



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 10:46 AM UTC

PDB ID : 6RAY / pdb_00006ray
EMDB ID : EMD-4787
Title : D. melanogaster CMG-DNA, State 2A
Authors : Eickhoff, P.; Martino, F.; Costa, A.
Deposited on : 2019-04-08
Resolution : 4.28 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

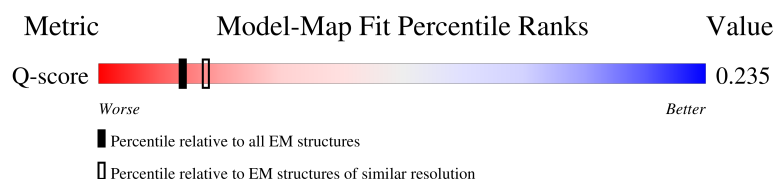
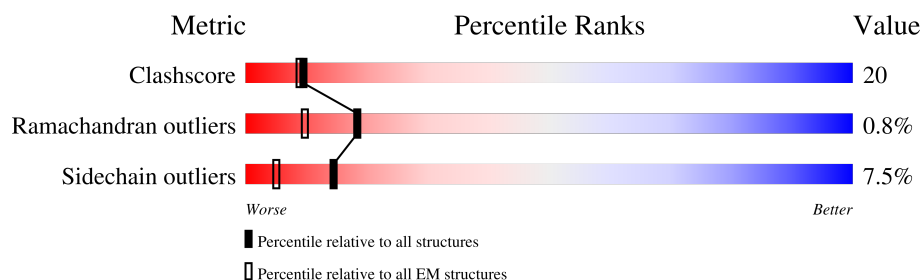
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.28 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	4493 (3.79 - 4.78)

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	3	819	 10% 43% 27% • 27%
2	4	866	 11% 41% 26% • • 29%
3	7	720	 10% 42% 32% 7% • 18%
4	6	817	 14% 47% 24% • 27%

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Mol	Chain	Length	Quality of chain
5	5	733	
6	A	575	
7	H	202	
8	L	203	
9	M	212	
10	N	228	
11	2	887	
12	X	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ATP	3	901	-	-	X	-
13	ATP	4	901	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 39071 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor Mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	600	Total	C	N	O	S	0	0
			4685	2927	839	893	26		

- Molecule 2 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	617	Total	C	N	O	S	0	0
			4901	3071	870	938	22		

- Molecule 3 is a protein called DNA replication licensing factor Mcm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	587	Total	C	N	O	S	0	0
			4577	2865	819	873	20		

- Molecule 4 is a protein called DNA replication licensing factor Mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	600	Total	C	N	O	S	0	0
			4748	2968	848	908	24		

- Molecule 5 is a protein called DNA replication licensing factor Mcm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	577	Total	C	N	O	S	0	0
			4505	2832	796	850	27		

- Molecule 6 is a protein called CDC45L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	567	Total	C	N	O	S	0	0
			4555	2885	788	860	22		

- Molecule 7 is a protein called IP07275p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	189	Total	C	N	O	S	0	0
			1504	961	263	273	7		

- Molecule 8 is a protein called Probable DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	177	Total	C	N	O	S	0	0
			1422	915	239	256	12		

- Molecule 9 is a protein called AT18545p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	167	Total	C	N	O	S	0	0
			1377	875	244	254	4		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	206	Total	C	N	O	S	0	0
			1627	1007	279	328	13		

- Molecule 11 is a protein called DNA replication licensing factor Mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	600	Total	C	N	O	S	0	0
			4731	2988	827	885	31		

- Molecule 12 is a DNA chain called DNA (5'-D(P*AP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	13	Total	C	N	O	P	0	0
			261	130	29	89	13		

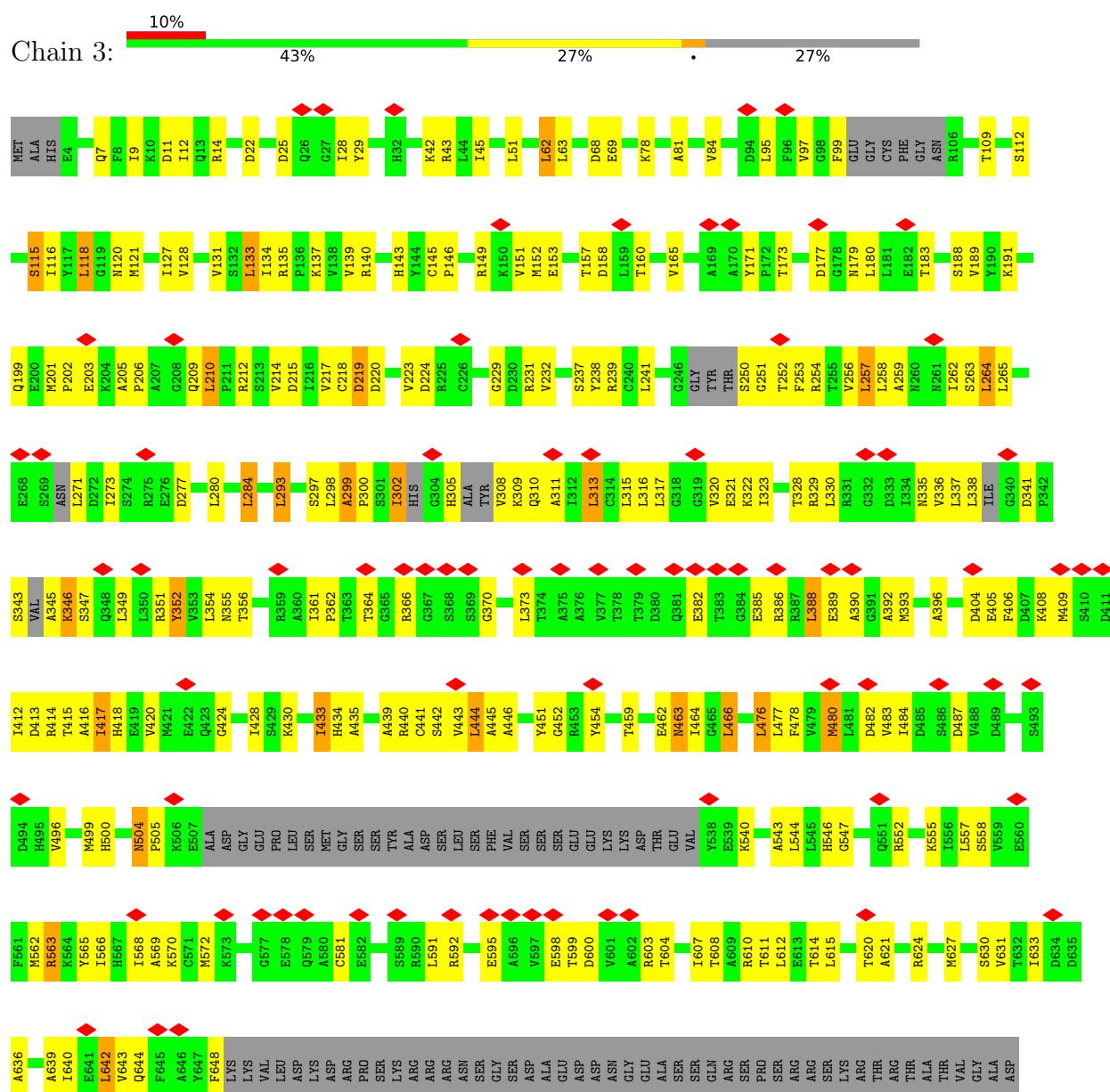
- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					AltConf
14	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	5	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

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

- Molecule 1: DNA replication licensing factor Mcm3



PHE
LEU
ILE

Chain 4:

LEU PRO ALA ALA THR SER PRO ALA ARG ALG GLY LEU GLY ASN MET SER GLU ASP LEU SER SER PRO LEU ASN TYR GLY THR PRO SER SER MET GLY SER ILE ARG THR PRO ARG ASP ASP ILE THR THR ASP LYS ASP ARG ILE ARG ASN

[illegible]

D190	V191	N192	Q193	P194	L195	K199	E201	E202	H204	T205	E207	E208	L211	N212	C215	Y226	T230	G239	M242	M243	T244	N245	F248	R251	T252	T253	A254	A255	L256	L257	E258	H259	Q260	T261	Q262	VAL	ARG	PRO	F266	N267	M268	T269	D270	T271	R272	N273
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S276	L277	M282	L285	L286	S287	L288	G290	G291	V292	S295	L299	P300	E301	A305	F306	F307	E319	V320	D321	Q327	P328	T329	L330	C331	T332	C333	C334	N335	T336	L342	T343	T350	D351	L354	V355	A356	L357	Q358	E359	S360	P361	M364	A365	A366	Q367	G368
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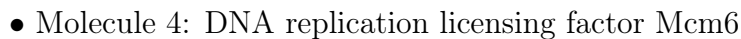
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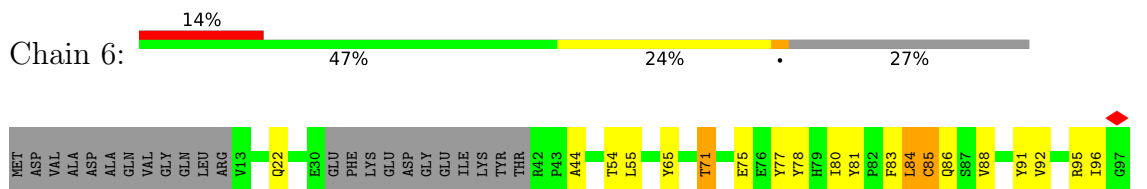
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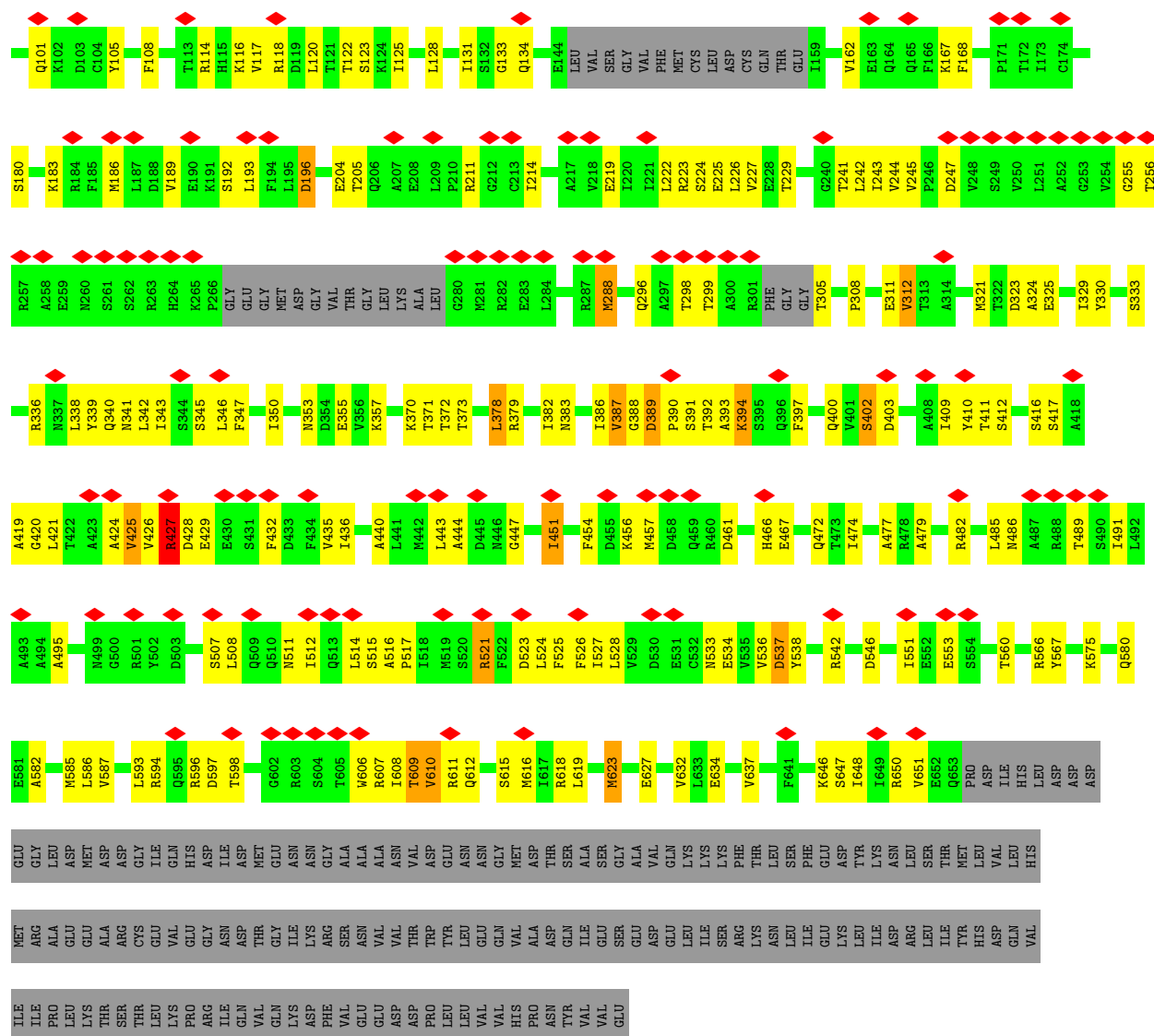
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Chain 7:

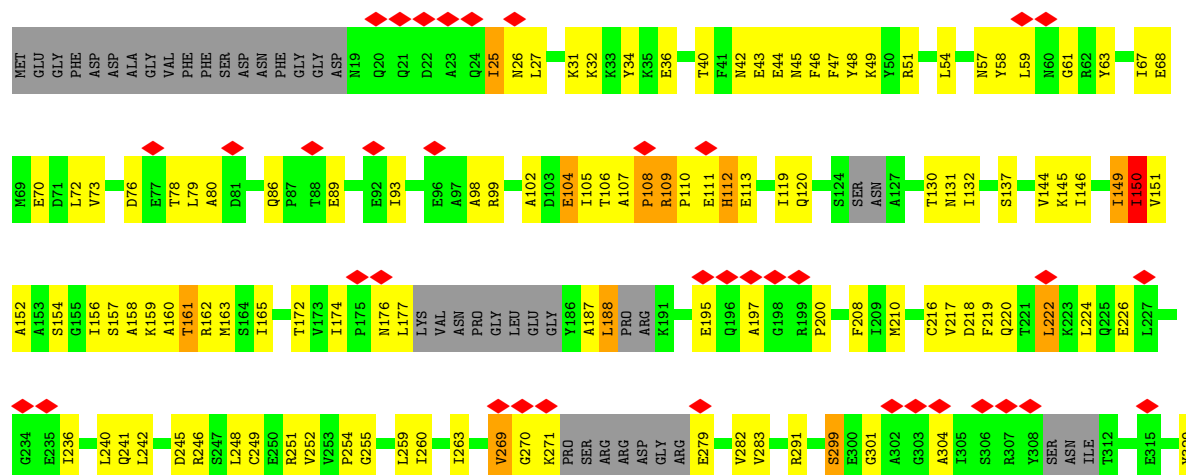


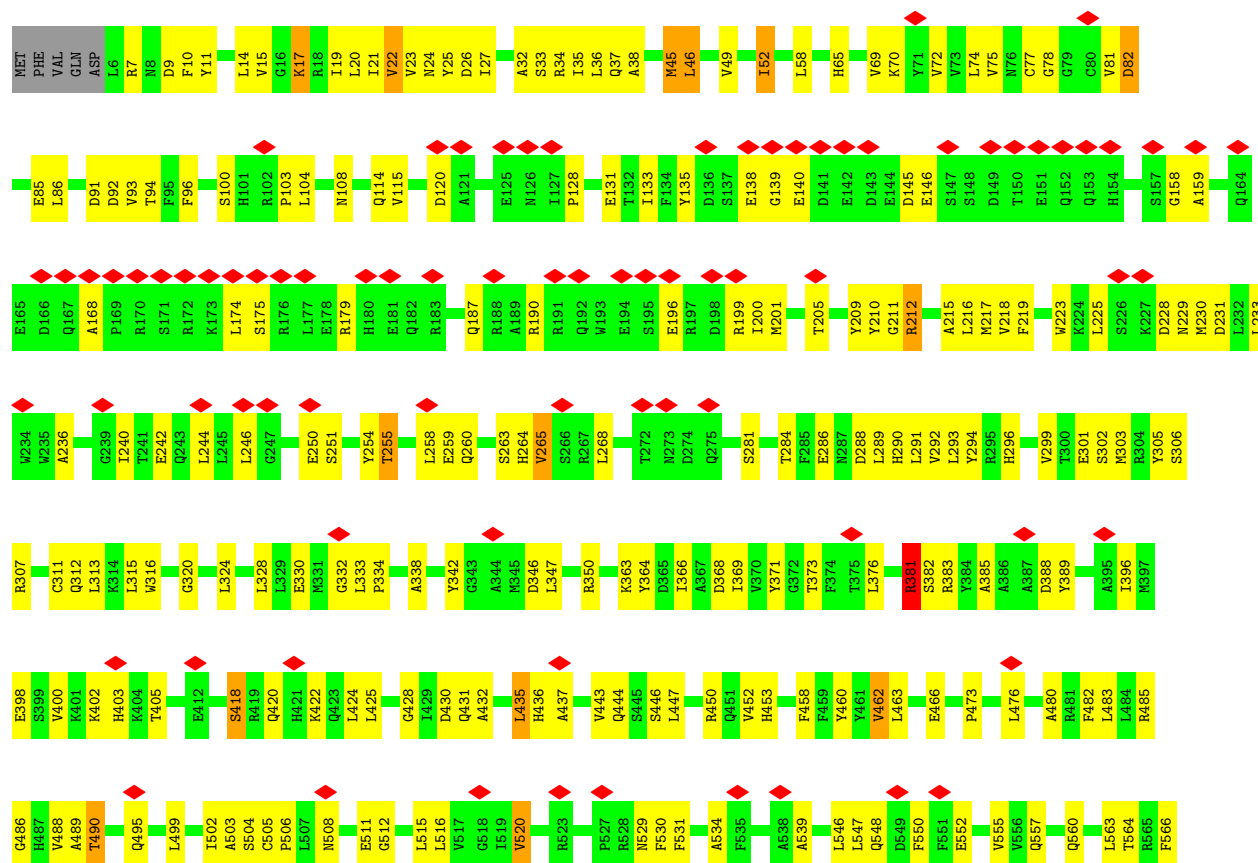
Chain 6:





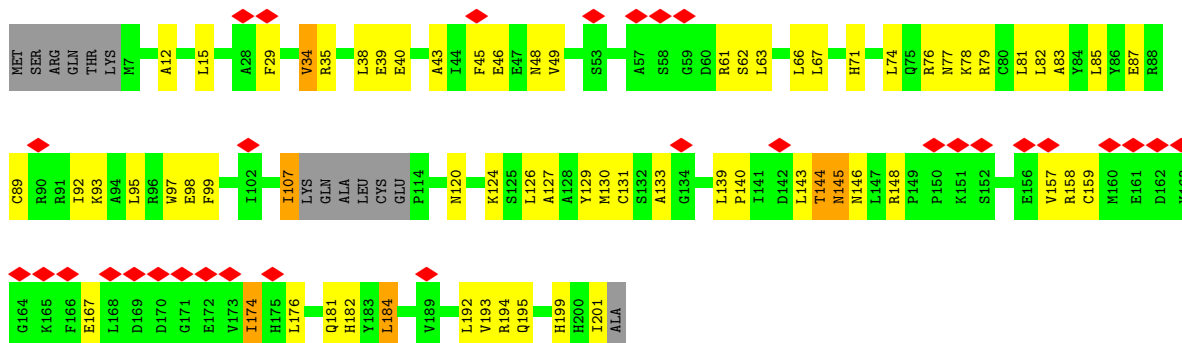
• Molecule 5: DNA replication licensing factor Mcm5



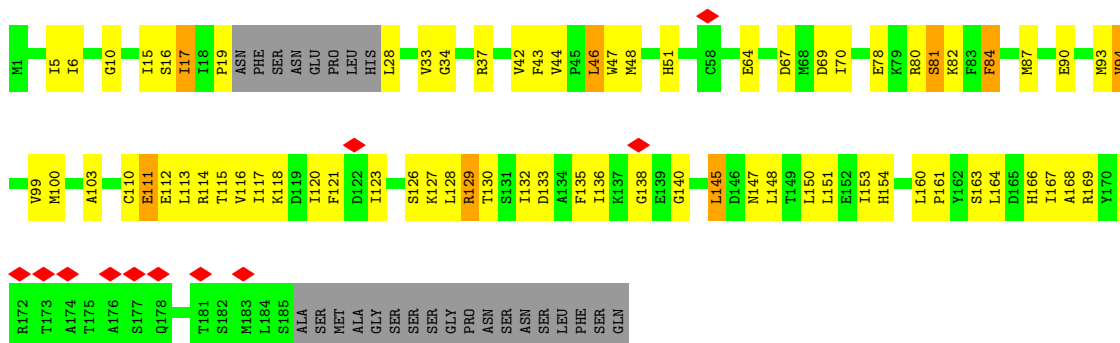




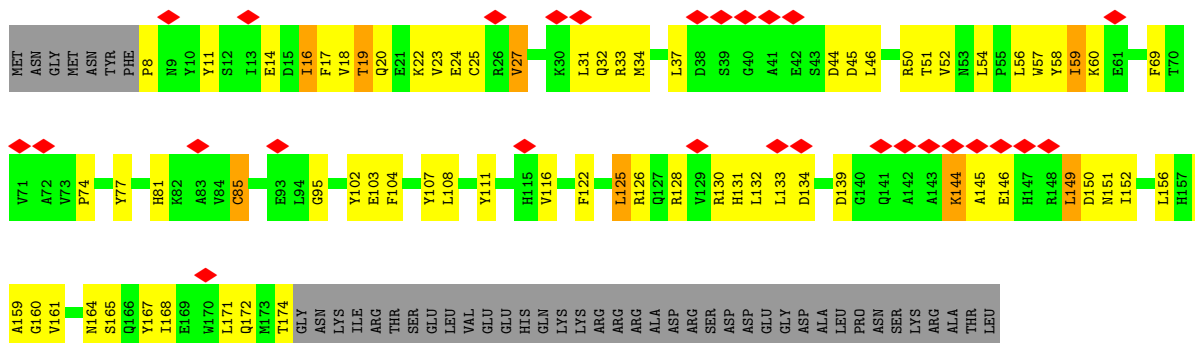
• Molecule 7: IP07275p



• Molecule 8: Probable DNA replication complex GINS protein PSF2

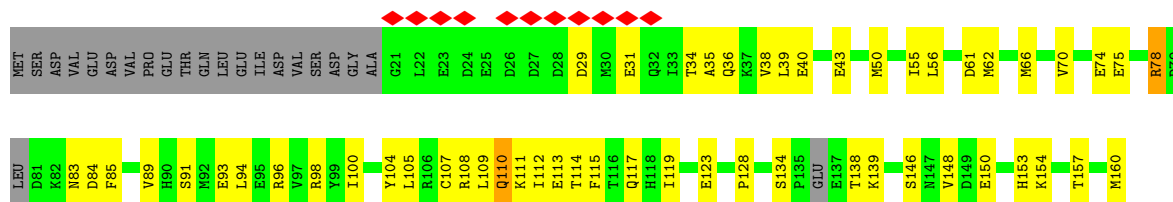


• Molecule 9: AT18545p

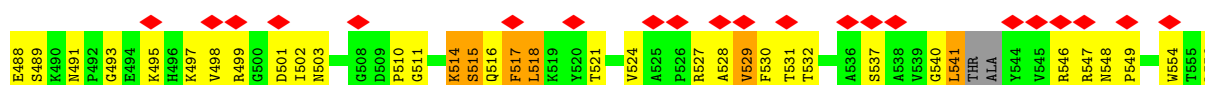
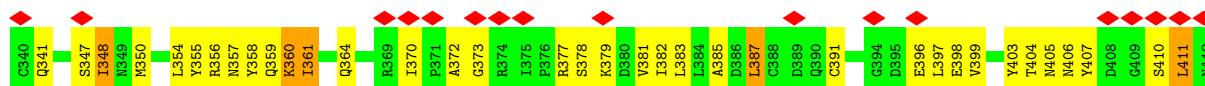
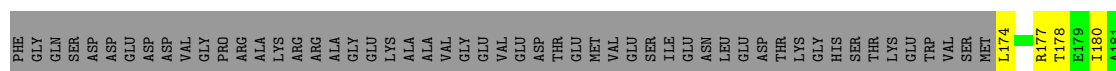
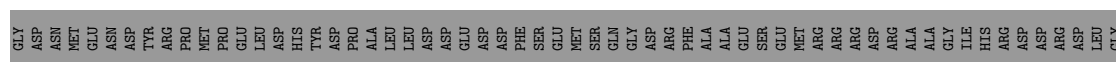
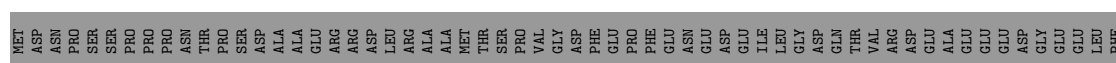


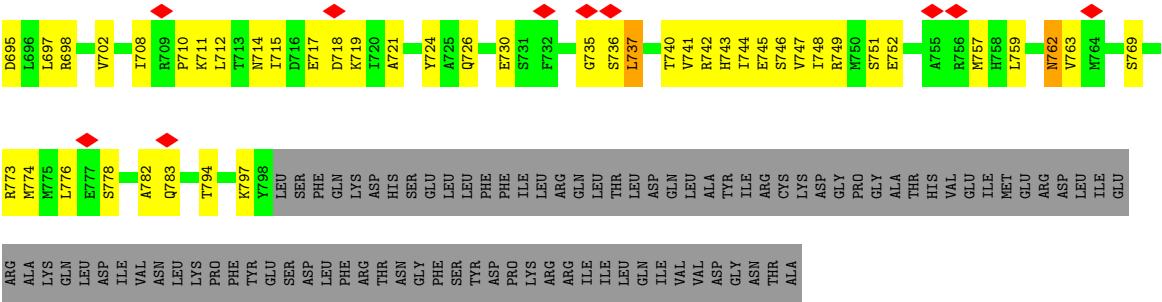
• Molecule 10: DNA replication complex GINS protein SLD5



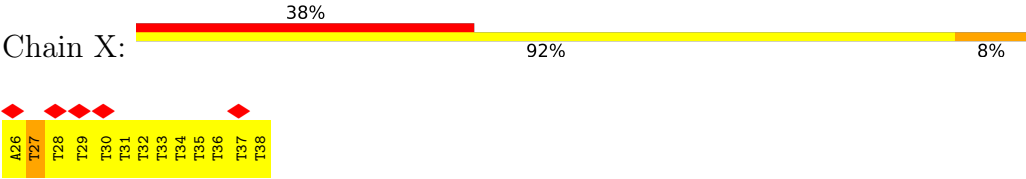


• Molecule 11: DNA replication licensing factor Mcm2





● Molecule 12: DNA (5'-D(P*AP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52214	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	3	0.53	0/4747	0.93	6/6394 (0.1%)
2	4	0.72	3/4986 (0.1%)	1.17	40/6744 (0.6%)
3	7	0.75	6/4636 (0.1%)	1.18	31/6246 (0.5%)
4	6	0.59	1/4819 (0.0%)	0.95	7/6502 (0.1%)
5	5	0.57	0/4571	1.11	16/6151 (0.3%)
6	A	0.48	0/4647	0.81	0/6283
7	H	0.60	0/1538	1.01	0/2077
8	L	0.66	0/1454	0.84	0/1966
9	M	0.58	0/1409	0.82	1/1909 (0.1%)
10	N	0.58	0/1647	0.90	1/2226 (0.0%)
11	2	0.56	0/4813	1.05	21/6499 (0.3%)
12	X	0.50	0/287	1.18	2/441 (0.5%)
All	All	0.61	10/39554 (0.0%)	1.02	125/53438 (0.2%)

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	3	0	14
2	4	2	10
3	7	0	7
4	6	0	6
5	5	1	12
6	A	0	6
7	H	0	3
8	L	0	2
9	M	0	2
11	2	1	8
All	All	4	70

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	254	THR	C-N	25.49	1.67	1.33
2	4	588	VAL	C-N	23.32	1.66	1.33
4	6	108	PHE	C-N	15.80	1.52	1.33
3	7	267	PRO	C-N	14.07	1.54	1.33
2	4	271	THR	C-N	12.01	1.49	1.33
3	7	619	LEU	C-N	11.02	1.50	1.33
2	4	272	ARG	C-N	10.66	1.47	1.33
3	7	629	ASP	C-N	-9.97	1.22	1.33
3	7	431	GLY	C-N	-9.28	1.18	1.33
3	7	250	PRO	C-N	8.15	1.44	1.33

