



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 12:31 AM UTC

PDB ID : 6MWX / pdb_00006mwx
EMDB ID : EMD-9279
Title : CryoEM structure of Chimeric Eastern Equine Encephalitis Virus with Fab of
EEEV-69 Antibody
Authors : Hasan, S.S.; Sun, C.; Kim, A.S.; Watanabe, Y.; Chen, C.L.; Klose, T.; Buda,
G.; Crispin, M.; Diamond, M.S.; Klimstra, W.B.; Rossmann, M.G.
Deposited on : 2018-10-30
Resolution : 8.20 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:

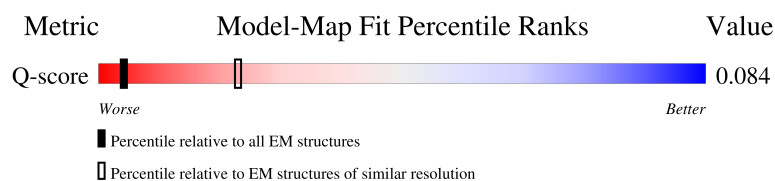
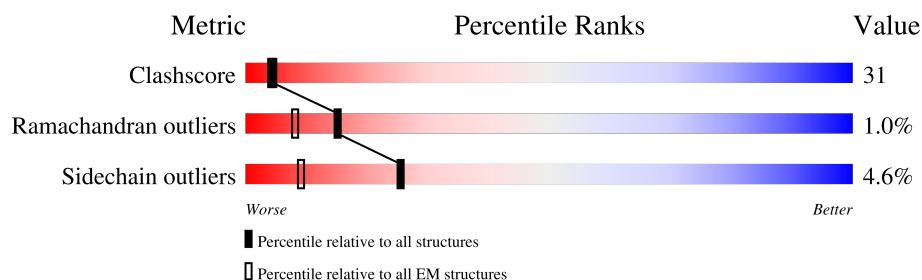
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (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 8.20 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.



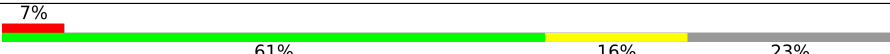
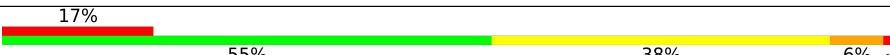
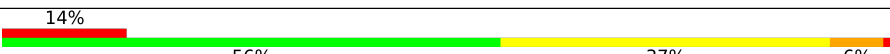
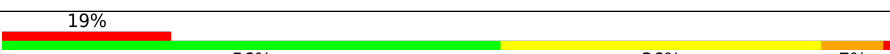
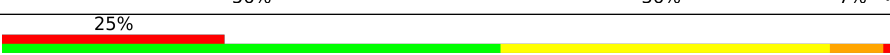
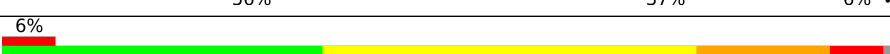
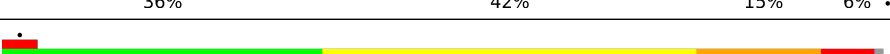
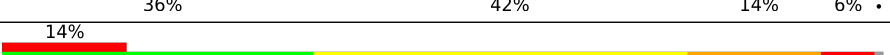
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	337 (7.70 - 8.70)

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	441	
1	E	441	
1	I	441	
1	M	441	

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Mol	Chain	Length	Quality of chain
2	B	420	
2	F	420	
2	J	420	
2	N	420	
3	C	218	
3	G	218	
3	K	218	
3	O	218	
4	D	214	
4	H	214	
4	L	214	
4	P	214	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35528 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 E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	E	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	I	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		
1	M	400	Total	C	N	O	S	0	0
			3063	1940	511	592	20		

- Molecule 2 is a protein called E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	325	Total	C	N	O	S	0	0
			2550	1601	471	462	16		
2	F	325	Total	C	N	O	S	0	0
			2550	1601	471	462	16		
2	J	325	Total	C	N	O	S	0	0
			2550	1601	471	462	16		
2	N	325	Total	C	N	O	S	0	0
			2550	1601	471	462	16		

- Molecule 3 is a protein called EEEV-69 antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	G	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	K	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		
3	O	218	Total	C	N	O	S	0	0
			1671	1066	272	326	7		

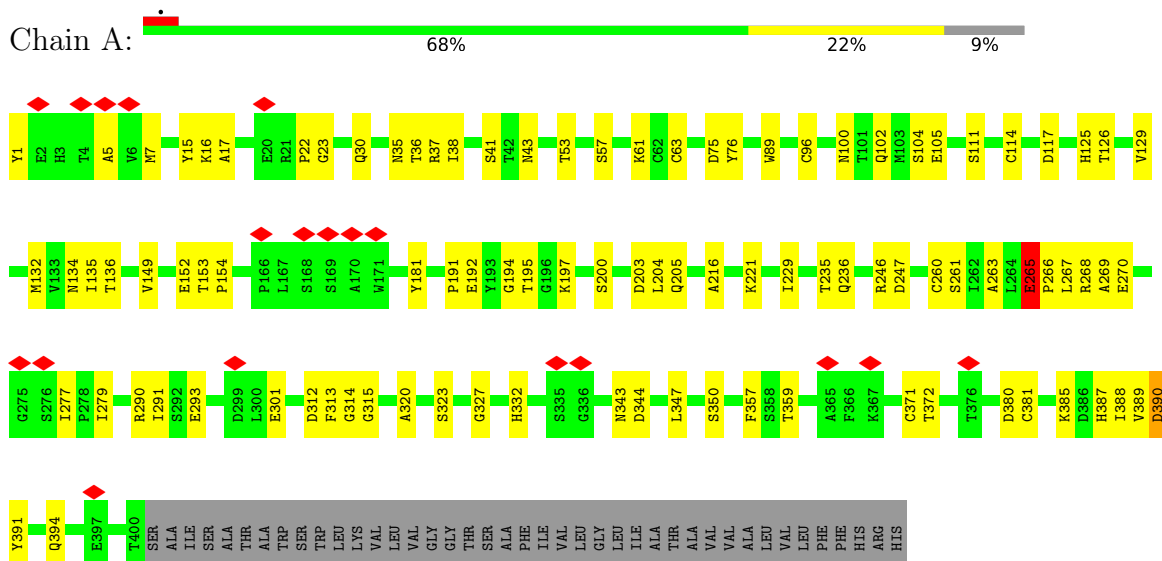
- Molecule 4 is a protein called EEEV-69 antibody light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	211	Total 1598	C 999	N 270	O 322	S 7	0	0
4	H	211	Total 1598	C 999	N 270	O 322	S 7	0	0
4	L	211	Total 1598	C 999	N 270	O 322	S 7	0	0
4	P	211	Total 1598	C 999	N 270	O 322	S 7	0	0

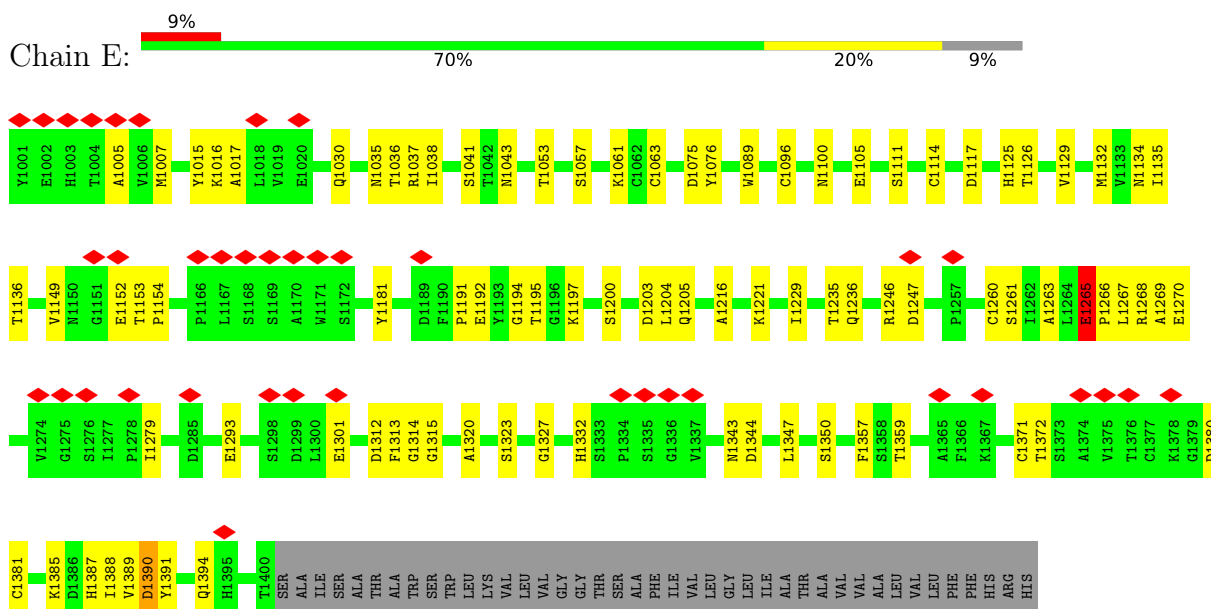
3 Residue-property plots

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

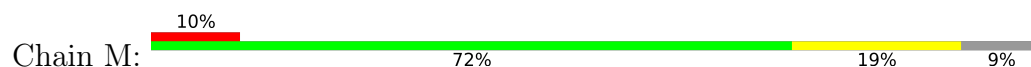
• Molecule 1: E1



• Molecule 1: E1

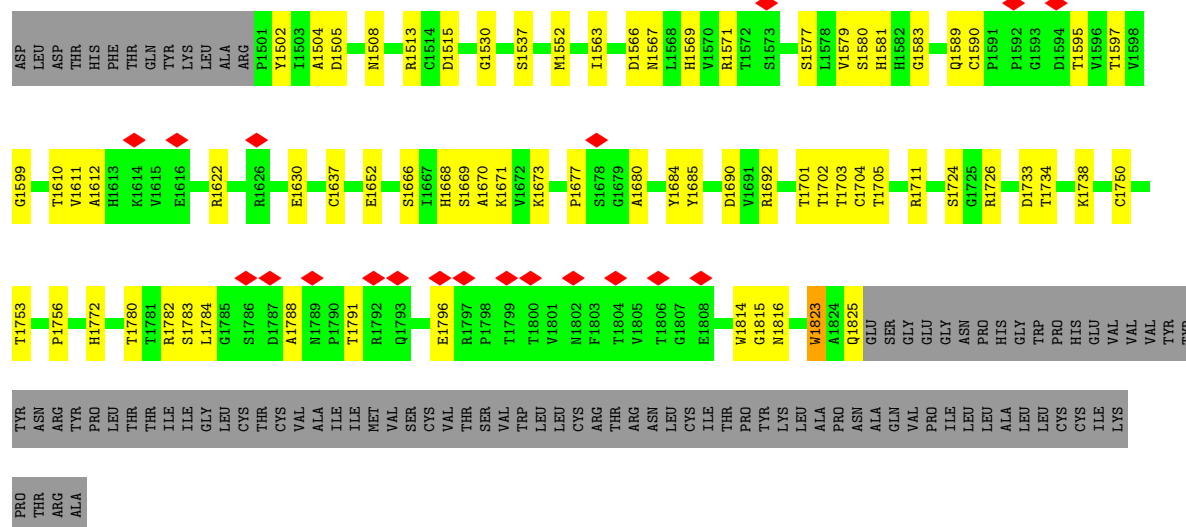


Chain I: 5% 71% 19% 9%

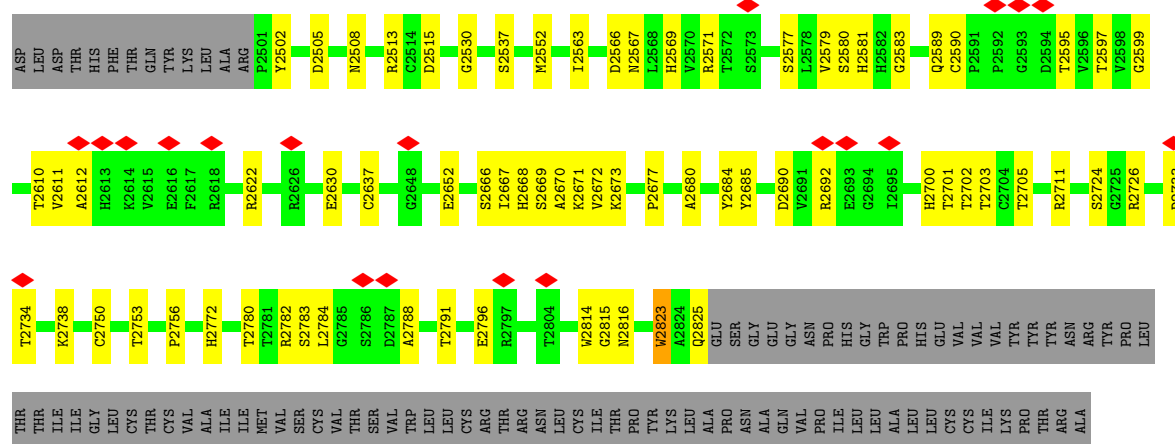


VAL SER CYS VAL THR SER VAL TRP LEU LEU CYS VAL ARG THR ARG ASN LEU CYS ILE THR PRO TYR LEU LEU ALA PRO ASN ALA GLN VAL PRO ILE LEU ALA LEU LEU CYS CYS ILE LEU PRO THR ARG ALA

• Molecule 2: E2

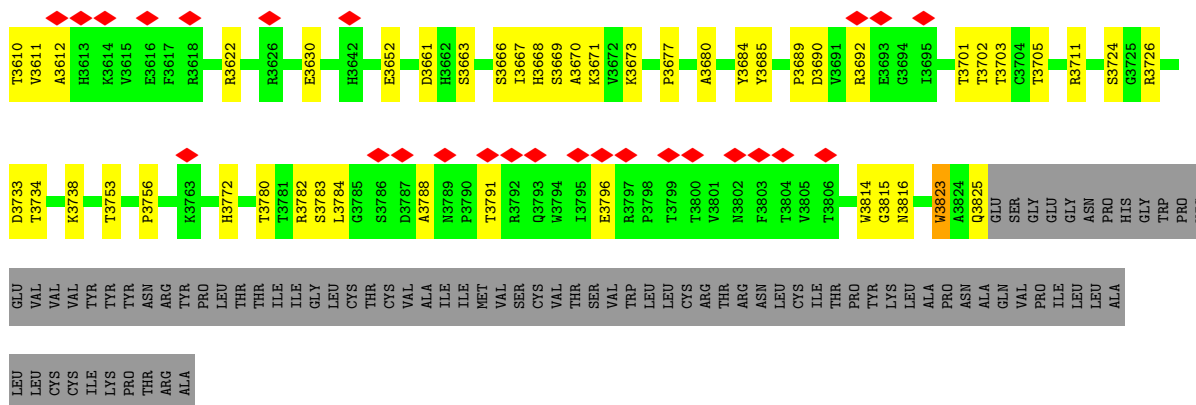


• Molecule 2: E2

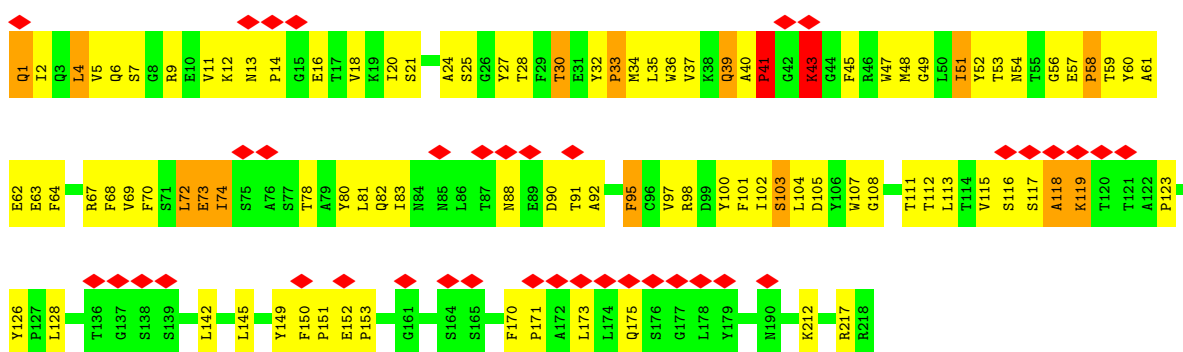


• Molecule 2: E2

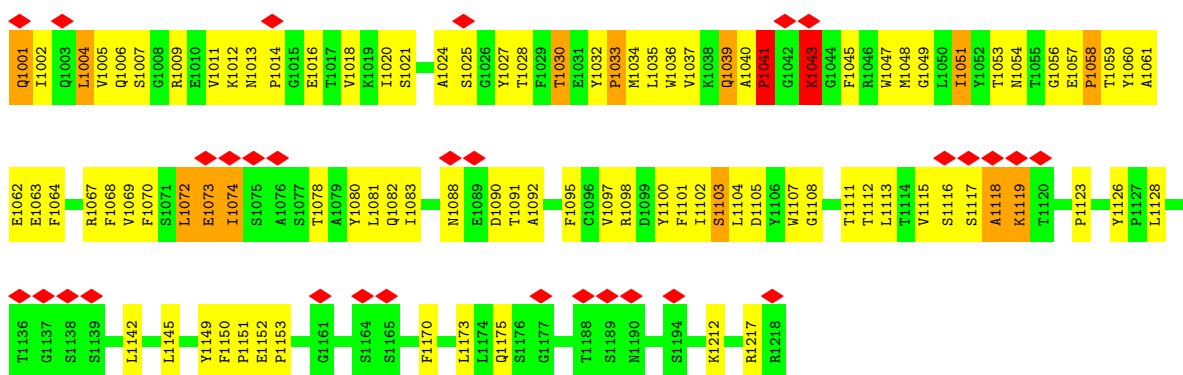




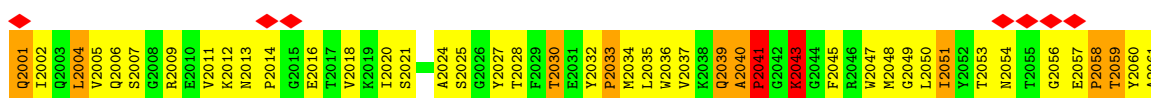
• Molecule 3: EEEV-69 antibody heavy chain

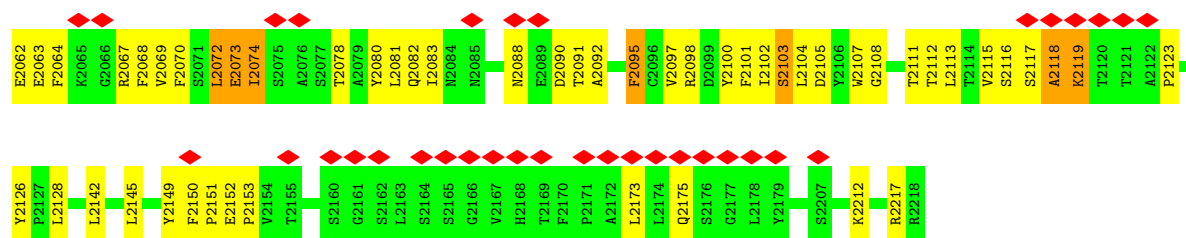


• Molecule 3: EEEV-69 antibody heavy chain

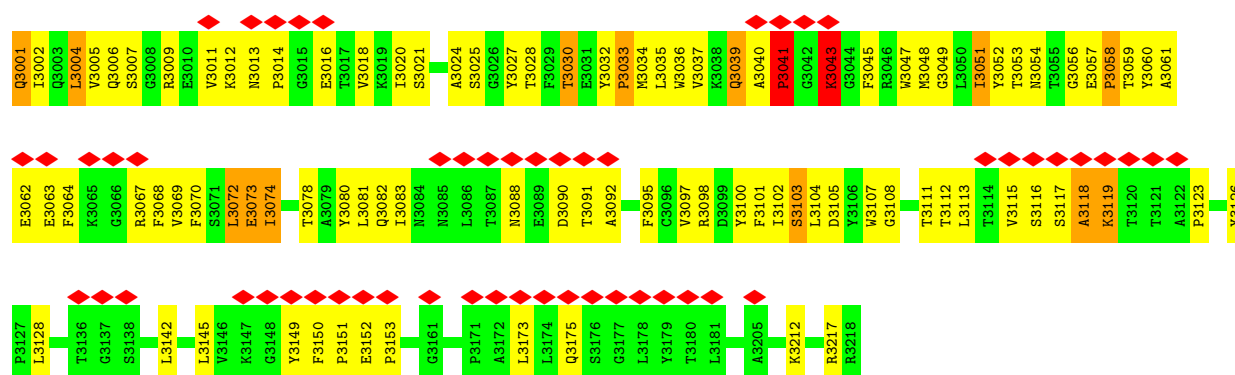


• Molecule 3: EEEV-69 antibody heavy chain

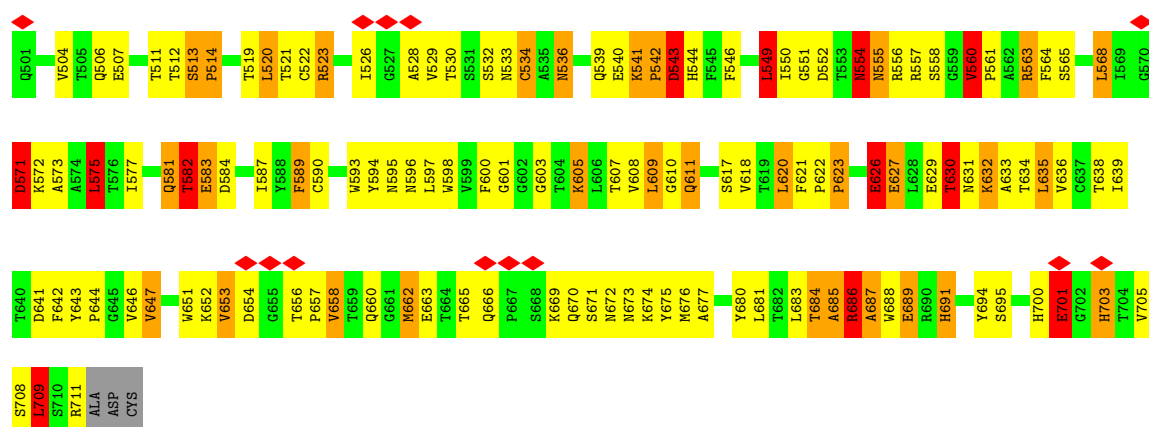




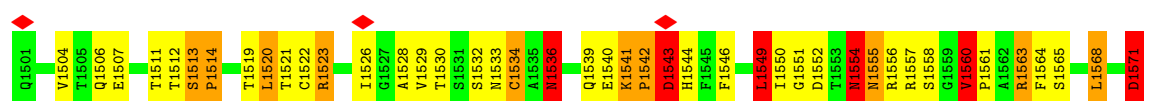
• Molecule 3: EEEV-69 antibody heavy chain

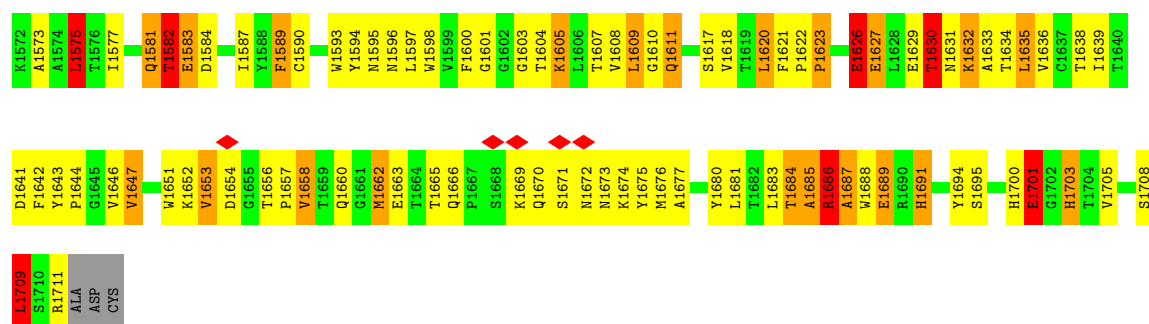


• Molecule 4: EEEV-69 antibody light chain

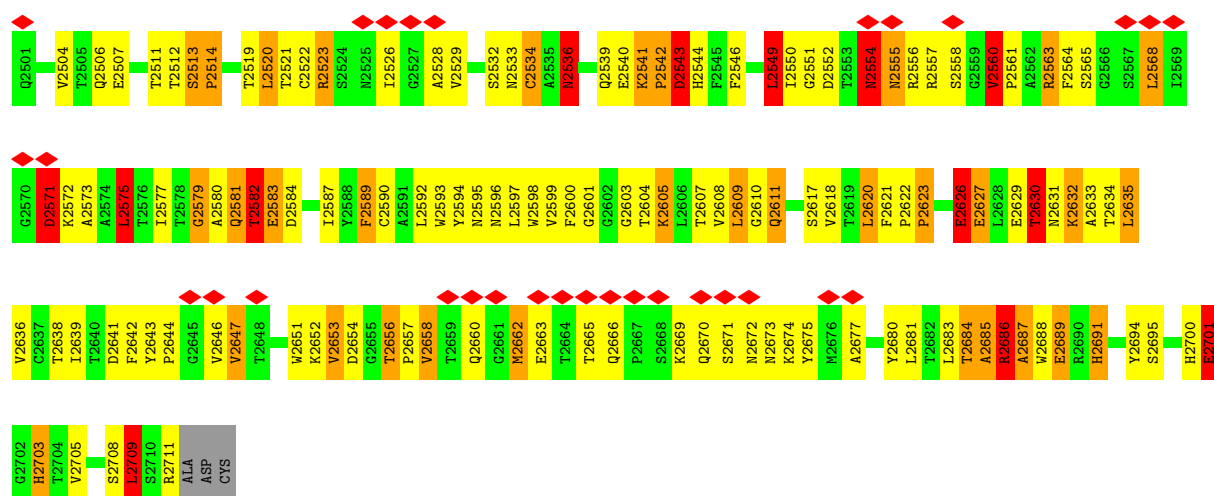


• Molecule 4: EEEV-69 antibody light chain

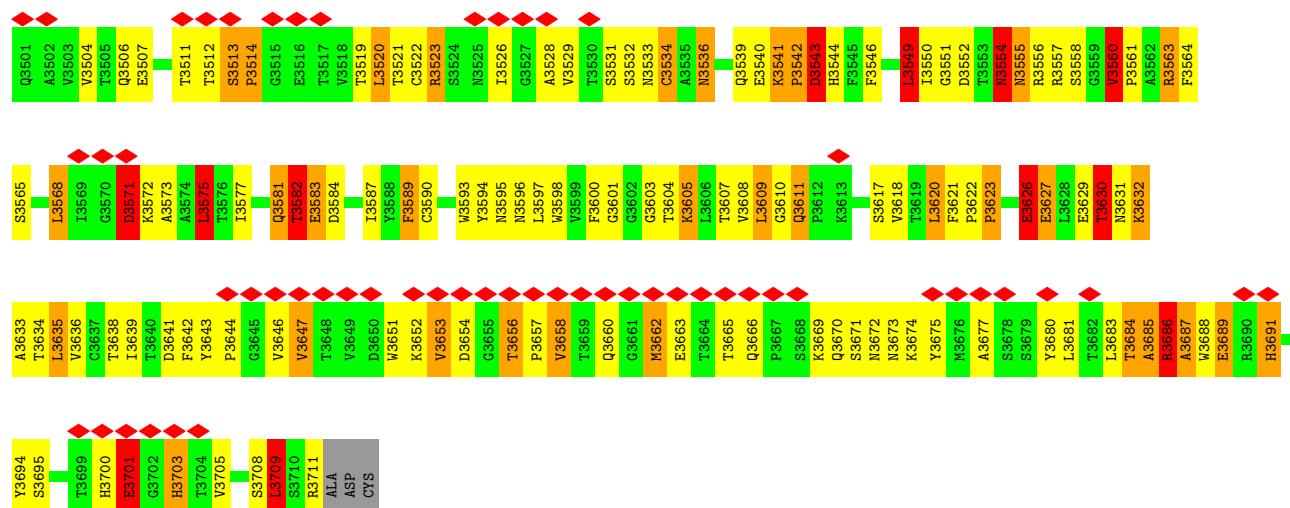




• Molecule 4: EEEV-69 antibody light chain



• Molecule 4: EEEV-69 antibody light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5964	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 ($e^-/\text{\AA}^2$)	31	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	5.247	Depositor
Minimum map value	-6.052	Depositor
Average map value	0.060	Depositor
Map value standard deviation	0.760	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	907.2, 907.2, 907.2	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.62, 1.62, 1.62	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	0.44	0/3147	0.63	1/4294 (0.0%)
1	E	0.44	0/3147	0.63	1/4294 (0.0%)
1	I	0.44	0/3147	0.63	1/4294 (0.0%)
1	M	0.44	0/3147	0.63	1/4294 (0.0%)
2	B	0.43	0/2624	0.64	2/3571 (0.1%)
2	F	0.43	0/2624	0.64	2/3571 (0.1%)
2	J	0.43	0/2624	0.64	2/3571 (0.1%)
2	N	0.43	0/2624	0.64	2/3571 (0.1%)
3	C	0.84	5/1714 (0.3%)	1.15	13/2340 (0.6%)
3	G	0.84	5/1714 (0.3%)	1.15	12/2340 (0.5%)
3	K	0.84	5/1714 (0.3%)	1.15	13/2340 (0.6%)
3	O	0.84	5/1714 (0.3%)	1.15	12/2340 (0.5%)
4	D	1.18	4/1634 (0.2%)	1.94	56/2232 (2.5%)
4	H	1.19	4/1634 (0.2%)	1.94	55/2232 (2.5%)
4	L	1.19	4/1634 (0.2%)	1.94	56/2232 (2.5%)
4	P	1.19	4/1634 (0.2%)	1.93	55/2232 (2.5%)
All	All	0.71	36/36476 (0.1%)	1.08	284/49748 (0.6%)

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	1
1	E	0	1
1	I	0	1
1	M	0	1
All	All	0	4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	58	PRO	N-CD	17.56	1.72	1.47
3	G	1058	PRO	N-CD	17.55	1.72	1.47
3	K	2058	PRO	N-CD	17.51	1.72	1.47
3	O	3058	PRO	N-CD	17.50	1.72	1.47
3	K	2041	PRO	N-CD	14.12	1.67	1.47
3	C	41	PRO	N-CD	14.05	1.67	1.47
3	G	1041	PRO	N-CD	14.03	1.67	1.47
3	O	3041	PRO	N-CD	14.01	1.67	1.47
4	L	2514	PRO	N-CD	13.29	1.66	1.47
4	H	1514	PRO	N-CD	13.25	1.66	1.47
4	P	3514	PRO	N-CD	13.23	1.66	1.47
4	D	514	PRO	N-CD	13.20	1.66	1.47
3	O	3014	PRO	N-CD	9.53	1.61	1.47
3	G	1014	PRO	N-CD	9.50	1.61	1.47
3	C	14	PRO	N-CD	9.45	1.60	1.47
3	K	2014	PRO	N-CD	9.44	1.60	1.47
4	P	3544	HIS	CG-CD2	9.28	1.46	1.35
4	H	1544	HIS	CG-CD2	9.26	1.46	1.35
4	L	2544	HIS	CG-CD2	9.23	1.46	1.35
4	D	544	HIS	CG-CD2	9.23	1.46	1.35
4	H	1542	PRO	N-CD	6.96	1.57	1.47
4	L	2542	PRO	N-CD	6.95	1.57	1.47
4	P	3542	PRO	N-CD	6.89	1.57	1.47
4	D	542	PRO	N-CD	6.87	1.57	1.47
3	K	2033	PRO	N-CD	6.17	1.56	1.47
3	C	33	PRO	N-CD	6.16	1.56	1.47
3	G	1033	PRO	N-CD	6.13	1.56	1.47
3	O	3033	PRO	N-CD	6.11	1.56	1.47
3	K	2108	GLY	C-N	5.13	1.41	1.33
3	C	108	GLY	C-N	5.12	1.41	1.33
4	H	1544	HIS	CD2-NE2	-5.11	1.32	1.37
4	L	2544	HIS	CD2-NE2	-5.10	1.32	1.37
3	G	1108	GLY	C-N	5.10	1.41	1.33
4	P	3544	HIS	CD2-NE2	-5.07	1.32	1.37
3	O	3108	GLY	C-N	5.06	1.41	1.33
4	D	544	HIS	CD2-NE2	-5.01	1.32	1.37

