



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:47 PM UTC

PDB ID : 6RAZ / pdb_00006raz
EMDB ID : EMD-4788
Title : D. melanogaster CMG-DNA, State 2B
Authors : Eickhoff, P.; Martino, F.; Costa, A.
Deposited on : 2019-04-08
Resolution : 4.46 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:

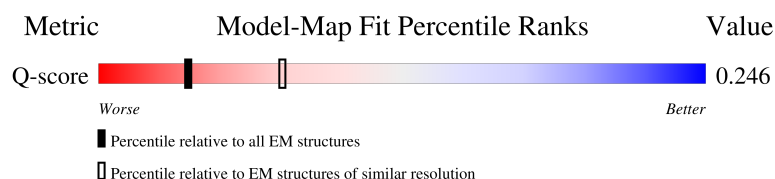
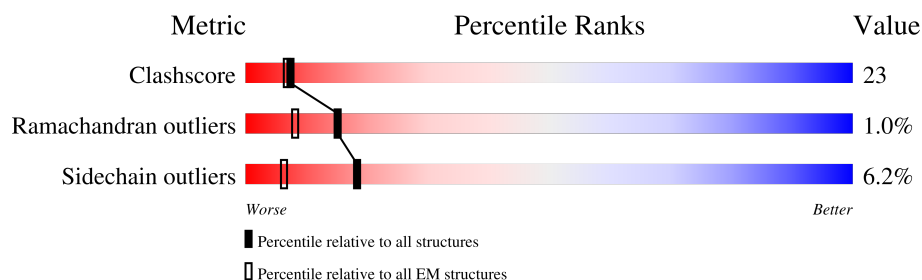
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.46 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.



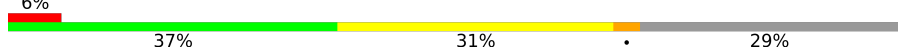
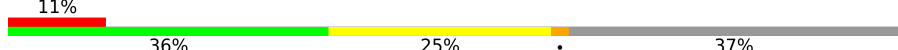
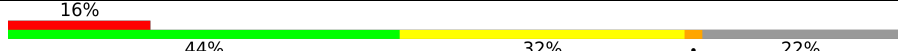
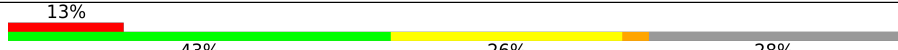
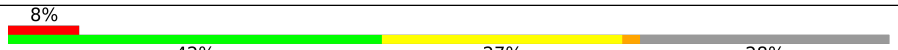
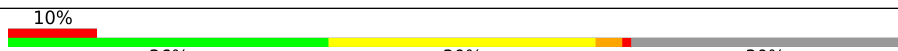
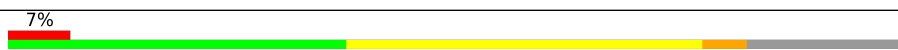
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3001 (3.96 - 4.96)

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	X	21	
2	Y	2	
3	A	575	
4	H	202	

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Mol	Chain	Length	Quality of chain
5	L	203	
6	M	212	
7	N	228	
8	2	887	
9	5	733	
10	6	817	
11	3	819	
12	4	866	
13	7	720	

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
15	ATP	7	801	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 38294 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 DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	21	Total	C	N	O	P	0	0
			425	209	58	137	21		

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	2	Total	C	N	O	P	0	0
			41	19	8	12	2		

- Molecule 3 is a protein called CDC45L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	519	Total	C	N	O	S	0	0
			4190	2685	718	765	22		

- Molecule 4 is a protein called IP07275p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	195	Total	C	N	O	S	0	0
			1583	1007	279	289	8		

- Molecule 5 is a protein called Probable DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	179	Total	C	N	O	S	0	0
			1457	939	243	262	13		

- Molecule 6 is a protein called AT18545p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	150	Total	C	N	O	S	0	0
			1259	806	220	229	4		

- Molecule 7 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	206	Total	C	N	O	S	0	0
			1661	1032	283	333	13		

- Molecule 8 is a protein called DNA replication licensing factor Mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	559	Total	C	N	O	S	0	0
			4442	2811	781	823	27		

- Molecule 9 is a protein called DNA replication licensing factor Mcm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	5	571	Total	C	N	O	S	0	0
			4459	2801	790	841	27		

- Molecule 10 is a protein called DNA replication licensing factor Mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	6	588	Total	C	N	O	S	0	0
			4609	2891	804	892	22		

- Molecule 11 is a protein called DNA replication licensing factor Mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3	590	Total	C	N	O	S	0	0
			4585	2857	825	877	26		

- Molecule 12 is a protein called DNA replication licensing factor MCM4.

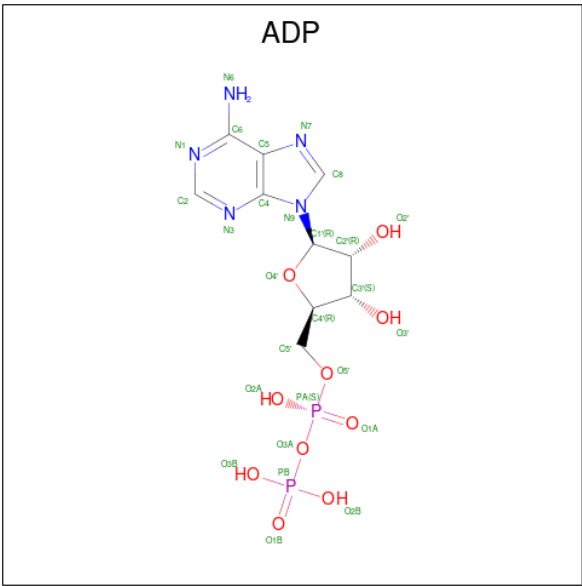
Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	606	Total	C	N	O	S	0	0
			4811	3022	854	913	22		

- Molecule 13 is a protein called DNA replication licensing factor Mcm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	601	Total	C	N	O	S	0	0
			4594	2876	818	875	25		

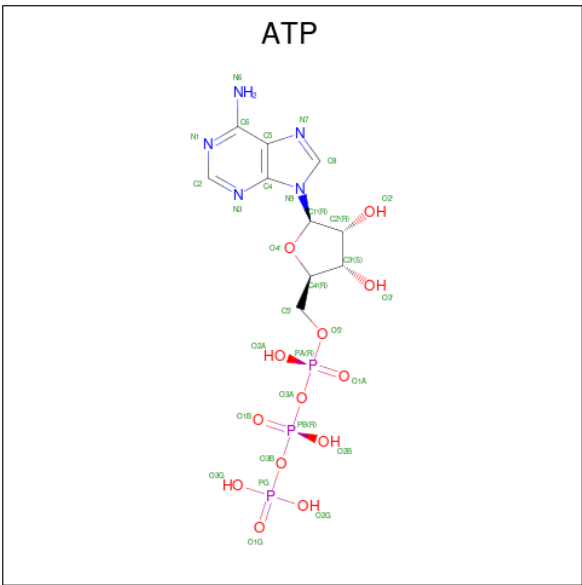
- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	6	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

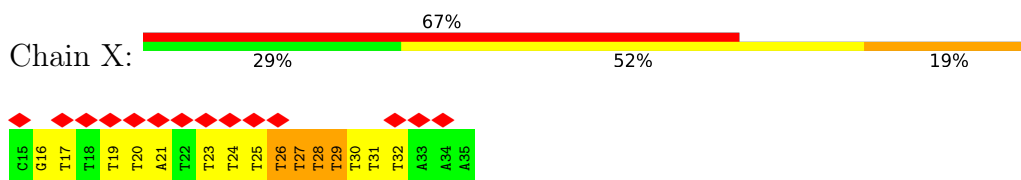


Mol	Chain	Residues	Atoms					AltConf
15	6	1	Total 31	C 10	N 5	O 13	P 3	0
15	3	1	Total 31	C 10	N 5	O 13	P 3	0
15	4	1	Total 31	C 10	N 5	O 13	P 3	0
15	7	1	Total 31	C 10	N 5	O 13	P 3	0

