



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:42 PM UTC

PDB ID : 5YZ0 / pdb_00005yz0
EMDB ID : EMD-6862
Title : Cryo-EM Structure of human ATR-ATRIP complex
Authors : Rao, Q.; Liu, M.; Tian, Y.; Wu, Z.; Wang, H.; Wang, J.; Xu, Y.
Deposited on : 2017-12-11
Resolution : 4.70 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:

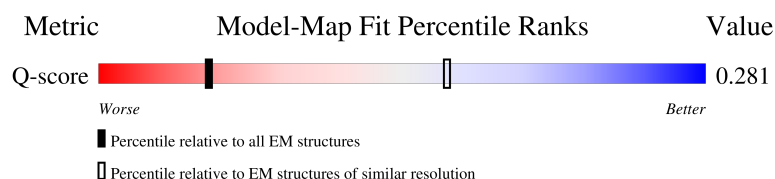
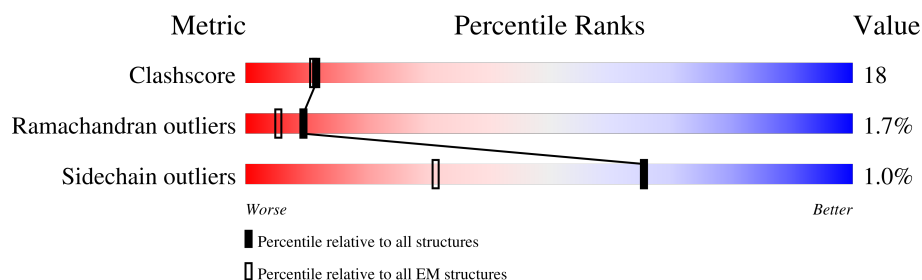
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.70 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	1989 (4.20 - 5.20)

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	2644	
1	B	2644	
2	C	791	
2	D	791	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33371 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 Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2362	Total	C	N	O	S	0	0
			15007	9318	2785	2842	62		
1	B	2362	Total	C	N	O	S	0	0
			15007	9318	2785	2842	62		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	362	Total	C	N	O	0	0
			1785	1061	362	362		
2	D	318	Total	C	N	O	0	0
			1572	936	318	318		

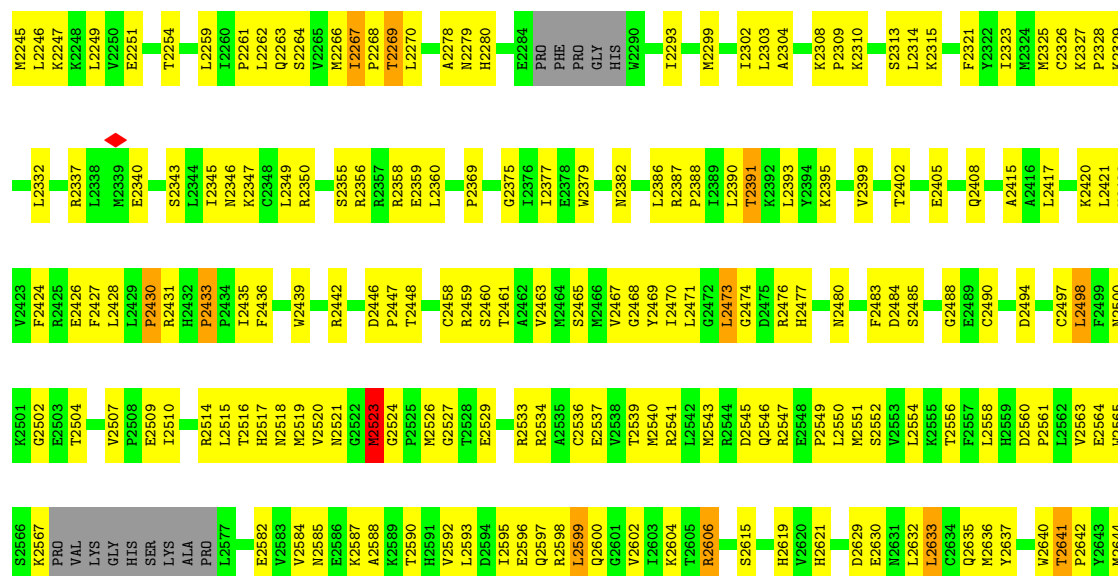
3 Residue-property plots

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: Serine/threonine-protein kinase ATR



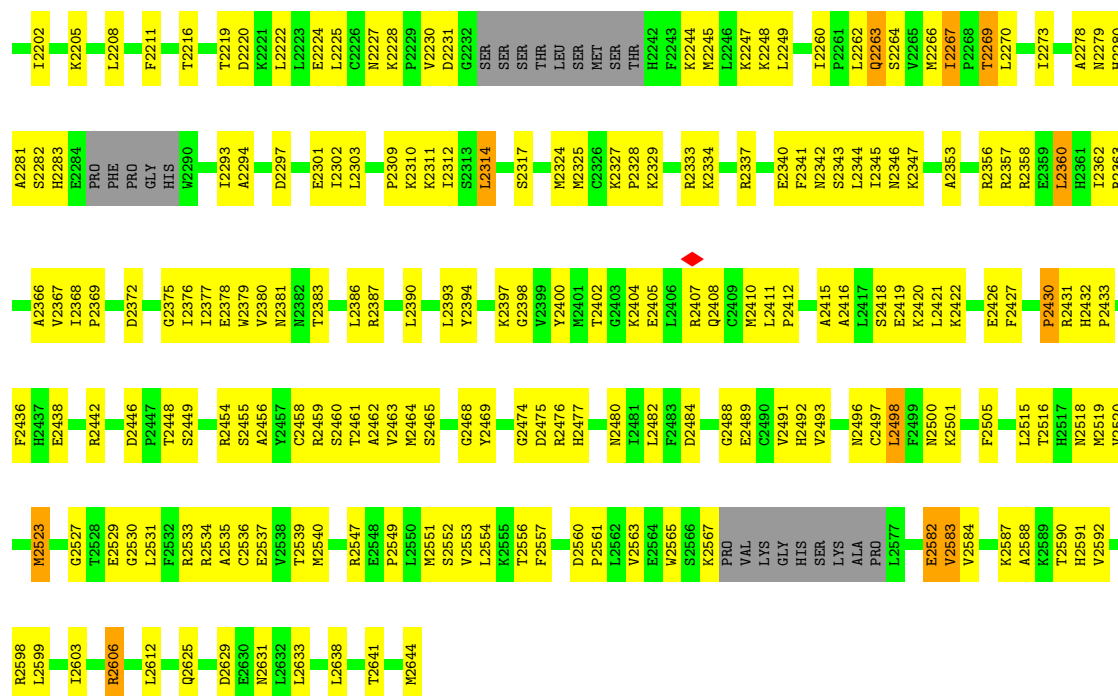




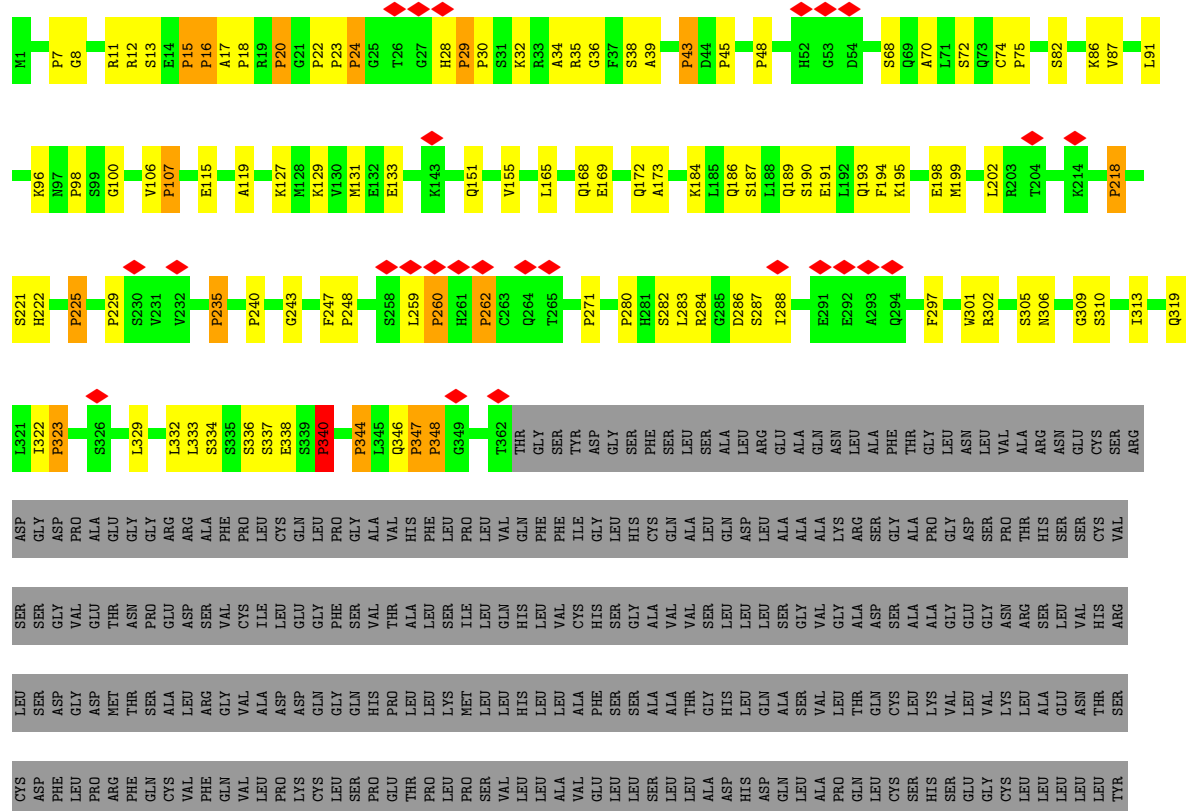
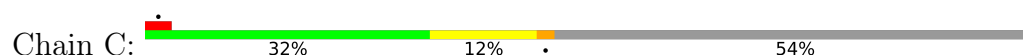
• Molecule 1: Serine/threonine-protein kinase ATR



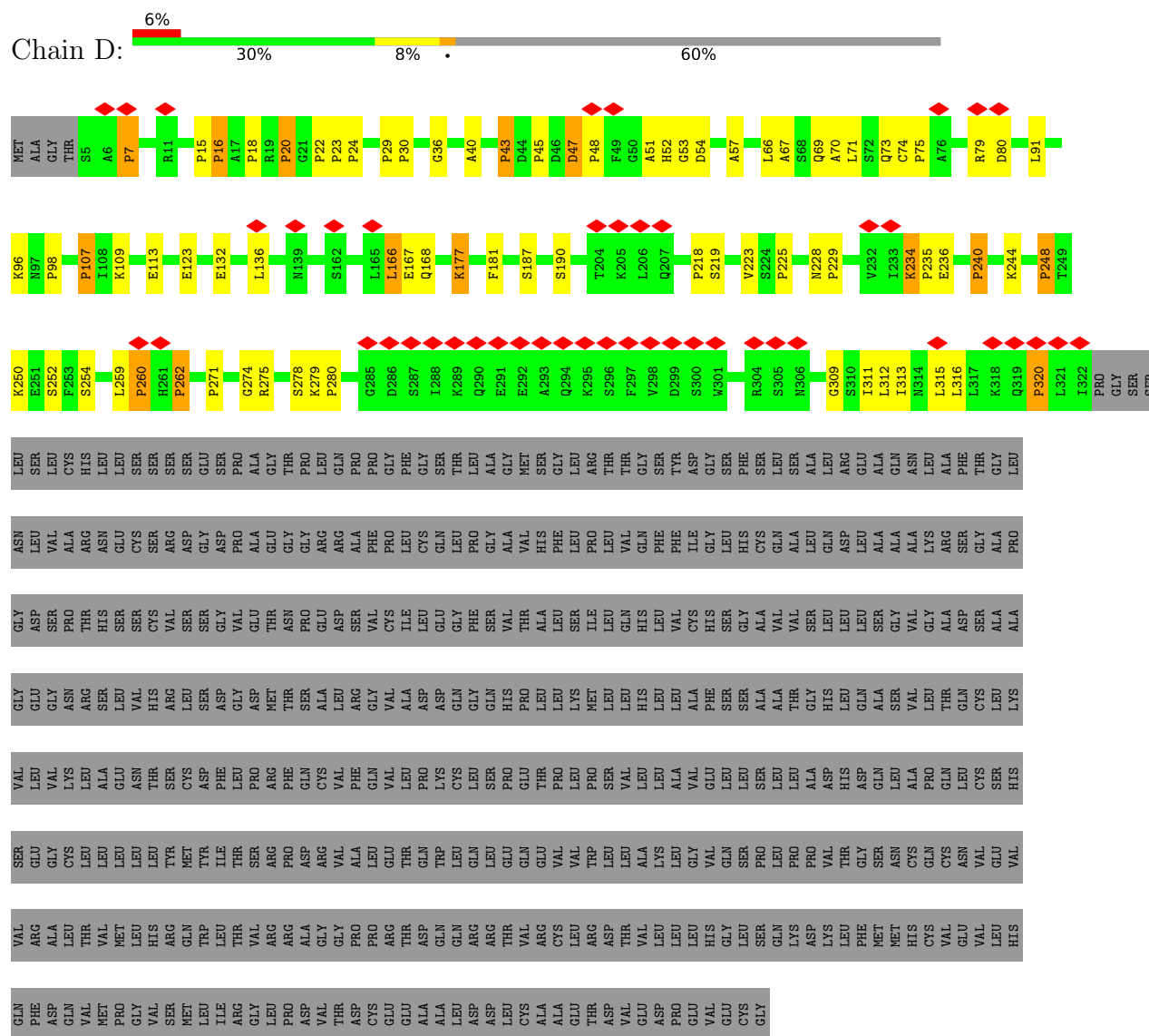




• Molecule 2: ATR-interacting protein



- Molecule 2: ATR-interacting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	312.0, 312.0, 312.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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	0.42	1/15191 (0.0%)	0.87	71/20804 (0.3%)
1	B	0.44	0/15191	0.90	65/20804 (0.3%)
2	C	0.32	0/1784	1.08	36/2481 (1.5%)
2	D	0.33	0/1571	1.13	27/2187 (1.2%)
All	All	0.42	1/33737 (0.0%)	0.91	199/46276 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	48
1	B	0	59
2	C	0	3
2	D	0	3
All	All	0	113