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1701	GLU	CB-CG-CD	12.69	134.18	112.60
4	D	701	GLU	CB-CG-CD	12.68	134.16	112.60
4	L	2701	GLU	CB-CG-CD	12.67	134.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	3701	GLU	CB-CG-CD	12.67	134.13	112.60
4	H	1658	VAL	N-CA-C	-8.96	100.08	110.21
4	D	658	VAL	N-CA-C	-8.96	100.09	110.21
4	L	2658	VAL	N-CA-C	-8.95	100.09	110.21
4	P	3658	VAL	N-CA-C	-8.95	100.10	110.21
4	D	703	HIS	CA-CB-CG	-8.63	105.17	113.80
4	H	1703	HIS	CA-CB-CG	-8.61	105.19	113.80
4	L	2703	HIS	CA-CB-CG	-8.61	105.19	113.80
4	P	3703	HIS	CA-CB-CG	-8.58	105.22	113.80
4	D	575	LEU	CA-C-O	-8.13	111.60	120.30
4	H	1575	LEU	CA-C-O	-8.09	111.64	120.30
4	P	3575	LEU	CA-C-O	-8.08	111.65	120.30
4	L	2575	LEU	CA-C-O	-8.07	111.67	120.30
4	H	1674	LYS	CA-C-O	-7.86	111.67	121.88
4	P	3674	LYS	CA-C-O	-7.85	111.68	121.88
4	D	674	LYS	CA-C-O	-7.84	111.69	121.88
4	L	2674	LYS	CA-C-O	-7.83	111.70	121.88
4	P	3658	VAL	CB-CA-C	7.74	120.12	111.45
4	D	658	VAL	CB-CA-C	7.74	120.11	111.45
4	H	1658	VAL	CB-CA-C	7.72	120.10	111.45
4	L	2658	VAL	CB-CA-C	7.72	120.10	111.45
4	L	2627	GLU	CB-CG-CD	7.45	125.27	112.60
4	H	1627	GLU	CB-CG-CD	7.44	125.25	112.60
4	D	627	GLU	CB-CG-CD	7.43	125.24	112.60
4	P	3627	GLU	CB-CG-CD	7.42	125.21	112.60
4	H	1589	PHE	CA-C-O	-7.24	113.04	120.71
4	D	589	PHE	CA-C-O	-7.21	113.07	120.71
4	L	2589	PHE	CA-C-O	-7.20	113.08	120.71
4	P	3589	PHE	CA-C-O	-7.19	113.09	120.71
4	P	3541	LYS	CA-C-O	-7.02	113.60	120.97
4	D	541	LYS	CA-C-O	-7.01	113.61	120.97
4	H	1541	LYS	CA-C-O	-7.00	113.62	120.97
4	L	2541	LYS	CA-C-O	-6.99	113.63	120.97
4	H	1701	GLU	N-CA-CB	6.91	122.16	110.49
4	D	701	GLU	N-CA-CB	6.89	122.14	110.49
4	P	3701	GLU	N-CA-CB	6.89	122.13	110.49
4	L	2701	GLU	N-CA-CB	6.88	122.11	110.49
4	L	2687	ALA	N-CA-C	-6.87	103.79	111.28
1	A	265	GLU	N-CA-C	-6.83	94.71	109.81
1	I	2265	GLU	N-CA-C	-6.83	94.71	109.81
4	D	687	ALA	N-CA-C	-6.82	103.84	111.28
4	H	1687	ALA	N-CA-C	-6.82	103.84	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	3265	GLU	N-CA-C	-6.82	94.74	109.81
1	E	1265	GLU	N-CA-C	-6.81	94.75	109.81
4	P	3687	ALA	N-CA-C	-6.80	103.87	111.28
4	D	634	THR	CA-CB-OG1	-6.76	99.45	109.60
4	H	1634	THR	CA-CB-OG1	-6.74	99.49	109.60
4	P	3634	THR	CA-CB-OG1	-6.74	99.48	109.60
4	L	2634	THR	CA-CB-OG1	-6.73	99.51	109.60
3	K	2004	LEU	N-CA-C	-6.68	97.53	108.41
3	G	1004	LEU	N-CA-C	-6.65	97.57	108.41
3	C	4	LEU	N-CA-C	-6.63	97.59	108.41
4	H	1686	ARG	N-CA-C	6.63	118.30	111.14
4	P	3686	ARG	N-CA-C	6.63	118.30	111.14
3	O	3004	LEU	N-CA-C	-6.63	97.60	108.41
4	D	686	ARG	N-CA-C	6.62	118.29	111.14
4	L	2686	ARG	N-CA-C	6.61	118.27	111.14
3	C	43	LYS	N-CA-C	6.51	124.67	110.80
3	K	2043	LYS	N-CA-C	6.50	124.65	110.80
3	K	2030	THR	N-CA-C	6.50	120.47	112.54
3	G	1043	LYS	N-CA-C	6.50	124.64	110.80
3	O	3030	THR	N-CA-C	6.49	120.46	112.54
3	O	3043	LYS	N-CA-C	6.49	124.61	110.80
3	G	1030	THR	N-CA-C	6.48	120.44	112.54
4	P	3541	LYS	N-CA-C	-6.47	101.92	110.40
4	L	2541	LYS	N-CA-C	-6.47	101.92	110.40
4	D	541	LYS	N-CA-C	-6.46	101.93	110.40
3	C	30	THR	N-CA-C	6.46	120.42	112.54
4	H	1541	LYS	N-CA-C	-6.46	101.94	110.40
4	D	582	THR	CA-C-O	6.39	127.32	120.10
4	H	1582	THR	CA-C-O	6.38	127.31	120.10
4	L	2582	THR	CA-C-O	6.38	127.31	120.10
4	P	3582	THR	CA-C-O	6.37	127.30	120.10
4	H	1560	VAL	N-CA-C	-6.16	101.17	107.89
4	P	3560	VAL	N-CA-C	-6.16	101.18	107.89
4	D	560	VAL	N-CA-C	-6.15	101.19	107.89
4	L	2560	VAL	N-CA-C	-6.14	101.20	107.89
4	D	635	LEU	CA-CB-CG	6.08	137.59	116.30
4	P	3635	LEU	CA-CB-CG	6.08	137.58	116.30
4	L	2635	LEU	CA-CB-CG	6.08	137.56	116.30
4	H	1635	LEU	CA-CB-CG	6.07	137.56	116.30
4	D	677	ALA	O-C-N	6.02	129.42	123.46
4	H	1677	ALA	O-C-N	5.99	129.39	123.46
4	L	2677	ALA	O-C-N	5.93	129.34	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1600	PHE	CA-C-O	-5.93	114.28	121.28
4	P	3677	ALA	O-C-N	5.93	129.33	123.46
4	D	600	PHE	CA-C-O	-5.92	114.30	121.28
4	D	536	ASN	CA-C-O	-5.91	114.43	121.11
4	L	2600	PHE	CA-C-O	-5.91	114.31	121.28
4	P	3600	PHE	CA-C-O	-5.90	114.31	121.28
4	L	2685	ALA	CA-C-N	5.90	128.46	120.44
4	L	2685	ALA	C-N-CA	5.90	128.46	120.44
4	D	511	THR	CA-C-O	-5.88	114.01	120.36
4	H	1685	ALA	CA-C-N	5.87	128.43	120.44
4	H	1685	ALA	C-N-CA	5.87	128.43	120.44
4	P	3685	ALA	CA-C-N	5.87	128.43	120.44
4	P	3685	ALA	C-N-CA	5.87	128.43	120.44
4	L	2536	ASN	CA-C-O	-5.87	114.48	121.11
4	D	685	ALA	CA-C-N	5.86	128.42	120.44
4	D	685	ALA	C-N-CA	5.86	128.42	120.44
4	P	3536	ASN	CA-C-O	-5.86	114.49	121.11
4	H	1536	ASN	CA-C-O	-5.85	114.50	121.11
4	L	2511	THR	CA-C-O	-5.85	114.04	120.36
4	H	1511	THR	CA-C-O	-5.84	114.05	120.36
4	P	3511	THR	CA-C-O	-5.82	114.07	120.36
4	D	554	ASN	CA-C-O	-5.82	113.46	119.51
3	C	34	MET	N-CA-C	5.80	118.36	108.90
4	P	3641	ASP	CA-C-O	-5.80	114.81	121.54
2	J	2685	TYR	CA-CB-CG	5.79	124.33	113.90
4	L	2554	ASN	CA-C-O	-5.79	113.49	119.51
4	L	2641	ASP	CA-C-O	-5.79	114.82	121.54
2	F	1685	TYR	CA-CB-CG	5.79	124.32	113.90
3	K	2034	MET	N-CA-C	5.79	118.34	108.90
3	G	1034	MET	N-CA-C	5.78	118.33	108.90
4	P	3554	ASN	CA-C-O	-5.78	113.50	119.51
2	B	685	TYR	CA-CB-CG	5.78	124.30	113.90
4	H	1554	ASN	CA-C-O	-5.77	113.51	119.51
4	H	1641	ASP	CA-C-O	-5.77	114.84	121.54
2	N	3685	TYR	CA-CB-CG	5.75	124.26	113.90
3	O	3034	MET	N-CA-C	5.75	118.28	108.90
4	D	641	ASP	CA-C-O	-5.75	114.87	121.54
3	K	2039	GLN	N-CA-C	-5.72	98.01	108.02
4	D	611	GLN	CA-C-N	-5.71	114.08	119.90
4	D	611	GLN	C-N-CA	-5.71	114.08	119.90
3	G	1039	GLN	N-CA-C	-5.70	98.04	108.02
4	P	3611	GLN	CA-C-N	-5.70	114.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	3611	GLN	C-N-CA	-5.70	114.08	119.90
3	C	39	GLN	N-CA-C	-5.69	98.06	108.02
4	H	1611	GLN	CA-C-N	-5.69	114.09	119.90
4	H	1611	GLN	C-N-CA	-5.69	114.09	119.90
3	O	3039	GLN	N-CA-C	-5.69	98.06	108.02
4	L	2611	GLN	CA-C-N	-5.65	114.14	119.90
4	L	2611	GLN	C-N-CA	-5.65	114.14	119.90
4	H	1647	VAL	N-CA-CB	5.62	120.72	112.35
4	P	3647	VAL	N-CA-CB	5.59	120.68	112.35
4	L	2653	VAL	O-C-N	5.58	129.31	122.95
4	L	2677	ALA	CA-C-O	-5.57	114.97	121.10
4	D	647	VAL	N-CA-CB	5.57	120.64	112.35
4	L	2647	VAL	N-CA-CB	5.57	120.64	112.35
4	P	3656	THR	CA-CB-OG1	-5.57	101.25	109.60
4	L	2656	THR	CA-CB-OG1	-5.57	101.25	109.60
4	D	677	ALA	CA-C-O	-5.56	114.98	121.10
4	P	3677	ALA	CA-C-O	-5.56	114.99	121.10
4	H	1677	ALA	CA-C-O	-5.55	114.99	121.10
4	D	656	THR	CA-CB-OG1	-5.55	101.28	109.60
4	H	1656	THR	CA-CB-OG1	-5.54	101.29	109.60
4	H	1563	ARG	N-CA-C	-5.53	106.38	113.01
4	P	3634	THR	CA-CB-CG2	5.52	119.89	110.50
4	H	1653	VAL	O-C-N	5.52	129.24	122.95
4	D	634	THR	CA-CB-CG2	5.52	119.88	110.50
4	D	653	VAL	O-C-N	5.51	129.24	122.95
4	P	3653	VAL	O-C-N	5.51	129.24	122.95
4	L	2563	ARG	N-CA-C	-5.51	106.40	113.01
3	O	3111	THR	N-CA-C	-5.51	99.31	108.34
3	C	111	THR	N-CA-C	-5.51	99.31	108.34
4	H	1634	THR	CA-CB-CG2	5.50	119.85	110.50
4	P	3563	ARG	N-CA-C	-5.50	106.41	113.01
3	G	1111	THR	N-CA-C	-5.50	99.32	108.34
4	L	2634	THR	CA-CB-CG2	5.50	119.85	110.50
3	K	2111	THR	N-CA-C	-5.50	99.33	108.34
4	D	563	ARG	N-CA-C	-5.49	106.42	113.01
4	H	1701	GLU	CA-C-N	5.49	132.17	121.41
4	H	1701	GLU	C-N-CA	5.49	132.17	121.41
4	L	2607	THR	CA-C-O	-5.49	114.40	120.38
4	D	617	SER	O-C-N	5.48	130.04	123.13
4	P	3701	GLU	CA-C-N	5.48	132.15	121.41
4	P	3701	GLU	C-N-CA	5.48	132.15	121.41
4	L	2617	SER	O-C-N	5.47	130.03	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2701	GLU	CA-C-N	5.47	132.14	121.41
4	L	2701	GLU	C-N-CA	5.47	132.14	121.41
4	D	607	THR	CA-C-O	-5.47	114.41	120.38
4	D	534	CYS	CA-C-O	-5.46	115.64	122.03
4	H	1607	THR	CA-C-O	-5.46	114.43	120.38
4	D	701	GLU	CA-C-N	5.45	132.09	121.41
4	D	701	GLU	C-N-CA	5.45	132.09	121.41
4	H	1617	SER	O-C-N	5.45	130.00	123.13
4	P	3607	THR	CA-C-O	-5.44	114.45	120.38
4	P	3534	CYS	CA-C-O	-5.44	115.67	122.03
4	L	2534	CYS	CA-C-O	-5.43	115.67	122.03
4	P	3617	SER	O-C-N	5.43	129.97	123.13
4	H	1534	CYS	CA-C-O	-5.42	115.69	122.03
4	D	543	ASP	CA-C-O	-5.40	112.79	120.51
4	L	2543	ASP	CA-C-O	-5.40	112.79	120.51
4	H	1543	ASP	CA-C-O	-5.39	112.80	120.51
4	P	3543	ASP	CA-C-O	-5.37	112.83	120.51
4	H	1529	VAL	CA-C-O	-5.35	114.74	121.11
4	P	3529	VAL	CA-C-O	-5.35	114.74	121.11
4	L	2529	VAL	CA-C-O	-5.34	114.75	121.11
4	D	529	VAL	CA-C-O	-5.31	114.79	121.11
4	H	1646	VAL	CA-C-O	-5.22	114.74	120.43
4	D	555	ASN	CA-C-O	-5.21	114.79	120.36
4	L	2513	SER	O-C-N	5.21	126.62	121.57
4	P	3555	ASN	CA-C-O	-5.21	114.79	120.36
4	H	1571	ASP	CA-C-N	-5.21	113.78	122.21
4	H	1571	ASP	C-N-CA	-5.21	113.78	122.21
4	P	3630	THR	CA-CB-CG2	5.21	119.35	110.50
4	L	2630	THR	CA-CB-CG2	5.20	119.34	110.50
4	P	3571	ASP	CA-C-N	-5.20	113.78	122.21
4	P	3571	ASP	C-N-CA	-5.20	113.78	122.21
4	D	630	THR	CA-CB-CG2	5.20	119.34	110.50
4	L	2571	ASP	CA-C-N	-5.20	113.79	122.21
4	L	2571	ASP	C-N-CA	-5.20	113.79	122.21
4	D	513	SER	O-C-N	5.20	126.61	121.57
4	H	1513	SER	O-C-N	5.20	126.61	121.57
4	D	571	ASP	CA-C-N	-5.19	113.80	122.21
4	D	571	ASP	C-N-CA	-5.19	113.80	122.21
4	H	1630	THR	CA-CB-CG2	5.19	119.33	110.50
4	D	675	TYR	O-C-N	5.19	130.05	122.94
3	O	3040	ALA	CA-C-N	5.19	126.33	119.84
3	O	3040	ALA	C-N-CA	5.19	126.33	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	3513	SER	O-C-N	5.19	126.60	121.57
4	H	1675	TYR	O-C-N	5.18	130.04	122.94
3	K	2040	ALA	CA-C-N	5.17	126.31	119.84
3	K	2040	ALA	C-N-CA	5.17	126.31	119.84
4	P	3646	VAL	CA-C-O	-5.17	114.79	120.43
4	D	646	VAL	CA-C-O	-5.17	114.79	120.43
4	P	3675	TYR	O-C-N	5.16	130.01	122.94
4	L	2646	VAL	CA-C-O	-5.15	114.81	120.43
4	L	2675	TYR	O-C-N	5.15	130.00	122.94
3	K	2056	GLY	O-C-N	-5.15	116.43	122.50
4	L	2568	LEU	N-CA-C	-5.15	100.51	108.90
3	G	1040	ALA	CA-C-N	5.14	126.27	119.84
3	G	1040	ALA	C-N-CA	5.14	126.27	119.84
4	H	1555	ASN	CA-C-O	-5.14	114.86	120.36
4	P	3568	LEU	N-CA-C	-5.14	100.52	108.90
4	P	3709	LEU	CB-CA-C	5.14	118.96	109.71
4	D	709	LEU	CB-CA-C	5.13	118.95	109.71
4	H	1623	PRO	CA-C-O	-5.13	115.49	121.34
4	H	1568	LEU	N-CA-C	-5.13	100.53	108.90
3	O	3056	GLY	O-C-N	-5.13	116.44	122.50
3	C	74	ILE	CA-C-O	5.13	127.19	120.78
4	D	568	LEU	N-CA-C	-5.13	100.53	108.90
3	G	1074	ILE	CA-C-O	5.13	127.19	120.78
3	K	2074	ILE	CA-C-O	5.13	127.19	120.78
3	C	40	ALA	CA-C-N	5.13	126.25	119.84
3	C	40	ALA	C-N-CA	5.13	126.25	119.84
4	H	1709	LEU	CB-CA-C	5.13	118.94	109.71
4	L	2555	ASN	CA-C-O	-5.13	114.87	120.36
3	C	1	GLN	CA-C-O	-5.13	112.09	120.80
3	C	56	GLY	O-C-N	-5.12	116.45	122.50
3	G	1056	GLY	O-C-N	-5.12	116.45	122.50
4	L	2623	PRO	CA-C-O	-5.12	115.50	121.34
3	G	1001	GLN	CA-C-O	-5.12	112.10	120.80
3	O	3074	ILE	CA-C-O	5.11	127.17	120.78
3	K	2001	GLN	CA-C-O	-5.11	112.12	120.80
4	L	2709	LEU	CB-CA-C	5.10	118.89	109.71
4	D	549	LEU	CA-C-N	5.10	130.80	122.69
4	D	549	LEU	C-N-CA	5.10	130.80	122.69
3	O	3001	GLN	CA-C-O	-5.10	112.13	120.80
3	G	1059	THR	N-CA-C	-5.10	101.38	109.59
4	P	3623	PRO	CA-C-O	-5.10	115.53	121.34
3	C	59	THR	N-CA-C	-5.09	101.39	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2059	THR	N-CA-C	-5.09	101.39	109.59
4	L	2623	PRO	N-CA-C	-5.09	103.20	111.14
4	D	623	PRO	CA-C-O	-5.09	115.54	121.34
4	D	623	PRO	N-CA-C	-5.09	103.20	111.14
4	L	2549	LEU	CA-C-N	5.09	130.78	122.69
4	L	2549	LEU	C-N-CA	5.09	130.78	122.69
3	O	3059	THR	N-CA-C	-5.09	101.40	109.59
4	H	1623	PRO	N-CA-C	-5.08	103.21	111.14
4	P	3549	LEU	CA-C-N	5.07	130.76	122.69
4	P	3549	LEU	C-N-CA	5.07	130.76	122.69
4	P	3623	PRO	N-CA-C	-5.07	103.23	111.14
4	H	1626	GLU	CB-CG-CD	5.07	121.22	112.60
2	J	2823	TRP	CA-CB-CG	5.07	123.23	113.60
4	D	647	VAL	CA-CB-CG1	5.07	119.02	110.40
4	L	2647	VAL	CA-CB-CG1	5.07	119.01	110.40
4	L	2626	GLU	CB-CG-CD	5.06	121.20	112.60
2	N	3823	TRP	CA-CB-CG	5.06	123.21	113.60
4	D	626	GLU	CB-CG-CD	5.05	121.19	112.60
2	F	1823	TRP	CA-CB-CG	5.05	123.20	113.60
4	H	1647	VAL	CA-CB-CG1	5.05	118.99	110.40
2	B	823	TRP	CA-CB-CG	5.05	123.20	113.60
4	H	1549	LEU	CA-C-N	5.05	130.72	122.69
4	H	1549	LEU	C-N-CA	5.05	130.72	122.69
4	P	3626	GLU	CB-CG-CD	5.04	121.17	112.60
4	P	3647	VAL	CA-CB-CG1	5.03	118.96	110.40
3	K	2095	PHE	O-C-N	-5.02	116.84	123.21
3	C	95	PHE	O-C-N	-5.01	116.85	123.21
4	L	2579	GLY	N-CA-C	-5.01	101.30	113.18
4	D	560	VAL	O-C-N	5.00	125.91	121.41

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	LYS	Peptide
1	E	1385	LYS	Peptide
1	I	2385	LYS	Peptide
1	M	3385	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	3063	0	2950	93	0
1	E	3063	0	2947	74	0
1	I	3063	0	2947	75	0
1	M	3063	0	2947	58	0
2	B	2550	0	2489	169	0
2	F	2550	0	2487	109	0
2	J	2550	0	2487	266	0
2	N	2550	0	2492	90	0
3	C	1671	0	1640	231	0
3	G	1671	0	1638	208	0
3	K	1671	0	1637	266	0
3	O	1671	0	1637	227	0
4	D	1598	0	1522	289	0
4	H	1598	0	1517	238	0
4	L	1598	0	1523	358	0
4	P	1598	0	1524	210	0
All	All	35528	0	34384	2158	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 31.