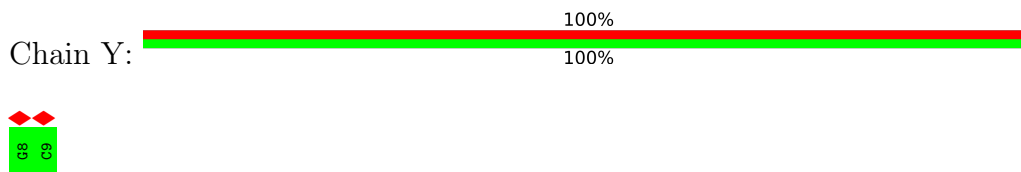
3 Residue-property plots

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

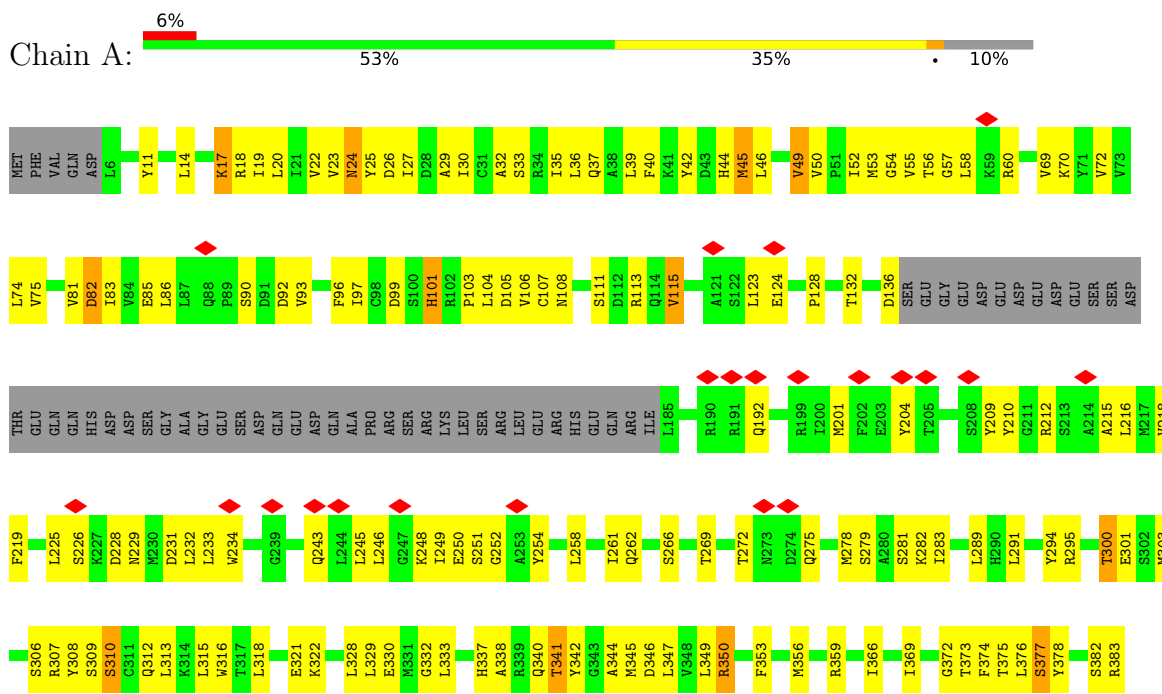
• Molecule 1: DNA

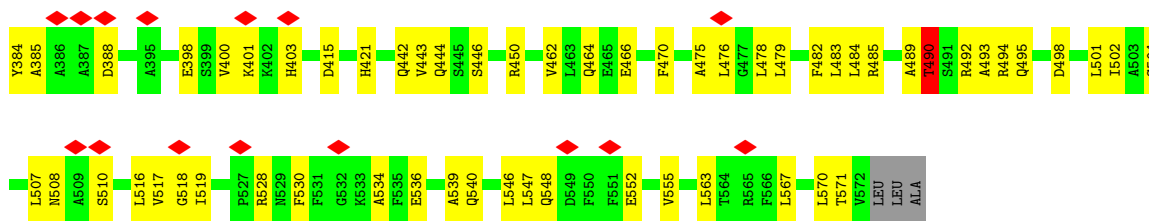


• Molecule 2: DNA

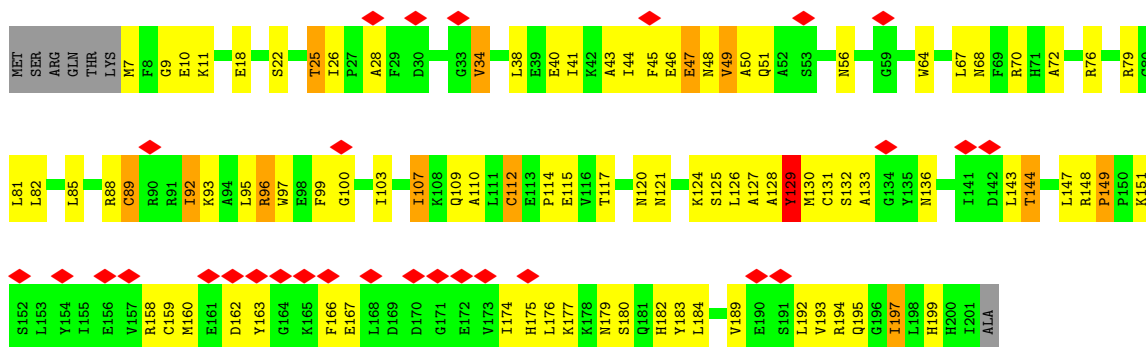


• Molecule 3: CDC45L

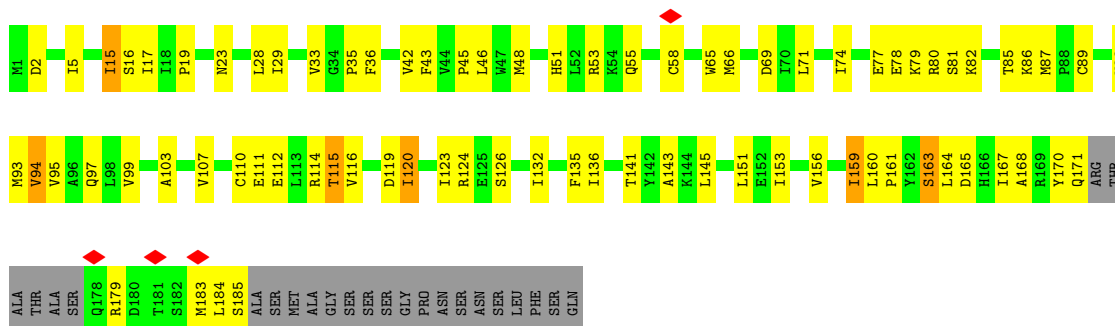




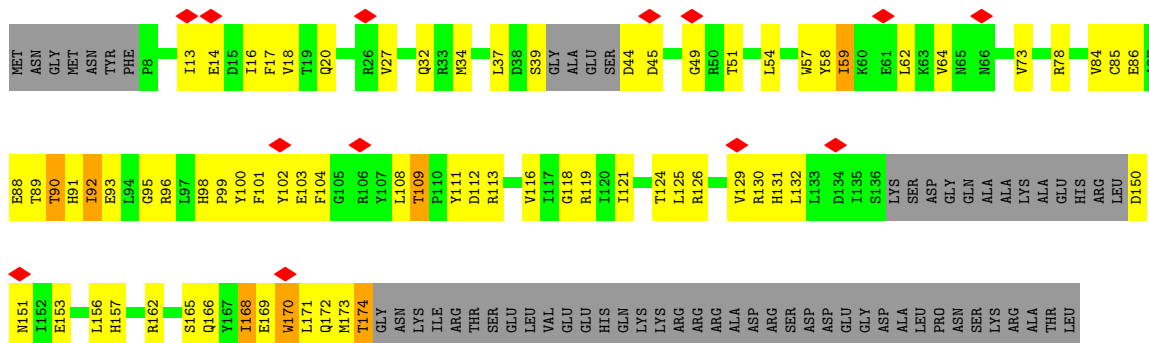
• Molecule 4: IP07275p



• Molecule 5: Probable DNA replication complex GINS protein PSF2



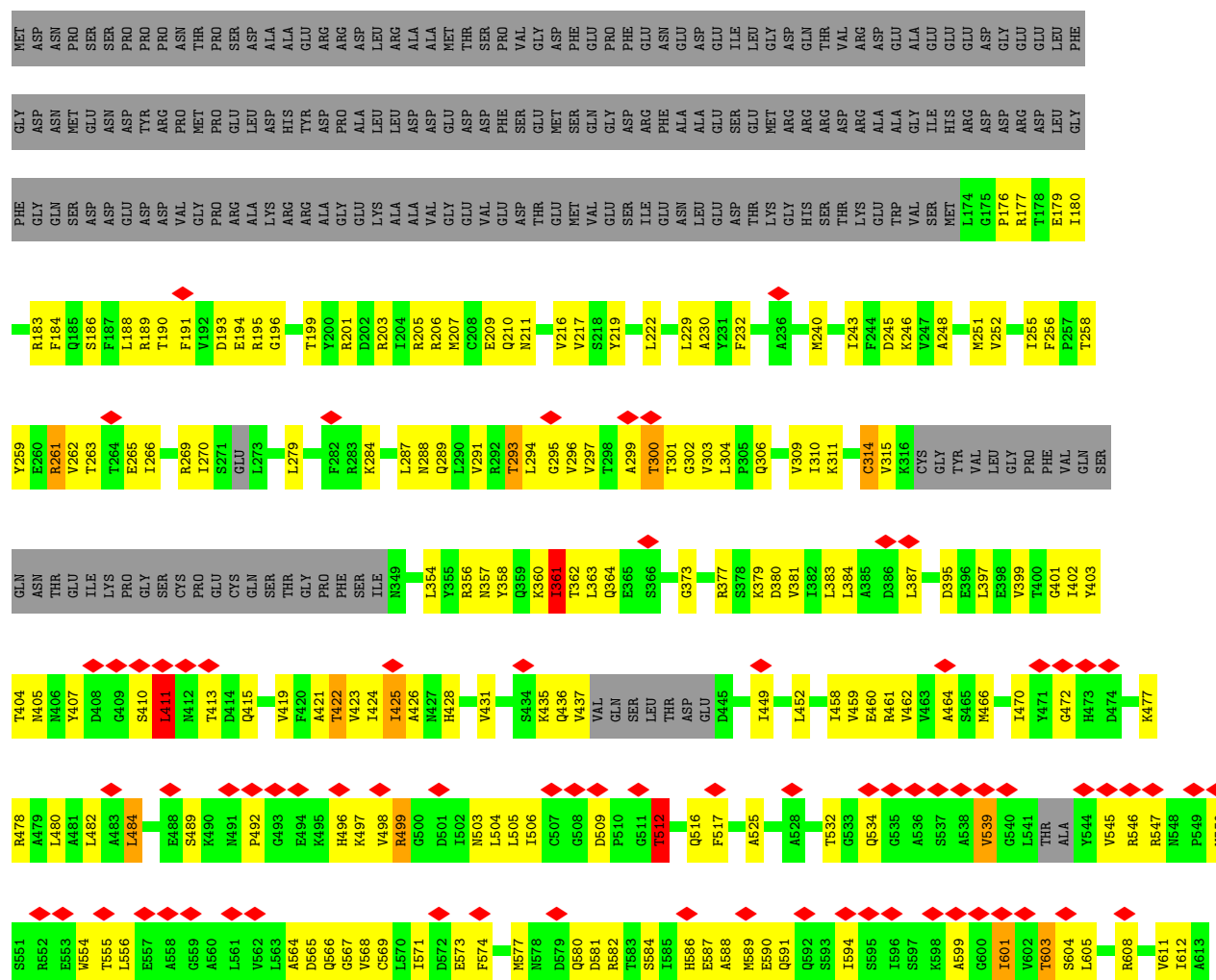
• Molecule 6: AT18545p

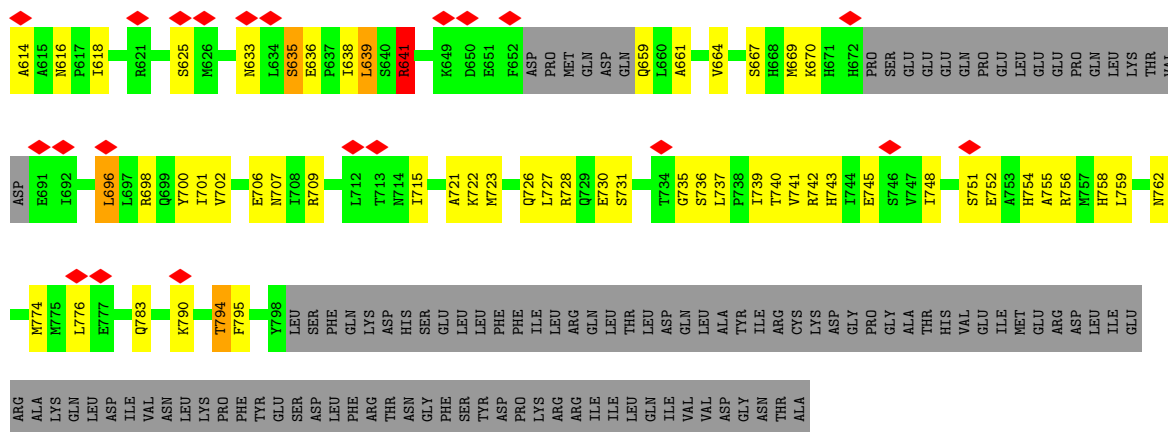


Chain N: 9% 54% 34% 10%

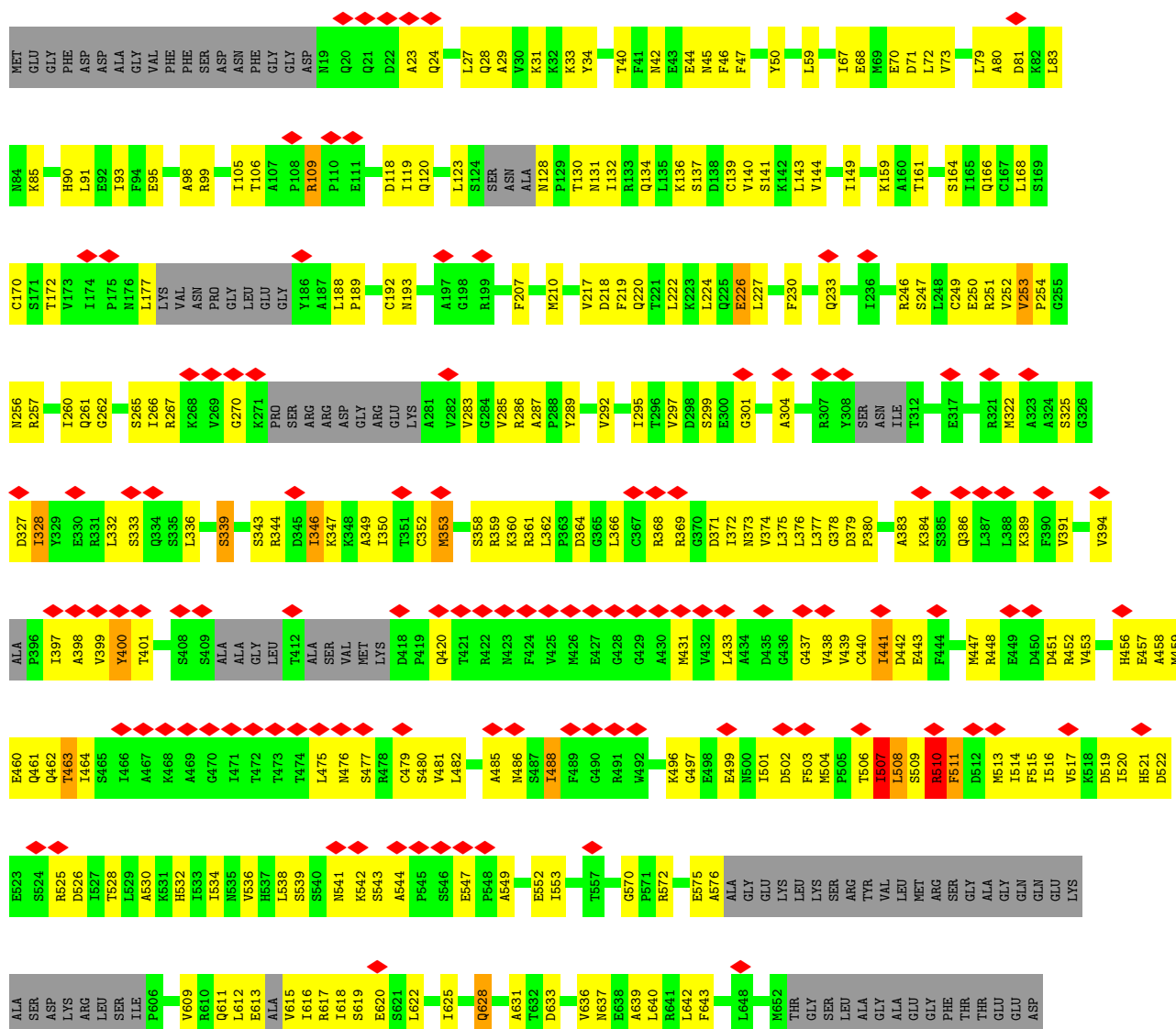
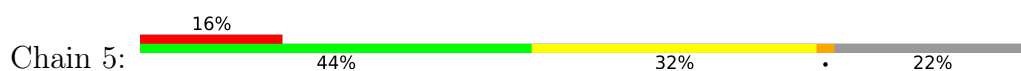


Chain 2: 11% 36% 25% 37%





• Molecule 9: DNA replication licensing factor Mcm5







VAL	K596	R532	L533	A534	K535	H536	I537	T538	V539	V540	H541	S544	K545	Q546	P547	P548	T549	R550	V551	K552	A553	L554	D555	M556	N557	L558	M559	R560	R561	N564	L565	C566	K567	R568	N570	P571	T572	I573	P574	D575	E576	L577	T578	T581	V582	G583	A584	Y585	V586	E587	L588	R589	R590	E591	A592	R593																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
ARG		T466	I467	S468	I469	A470	K471	A472	G473	L474	M475	T476	T477	L478	N479	A480	R481	V482	S483	I484	L485	A486	A487	A488	N489	P490	A491	F492	Y495	R499	T500	V501	E502	Q503	N504	I505	A509	A510	L511	L512	S513	R514	F515	D516	L517	L518	W519	L520	I521	K524	P525	D526	R527	D528	N529	L531																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
GLU		Q402	Y403	T404	T405	G406	R407	G408	S409	S410	G411	V412	G413	L414	T415	A416	A417	K420	D421	P422	L423	T424	G425	E426	M427	T428	L429	E430	G431	G432	A433	L434	V435	L436	A437	D438	Q439	G440	V441	C442	C443	E446	F447	D448	K449	M450	A451	D452	Q453	D454	R455	H459	E460	V461	M462	E463	Q464	Q465																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
LEU		T338	S339	L340	A341	P342	E343	I344	Y345		D349	V350	K351	L354	L355	L356	L357	L358	V359	G360	G361	V362	D363	K364	R365	P366	D367	G368	M369	K370	I371	R372	G373	N374	I375	N376	I377	C378	L379	M380	G381	D382	P383	G384	V385	A386	K387	S388	Q389	L390	L391	G392	Y393	I394	L397	A398	V399	R400	S401																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
ALA		G275	G276	F277	L278	L279	L280	M281	R282	T283	G284	F285	A286	Q287	M288	L289	Q290	G291	L292	L293	S294	E295	T296	F297	L298	Q299	R302	I303	I304	C305	I306	ASN	LYS	ASN	ASP	GLU	ILE	SER	ASP	LYS	ASP	ALA	GLU	LEU	THR	P321	E322	E323	L324	E325	E326	L327	A328	Q329	Y333	E334	R335	L336	A337																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61082	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	0.039	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	X	0.36	0/471	1.12	7/725 (1.0%)
2	Y	0.17	0/45	0.37	0/67
3	A	0.45	0/4280	0.77	0/5790
4	H	0.49	0/1618	0.85	2/2184 (0.1%)
5	L	0.55	0/1492	0.76	0/2017
6	M	0.55	0/1288	0.85	0/1745
7	N	0.47	0/1685	0.77	0/2277
8	2	0.45	0/4515	0.91	8/6089 (0.1%)
9	5	0.57	1/4526 (0.0%)	1.04	14/6092 (0.2%)
10	6	0.48	0/4678	0.91	7/6319 (0.1%)
11	3	0.49	0/4641	0.88	4/6251 (0.1%)
12	4	0.78	1/4896 (0.0%)	1.10	28/6626 (0.4%)
13	7	0.45	2/4661 (0.0%)	0.79	1/6297 (0.0%)
All	All	0.53	4/38796 (0.0%)	0.91	71/52479 (0.1%)

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
3	A	0	4
4	H	0	6
5	L	0	1
6	M	0	2
7	N	0	2
8	2	0	5
9	5	0	15
10	6	0	6
11	3	0	12
12	4	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	7	0	1
All	All	0	66

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	4	491	LYS	C-N	-43.85	0.72	1.33
9	5	507	ILE	C-N	-20.79	1.04	1.33
13	7	220	LEU	C-N	8.39	1.45	1.33
13	7	249	ILE	N-CA	5.22	1.50	1.45

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	4	491	LYS	O-C-N	-24.74	94.09	123.29
9	5	507	ILE	CA-C-N	-22.87	77.85	121.54
9	5	507	ILE	C-N-CA	-22.87	77.85	121.54
8	2	641	ARG	CD-NE-CZ	12.43	141.81	124.40
1	X	27	DT	P-O3'-C3'	11.54	137.50	120.20
9	5	510	ARG	CD-NE-CZ	11.37	140.31	124.40
9	5	270	GLY	CA-C-N	11.21	141.87	121.70
9	5	270	GLY	C-N-CA	11.21	141.87	121.70
12	4	365	ALA	CA-C-N	10.21	139.64	121.97
12	4	365	ALA	C-N-CA	10.21	139.64	121.97
12	4	295	SER	CA-C-N	10.10	138.87	121.29
12	4	295	SER	C-N-CA	10.10	138.87	121.29
1	X	27	DT	O3'-P-O5'	10.06	119.10	104.00
12	4	491	LYS	CA-C-N	9.27	139.25	121.54
12	4	491	LYS	C-N-CA	9.27	139.25	121.54
12	4	648	LEU	CA-C-N	8.68	134.75	123.13
12	4	648	LEU	C-N-CA	8.68	134.75	123.13
11	3	610	ARG	CD-NE-CZ	8.51	136.31	124.40
12	4	646	PHE	CA-C-N	8.35	132.39	120.79
12	4	646	PHE	C-N-CA	8.35	132.39	120.79
12	4	706	ASP	CA-C-N	8.25	136.91	121.81
12	4	706	ASP	C-N-CA	8.25	136.91	121.81
1	X	27	DT	C4'-C3'-O3'	8.23	122.34	110.00
9	5	507	ILE	O-C-N	-7.93	112.66	122.57
10	6	533	ASN	CA-C-N	7.88	133.21	120.60
10	6	533	ASN	C-N-CA	7.88	133.21	120.60
8	2	410	SER	CA-C-N	7.83	135.39	122.07
8	2	410	SER	C-N-CA	7.83	135.39	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	149	ILE	CA-C-N	7.79	131.18	120.35
9	5	149	ILE	C-N-CA	7.79	131.18	120.35
11	3	610	ARG	NE-CZ-NH2	-7.32	112.61	119.20
9	5	511	PHE	O-C-N	-6.96	114.75	123.17
9	5	511	PHE	CA-C-N	6.83	134.59	121.54
9	5	511	PHE	C-N-CA	6.83	134.59	121.54
12	4	575	ILE	CG1-CB-CG2	6.72	130.85	110.70
13	7	327	LEU	CA-CB-CG	6.66	139.62	116.30
12	4	512	GLY	CA-C-N	6.61	137.93	121.80
12	4	512	GLY	C-N-CA	6.61	137.93	121.80
8	2	196	GLY	N-CA-C	6.57	123.12	112.61
8	2	601	ILE	CG1-CB-CG2	6.10	128.99	110.70
1	X	29	DT	C5'-C4'-O4'	-6.03	100.36	109.40
12	4	535	THR	OG1-CB-CG2	6.02	121.33	109.30
12	4	762	GLU	CA-C-N	5.97	128.21	120.44
12	4	762	GLU	C-N-CA	5.97	128.21	120.44
1	X	26	DT	O3'-P-O5'	5.86	112.79	104.00
12	4	572	VAL	CG1-CB-CG2	5.85	123.67	110.80
11	3	387	ARG	CA-C-N	5.81	132.63	121.54
11	3	387	ARG	C-N-CA	5.81	132.63	121.54
10	6	220	ILE	CA-C-N	5.76	130.74	122.45
10	6	220	ILE	C-N-CA	5.76	130.74	122.45
8	2	195	ARG	CA-CB-CG	-5.60	102.89	114.10
10	6	223	ARG	CA-C-N	5.57	127.68	120.44
10	6	223	ARG	C-N-CA	5.57	127.68	120.44
9	5	252	VAL	CG1-CB-CG2	5.55	123.02	110.80
12	4	230	ILE	CG1-CB-CG2	5.49	127.16	110.70
8	2	411	LEU	CB-CG-CD1	5.45	127.06	110.70
12	4	513	ASP	C-N-CD	-5.45	102.64	125.00
12	4	692	TYR	CA-CB-CG	5.42	123.66	113.90
9	5	224	LEU	N-CA-C	5.38	117.58	109.23
10	6	162	VAL	CG1-CB-CG2	5.37	122.62	110.80
9	5	507	ILE	N-CA-CB	-5.36	102.38	111.23
12	4	486	LEU	CA-C-O	-5.35	112.86	120.51
12	4	615	ILE	CG1-CB-CG2	5.28	126.55	110.70
1	X	28	DT	P-O5'-C5'	5.25	127.88	120.00
4	H	96	ARG	CA-CB-CG	5.15	124.41	114.10
12	4	693	ILE	CG1-CB-CG2	5.15	126.16	110.70
1	X	29	DT	P-O3'-C3'	5.15	127.92	120.20
4	H	129	TYR	CA-CB-CG	5.08	123.05	113.90
12	4	488	GLY	N-CA-C	5.07	125.20	113.18
8	2	599	ALA	N-CA-C	-5.05	100.04	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	4	450	LEU	CB-CG-CD1	5.03	125.80	110.70

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	2	261	ARG	Peptide
8	2	311	LYS	Peptide
8	2	361	ILE	Peptide
8	2	459	VAL	Peptide
8	2	641	ARG	Sidechain
11	3	201	MET	Peptide
11	3	219	ASP	Peptide
11	3	222	LEU	Peptide
11	3	257	LEU	Peptide
11	3	28	ILE	Peptide
11	3	387	ARG	Sidechain
11	3	392	ALA	Peptide
11	3	462	GLU	Peptide
11	3	473	ARG	Sidechain
11	3	501	ARG	Peptide
11	3	546	HIS	Peptide
11	3	610	ARG	Sidechain
12	4	327	GLN	Peptide
12	4	343	ILE	Peptide
12	4	384	LYS	Peptide
12	4	473	TYR	Peptide
12	4	484	LEU	Peptide
12	4	487	PHE	Peptide
12	4	488	GLY	Peptide
12	4	493	LYS	Peptide
12	4	499	ARG	Peptide
12	4	629	ARG	Peptide
12	4	645	ARG	Sidechain
12	4	750	ARG	Peptide
9	5	109	ARG	Peptide
9	5	193	ASN	Peptide
9	5	251	ARG	Sidechain
9	5	286	ARG	Peptide
9	5	292	VAL	Peptide
9	5	304	ALA	Peptide
9	5	400	TYR	Peptide

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Mol	Chain	Res	Type	Group
9	5	44	GLU	Peptide
9	5	458	ALA	Peptide
9	5	488	ILE	Peptide
9	5	497	GLY	Peptide
9	5	507	ILE	Mainchain
9	5	510	ARG	Sidechain
9	5	552	GLU	Peptide
9	5	628	GLN	Peptide
10	6	106	VAL	Peptide
10	6	312	VAL	Peptide
10	6	373	THR	Peptide
10	6	488	ARG	Peptide
10	6	549	SER	Peptide
10	6	611	ARG	Sidechain
13	7	474	ILE	Peptide
3	A	101	HIS	Peptide
3	A	294	TYR	Peptide
3	A	490	THR	Peptide
3	A	82	ASP	Peptide
4	H	112	CYS	Peptide
4	H	147	LEU	Peptide
4	H	148	ARG	Peptide
4	H	180	SER	Peptide
4	H	197	ILE	Peptide
4	H	34	VAL	Peptide
5	L	145	LEU	Peptide
6	M	96	ARG	Peptide
6	M	98	HIS	Peptide
7	N	154	LYS	Peptide
7	N	180	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	425	0	247	26	0
2	Y	41	0	23	0	0
3	A	4190	0	4167	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1583	0	1567	64	0
5	L	1457	0	1476	65	0
6	M	1259	0	1233	59	0
7	N	1661	0	1609	67	0
8	2	4442	0	4503	176	0
9	5	4459	0	4452	215	0
10	6	4609	0	4509	221	0
11	3	4585	0	4624	204	0
12	4	4811	0	4768	251	0
13	7	4594	0	4509	391	0
14	5	27	0	11	5	0
14	6	27	0	12	5	0
15	3	31	0	12	7	0
15	4	31	0	10	5	0
15	6	31	0	11	6	0
15	7	31	0	9	11	0
All	All	38294	0	37752	1769	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 23.