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2641	THR	C-O	5.52	1.26	1.23

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	24	PRO	N-CA-CB	10.51	109.85	102.81
2	D	235	PRO	N-CA-CB	9.03	111.00	101.88
1	A	358	PRO	N-CA-CB	8.32	111.99	103.25
1	A	1189	PRO	N-CA-CB	8.22	111.88	103.25
2	D	107	PRO	N-CA-CB	8.19	111.85	103.25
2	C	24	PRO	N-CA-CB	8.01	111.66	103.25
2	C	323	PRO	N-CA-CB	7.93	111.58	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	765	PRO	N-CA-CB	7.91	111.56	103.25
1	B	193	PRO	N-CA-CB	7.86	111.50	103.25
2	C	23	PRO	N-CA-CB	7.85	110.70	103.08
2	C	348	PRO	N-CA-CB	7.80	111.45	103.25
2	D	320	PRO	N-CA-CB	7.73	111.36	103.25
2	C	347	PRO	N-CA-CB	7.72	110.57	103.08
2	C	20	PRO	N-CA-CB	7.72	111.35	103.25
2	C	15	PRO	N-CA-CB	7.70	110.55	103.08
1	A	193	PRO	N-CA-CB	7.64	111.28	103.25
1	B	1000	PRO	N-CA-CB	7.59	110.52	103.46
1	B	358	PRO	N-CA-CB	7.57	111.20	103.25
2	D	22	PRO	N-CA-CB	7.55	110.40	103.08
2	D	260	PRO	N-CA-CB	7.53	111.16	103.25
2	D	23	PRO	N-CA-CB	7.53	110.38	103.08
2	D	30	PRO	N-CA-CB	7.52	110.48	103.41
1	B	1189	PRO	N-CA-CB	7.51	111.14	103.25
1	A	765	PRO	N-CA-CB	7.49	111.11	103.25
1	B	445	PRO	N-CA-CB	7.47	111.10	103.25
1	B	597	PRO	N-CA-CB	7.45	111.07	103.25
1	B	1437	GLY	CA-C-N	7.41	129.10	119.84
1	B	1437	GLY	C-N-CA	7.41	129.10	119.84
2	D	240	PRO	N-CA-CB	7.39	111.35	103.52
1	A	630	PRO	N-CA-CB	7.38	110.60	103.51
1	B	395	PRO	N-CA-CB	7.38	110.93	102.88
2	C	320	PRO	N-CA-CB	7.33	111.13	102.85
2	C	22	PRO	N-CA-CB	7.29	110.15	103.08
2	D	7	PRO	N-CA-CB	7.28	110.89	103.25
1	B	1447	PRO	N-CA-CB	7.21	110.44	103.51
2	C	340	PRO	N-CA-CB	7.17	110.78	103.25
2	D	15	PRO	N-CA-CB	7.16	110.02	103.08
1	A	1116	PRO	N-CA-CB	7.14	111.09	103.52
1	B	528	PRO	N-CA-CB	7.13	110.36	103.51
1	A	953	PRO	N-CA-CB	7.13	110.86	103.38
1	A	597	PRO	N-CA-CB	7.13	110.73	103.25
1	B	953	PRO	N-CA-CB	7.12	110.72	103.25
2	D	45	PRO	N-CA-CB	7.11	110.34	103.51
2	C	344	PRO	N-CA-CB	7.10	110.71	103.25
2	C	75	PRO	N-CA-CB	7.09	110.70	103.25
1	B	950	PRO	N-CA-CB	7.09	110.69	103.25
1	A	731	PRO	N-CA-CB	7.07	111.02	103.52
1	A	445	PRO	N-CA-CB	7.05	110.65	103.25
1	B	1164	PRO	N-CA-CB	7.02	110.62	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1456	PRO	N-CA-CB	6.97	110.48	102.88
1	B	886	PRO	N-CA-CB	6.96	110.56	103.25
1	A	395	PRO	N-CA-CB	6.94	110.17	103.51
1	A	1106	PRO	N-CA-CB	6.94	110.88	103.52
2	C	260	PRO	N-CA-CB	6.94	110.54	103.25
1	B	630	PRO	N-CA-CB	6.93	110.87	103.52
2	C	262	PRO	N-CA-CB	6.89	110.49	103.25
2	D	271	PRO	N-CA-CB	6.89	110.48	103.25
1	B	429	PRO	N-CA-CB	6.89	110.82	103.52
1	B	139	PRO	N-CA-CB	6.88	110.82	103.52
2	D	98	PRO	N-CA-CB	6.88	110.48	103.25
1	A	440	PRO	N-CA-CB	6.88	110.82	103.52
1	B	777	PRO	N-CA-CB	6.88	110.81	103.52
1	A	13	PRO	N-CA-CB	6.88	110.81	103.52
1	B	242	PRO	N-CA-CB	6.87	110.10	103.51
1	A	644	PRO	N-CA-CB	6.87	110.10	103.51
1	A	777	PRO	N-CA-CB	6.86	110.79	103.52
1	B	731	PRO	N-CA-CB	6.83	110.76	103.52
1	B	1106	PRO	N-CA-CB	6.81	110.41	103.25
1	A	932	PRO	N-CA-CB	6.79	110.38	103.25
1	B	1116	PRO	N-CA-CB	6.79	110.54	102.60
2	D	75	PRO	N-CA-CB	6.79	110.34	102.33
1	A	1477	PRO	N-CA-CB	6.78	110.36	103.25
1	B	1477	PRO	N-CA-CB	6.76	110.35	103.25
2	D	218	PRO	N-CA-CB	6.75	110.68	103.52
2	C	280	PRO	N-CA-CB	6.75	109.99	103.51
1	A	985	PRO	N-CA-CB	6.75	110.67	103.52
1	B	440	PRO	N-CA-CB	6.75	109.99	103.51
1	A	304	PRO	N-CA-CB	6.73	110.32	103.25
1	A	63	PRO	N-CA-CB	6.70	110.62	103.52
2	C	235	PRO	N-CA-CB	6.70	110.28	103.25
1	A	1437	GLY	CA-C-N	6.69	128.21	119.84
1	A	1437	GLY	C-N-CA	6.69	128.21	119.84
1	A	775	PRO	N-CA-CB	6.69	110.61	103.52
1	B	294	PRO	N-CA-CB	6.68	110.61	103.52
1	B	985	PRO	N-CA-CB	6.68	110.60	103.52
2	C	43	PRO	N-CA-CB	6.67	110.58	103.52
1	B	444	ALA	CA-C-N	6.66	128.17	119.84
1	B	444	ALA	C-N-CA	6.66	128.17	119.84
2	C	45	PRO	N-CA-CB	6.66	109.52	103.20
1	A	33	PRO	N-CA-CB	6.65	110.57	103.52
2	D	20	PRO	N-CA-CB	6.64	110.22	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1110	PRO	N-CA-CB	6.63	110.62	103.33
1	B	932	PRO	N-CA-CB	6.61	110.19	103.25
2	C	225	PRO	N-CA-CB	6.61	110.53	103.39
2	D	262	PRO	N-CA-CB	6.60	110.18	103.25
1	A	172	PRO	N-CA-CB	6.59	110.17	103.25
1	B	114	PRO	N-CA-CB	6.56	110.47	103.52
1	A	886	PRO	N-CA-CB	6.55	110.24	103.23
1	B	262	PRO	N-CA-CB	6.55	110.13	103.25
1	A	485	PRO	N-CA-CB	6.55	110.78	103.44
1	A	528	PRO	N-CA-CB	6.54	110.12	103.25
1	A	262	PRO	N-CA-CB	6.54	110.11	103.25
1	B	33	PRO	N-CA-CB	6.52	110.10	103.25
1	B	80	PRO	N-CA-CB	6.52	110.43	103.52
2	C	107	PRO	N-CA-CB	6.52	110.09	103.25
1	A	2527	GLY	N-CA-C	-6.51	106.59	114.66
1	B	1008	PRO	N-CA-CB	6.51	110.08	103.25
1	B	1456	PRO	N-CA-CB	6.50	109.97	102.88
2	C	16	PRO	N-CA-CB	6.49	110.40	103.52
1	A	1164	PRO	N-CA-CB	6.48	110.05	103.25
2	C	29	PRO	N-CA-CB	6.48	109.36	103.08
2	D	225	PRO	N-CA-CB	6.48	110.38	103.52
1	B	192	ALA	CA-C-N	6.46	127.92	119.84
1	B	192	ALA	C-N-CA	6.46	127.92	119.84
1	A	1125	PRO	N-CA-CB	6.43	110.34	103.52
2	D	48	PRO	N-CA-CB	6.42	109.96	102.76
2	D	16	PRO	N-CA-CB	6.41	110.31	103.52
1	A	689	PRO	N-CA-CB	6.41	110.31	103.52
2	D	248	PRO	N-CA-CB	6.40	110.30	103.52
1	A	80	PRO	N-CA-CB	6.39	110.30	103.52
1	A	816	PRO	N-CA-CB	6.39	110.29	103.52
1	A	1008	PRO	N-CA-CB	6.39	110.29	103.52
2	C	218	PRO	N-CA-CB	6.38	110.28	103.52
1	A	114	PRO	N-CA-CB	6.37	110.27	103.52
2	D	29	PRO	N-CA-CB	6.37	109.26	103.08
2	D	43	PRO	N-CA-CB	6.37	109.94	103.25
1	B	63	PRO	N-CA-CB	6.37	110.57	103.44
1	B	775	PRO	N-CA-CB	6.37	109.93	103.25
2	C	229	PRO	N-CA-CB	6.36	109.93	103.25
1	A	429	PRO	N-CA-CB	6.36	110.26	103.52
1	B	816	PRO	N-CA-CB	6.36	110.26	103.52
1	B	13	PRO	N-CA-CB	6.35	110.25	103.52
1	A	294	PRO	N-CA-CB	6.34	110.24	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	98	PRO	N-CA-CB	6.34	110.24	103.52
1	B	1125	PRO	N-CA-CB	6.33	110.23	103.52
1	B	172	PRO	N-CA-CB	6.33	109.89	103.25
2	C	240	PRO	N-CA-CB	6.32	110.29	103.33
1	A	139	PRO	N-CA-CB	6.31	110.21	103.52
1	A	242	PRO	N-CA-CB	6.29	110.19	103.39
1	A	2326	CYS	CA-C-N	-6.29	109.95	122.40
1	A	2326	CYS	C-N-CA	-6.29	109.95	122.40
2	C	7	PRO	N-CA-CB	6.29	110.18	103.52
1	A	315	PRO	N-CA-CB	6.26	110.45	103.44
1	A	1447	PRO	N-CA-CB	6.26	109.83	103.25
1	A	950	PRO	N-CA-CB	6.21	109.77	103.25
2	D	229	PRO	N-CA-CB	6.21	110.16	103.33
1	B	1110	PRO	N-CA-CB	6.18	110.36	103.44
1	B	644	PRO	N-CA-CB	6.14	109.70	103.25
2	C	18	PRO	N-CA-CB	6.14	110.32	103.44
1	A	265	PRO	N-CA-CB	6.13	110.31	103.44
2	C	48	PRO	N-CA-CB	6.11	109.99	103.39
1	A	1000	PRO	N-CA-CB	6.11	110.00	103.52
1	A	2230	VAL	CA-C-N	6.07	130.35	121.31
1	A	2230	VAL	C-N-CA	6.07	130.35	121.31
1	A	2020	ALA	N-CA-C	-6.05	99.80	109.96
1	B	315	PRO	N-CA-CB	6.05	110.21	103.44
1	B	304	PRO	N-CA-CB	6.05	110.21	103.44
2	D	280	PRO	N-CA-CB	6.00	110.16	103.44
1	A	192	ALA	CA-C-N	5.98	127.32	119.84
1	A	192	ALA	C-N-CA	5.98	127.32	119.84
2	C	30	PRO	N-CA-CB	5.98	109.84	103.39
2	D	18	PRO	N-CA-CB	5.94	110.10	103.44
2	C	271	PRO	N-CA-CB	5.93	110.08	103.44
1	A	444	ALA	CA-C-N	5.90	127.22	119.84
1	A	444	ALA	C-N-CA	5.90	127.22	119.84
1	B	2583	VAL	CA-C-N	5.87	132.53	121.97
1	B	2583	VAL	C-N-CA	5.87	132.53	121.97
1	B	485	PRO	N-CA-CB	5.86	110.00	103.44
1	B	689	PRO	N-CA-CB	5.86	110.00	103.44
1	B	2112	ARG	CA-C-N	5.83	128.41	120.77
1	B	2112	ARG	C-N-CA	5.83	128.41	120.77
1	B	265	PRO	N-CA-CB	5.77	109.90	103.44
2	C	248	PRO	N-CA-CB	5.76	109.89	103.44
1	A	2527	GLY	CA-C-N	5.71	129.39	120.82
1	A	2527	GLY	C-N-CA	5.71	129.39	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1151	ALA	CA-C-N	5.70	132.43	121.54
1	A	1151	ALA	C-N-CA	5.70	132.43	121.54
2	C	165	LEU	CA-C-N	5.66	132.34	121.54
2	C	165	LEU	C-N-CA	5.66	132.34	121.54
1	A	22	THR	CA-C-N	5.59	126.82	119.84
1	A	22	THR	C-N-CA	5.59	126.82	119.84
1	B	1997	LEU	CA-C-N	5.54	127.75	120.60
1	B	1997	LEU	C-N-CA	5.54	127.75	120.60
1	B	1151	ALA	CA-C-N	5.50	132.05	121.54
1	B	1151	ALA	C-N-CA	5.50	132.05	121.54
1	A	518	LYS	CA-C-N	5.44	131.93	121.54
1	A	518	LYS	C-N-CA	5.44	131.93	121.54
1	A	1921	GLY	N-CA-C	-5.40	107.75	115.64
1	A	23	PRO	N-CA-CB	5.27	108.79	103.25
2	C	322	ILE	CA-C-N	5.26	126.42	119.84
2	C	322	ILE	C-N-CA	5.26	126.42	119.84
1	B	2433	PRO	N-CA-C	5.17	117.01	110.70
1	A	1637	PRO	CA-C-N	5.17	131.00	121.70
1	A	1637	PRO	C-N-CA	5.17	131.00	121.70
1	B	2171	TYR	CB-CA-C	-5.15	106.52	111.00
1	A	1438	PRO	N-CA-CB	5.09	108.60	103.25
1	B	1165	LYS	CA-C-N	-5.06	115.53	121.90
1	B	1165	LYS	C-N-CA	-5.06	115.53	121.90
1	B	2314	LEU	N-CA-C	-5.01	108.44	114.75

There are no chirality outliers.

All (113) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1032	ASN	Peptide
1	A	1119	MET	Peptide
1	A	1139	LEU	Peptide
1	A	1147	ASP	Peptide
1	A	1148	LYS	Peptide
1	A	1152	LEU	Peptide
1	A	1185	LYS	Peptide
1	A	1186	ASP	Peptide
1	A	1437	GLY	Peptide
1	A	1540	CYS	Peptide
1	A	1541	ASN	Peptide
1	A	1649	LYS	Peptide
1	A	1650	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	1732	GLN	Peptide
1	A	1776	GLU	Peptide
1	A	1813	LYS	Peptide
1	A	1837	ALA	Peptide
1	A	1846	ARG	Peptide
1	A	1920	VAL	Peptide
1	A	1941	TYR	Peptide
1	A	1984	PHE	Peptide
1	A	1987	ASN	Peptide
1	A	1989	THR	Peptide
1	A	2010	MET	Peptide
1	A	2011	GLU	Peptide
1	A	2016	PHE	Peptide
1	A	2019	ASN	Peptide
1	A	2038	GLY	Peptide
1	A	2186	SER	Peptide
1	A	22	THR	Peptide
1	A	2205	LYS	Peptide
1	A	2228	LYS	Peptide
1	A	2263	GLN	Peptide
1	A	2267	ILE	Peptide
1	A	2269	THR	Peptide
1	A	2280	HIS	Peptide
1	A	2391	THR	Peptide
1	A	2433	PRO	Peptide
1	A	2446	ASP	Peptide
1	A	2498	LEU	Peptide
1	A	2523	MET	Peptide
1	A	2550	LEU	Peptide
1	A	2564	GLU	Peptide
1	A	2599	LEU	Peptide
1	A	2606	ARG	Peptide
1	A	384	GLY	Peptide
1	A	866	LYS	Peptide
1	A	933	ILE	Peptide
1	B	1033	PHE	Peptide
1	B	1147	ASP	Peptide
1	B	1148	LYS	Peptide
1	B	1152	LEU	Peptide
1	B	1167	VAL	Peptide
1	B	1185	LYS	Peptide
1	B	1186	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	1418	ALA	Peptide
1	B	1435	THR	Peptide
1	B	1437	GLY	Peptide
1	B	1469	THR	Peptide
1	B	1556	LEU	Peptide
1	B	1636	ILE	Peptide
1	B	1637	PRO	Peptide
1	B	1649	LYS	Peptide
1	B	1651	TYR	Peptide
1	B	1668	ASN	Peptide
1	B	1700	PRO	Peptide
1	B	1732	GLN	Peptide
1	B	1769	GLU	Peptide
1	B	1774	ARG	Peptide
1	B	1776	GLU	Peptide
1	B	1837	ALA	Peptide
1	B	1846	ARG	Peptide
1	B	1847	GLY	Peptide
1	B	1901	LEU	Peptide
1	B	1907	LEU	Peptide
1	B	1920	VAL	Peptide
1	B	1941	TYR	Peptide
1	B	1954	GLU	Peptide
1	B	1984	PHE	Peptide
1	B	1985	PRO	Peptide
1	B	1989	THR	Peptide
1	B	2010	MET	Peptide
1	B	2014	ALA	Peptide
1	B	2019	ASN	Peptide
1	B	2038	GLY	Peptide
1	B	2070	LEU	Peptide
1	B	2081	GLN	Peptide
1	B	2083	ILE	Peptide
1	B	2084	TYR	Peptide
1	B	2100	LYS	Peptide
1	B	2167	VAL	Peptide
1	B	2186	SER	Peptide
1	B	2263	GLN	Peptide
1	B	2267	ILE	Peptide
1	B	2269	THR	Peptide
1	B	2280	HIS	Peptide
1	B	2427	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	2432	HIS	Peptide
1	B	2446	ASP	Peptide
1	B	2498	LEU	Peptide
1	B	2582	GLU	Peptide
1	B	2603	ILE	Peptide
1	B	2606	ARG	Peptide
1	B	443	ARG	Peptide
1	B	445	PRO	Peptide
1	B	849	ARG	Peptide
1	B	967	GLN	Peptide
2	C	184	LYS	Peptide
2	C	186	GLN	Peptide
2	C	28	HIS	Peptide
2	D	166	LEU	Peptide
2	D	177	LYS	Peptide
2	D	234	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15007	0	11392	465	0
1	B	15007	0	11392	491	0
2	C	1785	0	791	44	0
2	D	1572	0	689	26	0
All	All	33371	0	24264	1020	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 18.

