:CG	2.94	0.43
1:A:2174:SER:HB3	1:A:2218:PHE:CD1	2.53	0.43
1:A:3281:CYS:HB2	1:A:3329:LEU:HD13	2.01	0.43
1:A:374:LYS:HD2	1:A:423:TYR:HB3	2.00	0.43
1:A:745:VAL:O	1:A:749:VAL:HG23	2.18	0.43
1:A:1217:VAL:HG12	1:A:1221:ILE:CD1	2.48	0.43
1:A:1279:LEU:HD23	1:A:1279:LEU:HA	1.87	0.43
1:A:1321:ARG:O	1:A:1323:SER:N	2.52	0.43
1:A:1935:GLU:HG2	1:A:1936:ARG:N	2.31	0.43
1:A:2237:ILE:O	1:A:2240:THR:OG1	2.35	0.43
1:A:2482:ASP:HA	1:A:2485:ARG:HH21	1.82	0.43
1:A:1030:GLY:O	1:A:1033:ILE:HG22	2.18	0.43
1:A:1874:TYR:HE2	1:A:1940:TYR:HE1	1.67	0.43
1:A:2280:VAL:HG22	1:A:2285:LEU:HB2	2.00	0.43
1:A:3006:ALA:HB1	1:A:3008:TRP:NE1	2.34	0.43
1:A:3077:ILE:HA	1:A:3080:LEU:HD23	2.01	0.43
1:A:3082:TYR:O	1:A:3086:LEU:HG	2.18	0.43
1:A:3480:LEU:O	1:A:3482:LEU:N	2.51	0.43
1:A:3583:LEU:HD22	1:A:3733:ARG:O	2.19	0.43
1:A:666:PHE:O	1:A:670:LEU:HB2	2.19	0.43
1:A:1915:LEU:HA	1:A:1918:LEU:HG	2.01	0.43
1:A:3189:PHE:O	1:A:3193:ILE:HG13	2.19	0.43
1:A:4016:PHE:O	1:A:4020:MET:HG2	2.19	0.43
1:A:1018:VAL:HG13	1:A:1018:VAL:O	2.19	0.43
1:A:1453:SER:O	1:A:1457:GLN:HG3	2.19	0.43
1:A:1668:PHE:HZ	1:A:1702:LEU:HD11	1.84	0.43
1:A:1722:PHE:CE2	1:A:1743:MET:HE1	2.54	0.43
1:A:1236:LEU:HD23	1:A:1236:LEU:HA	1.88	0.43
1:A:1605:PHE:CD1	1:A:1608:ARG:HD3	2.53	0.43
1:A:2184:TYR:O	1:A:2188:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2466:SER:OG	1:A:2469:CYS:N	2.26	0.43
1:A:3298:LEU:HD13	1:A:3298:LEU:HA	1.77	0.43
1:A:3493:TRP:CD2	1:A:3711:PRO:HB3	2.53	0.43
1:A:3949:ALA:HA	1:A:3953:LEU:HG	2.01	0.43
1:A:176:GLU:HG3	1:A:223:CYS:HB3	1.99	0.43
1:A:585:ILE:HG13	1:A:611:ASN:O	2.18	0.43
1:A:2517:LEU:HA	1:A:2517:LEU:HD23	1.73	0.43
1:A:2898:LEU:HD21	1:A:3972:LEU:HG	2.00	0.43
1:A:172:GLU:CG	1:A:223:CYS:HB2	2.48	0.42
1:A:254:LYS:C	1:A:300:TRP:HH2	2.27	0.42
1:A:432:THR:O	1:A:436:GLU:HG2	2.18	0.42
1:A:722:LYS:HB3	1:A:723:ASP:H	1.63	0.42
1:A:1539:SER:HA	1:A:1551:ILE:O	2.19	0.42
1:A:2341:LEU:O	1:A:2345:VAL:HG23	2.19	0.42
1:A:3016:THR:OG1	1:A:3040:TYR:HB3	2.18	0.42
1:A:3100:LYS:HG2	1:A:3104:GLN:HE22	1.84	0.42
1:A:3428:GLU:OE2	1:A:3474:ARG:HD3	2.19	0.42
1:A:4045:CYS:O	1:A:4049:ARG:HG3	2.19	0.42
1:A:965:THR:HG22	1:A:969:LEU:CD1	2.49	0.42
1:A:1210:ASP:O	1:A:1214:GLU:OE1	2.37	0.42
1:A:1225:GLU:HB3	1:A:1236:LEU:HG	2.01	0.42
1:A:1779:GLN:O	1:A:1783:ARG:HG3	2.18	0.42
1:A:2094:MET:CA	1:A:2097:LEU:HD23	2.46	0.42
1:A:2272:VAL:O	1:A:2276:LEU:HG	2.19	0.42
1:A:2428:ASP:N	1:A:2432:GLN:HE21	2.17	0.42
1:A:3618:GLY:C	1:A:3633:ILE:HG23	2.44	0.42
1:A:4014:LYS:O	1:A:4018:GLN:HG2	2.19	0.42
1:A:340:TYR:O	1:A:344:GLN:HG2	2.19	0.42
1:A:897:PRO:O	1:A:2566:THR:HG22	2.19	0.42
1:A:1575:LEU:H	1:A:1575:LEU:HD23	1.83	0.42
1:A:2318:ALA:HA	1:A:2321:GLU:OE2	2.18	0.42
1:A:2520:ILE:HA	1:A:2523:ASN:HD21	1.84	0.42
1:A:3614:TYR:HA	1:A:3617:LEU:O	2.19	0.42
1:A:1482:GLU:HA	1:A:1486:LEU:HD13	2.01	0.42
1:A:1690:GLY:O	1:A:1745:LYS:HD2	2.20	0.42
1:A:1750:LEU:CD2	1:A:1785:ILE:HG21	2.49	0.42
1:A:1752:LEU:HD23	1:A:1752:LEU:HA	1.87	0.42
1:A:2104:MET:HA	1:A:2107:SER:HB3	2.02	0.42
1:A:3451:LEU:HD21	1:A:3487:ILE:HA	2.02	0.42
1:A:3797:THR:HG22	1:A:3798:SER:N	2.35	0.42
1:A:3855:TYR:O	1:A:3858:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3964:THR:HB	1:A:4128:MET:C	2.44	0.42
1:A:859:LEU:HD21	1:A:870:LEU:HD13	2.02	0.42
1:A:984:TYR:O	1:A:988:VAL:HG23	2.20	0.42
1:A:1627:LYS:HE3	1:A:1670:GLU:CD	2.44	0.42
1:A:1653:LEU:HA	1:A:1653:LEU:HD23	1.83	0.42
1:A:1668:PHE:HA	1:A:1671:VAL:HG12	2.01	0.42
1:A:3285:HIS:CD2	1:A:3298:LEU:HD11	2.45	0.42
1:A:3681:LYS:NZ	1:A:3722:PHE:HB3	2.34	0.42
1:A:3750:PHE:CE2	1:A:3804:GLU:HA	2.52	0.42
1:A:128:LEU:O	1:A:131:LEU:HG	2.20	0.42
1:A:225:LYS:HZ1	1:A:267:VAL:HG13	1.84	0.42
1:A:722:LYS:HG3	1:A:726:LEU:CD2	2.49	0.42
1:A:1202:ARG:HH22	1:A:1210:ASP:HB2	1.85	0.42
1:A:1476:HIS:CD2	1:A:1521:PHE:HD2	2.37	0.42
1:A:1607:GLU:HG3	1:A:1611:GLN:OE1	2.19	0.42
1:A:2277:LEU:O	1:A:2281:MET:HG2	2.20	0.42
1:A:2481:HIS:CD2	1:A:2485:ARG:HH12	2.38	0.42
1:A:3034:PRO:HG2	1:A:3037:GLN:HG3	2.02	0.42
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.52	0.42
1:A:183:GLU:HA	1:A:233:ASN:ND2	2.34	0.42
1:A:722:LYS:HB2	1:A:722:LYS:HE3	1.45	0.42
1:A:1689:LYS:O	1:A:1693:VAL:HG13	2.20	0.42
1:A:1718:ILE:O	1:A:1722:PHE:HB2	2.20	0.42
1:A:1808:ASP:CG	1:A:1809:ASP:H	2.27	0.42
1:A:2385:LEU:HD21	1:A:2389:PHE:HE2	1.85	0.42
1:A:2514:ASN:HB3	1:A:2517:LEU:HB2	2.01	0.42
1:A:2887:PRO:HG2	1:A:3895:GLU:HG3	2.01	0.42
1:A:200:PHE:HE1	1:A:224:LEU:HD22	1.84	0.42
1:A:1871:MET:HE2	1:A:1871:MET:HB3	1.94	0.42
1:A:2091:HIS:CE1	1:A:2093:CYS:SG	3.13	0.42
1:A:2361:ILE:HD11	1:A:2393:LEU:HD22	2.02	0.42
1:A:2375:ALA:HA	1:A:2378:PHE:HB2	2.02	0.42
1:A:4121:TRP:CD1	1:A:4123:GLY:H	2.37	0.42
1:A:364:ARG:O	1:A:368:LEU:HD23	2.19	0.42
1:A:546:ALA:HA	1:A:550:PHE:CE1	2.55	0.42
1:A:967:PRO:HA	1:A:1014:LEU:HD11	2.01	0.42
1:A:1607:GLU:HG3	1:A:1607:GLU:O	2.19	0.42
1:A:2218:PHE:HD2	1:A:2219:LEU:HD12	1.85	0.42
1:A:22:ALA:HB3	1:A:34:LEU:HD21	2.00	0.41
1:A:291:VAL:HG12	1:A:340:TYR:CE2	2.55	0.41
1:A:1086:TYR:C	1:A:1088:GLU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:SER:O	1:A:1325:GLN:N	2.53	0.41
1:A:1884:LEU:HD23	1:A:1884:LEU:HA	1.75	0.41
1:A:1935:GLU:OE1	1:A:1935:GLU:N	2.36	0.41
1:A:1980:ASN:OD1	1:A:1981:LEU:N	2.53	0.41
1:A:2207:LYS:HA	1:A:2210:VAL:HB	2.02	0.41
1:A:2356:MET:C	1:A:2358:ASP:N	2.78	0.41
1:A:3542:PHE:HE2	1:A:3551:ASN:HB2	1.85	0.41
1:A:366:TYR:CD1	1:A:384:MET:HE3	2.55	0.41
1:A:933:LEU:O	1:A:937:MET:HG3	2.20	0.41
1:A:1334:LYS:O	1:A:1338:VAL:HG23	2.19	0.41
1:A:1765:VAL:HG22	1:A:1768:ARG:HH21	1.86	0.41
1:A:2269:ASP:O	1:A:2272:VAL:HG22	2.20	0.41
1:A:2281:MET:SD	1:A:2287:PRO:HG3	2.60	0.41
1:A:630:CYS:O	1:A:635:PRO:HD3	2.20	0.41
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	2.03	0.41
1:A:1484:LEU:HD11	1:A:1527:ARG:NH1	2.34	0.41
1:A:2212:ALA:O	1:A:2215:LEU:HB3	2.20	0.41
1:A:2547:SER:O	1:A:2549:LYS:N	2.54	0.41
1:A:2576:MET:HB3	1:A:2787:HIS:CD2	2.55	0.41
1:A:2790:LEU:C	1:A:2793:PRO:HD2	2.45	0.41
1:A:3100:LYS:HB3	1:A:3100:LYS:HE3	1.85	0.41
1:A:3459:ASN:OD1	1:A:3459:ASN:N	2.51	0.41