All (1769) 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)
11:3:422:GLU:HG3	11:3:473:ARG:NH1	1.24	1.41
9:5:460:GLU:CG	9:5:510:ARG:HD2	1.54	1.34
11:3:418:HIS:NE2	11:3:473:ARG:NH2	1.77	1.31
10:6:611:ARG:NH1	14:6:901:ADP:O1B	1.64	1.30
9:5:506:THR:O	9:5:509:SER:CB	1.81	1.29
9:5:506:THR:O	9:5:509:SER:HB2	1.23	1.27
11:3:418:HIS:CD2	11:3:473:ARG:CZ	2.20	1.24
10:6:544:ILE:CG2	10:6:547:LEU:HD23	1.69	1.21
13:7:404:THR:HG21	13:7:414:LEU:CD2	1.72	1.17
10:6:544:ILE:HG23	10:6:547:LEU:HD23	1.21	1.16
10:6:544:ILE:CG1	10:6:547:LEU:HD22	1.79	1.13
10:6:544:ILE:HG12	10:6:547:LEU:CD2	1.80	1.11
11:3:422:GLU:CG	11:3:473:ARG:NH1	2.14	1.09
10:6:611:ARG:HH11	14:6:901:ADP:PB	1.77	1.07
9:5:460:GLU:OE2	9:5:510:ARG:CZ	2.03	1.07
11:3:422:GLU:OE2	11:3:473:ARG:NH2	1.87	1.07
3:A:289:LEU:HD13	3:A:291:LEU:HD12	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:544:ILE:HG12	10:6:547:LEU:HD22	1.07	1.06
11:3:418:HIS:CD2	11:3:473:ARG:NH1	2.24	1.05
12:4:494:HIS:NE2	12:4:502:PHE:HB2	1.73	1.03
13:7:474:ILE:HG21	13:7:476:THR:HG23	1.39	1.01
10:6:544:ILE:HG23	10:6:547:LEU:CD2	1.90	1.01
13:7:379:LEU:HD13	13:7:387:LYS:HD3	1.40	1.01
9:5:460:GLU:HG2	9:5:510:ARG:CD	1.91	1.00
9:5:375:LEU:HD21	9:5:511:PHE:CD2	1.98	0.98
11:3:422:GLU:CD	11:3:473:ARG:HH22	1.72	0.97
9:5:391:VAL:HA	9:5:394:VAL:HG22	1.44	0.96
11:3:422:GLU:HG3	11:3:473:ARG:CZ	1.94	0.96
9:5:460:GLU:CG	9:5:510:ARG:CD	2.43	0.96
9:5:460:GLU:HG2	9:5:510:ARG:HD2	0.96	0.96
10:6:544:ILE:HA	10:6:547:LEU:HB2	1.47	0.96
9:5:439:VAL:HG23	9:5:481:VAL:HG13	1.45	0.95
11:3:422:GLU:HG3	11:3:473:ARG:HH12	1.25	0.95
13:7:404:THR:HG21	13:7:414:LEU:HD21	1.48	0.94
12:4:502:PHE:CE2	12:4:737:GLU:OE1	2.21	0.94
9:5:622:LEU:HD22	9:5:636:VAL:HG22	1.49	0.93
11:3:612:LEU:HD23	11:3:615:LEU:HD12	1.48	0.93
13:7:386:ALA:HB1	13:7:389:GLN:HB2	1.52	0.92
9:5:369:ARG:NH2	9:5:510:ARG:HB2	1.84	0.92
12:4:494:HIS:NE2	12:4:502:PHE:CB	2.32	0.91
9:5:506:THR:O	9:5:509:SER:HB3	1.70	0.91
12:4:590:HIS:O	12:4:590:HIS:CG	2.23	0.91
10:6:546:ASP:HB3	10:6:553:GLU:HA	1.52	0.91
11:3:418:HIS:HD2	11:3:473:ARG:CZ	1.83	0.90
12:4:494:HIS:CE1	12:4:502:PHE:H	1.92	0.87
13:7:416:ALA:HA	13:7:431:GLY:HA2	1.54	0.87
10:6:232:ALA:HB2	10:6:443:LEU:HB3	1.57	0.87
11:3:418:HIS:NE2	11:3:473:ARG:CZ	2.33	0.87
11:3:422:GLU:CD	11:3:473:ARG:NH2	2.33	0.86
10:6:421:LEU:HD12	10:6:422:THR:HG23	1.58	0.86
13:7:462:MET:HG3	13:7:514:ARG:HG3	1.56	0.85
9:5:460:GLU:CD	9:5:510:ARG:CD	2.48	0.85
13:7:387:LYS:CD	13:7:487:ALA:HB1	2.06	0.85
13:7:467:ILE:HG22	13:7:467:ILE:O	1.74	0.85
7:N:110:GLN:O	7:N:114:THR:OG1	1.94	0.85
11:3:394:VAL:HA	11:3:397:ASP:OD1	1.76	0.84
12:4:502:PHE:HE2	12:4:737:GLU:CD	1.84	0.84
1:X:27:DT:H1'	1:X:28:DT:H5'	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3:600:ASP:O	11:3:604:THR:OG1	1.96	0.83
9:5:375:LEU:HD21	9:5:511:PHE:CG	2.12	0.83
9:5:375:LEU:CD2	9:5:511:PHE:CD2	2.60	0.83
10:6:345:SER:O	10:6:557:ARG:NH2	2.12	0.83
10:6:544:ILE:CG2	10:6:547:LEU:CD2	2.49	0.83
9:5:339:SER:O	9:5:542:LYS:NZ	2.12	0.83
13:7:438:ASP:HB3	13:7:439:GLN:HE21	1.43	0.82
13:7:387:LYS:HA	13:7:390:LEU:HD21	1.59	0.82
4:H:114:PRO:O	4:H:117:THR:OG1	1.97	0.82
8:2:435:LYS:NZ	8:2:525:ALA:O	2.13	0.82
9:5:459:MET:HE3	9:5:510:ARG:HG3	1.59	0.82
13:7:467:ILE:O	13:7:467:ILE:CG2	2.27	0.81
8:2:186:SER:O	8:2:190:THR:OG1	1.98	0.81
13:7:588:LEU:HD22	13:7:589:ARG:HD2	1.63	0.81
9:5:456:HIS:CD2	9:5:460:GLU:OE2	2.34	0.81
11:3:263:SER:O	11:3:264:LEU:HG	1.81	0.81
13:7:416:ALA:HB1	13:7:429:LEU:HB2	1.63	0.81
12:4:199:LYS:O	12:4:203:ILE:N	2.14	0.81
13:7:387:LYS:HD2	13:7:487:ALA:HB1	1.63	0.80
9:5:460:GLU:CD	9:5:510:ARG:HD2	2.05	0.80
10:6:544:ILE:HG21	10:6:547:LEU:HD23	1.63	0.80
12:4:686:MET:O	12:4:690:ARG:NH2	2.15	0.80
13:7:383:PRO:HD2	13:7:385:VAL:HG12	1.62	0.80
8:2:641:ARG:NH1	14:5:801:ADP:O1B	2.15	0.80
10:6:611:ARG:NH1	14:6:901:ADP:PB	2.47	0.80
8:2:516:GLN:OE1	14:6:901:ADP:O2A	1.99	0.80
9:5:477:SER:HG	9:5:479:CYS:HG	1.23	0.80
3:A:306:SER:O	3:A:310:SER:OG	2.01	0.79
8:2:296:VAL:O	8:2:364:GLN:N	2.15	0.79
12:4:497:LEU:HD21	12:4:499:ARG:HE	1.46	0.79
12:4:672:TYR:OH	13:7:571:PRO:O	2.00	0.79
12:4:502:PHE:CE2	12:4:737:GLU:CD	2.61	0.79
13:7:439:GLN:HE22	13:7:481:ARG:HD2	1.48	0.79
11:3:422:GLU:CG	11:3:473:ARG:CZ	2.58	0.79
3:A:210:TYR:OH	3:A:552:GLU:OE1	2.01	0.78
9:5:377:LEU:HA	9:5:485:ALA:HB3	1.64	0.78
12:4:531:ARG:NH1	12:4:569:ASP:O	2.16	0.78
7:N:114:THR:O	7:N:117:GLN:NE2	2.15	0.78
9:5:572:ARG:NH2	11:3:500:HIS:O	2.17	0.78
13:7:409:SER:HB3	13:7:414:LEU:HG	1.64	0.78
12:4:623:GLU:OE2	12:4:635:ASN:ND2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:360:LYS:NZ	9:5:570:GLY:O	2.15	0.78
8:2:625:SER:OG	8:2:783:GLN:O	2.01	0.77
13:7:637:LEU:O	13:7:640:SER:OG	2.01	0.77
8:2:379:LYS:NZ	8:2:380:ASP:O	2.16	0.77
10:6:558:ALA:O	10:6:559:TYR:HB2	1.85	0.77
8:2:577:MET:O	8:2:582:ARG:NH1	2.18	0.77
8:2:728:ARG:NH1	9:5:519:ASP:O	2.17	0.77
3:A:81:VAL:O	3:A:108:ASN:ND2	2.18	0.77
10:6:394:LYS:HZ2	10:6:394:LYS:HB3	1.49	0.77
12:4:670:SER:O	12:4:674:VAL:N	2.16	0.77
5:L:170:TYR:OH	5:L:183:MET:SD	2.42	0.77
9:5:459:MET:CE	9:5:510:ARG:CG	2.62	0.77
13:7:340:LEU:HD13	13:7:559:MET:HE1	1.67	0.76
10:6:174:CYS:HB2	10:6:177:PRO:O	1.85	0.76
9:5:506:THR:HB	9:5:510:ARG:HH22	1.50	0.76
11:3:422:GLU:CG	11:3:473:ARG:HH12	1.90	0.76
10:6:393:ALA:HB2	15:6:902:ATP:H2'	1.66	0.76
11:3:425:ARG:NH2	11:3:436:SER:OG	2.17	0.76
7:N:81:ASP:OD1	7:N:82:LYS:NZ	2.17	0.76
3:A:22:VAL:HG12	3:A:29:ALA:HB1	1.67	0.76
3:A:356:MET:SD	3:A:359:ARG:NH2	2.58	0.76
5:L:93:MET:HB2	5:L:151:LEU:HD22	1.68	0.76
9:5:358:SER:OG	9:5:620:GLU:OE1	2.05	0.76
8:2:565:ASP:O	9:5:233:GLN:NE2	2.19	0.75
13:7:467:ILE:HG21	13:7:478:LEU:HD12	1.67	0.75
11:3:298:LEU:HB2	11:3:309:LYS:HZ1	1.51	0.75
3:A:234:TRP:HZ2	3:A:376:LEU:HD23	1.52	0.75
13:7:404:THR:HG21	13:7:414:LEU:HD22	1.63	0.74
8:2:754:HIS:O	8:2:758:HIS:ND1	2.20	0.74
9:5:520:ILE:O	9:5:525:ARG:NH2	2.19	0.74
12:4:521:MET:O	12:4:525:VAL:HG23	1.88	0.74
13:7:402:GLN:HG2	13:7:433:ALA:HB1	1.66	0.74
13:7:452:ASP:HA	13:7:455:ARG:HH11	1.52	0.74
12:4:490:THR:HG21	12:4:702:PRO:HD2	1.70	0.74
8:2:364:GLN:NE2	8:2:377:ARG:O	2.21	0.73
12:4:494:HIS:CE1	12:4:502:PHE:N	2.55	0.73
13:7:386:ALA:HB2	15:7:801:ATP:H3'	1.68	0.73
3:A:17:LYS:NZ	4:H:183:TYR:OH	2.21	0.73
9:5:159:LYS:O	9:5:217:VAL:N	2.21	0.73
5:L:94:VAL:HB	5:L:151:LEU:HD21	1.68	0.73
12:4:538:ARG:N	12:4:581:MET:SD	2.61	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:232:ALA:CB	10:6:443:LEU:HB3	2.18	0.73
15:4:901:ATP:O4'	13:7:604:ARG:NH1	2.13	0.73
13:7:409:SER:CB	13:7:414:LEU:HG	2.19	0.73
11:3:430:LYS:N	13:7:408:GLY:O	2.22	0.73
9:5:384:LYS:HD2	9:5:517:VAL:HG21	1.71	0.73
13:7:350:VAL:HG22	13:7:519:TRP:HZ3	1.53	0.73
3:A:466:GLU:OE1	3:A:508:ASN:N	2.22	0.73
8:2:460:GLU:O	8:2:464:ALA:N	2.21	0.72
12:4:514:PRO:HG2	12:4:516:THR:HG23	1.71	0.72
8:2:304:LEU:O	8:2:358:TYR:N	2.22	0.72
10:6:59:PHE:N	10:6:109:THR:O	2.19	0.72
7:N:65:LEU:O	7:N:69:GLN:NE2	2.23	0.72
11:3:626:ARG:NH1	11:3:635:ASP:OD2	2.22	0.72
5:L:79:LYS:O	5:L:82:LYS:NZ	2.23	0.72
8:2:436:GLN:O	8:2:698:ARG:NH2	2.23	0.72
13:7:376:ASN:N	13:7:516:ASP:OD2	2.21	0.72
10:6:118:ARG:HH12	10:6:213:CYS:CB	2.01	0.72
10:6:546:ASP:CB	10:6:553:GLU:HA	2.19	0.72
10:6:426:VAL:O	10:6:427:ARG:NE	2.23	0.72
8:2:184:PHE:O	8:2:188:LEU:HD12	1.90	0.72
9:5:456:HIS:NE2	9:5:460:GLU:OE2	2.23	0.72
11:3:490:GLN:NE2	11:3:493:SER:OG	2.22	0.72
12:4:516:THR:C	15:4:901:ATP:H5'1	2.14	0.72
3:A:104:LEU:O	3:A:204:TYR:OH	2.08	0.71
10:6:475:SER:OG	10:6:483:ALA:O	2.04	0.71
10:6:478:ARG:O	10:6:482:ARG:NH2	2.22	0.71
10:6:120:LEU:HD23	10:6:120:LEU:C	2.15	0.71
12:4:482:ILE:HA	12:4:485:GLN:HE21	1.54	0.71
7:N:79:ASP:O	7:N:82:LYS:NZ	2.22	0.71
10:6:373:THR:OG1	10:6:376:THR:O	2.07	0.71
3:A:281:SER:O	3:A:376:LEU:HD21	1.90	0.71
9:5:460:GLU:CD	9:5:510:ARG:CZ	2.63	0.71
11:3:454:TYR:O	11:3:463:ASN:ND2	2.24	0.71
8:2:306:GLN:OE1	8:2:356:ARG:NH2	2.22	0.71
12:4:299:ILE:O	12:4:352:LYS:NZ	2.20	0.71
4:H:45:PHE:O	4:H:49:VAL:N	2.23	0.71
9:5:534:ILE:O	9:5:538:LEU:N	2.23	0.71
12:4:507:HIS:HB3	12:4:615:ILE:HB	1.72	0.71
11:3:470:LEU:HA	11:3:473:ARG:HG2	1.73	0.71
12:4:500:GLN:HG3	12:4:502:PHE:HD1	1.55	0.71
1:X:26:DT:O2	12:4:556:ARG:NH2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:404:THR:CG2	13:7:414:LEU:HD21	2.21	0.71
3:A:36:LEU:HD13	3:A:39:LEU:HB3	1.71	0.70
3:A:485:ARG:O	3:A:490:THR:OG1	2.09	0.70
10:6:423:ALA:N	10:6:438:ALA:O	2.25	0.70
11:3:335:ASN:OD1	11:3:443:VAL:N	2.24	0.70
3:A:494:ARG:NE	3:A:498:ASP:OD2	2.22	0.70
9:5:459:MET:CE	9:5:510:ARG:HG3	2.21	0.70
13:7:472:ALA:HB3	13:7:474:ILE:HD11	1.73	0.70
9:5:477:SER:OG	9:5:479:CYS:SG	2.43	0.70
4:H:112:CYS:SG	7:N:154:LYS:NZ	2.62	0.70
10:6:544:ILE:HG23	10:6:547:LEU:HB3	1.72	0.70
11:3:333:ASP:OD2	11:3:442:SER:OG	2.07	0.70
10:6:544:ILE:HG23	10:6:547:LEU:CB	2.22	0.69
8:2:509:ASP:O	8:2:512:THR:OG1	2.10	0.69
12:4:642:LEU:HD22	12:4:645:ARG:NH2	2.08	0.69
8:2:566:GLN:N	8:2:608:ARG:O	2.25	0.69
10:6:612:GLN:O	10:6:615:SER:OG	2.10	0.69
12:4:744:GLU:OE1	12:4:744:GLU:N	2.25	0.69
8:2:296:VAL:N	8:2:364:GLN:O	2.26	0.69
13:7:234:GLU:HG3	13:7:255:ILE:O	1.92	0.69
13:7:387:LYS:O	13:7:391:LEU:HG	1.91	0.69
11:3:412:ILE:O	11:3:415:THR:OG1	2.09	0.69
13:7:465:GLN:HA	13:7:480:ALA:N	2.06	0.69
7:N:143:GLU:O	7:N:147:ASN:ND2	2.25	0.69
10:6:540:ILE:O	10:6:544:ILE:HD12	1.92	0.69
3:A:301:GLU:OE1	3:A:301:GLU:N	2.26	0.69
11:3:298:LEU:HB2	11:3:309:LYS:NZ	2.08	0.69
13:7:528:ASP:HA	13:7:531:LEU:HD11	1.74	0.69
3:A:492:ARG:NH1	3:A:495:GLN:OE1	2.25	0.69
4:H:51:GLN:OE1	4:H:56:ASN:ND2	2.25	0.69
8:2:571:ILE:O	8:2:614:ALA:N	2.26	0.68
6:M:32:GLN:NE2	6:M:44:ASP:O	2.26	0.68
8:2:735:GLY:O	8:2:783:GLN:NE2	2.27	0.68
11:3:309:LYS:HA	11:3:312:ILE:HD12	1.75	0.68
12:4:710:GLN:HA	12:4:713:ILE:HB	1.75	0.68
13:7:585:TYR:OH	13:7:589:ARG:NH1	2.26	0.68
6:M:173:MET:N	6:M:173:MET:SD	2.67	0.68
8:2:299:ALA:O	8:2:362:THR:OG1	2.07	0.68
9:5:496:LYS:NZ	9:5:499:GLU:OE1	2.26	0.68
11:3:507:GLU:O	11:3:544:LEU:N	2.26	0.68
13:7:379:LEU:O	13:7:488:ALA:N	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:380:MET:SD	13:7:520:LEU:HG	2.34	0.68
4:H:93:LYS:NZ	7:N:113:GLU:OE1	2.27	0.68
8:2:667:SER:O	8:2:670:LYS:NZ	2.23	0.67
11:3:299:ALA:HB3	11:3:309:LYS:HD2	1.75	0.67
10:6:646:LYS:O	10:6:650:ARG:N	2.27	0.67
12:4:670:SER:OG	13:7:578:THR:OG1	2.12	0.67
13:7:160:LEU:HA	13:7:275:GLY:O	1.94	0.67
1:X:26:DT:H4'	10:6:425:VAL:HG21	1.76	0.67
4:H:47:GLU:OE1	4:H:47:GLU:N	2.27	0.67
8:2:452:LEU:O	8:2:461:ARG:NH2	2.27	0.67
10:6:557:ARG:NH2	10:6:559:TYR:O	2.27	0.67
13:7:355:LEU:O	13:7:359:VAL:HG23	1.94	0.67
5:L:93:MET:N	5:L:93:MET:SD	2.68	0.67
12:4:200:LEU:HD21	12:4:248:PHE:HA	1.74	0.67
4:H:167:GLU:HG2	4:H:176:LEU:HD22	1.76	0.67
4:H:79:ARG:NH1	4:H:82:LEU:HD22	2.10	0.67
5:L:151:LEU:HD23	6:M:170:TRP:CH2	2.30	0.67
12:4:472:ILE:HG22	12:4:474:GLU:H	1.59	0.67
3:A:74:LEU:HB3	3:A:97:ILE:HG22	1.77	0.67
13:7:450:MET:HG2	13:7:454:ASP:OD2	1.94	0.67
6:M:88:GLU:OE2	6:M:92:ILE:N	2.28	0.66
6:M:129:VAL:HG12	6:M:130:ARG:NH1	2.10	0.66
13:7:604:ARG:HG3	13:7:607:LEU:HD23	1.77	0.66
4:H:64:TRP:O	4:H:68:ASN:ND2	2.28	0.66
12:4:454:LEU:O	12:4:460:ILE:HD11	1.95	0.66
12:4:512:GLY:N	12:4:619:ALA:O	2.28	0.66
6:M:34:MET:N	6:M:39:SER:OG	2.29	0.66
8:2:379:LYS:NZ	8:2:422:THR:O	2.20	0.66
8:2:413:THR:N	10:6:168:PHE:O	2.28	0.66
9:5:460:GLU:CD	9:5:510:ARG:NE	2.54	0.66
10:6:394:LYS:HB3	10:6:394:LYS:NZ	2.10	0.66
8:2:219:TYR:OH	8:2:229:LEU:O	2.08	0.66
8:2:790:LYS:O	8:2:794:THR:OG1	2.14	0.66
12:4:202:GLU:O	12:4:206:LEU:HD22	1.95	0.66
8:2:436:GLN:HE21	8:2:437:VAL:HG22	1.61	0.66
11:3:336:VAL:O	11:3:444:LEU:HD22	1.96	0.66
13:7:571:PRO:HG3	13:7:617:ALA:HB3	1.77	0.66
4:H:143:LEU:HD12	4:H:144:THR:HG23	1.78	0.65
7:N:83:ASN:OD1	7:N:84:ASP:N	2.29	0.65
9:5:459:MET:HE1	9:5:510:ARG:HG2	1.77	0.65
8:2:503:ASN:ND2	8:2:589:MET:SD	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:507:ILE:O	9:5:509:SER:N	2.13	0.65
12:4:163:GLN:O	12:4:167:LYS:HG2	1.96	0.65
3:A:398:GLU:HG3	3:A:400:VAL:HG23	1.77	0.65
4:H:85:LEU:HD11	4:H:115:GLU:HG2	1.77	0.65
7:N:200:GLU:N	7:N:200:GLU:OE1	2.30	0.65
10:6:370:LYS:HD3	10:6:372:THR:HG23	1.77	0.65
3:A:23:VAL:HA	3:A:52:ILE:HD13	1.77	0.65
9:5:384:LYS:NZ	9:5:485:ALA:O	2.23	0.65
7:N:220:ILE:O	7:N:223:ASN:ND2	2.30	0.65
9:5:266:ILE:O	9:5:289:TYR:OH	2.13	0.65
10:6:421:LEU:O	10:6:440:ALA:N	2.29	0.65