All (1020) 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:1637:PRO:HB2	1:A:1638:GLN:HG2	1.62	0.78
1:B:2333:ARG:HH11	1:B:2337:ARG:HH21	1.36	0.74
1:A:1964:TRP:HE1	1:A:2010:MET:HG3	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1559:ASP:HB3	1:A:1574:CYS:HB3	1.71	0.72
1:A:1670:GLN:HE22	1:A:1697:LYS:HE3	1.56	0.71
1:B:2037:ASP:H	1:B:2042:LEU:HD11	1.56	0.69
1:A:2211:PHE:HE1	1:A:2259:LEU:H	1.41	0.68
1:B:2302:ILE:HG12	1:B:2310:LYS:HG2	1.76	0.68
1:A:2358:ARG:HB3	1:A:2459:ARG:HD3	1.77	0.67
1:A:2043:ALA:H	1:A:2076:LEU:HD13	1.58	0.67
1:B:1900:ILE:HD13	1:B:2357:ARG:HH11	1.59	0.67
1:A:2225:LEU:O	1:A:2310:LYS:NZ	2.28	0.67
1:A:2606:ARG:NH1	1:B:2022:MET:SD	2.69	0.65
1:A:1699:GLU:O	1:A:1705:GLN:NE2	2.30	0.65
1:A:1932:ARG:NH2	1:A:1958:GLU:O	2.30	0.65
1:B:2325:MET:HB2	1:B:2377:ILE:HB	1.79	0.65
1:A:2302:ILE:HG12	1:A:2310:LYS:HG2	1.79	0.64
1:A:2477:HIS:H	1:A:2480:ASN:HD22	1.46	0.64
1:B:1699:GLU:O	1:B:1705:GLN:NE2	2.31	0.63
1:B:2105:GLU:HA	1:B:2109:ARG:HB2	1.80	0.63
1:B:2475:ASP:O	1:B:2480:ASN:ND2	2.32	0.63
1:A:1770:LEU:HA	1:A:1774:ARG:HB2	1.79	0.63
1:B:1184:PHE:O	1:B:1844:TYR:OH	2.15	0.63
1:A:2264:SER:O	1:A:2267:ILE:N	2.29	0.63
1:B:2301:GLU:HB2	1:B:2311:LYS:HB2	1.81	0.63
1:A:2325:MET:HB2	1:A:2377:ILE:HB	1.80	0.62
1:B:2038:GLY:HA2	1:B:2079:GLY:HA3	1.80	0.62
1:A:1758:GLY:HA2	1:B:1757:ASN:HB2	1.82	0.62
1:A:1961:LYS:HE2	1:A:2003:MET:HB2	1.82	0.62
1:A:2113:VAL:O	1:A:2117:ASN:ND2	2.32	0.62
1:B:1770:LEU:HA	1:B:1774:ARG:HB2	1.82	0.62
1:A:1595:LYS:HD3	1:A:1626:TYR:HB2	1.82	0.61
1:A:2510:ILE:HB	1:A:2632:LEU:HD11	1.82	0.61
1:B:2498:LEU:H	1:B:2501:LYS:HD3	1.65	0.61
1:B:2222:LEU:HD13	1:B:2376:ILE:HD11	1.82	0.61
1:B:862:ASN:HA	1:B:867:ASP:H	1.64	0.61
1:A:769:LEU:O	1:A:773:LYS:N	2.31	0.61
1:B:2219:THR:HA	1:B:2222:LEU:HB2	1.81	0.61
1:B:2410:MET:HE1	1:B:2420:LYS:HG2	1.82	0.61
1:A:2514:ARG:NH2	1:A:2641:THR:O	2.34	0.61
1:B:2105:GLU:O	1:B:2112:ARG:NH2	2.33	0.61
1:A:1757:ASN:HA	1:A:1760:HIS:HD2	1.66	0.60
1:A:1670:GLN:NE2	1:A:1695:ILE:O	2.33	0.60
1:B:1746:LEU:HD22	1:B:1748:GLN:HE21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1932:ARG:NH2	1:B:1958:GLU:O	2.35	0.60
1:B:2342:ASN:HA	1:B:2345:ILE:HD12	1.83	0.60
1:A:1864:ILE:HG22	1:A:1868:PHE:HB2	1.82	0.60
1:A:1901:LEU:HA	1:A:1904:ARG:HB3	1.83	0.60
1:A:1977:GLN:NE2	1:A:1981:GLU:OE2	2.35	0.60
1:A:2244:LYS:HG2	1:A:2299:MET:HG2	1.84	0.59
1:B:2043:ALA:HB1	1:B:2072:PHE:HB3	1.84	0.59
1:A:2424:PHE:O	1:A:2428:LEU:N	2.35	0.59
1:B:155:ASP:O	1:B:159:LEU:N	2.35	0.59
1:A:1949:GLU:O	1:A:1953:ALA:N	2.35	0.59
1:B:2421:LEU:HD21	1:B:2631:ASN:HA	1.83	0.59
1:B:2482:LEU:HB2	1:B:2491:VAL:HB	1.83	0.59
1:A:150:LEU:HA	1:A:154:GLU:H	1.67	0.59
1:B:1995:ASN:O	1:B:2001:ARG:NE	2.35	0.59
1:B:2094:TRP:HA	1:B:2097:TYR:HB2	1.85	0.59
1:A:1776:GLU:O	1:A:1779:TRP:N	2.34	0.59
1:B:1670:GLN:NE2	1:B:1695:ILE:O	2.36	0.59
1:B:1057:LYS:O	1:B:1061:GLU:N	2.35	0.59
1:B:1997:LEU:O	1:B:2001:ARG:N	2.30	0.59
1:B:2109:ARG:O	1:B:2112:ARG:NH2	2.36	0.59
1:B:2262:LEU:HD22	1:B:2314:LEU:HD11	1.84	0.59
1:B:2383:THR:HB	1:B:2482:LEU:HB3	1.83	0.59
1:B:2012:GLU:HG2	1:B:2015:ASN:HD21	1.67	0.58
1:A:1184:PHE:O	1:A:1844:TYR:OH	2.19	0.58
1:A:1827:ARG:NH2	1:A:1861:GLU:OE1	2.36	0.58
1:B:1779:TRP:O	1:B:1913:ARG:NH1	2.35	0.58
1:B:2539:THR:OG1	1:B:2540:MET:N	2.35	0.58
1:B:2089:ARG:NH1	1:B:2552:SER:OG	2.36	0.58
1:B:1756:VAL:O	1:B:1774:ARG:NH1	2.37	0.58
1:B:2089:ARG:O	1:B:2093:LEU:N	2.36	0.58
1:A:1944:LEU:HD13	1:A:1973:LEU:HD13	1.85	0.58
1:B:2190:ARG:NH1	1:B:2372:ASP:OD2	2.36	0.58
1:A:1536:VAL:O	1:A:1545:GLN:NE2	2.37	0.58
1:A:2224:GLU:HA	1:A:2227:ASN:HB2	1.85	0.58
1:A:1971:GLN:HE21	1:A:2013:THR:HG22	1.69	0.58
1:B:703:VAL:O	1:B:707:PHE:N	2.34	0.58
1:B:1593:ARG:HD3	1:B:2442:ARG:HG2	1.86	0.58
1:A:1942:ASN:HB3	1:A:1944:LEU:HG	1.86	0.57
1:A:1750:SER:OG	1:B:1723:ASP:OD1	2.23	0.57
1:A:2565:TRP:HB3	1:A:2567:LYS:HE3	1.86	0.57
1:A:2093:LEU:HD21	1:A:2556:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2205:LYS:HB3	1:A:2208:LEU:HB2	1.87	0.57
1:A:2151:HIS:O	1:A:2193:ARG:NH1	2.36	0.57
1:B:713:GLN:O	1:B:717:THR:N	2.38	0.57
1:B:2139:LEU:HB3	1:B:2270:LEU:HD13	1.86	0.57
1:A:1106:PRO:O	1:A:1110:PRO:N	2.37	0.57
2:D:309:GLY:O	2:D:313:ILE:N	2.37	0.57
1:A:1741:LYS:O	1:A:1745:GLY:N	2.37	0.57
1:A:2270:LEU:O	1:A:2347:LYS:NZ	2.35	0.57
1:A:1745:GLY:O	1:A:1946:ASN:ND2	2.38	0.57
1:B:2043:ALA:O	1:B:2047:ASP:N	2.31	0.57
1:B:2527:GLY:HA2	1:B:2530:GLY:HA3	1.87	0.57
1:B:400:LEU:O	1:B:404:SER:N	2.37	0.56
1:B:1901:LEU:O	1:B:1905:ARG:NH1	2.38	0.56
2:C:340:PRO:O	2:C:344:PRO:N	2.38	0.56
1:A:155:ASP:O	1:A:159:LEU:N	2.38	0.56
1:A:1406:ALA:O	1:A:1410:ASN:N	2.38	0.56
1:A:2516:THR:HG23	1:A:2519:MET:H	1.70	0.56
1:B:710:ILE:O	1:B:714:LEU:N	2.37	0.56
1:B:1771:ASN:HB3	1:B:1797:SER:HA	1.88	0.56
1:B:1935:GLY:HA2	1:B:1938:GLN:HB2	1.87	0.56
1:B:2264:SER:O	1:B:2267:ILE:N	2.36	0.56
1:B:1623:TYR:HA	1:B:1626:TYR:HB3	1.87	0.56
1:B:2155:GLU:HA	1:B:2158:VAL:HB	1.87	0.56
1:A:1650:ALA:HA	1:A:1651:TYR:CG	2.40	0.56
1:A:1756:VAL:O	1:A:1774:ARG:NH1	2.39	0.56
1:A:2387:ARG:HA	1:A:2390:LEU:HB2	1.86	0.56
1:B:914:LEU:O	1:B:918:LYS:N	2.39	0.56
1:B:2081:GLN:NE2	1:B:2279:ASN:OD1	2.39	0.56
1:A:1775:VAL:HG11	1:A:1802:VAL:HA	1.87	0.56
1:B:1595:LYS:HD3	1:B:1626:TYR:HB2	1.88	0.56
1:B:2093:LEU:O	1:B:2097:TYR:N	2.26	0.56
1:A:2515:LEU:HD12	1:A:2519:MET:HB3	1.88	0.56
1:B:707:PHE:O	1:B:711:LEU:N	2.39	0.56
2:C:187:SER:O	2:C:191:GLU:N	2.37	0.56
1:A:1701:SER:HG	1:A:1704:GLU:H	1.50	0.56
1:A:2533:ARG:HH22	1:A:2621:HIS:HB2	1.70	0.56
1:B:1913:ARG:O	1:B:1917:ASN:N	2.37	0.56
1:B:1448:GLU:O	1:B:1452:GLU:N	2.37	0.56
1:B:2402:THR:HB	1:B:2405:GLU:HB3	1.88	0.56
2:C:11:ARG:O	2:C:15:PRO:N	2.39	0.56
1:B:2090:MET:HA	1:B:2093:LEU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2103:GLU:O	1:A:2107:ALA:N	2.38	0.55
1:A:1102:SER:O	1:A:1106:PRO:N	2.39	0.55
1:A:1930:VAL:O	1:A:1934:ALA:N	2.37	0.55
1:B:1022:ASN:O	1:B:1026:ARG:N	2.33	0.55
1:A:1978:LYS:O	1:A:1982:LEU:N	2.38	0.55
1:A:924:SER:O	1:A:928:GLN:N	2.37	0.55
1:A:2427:PHE:HA	1:A:2430:PRO:HD2	1.88	0.55
1:A:2140:THR:HA	1:A:2270:LEU:HD13	1.88	0.55
1:B:2404:LYS:O	1:B:2408:GLN:N	2.39	0.55
1:B:2090:MET:HE3	1:B:2094:TRP:HE1	1.72	0.55
1:A:1901:LEU:O	1:A:1905:ARG:NE	2.28	0.55
1:B:1756:VAL:HG13	1:B:1774:ARG:HD3	1.87	0.55
1:B:2202:ILE:HA	1:B:2205:LYS:HB2	1.87	0.55
1:A:2074:ARG:HD3	1:A:2129:HIS:HB3	1.89	0.55
1:B:2534:ARG:NH1	1:B:2537:GLU:OE1	2.40	0.55
1:A:1132:ALA:O	1:A:1136:MET:N	2.39	0.55
1:A:2019:ASN:H	1:B:2606:ARG:HH21	1.55	0.55
1:A:2402:THR:HB	1:A:2405:GLU:HB3	1.88	0.55
1:B:1619:SER:O	1:B:1623:TYR:N	2.37	0.55
1:B:2529:GLU:HB3	1:B:2533:ARG:HD2	1.89	0.55
1:A:34:ARG:O	1:A:38:CYS:N	2.39	0.54
1:A:549:SER:O	1:A:553:SER:N	2.34	0.54
1:A:921:LYS:O	1:A:925:PHE:N	2.38	0.54
1:B:425:ASP:O	1:B:429:PRO:N	2.40	0.54
1:B:2273:ILE:HD11	1:B:2282:SER:H	1.72	0.54
1:B:2411:LEU:HB2	1:B:2415:ALA:HB2	1.89	0.54
1:B:2418:SER:HA	1:B:2421:LEU:HD12	1.88	0.54
1:A:2245:MET:HA	1:A:2249:LEU:HB2	1.88	0.54
1:B:917:ALA:O	1:B:921:LYS:N	2.40	0.54
1:B:2518:ASN:ND2	1:B:2644:MET:O	2.40	0.54
1:B:1427:ILE:O	1:B:1431:ARG:N	2.40	0.54
1:B:1508:SER:O	1:B:1512:THR:N	2.37	0.54
1:B:1741:LYS:O	1:B:1745:GLY:N	2.41	0.54
1:A:940:SER:O	1:A:944:SER:N	2.40	0.54
1:A:1504:HIS:HA	1:A:1507:ALA:HB3	1.90	0.54
1:A:1752:VAL:HA	1:A:1755:GLN:HB3	1.90	0.54
1:A:2065:ILE:O	1:A:2069:VAL:N	2.39	0.54
1:A:2476:ARG:NH2	1:A:2494:ASP:O	2.41	0.54
1:A:1932:ARG:NH2	1:A:1957:VAL:O	2.37	0.54
1:B:506:HIS:O	1:B:510:GLN:N	2.39	0.54
1:B:2266:MET:O	1:B:2269:THR:OG1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2547:ARG:O	1:B:2551:MET:N	2.34	0.54
1:A:2071:HIS:O	1:A:2075:SER:N	2.41	0.54
1:A:2213:GLY:O	1:A:2216:THR:OG1	2.25	0.54
1:A:2587:LYS:O	1:A:2590:THR:OG1	2.22	0.54
1:B:2456:ALA:O	1:B:2460:SER:N	2.31	0.54
1:B:2245:MET:HA	1:B:2249:LEU:HB2	1.88	0.54
1:B:2465:SER:O	1:B:2469:TYR:N	2.38	0.54
1:A:1057:LYS:O	1:A:1061:GLU:N	2.37	0.54
1:B:758:LEU:O	1:B:762:VAL:N	2.39	0.54
1:B:1531:HIS:O	1:B:1535:TYR:N	2.37	0.54
1:A:1108:GLN:O	1:A:1112:ASP:N	2.38	0.53
1:A:2405:GLU:HA	1:A:2408:GLN:HG3	1.90	0.53
1:A:2561:PRO:HB2	1:A:2582:GLU:HB3	1.89	0.53
1:B:270:PHE:O	1:B:274:LEU:N	2.37	0.53
1:A:2332:LEU:HB2	1:A:2369:PRO:HB3	1.91	0.53
1:B:2129:HIS:HA	1:B:2132:TYR:HB2	1.89	0.53
2:C:190:SER:O	2:C:194:PHE:N	2.41	0.53
1:B:1586:ASP:O	1:B:1589:THR:OG1	2.26	0.53
2:D:248:PRO:O	2:D:252:SER:N	2.39	0.53
2:D:312:LEU:O	2:D:316:LEU:N	2.41	0.53
1:A:485:PRO:O	1:A:489:MET:N	2.39	0.53
1:B:161:ARG:O	1:B:165:MET:N	2.42	0.53
1:B:857:ALA:O	1:B:861:ARG:N	2.39	0.53
1:B:2629:ASP:O	1:B:2633:LEU:N	2.39	0.53
1:B:406:GLU:O	1:B:410:GLU:N	2.40	0.53
1:B:1775:VAL:HG11	1:B:1802:VAL:HG22	1.91	0.53
1:B:2225:LEU:O	1:B:2310:LYS:NZ	2.40	0.53
1:A:1060:THR:O	1:A:1064:LEU:N	2.38	0.53
1:A:1575:GLN:O	1:A:1578:THR:OG1	2.26	0.53
1:A:1787:VAL:HG12	1:A:1809:LEU:HD11	1.91	0.53
1:A:1925:LEU:HA	1:A:1957:VAL:HG11	1.91	0.53
1:A:2089:ARG:NH1	1:A:2552:SER:OG	2.39	0.53
1:A:2105:GLU:HA	1:A:2109:ARG:HB2	1.89	0.53
1:A:2391:THR:O	1:A:2395:LYS:N	2.37	0.53
1:B:755:SER:O	1:B:759:LYS:N	2.38	0.53
1:B:892:LEU:O	1:B:896:LEU:N	2.41	0.53
1:B:1451:ARG:O	1:B:1455:GLU:N	2.37	0.53
1:B:1577:SER:O	1:B:1580:THR:OG1	2.24	0.53
1:B:1780:LYS:HA	1:B:1913:ARG:HH22	1.74	0.53
1:A:470:ALA:O	1:A:474:GLN:N	2.41	0.53
1:A:1025:ARG:O	1:A:1029:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:SER:O	1:A:1107:TYR:N	2.35	0.53
1:A:2588:ALA:O	1:A:2592:VAL:N	2.38	0.53
1:B:411:ILE:O	1:B:415:THR:N	2.41	0.53
1:B:510:GLN:O	1:B:514:CYS:N	2.41	0.53
1:B:2113:VAL:O	1:B:2117:ASN:ND2	2.42	0.53
1:B:2224:GLU:HA	1:B:2227:ASN:HB2	1.89	0.53
1:A:2173:GLN:HA	1:A:2176:MET:HG2	1.91	0.53
1:A:447:GLN:O	1:A:451:ILE:N	2.40	0.53
1:A:1486:ASN:O	1:A:1490:TRP:N	2.38	0.53
1:A:1702:LEU:HD11	1:A:1728:LEU:HB2	1.90	0.53
1:A:2529:GLU:HB3	1:A:2533:ARG:HD2	1.91	0.53
1:B:1471:TRP:O	1:B:1475:LYS:N	2.38	0.53
1:B:1492:ALA:O	1:B:1496:GLY:N	2.37	0.53
1:B:1942:ASN:HB3	1:B:1944:LEU:HG	1.90	0.53
1:A:957:ALA:O	1:A:961:LYS:N	2.42	0.53
1:A:2106:LYS:HG2	1:A:2116:ARG:HH21	1.74	0.53
1:A:2417:LEU:O	1:A:2421:LEU:N	2.36	0.53
1:B:99:PHE:O	1:B:103:ILE:N	2.41	0.53
2:C:168:GLN:O	2:C:172:GLN:N	2.38	0.53
1:A:1831:ILE:O	1:A:1835:SER:N	2.42	0.52
1:B:1821:ASP:O	1:B:1825:LEU:N	2.43	0.52
1:B:2089:ARG:HG2	1:B:2144:GLN:HE22	1.74	0.52
1:B:2454:ARG:HD2	1:B:2523:MET:HA	1.90	0.52
1:B:2587:LYS:O	1:B:2590:THR:OG1	2.21	0.52
1:A:1577:SER:O	1:A:1580:THR:OG1	2.24	0.52
1:A:2043:ALA:O	1:A:2047:ASP:N	2.37	0.52
1:A:2159:VAL:O	1:A:2163:ILE:N	2.38	0.52
1:A:2539:THR:OG1	1:A:2540:MET:N	2.43	0.52
1:B:407:ILE:O	1:B:411:ILE:N	2.39	0.52
1:B:733:SER:O	1:B:737:HIS:N	2.40	0.52
2:D:275:ARG:O	2:D:279:LYS:N	2.40	0.52
1:A:1437:GLY:O	1:A:1439:GLY:N	2.42	0.52
1:A:2417:LEU:HA	1:A:2420:LYS:HB2	1.90	0.52
1:B:910:GLU:O	1:B:914:LEU:N	2.40	0.52
1:B:1595:LYS:O	1:B:1599:LEU:N	2.41	0.52
1:B:2077:GLN:HE22	1:B:2088:PRO:HD3	1.74	0.52
1:A:702:ILE:O	1:A:706:GLU:N	2.42	0.52
1:A:1001:ASP:O	1:A:1005:LYS:N	2.41	0.52
1:A:1621:VAL:O	1:A:1625:ASP:N	2.39	0.52
1:B:706:GLU:O	1:B:710:ILE:N	2.42	0.52
1:B:2422:LYS:O	1:B:2426:GLU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2549:PRO:O	1:B:2552:SER:OG	2.25	0.52
1:A:9:ALA:O	1:A:13:PRO:N	2.42	0.52
1:A:160:HIS:O	1:A:164:VAL:N	2.42	0.52
1:A:397:TYR:O	1:A:401:LYS:N	2.42	0.52
1:A:914:LEU:O	1:A:918:LYS:N	2.39	0.52
1:A:2194:CYS:HA	1:A:2197:ILE:HD12	1.91	0.52
1:B:286:ASP:O	1:B:290:LEU:N	2.40	0.52
1:B:646:ARG:O	1:B:650:GLU:N	2.42	0.52
1:B:1054:HIS:O	1:B:1058:ASN:N	2.37	0.52
1:B:2464:MET:O	1:B:2468:GLY:N	2.36	0.52
2:C:297:PHE:O	2:C:301:TRP:N	2.42	0.52
1:A:346:LEU:O	1:A:350:LEU:N	2.42	0.52
1:A:571:ASP:O	1:A:575:TYR:N	2.42	0.52
1:B:1108:GLN:O	1:B:1112:ASP:N	2.42	0.52
1:A:960:ARG:O	1:A:964:VAL:N	2.41	0.52
1:B:1638:GLN:OE1	1:B:1660:SER:OG	2.27	0.52
1:B:2244:LYS:HB2	1:B:2247:LYS:HG3	1.91	0.52
1:A:1043:SER:O	1:A:1047:ASP:N	2.43	0.52
1:B:943:SER:O	1:B:947:THR:N	2.43	0.52
1:B:976:SER:O	1:B:980:ASN:N	2.39	0.52
1:A:2173:GLN:HB3	1:A:2261:PRO:HG3	1.92	0.52
1:A:2303:LEU:HB2	1:A:2309:PRO:HG2	1.91	0.52
1:B:1102:SER:O	1:B:1106:PRO:N	2.43	0.52
1:B:2267:ILE:HD13	1:B:2283:HIS:HB3	1.91	0.52
1:A:316:VAL:O	1:A:320:MET:N	2.40	0.51
1:A:673:SER:O	1:A:677:ILE:N	2.44	0.51
1:B:921:LYS:O	1:B:925:PHE:N	2.43	0.51
1:A:30:VAL:O	1:A:34:ARG:N	2.42	0.51
1:B:253:THR:O	1:B:257:GLN:N	2.41	0.51
1:B:508:SER:O	1:B:512:MET:N	2.42	0.51
1:B:800:THR:O	1:B:804:ALA:N	2.42	0.51
1:B:2171:TYR:OH	1:B:2281:ALA:O	2.28	0.51
1:A:2415:ALA:HB3	1:A:2420:LYS:HE3	1.92	0.51
1:B:1659:GLU:HA	1:B:1662:ILE:HD12	1.92	0.51
1:B:2065:ILE:HG12	1:B:2068:ILE:HD12	1.92	0.51
1:B:2162:GLU:O	1:B:2166:LYS:N	2.34	0.51
1:A:313:ILE:O	1:A:317:TYR:N	2.40	0.51
1:A:917:ALA:O	1:A:921:LYS:N	2.39	0.51
1:A:2345:ILE:O	1:A:2349:LEU:N	2.36	0.51
1:B:880:ALA:O	1:B:884:LEU:N	2.41	0.51
1:B:1710:GLU:OE2	1:B:1722:TYR:OH	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2190:ARG:HH21	1:B:2582:GLU:HG2	1.74	0.51
1:A:59:THR:O	1:A:63:PRO:N	2.42	0.51
1:A:1905:ARG:HA	1:A:1908:LEU:HB3	1.93	0.51
1:B:853:ALA:O	1:B:857:ALA:N	2.42	0.51
1:B:961:LYS:O	1:B:965:ALA:N	2.42	0.51
1:B:1841:ARG:HH22	1:B:2449:SER:HA	1.75	0.51
2:C:35:ARG:O	2:C:39:ALA:N	2.40	0.51
1:A:1841:ARG:NH2	1:A:2448:THR:OG1	2.40	0.51
1:B:123:ILE:O	1:B:126:VAL:N	2.41	0.51
1:B:212:VAL:O	1:B:216:ILE:N	2.38	0.51
1:B:487:ILE:O	1:B:491:GLU:N	2.43	0.51
1:B:1001:ASP:O	1:B:1005:LYS:N	2.36	0.51
1:B:1759:VAL:HB	1:B:1774:ARG:HH12	1.75	0.51
1:B:1801:SER:O	1:B:1805:GLY:N	2.44	0.51
1:A:451:ILE:O	1:A:455:ASP:N	2.41	0.51
1:A:1507:ALA:O	1:A:1511:PHE:N	2.40	0.51
1:B:1422:GLN:O	1:B:1426:SER:N	2.44	0.51
1:B:2023:LYS:O	1:B:2027:ASP:N	2.41	0.51
1:A:710:ILE:O	1:A:714:LEU:N	2.43	0.51
1:A:773:LYS:O	1:A:777:PRO:N	2.43	0.51
1:B:96:CYS:O	1:B:100:SER:N	2.43	0.51
1:B:341:LEU:O	1:B:345:ALA:N	2.40	0.51
1:B:484:ASN:O	1:B:488:GLU:N	2.41	0.51
1:B:1687:ASP:OD2	1:B:2459:ARG:NH2	2.40	0.51
1:B:2303:LEU:HB2	1:B:2309:PRO:HG2	1.92	0.51
2:D:91:LEU:O	2:D:96:LYS:N	2.41	0.51
1:A:136:SER:O	1:A:140:ALA:N	2.41	0.51
1:A:400:LEU:O	1:A:404:SER:N	2.40	0.51
1:A:1187:ASP:HB2	1:A:2356:ARG:NE	2.26	0.51
1:A:1687:ASP:OD2	1:A:2358:ARG:NE	2.42	0.51
1:A:1933:LYS:HA	1:A:1936:HIS:HB2	1.93	0.51
1:A:2262:LEU:HD21	1:A:2293:ILE:HG13	1.93	0.51
1:A:2593:LEU:HB3	1:A:2597:GLN:HE22	1.75	0.51
1:B:2294:ALA:HB3	1:B:2317:SER:HA	1.92	0.51
2:C:194:PHE:O	2:C:198:GLU:N	2.42	0.51
1:A:918:LYS:O	1:A:922:LEU:N	2.39	0.50
1:A:1969:VAL:O	1:A:1973:LEU:N	2.37	0.50
1:A:2018:SER:OG	1:A:2019:ASN:ND2	2.44	0.50
1:A:2090:MET:HA	1:A:2093:LEU:HB2	1.92	0.50
1:B:403:GLU:O	1:B:407:ILE:N	2.42	0.50
1:B:1905:ARG:HH21	1:B:1938:GLN:HE21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2520:VAL:HA	1:B:2523:MET:HE3	1.92	0.50
2:C:13:SER:O	2:C:17:ALA:N	2.40	0.50
1:A:937:LEU:O	1:A:941:LEU:N	2.44	0.50
1:B:2130:THR:HG21	1:B:2163:ILE:HG12	1.94	0.50
1:A:311:ARG:O	1:A:315:PRO:N	2.45	0.50
1:A:1756:VAL:HG13	1:A:1774:ARG:HD3	1.92	0.50
1:A:2551:MET:HE1	1:A:2595:ILE:HB	1.93	0.50