All (2158) 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)
3:K:2032:TYR:HE1	3:K:2100:TYR:CD1	1.00	1.70
3:C:32:TYR:HE1	3:C:100:TYR:CD1	1.00	1.67
3:K:2118:ALA:HB3	3:K:2150:PHE:CE2	1.17	1.63
3:G:1118:ALA:HB3	3:G:1150:PHE:CE2	1.17	1.63
3:O:3118:ALA:HB3	3:O:3150:PHE:CE2	1.17	1.63
3:C:118:ALA:HB3	3:C:150:PHE:CE2	1.17	1.62
3:G:1032:TYR:HE1	3:G:1100:TYR:CD1	1.00	1.61
3:O:3032:TYR:CE1	3:O:3100:TYR:CD1	1.86	1.61
3:O:3032:TYR:HE1	3:O:3100:TYR:CD1	1.00	1.60
3:G:1032:TYR:CE1	3:G:1100:TYR:CD1	1.86	1.59
3:C:32:TYR:CE1	3:C:100:TYR:CD1	1.86	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1035:LEU:HD13	3:G:1104:LEU:CD2	1.36	1.55
3:O:3035:LEU:CD1	3:O:3104:LEU:HD21	1.36	1.55
2:B:671:LYS:CA	4:D:595:ASN:N	1.67	1.55
2:B:671:LYS:HE2	4:D:594:TYR:C	1.12	1.54
3:C:35:LEU:CD1	3:C:104:LEU:HD21	1.36	1.54
3:O:3035:LEU:HD13	3:O:3104:LEU:CD2	1.36	1.54
3:C:35:LEU:HD13	3:C:104:LEU:CD2	1.36	1.54
3:G:1045:PHE:CZ	4:H:1546:PHE:CZ	1.96	1.54
3:K:2032:TYR:CE1	3:K:2100:TYR:CD1	1.86	1.54
3:K:2035:LEU:HD13	3:K:2104:LEU:CD2	1.36	1.54
2:B:671:LYS:HA	4:D:595:ASN:CA	1.10	1.53
2:J:2669:SER:CB	4:L:2592:LEU:HB3	1.07	1.53
3:K:2035:LEU:CD1	3:K:2104:LEU:HD21	1.36	1.53
3:G:1045:PHE:CZ	4:H:1546:PHE:HZ	1.25	1.52
3:C:45:PHE:CZ	4:D:546:PHE:CZ	1.96	1.52
3:G:1035:LEU:CD1	3:G:1104:LEU:HD21	1.36	1.51
2:J:2705:THR:HA	4:L:2596:ASN:ND2	1.22	1.51
3:O:3118:ALA:CB	3:O:3150:PHE:CE2	1.93	1.50
2:F:1702:THR:CA	4:H:1593:TRP:NE1	1.70	1.50
3:O:3045:PHE:CZ	4:P:3546:PHE:CZ	1.96	1.50
3:G:1118:ALA:CB	3:G:1150:PHE:CE2	1.93	1.49
3:K:2045:PHE:CZ	4:L:2546:PHE:CZ	1.96	1.49
3:K:2045:PHE:CZ	4:L:2546:PHE:HZ	1.25	1.49
2:F:1703:THR:C	4:H:1595:ASN:HB3	1.29	1.49
3:K:2118:ALA:CB	3:K:2150:PHE:CE2	1.93	1.49
2:J:2705:THR:CA	4:L:2596:ASN:ND2	1.72	1.49
2:B:692:ARG:HH22	3:C:57:GLU:CD	1.21	1.48
2:B:668:HIS:HE1	3:C:102:ILE:CG2	1.23	1.47
2:J:2668:HIS:CE1	4:L:2598:TRP:CH2	2.03	1.46
3:O:3045:PHE:CZ	4:P:3546:PHE:HZ	1.25	1.46
3:C:45:PHE:CZ	4:D:546:PHE:HZ	1.25	1.46
3:C:118:ALA:CB	3:C:150:PHE:CE2	1.92	1.46
3:K:2041:PRO:CD	3:K:2041:PRO:N	1.67	1.42
3:O:3102:ILE:CB	4:P:3552:ASP:HB2	1.49	1.42
3:C:102:ILE:CB	4:D:552:ASP:HB2	1.49	1.41
2:F:1669:SER:C	4:H:1533:ASN:OD1	1.63	1.40
3:G:1102:ILE:CB	4:H:1552:ASP:HB2	1.49	1.40
3:K:2102:ILE:CB	4:L:2552:ASP:HB2	1.49	1.40
2:B:668:HIS:CE1	3:C:102:ILE:CG2	2.04	1.40
2:J:2669:SER:CB	4:L:2592:LEU:CB	1.97	1.39
2:B:671:LYS:CE	4:D:594:TYR:C	1.96	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3058:PRO:CD	3:O:3058:PRO:N	1.72	1.38
2:J:2667:ILE:HD13	4:L:2595:ASN:CG	0.97	1.38
3:K:2058:PRO:CD	3:K:2058:PRO:N	1.72	1.37
3:K:2078:THR:HG21	3:K:2080:TYR:CZ	1.59	1.36
2:B:671:LYS:CA	4:D:595:ASN:HA	1.54	1.36
3:C:78:THR:HG21	3:C:80:TYR:CZ	1.59	1.36
3:G:1078:THR:HG21	3:G:1080:TYR:CZ	1.59	1.35
3:C:45:PHE:CE2	4:D:546:PHE:CZ	2.14	1.35
2:F:1670:ALA:N	4:H:1533:ASN:OD1	1.59	1.35
3:G:1045:PHE:CE2	4:H:1546:PHE:CZ	2.14	1.34
2:J:2668:HIS:NE2	4:L:2598:TRP:CZ3	1.91	1.34
2:J:2671:LYS:CA	4:L:2596:ASN:H	1.28	1.34
3:K:2045:PHE:CE2	4:L:2546:PHE:CZ	2.14	1.34
3:G:1058:PRO:CD	3:G:1058:PRO:N	1.72	1.34
3:O:3078:THR:HG21	3:O:3080:TYR:CZ	1.59	1.34
2:B:692:ARG:NH2	3:C:57:GLU:CD	1.85	1.34
3:O:3045:PHE:CE2	4:P:3546:PHE:CZ	2.14	1.33
2:B:671:LYS:HA	4:D:595:ASN:N	1.03	1.33
2:F:1703:THR:O	4:H:1595:ASN:CB	1.76	1.31
2:B:671:LYS:HE2	4:D:595:ASN:N	1.40	1.31
2:B:701:THR:O	4:D:593:TRP:HZ2	1.11	1.31
2:B:668:HIS:CE1	3:C:102:ILE:HG23	1.61	1.30
3:G:1032:TYR:OH	3:G:1100:TYR:CZ	1.68	1.30
2:J:2671:LYS:HB3	4:L:2596:ASN:N	1.44	1.30
2:N:3669:SER:CB	4:P:3534:CYS:SG	2.16	1.30
3:G:1032:TYR:OH	3:G:1100:TYR:CE1	1.84	1.30
3:C:32:TYR:OH	3:C:100:TYR:CE1	1.84	1.30
3:C:2:ILE:CD1	3:C:98:ARG:NH1	1.95	1.29
2:N:3689:PRO:HB2	3:O:3057:GLU:OE2	1.18	1.29
3:O:3002:ILE:CD1	3:O:3098:ARG:NH1	1.95	1.29
2:F:1702:THR:CA	4:H:1593:TRP:HE1	1.34	1.29
3:K:2032:TYR:OH	3:K:2100:TYR:CE1	1.84	1.29
3:K:2002:ILE:CD1	3:K:2098:ARG:NH1	1.95	1.29
2:N:3669:SER:O	4:P:3533:ASN:CA	1.79	1.29
3:G:1002:ILE:CD1	3:G:1098:ARG:NH1	1.95	1.29
2:F:1703:THR:C	4:H:1595:ASN:CB	2.04	1.29
3:O:3032:TYR:OH	3:O:3100:TYR:CZ	1.68	1.28
2:B:702:THR:O	4:D:596:ASN:C	1.77	1.28
2:J:2668:HIS:NE2	4:L:2598:TRP:CH2	2.00	1.27
3:C:32:TYR:OH	3:C:100:TYR:CZ	1.68	1.27
2:B:692:ARG:NH2	3:C:57:GLU:OE2	1.66	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2032:TYR:OH	3:K:2100:TYR:CZ	1.68	1.26
2:J:2701:THR:N	4:L:2593:TRP:CZ2	2.00	1.26
3:O:3032:TYR:OH	3:O:3100:TYR:CE1	1.84	1.26
2:B:690:ASP:OD1	3:C:52:TYR:OH	1.53	1.26
3:C:32:TYR:CE1	3:C:100:TYR:CG	2.24	1.25
3:C:58:PRO:CD	3:C:58:PRO:N	1.72	1.25
3:K:2032:TYR:CE1	3:K:2100:TYR:CG	2.24	1.25
2:N:3669:SER:HB2	4:P:3534:CYS:SG	1.57	1.25
3:C:102:ILE:HB	4:D:552:ASP:CB	1.66	1.25
3:G:1032:TYR:CE1	3:G:1100:TYR:CG	2.24	1.25
3:K:2045:PHE:HZ	4:L:2546:PHE:CZ	1.43	1.24
2:J:2700:HIS:CE1	3:K:2050:LEU:HD13	1.69	1.24
3:O:3032:TYR:CE1	3:O:3100:TYR:CG	2.24	1.24
2:B:702:THR:O	4:D:596:ASN:CA	1.85	1.24
3:K:2102:ILE:HB	4:L:2552:ASP:CB	1.66	1.24
3:O:3102:ILE:HB	4:P:3552:ASP:CB	1.66	1.23
3:C:21:SER:OG	3:C:80:TYR:HE2	1.21	1.23
3:G:1021:SER:OG	3:G:1080:TYR:HE2	1.21	1.23
3:G:1102:ILE:HB	4:H:1552:ASP:CB	1.66	1.22
2:N:3668:HIS:HE2	3:O:3102:ILE:CA	1.51	1.22
3:C:217:ARG:NH2	4:D:622:PRO:HD2	1.55	1.22
3:C:45:PHE:HZ	4:D:546:PHE:CZ	1.43	1.21
3:K:2217:ARG:NH2	4:L:2622:PRO:HD2	1.55	1.21
3:O:3217:ARG:NH2	4:P:3622:PRO:HD2	1.55	1.20
2:B:702:THR:O	4:D:596:ASN:HA	1.35	1.20
2:B:701:THR:O	4:D:593:TRP:CZ2	1.94	1.20
3:G:1021:SER:OG	3:G:1080:TYR:CE2	1.92	1.20
2:J:2673:LYS:HB2	4:L:2593:TRP:CD1	1.77	1.20
2:N:3669:SER:O	4:P:3533:ASN:HA	1.05	1.19
3:G:1045:PHE:HZ	4:H:1546:PHE:CZ	1.43	1.19
3:G:1217:ARG:NH2	4:H:1622:PRO:HD2	1.55	1.19
2:J:2667:ILE:HD13	4:L:2595:ASN:OD1	1.43	1.19
3:K:2021:SER:OG	3:K:2080:TYR:CE2	1.91	1.19
2:J:2669:SER:OG	4:L:2592:LEU:HB3	1.42	1.18
3:O:3078:THR:CG2	3:O:3080:TYR:CZ	2.26	1.18
3:O:3021:SER:OG	3:O:3080:TYR:CE2	1.92	1.18
3:C:78:THR:CG2	3:C:80:TYR:CZ	2.26	1.18
3:K:2078:THR:CG2	3:K:2080:TYR:CZ	2.26	1.18
2:N:3703:THR:N	3:O:3052:TYR:OH	1.75	1.17
4:D:514:PRO:HG3	4:D:609:LEU:O	1.45	1.17
4:D:514:PRO:CG	4:D:609:LEU:O	1.93	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1078:THR:CG2	3:G:1080:TYR:CZ	2.26	1.16
2:F:1703:THR:O	4:H:1595:ASN:HB2	1.35	1.16
2:N:3671:LYS:NZ	4:P:3596:ASN:HA	1.57	1.16
2:N:3705:THR:CB	4:P:3595:ASN:HB3	1.72	1.16
4:P:3514:PRO:CG	4:P:3609:LEU:O	1.93	1.16
3:O:3021:SER:OG	3:O:3080:TYR:HE2	1.21	1.16
3:C:21:SER:OG	3:C:80:TYR:CE2	1.91	1.16
4:H:1514:PRO:HG3	4:H:1609:LEU:O	1.45	1.16
4:H:1514:PRO:CG	4:H:1609:LEU:O	1.93	1.16
2:J:2701:THR:N	4:L:2593:TRP:HZ2	1.37	1.16
3:K:2032:TYR:HE1	3:K:2100:TYR:CG	1.61	1.16
4:L:2514:PRO:HG3	4:L:2609:LEU:O	1.45	1.16
2:F:1703:THR:HG23	4:H:1596:ASN:HB3	1.24	1.15
2:J:2671:LYS:CB	4:L:2596:ASN:N	2.07	1.15
2:B:671:LYS:HD3	4:D:595:ASN:C	1.49	1.15
2:B:671:LYS:NZ	4:D:597:LEU:H	1.42	1.15
2:J:2669:SER:N	4:L:2533:ASN:HD22	1.45	1.15
4:L:2514:PRO:CG	4:L:2609:LEU:O	1.93	1.14
3:O:3002:ILE:HD11	3:O:3098:ARG:NH1	1.62	1.14
3:O:3045:PHE:HZ	4:P:3546:PHE:CZ	1.43	1.14
4:P:3514:PRO:HG3	4:P:3609:LEU:O	1.45	1.14
2:F:1704:CYS:N	4:H:1595:ASN:HB3	1.61	1.14
2:J:2700:HIS:HB2	4:L:2593:TRP:CZ2	1.82	1.14
2:N:3705:THR:HB	4:P:3595:ASN:HB3	1.17	1.14
2:J:2671:LYS:CB	4:L:2596:ASN:H	1.57	1.14
3:O:3032:TYR:HE1	3:O:3100:TYR:CG	1.61	1.13
3:C:32:TYR:HE1	3:C:100:TYR:CG	1.61	1.13
2:F:1668:HIS:O	4:H:1533:ASN:N	1.80	1.13
3:G:1002:ILE:HD11	3:G:1098:ARG:HH12	1.12	1.12
3:G:1102:ILE:HG22	4:H:1534:CYS:HB3	1.25	1.12
3:C:2:ILE:HD11	3:C:98:ARG:HH12	1.12	1.11
3:C:102:ILE:HG13	4:D:552:ASP:CG	1.76	1.11
3:K:2002:ILE:HD11	3:K:2098:ARG:HH12	1.12	1.11
3:K:2021:SER:OG	3:K:2080:TYR:HE2	1.21	1.11
2:J:2669:SER:HB3	4:L:2592:LEU:HB3	1.18	1.11
3:K:2102:ILE:HG13	4:L:2552:ASP:CG	1.76	1.11
2:B:671:LYS:HD2	4:D:593:TRP:CH2	1.46	1.11
3:G:1102:ILE:HG13	4:H:1552:ASP:CG	1.76	1.11
3:G:1035:LEU:CD2	3:G:1037:VAL:CG2	2.29	1.10
2:J:2669:SER:HB2	4:L:2592:LEU:HB3	1.19	1.10
3:C:35:LEU:CD2	3:C:37:VAL:HG23	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:THR:HG23	4:D:596:ASN:HD22	1.03	1.10
3:G:1032:TYR:HE1	3:G:1100:TYR:CG	1.61	1.10
3:O:3102:ILE:HG22	4:P:3534:CYS:HB3	1.25	1.10
2:B:702:THR:HA	4:D:593:TRP:CH2	1.85	1.10
3:C:35:LEU:CD2	3:C:37:VAL:CG2	2.29	1.10
3:K:2035:LEU:CD2	3:K:2037:VAL:CG2	2.29	1.10
2:B:705:THR:HB	4:D:595:ASN:HD22	0.98	1.09
2:J:2702:THR:CA	4:L:2596:ASN:O	1.95	1.09
3:O:3035:LEU:CD2	3:O:3037:VAL:CG2	2.29	1.09
2:B:671:LYS:HE2	4:D:594:TYR:O	1.52	1.09
3:K:2035:LEU:CD2	3:K:2037:VAL:HG23	1.80	1.09
3:O:3118:ALA:HB3	3:O:3150:PHE:CZ	1.88	1.09
2:B:671:LYS:NZ	4:D:597:LEU:N	1.92	1.09
3:C:102:ILE:HG22	4:D:534:CYS:HB3	1.25	1.09
3:C:118:ALA:HB3	3:C:150:PHE:CZ	1.88	1.09
3:G:1035:LEU:CD2	3:G:1037:VAL:HG23	1.80	1.09
2:J:2668:HIS:CE1	4:L:2598:TRP:CZ3	2.37	1.09
3:O:3035:LEU:CD2	3:O:3037:VAL:HG23	1.80	1.09
3:O:3102:ILE:HG13	4:P:3552:ASP:CG	1.75	1.09
3:K:2118:ALA:HB3	3:K:2150:PHE:CZ	1.88	1.08
3:C:2:ILE:HD11	3:C:98:ARG:NH1	1.62	1.07
2:J:2669:SER:OG	4:L:2533:ASN:HB3	1.53	1.07
3:K:2102:ILE:HG22	4:L:2534:CYS:HB3	1.25	1.07
3:G:1118:ALA:HB3	3:G:1150:PHE:CZ	1.88	1.06
3:K:2102:ILE:HG21	4:L:2552:ASP:OD1	1.55	1.06
3:G:1002:ILE:HD11	3:G:1098:ARG:NH1	1.62	1.06
3:K:2102:ILE:CB	4:L:2552:ASP:CB	2.30	1.06
3:C:102:ILE:HG21	4:D:552:ASP:OD1	1.55	1.06
3:K:2039:GLN:NE2	3:K:2045:PHE:CE1	2.24	1.06
2:B:671:LYS:CA	4:D:595:ASN:CA	2.02	1.05
2:F:1703:THR:CG2	4:H:1596:ASN:HB3	1.86	1.05
2:J:2692:ARG:NH1	3:K:2057:GLU:CD	2.14	1.05
2:N:3668:HIS:NE2	3:O:3102:ILE:CA	2.01	1.05
2:N:3702:THR:C	3:O:3052:TYR:OH	1.95	1.05
3:G:1039:GLN:NE2	3:G:1045:PHE:CE1	2.24	1.05
3:G:1102:ILE:HG21	4:H:1552:ASP:OD1	1.55	1.05
2:J:2671:LYS:CA	4:L:2596:ASN:N	2.11	1.05
2:B:702:THR:O	4:D:596:ASN:O	1.74	1.05
3:O:3002:ILE:HD11	3:O:3098:ARG:HH12	1.12	1.05
3:O:3039:GLN:NE2	3:O:3045:PHE:CE1	2.24	1.05
2:N:3671:LYS:HZ1	4:P:3596:ASN:HA	0.93	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:GLN:NE2	3:C:45:PHE:CE1	2.24	1.04
3:O:3102:ILE:HG21	4:P:3552:ASP:OD1	1.55	1.04
2:B:671:LYS:CD	4:D:595:ASN:C	2.25	1.04
3:G:1045:PHE:CE2	4:H:1546:PHE:CE1	2.46	1.04
4:H:1514:PRO:HD3	4:H:1609:LEU:CB	1.88	1.04
2:J:2669:SER:HB2	4:L:2592:LEU:CB	1.75	1.04
2:J:2701:THR:HB	4:L:2596:ASN:HA	1.39	1.04
2:B:669:SER:OG	4:D:530:THR:O	1.74	1.04
2:J:2702:THR:C	4:L:2596:ASN:O	2.00	1.04
4:P:3514:PRO:HD3	4:P:3609:LEU:CB	1.87	1.04
2:J:2701:THR:HB	4:L:2595:ASN:O	1.58	1.04
4:L:2514:PRO:HD3	4:L:2609:LEU:CB	1.87	1.04
3:C:102:ILE:CB	4:D:552:ASP:CB	2.30	1.03
2:F:1702:THR:HA	4:H:1593:TRP:NE1	0.75	1.03
2:J:2671:LYS:NZ	4:L:2596:ASN:OD1	1.92	1.03
3:K:2045:PHE:CE2	4:L:2546:PHE:CE1	2.46	1.03
2:F:1703:THR:HG23	4:H:1596:ASN:CB	1.87	1.03
3:O:3045:PHE:CE2	4:P:3546:PHE:CE1	2.46	1.03
3:C:45:PHE:CE2	4:D:546:PHE:CE1	2.46	1.03
2:J:2671:LYS:HB3	4:L:2596:ASN:CA	1.76	1.03
2:J:2668:HIS:NE2	4:L:2598:TRP:CZ2	2.26	1.03
2:J:2692:ARG:NH1	3:K:2057:GLU:CG	2.22	1.03
2:N:3670:ALA:O	4:P:3595:ASN:HA	1.58	1.03
4:D:514:PRO:HD3	4:D:609:LEU:CB	1.87	1.02
2:B:702:THR:O	4:D:593:TRP:CH2	2.11	1.02
3:G:1045:PHE:CZ	4:H:1546:PHE:CE1	2.48	1.02
2:B:705:THR:O	4:D:595:ASN:CG	2.01	1.02
2:J:2670:ALA:CB	4:L:2599:VAL:HG23	1.90	1.02
3:K:2002:ILE:HD11	3:K:2098:ARG:NH1	1.62	1.01
2:J:2668:HIS:NE2	4:L:2598:TRP:CE3	2.11	1.01
3:C:45:PHE:CZ	4:D:546:PHE:CE1	2.48	1.01
2:J:2667:ILE:CG1	4:L:2595:ASN:HD21	1.73	1.01
2:J:2669:SER:HB2	4:L:2592:LEU:C	1.84	1.00
2:N:3689:PRO:CB	3:O:3057:GLU:OE2	2.09	1.00
2:B:667:ILE:HB	4:D:532:SER:OG	1.61	1.00
2:J:2700:HIS:HB2	4:L:2593:TRP:CE2	1.96	1.00
3:K:2045:PHE:CZ	4:L:2546:PHE:CE1	2.48	1.00
3:O:3102:ILE:CB	4:P:3552:ASP:CB	2.30	1.00
3:O:3045:PHE:CZ	4:P:3546:PHE:CE1	2.48	1.00
2:N:3668:HIS:NE2	3:O:3102:ILE:HA	1.11	1.00
2:B:671:LYS:CE	4:D:594:TYR:O	2.08	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:THR:HG22	4:D:594:TYR:O	1.59	1.00
3:C:35:LEU:HD21	3:C:37:VAL:HG22	1.43	1.00
2:B:702:THR:O	4:D:593:TRP:HH2	1.44	1.00
2:F:1703:THR:HA	4:H:1596:ASN:CB	1.91	0.99
2:F:1703:THR:HA	4:H:1596:ASN:HB3	1.44	0.99
2:B:668:HIS:HE1	3:C:102:ILE:HG22	1.20	0.99
3:G:1102:ILE:CB	4:H:1552:ASP:CB	2.30	0.99
2:J:2703:THR:OG1	3:K:2059:THR:HG23	1.60	0.99
3:G:1032:TYR:CZ	3:G:1100:TYR:CE1	2.50	0.99
3:C:32:TYR:CZ	3:C:100:TYR:CE1	2.50	0.99
2:F:1671:LYS:HB2	4:H:1532:SER:O	1.63	0.99
3:O:3217:ARG:HH21	4:P:3622:PRO:HD2	1.18	0.98
2:B:705:THR:HG23	4:D:596:ASN:ND2	1.77	0.98
2:J:2702:THR:CB	3:K:2047:TRP:HH2	1.74	0.98
4:H:1563:ARG:NH2	4:H:1584:ASP:OD1	1.96	0.98
3:K:2032:TYR:CZ	3:K:2100:TYR:CE1	2.50	0.98
3:O:3032:TYR:CZ	3:O:3100:TYR:CE1	2.50	0.98
3:G:1097:VAL:HG11	3:G:1104:LEU:HD23	1.45	0.98
2:J:2669:SER:HA	4:L:2594:TYR:CE1	1.94	0.98
3:G:1035:LEU:HD21	3:G:1037:VAL:HG22	1.43	0.98
2:N:3705:THR:HB	4:P:3595:ASN:CB	1.76	0.98
1:A:290:ARG:HH22	1:I:2356:HIS:CE1	1.80	0.98
3:K:2011:VAL:HG11	3:K:2151:PRO:CB	1.93	0.98
2:J:2700:HIS:NE2	3:K:2050:LEU:HD13	1.76	0.98
2:B:671:LYS:HA	4:D:595:ASN:HA	1.00	0.97
3:C:11:VAL:HG11	3:C:151:PRO:CB	1.93	0.97
3:K:2011:VAL:HG21	3:K:2152:GLU:H	1.29	0.97
3:K:2032:TYR:CE1	3:K:2100:TYR:CE1	2.52	0.97
3:G:1102:ILE:CG2	4:H:1534:CYS:HB3	1.94	0.97
1:A:291:ILE:CG2	1:I:2316:ILE:HD13	1.94	0.97
3:G:1011:VAL:HG11	3:G:1151:PRO:CB	1.93	0.97
3:O:3011:VAL:HG11	3:O:3151:PRO:CB	1.93	0.97
4:L:2563:ARG:NH2	4:L:2584:ASP:OD1	1.96	0.97
4:H:1631:ASN:HA	4:H:1685:ALA:HB2	1.47	0.97
2:J:2670:ALA:HB2	4:L:2599:VAL:CG2	1.95	0.97
3:K:2217:ARG:HH21	4:L:2622:PRO:HD2	1.18	0.97
4:P:3563:ARG:NH2	4:P:3584:ASP:OD1	1.96	0.97
3:O:3035:LEU:HD21	3:O:3037:VAL:HG22	1.43	0.97
3:O:3097:VAL:HG11	3:O:3104:LEU:HD23	1.45	0.97
4:H:1513:SER:OG	4:H:1609:LEU:HD22	1.65	0.97
3:K:2035:LEU:HD21	3:K:2037:VAL:HG22	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:VAL:HG11	3:C:104:LEU:HD23	1.45	0.97
4:L:2631:ASN:HA	4:L:2685:ALA:HB2	1.47	0.96
4:P:3631:ASN:HA	4:P:3685:ALA:HB2	1.47	0.96
1:A:291:ILE:HG21	1:I:2316:ILE:HD13	1.47	0.96
4:D:563:ARG:NH2	4:D:584:ASP:OD1	1.96	0.96
3:O:3032:TYR:CE1	3:O:3100:TYR:CE1	2.52	0.96
3:C:32:TYR:CE1	3:C:100:TYR:CE1	2.52	0.96
2:F:1703:THR:HA	4:H:1596:ASN:CA	1.82	0.96
2:B:705:THR:HB	4:D:595:ASN:ND2	1.73	0.96
4:D:513:SER:OG	4:D:609:LEU:HD22	1.65	0.96
2:J:2666:SER:CB	4:L:2532:SER:HB2	1.95	0.96
3:K:2102:ILE:CG2	4:L:2534:CYS:HB3	1.94	0.96
3:O:3102:ILE:CG2	4:P:3534:CYS:HB3	1.94	0.96
2:J:2673:LYS:HD3	4:L:2593:TRP:CD1	1.99	0.96
3:G:1032:TYR:CE1	3:G:1100:TYR:CE1	2.52	0.96
2:J:2668:HIS:HE1	4:L:2598:TRP:CH2	1.78	0.95
3:G:1045:PHE:HE2	4:H:1546:PHE:CZ	1.80	0.95
2:B:692:ARG:NH2	3:C:57:GLU:OE1	1.93	0.95
3:K:2097:VAL:HG11	3:K:2104:LEU:HD23	1.45	0.95
4:P:3513:SER:OG	4:P:3609:LEU:HD22	1.65	0.95
3:C:11:VAL:HG21	3:C:152:GLU:H	1.29	0.95
2:J:2669:SER:HB3	4:L:2592:LEU:CB	1.81	0.95
3:O:3011:VAL:HG21	3:O:3152:GLU:H	1.29	0.95
3:C:217:ARG:HH21	4:D:622:PRO:HD2	1.19	0.95
2:B:671:LYS:CE	4:D:597:LEU:H	1.78	0.95
2:J:2668:HIS:NE2	4:L:2598:TRP:CD2	2.34	0.95
2:F:1673:LYS:HB2	4:H:1532:SER:HB3	1.46	0.95
3:G:1011:VAL:HG21	3:G:1152:GLU:H	1.30	0.95
2:F:1670:ALA:N	4:H:1533:ASN:CG	2.11	0.94
3:K:2102:ILE:HG23	4:L:2534:CYS:SG	2.07	0.94
2:J:2667:ILE:CG1	4:L:2595:ASN:ND2	2.30	0.94
4:L:2513:SER:OG	4:L:2609:LEU:HD22	1.65	0.94
3:G:1102:ILE:HG23	4:H:1534:CYS:SG	2.07	0.94
4:D:631:ASN:HA	4:D:685:ALA:HB2	1.47	0.94
3:O:3118:ALA:HB1	3:O:3150:PHE:CE2	2.03	0.94
3:G:1035:LEU:HD22	3:G:1037:VAL:HG23	1.48	0.94
2:J:2671:LYS:HA	4:L:2596:ASN:H	1.31	0.94
4:P:3694:TYR:HB2	4:P:3709:LEU:HD22	1.50	0.94
3:C:118:ALA:HB1	3:C:150:PHE:CE2	2.03	0.94
3:G:1217:ARG:HH21	4:H:1622:PRO:HD2	1.18	0.94
3:K:2032:TYR:CZ	3:K:2100:TYR:CD1	2.56	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2666:SER:HB2	4:L:2532:SER:CB	1.98	0.94
3:O:3102:ILE:HG23	4:P:3534:CYS:SG	2.07	0.94
3:K:2045:PHE:HE2	4:L:2546:PHE:CZ	1.80	0.93
3:G:1118:ALA:HB1	3:G:1150:PHE:CE2	2.03	0.93
4:H:1694:TYR:HB2	4:H:1709:LEU:HD22	1.50	0.93
2:J:2668:HIS:H	4:L:2595:ASN:H	1.15	0.93
3:G:1032:TYR:CZ	3:G:1100:TYR:CD1	2.56	0.93
2:J:2670:ALA:CB	4:L:2599:VAL:CG2	2.44	0.93
2:N:3671:LYS:HZ1	4:P:3596:ASN:CA	1.80	0.93
4:D:694:TYR:HB2	4:D:709:LEU:HD22	1.50	0.93
3:C:32:TYR:CZ	3:C:100:TYR:CD1	2.56	0.93
2:J:2700:HIS:CE1	3:K:2050:LEU:CD1	2.51	0.93
2:B:671:LYS:HD2	4:D:593:TRP:CZ3	1.99	0.93
3:O:3035:LEU:HD22	3:O:3037:VAL:HG23	1.48	0.93
3:C:35:LEU:HD22	3:C:37:VAL:HG23	1.48	0.93
4:L:2694:TYR:HB2	4:L:2709:LEU:HD22	1.50	0.93
2:B:702:THR:C	4:D:596:ASN:HA	1.94	0.93
2:J:2705:THR:CG2	4:L:2596:ASN:ND2	2.32	0.93
3:K:2097:VAL:CG1	3:K:2104:LEU:HD23	1.98	0.93
2:J:2667:ILE:HG22	4:L:2594:TYR:HA	1.49	0.92
2:J:2692:ARG:NH2	3:K:2057:GLU:HG2	1.83	0.92
3:K:2078:THR:HG21	3:K:2080:TYR:OH	1.69	0.92
3:G:1097:VAL:CG1	3:G:1104:LEU:HD23	1.98	0.92
2:F:1702:THR:N	4:H:1593:TRP:HE1	1.67	0.92
3:O:3045:PHE:HE2	4:P:3546:PHE:CZ	1.80	0.92
3:O:3097:VAL:CG1	3:O:3104:LEU:HD23	1.98	0.92
3:C:102:ILE:HG23	4:D:534:CYS:SG	2.07	0.92
3:O:3032:TYR:CZ	3:O:3100:TYR:CD1	2.56	0.92
3:G:1035:LEU:HD21	3:G:1037:VAL:CG2	1.98	0.92
3:K:2035:LEU:HD22	3:K:2037:VAL:HG23	1.48	0.92
2:B:705:THR:O	4:D:595:ASN:ND2	2.02	0.92
3:C:78:THR:HG21	3:C:80:TYR:OH	1.69	0.92
3:C:97:VAL:CG1	3:C:104:LEU:HD23	1.98	0.92
3:C:45:PHE:HE2	4:D:546:PHE:CZ	1.80	0.92
2:J:2667:ILE:CD1	4:L:2595:ASN:ND2	0.79	0.92
3:G:1032:TYR:HE1	3:G:1100:TYR:HD1	1.13	0.91
3:G:1118:ALA:CB	3:G:1150:PHE:CZ	2.51	0.91
2:J:2702:THR:HA	4:L:2596:ASN:O	1.70	0.91
3:K:2118:ALA:HB1	3:K:2150:PHE:CE2	2.03	0.91
3:G:1078:THR:HG21	3:G:1080:TYR:OH	1.69	0.91
2:J:2666:SER:OG	4:L:2532:SER:HB2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2668:HIS:NE2	4:L:2598:TRP:CE2	2.38	0.91
3:O:3032:TYR:HE1	3:O:3100:TYR:HD1	1.13	0.91
2:J:2670:ALA:HB3	4:L:2599:VAL:HG23	1.52	0.90
3:K:2032:TYR:HE1	3:K:2100:TYR:HD1	1.13	0.90
2:F:1703:THR:O	4:H:1595:ASN:HB3	1.52	0.90
2:J:2669:SER:HG	4:L:2533:ASN:HB3	1.28	0.90
2:J:2670:ALA:HB2	4:L:2599:VAL:HG21	1.53	0.90
3:O:3078:THR:HG21	3:O:3080:TYR:OH	1.69	0.90
4:P:3552:ASP:HB3	4:P:3555:ASN:ND2	1.87	0.90
2:J:2671:LYS:HG3	4:L:2593:TRP:CZ3	2.05	0.90
2:J:2667:ILE:CG2	4:L:2594:TYR:HA	2.01	0.90
2:J:2673:LYS:HB2	4:L:2593:TRP:HD1	1.30	0.90
2:B:667:ILE:CA	4:D:532:SER:CB	1.96	0.90
3:C:11:VAL:HG11	3:C:151:PRO:HB3	1.53	0.90
2:B:671:LYS:N	4:D:595:ASN:N	1.96	0.90
3:O:3011:VAL:HG11	3:O:3151:PRO:HB3	1.53	0.90
3:G:1011:VAL:HG11	3:G:1151:PRO:HB3	1.53	0.89
3:G:1011:VAL:HG21	3:G:1152:GLU:N	1.87	0.89
2:J:2666:SER:HB2	4:L:2532:SER:HB2	1.54	0.89
2:J:2702:THR:HB	3:K:2047:TRP:HH2	1.34	0.89
3:K:2011:VAL:HG21	3:K:2152:GLU:N	1.87	0.89
3:G:1173:LEU:HD12	4:H:1665:THR:HG22	1.54	0.89
2:J:2668:HIS:HE2	4:L:2598:TRP:CZ3	1.29	0.89
3:O:3035:LEU:HD21	3:O:3037:VAL:CG2	1.98	0.89
4:D:694:TYR:HB2	4:D:709:LEU:CD2	2.03	0.89
3:K:2173:LEU:HD12	4:L:2665:THR:HG22	1.54	0.89
4:D:552:ASP:HB3	4:D:555:ASN:ND2	1.87	0.89
4:H:1694:TYR:HB2	4:H:1709:LEU:CD2	2.03	0.88
3:C:11:VAL:HG21	3:C:152:GLU:N	1.87	0.88
3:K:2011:VAL:HG11	3:K:2151:PRO:HB3	1.53	0.88
4:L:2554:ASN:HD22	4:L:2554:ASN:C	1.81	0.88
3:C:35:LEU:HD21	3:C:37:VAL:CG2	1.98	0.88
3:O:3011:VAL:HG21	3:O:3152:GLU:N	1.87	0.88
4:H:1552:ASP:HB3	4:H:1555:ASN:ND2	1.87	0.88
4:L:2552:ASP:HB3	4:L:2555:ASN:ND2	1.87	0.88
4:H:1554:ASN:C	4:H:1554:ASN:HD22	1.81	0.88
2:J:2668:HIS:CE1	4:L:2598:TRP:CZ2	2.61	0.88
2:J:2692:ARG:CZ	3:K:2057:GLU:OE2	2.21	0.88
2:J:2701:THR:CB	4:L:2596:ASN:HA	1.96	0.88
3:C:173:LEU:HD12	4:D:665:THR:HG22	1.54	0.87
2:F:1671:LYS:O	4:H:1532:SER:OG	1.91	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2667:ILE:CD1	4:L:2595:ASN:CG	1.78	0.87
3:O:3173:LEU:HD12	4:P:3665:THR:HG22	1.54	0.87
2:F:1703:THR:CA	4:H:1596:ASN:HB3	2.04	0.87
2:F:1671:LYS:HG3	4:H:1593:TRP:CD1	2.09	0.87
3:K:2118:ALA:CB	3:K:2150:PHE:CZ	2.51	0.87
4:L:2694:TYR:HB2	4:L:2709:LEU:CD2	2.03	0.87
4:P:3694:TYR:HB2	4:P:3709:LEU:CD2	2.03	0.87
2:J:2672:VAL:CG1	4:L:2595:ASN:O	2.23	0.87
2:F:1670:ALA:HB1	4:H:1594:TYR:CE1	2.09	0.87
3:O:3011:VAL:CB	3:O:3151:PRO:HB2	2.05	0.87
1:A:290:ARG:NH2	1:I:2356:HIS:CE1	2.43	0.86
3:C:32:TYR:HE1	3:C:100:TYR:HD1	1.13	0.86
4:P:3554:ASN:C	4:P:3554:ASN:HD22	1.81	0.86
2:J:2692:ARG:CZ	3:K:2057:GLU:CD	2.48	0.86
3:C:11:VAL:CB	3:C:151:PRO:HB2	2.05	0.86
3:G:1011:VAL:CB	3:G:1151:PRO:HB2	2.05	0.86
3:O:3070:PHE:HE1	3:O:3081:LEU:HD13	1.40	0.86
4:D:554:ASN:HD22	4:D:554:ASN:C	1.81	0.86
3:K:2011:VAL:CB	3:K:2151:PRO:HB2	2.05	0.86
3:K:2035:LEU:HD21	3:K:2037:VAL:CG2	1.98	0.86
2:B:671:LYS:HZ1	4:D:597:LEU:H	1.17	0.86
2:N:3671:LYS:NZ	4:P:3596:ASN:CA	2.37	0.86
2:B:671:LYS:CE	4:D:595:ASN:N	2.26	0.85
2:B:702:THR:HA	4:D:593:TRP:CZ2	2.09	0.85
3:G:1035:LEU:HD22	3:G:1037:VAL:CG2	2.05	0.85
3:G:1039:GLN:NE2	3:G:1045:PHE:CZ	2.44	0.85
1:A:291:ILE:HG21	1:I:2316:ILE:CD1	2.06	0.85
3:K:2070:PHE:HE1	3:K:2081:LEU:HD13	1.40	0.85
4:P:3513:SER:HA	4:P:3609:LEU:HB2	1.59	0.85
2:B:702:THR:CA	4:D:593:TRP:CH2	2.59	0.85
3:G:1070:PHE:HE1	3:G:1081:LEU:HD13	1.40	0.85
3:C:39:GLN:NE2	3:C:45:PHE:CZ	2.44	0.85
2:B:671:LYS:HZ1	4:D:597:LEU:N	1.71	0.85
3:C:70:PHE:HE1	3:C:81:LEU:HD13	1.40	0.85
2:J:2670:ALA:H	4:L:2594:TYR:N	1.72	0.85
2:F:1670:ALA:HB1	4:H:1594:TYR:CD1	2.11	0.85
4:L:2513:SER:HA	4:L:2609:LEU:HB2	1.59	0.85
3:O:3118:ALA:CB	3:O:3150:PHE:CZ	2.51	0.85
3:O:3039:GLN:NE2	3:O:3045:PHE:CZ	2.44	0.84
2:B:667:ILE:CB	4:D:532:SER:OG	2.24	0.84
3:C:35:LEU:HD22	3:C:37:VAL:CG2	2.04	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:VAL:HG11	3:C:151:PRO:HB2	1.60	0.84
3:C:78:THR:CG2	3:C:80:TYR:CE1	2.61	0.84
3:O:3175:GLN:HG3	4:P:3663:GLU:OE2	1.78	0.84
3:C:118:ALA:CB	3:C:150:PHE:CZ	2.51	0.84
3:G:1011:VAL:HG11	3:G:1151:PRO:HB2	1.60	0.84
3:C:102:ILE:HG21	4:D:552:ASP:CG	2.02	0.84
2:F:1701:THR:O	4:H:1595:ASN:HA	1.78	0.84
4:H:1582:THR:OG1	4:H:1610:GLY:HA3	1.78	0.84
3:K:2039:GLN:NE2	3:K:2045:PHE:CZ	2.44	0.84
3:G:1078:THR:CG2	3:G:1080:TYR:CE1	2.61	0.84
2:J:2668:HIS:CD2	4:L:2593:TRP:CE3	2.65	0.83
2:N:3670:ALA:O	4:P:3595:ASN:CA	2.25	0.83
1:A:125:HIS:CE1	1:E:1126:THR:HG22	2.13	0.83
3:G:1037:VAL:HG21	3:G:1107:TRP:CH2	2.13	0.83
3:O:3091:THR:HG22	3:O:3115:VAL:H	1.43	0.83
2:B:671:LYS:C	4:D:595:ASN:HA	2.02	0.83
2:J:2692:ARG:HH12	3:K:2057:GLU:CG	1.90	0.83
3:O:3037:VAL:HG21	3:O:3107:TRP:CH2	2.13	0.83
1:A:126:THR:HG22	1:E:1125:HIS:CE1	2.13	0.83
3:K:2175:GLN:HG3	4:L:2663:GLU:OE2	1.78	0.83
4:P:3653:VAL:HG23	4:P:3658:VAL:HG21	1.60	0.83
2:J:2667:ILE:CD1	4:L:2595:ASN:HD21	0.50	0.83
3:C:37:VAL:HG21	3:C:107:TRP:CH2	2.13	0.83
4:D:582:THR:OG1	4:D:610:GLY:HA3	1.78	0.83
2:F:1669:SER:CA	4:H:1533:ASN:OD1	2.25	0.83
3:K:2011:VAL:HG11	3:K:2151:PRO:HB2	1.60	0.83
3:O:3102:ILE:HG21	4:P:3552:ASP:CG	2.03	0.83
3:C:175:GLN:HG3	4:D:663:GLU:OE2	1.78	0.83
4:D:513:SER:HA	4:D:609:LEU:HB2	1.59	0.83
4:D:683:LEU:HD11	4:D:694:TYR:HE2	1.44	0.83
3:G:1102:ILE:HG21	4:H:1552:ASP:CG	2.03	0.83
2:J:2701:THR:C	4:L:2593:TRP:HH2	1.85	0.83
2:J:2702:THR:HB	3:K:2047:TRP:CH2	2.13	0.83
3:K:2091:THR:HG22	3:K:2115:VAL:H	1.43	0.83
4:L:2683:LEU:HD11	4:L:2694:TYR:HE2	1.44	0.83
4:H:1513:SER:HA	4:H:1609:LEU:HB2	1.59	0.83
4:H:1683:LEU:HD11	4:H:1694:TYR:HE2	1.44	0.83
3:O:3030:THR:HG23	3:O:3054:ASN:HD22	1.44	0.83
4:D:653:VAL:HG23	4:D:658:VAL:HG21	1.60	0.83
3:K:2078:THR:CG2	3:K:2080:TYR:CE1	2.61	0.83
3:K:2102:ILE:HG21	4:L:2552:ASP:CG	2.03	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:3667:ILE:CG2	4:P:3532:SER:HB2	2.09	0.83
4:P:3683:LEU:HD11	4:P:3694:TYR:HE2	1.44	0.83
3:G:1175:GLN:HG3	4:H:1663:GLU:OE2	1.78	0.82
3:K:2078:THR:HG21	3:K:2080:TYR:CE2	2.14	0.82
4:P:3582:THR:OG1	4:P:3610:GLY:HA3	1.78	0.82
2:N:3669:SER:OG	4:P:3531:SER:O	1.95	0.82
3:C:30:THR:HG23	3:C:54:ASN:HD22	1.44	0.82
3:O:3078:THR:CG2	3:O:3080:TYR:CE1	2.61	0.82
2:J:2666:SER:CB	4:L:2532:SER:CB	2.56	0.82
3:K:2037:VAL:HG21	3:K:2107:TRP:CH2	2.13	0.82
3:O:3102:ILE:CG2	4:P:3534:CYS:SG	2.68	0.82
3:C:98:ARG:NH2	3:C:105:ASP:OD2	2.13	0.82
3:G:1102:ILE:HG13	4:H:1552:ASP:OD2	1.80	0.82
4:L:2582:THR:OG1	4:L:2610:GLY:HA3	1.78	0.82
2:B:705:THR:CB	4:D:595:ASN:HD22	1.84	0.82
2:B:671:LYS:HE2	4:D:595:ASN:CA	2.07	0.82
2:F:1671:LYS:O	4:H:1532:SER:CB	2.28	0.82
2:J:2702:THR:HG22	3:K:2047:TRP:CZ2	2.14	0.82
4:H:1653:VAL:HG23	4:H:1658:VAL:HG21	1.60	0.82
3:K:2102:ILE:HG13	4:L:2552:ASP:OD2	1.80	0.82
3:K:2102:ILE:HG22	3:K:2102:ILE:O	1.79	0.82
3:O:3102:ILE:HG13	4:P:3552:ASP:OD2	1.80	0.82
3:G:1011:VAL:HG21	3:G:1151:PRO:HB2	1.62	0.81
2:B:672:VAL:N	4:D:595:ASN:HA	1.95	0.81
3:C:11:VAL:HG21	3:C:151:PRO:HB2	1.62	0.81
3:C:78:THR:HG21	3:C:80:TYR:CE2	2.14	0.81
3:G:1030:THR:HG23	3:G:1054:ASN:HD22	1.44	0.81
3:G:1078:THR:HG21	3:G:1080:TYR:CE2	2.14	0.81
2:J:2705:THR:CB	4:L:2596:ASN:ND2	2.43	0.81
3:O:3078:THR:HG21	3:O:3080:TYR:CE2	2.14	0.81
2:J:2700:HIS:HB2	4:L:2593:TRP:CH2	2.15	0.81
3:O:3098:ARG:NH2	3:O:3105:ASP:OD2	2.13	0.81
2:J:2667:ILE:CG2	4:L:2594:TYR:HD1	1.94	0.81
3:K:2035:LEU:HD22	3:K:2037:VAL:CG2	2.05	0.81
3:K:2098:ARG:NH2	3:K:2105:ASP:OD2	2.13	0.81
3:O:3011:VAL:HG21	3:O:3151:PRO:HB2	1.62	0.81
3:K:2102:ILE:CG2	4:L:2534:CYS:SG	2.68	0.81
2:B:670:ALA:HA	4:D:594:TYR:CD1	2.16	0.81
4:L:2653:VAL:HG23	4:L:2658:VAL:HG21	1.60	0.81
3:G:1102:ILE:CG2	4:H:1534:CYS:SG	2.68	0.81
3:G:1102:ILE:HG22	3:G:1102:ILE:O	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2668:HIS:HA	4:L:2533:ASN:HA	1.63	0.80
3:O:3011:VAL:HG11	3:O:3151:PRO:HB2	1.60	0.80
3:C:91:THR:HG22	3:C:115:VAL:H	1.43	0.80
3:G:1102:ILE:CG1	4:H:1552:ASP:HB2	2.12	0.80
1:A:389:VAL:O	2:B:823:TRP:N	2.13	0.80
2:B:668:HIS:CE1	3:C:102:ILE:HG22	1.97	0.80
1:M:3389:VAL:O	2:N:3823:TRP:N	2.13	0.80
2:J:2700:HIS:CB	4:L:2593:TRP:CZ2	2.63	0.80
3:K:2011:VAL:HG21	3:K:2151:PRO:HB2	1.62	0.80
3:G:1098:ARG:NH2	3:G:1105:ASP:OD2	2.13	0.80
3:K:2030:THR:HG23	3:K:2054:ASN:HD22	1.44	0.80
3:O:3102:ILE:CG1	4:P:3552:ASP:HB2	2.12	0.80
3:C:102:ILE:HG13	4:D:552:ASP:OD2	1.80	0.80
2:J:2690:ASP:OD1	3:K:2059:THR:OG1	1.98	0.80
1:E:1389:VAL:O	2:F:1823:TRP:N	2.13	0.80
3:G:1102:ILE:CG2	4:H:1534:CYS:CB	2.60	0.80
2:J:2692:ARG:CZ	3:K:2057:GLU:HG2	2.11	0.80
2:J:2701:THR:HB	4:L:2596:ASN:CA	2.11	0.80
3:C:102:ILE:CG2	4:D:552:ASP:HA	2.12	0.80
3:C:102:ILE:HG22	3:C:102:ILE:O	1.79	0.80
4:H:1514:PRO:HD3	4:H:1609:LEU:HB2	1.62	0.80
2:B:668:HIS:HE1	3:C:102:ILE:HG21	1.44	0.79
2:F:1668:HIS:C	4:H:1530:THR:C	2.50	0.79
3:K:2102:ILE:CG2	4:L:2534:CYS:CB	2.60	0.79
3:K:2102:ILE:CG2	4:L:2552:ASP:HA	2.12	0.79
2:N:3667:ILE:HG21	4:P:3532:SER:HB2	1.64	0.79
2:B:705:THR:CG2	4:D:596:ASN:ND2	2.44	0.79
2:J:2669:SER:HB2	4:L:2592:LEU:CA	2.11	0.79
3:O:3102:ILE:CG2	4:P:3534:CYS:CB	2.60	0.79
3:G:1091:THR:HG22	3:G:1115:VAL:H	1.43	0.79
3:G:1102:ILE:CG1	4:H:1552:ASP:CG	2.56	0.79
2:J:2702:THR:CB	3:K:2047:TRP:CH2	2.64	0.79
2:F:1670:ALA:CB	4:H:1594:TYR:CE1	2.66	0.79
3:G:1020:ILE:HD11	3:G:1113:LEU:HD11	1.65	0.79
2:J:2673:LYS:CB	4:L:2593:TRP:CD1	2.64	0.79
4:P:3514:PRO:HD3	4:P:3609:LEU:HB2	1.62	0.79
3:C:102:ILE:CG1	4:D:552:ASP:HB2	2.12	0.79
4:L:2514:PRO:HD3	4:L:2609:LEU:HB2	1.62	0.79
4:D:514:PRO:HD3	4:D:609:LEU:HB2	1.62	0.79
3:O:3102:ILE:HG22	3:O:3102:ILE:O	1.79	0.79
3:O:3020:ILE:HD11	3:O:3113:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2102:ILE:CG1	4:L:2552:ASP:HB2	2.12	0.79
3:C:2:ILE:HD12	3:C:98:ARG:NH1	1.98	0.78
1:I:2389:VAL:O	2:J:2823:TRP:N	2.13	0.78
2:B:672:VAL:N	4:D:595:ASN:OD1	2.16	0.78
3:C:20:ILE:HD11	3:C:113:LEU:HD11	1.65	0.78
3:C:102:ILE:CG1	4:D:552:ASP:CG	2.56	0.78
3:G:1102:ILE:CG2	4:H:1552:ASP:HA	2.12	0.78
2:J:2705:THR:HG22	4:L:2596:ASN:ND2	1.98	0.78
4:L:2519:THR:C	4:L:2520:LEU:HD23	2.09	0.78
4:L:2695:SER:HB2	4:L:2708:SER:OG	1.83	0.78
3:O:3102:ILE:CG2	4:P:3552:ASP:HA	2.12	0.78
4:D:695:SER:HB2	4:D:708:SER:OG	1.83	0.78
3:O:3102:ILE:CG1	4:P:3552:ASP:CG	2.56	0.78
2:B:705:THR:CG2	4:D:596:ASN:HD22	1.90	0.78
4:D:542:PRO:O	4:D:543:ASP:HB2	1.83	0.78
2:B:668:HIS:O	4:D:533:ASN:C	2.05	0.78
4:P:3519:THR:C	4:P:3520:LEU:HD23	2.09	0.78
4:P:3695:SER:HB2	4:P:3708:SER:OG	1.83	0.78
4:P:3520:LEU:HD23	4:P:3520:LEU:N	1.99	0.78
3:C:48:MET:HG2	3:C:64:PHE:CZ	2.19	0.78
2:J:2669:SER:CA	4:L:2533:ASN:HD22	1.96	0.78
2:J:2705:THR:N	4:L:2596:ASN:ND2	1.91	0.78
3:K:2021:SER:OG	3:K:2080:TYR:CD2	2.37	0.78
3:G:1102:ILE:CG2	4:H:1552:ASP:CB	2.62	0.78
4:L:2520:LEU:HD23	4:L:2520:LEU:N	1.99	0.78
3:K:2070:PHE:CE1	3:K:2081:LEU:HD13	2.19	0.77
3:K:2102:ILE:CG2	4:L:2552:ASP:CB	2.62	0.77
3:O:3102:ILE:CG2	4:P:3552:ASP:CB	2.62	0.77
3:K:2011:VAL:CG1	3:K:2151:PRO:HB2	2.14	0.77
3:K:2048:MET:HG2	3:K:2064:PHE:CZ	2.19	0.77
2:N:3669:SER:OG	4:P:3534:CYS:SG	2.42	0.77
3:C:70:PHE:CE1	3:C:81:LEU:HD13	2.19	0.77
3:C:78:THR:HG22	3:C:80:TYR:CE1	2.20	0.77
3:G:1021:SER:OG	3:G:1080:TYR:CD2	2.37	0.77
4:H:1695:SER:HB2	4:H:1708:SER:OG	1.83	0.77
3:O:3035:LEU:HD22	3:O:3037:VAL:CG2	2.05	0.77
4:D:519:THR:C	4:D:520:LEU:HD23	2.09	0.77
3:G:1048:MET:HG2	3:G:1064:PHE:CZ	2.19	0.77
4:H:1542:PRO:O	4:H:1543:ASP:HB2	1.83	0.77
3:O:3070:PHE:CE1	3:O:3081:LEU:HD13	2.19	0.77
3:C:45:PHE:CE1	4:D:589:PHE:CE2	2.73	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:520:LEU:HD23	4:D:520:LEU:N	1.99	0.77
3:G:1070:PHE:CE1	3:G:1081:LEU:HD13	2.19	0.77
2:J:2673:LYS:HA	4:L:2593:TRP:HE1	1.50	0.77
4:L:2514:PRO:HD3	4:L:2609:LEU:CA	2.15	0.77
3:O:3048:MET:HG2	3:O:3064:PHE:CZ	2.19	0.77
3:O:3217:ARG:NH2	4:P:3622:PRO:CD	2.45	0.77
4:D:685:ALA:O	4:D:688:TRP:HB3	1.85	0.77
2:J:2692:ARG:CZ	3:K:2057:GLU:CG	2.63	0.77
3:K:2045:PHE:CE1	4:L:2589:PHE:CE2	2.73	0.77
3:C:102:ILE:CG2	4:D:552:ASP:CB	2.62	0.77
4:D:514:PRO:HD3	4:D:609:LEU:CA	2.15	0.77
3:G:1002:ILE:HD12	3:G:1098:ARG:NH1	1.98	0.77
4:H:1519:THR:C	4:H:1520:LEU:HD23	2.09	0.77
4:H:1520:LEU:HD23	4:H:1520:LEU:N	1.99	0.77
2:N:3684:TYR:OH	2:N:3701:THR:OG1	2.03	0.77
3:O:3011:VAL:CG1	3:O:3151:PRO:HB2	2.14	0.77
2:F:1670:ALA:H	4:H:1533:ASN:CG	1.88	0.76
3:G:1045:PHE:CE1	4:H:1589:PHE:CE2	2.73	0.76
2:J:2756:PRO:O	2:J:2814:TRP:NE1	2.18	0.76
3:K:2020:ILE:HD11	3:K:2113:LEU:HD11	1.65	0.76
4:L:2685:ALA:O	4:L:2688:TRP:HB3	1.85	0.76
1:A:22:PRO:HA	1:I:2306:GLU:OE2	1.85	0.76
3:G:1078:THR:HG22	3:G:1080:TYR:CE1	2.20	0.76
2:N:3692:ARG:O	2:N:3711:ARG:NH2	2.19	0.76
4:H:1685:ALA:O	4:H:1688:TRP:HB3	1.85	0.76
2:J:2595:THR:OG1	2:J:2611:VAL:O	2.04	0.76
3:K:2102:ILE:CG1	4:L:2552:ASP:CG	2.56	0.76
2:B:667:ILE:N	4:D:532:SER:CB	2.48	0.76
2:B:684:TYR:OH	2:B:701:THR:OG1	2.03	0.76
2:F:1692:ARG:O	2:F:1711:ARG:NH2	2.19	0.76
2:J:2669:SER:CA	4:L:2594:TYR:CE1	2.44	0.76
4:L:2542:PRO:O	4:L:2543:ASP:HB2	1.83	0.76
3:O:3045:PHE:CE1	4:P:3589:PHE:CE2	2.73	0.76
4:P:3514:PRO:CD	4:P:3609:LEU:O	2.34	0.76
2:B:692:ARG:O	2:B:711:ARG:NH2	2.19	0.76
3:C:11:VAL:CG2	3:C:151:PRO:HB2	2.16	0.76
4:P:3542:PRO:O	4:P:3543:ASP:HB2	1.83	0.76
3:G:1011:VAL:CG2	3:G:1151:PRO:HB2	2.16	0.76
3:K:2011:VAL:CG2	3:K:2151:PRO:HB2	2.16	0.76
2:N:3595:THR:OG1	2:N:3611:VAL:O	2.04	0.76
2:B:595:THR:OG1	2:B:611:VAL:O	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:SER:CB	3:C:80:TYR:CE2	2.69	0.76
3:G:1011:VAL:CG1	3:G:1151:PRO:HB2	2.14	0.76
2:J:2672:VAL:HG13	4:L:2595:ASN:O	1.85	0.76
3:O:3011:VAL:CG2	3:O:3151:PRO:HB2	2.16	0.76
3:O:3078:THR:HG22	3:O:3080:TYR:CE1	2.20	0.76
3:O:3097:VAL:HG11	3:O:3104:LEU:CD2	2.16	0.76
4:P:3514:PRO:HD3	4:P:3609:LEU:CA	2.15	0.76
4:P:3685:ALA:O	4:P:3688:TRP:HB3	1.85	0.76
2:F:1595:THR:OG1	2:F:1611:VAL:O	2.04	0.76
4:H:1514:PRO:HD3	4:H:1609:LEU:CA	2.15	0.76
2:J:2673:LYS:CA	4:L:2593:TRP:HE1	1.99	0.76
2:J:2692:ARG:HH22	3:K:2057:GLU:HG2	1.50	0.76
2:J:2692:ARG:O	2:J:2711:ARG:NH2	2.19	0.76
3:O:3002:ILE:HD12	3:O:3098:ARG:NH1	1.98	0.76
3:C:11:VAL:CG1	3:C:151:PRO:HB2	2.14	0.76
2:F:1756:PRO:O	2:F:1814:TRP:NE1	2.18	0.76
2:J:2753:THR:OG1	2:J:2816:ASN:ND2	2.20	0.76
2:N:3756:PRO:O	2:N:3814:TRP:NE1	2.18	0.76
3:C:217:ARG:NH2	4:D:622:PRO:CD	2.45	0.75
2:B:756:PRO:O	2:B:814:TRP:NE1	2.18	0.75
4:D:514:PRO:CD	4:D:609:LEU:O	2.34	0.75
3:K:2217:ARG:NH2	4:L:2622:PRO:CD	2.45	0.75
3:G:1217:ARG:NH2	4:H:1622:PRO:CD	2.45	0.75
4:L:2514:PRO:CD	4:L:2609:LEU:O	2.34	0.75
2:N:3753:THR:OG1	2:N:3816:ASN:ND2	2.20	0.75
3:O:3021:SER:CB	3:O:3080:TYR:CE2	2.69	0.75
2:B:705:THR:CG2	4:D:594:TYR:O	2.33	0.75
3:C:97:VAL:HG11	3:C:104:LEU:CD2	2.16	0.75
3:K:2002:ILE:HD12	3:K:2098:ARG:NH1	1.98	0.75
3:K:2078:THR:HG22	3:K:2080:TYR:CE1	2.20	0.75
3:G:1102:ILE:HG21	4:H:1552:ASP:HA	1.69	0.75
4:H:1514:PRO:CD	4:H:1609:LEU:O	2.34	0.75
1:A:291:ILE:CG2	1:I:2316:ILE:CD1	2.63	0.75
2:J:2669:SER:N	4:L:2533:ASN:ND2	2.29	0.75
3:K:2021:SER:CB	3:K:2080:TYR:CE2	2.69	0.75
2:B:705:THR:C	4:D:595:ASN:ND2	2.43	0.75
3:G:1021:SER:CB	3:G:1080:TYR:CE2	2.69	0.75
2:J:2701:THR:HG22	4:L:2596:ASN:HB2	1.67	0.75
3:K:2002:ILE:HD13	3:K:2098:ARG:NH1	2.00	0.75
4:L:2514:PRO:CD	4:L:2609:LEU:CB	2.65	0.75
4:P:3552:ASP:HB3	4:P:3555:ASN:HD22	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:552:ASP:HB3	4:D:555:ASN:HD22	1.51	0.75
3:G:1097:VAL:CG2	3:G:1107:TRP:CE3	2.70	0.75
3:K:2097:VAL:CG2	3:K:2107:TRP:CE3	2.70	0.75
3:C:2:ILE:HD13	3:C:98:ARG:NH1	2.00	0.74
2:J:2702:THR:CA	3:K:2047:TRP:HH2	1.99	0.74
4:P:3631:ASN:CA	4:P:3685:ALA:HB2	2.17	0.74
2:B:668:HIS:HB3	4:D:593:TRP:HD1	1.51	0.74
3:O:3021:SER:OG	3:O:3080:TYR:CD2	2.37	0.74
3:G:1024:ALA:HB1	3:G:1027:TYR:CE1	2.22	0.74
4:H:1514:PRO:CD	4:H:1609:LEU:CB	2.65	0.74
3:O:3097:VAL:HG21	3:O:3107:TRP:CE3	2.22	0.74
4:H:1631:ASN:CA	4:H:1685:ALA:HB2	2.17	0.74