12:4:517:SER:O	12:4:521:MET:HE2	1.96	0.65
3:A:246:LEU:HD23	3:A:250:GLU:HA	1.79	0.64
3:A:254:TYR:OH	3:A:372:GLY:N	2.29	0.64
13:7:452:ASP:HA	13:7:455:ARG:NH1	2.12	0.64
9:5:81:ASP:O	9:5:85:LYS:HG2	1.97	0.64
11:3:610:ARG:CB	15:7:801:ATP:H5'2	2.27	0.64
12:4:507:HIS:O	12:4:508:LEU:HD23	1.97	0.64
6:M:153:GLU:HG2	6:M:156:LEU:HD11	1.79	0.64
8:2:189:ARG:NH2	8:2:251:MET:SD	2.70	0.64
12:4:158:ASN:O	12:4:228:GLN:NE2	2.31	0.64
12:4:670:SER:O	12:4:674:VAL:HG13	1.97	0.64
13:7:380:MET:SD	13:7:490:PRO:HG3	2.38	0.64
13:7:244:VAL:HG11	13:7:250:PRO:HG3	1.77	0.64
9:5:514:ILE:HG22	9:5:516:ILE:HD11	1.80	0.64
12:4:514:PRO:HG2	12:4:516:THR:CG2	2.27	0.64
13:7:402:GLN:CG	13:7:433:ALA:HB1	2.28	0.64
6:M:54:LEU:HD23	6:M:58:TYR:OH	1.98	0.64
6:M:84:VAL:O	6:M:88:GLU:N	2.26	0.64
8:2:289:GLN:O	8:2:291:VAL:HG23	1.98	0.64
11:3:273:ILE:HG23	11:3:277:ASP:HB3	1.80	0.64
3:A:228:ASP:OD2	3:A:282:LYS:NZ	2.28	0.64
13:7:365:ARG:HG2	13:7:370:LYS:HD3	1.79	0.64
1:X:27:DT:H2"	1:X:28:DT:H71	1.80	0.64
9:5:391:VAL:HA	9:5:394:VAL:CG2	2.22	0.64
5:L:28:LEU:HD22	5:L:35:PRO:HD3	1.80	0.64
8:2:742:ARG:NH1	14:5:801:ADP:O1A	2.30	0.63
10:6:103:ASP:CG	10:6:104:CYS:H	2.06	0.63
13:7:374:ASN:OD1	13:7:464:GLN:NE2	2.30	0.63
9:5:461:GLN:NE2	11:3:347:SER:HB3	2.14	0.63
12:4:410:SER:OG	13:7:200:PHE:O	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:490:THR:HG21	12:4:702:PRO:CD	2.29	0.63
3:A:53:MET:N	3:A:53:MET:SD	2.70	0.63
4:H:112:CYS:O	4:H:115:GLU:N	2.29	0.63
5:L:48:MET:O	5:L:51:HIS:N	2.31	0.63
8:2:300:THR:OG1	8:2:301:THR:N	2.30	0.63
8:2:776:LEU:HD11	8:2:795:PHE:CD1	2.33	0.63
9:5:460:GLU:CB	9:5:510:ARG:HD2	2.27	0.63
5:L:15:ILE:HG12	5:L:46:LEU:HD21	1.79	0.63
10:6:586:LEU:HD22	10:6:637:VAL:HG11	1.79	0.63
12:4:736:LEU:HA	12:4:739:LEU:HD12	1.80	0.63
13:7:343:GLU:HB2	13:7:389:GLN:NE2	2.13	0.63
5:L:110:CYS:N	5:L:111:GLU:OE1	2.31	0.63
9:5:539:SER:OG	9:5:541:ASN:ND2	2.32	0.63
12:4:272:ARG:HD2	12:4:273:ASN:N	2.14	0.63
12:4:301:GLU:N	12:4:350:THR:O	2.31	0.63
13:7:459:HIS:HA	13:7:462:MET:HG2	1.81	0.63
8:2:203:ARG:NH1	8:2:216:VAL:O	2.31	0.63
10:6:637:VAL:O	10:6:641:PHE:N	2.31	0.63
4:H:162:ASP:OD1	4:H:163:TYR:N	2.32	0.63
9:5:343:SER:O	9:5:347:LYS:N	2.31	0.63
13:7:62:LEU:HA	13:7:65:ALA:HB3	1.80	0.63
13:7:413:GLY:O	13:7:432:GLY:HA3	1.99	0.63
8:2:248:ALA:HB1	8:2:266:ILE:HD13	1.81	0.62
8:2:306:GLN:NE2	9:5:283:VAL:HB	2.14	0.62
11:3:302:ILE:HA	15:3:901:ATP:H2	1.64	0.62
11:3:420:VAL:O	11:3:424:GLY:N	2.32	0.62
13:7:574:PRO:HD2	13:7:625:VAL:O	1.98	0.62
5:L:23:ASN:N	5:L:36:PHE:O	2.32	0.62
12:4:665:ALA:HB1	13:7:582:VAL:HG12	1.81	0.62
12:4:673:TYR:OH	13:7:574:PRO:HA	1.99	0.62
7:N:86:ARG:O	7:N:90:HIS:ND1	2.32	0.62
10:6:470:GLU:N	10:6:472:GLN:OE1	2.33	0.62
6:M:171:LEU:HD23	9:5:46:PHE:CB	2.30	0.62
9:5:33:LYS:HE2	9:5:79:LEU:HD11	1.82	0.62
11:3:610:ARG:HB3	15:7:801:ATP:H5'2	1.80	0.62
6:M:171:LEU:HD23	9:5:46:PHE:HB2	1.79	0.62
9:5:369:ARG:HH22	9:5:510:ARG:HB2	1.59	0.62
3:A:291:LEU:HD11	3:A:369:ILE:CG2	2.30	0.62
3:A:375:THR:OG1	3:A:384:TYR:O	2.14	0.62
8:2:222:LEU:HD21	8:2:229:LEU:HB2	1.80	0.62
8:2:745:GLU:HA	8:2:748:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:67:ILE:HG22	9:5:68:GLU:H	1.64	0.62
4:H:10:GLU:HG2	6:M:16:ILE:HG21	1.81	0.62
7:N:110:GLN:OE1	7:N:110:GLN:N	2.30	0.62
13:7:546:GLN:HB3	13:7:547:PRO:HD3	1.81	0.62
7:N:177:LEU:O	7:N:214:GLN:N	2.32	0.62
8:2:776:LEU:HD13	8:2:794:THR:HB	1.81	0.61
10:6:421:LEU:CD1	10:6:422:THR:HG23	2.29	0.61
10:6:474:ILE:HD13	10:6:485:LEU:CB	2.29	0.61
11:3:342:PRO:HG3	11:3:449:PRO:HD2	1.80	0.61
11:3:370:GLY:O	11:3:392:ALA:N	2.33	0.61
13:7:400:ARG:NH2	13:7:437:ALA:HA	2.15	0.61
13:7:433:ALA:HA	13:7:436:LEU:CD2	2.30	0.61
11:3:116:ILE:HG23	11:3:117:TYR:N	2.14	0.61
3:A:99:ASP:OD1	3:A:101:HIS:N	2.30	0.61
10:6:538:TYR:OH	12:4:714:GLN:O	2.16	0.61
13:7:381:GLY:N	13:7:490:PRO:HD3	2.15	0.61
13:7:510:ALA:O	13:7:514:ARG:HG2	2.00	0.61
3:A:278:MET:SD	3:A:279:SER:N	2.73	0.61
5:L:65:TRP:HZ3	5:L:66:MET:HE2	1.65	0.61
12:4:482:ILE:HA	12:4:485:GLN:NE2	2.15	0.61
12:4:642:LEU:HD22	12:4:645:ARG:HH21	1.65	0.61
13:7:626:GLU:N	13:7:629:ASP:OD2	2.29	0.61
12:4:305:ALA:HB2	12:4:325:ILE:HD11	1.80	0.61
13:7:546:GLN:O	13:7:548:PRO:HD3	2.00	0.61
3:A:536:GLU:O	3:A:540:GLN:N	2.34	0.61
8:2:300:THR:OG1	8:2:360:LYS:O	2.16	0.61
1:X:29:DT:H1'	1:X:30:DT:C5'	2.30	0.61
7:N:64:GLU:N	7:N:64:GLU:OE2	2.34	0.61
8:2:496:HIS:ND1	8:2:497:LYS:O	2.33	0.61
9:5:132:ILE:HD13	9:5:226:GLU:HB3	1.83	0.61
12:4:492:LYS:NZ	12:4:740:ILE:O	2.34	0.61
3:A:446:SER:O	3:A:450:ARG:N	2.34	0.61
9:5:439:VAL:CG2	9:5:481:VAL:HG13	2.28	0.61
13:7:339:SER:OG	13:7:554:LEU:N	2.34	0.61
13:7:415:THR:HA	13:7:435:VAL:HG23	1.83	0.61
13:7:448:ASP:CG	13:7:488:ALA:HB1	2.25	0.61
3:A:49:VAL:HG12	3:A:50:VAL:H	1.65	0.61
10:6:165:GLN:OE1	10:6:166:PHE:N	2.33	0.61
3:A:373:THR:HG22	3:A:374:PHE:H	1.66	0.60
11:3:429:SER:HB2	11:3:434:HIS:HA	1.83	0.60
12:4:551:LYS:CE	13:7:422:PRO:HA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:49:THR:O	13:7:50:ILE:HD13	2.01	0.60
3:A:366:ILE:HB	3:A:369:ILE:HD11	1.83	0.60
10:6:544:ILE:CG1	10:6:547:LEU:CD2	2.58	0.60
13:7:482:VAL:HG23	13:7:483:SER:O	2.01	0.60
13:7:363:ASP:HB2	13:7:370:LYS:NZ	2.15	0.60
6:M:174:THR:HG21	9:5:47:PHE:CG	2.35	0.60
9:5:359:ARG:NH1	9:5:477:SER:O	2.35	0.60
9:5:372:ILE:HD12	9:5:618:ILE:HD11	1.83	0.60
11:3:443:VAL:O	11:3:444:LEU:HD23	2.00	0.60
12:4:305:ALA:CB	12:4:325:ILE:HD11	2.31	0.60
12:4:648:LEU:HD11	12:4:770:ALA:HB3	1.83	0.60
12:4:174:ARG:NH1	12:4:220:THR:OG1	2.34	0.60
5:L:132:ILE:O	6:M:130:ARG:NH1	2.33	0.60
8:2:702:VAL:O	8:2:706:GLU:N	2.34	0.60
11:3:239:ARG:O	11:3:255:THR:OG1	2.15	0.60
1:X:29:DT:H2"	1:X:30:DT:OP2	2.00	0.60
7:N:101:MET:HE2	7:N:101:MET:HA	1.84	0.60
9:5:389:LYS:HA	9:5:400:TYR:CE2	2.36	0.60
10:6:627:GLU:OE2	10:6:636:HIS:NE2	2.34	0.60
13:7:345:TYR:O	13:7:532:ARG:NH2	2.34	0.60
13:7:585:TYR:CE1	13:7:589:ARG:HD3	2.37	0.60
13:7:612:LEU:HD21	13:7:633:ALA:HB1	1.84	0.60
10:6:48:GLU:N	10:6:48:GLU:OE2	2.34	0.60
13:7:572:THR:O	13:7:625:VAL:N	2.35	0.60
9:5:72:LEU:HD21	9:5:80:ALA:N	2.16	0.60
13:7:386:ALA:HB2	15:7:801:ATP:C3'	2.31	0.60
8:2:584:SER:O	8:2:594:ILE:HG21	2.02	0.59
10:6:473:THR:HA	10:6:474:ILE:HD12	1.83	0.59
13:7:390:LEU:O	13:7:394:ILE:HG22	2.02	0.59
3:A:340:GLN:OE1	9:5:128:ASN:ND2	2.34	0.59
3:A:462:VAL:HG23	3:A:504:SER:CB	2.32	0.59
5:L:29:ILE:HD13	7:N:90:HIS:NE2	2.17	0.59
12:4:673:TYR:CZ	13:7:574:PRO:HA	2.37	0.59
13:7:38:VAL:O	13:7:42:HIS:N	2.35	0.59
3:A:442:GLN:OE1	3:A:442:GLN:N	2.36	0.59
9:5:377:LEU:HG	9:5:485:ALA:CB	2.32	0.59
11:3:418:HIS:HD2	11:3:473:ARG:NH1	1.85	0.59
12:4:153:VAL:HG23	12:4:159:VAL:O	2.01	0.59
12:4:211:LEU:HD23	12:4:212:ASN:N	2.17	0.59
9:5:227:LEU:HD12	9:5:230:PHE:CE1	2.38	0.59
11:3:341:ASP:OD1	11:3:341:ASP:N	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:720:ARG:NE	12:4:731:ALA:O	2.36	0.59
12:4:747:ALA:HB1	12:4:752:SER:O	2.02	0.59
13:7:571:PRO:HA	13:7:623:ASP:HA	1.85	0.59
8:2:489:SER:O	8:2:497:LYS:NZ	2.22	0.59
10:6:103:ASP:OD1	10:6:104:CYS:N	2.34	0.59
10:6:339:TYR:CD2	10:6:343:ILE:HD11	2.37	0.59
11:3:458:LYS:NZ	11:3:461:MET:O	2.36	0.59
12:4:169:LYS:HD3	12:4:172:ILE:HD11	1.85	0.59
12:4:179:SER:O	12:4:184:GLU:N	2.36	0.59
9:5:460:GLU:OE2	9:5:510:ARG:NE	2.35	0.59
11:3:302:ILE:HA	15:3:901:ATP:C2	2.37	0.59
11:3:317:LEU:HD13	11:3:621:ALA:HB1	1.83	0.59
3:A:342:TYR:OH	3:A:350:ARG:O	2.10	0.59
8:2:383:LEU:O	8:2:384:LEU:HD12	2.02	0.59
9:5:81:ASP:OD1	9:5:85:LYS:HE3	2.03	0.59
10:6:54:THR:HG21	10:6:225:GLU:HB3	1.83	0.59
13:7:363:ASP:HB2	13:7:370:LYS:HZ1	1.67	0.59
13:7:441:VAL:HA	13:7:483:SER:O	2.02	0.59
5:L:29:ILE:HG23	5:L:33:VAL:HG11	1.83	0.59
9:5:431:MET:HG2	9:5:475:LEU:HD21	1.85	0.59
9:5:616:ILE:O	9:5:619:SER:OG	2.12	0.59
11:3:585:ALA:HB1	13:7:531:LEU:HA	1.85	0.59
7:N:218:ASP:O	7:N:222:ASN:ND2	2.36	0.59
12:4:633:ILE:HD13	12:4:729:ILE:HG21	1.84	0.59
8:2:411:LEU:HD13	10:6:170:ASN:HB2	1.84	0.58
10:6:361:LEU:HD11	10:6:626:LEU:HD21	1.84	0.58
3:A:56:THR:OG1	3:A:57:GLY:N	2.35	0.58
4:H:7:MET:N	4:H:11:LYS:HZ3	2.01	0.58
7:N:177:LEU:HD12	7:N:214:GLN:OE1	2.03	0.58
8:2:737:LEU:O	8:2:739:ILE:N	2.35	0.58
9:5:547:GLU:OE1	9:5:547:GLU:N	2.36	0.58
9:5:628:GLN:OE1	9:5:631:ALA:HB2	2.04	0.58
7:N:51:CYS:SG	7:N:181:VAL:HG12	2.43	0.58
10:6:544:ILE:HG23	10:6:547:LEU:CG	2.33	0.58
12:4:219:LYS:O	12:4:223:GLN:NE2	2.37	0.58
1:X:26:DT:H4'	10:6:425:VAL:CG2	2.32	0.58
3:A:333:LEU:HD12	3:A:349:LEU:HD13	1.84	0.58
5:L:78:GLU:CD	5:L:85:THR:HG21	2.28	0.58
12:4:294:ARG:HB3	12:4:355:VAL:HG13	1.84	0.58
12:4:314:PHE:HE2	12:4:337:ASN:HD22	1.51	0.58
13:7:99:LEU:O	13:7:103:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:22:VAL:HG23	3:A:49:VAL:HG13	1.83	0.58
3:A:492:ARG:NH2	3:A:493:ALA:HB3	2.18	0.58
3:A:501:LEU:HD12	3:A:502:ILE:H	1.67	0.58
13:7:147:HIS:O	13:7:163:VAL:HG12	2.04	0.58
4:H:159:CYS:O	4:H:199:HIS:NE2	2.37	0.58
11:3:325:PRO:CD	13:7:544:SER:HB3	2.34	0.58
12:4:516:THR:HG21	12:4:652:VAL:CG1	2.34	0.58
3:A:289:LEU:HD22	3:A:369:ILE:HG22	1.86	0.58
5:L:153:ILE:HD11	7:N:182:PHE:CD2	2.38	0.58
12:4:301:GLU:O	12:4:350:THR:N	2.37	0.58
12:4:378:HIS:O	12:4:382:VAL:HG13	2.04	0.58
13:7:382:ASP:OD1	13:7:382:ASP:N	2.37	0.58
13:7:464:GLN:HE21	13:7:481:ARG:HA	1.68	0.58
9:5:368:ARG:NH2	9:5:620:GLU:OE2	2.37	0.58
10:6:196:ASP:N	10:6:196:ASP:OD1	2.37	0.58
10:6:586:LEU:HB3	10:6:616:MET:HE2	1.85	0.58
8:2:413:THR:OG1	10:6:168:PHE:N	2.37	0.58
11:3:231:ARG:C	11:3:232:VAL:CG1	2.77	0.58
13:7:604:ARG:H	13:7:604:ARG:HD2	1.69	0.58
6:M:121:ILE:O	6:M:124:THR:OG1	2.21	0.57
10:6:474:ILE:HD13	10:6:485:LEU:HB2	1.86	0.57
4:H:46:GLU:HA	4:H:49:VAL:HG12	1.86	0.57
9:5:260:ILE:HG22	9:5:295:ILE:HG22	1.86	0.57
9:5:459:MET:CE	9:5:510:ARG:HG2	2.33	0.57
10:6:399:LYS:O	10:6:402:SER:OG	2.22	0.57
12:4:276:SER:C	12:4:277:LEU:HD22	2.29	0.57
6:M:102:TYR:CD1	6:M:125:LEU:HD21	2.39	0.57
10:6:379:ARG:HD3	10:6:469:MET:HE3	1.86	0.57
11:3:349:LEU:O	11:3:351:ARG:N	2.36	0.57
3:A:83:ILE:HD11	3:A:115:VAL:HG11	1.86	0.57
7:N:179:SER:O	7:N:181:VAL:HG13	2.03	0.57
10:6:544:ILE:HA	10:6:547:LEU:CB	2.28	0.57
13:7:555:ASP:OD1	13:7:558:LEU:HB2	2.04	0.57
1:X:29:DT:H1'	1:X:30:DT:H5''	1.85	0.57
8:2:498:VAL:HG12	8:2:499:ARG:HB2	1.87	0.57
8:2:601:ILE:HG12	8:2:603:THR:HG23	1.85	0.57
13:7:62:LEU:HD23	13:7:65:ALA:HB3	1.86	0.57
13:7:604:ARG:HA	13:7:607:LEU:HB3	1.86	0.57
11:3:384:GLY:CA	11:3:387:ARG:HB2	2.34	0.57
3:A:462:VAL:HG22	3:A:464:GLN:OE1	2.04	0.57
3:A:546:LEU:O	3:A:547:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:431:MET:HE3	9:5:464:ILE:HD11	1.86	0.57
11:3:256:VAL:C	11:3:257:LEU:HD12	2.29	0.57
13:7:129:GLU:O	13:7:228:LYS:HE3	2.05	0.57
7:N:194:VAL:HG21	7:N:219:LEU:HD11	1.86	0.57
11:3:585:ALA:HB2	13:7:534:ALA:HB3	1.87	0.57
13:7:356:LEU:HD12	13:7:616:LEU:HD11	1.86	0.57
13:7:404:THR:CG2	13:7:414:LEU:CD2	2.65	0.57
9:5:543:SER:OG	9:5:544:ALA:N	2.38	0.57
12:4:225:LEU:HD11	12:4:240:PHE:HZ	1.68	0.57
13:7:465:GLN:N	13:7:480:ALA:O	2.34	0.57
13:7:567:LYS:O	13:7:618:ARG:NH2	2.38	0.57
13:7:612:LEU:HD11	13:7:633:ALA:HA	1.87	0.57
3:A:567:LEU:O	3:A:571:THR:N	2.37	0.57
5:L:179:ARG:HD2	5:L:184:LEU:HD13	1.86	0.57
10:6:135:VAL:O	10:6:135:VAL:HG12	2.04	0.57
10:6:561:ARG:HH22	12:4:499:ARG:HH22	1.53	0.57
11:3:43:ARG:NH2	11:3:260:ASN:O	2.35	0.57
11:3:612:LEU:HD23	11:3:615:LEU:CD1	2.31	0.57
12:4:578:PHE:O	12:4:586:ARG:NE	2.38	0.57
3:A:295:ARG:NH1	3:A:385:ALA:HB2	2.19	0.56
4:H:128:ALA:HB1	7:N:136:GLU:HB3	1.86	0.56
7:N:61:ASP:O	7:N:65:LEU:HD13	2.04	0.56
8:2:179:GLU:OE1	8:2:183:ARG:NH1	2.38	0.56
8:2:248:ALA:O	8:2:252:VAL:HG23	2.05	0.56
10:6:141:VAL:HG12	10:6:143:PRO:HD3	1.86	0.56
13:7:631:ALA:HA	13:7:634:LEU:HD21	1.86	0.56
3:A:26:ASP:OD1	3:A:27:ILE:N	2.37	0.56
3:A:72:VAL:O	3:A:96:PHE:N	2.37	0.56
4:H:85:LEU:O	4:H:89:CYS:N	2.39	0.56
5:L:71:LEU:HA	5:L:74:ILE:HG22	1.87	0.56
9:5:50:TYR:OH	9:5:71:ASP:OD2	2.23	0.56
11:3:271:LEU:HB3	11:3:273:ILE:HD12	1.86	0.56
11:3:346:LYS:NZ	15:3:901:ATP:O1G	2.38	0.56
12:4:519:SER:O	12:4:523:GLN:N	2.36	0.56
13:7:350:VAL:O	13:7:354:LEU:HG	2.05	0.56
13:7:375:ILE:HD13	13:7:611:ARG:HD3	1.87	0.56
13:7:379:LEU:CB	13:7:487:ALA:HA	2.36	0.56
13:7:400:ARG:HH22	13:7:436:LEU:HD12	1.71	0.56
13:7:407:ARG:HH12	13:7:410:SER:HB2	1.70	0.56
3:A:243:GLN:CD	3:A:249:ILE:HD13	2.31	0.56
7:N:200:GLU:O	7:N:203:MET:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:549:ALA:HB3	9:5:553:ILE:HG23	1.87	0.56