1:B:1773:TYR:O	1:B:1777:ALA:N	2.40	0.50
1:A:567:VAL:O	1:A:571:ASP:N	2.44	0.50
1:A:2520:VAL:HA	1:A:2523:MET:HE3	1.93	0.50
1:B:1654:ALA:O	1:B:1658:PHE:N	2.44	0.50
1:B:2346:ASN:HD21	1:B:2362:ILE:HB	1.75	0.50
1:A:779:LYS:O	1:A:783:ILE:N	2.43	0.50
1:A:1749:LEU:HD11	1:A:1780:LYS:HD2	1.92	0.50
1:A:1997:LEU:O	1:A:2001:ARG:N	2.35	0.50
1:B:319:ASN:O	1:B:323:GLU:N	2.40	0.50
1:B:778:VAL:O	1:B:782:PHE:N	2.44	0.50
1:A:1807:LEU:O	1:A:1811:ALA:N	2.45	0.50
1:A:2470:ILE:HG13	1:A:2471:LEU:HD22	1.94	0.50
1:B:202:LEU:O	1:B:206:GLU:N	2.40	0.50
1:A:401:LYS:O	1:A:405:MET:N	2.41	0.50
1:A:982:PHE:O	1:A:986:ASP:N	2.43	0.50
1:B:105:THR:O	1:B:109:ARG:N	2.45	0.50
1:B:1106:PRO:O	1:B:1110:PRO:N	2.45	0.50
1:B:1575:GLN:O	1:B:1578:THR:OG1	2.29	0.50
1:B:1597:GLN:O	1:B:1601:ALA:N	2.42	0.50
1:B:1788:GLU:OE2	1:B:1813:LYS:NZ	2.44	0.50
1:B:2515:LEU:HD12	1:B:2519:MET:HB3	1.94	0.50
2:C:16:PRO:O	2:C:20:PRO:N	2.45	0.50
1:A:1477:PRO:O	1:A:1481:SER:N	2.44	0.50
1:A:2103:GLU:HA	1:A:2106:LYS:HB2	1.94	0.50
1:A:2386:LEU:HD11	1:A:2436:PHE:HE1	1.77	0.50
1:B:350:LEU:O	1:B:354:LEU:N	2.45	0.50
1:B:2394:TYR:O	1:B:2398:GLY:N	2.45	0.50
1:A:2502:GLY:O	1:A:2509:GLU:N	2.44	0.50
1:B:288:LEU:O	1:B:292:GLU:N	2.41	0.50
1:B:984:PHE:O	1:B:988:ASN:N	2.41	0.50
1:B:1998:ILE:HA	1:B:2001:ARG:HD2	1.94	0.50
1:B:2184:LYS:NZ	1:B:2220:ASP:OD1	2.45	0.50
1:A:33:PRO:O	1:A:37:LEU:N	2.43	0.49
1:A:266:ALA:O	1:A:270:PHE:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LYS:O	1:A:549:SER:N	2.37	0.49
1:A:961:LYS:O	1:A:965:ALA:N	2.42	0.49
1:A:981:VAL:O	1:A:985:PRO:N	2.45	0.49
1:A:2131:ASN:OD1	1:A:2166:LYS:NZ	2.37	0.49
1:A:2474:GLY:N	1:A:2497:CYS:O	2.37	0.49
1:B:316:VAL:O	1:B:320:MET:N	2.41	0.49
1:B:1546:GLN:O	1:B:1550:ALA:N	2.45	0.49
1:A:1409:ASP:O	1:A:1413:ALA:N	2.40	0.49
1:A:2106:LYS:NZ	1:A:2154:ASP:OD1	2.44	0.49
1:B:983:ASP:O	1:B:987:LEU:N	2.40	0.49
1:B:1026:ARG:O	1:B:1030:ILE:N	2.35	0.49
1:B:1737:HIS:HE1	1:B:1772:THR:HG21	1.76	0.49
1:B:2363:ARG:HH21	1:B:2380:VAL:HG11	1.77	0.49
1:B:2397:LYS:NZ	1:B:2438:GLU:OE2	2.40	0.49
2:C:333:LEU:O	2:C:337:SER:N	2.41	0.49
1:A:351:GLN:O	1:A:355:LYS:N	2.45	0.49
1:A:782:PHE:O	1:A:786:LEU:N	2.42	0.49
1:A:1022:ASN:O	1:A:1026:ARG:N	2.45	0.49
1:B:162:ARG:O	1:B:166:GLY:N	2.43	0.49
1:B:804:ALA:O	1:B:808:THR:N	2.45	0.49
1:B:1019:LYS:O	1:B:1023:VAL:N	2.44	0.49
1:B:2270:LEU:HA	1:B:2283:HIS:HE1	1.77	0.49
1:B:2344:LEU:HD12	1:B:2347:LYS:HD2	1.93	0.49
1:B:2560:ASP:HB3	1:B:2563:VAL:HB	1.94	0.49
2:D:219:SER:O	2:D:223:VAL:N	2.44	0.49
1:A:1495:ALA:O	1:A:1499:ILE:N	2.42	0.49
1:A:2023:LYS:O	1:A:2027:ASP:N	2.43	0.49
1:A:2093:LEU:O	1:A:2097:TYR:N	2.35	0.49
1:B:1926:GLN:HA	1:B:1929:ARG:HB2	1.93	0.49
1:B:2405:GLU:HA	1:B:2408:GLN:HB2	1.94	0.49
2:C:302:ARG:O	2:C:306:ASN:N	2.45	0.49
1:A:2509:GLU:HA	1:A:2636:MET:HE1	1.93	0.49
1:B:1016:THR:O	1:B:1020:GLN:N	2.44	0.49
2:C:332:LEU:O	2:C:336:SER:N	2.43	0.49
1:A:195:GLN:O	1:A:199:MET:N	2.45	0.49
1:A:2484:ASP:HB2	1:A:2488:GLY:H	1.78	0.49
1:B:549:SER:O	1:B:553:SER:N	2.44	0.49
1:B:631:GLN:O	1:B:635:ARG:N	2.45	0.49
1:B:775:PRO:O	1:B:779:LYS:N	2.43	0.49
1:B:1523:LYS:HA	1:B:1526:ILE:HD12	1.94	0.49
1:B:1949:GLU:O	1:B:1953:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2036:GLU:HB3	1:B:2039:HIS:CD2	2.47	0.49
1:A:1592:ALA:O	1:A:1596:PHE:N	2.40	0.49
2:C:306:ASN:O	2:C:310:SER:N	2.45	0.49
1:A:174:VAL:O	1:A:178:PHE:N	2.46	0.49
1:A:343:LYS:O	1:A:347:CYS:N	2.42	0.49
1:B:731:PRO:O	1:B:735:HIS:N	2.40	0.49
1:B:1579:GLN:HA	1:B:1582:PHE:HD2	1.78	0.49
1:B:1589:THR:OG1	1:B:1590:GLN:N	2.46	0.49
1:B:2387:ARG:HE	1:B:2641:THR:HG21	1.76	0.49
2:C:82:SER:O	2:C:86:LYS:N	2.45	0.49
1:A:347:CYS:O	1:A:351:GLN:N	2.44	0.49
1:A:2214:ASP:O	1:A:2218:LEU:N	2.44	0.49
1:B:729:THR:O	1:B:733:SER:N	2.38	0.49
1:A:373:ARG:O	1:A:377:LYS:N	2.43	0.49
1:B:266:ALA:O	1:B:270:PHE:N	2.44	0.49
1:B:709:SER:O	1:B:713:GLN:N	2.44	0.49
1:B:2147:SER:HB2	1:B:2561:PRO:HD2	1.95	0.49
1:A:10:SER:O	1:A:14:ALA:N	2.43	0.48
1:A:1053:LEU:O	1:A:1057:LYS:N	2.43	0.48
1:A:2554:LEU:O	1:A:2558:LEU:N	2.44	0.48
1:B:397:TYR:O	1:B:401:LYS:N	2.45	0.48
1:B:2198:LEU:O	1:B:2202:ILE:N	2.38	0.48
2:C:20:PRO:O	2:C:24:PRO:N	2.46	0.48
2:C:336:SER:O	2:C:340:PRO:N	2.46	0.48
1:B:437:SER:O	1:B:441:SER:N	2.45	0.48
1:B:833:GLU:O	1:B:837:SER:N	2.47	0.48
1:B:920:VAL:O	1:B:924:SER:N	2.42	0.48
1:B:2070:LEU:HD22	1:B:2091:LEU:HD23	1.95	0.48
1:A:564:ASP:O	1:A:568:LYS:N	2.43	0.48
1:B:2459:ARG:HG2	1:B:2535:ALA:HB2	1.95	0.48
1:A:489:MET:O	1:A:493:ILE:N	2.44	0.48
1:A:553:SER:O	1:A:557:LEU:N	2.42	0.48
1:A:1808:LEU:HA	1:A:1811:ALA:HB3	1.96	0.48
1:A:2268:PRO:HG2	1:A:2269:THR:HG23	1.96	0.48
1:A:2355:SER:O	1:A:2359:GLU:N	2.47	0.48
1:B:2363:ARG:NH1	1:B:2484:ASP:OD2	2.47	0.48
2:C:329:LEU:O	2:C:333:LEU:N	2.46	0.48
2:D:66:LEU:O	2:D:70:ALA:N	2.43	0.48
1:A:1618:VAL:O	1:A:1622:ASP:N	2.41	0.48
1:A:2382:ASN:O	1:A:2485:SER:N	2.45	0.48
1:A:2460:SER:OG	1:A:2461:THR:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:O	1:B:114:PRO:N	2.46	0.48
1:B:683:ASN:O	1:B:687:ARG:N	2.43	0.48
1:B:1390:SER:O	1:B:1394:TYR:N	2.43	0.48
1:A:275:GLU:O	1:A:279:HIS:N	2.46	0.48
1:A:1620:THR:O	1:A:1624:GLU:N	2.41	0.48
1:A:2395:LYS:HA	1:A:2399:VAL:HG23	1.95	0.48
1:B:702:ILE:O	1:B:706:GLU:N	2.45	0.48
1:A:1623:TYR:HA	1:A:1626:TYR:HB3	1.95	0.48
1:A:2469:TYR:CZ	1:A:2598:ARG:HD3	2.49	0.48
1:B:59:THR:O	1:B:63:PRO:N	2.47	0.48
1:B:1009:ALA:HA	1:B:1012:ALA:HB2	1.95	0.48
1:A:1801:SER:O	1:A:1805:GLY:N	2.42	0.48
1:A:2536:CYS:O	1:A:2539:THR:OG1	2.27	0.48
1:A:2558:LEU:HB3	1:A:2588:ALA:HB1	1.94	0.48
1:B:102:TRP:O	1:B:106:ARG:N	2.44	0.48
1:B:1804:LEU:HD12	1:B:1807:LEU:HD12	1.95	0.48
1:B:2262:LEU:HD21	1:B:2293:ILE:HA	1.96	0.48
2:C:96:LYS:O	2:C:100:GLY:N	2.43	0.48
1:A:670:SER:O	1:A:674:GLY:N	2.43	0.48
1:A:1824:LYS:HA	1:A:1827:ARG:HB2	1.95	0.48
1:A:2044:LYS:HZ1	1:A:2086:SER:HG	1.59	0.48
1:A:2133:LEU:HD21	1:A:2137:GLN:HB2	1.94	0.48
1:B:874:GLY:O	1:B:878:ARG:N	2.41	0.48
1:B:2431:ARG:HD3	1:B:2644:MET:HA	1.96	0.48
1:A:1127:LEU:O	1:A:1131:LEU:N	2.45	0.48
1:A:2174:GLN:HE21	1:A:2267:ILE:HG22	1.78	0.48
1:A:2534:ARG:NH1	1:A:2537:GLU:OE1	2.47	0.48
1:B:215:ARG:HA	1:B:218:ALA:HB3	1.94	0.48
1:B:875:ASP:O	1:B:879:ALA:N	2.43	0.48
1:B:1841:ARG:NH1	1:B:2448:THR:O	2.47	0.48
1:B:1487:PHE:O	1:B:1491:SER:N	2.41	0.47
1:B:2536:CYS:O	1:B:2539:THR:OG1	2.32	0.47
2:C:218:PRO:O	2:C:222:HIS:N	2.46	0.47
2:D:236:GLU:O	2:D:240:PRO:N	2.47	0.47
1:A:27:ASN:O	1:A:31:GLN:N	2.44	0.47
1:A:1188:PHE:HA	1:A:2350:ARG:HD3	1.96	0.47
1:A:2096:ASP:O	1:A:2099:THR:OG1	2.25	0.47
1:B:1056:LEU:O	1:B:1060:THR:N	2.47	0.47
2:C:115:GLU:O	2:C:119:ALA:N	2.47	0.47
2:D:36:GLY:O	2:D:40:ALA:N	2.46	0.47
1:A:14:ALA:O	1:A:18:LEU:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:LEU:O	1:A:1404:TYR:N	2.46	0.47
1:A:1734:ILE:O	1:A:1738:GLY:N	2.45	0.47
1:A:2597:GLN:HB3	1:A:2602:VAL:HB	1.96	0.47
1:B:136:SER:O	1:B:140:ALA:N	2.44	0.47
1:B:1642:ALA:O	1:B:1645:SER:OG	2.22	0.47
1:B:2139:LEU:HD13	1:B:2270:LEU:HD22	1.97	0.47
1:B:2390:LEU:HA	1:B:2393:LEU:HD12	1.96	0.47
1:B:125:GLU:O	1:B:129:SER:N	2.42	0.47
1:B:159:LEU:O	1:B:163:ASN:N	2.43	0.47
1:B:323:GLU:O	1:B:327:VAL:N	2.47	0.47
1:B:1154:SER:O	1:B:1158:LEU:N	2.45	0.47
1:B:1187:ASP:HB2	1:B:2356:ARG:HD3	1.97	0.47
1:B:2358:ARG:HB3	1:B:2459:ARG:HD3	1.96	0.47
1:A:1054:HIS:O	1:A:1058:ASN:N	2.43	0.47
1:A:1752:VAL:O	1:A:1756:VAL:N	2.46	0.47
1:A:2226:CYS:SG	1:A:2327:LYS:N	2.87	0.47
1:A:2427:PHE:HD1	1:A:2430:PRO:HG2	1.79	0.47
1:B:55:LEU:O	1:B:59:THR:N	2.48	0.47
1:B:1477:PRO:O	1:B:1481:SER:N	2.37	0.47
1:A:2629:ASP:O	1:A:2633:LEU:N	2.42	0.47
1:B:1529:LEU:HA	1:B:1532:ILE:HD12	1.96	0.47
1:B:2038:GLY:H	1:B:2039:HIS:HD2	1.61	0.47
1:B:2474:GLY:O	1:B:2476:ARG:NE	2.33	0.47
1:B:2477:HIS:H	1:B:2480:ASN:ND2	2.13	0.47
1:A:31:GLN:O	1:A:35:GLN:N	2.44	0.47
1:A:292:GLU:O	1:A:296:SER:N	2.41	0.47
1:A:481:GLY:HA2	1:A:482:LEU:HA	1.63	0.47
1:A:727:SER:O	1:A:731:PRO:N	2.48	0.47
1:A:1474:VAL:O	1:A:1478:ILE:N	2.44	0.47
1:A:2500:ASN:O	1:A:2504:THR:N	2.47	0.47
1:B:980:ASN:O	1:B:984:PHE:N	2.43	0.47
1:B:1018:GLY:O	1:B:1022:ASN:N	2.44	0.47
1:B:1549:TYR:HA	1:B:1552:ILE:HD12	1.94	0.47
1:B:1702:LEU:HD21	1:B:1728:LEU:HD12	1.97	0.47
1:B:1850:TYR:HA	1:B:1853:ARG:HB2	1.96	0.47
1:B:1900:ILE:HD11	1:B:2357:ARG:HB2	1.96	0.47
1:B:2076:LEU:HG	1:B:2080:ASN:HD21	1.80	0.47
1:B:2102:TYR:O	1:B:2106:LYS:N	2.42	0.47
1:B:2334:LYS:NZ	1:B:2496:ASN:O	2.48	0.47
1:B:2484:ASP:O	1:B:2488:GLY:N	2.47	0.47
2:D:47:ASP:HA	2:D:57:ALA:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:CYS:O	1:A:132:PHE:N	2.44	0.47
1:A:1850:TYR:HA	1:A:1853:ARG:HB2	1.95	0.47
1:A:2053:VAL:O	1:A:2057:LYS:N	2.48	0.47
1:B:662:SER:O	1:B:666:VAL:N	2.42	0.47
2:C:282:SER:O	2:C:286:ASP:N	2.47	0.47
2:C:283:LEU:O	2:C:287:SER:N	2.43	0.47
1:A:623:ARG:O	1:A:627:SER:N	2.47	0.47
1:A:1529:LEU:HD23	1:A:1532:ILE:HD12	1.97	0.47
1:B:481:GLY:HA2	1:B:482:LEU:HA	1.65	0.47
1:B:501:ALA:O	1:B:505:VAL:N	2.47	0.47
1:B:2516:THR:HG23	1:B:2518:ASN:H	1.79	0.47
1:B:2590:THR:OG1	1:B:2591:HIS:N	2.48	0.47
1:A:270:PHE:O	1:A:274:LEU:N	2.47	0.47
1:A:2266:MET:O	1:A:2269:THR:OG1	2.30	0.47
1:B:604:ASP:O	1:B:608:LEU:N	2.46	0.47
1:B:1752:VAL:HA	1:B:1755:GLN:HB3	1.95	0.47
1:B:1991:PRO:HB2	1:B:1992:GLU:HG3	1.96	0.47
1:B:2561:PRO:HB2	1:B:2582:GLU:HB3	1.97	0.47
1:A:146:THR:O	1:A:150:LEU:N	2.43	0.46
1:A:520:CYS:O	1:A:524:SER:N	2.47	0.46
1:A:1793:ALA:HB1	1:A:1796:LYS:HB2	1.97	0.46
1:A:2044:LYS:HZ3	1:A:2087:MET:HG2	1.81	0.46
1:B:940:SER:O	1:B:944:SER:N	2.43	0.46
1:B:1053:LEU:O	1:B:1057:LYS:N	2.38	0.46
1:B:1385:THR:O	1:B:1389:ASP:N	2.43	0.46
1:B:1717:ASP:OD1	1:B:1717:ASP:N	2.39	0.46
1:B:2096:ASP:O	1:B:2099:THR:OG1	2.30	0.46
2:C:195:LYS:O	2:C:199:MET:N	2.48	0.46
2:D:274:GLY:O	2:D:278:SER:N	2.43	0.46
1:A:73:GLN:HA	1:A:74:HIS:HA	1.60	0.46
1:B:1447:PRO:O	1:B:1451:ARG:N	2.44	0.46
2:C:169:GLU:O	2:C:173:ALA:N	2.49	0.46
1:A:225:GLN:O	1:A:229:LEU:N	2.47	0.46
1:A:1385:THR:O	1:A:1389:ASP:N	2.45	0.46
1:B:2366:ALA:N	1:B:2378:GLU:OE1	2.47	0.46
2:C:32:LYS:O	2:C:36:GLY:N	2.40	0.46
1:A:100:SER:O	1:A:104:ILE:N	2.44	0.46
1:A:833:GLU:O	1:A:837:SER:N	2.49	0.46
1:B:714:LEU:O	1:B:718:LEU:N	2.44	0.46
1:B:1905:ARG:HH22	1:B:1943:ALA:HB3	1.80	0.46
2:C:12:ARG:O	2:C:16:PRO:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:ALA:O	2:C:74:CYS:N	2.44	0.46
2:D:311:ILE:O	2:D:315:LEU:N	2.49	0.46
1:A:297:LYS:O	1:A:301:THR:N	2.46	0.46
1:A:874:GLY:O	1:A:878:ARG:N	2.47	0.46
1:A:1021:LEU:O	1:A:1025:ARG:N	2.40	0.46
1:A:1778:ALA:HA	1:A:1781:LEU:HB3	1.96	0.46
1:A:1959:ARG:H	1:A:1959:ARG:HD2	1.81	0.46
1:A:2074:ARG:O	1:A:2077:GLN:N	2.39	0.46
1:B:274:LEU:O	1:B:278:LYS:N	2.45	0.46
2:C:221:SER:O	2:C:225:PRO:N	2.48	0.46
2:C:284:ARG:O	2:C:288:ILE:N	2.49	0.46
1:A:404:SER:O	1:A:408:ILE:N	2.42	0.46
1:A:508:SER:O	1:A:512:MET:N	2.44	0.46
1:A:2053:VAL:HA	1:A:2056:ASN:HB2	1.97	0.46
1:A:2313:SER:HA	1:A:2323:ILE:HA	1.97	0.46
1:A:2417:LEU:HB3	1:A:2635:GLN:HE21	1.81	0.46
1:B:371:TYR:O	1:B:375:ILE:N	2.48	0.46
1:B:507:CYS:O	1:B:511:ASN:N	2.45	0.46
1:B:982:PHE:O	1:B:986:ASP:N	2.42	0.46
1:B:1060:THR:O	1:B:1064:LEU:N	2.49	0.46
1:B:2027:ASP:O	1:B:2031:CYS:N	2.45	0.46
1:B:2096:ASP:HA	1:B:2099:THR:HG23	1.97	0.46
1:A:409:GLU:O	1:A:413:CYS:N	2.47	0.46
1:A:711:LEU:O	1:A:715:VAL:N	2.41	0.46
1:A:925:PHE:O	1:A:929:TYR:N	2.47	0.46
1:A:1389:ASP:O	1:A:1393:ALA:N	2.48	0.46
1:A:1508:SER:O	1:A:1512:THR:N	2.44	0.46
1:A:1623:TYR:O	1:A:1627:GLN:N	2.43	0.46
1:A:1928:ALA:O	1:A:1932:ARG:N	2.40	0.46
1:A:1979:GLY:O	1:A:1983:CYS:N	2.49	0.46
1:A:2157:PHE:HA	1:A:2160:LEU:HB2	1.96	0.46
1:B:979:ALA:O	1:B:983:ASP:N	2.46	0.46
1:B:1650:ALA:HA	1:B:1651:TYR:HA	1.71	0.46
1:B:2103:GLU:OE2	1:B:2152:SER:OG	2.24	0.46
1:B:2455:SER:O	1:B:2459:ARG:NH1	2.43	0.46
1:A:783:ILE:O	1:A:787:HIS:N	2.48	0.46
1:A:1598:ALA:O	1:A:1602:GLU:N	2.48	0.46
1:A:1801:SER:HA	1:A:1804:LEU:HB3	1.98	0.46
1:A:2190:ARG:O	1:A:2194:CYS:N	2.45	0.46
1:B:2407:ARG:NH2	1:B:2638:LEU:O	2.48	0.46
1:B:2412:PRO:O	1:B:2415:ALA:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:O	1:A:572:ALA:N	2.45	0.46
1:A:703:VAL:O	1:A:707:PHE:N	2.38	0.46
1:A:2507:VAL:HB	1:A:2637:TYR:HB2	1.98	0.46
1:B:1709:HIS:NE2	1:B:1714:LEU:O	2.48	0.46
1:B:2032:LEU:HA	1:B:2035:TRP:HD1	1.81	0.46
1:A:1429:ASP:O	1:A:1433:MET:N	2.47	0.46
1:A:1630:THR:HA	1:A:1633:LEU:HB2	1.97	0.46
1:A:2596:GLU:O	1:A:2600:GLN:N	2.49	0.46
1:B:36:ILE:O	1:B:40:PHE:N	2.47	0.46
1:B:314:GLU:O	1:B:318:LEU:N	2.45	0.46
1:B:2009:PHE:CZ	1:B:2042:LEU:HA	2.51	0.46
1:B:2469:TYR:O	1:B:2598:ARG:NH1	2.49	0.46
1:A:2089:ARG:NH2	1:A:2549:PRO:O	2.49	0.45
1:A:2468:GLY:HA3	1:A:2473:LEU:HD22	1.97	0.45
1:A:2470:ILE:HD12	1:A:2599:LEU:HD11	1.98	0.45
1:B:888:ALA:HA	1:B:889:LEU:HA	1.68	0.45
1:B:2182:VAL:O	1:B:2185:SER:OG	2.34	0.45
1:A:310:TYR:O	1:A:314:GLU:N	2.46	0.45
1:A:733:SER:O	1:A:737:HIS:N	2.42	0.45
1:A:1619:SER:O	1:A:1623:TYR:N	2.40	0.45
1:A:2518:ASN:ND2	1:A:2644:MET:O	2.49	0.45
1:B:2297:ASP:OD1	1:B:2297:ASP:N	2.48	0.45
2:D:70:ALA:O	2:D:74:CYS:N	2.44	0.45
1:A:319:ASN:O	1:A:323:GLU:N	2.47	0.45
1:A:1005:LYS:O	1:A:1009:ALA:N	2.41	0.45
1:A:2184:LYS:NZ	1:A:2219:THR:OG1	2.43	0.45
1:A:2558:LEU:HD22	1:A:2588:ALA:HA	1.99	0.45
1:B:488:GLU:O	1:B:492:GLY:N	2.42	0.45
1:B:1899:PRO:HD2	1:B:2353:ALA:HB2	1.97	0.45
1:B:2565:TRP:HB3	1:B:2567:LYS:HE3	1.98	0.45
1:A:507:CYS:O	1:A:511:ASN:N	2.49	0.45
1:A:659:ALA:O	1:A:663:SER:N	2.49	0.45
1:A:2615:SER:O	1:A:2619:HIS:N	2.47	0.45
1:B:2464:MET:HG2	1:B:2492:HIS:CD2	2.52	0.45
1:A:11:MET:O	1:A:15:LEU:N	2.49	0.45
1:A:1717:ASP:OD1	1:A:1717:ASP:N	2.42	0.45
1:A:1779:TRP:HZ2	1:A:1804:LEU:HG	1.82	0.45
1:B:896:LEU:O	1:B:900:SER:N	2.47	0.45
1:B:1799:THR:H	1:B:1802:VAL:HB	1.82	0.45
1:B:2042:LEU:HB2	1:B:2076:LEU:HD13	1.98	0.45
1:A:889:LEU:O	1:A:893:LEU:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1587:HIS:O	1:A:1591:TRP:N	2.41	0.45
1:A:1996:MET:SD	1:A:2001:ARG:NH2	2.89	0.45
1:A:2219:THR:HA	1:A:2222:LEU:HB2	1.99	0.45
1:A:2556:THR:O	1:A:2560:ASP:N	2.50	0.45
1:B:769:LEU:O	1:B:773:LYS:N	2.41	0.45
1:B:960:ARG:O	1:B:964:VAL:N	2.45	0.45
1:B:1103:SER:O	1:B:1107:TYR:N	2.41	0.45
1:B:2084:TYR:OH	1:B:2137:GLN:O	2.29	0.45
1:A:2386:LEU:HD13	1:A:2483:PHE:HE2	1.81	0.45
1:A:2547:ARG:CZ	1:A:2600:GLN:HG2	2.47	0.45
1:B:73:GLN:HA	1:B:74:HIS:HA	1.70	0.45
1:B:160:HIS:O	1:B:164:VAL:N	2.47	0.45
1:B:760:ALA:O	1:B:764:LYS:N	2.44	0.45
1:B:1669:ILE:HG22	1:B:1673:LEU:HD23	1.98	0.45
1:A:785:ASN:O	1:A:789:LEU:N	2.50	0.45
1:A:1998:ILE:HA	1:A:2001:ARG:HB2	1.99	0.45
1:A:2516:THR:OG1	1:A:2517:HIS:N	2.49	0.45
1:B:877:GLY:O	1:B:881:LYS:N	2.49	0.45
1:B:1780:LYS:HA	1:B:1913:ARG:HH12	1.82	0.45
1:B:2341:PHE:HD1	1:B:2553:VAL:HG11	1.81	0.45
1:A:317:TYR:O	1:A:321:LEU:N	2.44	0.45
1:A:2427:PHE:O	1:A:2431:ARG:NH1	2.50	0.45
1:B:1947:ALA:O	1:B:1950:SER:N	2.49	0.45
1:B:2244:LYS:H	1:B:2247:LYS:HD2	1.82	0.45
1:B:2367:VAL:HG22	1:B:2377:ILE:HA	1.98	0.45
1:A:665:GLU:O	1:A:669:ALA:N	2.40	0.45