1:A:3759:ARG:O	1:A:3763:ARG:HG2	2.20	0.41
1:A:3985:VAL:HG21	1:A:4101:GLU:HG3	2.01	0.41
1:A:1240:THR:HG23	1:A:1296:PHE:CD1	2.54	0.41
1:A:1395:LEU:O	1:A:1398:VAL:HG12	2.20	0.41
1:A:2164:TRP:O	1:A:2167:PRO:HD2	2.19	0.41
1:A:2397:CYS:HA	1:A:2400:VAL:HG12	2.03	0.41
1:A:3495:PHE:HB3	1:A:3502:MET:CE	2.48	0.41
1:A:3495:PHE:CG	1:A:3502:MET:HE1	2.55	0.41
1:A:3911:ILE:HD13	1:A:3911:ILE:HG21	1.83	0.41
1:A:115:TYR:HD1	1:A:130:LEU:HD22	1.85	0.41
1:A:172:GLU:H	1:A:172:GLU:CD	2.28	0.41
1:A:1339:VAL:O	1:A:1343:GLU:OE1	2.39	0.41
1:A:1641:THR:O	1:A:1645:VAL:HG23	2.21	0.41
1:A:2211:LEU:HA	1:A:2214:ARG:HE	1.85	0.41
1:A:3582:GLU:HG2	1:A:3583:LEU:N	2.36	0.41
1:A:3730:ALA:HA	1:A:3734:ARG:NH2	2.35	0.41
1:A:3886:ALA:O	1:A:3890:MET:HG2	2.19	0.41
1:A:3917:ILE:HD12	1:A:3991:PHE:HD2	1.85	0.41
1:A:1633:TRP:CZ2	1:A:1674:THR:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3107:ILE:HD13	1:A:3135:LEU:CD2	2.50	0.41
1:A:3413:TYR:CD1	1:A:3449:LYS:HD2	2.56	0.41
1:A:3567:VAL:HB	1:A:3696:ARG:O	2.21	0.41
1:A:3686:TRP:C	1:A:3688:SER:N	2.78	0.41
1:A:3729:MET:HG3	1:A:3737:ARG:HH21	1.85	0.41
1:A:107:ILE:HG21	1:A:137:THR:HG21	2.01	0.41
1:A:175:TYR:HB3	1:A:227:LEU:CD2	2.46	0.41
1:A:294:PHE:O	1:A:298:LEU:HD23	2.21	0.41
1:A:803:SER:OG	1:A:848:LEU:HD21	2.20	0.41
1:A:1211:VAL:HA	1:A:1214:GLU:OE2	2.21	0.41
1:A:1379:PRO:HB2	1:A:1384:PHE:CD2	2.55	0.41
1:A:1646:LEU:HD13	1:A:1678:LEU:HD13	2.03	0.41
1:A:2088:LEU:HD12	1:A:2152:ASN:HD21	1.85	0.41
1:A:2093:CYS:CA	1:A:2096:PRO:HG2	2.50	0.41
1:A:938:VAL:HA	1:A:941:MET:HE3	2.02	0.41
1:A:1297:PHE:CZ	1:A:1301:ILE:HG21	2.56	0.41
1:A:1448:LEU:HD21	1:A:1514:LEU:HD11	2.02	0.41
1:A:1688:LEU:HA	1:A:1691:GLN:OE1	2.21	0.41
1:A:2205:VAL:O	1:A:2208:ASP:HB3	2.21	0.41
1:A:2364:LEU:HD11	1:A:2375:ALA:HB2	2.02	0.41
1:A:2786:LYS:O	1:A:2787:HIS:C	2.63	0.41
1:A:3182:ILE:HG21	1:A:3182:ILE:HD13	1.84	0.41
1:A:3256:MET:SD	1:A:3283:LEU:HD21	2.61	0.41
1:A:3269:ARG:C	1:A:3271:ASP:H	2.28	0.41
1:A:3963:LEU:HB3	1:A:4112:THR:HG22	2.03	0.41
1:A:415:GLN:HG2	1:A:460:ALA:HA	2.03	0.41
1:A:851:ILE:HD13	1:A:851:ILE:HA	1.88	0.41
1:A:1009:LEU:O	1:A:1013:ILE:HG13	2.21	0.41
1:A:1082:PHE:C	1:A:1084:ASN:N	2.79	0.41
1:A:1135:CYS:HB2	1:A:1194:PHE:CZ	2.55	0.41
1:A:1154:PRO:HD2	1:A:1157:PHE:CD2	2.56	0.41
1:A:1583:MET:HA	1:A:1586:SER:HB2	2.03	0.41
1:A:1753:SER:OG	1:A:1755:SER:HB2	2.20	0.41
1:A:1761:LEU:HD23	1:A:1761:LEU:HA	1.85	0.41
1:A:2098:THR:O	1:A:2101:VAL:HG22	2.21	0.41
1:A:2260:PHE:HA	1:A:2270:ASN:HA	2.03	0.41
1:A:2334:LYS:O	1:A:2336:ILE:N	2.53	0.41
1:A:2334:LYS:HB2	1:A:2338:GLU:HB3	2.03	0.41
1:A:2349:LEU:HA	1:A:2352:HIS:HE1	1.84	0.41
1:A:2560:ASN:O	1:A:2564:GLU:HG2	2.21	0.41
1:A:2933:ILE:HD13	1:A:2933:ILE:HG21	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3259:LEU:HD23	1:A:3259:LEU:HA	1.90	0.41
1:A:3293:CYS:HA	1:A:3296:GLN:CD	2.45	0.41
1:A:3763:ARG:HB2	1:A:4005:PHE:CE1	2.56	0.41
1:A:3913:ILE:HD12	1:A:3913:ILE:HA	1.93	0.41
1:A:178:LEU:HD23	1:A:178:LEU:H	1.85	0.41
1:A:203:GLU:O	1:A:206:THR:OG1	2.24	0.41
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.88	0.41
1:A:721:TYR:CD2	1:A:725:LEU:HD21	2.55	0.41
1:A:1104:LEU:HA	1:A:1134:LEU:HD13	2.03	0.41
1:A:1365:ASN:OD1	1:A:1366:THR:N	2.53	0.41
1:A:1445:ARG:HG3	1:A:1510:LEU:HD13	2.03	0.41
1:A:1104:LEU:HD23	1:A:1168:LEU:HD21	2.03	0.40
1:A:1577:LEU:H	1:A:1577:LEU:HD23	1.84	0.40
1:A:2205:VAL:HA	1:A:2206:PRO:HD3	1.95	0.40
1:A:2494:ASP:HA	1:A:2497:GLU:HG2	2.03	0.40
1:A:2930:TYR:HA	1:A:2933:ILE:HG22	2.03	0.40
1:A:3003:ASN:OD1	1:A:3046:ARG:NH1	2.55	0.40
1:A:3424:LEU:HD21	1:A:3442:TYR:HB3	2.03	0.40
1:A:3859:TYR:CE1	1:A:4119:ARG:HD3	2.56	0.40
1:A:620:PHE:HE1	1:A:663:ILE:HD12	1.86	0.40
1:A:2361:ILE:HD11	1:A:2393:LEU:HB3	2.02	0.40
1:A:2436:LEU:CD1	1:A:2461:PHE:CE1	2.93	0.40
1:A:2928:LYS:HE3	1:A:2928:LYS:HB2	1.77	0.40
1:A:3065:ILE:HA	1:A:3065:ILE:HD13	1.81	0.40
1:A:3535:ILE:O	1:A:3538:GLU:HG2	2.21	0.40
1:A:3811:THR:HG22	1:A:3929:MET:HG2	2.02	0.40
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.83	0.40
1:A:1864:ASP:OD1	1:A:1865:THR:N	2.54	0.40
1:A:2121:ASP:OD1	1:A:2121:ASP:N	2.49	0.40
1:A:2227:LYS:HB2	1:A:2230:VAL:HG12	2.02	0.40
1:A:2455:LEU:HD12	1:A:2455:LEU:HA	1.88	0.40
1:A:3266:SER:O	1:A:3267:LYS:HB2	2.21	0.40
1:A:3620:PRO:HA	1:A:3633:ILE:HG21	2.02	0.40
1:A:3723:ASP:HB3	1:A:3739:ILE:HB	2.03	0.40
1:A:153:PHE:HA	1:A:156:PHE:CD2	2.57	0.40
1:A:712:LYS:HE3	1:A:712:LYS:HB2	1.88	0.40
1:A:1238:GLN:O	1:A:1256:TRP:NE1	2.54	0.40
1:A:1718:ILE:HG13	1:A:1719:VAL:N	2.35	0.40
1:A:2146:LEU:O	1:A:2150:VAL:HG23	2.21	0.40
1:A:2969:ALA:HB2	1:A:3001:CYS:HB3	2.04	0.40
1:A:3080:LEU:O	1:A:3080:LEU:HG	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3262:LEU:O	1:A:3276:TRP:NE1	2.53	0.40
1:A:3552:LYS:O	1:A:3555:VAL:HG22	2.22	0.40
1:A:3620:PRO:CA	1:A:3633:ILE:HG21	2.52	0.40
1:A:156:PHE:HA	1:A:159:GLU:HG2	2.02	0.40
1:A:217:LEU:O	1:A:220:LEU:HB3	2.21	0.40
1:A:468:LEU:HD13	1:A:478:CYS:HB3	2.03	0.40
1:A:609:ALA:HA	1:A:612:LEU:HD12	2.03	0.40
1:A:1015:ASP:O	1:A:1026:ARG:HG2	2.21	0.40
1:A:1031:ARG:HE	1:A:1031:ARG:HB3	1.52	0.40
1:A:1212:LEU:CD1	1:A:1217:VAL:HA	2.50	0.40
1:A:1333:SER:O	1:A:1336:THR:HG22	2.22	0.40
1:A:2424:MET:HE2	1:A:2424:MET:HB3	1.91	0.40
1:A:2978:LYS:HD2	1:A:2981:TRP:CZ2	2.57	0.40
1:A:3531:TYR:O	1:A:3535:ILE:HG13	2.21	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%)	3230 (90%)	365 (10%)	7 (0%)	43	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1019	ASP
1	A	3692	VAL
1	A	3495	PHE
1	A	2787	HIS
1	A	3406	ALA
1	A	3695	LEU
1	A	1813	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3194/3671 (87%)	3170 (99%)	24 (1%)	73 85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	722	LYS
1	A	1019	ASP
1	A	1884	LEU
1	A	1975	LEU
1	A	1976	LEU
1	A	2097	LEU
1	A	2460	GLU
1	A	2462	VAL
1	A	2555	LEU
1	A	3080	LEU
1	A	3493	TRP
1	A	3494	GLN
1	A	3692	VAL
1	A	3694	PHE
1	A	3695	LEU
1	A	3696	ARG
1	A	3729	MET
1	A	3751	LEU
1	A	3803	ILE
1	A	3898	LEU
1	A	3963	LEU
1	A	3971	MET
1	A	3972	LEU
1	A	4023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN

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Mol	Chain	Res	Type
1	A	344	GLN
1	A	356	ASN
1	A	437	HIS
1	A	442	GLN
1	A	484	HIS
1	A	613	HIS
1	A	739	ASN
1	A	1048	GLN
1	A	1083	ASN
1	A	1574	ASN
1	A	1614	GLN
1	A	1771	GLN
1	A	2103	HIS
1	A	2233	HIS
1	A	2234	ASN
1	A	2305	ASN
1	A	2348	GLN
1	A	2352	HIS
1	A	2365	ASN
1	A	2432	GLN
1	A	2523	ASN
1	A	2784	GLN
1	A	2831	ASN
1	A	2971	GLN
1	A	3084	GLN
1	A	3166	ASN
1	A	3326	GLN
1	A	3390	GLN
1	A	3494	GLN
1	A	3501	HIS
1	A	3527	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	1IX	A	6101	-	38,38,38	2.96	15 (39%)	53,54,54	2.65	23 (43%)

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	1IX	A	6101	-	-	4/18/26/26	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	1IX	O29-C30	-10.87	1.00	1.42
2	A	6101	1IX	C12-C13	5.36	1.46	1.37
2	A	6101	1IX	C21-C20	-5.35	1.34	1.42
2	A	6101	1IX	C14-C16	5.18	1.55	1.49
2	A	6101	1IX	C16-N17	-4.23	1.28	1.32
2	A	6101	1IX	C20-N19	-4.04	1.30	1.37
2	A	6101	1IX	C11-CL1	3.96	1.83	1.73
2	A	6101	1IX	C27-N26	-3.93	1.40	1.46
2	A	6101	1IX	C14-C13	-3.45	1.32	1.39
2	A	6101	1IX	C11-C10	-2.65	1.36	1.39
2	A	6101	1IX	C06-N05	-2.49	1.29	1.33
2	A	6101	1IX	C06-C09	-2.34	1.51	1.52
2	A	6101	1IX	C18-N17	-2.19	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	1IX	C25-C20	2.18	1.45	1.41
2	A	6101	1IX	C24-N26	2.06	1.44	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6101	1IX	C30-O29-C28	7.98	135.69	109.88
2	A	6101	1IX	C10-C09-C06	-6.43	105.09	111.20
2	A	6101	1IX	C18-N19-C20	5.55	121.74	115.43
2	A	6101	1IX	C21-C20-N19	-4.75	117.78	122.82
2	A	6101	1IX	C21-C16-N17	-4.69	119.95	123.04
2	A	6101	1IX	N19-C18-N17	-4.37	122.74	128.67
2	A	6101	1IX	C12-C11-C10	-3.63	118.54	122.46
2	A	6101	1IX	C07-C06-N05	-3.62	119.07	122.36
2	A	6101	1IX	C03-N04-N05	3.53	123.08	118.42
2	A	6101	1IX	C16-C21-C20	3.49	118.89	115.90
2	A	6101	1IX	C01-O02-C03	-3.11	112.70	117.33
2	A	6101	1IX	C14-C16-N17	3.10	120.70	115.17
2	A	6101	1IX	C11-C12-C13	3.01	120.69	118.42
2	A	6101	1IX	C15-C10-C11	2.77	119.77	117.14
2	A	6101	1IX	C30-C31-N26	2.77	115.16	109.93
2	A	6101	1IX	C31-N26-C24	2.76	125.63	118.11
2	A	6101	1IX	C25-C20-N19	2.43	120.81	118.01
2	A	6101	1IX	C15-C10-C09	-2.37	116.36	120.20
2	A	6101	1IX	C28-C27-N26	2.22	114.13	109.93
2	A	6101	1IX	C12-C11-CL1	2.17	122.00	118.45
2	A	6101	1IX	O02-C03-C08	2.13	120.54	116.77
2	A	6101	1IX	C12-C13-C14	-2.10	120.23	123.59
2	A	6101	1IX	C08-C03-N04	-2.04	120.22	124.57