10:6:120:LEU:HD23	10:6:120:LEU:O	2.05	0.56
3:A:83:ILE:HD11	3:A:115:VAL:CG1	2.36	0.56
4:H:34:VAL:HG12	4:H:38:LEU:CD1	2.35	0.56
8:2:499:ARG:NH2	9:5:386:GLN:OE1	2.39	0.56
12:4:620:ASN:OD1	12:4:620:ASN:N	2.36	0.56
9:5:481:VAL:HG12	9:5:482:LEU:O	2.06	0.56
13:7:448:ASP:HA	13:7:455:ARG:HH21	1.70	0.56
9:5:398:ALA:HB2	9:5:438:VAL:O	2.04	0.56
9:5:440:CYS:C	9:5:441:ILE:HD12	2.31	0.56
13:7:461:VAL:O	13:7:461:VAL:HG12	2.04	0.56
9:5:27:LEU:O	9:5:31:LYS:N	2.34	0.56
9:5:507:ILE:HG22	9:5:508:LEU:N	2.21	0.56
13:7:334:GLU:OE1	13:7:334:GLU:N	2.31	0.56
13:7:516:ASP:OD1	13:7:517:LEU:N	2.39	0.56
8:2:269:ARG:NH2	8:2:387:LEU:HD21	2.20	0.56
8:2:580:GLN:OE1	9:5:448:ARG:NH1	2.38	0.56
10:6:393:ALA:H	15:6:902:ATP:H5'1	1.70	0.56
11:3:397:ASP:HB2	13:7:246:VAL:HG23	1.87	0.56
9:5:375:LEU:HD21	9:5:511:PHE:HB3	1.88	0.56
12:4:287:SER:OG	12:4:393:VAL:O	2.11	0.56
13:7:433:ALA:HA	13:7:436:LEU:HG	1.88	0.56
13:7:588:LEU:CD2	13:7:589:ARG:HD2	2.34	0.56
8:2:303:VAL:O	8:2:304:LEU:HD23	2.06	0.55
8:2:574:PHE:HA	8:2:577:MET:HE2	1.87	0.55
8:2:752:GLU:OE2	8:2:756:ARG:NH1	2.39	0.55
12:4:203:ILE:O	12:4:207:GLU:N	2.38	0.55
13:7:345:TYR:CD2	13:7:532:ARG:HD3	2.40	0.55
3:A:476:LEU:HD23	3:A:517:VAL:HG12	1.88	0.55
4:H:48:ASN:O	4:H:70:ARG:NH1	2.39	0.55
11:3:377:VAL:O	11:3:377:VAL:HG12	2.05	0.55
3:A:443:VAL:HA	3:A:483:LEU:HD21	1.89	0.55
5:L:28:LEU:HD11	5:L:33:VAL:HG13	1.89	0.55
13:7:604:ARG:HD2	13:7:604:ARG:N	2.21	0.55
3:A:17:LYS:HG3	3:A:69:VAL:HG13	1.86	0.55
11:3:572:MET:O	11:3:624:ARG:NH1	2.40	0.55
13:7:359:VAL:O	13:7:567:LYS:HG2	2.05	0.55
13:7:381:GLY:H	13:7:490:PRO:HD3	1.71	0.55
3:A:262:GLN:O	3:A:266:SER:N	2.34	0.55
5:L:114:ARG:NH1	9:5:42:ASN:OD1	2.39	0.55
8:2:206:ARG:O	8:2:210:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:310:SER:OG	10:6:311:GLU:N	2.39	0.55
11:3:633:ILE:O	11:3:636:ALA:HB3	2.06	0.55
12:4:464:LEU:HG	12:4:465:ALA:N	2.21	0.55
13:7:366:PRO:O	13:7:369:MET:HG2	2.06	0.55
13:7:626:GLU:O	13:7:629:ASP:HB2	2.06	0.55
3:A:332:GLY:O	8:2:261:ARG:NH2	2.40	0.55
7:N:55:ILE:HD11	7:N:132:ARG:O	2.06	0.55
9:5:143:LEU:HD12	9:5:262:GLY:O	2.06	0.55
10:6:70:ALA:HA	10:6:73:ILE:HG22	1.87	0.55
10:6:329:ILE:HD11	10:6:566:ARG:NH1	2.21	0.55
10:6:561:ARG:NH2	12:4:499:ARG:HH22	2.05	0.55
13:7:376:ASN:HD22	13:7:484:ILE:H	1.54	0.55
4:H:88:ARG:O	4:H:92:ILE:HD12	2.06	0.55
7:N:219:LEU:O	7:N:223:ASN:N	2.39	0.55
13:7:417:ALA:O	13:7:429:LEU:HA	2.05	0.55
13:7:462:MET:SD	13:7:514:ARG:HB3	2.46	0.55
3:A:303:MET:O	3:A:315:LEU:HD13	2.07	0.55
5:L:141:THR:HG21	7:N:199:GLU:HB2	1.89	0.55
7:N:68:SER:OG	7:N:69:GLN:NE2	2.40	0.55
10:6:340:GLN:HA	10:6:343:ILE:HD12	1.88	0.55
11:3:310:GLN:O	11:3:313:LEU:HD23	2.07	0.55
11:3:463:ASN:N	11:3:464:ILE:HD12	2.22	0.55
12:4:694:ALA:HA	12:4:697:ARG:HH12	1.71	0.55
13:7:585:TYR:CZ	13:7:589:ARG:HD3	2.41	0.55
6:M:156:LEU:HD12	6:M:157:HIS:N	2.22	0.55
6:M:172:GLN:CD	9:5:45:ASN:HA	2.32	0.55
8:2:262:VAL:HG12	8:2:263:THR:HG23	1.88	0.55
10:6:421:LEU:HD12	10:6:422:THR:H	1.72	0.55
11:3:568:ILE:HG23	11:3:627:MET:HE1	1.89	0.55
12:4:545:LEU:HD23	12:4:565:LEU:HD13	1.88	0.55
13:7:31:PHE:O	13:7:35:SER:OG	2.23	0.55
13:7:429:LEU:HD23	13:7:429:LEU:H	1.72	0.55
4:H:18:GLU:OE2	4:H:88:ARG:NH2	2.39	0.55
4:H:167:GLU:HG3	4:H:174:ILE:HD11	1.89	0.55
7:N:107:CYS:SG	7:N:111:LYS:NZ	2.66	0.55
9:5:29:ALA:HB1	9:5:34:TYR:CD2	2.41	0.55
10:6:139:HIS:CE1	10:6:430:GLU:HG3	2.42	0.55
11:3:350:LEU:H	11:3:350:LEU:HD23	1.72	0.55
12:4:261:ILE:HG22	12:4:262:GLN:O	2.07	0.55
12:4:492:LYS:HZ3	12:4:740:ILE:HG13	1.72	0.55
12:4:538:ARG:NH2	13:7:453:GLN:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:387:LYS:HA	13:7:390:LEU:CD2	2.32	0.55
5:L:97:GLN:NE2	6:M:172:GLN:OE1	2.40	0.54
6:M:168:ILE:HG23	9:5:47:PHE:CZ	2.41	0.54
8:2:604:SER:OG	8:2:605:LEU:N	2.38	0.54
11:3:549:SER:OG	11:3:550:ARG:NH2	2.40	0.54
12:4:497:LEU:HD21	12:4:499:ARG:NE	2.19	0.54
13:7:208:SER:O	13:7:212:ARG:N	2.40	0.54
13:7:323:GLU:HG2	13:7:323:GLU:O	2.06	0.54
13:7:382:ASP:OD1	13:7:490:PRO:HD2	2.07	0.54
3:A:248:LYS:C	3:A:249:ILE:HD12	2.32	0.54
8:2:288:ASN:N	8:2:403:TYR:O	2.36	0.54
9:5:322:MET:O	9:5:325:SER:OG	2.12	0.54
12:4:518:LYS:HA	12:4:521:MET:HE2	1.89	0.54
12:4:693:ILE:O	12:4:697:ARG:NH1	2.39	0.54
13:7:372:ARG:NH2	13:7:462:MET:O	2.39	0.54
4:H:95:LEU:HD13	4:H:99:PHE:CZ	2.43	0.54
9:5:364:ASP:OD2	11:3:301:SER:HB3	2.08	0.54
11:3:238:TYR:CD2	11:3:257:LEU:HD11	2.42	0.54
12:4:633:ILE:HD11	12:4:640:HIS:HA	1.89	0.54
3:A:382:SER:OG	3:A:383:ARG:N	2.39	0.54
13:7:237:MET:O	13:7:252:SER:HA	2.07	0.54
13:7:532:ARG:HD2	13:7:533:LEU:N	2.22	0.54
3:A:309:SER:CB	3:A:315:LEU:HD11	2.38	0.54
9:5:120:GLN:NE2	9:5:247:SER:OG	2.39	0.54
12:4:521:MET:HE3	12:4:522:LEU:CD1	2.38	0.54
8:2:199:THR:O	8:2:203:ARG:N	2.31	0.54
12:4:271:THR:HG21	12:4:288:ILE:CD1	2.38	0.54
12:4:298:VAL:C	12:4:299:ILE:HD12	2.32	0.54
13:7:380:MET:O	13:7:521:ILE:HG22	2.08	0.54
13:7:402:GLN:NE2	13:7:436:LEU:HD11	2.23	0.54
6:M:86:GLU:OE1	6:M:119:ARG:NH1	2.41	0.54
7:N:158:GLN:OE1	7:N:158:GLN:N	2.38	0.54
7:N:118:HIS:ND1	7:N:172:ILE:HG23	2.23	0.54
10:6:387:VAL:HG12	10:6:388:GLY:H	1.73	0.54
11:3:388:LEU:O	11:3:388:LEU:HG	2.08	0.54
12:4:274:MET:HE3	12:4:371:HIS:HD2	1.71	0.54
12:4:728:GLN:CD	12:4:776:THR:HG21	2.33	0.54
13:7:500:THR:O	13:7:504:ASN:N	2.31	0.54
13:7:526:ASP:HB3	13:7:529:ASN:HB3	1.90	0.54
1:X:25:DT:H2''	1:X:26:DT:H72	1.88	0.54
1:X:27:DT:C1'	1:X:28:DT:H5'	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:370:LYS:CD	10:6:372:THR:HG23	2.37	0.54
11:3:463:ASN:H	11:3:464:ILE:HD12	1.72	0.54
12:4:540:SER:OG	13:7:470:ALA:N	2.30	0.54
3:A:346:ASP:OD1	3:A:347:LEU:HD23	2.08	0.54
8:2:413:THR:HG1	10:6:168:PHE:C	2.14	0.54
8:2:564:ALA:O	8:2:567:GLY:N	2.40	0.54
10:6:139:HIS:HB2	10:6:199:LYS:O	2.06	0.54
13:7:387:LYS:HD2	13:7:487:ALA:CB	2.36	0.54
13:7:433:ALA:HA	13:7:436:LEU:HD21	1.89	0.54
13:7:509:ALA:HA	13:7:512:LEU:HD13	1.88	0.54
3:A:74:LEU:CB	3:A:97:ILE:HG22	2.38	0.53
3:A:462:VAL:HG23	3:A:504:SER:HB2	1.90	0.53
9:5:343:SER:O	9:5:343:SER:OG	2.24	0.53
10:6:557:ARG:NH1	10:6:561:ARG:HD3	2.23	0.53
12:4:493:LYS:HZ1	12:4:495:ALA:HB2	1.72	0.53
13:7:581:ILE:HG13	13:7:582:VAL:N	2.23	0.53
3:A:309:SER:OG	3:A:315:LEU:HD11	2.08	0.53
9:5:375:LEU:HD22	9:5:511:PHE:CD2	2.42	0.53
10:6:321:MET:HA	10:6:324:ALA:HB2	1.91	0.53
12:4:595:GLN:O	12:4:597:THR:HG23	2.09	0.53
13:7:577:LEU:O	13:7:581:ILE:HG23	2.08	0.53
10:6:54:THR:HG21	10:6:225:GLU:CB	2.38	0.53
13:7:364:LYS:H	13:7:371:ILE:HG12	1.73	0.53
4:H:9:GLY:O	4:H:76:ARG:NE	2.42	0.53
5:L:87:MET:HE1	5:L:124:ARG:HH12	1.74	0.53
8:2:509:ASP:N	8:2:512:THR:OG1	2.42	0.53
8:2:741:VAL:HG21	14:5:801:ADP:H1'	1.90	0.53
10:6:80:ILE:O	10:6:83:PHE:N	2.41	0.53
10:6:226:LEU:O	10:6:229:THR:HG22	2.07	0.53
13:7:381:GLY:HA3	13:7:521:ILE:CG2	2.37	0.53
13:7:433:ALA:O	13:7:436:LEU:HG	2.08	0.53
8:2:741:VAL:O	8:2:745:GLU:N	2.37	0.53
9:5:72:LEU:HD21	9:5:79:LEU:HB2	1.91	0.53
11:3:336:VAL:HG11	11:3:476:LEU:HD12	1.91	0.53
12:4:293:ILE:HD11	12:4:356:LYS:HB3	1.90	0.53
12:4:305:ALA:CB	12:4:325:ILE:CD1	2.86	0.53
12:4:509:LEU:C	12:4:510:LEU:HD22	2.34	0.53
13:7:403:TYR:HE1	13:7:405:THR:HG22	1.73	0.53
5:L:112:GLU:O	5:L:116:VAL:HG13	2.09	0.53
8:2:407:TYR:HE2	9:5:283:VAL:HG13	1.74	0.53
3:A:234:TRP:CZ2	3:A:376:LEU:HD23	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:160:MET:N	4:H:197:ILE:O	2.41	0.53
10:6:446:ASN:OD1	10:6:488:ARG:NH2	2.41	0.53
13:7:446:GLU:CD	13:7:488:ALA:HA	2.34	0.53
13:7:590:ARG:CZ	13:7:591:GLU:HG2	2.39	0.53
8:2:436:GLN:NE2	8:2:437:VAL:HG22	2.23	0.53
8:2:573:GLU:OE2	8:2:616:ASN:ND2	2.42	0.53
11:3:552:ARG:NH2	11:3:557:LEU:HD13	2.23	0.53
12:4:712:LEU:HD23	12:4:712:LEU:O	2.09	0.53
13:7:574:PRO:O	13:7:577:LEU:HD23	2.09	0.53
9:5:217:VAL:HG12	9:5:218:ASP:H	1.73	0.53
11:3:137:LYS:NZ	13:7:293:LEU:HA	2.22	0.53
12:4:575:ILE:O	12:4:617:ALA:HA	2.09	0.53
13:7:451:ALA:HB3	13:7:454:ASP:OD2	2.08	0.53
9:5:431:MET:CE	9:5:464:ILE:HD11	2.38	0.52
13:7:416:ALA:CA	13:7:431:GLY:HA2	2.35	0.52
13:7:449:LYS:HE2	13:7:489:ASN:OD1	2.09	0.52
1:X:16:DG:H2''	1:X:17:DT:C6	2.45	0.52
7:N:83:ASN:OD1	7:N:85:PHE:N	2.41	0.52
9:5:488:ILE:HD11	9:5:499:GLU:O	2.10	0.52
12:4:502:PHE:CD2	12:4:737:GLU:OE1	2.63	0.52
1:X:24:DT:H5''	8:2:554:TRP:HD1	1.74	0.52
1:X:31:DT:H2''	1:X:32:DT:O5'	2.10	0.52
3:A:50:VAL:HB	3:A:52:ILE:HD11	1.91	0.52
10:6:146:VAL:HG22	10:6:164:GLN:CG	2.38	0.52
11:3:135:ARG:O	11:3:193:HIS:HB3	2.09	0.52
12:4:585:THR:HG22	12:4:586:ARG:HG2	1.91	0.52
13:7:379:LEU:HB2	13:7:487:ALA:HA	1.91	0.52
3:A:11:TYR:HA	3:A:14:LEU:HD13	1.91	0.52
8:2:219:TYR:OH	8:2:230:ALA:HB2	2.09	0.52
11:3:171:TYR:CD1	11:3:183:THR:HG22	2.45	0.52
12:4:542:ALA:HB2	12:4:585:THR:HG23	1.91	0.52
12:4:551:LYS:HE3	13:7:422:PRO:HA	1.92	0.52
13:7:511:LEU:HD12	13:7:512:LEU:N	2.24	0.52
9:5:375:LEU:HD21	9:5:511:PHE:CB	2.39	0.52
9:5:459:MET:HE3	9:5:510:ARG:CG	2.26	0.52
9:5:637:ASN:ND2	9:5:640:LEU:HD22	2.24	0.52
10:6:122:THR:HG23	12:4:351:ASP:CG	2.35	0.52
12:4:285:LEU:C	12:4:286:ILE:HD12	2.35	0.52
13:7:584:ALA:HA	13:7:587:GLU:OE1	2.09	0.52
3:A:132:THR:HG23	3:A:192:GLN:OE1	2.09	0.52
3:A:308:TYR:O	3:A:312:GLN:NE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:342:LEU:HD21	10:6:559:TYR:HE2	1.75	0.52
12:4:535:THR:N	12:4:574:CYS:O	2.42	0.52
13:7:462:MET:HG3	13:7:514:ARG:CG	2.34	0.52
3:A:269:THR:O	3:A:272:THR:OG1	2.24	0.52
8:2:554:TRP:O	8:2:556:LEU:HD12	2.10	0.52
8:2:590:GLU:HB2	8:2:641:ARG:HE	1.73	0.52
8:2:707:ASN:O	8:2:709:ARG:NH1	2.43	0.52
9:5:349:ALA:HB2	9:5:642:LEU:CD2	2.40	0.52
9:5:374:VAL:HG12	9:5:375:LEU:H	1.74	0.52
9:5:447:MET:HE2	9:5:451:ASP:OD2	2.10	0.52
11:3:407:ASP:N	11:3:407:ASP:OD1	2.42	0.52
13:7:472:ALA:HB3	13:7:474:ILE:CD1	2.39	0.52
13:7:538:THR:HA	13:7:541:HIS:HD2	1.73	0.52
3:A:35:ILE:HD12	3:A:36:LEU:HD23	1.92	0.52
4:H:107:ILE:HD12	4:H:110:ALA:H	1.74	0.52
9:5:536:VAL:HG13	9:5:542:LYS:HE2	1.92	0.52
12:4:590:HIS:O	12:4:590:HIS:CD2	2.61	0.52
13:7:340:LEU:CD1	13:7:559:MET:HE1	2.37	0.52
13:7:606:LEU:HA	13:7:609:ILE:HG12	1.91	0.52
13:7:613:SER:CB	13:7:630:VAL:HG22	2.39	0.52
3:A:507:LEU:HD22	3:A:510:SER:OG	2.10	0.52
7:N:61:ASP:OD1	7:N:62:MET:N	2.42	0.52
9:5:72:LEU:HD21	9:5:80:ALA:H	1.74	0.52
11:3:241:LEU:N	11:3:242:PRO:HD2	2.25	0.52
11:3:320:VAL:HB	11:3:620:THR:HG21	1.90	0.52
12:4:503:ARG:HG2	12:4:596:GLN:HE22	1.74	0.52
12:4:763:ALA:O	12:4:767:HIS:N	2.37	0.52
13:7:365:ARG:HD2	13:7:370:LYS:HA	1.92	0.52
13:7:528:ASP:HA	13:7:531:LEU:CD1	2.39	0.52
3:A:567:LEU:O	3:A:570:LEU:N	2.43	0.51
7:N:171:ARG:C	7:N:172:ILE:HD12	2.35	0.51
9:5:227:LEU:HD12	9:5:230:PHE:CD1	2.44	0.51
10:6:612:GLN:OE1	10:6:612:GLN:N	2.43	0.51
11:3:353:VAL:CG2	11:3:357:ALA:HB2	2.40	0.51
12:4:571:GLY:O	12:4:613:THR:OG1	2.28	0.51
13:7:340:LEU:HD13	13:7:559:MET:CE	2.39	0.51
13:7:532:ARG:NH2	13:7:533:LEU:HD13	2.25	0.51
13:7:571:PRO:HB3	13:7:623:ASP:HA	1.92	0.51
5:L:19:PRO:HD3	5:L:42:VAL:HG22	1.93	0.51
8:2:516:GLN:NE2	14:6:901:ADP:O1A	2.40	0.51
8:2:696:LEU:O	8:2:698:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:132:ILE:HD13	9:5:226:GLU:CB	2.38	0.51
9:5:325:SER:OG	9:5:327:ASP:OD1	2.29	0.51
9:5:378:GLY:HA3	9:5:517:VAL:HB	1.91	0.51
11:3:331:ARG:NH2	11:3:420:VAL:O	2.44	0.51
11:3:384:GLY:HA3	11:3:387:ARG:HB2	1.91	0.51
12:4:216:ALA:HB2	12:4:268:ALA:CB	2.40	0.51
12:4:516:THR:O	15:4:901:ATP:H5'1	2.10	0.51
12:4:704:LEU:HD12	12:4:755:VAL:HG11	1.91	0.51
13:7:375:ILE:CD1	13:7:611:ARG:HD3	2.39	0.51
5:L:29:ILE:HD13	7:N:90:HIS:CE1	2.46	0.51
9:5:461:GLN:CD	11:3:347:SER:HB3	2.35	0.51
9:5:549:ALA:HB3	9:5:553:ILE:CG2	2.40	0.51
10:6:403:ASP:OD1	10:6:403:ASP:N	2.44	0.51
11:3:70:GLN:HG3	11:3:71:LEU:H	1.76	0.51
11:3:252:THR:HG22	11:3:253:PHE:H	1.75	0.51
12:4:538:ARG:HH21	13:7:453:GLN:HB2	1.75	0.51
3:A:231:ASP:N	3:A:231:ASP:OD1	2.41	0.51
5:L:95:VAL:O	5:L:99:VAL:HG23	2.11	0.51
6:M:102:TYR:N	6:M:103:GLU:OE1	2.43	0.51
8:2:248:ALA:CB	8:2:266:ILE:HD13	2.40	0.51
9:5:99:ARG:NH1	9:5:118:ASP:OD1	2.44	0.51
9:5:522:ASP:O	9:5:526:ASP:N	2.42	0.51
11:3:310:GLN:NE2	11:3:311:ALA:HB2	2.25	0.51
11:3:422:GLU:CD	11:3:473:ARG:HH12	2.17	0.51
12:4:468:ILE:HD13	12:4:482:ILE:HG21	1.93	0.51
4:H:34:VAL:HG12	4:H:38:LEU:HD11	1.92	0.51
9:5:400:TYR:O	9:5:401:THR:HG23	2.10	0.51
11:3:35:ASP:O	11:3:88:TYR:OH	2.24	0.51
11:3:426:VAL:HB	11:3:437:LEU:HD21	1.91	0.51
12:4:271:THR:HG21	12:4:288:ILE:HG12	1.93	0.51