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	270	GLY	CA-C-N	18.94	155.79	121.70
5	5	270	GLY	C-N-CA	18.94	155.79	121.70
3	7	431	GLY	CA-C-N	18.33	144.56	122.19
3	7	431	GLY	C-N-CA	18.33	144.56	122.19
3	7	267	PRO	O-C-N	17.48	146.24	122.64
3	7	629	ASP	O-C-N	-17.05	100.55	122.37
5	5	425	VAL	CB-CA-C	-16.34	84.50	111.29
3	7	567	LYS	N-CA-C	15.67	128.35	111.28
3	7	431	GLY	O-C-N	-15.52	102.53	122.70
2	4	424	PHE	N-CA-C	14.27	133.18	113.21
3	7	152	VAL	N-CA-C	-14.14	89.84	108.93
4	6	427	ARG	CD-NE-CZ	12.68	142.15	124.40
5	5	419	PRO	CB-CA-C	12.23	130.99	111.31
5	5	610	ARG	CD-NE-CZ	12.08	141.31	124.40
3	7	216	ALA	N-CA-C	-11.72	92.72	110.30
11	2	316	LYS	CA-C-N	11.45	146.29	122.58
11	2	316	LYS	C-N-CA	11.45	146.29	122.58
11	2	641	ARG	CD-NE-CZ	11.14	140.00	124.40
2	4	643	LEU	CA-C-N	10.88	141.01	122.95
2	4	643	LEU	C-N-CA	10.88	141.01	122.95
3	7	216	ALA	CB-CA-C	10.71	124.94	110.06
5	5	425	VAL	N-CA-C	10.48	131.14	109.34
3	7	267	PRO	CA-C-N	-10.45	100.93	121.41
3	7	267	PRO	C-N-CA	-10.45	100.93	121.41
3	7	567	LYS	CB-CA-C	-10.22	93.82	110.79
2	4	608	GLN	CA-C-N	10.22	141.33	122.02
2	4	608	GLN	C-N-CA	10.22	141.33	122.02
3	7	622	SER	N-CA-C	-9.65	90.24	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6	580	GLN	CA-C-N	9.46	132.96	120.28
4	6	580	GLN	C-N-CA	9.46	132.96	120.28
1	3	480	MET	CB-CG-SD	9.33	140.69	112.70
3	7	628	ASP	CA-C-N	-9.04	107.65	122.65
3	7	628	ASP	C-N-CA	-9.04	107.65	122.65
3	7	604	ARG	CD-NE-CZ	8.94	136.92	124.40
2	4	288	ILE	CA-C-N	8.84	136.87	122.29
2	4	288	ILE	C-N-CA	8.84	136.87	122.29
2	4	365	ALA	CA-C-N	8.82	138.40	121.54
2	4	365	ALA	C-N-CA	8.82	138.40	121.54
3	7	619	LEU	CA-C-N	-8.79	108.28	122.26
3	7	619	LEU	C-N-CA	-8.79	108.28	122.26
2	4	631	ASN	CA-C-N	8.74	132.43	120.46
2	4	631	ASN	C-N-CA	8.74	132.43	120.46
5	5	149	ILE	CA-C-N	8.67	132.41	120.35
5	5	149	ILE	C-N-CA	8.67	132.41	120.35
2	4	295	SER	CA-C-N	8.65	136.34	121.29
2	4	295	SER	C-N-CA	8.65	136.34	121.29
12	X	27	DT	C5'-C4'-O4'	8.35	121.92	109.40
4	6	108	PHE	CA-C-N	-8.21	107.88	122.32
4	6	108	PHE	C-N-CA	-8.21	107.88	122.32
3	7	152	VAL	CB-CA-C	8.17	124.44	111.69
3	7	566	CYS	CB-CA-C	-8.11	95.39	109.02
3	7	383	PRO	N-CA-C	-7.92	96.16	112.47
2	4	593	MET	N-CA-C	7.81	120.48	111.11
3	7	622	SER	CB-CA-C	7.72	125.79	110.42
4	6	533	ASN	CA-C-N	7.24	130.95	120.38
4	6	533	ASN	C-N-CA	7.24	130.95	120.38
11	2	410	SER	CA-C-N	7.23	133.88	122.17
11	2	410	SER	C-N-CA	7.23	133.88	122.17
3	7	566	CYS	CA-C-N	7.06	129.74	120.28
3	7	566	CYS	C-N-CA	7.06	129.74	120.28
3	7	383	PRO	CA-C-N	7.04	135.21	121.41
3	7	383	PRO	C-N-CA	7.04	135.21	121.41
11	2	332	ILE	N-CA-C	-7.01	106.08	111.62
11	2	322	GLY	N-CA-C	7.01	126.63	112.34
5	5	510	ARG	NE-CZ-NH2	-6.90	112.99	119.20
5	5	471	ILE	CG1-CB-CG2	6.90	131.39	110.70
2	4	472	ILE	CG1-CB-CG2	6.81	131.13	110.70
5	5	150	ILE	CG1-CB-CG2	6.67	130.72	110.70
2	4	421	VAL	N-CA-C	6.64	117.84	107.28
11	2	339	GLU	CA-CB-CG	6.59	127.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	595	GLN	CB-CA-C	6.52	121.76	110.68
5	5	510	ARG	CD-NE-CZ	6.52	133.52	124.40
11	2	325	VAL	CG1-CB-CG2	6.37	124.81	110.80
11	2	348	ILE	CG1-CB-CG2	6.25	129.46	110.70
2	4	513	ASP	N-CA-C	-6.17	96.18	109.81
2	4	652	VAL	CG1-CB-CG2	6.00	124.00	110.80
1	3	205	ALA	N-CA-C	5.96	116.45	109.60
2	4	532	SER	N-CA-C	5.95	118.43	108.96
11	2	360	LYS	CA-C-N	5.92	128.60	122.27
11	2	360	LYS	C-N-CA	5.92	128.60	122.27
2	4	392	THR	OG1-CB-CG2	5.91	121.11	109.30
11	2	310	ILE	CG1-CB-CG2	5.90	128.40	110.70
2	4	271	THR	CA-C-N	5.87	133.63	122.60
2	4	271	THR	C-N-CA	5.87	133.63	122.60
11	2	601	ILE	CG1-CB-CG2	5.81	128.13	110.70
2	4	599	SER	N-CA-C	-5.69	98.68	110.80
2	4	572	VAL	CG1-CB-CG2	5.65	123.23	110.80
2	4	589	LEU	N-CA-C	-5.63	98.81	110.80
11	2	641	ARG	NE-CZ-NH2	-5.61	114.15	119.20
2	4	599	SER	CB-CA-C	5.61	121.58	110.42
10	N	215	LEU	CB-CG-CD1	5.59	127.47	110.70
11	2	187	PHE	N-CA-CB	5.55	119.02	110.81
5	5	252	VAL	CG1-CB-CG2	5.53	122.97	110.80
2	4	424	PHE	CA-C-N	5.51	133.14	122.07
2	4	424	PHE	C-N-CA	5.51	133.14	122.07
11	2	515	SER	N-CA-C	5.48	116.93	111.07
5	5	610	ARG	NE-CZ-NH1	-5.47	116.03	121.50
3	7	627	LYS	O-C-N	5.47	129.50	122.39
11	2	602	VAL	CA-CB-CG1	5.46	119.68	110.40
9	M	144	LYS	CB-CA-C	5.39	119.34	110.83
3	7	509	ALA	CA-C-N	5.39	127.50	120.28
3	7	509	ALA	C-N-CA	5.39	127.50	120.28
12	X	27	DT	C5'-C4'-C3'	5.37	122.95	114.90
2	4	588	VAL	O-C-N	5.32	129.46	122.12
11	2	459	VAL	CG1-CB-CG2	-5.32	99.10	110.80
5	5	365	GLY	N-CA-C	5.30	119.05	112.64
2	4	513	ASP	CB-CA-C	-5.28	99.76	110.17
1	3	133	LEU	CB-CA-C	-5.25	98.74	110.19
1	3	418	HIS	CA-CB-CG	5.24	119.04	113.80
2	4	593	MET	CB-CA-C	-5.22	102.45	110.81
2	4	620	ASN	CB-CA-C	5.22	117.13	110.76
2	4	507	HIS	CB-CA-C	5.22	117.65	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	575	ILE	CA-CB-CG2	5.16	119.27	110.50
11	2	517	PHE	CB-CA-C	-5.15	100.63	110.57
11	2	196	GLY	N-CA-C	5.13	120.82	112.61
2	4	382	VAL	N-CA-C	5.13	114.58	106.32
1	3	210	LEU	CB-CG-CD2	5.12	126.05	110.70
2	4	636	VAL	CG1-CB-CG2	5.08	121.99	110.80
3	7	509	ALA	CB-CA-C	-5.06	99.87	109.95
5	5	200	PRO	N-CA-C	5.05	119.49	111.26
1	3	293	LEU	CB-CG-CD2	5.04	125.82	110.70
2	4	343	ILE	CG1-CB-CG2	5.04	125.81	110.70
3	7	566	CYS	N-CA-C	5.02	120.79	114.31
2	4	375	LEU	CB-CG-CD2	5.02	125.76	110.70
2	4	543	VAL	CA-CB-CG1	5.01	118.91	110.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	4	472	ILE	CB
2	4	575	ILE	CB
5	5	464	ILE	CB
11	2	310	ILE	CB

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	2	310	ILE	Peptide
11	2	361	ILE	Peptide
11	2	484	LEU	Peptide
11	2	514	LYS	Mainchain
11	2	641	ARG	Sidechain
11	2	648	VAL	Peptide
11	2	735	GLY	Peptide
11	2	737	LEU	Peptide
1	3	219	ASP	Peptide
1	3	223	VAL	Peptide
1	3	257	LEU	Peptide
1	3	259	ALA	Peptide
1	3	28	ILE	Peptide
1	3	440	ARG	Peptide
1	3	444	LEU	Peptide
1	3	451	TYR	Peptide
1	3	462	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	3	463	ASN	Peptide
1	3	546	HIS	Peptide
1	3	555	LYS	Peptide
1	3	563	ARG	Sidechain
1	3	69	GLU	Peptide
2	4	176	ILE	Peptide
2	4	327	GLN	Peptide
2	4	343	ILE	Peptide
2	4	510	LEU	Peptide
2	4	531	ARG	Peptide
2	4	532	SER	Peptide
2	4	538	ARG	Sidechain
2	4	556	ARG	Sidechain
2	4	590	HIS	Mainchain
2	4	734	ARG	Sidechain
5	5	109	ARG	Peptide
5	5	112	HIS	Peptide
5	5	269	VAL	Peptide
5	5	299	SER	Peptide
5	5	304	ALA	Peptide
5	5	32	LYS	Peptide
5	5	365	GLY	Peptide
5	5	44	GLU	Peptide
5	5	468	LYS	Peptide
5	5	510	ARG	Sidechain
5	5	610	ARG	Peptide,Sidechain
4	6	118	ARG	Sidechain
4	6	312	VAL	Peptide
4	6	379	ARG	Sidechain
4	6	427	ARG	Sidechain
4	6	521	ARG	Sidechain
4	6	546	ASP	Peptide
3	7	372	ARG	Sidechain
3	7	400	ARG	Sidechain
3	7	432	GLY	Mainchain
3	7	604	ARG	Sidechain
3	7	611	ARG	Sidechain
3	7	620	ARG	Mainchain
3	7	629	ASP	Mainchain
6	A	22	VAL	Peptide
6	A	346	ASP	Peptide
6	A	381	ARG	Peptide