1:A:2198:LEU:O	1:A:2202:ILE:N	2.41	0.45
1:B:410:GLU:O	1:B:414:GLN:N	2.39	0.45
1:B:1486:ASN:O	1:B:1490:TRP:N	2.41	0.45
1:B:1526:ILE:HA	1:B:1529:LEU:HD12	1.99	0.45
1:B:2216:THR:O	1:B:2220:ASP:N	2.38	0.45
1:A:403:GLU:O	1:A:407:ILE:N	2.46	0.44
1:A:1823:LEU:HB3	1:A:1827:ARG:HE	1.82	0.44
1:A:1826:VAL:HA	1:A:1829:GLU:HB2	1.98	0.44
1:A:2636:MET:HB2	1:A:2642:PRO:HG3	1.99	0.44
1:B:752:GLU:O	1:B:756:SER:N	2.48	0.44
1:B:1819:PHE:O	1:B:1822:SER:OG	2.33	0.44
1:B:1995:ASN:O	1:B:1997:LEU:N	2.50	0.44
1:B:2208:LEU:HA	1:B:2211:PHE:HD2	1.82	0.44
1:B:2554:LEU:HA	1:B:2557:PHE:HB3	1.99	0.44
1:A:314:GLU:O	1:A:318:LEU:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:ILE:HG22	1:A:1737:HIS:HB2	1.98	0.44
1:A:1859:GLU:O	1:A:1863:SER:OG	2.33	0.44
1:B:1623:TYR:O	1:B:1627:GLN:N	2.45	0.44
1:B:2475:ASP:HB2	1:B:2497:CYS:HB2	1.99	0.44
1:A:244:ILE:O	1:A:248:ALA:N	2.47	0.44
1:A:339:SER:O	1:A:343:LYS:N	2.42	0.44
1:A:1591:TRP:HA	1:A:1594:HIS:HB2	1.99	0.44
1:A:2142:PHE:HE2	1:A:2178:MET:HB2	1.83	0.44
1:A:2147:SER:HB3	1:A:2337:ARG:HH22	1.82	0.44
1:B:1002:LEU:O	1:B:1006:ALA:N	2.43	0.44
1:B:1188:PHE:HA	1:B:2356:ARG:HH12	1.82	0.44
1:B:2460:SER:OG	1:B:2461:THR:N	2.51	0.44
1:A:1995:ASN:O	1:A:2001:ARG:NE	2.48	0.44
1:A:2460:SER:HB2	1:A:2490:CYS:H	1.81	0.44
1:A:2541:ARG:NH1	1:A:2545:ASP:OD1	2.50	0.44
1:B:100:SER:O	1:B:104:ILE:N	2.40	0.44
1:B:732:PHE:O	1:B:736:GLY:N	2.43	0.44
1:B:2085:GLN:HE22	1:B:2140:THR:HB	1.83	0.44
1:B:2114:GLN:O	1:B:2118:ASP:N	2.39	0.44
1:A:1642:ALA:O	1:A:1646:PHE:N	2.47	0.44
1:A:2386:LEU:HA	1:A:2386:LEU:HD12	1.78	0.44
1:B:1628:SER:HA	1:B:1631:ARG:HB2	2.00	0.44
1:B:2074:ARG:HH22	1:B:2126:ILE:HG12	1.83	0.44
2:D:240:PRO:O	2:D:244:LYS:N	2.46	0.44
1:A:426:GLY:O	1:A:430:LYS:N	2.44	0.44
1:B:924:SER:O	1:B:928:GLN:N	2.47	0.44
1:A:161:ARG:O	1:A:165:MET:N	2.47	0.44
1:A:1105:ASP:O	1:A:1109:GLY:N	2.44	0.44
1:A:1723:ASP:OD1	1:B:1750:SER:OG	2.25	0.44
1:A:1836:ALA:O	1:A:1838:SER:N	2.50	0.44
1:A:2251:GLU:O	1:A:2254:THR:OG1	2.34	0.44
1:A:2546:GLN:HB3	1:A:2549:PRO:HG2	1.99	0.44
1:B:343:LYS:O	1:B:347:CYS:N	2.50	0.44
1:B:981:VAL:O	1:B:985:PRO:N	2.51	0.44
1:B:1426:SER:O	1:B:1430:CYS:N	2.44	0.44
1:B:1714:LEU:HD22	1:B:1716:ARG:HH21	1.83	0.44
1:B:1926:GLN:HA	1:B:1929:ARG:HD2	2.00	0.44
2:C:34:ALA:O	2:C:38:SER:N	2.45	0.44
2:C:151:GLN:O	2:C:155:VAL:N	2.51	0.44
1:A:755:SER:O	1:A:759:LYS:N	2.51	0.44
1:A:1673:LEU:HD21	1:A:2526:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2211:PHE:HA	1:A:2214:ASP:HB2	1.99	0.44
1:B:564:ASP:O	1:B:568:LYS:N	2.42	0.44
1:B:916:ALA:O	1:B:920:VAL:N	2.49	0.44
1:B:1391:SER:O	1:B:1395:GLY:N	2.51	0.44
1:B:2119:LEU:HD21	1:B:2156:VAL:HG23	2.00	0.44
1:B:2278:ALA:HA	1:B:2279:ASN:HA	1.58	0.44
2:D:52:HIS:HA	2:D:53:GLY:HA2	1.55	0.44
1:A:1410:ASN:O	1:A:1414:GLN:N	2.51	0.44
1:A:1743:MET:HB3	1:A:1752:VAL:HG22	2.00	0.44
1:A:2343:SER:HA	1:A:2346:ASN:HB2	2.00	0.44
1:B:1696:ARG:HD3	1:B:1699:GLU:HA	2.00	0.44
1:B:2076:LEU:O	1:B:2079:GLY:N	2.51	0.44
1:B:2379:TRP:NE1	1:B:2381:ASN:OD1	2.42	0.44
1:A:1388:GLU:O	1:A:1392:PHE:N	2.50	0.43
1:A:1579:GLN:HA	1:A:1582:PHE:HD2	1.82	0.43
1:B:64:THR:O	1:B:68:LEU:N	2.49	0.43
1:B:65:SER:O	1:B:69:LEU:N	2.45	0.43
1:B:757:GLN:O	1:B:761:SER:N	2.47	0.43
1:A:1848:TYR:HA	1:A:1851:ILE:HD12	1.99	0.43
1:A:2096:ASP:HB3	1:A:2148:ARG:HD2	1.99	0.43
1:A:2382:ASN:HB3	1:A:2485:SER:H	1.83	0.43
1:B:801:ASP:O	1:B:805:VAL:N	2.43	0.43
1:B:1778:ALA:HA	1:B:1781:LEU:HB3	1.99	0.43
1:A:839:ASP:HA	1:A:840:GLY:HA2	1.77	0.43
1:A:2521:ASN:HA	1:A:2524:GLY:HA2	1.99	0.43
1:B:342:LEU:O	1:B:346:LEU:N	2.47	0.43
1:B:1786:LEU:HB3	1:B:1790:TYR:CE2	2.53	0.43
1:B:2464:MET:HG2	1:B:2492:HIS:CG	2.52	0.43
2:D:166:LEU:O	2:D:168:GLN:N	2.36	0.43
1:A:2244:LYS:HB2	1:A:2247:LYS:H	1.83	0.43
1:A:2428:LEU:O	1:A:2431:ARG:N	2.50	0.43
1:A:2477:HIS:H	1:A:2480:ASN:ND2	2.12	0.43
1:A:2551:MET:HE2	1:A:2596:GLU:HG3	2.00	0.43
1:B:201:ASN:O	1:B:205:ILE:N	2.43	0.43
1:B:754:SER:O	1:B:758:LEU:N	2.47	0.43
1:B:2043:ALA:HB3	1:B:2076:LEU:HB2	2.00	0.43
2:C:39:ALA:O	2:C:43:PRO:N	2.51	0.43
1:A:1396:LEU:HA	1:A:1591:TRP:CD1	2.53	0.43
1:A:1643:VAL:O	1:A:1647:ARG:N	2.42	0.43
1:B:671:CYS:O	1:B:675:PHE:N	2.43	0.43
1:B:1541:ASN:O	1:B:1544:ASP:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2040:PHE:HA	1:B:2080:ASN:OD1	2.19	0.43
1:B:2066:ARG:CZ	1:B:2098:GLY:HA2	2.48	0.43
1:A:268:THR:O	1:A:272:SER:N	2.46	0.43
1:B:426:GLY:O	1:B:430:LYS:N	2.45	0.43
1:B:1932:ARG:O	1:B:1935:GLY:N	2.49	0.43
1:B:1975:VAL:HG12	1:B:1978:LYS:H	1.82	0.43
1:B:2340:GLU:O	1:B:2343:SER:OG	2.35	0.43
2:C:243:GLY:O	2:C:247:PHE:N	2.48	0.43
1:A:29:VAL:O	1:A:33:PRO:N	2.52	0.43
1:B:26:TYR:O	1:B:30:VAL:N	2.52	0.43
1:B:77:LYS:O	1:B:81:LEU:N	2.44	0.43
1:B:2059:GLU:HA	1:B:2060:LYS:HA	1.71	0.43
1:A:341:LEU:O	1:A:345:ALA:N	2.47	0.43
1:A:1386:GLY:O	1:A:1390:SER:N	2.43	0.43
1:A:1440:HIS:O	1:A:1444:ARG:N	2.51	0.43
1:A:1719:THR:OG1	1:B:1748:GLN:NE2	2.52	0.43
1:A:1730:PRO:HG2	1:A:1732:GLN:HG3	2.01	0.43
1:A:2077:GLN:HA	1:A:2080:ASN:CG	2.44	0.43
1:B:1745:GLY:O	1:B:1946:ASN:ND2	2.52	0.43
1:B:2260:ILE:HB	1:B:2293:ILE:HD11	2.01	0.43
1:B:2263:GLN:HG2	1:B:2368:ILE:HD12	2.00	0.43
2:D:177:LYS:O	2:D:181:PHE:N	2.51	0.43
1:A:984:PHE:O	1:A:988:ASN:N	2.46	0.43
1:A:2563:VAL:HG11	1:A:2585:ASN:HD21	1.84	0.43
1:B:701:ASP:O	1:B:705:LYS:N	2.43	0.43
1:B:1677:GLN:HG2	1:B:1692:VAL:HG21	2.00	0.43
2:C:8:GLY:O	2:C:12:ARG:N	2.47	0.43
2:C:129:LYS:O	2:C:133:GLU:N	2.51	0.43
2:D:69:GLN:O	2:D:73:GLN:N	2.42	0.43
1:A:2393:LEU:HD22	1:A:2442:ARG:HH11	1.84	0.43
1:B:509:HIS:O	1:B:513:ASN:N	2.45	0.43
1:B:665:GLU:O	1:B:669:ALA:N	2.42	0.43
1:B:672:VAL:O	1:B:676:PHE:N	2.48	0.43
1:B:1024:ASN:O	1:B:1028:ILE:N	2.52	0.43
1:B:1932:ARG:HH21	1:B:1962:TRP:HB2	1.84	0.43
1:B:2162:GLU:HB3	1:B:2166:LYS:HE3	2.00	0.43
1:B:2484:ASP:HB2	1:B:2489:GLU:H	1.84	0.43
2:C:334:SER:O	2:C:338:GLU:N	2.46	0.43
1:B:1387:VAL:O	1:B:1391:SER:N	2.52	0.42
1:B:1449:HIS:O	1:B:1453:ILE:N	2.42	0.42
1:B:2458:CYS:SG	1:B:2531:LEU:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2500:ASN:OD1	1:B:2598:ARG:NH2	2.52	0.42
1:B:1996:MET:SD	1:B:2001:ARG:NH2	2.92	0.42
1:B:2043:ALA:HA	1:B:2046:TYR:HB3	2.01	0.42
1:A:97:ILE:O	1:A:101:ASN:N	2.45	0.42
1:A:852:GLU:O	1:A:856:HIS:N	2.43	0.42
1:A:1779:TRP:CZ2	1:A:1804:LEU:HG	2.54	0.42
1:A:1922:GLU:HB3	1:A:1925:LEU:HG	2.02	0.42
1:B:2044:LYS:HE2	1:B:2083:ILE:HG22	2.00	0.42
1:B:2089:ARG:NH2	1:B:2553:VAL:HG22	2.33	0.42
1:B:2103:GLU:HG3	1:B:2153:HIS:CE1	2.55	0.42
2:D:250:LYS:O	2:D:254:SER:N	2.47	0.42
1:A:1702:LEU:HD23	1:A:1724:ARG:NH1	2.35	0.42
1:A:2103:GLU:HG2	1:A:2106:LYS:HE3	2.01	0.42
1:A:2471:LEU:HD13	1:A:2471:LEU:HA	1.84	0.42
1:B:708:ALA:O	1:B:712:GLY:N	2.44	0.42
1:B:1531:HIS:HA	1:B:1534:VAL:HB	2.00	0.42
1:B:1533:LEU:HD12	1:B:1584:MET:HB3	2.01	0.42
1:B:1620:THR:O	1:B:1624:GLU:N	2.47	0.42
1:B:1650:ALA:HB1	1:B:1651:TYR:CD1	2.54	0.42
1:B:1753:ILE:HA	1:B:1756:VAL:HG23	2.01	0.42
1:B:2012:GLU:HG2	1:B:2015:ASN:ND2	2.32	0.42
1:B:2228:LYS:O	1:B:2230:VAL:N	2.52	0.42
1:A:671:CYS:O	1:A:675:PHE:N	2.40	0.42
1:A:888:ALA:HA	1:A:889:LEU:HA	1.85	0.42
1:A:1002:LEU:O	1:A:1006:ALA:N	2.51	0.42
1:A:1624:GLU:HA	1:A:1627:GLN:HB2	2.02	0.42
1:B:2074:ARG:NH2	1:B:2126:ILE:HG12	2.35	0.42
1:B:2553:VAL:O	1:B:2556:THR:OG1	2.33	0.42
1:A:1670:GLN:HE21	1:A:1695:ILE:HG22	1.85	0.42
1:A:2228:LYS:O	1:A:2230:VAL:N	2.53	0.42
1:B:2103:GLU:HA	1:B:2106:LYS:HB2	2.02	0.42
1:A:219:ILE:O	1:A:223:ARG:N	2.46	0.42
1:A:706:GLU:O	1:A:710:ILE:N	2.51	0.42
1:A:1947:ALA:C	1:A:1951:ARG:HE	2.27	0.42
1:A:2011:GLU:H	1:A:2011:GLU:HG3	1.67	0.42
1:B:322:LEU:O	1:B:326:CYS:N	2.47	0.42
1:B:1004:ALA:O	1:B:1008:PRO:N	2.53	0.42
1:B:1670:GLN:HA	1:B:1673:LEU:HB2	2.02	0.42
1:A:1387:VAL:O	1:A:1391:SER:N	2.48	0.42
1:A:1702:LEU:HD22	1:A:1725:ALA:HA	2.01	0.42
1:A:2304:ALA:O	1:A:2308:LYS:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2325:MET:HG2	1:A:2379:TRP:HB2	2.01	0.42
1:A:1533:LEU:HA	1:A:1536:VAL:HB	2.02	0.42
1:A:2102:TYR:HE1	1:A:2115:MET:HE3	1.84	0.42
1:B:1785:ASP:O	1:B:1789:ASN:ND2	2.52	0.42
1:B:1831:ILE:HG12	1:B:1854:LEU:HD11	2.01	0.42
1:B:2151:HIS:HB3	1:B:2153:HIS:HD2	1.84	0.42
1:B:2172:PRO:HG3	1:B:2208:LEU:HD13	2.01	0.42
1:B:2400:TYR:CD2	1:B:2430:PRO:HA	2.55	0.42
1:A:130:LEU:O	1:A:134:PHE:N	2.53	0.42
1:A:320:MET:O	1:A:324:LYS:N	2.42	0.42
1:A:338:LYS:O	1:A:342:LEU:N	2.43	0.42
1:A:1491:SER:O	1:A:1495:ALA:N	2.45	0.42
1:A:2436:PHE:CE2	1:A:2518:ASN:HB3	2.55	0.42
1:B:876:ILE:O	1:B:880:ALA:N	2.45	0.42
2:C:189:GLN:O	2:C:193:GLN:N	2.48	0.42
2:C:198:GLU:O	2:C:202:LEU:N	2.51	0.42
2:D:79:ARG:HA	2:D:80:ASP:HA	1.84	0.42
1:A:162:ARG:O	1:A:166:GLY:N	2.50	0.41
1:A:566:VAL:O	1:A:570:TYR:N	2.47	0.41
1:A:1000:PRO:O	1:A:1004:ALA:N	2.47	0.41
1:A:2221:LYS:NZ	1:A:2251:GLU:O	2.38	0.41
1:A:2327:LYS:HD3	1:A:2328:PRO:HD2	2.01	0.41
1:B:1430:CYS:O	1:B:1434:GLU:N	2.52	0.41
1:B:1725:ALA:O	1:B:1729:GLU:N	2.52	0.41
1:A:1919:MET:HB3	1:A:1920:VAL:H	1.68	0.41
1:A:2458:CYS:O	1:A:2461:THR:N	2.53	0.41
1:A:2514:ARG:HD3	1:A:2640:TRP:CZ2	2.55	0.41
1:B:2599:LEU:HA	1:B:2599:LEU:HD23	1.80	0.41
1:A:1061:GLU:O	1:A:1065:GLY:N	2.47	0.41
1:A:2201:ALA:O	1:A:2205:LYS:HG3	2.20	0.41
1:A:2315:LYS:HA	1:A:2321:PHE:HA	2.02	0.41
1:A:2360:LEU:HD13	1:A:2463:VAL:HG21	2.01	0.41
1:B:522:HIS:O	1:B:526:LYS:N	2.53	0.41
1:B:2023:LYS:HA	1:B:2026:LYS:HB2	2.01	0.41
1:A:450:GLU:O	1:A:454:VAL:N	2.51	0.41
1:A:2388:PRO:O	1:A:2391:THR:OG1	2.25	0.41
1:B:727:SER:O	1:B:731:PRO:N	2.53	0.41
1:B:2136:TYR:OH	1:B:2282:SER:O	2.36	0.41
2:C:87:VAL:O	2:C:91:LEU:N	2.53	0.41
1:A:2350:ARG:HG2	1:A:2356:ARG:HH21	1.84	0.41
1:B:1437:GLY:O	1:B:1439:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2071:HIS:O	1:B:2075:SER:N	2.39	0.41
1:B:2112:ARG:HD3	1:B:2116:ARG:CZ	2.50	0.41
1:B:2416:ALA:HB3	1:B:2419:GLU:HG3	2.02	0.41
1:A:909:THR:HA	1:A:910:GLU:HA	1.78	0.41
1:A:1526:ILE:HA	1:A:1529:LEU:HD12	2.03	0.41
1:A:2099:THR:HA	1:A:2102:TYR:HD2	1.85	0.41
1:B:756:SER:O	1:B:760:ALA:N	2.45	0.41
1:B:1618:VAL:O	1:B:1622:ASP:N	2.47	0.41
1:B:1650:ALA:HB1	1:B:1651:TYR:CG	2.55	0.41
2:C:127:LYS:O	2:C:131:MET:N	2.46	0.41
2:C:305:SER:O	2:C:309:GLY:N	2.47	0.41
2:D:67:ALA:O	2:D:71:LEU:N	2.45	0.41
1:A:1973:LEU:HG	1:A:1974:ILE:HG13	2.02	0.41
1:A:2313:SER:HB2	1:A:2323:ILE:HG13	2.02	0.41
1:A:2433:PRO:HB3	1:A:2517:HIS:HD2	1.85	0.41
1:A:2467:VAL:HG22	1:A:2543:MET:HE3	2.03	0.41
1:B:759:LYS:O	1:B:763:CYS:N	2.48	0.41
1:B:2463:VAL:HG22	1:B:2539:THR:HG22	2.02	0.41
1:B:2612:LEU:HD23	1:B:2612:LEU:HA	1.91	0.41
2:C:309:GLY:O	2:C:313:ILE:N	2.46	0.41
2:D:187:SER:O	2:D:190:SER:N	2.48	0.41
1:A:1513:CYS:O	1:A:1517:MET:N	2.54	0.41
1:A:1523:LYS:HA	1:A:1526:ILE:HD12	2.02	0.41
1:A:1615:ASP:O	1:A:1619:SER:N	2.49	0.41
1:A:1750:SER:HA	1:A:1753:ILE:HD12	2.02	0.41
1:A:2369:PRO:HA	1:A:2375:GLY:HA3	2.01	0.41
1:A:2470:ILE:HG21	1:A:2599:LEU:HD21	2.03	0.41
1:A:2558:LEU:HD23	1:A:2558:LEU:HA	1.89	0.41
1:B:254:GLU:O	1:B:258:LEU:N	2.52	0.41
1:B:1410:ASN:O	1:B:1414:GLN:N	2.53	0.41
1:A:371:TYR:O	1:A:375:ILE:N	2.47	0.41
1:A:713:GLN:O	1:A:717:THR:N	2.54	0.41
1:A:2020:ALA:HB3	1:A:2025:TYR:CZ	2.56	0.41
1:A:2142:PHE:HA	1:A:2145:LEU:HD12	2.02	0.41
1:A:2422:LYS:O	1:A:2426:GLU:N	2.33	0.41
1:A:2498:LEU:HD23	1:A:2498:LEU:HA	1.89	0.41
1:B:84:VAL:O	1:B:88:GLY:N	2.52	0.41
1:B:704:LYS:O	1:B:708:ALA:N	2.50	0.41
1:B:859:ILE:O	1:B:863:ASN:N	2.52	0.41
1:B:1126:LYS:O	1:B:1130:ILE:N	2.48	0.41
1:B:1677:GLN:O	1:B:1681:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1750:SER:HA	1:B:1753:ILE:HD12	2.01	0.41
1:B:2103:GLU:HG2	1:B:2106:LYS:HD2	2.03	0.41
1:B:2135:PRO:HA	1:B:2138:PHE:HD2	1.85	0.41
1:B:2231:ASP:OD1	1:B:2248:LYS:NZ	2.53	0.41
1:B:2312:ILE:O	1:B:2324:MET:N	2.51	0.41
1:B:2386:LEU:HD11	1:B:2436:PHE:CZ	2.55	0.41
1:B:2588:ALA:O	1:B:2592:VAL:N	2.36	0.41
1:B:2625:GLN:O	1:B:2629:ASP:N	2.54	0.41
1:A:1582:PHE:O	1:A:1586:ASP:N	2.49	0.41
1:A:2465:SER:O	1:A:2469:TYR:N	2.48	0.41
1:B:687:ARG:O	1:B:691:ILE:N	2.44	0.41
1:B:1933:LYS:HA	1:B:1936:HIS:HB2	2.03	0.41
1:B:2008:ARG:HD2	1:B:2032:LEU:HD21	2.03	0.41
1:B:2035:TRP:HB3	1:B:2036:GLU:HG3	2.03	0.41
1:B:2360:LEU:HB3	1:B:2459:ARG:HB3	2.03	0.41
1:A:2039:HIS:HB3	1:A:2041:TYR:CE2	2.56	0.40
1:B:101:ASN:O	1:B:105:THR:N	2.52	0.40
1:B:135:LYS:O	1:B:139:PRO:N	2.54	0.40
1:B:730:GLU:O	1:B:734:GLU:N	2.47	0.40
1:B:1530:PRO:HB3	1:B:1587:HIS:CG	2.56	0.40
1:B:2205:LYS:O	1:B:2208:LEU:N	2.53	0.40
1:B:2369:PRO:HA	1:B:2375:GLY:HA3	2.03	0.40
1:B:2462:ALA:HA	1:B:2465:SER:HB2	2.03	0.40
1:A:565:LYS:O	1:A:569:ILE:N	2.49	0.40
1:A:681:GLN:O	1:A:685:CYS:N	2.54	0.40
1:A:1141:SER:O	1:A:1145:ILE:N	2.54	0.40
1:A:1475:LYS:O	1:A:1479:TYR:N	2.49	0.40
1:A:1814:ARG:H	1:A:1814:ARG:HD2	1.86	0.40
1:A:1901:LEU:HD11	1:A:1938:GLN:HG2	2.04	0.40
1:A:2059:GLU:HA	1:A:2060:LYS:HA	1.82	0.40
1:A:2346:ASN:HA	1:A:2349:LEU:HB2	2.03	0.40
1:A:2630:GLU:HA	1:A:2633:LEU:HB3	2.04	0.40
1:B:198:SER:O	1:B:202:LEU:N	2.50	0.40
1:B:215:ARG:O	1:B:219:ILE:N	2.41	0.40
1:B:2157:PHE:O	1:B:2161:MET:HG2	2.20	0.40
2:D:51:ALA:O	2:D:54:ASP:N	2.54	0.40
1:A:402:MET:O	1:A:406:GLU:N	2.49	0.40
1:A:407:ILE:O	1:A:411:ILE:N	2.44	0.40
1:A:1487:PHE:O	1:A:1491:SER:N	2.46	0.40
1:A:1622:ASP:O	1:A:1626:TYR:N	2.41	0.40
1:B:313:ILE:O	1:B:317:TYR:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ILE:O	1:B:497:LEU:N	2.53	0.40
1:B:711:LEU:O	1:B:715:VAL:N	2.44	0.40
1:B:1726:ILE:H	1:B:1726:ILE:HG13	1.73	0.40
1:B:1952:LEU:HD13	1:B:1952:LEU:HA	1.90	0.40
1:B:2120:GLY:HA2	1:B:2123:ASN:HB2	2.04	0.40
1:B:2501:LYS:O	1:B:2505:PHE:N	2.55	0.40
2:D:109:LYS:O	2:D:113:GLU:N	2.49	0.40
2:D:132:GLU:O	2:D:136:LEU:N	2.54	0.40
1:A:61:SER:O	1:A:65:SER:N	2.50	0.40
1:A:127:ILE:O	1:A:131:LEU:N	2.53	0.40
1:A:920:VAL:O	1:A:924:SER:N	2.51	0.40
1:A:2088:PRO:HA	1:A:2091:LEU:HD12	2.03	0.40
1:A:2102:TYR:CE1	1:A:2115:MET:HB3	2.57	0.40
1:A:2278:ALA:HA	1:A:2279:ASN:HA	1.60	0.40
1:A:2435:ILE:O	1:A:2439:TRP:N	2.34	0.40
1:A:2484:ASP:HB2	1:A:2488:GLY:N	2.37	0.40
1:B:79:SER:O	1:B:83:PHE:N	2.55	0.40
1:B:1478:ILE:HA	1:B:1482:LYS:H	1.85	0.40
1:B:1744:LEU:C	1:B:1747:GLY:H	2.29	0.40
1:B:1919:MET:HB3	1:B:1920:VAL:H	1.67	0.40
1:B:1925:LEU:HA	1:B:1957:VAL:HG11	2.02	0.40
2:C:68:SER:O	2:C:72:SER:N	2.49	0.40
2:D:16:PRO:O	2:D:20:PRO:N	2.54	0.40
1:A:406:GLU:O	1:A:410:GLU:N	2.51	0.40
1:A:1426:SER:O	1:A:1430:CYS:N	2.53	0.40
1:A:1841:ARG:H	1:A:1841:ARG:HG2	1.65	0.40
1:A:2160:LEU:HA	1:A:2163:ILE:HD12	2.03	0.40
1:A:2244:LYS:HB3	1:A:2246:LEU:H	1.87	0.40
1:A:2340:GLU:O	1:A:2343:SER:OG	2.33	0.40
1:B:262:PRO:O	1:B:266:ALA:N	2.49	0.40
1:B:1637:PRO:HA	1:B:1638:GLN:HA	1.89	0.40
1:B:2100:LYS:HE3	1:B:2151:HIS:CE1	2.56	0.40
1:B:2327:LYS:HD3	1:B:2328:PRO:HD2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2344/2644 (89%)	1962 (84%)	350 (15%)	32 (1%)	9	39
1	B	2344/2644 (89%)	1953 (83%)	358 (15%)	33 (1%)	9	39
2	C	360/791 (46%)	284 (79%)	63 (18%)	13 (4%)	2	20
2	D	316/791 (40%)	240 (76%)	64 (20%)	12 (4%)	2	19
All	All	5364/6870 (78%)	4439 (83%)	835 (16%)	90 (2%)	9	35