3:K:2097:VAL:HG21	3:K:2107:TRP:CE3	2.23	0.74
4:L:2552:ASP:HB3	4:L:2555:ASN:HD22	1.51	0.74
4:L:2631:ASN:CA	4:L:2685:ALA:HB2	2.17	0.74
3:O:3097:VAL:CG2	3:O:3107:TRP:CE3	2.70	0.74
3:O:3102:ILE:HG21	4:P:3552:ASP:HA	1.69	0.74
2:B:753:THR:OG1	2:B:816:ASN:ND2	2.19	0.74
3:G:1002:ILE:HD13	3:G:1098:ARG:NH1	2.00	0.74
2:J:2700:HIS:HE1	3:K:2050:LEU:HD13	1.43	0.74
3:K:2097:VAL:HG11	3:K:2104:LEU:CD2	2.16	0.74
3:C:97:VAL:CG2	3:C:107:TRP:CE3	2.70	0.74
2:F:1753:THR:OG1	2:F:1816:ASN:ND2	2.20	0.74
3:K:2102:ILE:HG21	4:L:2552:ASP:HA	1.69	0.74
1:A:30:GLN:OE1	1:A:136:THR:OG1	2.06	0.74
3:C:24:ALA:HB1	3:C:27:TYR:CE1	2.22	0.74
3:O:3002:ILE:HD13	3:O:3098:ARG:NH1	2.00	0.74
3:O:3024:ALA:HB1	3:O:3027:TYR:CE1	2.22	0.74
2:B:702:THR:C	4:D:593:TRP:HH2	1.95	0.74
3:C:97:VAL:HG21	3:C:107:TRP:CE3	2.23	0.74
3:C:102:ILE:HB	4:D:552:ASP:HB2	0.75	0.74
1:E:1030:GLN:OE1	1:E:1136:THR:OG1	2.06	0.74
1:M:3030:GLN:OE1	1:M:3136:THR:OG1	2.06	0.74
2:B:702:THR:C	4:D:593:TRP:CH2	2.65	0.73
3:G:1097:VAL:HG11	3:G:1104:LEU:CD2	2.16	0.73
2:J:2667:ILE:HG21	4:L:2594:TYR:HD1	1.52	0.73
3:K:2024:ALA:HB1	3:K:2027:TYR:CE1	2.22	0.73
4:P:3514:PRO:CD	4:P:3609:LEU:CB	2.65	0.73
4:D:631:ASN:CA	4:D:685:ALA:HB2	2.17	0.73
3:G:1039:GLN:CD	3:G:1045:PHE:CZ	2.66	0.73
2:J:2667:ILE:CD1	4:L:2595:ASN:HD22	1.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2126:TYR:CE2	4:L:2627:GLU:HG3	2.23	0.73
3:C:126:TYR:CE2	4:D:627:GLU:HG3	2.23	0.73
3:G:1126:TYR:CE2	4:H:1627:GLU:HG3	2.23	0.73
2:J:2671:LYS:HB2	4:L:2593:TRP:CD2	2.22	0.73
3:O:3039:GLN:CD	3:O:3045:PHE:CZ	2.66	0.73
3:C:39:GLN:CD	3:C:45:PHE:CZ	2.66	0.73
3:G:1097:VAL:HG21	3:G:1107:TRP:CE3	2.23	0.73
3:K:2039:GLN:CD	3:K:2045:PHE:CZ	2.66	0.73
3:C:102:ILE:HG21	4:D:552:ASP:HA	1.69	0.73
2:F:1669:SER:CB	4:H:1533:ASN:OD1	2.37	0.73
2:F:1684:TYR:OH	2:F:1701:THR:OG1	2.03	0.73
2:J:2692:ARG:HG2	3:K:2057:GLU:OE2	1.88	0.73
3:O:3032:TYR:HH	3:O:3100:TYR:CE1	1.46	0.73
2:J:2692:ARG:HH12	3:K:2057:GLU:HG3	1.52	0.73
3:G:1011:VAL:CG1	3:G:1151:PRO:CB	2.67	0.73
4:H:1552:ASP:HB3	4:H:1555:ASN:HD22	1.51	0.73
3:O:3011:VAL:CG1	3:O:3151:PRO:CB	2.67	0.73
3:C:11:VAL:CG1	3:C:151:PRO:CB	2.67	0.72
2:F:1701:THR:C	4:H:1593:TRP:HE1	1.97	0.72
2:J:2667:ILE:HD12	4:L:2595:ASN:HD22	0.98	0.72
3:O:3126:TYR:CE2	4:P:3627:GLU:HG3	2.23	0.72
3:C:102:ILE:HG22	4:D:534:CYS:CB	2.13	0.72
2:F:1783:SER:OG	2:F:1788:ALA:O	2.06	0.72
2:J:2667:ILE:O	4:L:2532:SER:O	2.08	0.72
3:G:1102:ILE:HB	4:H:1552:ASP:HB2	0.75	0.72
3:K:2011:VAL:CG1	3:K:2151:PRO:CB	2.67	0.72
2:B:622:ARG:NH2	2:B:815:GLY:O	2.23	0.72
2:F:1622:ARG:NH2	2:F:1815:GLY:O	2.23	0.72
2:N:3705:THR:CB	4:P:3595:ASN:CB	2.49	0.72
2:J:2684:TYR:OH	2:J:2701:THR:OG1	2.03	0.72
2:N:3622:ARG:NH2	2:N:3815:GLY:O	2.23	0.72
2:N:3669:SER:C	4:P:3533:ASN:CA	2.57	0.72
4:D:514:PRO:CD	4:D:609:LEU:CB	2.65	0.71
1:I:2030:GLN:OE1	1:I:2136:THR:OG1	2.06	0.71
2:J:2667:ILE:HD11	4:L:2595:ASN:HD21	0.54	0.71
2:N:3705:THR:OG1	4:P:3595:ASN:HB3	1.91	0.71
2:N:3783:SER:OG	2:N:3788:ALA:O	2.06	0.71
2:B:667:ILE:N	4:D:532:SER:HB3	2.04	0.71
2:B:671:LYS:CE	4:D:597:LEU:N	2.48	0.71
3:C:2:ILE:HD12	3:C:98:ARG:CZ	2.21	0.71
3:O:3102:ILE:CG2	4:P:3552:ASP:CA	2.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:670:ALA:CA	4:D:594:TYR:CD1	2.74	0.71
2:F:1703:THR:CB	4:H:1596:ASN:HB3	2.20	0.71
2:J:2701:THR:N	4:L:2593:TRP:CH2	2.45	0.71
2:J:2701:THR:CB	4:L:2595:ASN:O	2.35	0.71
2:B:670:ALA:HB2	4:D:594:TYR:CD2	2.18	0.71
2:J:2622:ARG:NH2	2:J:2815:GLY:O	2.23	0.71
2:J:2701:THR:C	4:L:2593:TRP:CH2	2.68	0.71
2:J:2702:THR:HA	3:K:2047:TRP:CH2	2.25	0.71
3:K:2102:ILE:CG2	4:L:2552:ASP:CA	2.69	0.71
1:A:76:TYR:OH	1:A:105:GLU:OE1	2.08	0.71
2:B:671:LYS:HE3	4:D:594:TYR:C	2.11	0.71
3:G:1102:ILE:CG2	4:H:1552:ASP:CA	2.69	0.71
2:J:2701:THR:O	4:L:2593:TRP:CH2	2.43	0.71
3:O:3002:ILE:HD12	3:O:3098:ARG:CZ	2.21	0.71
3:C:102:ILE:CG2	4:D:552:ASP:CA	2.69	0.71
1:E:1076:TYR:OH	1:E:1105:GLU:OE1	2.08	0.71
3:K:2002:ILE:HD12	3:K:2098:ARG:CZ	2.21	0.70
1:M:3076:TYR:OH	1:M:3105:GLU:OE1	2.08	0.70
3:C:102:ILE:CG2	4:D:534:CYS:SG	2.68	0.70
3:G:1002:ILE:HD12	3:G:1098:ARG:CZ	2.21	0.70
4:H:1542:PRO:HB3	4:H:1669:LYS:HD3	1.74	0.70
2:J:2670:ALA:HB1	4:L:2597:LEU:HD11	1.72	0.70
2:J:2673:LYS:HB2	4:L:2593:TRP:NE1	2.05	0.70
4:L:2542:PRO:HB3	4:L:2669:LYS:HD3	1.73	0.70
1:A:1:TYR:HA	1:I:2385:LYS:HZ2	1.55	0.70
4:D:542:PRO:HB3	4:D:669:LYS:HD3	1.73	0.70
1:I:2076:TYR:OH	1:I:2105:GLU:OE1	2.08	0.70
2:J:2671:LYS:CE	4:L:2596:ASN:OD1	2.39	0.70
4:P:3593:TRP:CH2	4:P:3596:ASN:C	2.70	0.70
2:F:1669:SER:O	4:H:1528:ALA:O	2.10	0.70
3:K:2060:TYR:OH	3:K:2069:VAL:HA	1.92	0.70
1:A:126:THR:HG22	1:E:1125:HIS:HE1	1.57	0.70
3:K:2102:ILE:HG22	4:L:2534:CYS:CB	2.13	0.70
4:L:2557:ARG:HD2	4:L:2558:SER:O	1.92	0.70
3:O:3030:THR:HG23	3:O:3054:ASN:ND2	2.07	0.70
2:J:2669:SER:HA	4:L:2533:ASN:ND2	2.06	0.70
3:C:2:ILE:CD1	3:C:98:ARG:CZ	2.70	0.69
3:G:1002:ILE:CD1	3:G:1098:ARG:CZ	2.70	0.69
4:H:1593:TRP:CH2	4:H:1596:ASN:C	2.70	0.69
3:K:2102:ILE:HB	4:L:2552:ASP:HB2	0.75	0.69
4:P:3542:PRO:HB3	4:P:3669:LYS:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:THR:HG23	3:C:54:ASN:ND2	2.07	0.69
2:J:2700:HIS:HE1	3:K:2050:LEU:CD1	1.97	0.69
2:B:702:THR:CA	4:D:593:TRP:CZ2	2.73	0.69
4:D:593:TRP:CH2	4:D:596:ASN:C	2.70	0.69
2:J:2783:SER:OG	2:J:2788:ALA:O	2.06	0.69
3:K:2002:ILE:CD1	3:K:2098:ARG:CZ	2.70	0.69
3:O:3002:ILE:CD1	3:O:3098:ARG:CZ	2.70	0.69
1:A:111:SER:N	1:A:114:CYS:SG	2.66	0.69
3:G:1030:THR:HG23	3:G:1054:ASN:ND2	2.07	0.69
4:H:1557:ARG:HD2	4:H:1558:SER:O	1.92	0.69
1:M:3111:SER:N	1:M:3114:CYS:SG	2.66	0.69
1:E:1111:SER:N	1:E:1114:CYS:SG	2.66	0.69
3:G:1060:TYR:OH	3:G:1069:VAL:HA	1.92	0.69
2:J:2667:ILE:HD11	4:L:2595:ASN:ND2	1.14	0.69
2:J:2671:LYS:HB2	4:L:2593:TRP:CE3	2.28	0.69
1:M:3359:THR:O	1:M:3394:GLN:NE2	2.26	0.69
4:P:3557:ARG:HD2	4:P:3558:SER:O	1.92	0.69
1:A:1:TYR:H1	1:I:2385:LYS:HD2	1.57	0.69
2:B:552:MET:N	2:B:563:ILE:O	2.26	0.69
4:L:2593:TRP:CH2	4:L:2596:ASN:C	2.70	0.69
2:N:3671:LYS:HG2	4:P:3593:TRP:CE2	2.27	0.69
2:N:3703:THR:OG1	3:O:3052:TYR:CE2	2.46	0.69
3:O:3078:THR:HG22	3:O:3080:TYR:CZ	2.25	0.69
1:A:125:HIS:HE1	1:E:1126:THR:HG22	1.57	0.69
2:J:2669:SER:CA	4:L:2533:ASN:ND2	2.56	0.69
3:C:60:TYR:OH	3:C:69:VAL:HA	1.92	0.68
4:D:557:ARG:HD2	4:D:558:SER:O	1.92	0.68
1:E:1359:THR:O	1:E:1394:GLN:NE2	2.26	0.68
3:G:1078:THR:HG22	3:G:1080:TYR:CZ	2.25	0.68
2:J:2667:ILE:HD12	4:L:2595:ASN:ND2	1.02	0.68
3:O:3102:ILE:HB	4:P:3552:ASP:HB2	0.75	0.68
2:J:2552:MET:N	2:J:2563:ILE:O	2.26	0.68
2:J:2668:HIS:CD2	4:L:2593:TRP:HE3	2.09	0.68
3:K:2102:ILE:HG21	4:L:2552:ASP:CB	2.23	0.68
1:I:2359:THR:O	1:I:2394:GLN:NE2	2.26	0.68
1:I:2391:TYR:OH	2:J:2784:LEU:HD11	1.94	0.68
3:K:2030:THR:HG23	3:K:2054:ASN:ND2	2.07	0.68
2:N:3552:MET:N	2:N:3563:ILE:O	2.26	0.68
3:O:3060:TYR:OH	3:O:3069:VAL:HA	1.92	0.68
2:J:2668:HIS:CD2	4:L:2598:TRP:CD2	2.81	0.68
1:A:359:THR:O	1:A:394:GLN:NE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:672:VAL:H	4:D:595:ASN:HA	1.56	0.68
1:I:2111:SER:N	1:I:2114:CYS:SG	2.66	0.68
1:A:391:TYR:OH	2:B:784:LEU:HD11	1.94	0.68
2:F:1703:THR:CA	4:H:1596:ASN:CA	2.67	0.68
1:M:3391:TYR:OH	2:N:3784:LEU:HD11	1.94	0.68
2:B:671:LYS:NZ	4:D:596:ASN:CG	2.52	0.67
2:J:2701:THR:H	4:L:2593:TRP:HZ2	0.69	0.67
3:O:3102:ILE:HG21	4:P:3552:ASP:CB	2.23	0.67
3:K:2128:LEU:HB3	4:L:2621:PHE:CD2	2.30	0.67
2:F:1552:MET:N	2:F:1563:ILE:O	2.26	0.67
2:B:671:LYS:NZ	4:D:594:TYR:O	2.28	0.67
3:C:41:PRO:HD3	3:C:92:ALA:HA	1.77	0.67
3:K:2041:PRO:HD3	3:K:2092:ALA:HA	1.77	0.67
3:G:1102:ILE:HG21	4:H:1552:ASP:CB	2.23	0.67
2:J:2673:LYS:HE2	4:L:2534:CYS:SG	2.35	0.67
2:B:667:ILE:CA	4:D:532:SER:OG	2.40	0.66
2:B:671:LYS:CB	4:D:595:ASN:HA	2.23	0.66
2:J:2700:HIS:HE2	3:K:2050:LEU:HD13	1.57	0.66
3:O:3128:LEU:HB3	4:P:3621:PHE:CD2	2.30	0.66
1:A:41:SER:OG	1:E:1043:ASN:OD1	2.07	0.66
3:C:128:LEU:HB3	4:D:621:PHE:CD2	2.30	0.66
2:J:2667:ILE:CG2	4:L:2594:TYR:CD1	2.77	0.66
4:P:3672:ASN:O	4:P:3673:ASN:HB2	1.95	0.66
1:E:1391:TYR:OH	2:F:1784:LEU:HD11	1.94	0.66
2:J:2673:LYS:CD	4:L:2593:TRP:CD1	2.77	0.66
2:B:668:HIS:HD2	4:D:593:TRP:CB	2.08	0.66
2:B:783:SER:OG	2:B:788:ALA:O	2.06	0.66
3:G:1128:LEU:HB3	4:H:1621:PHE:CD2	2.30	0.66
2:J:2671:LYS:HD3	4:L:2596:ASN:OD1	1.94	0.66
3:K:2073:GLU:OE1	3:K:2080:TYR:CZ	2.49	0.66
3:K:2078:THR:HG22	3:K:2080:TYR:CZ	2.25	0.66
3:C:102:ILE:HG21	4:D:552:ASP:CB	2.23	0.66
3:C:78:THR:HG22	3:C:80:TYR:CZ	2.25	0.66
2:B:671:LYS:CB	4:D:595:ASN:N	2.58	0.66
2:J:2703:THR:N	3:K:2059:THR:CG2	2.58	0.66
4:L:2506:GLN:CD	4:L:2590:CYS:SG	2.79	0.66
4:L:2672:ASN:O	4:L:2673:ASN:HB2	1.95	0.66
3:O:3073:GLU:OE1	3:O:3080:TYR:CZ	2.49	0.66
4:P:3506:GLN:CD	4:P:3590:CYS:SG	2.79	0.66
3:C:73:GLU:OE1	3:C:80:TYR:CZ	2.49	0.66
4:D:506:GLN:CD	4:D:590:CYS:SG	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1683:LEU:HD11	4:H:1694:TYR:CE2	2.29	0.65
2:J:2702:THR:HG21	3:K:2050:LEU:HB3	1.77	0.65
3:O:3041:PRO:HD3	3:O:3092:ALA:HA	1.77	0.65
4:H:1672:ASN:O	4:H:1673:ASN:HB2	1.95	0.65
2:J:2668:HIS:HD2	4:L:2593:TRP:HE3	1.43	0.65
4:L:2652:LYS:HG2	4:L:2657:PRO:HA	1.79	0.65
3:G:1118:ALA:CB	3:G:1150:PHE:HE2	1.65	0.65
3:C:102:ILE:CG1	4:D:552:ASP:CB	2.73	0.65
3:G:1073:GLU:OE1	3:G:1080:TYR:CZ	2.49	0.65
3:K:2102:ILE:CG1	4:L:2552:ASP:CB	2.73	0.65
3:G:1041:PRO:HD3	3:G:1092:ALA:HA	1.77	0.65
4:H:1506:GLN:CD	4:H:1590:CYS:SG	2.79	0.65
4:L:2631:ASN:HA	4:L:2685:ALA:CB	2.25	0.65
4:D:672:ASN:O	4:D:673:ASN:HB2	1.95	0.65
2:F:1671:LYS:O	4:H:1532:SER:HB2	1.96	0.65
4:H:1652:LYS:HG2	4:H:1657:PRO:HA	1.79	0.65
4:D:683:LEU:HD11	4:D:694:TYR:CE2	2.29	0.65
3:G:1102:ILE:CG1	4:H:1552:ASP:CB	2.73	0.65
4:P:3610:GLY:O	4:P:3611:GLN:HG3	1.97	0.65
3:G:1102:ILE:HG22	4:H:1534:CYS:CB	2.13	0.65
4:H:1610:GLY:O	4:H:1611:GLN:HG3	1.97	0.65
2:J:2667:ILE:HA	4:L:2595:ASN:OD1	1.97	0.65
4:D:513:SER:OG	4:D:609:LEU:CD2	2.44	0.64
4:D:564:PHE:CE1	4:D:577:ILE:HG12	2.33	0.64
3:K:2006:GLN:HE22	3:K:2095:PHE:HA	1.62	0.64
4:P:3564:PHE:CE1	4:P:3577:ILE:HG12	2.33	0.64
4:D:581:GLN:HB3	4:D:583:GLU:HG2	1.80	0.64
3:K:2073:GLU:OE1	3:K:2080:TYR:CE1	2.51	0.64
3:O:3006:GLN:HE22	3:O:3095:PHE:HA	1.62	0.64
4:P:3581:GLN:HB3	4:P:3583:GLU:HG2	1.80	0.64
2:J:2692:ARG:NH1	3:K:2057:GLU:HG2	2.10	0.64
2:B:671:LYS:CB	4:D:595:ASN:CA	2.75	0.64
4:H:1581:GLN:HB3	4:H:1583:GLU:HG2	1.80	0.64
2:N:3671:LYS:HZ2	4:P:3596:ASN:C	2.05	0.64
2:N:3703:THR:OG1	3:O:3052:TYR:HE2	1.78	0.64
4:D:568:LEU:HD23	4:D:573:ALA:HA	1.80	0.64
4:D:610:GLY:O	4:D:611:GLN:HG3	1.97	0.64
3:K:2040:ALA:C	3:K:2041:PRO:CD	2.63	0.64
4:L:2581:GLN:HB3	4:L:2583:GLU:HG2	1.80	0.64
4:L:2610:GLY:O	4:L:2611:GLN:HG3	1.97	0.64
3:C:6:GLN:HE22	3:C:95:PHE:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1564:PHE:CE1	4:H:1577:ILE:HG12	2.33	0.64
4:P:3568:LEU:HD23	4:P:3573:ALA:HA	1.80	0.64
4:H:1514:PRO:HD3	4:H:1609:LEU:HB3	1.79	0.64
4:D:631:ASN:HA	4:D:685:ALA:CB	2.25	0.64
4:P:3652:LYS:HG2	4:P:3657:PRO:HA	1.79	0.64
3:C:73:GLU:OE1	3:C:80:TYR:CE1	2.51	0.63
4:D:514:PRO:HD3	4:D:609:LEU:C	2.23	0.63
2:F:1669:SER:HB2	4:H:1533:ASN:OD1	1.98	0.63
3:O:3073:GLU:OE1	3:O:3080:TYR:CE1	2.51	0.63
4:P:3631:ASN:HA	4:P:3685:ALA:CB	2.25	0.63
4:H:1647:VAL:HG12	4:H:1700:HIS:HB2	1.80	0.63
2:J:2670:ALA:HB3	4:L:2597:LEU:HD12	1.80	0.63
4:L:2568:LEU:HD23	4:L:2573:ALA:HA	1.80	0.63
4:P:3647:VAL:HG12	4:P:3700:HIS:HB2	1.81	0.63
4:H:1568:LEU:HD23	4:H:1573:ALA:HA	1.80	0.63
2:J:2667:ILE:HG22	4:L:2594:TYR:CD1	2.33	0.63
2:B:670:ALA:N	4:D:533:ASN:HA	2.12	0.63
4:L:2683:LEU:HD11	4:L:2694:TYR:CE2	2.29	0.63
4:P:3514:PRO:HD3	4:P:3609:LEU:C	2.23	0.63
1:A:126:THR:CG2	1:E:1125:HIS:HE1	2.11	0.63
3:C:118:ALA:CB	3:C:150:PHE:HE2	1.65	0.63
3:K:2030:THR:O	3:K:2030:THR:CG2	2.46	0.63
3:G:1030:THR:CG2	3:G:1030:THR:O	2.46	0.63
2:J:2702:THR:O	4:L:2596:ASN:O	2.16	0.63
4:D:652:LYS:HG2	4:D:657:PRO:HA	1.79	0.63
2:F:1668:HIS:O	4:H:1532:SER:C	2.40	0.63
3:G:1006:GLN:HE22	3:G:1095:PHE:HA	1.62	0.63
4:H:1514:PRO:HD3	4:H:1609:LEU:C	2.23	0.63
2:J:2692:ARG:CG	3:K:2057:GLU:OE2	2.46	0.63
3:K:2035:LEU:HG	3:K:2047:TRP:CD1	2.34	0.63
4:L:2564:PHE:CE1	4:L:2577:ILE:HG12	2.33	0.63
4:P:3513:SER:OG	4:P:3609:LEU:CD2	2.44	0.63
2:B:670:ALA:CB	4:D:594:TYR:CD1	2.55	0.62
4:H:1561:PRO:HG2	4:H:1563:ARG:NH1	2.14	0.62
2:J:2702:THR:HG22	3:K:2047:TRP:CH2	2.34	0.62
4:L:2514:PRO:HD3	4:L:2609:LEU:C	2.23	0.62
1:A:125:HIS:HE1	1:E:1126:THR:CG2	2.11	0.62
4:D:647:VAL:HG12	4:D:700:HIS:HB2	1.81	0.62
2:J:2701:THR:HG22	4:L:2596:ASN:CB	2.29	0.62
3:O:3035:LEU:HG	3:O:3047:TRP:CD1	2.34	0.62
3:O:3102:ILE:CG1	4:P:3552:ASP:CB	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2703:THR:N	3:K:2059:THR:HG21	2.13	0.62
3:G:1072:LEU:HD13	3:G:1074:ILE:HG13	1.81	0.62
4:H:1514:PRO:HD3	4:H:1609:LEU:O	2.00	0.62
3:G:1035:LEU:HG	3:G:1047:TRP:CD1	2.34	0.62
3:C:35:LEU:HG	3:C:47:TRP:CD1	2.35	0.62
3:C:72:LEU:HD13	3:C:74:ILE:HG13	1.81	0.62
2:J:2671:LYS:HD3	4:L:2596:ASN:CG	2.25	0.62
3:C:30:THR:O	3:C:30:THR:CG2	2.46	0.62
4:D:561:PRO:HG2	4:D:563:ARG:NH1	2.14	0.62
3:G:1073:GLU:OE1	3:G:1080:TYR:CE1	2.51	0.62
3:O:3118:ALA:CB	3:O:3150:PHE:CD2	2.77	0.62
4:D:631:ASN:C	4:D:685:ALA:HB2	2.25	0.62
2:J:2669:SER:HB3	4:L:2592:LEU:HB2	1.78	0.62
3:O:3072:LEU:HD13	3:O:3074:ILE:HG13	1.81	0.62
4:H:1513:SER:OG	4:H:1609:LEU:CD2	2.44	0.62
3:K:2118:ALA:CB	3:K:2150:PHE:HE2	1.65	0.62
3:O:3011:VAL:HG23	3:O:3152:GLU:O	2.00	0.62
4:P:3631:ASN:C	4:P:3685:ALA:HB2	2.25	0.62
2:F:1505:ASP:O	2:F:1726:ARG:NH1	2.32	0.61
3:K:2011:VAL:HG23	3:K:2152:GLU:O	2.00	0.61
4:L:2514:PRO:HD3	4:L:2609:LEU:O	2.00	0.61
2:N:3505:ASP:O	2:N:3726:ARG:NH1	2.33	0.61
2:J:2671:LYS:CD	4:L:2596:ASN:OD1	2.48	0.61
3:K:2009:ARG:HG2	3:K:2112:THR:H	1.65	0.61
4:P:3683:LEU:HD11	4:P:3694:TYR:CE2	2.29	0.61
2:J:2692:ARG:NE	3:K:2057:GLU:OE2	2.33	0.61
1:A:43:ASN:OD1	1:E:1041:SER:OG	2.07	0.61
4:P:3514:PRO:HD3	4:P:3609:LEU:HB3	1.79	0.61
2:B:671:LYS:C	4:D:595:ASN:OD1	2.43	0.61
2:F:1702:THR:HA	4:H:1593:TRP:HE1	0.80	0.61
1:I:2053:THR:OG1	1:I:2236:GLN:OE1	2.18	0.61
2:J:2671:LYS:CG	4:L:2593:TRP:CZ3	2.81	0.61
2:J:2702:THR:CA	3:K:2047:TRP:CH2	2.82	0.61
3:K:2072:LEU:HD13	3:K:2074:ILE:HG13	1.81	0.61
2:B:505:ASP:O	2:B:726:ARG:NH1	2.32	0.61
4:D:514:PRO:CD	4:D:609:LEU:HB3	2.31	0.61
4:L:2647:VAL:HG12	4:L:2700:HIS:HB2	1.80	0.61
3:O:3030:THR:O	3:O:3030:THR:CG2	2.46	0.61
4:P:3662:MET:HA	4:P:3680:TYR:O	2.01	0.61
4:H:1513:SER:HG	4:H:1609:LEU:HD22	1.65	0.61
3:O:3009:ARG:HG2	3:O:3112:THR:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:3561:PRO:HG2	4:P:3563:ARG:NH1	2.14	0.61
4:H:1631:ASN:C	4:H:1685:ALA:HB2	2.25	0.61
4:L:2561:PRO:HG2	4:L:2563:ARG:NH1	2.14	0.61
1:A:53:THR:OG1	1:A:236:GLN:OE1	2.18	0.61
3:C:9:ARG:HG2	3:C:112:THR:H	1.65	0.61
4:D:662:MET:HA	4:D:680:TYR:O	2.01	0.61
3:G:1011:VAL:HG23	3:G:1152:GLU:O	2.00	0.61
4:H:1662:MET:HA	4:H:1680:TYR:O	2.01	0.61
2:J:2702:THR:HG22	3:K:2047:TRP:HZ2	1.62	0.61
2:B:668:HIS:CD2	4:D:593:TRP:HB3	2.36	0.61
3:C:11:VAL:HG23	3:C:152:GLU:O	2.00	0.61
4:H:1631:ASN:HA	4:H:1685:ALA:CB	2.25	0.61
4:L:2662:MET:HA	4:L:2680:TYR:O	2.01	0.61
2:J:2667:ILE:HG23	4:L:2594:TYR:HA	1.83	0.60
4:L:2513:SER:OG	4:L:2609:LEU:CD2	2.44	0.60
3:O:3102:ILE:HG21	4:P:3552:ASP:CA	2.31	0.60
3:G:1102:ILE:HG21	4:H:1552:ASP:CA	2.31	0.60
1:M:3053:THR:OG1	1:M:3236:GLN:OE1	2.18	0.60
4:P:3514:PRO:HD3	4:P:3609:LEU:O	2.00	0.60
3:C:102:ILE:HG21	4:D:552:ASP:CA	2.31	0.60
4:D:514:PRO:HD3	4:D:609:LEU:O	2.00	0.60
2:F:1581:HIS:NE2	2:F:1583:GLY:O	2.34	0.60
2:F:1671:LYS:HG3	4:H:1593:TRP:HD1	1.59	0.60
4:L:2631:ASN:C	4:L:2685:ALA:HB2	2.25	0.60
2:F:1671:LYS:CB	4:H:1532:SER:O	2.46	0.60
3:G:1009:ARG:O	3:G:1153:PRO:HD3	2.02	0.60
4:H:1514:PRO:CD	4:H:1609:LEU:HB3	2.31	0.60
2:J:2505:ASP:O	2:J:2726:ARG:NH1	2.32	0.60
3:O:3118:ALA:HB1	3:O:3150:PHE:CD2	2.36	0.60
3:C:118:ALA:CB	3:C:150:PHE:CD2	2.77	0.60
3:C:118:ALA:HB1	3:C:150:PHE:CD2	2.36	0.60
2:J:2668:HIS:CD2	4:L:2598:TRP:CE2	2.90	0.60
2:J:2669:SER:OG	4:L:2592:LEU:CB	2.26	0.60
3:O:3145:LEU:HD13	4:P:3680:TYR:HE2	1.67	0.60
2:B:581:HIS:NE2	2:B:583:GLY:O	2.34	0.60
3:C:97:VAL:HG21	3:C:107:TRP:CZ3	2.36	0.60
3:K:2009:ARG:O	3:K:2153:PRO:HD3	2.02	0.60
2:J:2668:HIS:HD2	4:L:2593:TRP:CE3	2.15	0.60
3:G:1009:ARG:HG2	3:G:1112:THR:H	1.66	0.60
2:N:3581:HIS:NE2	2:N:3583:GLY:O	2.34	0.60
3:O:3009:ARG:O	3:O:3153:PRO:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1118:ALA:HB1	3:G:1150:PHE:CD2	2.36	0.60
4:H:1686:ARG:HH11	4:H:1686:ARG:HG3	1.67	0.60
3:K:2097:VAL:HG21	3:K:2107:TRP:CZ3	2.36	0.60
4:L:2514:PRO:CD	4:L:2609:LEU:HB3	2.31	0.60
3:O:3097:VAL:HG21	3:O:3107:TRP:CZ3	2.36	0.60
1:E:1053:THR:OG1	1:E:1236:GLN:OE1	2.18	0.60
3:K:2102:ILE:CG2	4:L:2552:ASP:CG	2.75	0.60
1:M:3057:SER:OG	2:N:3724:SER:O	2.16	0.60
1:A:23:GLY:H	1:I:2306:GLU:HG2	1.66	0.59
2:B:671:LYS:CD	4:D:596:ASN:CA	2.65	0.59
2:J:2670:ALA:CB	4:L:2599:VAL:HG21	2.22	0.59
3:K:2021:SER:HA	3:K:2080:TYR:CD2	2.37	0.59
4:L:2528:ALA:HA	4:L:2571:ASP:HB2	1.85	0.59
4:P:3514:PRO:CD	4:P:3609:LEU:HB3	2.31	0.59
4:H:1514:PRO:CD	4:H:1609:LEU:HB2	2.31	0.59
3:K:2073:GLU:CD	3:K:2080:TYR:CE1	2.80	0.59
3:C:21:SER:HA	3:C:80:TYR:CD2	2.37	0.59
4:H:1528:ALA:HA	4:H:1571:ASP:HB2	1.84	0.59
4:L:2686:ARG:HH11	4:L:2686:ARG:HG3	1.67	0.59
4:D:541:LYS:HE2	4:D:583:GLU:O	2.02	0.59
3:G:1021:SER:HA	3:G:1080:TYR:CD2	2.37	0.59
3:G:1097:VAL:HG21	3:G:1107:TRP:CZ3	2.36	0.59
3:G:1102:ILE:CG2	3:G:1102:ILE:O	2.51	0.59
4:H:1541:LYS:HE2	4:H:1583:GLU:O	2.02	0.59
2:J:2700:HIS:CB	4:L:2593:TRP:CE2	2.81	0.59
3:K:2118:ALA:HB1	3:K:2150:PHE:CD2	2.36	0.59
3:G:1073:GLU:CD	3:G:1080:TYR:CE1	2.80	0.59
3:K:2032:TYR:CE1	3:K:2100:TYR:HD1	1.97	0.59
3:K:2145:LEU:HD13	4:L:2680:TYR:HE2	1.67	0.59
2:B:668:HIS:HB3	4:D:593:TRP:CD1	2.34	0.59
3:G:1032:TYR:CE1	3:G:1100:TYR:HD1	1.97	0.59
3:G:1102:ILE:CG2	4:H:1552:ASP:CG	2.75	0.59
3:G:1145:LEU:HD13	4:H:1680:TYR:HE2	1.66	0.59
4:D:686:ARG:HH11	4:D:686:ARG:HG3	1.67	0.59
4:P:3541:LYS:HE2	4:P:3583:GLU:O	2.02	0.59
3:C:145:LEU:HD13	4:D:680:TYR:HE2	1.67	0.59
4:P:3689:GLU:HA	4:P:3711:ARG:NH2	2.18	0.59
1:A:125:HIS:CE1	1:E:1126:THR:CG2	2.86	0.59
3:C:73:GLU:CD	3:C:80:TYR:CE1	2.81	0.59
2:J:2671:LYS:CB	4:L:2593:TRP:CH2	2.86	0.58
4:L:2689:GLU:HA	4:L:2711:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2668:HIS:CE1	4:L:2534:CYS:HB2	2.38	0.58
4:L:2700:HIS:O	4:L:2701:GLU:C	2.46	0.58
1:M:3038:ILE:HD12	1:M:3269:ALA:HB3	1.86	0.58
2:N:3669:SER:C	4:P:3593:TRP:HB3	2.28	0.58
3:O:3073:GLU:CD	3:O:3080:TYR:CE1	2.80	0.58
4:P:3686:ARG:HG3	4:P:3686:ARG:HH11	1.67	0.58
3:C:9:ARG:O	3:C:153:PRO:HD3	2.02	0.58
1:A:291:ILE:HG23	1:I:2316:ILE:HD13	1.82	0.58
2:B:577:SER:O	2:B:589:GLN:N	2.37	0.58
3:O:3021:SER:HA	3:O:3080:TYR:CD2	2.37	0.58
4:P:3528:ALA:HA	4:P:3571:ASP:HB2	1.84	0.58
4:D:528:ALA:HA	4:D:571:ASP:HB2	1.84	0.58
4:D:689:GLU:HA	4:D:711:ARG:NH2	2.18	0.58
2:J:2581:HIS:NE2	2:J:2583:GLY:O	2.34	0.58
1:A:38:ILE:HD12	1:A:269:ALA:HB3	1.85	0.58
2:F:1569:HIS:N	2:F:1599:GLY:O	2.37	0.58
2:F:1668:HIS:O	4:H:1530:THR:O	2.21	0.58
2:J:2667:ILE:CG2	4:L:2594:TYR:CA	2.78	0.58
3:O:3102:ILE:CG2	4:P:3552:ASP:CG	2.75	0.58
2:B:668:HIS:O	4:D:593:TRP:HB3	2.03	0.58
1:E:1038:ILE:HD12	1:E:1269:ALA:HB3	1.85	0.58
4:L:2541:LYS:HE2	4:L:2583:GLU:O	2.02	0.58
4:D:514:PRO:CD	4:D:609:LEU:HB2	2.31	0.58
4:D:688:TRP:CZ2	4:D:711:ARG:HG3	2.39	0.58
3:O:3045:PHE:HE1	4:P:3589:PHE:CE2	2.22	0.58
3:O:3102:ILE:CG2	3:O:3102:ILE:O	2.51	0.58
3:C:102:ILE:CB	4:D:552:ASP:CG	2.77	0.58
4:H:1688:TRP:CZ2	4:H:1711:ARG:HG3	2.39	0.58
4:L:2514:PRO:HD3	4:L:2609:LEU:HB3	1.79	0.58
2:J:2667:ILE:HG23	4:L:2594:TYR:CA	2.33	0.57
3:C:21:SER:CB	3:C:80:TYR:HE2	2.13	0.57
4:D:700:HIS:O	4:D:701:GLU:C	2.46	0.57
2:F:1508:ASN:OD1	2:F:1610:THR:OG1	2.11	0.57
4:H:1689:GLU:HA	4:H:1711:ARG:NH2	2.18	0.57
2:J:2670:ALA:H	4:L:2593:TRP:C	2.11	0.57
3:K:2145:LEU:CD1	4:L:2680:TYR:HE2	2.18	0.57
1:M:3391:TYR:CZ	2:N:3784:LEU:HD11	2.40	0.57
3:O:3102:ILE:HG13	4:P:3552:ASP:CB	2.34	0.57
3:C:145:LEU:CD1	4:D:680:TYR:HE2	2.17	0.57
1:E:1387:HIS:CD2	2:F:1825:GLN:HE21	2.22	0.57
1:I:2391:TYR:CZ	2:J:2784:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3145:LEU:CD1	4:P:3680:TYR:HE2	2.18	0.57
4:P:3611:GLN:HG3	4:P:3611:GLN:O	2.05	0.57
2:B:569:HIS:N	2:B:599:GLY:O	2.37	0.57
1:E:1391:TYR:CZ	2:F:1784:LEU:HD11	2.40	0.57
3:G:1061:ALA:HB3	3:G:1064:PHE:HD2	1.70	0.57
3:O:3061:ALA:HB3	3:O:3064:PHE:HD2	1.70	0.57
2:F:1703:THR:HG23	4:H:1596:ASN:HB2	1.82	0.57
4:H:1700:HIS:O	4:H:1701:GLU:C	2.46	0.57
2:J:2702:THR:C	3:K:2059:THR:CG2	2.77	0.57
2:F:1668:HIS:O	4:H:1533:ASN:CG	2.48	0.57
3:G:1045:PHE:HE1	4:H:1589:PHE:CE2	2.22	0.57
3:G:1100:TYR:CE2	3:G:1101:PHE:CZ	2.93	0.57
3:G:1145:LEU:CD1	4:H:1680:TYR:HE2	2.17	0.57
3:K:2100:TYR:CE2	3:K:2101:PHE:CZ	2.93	0.57
1:M:3387:HIS:CD2	2:N:3825:GLN:HE21	2.22	0.57
2:J:2700:HIS:CD2	4:L:2593:TRP:CH2	2.93	0.57
4:P:3688:TRP:CZ2	4:P:3711:ARG:HG3	2.39	0.57
3:G:1030:THR:CG2	3:G:1054:ASN:HD22	2.17	0.57
3:K:2102:ILE:HG21	4:L:2552:ASP:CA	2.31	0.57
2:N:3577:SER:O	2:N:3589:GLN:N	2.37	0.57
4:P:3700:HIS:O	4:P:3701:GLU:C	2.46	0.57
1:A:1:TYR:N	1:I:2385:LYS:HD2	2.18	0.57
2:B:671:LYS:HE3	4:D:594:TYR:H	1.70	0.57
1:I:2038:ILE:HD12	1:I:2269:ALA:HB3	1.85	0.57
2:J:2671:LYS:HB2	4:L:2593:TRP:CE2	2.39	0.57
3:K:2117:SER:O	3:K:2118:ALA:HB2	2.05	0.57
2:N:3508:ASN:OD1	2:N:3610:THR:OG1	2.11	0.57
3:K:2037:VAL:HG21	3:K:2107:TRP:HH2	1.70	0.56
4:L:2557:ARG:HE	4:L:2560:VAL:HG23	1.70	0.56
4:L:2653:VAL:HG23	4:L:2658:VAL:CG2	2.35	0.56
1:A:391:TYR:CZ	2:B:784:LEU:HD11	2.40	0.56
2:B:673:LYS:HZ3	3:C:102:ILE:HD12	1.70	0.56
3:C:61:ALA:HB3	3:C:64:PHE:HD2	1.70	0.56
4:D:684:THR:O	4:D:685:ALA:C	2.48	0.56
3:G:1117:SER:O	3:G:1118:ALA:HB2	2.05	0.56
4:H:1557:ARG:HE	4:H:1560:VAL:HG23	1.70	0.56
3:K:2030:THR:CG2	3:K:2054:ASN:HD22	2.17	0.56
2:N:3569:HIS:N	2:N:3599:GLY:O	2.37	0.56
3:O:3100:TYR:CE2	3:O:3101:PHE:CZ	2.93	0.56
3:O:3102:ILE:CB	4:P:3552:ASP:CG	2.77	0.56
2:B:668:HIS:HD2	4:D:593:TRP:HB3	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:TYR:CE2	3:C:101:PHE:CZ	2.93	0.56
3:C:117:SER:O	3:C:118:ALA:HB2	2.05	0.56
2:J:2666:SER:OG	4:L:2532:SER:CB	2.48	0.56
2:J:2702:THR:CG2	3:K:2050:LEU:HB3	2.35	0.56
2:J:2702:THR:CG2	3:K:2047:TRP:CH2	2.89	0.56
3:K:2011:VAL:HB	3:K:2151:PRO:HB2	1.87	0.56
4:L:2688:TRP:CZ2	4:L:2711:ARG:HG3	2.39	0.56
2:N:3530:GLY:O	2:N:3590:CYS:N	2.38	0.56
2:N:3667:ILE:HB	4:P:3532:SER:HB3	1.85	0.56
1:A:387:HIS:CD2	2:B:825:GLN:HE21	2.22	0.56
2:F:1530:GLY:O	2:F:1590:CYS:N	2.38	0.56
4:P:3653:VAL:CG2	4:P:3658:VAL:HG21	2.35	0.56
2:B:671:LYS:HE3	4:D:597:LEU:H	1.69	0.56
2:B:702:THR:CA	4:D:593:TRP:HH2	2.10	0.56
2:F:1577:SER:O	2:F:1589:GLN:N	2.37	0.56
4:H:1611:GLN:HG3	4:H:1611:GLN:O	2.05	0.56
2:J:2569:HIS:N	2:J:2599:GLY:O	2.37	0.56
2:J:2671:LYS:HB3	4:L:2593:TRP:CH2	2.39	0.56
2:J:2671:LYS:CB	4:L:2593:TRP:CZ3	2.88	0.56
4:P:3684:THR:O	4:P:3685:ALA:C	2.48	0.56
2:B:671:LYS:CD	4:D:595:ASN:CA	2.84	0.56
2:J:2672:VAL:CG1	4:L:2595:ASN:C	2.74	0.56
3:K:2021:SER:CB	3:K:2080:TYR:HE2	2.13	0.56
4:L:2684:THR:O	4:L:2685:ALA:C	2.48	0.56
3:O:3117:SER:O	3:O:3118:ALA:HB2	2.05	0.56
4:D:611:GLN:HG3	4:D:611:GLN:O	2.05	0.56
4:D:620:LEU:HD23	4:D:636:VAL:O	2.06	0.56
2:F:1705:THR:N	4:H:1595:ASN:ND2	2.12	0.56
4:H:1684:THR:O	4:H:1685:ALA:C	2.48	0.56
2:B:692:ARG:CZ	3:C:57:GLU:OE1	2.52	0.56
3:C:11:VAL:HB	3:C:151:PRO:HB2	1.87	0.56
3:C:102:ILE:CG2	4:D:534:CYS:HB3	1.94	0.56
4:D:653:VAL:CG2	4:D:658:VAL:HG21	2.35	0.56
3:G:1011:VAL:HB	3:G:1151:PRO:HB2	1.87	0.56
4:H:1620:LEU:HD23	4:H:1636:VAL:O	2.06	0.56
3:K:2045:PHE:CE1	4:L:2589:PHE:CZ	2.94	0.56
3:K:2061:ALA:HB3	3:K:2064:PHE:HD2	1.70	0.56
1:M:3194:GLY:N	1:M:3205:GLN:OE1	2.39	0.56
3:O:3118:ALA:HB3	3:O:3150:PHE:HE2	0.78	0.56
1:I:2057:SER:OG	2:J:2724:SER:O	2.16	0.56
1:I:2194:GLY:N	1:I:2205:GLN:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2387:HIS:CD2	2:J:2825:GLN:HE21	2.22	0.56
2:J:2530:GLY:O	2:J:2590:CYS:N	2.38	0.56
3:K:2118:ALA:HB3	3:K:2150:PHE:HE2	0.78	0.56
3:C:118:ALA:HB3	3:C:150:PHE:HE2	0.78	0.55
2:F:1670:ALA:CB	4:H:1594:TYR:CD1	2.88	0.55
4:L:2611:GLN:HG3	4:L:2611:GLN:O	2.05	0.55
3:C:45:PHE:CE1	4:D:589:PHE:CZ	2.94	0.55
4:D:620:LEU:HD21	4:D:651:TRP:HH2	1.72	0.55
1:E:1194:GLY:N	1:E:1205:GLN:OE1	2.39	0.55
1:E:1221:LYS:O	1:E:1235:THR:OG1	2.19	0.55
3:G:1126:TYR:CZ	4:H:1627:GLU:HG3	2.41	0.55
3:K:2126:TYR:CZ	4:L:2627:GLU:HG3	2.41	0.55
3:O:3035:LEU:HD23	3:O:3037:VAL:HG23	1.82	0.55
3:C:102:ILE:CG2	4:D:552:ASP:CG	2.75	0.55
3:G:1045:PHE:CE1	4:H:1589:PHE:CZ	2.94	0.55
3:K:2032:TYR:CZ	3:K:2100:TYR:CZ	2.84	0.55
4:L:2620:LEU:HD23	4:L:2636:VAL:O	2.06	0.55
4:D:689:GLU:HA	4:D:711:ARG:HH21	1.72	0.55
3:C:35:LEU:HD23	3:C:37:VAL:HG23	1.82	0.55
4:L:2620:LEU:HD21	4:L:2651:TRP:HH2	1.72	0.55
2:N:3671:LYS:CG	4:P:3593:TRP:CE2	2.90	0.55
3:O:3126:TYR:CZ	4:P:3627:GLU:HG3	2.41	0.55
4:P:3689:GLU:HA	4:P:3711:ARG:HH21	1.72	0.55
1:A:194:GLY:N	1:A:205:GLN:OE1	2.39	0.55
4:D:653:VAL:HG23	4:D:658:VAL:CG2	2.35	0.55
4:H:1620:LEU:HD21	4:H:1651:TRP:HH2	1.72	0.55
2:J:2577:SER:O	2:J:2589:GLN:N	2.37	0.55
3:O:3011:VAL:HB	3:O:3151:PRO:HB2	1.87	0.55
4:P:3557:ARG:HE	4:P:3560:VAL:HG23	1.70	0.55
4:P:3689:GLU:HA	4:P:3711:ARG:HE	1.72	0.55
3:G:1032:TYR:CE1	3:G:1100:TYR:CB	2.89	0.55
4:H:1689:GLU:HA	4:H:1711:ARG:HH21	1.72	0.55
2:J:2692:ARG:HG2	3:K:2057:GLU:CD	2.31	0.55
2:N:3670:ALA:O	4:P:3595:ASN:N	2.39	0.55
2:N:3670:ALA:HB1	4:P:3594:TYR:N	2.22	0.55
4:D:565:SER:O	4:D:575:LEU:HD23	2.07	0.55
3:O:3045:PHE:CE1	4:P:3589:PHE:CZ	2.94	0.55
3:O:3118:ALA:CB	3:O:3150:PHE:HE2	1.65	0.55
4:D:557:ARG:HE	4:D:560:VAL:HG23	1.71	0.55
4:D:689:GLU:HA	4:D:711:ARG:HE	1.72	0.55
2:F:1704:CYS:CA	4:H:1595:ASN:HB3	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2502:TYR:N	2:J:2537:SER:O	2.40	0.55
3:K:2032:TYR:CE1	3:K:2100:TYR:CB	2.89	0.55
4:L:2514:PRO:CD	4:L:2609:LEU:HB2	2.31	0.55
4:P:3620:LEU:HD23	4:P:3636:VAL:O	2.06	0.55
2:N:3502:TYR:N	2:N:3537:SER:O	2.40	0.54
4:P:3565:SER:O	4:P:3575:LEU:HD23	2.07	0.54
3:C:37:VAL:HG21	3:C:107:TRP:HH2	1.70	0.54
3:C:45:PHE:HE1	4:D:589:PHE:CE2	2.22	0.54
3:C:102:ILE:HG22	4:D:552:ASP:HA	1.89	0.54
3:C:126:TYR:CZ	4:D:627:GLU:HG3	2.41	0.54
2:J:2508:ASN:OD1	2:J:2610:THR:OG1	2.11	0.54
4:H:1565:SER:O	4:H:1575:LEU:HD23	2.07	0.54
2:J:2669:SER:OG	4:L:2533:ASN:CB	2.42	0.54
3:O:3032:TYR:CE1	3:O:3100:TYR:CB	2.89	0.54
3:K:2102:ILE:CB	4:L:2552:ASP:CG	2.77	0.54
2:N:3652:GLU:OE2	2:N:3738:LYS:NZ	2.41	0.54
2:B:508:ASN:OD1	2:B:610:THR:OG1	2.11	0.54
2:B:530:GLY:O	2:B:590:CYS:N	2.38	0.54
2:F:1677:PRO:HD2	2:F:1680:ALA:HB3	1.90	0.54
3:G:1118:ALA:HB3	3:G:1150:PHE:HE2	0.78	0.54
4:P:3620:LEU:HD21	4:P:3651:TRP:HH2	1.72	0.54
3:C:30:THR:CG2	3:C:54:ASN:HD22	2.17	0.54
2:F:1502:TYR:N	2:F:1537:SER:O	2.40	0.54
2:B:502:TYR:N	2:B:537:SER:O	2.40	0.54
3:C:32:TYR:CE1	3:C:100:TYR:CB	2.89	0.54
1:E:1061:LYS:NZ	1:E:1063:CYS:O	2.41	0.54
4:H:1507:GLU:OE2	4:H:1521:THR:OG1	2.23	0.54
1:I:2197:LYS:O	1:I:2200:SER:OG	2.18	0.54
3:K:2102:ILE:HG13	4:L:2552:ASP:CB	2.34	0.54
1:M:3371:CYS:O	1:M:3372:THR:OG1	2.25	0.54
3:O:3045:PHE:HZ	4:P:3546:PHE:HZ	0.61	0.54
3:C:102:ILE:CG2	3:C:102:ILE:O	2.51	0.54
3:K:2045:PHE:HE1	4:L:2589:PHE:CE2	2.22	0.54
4:L:2654:ASP:OD2	4:L:2691:HIS:HB3	2.08	0.54
1:M:3061:LYS:NZ	1:M:3063:CYS:O	2.41	0.54
4:P:3653:VAL:HG23	4:P:3658:VAL:CG2	2.35	0.54
4:P:3689:GLU:HA	4:P:3711:ARG:NE	2.23	0.54
2:F:1671:LYS:NZ	4:H:1595:ASN:CB	2.71	0.54
3:O:3011:VAL:CG2	3:O:3152:GLU:HB2	2.38	0.54
2:B:652:GLU:OE2	2:B:738:LYS:NZ	2.41	0.54
4:D:654:ASP:OD2	4:D:691:HIS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1102:ILE:HG22	4:H:1552:ASP:HA	1.89	0.54
3:G:1118:ALA:CB	3:G:1150:PHE:CD2	2.77	0.54
4:H:1654:ASP:OD2	4:H:1691:HIS:HB3	2.08	0.54
2:J:2652:GLU:OE2	2:J:2738:LYS:NZ	2.41	0.54
2:F:1671:LYS:HG2	4:H:1593:TRP:O	2.08	0.53
4:H:1689:GLU:HA	4:H:1711:ARG:NE	2.23	0.53
2:J:2690:ASP:OD2	2:J:2702:THR:N	2.42	0.53
4:L:2689:GLU:HA	4:L:2711:ARG:HE	1.72	0.53
2:B:690:ASP:OD2	2:B:702:THR:N	2.41	0.53
3:G:1011:VAL:CG2	3:G:1152:GLU:HB2	2.38	0.53
1:I:2061:LYS:NZ	1:I:2063:CYS:O	2.41	0.53
2:J:2700:HIS:HD2	4:L:2593:TRP:CH2	2.26	0.53
3:K:2078:THR:CG2	3:K:2080:TYR:CE2	2.84	0.53
2:B:670:ALA:HB2	4:D:594:TYR:CD1	2.29	0.53
4:D:689:GLU:HA	4:D:711:ARG:NE	2.23	0.53
1:E:1035:ASN:OD1	1:E:1036:THR:N	2.42	0.53
1:I:2221:LYS:O	1:I:2235:THR:OG1	2.19	0.53
3:K:2039:GLN:CD	3:K:2045:PHE:CE1	2.87	0.53
3:K:2128:LEU:HB3	4:L:2621:PHE:CG	2.44	0.53
4:L:2689:GLU:HA	4:L:2711:ARG:HH21	1.72	0.53
1:A:61:LYS:NZ	1:A:63:CYS:O	2.41	0.53
1:A:291:ILE:HG23	1:I:2316:ILE:CD1	2.38	0.53
2:B:667:ILE:H	4:D:532:SER:HB3	1.73	0.53
3:C:128:LEU:HB3	4:D:621:PHE:CG	2.44	0.53
4:H:1689:GLU:HA	4:H:1711:ARG:HE	1.72	0.53
2:J:2672:VAL:HG12	4:L:2595:ASN:O	2.07	0.53
2:J:2700:HIS:CA	4:L:2593:TRP:CZ2	2.90	0.53
3:K:2011:VAL:CG2	3:K:2152:GLU:HB2	2.38	0.53
2:J:2667:ILE:O	4:L:2532:SER:C	2.51	0.53
3:K:2217:ARG:HH21	4:L:2622:PRO:CD	2.08	0.53
3:O:3128:LEU:HB3	4:P:3621:PHE:CG	2.44	0.53
1:A:192:GLU:HG2	1:E:1153:THR:OG1	2.09	0.53
4:D:683:LEU:HD22	4:D:687:ALA:HB1	1.91	0.53
4:H:1683:LEU:HD22	4:H:1687:ALA:HB1	1.91	0.53
2:J:2670:ALA:CB	4:L:2597:LEU:CD1	2.87	0.53
2:J:2673:LYS:CB	4:L:2593:TRP:NE1	2.69	0.53
4:L:2565:SER:O	4:L:2575:LEU:HD23	2.07	0.53
4:L:2689:GLU:HA	4:L:2711:ARG:NE	2.23	0.53
1:A:343:ASN:OD1	1:A:344:ASP:N	2.42	0.53
2:B:702:THR:C	4:D:593:TRP:CZ2	2.87	0.53
3:C:11:VAL:CG2	3:C:152:GLU:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2118:ALA:CB	3:K:2150:PHE:CD2	2.77	0.53
4:D:504:VAL:CG1	4:D:522:CYS:SG	2.97	0.53
2:F:1652:GLU:OE2	2:F:1738:LYS:NZ	2.41	0.53
4:H:1504:VAL:CG1	4:H:1522:CYS:SG	2.97	0.53
4:P:3504:VAL:CG1	4:P:3522:CYS:SG	2.97	0.53
4:D:514:PRO:HD3	4:D:609:LEU:HB3	1.79	0.53
3:G:1033:PRO:HA	3:G:1053:THR:HG23	1.91	0.53
3:G:1102:ILE:CB	4:H:1552:ASP:CG	2.77	0.53
3:O:3033:PRO:HB2	3:O:3051:ILE:O	2.09	0.53
1:A:125:HIS:CD2	1:E:1041:SER:CB	2.92	0.52
3:C:33:PRO:HA	3:C:53:THR:HG23	1.91	0.52
1:I:2005:ALA:N	1:I:2279:ILE:O	2.42	0.52
1:M:3035:ASN:OD1	1:M:3036:THR:N	2.42	0.52
3:O:3102:ILE:HG22	4:P:3552:ASP:HA	1.89	0.52
1:A:41:SER:CB	1:E:1125:HIS:CD2	2.92	0.52
3:C:217:ARG:HH21	4:D:622:PRO:CD	2.08	0.52
2:F:1690:ASP:OD2	2:F:1702:THR:N	2.42	0.52
1:I:2035:ASN:OD1	1:I:2036:THR:N	2.42	0.52
2:J:2670:ALA:CB	4:L:2597:LEU:HD11	2.38	0.52
2:J:2677:PRO:HD2	2:J:2680:ALA:HB3	1.90	0.52
2:J:2700:HIS:HB2	4:L:2593:TRP:CD2	2.44	0.52
1:M:3343:ASN:OD1	1:M:3344:ASP:N	2.42	0.52
4:P:3630:THR:HG22	4:P:3632:LYS:HB2	1.91	0.52
3:C:30:THR:O	3:C:30:THR:HG22	2.09	0.52
3:C:33:PRO:HB2	3:C:51:ILE:O	2.09	0.52
3:C:212:LYS:CE	4:D:626:GLU:OE1	2.58	0.52
1:E:1315:GLY:O	1:E:1357:PHE:N	2.42	0.52
2:J:2667:ILE:HA	4:L:2595:ASN:CG	2.34	0.52
3:K:2030:THR:O	3:K:2030:THR:HG22	2.09	0.52
3:K:2033:PRO:HB2	3:K:2051:ILE:O	2.09	0.52
4:L:2630:THR:HG22	4:L:2632:LYS:HB2	1.91	0.52
4:L:2683:LEU:HD22	4:L:2687:ALA:HB1	1.91	0.52
1:M:3260:CYS:H	2:N:3782:ARG:HH22	1.57	0.52
3:O:3212:LYS:CE	4:P:3626:GLU:OE1	2.58	0.52
4:P:3654:ASP:OD2	4:P:3691:HIS:HB3	2.08	0.52
2:B:671:LYS:HD2	4:D:596:ASN:C	2.35	0.52
2:B:671:LYS:CD	4:D:595:ASN:N	2.72	0.52
2:B:677:PRO:HD2	2:B:680:ALA:HB3	1.90	0.52
3:C:102:ILE:HG13	4:D:552:ASP:CB	2.34	0.52
1:E:1005:ALA:N	1:E:1279:ILE:O	2.42	0.52
3:G:1039:GLN:CD	3:G:1045:PHE:CE1	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1630:THR:HG22	4:H:1632:LYS:HB2	1.91	0.52
4:H:1653:VAL:CG2	4:H:1658:VAL:HG21	2.35	0.52
4:L:2514:PRO:HG2	4:L:2609:LEU:O	2.03	0.52
1:E:1343:ASN:OD1	1:E:1344:ASP:N	2.42	0.52
3:G:1217:ARG:HH21	4:H:1622:PRO:CD	2.08	0.52
1:I:2343:ASN:OD1	1:I:2344:ASP:N	2.42	0.52
4:L:2504:VAL:CG1	4:L:2522:CYS:SG	2.97	0.52
1:A:153:THR:OG1	1:E:1192:GLU:HG2	2.09	0.52
2:J:2700:HIS:C	4:L:2593:TRP:CZ2	2.84	0.52
2:J:2701:THR:O	4:L:2593:TRP:HH2	1.83	0.52
2:N:3667:ILE:HB	4:P:3532:SER:CB	2.39	0.52
1:A:315:GLY:O	1:A:357:PHE:N	2.42	0.52
3:K:2102:ILE:CG2	3:K:2102:ILE:O	2.51	0.52
4:L:2520:LEU:N	4:L:2520:LEU:CD2	2.70	0.52
1:A:35:ASN:OD1	1:A:36:THR:N	2.42	0.52
2:B:701:THR:C	4:D:593:TRP:CZ2	2.82	0.52
4:L:2653:VAL:CG2	4:L:2658:VAL:HG21	2.35	0.52
2:N:3677:PRO:HD2	2:N:3680:ALA:HB3	1.90	0.52
3:O:3021:SER:CB	3:O:3080:TYR:HE2	2.13	0.52
2:B:670:ALA:CB	4:D:594:TYR:CD2	2.66	0.52
1:I:2260:CYS:H	2:J:2782:ARG:HH22	1.58	0.52
3:K:2033:PRO:HA	3:K:2053:THR:HG23	1.91	0.52
3:K:2097:VAL:CG2	3:K:2107:TRP:CD2	2.93	0.52
3:K:2212:LYS:CE	4:L:2626:GLU:OE1	2.58	0.52
1:M:3315:GLY:O	1:M:3357:PHE:N	2.42	0.52
3:O:3097:VAL:CG2	3:O:3107:TRP:CD2	2.93	0.52
3:C:35:LEU:HD23	3:C:36:TRP:N	2.25	0.52
3:G:1045:PHE:HZ	4:H:1546:PHE:HZ	0.62	0.52
3:G:1128:LEU:HB3	4:H:1621:PHE:CG	2.44	0.52
2:J:2702:THR:CG2	3:K:2047:TRP:CZ2	2.92	0.52
1:M:3005:ALA:N	1:M:3279:ILE:O	2.42	0.52
2:N:3690:ASP:OD2	2:N:3702:THR:N	2.42	0.52
3:O:3035:LEU:HD23	3:O:3036:TRP:N	2.25	0.52
3:C:97:VAL:CG2	3:C:107:TRP:CD2	2.93	0.51
4:D:554:ASN:C	4:D:554:ASN:ND2	2.54	0.51
4:D:630:THR:HG22	4:D:632:LYS:HB2	1.91	0.51
3:O:3107:TRP:HB2	4:P:3546:PHE:CB	2.40	0.51
4:P:3542:PRO:HB2	4:P:3669:LYS:HB2	1.92	0.51
3:G:1078:THR:CG2	3:G:1080:TYR:CE2	2.84	0.51
3:G:1212:LYS:CE	4:H:1626:GLU:OE1	2.58	0.51
3:K:2002:ILE:CD1	3:K:2098:ARG:HH12	1.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3221:LYS:O	1:M:3235:THR:OG1	2.19	0.51
3:C:39:GLN:CD	3:C:45:PHE:CE1	2.86	0.51
3:C:107:TRP:HB2	4:D:546:PHE:CB	2.40	0.51
1:E:1260:CYS:H	2:F:1782:ARG:HH22	1.58	0.51