There are no chirality outliers.

All (4) torsion outliers are listed below:

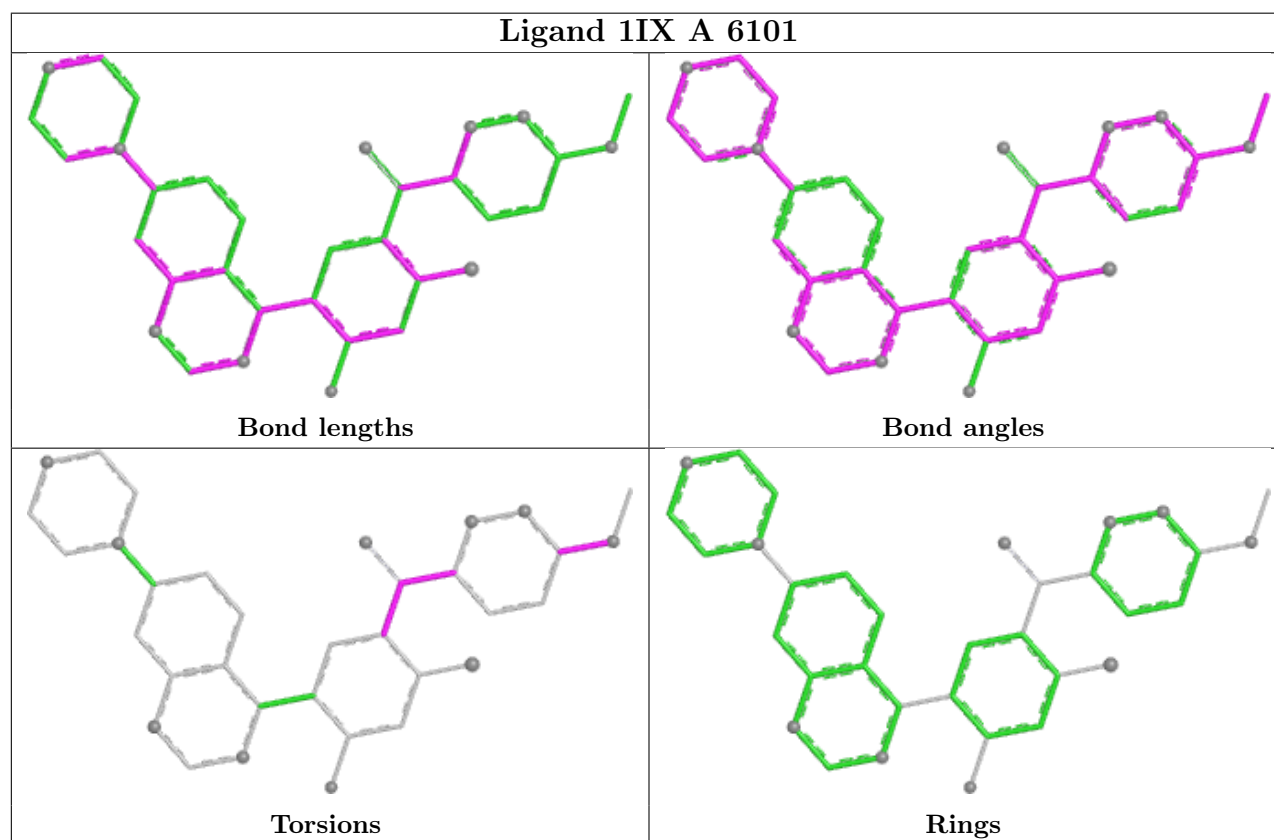
Mol	Chain	Res	Type	Atoms
2	A	6101	1IX	N04-C03-O02-C01
2	A	6101	1IX	C08-C03-O02-C01
2	A	6101	1IX	C06-C09-C10-C11
2	A	6101	1IX	N05-C06-C09-O34