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Mol	Chain	Res	Type	Group
6	A	46	LEU	Peptide
6	A	490	THR	Peptide
6	A	82	ASP	Peptide
7	H	146	ASN	Peptide
7	H	148	ARG	Peptide
7	H	61	ARG	Peptide
8	L	145	LEU	Peptide
8	L	81	SER	Peptide
9	M	107	TYR	Peptide
9	M	16	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	4685	0	4739	181	0
2	4	4901	0	4838	216	0
3	7	4577	0	4548	272	0
4	6	4748	0	4725	181	0
5	5	4505	0	4512	189	0
6	A	4555	0	4468	162	0
7	H	1504	0	1460	49	0
8	L	1422	0	1443	61	0
9	M	1377	0	1346	60	0
10	N	1627	0	1565	53	0
11	2	4731	0	4766	231	0
12	X	261	0	156	24	0
13	2	31	0	12	4	0
13	3	31	0	12	10	0
13	4	31	0	12	14	0
13	6	31	0	11	5	0
14	5	27	0	12	2	0
14	7	27	0	12	8	0
All	All	39071	0	38637	1550	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1550) 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)
4:6:466:HIS:CD2	4:6:521:ARG:NH2	2.03	1.25
5:5:425:VAL:CG2	5:5:425:VAL:O	1.78	1.24
2:4:590:HIS:NE2	13:6:901:ATP:O2G	1.75	1.19
4:6:587:VAL:HG11	11:2:658:GLN:HB3	1.32	1.10
2:4:393:VAL:HG13	2:4:423:HIS:O	1.51	1.08
2:4:535:THR:HG22	2:4:536:SER:H	1.20	1.07
5:5:384:LYS:NZ	5:5:486:ASN:OD1	1.92	1.02
2:4:603:ALA:HB2	4:6:419:ALA:HB1	1.38	1.01
11:2:586:HIS:CE1	11:2:641:ARG:HE	1.81	0.98
2:4:590:HIS:CE1	13:6:901:ATP:O2G	2.16	0.97
4:6:482:ARG:NH1	11:2:530:PHE:O	1.98	0.96
4:6:466:HIS:CG	4:6:521:ARG:NH2	2.34	0.95
5:5:553:ILE:HG23	5:5:554:SER:N	1.80	0.95
3:7:372:ARG:NH1	3:7:611:ARG:HH22	1.64	0.94
6:A:34:ARG:NH2	6:A:37:GLN:OE1	2.02	0.92
11:2:586:HIS:HE1	11:2:641:ARG:NH2	1.68	0.90
13:4:901:ATP:O1A	3:7:604:ARG:NH1	2.06	0.89
1:3:347:SER:N	13:3:901:ATP:O1B	2.07	0.87
4:6:466:HIS:CD2	4:6:521:ARG:HH22	1.89	0.87
2:4:519:SER:OG	13:4:901:ATP:O1G	1.92	0.85
4:6:586:LEU:HD21	4:6:637:VAL:HG22	1.59	0.85
4:6:482:ARG:HD3	11:2:530:PHE:O	1.75	0.85
4:6:587:VAL:HG11	11:2:658:GLN:CB	2.08	0.83
5:5:553:ILE:HG23	5:5:554:SER:H	1.40	0.83
11:2:529:VAL:HG21	11:2:563:LEU:HD21	1.58	0.83
3:7:419:MET:HE3	12:X:36:DT:H4'	1.60	0.83
5:5:425:VAL:O	5:5:425:VAL:HG23	0.99	0.83
3:7:575:ASP:O	3:7:578:THR:OG1	1.97	0.82
3:7:464:GLN:O	3:7:466:THR:HG23	1.81	0.81
4:6:466:HIS:CD2	4:6:521:ARG:HH21	1.94	0.81
5:5:536:VAL:HG21	14:5:801:ADP:H2	1.45	0.80
4:6:482:ARG:CZ	11:2:531:THR:OG1	2.30	0.80
1:3:237:SER:N	1:3:258:LEU:O	2.15	0.79
3:7:372:ARG:HH12	3:7:611:ARG:HH22	1.31	0.79
11:2:586:HIS:CE1	11:2:641:ARG:HH21	2.00	0.78
2:4:590:HIS:O	2:4:590:HIS:CD2	2.37	0.78
3:7:621:LEU:O	3:7:622:SER:C	2.26	0.78
6:A:58:LEU:HD21	6:A:86:LEU:HD21	1.67	0.77
6:A:205:THR:HG22	6:A:205:THR:O	1.83	0.76
11:2:586:HIS:CE1	11:2:641:ARG:NH2	2.53	0.76
3:7:617:ALA:O	3:7:621:LEU:N	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:572:MET:O	1:3:624:ARG:NH2	2.19	0.76
6:A:21:ILE:HG23	6:A:52:ILE:HD11	1.67	0.76
11:2:248:ALA:HB1	11:2:266:ILE:HD13	1.67	0.76
6:A:486:GLY:O	6:A:490:THR:OG1	2.04	0.76
11:2:726:GLN:O	11:2:730:GLU:N	2.18	0.75
6:A:217:MET:SD	6:A:217:MET:N	2.59	0.75
11:2:281:THR:O	11:2:283:ARG:HG3	1.86	0.75
5:5:111:GLU:O	8:L:130:THR:HG21	1.87	0.75
1:3:484:ILE:HG21	5:5:608:THR:HG22	1.70	0.74
11:2:304:LEU:O	11:2:358:TYR:N	2.20	0.74
11:2:747:VAL:O	11:2:751:SER:OG	2.04	0.74
5:5:623:ALA:O	5:5:628:GLN:N	2.20	0.74
12:X:27:DT:H2''	12:X:28:DT:O5'	1.88	0.74
10:N:188:ALA:HB3	10:N:192:VAL:HG11	1.70	0.74
10:N:189:VAL:HG23	10:N:205:ALA:H	1.53	0.74
5:5:389:LYS:HG2	5:5:400:TYR:CE1	2.21	0.73
6:A:254:TYR:HH	6:A:371:TYR:HD1	1.35	0.73
1:3:335:ASN:OD1	1:3:443:VAL:N	2.20	0.73
2:4:583:ASP:O	2:4:587:SER:HB3	1.88	0.73
1:3:302:ILE:HA	13:3:901:ATP:H2	1.52	0.73
11:2:586:HIS:HE1	11:2:641:ARG:CZ	2.02	0.73
5:5:528:THR:O	5:5:532:HIS:N	2.23	0.72
1:3:347:SER:OG	13:3:901:ATP:O2G	2.05	0.72
4:6:427:ARG:NH2	12:X:31:DT:OP2	2.19	0.72
7:H:167:GLU:HG2	7:H:176:LEU:HD22	1.70	0.72
4:6:350:ILE:O	4:6:357:LYS:NZ	2.21	0.71
2:4:645:ARG:HG2	2:4:646:PHE:CE1	2.24	0.71
4:6:382:ILE:HG12	4:6:618:ARG:NH1	2.06	0.71
4:6:466:HIS:HB3	4:6:521:ARG:CZ	2.21	0.71
1:3:302:ILE:HA	13:3:901:ATP:C2	2.26	0.71
3:7:624:SER:O	3:7:625:VAL:C	2.34	0.71
8:L:93:MET:HE2	8:L:151:LEU:HD13	1.73	0.71
3:7:387:LYS:N	14:7:801:ADP:O2B	2.23	0.70
1:3:389:GLU:O	1:3:389:GLU:HG2	1.91	0.70
1:3:305:HIS:HB3	1:3:308:VAL:HG21	1.71	0.70
1:3:373:LEU:O	1:3:390:ALA:HB3	1.91	0.70
11:2:511:GLY:HA2	13:2:901:ATP:H5'2	1.72	0.70
3:7:609:ILE:HG13	3:7:633:ALA:HB1	1.72	0.70
10:N:219:LEU:O	10:N:223:ASN:N	2.25	0.70
2:4:485:GLN:NE2	2:4:506:ILE:HD11	2.05	0.70
8:L:164:LEU:O	8:L:168:ALA:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:45:ASN:HA	9:M:172:GLN:CB	2.21	0.70
5:5:553:ILE:CG2	5:5:554:SER:N	2.54	0.70
1:3:22:ASP:O	1:3:25:ASP:N	2.24	0.70
4:6:311:GLU:O	4:6:566:ARG:NE	2.25	0.70
5:5:439:VAL:HG23	5:5:481:VAL:HG13	1.74	0.69
6:A:281:SER:O	6:A:376:LEU:HD21	1.92	0.69
4:6:393:ALA:HA	13:6:901:ATP:H5'1	1.73	0.69
11:2:397:LEU:HD13	11:2:431:VAL:HA	1.74	0.69
7:H:167:GLU:HG3	7:H:176:LEU:HD13	1.75	0.69
1:3:416:ALA:O	1:3:420:VAL:HG23	1.90	0.69
2:4:522:LEU:CD1	2:4:616:LEU:HG	2.22	0.69
4:6:325:GLU:OE1	4:6:566:ARG:NH1	2.26	0.69
11:2:586:HIS:CE1	11:2:641:ARG:NE	2.58	0.69
2:4:651:LEU:HD23	2:4:770:ALA:HB2	1.73	0.69
4:6:222:LEU:HD12	4:6:226:LEU:HB2	1.74	0.69
11:2:248:ALA:O	11:2:252:VAL:HG23	1.93	0.69
11:2:470:ILE:HG21	13:2:901:ATP:H2	1.56	0.69
2:4:468:ILE:HD11	2:4:486:LEU:HD21	1.75	0.69
11:2:296:VAL:O	11:2:364:GLN:N	2.26	0.69
2:4:609:LEU:HD23	2:4:609:LEU:H	1.58	0.69
11:2:204:ILE:HA	11:2:207:MET:HE3	1.75	0.69
11:2:383:LEU:HD12	11:2:387:LEU:O	1.93	0.69
11:2:714:ASN:OD1	11:2:717:GLU:N	2.26	0.69
11:2:752:GLU:N	11:2:752:GLU:OE1	2.25	0.69
1:3:145:CYS:O	1:3:149:ARG:N	2.24	0.68
2:4:199:LYS:O	2:4:203:ILE:N	2.26	0.68
9:M:31:LEU:O	9:M:32:GLN:HG3	1.93	0.68
12:X:26:DA:H1'	12:X:27:DT:H5'	1.75	0.68
2:4:645:ARG:HG2	2:4:646:PHE:CD1	2.28	0.68
7:H:85:LEU:O	7:H:89:CYS:N	2.26	0.68
8:L:48:MET:O	8:L:51:HIS:N	2.27	0.68
11:2:199:THR:O	11:2:203:ARG:N	2.26	0.68
11:2:233:LEU:HB2	11:2:290:LEU:HD21	1.76	0.68
5:5:46:PHE:HB3	9:M:171:LEU:HD23	1.73	0.68
11:2:712:LEU:HD13	11:2:715:ILE:HG21	1.74	0.68
9:M:34:MET:HB3	9:M:37:LEU:HD13	1.73	0.68
11:2:622:TYR:CE1	11:2:631:ASN:ND2	2.62	0.68
7:H:143:LEU:HD12	7:H:144:THR:HG23	1.75	0.68
1:3:382:GLU:HG2	12:X:27:DT:H5''	1.75	0.68
3:7:355:LEU:O	3:7:359:VAL:HG23	1.94	0.68
4:6:482:ARG:NH1	11:2:531:THR:OG1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:508:LEU:HD13	4:6:651:VAL:HG12	1.76	0.68
9:M:14:GLU:HB3	9:M:17:PHE:HB2	1.75	0.68
1:3:608:THR:O	1:3:611:THR:OG1	2.12	0.68
9:M:33:ARG:HE	9:M:44:ASP:HB3	1.59	0.67
9:M:156:LEU:O	9:M:160:GLY:N	2.27	0.67
2:4:372:ASN:OD1	2:4:372:ASN:N	2.27	0.67
11:2:515:SER:OG	13:2:901:ATP:O1B	2.10	0.67
1:3:412:ILE:O	1:3:415:THR:OG1	2.13	0.67
1:3:134:ILE:O	1:3:135:ARG:NE	2.28	0.67
2:4:590:HIS:O	2:4:590:HIS:HD2	1.76	0.67
1:3:404:ASP:HA	1:3:446:ALA:HB2	1.75	0.67
11:2:337:CYS:O	11:2:341:GLN:HA	1.95	0.66
3:7:383:PRO:C	3:7:385:VAL:H	2.04	0.66
1:3:592:ARG:NH2	3:7:525:PRO:HA	2.10	0.66
11:2:634:LEU:HD12	11:2:639:LEU:HD13	1.77	0.66
5:5:59:LEU:HD12	9:M:134:ASP:O	1.95	0.66
2:4:393:VAL:CG1	2:4:423:HIS:O	2.39	0.66
5:5:163:MET:O	5:5:172:THR:N	2.28	0.66
6:A:342:TYR:OH	6:A:350:ARG:O	2.12	0.66
9:M:122:PHE:O	9:M:126:ARG:N	2.28	0.66
6:A:254:TYR:OH	6:A:371:TYR:HD1	1.78	0.66
10:N:85:PHE:O	10:N:89:VAL:HG23	1.96	0.66
11:2:774:MET:O	11:2:778:SER:N	2.28	0.66
2:4:191:VAL:HG12	2:4:193:GLN:HB3	1.75	0.66
2:4:535:THR:HG22	2:4:536:SER:N	2.01	0.66
11:2:361:ILE:HG21	11:2:381:VAL:CG2	2.25	0.66
2:4:526:PHE:HE1	2:4:532:SER:HA	1.60	0.66
3:7:230:VAL:HG22	3:7:259:GLY:HA2	1.77	0.66
4:6:482:ARG:CD	11:2:530:PHE:O	2.42	0.66
9:M:27:VAL:CG2	9:M:52:VAL:HG21	2.25	0.66
6:A:301:GLU:N	6:A:301:GLU:OE1	2.29	0.66
6:A:389:TYR:OH	6:A:422:LYS:NZ	2.26	0.65
1:3:566:ILE:O	1:3:570:LYS:N	2.29	0.65
5:5:360:LYS:NZ	5:5:570:GLY:O	2.29	0.65
4:6:242:LEU:HD21	4:6:288:MET:HG2	1.79	0.65
11:2:249:LYS:HE3	11:2:266:ILE:HG22	1.79	0.65
1:3:351:ARG:HE	1:3:354:LEU:HD13	1.62	0.65
3:7:505:ILE:HG22	3:7:506:GLN:N	2.10	0.65
5:5:46:PHE:CB	9:M:171:LEU:HD23	2.27	0.65
10:N:75:GLU:HA	10:N:78:ARG:HB2	1.77	0.65
11:2:742:ARG:O	11:2:746:SER:OG	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:335:ASN:ND2	1:3:442:SER:OG	2.29	0.65
2:4:203:ILE:O	2:4:207:GLU:N	2.30	0.65
1:3:305:HIS:HB3	1:3:308:VAL:CG2	2.27	0.65
3:7:336:LEU:O	3:7:340:LEU:N	2.27	0.65
11:2:712:LEU:HD11	11:2:763:VAL:HB	1.79	0.65
1:3:592:ARG:HH22	3:7:525:PRO:HA	1.61	0.65
1:3:128:VAL:O	1:3:229:GLY:N	2.30	0.64
2:4:538:ARG:N	2:4:581:MET:SD	2.66	0.64
6:A:254:TYR:CZ	6:A:371:TYR:HD1	2.15	0.64
7:H:45:PHE:O	7:H:49:VAL:N	2.30	0.64
11:2:382:ILE:N	11:2:424:ILE:O	2.29	0.64
1:3:115:SER:OG	5:5:218:ASP:OD1	2.15	0.64
3:7:402:GLN:CD	3:7:436:LEU:HD11	2.23	0.64
3:7:435:VAL:HG22	3:7:478:LEU:HD22	1.79	0.64
4:6:424:ALA:HB1	12:X:32:DT:OP1	1.98	0.64
8:L:116:VAL:O	8:L:120:ILE:HG22	1.96	0.64
4:6:382:ILE:HG22	4:6:383:ASN:O	1.97	0.64
5:5:574:SER:N	5:5:631:ALA:O	2.30	0.64
11:2:189:ARG:NH2	11:2:251:MET:SD	2.69	0.64
1:3:496:VAL:HA	1:3:499:MET:HE2	1.77	0.64
2:4:685:ASP:O	2:4:690:ARG:NH2	2.29	0.64
2:4:487:PHE:CD2	2:4:749:VAL:HG23	2.32	0.64
1:3:439:ALA:HB1	1:3:441:CYS:SG	2.38	0.64
3:7:500:THR:HG22	3:7:503:GLN:OE1	1.98	0.64
5:5:640:LEU:O	5:5:644:GLN:NE2	2.30	0.64
2:4:291:MET:N	2:4:358:GLN:O	2.30	0.64
2:4:603:ALA:HB2	4:6:419:ALA:CB	2.24	0.64
7:H:83:ALA:O	7:H:87:GLU:N	2.31	0.64
1:3:137:LYS:O	1:3:191:LYS:N	2.31	0.64
7:H:35:ARG:O	7:H:39:GLU:N	2.29	0.64
11:2:398:GLU:N	11:2:430:VAL:O	2.31	0.64
1:3:366:ARG:NH2	1:3:408:LYS:O	2.31	0.64
3:7:556:MET:HE1	3:7:560:ARG:HH21	1.63	0.64
4:6:22:GLN:NE2	4:6:83:PHE:O	2.31	0.64
1:3:612:LEU:HA	1:3:615:LEU:HD12	1.79	0.64
3:7:338:THR:HG21	3:7:551:VAL:HB	1.78	0.63
3:7:556:MET:O	3:7:560:ARG:HG2	1.98	0.63
4:6:597:ASP:OD2	4:6:608:ILE:HG21	1.97	0.63
11:2:458:ILE:HD11	11:2:757:MET:HG2	1.80	0.63
1:3:558:SER:O	1:3:562:MET:HB2	1.98	0.63
11:2:571:ILE:HD13	11:2:577:MET:HE1	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:300:PRO:HG2	5:5:364:ASP:OD2	1.97	0.63
13:4:901:ATP:O1A	3:7:604:ARG:HD2	1.98	0.63
5:5:384:LYS:NZ	5:5:486:ASN:CG	2.57	0.63
4:6:340:GLN:HA	4:6:343:ILE:HD12	1.79	0.63
2:4:526:PHE:CE1	2:4:532:SER:HA	2.33	0.63
5:5:47:PHE:CD2	9:M:174:THR:HG21	2.34	0.63
5:5:157:SER:OG	5:5:158:ALA:N	2.28	0.63
9:M:122:PHE:O	9:M:125:LEU:N	2.31	0.63
2:4:248:PHE:CG	2:4:257:LEU:HD21	2.34	0.63
5:5:360:LYS:O	5:5:368:ARG:NH2	2.31	0.63
5:5:372:ILE:HG22	5:5:617:ARG:HD3	1.80	0.63
11:2:540:GLY:O	11:2:559:GLY:N	2.32	0.63
2:4:176:ILE:HD12	2:4:181:GLU:HB3	1.80	0.63
1:3:600:ASP:O	1:3:604:THR:OG1	2.17	0.62
4:6:330:TYR:O	4:6:333:SER:OG	2.17	0.62
6:A:74:LEU:N	6:A:96:PHE:O	2.32	0.62
1:3:430:LYS:HB2	3:7:410:SER:HB3	1.79	0.62
2:4:641:THR:HG21	4:6:390:PRO:HG2	1.80	0.62
3:7:416:ALA:HB1	3:7:429:LEU:O	1.98	0.62
4:6:81:TYR:OH	4:6:223:ARG:NH2	2.32	0.62
5:5:279:GLU:OE2	11:2:406:ASN:ND2	2.32	0.62
2:4:417:THR:HG21	3:7:174:LYS:CD	2.29	0.62
1:3:203:GLU:OE2	1:3:203:GLU:N	2.32	0.62
4:6:44:ALA:HB2	4:6:55:LEU:HD11	1.81	0.62
11:2:529:VAL:CG2	11:2:563:LEU:HD21	2.30	0.62
1:3:420:VAL:O	1:3:424:GLY:N	2.32	0.62
2:4:519:SER:HA	2:4:522:LEU:HD23	1.81	0.62
10:N:182:PHE:HB3	10:N:228:ILE:HD12	1.80	0.62
11:2:541:LEU:O	11:2:559:GLY:HA3	1.99	0.62
3:7:382:ASP:OD2	3:7:490:PRO:HD2	1.99	0.62
3:7:402:GLN:HE21	3:7:402:GLN:HA	1.64	0.62
11:2:644:VAL:O	11:2:645:LEU:HD22	1.99	0.62
3:7:546:GLN:HB2	3:7:547:PRO:HD3	1.82	0.62
3:7:465:GLN:HG2	3:7:479:ASN:HA	1.81	0.62
4:6:167:LYS:HA	11:2:413:THR:HG23	1.81	0.62
4:6:243:ILE:HG22	4:6:244:VAL:H	1.65	0.62
11:2:248:ALA:CB	11:2:266:ILE:HD13	2.29	0.62
1:3:354:LEU:HD12	1:3:362:PRO:HG3	1.82	0.62
2:4:588:VAL:O	2:4:590:HIS:N	2.32	0.62
2:4:658:GLU:CG	3:7:586:VAL:HG13	2.30	0.62
5:5:76:ASP:HB2	5:5:78:THR:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:577:GLU:HG2	3:7:459:HIS:NE2	2.14	0.61
7:H:46:GLU:HA	7:H:49:VAL:HG12	1.83	0.61
3:7:173:VAL:HA	3:7:232:PHE:O	2.00	0.61
4:6:461:ASP:N	4:6:461:ASP:OD1	2.33	0.61
4:6:587:VAL:CG1	11:2:658:GLN:HB3	2.21	0.61
5:5:43:GLU:OE1	6:A:381:ARG:NH2	2.33	0.61
5:5:536:VAL:HG21	14:5:801:ADP:C2	2.33	0.61
6:A:512:GLY:O	6:A:560:GLN:NE2	2.33	0.61
8:L:69:ASP:OD2	8:L:70:ILE:HG12	2.00	0.61
9:M:8:PRO:N	9:M:11:TYR:HH	1.99	0.61
1:3:299:ALA:H	1:3:300:PRO:HD3	1.65	0.61
3:7:305:CYS:O	3:7:309:ASN:HB2	1.99	0.61
4:6:383:ASN:ND2	4:6:521:ARG:O	2.33	0.61
2:4:535:THR:CG2	2:4:536:SER:H	2.02	0.61
3:7:50:ILE:O	3:7:139:LYS:HB3	1.99	0.61
3:7:386:ALA:HB1	14:7:801:ADP:H5'2	1.83	0.61
4:6:425:VAL:HG13	12:X:31:DT:H5''	1.82	0.61
1:3:568:ILE:HG13	1:3:572:MET:HE3	1.83	0.61
4:6:196:ASP:OD1	4:6:196:ASP:N	2.34	0.61
5:5:107:ALA:HB2	5:5:112:HIS:O	2.01	0.61
9:M:56:LEU:HD11	9:M:60:LYS:HA	1.83	0.61
10:N:123:GLU:N	10:N:123:GLU:OE1	2.34	0.61
4:6:427:ARG:HB2	12:X:31:DT:OP1	2.01	0.61
3:7:477:THR:HG22	3:7:479:ASN:H	1.66	0.60
2:4:351:ASP:OD1	4:6:122:THR:HG23	2.01	0.60
2:4:632:ILE:HD12	2:4:632:ILE:H	1.66	0.60
11:2:202:ASP:OD1	11:2:202:ASP:N	2.34	0.60
1:3:309:LYS:HE3	1:3:349:LEU:HD11	1.82	0.60
3:7:526:ASP:HB2	3:7:529:ASN:HB3	1.83	0.60
6:A:20:LEU:O	6:A:49:VAL:HG22	2.01	0.60
9:M:54:LEU:HD23	9:M:58:TYR:OH	1.99	0.60
11:2:283:ARG:HB2	11:2:285:LEU:HD23	1.82	0.60
11:2:396:GLU:O	11:2:397:LEU:HD22	2.02	0.60
2:4:599:SER:OG	4:6:412:SER:N	2.30	0.60
2:4:411:VAL:O	3:7:200:PHE:N	2.33	0.60
2:4:613:THR:HG22	2:4:614:SER:H	1.66	0.60
2:4:497:LEU:HD11	2:4:499:ARG:HE	1.67	0.60
4:6:329:ILE:HD12	4:6:566:ARG:NH2	2.17	0.60
6:A:452:VAL:HG11	6:A:488:VAL:HG21	1.83	0.60
1:3:336:VAL:O	1:3:444:LEU:HD22	2.02	0.60
2:4:591:GLU:O	2:4:591:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:371:THR:HG23	4:6:575:LYS:CE	2.32	0.60
4:6:507:SER:O	4:6:511:ASN:N	2.35	0.60
4:6:609:THR:OG1	4:6:610:VAL:N	2.34	0.60
6:A:93:VAL:N	6:A:114:GLN:OE1	2.35	0.60
2:4:586:ARG:O	2:4:589:LEU:N	2.16	0.60
5:5:618:ILE:O	5:5:621:SER:OG	2.13	0.60
1:3:177:ASP:HB3	1:3:179:ASN:CG	2.27	0.60
1:3:210:LEU:HG	1:3:210:LEU:O	2.01	0.60
3:7:306:ILE:O	3:7:312:ILE:HG13	2.02	0.60
3:7:618:ARG:O	3:7:621:LEU:HD23	2.01	0.60
9:M:16:ILE:O	9:M:20:GLN:OE1	2.19	0.60
11:2:184:PHE:O	11:2:188:LEU:HD12	2.02	0.60
1:3:309:LYS:CE	1:3:349:LEU:HD11	2.32	0.60
2:4:425:ARG:H	2:4:425:ARG:HD3	1.67	0.60
3:7:9:ASP:OD1	3:7:62:LEU:HD11	2.02	0.60
3:7:241:SER:HA	3:7:244:VAL:HG22	1.84	0.60
4:6:355:GLU:OE2	4:6:646:LYS:NZ	2.26	0.60
2:4:717:VAL:HG23	4:6:538:TYR:OH	2.01	0.59
6:A:11:TYR:HD1	6:A:14:LEU:HD22	1.67	0.59
11:2:589:MET:CB	11:2:641:ARG:HB3	2.32	0.59
3:7:402:GLN:HA	3:7:402:GLN:NE2	2.17	0.59
3:7:535:LYS:HA	3:7:538:THR:OG1	2.02	0.59
6:A:264:HIS:O	6:A:268:LEU:N	2.34	0.59
6:A:299:VAL:O	6:A:302:SER:OG	2.15	0.59
9:M:102:TYR:CE1	9:M:125:LEU:HD11	2.37	0.59
11:2:199:THR:OG1	11:2:203:ARG:NH2	2.34	0.59
3:7:621:LEU:C	3:7:622:SER:O	2.39	0.59
4:6:607:ARG:HG3	11:2:621:ARG:HE	1.66	0.59
11:2:234:PRO:HB3	11:2:290:LEU:HD23	1.84	0.59
11:2:278:GLU:HB2	11:2:281:THR:HG21	1.85	0.59
2:4:375:LEU:HD13	2:4:419:VAL:HB	1.84	0.59
5:5:137:SER:CB	11:2:354:LEU:HA	2.32	0.59
2:4:712:LEU:HA	2:4:715:ALA:HB3	1.82	0.59
3:7:412:VAL:HG12	3:7:412:VAL:O	2.02	0.59
3:7:421:ASP:HB3	3:7:422:PRO:CD	2.32	0.59
1:3:563:ARG:CB	1:3:566:ILE:HD12	2.33	0.59
2:4:522:LEU:HD11	2:4:616:LEU:HG	1.84	0.59
6:A:502:ILE:CG2	6:A:516:LEU:HD11	2.32	0.59
8:L:138:GLY:O	8:L:140:GLY:N	2.35	0.59
10:N:211:ILE:HD13	10:N:216:VAL:HG21	1.83	0.59
11:2:361:ILE:HG21	11:2:381:VAL:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:158:ASP:HA	1:3:165:VAL:HG22	1.85	0.59
2:4:462:ASP:O	2:4:466:ARG:HG3	2.02	0.59
3:7:566:CYS:O	3:7:618:ARG:CB	2.50	0.59
1:3:252:THR:HG22	1:3:253:PHE:H	1.66	0.59
1:3:499:MET:HE3	1:3:500:HIS:CE1	2.38	0.59
3:7:446:GLU:N	3:7:487:ALA:O	2.35	0.59
5:5:379:ASP:HB2	5:5:380:PRO:HD2	1.85	0.59
6:A:515:LEU:HD23	6:A:516:LEU:N	2.18	0.59
1:3:293:LEU:O	1:3:297:SER:OG	2.17	0.58
2:4:479:LYS:HG2	2:4:482:ILE:HD12	1.85	0.58
2:4:658:GLU:HG3	3:7:586:VAL:HG13	1.83	0.58
4:6:394:LYS:N	13:6:901:ATP:O2B	2.36	0.58
5:5:172:THR:O	5:5:174:ILE:HG23	2.02	0.58
5:5:622:LEU:HD12	5:5:625:ILE:HB	1.86	0.58
2:4:165:LYS:NZ	2:4:242:MET:SD	2.71	0.58
2:4:169:LYS:HG3	2:4:170:SER:N	2.18	0.58
2:4:598:LEU:O	2:4:599:SER:C	2.46	0.58
6:A:330:GLU:OE2	6:A:364:TYR:OH	2.11	0.58
6:A:485:ARG:HA	6:A:489:ALA:HB3	1.86	0.58
1:3:42:LYS:HG3	1:3:43:ARG:HG2	1.86	0.58
1:3:140:ARG:NE	1:3:153:GLU:OE2	2.35	0.58
4:6:427:ARG:NE	12:X:30:DT:H4'	2.17	0.58
9:M:108:LEU:O	9:M:111:TYR:N	2.34	0.58
11:2:594:ILE:HD11	11:2:605:LEU:HB2	1.84	0.58
3:7:379:LEU:CD2	3:7:519:TRP:HB3	2.33	0.58
5:5:442:ASP:OD2	5:5:484:ALA:HB3	2.04	0.58
8:L:15:ILE:CD1	8:L:46:LEU:HD11	2.34	0.58
3:7:533:LEU:O	3:7:533:LEU:HD12	2.02	0.58
2:4:542:ALA:HB2	2:4:584:SER:O	2.03	0.58
3:7:214:ASN:OD1	3:7:214:ASN:N	2.36	0.58
5:5:519:ASP:O	11:2:724:TYR:OH	2.21	0.58
6:A:82:ASP:O	6:A:85:GLU:N	2.34	0.58
6:A:265:VAL:HA	6:A:268:LEU:HG	1.86	0.58
8:L:123:ILE:O	8:L:126:SER:N	2.36	0.58
1:3:139:VAL:HG21	1:3:189:VAL:HG23	1.85	0.58
5:5:152:ALA:HA	5:5:254:PRO:CG	2.34	0.58
6:A:210:TYR:OH	6:A:552:GLU:OE1	2.20	0.58
1:3:271:LEU:HB3	1:3:273:ILE:HD12	1.84	0.58
5:5:382:THR:HG21	5:5:517:VAL:HG12	1.85	0.58
5:5:530:ALA:CB	11:2:721:ALA:HB2	2.33	0.58
2:4:375:LEU:HD12	2:4:421:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:487:PHE:CE2	2:4:749:VAL:HG23	2.39	0.58
2:4:590:HIS:CE1	2:4:645:ARG:HH22	2.21	0.57
6:A:49:VAL:O	7:H:158:ARG:NH2	2.36	0.57
7:H:127:ALA:HA	7:H:130:MET:HE3	1.86	0.57
11:2:308:SER:HB3	11:2:354:LEU:HD22	1.86	0.57
11:2:585:ILE:HG22	11:2:589:MET:HE1	1.86	0.57
3:7:625:VAL:HG13	3:7:629:ASP:HB2	1.85	0.57
4:6:394:LYS:CB	4:6:394:LYS:NZ	2.67	0.57
6:A:81:VAL:O	6:A:108:ASN:ND2	2.35	0.57
8:L:87:MET:HE2	8:L:148:LEU:C	2.29	0.57
10:N:107:CYS:O	10:N:111:LYS:N	2.37	0.57
2:4:226:TYR:CZ	2:4:230:ILE:HD11	2.39	0.57
2:4:509:LEU:HD23	2:4:617:ALA:HB2	1.86	0.57
3:7:344:ILE:HG13	14:7:801:ADP:C2	2.40	0.57
6:A:385:ALA:HB3	6:A:388:ASP:HB2	1.86	0.57
11:2:301:THR:HG22	11:2:360:LYS:HB3	1.85	0.57
1:3:127:ILE:HD11	1:3:201:MET:SD	2.45	0.57
4:6:227:VAL:O	4:6:229:THR:HG23	2.04	0.57
4:6:523:ASP:OD1	4:6:615:SER:OG	2.16	0.57
6:A:212:ARG:NH1	6:A:216:LEU:HD23	2.19	0.57
8:L:100:MET:HE1	8:L:114:ARG:HG3	1.86	0.57
10:N:100:ILE:O	10:N:104:TYR:N	2.37	0.57
2:4:717:VAL:N	4:6:538:TYR:OH	2.38	0.57
5:5:154:SER:HB2	5:5:220:GLN:O	2.05	0.57
2:4:248:PHE:CD2	2:4:257:LEU:HD21	2.39	0.57
3:7:344:ILE:HG23	14:7:801:ADP:N6	2.19	0.57
3:7:369:MET:SD	3:7:370:LYS:N	2.77	0.57
8:L:112:GLU:O	8:L:116:VAL:HG13	2.05	0.57
11:2:470:ILE:HG22	11:2:471:TYR:H	1.70	0.57
11:2:511:GLY:CA	13:2:901:ATP:H5'2	2.33	0.57
2:4:215:CYS:HG	2:4:266:PHE:N	2.02	0.57
4:6:427:ARG:HE	12:X:30:DT:H4'	1.68	0.57
10:N:112:ILE:HG23	10:N:119:ILE:HD13	1.85	0.57
2:4:248:PHE:HZ	2:4:255:ALA:HB3	1.69	0.57
11:2:177:ARG:HA	11:2:180:ILE:HD12	1.87	0.57
2:4:276:SER:C	2:4:277:LEU:HD22	2.30	0.56
2:4:516:THR:HG23	2:4:518:LYS:HG3	1.86	0.56
3:7:619:LEU:HG	3:7:619:LEU:O	2.05	0.56
3:7:49:THR:O	3:7:50:ILE:HD13	2.05	0.56
3:7:370:LYS:HG3	3:7:371:ILE:H	1.70	0.56
5:5:460:GLU:HB3	5:5:461:GLN:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:305:TYR:CZ	6:A:437:ALA:HB2	2.40	0.56
11:2:660:LEU:O	11:2:664:VAL:HG23	2.06	0.56
2:4:670:SER:O	2:4:674:VAL:N	2.35	0.56
4:6:117:VAL:HG21	4:6:204:GLU:HG3	1.86	0.56
4:6:466:HIS:CG	4:6:521:ARG:CZ	2.88	0.56
5:5:349:ALA:HB2	5:5:642:LEU:CD2	2.35	0.56
5:5:349:ALA:HB2	5:5:642:LEU:HD21	1.88	0.56
6:A:328:LEU:O	6:A:332:GLY:N	2.35	0.56
10:N:114:THR:O	10:N:117:GLN:NE2	2.36	0.56
11:2:304:LEU:N	11:2:358:TYR:O	2.36	0.56
11:2:541:LEU:HD11	11:2:585:ILE:HD11	1.88	0.56
2:4:666:SER:CA	3:7:582:VAL:HG11	2.35	0.56
5:5:369:ARG:HB2	5:5:617:ARG:HH21	1.69	0.56
11:2:466:MET:CE	11:2:480:LEU:HD12	2.35	0.56
2:4:759:ASP:OD1	2:4:760:VAL:N	2.39	0.56
3:7:505:ILE:CG2	3:7:506:GLN:H	2.17	0.56
3:7:606:LEU:HD12	3:7:607:LEU:N	2.20	0.56
5:5:130:THR:HG22	5:5:131:ASN:H	1.71	0.56
1:3:428:ILE:HG22	3:7:409:SER:OG	2.06	0.56
3:7:372:ARG:NH1	3:7:611:ARG:NH2	2.45	0.56
4:6:421:LEU:HD11	4:6:474:ILE:CD1	2.36	0.56
4:6:329:ILE:HD11	4:6:567:TYR:HB2	1.88	0.56
4:6:353:ASN:H	4:6:528:LEU:HD13	1.71	0.56
6:A:462:VAL:HG23	6:A:504:SER:CB	2.36	0.56
10:N:183:LEU:HD11	10:N:211:ILE:HG12	1.87	0.56
1:3:476:LEU:HD13	1:3:478:PHE:CZ	2.40	0.56
2:4:248:PHE:CD2	2:4:257:LEU:HD11	2.41	0.56
2:4:450:LEU:HD12	2:4:450:LEU:H	1.71	0.56
2:4:592:VAL:O	2:4:596:GLN:HG2	2.06	0.56
3:7:107:LEU:O	3:7:107:LEU:HG	2.05	0.56
5:5:27:LEU:O	5:5:31:LYS:N	2.37	0.56
5:5:217:VAL:HG12	5:5:218:ASP:H	1.71	0.56
11:2:712:LEU:HD13	11:2:715:ILE:CG2	2.36	0.56
2:4:665:ALA:O	2:4:669:VAL:N	2.38	0.56
6:A:288:ASP:O	6:A:371:TYR:N	2.30	0.56
8:L:167:ILE:HG22	8:L:171:GLN:CG	2.36	0.56
1:3:483:VAL:HG12	1:3:484:ILE:O	2.06	0.55
6:A:15:VAL:HG13	6:A:45:MET:HE1	1.87	0.55
11:2:663:PHE:O	11:2:667:SER:HB3	2.06	0.55
2:4:513:ASP:HB2	2:4:514:PRO:HD3	1.88	0.55
2:4:696:ALA:HA	2:4:700:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:379:LEU:N	3:7:486:ALA:O	2.40	0.55
6:A:400:VAL:HG11	6:A:405:THR:HG21	1.88	0.55
1:3:238:TYR:C	1:3:239:ARG:HG2	2.31	0.55
3:7:505:ILE:CG2	3:7:506:GLN:N	2.68	0.55
4:6:387:VAL:HG12	4:6:388:GLY:H	1.70	0.55
4:6:466:HIS:CB	4:6:521:ARG:CZ	2.84	0.55
5:5:151:VAL:HG22	5:5:224:LEU:HA	1.86	0.55
8:L:153:ILE:HD11	10:N:182:PHE:CE1	2.41	0.55
1:3:347:SER:HB3	5:5:461:GLN:OE1	2.06	0.55
13:4:901:ATP:O1A	3:7:604:ARG:CZ	2.54	0.55
4:6:482:ARG:NH1	11:2:529:VAL:HG12	2.22	0.55
9:M:14:GLU:O	9:M:17:PHE:N	2.39	0.55
1:3:443:VAL:O	1:3:444:LEU:HD23	2.06	0.55
2:4:176:ILE:HD12	2:4:181:GLU:CB	2.36	0.55
6:A:443:VAL:HG13	6:A:483:LEU:HG	1.89	0.55
11:2:361:ILE:HD13	11:2:381:VAL:CG2	2.37	0.55
6:A:320:GLY:O	6:A:324:LEU:N	2.37	0.55
1:3:171:TYR:CE2	1:3:183:THR:HG22	2.41	0.55
2:4:273:ASN:HD21	2:4:361:PRO:HG3	1.72	0.55
2:4:598:LEU:O	2:4:600:ILE:HG23	2.07	0.55
3:7:261:VAL:HG12	3:7:261:VAL:O	2.05	0.55
3:7:400:ARG:HH22	3:7:436:LEU:HD13	1.72	0.55
4:6:355:GLU:OE1	4:6:650:ARG:NH2	2.38	0.55
4:6:420:GLY:C	4:6:440:ALA:HB3	2.32	0.55
5:5:240:LEU:HD12	5:5:242:LEU:HD21	1.88	0.55
5:5:352:CYS:SG	5:5:618:ILE:HD12	2.46	0.55
1:3:257:LEU:O	1:3:258:LEU:HD23	2.07	0.55
1:3:382:GLU:CG	12:X:27:DT:H5"	2.37	0.55
1:3:496:VAL:HG11	5:5:612:LEU:HD11	1.89	0.55
2:4:354:LEU:HD11	2:4:374:LEU:HB2	1.88	0.55
3:7:606:LEU:HD12	3:7:607:LEU:HD23	1.89	0.55
5:5:25:ILE:HD12	5:5:26:ASN:H	1.71	0.55
4:6:373:THR:HG22	11:2:670:LYS:CE	2.37	0.55
5:5:137:SER:CB	11:2:355:TYR:H	2.20	0.55
6:A:205:THR:O	6:A:205:THR:CG2	2.53	0.54
8:L:64:GLU:O	8:L:67:ASP:OD1	2.24	0.54
10:N:214:GLN:HB3	10:N:215:LEU:HD12	1.88	0.54
11:2:548:ASN:ND2	11:2:549:PRO:O	2.38	0.54
3:7:515:PHE:HB2	3:7:518:LEU:HD11	1.90	0.54
11:2:285:LEU:HD23	11:2:285:LEU:H	1.72	0.54
11:2:762:ASN:N	11:2:762:ASN:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:62:LEU:HD23	3:7:65:ALA:HB3	1.89	0.54
4:6:255:GLY:O	4:6:256:THR:C	2.48	0.54
5:5:337:ALA:HB1	5:5:340:ILE:HB	1.89	0.54
5:5:389:LYS:HE2	5:5:400:TYR:OH	2.06	0.54
6:A:158:GLY:HA2	6:A:168:ALA:HB1	1.89	0.54
9:M:104:PHE:CZ	9:M:108:LEU:HD23	2.41	0.54
2:4:205:THR:HG23	2:4:251:ARG:HH11	1.72	0.54
4:6:420:GLY:O	4:6:440:ALA:HB3	2.07	0.54
11:2:315:VAL:HB	11:2:347:SER:OG	2.06	0.54
1:3:310:GLN:N	1:3:310:GLN:OE1	2.41	0.54
2:4:376:TYR:O	2:4:421:VAL:HG21	2.08	0.54
11:2:794:THR:O	11:2:797:LYS:N	2.40	0.54
7:H:40:GLU:O	7:H:43:ALA:HB3	2.08	0.54
7:H:95:LEU:HD13	7:H:99:PHE:CZ	2.43	0.54
4:6:427:ARG:HH22	4:6:479:ALA:HB3	1.73	0.54
6:A:446:SER:O	6:A:450:ARG:N	2.40	0.54
13:3:901:ATP:H3'	13:3:901:ATP:O2A	2.07	0.54
3:7:465:GLN:HA	3:7:480:ALA:N	2.23	0.54
3:7:609:ILE:CG1	3:7:633:ALA:HB1	2.37	0.54
4:6:168:PHE:O	11:2:413:THR:OG1	2.23	0.54
8:L:15:ILE:HD11	8:L:46:LEU:HD11	1.89	0.54
4:6:308:PRO:HB2	4:6:312:VAL:HG21	1.88	0.54
5:5:152:ALA:HA	5:5:254:PRO:HG3	1.89	0.54
5:5:461:GLN:CB	5:5:463:THR:HG23	2.38	0.54
12:X:30:DT:H5''	12:X:30:DT:H6	1.73	0.54
1:3:42:LYS:HD3	1:3:95:LEU:HA	1.89	0.54
7:H:192:LEU:HD13	7:H:195:GLN:NE2	2.22	0.54
1:3:215:ASP:OD2	1:3:254:ARG:NH1	2.41	0.53
1:3:338:LEU:HD21	1:3:478:PHE:C	2.32	0.53
5:5:481:VAL:HG12	5:5:482:LEU:O	2.08	0.53
11:2:192:VAL:HG11	11:2:196:GLY:HA2	1.90	0.53
1:3:317:LEU:HD12	1:3:621:ALA:HB1	1.91	0.53
3:7:429:LEU:HD12	3:7:430:GLU:N	2.23	0.53
4:6:88:VAL:O	4:6:92:VAL:HG23	2.07	0.53
5:5:378:GLY:HA3	5:5:517:VAL:HB	1.91	0.53
5:5:512:ASP:O	5:5:514:ILE:HD12	2.08	0.53
6:A:17:LYS:H	6:A:17:LYS:HD3	1.73	0.53
6:A:313:LEU:CB	6:A:315:LEU:HD21	2.39	0.53
11:2:378:SER:O	11:2:379:LYS:HD2	2.08	0.53
2:4:199:LYS:O	2:4:202:GLU:N	2.41	0.53
2:4:685:ASP:N	2:4:685:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:222:LEU:HD12	4:6:226:LEU:CB	2.37	0.53
8:L:129:ARG:O	8:L:133:ASP:N	2.39	0.53
3:7:369:MET:HE3	3:7:370:LYS:O	2.09	0.53
3:7:435:VAL:HG12	3:7:436:LEU:N	2.22	0.53
4:6:54:THR:HG22	4:6:105:TYR:CD2	2.44	0.53
6:A:26:ASP:OD1	6:A:27:ILE:N	2.42	0.53
6:A:32:ALA:CB	6:A:215:ALA:HB2	2.39	0.53
6:A:260:GLN:O	6:A:264:HIS:N	2.41	0.53
2:4:516:THR:HG21	2:4:652:VAL:HG11	1.89	0.53
3:7:343:GLU:OE2	3:7:389:GLN:NE2	2.38	0.53
3:7:381:GLY:HA2	3:7:490:PRO:HD3	1.91	0.53
4:6:370:LYS:HG2	4:6:371:THR:H	1.74	0.53
8:L:93:MET:CE	8:L:151:LEU:HD13	2.39	0.53
11:2:296:VAL:N	11:2:364:GLN:O	2.42	0.53
3:7:441:VAL:HA	3:7:483:SER:O	2.09	0.53
5:5:460:GLU:HB3	5:5:461:GLN:CD	2.34	0.53
6:A:100:SER:O	6:A:211:GLY:N	2.40	0.53
11:2:180:ILE:HG21	11:2:243:ILE:HG21	1.89	0.53
5:5:130:THR:N	5:5:145:LYS:O	2.42	0.53
7:H:93:LYS:O	7:H:97:TRP:N	2.42	0.53
11:2:269:ARG:NH1	11:2:427:ASN:O	2.41	0.53
2:4:473:TYR:O	2:4:475:ASN:N	2.41	0.53
4:6:372:THR:HG21	4:6:378:LEU:CD2	2.39	0.53
6:A:511:GLU:O	6:A:560:GLN:NE2	2.42	0.53
8:L:129:ARG:HD3	9:M:133:LEU:CD1	2.38	0.53
4:6:372:THR:HG21	4:6:378:LEU:HD23	1.90	0.53
5:5:461:GLN:HB2	5:5:463:THR:HG23	1.91	0.53
9:M:45:ASP:OD1	9:M:45:ASP:N	2.42	0.53
11:2:573:GLU:OE1	11:2:573:GLU:N	2.41	0.53
3:7:215:LYS:O	3:7:216:ALA:C	2.51	0.53
1:3:109:THR:N	1:3:112:SER:OG	2.41	0.52
3:7:51:ASP:N	3:7:54:ASP:OD2	2.41	0.52
4:6:54:THR:HG21	4:6:225:GLU:HB3	1.90	0.52
11:2:488:GLU:O	11:2:497:LYS:NZ	2.39	0.52
1:3:459:THR:O	1:3:463:ASN:ND2	2.42	0.52
3:7:459:HIS:CE1	3:7:514:ARG:HH22	2.27	0.52
3:7:607:LEU:O	3:7:610:LEU:HB3	2.09	0.52
4:6:402:SER:OG	4:6:410:TYR:HB2	2.10	0.52
5:5:241:GLN:O	5:5:242:LEU:HD23	2.08	0.52
1:3:405:GLU:O	1:3:409:MET:N	2.42	0.52
1:3:413:ASP:O	1:3:416:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:522:LEU:HD11	2:4:616:LEU:HB3	1.90	0.52
2:4:708:ALA:HB2	2:4:757:LEU:HD12	1.91	0.52
3:7:344:ILE:HG23	14:7:801:ADP:C6	2.45	0.52
3:7:402:GLN:HG2	3:7:433:ALA:HB1	1.90	0.52
3:7:624:SER:O	3:7:626:GLU:N	2.43	0.52
6:A:139:GLY:N	6:A:140:GLU:OE1	2.42	0.52
6:A:547:LEU:HD12	6:A:557:GLN:HB3	1.91	0.52
8:L:78:GLU:O	8:L:81:SER:HB3	2.09	0.52
10:N:74:GLU:O	10:N:78:ARG:N	2.39	0.52
3:7:42:HIS:C	3:7:43:ARG:HD3	2.34	0.52
3:7:421:ASP:HB3	3:7:422:PRO:HD2	1.91	0.52
3:7:573:ILE:O	3:7:574:PRO:O	2.26	0.52
6:A:428:GLY:O	6:A:432:ALA:N	2.40	0.52
3:7:472:ALA:HB3	3:7:474:ILE:HD11	1.91	0.52
6:A:259:GLU:O	6:A:263:SER:N	2.38	0.52
6:A:289:LEU:O	6:A:290:HIS:ND1	2.42	0.52
7:H:67:LEU:O	7:H:71:HIS:N	2.40	0.52
8:L:150:LEU:HB3	8:L:151:LEU:HD12	1.92	0.52
11:2:744:ILE:HD12	11:2:747:VAL:HB	1.90	0.52
1:3:640:ILE:O	1:3:643:VAL:N	2.40	0.52
2:4:417:THR:CG2	3:7:174:LYS:HD2	2.40	0.52
3:7:381:GLY:CA	3:7:490:PRO:HD3	2.40	0.52
6:A:254:TYR:CD2	6:A:255:THR:HG23	2.45	0.52
9:M:31:LEU:O	9:M:32:GLN:CG	2.57	0.52
2:4:379:ASN:OD1	2:4:380:ASP:N	2.42	0.52
2:4:389:ASP:OD2	2:4:390:ARG:N	2.43	0.52
3:7:364:LYS:O	3:7:370:LYS:HD2	2.10	0.52
3:7:505:ILE:HG22	3:7:506:GLN:H	1.72	0.52
6:A:19:ILE:HD12	6:A:69:VAL:HG11	1.91	0.52
3:7:569:LYS:HG3	3:7:621:LEU:HA	1.92	0.52
11:2:184:PHE:HD2	11:2:247:VAL:HG21	1.74	0.52
11:2:269:ARG:HH12	11:2:387:LEU:HD11	1.75	0.52
2:4:509:LEU:HD23	2:4:617:ALA:CB	2.39	0.52
3:7:62:LEU:HA	3:7:65:ALA:HB3	1.91	0.52
4:6:523:ASP:HB2	4:6:524:LEU:HD12	1.92	0.52
5:5:444:PHE:HE2	5:5:483:ALA:HB1	1.75	0.52
6:A:366:ILE:HD12	6:A:369:ILE:HD11	1.92	0.52
9:M:131:HIS:HB3	9:M:132:LEU:HD12	1.92	0.52
11:2:466:MET:SD	11:2:481:ALA:HB2	2.50	0.52
11:2:518:LEU:HD22	11:2:570:LEU:HB3	1.91	0.52
1:3:406:PHE:H	1:3:446:ALA:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:592:ARG:NH2	3:7:530:ASP:OD2	2.38	0.52
2:4:755:VAL:HG22	2:4:756:GLU:O	2.09	0.52
3:7:382:ASP:CG	3:7:489:ASN:HB2	2.34	0.52
3:7:387:LYS:O	3:7:391:LEU:HD13	2.10	0.52
4:6:373:THR:HG22	11:2:670:LYS:HE3	1.92	0.52
4:6:482:ARG:CZ	11:2:531:THR:HG1	2.23	0.52
6:A:175:SER:O	6:A:179:ARG:NE	2.37	0.52
10:N:190:PRO:O	10:N:192:VAL:N	2.43	0.52
11:2:361:ILE:HG21	11:2:381:VAL:HG22	1.91	0.52
2:4:527:ASN:ND2	3:7:368:GLY:O	2.43	0.51
5:5:222:LEU:O	5:5:241:GLN:NE2	2.43	0.51
6:A:466:GLU:OE1	6:A:508:ASN:N	2.43	0.51
10:N:83:ASN:OD1	10:N:84:ASP:N	2.43	0.51
2:4:459:ASP:O	2:4:463:ARG:N	2.40	0.51
3:7:195:VAL:HG22	3:7:200:PHE:CE1	2.45	0.51
11:2:240:MET:HE2	11:2:240:MET:N	2.25	0.51
11:2:568:VAL:HG13	11:2:610:THR:HG22	1.92	0.51
1:3:338:LEU:HD22	1:3:480:MET:SD	2.50	0.51
2:4:331:CYS:O	2:4:332:THR:OG1	2.25	0.51
4:6:512:ILE:HG22	4:6:514:LEU:HG	1.93	0.51
6:A:480:ALA:HB2	6:A:503:ALA:HB2	1.92	0.51
7:H:129:TYR:HD1	10:N:109:LEU:HD11	1.75	0.51
9:M:23:VAL:O	9:M:54:LEU:N	2.43	0.51
9:M:74:PRO:O	9:M:77:TYR:N	2.44	0.51
2:4:582:ASN:N	2:4:585:THR:OG1	2.40	0.51
4:6:612:GLN:OE1	4:6:612:GLN:N	2.43	0.51
5:5:78:THR:HG23	5:5:79:LEU:CD2	2.40	0.51
5:5:86:GLN:HB3	5:5:89:GLU:OE1	2.10	0.51
5:5:384:LYS:HE2	5:5:485:ALA:O	2.10	0.51
6:A:550:PHE:CG	6:A:555:VAL:HG21	2.46	0.51
8:L:166:HIS:O	8:L:169:ARG:NE	2.43	0.51
9:M:161:VAL:HG12	9:M:165:SER:OG	2.10	0.51
2:4:519:SER:HG	13:4:901:ATP:PG	2.27	0.51
4:6:428:ASP:OD1	4:6:429:GLU:N	2.44	0.51
6:A:316:TRP:O	6:A:444:GLN:NE2	2.44	0.51
7:H:182:HIS:C	7:H:184:LEU:HD13	2.36	0.51
8:L:116:VAL:O	8:L:120:ILE:N	2.43	0.51
10:N:35:ALA:HB1	10:N:93:GLU:OE2	2.11	0.51
11:2:586:HIS:HE1	11:2:641:ARG:NE	2.02	0.51
3:7:380:MET:HE3	3:7:505:ILE:HD11	1.93	0.51
8:L:90:GLU:HG3	8:L:150:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:472:ILE:HD12	13:4:901:ATP:C2	2.46	0.51
4:6:180:SER:OG	4:6:183:LYS:HB2	2.11	0.51
7:H:12:ALA:CB	7:H:15:LEU:HD12	2.41	0.51
9:M:50:ARG:C	9:M:52:VAL:HG23	2.36	0.51
11:2:589:MET:HB3	11:2:641:ARG:HB3	1.92	0.51
1:3:630:SER:OG	1:3:631:VAL:N	2.44	0.51
1:3:280:LEU:O	1:3:284:LEU:HD23	2.11	0.51
1:3:284:LEU:HD23	1:3:284:LEU:H	1.76	0.51
1:3:321:GLU:OE2	1:3:322:LYS:N	2.43	0.51
2:4:581:MET:HE3	2:4:585:THR:HB	1.93	0.51
3:7:278:LEU:HD21	3:7:299:GLN:HG3	1.93	0.51
5:5:57:ASN:O	5:5:61:GLY:N	2.44	0.51
5:5:236:ILE:HD11	11:2:302:GLY:HA2	1.92	0.51
5:5:352:CYS:HA	5:5:625:ILE:HD11	1.92	0.51
6:A:292:VAL:HG21	6:A:306:SER:HA	1.92	0.51
6:A:452:VAL:HG11	6:A:488:VAL:CG2	2.40	0.51
7:H:98:GLU:HA	7:H:144:THR:HG21	1.93	0.51
10:N:61:ASP:OD1	10:N:62:MET:N	2.43	0.51
2:4:484:LEU:HD13	2:4:742:LEU:O	2.11	0.51
3:7:587:GLU:O	3:7:590:ARG:HG3	2.11	0.51
4:6:606:TRP:C	4:6:607:ARG:HE	2.18	0.51
5:5:195:GLU:O	5:5:197:ALA:N	2.41	0.51
8:L:15:ILE:HG12	8:L:46:LEU:HD21	1.93	0.51
11:2:528:ALA:O	11:2:529:VAL:HG23	2.11	0.51
2:4:411:VAL:HG22	3:7:201:THR:HA	1.93	0.50
2:4:519:SER:O	2:4:522:LEU:N	2.44	0.50
4:6:339:TYR:CD2	4:6:343:ILE:HD11	2.46	0.50
11:2:524:VAL:HG22	11:2:697:LEU:HD11	1.93	0.50
1:3:231:ARG:HD2	1:3:265:LEU:HD21	1.92	0.50
2:4:591:GLU:O	2:4:597:THR:O	2.28	0.50
11:2:248:ALA:HB3	11:2:266:ILE:HG21	1.94	0.50
11:2:489:SER:OG	11:2:491:ASN:OD1	2.30	0.50
11:2:776:LEU:HD13	11:2:794:THR:OG1	2.11	0.50
2:4:507:HIS:CD2	2:4:615:ILE:HG22	2.46	0.50
2:4:666:SER:HB3	3:7:582:VAL:HG21	1.93	0.50
2:4:709:GLN:OE1	2:4:709:GLN:N	2.44	0.50
3:7:573:ILE:O	3:7:573:ILE:HG12	2.09	0.50
5:5:42:ASN:OD1	8:L:114:ARG:NH2	2.44	0.50
5:5:536:VAL:HG13	11:2:495:LYS:HE2	1.93	0.50
7:H:95:LEU:HD13	7:H:99:PHE:HZ	1.75	0.50
7:H:193:VAL:HG23	7:H:194:ARG:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:94:VAL:CG1	8:L:151:LEU:HD21	2.41	0.50
9:M:139:ASP:OD2	9:M:144:LYS:NZ	2.41	0.50
9:M:145:ALA:N	9:M:146:GLU:OE1	2.43	0.50
11:2:310:ILE:HD13	11:2:327:SER:CB	2.42	0.50
4:6:615:SER:O	4:6:619:LEU:HD13	2.11	0.50
5:5:145:LYS:NZ	5:5:259:LEU:HD22	2.26	0.50
10:N:171:ARG:C	10:N:172:ILE:HD12	2.36	0.50
11:2:397:LEU:CD1	11:2:431:VAL:HG22	2.42	0.50
1:3:329:ARG:C	1:3:330:LEU:HD12	2.37	0.50
6:A:35:ILE:O	6:A:38:ALA:HB3	2.12	0.50
10:N:153:HIS:O	10:N:157:THR:HG21	2.11	0.50
5:5:70:GLU:HA	5:5:73:VAL:HG22	1.93	0.50
5:5:109:ARG:O	5:5:111:GLU:N	2.42	0.50
5:5:504:MET:SD	5:5:504:MET:N	2.85	0.50
12:X:34:DT:H2''	12:X:35:DT:H5'	1.93	0.50
2:4:517:SER:CB	13:4:901:ATP:H2'	2.41	0.50
3:7:382:ASP:OD1	3:7:489:ASN:HB2	2.12	0.50
4:6:387:VAL:HB	4:6:527:ILE:HD12	1.94	0.50
4:6:525:PHE:HB3	4:6:527:ILE:HD11	1.92	0.50
5:5:49:LYS:HG3	5:5:51:ARG:HD3	1.94	0.50
7:H:63:LEU:O	7:H:67:LEU:N	2.39	0.50
8:L:94:VAL:HG12	8:L:151:LEU:HD21	1.93	0.50
4:6:387:VAL:HG22	4:6:495:ALA:HB3	1.94	0.50
6:A:58:LEU:HD22	6:A:86:LEU:HD11	1.94	0.50
6:A:246:LEU:HD23	6:A:250:GLU:HA	1.94	0.50
3:7:271:ILE:HA	3:7:305:CYS:SG	2.52	0.50
5:5:520:ILE:O	5:5:525:ARG:NH2	2.45	0.50
6:A:424:LEU:HD12	6:A:425:LEU:N	2.26	0.50
10:N:93:GLU:O	10:N:96:ARG:N	2.45	0.50
11:2:641:ARG:N	11:2:641:ARG:HD3	2.26	0.50
2:4:447:ARG:HD3	2:4:450:LEU:HD13	1.94	0.49
13:4:901:ATP:O2A	13:4:901:ATP:H3'	2.12	0.49
3:7:497:PRO:HB3	3:7:644:LEU:HD11	1.93	0.49
4:6:373:THR:HG22	11:2:670:LYS:NZ	2.26	0.49
4:6:387:VAL:C	4:6:527:ILE:HG23	2.36	0.49
4:6:411:THR:O	4:6:451:ILE:HD13	2.12	0.49
11:2:370:ILE:HG22	11:2:372:ALA:N	2.27	0.49
1:3:346:LYS:NZ	13:3:901:ATP:O3G	2.42	0.49
2:4:583:ASP:HB2	4:6:456:LYS:NZ	2.27	0.49
3:7:152:VAL:HG21	3:7:163:VAL:HG11	1.92	0.49
4:6:394:LYS:NZ	4:6:394:LYS:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:346:ILE:N	5:5:346:ILE:HD12	2.27	0.49
7:H:93:LYS:NZ	10:N:113:GLU:OE1	2.46	0.49
11:2:210:GLN:HB3	11:2:212:MET:HE2	1.94	0.49
11:2:567:GLY:O	11:2:610:THR:N	2.45	0.49
1:3:149:ARG:NH1	3:7:5:ASP:OD1	2.46	0.49
1:3:413:ASP:O	1:3:417:ILE:N	2.41	0.49
3:7:402:GLN:CG	3:7:433:ALA:HB1	2.41	0.49
3:7:494:ARG:O	3:7:494:ARG:HG3	2.12	0.49
4:6:444:ALA:HB3	4:6:489:THR:HG22	1.93	0.49
5:5:104:GLU:HG2	5:5:105:ILE:HG13	1.94	0.49
6:A:333:LEU:CD2	6:A:338:ALA:HB2	2.42	0.49
2:4:543:VAL:HG11	12:X:34:DT:H5'	1.95	0.49
2:4:661:ASP:HB3	3:7:585:TYR:HE2	1.77	0.49
2:4:200:LEU:HD21	2:4:248:PHE:HA	1.95	0.49
2:4:509:LEU:HD13	2:4:646:PHE:HD2	1.78	0.49
2:4:646:PHE:HE1	2:4:734:ARG:HH11	1.59	0.49
6:A:313:LEU:HB2	6:A:315:LEU:HD21	1.93	0.49
11:2:303:VAL:HG22	11:2:359:GLN:HB2	1.94	0.49
12:X:32:DT:H2''	12:X:33:DT:C6	2.48	0.49
1:3:563:ARG:HB3	1:3:566:ILE:HD12	1.93	0.49
4:6:427:ARG:HG3	4:6:427:ARG:O	2.12	0.49
8:L:136:ILE:HG22	9:M:126:ARG:NH2	2.28	0.49
10:N:134:SER:O	10:N:138:THR:HG23	2.13	0.49
1:3:7:GLN:OE1	1:3:7:GLN:N	2.45	0.49
1:3:345:ALA:HA	13:3:901:ATP:O2A	2.13	0.49
2:4:307:PHE:CE1	2:4:342:LEU:HD12	2.48	0.49
3:7:60:GLU:O	3:7:63:ALA:HB3	2.13	0.49
4:6:321:MET:HA	4:6:324:ALA:HB2	1.95	0.49
5:5:132:ILE:HD12	5:5:226:GLU:HB3	1.94	0.49
5:5:282:VAL:HG13	5:5:283:VAL:HG23	1.94	0.49
6:A:446:SER:OG	6:A:447:LEU:N	2.46	0.49
6:A:476:LEU:HD22	6:A:505:CYS:HB2	1.94	0.49
8:L:127:LYS:O	8:L:130:THR:N	2.44	0.49
10:N:34:THR:HG22	10:N:36:GLN:H	1.78	0.49
11:2:307:LEU:O	11:2:356:ARG:NH2	2.43	0.49