2:J:2733:ASP:OD1	2:J:2734:THR:N	2.44	0.51
3:K:2102:ILE:HG22	4:L:2552:ASP:HA	1.89	0.51
4:P:3514:PRO:CD	4:P:3609:LEU:HB2	2.31	0.51
4:P:3683:LEU:HD22	4:P:3687:ALA:HB1	1.91	0.51
4:D:507:GLU:OE2	4:D:521:THR:OG1	2.23	0.51
3:G:1033:PRO:HB2	3:G:1051:ILE:O	2.09	0.51
3:G:1035:LEU:HD23	3:G:1036:TRP:N	2.25	0.51
3:G:1107:TRP:HB2	4:H:1546:PHE:CB	2.40	0.51
1:I:2117:ASP:OD1	1:I:2181:TYR:OH	2.20	0.51
2:J:2569:HIS:O	2:J:2599:GLY:N	2.44	0.51
3:C:21:SER:OG	3:C:80:TYR:CD2	2.37	0.51
4:H:1507:GLU:O	4:H:1604:THR:OG1	2.27	0.51
4:H:1653:VAL:HG23	4:H:1658:VAL:CG2	2.35	0.51
2:B:733:ASP:OD1	2:B:734:THR:N	2.44	0.51
3:G:1097:VAL:CG2	3:G:1107:TRP:CD2	2.93	0.51
3:O:3033:PRO:HA	3:O:3053:THR:HG23	1.91	0.51
4:P:3507:GLU:O	4:P:3604:THR:OG1	2.27	0.51
1:A:126:THR:CG2	1:E:1125:HIS:CE1	2.86	0.51
1:A:260:CYS:H	2:B:782:ARG:HH22	1.58	0.51
3:G:1030:THR:O	3:G:1030:THR:HG22	2.09	0.51
4:H:1643:TYR:HA	4:H:1644:PRO:C	2.36	0.51
3:C:32:TYR:CE1	3:C:100:TYR:HD1	1.97	0.51
1:E:1301:GLU:O	1:E:1320:ALA:N	2.43	0.51
3:K:2107:TRP:HB2	4:L:2546:PHE:CB	2.40	0.51
4:L:2589:PHE:CE1	4:L:2603:GLY:HA3	2.46	0.51
2:N:3669:SER:O	4:P:3533:ASN:C	2.51	0.51
1:A:389:VAL:HG12	1:A:390:ASP:H	1.76	0.51
2:B:702:THR:O	4:D:593:TRP:CZ2	2.62	0.51
3:C:13:ASN:OD1	3:C:116:SER:O	2.29	0.51
1:E:1389:VAL:HG12	1:E:1390:ASP:H	1.76	0.51
2:F:1668:HIS:O	4:H:1533:ASN:OD1	2.28	0.51
3:G:1032:TYR:CD1	3:G:1100:TYR:HB2	2.46	0.51
3:K:2035:LEU:HD23	3:K:2036:TRP:N	2.25	0.51
3:K:2045:PHE:HZ	4:L:2546:PHE:HZ	0.62	0.51
2:N:3569:HIS:O	2:N:3599:GLY:N	2.44	0.51
1:A:5:ALA:N	1:A:279:ILE:O	2.42	0.51
1:I:2315:GLY:O	1:I:2357:PHE:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2668:HIS:ND1	4:L:2534:CYS:HB2	2.26	0.51
4:P:3643:TYR:HA	4:P:3644:PRO:C	2.36	0.51
2:J:2668:HIS:HE2	4:L:2598:TRP:CD2	1.69	0.50
2:B:569:HIS:O	2:B:599:GLY:N	2.44	0.50
3:C:78:THR:CG2	3:C:80:TYR:CE2	2.84	0.50
2:F:1671:LYS:HD3	4:H:1595:ASN:CG	2.36	0.50
4:H:1514:PRO:HG2	4:H:1609:LEU:O	2.03	0.50
1:I:2371:CYS:O	1:I:2372:THR:OG1	2.25	0.50
4:L:2542:PRO:HB2	4:L:2669:LYS:HB2	1.92	0.50
4:L:2643:TYR:HA	4:L:2644:PRO:C	2.36	0.50
2:N:3733:ASP:OD1	2:N:3734:THR:N	2.44	0.50
3:C:32:TYR:CD1	3:C:100:TYR:HB2	2.46	0.50
4:D:542:PRO:HB2	4:D:669:LYS:HB2	1.92	0.50
4:D:643:TYR:HA	4:D:644:PRO:C	2.36	0.50
3:G:1013:ASN:OD1	3:G:1116:SER:O	2.29	0.50
4:H:1589:PHE:CE1	4:H:1603:GLY:HA3	2.46	0.50
2:F:1569:HIS:O	2:F:1599:GLY:N	2.44	0.50
2:F:1733:ASP:OD1	2:F:1734:THR:N	2.44	0.50
2:J:2671:LYS:HB3	4:L:2593:TRP:CZ2	2.46	0.50
2:J:2701:THR:HB	4:L:2595:ASN:C	2.35	0.50
3:K:2032:TYR:CD1	3:K:2100:TYR:HB2	2.46	0.50
1:M:3389:VAL:HG12	1:M:3390:ASP:H	1.76	0.50
1:E:1117:ASP:OD1	1:E:1181:TYR:OH	2.20	0.50
1:E:1197:LYS:O	1:E:1200:SER:OG	2.18	0.50
1:I:2203:ASP:OD1	1:I:2204:LEU:N	2.43	0.50
2:J:2673:LYS:CB	4:L:2593:TRP:HD1	2.12	0.50
3:K:2013:ASN:OD1	3:K:2116:SER:O	2.29	0.50
1:A:23:GLY:N	1:I:2306:GLU:HG2	2.27	0.50
1:I:2389:VAL:HG12	1:I:2390:ASP:H	1.76	0.50
1:A:388:ILE:HD12	1:A:388:ILE:O	2.12	0.50
2:B:671:LYS:HG2	4:D:594:TYR:N	2.27	0.50
4:D:589:PHE:CE1	4:D:603:GLY:HA3	2.46	0.50
3:O:3032:TYR:CD1	3:O:3100:TYR:HB2	2.46	0.50
4:P:3589:PHE:CE1	4:P:3603:GLY:HA3	2.46	0.50
1:A:15:TYR:O	1:A:17:ALA:N	2.44	0.50
4:H:1554:ASN:C	4:H:1554:ASN:ND2	2.54	0.50
1:I:2007:MET:SD	1:I:2279:ILE:HD12	2.52	0.50
3:K:2035:LEU:HD23	3:K:2037:VAL:HG23	1.82	0.50
1:M:3203:ASP:OD1	1:M:3204:LEU:N	2.43	0.50
1:E:1203:ASP:OD1	1:E:1204:LEU:N	2.43	0.49
1:I:2015:TYR:O	1:I:2017:ALA:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1388:ILE:HD12	1:E:1388:ILE:O	2.12	0.49
4:H:1549:LEU:HD12	4:H:1560:VAL:CG2	2.42	0.49
3:O:3102:ILE:HG22	4:P:3534:CYS:CB	2.13	0.49
4:P:3549:LEU:HD12	4:P:3560:VAL:HG21	1.93	0.49
1:E:1057:SER:OG	2:F:1724:SER:O	2.16	0.49
2:F:1668:HIS:C	4:H:1530:THR:O	2.55	0.49
3:G:1035:LEU:HD23	3:G:1037:VAL:HG23	1.82	0.49
2:N:3705:THR:CG2	4:P:3596:ASN:HB3	2.42	0.49
3:O:3078:THR:CG2	3:O:3080:TYR:CE2	2.84	0.49
1:E:1007:MET:SD	1:E:1279:ILE:HD12	2.52	0.49
4:H:1542:PRO:HB2	4:H:1669:LYS:HB2	1.92	0.49
3:O:3002:ILE:HA	3:O:3025:SER:O	2.13	0.49
3:O:3037:VAL:HG21	3:O:3107:TRP:HH2	1.70	0.49
1:E:1015:TYR:O	1:E:1017:ALA:N	2.44	0.49
2:F:1668:HIS:N	2:F:1671:LYS:O	2.43	0.49
2:J:2672:VAL:HG23	4:L:2595:ASN:OD1	2.07	0.49
1:M:3015:TYR:O	1:M:3017:ALA:N	2.44	0.49
3:O:3030:THR:CG2	3:O:3054:ASN:HD22	2.17	0.49
1:A:89:TRP:N	2:B:515:ASP:OD2	2.46	0.49
2:B:671:LYS:HE3	4:D:594:TYR:N	2.26	0.49
4:D:549:LEU:HD12	4:D:560:VAL:HG21	1.93	0.49
2:J:2670:ALA:HB3	4:L:2597:LEU:CD1	2.42	0.49
1:A:203:ASP:OD1	1:A:204:LEU:N	2.43	0.49
4:H:1549:LEU:HD12	4:H:1560:VAL:HG21	1.93	0.49
4:L:2549:LEU:HD12	4:L:2560:VAL:CG2	2.42	0.49
4:D:549:LEU:HD12	4:D:560:VAL:CG2	2.42	0.49
2:F:1796:GLU:N	2:F:1796:GLU:OE1	2.45	0.49
2:J:2796:GLU:OE1	2:J:2796:GLU:N	2.45	0.49
1:M:3007:MET:SD	1:M:3279:ILE:HD12	2.52	0.49
3:O:3013:ASN:OD1	3:O:3116:SER:O	2.29	0.49
3:O:3057:GLU:C	3:O:3058:PRO:CD	2.74	0.49
4:P:3506:GLN:OE1	4:P:3601:GLY:HA3	2.13	0.49
1:A:7:MET:SD	1:A:279:ILE:HD12	2.52	0.49
1:A:265:GLU:OE1	1:A:268:ARG:NH2	2.46	0.49
3:C:35:LEU:HB3	3:C:97:VAL:HB	1.95	0.49
3:C:48:MET:HG2	3:C:64:PHE:CE1	2.48	0.49
3:G:1048:MET:HG2	3:G:1064:PHE:CE1	2.47	0.49
4:H:1506:GLN:OE1	4:H:1601:GLY:HA3	2.13	0.49
1:I:2265:GLU:OE1	1:I:2268:ARG:NH2	2.46	0.49
2:J:2669:SER:CB	4:L:2592:LEU:HB2	2.26	0.49
4:D:512:THR:HG22	4:D:608:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2388:ILE:HD12	1:I:2388:ILE:O	2.12	0.49
2:J:2669:SER:HB2	4:L:2593:TRP:N	2.25	0.49
3:K:2011:VAL:CB	3:K:2151:PRO:CB	2.86	0.49
1:E:1265:GLU:OE1	1:E:1268:ARG:NH2	2.46	0.48
3:G:1037:VAL:HG21	3:G:1107:TRP:HH2	1.70	0.48
4:H:1542:PRO:HB3	4:H:1669:LYS:CD	2.42	0.48
2:J:2703:THR:OG1	3:K:2059:THR:CG2	2.47	0.48
4:L:2512:THR:HG22	4:L:2608:VAL:HG22	1.95	0.48
1:M:3388:ILE:HD12	1:M:3388:ILE:O	2.12	0.48
3:O:3039:GLN:CD	3:O:3045:PHE:CE1	2.86	0.48
4:P:3597:LEU:HD12	4:P:3597:LEU:C	2.38	0.48
3:C:2:ILE:HA	3:C:25:SER:O	2.13	0.48
2:F:1671:LYS:NZ	4:H:1595:ASN:HB2	2.28	0.48
3:G:1011:VAL:CB	3:G:1151:PRO:CB	2.86	0.48
1:I:2260:CYS:H	2:J:2782:ARG:NH2	2.11	0.48
2:J:2701:THR:CG2	4:L:2596:ASN:CB	2.92	0.48
3:O:3035:LEU:HB3	3:O:3097:VAL:HB	1.95	0.48
2:B:780:THR:OG1	2:B:791:THR:O	2.30	0.48
2:B:796:GLU:OE1	2:B:796:GLU:N	2.46	0.48
3:C:18:VAL:O	3:C:82:GLN:HA	2.14	0.48
4:D:597:LEU:C	4:D:597:LEU:HD12	2.38	0.48
1:E:1371:CYS:O	1:E:1372:THR:OG1	2.25	0.48
4:L:2549:LEU:HD12	4:L:2560:VAL:HG21	1.93	0.48
1:M:3268:ARG:NE	1:M:3270:GLU:OE2	2.46	0.48
4:P:3554:ASN:C	4:P:3554:ASN:ND2	2.54	0.48
2:B:671:LYS:CG	4:D:595:ASN:N	2.76	0.48
1:E:1096:CYS:O	1:E:1100:ASN:ND2	2.46	0.48
1:E:1268:ARG:NE	1:E:1270:GLU:OE2	2.47	0.48
1:M:3037:ARG:HH12	1:M:3132:MET:HG3	1.79	0.48
1:M:3265:GLU:OE1	1:M:3268:ARG:NH2	2.46	0.48
2:N:3796:GLU:OE1	2:N:3796:GLU:N	2.46	0.48
1:E:1260:CYS:H	2:F:1782:ARG:NH2	2.11	0.48
4:H:1512:THR:HG22	4:H:1608:VAL:HG22	1.95	0.48
1:M:3197:LYS:O	1:M:3200:SER:OG	2.18	0.48
3:O:3048:MET:HG2	3:O:3064:PHE:CE1	2.48	0.48
4:P:3549:LEU:HD12	4:P:3560:VAL:CG2	2.42	0.48
1:A:371:CYS:O	1:A:372:THR:OG1	2.25	0.48
3:K:2002:ILE:HA	3:K:2025:SER:O	2.13	0.48
1:M:3129:VAL:HG22	1:M:3149:VAL:HG11	1.96	0.48
1:M:3301:GLU:O	1:M:3320:ALA:N	2.43	0.48
1:A:57:SER:OG	2:B:724:SER:O	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:NE	1:A:270:GLU:OE2	2.47	0.48
4:D:506:GLN:OE1	4:D:601:GLY:HA3	2.13	0.48
4:H:1597:LEU:C	4:H:1597:LEU:HD12	2.38	0.48
2:J:2667:ILE:HG23	4:L:2594:TYR:C	2.39	0.48
2:J:2672:VAL:HG12	4:L:2595:ASN:C	2.38	0.48
4:L:2506:GLN:OE1	4:L:2601:GLY:HA3	2.13	0.48
1:A:37:ARG:HH12	1:A:132:MET:HG3	1.79	0.48
3:G:1002:ILE:HA	3:G:1025:SER:O	2.13	0.48
3:G:1018:VAL:O	3:G:1082:GLN:HA	2.14	0.48
3:G:1035:LEU:HG	3:G:1047:TRP:NE1	2.29	0.48
1:I:2037:ARG:HH12	1:I:2132:MET:HG3	1.79	0.48
4:L:2597:LEU:HD12	4:L:2597:LEU:C	2.38	0.48
3:O:3002:ILE:CD1	3:O:3098:ARG:HH12	1.83	0.48
3:O:3030:THR:O	3:O:3030:THR:HG22	2.09	0.48
1:A:260:CYS:H	2:B:782:ARG:NH2	2.11	0.48
1:A:301:GLU:O	1:A:320:ALA:N	2.43	0.48
1:I:2268:ARG:NE	1:I:2270:GLU:OE2	2.46	0.48
4:P:3512:THR:HG22	4:P:3608:VAL:HG22	1.95	0.48
3:K:2035:LEU:HB3	3:K:2097:VAL:HB	1.95	0.47
3:K:2048:MET:HG2	3:K:2064:PHE:CE1	2.48	0.47
3:O:3018:VAL:O	3:O:3082:GLN:HA	2.14	0.47
3:O:3097:VAL:HG21	3:O:3107:TRP:CD2	2.49	0.47
3:C:24:ALA:HB1	3:C:27:TYR:HE1	1.75	0.47
1:I:2323:SER:N	1:I:2350:SER:OG	2.47	0.47
4:L:2554:ASN:C	4:L:2554:ASN:ND2	2.54	0.47
1:M:3260:CYS:H	2:N:3782:ARG:NH2	2.11	0.47
3:C:45:PHE:HZ	4:D:546:PHE:HZ	0.62	0.47
1:E:1089:TRP:N	2:F:1515:ASP:OD2	2.46	0.47
4:L:2689:GLU:HA	4:L:2711:ARG:CZ	2.44	0.47
2:N:3705:THR:HG21	4:P:3596:ASN:CB	2.42	0.47
3:C:48:MET:HE1	3:C:81:LEU:HD21	1.97	0.47
3:C:97:VAL:HG21	3:C:107:TRP:CD2	2.50	0.47
3:K:2035:LEU:HG	3:K:2047:TRP:NE1	2.29	0.47
3:K:2107:TRP:CB	4:L:2546:PHE:HB2	2.45	0.47
4:L:2656:THR:HA	4:L:2657:PRO:HD2	1.63	0.47
1:M:3096:CYS:O	1:M:3100:ASN:ND2	2.46	0.47
2:N:3705:THR:HG21	4:P:3596:ASN:HB3	1.96	0.47
1:A:221:LYS:O	1:A:235:THR:OG1	2.19	0.47
2:B:671:LYS:CE	4:D:594:TYR:CA	2.86	0.47
1:I:2129:VAL:HG22	1:I:2149:VAL:HG11	1.96	0.47
1:I:2312:ASP:OD1	1:I:2313:PHE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2018:VAL:O	3:K:2082:GLN:HA	2.14	0.47
3:K:2097:VAL:HG21	3:K:2107:TRP:CD2	2.49	0.47
4:L:2507:GLU:O	4:L:2604:THR:OG1	2.27	0.47
1:M:3312:ASP:OD1	1:M:3313:PHE:N	2.48	0.47
4:P:3703:HIS:ND1	4:P:3703:HIS:N	2.62	0.47
2:B:671:LYS:HD2	4:D:597:LEU:N	2.29	0.47
3:G:1035:LEU:HB3	3:G:1097:VAL:HB	1.95	0.47
1:A:312:ASP:OD1	1:A:313:PHE:N	2.48	0.47
1:A:390:ASP:O	2:B:823:TRP:HB3	2.15	0.47
3:G:1048:MET:HE1	3:G:1081:LEU:HD21	1.96	0.47
3:G:1103:SER:HA	4:H:1598:TRP:CH2	2.50	0.47
1:I:2390:ASP:O	2:J:2823:TRP:HB3	2.14	0.47
2:J:2673:LYS:CB	4:L:2593:TRP:HE1	2.28	0.47
2:J:2702:THR:HG21	3:K:2059:THR:HB	1.69	0.47
2:J:2780:THR:OG1	2:J:2791:THR:O	2.30	0.47
3:K:2048:MET:HE1	3:K:2081:LEU:HD21	1.97	0.47
1:M:3391:TYR:CE2	2:N:3784:LEU:HD11	2.49	0.47
2:N:3669:SER:C	4:P:3533:ASN:C	2.82	0.47
2:N:3671:LYS:HZ2	4:P:3596:ASN:CA	2.19	0.47
3:O:3035:LEU:HG	3:O:3047:TRP:NE1	2.29	0.47
1:A:323:SER:N	1:A:350:SER:OG	2.47	0.47
4:D:703:HIS:ND1	4:D:703:HIS:N	2.62	0.47
1:E:1037:ARG:HH12	1:E:1132:MET:HG3	1.79	0.47
1:E:1129:VAL:HG22	1:E:1149:VAL:HG11	1.96	0.47
1:I:2391:TYR:CE2	2:J:2784:LEU:HD11	2.49	0.47
3:K:2097:VAL:HG22	3:K:2107:TRP:CE3	2.49	0.47
4:L:2549:LEU:HA	4:L:2560:VAL:HG21	1.97	0.47
4:L:2703:HIS:ND1	4:L:2703:HIS:N	2.62	0.47
1:A:246:ARG:NH1	1:A:247:ASP:OD2	2.48	0.47
1:E:1312:ASP:OD1	1:E:1313:PHE:N	2.48	0.47
1:E:1391:TYR:CE2	2:F:1784:LEU:HD11	2.49	0.47
2:J:2670:ALA:O	4:L:2594:TYR:O	2.23	0.47
3:K:2030:THR:CG2	3:K:2054:ASN:ND2	2.78	0.47
3:O:3048:MET:HE1	3:O:3081:LEU:HD21	1.97	0.47
1:A:16:LYS:O	1:A:332:HIS:ND1	2.48	0.47
1:A:129:VAL:HG22	1:A:149:VAL:HG11	1.96	0.47
1:A:197:LYS:O	1:A:200:SER:OG	2.18	0.47
3:C:35:LEU:HD23	3:C:35:LEU:C	2.40	0.47
3:C:97:VAL:HG22	3:C:107:TRP:CE3	2.49	0.47
3:C:107:TRP:CB	4:D:546:PHE:HB2	2.45	0.47
4:D:514:PRO:HG2	4:D:609:LEU:O	2.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1097:VAL:HG21	3:G:1107:TRP:CD2	2.50	0.47
3:K:2045:PHE:HE1	4:L:2589:PHE:CZ	2.33	0.47
1:M:3016:LYS:O	1:M:3332:HIS:ND1	2.48	0.47
1:M:3390:ASP:O	2:N:3823:TRP:HB3	2.14	0.47
4:P:3689:GLU:HA	4:P:3711:ARG:CZ	2.44	0.47
1:A:391:TYR:CE2	2:B:784:LEU:HD11	2.49	0.46
1:E:1016:LYS:O	1:E:1332:HIS:ND1	2.48	0.46
1:E:1229:ILE:HG21	2:F:1513:ARG:HE	1.80	0.46
3:G:1107:TRP:CB	4:H:1546:PHE:HB2	2.45	0.46
1:I:2089:TRP:N	2:J:2515:ASP:OD2	2.46	0.46
2:J:2671:LYS:HB2	4:L:2593:TRP:CZ3	2.48	0.46
3:O:3107:TRP:CB	4:P:3546:PHE:HB2	2.45	0.46
3:C:35:LEU:HG	3:C:47:TRP:NE1	2.29	0.46
4:D:689:GLU:HA	4:D:711:ARG:CZ	2.44	0.46
1:E:1323:SER:N	1:E:1350:SER:OG	2.47	0.46
4:H:1703:HIS:ND1	4:H:1703:HIS:N	2.62	0.46
3:K:2024:ALA:HB1	3:K:2027:TYR:HE1	1.75	0.46
3:K:2035:LEU:HD23	3:K:2035:LEU:C	2.40	0.46
4:L:2542:PRO:HB3	4:L:2669:LYS:CD	2.42	0.46
4:P:3507:GLU:OE2	4:P:3521:THR:OG1	2.24	0.46
1:E:1390:ASP:O	2:F:1823:TRP:HB3	2.14	0.46
3:G:1024:ALA:HB1	3:G:1027:TYR:HE1	1.75	0.46
3:G:1035:LEU:HD23	3:G:1035:LEU:C	2.40	0.46
1:I:2016:LYS:O	1:I:2332:HIS:ND1	2.48	0.46
2:J:2668:HIS:CD2	4:L:2598:TRP:CE3	2.99	0.46
1:M:3323:SER:N	1:M:3350:SER:OG	2.47	0.46
4:P:3520:LEU:N	4:P:3520:LEU:CD2	2.70	0.46
2:B:671:LYS:HE3	4:D:597:LEU:O	2.16	0.46
1:E:1246:ARG:NH1	1:E:1247:ASP:OD2	2.48	0.46
4:H:1689:GLU:HA	4:H:1711:ARG:CZ	2.44	0.46
3:O:3012:LYS:HD2	3:O:3016:GLU:OE1	2.16	0.46
3:O:3102:ILE:HB	4:P:3552:ASP:CA	2.40	0.46
4:D:549:LEU:HA	4:D:560:VAL:HG21	1.97	0.46
4:H:1549:LEU:HA	4:H:1560:VAL:HG21	1.97	0.46
1:I:2229:ILE:HG21	2:J:2513:ARG:HE	1.80	0.46
3:O:3097:VAL:CG1	3:O:3104:LEU:HB3	2.46	0.46
3:O:3097:VAL:HG22	3:O:3107:TRP:CD2	2.51	0.46
1:A:229:ILE:HG21	2:B:513:ARG:HE	1.80	0.46
3:C:12:LYS:HD2	3:C:16:GLU:OE1	2.16	0.46
2:F:1612:ALA:HB3	2:J:2630:GLU:OE1	2.16	0.46
3:C:103:SER:HA	4:D:598:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1780:THR:OG1	2:F:1791:THR:O	2.30	0.46
3:K:2047:TRP:NE1	3:K:2049:GLY:O	2.49	0.46
3:K:2103:SER:HA	4:L:2598:TRP:CH2	2.50	0.46
4:L:2557:ARG:CD	4:L:2558:SER:O	2.63	0.46
1:M:3246:ARG:NH1	1:M:3247:ASP:OD2	2.48	0.46
3:O:3035:LEU:HD23	3:O:3035:LEU:C	2.40	0.46
2:B:703:THR:HA	4:D:596:ASN:HB2	1.78	0.46
3:C:2:ILE:CD1	3:C:98:ARG:HH11	2.15	0.46
3:C:67:ARG:HH22	3:C:90:ASP:CG	2.24	0.46
3:G:1057:GLU:C	3:G:1058:PRO:CD	2.74	0.46
4:H:1557:ARG:CD	4:H:1558:SER:O	2.63	0.46
2:J:2612:ALA:HB3	2:N:3630:GLU:OE1	2.16	0.46
1:M:3089:TRP:N	2:N:3515:ASP:OD2	2.46	0.46
3:O:3045:PHE:HE1	4:P:3589:PHE:CZ	2.33	0.46
4:P:3582:THR:HG1	4:P:3610:GLY:HA3	1.78	0.46
3:C:97:VAL:HG22	3:C:107:TRP:CD2	2.51	0.46
3:G:1072:LEU:HD13	3:G:1074:ILE:CG1	2.46	0.46
1:I:2246:ARG:NH1	1:I:2247:ASP:OD2	2.48	0.46
3:K:2011:VAL:CG2	3:K:2152:GLU:N	2.70	0.46
3:K:2012:LYS:HD2	3:K:2016:GLU:OE1	2.16	0.46
1:M:3229:ILE:HG21	2:N:3513:ARG:HE	1.80	0.46
2:N:3780:THR:OG1	2:N:3791:THR:O	2.30	0.46
4:P:3549:LEU:HA	4:P:3560:VAL:HG21	1.97	0.46
3:C:33:PRO:CB	3:C:51:ILE:O	2.64	0.46
3:C:47:TRP:NE1	3:C:49:GLY:O	2.49	0.46
4:H:1563:ARG:CZ	4:H:1564:PHE:HE2	2.29	0.46
3:O:3047:TRP:NE1	3:O:3049:GLY:O	2.49	0.46
3:C:97:VAL:CG1	3:C:104:LEU:HB3	2.46	0.45
1:E:1391:TYR:CZ	2:F:1784:LEU:CD1	2.99	0.45
3:G:1047:TRP:NE1	3:G:1049:GLY:O	2.49	0.45
3:G:1097:VAL:HG22	3:G:1107:TRP:CD2	2.51	0.45
4:H:1653:VAL:H	4:H:1658:VAL:HG23	1.81	0.45
3:O:3032:TYR:CZ	3:O:3100:TYR:CZ	2.84	0.45
3:O:3103:SER:HA	4:P:3598:TRP:CH2	2.50	0.45
1:E:1263:ALA:HB3	1:E:1268:ARG:HE	1.81	0.45
3:O:3097:VAL:HG22	3:O:3107:TRP:CE3	2.49	0.45
2:F:1668:HIS:NE2	4:H:1534:CYS:SG	2.90	0.45
3:G:1097:VAL:CG1	3:G:1104:LEU:HB3	2.46	0.45
1:M:3117:ASP:OD1	1:M:3181:TYR:OH	2.20	0.45
1:A:327:GLY:O	1:A:347:LEU:N	2.50	0.45
3:C:72:LEU:HD13	3:C:74:ILE:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1067:ARG:HH22	3:G:1090:ASP:CG	2.24	0.45
1:M:3263:ALA:HB3	1:M:3268:ARG:HE	1.81	0.45
2:N:3661:ASP:OD1	2:N:3663:SER:OG	2.28	0.45
1:A:125:HIS:CD2	1:E:1041:SER:HB2	2.52	0.45
2:B:566:ASP:OD1	2:B:567:ASN:N	2.50	0.45
2:B:670:ALA:HA	4:D:594:TYR:HD1	1.74	0.45
2:F:1772:HIS:HE1	1:M:3246:ARG:HH22	1.63	0.45
2:J:2671:LYS:CB	4:L:2593:TRP:CZ2	2.99	0.45
3:K:2067:ARG:HH22	3:K:2090:ASP:CG	2.24	0.45
1:M:3261:SER:O	1:M:3270:GLU:N	2.50	0.45
4:P:3514:PRO:HG2	4:P:3609:LEU:O	2.03	0.45
4:P:3686:ARG:H	4:P:3686:ARG:HG2	1.64	0.45
1:A:263:ALA:HB3	1:A:268:ARG:HE	1.81	0.45
1:E:1246:ARG:HH22	2:J:2772:HIS:HE1	1.63	0.45
2:F:1579:VAL:O	2:F:1580:SER:OG	2.33	0.45
1:I:2096:CYS:O	1:I:2100:ASN:ND2	2.46	0.45
1:I:2263:ALA:HB3	1:I:2268:ARG:HE	1.81	0.45
1:I:2380:ASP:OD1	1:I:2381:CYS:N	2.50	0.45
3:K:2033:PRO:CB	3:K:2051:ILE:O	2.64	0.45
3:K:2047:TRP:CZ2	3:K:2049:GLY:HA2	2.52	0.45
1:A:96:CYS:O	1:A:100:ASN:ND2	2.46	0.45
1:A:261:SER:O	1:A:270:GLU:N	2.50	0.45
2:F:1566:ASP:OD1	2:F:1567:ASN:N	2.50	0.45
2:F:1630:GLU:OE1	2:N:3612:ALA:HB3	2.16	0.45
2:F:1671:LYS:HD3	4:H:1595:ASN:OD1	2.17	0.45
1:I:2261:SER:O	1:I:2270:GLU:N	2.50	0.45
3:K:2097:VAL:HG22	3:K:2107:TRP:CD2	2.51	0.45
1:A:391:TYR:CZ	2:B:784:LEU:CD1	3.00	0.45
3:G:1012:LYS:HD2	3:G:1016:GLU:OE1	2.16	0.45
3:G:1030:THR:CG2	3:G:1054:ASN:ND2	2.78	0.45
3:G:1047:TRP:CZ2	3:G:1049:GLY:HA2	2.52	0.45
2:J:2690:ASP:CG	3:K:2059:THR:HG1	2.17	0.45
2:B:671:LYS:CD	4:D:593:TRP:CZ3	2.82	0.45
3:C:107:TRP:CB	4:D:546:PHE:CB	2.95	0.45
3:K:2097:VAL:CG1	3:K:2104:LEU:HB3	2.46	0.45
3:K:2102:ILE:O	4:L:2534:CYS:HB3	2.17	0.45
4:L:2507:GLU:OE2	4:L:2521:THR:OG1	2.23	0.45
1:M:3391:TYR:CZ	2:N:3784:LEU:CD1	2.99	0.45
3:O:3024:ALA:HB1	3:O:3027:TYR:HE1	1.75	0.45
3:O:3103:SER:OG	4:P:3551:GLY:HA3	2.17	0.45
4:P:3557:ARG:CD	4:P:3558:SER:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LYS:O	3:C:115:VAL:HA	2.17	0.45
3:C:30:THR:CG2	3:C:54:ASN:ND2	2.78	0.45
4:D:563:ARG:CZ	4:D:564:PHE:HE2	2.30	0.45
3:G:1102:ILE:O	4:H:1534:CYS:HB3	2.17	0.45
2:J:2667:ILE:CA	4:L:2595:ASN:OD1	2.65	0.45
1:M:3380:ASP:OD1	1:M:3381:CYS:N	2.50	0.45
3:O:3033:PRO:CB	3:O:3051:ILE:O	2.64	0.45
3:O:3047:TRP:CZ2	3:O:3049:GLY:HA2	2.52	0.45
1:A:41:SER:HB2	1:E:1125:HIS:CD2	2.52	0.44
1:A:117:ASP:OD1	1:A:181:TYR:OH	2.20	0.44
4:D:557:ARG:HD2	4:D:558:SER:N	2.33	0.44
4:H:1539:GLN:NE2	4:H:1541:LYS:HE3	2.32	0.44
1:I:2246:ARG:HH22	2:N:3772:HIS:HE1	1.63	0.44
2:J:2668:HIS:N	4:L:2594:TYR:HA	2.32	0.44
3:K:2104:LEU:N	4:L:2536:ASN:OD1	2.43	0.44
3:K:2107:TRP:CB	4:L:2546:PHE:CB	2.95	0.44
2:N:3566:ASP:OD1	2:N:3567:ASN:N	2.50	0.44
3:O:3011:VAL:CB	3:O:3151:PRO:CB	2.86	0.44
3:O:3107:TRP:CB	4:P:3546:PHE:CB	2.95	0.44
2:B:671:LYS:HE3	4:D:594:TYR:CA	2.46	0.44
3:G:1033:PRO:CB	3:G:1051:ILE:O	2.64	0.44
3:G:1103:SER:OG	4:H:1551:GLY:HA3	2.17	0.44
3:K:2078:THR:CG2	3:K:2080:TYR:OH	2.48	0.44
4:L:2539:GLN:NE2	4:L:2541:LYS:HE3	2.32	0.44
4:L:2563:ARG:CZ	4:L:2564:PHE:HE2	2.29	0.44
4:P:3563:ARG:CZ	4:P:3564:PHE:HE2	2.30	0.44
4:P:3653:VAL:H	4:P:3658:VAL:HG23	1.81	0.44
2:B:571:ARG:HG3	2:B:597:THR:OG1	2.18	0.44
1:I:2391:TYR:CZ	2:J:2784:LEU:CD1	2.99	0.44
2:J:2566:ASP:OD1	2:J:2567:ASN:N	2.50	0.44
3:O:3102:ILE:O	4:P:3534:CYS:HB3	2.17	0.44
4:P:3557:ARG:HD2	4:P:3558:SER:N	2.32	0.44
3:C:103:SER:OG	4:D:551:GLY:HA3	2.17	0.44
4:D:653:VAL:H	4:D:658:VAL:HG23	1.81	0.44
4:L:2523:ARG:HG3	4:L:2523:ARG:NH1	2.32	0.44
4:L:2638:THR:C	4:L:2639:ILE:HG13	2.43	0.44
4:L:2689:GLU:O	4:L:2689:GLU:HG3	2.18	0.44
1:M:3301:GLU:OE1	1:M:3303:LYS:NZ	2.40	0.44
4:D:539:GLN:NE2	4:D:541:LYS:HE3	2.32	0.44
4:D:542:PRO:HB3	4:D:669:LYS:CD	2.42	0.44
1:E:1380:ASP:OD1	1:E:1381:CYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1571:ARG:HG3	2:F:1597:THR:OG1	2.18	0.44
2:J:2571:ARG:HG3	2:J:2597:THR:OG1	2.18	0.44
3:K:2103:SER:OG	4:L:2551:GLY:HA3	2.17	0.44
4:L:2653:VAL:H	4:L:2658:VAL:HG23	1.81	0.44
4:L:2683:LEU:HD22	4:L:2687:ALA:CB	2.48	0.44
2:N:3571:ARG:HG3	2:N:3597:THR:OG1	2.18	0.44
3:O:3011:VAL:CG2	3:O:3152:GLU:N	2.70	0.44
4:D:523:ARG:NH1	4:D:523:ARG:HG3	2.32	0.44
3:K:2012:LYS:O	3:K:2115:VAL:HA	2.17	0.44
3:K:2123:PRO:HB3	3:K:2149:TYR:HB3	2.00	0.44
4:L:2557:ARG:HD2	4:L:2558:SER:N	2.33	0.44
1:M:3327:GLY:O	1:M:3347:LEU:N	2.50	0.44
3:O:3123:PRO:HB3	3:O:3149:TYR:HB3	2.00	0.44
4:P:3638:THR:C	4:P:3639:ILE:HG13	2.43	0.44
3:C:123:PRO:HB3	3:C:149:TYR:HB3	2.00	0.44
4:H:1523:ARG:HG3	4:H:1523:ARG:NH1	2.32	0.44
2:J:2701:THR:CB	4:L:2596:ASN:CA	2.80	0.44
3:K:2100:TYR:CD2	3:K:2101:PHE:CE2	3.06	0.44
3:O:3067:ARG:HH22	3:O:3090:ASP:CG	2.24	0.44
1:E:1261:SER:O	1:E:1270:GLU:N	2.50	0.44
3:G:1100:TYR:CD2	3:G:1101:PHE:CE2	3.06	0.44
4:H:1557:ARG:HD2	4:H:1558:SER:N	2.33	0.44
2:B:671:LYS:HD3	4:D:595:ASN:O	2.07	0.44
3:C:100:TYR:CD2	3:C:101:PHE:CE2	3.06	0.44
4:H:1638:THR:C	4:H:1639:ILE:HG13	2.43	0.44
1:I:2312:ASP:O	1:I:2314:GLY:N	2.50	0.44
4:P:3556:ARG:HD3	4:P:3560:VAL:HG12	2.00	0.44
3:C:102:ILE:O	4:D:534:CYS:HB3	2.17	0.43
3:G:1123:PRO:HB3	3:G:1149:TYR:HB3	2.00	0.43
4:P:3539:GLN:NE2	4:P:3541:LYS:HE3	2.32	0.43
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.52	0.43
4:D:514:PRO:CD	4:D:609:LEU:C	2.89	0.43
1:E:1327:GLY:O	1:E:1347:LEU:N	2.50	0.43
4:H:1669:LYS:HB3	4:H:1669:LYS:HE2	1.73	0.43
1:I:2152:GLU:OE1	1:I:2152:GLU:N	2.52	0.43
3:O:3032:TYR:CE1	3:O:3100:TYR:HD1	1.97	0.43
4:P:3542:PRO:HB3	4:P:3669:LYS:CD	2.42	0.43
1:A:1:TYR:HA	1:I:2385:LYS:NZ	2.30	0.43
3:K:2072:LEU:HD13	3:K:2074:ILE:CG1	2.46	0.43
2:B:671:LYS:CD	4:D:597:LEU:N	2.81	0.43
1:E:1312:ASP:O	1:E:1314:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1107:TRP:HB2	4:H:1546:PHE:HB2	2.01	0.43
3:G:1107:TRP:CB	4:H:1546:PHE:CB	2.95	0.43
2:N:3703:THR:CA	3:O:3052:TYR:OH	2.62	0.43
3:O:3002:ILE:HD13	3:O:3098:ARG:HH11	1.81	0.43
3:O:3012:LYS:O	3:O:3115:VAL:HA	2.17	0.43
4:P:3523:ARG:HG3	4:P:3523:ARG:NH1	2.32	0.43
1:A:291:ILE:HG21	1:I:2316:ILE:HD11	1.94	0.43
4:H:1556:ARG:HD3	4:H:1560:VAL:HG12	2.00	0.43
4:H:1662:MET:HB2	4:H:1662:MET:HE3	1.59	0.43
4:H:1683:LEU:HD22	4:H:1687:ALA:CB	2.48	0.43
2:J:2700:HIS:CB	4:L:2593:TRP:CH2	2.94	0.43
3:K:2040:ALA:CA	3:K:2041:PRO:CD	2.96	0.43
1:A:152:GLU:OE1	1:A:152:GLU:N	2.52	0.43
1:A:380:ASP:OD1	1:A:381:CYS:N	2.50	0.43
4:D:683:LEU:CD1	4:D:694:TYR:CE2	3.01	0.43
1:I:2301:GLU:O	1:I:2320:ALA:N	2.43	0.43
3:K:2102:ILE:HB	4:L:2552:ASP:CA	2.40	0.43
3:C:68:PHE:CD1	3:C:83:ILE:HG12	2.54	0.43
4:D:549:LEU:HD12	4:D:549:LEU:HA	1.85	0.43
3:G:1012:LYS:O	3:G:1115:VAL:HA	2.17	0.43
3:G:1175:GLN:CG	4:H:1663:GLU:OE2	2.60	0.43
1:M:3312:ASP:O	1:M:3314:GLY:N	2.51	0.43
3:O:3100:TYR:CD2	3:O:3101:PHE:CE2	3.06	0.43
4:P:3623:PRO:CG	4:P:3633:ALA:HB1	2.49	0.43
4:P:3683:LEU:HD22	4:P:3687:ALA:CB	2.48	0.43
2:B:668:HIS:CD2	4:D:593:TRP:CB	2.94	0.43
3:C:173:LEU:HD12	4:D:665:THR:CG2	2.39	0.43
3:C:175:GLN:CG	4:D:663:GLU:OE2	2.60	0.43
4:D:669:LYS:HB3	4:D:669:LYS:HE2	1.73	0.43
3:G:1097:VAL:HG22	3:G:1107:TRP:CE3	2.49	0.43
4:H:1514:PRO:CD	4:H:1609:LEU:C	2.89	0.43
2:J:2666:SER:CB	4:L:2532:SER:HB3	2.46	0.43
4:L:2556:ARG:HD3	4:L:2560:VAL:HG12	2.00	0.43
3:O:3107:TRP:HB2	4:P:3546:PHE:HB2	2.01	0.43
1:A:154:PRO:HD2	1:E:1195:THR:HB	2.00	0.43
1:A:195:THR:HB	1:E:1154:PRO:HD2	2.01	0.43
2:B:701:THR:C	4:D:593:TRP:HZ2	2.06	0.43
3:C:11:VAL:CG2	3:C:152:GLU:N	2.70	0.43
3:C:102:ILE:HB	4:D:552:ASP:CA	2.40	0.43
4:D:526:ILE:O	4:D:526:ILE:HG22	2.19	0.43
2:N:3666:SER:N	2:N:3673:LYS:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3078:THR:HB	3:O:3080:TYR:CE1	2.54	0.43
1:A:7:MET:O	1:A:277:ILE:N	2.48	0.43
3:G:1045:PHE:HE1	4:H:1589:PHE:CZ	2.33	0.43
4:H:1623:PRO:CG	4:H:1633:ALA:HB1	2.49	0.43
1:M:3152:GLU:N	1:M:3152:GLU:OE1	2.52	0.43
4:P:3526:ILE:O	4:P:3526:ILE:HG22	2.19	0.43
4:P:3689:GLU:O	4:P:3689:GLU:HG3	2.18	0.43
1:A:312:ASP:O	1:A:314:GLY:N	2.51	0.42
4:D:556:ARG:HD3	4:D:560:VAL:HG12	2.00	0.42
4:D:620:LEU:HD23	4:D:620:LEU:HA	1.89	0.42
4:D:638:THR:C	4:D:639:ILE:HG13	2.42	0.42
3:K:2039:GLN:OE1	3:K:2045:PHE:CZ	2.72	0.42
1:M:3007:MET:O	1:M:3277:ILE:N	2.48	0.42
3:O:3217:ARG:HH21	4:P:3622:PRO:CD	2.08	0.42
3:G:1039:GLN:OE1	3:G:1045:PHE:CZ	2.72	0.42
3:K:2040:ALA:HA	3:K:2041:PRO:CD	2.49	0.42
3:K:2078:THR:HB	3:K:2080:TYR:CE1	2.54	0.42
3:K:2088:ASN:O	3:K:2091:THR:HG23	2.19	0.42
4:L:2526:ILE:HG22	4:L:2526:ILE:O	2.19	0.42
4:L:2582:THR:HG1	4:L:2610:GLY:HA3	1.81	0.42
1:M:3102:GLN:NE2	1:M:3104:SER:OG	2.47	0.42
2:N:3671:LYS:HZ1	2:N:3705:THR:HG22	1.84	0.42
3:O:3037:VAL:HB	3:O:3107:TRP:HZ3	1.84	0.42
4:P:3656:THR:HA	4:P:3657:PRO:HD2	1.62	0.42
3:C:4:LEU:HD23	3:C:24:ALA:HA	2.02	0.42
3:C:78:THR:HB	3:C:80:TYR:CE1	2.54	0.42
4:D:623:PRO:CG	4:D:633:ALA:HB1	2.49	0.42
3:G:1068:PHE:CD1	3:G:1083:ILE:HG12	2.54	0.42
4:H:1542:PRO:CB	4:H:1669:LYS:CD	2.95	0.42
4:H:1582:THR:HG1	4:H:1610:GLY:HA3	1.80	0.42
3:K:2068:PHE:CD1	3:K:2083:ILE:HG12	2.54	0.42
3:O:3088:ASN:O	3:O:3091:THR:HG23	2.19	0.42
4:D:561:PRO:CG	4:D:563:ARG:NH1	2.82	0.42
4:D:683:LEU:HD22	4:D:687:ALA:CB	2.48	0.42
2:F:1671:LYS:C	4:H:1532:SER:HB2	2.44	0.42
2:J:2692:ARG:NH1	3:K:2057:GLU:HG3	2.13	0.42
4:P:3540:GLU:HB2	4:P:3546:PHE:CE1	2.55	0.42
2:B:705:THR:O	4:D:595:ASN:OD1	2.33	0.42
4:D:689:GLU:O	4:D:689:GLU:HG3	2.18	0.42
1:E:1152:GLU:OE1	1:E:1152:GLU:N	2.52	0.42
4:L:2639:ILE:HG22	4:L:2642:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:3068:PHE:CD1	3:O:3083:ILE:HG12	2.54	0.42
4:P:3639:ILE:HG22	4:P:3642:PHE:CD2	2.54	0.42
2:B:666:SER:N	2:B:673:LYS:O	2.52	0.42
2:F:1669:SER:HA	4:H:1530:THR:HG23	1.42	0.42
3:G:1013:ASN:CG	3:G:1117:SER:HA	2.44	0.42
3:G:1078:THR:HB	3:G:1080:TYR:CE1	2.54	0.42
4:H:1689:GLU:O	4:H:1689:GLU:HG3	2.18	0.42
3:K:2018:VAL:HG11	3:K:2113:LEU:HD13	2.02	0.42
3:C:13:ASN:CG	3:C:117:SER:HA	2.45	0.42
4:D:557:ARG:CD	4:D:558:SER:O	2.63	0.42
4:D:639:ILE:HG22	4:D:642:PHE:CD2	2.54	0.42
3:G:1004:LEU:HD23	3:G:1024:ALA:HA	2.02	0.42
4:H:1540:GLU:HB2	4:H:1546:PHE:CE1	2.55	0.42
2:J:2505:ASP:OD2	2:J:2513:ARG:NH2	2.53	0.42
3:K:2004:LEU:HD23	3:K:2024:ALA:HA	2.02	0.42
4:L:2540:GLU:HB2	4:L:2546:PHE:CE1	2.54	0.42
3:O:3013:ASN:CG	3:O:3117:SER:HA	2.45	0.42
4:D:540:GLU:HB2	4:D:546:PHE:CE1	2.54	0.42
2:F:1666:SER:N	2:F:1673:LYS:O	2.52	0.42
4:H:1593:TRP:CZ3	4:H:1597:LEU:CA	3.03	0.42
3:C:18:VAL:HG11	3:C:113:LEU:HD13	2.02	0.42
3:C:37:VAL:HB	3:C:107:TRP:HZ3	1.84	0.42
4:D:587:ILE:HG12	4:D:605:LYS:HG3	2.02	0.42
3:G:1037:VAL:HB	3:G:1107:TRP:HZ3	1.84	0.42
3:G:1088:ASN:O	3:G:1091:THR:HG23	2.19	0.42
4:H:1587:ILE:HG12	4:H:1605:LYS:HG3	2.02	0.42
4:H:1639:ILE:HG22	4:H:1642:PHE:CD2	2.54	0.42
2:N:3505:ASP:OD2	2:N:3513:ARG:NH2	2.53	0.42
3:O:3072:LEU:HD13	3:O:3074:ILE:CG1	2.46	0.42
2:B:673:LYS:HZ3	3:C:102:ILE:CD1	2.33	0.42
1:I:2327:GLY:O	1:I:2347:LEU:N	2.50	0.42
2:J:2637:CYS:SG	2:J:2750:CYS:N	2.93	0.42
3:K:2037:VAL:HB	3:K:2107:TRP:HZ3	1.84	0.42
3:K:2057:GLU:C	3:K:2058:PRO:CD	2.74	0.42
3:K:2100:TYR:HE2	3:K:2101:PHE:CZ	2.38	0.42
4:L:2587:ILE:HG12	4:L:2605:LYS:HG3	2.02	0.42
4:L:2623:PRO:CG	4:L:2633:ALA:HB1	2.49	0.42
1:M:3038:ILE:HG23	1:M:3129:VAL:HG12	2.02	0.42
1:M:3075:ASP:HB2	1:M:3216:ALA:HB3	2.02	0.42
4:P:3556:ARG:HD3	4:P:3560:VAL:O	2.20	0.42
4:P:3583:GLU:HG2	4:P:3583:GLU:H	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:TRP:HB2	4:D:546:PHE:HB2	2.01	0.41
2:J:2666:SER:N	2:J:2673:LYS:O	2.52	0.41
3:K:2107:TRP:HB2	4:L:2546:PHE:HB2	2.01	0.41
4:L:2683:LEU:CD1	4:L:2694:TYR:CE2	3.01	0.41
3:O:3030:THR:CG2	3:O:3054:ASN:ND2	2.78	0.41
3:C:45:PHE:HE1	4:D:589:PHE:CZ	2.33	0.41
4:L:2504:VAL:HG13	4:L:2522:CYS:SG	2.60	0.41
1:A:23:GLY:N	1:I:2306:GLU:CG	2.84	0.41
2:B:556:ASN:O	2:B:559:THR:OG1	2.30	0.41
4:D:593:TRP:CZ3	4:D:597:LEU:CA	3.03	0.41
3:G:1018:VAL:HG11	3:G:1113:LEU:HD13	2.02	0.41
4:H:1526:ILE:O	4:H:1526:ILE:HG22	2.19	0.41
1:I:2038:ILE:HG23	1:I:2129:VAL:HG12	2.02	0.41
3:K:2013:ASN:CG	3:K:2117:SER:HA	2.45	0.41
1:M:3391:TYR:CE2	2:N:3784:LEU:CD1	3.04	0.41
4:P:3556:ARG:C	4:P:3557:ARG:O	2.62	0.41
3:C:107:TRP:CG	4:D:546:PHE:HB3	2.55	0.41
4:D:504:VAL:HG13	4:D:522:CYS:SG	2.60	0.41
1:E:1134:ASN:OD1	1:E:1135:ILE:N	2.54	0.41
3:G:1104:LEU:N	4:H:1536:ASN:OD1	2.43	0.41
4:H:1581:GLN:C	4:H:1608:VAL:HG11	2.46	0.41
1:I:2150:ASN:CG	1:I:2153:THR:HG1	2.21	0.41
2:J:2666:SER:HB2	4:L:2532:SER:OG	2.20	0.41
4:L:2689:GLU:CA	4:L:2711:ARG:HH21	2.33	0.41
3:O:3078:THR:CG2	3:O:3080:TYR:OH	2.48	0.41
3:O:3107:TRP:CG	4:P:3546:PHE:HB3	2.56	0.41
4:P:3587:ILE:HG12	4:P:3605:LYS:HG3	2.02	0.41
2:B:705:THR:HG22	4:D:595:ASN:HB2	1.26	0.41
3:C:39:GLN:OE1	3:C:45:PHE:CZ	2.72	0.41
3:C:57:GLU:C	3:C:58:PRO:CD	2.74	0.41
3:C:88:ASN:O	3:C:91:THR:HG23	2.19	0.41
4:D:521:THR:HG21	4:D:572:LYS:HE2	2.03	0.41
4:D:621:PHE:HA	4:D:622:PRO:HD3	1.88	0.41
3:G:1011:VAL:CG2	3:G:1152:GLU:N	2.70	0.41
3:G:1107:TRP:CG	4:H:1546:PHE:HB3	2.55	0.41
1:I:2075:ASP:HB2	1:I:2216:ALA:HB3	2.02	0.41
3:K:2002:ILE:HD13	3:K:2098:ARG:HH11	1.81	0.41
4:L:2689:GLU:CA	4:L:2711:ARG:NH2	2.84	0.41
3:O:3039:GLN:OE1	3:O:3045:PHE:CZ	2.72	0.41
4:P:3689:GLU:CA	4:P:3711:ARG:NH2	2.84	0.41
1:A:75:ASP:HB2	1:A:216:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:VAL:CB	3:C:151:PRO:CB	2.86	0.41
1:E:1391:TYR:CE2	2:F:1784:LEU:CD1	3.04	0.41
2:F:1505:ASP:OD2	2:F:1513:ARG:NH2	2.53	0.41
3:G:1119:LYS:O	3:G:1150:PHE:HD2	2.04	0.41
3:K:2107:TRP:CG	4:L:2546:PHE:HB3	2.55	0.41
4:L:2561:PRO:HG2	4:L:2563:ARG:HH12	1.85	0.41
3:O:3004:LEU:HD23	3:O:3024:ALA:HA	2.01	0.41
4:P:3504:VAL:HG13	4:P:3522:CYS:SG	2.60	0.41
4:P:3581:GLN:C	4:P:3608:VAL:HG11	2.46	0.41
1:A:293:GLU:N	1:A:293:GLU:OE1	2.54	0.41
2:B:637:CYS:SG	2:B:750:CYS:N	2.93	0.41
4:D:662:MET:HE3	4:D:662:MET:HB2	1.59	0.41
4:H:1561:PRO:HG2	4:H:1563:ARG:HH12	1.85	0.41
2:J:2571:ARG:N	2:J:2597:THR:O	2.52	0.41
3:K:2175:GLN:CG	4:L:2663:GLU:OE2	2.60	0.41
4:L:2581:GLN:C	4:L:2608:VAL:HG11	2.46	0.41
4:L:2662:MET:HE3	4:L:2662:MET:HB2	1.59	0.41
3:O:3078:THR:CB	3:O:3080:TYR:CE1	3.04	0.41
1:A:134:ASN:OD1	1:A:135:ILE:N	2.54	0.41
2:B:671:LYS:HD2	4:D:596:ASN:CA	2.48	0.41
4:D:581:GLN:C	4:D:608:VAL:HG11	2.46	0.41
1:E:1265:GLU:O	1:E:1267:LEU:N	2.54	0.41
3:G:1078:THR:CB	3:G:1080:TYR:CE1	3.04	0.41
4:H:1504:VAL:HG13	4:H:1522:CYS:SG	2.60	0.41
3:K:2011:VAL:CG2	3:K:2152:GLU:O	2.68	0.41
4:L:2556:ARG:HD3	4:L:2560:VAL:O	2.20	0.41
4:L:2669:LYS:HB3	4:L:2669:LYS:HE2	1.73	0.41
1:A:391:TYR:CE2	2:B:784:LEU:CD1	3.04	0.41
2:B:502:TYR:HE2	2:B:504:ALA:HB2	1.86	0.41
2:B:505:ASP:OD2	2:B:513:ARG:NH2	2.53	0.41
4:D:556:ARG:HD3	4:D:560:VAL:O	2.20	0.41
1:E:1075:ASP:HB2	1:E:1216:ALA:HB3	2.02	0.41
1:E:1293:GLU:OE1	1:E:1293:GLU:N	2.54	0.41
2:F:1637:CYS:SG	2:F:1750:CYS:N	2.93	0.41
2:F:1668:HIS:O	4:H:1533:ASN:CB	2.69	0.41
2:F:1670:ALA:CB	4:H:1594:TYR:HE1	2.27	0.41
1:I:2134:ASN:OD1	1:I:2135:ILE:N	2.54	0.41
1:I:2293:GLU:OE1	1:I:2293:GLU:N	2.54	0.41
3:K:2091:THR:O	3:K:2092:ALA:HB2	2.21	0.41
4:L:2689:GLU:OE2	4:L:2711:ARG:NH2	2.54	0.41
4:P:3521:THR:HG21	4:P:3572:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:3662:MET:HB2	4:P:3662:MET:HE3	1.59	0.41
1:A:102:GLN:NE2	1:A:104:SER:OG	2.47	0.41
2:B:668:HIS:CE1	3:C:102:ILE:HG21	2.29	0.41
3:C:100:TYR:HE2	3:C:101:PHE:CZ	2.38	0.41
3:C:119:LYS:O	3:C:150:PHE:HD2	2.04	0.41
2:F:1502:TYR:HE2	2:F:1504:ALA:HB2	1.86	0.41
1:I:2265:GLU:O	1:I:2267:LEU:N	2.54	0.41
3:K:2045:PHE:HE2	4:L:2546:PHE:CE1	2.16	0.41
3:K:2078:THR:CB	3:K:2080:TYR:CE1	3.04	0.41
4:L:2561:PRO:CG	4:L:2563:ARG:NH1	2.82	0.41
3:O:3032:TYR:CE1	3:O:3100:TYR:HB2	2.56	0.41
3:O:3057:GLU:HA	3:O:3058:PRO:CD	2.51	0.41
4:P:3593:TRP:CZ3	4:P:3597:LEU:CA	3.03	0.41
1:A:265:GLU:O	1:A:267:LEU:N	2.54	0.40
3:C:67:ARG:NH1	3:C:90:ASP:OD2	2.52	0.40
4:D:561:PRO:HG2	4:D:563:ARG:HH12	1.85	0.40
4:D:582:THR:HG1	4:D:610:GLY:HA3	1.83	0.40
3:G:1170:PHE:HE1	4:H:1676:MET:HB2	1.87	0.40
3:K:2067:ARG:NH1	3:K:2090:ASP:OD2	2.52	0.40
3:K:2119:LYS:O	3:K:2150:PHE:HD2	2.04	0.40
1:M:3265:GLU:O	1:M:3267:LEU:N	2.54	0.40
3:O:3018:VAL:HG11	3:O:3113:LEU:HD13	2.02	0.40
1:A:38:ILE:HG23	1:A:129:VAL:HG12	2.02	0.40
3:C:11:VAL:CG2	3:C:152:GLU:O	2.68	0.40
3:C:170:PHE:HA	3:C:171:PRO:HD3	1.95	0.40
3:C:170:PHE:HE1	4:D:676:MET:HB2	1.87	0.40
4:D:689:GLU:CA	4:D:711:ARG:NH2	2.84	0.40
4:H:1689:GLU:OE2	4:H:1711:ARG:NH2	2.54	0.40
2:N:3502:TYR:HE2	2:N:3504:ALA:HB2	1.86	0.40
3:O:3145:LEU:CD1	4:P:3680:TYR:CE2	3.03	0.40
3:C:78:THR:CG2	3:C:80:TYR:OH	2.48	0.40
1:E:1038:ILE:HG23	1:E:1129:VAL:HG12	2.02	0.40
2:F:1702:THR:O	4:H:1593:TRP:CE2	2.74	0.40
3:G:1175:GLN:NE2	4:H:1663:GLU:HG3	2.37	0.40
1:I:2391:TYR:CE2	2:J:2784:LEU:CD1	3.04	0.40
2:J:2579:VAL:O	2:J:2580:SER:OG	2.33	0.40
2:J:2672:VAL:HG12	4:L:2596:ASN:HB3	2.04	0.40
4:L:2521:THR:HG21	4:L:2572:LYS:HE2	2.03	0.40
3:O:3150:PHE:HA	3:O:3151:PRO:HA	1.84	0.40
4:P:3689:GLU:CA	4:P:3711:ARG:HH21	2.33	0.40
1:A:22:PRO:CA	1:I:2306:GLU:OE2	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:673:LYS:NZ	3:C:102:ILE:CD1	2.84	0.40
3:C:57:GLU:HA	3:C:58:PRO:CD	2.52	0.40
3:C:175:GLN:NE2	4:D:663:GLU:HG3	2.37	0.40
3:G:1011:VAL:CG2	3:G:1152:GLU:O	2.68	0.40
4:H:1556:ARG:HD3	4:H:1560:VAL:O	2.20	0.40
4:L:2514:PRO:CD	4:L:2609:LEU:C	2.89	0.40
4:L:2579:GLY:O	4:L:2580:ALA:C	2.64	0.40
1:M:3293:GLU:OE1	1:M:3293:GLU:N	2.54	0.40
2:N:3571:ARG:N	2:N:3597:THR:O	2.52	0.40
3:O:3119:LYS:O	3:O:3150:PHE:HD2	2.04	0.40
3:O:3175:GLN:NE2	4:P:3663:GLU:HG3	2.37	0.40
4:H:1689:GLU:CA	4:H:1711:ARG:NH2	2.83	0.40
3:K:2057:GLU:HA	3:K:2058:PRO:CD	2.52	0.40
4:L:2583:GLU:HG2	4:L:2583:GLU:H	1.59	0.40
3:O:3091:THR:O	3:O:3092:ALA:HB2	2.21	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	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	12	49
1	E	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	12	49
1	I	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	12	49
1	M	398/441 (90%)	322 (81%)	72 (18%)	4 (1%)	12	49
2	B	323/420 (77%)	258 (80%)	65 (20%)	0	100	100
2	F	323/420 (77%)	258 (80%)	65 (20%)	0	100	100
2	J	323/420 (77%)	259 (80%)	64 (20%)	0	100	100
2	N	323/420 (77%)	258 (80%)	65 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	5	28
3	G	216/218 (99%)	195 (90%)	16 (7%)	5 (2%)	5	28
3	K	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	5	28
3	O	216/218 (99%)	196 (91%)	15 (7%)	5 (2%)	5	28
4	D	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	12	49
4	H	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	12	49
4	L	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	12	49
4	P	209/214 (98%)	188 (90%)	19 (9%)	2 (1%)	12	49
All	All	4584/5172 (89%)	3856 (84%)	684 (15%)	44 (1%)	15	49