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	1IX	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	82.32

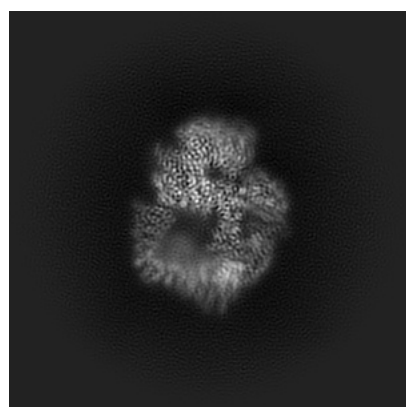
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13069. These allow visual inspection of the internal detail of the map and identification of artifacts.

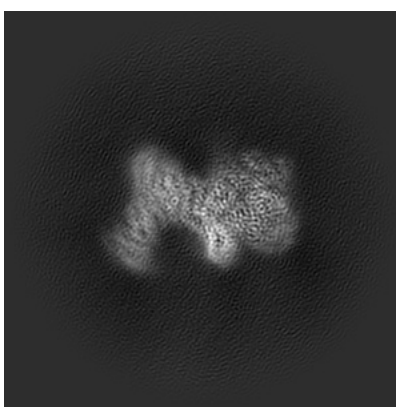
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

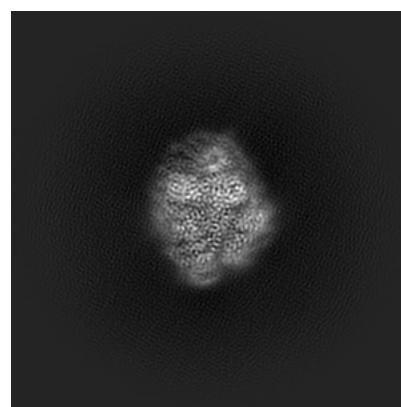
6.1.1 Primary map



X



Y

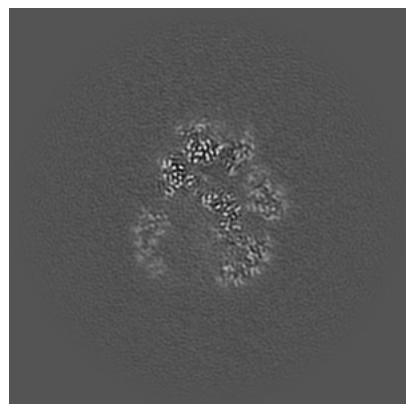


Z

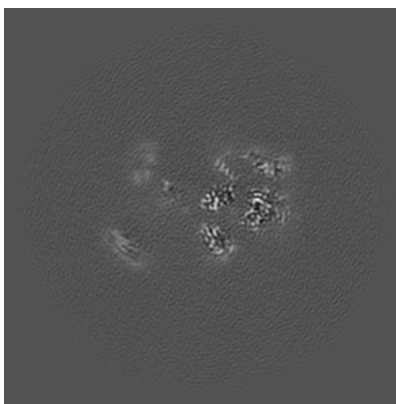
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

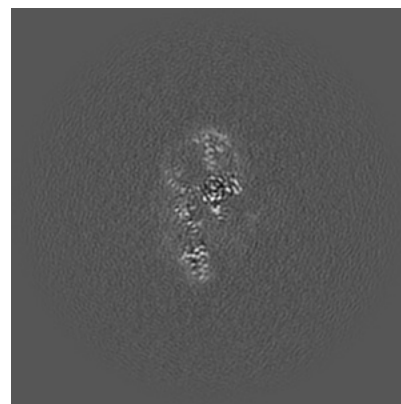
6.2.1 Primary map



X Index: 130



Y Index: 130

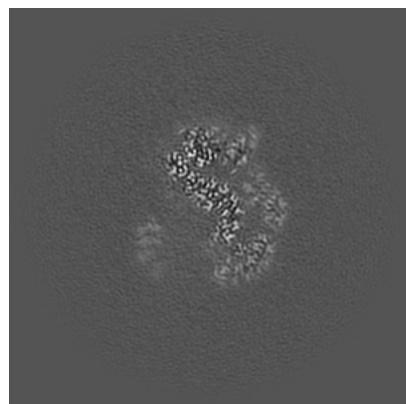


Z Index: 130

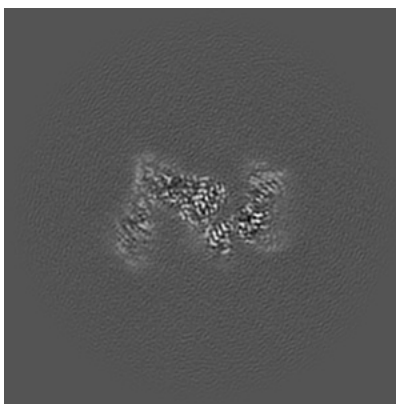
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

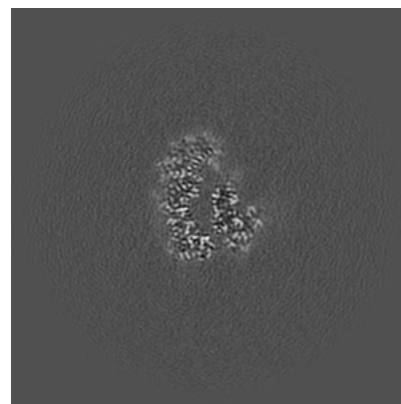
6.3.1 Primary map



X Index: 134



Y Index: 142

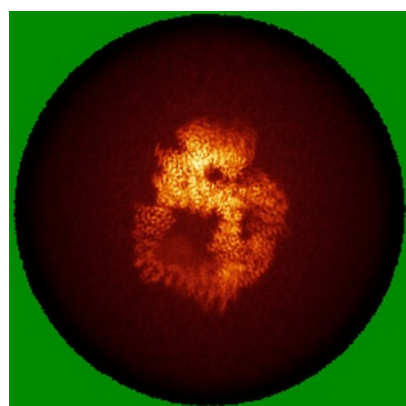


Z Index: 141

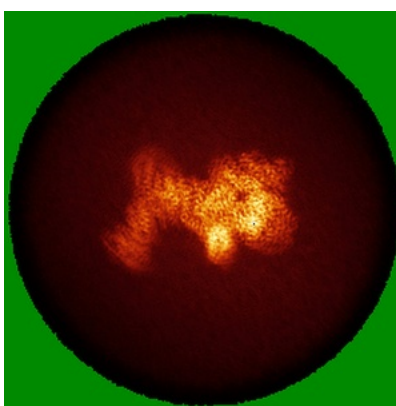
The images above show the largest variance slices of the map in three orthogonal directions.