1:3:464:ILE:HB	1:3:466:LEU:HD22	1.94	0.49
1:3:644:GLN:O	1:3:648:PHE:N	2.46	0.49
2:4:548:TYR:HD1	2:4:550:THR:HG1	1.58	0.49
3:7:365:ARG:O	3:7:365:ARG:HD3	2.12	0.49
1:3:146:PRO:HB2	1:3:180:LEU:HD13	1.95	0.49
5:5:163:MET:SD	5:5:172:THR:OG1	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:30:DT:H2''	12:X:31:DT:OP1	2.12	0.49
6:A:443:VAL:HG13	6:A:483:LEU:CG	2.42	0.49
1:3:313:LEU:HA	1:3:316:LEU:HD12	1.94	0.48
1:3:430:LYS:HB2	3:7:410:SER:CB	2.42	0.48
3:7:340:LEU:HA	3:7:559:MET:HE1	1.94	0.48
3:7:419:MET:HB2	12:X:36:DT:OP1	2.13	0.48
3:7:569:LYS:HA	3:7:569:LYS:HD3	1.51	0.48
4:6:341:ASN:O	4:6:345:SER:OG	2.23	0.48
6:A:244:LEU:HD12	6:A:251:SER:HB2	1.95	0.48
8:L:94:VAL:HB	8:L:151:LEU:HD21	1.95	0.48
9:M:24:GLU:N	9:M:24:GLU:OE1	2.45	0.48
11:2:560:ALA:HB1	11:2:563:LEU:HD23	1.94	0.48
1:3:504:ASN:O	1:3:543:ALA:HB2	2.14	0.48
4:6:411:THR:HG23	4:6:451:ILE:CD1	2.43	0.48
5:5:271:LYS:HD2	5:5:283:VAL:HG12	1.95	0.48
5:5:460:GLU:OE2	5:5:510:ARG:HG3	2.13	0.48
6:A:564:THR:O	6:A:568:ASP:N	2.40	0.48
11:2:192:VAL:HG13	11:2:198:TYR:HB2	1.95	0.48
11:2:357:ASN:OD1	11:2:385:ALA:HB1	2.13	0.48
11:2:502:ILE:HB	11:2:610:THR:HG23	1.95	0.48
3:7:241:SER:HA	3:7:244:VAL:CG2	2.44	0.48
5:5:152:ALA:HA	5:5:254:PRO:HG2	1.96	0.48
6:A:240:ILE:CG2	6:A:244:LEU:HD22	2.43	0.48
6:A:483:LEU:O	6:A:486:GLY:N	2.45	0.48
7:H:74:LEU:O	7:H:77:ASN:N	2.46	0.48
11:2:439:GLN:HE21	11:2:439:GLN:HA	1.77	0.48
1:3:591:LEU:HD23	1:3:607:ILE:CD1	2.43	0.48
2:4:373:VAL:HG13	2:4:374:LEU:N	2.26	0.48
2:4:522:LEU:HD11	2:4:616:LEU:CB	2.44	0.48
2:4:573:CYS:SG	2:4:575:ILE:HG22	2.53	0.48
6:A:23:VAL:HG11	6:A:75:VAL:HB	1.95	0.48
6:A:219:PHE:O	6:A:223:TRP:N	2.47	0.48
7:H:129:TYR:CD1	10:N:109:LEU:HD21	2.48	0.48
11:2:527:ARG:HB3	11:2:564:ALA:HA	1.95	0.48
3:7:449:LYS:HE2	3:7:489:ASN:OD1	2.14	0.48
4:6:425:VAL:HG22	4:6:426:VAL:H	1.78	0.48
6:A:33:SER:O	6:A:36:LEU:N	2.38	0.48
7:H:126:LEU:O	7:H:129:TYR:HB3	2.13	0.48
1:3:131:VAL:HG11	1:3:224:ASP:OD1	2.14	0.48
1:3:433:ILE:HG23	1:3:434:HIS:N	2.29	0.48
2:4:666:SER:N	3:7:582:VAL:HG11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:901:ATP:C4'	3:7:603:ALA:HB3	2.44	0.48
5:5:63:TYR:HA	5:5:119:ILE:HG22	1.94	0.48
5:5:362:LEU:HB3	5:5:363:PRO:HD2	1.96	0.48
11:2:501:ASP:O	11:2:749:ARG:NE	2.47	0.48
1:3:355:ASN:OD1	1:3:356:THR:HG23	2.14	0.48
1:3:600:ASP:OD1	1:3:603:ARG:NH1	2.47	0.48
2:4:420:ASP:OD1	2:4:421:VAL:N	2.47	0.48
2:4:432:LEU:HB2	2:4:488:GLY:HA2	1.96	0.48
3:7:238:GLN:HB2	3:7:252:SER:HB2	1.94	0.48
3:7:383:PRO:HD2	3:7:385:VAL:HB	1.95	0.48
3:7:591:GLU:O	3:7:591:GLU:HG2	2.13	0.48
5:5:47:PHE:CZ	9:M:171:LEU:HD22	2.49	0.48
8:L:160:LEU:HD12	8:L:161:PRO:CD	2.44	0.48
11:2:370:ILE:HG22	11:2:372:ALA:H	1.77	0.48
11:2:718:ASP:O	11:2:721:ALA:HB3	2.14	0.48
2:4:177:ASP:HB2	2:4:195:LEU:HD21	1.95	0.48
3:7:365:ARG:NH2	3:7:368:GLY:HA2	2.28	0.48
3:7:556:MET:HE1	3:7:560:ARG:NH2	2.28	0.48
4:6:329:ILE:HD12	4:6:566:ARG:CZ	2.43	0.48
4:6:347:PHE:HB3	4:6:350:ILE:HD13	1.96	0.48
8:L:135:PHE:O	9:M:130:ARG:NH1	2.47	0.48
2:4:319:GLU:OE1	2:4:319:GLU:N	2.42	0.48
3:7:324:LEU:HD23	3:7:325:GLU:H	1.78	0.48
4:6:382:ILE:CG2	4:6:383:ASN:N	2.77	0.48
5:5:538:LEU:HD23	11:2:711:LYS:HE3	1.95	0.48
11:2:300:THR:OG1	11:2:301:THR:N	2.47	0.48
1:3:206:PRO:HG2	1:3:209:GLN:HG2	1.96	0.48
1:3:250:SER:OG	1:3:251:GLY:N	2.45	0.48
2:4:723:GLY:HA3	2:4:730:SER:OG	2.14	0.48
3:7:585:TYR:CZ	3:7:606:LEU:HD23	2.49	0.48
5:5:63:TYR:CA	5:5:119:ILE:HG22	2.44	0.48
5:5:72:LEU:HD22	5:5:80:ALA:HB2	1.95	0.48
5:5:120:GLN:OE1	5:5:246:ARG:NE	2.47	0.48
5:5:150:ILE:HG23	5:5:255:GLY:H	1.78	0.48
5:5:165:ILE:HG23	5:5:208:PHE:O	2.14	0.48
5:5:240:LEU:CD1	5:5:242:LEU:HD21	2.44	0.48
5:5:532:HIS:O	5:5:532:HIS:ND1	2.43	0.48
9:M:50:ARG:O	9:M:52:VAL:HG23	2.14	0.48
10:N:146:SER:O	10:N:150:GLU:HG2	2.14	0.48
11:2:337:CYS:O	11:2:339:GLU:N	2.47	0.48
11:2:698:ARG:O	11:2:702:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:529:ASN:O	3:7:532:ARG:HB2	2.14	0.47
4:6:444:ALA:HB1	4:6:447:GLY:CA	2.44	0.47
6:A:58:LEU:CD2	6:A:86:LEU:HD21	2.40	0.47
6:A:72:VAL:O	6:A:96:PHE:N	2.47	0.47
11:2:578:ASN:C	11:2:582:ARG:HE	2.22	0.47
1:3:219:ASP:OD1	1:3:220:ASP:N	2.47	0.47
2:4:301:GLU:O	2:4:350:THR:N	2.47	0.47
3:7:359:VAL:HG12	3:7:360:GLY:O	2.14	0.47
3:7:587:GLU:HA	3:7:590:ARG:CG	2.44	0.47
3:7:593:ARG:HD2	3:7:593:ARG:O	2.14	0.47
4:6:78:TYR:CE1	4:6:125:ILE:HD11	2.49	0.47
4:6:427:ARG:NH2	4:6:479:ALA:HB3	2.28	0.47
4:6:444:ALA:HB3	4:6:489:THR:CG2	2.43	0.47
4:6:521:ARG:HH11	11:2:510:PRO:CB	2.27	0.47
5:5:442:ASP:OD2	5:5:484:ALA:CB	2.61	0.47
5:5:538:LEU:HD11	11:2:712:LEU:O	2.14	0.47
6:A:135:TYR:CZ	6:A:159:ALA:HB2	2.49	0.47
6:A:231:ASP:OD1	6:A:231:ASP:N	2.45	0.47
4:6:416:SER:OG	4:6:417:SER:N	2.47	0.47
5:5:418:ASP:OD1	5:5:418:ASP:N	2.47	0.47
5:5:549:ALA:HB1	5:5:552:GLU:OE1	2.13	0.47
5:5:622:LEU:CD2	5:5:636:VAL:HG22	2.43	0.47
6:A:504:SER:HA	6:A:516:LEU:HD12	1.96	0.47
8:L:151:LEU:O	8:L:154:HIS:NE2	2.47	0.47
9:M:20:GLN:O	9:M:22:LYS:HD3	2.13	0.47
9:M:34:MET:CB	9:M:37:LEU:HD13	2.42	0.47
9:M:95:GLY:O	9:M:149:LEU:N	2.47	0.47
11:2:178:THR:O	11:2:182:ASN:OD1	2.33	0.47
4:6:537:ASP:N	4:6:537:ASP:OD1	2.45	0.47
5:5:36:GLU:O	5:5:40:THR:N	2.47	0.47
6:A:502:ILE:HG23	6:A:516:LEU:HD11	1.96	0.47
11:2:404:THR:OG1	11:2:423:VAL:HG23	2.14	0.47
1:3:328:THR:CG2	3:7:396:ARG:HE	2.27	0.47
1:3:484:ILE:CG2	5:5:608:THR:HG22	2.41	0.47
2:4:503:ARG:O	2:4:741:ARG:NH2	2.43	0.47
3:7:482:VAL:HG22	3:7:483:SER:O	2.13	0.47
3:7:524:LYS:HB3	3:7:525:PRO:CD	2.44	0.47
4:6:91:TYR:O	4:6:95:ARG:NH2	2.47	0.47
4:6:521:ARG:HH11	11:2:510:PRO:HB2	1.79	0.47
5:5:150:ILE:CG2	5:5:254:PRO:HA	2.45	0.47
6:A:201:MET:O	6:A:205:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:333:LEU:HD21	6:A:338:ALA:HB2	1.96	0.47
7:H:12:ALA:H	7:H:76:ARG:NH2	2.12	0.47
10:N:91:SER:O	10:N:94:LEU:N	2.48	0.47
11:2:435:LYS:HE3	11:2:435:LYS:HB2	1.67	0.47
1:3:212:ARG:NH1	5:5:156:ILE:HD12	2.29	0.47
2:4:519:SER:OG	13:4:901:ATP:PG	2.71	0.47
2:4:609:LEU:H	2:4:609:LEU:CD2	2.27	0.47
3:7:555:ASP:O	3:7:559:MET:HG3	2.15	0.47
4:6:219:GLU:N	4:6:219:GLU:OE2	2.47	0.47
8:L:133:ASP:OD2	9:M:133:LEU:HD12	2.15	0.47
9:M:150:ASP:OD1	9:M:151:ASN:N	2.47	0.47
1:3:81:ALA:HA	1:3:84:VAL:HG22	1.97	0.47
2:4:417:THR:HG21	3:7:174:LYS:HD3	1.97	0.47
2:4:548:TYR:OH	12:X:33:DT:O2	2.17	0.47
3:7:537:ILE:O	3:7:540:VAL:HG12	2.14	0.47
3:7:588:LEU:CD2	3:7:589:ARG:HD2	2.45	0.47
4:6:417:SER:OG	4:6:419:ALA:N	2.43	0.47
5:5:25:ILE:HD12	5:5:26:ASN:N	2.30	0.47
6:A:382:SER:O	6:A:383:ARG:NH2	2.46	0.47
9:M:19:THR:OG1	9:M:57:TRP:N	2.47	0.47
10:N:105:LEU:O	10:N:109:LEU:HD13	2.15	0.47
11:2:243:ILE:O	11:2:247:VAL:HG23	2.14	0.47
12:X:33:DT:C6	12:X:34:DT:H72	2.50	0.47
13:3:901:ATP:O1A	5:5:610:ARG:NH2	2.48	0.47
3:7:515:PHE:HB2	3:7:518:LEU:CD1	2.44	0.47
5:5:329:TYR:HA	5:5:351:THR:HG21	1.96	0.47
6:A:35:ILE:HD12	6:A:218:VAL:HG11	1.97	0.47
6:A:140:GLU:OE1	6:A:140:GLU:N	2.47	0.47
6:A:539:ALA:CB	6:A:546:LEU:HD22	2.44	0.47
7:H:29:PHE:HB2	7:H:107:ILE:HD11	1.97	0.47
7:H:167:GLU:HG3	7:H:174:ILE:HD11	1.97	0.47
10:N:105:LEU:HB3	10:N:109:LEU:HD13	1.96	0.47
11:2:577:MET:O	11:2:582:ARG:NH2	2.47	0.47
1:3:642:LEU:HD12	1:3:643:VAL:HG23	1.97	0.47
2:4:430:LYS:NZ	2:4:437:GLU:OE1	2.48	0.47
2:4:533:GLN:C	2:4:533:GLN:HE21	2.23	0.47
3:7:11:GLU:N	3:7:11:GLU:OE1	2.47	0.47
3:7:209:ASP:HA	3:7:212:ARG:HB2	1.95	0.47
3:7:573:ILE:O	3:7:574:PRO:C	2.58	0.47
7:H:77:ASN:O	7:H:81:LEU:HD13	2.15	0.47
7:H:78:LYS:O	7:H:82:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:498:VAL:O	11:2:499:ARG:HG3	2.14	0.47
1:3:11:ASP:OD1	1:3:14:ARG:NH2	2.42	0.47
2:4:461:TYR:HA	2:4:483:LEU:HD13	1.97	0.47
3:7:573:ILE:C	3:7:574:PRO:O	2.58	0.47
5:5:444:PHE:O	5:5:452:ARG:NH1	2.48	0.47
7:H:159:CYS:O	7:H:199:HIS:NE2	2.48	0.47
8:L:80:ARG:O	8:L:82:LYS:N	2.42	0.47
1:3:232:VAL:HA	1:3:265:LEU:HD22	1.97	0.46
1:3:366:ARG:O	5:5:453:VAL:HG21	2.14	0.46
3:7:256:MET:O	3:7:299:GLN:HA	2.15	0.46
3:7:560:ARG:HA	3:7:563:ILE:HB	1.98	0.46
4:6:393:ALA:CA	13:6:901:ATP:H5'1	2.44	0.46
5:5:72:LEU:HD21	5:5:80:ALA:N	2.29	0.46
6:A:24:ASN:OD1	6:A:25:TYR:N	2.47	0.46
1:3:118:LEU:HD22	1:3:238:TYR:CZ	2.50	0.46
2:4:583:ASP:OD2	2:4:584:SER:N	2.48	0.46
3:7:343:GLU:HB2	3:7:344:ILE:HD12	1.97	0.46
3:7:405:THR:HG23	3:7:407:ARG:H	1.80	0.46
9:M:19:THR:HG1	9:M:56:LEU:HB3	1.80	0.46
11:2:184:PHE:CD2	11:2:247:VAL:HG21	2.50	0.46
11:2:503:ASN:O	11:2:644:VAL:N	2.41	0.46
11:2:740:THR:HG23	11:2:743:HIS:H	1.80	0.46
2:4:387:PRO:HG2	2:4:567:LEU:HD13	1.98	0.46
3:7:415:THR:OG1	3:7:416:ALA:N	2.47	0.46
3:7:441:VAL:HG23	3:7:483:SER:O	2.15	0.46
4:6:80:ILE:O	4:6:83:PHE:N	2.44	0.46
6:A:303:MET:O	6:A:315:LEU:HD13	2.15	0.46
11:2:449:ILE:HD13	11:2:692:ILE:HG23	1.96	0.46
2:4:393:VAL:HG12	2:4:394:THR:O	2.15	0.46
3:7:200:PHE:C	3:7:201:THR:HG22	2.41	0.46
4:6:329:ILE:HD11	4:6:567:TYR:CB	2.45	0.46
5:5:606:PRO:HD2	5:5:647:THR:HG23	1.98	0.46
6:A:504:SER:CA	6:A:516:LEU:HD12	2.45	0.46
1:3:143:HIS:O	1:3:152:MET:N	2.47	0.46
3:7:380:MET:O	3:7:520:LEU:HD12	2.15	0.46
3:7:415:THR:HG23	3:7:416:ALA:H	1.81	0.46
5:5:509:SER:HB2	5:5:510:ARG:HD2	1.97	0.46
6:A:133:ILE:HD11	6:A:200:ILE:HD13	1.96	0.46
1:3:308:VAL:O	1:3:311:ALA:HB3	2.16	0.46
2:4:354:LEU:HD12	2:4:355:VAL:H	1.80	0.46
3:7:341:ALA:HA	3:7:343:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:621:LEU:O	3:7:622:SER:O	2.33	0.46
5:5:159:LYS:HD2	5:5:219:PHE:CE2	2.50	0.46
5:5:369:ARG:CZ	5:5:369:ARG:HB3	2.44	0.46
6:A:418:SER:OG	6:A:420:GLN:N	2.48	0.46
11:2:745:GLU:O	11:2:748:ILE:HG22	2.16	0.46
3:7:416:ALA:HB2	3:7:431:GLY:HA2	1.98	0.46
3:7:544:SER:HB3	3:7:545:LYS:HD2	1.97	0.46
4:6:71:THR:HG22	4:6:75:GLU:OE2	2.16	0.46
5:5:462:GLN:NE2	5:5:477:SER:O	2.49	0.46
6:A:78:GLY:HA3	6:A:104:LEU:HD21	1.97	0.46
11:2:249:LYS:CE	11:2:266:ILE:HG22	2.42	0.46
11:2:313:ASP:OD1	11:2:313:ASP:N	2.47	0.46
11:2:337:CYS:H	11:2:341:GLN:HA	1.81	0.46
1:3:137:LYS:CG	3:7:292:LEU:HB2	2.46	0.46
1:3:171:TYR:CD2	1:3:183:THR:HG22	2.51	0.46
4:6:516:ALA:HB3	4:6:517:PRO:HD3	1.98	0.46
5:5:567:THR:O	5:5:567:THR:HG22	2.16	0.46
5:5:637:ASN:ND2	5:5:640:LEU:HD22	2.31	0.46
9:M:56:LEU:HD12	9:M:56:LEU:O	2.15	0.46
3:7:356:LEU:O	3:7:359:VAL:HB	2.16	0.46
5:5:34:TYR:OH	5:5:79:LEU:HD13	2.16	0.46
5:5:78:THR:HG23	5:5:79:LEU:HD23	1.98	0.46
5:5:521:HIS:O	5:5:521:HIS:ND1	2.49	0.46
5:5:612:LEU:HA	5:5:615:VAL:HG12	1.97	0.46
11:2:411:LEU:O	11:2:411:LEU:HG	2.15	0.46
1:3:370:GLY:O	1:3:392:ALA:N	2.49	0.46
2:4:292:VAL:HG11	2:4:387:PRO:HA	1.98	0.46
3:7:66:VAL:HG22	3:7:73:TYR:CE2	2.51	0.46
3:7:630:VAL:O	3:7:633:ALA:HB3	2.15	0.46
4:6:84:LEU:O	4:6:88:VAL:HG23	2.16	0.46
6:A:27:ILE:HD12	6:A:242:GLU:HG3	1.96	0.46
11:2:184:PHE:HA	11:2:187:PHE:CE1	2.51	0.46
11:2:219:TYR:HB3	11:2:274:PRO:HD3	1.97	0.46
11:2:458:ILE:HB	11:2:462:VAL:HG23	1.97	0.45
11:2:737:LEU:O	11:2:737:LEU:HD23	2.16	0.45
1:3:133:LEU:HD23	1:3:133:LEU:O	2.16	0.45
2:4:376:TYR:O	2:4:421:VAL:HG11	2.16	0.45
3:7:151:GLU:O	3:7:152:VAL:C	2.58	0.45
5:5:335:SER:HB3	5:5:552:GLU:HB3	1.98	0.45
6:A:431:GLN:O	6:A:435:LEU:HD23	2.17	0.45
6:A:458:PHE:CA	6:A:499:LEU:HD13	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:112:ILE:CG2	10:N:119:ILE:HD13	2.46	0.45
11:2:287:LEU:HD22	11:2:403:TYR:CD2	2.51	0.45
11:2:405:ASN:C	11:2:423:VAL:HG22	2.41	0.45
1:3:68:ASP:OD1	1:3:68:ASP:N	2.48	0.45
13:4:901:ATP:O1A	3:7:604:ARG:CD	2.64	0.45
5:5:331:ARG:HB3	5:5:332:LEU:HD12	1.97	0.45
11:2:383:LEU:HD23	11:2:383:LEU:N	2.31	0.45
1:3:256:VAL:HG13	1:3:258:LEU:HD21	1.97	0.45
2:4:342:LEU:O	2:4:343:ILE:HG23	2.16	0.45
2:4:425:ARG:H	2:4:425:ARG:CD	2.30	0.45
4:6:417:SER:HG	4:6:419:ALA:H	1.64	0.45
5:5:72:LEU:HD21	5:5:79:LEU:HB2	1.99	0.45
1:3:127:ILE:N	1:3:199:GLN:O	2.46	0.45
1:3:505:PRO:HD3	1:3:540:LYS:HG3	1.97	0.45
2:4:738:SER:HA	2:4:741:ARG:HD2	1.99	0.45
3:7:38:VAL:O	3:7:41:ALA:HB3	2.16	0.45
5:5:67:ILE:HG22	5:5:68:GLU:N	2.32	0.45
7:H:182:HIS:O	7:H:184:LEU:HD13	2.16	0.45
8:L:47:TRP:CD1	8:L:48:MET:HE1	2.51	0.45
9:M:102:TYR:HB2	9:M:103:GLU:OE1	2.17	0.45
10:N:219:LEU:HB3	10:N:225:ALA:HB3	1.99	0.45
2:4:601:ALA:O	2:4:602:LYS:HG2	2.17	0.45
2:4:703:THR:O	2:4:755:VAL:N	2.50	0.45
4:6:421:LEU:HD11	4:6:474:ILE:HD11	1.99	0.45
5:5:637:ASN:CG	5:5:640:LEU:HD13	2.41	0.45
6:A:289:LEU:HD22	6:A:369:ILE:HG22	1.98	0.45
8:L:6:ILE:O	8:L:10:GLY:N	2.37	0.45
10:N:194:VAL:HG21	10:N:219:LEU:HD21	1.99	0.45
12:X:31:DT:H6	12:X:31:DT:H2'	1.47	0.45
1:3:591:LEU:HD23	1:3:607:ILE:HD12	1.98	0.45
1:3:611:THR:O	1:3:614:THR:N	2.49	0.45
3:7:305:CYS:H	3:7:309:ASN:ND2	2.15	0.45
4:6:382:ILE:HG22	4:6:383:ASN:N	2.32	0.45
6:A:145:ASP:OD1	6:A:146:GLU:N	2.48	0.45
6:A:284:THR:OG1	6:A:286:GLU:OE2	2.26	0.45
1:3:217:VAL:HB	1:3:258:LEU:HD22	1.99	0.45
3:7:312:ILE:HD12	3:7:312:ILE:HG23	1.52	0.45
5:5:452:ARG:O	5:5:455:ILE:HG12	2.16	0.45
5:5:460:GLU:OE2	5:5:510:ARG:CG	2.65	0.45
5:5:565:CYS:C	5:5:567:THR:H	2.24	0.45
6:A:291:LEU:HD23	6:A:292:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:432:ALA:O	6:A:436:HIS:ND1	2.49	0.45
11:2:222:LEU:HD21	11:2:229:LEU:CB	2.47	0.45
2:4:645:ARG:HD3	2:4:646:PHE:CZ	2.52	0.45
5:5:530:ALA:HB2	11:2:721:ALA:HB2	1.99	0.45
5:5:540:SER:HA	11:2:493:GLY:HA2	1.99	0.45
6:A:233:LEU:O	6:A:236:ALA:HB3	2.16	0.45
8:L:93:MET:HB2	8:L:151:LEU:HD22	1.99	0.45
9:M:27:VAL:HG13	9:M:69:PHE:CE1	2.52	0.45
10:N:107:CYS:O	10:N:110:GLN:N	2.50	0.45
11:2:594:ILE:HD11	11:2:605:LEU:CB	2.46	0.45
1:3:139:VAL:CG2	1:3:189:VAL:HG23	2.47	0.45
2:4:364:MET:HE3	3:7:479:ASN:OD1	2.17	0.45
2:4:374:LEU:N	2:4:374:LEU:HD23	2.32	0.45
2:4:561:GLN:O	4:6:214:ILE:HD11	2.17	0.45
13:4:901:ATP:PA	3:7:604:ARG:HD2	2.57	0.45
4:6:296:GLN:O	4:6:298:THR:HG23	2.17	0.45
4:6:582:ALA:CB	4:6:634:GLU:HB3	2.47	0.45
7:H:78:LYS:O	7:H:81:LEU:N	2.50	0.45
7:H:79:ARG:NH1	7:H:82:LEU:HD22	2.32	0.45
8:L:16:SER:HA	8:L:43:PHE:HA	1.99	0.45
8:L:167:ILE:HG22	8:L:171:GLN:HG2	1.99	0.45
11:2:313:ASP:OD2	11:2:321:LEU:HD22	2.17	0.45
2:4:508:LEU:HD12	2:4:508:LEU:O	2.18	0.44
2:4:655:PRO:O	2:4:657:ASP:N	2.49	0.44
3:7:435:VAL:CG2	3:7:478:LEU:HD22	2.47	0.44
3:7:465:GLN:N	3:7:480:ALA:O	2.42	0.44
4:6:244:VAL:HG12	4:6:245:VAL:N	2.33	0.44
4:6:338:LEU:HD12	4:6:342:LEU:HD12	1.99	0.44
5:5:208:PHE:O	5:5:210:MET:HE2	2.17	0.44
6:A:103:PRO:HD3	6:A:209:TYR:O	2.17	0.44
6:A:307:ARG:O	6:A:311:CYS:N	2.50	0.44
10:N:115:PHE:CD2	10:N:119:ILE:HD12	2.52	0.44
10:N:150:GLU:O	10:N:153:HIS:CB	2.65	0.44
11:2:462:VAL:HG22	11:2:692:ILE:CD1	2.47	0.44
2:4:459:ASP:N	2:4:459:ASP:OD1	2.49	0.44
3:7:171:THR:HG22	3:7:172:GLU:H	1.82	0.44
5:5:161:THR:HG22	5:5:177:LEU:CD2	2.48	0.44
6:A:520:VAL:HG13	6:A:529:ASN:OD1	2.18	0.44
6:A:530:PHE:O	6:A:534:ALA:N	2.43	0.44
10:N:38:VAL:CG1	10:N:66:MET:HE1	2.47	0.44
11:2:331:GLU:OE2	11:2:331:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:359:GLN:O	11:2:383:LEU:HD21	2.17	0.44
11:2:476:ILE:HG22	11:2:646:CYS:SG	2.56	0.44
1:3:433:ILE:HG22	1:3:435:ALA:HB2	1.98	0.44
1:3:543:ALA:C	1:3:544:LEU:HD12	2.42	0.44
2:4:287:SER:HA	2:4:394:THR:HA	2.00	0.44
2:4:759:ASP:OD1	2:4:760:VAL:HG23	2.16	0.44
3:7:261:VAL:O	3:7:261:VAL:CG1	2.65	0.44
3:7:571:PRO:HG3	3:7:614:THR:O	2.17	0.44
8:L:5:ILE:HD13	10:N:50:MET:HE1	1.98	0.44
10:N:189:VAL:HB	10:N:205:ALA:HB2	1.99	0.44
11:2:216:VAL:HG22	11:2:269:ARG:HB2	2.00	0.44
11:2:439:GLN:HE21	11:2:439:GLN:CA	2.28	0.44
1:3:115:SER:O	1:3:118:LEU:HD21	2.17	0.44
1:3:118:LEU:HD22	1:3:238:TYR:CE1	2.53	0.44
3:7:193:GLN:HG2	3:7:200:PHE:HZ	1.83	0.44
4:6:454:PHE:HZ	4:6:491:ILE:HD11	1.81	0.44
7:H:83:ALA:HB1	7:H:87:GLU:HB2	1.98	0.44
8:L:127:LYS:O	8:L:130:THR:HB	2.17	0.44
2:4:400:THR:HG22	2:4:401:PRO:O	2.17	0.44
2:4:483:LEU:CG	2:4:749:VAL:HG21	2.48	0.44
2:4:499:ARG:O	2:4:501:ASN:N	2.49	0.44
3:7:370:LYS:C	3:7:371:ILE:HD12	2.43	0.44
5:5:34:TYR:CZ	5:5:79:LEU:HD13	2.53	0.44
6:A:382:SER:OG	6:A:383:ARG:N	2.50	0.44
6:A:566:PHE:O	6:A:569:SER:OG	2.33	0.44
7:H:45:PHE:HA	7:H:48:ASN:HD22	1.81	0.44
1:3:320:VAL:HB	1:3:620:THR:HG21	2.00	0.44
2:4:622:ALA:HB2	2:4:637:GLN:CG	2.48	0.44
4:6:336:ARG:H	4:6:336:ARG:HD3	1.82	0.44
5:5:34:TYR:CE1	5:5:79:LEU:HD13	2.52	0.44
6:A:70:LYS:O	6:A:94:THR:N	2.51	0.44
6:A:458:PHE:HA	6:A:499:LEU:HD13	2.00	0.44
6:A:548:GLN:NE2	6:A:555:VAL:O	2.47	0.44
9:M:149:LEU:HD23	9:M:149:LEU:H	1.83	0.44
10:N:198:ASP:HB3	10:N:215:LEU:HD22	2.00	0.44
11:2:563:LEU:O	11:2:564:ALA:HB3	2.18	0.44
1:3:9:ILE:HA	1:3:12:ILE:HD12	1.99	0.44
3:7:369:MET:HG3	3:7:370:LYS:O	2.17	0.44
3:7:535:LYS:HA	3:7:538:THR:HG1	1.83	0.44
4:6:477:ALA:HB1	11:2:537:SER:O	2.17	0.44
5:5:374:VAL:O	5:5:375:LEU:HD22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:254:TYR:OH	6:A:371:TYR:CD1	2.61	0.44
6:A:260:GLN:O	6:A:263:SER:N	2.51	0.44
10:N:107:CYS:SG	10:N:108:ARG:N	2.90	0.44
11:2:219:TYR:HB3	11:2:274:PRO:CD	2.48	0.44
11:2:546:ARG:NE	12:X:29:DT:OP1	2.51	0.44
11:2:639:LEU:HD12	11:2:642:PHE:CD2	2.53	0.44
2:4:622:ALA:HB2	2:4:637:GLN:HG3	1.99	0.44
2:4:708:ALA:CB	2:4:757:LEU:HD12	2.48	0.44
6:A:288:ASP:N	6:A:371:TYR:O	2.46	0.44
11:2:322:GLY:O	11:2:323:PRO:C	2.56	0.44
11:2:561:LEU:HD21	11:2:607:ALA:HB2	2.00	0.44
1:3:388:LEU:H	1:3:388:LEU:HD23	1.82	0.44
2:4:373:VAL:HG22	2:4:374:LEU:H	1.83	0.44
2:4:513:ASP:HB2	2:4:514:PRO:CD	2.48	0.44
2:4:746:HIS:HA	2:4:749:VAL:HG12	2.00	0.44
3:7:587:GLU:HA	3:7:590:ARG:HG2	2.00	0.44
4:6:425:VAL:HA	4:6:436:ILE:HG12	2.00	0.44
4:6:623:MET:O	4:6:627:GLU:N	2.50	0.44
6:A:424:LEU:HD12	6:A:425:LEU:CA	2.48	0.44
8:L:5:ILE:CD1	10:N:50:MET:HE1	2.48	0.44
11:2:233:LEU:HB2	11:2:290:LEU:CD2	2.45	0.44
11:2:417:PHE:HE2	11:2:419:VAL:HG22	1.83	0.44
1:3:321:GLU:HG3	1:3:323:ILE:HD11	2.00	0.43
2:4:307:PHE:HE1	2:4:342:LEU:HD12	1.82	0.43
2:4:487:PHE:HD2	2:4:749:VAL:HG23	1.79	0.43
2:4:647:ASP:OD1	2:4:648:LEU:N	2.50	0.43
3:7:321:PRO:O	3:7:324:LEU:HD22	2.18	0.43
3:7:376:ASN:OD1	3:7:484:ILE:HB	2.18	0.43
5:5:522:ASP:HB2	5:5:525:ARG:HG3	1.99	0.43
6:A:9:ASP:OD1	6:A:10:PHE:N	2.51	0.43
7:H:145:ASN:ND2	7:H:193:VAL:HG13	2.33	0.43
11:2:203:ARG:HA	11:2:206:ARG:HE	1.83	0.43
11:2:572:ASP:HA	11:2:614:ALA:HB3	1.99	0.43
1:3:214:VAL:HG12	1:3:215:ASP:N	2.33	0.43
1:3:237:SER:O	1:3:258:LEU:N	2.44	0.43
2:4:549:VAL:HG12	2:4:549:VAL:O	2.18	0.43
3:7:305:CYS:HB3	3:7:307:ASN:O	2.18	0.43
3:7:379:LEU:HD21	3:7:519:TRP:HB3	2.01	0.43
3:7:402:GLN:NE2	3:7:436:LEU:HD11	2.33	0.43
4:6:353:ASN:OD1	4:6:528:LEU:HD13	2.18	0.43
4:6:435:VAL:HG13	4:6:435:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:372:ILE:HD12	5:5:618:ILE:HD11	2.00	0.43
6:A:120:ASP:OD1	6:A:120:ASP:N	2.50	0.43
11:2:454:LYS:HE3	11:2:759:LEU:HD22	1.99	0.43
3:7:76:ILE:O	3:7:80:VAL:HG23	2.19	0.43
3:7:239:GLU:CD	3:7:240:HIS:H	2.27	0.43
4:6:85:CYS:SG	4:6:86:GLN:N	2.91	0.43
4:6:186:MET:HE3	4:6:189:VAL:CG1	2.48	0.43
5:5:248:LEU:O	5:5:251:ARG:HB3	2.18	0.43
6:A:196:GLU:O	6:A:199:ARG:N	2.49	0.43
11:2:484:LEU:HD22	11:2:521:THR:HG21	2.00	0.43
1:3:322:LYS:NZ	1:3:330:LEU:HD22	2.34	0.43
1:3:598:GLU:O	1:3:599:THR:OG1	2.34	0.43
2:4:245:ASN:OD1	2:4:257:LEU:HD22	2.18	0.43
6:A:291:LEU:HD22	6:A:294:TYR:HB2	1.99	0.43
6:A:480:ALA:HB2	6:A:503:ALA:CB	2.49	0.43
9:M:156:LEU:HA	9:M:159:ALA:HB3	2.00	0.43
1:3:277:ASP:OD1	1:3:280:LEU:HD12	2.18	0.43
1:3:337:LEU:HD13	1:3:445:ALA:C	2.43	0.43
1:3:552:ARG:NH2	1:3:557:LEU:HD22	2.34	0.43
3:7:48:ILE:HG22	3:7:49:THR:H	1.83	0.43
5:5:106:THR:HG21	5:5:113:GLU:CD	2.43	0.43
6:A:333:LEU:HD12	6:A:334:PRO:HD2	2.00	0.43
6:A:482:PHE:C	6:A:483:LEU:HD12	2.44	0.43
8:L:117:ILE:HG13	8:L:118:LYS:N	2.33	0.43
11:2:697:LEU:HD12	11:2:698:ARG:N	2.34	0.43
11:2:708:ILE:HG22	11:2:710:PRO:HD3	2.01	0.43
1:3:97:VAL:HG23	1:3:99:PHE:CE1	2.54	0.43
1:3:639:ALA:O	1:3:642:LEU:HD21	2.19	0.43
2:4:211:LEU:HD23	2:4:212:ASN:CA	2.48	0.43
2:4:368:GLN:NE2	2:4:368:GLN:HA	2.34	0.43
3:7:102:TYR:CB	3:7:106:ARG:HH12	2.32	0.43
3:7:524:LYS:HB3	3:7:525:PRO:HD2	2.01	0.43
4:6:95:ARG:HG2	4:6:96:ILE:HD12	1.99	0.43
4:6:466:HIS:HB3	4:6:521:ARG:NH1	2.33	0.43
9:M:128:ARG:HA	9:M:131:HIS:HB3	2.00	0.43
11:2:663:PHE:O	11:2:667:SER:CB	2.66	0.43
2:4:492:LYS:HE3	2:4:740:ILE:HD12	1.99	0.43
2:4:517:SER:HB3	13:4:901:ATP:H2'	1.99	0.43
2:4:649:ILE:HG22	2:4:770:ALA:HB1	2.01	0.43
3:7:311:GLU:OE1	3:7:322:GLU:OE1	2.37	0.43
4:6:224:SER:O	4:6:227:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:244:VAL:HG12	4:6:245:VAL:H	1.84	0.43
4:6:466:HIS:HD2	4:6:521:ARG:HH21	1.57	0.43
4:6:521:ARG:HG2	4:6:611:ARG:CZ	2.49	0.43
5:5:349:ALA:HB1	5:5:513:MET:SD	2.59	0.43
6:A:254:TYR:CE2	6:A:255:THR:HG23	2.54	0.43
6:A:568:ASP:O	6:A:571:THR:HG23	2.18	0.43
11:2:518:LEU:HD22	11:2:570:LEU:CB	2.49	0.43
1:3:338:LEU:HD11	1:3:478:PHE:HB2	2.01	0.43
2:4:497:LEU:HD11	2:4:499:ARG:NE	2.31	0.43
3:7:103:ILE:O	3:7:107:LEU:N	2.48	0.43
3:7:522:GLN:HG2	3:7:523:ASP:N	2.34	0.43
5:5:150:ILE:HG23	5:5:254:PRO:HA	2.01	0.43
5:5:606:PRO:O	5:5:608:THR:N	2.51	0.43
6:A:128:PRO:O	6:A:131:GLU:N	2.50	0.43
8:L:17:ILE:HD13	8:L:44:VAL:CG2	2.49	0.43
9:M:81:HIS:O	9:M:85:CYS:N	2.48	0.43
11:2:297:VAL:O	11:2:298:THR:HG23	2.18	0.43
1:3:45:ILE:HD12	1:3:45:ILE:H	1.83	0.43
1:3:232:VAL:HG22	1:3:264:LEU:HA	2.00	0.43
2:4:483:LEU:HG	2:4:749:VAL:HG21	2.00	0.43
8:L:160:LEU:O	8:L:164:LEU:N	2.51	0.43
2:4:658:GLU:CB	3:7:586:VAL:HG13	2.49	0.43
3:7:66:VAL:HG13	3:7:73:TYR:CG	2.54	0.43
4:6:299:THR:HG22	4:6:299:THR:O	2.19	0.43
4:6:400:GLN:HA	4:6:403:ASP:HB2	2.00	0.43
4:6:485:LEU:HD22	11:2:373:GLY:HA3	2.01	0.43
5:5:466:ILE:CG2	5:5:467:ALA:N	2.82	0.43
6:A:11:TYR:HA	6:A:14:LEU:HD13	2.00	0.43
2:4:525:VAL:O	2:4:529:VAL:HG12	2.18	0.42
3:7:278:LEU:O	3:7:278:LEU:HG	2.19	0.42
5:5:48:TYR:C	5:5:49:LYS:HD2	2.44	0.42
5:5:337:ALA:HB2	5:5:347:LYS:NZ	2.34	0.42
1:3:143:HIS:HB3	1:3:152:MET:SD	2.59	0.42
2:4:718:ASP:OD2	2:4:772:LYS:NZ	2.52	0.42
3:7:378:CYS:HA	3:7:486:ALA:HB3	2.00	0.42
3:7:546:GLN:O	3:7:548:PRO:HD3	2.19	0.42
4:6:593:LEU:O	4:6:596:ARG:N	2.46	0.42
5:5:522:ASP:O	5:5:526:ASP:N	2.47	0.42
8:L:81:SER:HB2	8:L:84:PHE:O	2.18	0.42
10:N:183:LEU:HD11	10:N:211:ILE:CG1	2.48	0.42
11:2:741:VAL:O	11:2:745:GLU:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:262:ILE:HG22	1:3:263:SER:N	2.34	0.42
3:7:497:PRO:HB3	3:7:644:LEU:CD1	2.49	0.42
3:7:585:TYR:CE1	3:7:606:LEU:HD23	2.54	0.42
3:7:593:ARG:HD2	3:7:593:ARG:C	2.43	0.42
8:L:163:SER:HG	8:L:164:LEU:HD12	1.83	0.42
9:M:31:LEU:CD2	9:M:46:LEU:HD13	2.49	0.42
1:3:354:LEU:HD12	1:3:362:PRO:CG	2.49	0.42
1:3:544:LEU:O	1:3:547:GLY:N	2.46	0.42
2:4:569:ASP:OD1	4:6:211:ARG:NE	2.41	0.42
2:4:666:SER:HB3	3:7:582:VAL:HG11	2.00	0.42
3:7:450:MET:O	3:7:451:ALA:HB2	2.19	0.42
3:7:511:LEU:O	3:7:515:PHE:CE2	2.73	0.42
4:6:372:THR:HG22	11:2:668:HIS:HA	2.00	0.42
6:A:563:LEU:O	6:A:567:LEU:N	2.48	0.42
9:M:51:THR:O	9:M:51:THR:HG23	2.19	0.42
11:2:465:SER:OG	11:2:691:GLU:OE1	2.37	0.42
1:3:361:ILE:HG22	1:3:362:PRO:O	2.19	0.42
1:3:409:MET:HE2	1:3:414:ARG:HG3	2.02	0.42
3:7:103:ILE:HA	3:7:106:ARG:HB2	2.02	0.42
3:7:370:LYS:HD2	3:7:370:LYS:HA	1.79	0.42
5:5:98:ALA:CB	5:5:119:ILE:HD11	2.49	0.42
5:5:160:ALA:HA	5:5:216:CYS:HA	2.02	0.42
6:A:46:LEU:HD22	7:H:201:ILE:HD13	2.01	0.42
6:A:281:SER:O	6:A:376:LEU:HD11	2.19	0.42
7:H:133:ALA:O	7:H:139:LEU:N	2.52	0.42
1:3:118:LEU:HD11	5:5:216:CYS:HB3	2.02	0.42
2:4:611:ALA:HA	4:6:211:ARG:NH2	2.34	0.42
4:6:389:ASP:O	4:6:392:THR:HG22	2.20	0.42
5:5:460:GLU:OE2	5:5:510:ARG:NH1	2.36	0.42
6:A:22:VAL:HG23	6:A:49:VAL:HG13	2.00	0.42
1:3:257:LEU:C	1:3:258:LEU:HD23	2.45	0.42
2:4:586:ARG:O	2:4:588:VAL:N	2.53	0.42
3:7:37:LEU:HD21	3:7:86:PRO:HG2	2.02	0.42
3:7:230:VAL:HG13	3:7:231:LYS:O	2.20	0.42
3:7:342:PRO:HD2	3:7:343:GLU:OE1	2.20	0.42
3:7:419:MET:HE3	12:X:36:DT:C4'	2.39	0.42
5:5:54:LEU:O	5:5:58:TYR:N	2.44	0.42
5:5:217:VAL:HG12	5:5:245:ASP:O	2.20	0.42
5:5:637:ASN:OD1	5:5:640:LEU:HD13	2.20	0.42
6:A:453:HIS:O	6:A:460:TYR:N	2.53	0.42
7:H:12:ALA:H	7:H:76:ARG:HH22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:92:ILE:O	7:H:95:LEU:HD12	2.19	0.42
7:H:182:HIS:HB2	7:H:184:LEU:CD1	2.49	0.42
8:L:111:GLU:O	8:L:115:THR:N	2.49	0.42
11:2:782:ALA:N	11:2:783:GLN:OE1	2.52	0.42
1:3:151:VAL:HG23	1:3:151:VAL:O	2.20	0.42
2:4:581:MET:CE	2:4:585:THR:HB	2.50	0.42
2:4:583:ASP:HB2	4:6:456:LYS:HZ1	1.83	0.42
3:7:349:ASP:OD2	3:7:350:VAL:HG22	2.19	0.42
3:7:357:LEU:HD13	3:7:485:LEU:HD21	2.01	0.42
4:6:347:PHE:O	4:6:357:LYS:NZ	2.47	0.42
5:5:86:GLN:HG2	5:5:89:GLU:OE1	2.20	0.42
6:A:32:ALA:HB1	6:A:215:ALA:HB2	2.02	0.42
6:A:65:HIS:CE1	7:H:181:GLN:HG2	2.55	0.42
6:A:296:HIS:O	6:A:296:HIS:ND1	2.52	0.42
6:A:312:GLN:O	6:A:313:LEU:HD23	2.18	0.42
6:A:313:LEU:HB3	6:A:315:LEU:HD21	2.01	0.42
6:A:400:VAL:CG1	6:A:405:THR:HG21	2.50	0.42
8:L:64:GLU:OE2	8:L:64:GLU:N	2.44	0.42
9:M:164:ASN:HA	9:M:167:TYR:HB3	2.02	0.42
11:2:287:LEU:HD22	11:2:403:TYR:HD2	1.83	0.42
1:3:120:ASN:OD1	1:3:121:MET:N	2.53	0.42
1:3:298:LEU:HG	1:3:352:TYR:CD1	2.55	0.42
3:7:372:ARG:CD	3:7:463:GLU:O	2.67	0.42
3:7:386:ALA:CB	14:7:801:ADP:H5'2	2.48	0.42
4:6:338:LEU:O	4:6:342:LEU:HD12	2.20	0.42
5:5:283:VAL:HG22	11:2:407:TYR:CE1	2.54	0.42
5:5:442:ASP:OD1	5:5:485:ALA:HA	2.19	0.42
6:A:174:LEU:HG	6:A:175:SER:H	1.85	0.42
8:L:93:MET:N	8:L:93:MET:SD	2.93	0.42
10:N:56:LEU:O	10:N:108:ARG:NH2	2.47	0.42
11:2:310:ILE:HD13	11:2:327:SER:HB2	2.02	0.42
1:3:633:ILE:O	1:3:636:ALA:HB3	2.20	0.42
2:4:354:LEU:HD12	2:4:355:VAL:N	2.34	0.42
3:7:228:LYS:C	3:7:228:LYS:CD	2.91	0.42
3:7:278:LEU:HD11	3:7:297:PHE:CZ	2.55	0.42
3:7:435:VAL:CG2	3:7:478:LEU:HD13	2.50	0.42
3:7:557:ASN:O	3:7:560:ARG:HG3	2.20	0.42
5:5:108:PRO:HB3	8:L:123:ILE:HG13	2.02	0.42
5:5:172:THR:O	5:5:172:THR:HG22	2.20	0.42
5:5:299:SER:O	5:5:301:GLY:N	2.49	0.42
6:A:228:ASP:O	6:A:230:MET:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:215:LEU:HD12	10:N:215:LEU:H	1.85	0.42
11:2:271:SER:HB3	11:2:428:HIS:ND1	2.35	0.42
2:4:260:GLN:HA	2:4:261:ILE:HD12	2.02	0.41
2:4:290:GLY:O	2:4:390:ARG:HD2	2.20	0.41
2:4:535:THR:CG2	2:4:536:SER:N	2.70	0.41
2:4:661:ASP:HB3	3:7:585:TYR:CE2	2.54	0.41
3:7:176:MET:O	3:7:230:VAL:N	2.53	0.41
3:7:381:GLY:O	3:7:387:LYS:HE3	2.20	0.41
3:7:402:GLN:HG3	3:7:403:TYR:N	2.35	0.41
4:6:77:TYR:CG	4:6:128:LEU:HD11	2.55	0.41
4:6:594:ARG:O	4:6:598:THR:N	2.44	0.41
11:2:382:ILE:HG22	11:2:383:LEU:N	2.35	0.41
1:3:201:MET:HE3	1:3:202:PRO:HD2	2.02	0.41
1:3:341:ASP:OD2	1:3:482:ASP:N	2.53	0.41
1:3:417:ILE:N	1:3:417:ILE:HD13	2.35	0.41
1:3:565:TYR:CG	1:3:569:ALA:HB2	2.56	0.41
2:4:623:GLU:OE2	2:4:623:GLU:N	2.53	0.41
3:7:228:LYS:HD2	3:7:229:PHE:O	2.20	0.41
3:7:606:LEU:CD1	3:7:607:LEU:HD23	2.50	0.41
3:7:627:LYS:O	3:7:631:ALA:HB2	2.20	0.41
4:6:133:GLY:C	4:6:134:GLN:HG2	2.44	0.41
4:6:435:VAL:N	4:6:436:ILE:HD12	2.35	0.41
4:6:523:ASP:CB	4:6:524:LEU:HD12	2.50	0.41
5:5:187:ALA:O	5:5:188:LEU:O	2.38	0.41
5:5:263:ILE:HG22	5:5:291:ARG:CB	2.50	0.41
11:2:436:GLN:HG2	11:2:437:VAL:N	2.34	0.41
1:3:310:GLN:O	1:3:313:LEU:HD23	2.20	0.41
1:3:406:PHE:CD2	1:3:445:ALA:HB1	2.55	0.41
2:4:282:MET:O	2:4:397:TYR:HB3	2.20	0.41
2:4:739:LEU:O	2:4:742:LEU:HD23	2.20	0.41
3:7:455:ARG:HG2	3:7:456:THR:N	2.35	0.41
3:7:465:GLN:HE21	3:7:465:GLN:HB3	1.60	0.41
3:7:563:ILE:HD13	3:7:563:ILE:HA	1.75	0.41
7:H:76:ARG:C	7:H:76:ARG:HD3	2.45	0.41
10:N:153:HIS:C	10:N:157:THR:HG21	2.45	0.41
11:2:214:SER:O	11:2:216:VAL:HG23	2.20	0.41
11:2:478:ARG:HD3	11:2:774:MET:HE2	2.02	0.41
11:2:556:LEU:O	11:2:556:LEU:HD12	2.20	0.41
1:3:62:LEU:HD12	1:3:63:LEU:HB2	2.02	0.41
2:4:378:HIS:O	2:4:382:VAL:HG13	2.19	0.41
3:7:198:LEU:HD23	3:7:198:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:269:ASP:O	3:7:271:ILE:HG23	2.20	0.41
4:6:467:GLU:O	4:6:472:GLN:N	2.43	0.41
6:A:100:SER:OG	6:A:212:ARG:O	2.25	0.41
6:A:463:LEU:HD23	6:A:506:PRO:HD2	2.03	0.41
11:2:398:GLU:O	11:2:430:VAL:N	2.45	0.41
2:4:483:LEU:HD11	2:4:749:VAL:HG21	2.02	0.41
3:7:205:ASP:HB3	3:7:206:CYS:H	1.59	0.41
3:7:233:GLN:HG2	3:7:234:GLU:N	2.35	0.41
3:7:245:PRO:HB2	3:7:248:HIS:HB2	2.02	0.41
3:7:397:LEU:HD12	3:7:556:MET:HB2	2.02	0.41
4:6:371:THR:HG23	4:6:575:LYS:HE3	2.02	0.41
5:5:627:LEU:HD12	5:5:627:LEU:N	2.35	0.41
6:A:22:VAL:CG2	6:A:49:VAL:HG13	2.51	0.41
7:H:74:LEU:C	7:H:74:LEU:HD23	2.45	0.41
7:H:192:LEU:HD13	7:H:195:GLN:HE21	1.84	0.41
8:L:110:CYS:HA	8:L:113:LEU:HD23	2.02	0.41
10:N:40:GLU:HA	10:N:43:GLU:CD	2.45	0.41
10:N:157:THR:HA	10:N:160:MET:HB3	2.01	0.41
11:2:602:VAL:HG12	11:2:602:VAL:O	2.20	0.41
1:3:165:VAL:HG21	5:5:208:PHE:CE2	2.55	0.41
2:4:333:ASN:CG	2:4:336:THR:HG1	2.24	0.41
2:4:515:GLY:O	13:4:901:ATP:H5'2	2.20	0.41
3:7:157:ILE:HD13	3:7:157:ILE:HA	1.66	0.41
3:7:164:ARG:HD2	3:7:164:ARG:O	2.21	0.41
3:7:228:LYS:HD2	3:7:229:PHE:N	2.36	0.41
5:5:415:VAL:HB	5:5:468:LYS:HD2	2.02	0.41
5:5:444:PHE:CE2	5:5:483:ALA:HB1	2.55	0.41
9:M:33:ARG:NE	9:M:44:ASP:HB3	2.30	0.41
11:2:215:PHE:HB3	11:2:268:VAL:HG12	2.03	0.41
11:2:548:ASN:ND2	11:2:554:TRP:HB3	2.35	0.41
1:3:382:GLU:OE1	12:X:27:DT:H4'	2.21	0.41
2:4:540:SER:OG	3:7:470:ALA:HB3	2.20	0.41
2:4:717:VAL:HG13	4:6:534:GLU:OE2	2.20	0.41
4:6:211:ARG:HD2	4:6:211:ARG:HA	1.94	0.41
5:5:106:THR:HG22	5:5:112:HIS:ND1	2.35	0.41
5:5:217:VAL:HG12	5:5:218:ASP:N	2.35	0.41
5:5:372:ILE:CG2	5:5:617:ARG:HD3	2.48	0.41
6:A:7:ARG:HB2	6:A:10:PHE:HB2	2.03	0.41
6:A:70:LYS:HA	6:A:93:VAL:HG13	2.02	0.41
6:A:91:ASP:OD1	6:A:92:ASP:N	2.49	0.41
7:H:34:VAL:HG12	7:H:38:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:15:ILE:HD13	8:L:46:LEU:HD11	2.02	0.41
9:M:146:GLU:OE1	9:M:146:GLU:N	2.54	0.41
9:M:149:LEU:N	9:M:149:LEU:HD23	2.35	0.41
11:2:279:LEU:HD13	11:2:282:PHE:HZ	1.85	0.41
11:2:306:GLN:O	11:2:307:LEU:HD23	2.20	0.41
2:4:205:THR:HG23	2:4:251:ARG:NH1	2.35	0.41
3:7:344:ILE:HG23	14:7:801:ADP:HN62	1.85	0.41
3:7:379:LEU:O	3:7:487:ALA:HA	2.20	0.41
3:7:401:SER:OG	3:7:402:GLN:N	2.54	0.41
4:6:241:THR:HG23	4:6:241:THR:O	2.21	0.41
5:5:540:SER:O	5:5:540:SER:OG	2.27	0.41
6:A:531:PHE:HA	6:A:534:ALA:HB3	2.02	0.41
8:L:19:PRO:HD3	8:L:42:VAL:HG22	2.03	0.41
11:2:357:ASN:OD1	11:2:357:ASN:N	2.53	0.41
11:2:502:ILE:HG22	11:2:503:ASN:N	2.36	0.41
1:3:118:LEU:N	1:3:118:LEU:HD23	2.35	0.41
1:3:206:PRO:HG2	1:3:209:GLN:CG	2.51	0.41
1:3:299:ALA:N	1:3:300:PRO:CD	2.84	0.41
1:3:464:ILE:HG21	1:3:466:LEU:HD13	2.03	0.41
2:4:425:ARG:HD3	2:4:425:ARG:N	2.33	0.41
2:4:533:GLN:C	2:4:533:GLN:NE2	2.79	0.41
2:4:732:TYR:HB3	4:6:391:SER:HB3	2.02	0.41
3:7:343:GLU:CD	3:7:343:GLU:H	2.29	0.41
3:7:369:MET:HE3	3:7:370:LYS:C	2.46	0.41
3:7:385:VAL:HG13	3:7:387:LYS:H	1.85	0.41
3:7:571:PRO:HB3	3:7:617:ALA:HB3	2.03	0.41
3:7:587:GLU:HA	3:7:590:ARG:HE	1.84	0.41
4:6:411:THR:HG23	4:6:451:ILE:HD11	2.03	0.41
4:6:454:PHE:HA	4:6:457:MET:HE2	2.02	0.41
4:6:485:LEU:HG	4:6:486:ASN:H	1.86	0.41
4:6:523:ASP:C	4:6:524:LEU:HD12	2.45	0.41
5:5:46:PHE:HB2	9:M:171:LEU:HD23	2.02	0.41
5:5:263:ILE:HG22	5:5:291:ARG:HB3	2.02	0.41
6:A:563:LEU:HD23	6:A:563:LEU:H	1.85	0.41
8:L:99:VAL:O	8:L:103:ALA:N	2.53	0.41
8:L:145:LEU:HB2	10:N:207:SER:HA	2.02	0.41
9:M:56:LEU:O	9:M:59:ILE:N	2.53	0.41
11:2:527:ARG:O	11:2:528:ALA:HB2	2.21	0.41
11:2:589:MET:CE	11:2:641:ARG:HB2	2.51	0.41
11:2:634:LEU:HD12	11:2:639:LEU:CD1	2.48	0.41
1:3:393:MET:O	1:3:396:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:595:GLU:C	1:3:604:THR:HG21	2.45	0.41
3:7:291:GLY:C	3:7:293:LEU:HD12	2.46	0.41
3:7:400:ARG:HD2	3:7:400:ARG:HA	1.62	0.41
3:7:590:ARG:HG3	3:7:591:GLU:H	1.85	0.41
5:5:102:ALA:O	5:5:106:THR:N	2.54	0.41
6:A:502:ILE:HG22	6:A:516:LEU:HD11	2.02	0.41
8:L:93:MET:HG2	8:L:121:PHE:CE1	2.56	0.41
9:M:25:CYS:HB2	9:M:54:LEU:HD11	2.03	0.41
11:2:321:LEU:HD11	11:2:339:GLU:N	2.35	0.41
11:2:397:LEU:HD13	11:2:431:VAL:HG22	2.03	0.41
1:3:343:SER:O	13:3:901:ATP:H5'2	2.22	0.40
2:4:763:ALA:O	2:4:767:HIS:ND1	2.45	0.40
3:7:231:LYS:H	3:7:231:LYS:HE2	1.86	0.40
3:7:637:LEU:O	3:7:640:SER:HB3	2.20	0.40
4:6:133:GLY:HA2	4:6:205:THR:HG22	2.02	0.40
4:6:386:ILE:HG22	4:6:394:LYS:HD2	2.04	0.40
5:5:611:GLN:O	5:5:615:VAL:HG12	2.21	0.40
6:A:138:GLU:OE2	6:A:190:ARG:NE	2.40	0.40
11:2:207:MET:HE1	11:2:215:PHE:CB	2.52	0.40
11:2:377:ARG:HA	11:2:377:ARG:NE	2.36	0.40
11:2:387:LEU:HD12	11:2:387:LEU:N	2.36	0.40
11:2:514:LYS:HB2	11:2:517:PHE:CE1	2.57	0.40
11:2:589:MET:HE2	11:2:641:ARG:HB2	2.04	0.40
11:2:620:GLY:HA3	11:2:621:ARG:HH21	1.85	0.40
1:3:299:ALA:H	1:3:300:PRO:CD	2.31	0.40
13:3:901:ATP:PA	5:5:610:ARG:HH21	2.45	0.40
2:4:387:PRO:HG2	2:4:567:LEU:HD22	2.04	0.40
2:4:745:ALA:O	2:4:749:VAL:N	2.53	0.40
3:7:343:GLU:C	3:7:344:ILE:HD12	2.47	0.40
3:7:594:ASN:OD1	3:7:594:ASN:N	2.54	0.40
4:6:647:SER:HA	4:6:650:ARG:HH11	1.85	0.40
5:5:162:ARG:HE	5:5:174:ILE:H	1.68	0.40
6:A:289:LEU:CD1	6:A:291:LEU:HD13	2.52	0.40
1:3:610:ARG:NH2	14:7:801:ADP:O3A	2.53	0.40
2:4:404:THR:HG23	2:4:412:LYS:HE2	2.04	0.40
2:4:417:THR:HG23	3:7:174:LYS:HD2	2.03	0.40
3:7:215:LYS:HE3	3:7:215:LYS:HB2	1.77	0.40
3:7:463:GLU:O	3:7:464:GLN:HB2	2.21	0.40
3:7:618:ARG:O	3:7:621:LEU:CD2	2.68	0.40
6:A:255:THR:HA	6:A:258:LEU:HD23	2.03	0.40
6:A:398:GLU:HG3	6:A:400:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:482:PHE:HB3	6:A:483:LEU:HD12	2.03	0.40
11:2:192:VAL:HG22	11:2:198:TYR:HB2	2.03	0.40
11:2:350:MET:SD	11:2:350:MET:N	2.94	0.40
11:2:454:LYS:CE	11:2:759:LEU:HD22	2.51	0.40
11:2:546:ARG:O	11:2:547:ARG:HG3	2.21	0.40
11:2:717:GLU:OE2	11:2:719:LYS:NZ	2.41	0.40
1:3:157:THR:HG22	1:3:158:ASP:H	1.85	0.40
1:3:540:LYS:CE	5:5:360:LYS:HD2	2.51	0.40
2:4:295:SER:OG	2:4:387:PRO:HD3	2.22	0.40
3:7:380:MET:HA	3:7:488:ALA:O	2.21	0.40
3:7:387:LYS:H	3:7:387:LYS:HG3	1.71	0.40
6:A:46:LEU:HD22	7:H:201:ILE:HG21	2.02	0.40
6:A:400:VAL:HG12	6:A:402:LYS:H	1.86	0.40
12:X:37:DT:H4'	12:X:38:DT:OP2	2.21	0.40
1:3:364:THR:HB	5:5:453:VAL:HG11	2.04	0.40
2:4:342:LEU:HD23	2:4:343:ILE:N	2.36	0.40
2:4:525:VAL:HG12	2:4:526:PHE:N	2.36	0.40
2:4:577:GLU:HG2	3:7:459:HIS:CE1	2.56	0.40
2:4:583:ASP:C	2:4:587:SER:HB3	2.46	0.40
2:4:713:ILE:HG21	4:6:542:ARG:CZ	2.52	0.40
3:7:382:ASP:CG	3:7:490:PRO:HD2	2.46	0.40
3:7:383:PRO:HB2	3:7:384:GLY:H	1.64	0.40
3:7:385:VAL:HG13	3:7:386:ALA:N	2.35	0.40
3:7:616:LEU:HD11	3:7:632:GLU:OE1	2.21	0.40
4:6:409:ILE:HG22	4:6:411:THR:HG22	2.04	0.40
4:6:482:ARG:NH1	11:2:529:VAL:CG1	2.84	0.40
4:6:551:ILE:O	4:6:551:ILE:HG23	2.22	0.40
5:5:466:ILE:HG22	5:5:467:ALA:N	2.36	0.40
8:L:28:LEU:HD13	8:L:34:GLY:C	2.46	0.40
8:L:128:LEU:O	8:L:132:ILE:HG12	2.22	0.40
9:M:27:VAL:HG22	9:M:52:VAL:HG21	2.00	0.40
10:N:29:ASP:HB3	10:N:31:GLU:OE2	2.21	0.40
10:N:168:ALA:HB3	10:N:171:ARG:CZ	2.52	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	3	582/819 (71%)	471 (81%)	108 (19%)	3 (0%)	24	62
2	4	611/866 (71%)	494 (81%)	108 (18%)	9 (2%)	8	38
3	7	561/720 (78%)	468 (83%)	83 (15%)	10 (2%)	6	33
4	6	590/817 (72%)	495 (84%)	93 (16%)	2 (0%)	36	71
5	5	555/733 (76%)	439 (79%)	109 (20%)	7 (1%)	9	41
6	A	565/575 (98%)	475 (84%)	89 (16%)	1 (0%)	43	77
7	H	185/202 (92%)	149 (80%)	35 (19%)	1 (0%)	24	62
8	L	173/203 (85%)	137 (79%)	36 (21%)	0	100	100
9	M	165/212 (78%)	129 (78%)	36 (22%)	0	100	100
10	N	200/228 (88%)	168 (84%)	32 (16%)	0	100	100
11	2	588/887 (66%)	482 (82%)	102 (17%)	4 (1%)	18	55
All	All	4775/6262 (76%)	3907 (82%)	831 (17%)	37 (1%)	18	52