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASP
3	C	43	LYS
4	D	543	ASP
1	E	1390	ASP
3	G	1043	LYS
4	H	1543	ASP
1	I	2390	ASP
3	K	2043	LYS
4	L	2543	ASP
1	M	3390	ASP
3	O	3043	LYS
4	P	3543	ASP
3	C	103	SER
3	G	1103	SER
3	K	2103	SER
3	O	3103	SER
3	C	41	PRO
4	D	701	GLU
3	G	1041	PRO
4	H	1701	GLU
3	K	2041	PRO
4	L	2701	GLU
3	O	3041	PRO
4	P	3701	GLU
1	A	265	GLU
1	A	266	PRO

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Mol	Chain	Res	Type
3	C	118	ALA
1	E	1265	GLU
1	E	1266	PRO
3	G	1118	ALA
1	I	2265	GLU
1	I	2266	PRO
3	K	2118	ALA
1	M	3265	GLU
1	M	3266	PRO
3	O	3118	ALA
3	C	119	LYS
3	G	1119	LYS
3	K	2119	LYS
3	O	3119	LYS
1	A	191	PRO
1	E	1191	PRO
1	I	2191	PRO
1	M	3191	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	339/370 (92%)	339 (100%)	0	100	100
1	E	339/370 (92%)	339 (100%)	0	100	100
1	I	339/370 (92%)	339 (100%)	0	100	100
1	M	339/370 (92%)	339 (100%)	0	100	100
2	B	282/367 (77%)	282 (100%)	0	100	100
2	F	282/367 (77%)	282 (100%)	0	100	100
2	J	282/367 (77%)	282 (100%)	0	100	100
2	N	282/367 (77%)	282 (100%)	0	100	100
3	C	188/188 (100%)	176 (94%)	12 (6%)	16	37
3	G	188/188 (100%)	176 (94%)	12 (6%)	16	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	188/188 (100%)	176 (94%)	12 (6%)	16	37
3	O	188/188 (100%)	176 (94%)	12 (6%)	16	37
4	D	178/183 (97%)	145 (82%)	33 (18%)	1	8
4	H	178/183 (97%)	145 (82%)	33 (18%)	1	8
4	L	178/183 (97%)	145 (82%)	33 (18%)	1	8
4	P	178/183 (97%)	145 (82%)	33 (18%)	1	8
All	All	3948/4432 (89%)	3768 (95%)	180 (5%)	25	45