12:4:636:VAL:CG1	12:4:638:LEU:HD23	2.40	0.51
13:7:400:ARG:HA	13:7:400:ARG:HH11	1.76	0.51
13:7:495:TYR:OH	13:7:644:LEU:HD22	2.09	0.51
4:H:68:ASN:O	4:H:72:ALA:N	2.39	0.51
4:H:95:LEU:HD13	4:H:99:PHE:HZ	1.75	0.51
10:6:214:ILE:O	10:6:216:ARG:N	2.43	0.51
10:6:580:GLN:NE2	10:6:632:VAL:O	2.44	0.51
12:4:516:THR:CA	15:4:901:ATP:H5'1	2.40	0.51
13:7:429:LEU:HD12	13:7:478:LEU:HD11	1.92	0.51
1:X:27:DT:H5''	10:6:424:ALA:CB	2.40	0.51
3:A:485:ARG:HA	3:A:489:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:65:LEU:O	7:N:68:SER:OG	2.23	0.51
7:N:157:THR:HG22	7:N:160:MET:HE2	1.93	0.51
8:2:517:PHE:CD2	8:2:614:ALA:HB2	2.44	0.51
9:5:168:LEU:HD12	9:5:170:CYS:SG	2.49	0.51
11:3:387:ARG:HH21	11:3:387:ARG:CG	2.24	0.51
12:4:177:ASP:CG	12:4:195:LEU:HD11	2.35	0.51
4:H:25:THR:OG1	4:H:25:THR:O	2.29	0.51
5:L:85:THR:OG1	5:L:86:LYS:N	2.44	0.51
7:N:93:GLU:OE1	7:N:94:LEU:N	2.44	0.51
13:7:433:ALA:HA	13:7:436:LEU:CG	2.41	0.51
3:A:32:ALA:HB1	3:A:215:ALA:HB2	1.93	0.51
10:6:370:LYS:HB3	10:6:378:LEU:HD11	1.93	0.51
11:3:340:GLY:HA2	11:3:480:MET:O	2.10	0.51
13:7:524:LYS:HB3	13:7:525:PRO:HD2	1.92	0.51
3:A:563:LEU:HD23	3:A:563:LEU:H	1.76	0.51
8:2:199:THR:HB	8:2:203:ARG:HE	1.75	0.51
8:2:489:SER:OG	8:2:608:ARG:NH2	2.44	0.51
8:2:698:ARG:O	8:2:701:ILE:HG12	2.11	0.51
10:6:526:PHE:HZ	10:6:643:LEU:HD12	1.75	0.51
10:6:585:MET:O	10:6:589:ASN:ND2	2.42	0.51
11:3:34:LYS:NZ	11:3:35:ASP:OD1	2.44	0.51
13:7:365:ARG:HD2	13:7:369:MET:C	2.36	0.51
6:M:99:PRO:O	6:M:101:PHE:N	2.43	0.50
8:2:659:GLN:N	8:2:659:GLN:OE1	2.44	0.50
9:5:453:VAL:HG22	9:5:457:GLU:OE1	2.10	0.50
11:3:353:VAL:HG22	11:3:357:ALA:HB2	1.93	0.50
11:3:579:GLN:OE1	11:3:579:GLN:N	2.43	0.50
13:7:397:LEU:HD12	13:7:560:ARG:NH1	2.27	0.50
3:A:29:ALA:O	3:A:33:SER:OG	2.19	0.50
3:A:104:LEU:C	3:A:204:TYR:HH	2.14	0.50
10:6:41:THR:O	10:6:45:ALA:N	2.38	0.50
10:6:288:MET:HE2	10:6:288:MET:HA	1.92	0.50
10:6:476:ILE:HD11	10:6:478:ARG:HG2	1.94	0.50
4:H:158:ARG:NH1	4:H:179:ASN:OD1	2.44	0.50
8:2:505:LEU:HD23	8:2:506:ILE:C	2.35	0.50
12:4:670:SER:C	12:4:674:VAL:HG13	2.37	0.50
13:7:46:VAL:O	13:7:135:GLU:N	2.44	0.50
13:7:151:GLU:O	13:7:153:LYS:N	2.44	0.50
13:7:365:ARG:HG2	13:7:370:LYS:CD	2.42	0.50
15:7:801:ATP:H3'	15:7:801:ATP:O2A	2.11	0.50
3:A:309:SER:O	3:A:313:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:111:GLU:O	5:L:115:THR:OG1	2.19	0.50
6:M:112:ASP:OD1	6:M:113:ARG:N	2.45	0.50
8:2:776:LEU:HD13	8:2:794:THR:CB	2.41	0.50
10:6:311:GLU:OE2	10:6:332:MET:HE1	2.11	0.50
13:7:146:ALA:N	13:7:162:THR:HG1	2.08	0.50
13:7:343:GLU:OE1	13:7:343:GLU:N	2.44	0.50
13:7:367:ASP:O	13:7:369:MET:HE3	2.11	0.50
13:7:567:LYS:HA	13:7:618:ARG:HB3	1.92	0.50
13:7:619:LEU:O	13:7:619:LEU:HG	2.11	0.50
1:X:26:DT:H2''	1:X:27:DT:H71	1.93	0.50
4:H:136:ASN:HA	7:N:63:LEU:HD11	1.94	0.50
8:2:232:PHE:O	8:2:240:MET:HE3	2.11	0.50
12:4:714:GLN:O	12:4:714:GLN:NE2	2.44	0.50
3:A:243:GLN:OE1	3:A:249:ILE:HD13	2.12	0.50
5:L:163:SER:OG	5:L:164:LEU:N	2.42	0.50
8:2:361:ILE:HG21	8:2:381:VAL:HB	1.93	0.50
11:3:476:LEU:HD13	11:3:478:PHE:CE2	2.47	0.50
12:4:176:ILE:HD12	12:4:181:GLU:HB3	1.92	0.50
12:4:722:VAL:HG23	12:4:730:SER:HB3	1.93	0.50
13:7:381:GLY:HA3	13:7:521:ILE:HG23	1.93	0.50
13:7:644:LEU:HD12	13:7:645:ASN:H	1.77	0.50
1:X:29:DT:H1'	1:X:30:DT:H5'	1.94	0.50
3:A:30:ILE:HD12	3:A:30:ILE:H	1.77	0.50
6:M:150:ASP:OD1	6:M:151:ASN:N	2.43	0.50
8:2:458:ILE:O	8:2:462:VAL:N	2.42	0.50
9:5:459:MET:HE1	9:5:510:ARG:CG	2.35	0.50
9:5:532:HIS:O	9:5:536:VAL:HG21	2.12	0.50
10:6:146:VAL:HG22	10:6:164:GLN:HG3	1.94	0.50
10:6:308:PRO:HG2	10:6:312:VAL:HG21	1.93	0.50
10:6:473:THR:CA	10:6:474:ILE:HD12	2.41	0.50
11:3:422:GLU:CD	11:3:473:ARG:NH1	2.68	0.50
12:4:468:ILE:CD1	12:4:482:ILE:HG21	2.42	0.50
13:7:266:GLN:OE1	13:7:267:PRO:HD2	2.12	0.50
13:7:344:ILE:HG23	15:7:801:ATP:N6	2.27	0.50
13:7:401:SER:OG	13:7:402:GLN:N	2.42	0.50
3:A:40:PHE:O	3:A:45:MET:N	2.43	0.50
3:A:307:ARG:O	3:A:310:SER:N	2.45	0.50
7:N:219:LEU:O	7:N:224:GLN:N	2.44	0.50
10:6:55:LEU:CD2	10:6:57:VAL:HG13	2.42	0.50
13:7:571:PRO:HG2	13:7:625:VAL:HG23	1.94	0.50
3:A:58:LEU:HD13	3:A:86:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:265:SER:OG	9:5:266:ILE:N	2.37	0.50
10:6:470:GLU:OE1	10:6:521:ARG:NH1	2.44	0.50
11:3:422:GLU:CD	11:3:473:ARG:CZ	2.82	0.50
12:4:290:GLY:N	12:4:357:LEU:HD21	2.27	0.50
13:7:325:GLU:O	13:7:328:ALA:HB3	2.12	0.50
13:7:358:LEU:O	13:7:358:LEU:HD12	2.12	0.50
3:A:328:LEU:O	3:A:332:GLY:N	2.45	0.49
7:N:178:MET:O	7:N:180:HIS:ND1	2.36	0.49
8:2:207:MET:O	8:2:211:ASN:N	2.45	0.49
8:2:484:LEU:HD13	8:2:701:ILE:HD12	1.93	0.49
8:2:504:LEU:HD23	8:2:505:LEU:N	2.27	0.49
9:5:79:LEU:O	9:5:83:LEU:N	2.39	0.49
9:5:383:ALA:HB2	14:5:801:ADP:C4	2.47	0.49
13:7:422:PRO:O	13:7:423:LEU:HD12	2.12	0.49
13:7:459:HIS:NE2	13:7:510:ALA:O	2.44	0.49
13:7:633:ALA:O	13:7:636:LEU:HG	2.11	0.49
13:7:645:ASN:CG	13:7:646:GLN:HG2	2.36	0.49
6:M:13:ILE:HD12	6:M:13:ILE:H	1.77	0.49
6:M:174:THR:HG21	9:5:47:PHE:CD1	2.47	0.49
8:2:193:ASP:OD1	8:2:194:GLU:N	2.45	0.49
8:2:251:MET:CE	8:2:255:ILE:HD11	2.43	0.49
12:4:314:PHE:HE2	12:4:337:ASN:ND2	2.10	0.49
3:A:291:LEU:HD11	3:A:369:ILE:HG23	1.94	0.49
6:M:168:ILE:HG23	9:5:47:PHE:HZ	1.77	0.49
8:2:397:LEU:HD13	8:2:431:VAL:HA	1.94	0.49
8:2:635:SER:HB3	8:2:638:ILE:HG22	1.94	0.49
10:6:201:ARG:HH11	12:4:605:ILE:HD11	1.77	0.49
10:6:402:SER:HA	10:6:408:ALA:HB3	1.95	0.49
11:3:132:SER:OG	11:3:195:THR:O	2.26	0.49
11:3:171:TYR:CE1	11:3:183:THR:HG22	2.47	0.49
13:7:345:TYR:HD2	13:7:532:ARG:HD3	1.75	0.49
5:L:65:TRP:CZ3	5:L:66:MET:HE2	2.45	0.49
5:L:167:ILE:HG22	5:L:171:GLN:CG	2.42	0.49
11:3:325:PRO:HG2	13:7:545:LYS:HD3	1.95	0.49
12:4:399:ALA:C	12:4:400:THR:HG23	2.37	0.49
13:7:394:ILE:CD1	13:7:398:ALA:HB2	2.42	0.49
13:7:402:GLN:OE1	13:7:402:GLN:HA	2.12	0.49
13:7:402:GLN:CD	13:7:436:LEU:HD11	2.38	0.49
13:7:468:SER:HA	13:7:476:THR:O	2.13	0.49
13:7:572:THR:OG1	13:7:623:ASP:O	2.21	0.49
3:A:337:HIS:O	3:A:345:MET:HE3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:109:THR:OG1	10:6:110:GLU:N	2.44	0.49
10:6:163:GLU:N	10:6:164:GLN:OE1	2.46	0.49
11:3:633:ILE:HG23	11:3:634:ASP:OD1	2.13	0.49
13:7:386:ALA:N	15:7:801:ATP:O2A	2.46	0.49
13:7:448:ASP:OD1	13:7:449:LYS:N	2.45	0.49
13:7:512:LEU:H	13:7:512:LEU:HD12	1.76	0.49
13:7:571:PRO:CB	13:7:623:ASP:HA	2.43	0.49
3:A:20:LEU:HD13	3:A:37:GLN:OE1	2.13	0.49
3:A:111:SER:O	3:A:113:ARG:N	2.42	0.49
5:L:78:GLU:O	5:L:81:SER:OG	2.13	0.49
8:2:755:ALA:O	8:2:759:LEU:N	2.42	0.49
9:5:168:LEU:CD2	9:5:188:LEU:HD11	2.43	0.49
10:6:18:GLY:O	10:6:22:GLN:N	2.45	0.49
10:6:201:ARG:NH1	12:4:605:ILE:HD11	2.27	0.49
12:4:225:LEU:HD11	12:4:240:PHE:CZ	2.47	0.49
13:7:431:GLY:HA3	13:7:435:VAL:HG11	1.95	0.49
3:A:82:ASP:O	3:A:85:GLU:N	2.34	0.49
10:6:122:THR:HG23	12:4:351:ASP:OD2	2.13	0.49
13:7:550:ARG:O	13:7:550:ARG:HD2	2.12	0.49
1:X:31:DT:H2"	1:X:32:DT:C5'	2.42	0.49
9:5:397:ILE:HG12	9:5:433:LEU:HG	1.95	0.49
9:5:442:ASP:OD1	9:5:443:GLU:N	2.45	0.49
11:3:57:GLN:OE1	11:3:57:GLN:N	2.42	0.49
12:4:651:LEU:HD12	12:4:652:VAL:N	2.28	0.49
13:7:302:ARG:HG3	13:7:304:ILE:HG13	1.94	0.49
13:7:619:LEU:C	13:7:621:LEU:HD12	2.38	0.49
7:N:157:THR:HA	7:N:160:MET:HB3	1.95	0.49
8:2:466:MET:HE2	8:2:480:LEU:HD22	1.93	0.49
12:4:291:MET:N	12:4:358:GLN:O	2.40	0.49
12:4:571:GLY:O	12:4:614:SER:OG	2.31	0.49
9:5:347:LYS:HD2	9:5:350:ILE:HD12	1.93	0.49
9:5:371:ASP:OD2	9:5:462:GLN:NE2	2.42	0.49
10:6:609:THR:OG1	10:6:610:VAL:N	2.45	0.49
13:7:386:ALA:HB1	13:7:389:GLN:CB	2.33	0.49
13:7:477:THR:HG23	13:7:478:LEU:H	1.78	0.49
13:7:612:LEU:HD11	13:7:633:ALA:CB	2.43	0.49
3:A:55:VAL:HG23	3:A:58:LEU:HD12	1.94	0.48
4:H:129:TYR:O	4:H:133:ALA:N	2.38	0.48
5:L:15:ILE:HD11	5:L:46:LEU:HD11	1.94	0.48
10:6:550:ASN:ND2	12:4:496:THR:OG1	2.46	0.48
13:7:107:LEU:HD12	13:7:110:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:234:GLU:HA	13:7:255:ILE:O	2.12	0.48
13:7:571:PRO:CA	13:7:623:ASP:HA	2.43	0.48
4:H:124:LYS:O	4:H:127:ALA:HB3	2.13	0.48
8:2:482:LEU:HD11	8:2:774:MET:HE1	1.95	0.48
10:6:117:VAL:O	10:6:216:ARG:NH1	2.47	0.48
10:6:336:ARG:NH1	10:6:627:GLU:OE1	2.46	0.48
11:3:127:ILE:O	11:3:198:ILE:HG23	2.13	0.48
11:3:335:ASN:ND2	11:3:442:SER:OG	2.47	0.48
12:4:415:TYR:O	13:7:174:LYS:HD2	2.13	0.48
12:4:471:SER:OG	13:7:367:ASP:OD2	2.31	0.48
13:7:386:ALA:HB2	15:7:801:ATP:H2'	1.94	0.48
3:A:19:ILE:HD12	3:A:69:VAL:HG11	1.94	0.48
9:5:299:SER:O	9:5:301:GLY:N	2.45	0.48
10:6:202:ILE:HD11	10:6:290:PHE:HZ	1.77	0.48
12:4:722:VAL:HG11	12:4:772:LYS:NZ	2.28	0.48
9:5:639:ALA:O	9:5:643:PHE:N	2.46	0.48
12:4:151:GLN:O	12:4:152:LEU:HD23	2.12	0.48
12:4:514:PRO:O	12:4:516:THR:N	2.46	0.48
3:A:23:VAL:HG11	3:A:75:VAL:O	2.14	0.48
3:A:212:ARG:NH1	3:A:216:LEU:HD22	2.29	0.48
6:M:14:GLU:O	6:M:17:PHE:N	2.45	0.48
6:M:103:GLU:OE1	6:M:103:GLU:N	2.46	0.48
7:N:34:THR:HG22	7:N:36:GLN:H	1.78	0.48
8:2:252:VAL:O	8:2:256:PHE:N	2.32	0.48
8:2:301:THR:OG1	8:2:302:GLY:N	2.44	0.48
9:5:267:ARG:HG2	9:5:287:ALA:HB1	1.94	0.48
10:6:419:ALA:O	12:4:603:ALA:HB2	2.13	0.48
10:6:557:ARG:HH12	10:6:561:ARG:HD3	1.79	0.48
12:4:558:LEU:HD23	12:4:558:LEU:H	1.79	0.48
13:7:173:VAL:HA	13:7:232:PHE:O	2.14	0.48
13:7:462:MET:SD	13:7:514:ARG:CB	3.02	0.48
3:A:475:ALA:HA	3:A:478:LEU:HD12	1.95	0.48
12:4:664:LEU:HD22	12:4:668:LEU:HD11	1.96	0.48
13:7:386:ALA:HB2	15:7:801:ATP:C2'	2.43	0.48
13:7:453:GLN:OE1	13:7:453:GLN:N	2.44	0.48
7:N:38:VAL:HG13	7:N:41:ILE:HD11	1.96	0.48
8:2:554:TRP:CZ3	8:2:556:LEU:HD13	2.49	0.48
8:2:669:MET:HE3	10:6:370:LYS:CE	2.44	0.48
9:5:373:ASN:ND2	9:5:481:VAL:O	2.47	0.48
10:6:84:LEU:O	10:6:88:VAL:HG23	2.13	0.48
10:6:471:GLN:O	10:6:473:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:367:ASP:N	13:7:367:ASP:OD1	2.47	0.48
13:7:570:ASN:HA	13:7:618:ARG:NH1	2.29	0.48
3:A:376:LEU:O	3:A:384:TYR:N	2.47	0.48
6:M:39:SER:OG	6:M:39:SER:O	2.24	0.48
11:3:450:VAL:HG23	11:3:464:ILE:O	2.14	0.48
12:4:173:MET:HE2	12:4:173:MET:HA	1.94	0.48
13:7:362:VAL:HG13	13:7:362:VAL:O	2.13	0.48
3:A:322:LYS:NZ	8:2:209:GLU:OE1	2.47	0.48
3:A:470:PHE:CZ	3:A:479:LEU:HD11	2.48	0.48
4:H:143:LEU:CD1	4:H:144:THR:HG23	2.41	0.48
4:H:182:HIS:O	4:H:184:LEU:N	2.47	0.48
6:M:18:VAL:N	6:M:20:GLN:OE1	2.45	0.48
8:2:670:LYS:HB2	10:6:372:THR:HG22	1.95	0.48
10:6:222:LEU:N	10:6:222:LEU:HD23	2.29	0.48
1:X:31:DT:H2'	1:X:32:DT:C6	2.49	0.48
7:N:77:MET:HE1	7:N:80:LEU:HD12	1.96	0.48
8:2:199:THR:OG1	8:2:203:ARG:NH2	2.47	0.48
9:5:361:ARG:O	9:5:362:LEU:HD23	2.14	0.48
11:3:317:LEU:CD1	11:3:621:ALA:HB1	2.43	0.48
11:3:386:ARG:O	11:3:386:ARG:HG2	2.14	0.48
11:3:590:ARG:NE	13:7:527:ARG:HH12	2.11	0.48
11:3:590:ARG:NH2	13:7:527:ARG:HH22	2.12	0.48
12:4:271:THR:HG21	12:4:288:ILE:HD11	1.96	0.48
12:4:308:SER:OG	12:4:309:CYS:N	2.43	0.48
13:7:338:THR:HG21	13:7:551:VAL:HB	1.96	0.48
13:7:495:TYR:CD1	13:7:520:LEU:HD11	2.49	0.48
13:7:613:SER:HB3	13:7:629:ASP:O	2.13	0.48
5:L:77:GLU:O	5:L:80:ARG:NH1	2.47	0.47
5:L:179:ARG:CD	5:L:184:LEU:HD13	2.44	0.47
8:2:284:LYS:NZ	10:6:194:PHE:O	2.43	0.47
10:6:138:THR:OG1	10:6:200:ILE:HG22	2.13	0.47
11:3:298:LEU:HB3	11:3:352:TYR:HB3	1.94	0.47
11:3:595:GLU:HG2	11:3:604:THR:HG23	1.96	0.47
12:4:339:CYS:SG	12:4:340:PHE:N	2.86	0.47
13:7:48:ILE:HG22	13:7:49:THR:H	1.79	0.47
13:7:358:LEU:HD13	13:7:358:LEU:HA	1.68	0.47
5:L:119:ASP:O	5:L:123:ILE:HD13	2.14	0.47
8:2:726:GLN:O	8:2:730:GLU:N	2.43	0.47
9:5:140:VAL:O	9:5:141:SER:OG	2.26	0.47
10:6:218:VAL:HG22	10:6:290:PHE:CE1	2.48	0.47
10:6:340:GLN:O	10:6:344:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:381:ASP:O	10:6:618:ARG:NH1	2.47	0.47
12:4:746:HIS:HB2	12:4:759:ASP:OD2	2.14	0.47
13:7:9:ASP:OD1	13:7:12:SER:OG	2.29	0.47
6:M:59:ILE:HA	6:M:62:LEU:HB2	1.97	0.47
8:2:251:MET:HE3	8:2:255:ILE:HD11	1.97	0.47
8:2:413:THR:OG1	10:6:168:PHE:O	2.22	0.47
9:5:90:HIS:O	9:5:93:ILE:HG22	2.14	0.47
11:3:585:ALA:HB2	13:7:534:ALA:CB	2.45	0.47
13:7:14:LYS:HE2	13:7:17:LEU:HD21	1.95	0.47
6:M:93:GLU:OE2	6:M:95:GLY:N	2.47	0.47
8:2:402:ILE:H	8:2:424:ILE:HG23	1.79	0.47
10:6:339:TYR:HD2	10:6:343:ILE:HD11	1.79	0.47
11:3:107:HIS:ND1	11:3:107:HIS:O	2.47	0.47
11:3:345:ALA:HB1	11:3:348:GLN:HE22	1.78	0.47
12:4:291:MET:HE3	12:4:390:ARG:HG2	1.96	0.47
13:7:596:LYS:HA	13:7:596:LYS:HE3	1.96	0.47
10:6:310:SER:O	10:6:312:VAL:N	2.47	0.47
10:6:544:ILE:CB	10:6:547:LEU:CD2	2.93	0.47
11:3:109:THR:C	11:3:111:ARG:N	2.72	0.47
11:3:221:ASP:OD1	11:3:221:ASP:N	2.47	0.47