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	7	383	PRO
4	6	425	VAL
11	2	314	CYS
2	4	488	GLY
2	4	538	ARG
3	7	625	VAL
2	4	589	LEU
2	4	605	ILE
3	7	574	PRO
2	4	500	GLN
5	5	458	ALA
11	2	564	ALA
11	2	625	SER

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Mol	Chain	Res	Type
1	3	352	TYR
3	7	424	THR
3	7	463	GLU
3	7	621	LEU
5	5	468	LYS
5	5	566	ARG
5	5	569	CYS
1	3	299	ALA
2	4	536	SER
2	4	551	LYS
3	7	132	LYS
3	7	464	GLN
3	7	623	ASP
4	6	632	VAL
5	5	553	ILE
11	2	624	PRO
1	3	452	GLY
5	5	110	PRO
2	4	253	PRO
2	4	674	VAL
3	7	384	GLY
7	H	140	PRO
5	5	108	PRO
6	A	473	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	3	513/699 (73%)	481 (94%)	32 (6%)	16	39
2	4	540/759 (71%)	497 (92%)	43 (8%)	11	32
3	7	492/630 (78%)	431 (88%)	61 (12%)	4	18
4	6	519/718 (72%)	479 (92%)	40 (8%)	12	33
5	5	491/630 (78%)	460 (94%)	31 (6%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	491/501 (98%)	465 (95%)	26 (5%)	20	43
7	H	156/176 (89%)	144 (92%)	12 (8%)	12	33
8	L	159/184 (86%)	150 (94%)	9 (6%)	18	41
9	M	148/188 (79%)	137 (93%)	11 (7%)	13	34
10	N	178/205 (87%)	163 (92%)	15 (8%)	10	31
11	2	526/781 (67%)	492 (94%)	34 (6%)	15	38
All	All	4213/5471 (77%)	3899 (92%)	314 (8%)	14	33