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

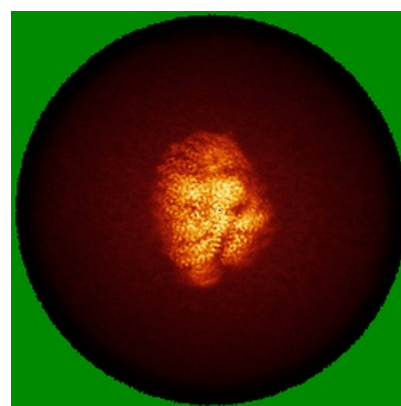
6.4.1 Primary map



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

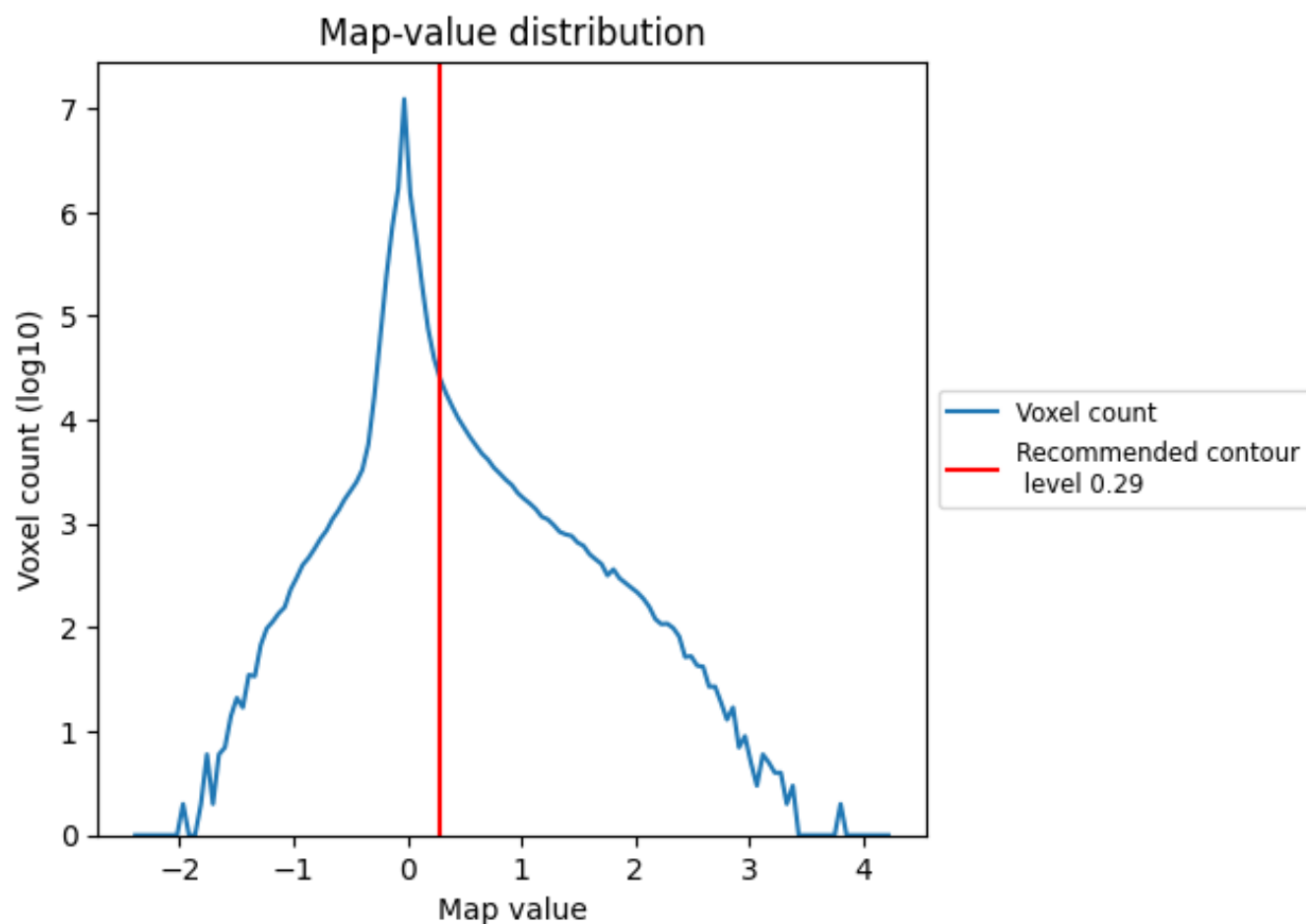
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

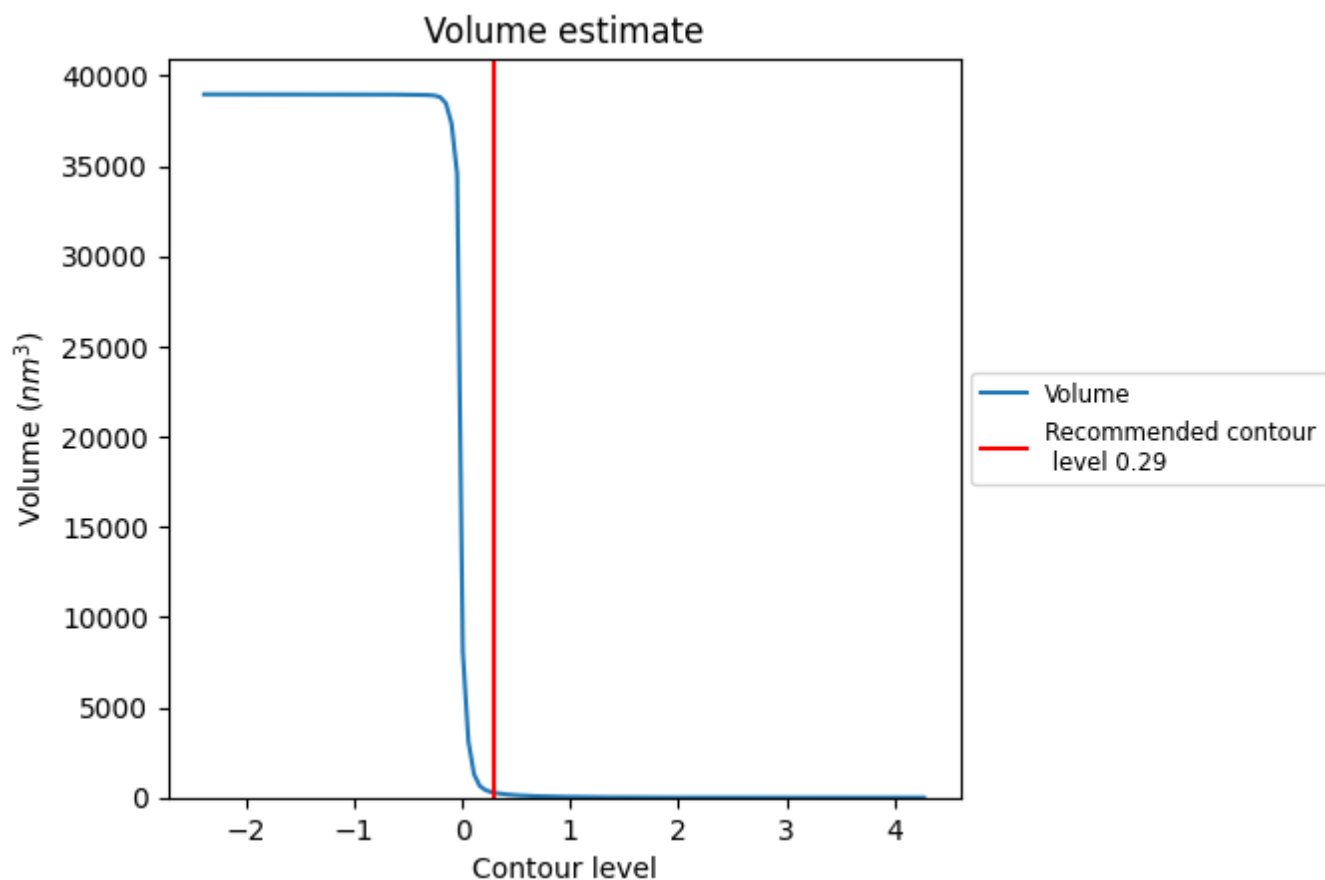
This section contains the results of statistical analysis of the map.