11:3:223:VAL:O	11:3:225:ARG:NH2	2.48	0.47
12:4:170:SER:O	12:4:174:ARG:N	2.42	0.47
12:4:305:ALA:HB2	12:4:325:ILE:CD1	2.44	0.47
13:7:504:ASN:OD1	13:7:505:ILE:HG13	2.15	0.47
6:M:27:VAL:O	6:M:49:GLY:N	2.47	0.47
7:N:153:HIS:O	7:N:157:THR:OG1	2.33	0.47
8:2:539:VAL:HA	8:2:581:ASP:OD1	2.14	0.47
9:5:220:GLN:HG2	9:5:222:LEU:HD23	1.96	0.47
10:6:413:GLY:N	10:6:452:ASP:O	2.46	0.47
11:3:109:THR:C	11:3:111:ARG:H	2.22	0.47
12:4:177:ASP:O	12:4:181:GLU:N	2.48	0.47
12:4:302:MET:HG3	12:4:303:ARG:N	2.29	0.47
12:4:508:LEU:HD21	12:4:647:ASP:OD1	2.13	0.47
13:7:499:ARG:HB3	13:7:504:ASN:HB3	1.96	0.47
13:7:538:THR:HA	13:7:541:HIS:CD2	2.50	0.47
13:7:572:THR:H	13:7:623:ASP:C	2.22	0.47
1:X:23:DT:H2"	1:X:24:DT:C5	2.49	0.47
3:A:32:ALA:O	3:A:35:ILE:HD11	2.15	0.47
3:A:57:GLY:HA2	3:A:60:ARG:HE	1.80	0.47
5:L:5:ILE:CD1	7:N:50:MET:HE1	2.44	0.47
5:L:53:ARG:NH1	5:L:58:CYS:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:78:GLU:CG	5:L:85:THR:HG21	2.45	0.47
11:3:241:LEU:H	11:3:242:PRO:HD2	1.79	0.47
11:3:637:HIS:HA	11:3:640:ILE:HG22	1.97	0.47
12:4:354:LEU:HD11	12:4:374:LEU:HB2	1.97	0.47
12:4:465:ALA:HB1	12:4:479:LYS:HB3	1.96	0.47
12:4:608:GLN:O	12:4:608:GLN:HG2	2.15	0.47
12:4:658:GLU:CB	13:7:586:VAL:HG13	2.45	0.47
6:M:34:MET:HG2	6:M:37:LEU:HD22	1.96	0.47
6:M:64:VAL:HG22	6:M:113:ARG:HD2	1.97	0.47
7:N:189:VAL:HG23	7:N:205:ALA:H	1.79	0.47
8:2:411:LEU:HD11	10:6:186:MET:HE1	1.95	0.47
8:2:478:ARG:CG	8:2:774:MET:HE2	2.45	0.47
10:6:185:PHE:HB3	10:6:187:LEU:HD23	1.96	0.47
10:6:345:SER:O	10:6:557:ARG:CZ	2.62	0.47
11:3:343:SER:HA	15:3:901:ATP:O3A	2.15	0.47
11:3:386:ARG:O	11:3:388:LEU:N	2.48	0.47
11:3:493:SER:OG	11:3:494:ASP:N	2.47	0.47
12:4:177:ASP:HB2	12:4:195:LEU:HD21	1.97	0.47
12:4:213:LEU:HD23	12:4:263:VAL:HG13	1.96	0.47
12:4:545:LEU:CD2	12:4:565:LEU:HD13	2.45	0.47
3:A:49:VAL:O	4:H:158:ARG:NH2	2.48	0.47
9:5:333:SER:OG	9:5:344:ARG:O	2.33	0.47
9:5:376:LEU:HD13	9:5:517:VAL:HG21	1.97	0.47
10:6:546:ASP:C	10:6:553:GLU:HB2	2.40	0.47
11:3:324:LEU:HD12	11:3:325:PRO:CD	2.44	0.47
4:H:174:ILE:HG22	4:H:184:LEU:HD11	1.97	0.47
8:2:591:GLN:HE21	9:5:389:LYS:HE2	1.79	0.47
10:6:315:GLU:C	10:6:324:ALA:HB1	2.40	0.47
11:3:310:GLN:HE21	11:3:311:ALA:HB2	1.78	0.47
12:4:204:HIS:CE1	12:4:255:ALA:HB1	2.49	0.47
12:4:263:VAL:HG12	12:4:266:PHE:CD1	2.50	0.47
12:4:272:ARG:HH22	12:4:276:SER:HB3	1.80	0.47
12:4:548:TYR:CE2	13:7:472:ALA:HA	2.49	0.47
13:7:526:ASP:OD2	13:7:529:ASN:HB2	2.15	0.47
6:M:129:VAL:HG12	6:M:130:ARG:HH11	1.80	0.46
9:5:188:LEU:HD13	9:5:207:PHE:CE2	2.50	0.46
9:5:377:LEU:HA	9:5:485:ALA:CB	2.40	0.46
10:6:53:CYS:O	10:6:105:TYR:CB	2.62	0.46
10:6:640:ALA:O	10:6:644:LEU:HD12	2.15	0.46
12:4:448:VAL:HA	12:4:451:LEU:HD23	1.97	0.46
12:4:550:THR:CG2	13:7:426:GLU:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:24:DT:H2"	1:X:25:DT:H71	1.97	0.46
3:A:132:THR:OG1	3:A:192:GLN:NE2	2.48	0.46
6:M:73:VAL:HG11	6:M:78:ARG:N	2.30	0.46
6:M:108:LEU:O	6:M:111:TYR:N	2.46	0.46
11:3:325:PRO:HG3	13:7:544:SER:HB3	1.97	0.46
12:4:213:LEU:HD21	12:4:263:VAL:HG22	1.96	0.46
13:7:569:LYS:HG3	13:7:621:LEU:HA	1.98	0.46
13:7:571:PRO:HG2	13:7:625:VAL:CG2	2.45	0.46
5:L:103:ALA:O	5:L:107:VAL:HG23	2.14	0.46
8:2:287:LEU:HD22	8:2:403:TYR:HD2	1.80	0.46
9:5:28:GLN:O	9:5:28:GLN:NE2	2.47	0.46
9:5:386:GLN:HA	9:5:389:LYS:HB3	1.98	0.46
9:5:457:GLU:O	9:5:463:THR:N	2.46	0.46
12:4:356:LYS:NZ	12:4:374:LEU:HD22	2.30	0.46
12:4:700:LEU:HD21	12:4:753:ASN:HB3	1.97	0.46
13:7:340:LEU:HD12	13:7:393:TYR:CE1	2.51	0.46
13:7:378:CYS:HA	13:7:486:ALA:HB3	1.97	0.46
13:7:416:ALA:CB	13:7:429:LEU:HB2	2.41	0.46
13:7:615:ALA:O	13:7:618:ARG:HG2	2.16	0.46
5:L:135:PHE:O	6:M:130:ARG:NH2	2.49	0.46
5:L:160:LEU:HD12	5:L:161:PRO:HG3	1.97	0.46
10:6:537:ASP:HA	10:6:540:ILE:HD13	1.97	0.46
11:3:382:GLU:O	13:7:422:PRO:HD2	2.15	0.46
12:4:709:GLN:OE1	12:4:709:GLN:N	2.47	0.46
13:7:165:GLY:C	13:7:166:ILE:HD12	2.40	0.46
13:7:409:SER:HB2	13:7:414:LEU:HG	1.95	0.46
3:A:58:LEU:CD1	3:A:86:LEU:HD21	2.45	0.46
4:H:107:ILE:HD12	4:H:109:GLN:H	1.81	0.46
6:M:131:HIS:HB3	6:M:132:LEU:HD12	1.96	0.46
8:2:259:TYR:O	8:2:261:ARG:N	2.45	0.46
8:2:573:GLU:OE1	8:2:573:GLU:N	2.49	0.46
10:6:531:GLU:OE2	10:6:533:ASN:N	2.49	0.46
11:3:255:THR:OG1	11:3:256:VAL:N	2.47	0.46
12:4:375:LEU:HD12	12:4:421:VAL:HG12	1.97	0.46
13:7:571:PRO:HD3	13:7:618:ARG:NE	2.30	0.46
13:7:612:LEU:HD11	13:7:633:ALA:CA	2.45	0.46
7:N:48:ASN:OD1	7:N:49:GLU:N	2.48	0.46
8:2:723:MET:HE2	8:2:723:MET:N	2.31	0.46
9:5:188:LEU:HD22	9:5:207:PHE:CZ	2.51	0.46
10:6:509:GLN:O	10:6:513:GLN:N	2.43	0.46
11:3:106:ARG:HB2	11:3:122:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:288:ILE:HG22	12:4:289:SER:H	1.80	0.46
13:7:500:THR:O	13:7:503:GLN:HB2	2.15	0.46
3:A:309:SER:HB2	3:A:315:LEU:HD11	1.97	0.46
8:2:590:GLU:HB2	8:2:641:ARG:HG2	1.98	0.46
9:5:534:ILE:HG23	9:5:538:LEU:HD12	1.97	0.46
11:3:338:LEU:HD23	11:3:479:VAL:C	2.41	0.46
11:3:499:MET:O	11:3:503:ARG:N	2.47	0.46
11:3:558:SER:O	11:3:562:MET:N	2.49	0.46
12:4:213:LEU:CD2	12:4:263:VAL:HG13	2.45	0.46
12:4:484:LEU:HD21	12:4:506:ILE:HD11	1.96	0.46
12:4:510:LEU:HG	12:4:521:MET:HE1	1.98	0.46
12:4:590:HIS:O	12:4:590:HIS:ND1	2.47	0.46
12:4:596:GLN:HB2	12:4:611:ALA:O	2.15	0.46
13:7:357:LEU:HD23	13:7:357:LEU:O	2.16	0.46
13:7:614:THR:OG1	13:7:625:VAL:HG21	2.15	0.46
13:7:634:LEU:HD12	13:7:635:ARG:N	2.31	0.46
3:A:546:LEU:C	3:A:547:LEU:HD23	2.41	0.46
4:H:193:VAL:HG23	4:H:194:ARG:N	2.31	0.46
5:L:141:THR:O	7:N:209:HIS:ND1	2.49	0.46
8:2:205:ARG:O	8:2:209:GLU:N	2.45	0.46
10:6:19:ILE:O	10:6:23:LYS:N	2.47	0.46
10:6:206:GLN:NE2	10:6:209:LEU:HD21	2.30	0.46
10:6:236:TYR:HB3	10:6:295:VAL:HG13	1.98	0.46
13:7:52:LEU:O	13:7:56:ALA:HB2	2.16	0.46
3:A:23:VAL:HG11	3:A:75:VAL:H	1.81	0.46
3:A:295:ARG:HH12	3:A:385:ALA:HB2	1.80	0.46
8:2:545:VAL:HG23	8:2:545:VAL:O	2.16	0.46
9:5:328:ILE:HG23	9:5:332:LEU:HD13	1.96	0.46
9:5:377:LEU:CA	9:5:485:ALA:HB3	2.40	0.46
11:3:387:ARG:CG	11:3:387:ARG:NH2	2.79	0.46
13:7:376:ASN:HB3	13:7:484:ILE:HG22	1.98	0.46
13:7:451:ALA:HB3	13:7:454:ASP:CG	2.41	0.46
13:7:636:LEU:HD12	13:7:637:LEU:N	2.31	0.46
5:L:167:ILE:HG22	5:L:171:GLN:CD	2.41	0.46
8:2:591:GLN:NE2	9:5:389:LYS:HE2	2.31	0.46
9:5:352:CYS:HA	9:5:625:ILE:HD11	1.98	0.46
10:6:26:GLN:NE2	10:6:30:GLU:OE1	2.45	0.46
10:6:428:ASP:O	10:6:430:GLU:N	2.46	0.46
11:3:610:ARG:HB2	15:7:801:ATP:H5'2	1.97	0.46
12:4:361:PRO:O	12:4:364:MET:HE2	2.16	0.46
13:7:406:GLY:C	13:7:450:MET:HE3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:412:VAL:O	13:7:417:ALA:HB2	2.16	0.46
13:7:439:GLN:NE2	13:7:481:ARG:HH11	2.13	0.46
7:N:77:MET:CE	7:N:80:LEU:HD12	2.46	0.45
8:2:361:ILE:O	8:2:362:THR:HG23	2.16	0.45
9:5:137:SER:O	9:5:140:VAL:HG23	2.16	0.45
10:6:341:ASN:OD1	10:6:341:ASN:N	2.49	0.45
12:4:694:ALA:HA	12:4:697:ARG:NH1	2.31	0.45
13:7:291:GLY:O	13:7:292:LEU:HB2	2.16	0.45
13:7:555:ASP:OD2	13:7:557:ASN:HB2	2.16	0.45
3:A:229:ASN:O	3:A:232:LEU:N	2.49	0.45
3:A:385:ALA:HB3	3:A:388:ASP:HB2	1.98	0.45
3:A:484:LEU:HD12	3:A:485:ARG:N	2.31	0.45
5:L:160:LEU:HD12	5:L:161:PRO:CD	2.47	0.45
6:M:168:ILE:HG22	6:M:169:GLU:OE1	2.16	0.45
8:2:288:ASN:ND2	8:2:403:TYR:O	2.50	0.45
9:5:164:SER:HA	9:5:172:THR:HG23	1.98	0.45
10:6:546:ASP:HB3	10:6:553:GLU:CA	2.36	0.45
11:3:368:SER:HA	11:3:371:VAL:HG23	1.98	0.45
12:4:201:GLU:O	12:4:205:THR:OG1	2.30	0.45
12:4:213:LEU:CD2	12:4:263:VAL:HG22	2.46	0.45
12:4:672:TYR:CE2	13:7:573:ILE:HG22	2.50	0.45
13:7:502:GLU:H	13:7:505:ILE:HD12	1.82	0.45
3:A:44:HIS:CE1	7:N:88:VAL:HG21	2.50	0.45
3:A:415:ASP:O	3:A:421:HIS:ND1	2.44	0.45
5:L:45:PRO:O	5:L:48:MET:HE2	2.17	0.45
5:L:123:ILE:O	5:L:126:SER:OG	2.31	0.45
8:2:472:GLY:O	8:2:477:LYS:NZ	2.44	0.45
10:6:393:ALA:HB2	15:6:902:ATP:C2'	2.40	0.45
11:3:114:THR:O	11:3:115:SER:OG	2.29	0.45
11:3:125:GLU:OE1	11:3:125:GLU:N	2.50	0.45
11:3:331:ARG:HE	11:3:423:GLN:C	2.24	0.45
12:4:372:ASN:OD1	12:4:372:ASN:N	2.49	0.45
12:4:633:ILE:HD13	12:4:729:ILE:HD13	1.97	0.45
12:4:657:ASP:OD1	12:4:658:GLU:N	2.49	0.45
13:7:407:ARG:HH12	13:7:410:SER:CB	2.28	0.45
13:7:533:LEU:HD21	15:7:801:ATP:N7	2.31	0.45
1:X:20:DT:H2''	13:7:285:PHE:CZ	2.51	0.45
10:6:149:VAL:HG22	10:6:159:ILE:O	2.17	0.45
10:6:385:CYS:HA	10:6:493:ALA:HB3	1.98	0.45
10:6:461:ASP:N	10:6:461:ASP:OD1	2.49	0.45
10:6:565:LEU:O	10:6:568:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:4:200:LEU:HD23	12:4:251:ARG:HB2	1.97	0.45
12:4:583:ASP:O	12:4:587:SER:OG	2.33	0.45
13:7:361:GLY:O	13:7:614:THR:HG22	2.16	0.45
3:A:229:ASN:CB	3:A:232:LEU:HD22	2.46	0.45
3:A:377:SER:OG	3:A:378:TYR:N	2.48	0.45
4:H:93:LYS:O	4:H:97:TRP:N	2.49	0.45
4:H:120:ASN:OD1	4:H:121:ASN:N	2.50	0.45
9:5:378:GLY:HA3	9:5:517:VAL:O	2.17	0.45
10:6:132:SER:HB3	10:6:236:TYR:O	2.17	0.45
11:3:356:THR:O	11:3:563:ARG:NH1	2.49	0.45
12:4:211:LEU:CD2	12:4:213:LEU:HB3	2.46	0.45
13:7:455:ARG:O	13:7:459:HIS:HB2	2.16	0.45
7:N:196:VAL:HG12	7:N:200:GLU:HB3	1.97	0.45
8:2:601:ILE:CG1	8:2:603:THR:HG23	2.47	0.45
9:5:40:THR:O	9:5:42:ASN:N	2.49	0.45
9:5:379:ASP:HB2	9:5:380:PRO:HD2	1.97	0.45
10:6:394:LYS:NZ	10:6:394:LYS:CB	2.76	0.45
11:3:404:ASP:HA	11:3:446:ALA:HB2	1.98	0.45
13:7:540:VAL:CG2	13:7:546:GLN:HB2	2.47	0.45
13:7:540:VAL:O	13:7:540:VAL:HG12	2.15	0.45
3:A:482:PHE:C	3:A:483:LEU:HD12	2.42	0.45
5:L:164:LEU:HA	5:L:167:ILE:HD12	1.98	0.45
5:L:165:ASP:O	5:L:168:ALA:N	2.49	0.45
8:2:509:ASP:HB3	8:2:512:THR:HG23	1.99	0.45
9:5:144:VAL:O	9:5:261:GLN:NE2	2.50	0.45
11:3:434:HIS:NE2	13:7:403:TYR:O	2.42	0.45
12:4:651:LEU:HD12	12:4:652:VAL:H	1.81	0.45
13:7:262:THR:HG23	13:7:263:ARG:N	2.31	0.45
13:7:378:CYS:HB3	13:7:518:LEU:HA	1.97	0.45
8:2:589:MET:SD	8:2:611:VAL:HG21	2.57	0.45
9:5:28:GLN:HA	9:5:31:LYS:HB3	1.99	0.45
10:6:341:ASN:O	10:6:345:SER:N	2.43	0.45
10:6:560:THR:O	10:6:564:VAL:HG23	2.17	0.45
10:6:627:GLU:OE2	10:6:635:ARG:NH1	2.50	0.45
11:3:565:TYR:CE1	11:3:627:MET:HE3	2.52	0.45
12:4:248:PHE:HB3	12:4:257:LEU:HD21	1.98	0.45
13:7:302:ARG:HD3	13:7:303:ILE:H	1.81	0.45
13:7:355:LEU:O	13:7:355:LEU:HD12	2.16	0.45
13:7:464:GLN:O	13:7:465:GLN:HG3	2.16	0.45
4:H:44:ILE:O	4:H:48:ASN:ND2	2.50	0.45
9:5:504:MET:HG3	9:5:507:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:397:PHE:O	10:6:401:VAL:HG23	2.17	0.45
11:3:496:VAL:HG12	11:3:500:HIS:NE2	2.31	0.45
13:7:400:ARG:NH2	13:7:436:LEU:HD12	2.32	0.45
3:A:92:ASP:OD1	3:A:113:ARG:NH2	2.49	0.45
3:A:105:ASP:OD1	3:A:106:VAL:N	2.49	0.45
5:L:16:SER:HA	5:L:43:PHE:HA	1.98	0.45
7:N:74:GLU:O	7:N:78:ARG:N	2.46	0.45
8:2:363:LEU:HD21	8:2:379:LYS:HB3	1.99	0.45
8:2:618:ILE:HD13	8:2:633:ASN:OD1	2.17	0.45
10:6:385:CYS:HB3	10:6:493:ALA:HB3	1.99	0.45
10:6:586:LEU:CD2	10:6:637:VAL:HG11	2.46	0.45
12:4:583:ASP:OD1	12:4:584:SER:N	2.49	0.45
12:4:685:ASP:O	12:4:689:LEU:HD22	2.17	0.45
13:7:455:ARG:HD2	13:7:455:ARG:N	2.32	0.45
13:7:473:GLY:C	13:7:474:ILE:HG13	2.42	0.45
13:7:644:LEU:HD12	13:7:645:ASN:N	2.31	0.45
4:H:22:SER:CB	4:H:26:ILE:HG23	2.46	0.44
4:H:131:CYS:SG	4:H:132:SER:N	2.90	0.44
5:L:5:ILE:HD11	7:N:50:MET:HE1	1.99	0.44
8:2:176:PRO:O	8:2:180:ILE:HD12	2.18	0.44
8:2:177:ARG:HD3	8:2:243:ILE:HD11	1.98	0.44
9:5:98:ALA:HB3	9:5:119:ILE:HD12	1.99	0.44
9:5:349:ALA:HB2	9:5:642:LEU:HD23	1.99	0.44
9:5:372:ILE:HG22	9:5:617:ARG:HH11	1.82	0.44
10:6:385:CYS:CB	10:6:493:ALA:HB3	2.47	0.44
13:7:261:VAL:O	13:7:264:MET:HG3	2.17	0.44
13:7:446:GLU:OE2	13:7:489:ASN:N	2.49	0.44
13:7:461:VAL:O	13:7:461:VAL:CG1	2.65	0.44
13:7:464:GLN:HE21	13:7:481:ARG:CA	2.30	0.44
3:A:530:PHE:O	3:A:534:ALA:N	2.48	0.44
8:2:177:ARG:CD	8:2:243:ILE:HD11	2.47	0.44
9:5:95:GLU:HA	9:5:119:ILE:HD11	2.00	0.44
9:5:374:VAL:O	9:5:482:LEU:HD12	2.16	0.44
9:5:506:THR:O	9:5:510:ARG:NH2	2.51	0.44
10:6:346:LEU:HD23	10:6:346:LEU:H	1.82	0.44
13:7:421:ASP:OD1	13:7:424:THR:HG22	2.18	0.44
3:A:245:LEU:HD23	3:A:248:LYS:HG2	1.99	0.44
8:2:361:ILE:HG22	8:2:381:VAL:O	2.18	0.44
8:2:383:LEU:HD12	8:2:387:LEU:O	2.17	0.44
9:5:23:ALA:HB3	9:5:24:GLN:NE2	2.32	0.44
9:5:260:ILE:HG22	9:5:295:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:139:HIS:HE1	10:6:430:GLU:HG3	1.82	0.44
11:3:418:HIS:CD2	11:3:473:ARG:NH2	2.43	0.44
12:4:582:ASN:ND2	12:4:584:SER:OG	2.46	0.44
13:7:97:ASP:OD1	13:7:98:ALA:N	2.50	0.44
13:7:381:GLY:CA	13:7:490:PRO:HD3	2.47	0.44
3:A:46:LEU:HD12	4:H:151:LYS:HB2	1.99	0.44
3:A:316:TRP:O	3:A:444:GLN:NE2	2.50	0.44
9:5:475:LEU:HD12	9:5:476:ASN:H	1.82	0.44
10:6:335:ASP:O	10:6:338:LEU:HD23	2.17	0.44