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	192	ALA
1	A	193	PRO
1	A	357	VAL
1	A	444	ALA
1	A	445	PRO
1	A	597	PRO
1	A	765	PRO
1	A	932	PRO
1	A	949	LEU
1	A	950	PRO
1	A	1189	PRO
1	A	1438	PRO
1	B	192	ALA
1	B	193	PRO
1	B	358	PRO
1	B	444	ALA
1	B	445	PRO
1	B	597	PRO
1	B	764	LYS
1	B	765	PRO
1	B	932	PRO

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Mol	Chain	Res	Type
1	B	1189	PRO
2	C	107	PRO
2	C	260	PRO
2	C	323	PRO
2	C	348	PRO
2	D	7	PRO
2	D	43	PRO
2	D	107	PRO
2	D	123	GLU
2	D	234	LYS
2	D	260	PRO
2	D	262	PRO
2	D	320	PRO
1	A	1847	GLY
1	A	2604	LYS
1	B	1847	GLY
2	C	262	PRO
2	D	167	GLU
1	A	1149	LYS
1	A	1942	ASN
1	B	155	ASP
1	B	261	LEU
1	B	262	PRO
1	B	950	PRO
1	B	1438	PRO
2	C	29	PRO
2	C	106	VAL
1	A	155	ASP
1	A	261	LEU
1	A	334	LEU
1	A	764	LYS
1	A	1446	PHE
1	B	44	ILE
1	B	387	VAL
1	B	1148	LYS
1	B	1942	ASN
2	C	235	PRO
2	C	259	LEU
1	A	1148	LYS
1	B	144	VAL
2	C	346	GLN
2	C	347	PRO