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.

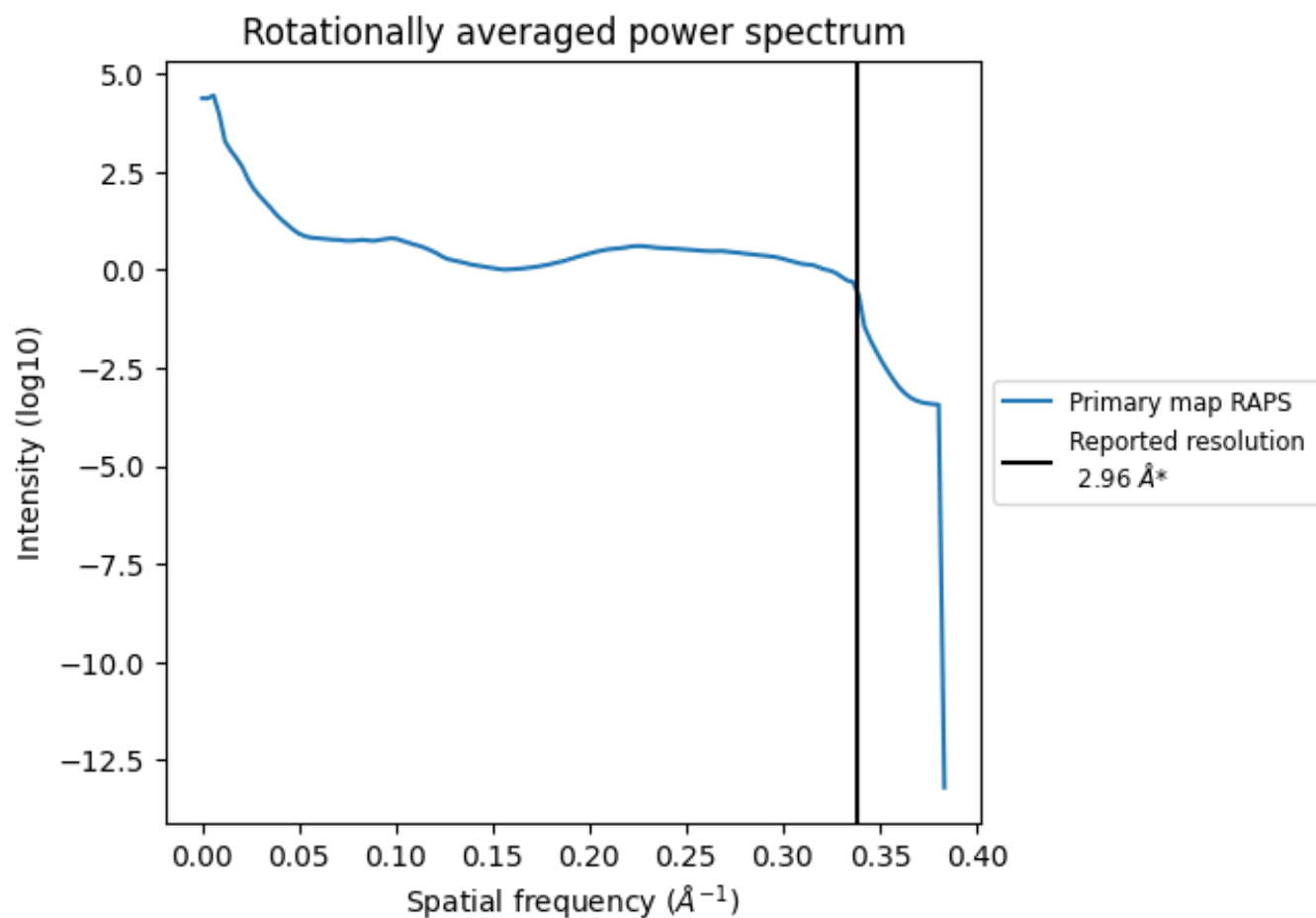
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm^3 ; this corresponds to an approximate mass of 252 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 0.338 Å⁻¹

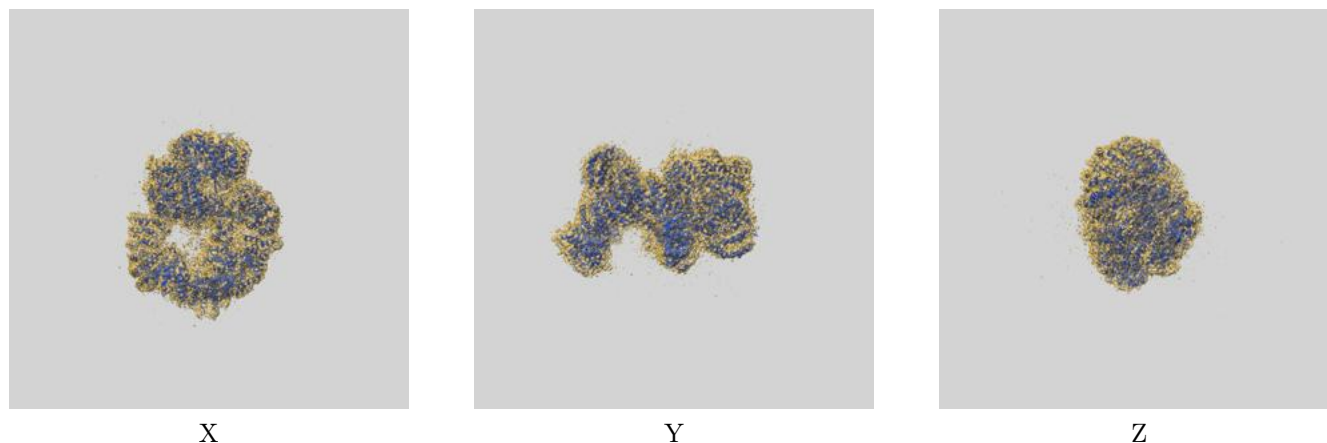
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