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	29	TYR
1	3	51	LEU
1	3	62	LEU
1	3	78	LYS
1	3	115	SER
1	3	116	ILE
1	3	118	LEU
1	3	160	THR
1	3	173	THR
1	3	188	SER
1	3	218	CYS
1	3	241	LEU
1	3	264	LEU
1	3	284	LEU
1	3	302	ILE
1	3	313	LEU
1	3	315	LEU
1	3	346	LYS
1	3	385	GLU
1	3	386	ARG
1	3	388	LEU
1	3	417	ILE
1	3	433	ILE
1	3	454	TYR
1	3	466	LEU
1	3	476	LEU
1	3	477	LEU
1	3	487	ASP
1	3	504	ASN

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Mol	Chain	Res	Type
1	3	581	CYS
1	3	627	MET
1	3	642	LEU
2	4	159	VAL
2	4	169	LYS
2	4	176	ILE
2	4	188	ASN
2	4	208	GLU
2	4	230	ILE
2	4	244	ILE
2	4	285	LEU
2	4	288	ILE
2	4	299	ILE
2	4	329	THR
2	4	357	LEU
2	4	359	GLU
2	4	372	ASN
2	4	373	VAL
2	4	375	LEU
2	4	376	TYR
2	4	427	VAL
2	4	450	LEU
2	4	472	ILE
2	4	503	ARG
2	4	507	HIS
2	4	510	LEU
2	4	519	SER
2	4	525	VAL
2	4	528	LEU
2	4	529	VAL
2	4	533	GLN
2	4	543	VAL
2	4	545	LEU
2	4	562	THR
2	4	607	CYS
2	4	608	GLN
2	4	609	LEU
2	4	613	THR
2	4	652	VAL
2	4	668	LEU
2	4	676	ARG
2	4	685	ASP

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Mol	Chain	Res	Type
2	4	699	HIS
2	4	705	SER
2	4	712	LEU
2	4	742	LEU
3	7	43	ARG
3	7	46	VAL
3	7	49	THR
3	7	51	ASP
3	7	79	ASP
3	7	109	MET
3	7	150	ARG
3	7	161	VAL
3	7	171	THR
3	7	195	VAL
3	7	198	LEU
3	7	201	THR
3	7	208	SER
3	7	212	ARG
3	7	213	VAL
3	7	214	ASN
3	7	215	LYS
3	7	219	ARG
3	7	230	VAL
3	7	231	LYS
3	7	244	VAL
3	7	246	VAL
3	7	248	HIS
3	7	255	ILE
3	7	269	ASP
3	7	271	ILE
3	7	277	PHE
3	7	302	ARG
3	7	304	ILE
3	7	333	TYR
3	7	338	THR
3	7	350	VAL
3	7	364	LYS
3	7	367	ASP
3	7	372	ARG
3	7	380	MET
3	7	387	LYS
3	7	404	THR

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Mol	Chain	Res	Type
3	7	414	LEU
3	7	415	THR
3	7	423	LEU
3	7	424	THR
3	7	434	LEU
3	7	435	VAL
3	7	455	ARG
3	7	456	THR
3	7	460	GLU
3	7	462	MET
3	7	465	GLN
3	7	474	ILE
3	7	499	ARG
3	7	522	GLN
3	7	540	VAL
3	7	551	VAL
3	7	569	LYS
3	7	573	ILE
3	7	586	VAL
3	7	600	PHE
3	7	601	THR
3	7	620	ARG
3	7	621	LEU
4	6	65	TYR
4	6	71	THR
4	6	84	LEU
4	6	85	CYS
4	6	101	GLN
4	6	114	ARG
4	6	116	LYS
4	6	120	LEU
4	6	123	SER
4	6	131	ILE
4	6	162	VAL
4	6	192	SER
4	6	193	LEU
4	6	196	ASP
4	6	247	ASP
4	6	288	MET
4	6	305	THR
4	6	323	ASP
4	6	346	LEU

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Mol	Chain	Res	Type
4	6	378	LEU
4	6	387	VAL
4	6	389	ASP
4	6	394	LYS
4	6	397	PHE
4	6	402	SER
4	6	432	PHE
4	6	443	LEU
4	6	451	ILE
4	6	515	SER
4	6	526	PHE
4	6	536	VAL
4	6	537	ASP
4	6	553	GLU
4	6	560	THR
4	6	585	MET
4	6	609	THR
4	6	610	VAL
4	6	616	MET
4	6	623	MET
4	6	648	ILE
5	5	25	ILE
5	5	93	ILE
5	5	99	ARG
5	5	104	GLU
5	5	144	VAL
5	5	146	ILE
5	5	149	ILE
5	5	150	ILE
5	5	161	THR
5	5	176	ASN
5	5	188	LEU
5	5	222	LEU
5	5	249	CYS
5	5	260	ILE
5	5	269	VAL
5	5	374	VAL
5	5	384	LYS
5	5	391	VAL
5	5	397	ILE
5	5	401	THR
5	5	418	ASP

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Mol	Chain	Res	Type
5	5	439	VAL
5	5	456	HIS
5	5	460	GLU
5	5	552	GLU
5	5	556	SER
5	5	563	HIS
5	5	572	ARG
5	5	573	LEU
5	5	640	LEU
5	5	644	GLN
6	A	17	LYS
6	A	45	MET
6	A	52	ILE
6	A	77	CYS
6	A	115	VAL
6	A	187	GLN
6	A	212	ARG
6	A	225	LEU
6	A	229	ASN
6	A	255	THR
6	A	265	VAL
6	A	293	LEU
6	A	347	LEU
6	A	363	LYS
6	A	368	ASP
6	A	373	THR
6	A	381	ARG
6	A	396	ILE
6	A	403	HIS
6	A	418	SER
6	A	430	ASP
6	A	435	LEU
6	A	462	VAL
6	A	495	GLN
6	A	520	VAL
6	A	570	LEU
7	H	34	VAL
7	H	62	SER
7	H	66	LEU
7	H	107	ILE
7	H	120	ASN
7	H	124	LYS

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Mol	Chain	Res	Type
7	H	131	CYS
7	H	144	THR
7	H	145	ASN
7	H	157	VAL
7	H	174	ILE
7	H	184	LEU
8	L	17	ILE
8	L	33	VAL
8	L	37	ARG
8	L	46	LEU
8	L	84	PHE
8	L	94	VAL
8	L	111	GLU
8	L	129	ARG
8	L	147	ASN
9	M	18	VAL
9	M	19	THR
9	M	27	VAL
9	M	59	ILE
9	M	85	CYS
9	M	116	VAL
9	M	125	LEU
9	M	149	LEU
9	M	152	ILE
9	M	158	GLU
9	M	168	ILE
10	N	39	LEU
10	N	55	ILE
10	N	70	VAL
10	N	78	ARG
10	N	98	ARG
10	N	110	GLN
10	N	128	PRO
10	N	139	LYS
10	N	148	VAL
10	N	154	LYS
10	N	192	VAL
10	N	198	ASP
10	N	207	SER
10	N	215	LEU
10	N	228	ILE
11	2	174	LEU

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Mol	Chain	Res	Type
11	2	202	ASP
11	2	204	ILE
11	2	233	LEU
11	2	245	ASP
11	2	327	SER
11	2	339	GLU
11	2	348	ILE
11	2	387	LEU
11	2	391	CYS
11	2	399	VAL
11	2	411	LEU
11	2	422	THR
11	2	430	VAL
11	2	439	GLN
11	2	446	ILE
11	2	448	THR
11	2	470	ILE
11	2	480	LEU
11	2	516	GLN
11	2	518	LEU
11	2	529	VAL
11	2	532	THR
11	2	541	LEU
11	2	563	LEU
11	2	601	ILE
11	2	609	CYS
11	2	621	ARG
11	2	632	VAL
11	2	695	ASP
11	2	736	SER
11	2	762	ASN
11	2	769	SER
11	2	773	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	32	HIS
1	3	49	ASN
1	3	70	GLN
1	3	92	HIS
2	4	326	ASN

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Mol	Chain	Res	Type
2	4	475	ASN
2	4	520	GLN
2	4	533	GLN
2	4	582	ASN
2	4	746	HIS
4	6	264	HIS
4	6	296	GLN
4	6	466	HIS
4	6	584	HIS
4	6	630	ASN
5	5	456	HIS
5	5	563	HIS
5	5	628	GLN
5	5	635	HIS
6	A	337	HIS
6	A	431	GLN
6	A	557	GLN
7	H	48	ASN
8	L	171	GLN
9	M	115	HIS
10	N	142	GLN
11	2	224	ASN
11	2	267	HIS
11	2	341	GLN
11	2	364	GLN
11	2	496	HIS
11	2	534	GLN
11	2	586	HIS

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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	ATP	6	901	-	32,33,33	1.25	3 (9%)	48,52,52	2.01	13 (27%)
13	ATP	4	901	-	32,33,33	1.50	6 (18%)	48,52,52	2.04	10 (20%)
13	ATP	3	901	-	32,33,33	1.32	5 (15%)	48,52,52	1.84	12 (25%)
13	ATP	2	901	-	32,33,33	1.41	4 (12%)	48,52,52	1.82	9 (18%)
14	ADP	7	801	-	28,29,29	1.41	3 (10%)	43,45,45	1.92	11 (25%)
14	ADP	5	801	-	28,29,29	1.47	4 (14%)	43,45,45	1.86	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ATP	6	901	-	-	5/22/38/38	0/3/3/3
13	ATP	4	901	-	-	5/22/38/38	0/3/3/3
13	ATP	3	901	-	-	4/22/38/38	0/3/3/3
13	ATP	2	901	-	-	5/22/38/38	0/3/3/3
14	ADP	7	801	-	-	2/16/32/32	0/3/3/3
14	ADP	5	801	-	-	2/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	5	801	ADP	C5-C4	5.09	1.48	1.39
13	4	901	ATP	C5-C4	5.07	1.48	1.39
14	7	801	ADP	C5-C4	4.88	1.47	1.39
13	2	901	ATP	C5-C4	4.86	1.47	1.39
13	6	901	ATP	C5-C4	4.11	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	901	ATP	C5-C4	4.01	1.46	1.39
13	2	901	ATP	C5-N7	-2.83	1.33	1.39
13	4	901	ATP	C5-C6	2.73	1.48	1.41
14	5	801	ADP	C5-N7	-2.68	1.34	1.39
14	7	801	ADP	C5-C6	2.66	1.48	1.41
13	3	901	ATP	C5-N7	-2.64	1.34	1.39
13	6	901	ATP	C5-N7	-2.63	1.34	1.39
14	5	801	ADP	C5-C6	2.62	1.48	1.41
13	4	901	ATP	C5-N7	-2.60	1.34	1.39
14	7	801	ADP	C5-N7	-2.57	1.34	1.39
13	4	901	ATP	PB-O3A	2.55	1.62	1.59
13	3	901	ATP	C4-N9	-2.48	1.32	1.37
13	2	901	ATP	C5-C6	2.47	1.47	1.41
13	4	901	ATP	C8-N7	2.39	1.36	1.31
13	6	901	ATP	C5-C6	2.38	1.47	1.41
13	2	901	ATP	C8-N9	-2.27	1.33	1.37
13	3	901	ATP	C8-N7	2.23	1.36	1.31
13	3	901	ATP	C5-C6	2.20	1.47	1.41
13	4	901	ATP	PA-O3A	2.14	1.61	1.59
14	5	801	ADP	C8-N7	2.14	1.35	1.31

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	4	901	ATP	C5-C4-N3	-6.80	117.36	126.72
13	6	901	ATP	C5-C4-N3	-6.53	117.73	126.72
13	2	901	ATP	C5-C4-N3	-6.49	117.78	126.72
14	5	801	ADP	C5-C4-N3	-6.46	117.82	126.72
14	7	801	ADP	C5-C4-N3	-6.32	118.02	126.72
13	3	901	ATP	C5-C4-N3	-5.75	118.80	126.72
13	6	901	ATP	N3-C4-N9	5.37	136.30	127.17
14	7	801	ADP	N3-C4-N9	5.29	136.16	127.17
13	2	901	ATP	N3-C4-N9	5.14	135.91	127.17
14	5	801	ADP	N3-C4-N9	4.96	135.60	127.17
13	4	901	ATP	N3-C4-N9	4.94	135.56	127.17
13	3	901	ATP	N3-C4-N9	4.31	134.49	127.17
13	4	901	ATP	O5'-C5'-C4'	3.98	122.55	108.99
13	4	901	ATP	C3'-C2'-C1'	3.96	108.95	101.46
13	6	901	ATP	C2-N3-C4	3.92	121.40	111.83
13	4	901	ATP	C2-N3-C4	3.91	121.37	111.83
14	7	801	ADP	C2-N3-C4	3.72	120.90	111.83
13	3	901	ATP	C2-N3-C4	3.71	120.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	801	ADP	C2-N3-C4	3.60	120.62	111.83
13	2	901	ATP	C2-N3-C4	3.50	120.37	111.83
13	3	901	ATP	C4-C5-N7	-3.40	106.69	110.58
14	5	801	ADP	C4-C5-N7	-3.36	106.74	110.58
13	2	901	ATP	O5'-C5'-C4'	3.27	120.12	108.99
13	2	901	ATP	C4-C5-N7	-3.26	106.85	110.58
13	4	901	ATP	C4-C5-N7	-3.24	106.87	110.58
14	7	801	ADP	C4-C5-N7	-3.13	107.00	110.58
13	6	901	ATP	N3-C2-N1	-3.04	123.98	128.58
13	6	901	ATP	C4-C5-N7	-3.01	107.14	110.58
13	6	901	ATP	C3'-C2'-C1'	3.00	107.15	101.46
13	3	901	ATP	N3-C2-N1	-2.97	124.09	128.58
13	4	901	ATP	N3-C2-N1	-2.93	124.14	128.58
14	7	801	ADP	N3-C2-N1	-2.92	124.16	128.58
13	6	901	ATP	O5'-C5'-C4'	2.91	118.89	108.99
13	3	901	ATP	C2'-C1'-N9	-2.73	106.52	113.30
14	5	801	ADP	N3-C2-N1	-2.59	124.67	128.58
13	6	901	ATP	C4-N9-C8	2.56	108.43	105.74
13	3	901	ATP	C4-N9-C8	2.56	108.42	105.74
13	4	901	ATP	C1'-N9-C8	-2.54	121.47	127.09
13	4	901	ATP	C2'-C1'-N9	-2.52	107.06	113.30
13	3	901	ATP	O3A-PB-O1B	-2.44	103.35	110.70
14	7	801	ADP	C1'-N9-C8	-2.41	121.75	127.09
13	6	901	ATP	C2'-C1'-N9	-2.41	107.32	113.30
13	3	901	ATP	C3'-C2'-C1'	2.38	105.97	101.46
13	2	901	ATP	N3-C2-N1	-2.35	125.03	128.58
13	3	901	ATP	C5-N7-C8	2.34	107.12	103.45
14	7	801	ADP	O2A-PA-O1A	2.33	123.29	112.44
14	7	801	ADP	C4-N9-C8	2.32	108.18	105.74
13	6	901	ATP	C5-N7-C8	2.31	107.08	103.45
13	6	901	ATP	O2A-PA-O1A	2.31	123.20	112.44
14	7	801	ADP	C5-N7-C8	2.28	107.03	103.45
14	5	801	ADP	C3'-C2'-C1'	2.25	105.72	101.46
14	5	801	ADP	O3B-PB-O2B	2.24	116.21	107.80
13	3	901	ATP	C6-C5-N7	2.17	136.28	132.09
13	2	901	ATP	C1'-N9-C8	-2.17	122.28	127.09
13	6	901	ATP	O3B-PG-O1G	-2.16	99.69	111.04
14	7	801	ADP	O2A-PA-O3A	-2.15	101.45	107.27
13	4	901	ATP	O2A-PA-O1A	2.15	122.43	112.44
14	5	801	ADP	C5-N7-C8	2.15	106.82	103.45
14	7	801	ADP	C3'-C2'-C1'	2.12	105.47	101.46
13	6	901	ATP	O2A-PA-O3A	-2.04	101.75	107.27

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	901	ATP	C3'-C2'-C1'	2.04	105.31	101.46
13	3	901	ATP	N9-C8-N7	-2.03	111.06	113.94
13	2	901	ATP	C2'-C3'-C4'	2.02	106.52	102.61

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	3	901	ATP	C5'-O5'-PA-O1A
13	3	901	ATP	C5'-O5'-PA-O2A
13	3	901	ATP	C5'-O5'-PA-O3A
13	4	901	ATP	C5'-O5'-PA-O1A
13	4	901	ATP	C5'-O5'-PA-O2A
13	4	901	ATP	C5'-O5'-PA-O3A
13	6	901	ATP	C5'-O5'-PA-O2A
13	6	901	ATP	C5'-O5'-PA-O3A
13	2	901	ATP	C5'-O5'-PA-O1A
13	2	901	ATP	C5'-O5'-PA-O2A
13	2	901	ATP	C5'-O5'-PA-O3A
14	5	801	ADP	C2'-C1'-N9-C8
14	7	801	ADP	C2'-C1'-N9-C4
14	5	801	ADP	C2'-C1'-N9-C4
14	7	801	ADP	C2'-C1'-N9-C8
13	4	901	ATP	C4'-C5'-O5'-PA
13	6	901	ATP	C5'-O5'-PA-O1A
13	3	901	ATP	C4'-C5'-O5'-PA
13	6	901	ATP	C4'-C5'-O5'-PA
13	2	901	ATP	C4'-C5'-O5'-PA
13	4	901	ATP	C2'-C1'-N9-C8
13	2	901	ATP	O4'-C4'-C5'-O5'
13	6	901	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 43 short contacts:

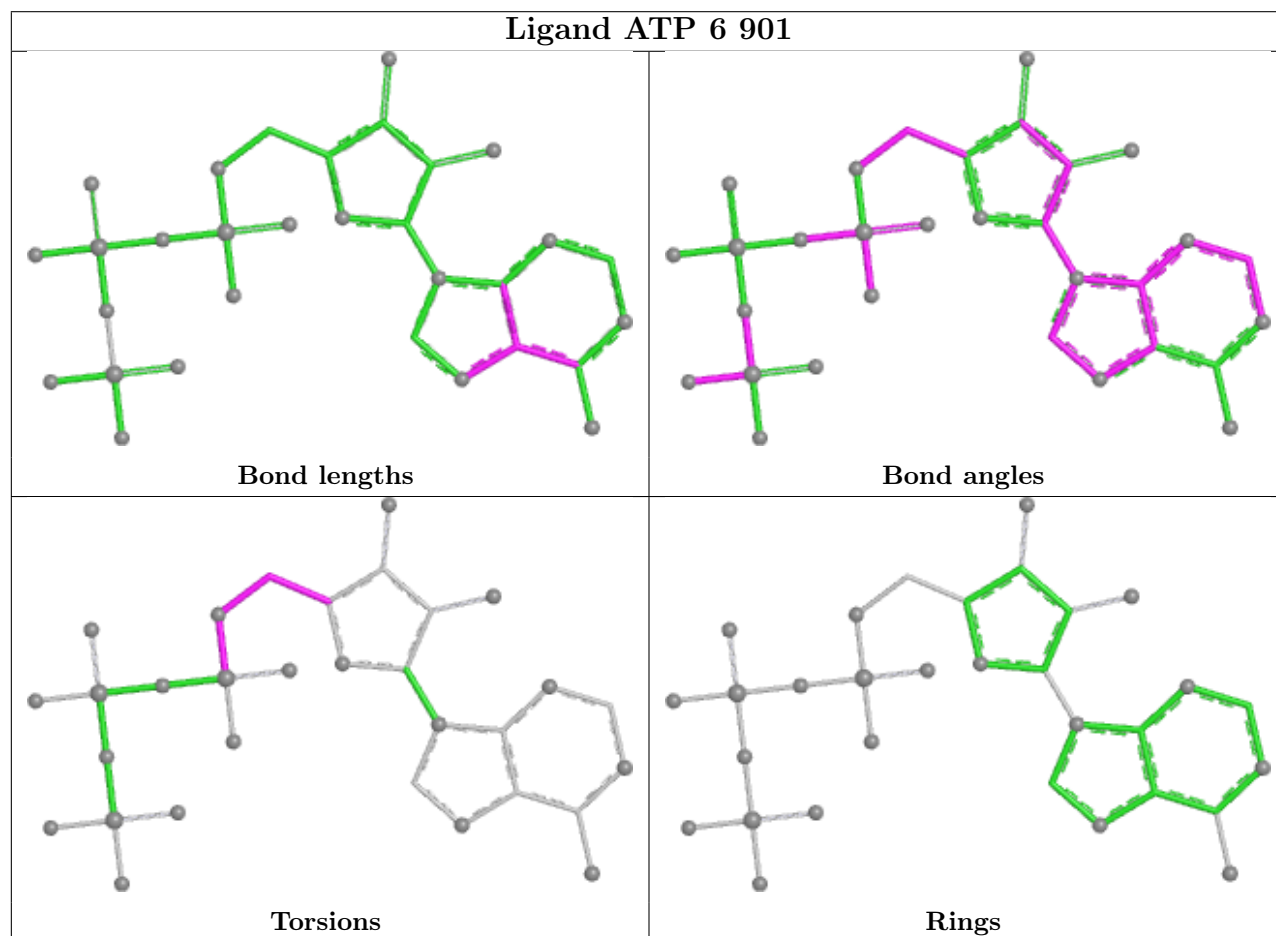
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	6	901	ATP	5	0
13	4	901	ATP	14	0
13	3	901	ATP	10	0
13	2	901	ATP	4	0
14	7	801	ADP	8	0

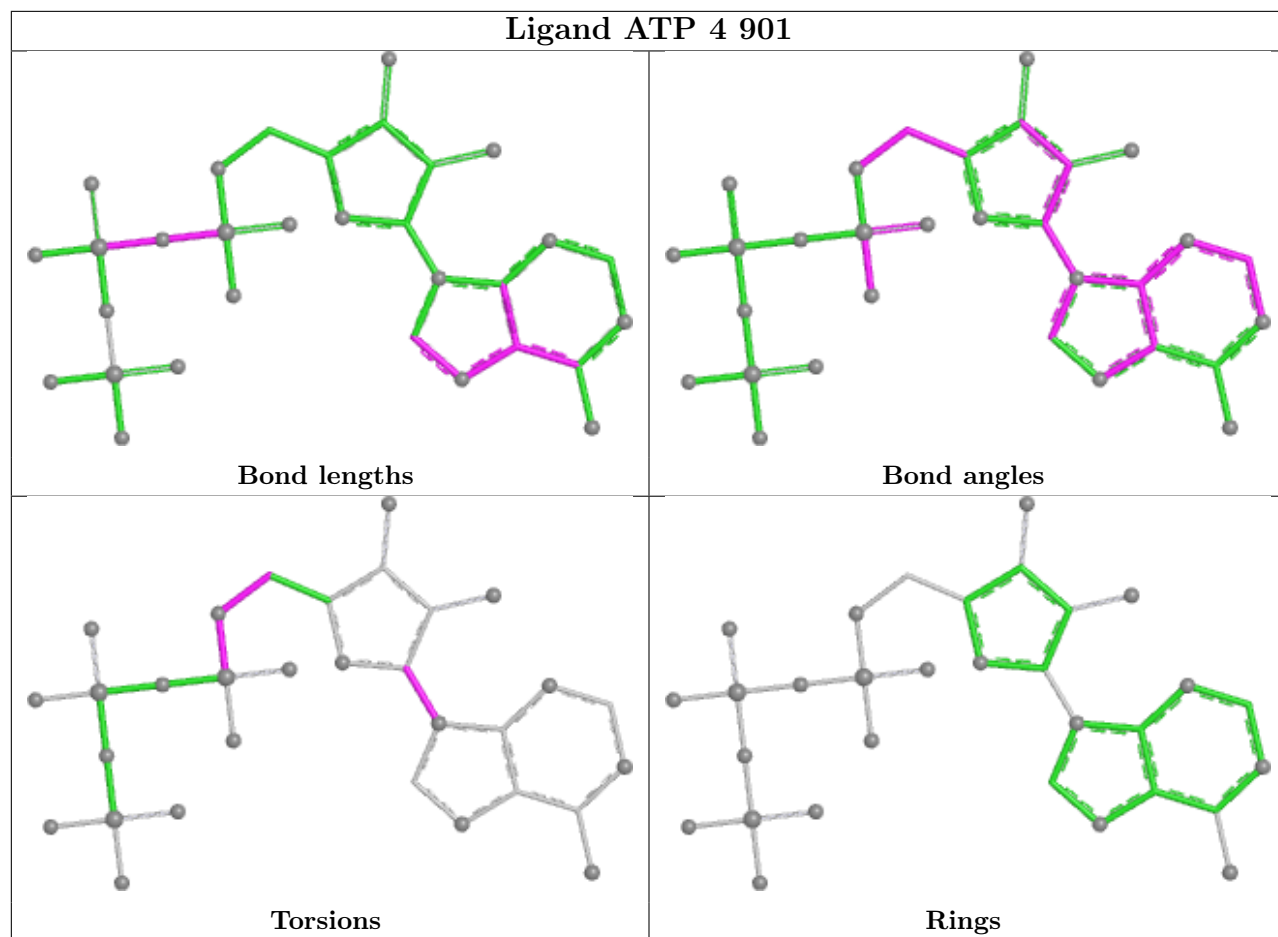
Continued on next page...

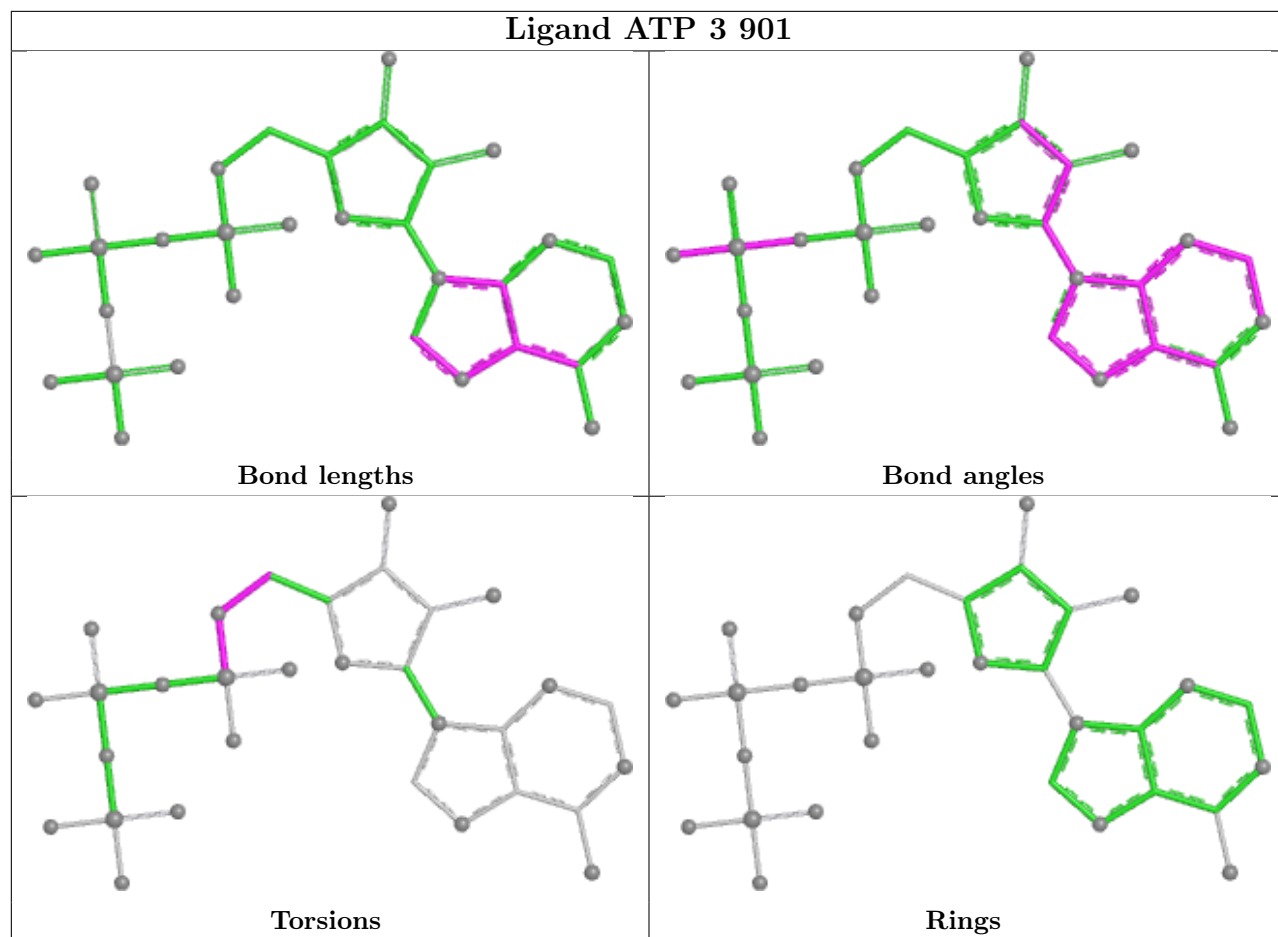
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	5	801	ADP	2	0

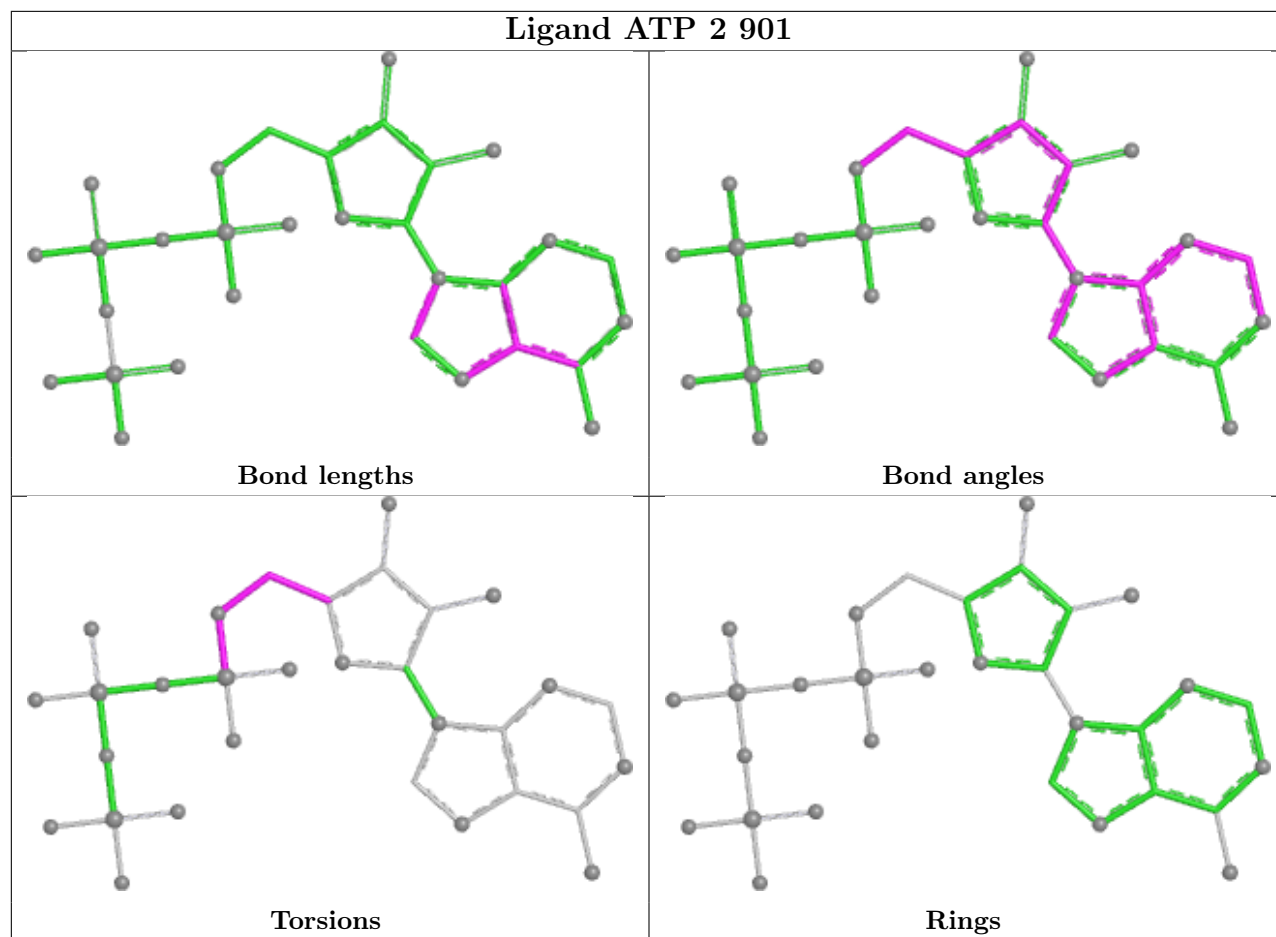
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



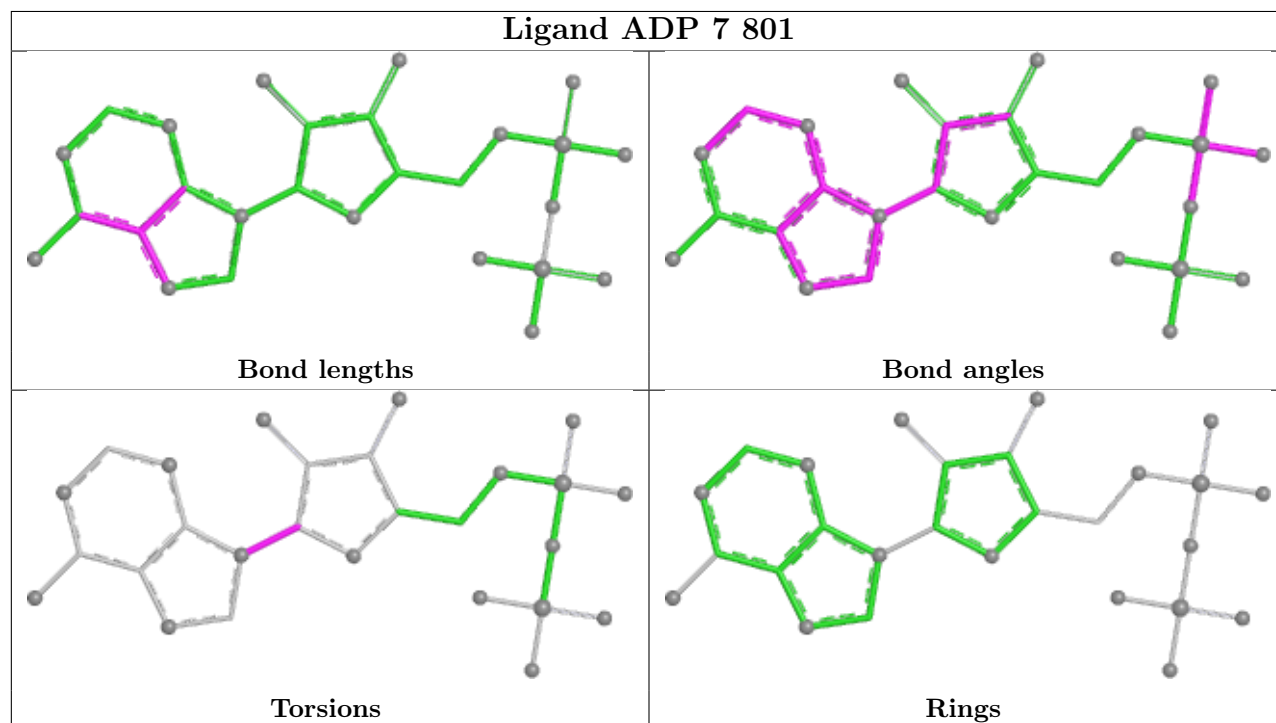


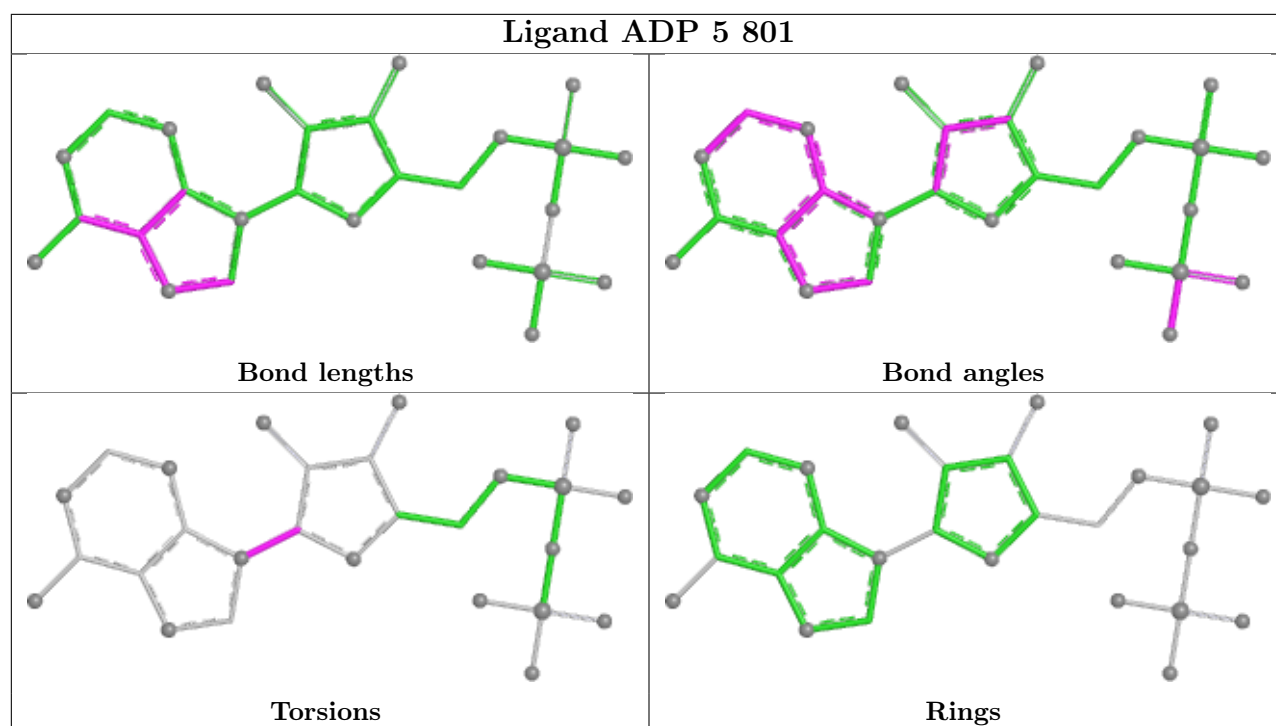


Ligand ATP 2 901



Ligand ADP 7 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	4	2
3	7	2
11	2	1
5	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	442:ILE	C	443:PHE	N	14.43
1	2	441:LEU	C	442:THR	N	10.58
1	5	405:GLY	C	408:SER	N	6.53
1	7	254:THR	C	255:ILE	N	1.67
1	4	588:VAL	C	589:LEU	N	1.66
1	7	431:GLY	C	432:GLY	N	1.17

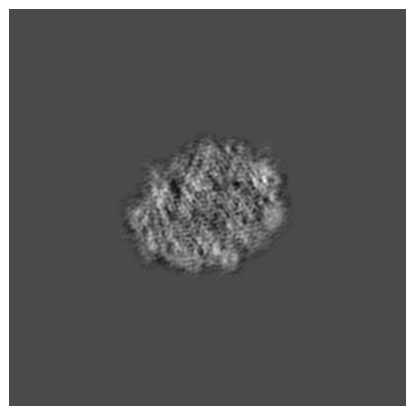
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4787. These allow visual inspection of the internal detail of the map and identification of artifacts.

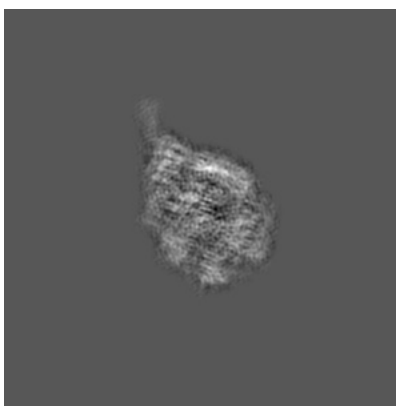
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

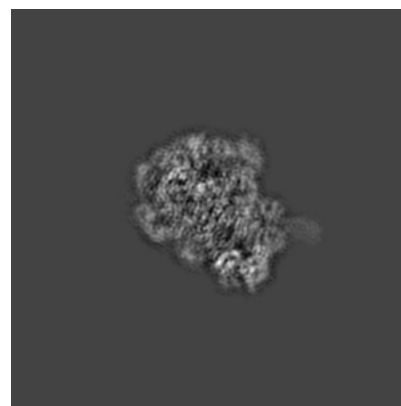
6.1.1 Primary map



X

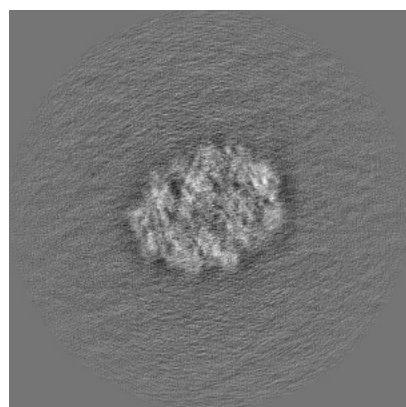


Y

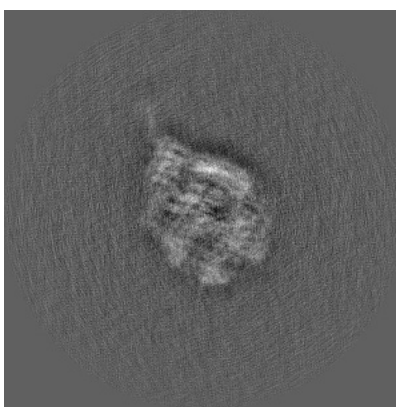


Z

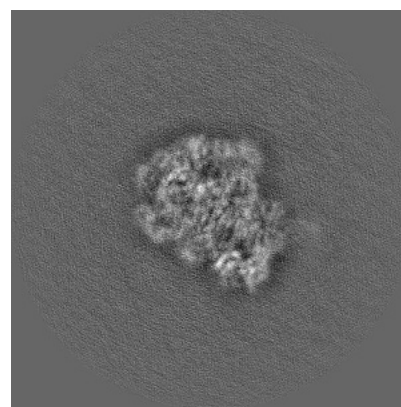
6.1.2 Raw map



X



Y

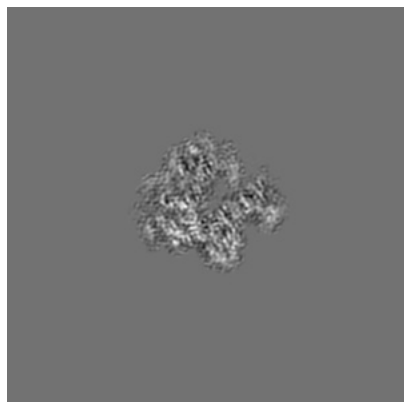


Z

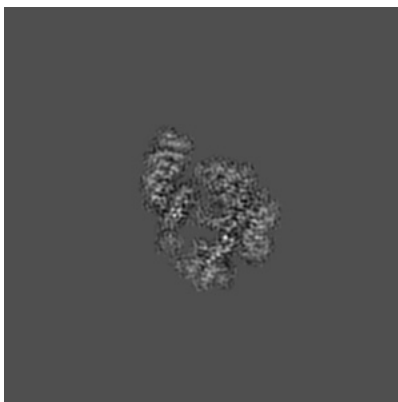
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

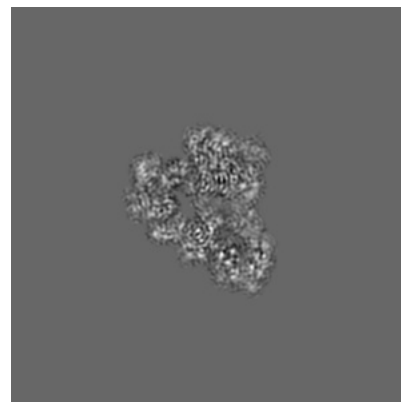
6.2.1 Primary map



X Index: 192

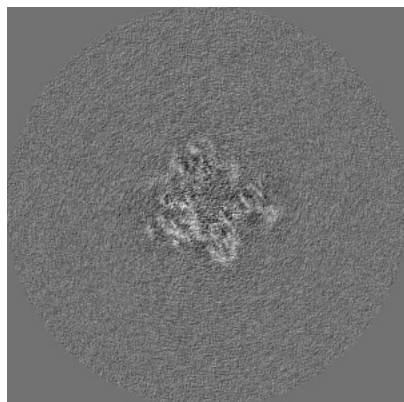


Y Index: 192

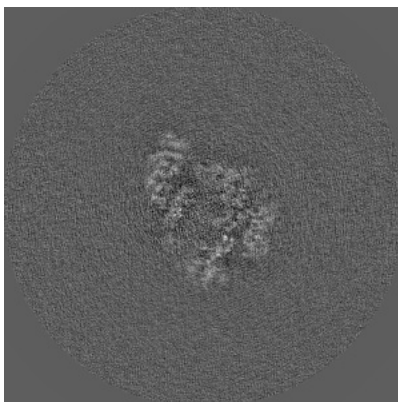


Z Index: 192

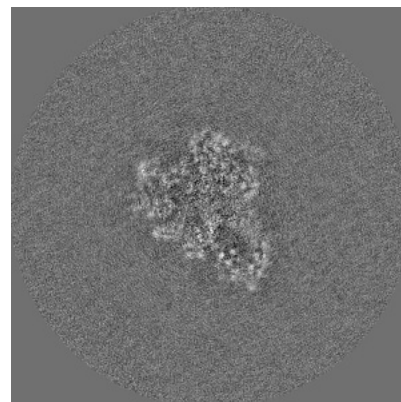
6.2.2 Raw map



X Index: 192



Y Index: 192

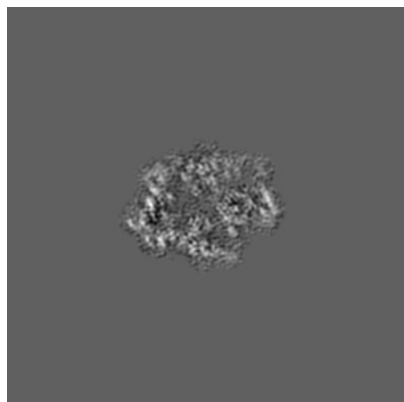


Z Index: 192

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

6.3 Largest variance slices [i](#)

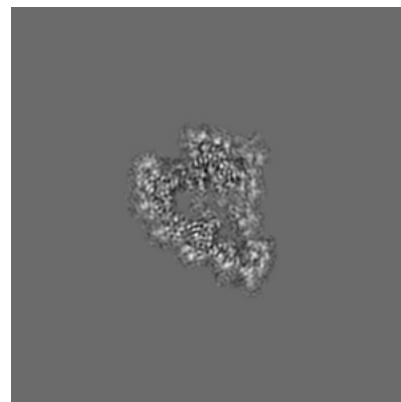
6.3.1 Primary map



X Index: 207

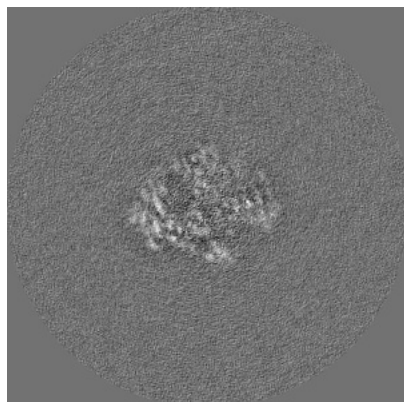


Y Index: 180

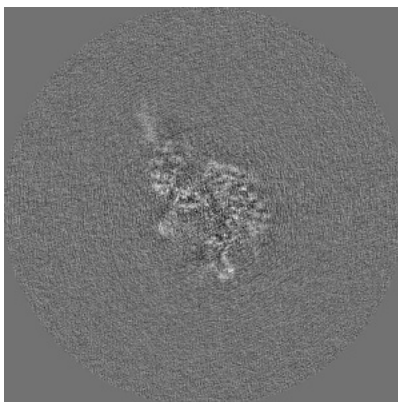


Z Index: 197

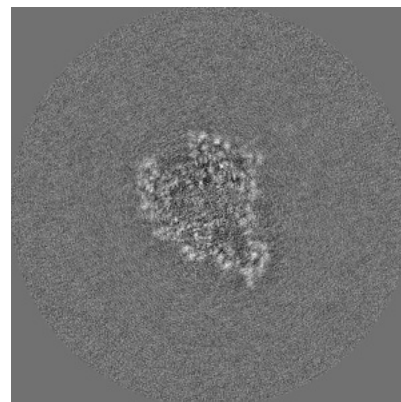
6.3.2 Raw map



X Index: 202



Y Index: 180

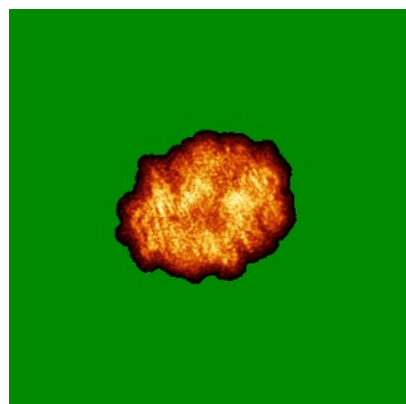


Z Index: 197

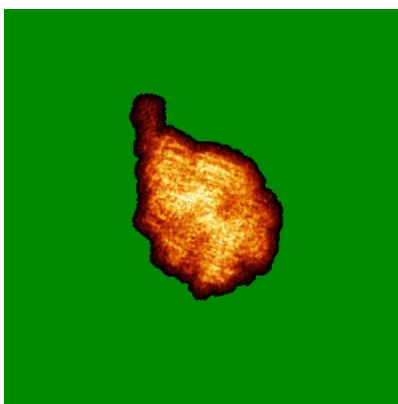
The images above show the largest variance slices of the map in three orthogonal directions.