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Mol	Chain	Res	Type
1	B	1186	ASP
1	B	1666	LYS
1	B	1700	PRO
1	A	387	VAL
1	A	1036	ILE
1	A	1167	VAL
1	B	775	PRO
1	B	1167	VAL
1	B	2583	VAL
2	C	319	GLN
2	D	47	ASP
2	D	259	LEU
1	A	358	PRO
1	A	385	ILE
1	B	357	VAL
1	A	123	ILE
1	A	304	PRO
1	A	1733	ILE
1	B	48	VAL
1	B	1733	ILE
1	B	2430	PRO
2	D	228	ASN
1	A	2447	PRO
2	C	340	PRO
1	B	23	PRO
1	B	1477	PRO

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	924/2363 (39%)	915 (99%)	9 (1%)	68	76
1	B	924/2363 (39%)	915 (99%)	9 (1%)	68	76
All	All	1848/4726 (39%)	1830 (99%)	18 (1%)	65	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1641	LEU
1	A	1673	LEU
1	A	2314	LEU
1	A	2329	LYS
1	A	2430	PRO
1	A	2473	LEU
1	A	2523	MET
1	A	2584	VAL
1	A	2633	LEU
1	B	1746	LEU
1	B	1781	LEU
1	B	1826	VAL
1	B	1901	LEU
1	B	2329	LYS
1	B	2360	LEU
1	B	2493	VAL
1	B	2523	MET
1	B	2584	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1531	HIS
1	A	1545	GLN
1	A	1670	GLN
1	A	1748	GLN
1	A	1755	GLN
1	A	1757	ASN
1	A	1760	HIS
1	A	1845	GLN
1	A	1942	ASN
1	A	1971	GLN
1	A	1987	ASN
1	A	2019	ASN
1	A	2117	ASN
1	A	2123	ASN
1	A	2144	GLN
1	A	2174	GLN
1	A	2199	ASN
1	A	2480	ASN
1	A	2496	ASN
1	A	2585	ASN
1	A	2591	HIS

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Mol	Chain	Res	Type
1	A	2597	GLN
1	A	2635	GLN
1	B	1587	HIS
1	B	1672	HIS
1	B	1737	HIS
1	B	1748	GLN
1	B	1789	ASN
1	B	1936	HIS
1	B	1937	HIS
1	B	1938	GLN
1	B	1942	ASN
1	B	2015	ASN
1	B	2039	HIS
1	B	2077	GLN
1	B	2085	GLN
1	B	2117	ASN
1	B	2123	ASN
1	B	2144	GLN
1	B	2153	HIS
1	B	2280	HIS
1	B	2480	ASN
1	B	2521	ASN
1	B	2591	HIS
1	B	2635	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

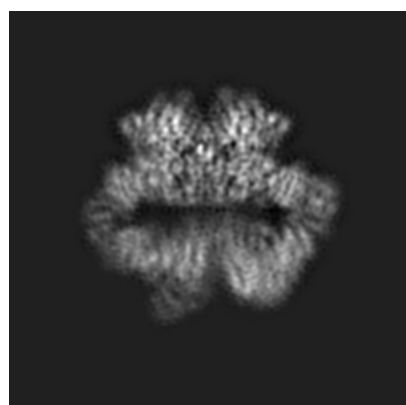
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6862. These allow visual inspection of the internal detail of the map and identification of artifacts.

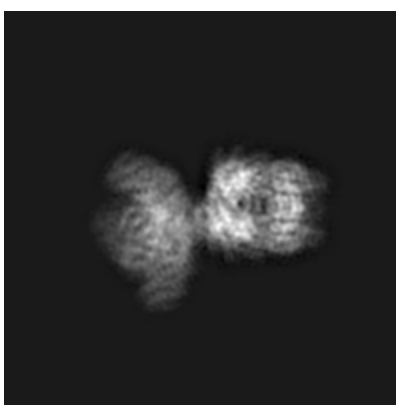
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

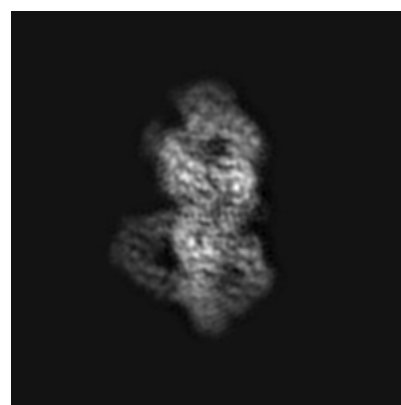
6.1.1 Primary map



X



Y

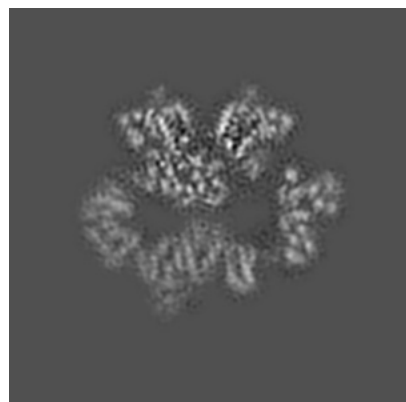


Z

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

6.2 Central slices [i](#)

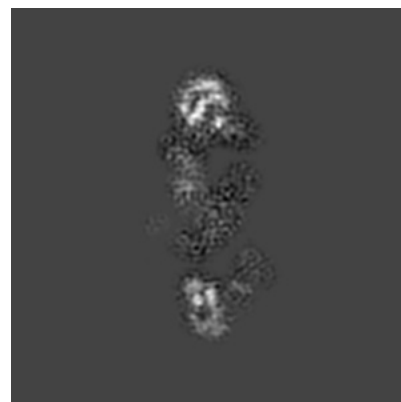
6.2.1 Primary map



X Index: 120



Y Index: 120

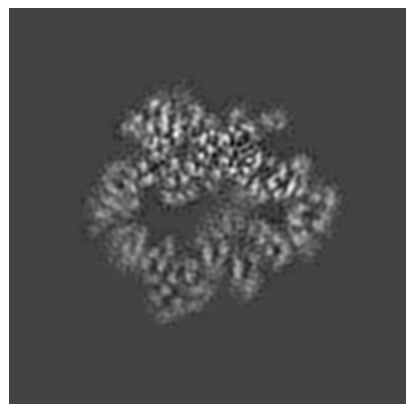


Z Index: 120

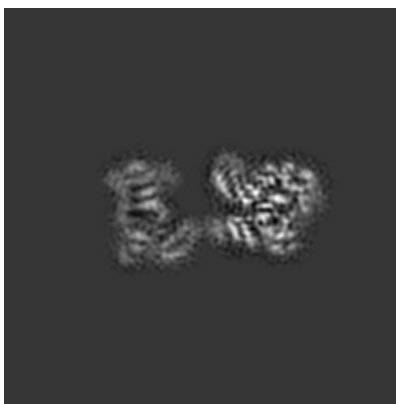
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

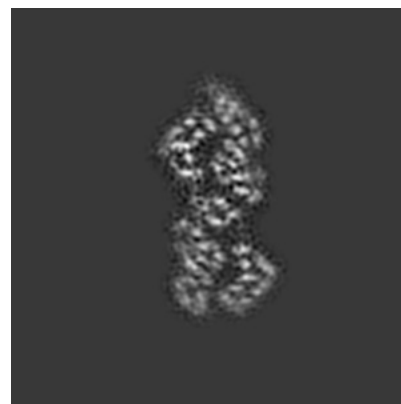
6.3.1 Primary map



X Index: 110



Y Index: 140

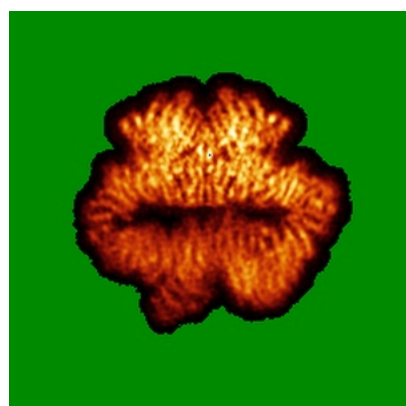


Z Index: 138

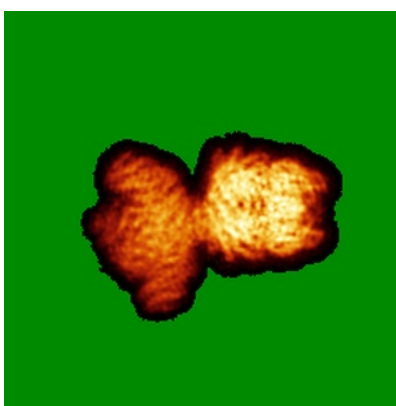
The images above show the largest variance slices of the map in three orthogonal directions.

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

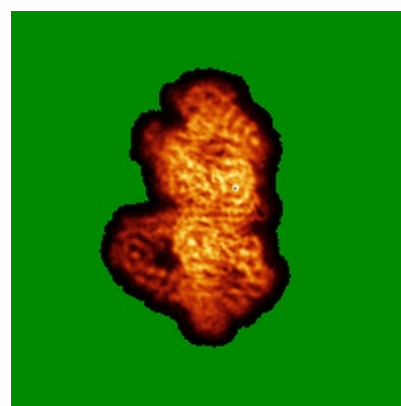
6.4.1 Primary map



X



Y

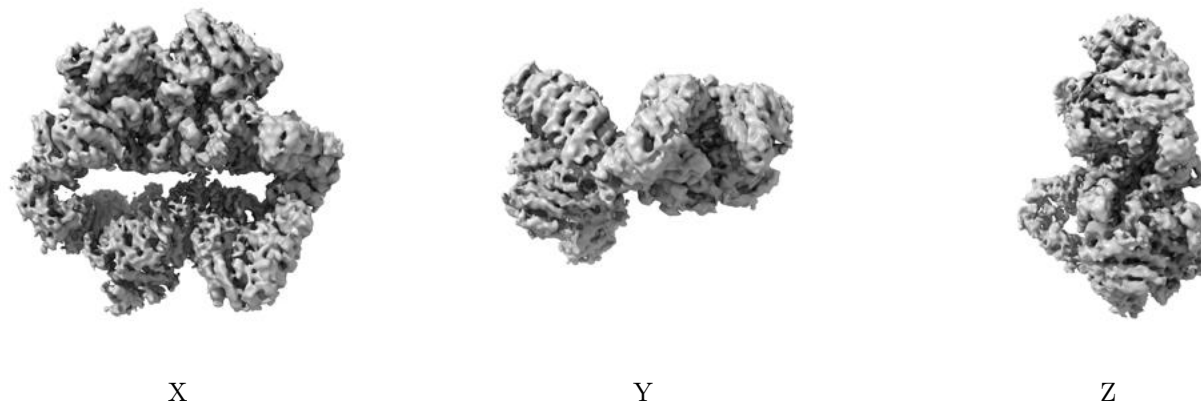


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

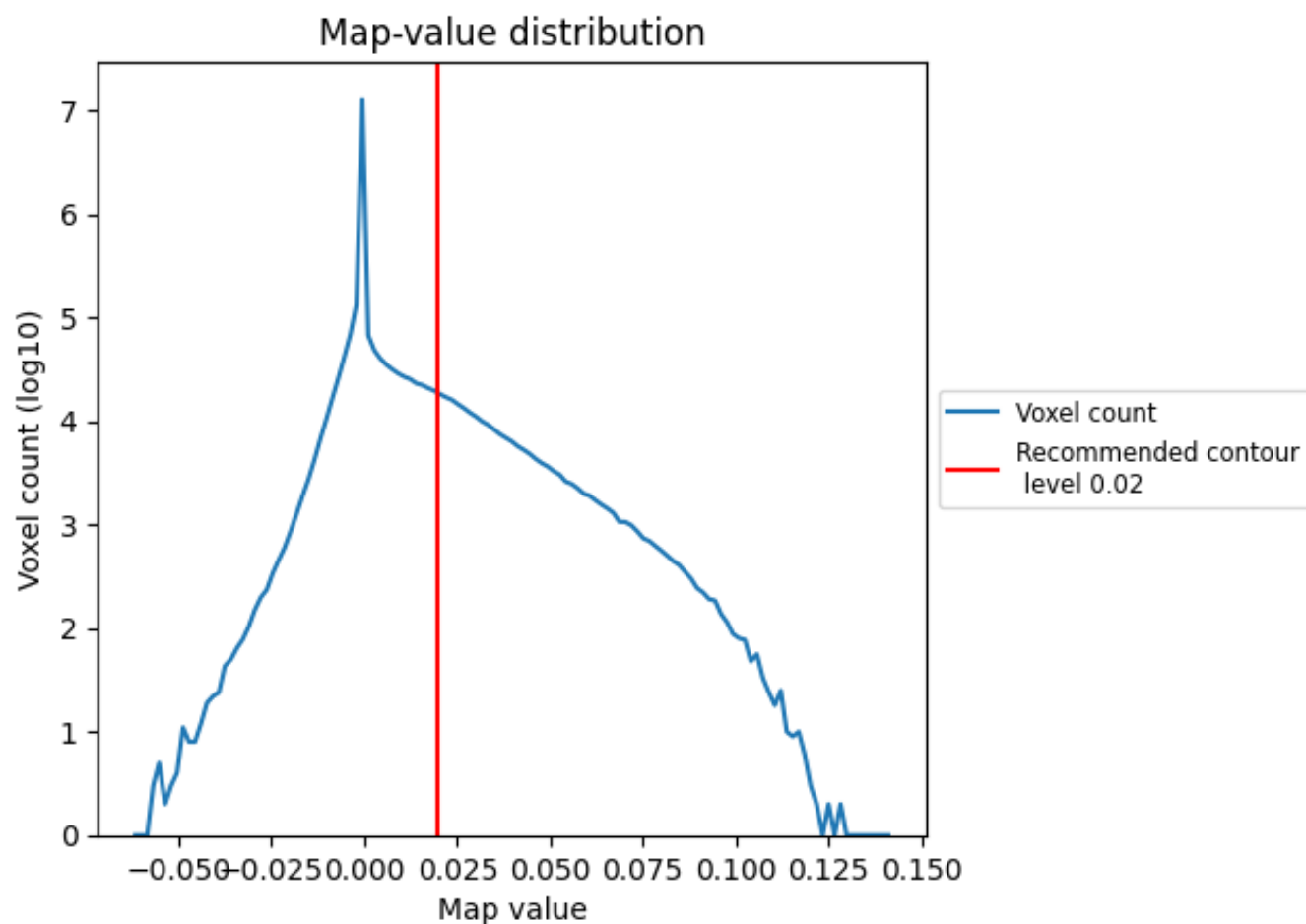
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

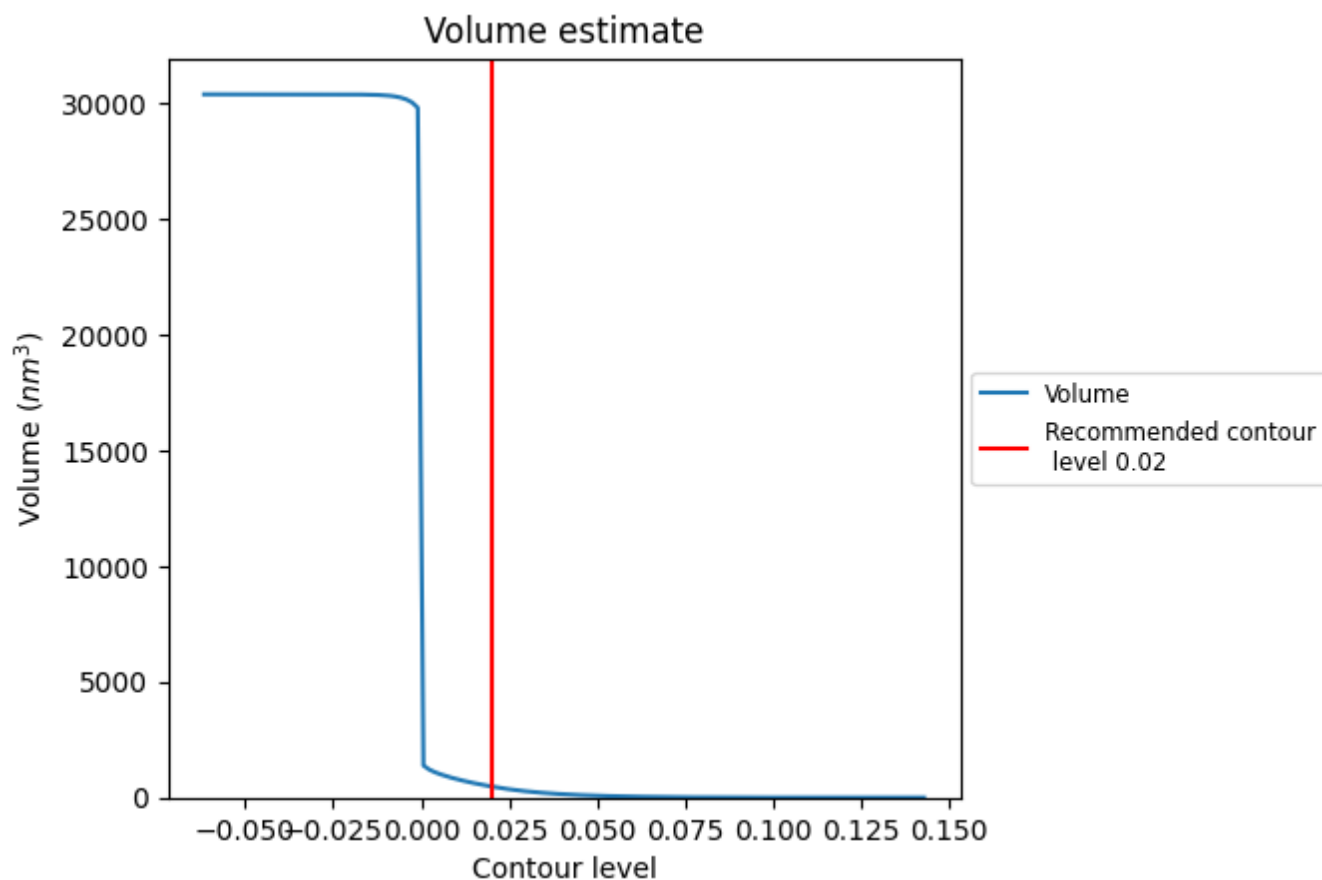
This section contains the results of statistical analysis of the map.