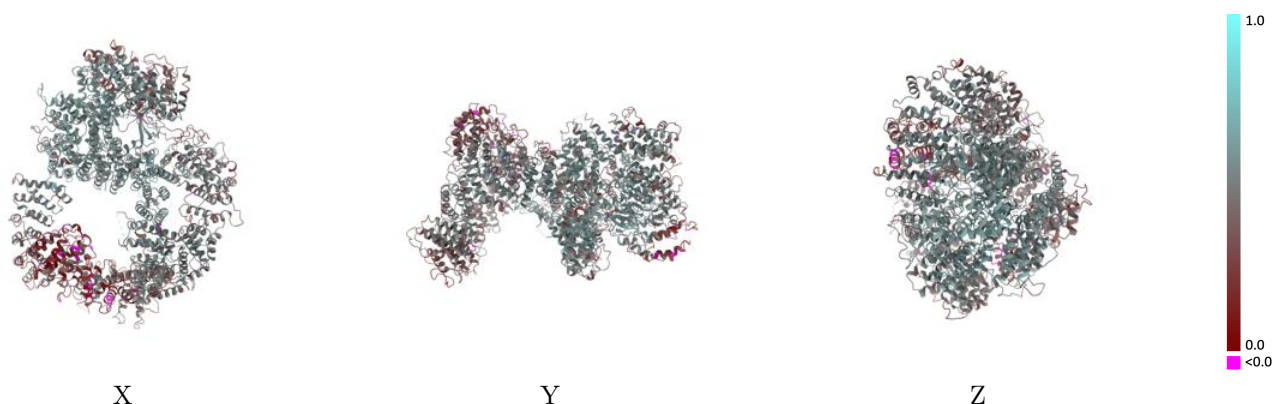
This section contains information regarding the fit between EMDB map EMD-13069 and PDB model 7OTY. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



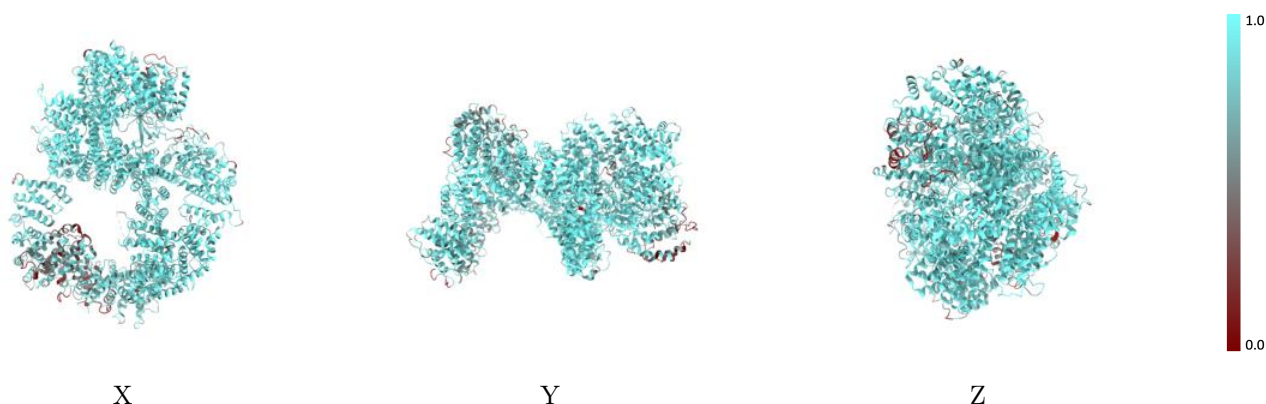
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



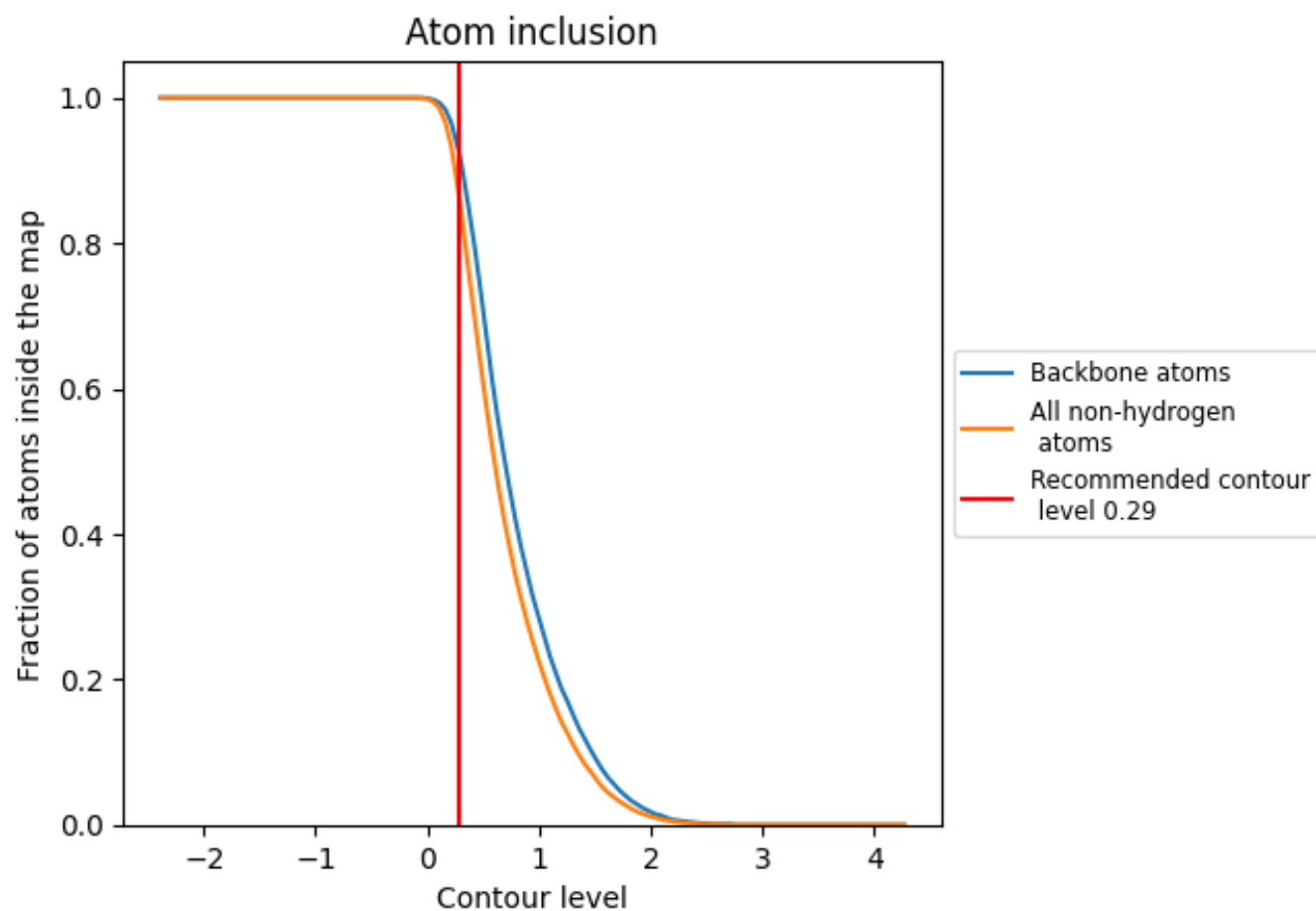
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.4620
A	0.8590	0.4620