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

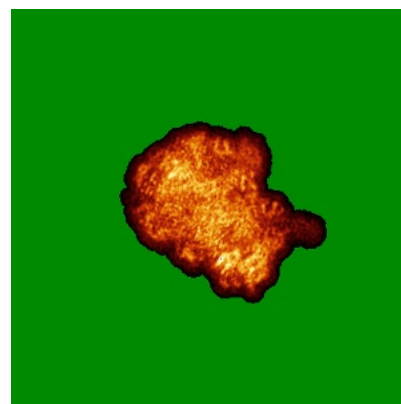
6.4.1 Primary map



X

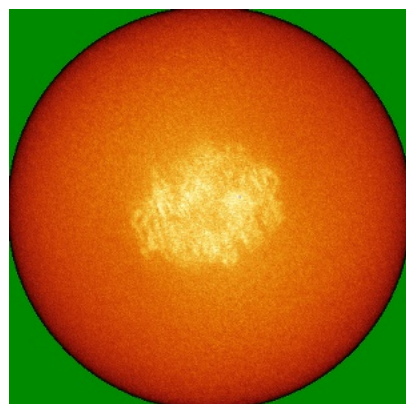


Y

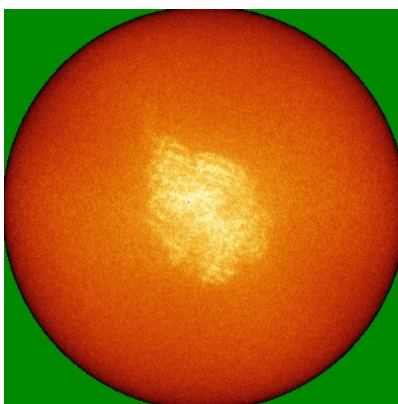


Z

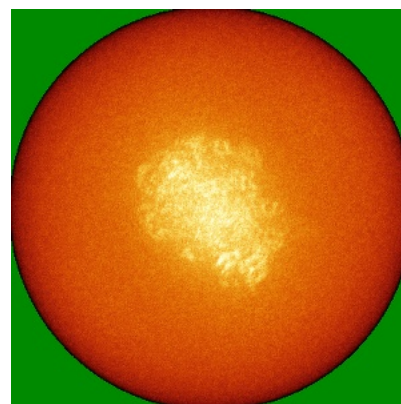
6.4.2 Raw map



X



Y

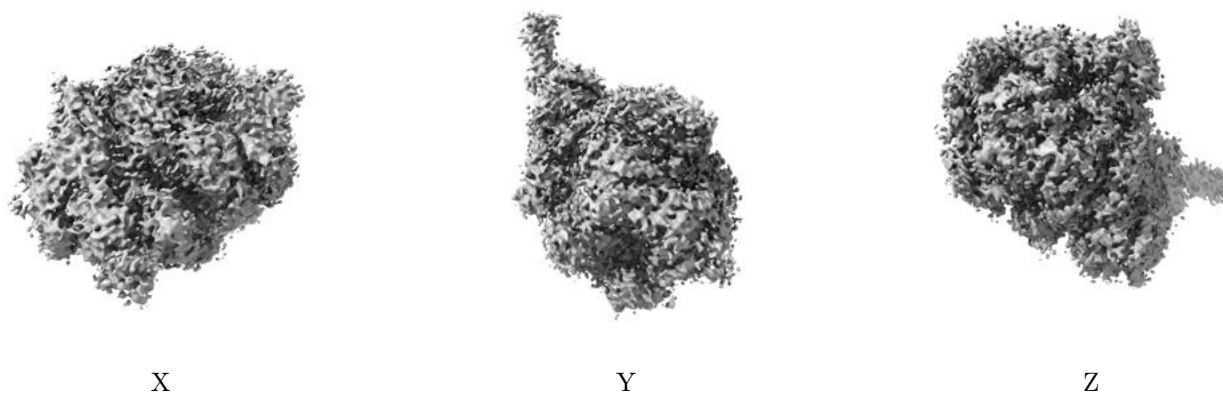


Z

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.

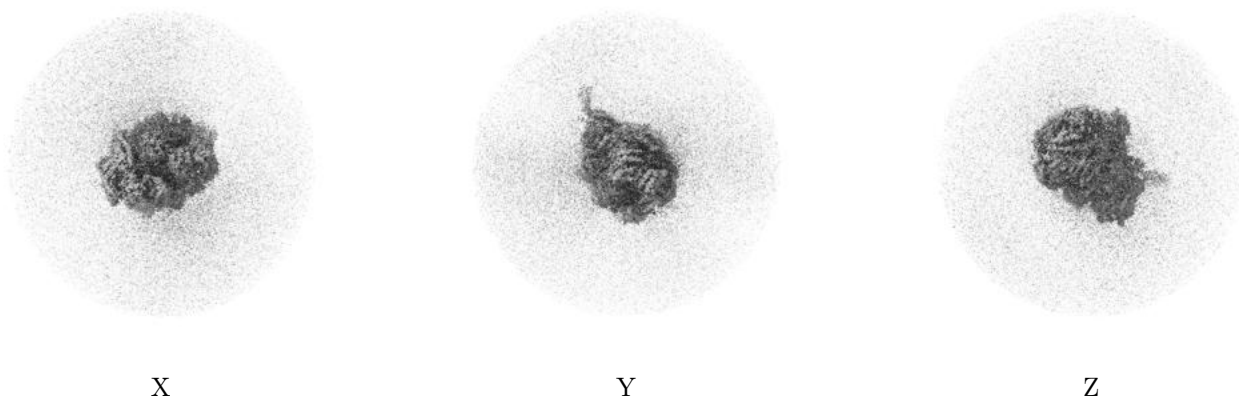
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

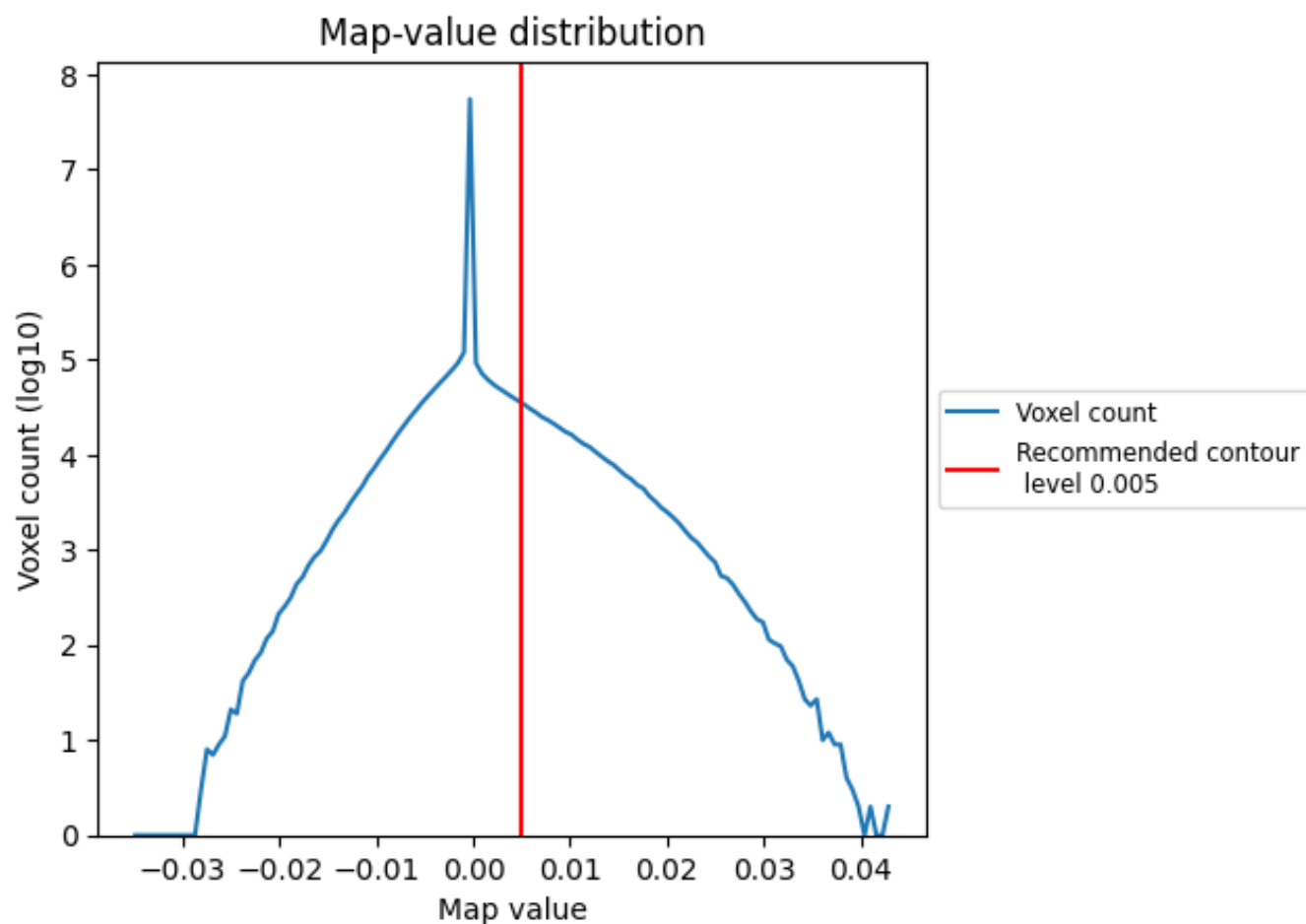
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

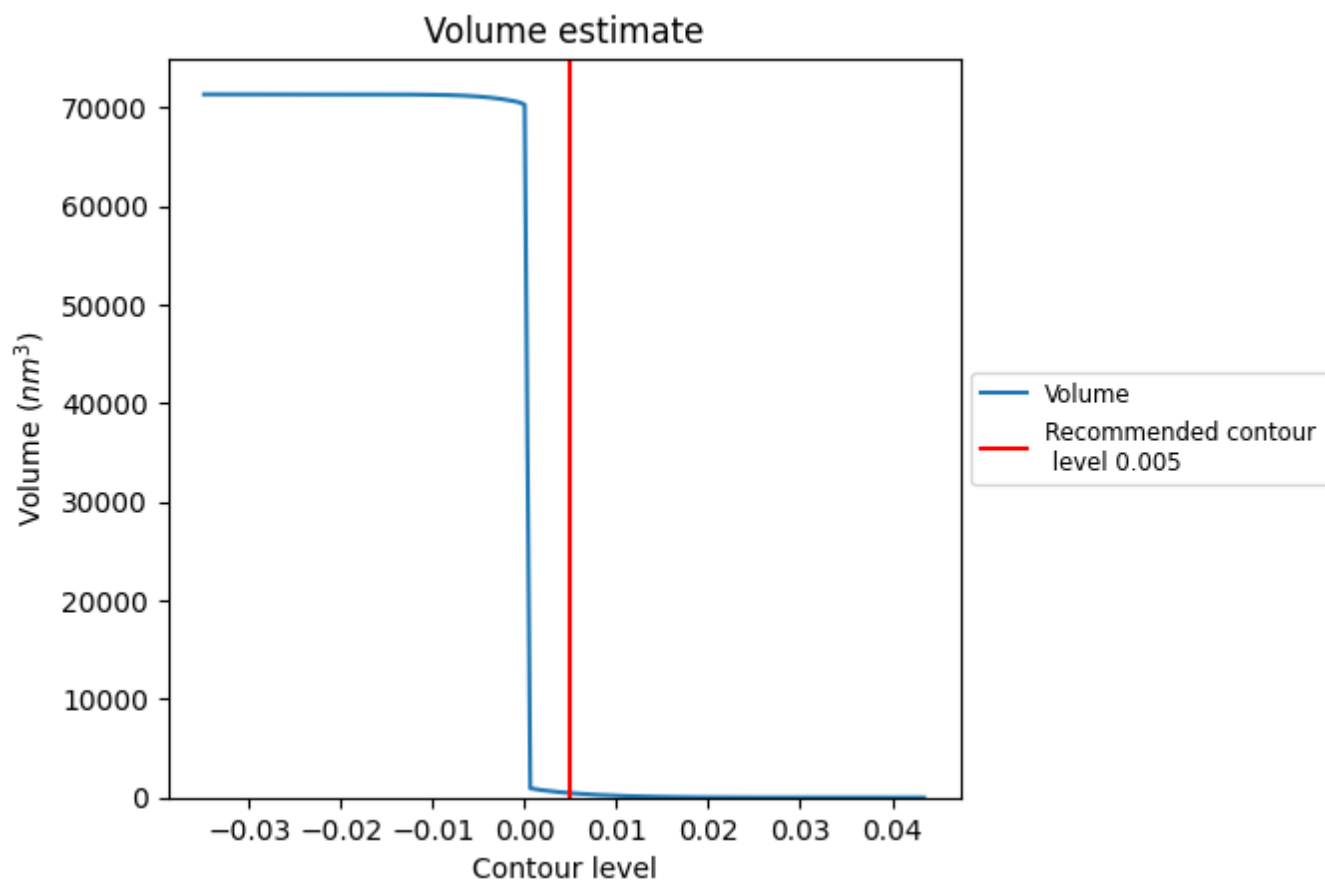
This section contains the results of statistical analysis of the map.

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.

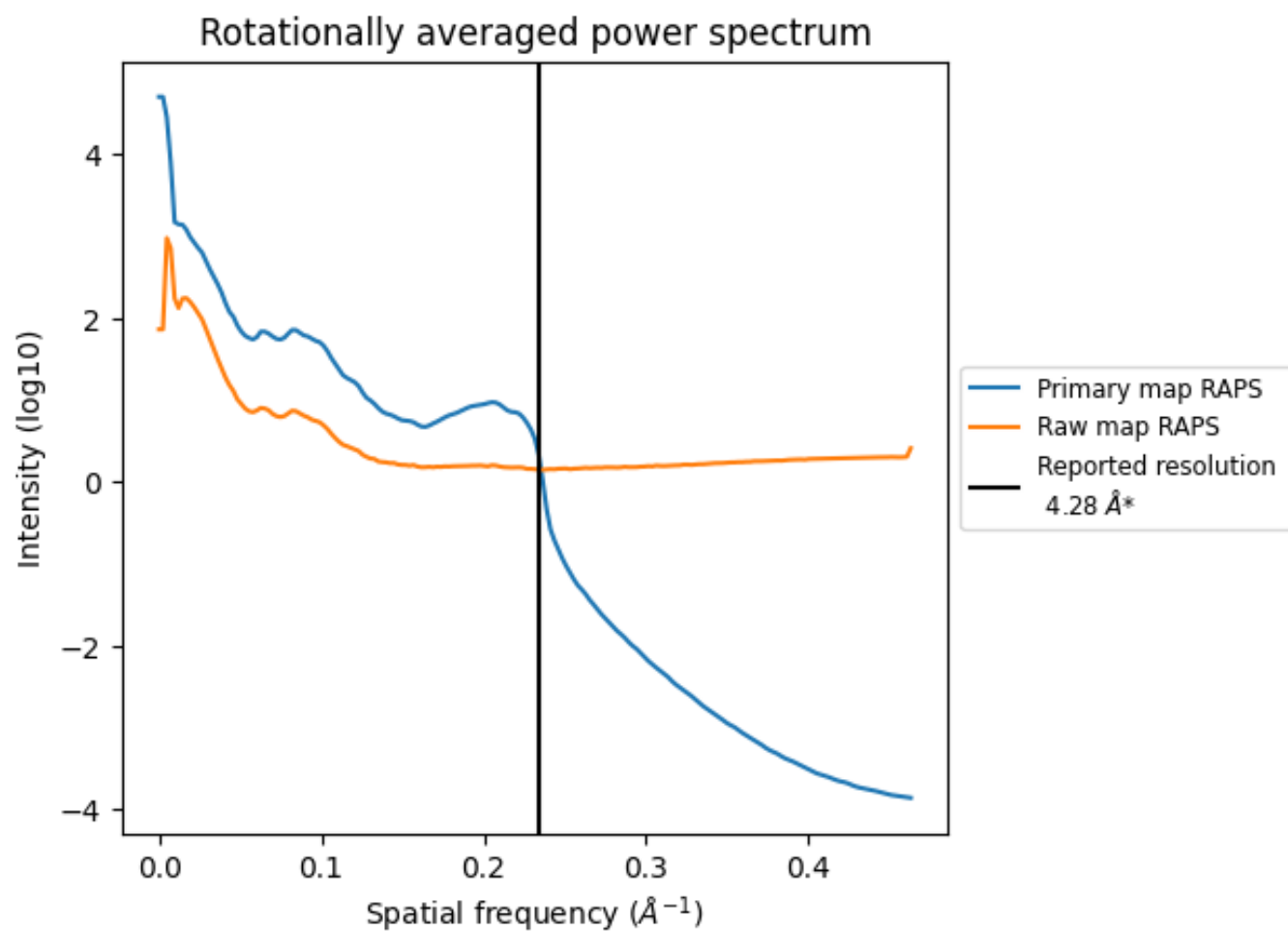
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 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 ⓘ

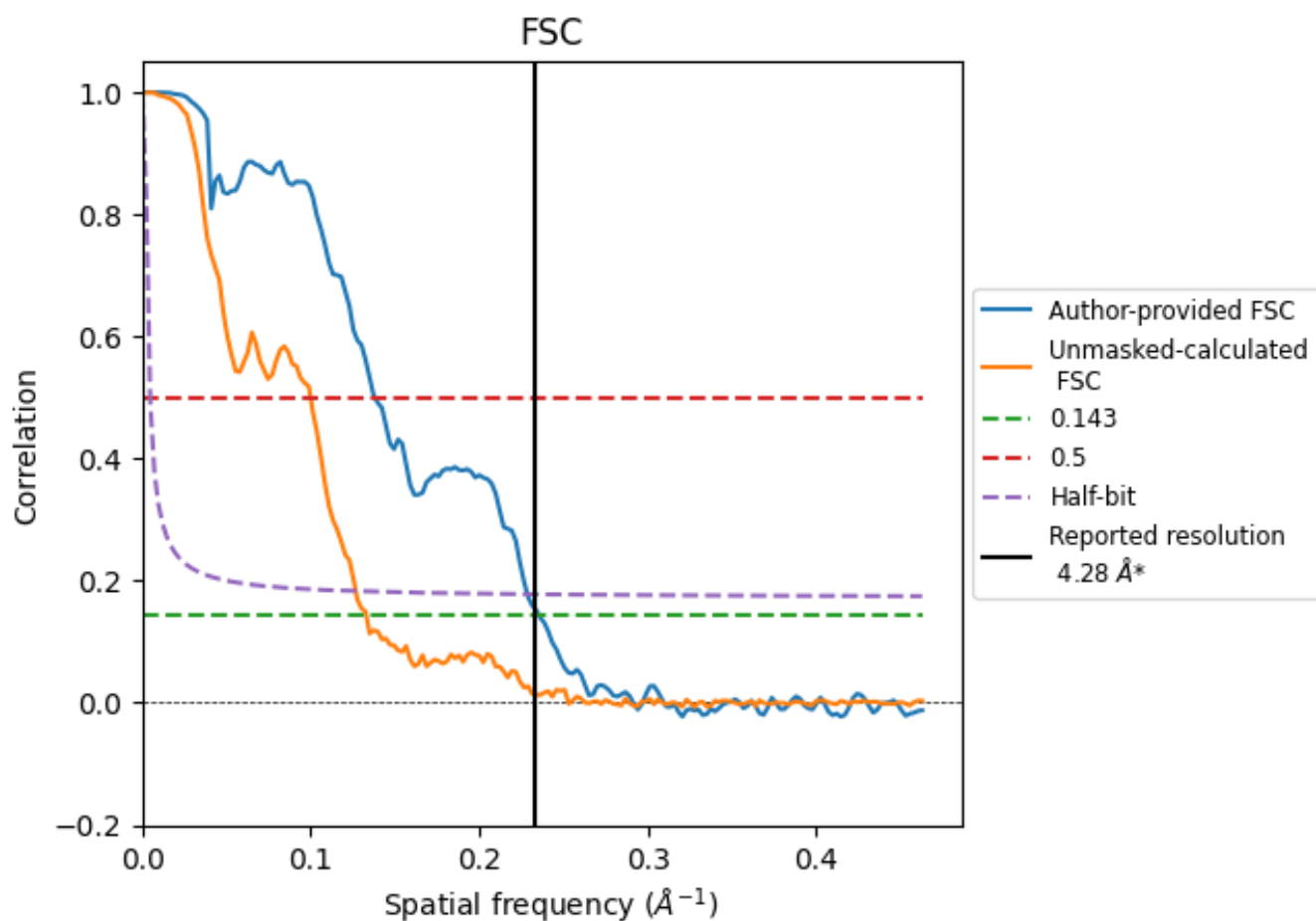


*Reported resolution corresponds to spatial frequency of 0.234 Å⁻¹

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 0.234 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

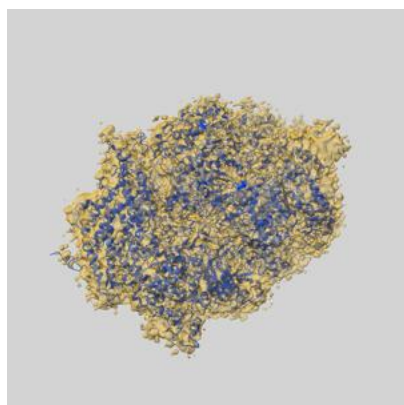
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.28	-	-
Author-provided FSC curve	4.24	7.24	4.37
Unmasked-calculated*	7.52	10.01	7.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.52 differs from the reported value 4.28 by more than 10 %

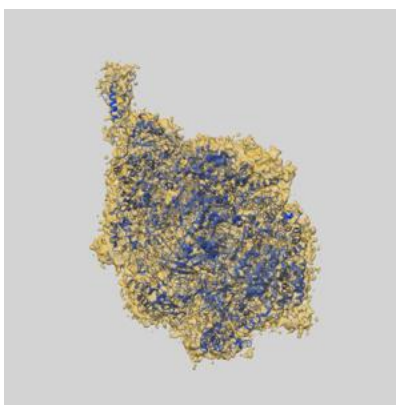
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4787 and PDB model 6RAY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

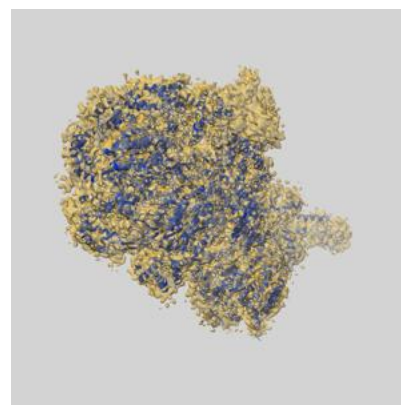
9.1 Map-model overlay [i](#)



X



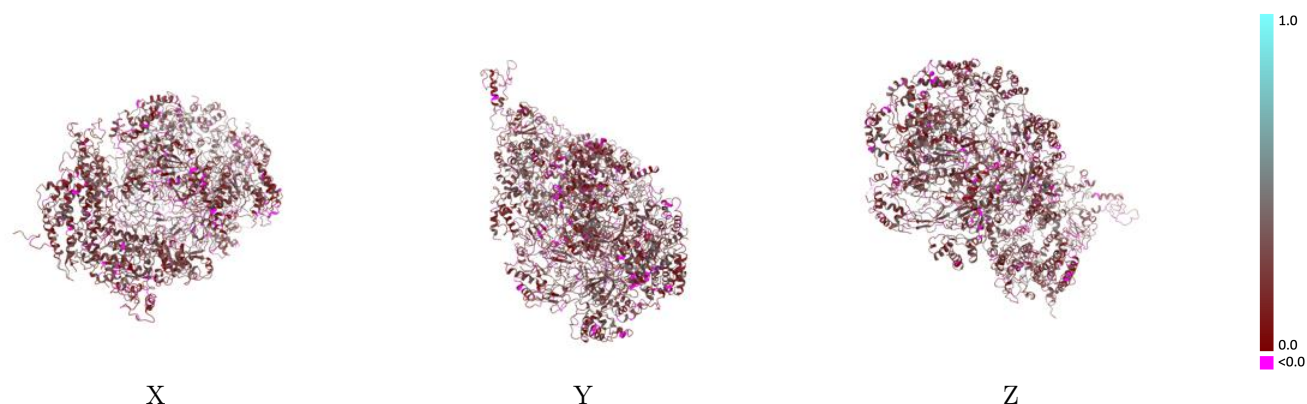
Y



Z

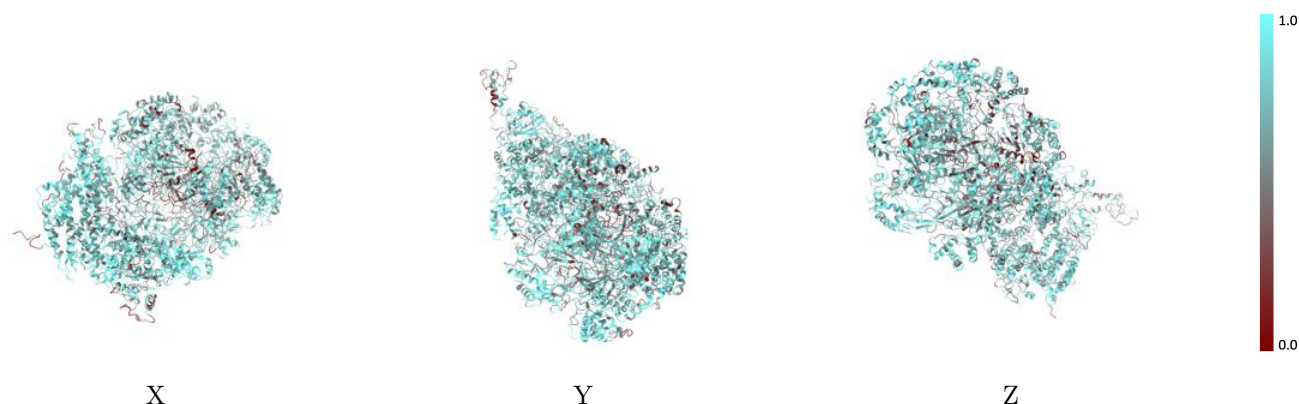
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



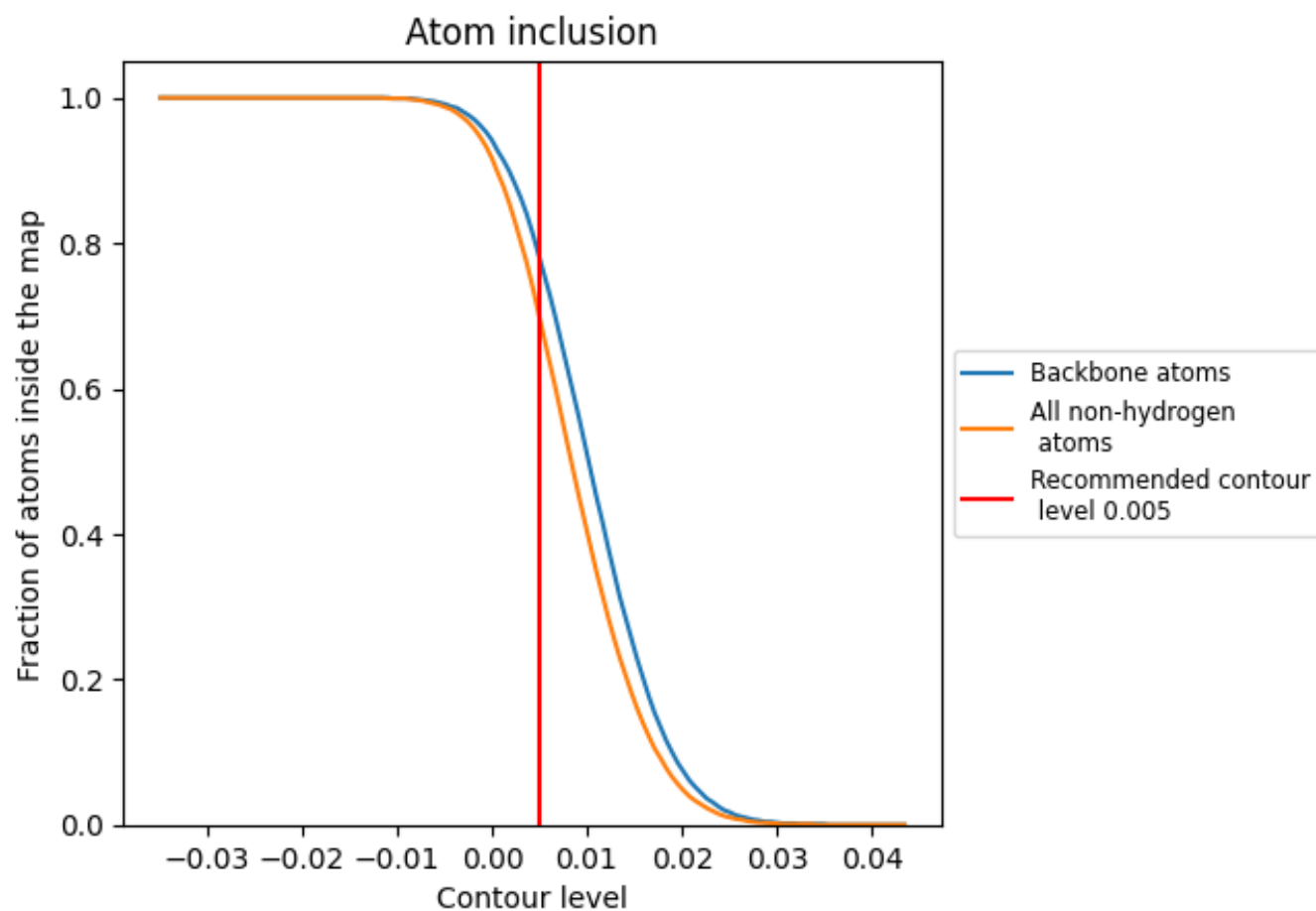
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6990	0.2350
2	0.6740	0.2130
3	0.7080	0.2460
4	0.7180	0.2440
5	0.6610	0.2370
6	0.6710	0.2230
7	0.7080	0.2600
A	0.7190	0.2350
H	0.7230	0.1890
L	0.7860	0.2630
M	0.6690	0.2200
N	0.7530	0.2390
X	0.5330	0.2370

1.0

0.0

<0.0