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1	GLN
3	C	5	VAL
3	C	7	SER
3	C	28	THR
3	C	41	PRO
3	C	43	LYS
3	C	51	ILE
3	C	62	GLU
3	C	63	GLU
3	C	72	LEU
3	C	73	GLU
3	C	142	LEU
4	D	520	LEU
4	D	523	ARG
4	D	536	ASN
4	D	549	LEU
4	D	550	ILE
4	D	554	ASN
4	D	560	VAL
4	D	571	ASP
4	D	575	LEU
4	D	581	GLN
4	D	582	THR
4	D	583	GLU
4	D	605	LYS
4	D	609	LEU
4	D	618	VAL
4	D	620	LEU
4	D	626	GLU

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Mol	Chain	Res	Type
4	D	629	GLU
4	D	630	THR
4	D	632	LYS
4	D	635	LEU
4	D	660	GLN
4	D	662	MET
4	D	666	GLN
4	D	670	GLN
4	D	671	SER
4	D	681	LEU
4	D	684	THR
4	D	686	ARG
4	D	689	GLU
4	D	691	HIS
4	D	705	VAL
4	D	709	LEU
3	G	1001	GLN
3	G	1005	VAL
3	G	1007	SER
3	G	1028	THR
3	G	1041	PRO
3	G	1043	LYS
3	G	1051	ILE
3	G	1062	GLU
3	G	1063	GLU
3	G	1072	LEU
3	G	1073	GLU
3	G	1142	LEU
4	H	1520	LEU
4	H	1523	ARG
4	H	1536	ASN
4	H	1549	LEU
4	H	1550	ILE
4	H	1554	ASN
4	H	1560	VAL
4	H	1571	ASP
4	H	1575	LEU
4	H	1581	GLN
4	H	1582	THR
4	H	1583	GLU
4	H	1605	LYS
4	H	1609	LEU

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Mol	Chain	Res	Type
4	H	1618	VAL
4	H	1620	LEU
4	H	1626	GLU
4	H	1629	GLU
4	H	1630	THR
4	H	1632	LYS
4	H	1635	LEU
4	H	1660	GLN
4	H	1662	MET
4	H	1666	GLN
4	H	1670	GLN
4	H	1671	SER
4	H	1681	LEU
4	H	1684	THR
4	H	1686	ARG
4	H	1689	GLU
4	H	1691	HIS
4	H	1705	VAL
4	H	1709	LEU
3	K	2001	GLN
3	K	2005	VAL
3	K	2007	SER
3	K	2028	THR
3	K	2041	PRO
3	K	2043	LYS
3	K	2051	ILE
3	K	2062	GLU
3	K	2063	GLU
3	K	2072	LEU
3	K	2073	GLU
3	K	2142	LEU
4	L	2520	LEU
4	L	2523	ARG
4	L	2536	ASN
4	L	2549	LEU
4	L	2550	ILE
4	L	2554	ASN
4	L	2560	VAL
4	L	2571	ASP
4	L	2575	LEU
4	L	2581	GLN
4	L	2582	THR

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Mol	Chain	Res	Type
4	L	2583	GLU
4	L	2605	LYS
4	L	2609	LEU
4	L	2618	VAL
4	L	2620	LEU
4	L	2626	GLU
4	L	2629	GLU
4	L	2630	THR
4	L	2632	LYS
4	L	2635	LEU
4	L	2660	GLN
4	L	2662	MET
4	L	2666	GLN
4	L	2670	GLN
4	L	2671	SER
4	L	2681	LEU
4	L	2684	THR
4	L	2686	ARG
4	L	2689	GLU
4	L	2691	HIS
4	L	2705	VAL
4	L	2709	LEU
3	O	3001	GLN
3	O	3005	VAL
3	O	3007	SER
3	O	3028	THR
3	O	3041	PRO
3	O	3043	LYS
3	O	3051	ILE
3	O	3062	GLU
3	O	3063	GLU
3	O	3072	LEU
3	O	3073	GLU
3	O	3142	LEU
4	P	3520	LEU
4	P	3523	ARG
4	P	3536	ASN
4	P	3549	LEU
4	P	3550	ILE
4	P	3554	ASN
4	P	3560	VAL
4	P	3571	ASP

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Mol	Chain	Res	Type
4	P	3575	LEU
4	P	3581	GLN
4	P	3582	THR
4	P	3583	GLU
4	P	3605	LYS
4	P	3609	LEU
4	P	3618	VAL
4	P	3620	LEU
4	P	3626	GLU
4	P	3629	GLU
4	P	3630	THR
4	P	3632	LYS
4	P	3635	LEU
4	P	3660	GLN
4	P	3662	MET
4	P	3666	GLN
4	P	3670	GLN
4	P	3671	SER
4	P	3681	LEU
4	P	3684	THR
4	P	3686	ARG
4	P	3689	GLU
4	P	3691	HIS
4	P	3705	VAL
4	P	3709	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	125	HIS
1	A	183	HIS
1	A	387	HIS
1	A	394	GLN
2	B	528	HIS
2	B	638	ASN
2	B	642	HIS
2	B	825	GLN
3	C	6	GLN
3	C	54	ASN
3	C	82	GLN
3	C	84	ASN

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Mol	Chain	Res	Type
3	C	109	GLN
3	C	168	HIS
4	D	554	ASN
4	D	555	ASN
4	D	596	ASN
4	D	673	ASN
1	E	1102	GLN
1	E	1125	HIS
1	E	1183	HIS
1	E	1387	HIS
1	E	1394	GLN
2	F	1528	HIS
2	F	1638	ASN
2	F	1642	HIS
2	F	1825	GLN
3	G	1003	GLN
3	G	1006	GLN
3	G	1054	ASN
3	G	1082	GLN
3	G	1084	ASN
3	G	1109	GLN
3	G	1168	HIS
4	H	1554	ASN
4	H	1555	ASN
4	H	1673	ASN
1	I	2077	GLN
1	I	2102	GLN
1	I	2183	HIS
1	I	2328	ASN
1	I	2387	HIS
1	I	2394	GLN
2	J	2528	HIS
2	J	2638	ASN
2	J	2700	HIS
2	J	2825	GLN
3	K	2006	GLN
3	K	2039	GLN
3	K	2054	ASN
3	K	2082	GLN
3	K	2084	ASN
3	K	2109	GLN
3	K	2168	HIS

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Mol	Chain	Res	Type
4	L	2533	ASN
4	L	2554	ASN
4	L	2555	ASN
4	L	2673	ASN
1	M	3077	GLN
1	M	3102	GLN
1	M	3183	HIS
1	M	3387	HIS
1	M	3394	GLN
2	N	3528	HIS
2	N	3638	ASN
2	N	3825	GLN
3	O	3003	GLN
3	O	3006	GLN
3	O	3054	ASN
3	O	3082	GLN
3	O	3084	ASN
3	O	3109	GLN
3	O	3168	HIS
3	O	3175	GLN
4	P	3554	ASN
4	P	3555	ASN
4	P	3673	ASN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

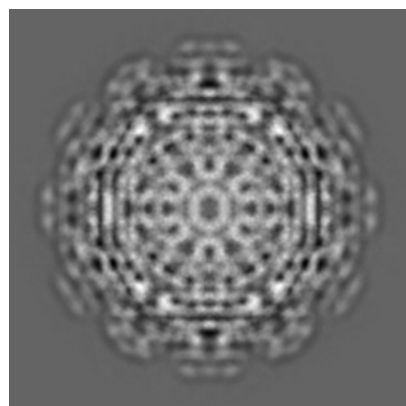
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9279. These allow visual inspection of the internal detail of the map and identification of artifacts.