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.

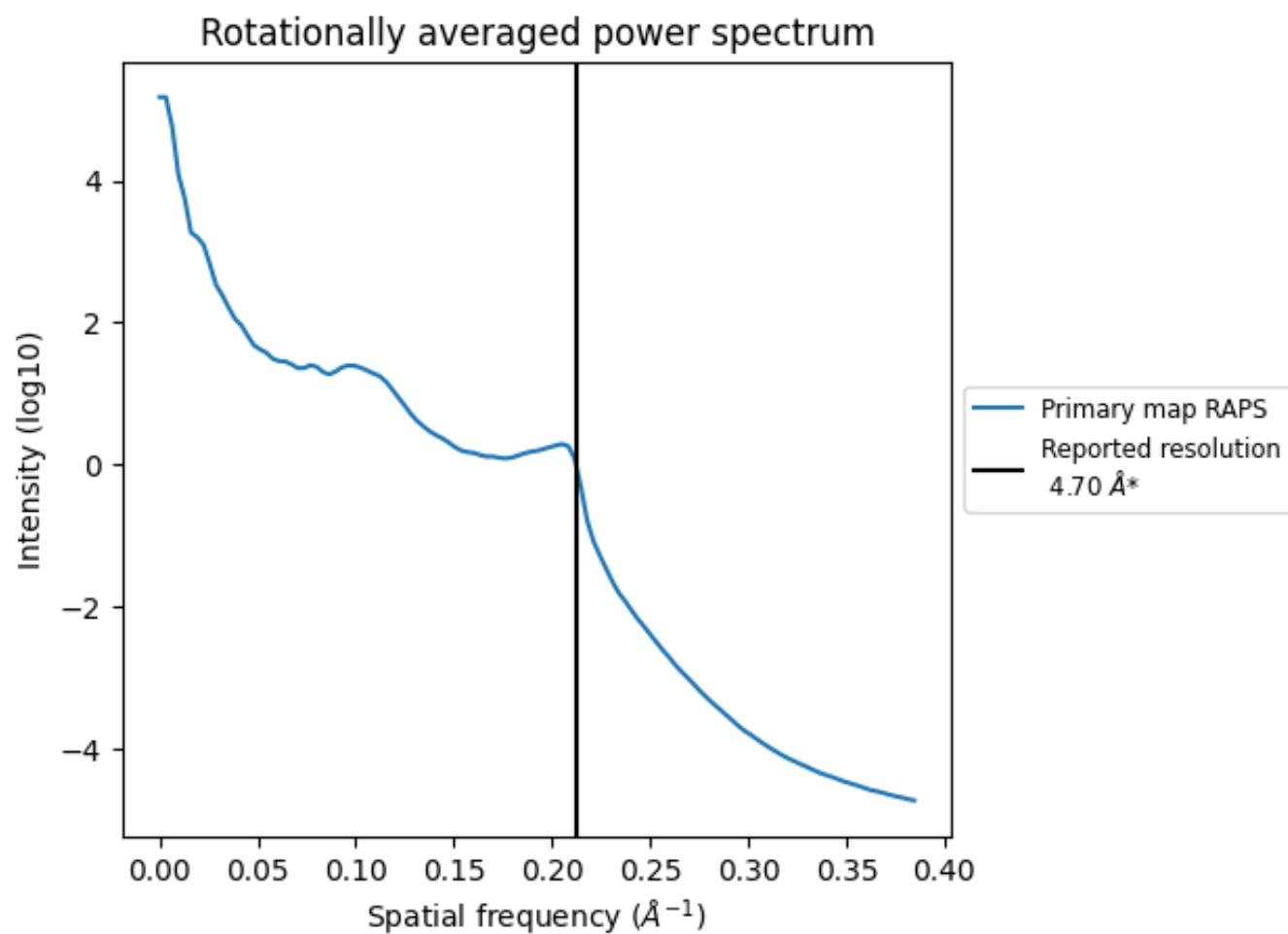
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 477 nm^3 ; this corresponds to an approximate mass of 431 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 ⓘ

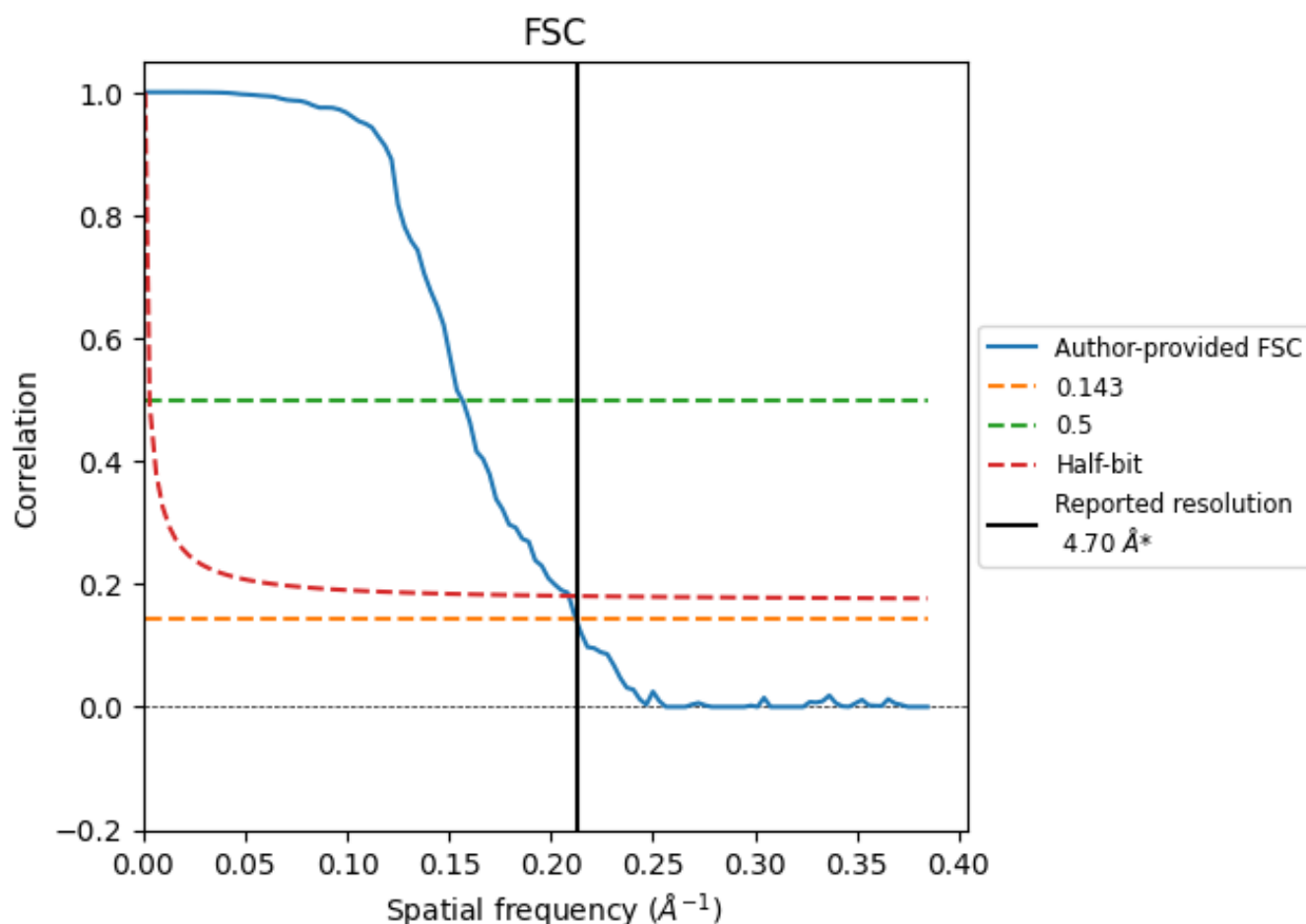


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

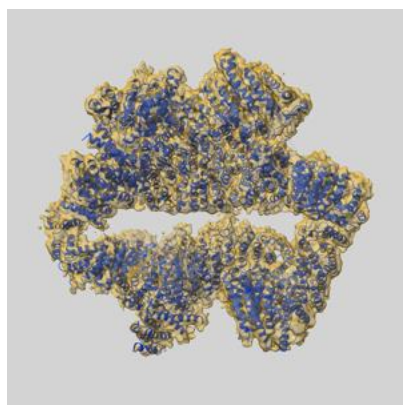
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.71	6.40	4.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

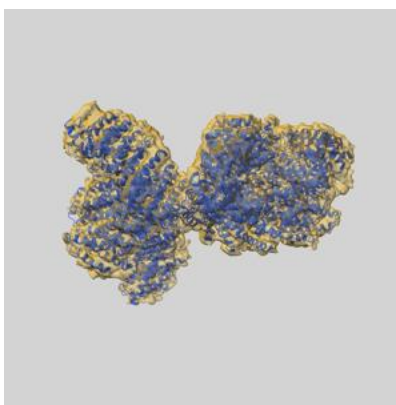
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6862 and PDB model 5YZ0. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

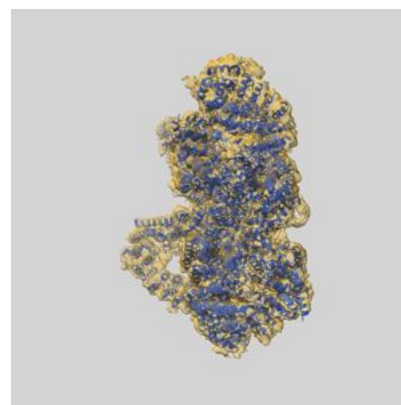
9.1 Map-model overlay [i](#)



X



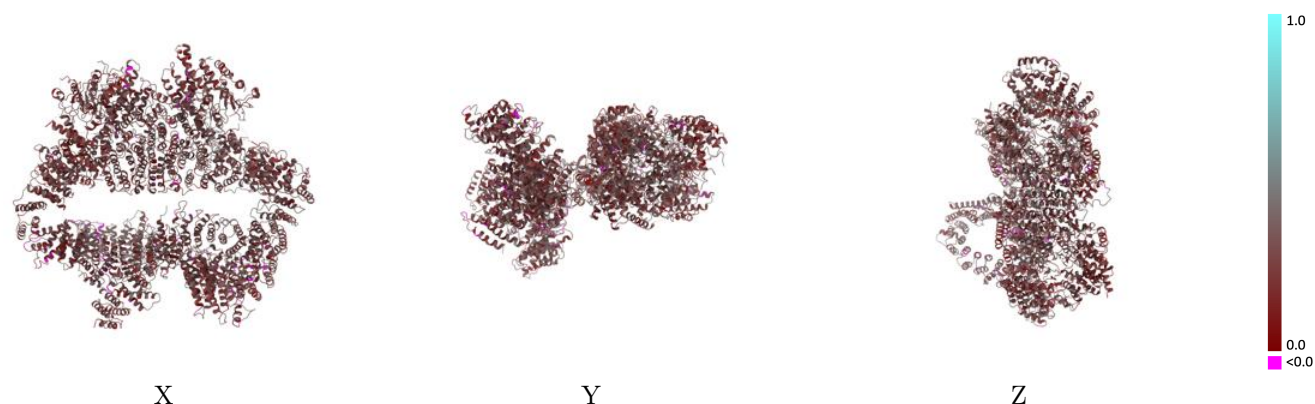
Y



Z

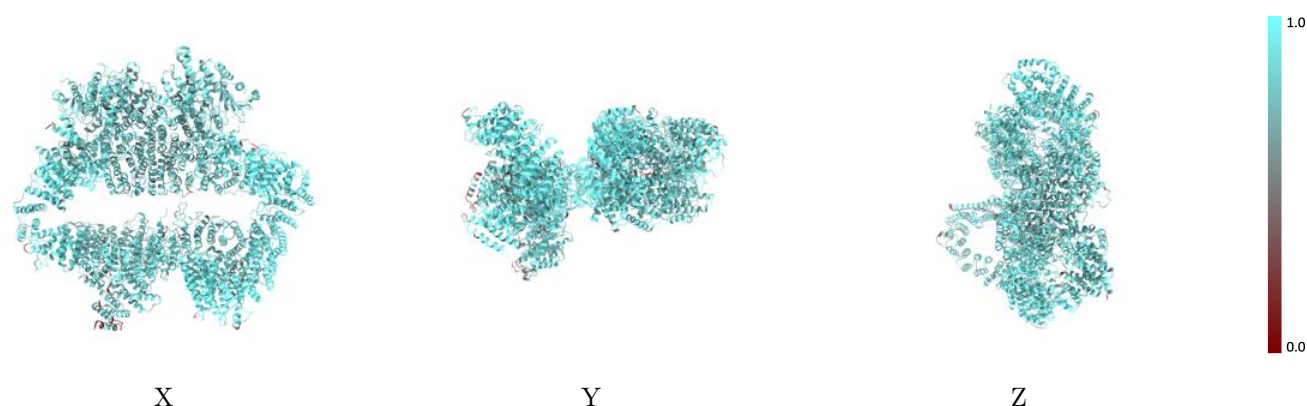
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



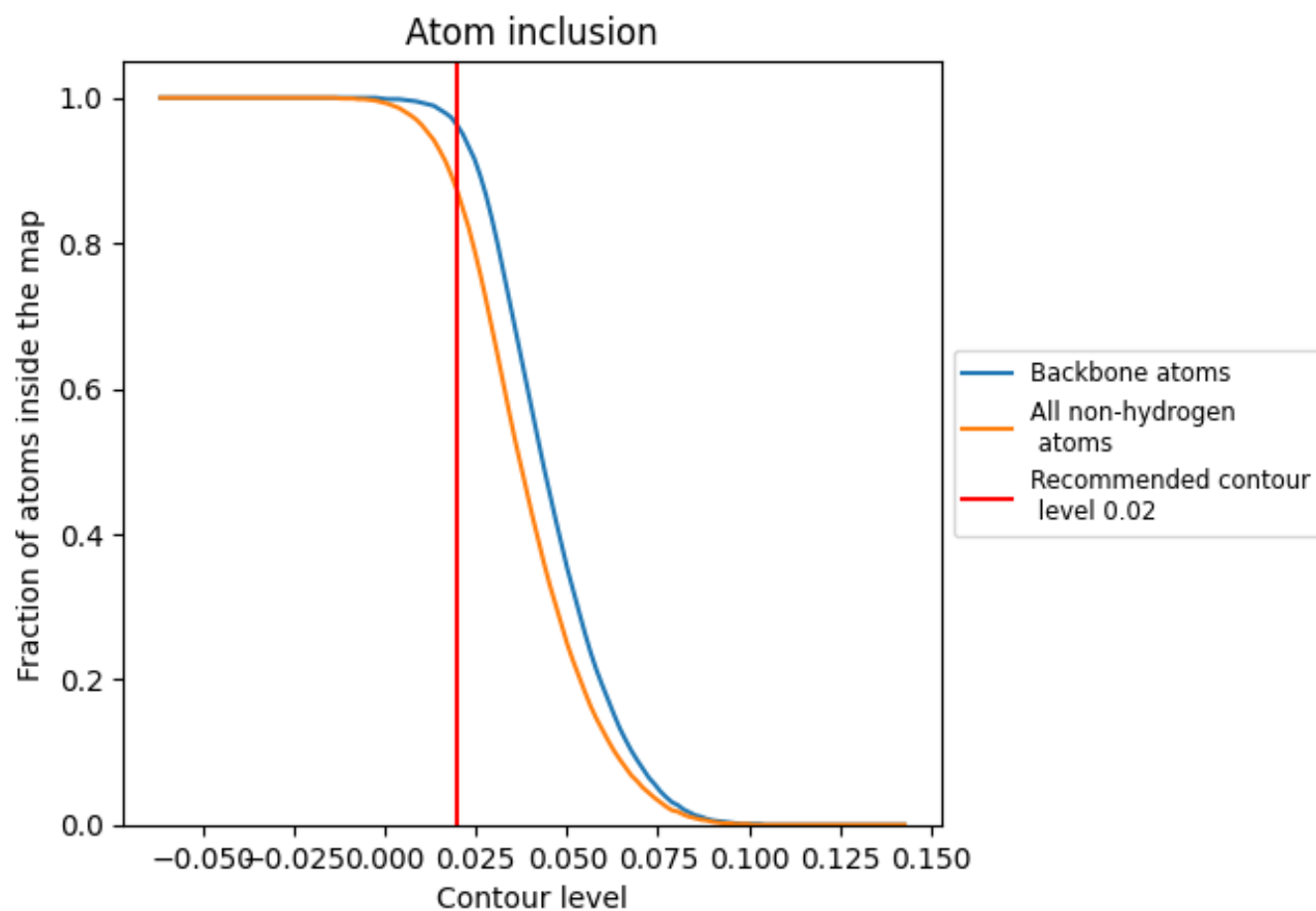
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8700	0.2810
A	0.8570	0.2760
B	0.8900	0.2880
C	0.8500	0.2820
D	0.8220	0.2630