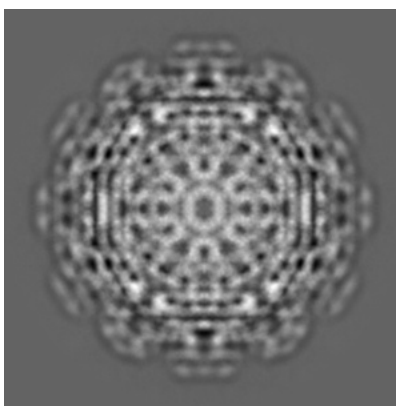
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

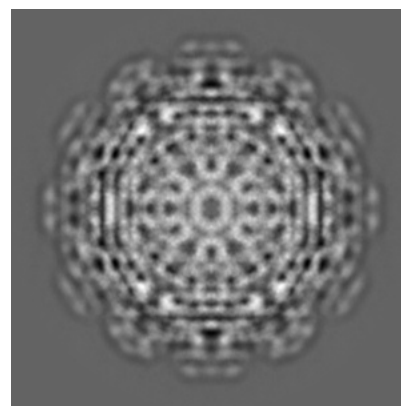
6.1.1 Primary map



X

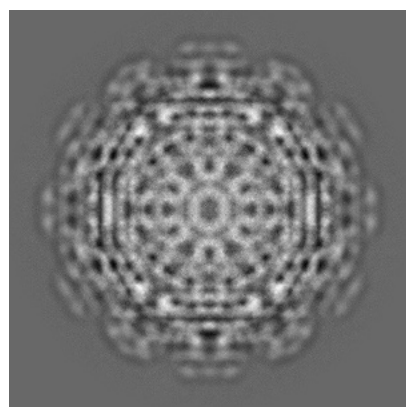


Y

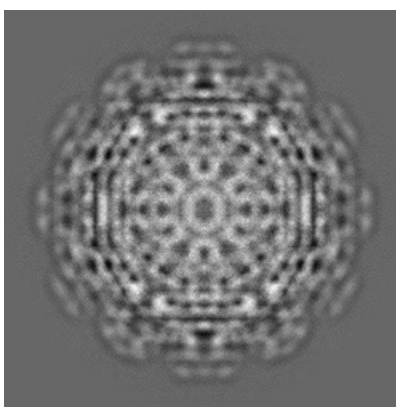


Z

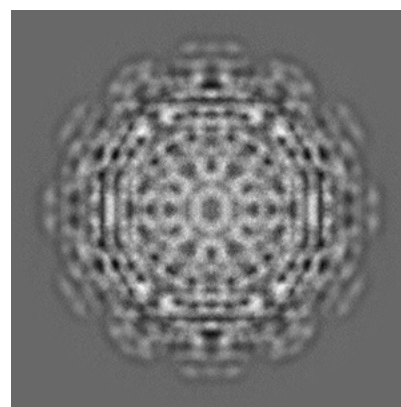
6.1.2 Raw map



X



Y

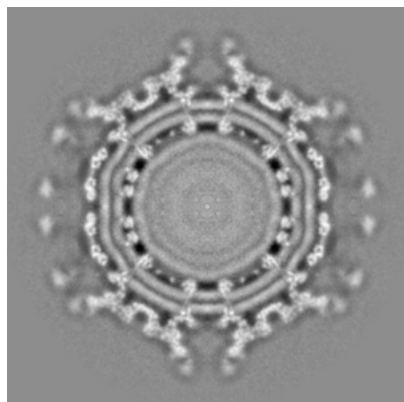


Z

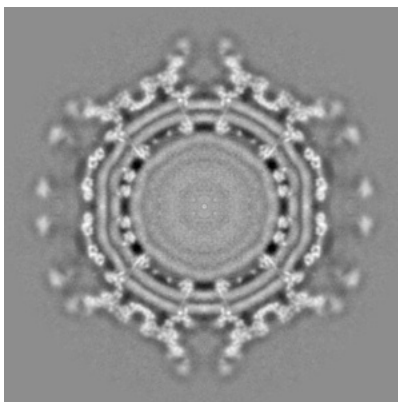
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

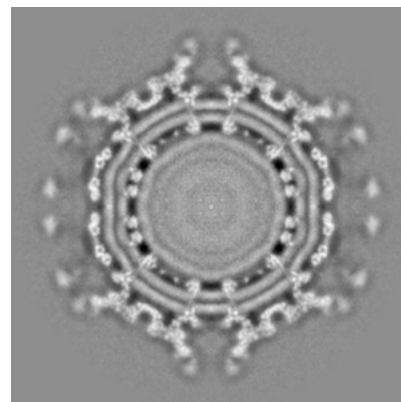
6.2.1 Primary map



X Index: 280

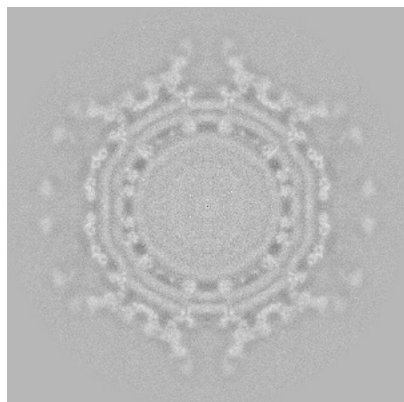


Y Index: 280

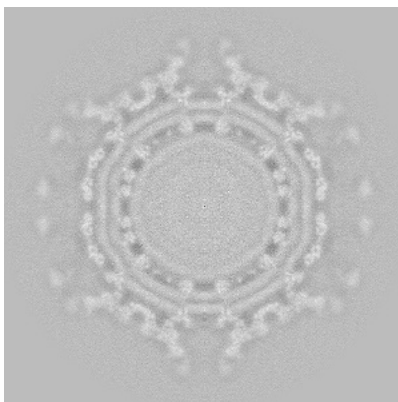


Z Index: 280

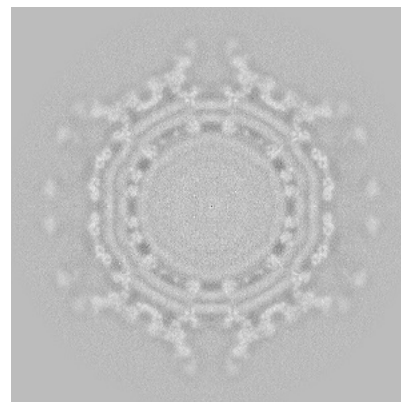
6.2.2 Raw map



X Index: 280



Y Index: 280

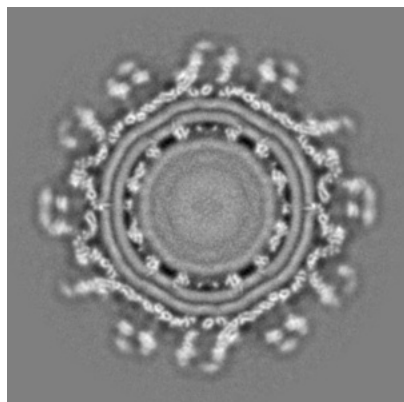


Z Index: 280

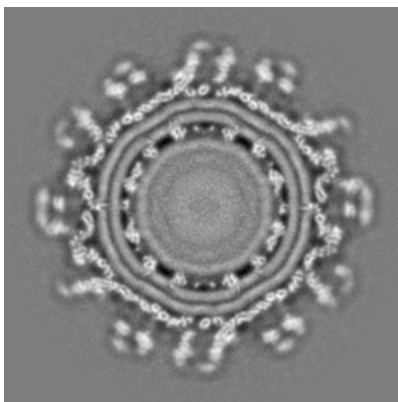
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

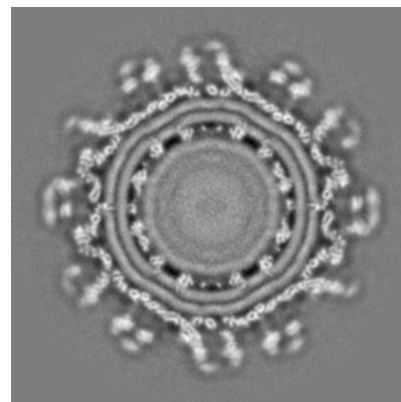
6.3.1 Primary map



X Index: 247

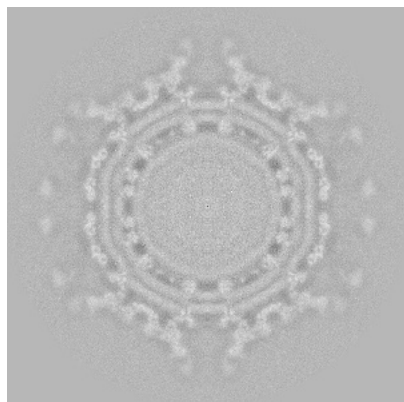


Y Index: 247

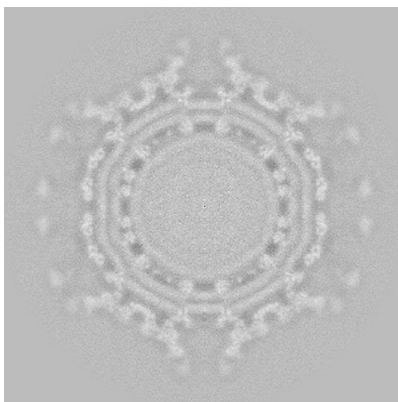


Z Index: 313

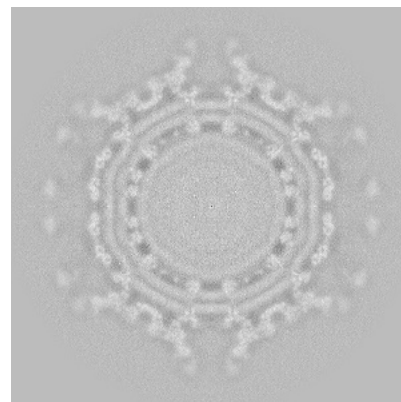
6.3.2 Raw map



X Index: 280



Y Index: 280

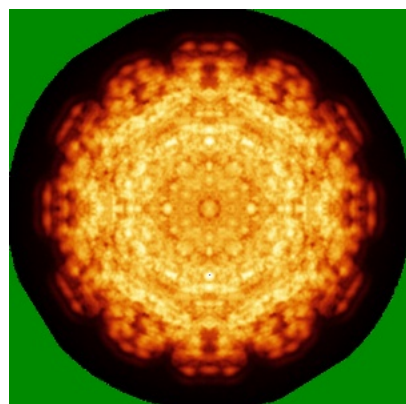


Z Index: 280

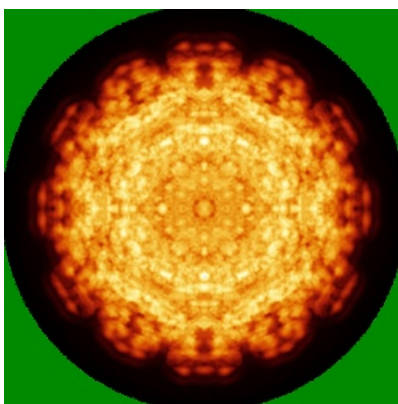
The images above show the largest variance slices of the map in three orthogonal directions.

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

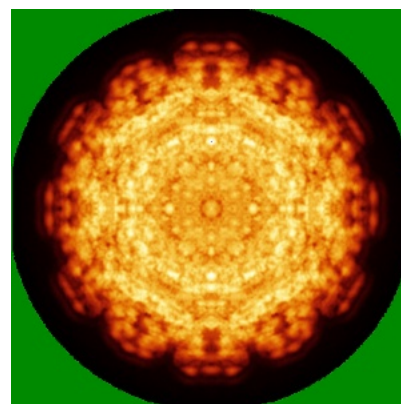
6.4.1 Primary map



X

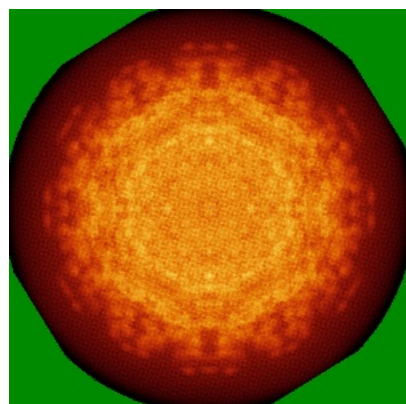


Y

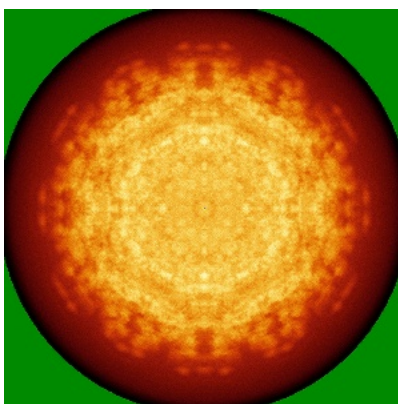


Z

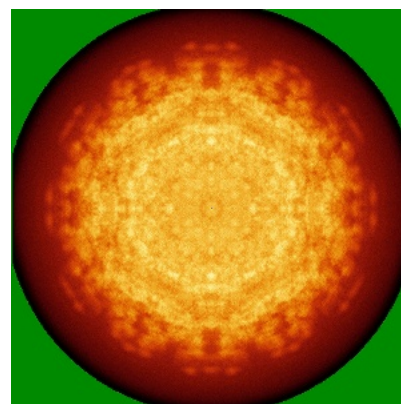
6.4.2 Raw map



X



Y

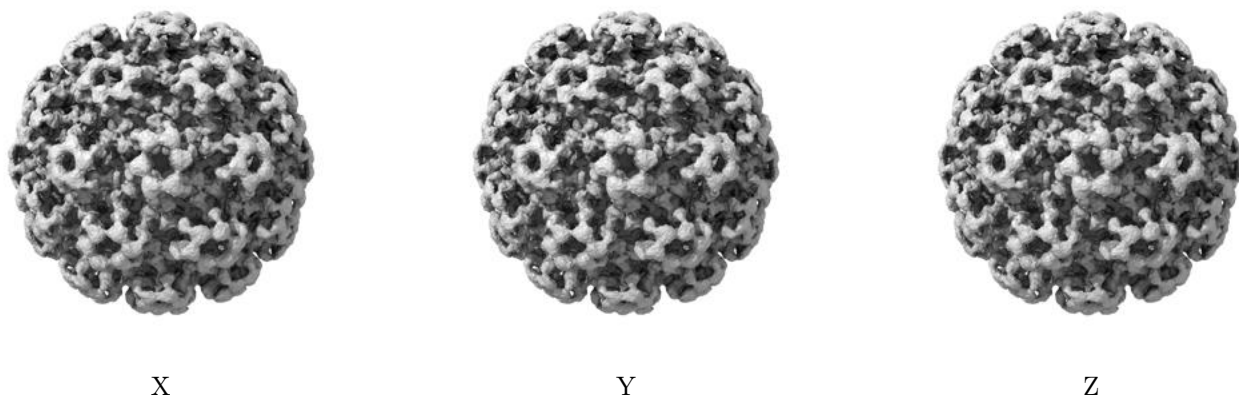


Z

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.

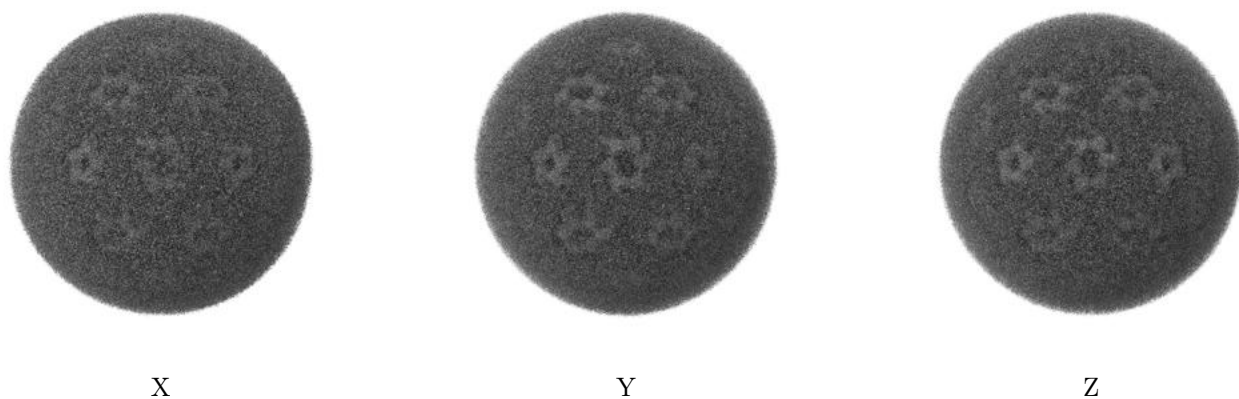
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

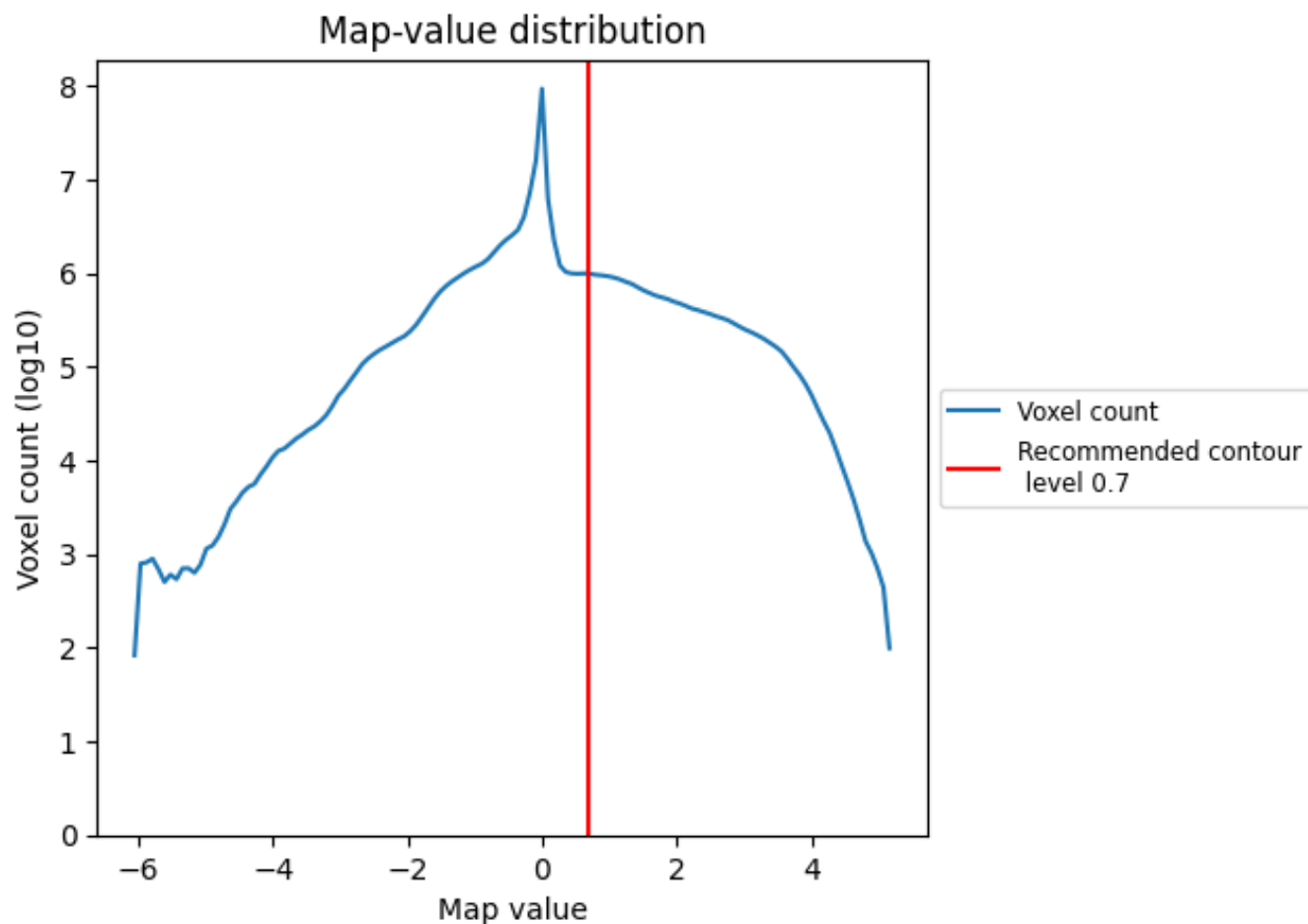
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

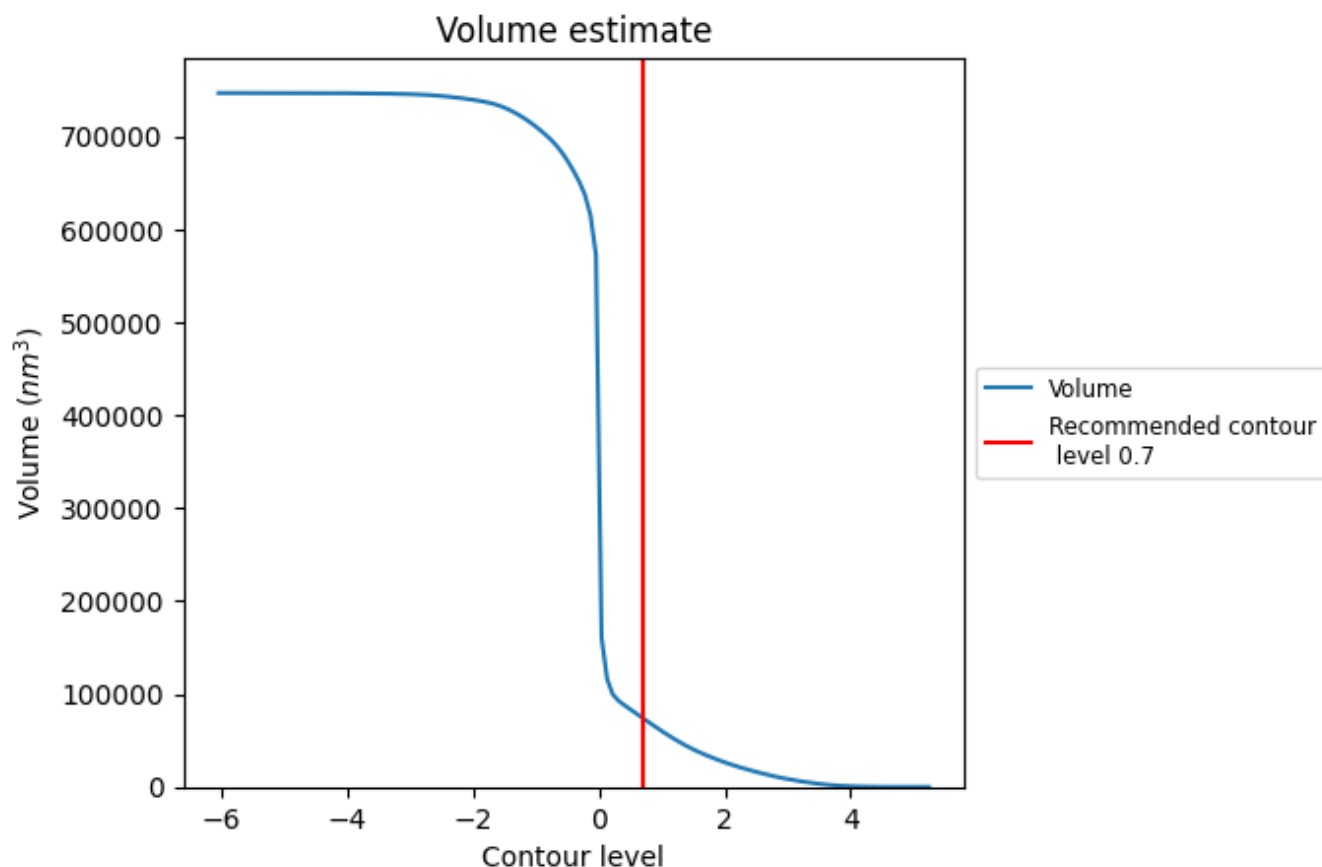
This section contains the results of statistical analysis of the map.

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.

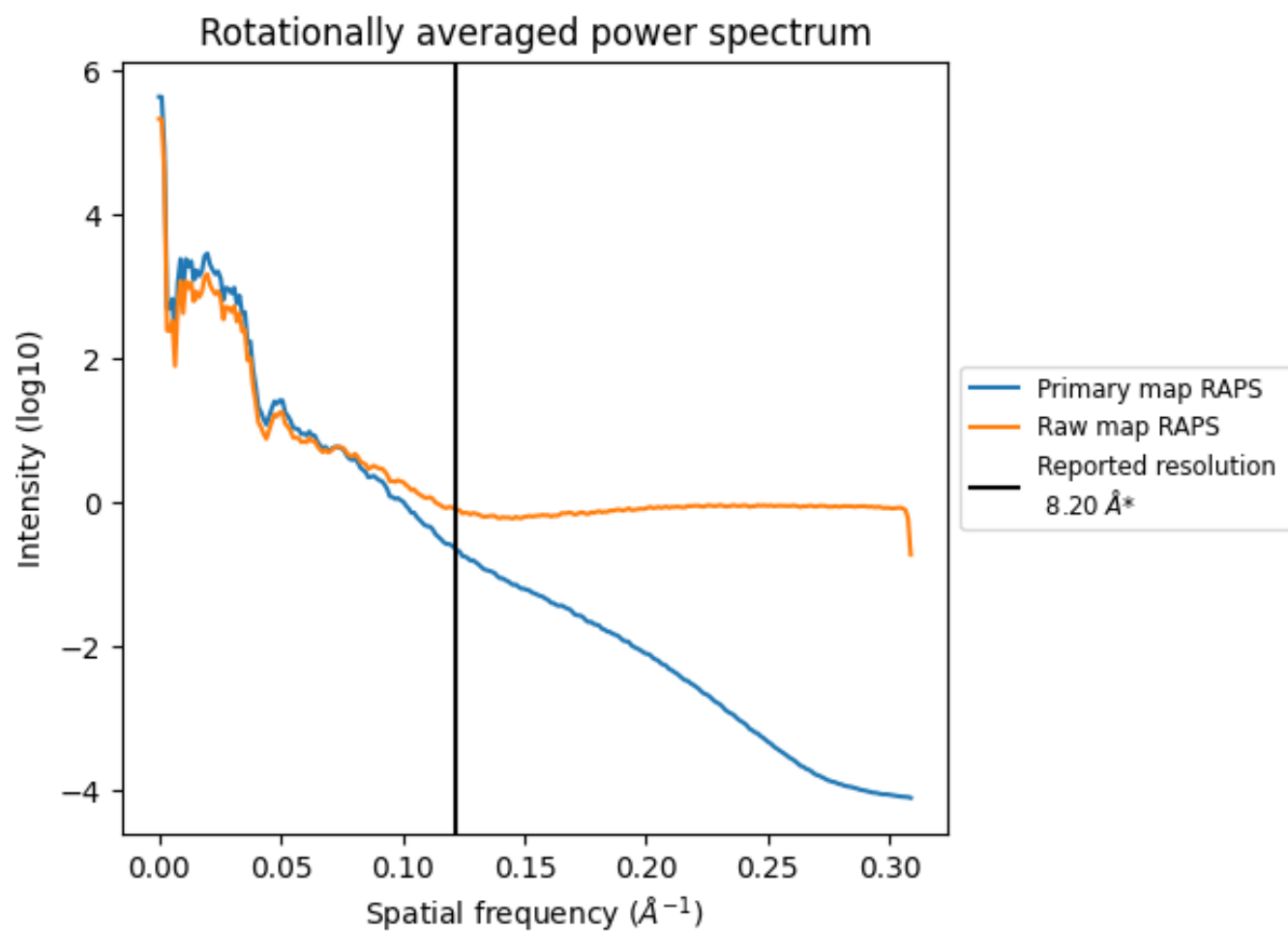
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73800 nm^3 ; this corresponds to an approximate mass of 66665 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 ⓘ

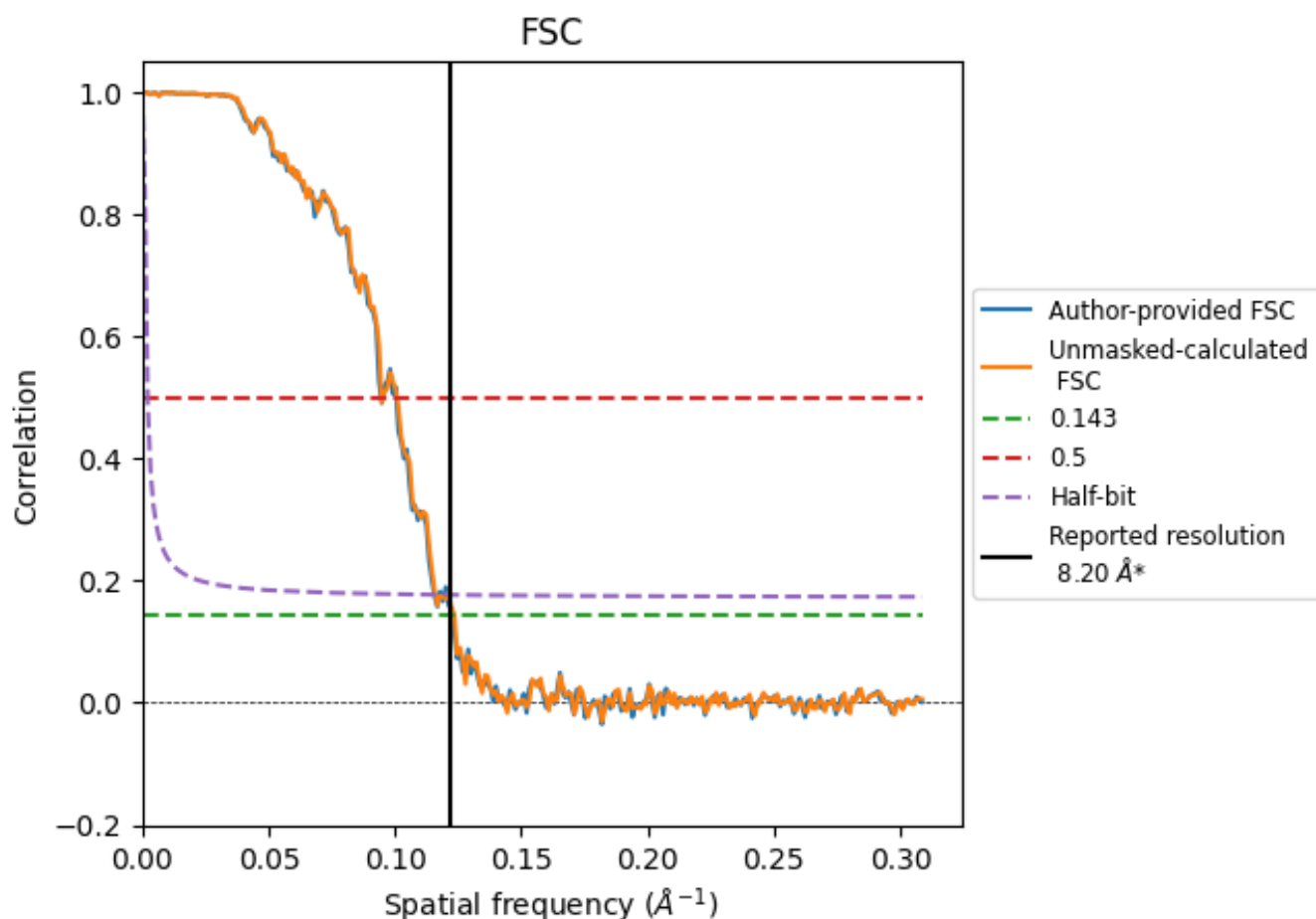


*Reported resolution corresponds to spatial frequency of 0.122 Å⁻¹

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 0.122 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	8.15	10.58	8.65
Unmasked-calculated*	8.10	10.56	8.61

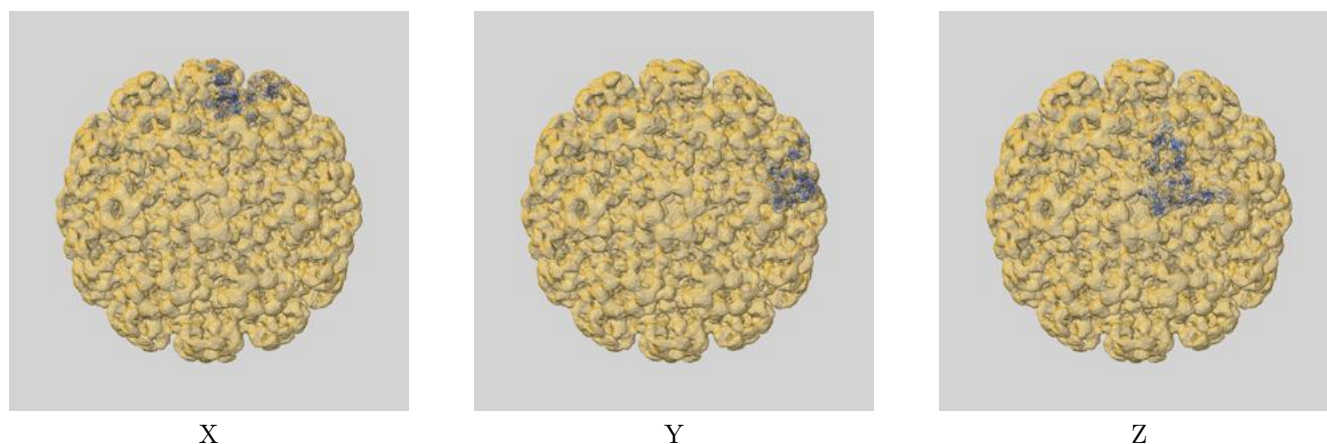
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

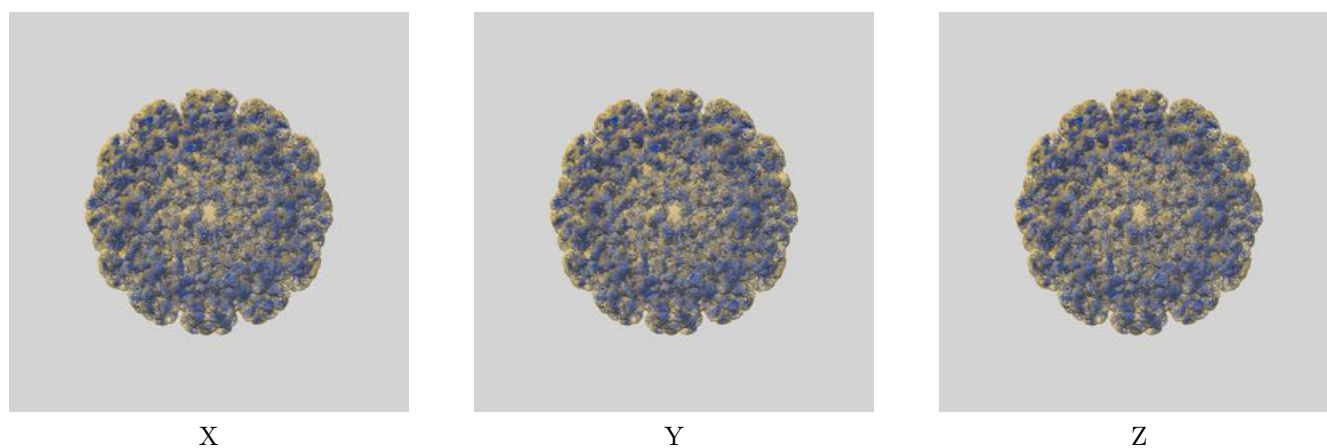
This section contains information regarding the fit between EMDB map EMD-9279 and PDB model 6MWX. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

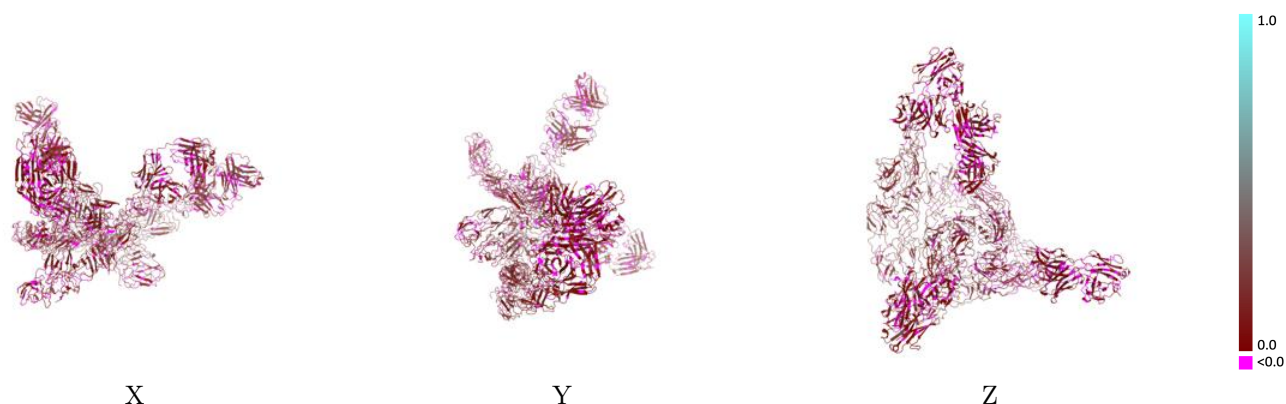


9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.7 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](#)



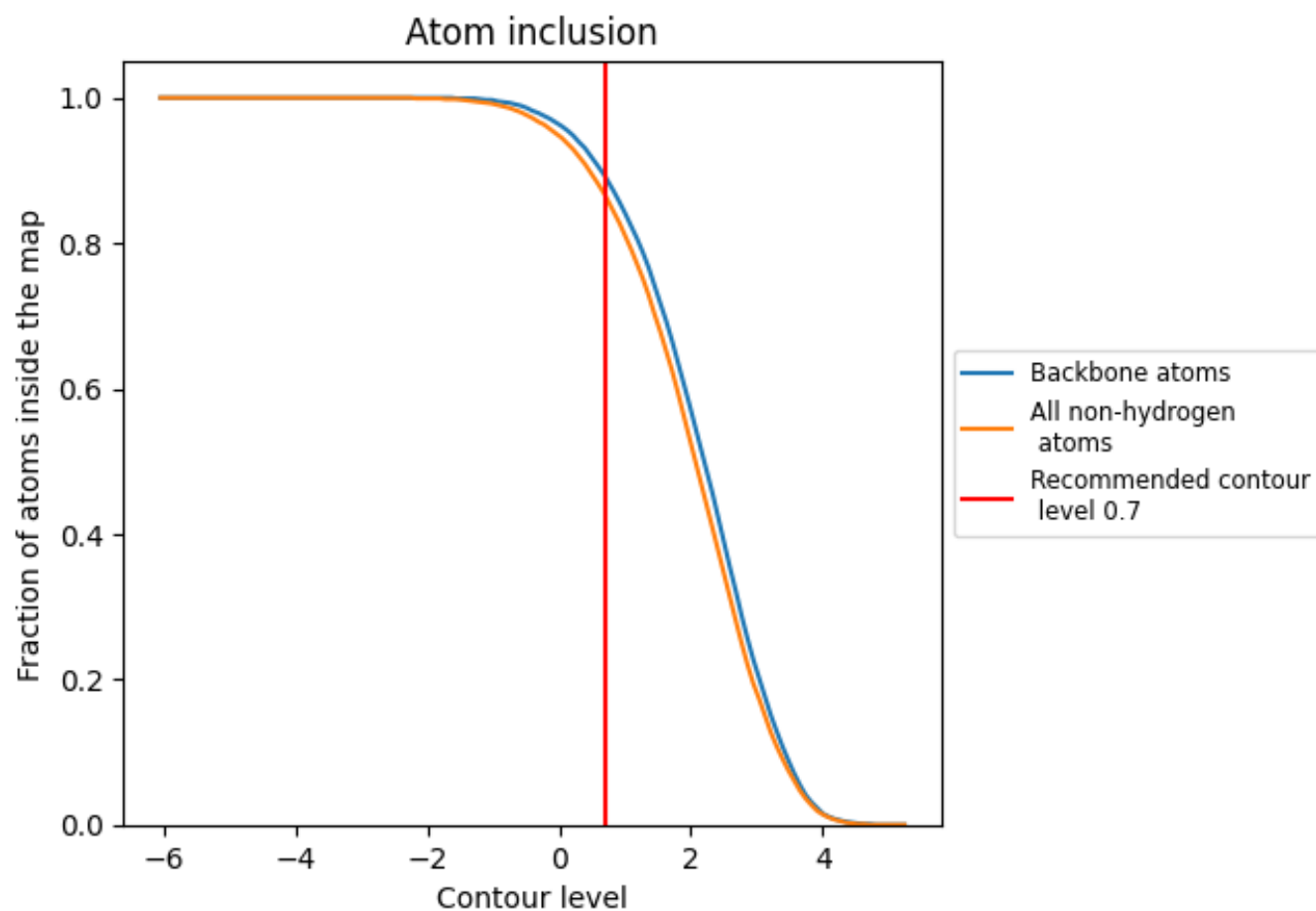
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.0840
A	 0.9170	 0.1240
B	 0.9290	 0.1190
C	 0.8100	 0.0450
D	 0.9040	 0.0750
E	 0.8630	 0.1050
F	 0.9010	 0.1020
G	 0.8410	 0.0640
H	 0.9340	 0.0730
I	 0.9080	 0.1070
J	 0.8920	 0.0800
K	 0.7950	 0.0430
L	 0.8480	 0.0570
M	 0.8590	 0.0840
N	 0.8580	 0.0800
O	 0.7500	 0.0470
P	 0.7080	 0.0460