11:3:324:LEU:HD12	11:3:325:PRO:HD2	1.99	0.44
12:4:485:GLN:C	12:4:486:LEU:HD12	2.42	0.44
13:7:364:LYS:O	13:7:371:ILE:HG12	2.18	0.44
6:M:109:THR:HG21	6:M:118:GLY:HA2	1.99	0.44
10:6:550:ASN:HB3	12:4:496:THR:HG21	1.99	0.44
10:6:623:MET:HE3	10:6:636:HIS:HB3	1.99	0.44
10:6:641:PHE:O	10:6:645:ASN:N	2.48	0.44
11:3:286:LYS:O	11:3:288:ASN:ND2	2.51	0.44
13:7:135:GLU:OE1	13:7:260:GLU:HG2	2.18	0.44
13:7:482:VAL:O	13:7:482:VAL:HG22	2.17	0.44
5:L:156:VAL:HA	5:L:159:ILE:HD11	1.98	0.44
8:2:295:GLY:HA3	8:2:363:LEU:HD12	2.00	0.44
11:3:402:CYS:O	11:3:403:ILE:HG23	2.18	0.44
11:3:557:LEU:HD23	11:3:557:LEU:H	1.81	0.44
13:7:356:LEU:O	13:7:359:VAL:HB	2.17	0.44
13:7:554:LEU:HB3	13:7:559:MET:HG3	1.99	0.44
3:A:90:SER:HA	3:A:93:VAL:HG12	2.00	0.44
8:2:740:THR:OG1	8:2:743:HIS:N	2.50	0.44
9:5:366:LEU:CD2	11:3:301:SER:HB2	2.48	0.44
9:5:461:GLN:HE22	11:3:347:SER:HB3	1.83	0.44
10:6:473:THR:C	10:6:474:ILE:HD12	2.43	0.44
11:3:386:ARG:O	11:3:386:ARG:CG	2.64	0.44
12:4:319:GLU:OE1	12:4:319:GLU:N	2.48	0.44
12:4:377:ALA:C	12:4:421:VAL:HG21	2.43	0.44
13:7:38:VAL:HA	13:7:41:ALA:HB3	2.00	0.44
13:7:302:ARG:CG	13:7:304:ILE:HG13	2.48	0.44
13:7:333:TYR:OH	13:7:616:LEU:HB3	2.17	0.44
13:7:593:ARG:O	13:7:596:LYS:NZ	2.38	0.44
3:A:228:ASP:CG	3:A:282:LYS:HZ1	2.22	0.44
6:M:64:VAL:HG22	6:M:113:ARG:CD	2.48	0.44
9:5:131:ASN:HB2	9:5:134:GLN:NE2	2.33	0.44
10:6:544:ILE:CA	10:6:547:LEU:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3:584:ILE:HD11	13:7:538:THR:HG21	2.00	0.44
12:4:211:LEU:HD23	12:4:212:ASN:C	2.43	0.44
12:4:647:ASP:OD1	12:4:647:ASP:N	2.50	0.44
13:7:365:ARG:HD2	13:7:370:LYS:CA	2.48	0.44
13:7:469:ILE:HG23	13:7:471:LYS:HB2	1.99	0.44
1:X:27:DT:H5''	10:6:424:ALA:HB1	2.00	0.44
4:H:175:HIS:O	4:H:177:LYS:N	2.51	0.44
8:2:297:VAL:N	8:2:395:ASP:O	2.39	0.44
10:6:421:LEU:HD12	10:6:422:THR:N	2.33	0.44
13:7:277:PHE:CZ	13:7:296:THR:HG21	2.53	0.44
13:7:327:LEU:CD2	13:7:565:LEU:HG	2.48	0.44
13:7:484:ILE:HA	13:7:484:ILE:HD13	1.69	0.44
1:X:26:DT:C2'	1:X:27:DT:H71	2.48	0.43
10:6:144:GLU:OE2	10:6:146:VAL:HG23	2.19	0.43
11:3:187:LEU:O	11:3:189:VAL:HG13	2.18	0.43
13:7:146:ALA:N	13:7:162:THR:OG1	2.51	0.43
13:7:387:LYS:O	13:7:390:LEU:HG	2.18	0.43
13:7:561:ARG:O	13:7:564:ASN:HB2	2.18	0.43
13:7:610:LEU:HD23	13:7:611:ARG:N	2.33	0.43
7:N:114:THR:CB	7:N:173:VAL:HG21	2.48	0.43
10:6:393:ALA:CB	15:6:902:ATP:H2'	2.41	0.43
10:6:430:GLU:OE2	12:4:557:GLN:NE2	2.51	0.43
11:3:134:ILE:CD1	11:3:194:GLN:CD	2.91	0.43
11:3:373:LEU:HD11	11:3:413:ASP:OD1	2.17	0.43
12:4:328:PRO:HG3	12:4:333:ASN:HD22	1.82	0.43
13:7:500:THR:N	13:7:503:GLN:HB2	2.34	0.43
3:A:300:THR:HG23	3:A:338:ALA:O	2.18	0.43
3:A:548:GLN:NE2	3:A:555:VAL:O	2.51	0.43
8:2:399:VAL:HG22	8:2:401:GLY:N	2.34	0.43
12:4:478:ILE:HD12	12:4:478:ILE:HA	1.89	0.43
12:4:700:LEU:HD11	12:4:753:ASN:CG	2.43	0.43
13:7:470:ALA:HA	13:7:474:ILE:O	2.17	0.43
13:7:608:GLY:O	13:7:611:ARG:HG2	2.18	0.43
5:L:136:ILE:HG22	6:M:126:ARG:NH2	2.34	0.43
7:N:114:THR:CA	7:N:173:VAL:HG21	2.48	0.43
7:N:153:HIS:HA	7:N:157:THR:HG21	1.99	0.43
8:2:293:THR:HG22	8:2:294:LEU:H	1.84	0.43
8:2:588:ALA:N	8:2:594:ILE:HG23	2.34	0.43
9:5:67:ILE:HG22	9:5:68:GLU:N	2.31	0.43
10:6:561:ARG:HH22	12:4:499:ARG:NH2	2.16	0.43
12:4:450:LEU:HG	12:4:451:LEU:N	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:48:ILE:HB	13:7:136:VAL:HG22	1.99	0.43
13:7:350:VAL:HG22	13:7:519:TRP:CZ3	2.43	0.43
13:7:359:VAL:HG11	13:7:616:LEU:HA	2.01	0.43
13:7:631:ALA:HA	13:7:634:LEU:CD2	2.48	0.43
1:X:21:DA:C6	13:7:287:GLN:HG3	2.53	0.43
3:A:42:TYR:OH	5:L:55:GLN:O	2.37	0.43
3:A:225:LEU:O	3:A:226:SER:OG	2.33	0.43
3:A:251:SER:OG	3:A:252:GLY:N	2.52	0.43
4:H:121:ASN:O	4:H:125:SER:N	2.51	0.43
8:2:547:ARG:HH22	8:2:603:THR:HG21	1.84	0.43
10:6:388:GLY:N	10:6:502:TYR:OH	2.52	0.43
11:3:507:GLU:O	11:3:545:LEU:N	2.52	0.43
12:4:421:VAL:HG23	12:4:421:VAL:O	2.19	0.43
12:4:609:LEU:C	12:4:609:LEU:HD12	2.44	0.43
13:7:526:ASP:HB3	13:7:529:ASN:CB	2.48	0.43
1:X:27:DT:OP2	10:6:478:ARG:NE	2.51	0.43
3:A:443:VAL:HG13	3:A:483:LEU:HD21	1.99	0.43
6:M:174:THR:OG1	9:5:45:ASN:ND2	2.46	0.43
11:3:140:ARG:HG3	11:3:155:LYS:HA	2.01	0.43
11:3:605:GLN:HB2	11:3:606:PRO:HD3	2.00	0.43
13:7:277:PHE:CE2	13:7:296:THR:HG21	2.54	0.43
13:7:359:VAL:HG12	13:7:360:GLY:O	2.18	0.43
4:H:28:ALA:HB1	4:H:107:ILE:HG21	2.01	0.43
7:N:189:VAL:HA	7:N:205:ALA:H	1.83	0.43
8:2:669:MET:HE3	10:6:370:LYS:HE3	2.00	0.43
9:5:397:ILE:HD11	9:5:433:LEU:HD11	1.99	0.43
9:5:462:GLN:O	9:5:464:ILE:HD12	2.19	0.43
10:6:151:MET:SD	10:6:152:CYS:N	2.91	0.43
10:6:561:ARG:O	10:6:565:LEU:HD23	2.18	0.43
15:6:902:ATP:O3B	12:4:734:ARG:NH1	2.50	0.43
11:3:231:ARG:C	11:3:232:VAL:HG12	2.44	0.43
11:3:349:LEU:O	11:3:349:LEU:HD12	2.19	0.43
12:4:517:SER:OG	15:4:901:ATP:H2'	2.18	0.43
3:A:329:LEU:C	3:A:329:LEU:HD23	2.44	0.43
8:2:550:VAL:HG13	8:2:555:THR:HA	2.01	0.43
8:2:722:LYS:O	8:2:726:GLN:N	2.51	0.43
9:5:349:ALA:HB1	9:5:513:MET:SD	2.59	0.43
9:5:353:MET:HE3	9:5:374:VAL:HG23	2.01	0.43
9:5:397:ILE:HD11	9:5:433:LEU:CD1	2.49	0.43
11:3:325:PRO:CG	13:7:544:SER:HB3	2.47	0.43
11:3:338:LEU:HD23	11:3:479:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3:458:LYS:O	11:3:459:THR:HG23	2.18	0.43
12:4:503:ARG:HG2	12:4:596:GLN:NE2	2.33	0.43
13:7:336:LEU:H	13:7:336:LEU:HD12	1.84	0.43
13:7:338:THR:HG22	13:7:551:VAL:HG11	2.00	0.43
13:7:443:CYS:HA	13:7:485:LEU:HB3	2.00	0.43
13:7:535:LYS:HA	13:7:535:LYS:HD2	1.76	0.43
3:A:283:ILE:CB	3:A:376:LEU:HD22	2.49	0.43
4:H:184:LEU:HD23	4:H:189:VAL:HG12	2.00	0.43
8:2:287:LEU:HD22	8:2:403:TYR:CD2	2.53	0.43
8:2:404:THR:HG23	8:2:423:VAL:HG23	2.00	0.43
13:7:233:GLN:OE1	13:7:263:ARG:HA	2.19	0.43
13:7:263:ARG:O	13:7:263:ARG:HG2	2.18	0.43
13:7:512:LEU:HD23	13:7:518:LEU:CD2	2.48	0.43
3:A:215:ALA:HB1	3:A:218:VAL:HB	2.00	0.43
3:A:275:GLN:N	3:A:275:GLN:OE1	2.52	0.43
10:6:117:VAL:HG23	10:6:118:ARG:HD3	2.01	0.43
10:6:157:THR:HB	10:6:187:LEU:HD11	2.01	0.43
11:3:121:MET:HE1	11:3:259:ALA:O	2.19	0.43
13:7:168:THR:HG23	13:7:236:LYS:O	2.19	0.43
13:7:479:ASN:HD22	13:7:479:ASN:HA	1.62	0.43
13:7:527:ARG:O	13:7:531:LEU:HD21	2.19	0.43
13:7:619:LEU:O	13:7:621:LEU:HD12	2.19	0.43
3:A:375:THR:HG21	3:A:383:ARG:NH1	2.34	0.42
9:5:611:GLN:O	9:5:615:VAL:HG12	2.19	0.42
10:6:353:ASN:HB3	10:6:528:LEU:HD13	2.00	0.42
10:6:508:LEU:HD11	10:6:650:ARG:O	2.18	0.42
11:3:302:ILE:HG23	15:3:901:ATP:N1	2.34	0.42
11:3:343:SER:HA	15:3:901:ATP:PB	2.59	0.42
11:3:361:ILE:HG22	11:3:362:PRO:O	2.19	0.42
12:4:288:ILE:HG22	12:4:289:SER:N	2.34	0.42
12:4:663:ARG:O	12:4:666:SER:OG	2.29	0.42
3:A:23:VAL:CA	3:A:52:ILE:HD13	2.46	0.42
3:A:103:PRO:HD3	3:A:209:TYR:O	2.19	0.42
7:N:147:ASN:OD1	7:N:148:VAL:N	2.52	0.42
8:2:504:LEU:HB3	8:2:612:ILE:HD13	2.01	0.42
8:2:721:ALA:HB2	9:5:530:ALA:CB	2.49	0.42
10:6:18:GLY:HA3	10:6:80:ILE:HD13	2.01	0.42
11:3:302:ILE:HG23	15:3:901:ATP:C2	2.54	0.42
11:3:579:GLN:NE2	11:3:631:VAL:O	2.51	0.42
12:4:482:ILE:O	12:4:482:ILE:HG22	2.18	0.42
12:4:669:VAL:HG21	13:7:581:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:233:GLN:CD	13:7:263:ARG:H	2.27	0.42
13:7:426:GLU:CD	13:7:427:MET:H	2.27	0.42
1:X:19:DT:C6	1:X:19:DT:H5''	2.55	0.42
3:A:510:SER:OG	3:A:510:SER:O	2.32	0.42
5:L:69:ASP:N	5:L:69:ASP:OD1	2.51	0.42
5:L:80:ARG:O	5:L:82:LYS:N	2.46	0.42
6:M:51:THR:O	6:M:51:THR:HG23	2.17	0.42
8:2:449:ILE:HD12	8:2:700:TYR:HB2	2.01	0.42
9:5:447:MET:HE2	9:5:451:ASP:CG	2.44	0.42
9:5:528:THR:O	9:5:532:HIS:N	2.52	0.42
10:6:40:TYR:CE2	10:6:57:VAL:HG12	2.54	0.42
10:6:226:LEU:HD12	10:6:226:LEU:N	2.34	0.42
11:3:12:ILE:HG22	11:3:16:TYR:CE2	2.54	0.42
13:7:365:ARG:NE	13:7:368:GLY:O	2.51	0.42
3:A:74:LEU:N	3:A:96:PHE:O	2.52	0.42
8:2:466:MET:HG2	8:2:477:LYS:HA	2.02	0.42
10:6:229:THR:O	10:6:229:THR:HG23	2.19	0.42
13:7:376:ASN:ND2	13:7:484:ILE:H	2.15	0.42
13:7:402:GLN:NE2	13:7:436:LEU:HD21	2.34	0.42
13:7:529:ASN:O	13:7:532:ARG:HG3	2.20	0.42
5:L:143:ALA:HB3	7:N:208:GLN:HG2	2.02	0.42
8:2:586:HIS:CE1	8:2:641:ARG:HH21	2.37	0.42
11:3:428:ILE:HA	13:7:408:GLY:HA3	2.01	0.42
12:4:491:LYS:CD	12:4:493:LYS:HG2	2.49	0.42
13:7:278:LEU:HA	13:7:278:LEU:HD23	1.84	0.42
3:A:507:LEU:HD22	3:A:510:SER:CB	2.49	0.42
4:H:192:LEU:HD22	4:H:195:GLN:NE2	2.35	0.42
5:L:156:VAL:O	5:L:156:VAL:HG12	2.19	0.42
6:M:100:TYR:O	6:M:104:PHE:N	2.52	0.42
8:2:245:ASP:OD1	8:2:246:LYS:N	2.52	0.42
8:2:425:ILE:HG22	8:2:426:ALA:H	1.84	0.42
9:5:397:ILE:HG23	9:5:437:GLY:HA3	2.01	0.42
9:5:521:HIS:ND1	9:5:521:HIS:O	2.53	0.42
10:6:416:SER:HA	12:4:601:ALA:O	2.20	0.42
11:3:143:HIS:NE2	11:3:172:PRO:O	2.52	0.42
11:3:477:LEU:HD21	11:3:605:GLN:NE2	2.35	0.42
6:M:58:TYR:O	6:M:62:LEU:HD12	2.19	0.42
6:M:90:THR:OG1	6:M:91:HIS:N	2.52	0.42
8:2:415:GLN:NE2	8:2:419:VAL:HG23	2.34	0.42
14:5:801:ADP:N3	14:5:801:ADP:H2'	2.34	0.42
10:6:70:ALA:O	10:6:74:ILE:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:584:HIS:O	10:6:585:MET:HE2	2.19	0.42
11:3:198:ILE:HD11	11:3:216:ILE:HD13	2.02	0.42
12:4:494:HIS:NE2	12:4:502:PHE:CA	2.83	0.42
12:4:633:ILE:CD1	12:4:729:ILE:HG21	2.48	0.42
13:7:387:LYS:O	13:7:391:LEU:CG	2.65	0.42
3:A:123:LEU:N	3:A:124:GLU:OE2	2.53	0.42
3:A:201:MET:HE2	3:A:201:MET:HA	2.02	0.42
7:N:38:VAL:CG1	7:N:66:MET:HE1	2.50	0.42
8:2:727:LEU:O	8:2:731:SER:OG	2.37	0.42
9:5:502:ASP:OD1	9:5:502:ASP:N	2.53	0.42
9:5:576:ALA:O	9:5:633:ASP:N	2.53	0.42
10:6:393:ALA:N	15:6:902:ATP:H5'1	2.34	0.42
11:3:287:ASN:O	11:3:290:ILE:HG23	2.19	0.42
11:3:293:LEU:O	11:3:297:SER:OG	2.34	0.42
12:4:494:HIS:NE2	12:4:502:PHE:HB3	2.28	0.42
13:7:62:LEU:HD22	13:7:73:TYR:CE2	2.55	0.42
13:7:341:ALA:HA	13:7:393:TYR:CZ	2.55	0.42
13:7:524:LYS:HB3	13:7:525:PRO:CD	2.50	0.42
13:7:612:LEU:HD11	13:7:633:ALA:HB2	2.02	0.42
3:A:22:VAL:CG1	3:A:29:ALA:HB1	2.42	0.42
9:5:253:VAL:HG22	9:5:254:PRO:HD2	2.01	0.42
9:5:507:ILE:CG2	9:5:508:LEU:N	2.63	0.42
10:6:412:SER:HB3	12:4:599:SER:HB3	2.01	0.42
11:3:362:PRO:HA	11:3:401:VAL:HG13	2.01	0.42
12:4:316:THR:O	12:4:317:THR:HG23	2.20	0.42
12:4:666:SER:CA	13:7:582:VAL:HG11	2.50	0.42
3:A:385:ALA:HB3	3:A:388:ASP:OD2	2.20	0.42
4:H:192:LEU:HD22	4:H:195:GLN:CD	2.45	0.42
4:H:192:LEU:HD13	4:H:195:GLN:HE21	1.85	0.42
5:L:78:GLU:HB2	9:5:109:ARG:CZ	2.50	0.42
6:M:165:SER:OG	6:M:166:GLN:NE2	2.52	0.42
8:2:191:PHE:O	8:2:201:ARG:NH1	2.40	0.42
8:2:309:VAL:HB	8:2:354:LEU:HD21	2.01	0.42
9:5:161:THR:HG22	9:5:177:LEU:HD21	2.02	0.42
9:5:166:GLN:HB2	9:5:210:MET:HE3	2.01	0.42
9:5:322:MET:HE1	9:5:553:ILE:HD11	2.01	0.42
9:5:612:LEU:HD23	9:5:613:GLU:N	2.34	0.42
11:3:427:THR:HG23	11:3:435:ALA:O	2.20	0.42
13:7:512:LEU:HB3	13:7:518:LEU:HD21	2.01	0.42
3:A:90:SER:CB	3:A:93:VAL:HG12	2.50	0.41
3:A:563:LEU:HD23	3:A:563:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:50:ALA:HB3	4:H:70:ARG:HH22	1.85	0.41
5:L:94:VAL:CB	5:L:151:LEU:HD21	2.42	0.41
8:2:405:ASN:ND2	8:2:421:ALA:O	2.49	0.41
9:5:369:ARG:HD3	9:5:617:ARG:NH2	2.35	0.41
11:3:136:PRO:HA	11:3:191:LYS:O	2.19	0.41
12:4:670:SER:O	12:4:673:TYR:N	2.53	0.41
12:4:736:LEU:O	12:4:740:ILE:HG23	2.20	0.41
13:7:166:ILE:HD11	13:7:270:HIS:HD2	1.85	0.41
13:7:361:GLY:HA3	13:7:618:ARG:HG3	2.02	0.41
6:M:45:ASP:OD1	6:M:45:ASP:N	2.53	0.41
6:M:102:TYR:CG	6:M:125:LEU:HD21	2.55	0.41
8:2:199:THR:CB	8:2:203:ARG:HE	2.33	0.41
10:6:174:CYS:CB	10:6:177:PRO:O	2.63	0.41
11:3:326:ASN:HD21	13:7:545:LYS:HE3	1.84	0.41
12:4:551:LYS:HD2	13:7:425:GLY:O	2.19	0.41
3:A:443:VAL:HG13	3:A:483:LEU:CG	2.51	0.41
4:H:184:LEU:HD23	4:H:189:VAL:CG1	2.50	0.41
9:5:188:LEU:HD13	9:5:207:PHE:CD2	2.56	0.41
9:5:364:ASP:CG	11:3:301:SER:HB3	2.45	0.41
9:5:374:VAL:HG12	9:5:375:LEU:N	2.36	0.41
11:3:340:GLY:HA3	11:3:480:MET:SD	2.60	0.41
11:3:418:HIS:O	11:3:473:ARG:NH1	2.53	0.41
12:4:666:SER:HA	13:7:582:VAL:HG11	2.02	0.41
13:7:299:GLN:HA	13:7:299:GLN:OE1	2.20	0.41
3:A:19:ILE:HD12	3:A:69:VAL:CG1	2.49	0.41
3:A:318:LEU:O	3:A:321:GLU:N	2.49	0.41
3:A:401:LYS:O	3:A:401:LYS:HD3	2.20	0.41
4:H:40:GLU:O	4:H:43:ALA:HB3	2.20	0.41
6:M:169:GLU:OE1	6:M:169:GLU:N	2.53	0.41
6:M:171:LEU:HD22	9:5:47:PHE:CE1	2.56	0.41
8:2:270:ILE:O	8:2:428:HIS:ND1	2.54	0.41
8:2:373:GLY:HA2	10:6:442:MET:HG3	2.03	0.41
8:2:478:ARG:HD3	8:2:774:MET:HE2	2.01	0.41
10:6:185:PHE:HD1	10:6:185:PHE:HA	1.78	0.41
10:6:317:MET:HE3	10:6:323:ASP:O	2.20	0.41
10:6:581:GLU:OE1	10:6:585:MET:HE3	2.21	0.41
11:3:279:MET:HA	11:3:279:MET:HE3	2.02	0.41
11:3:443:VAL:C	11:3:444:LEU:HD23	2.46	0.41
12:4:169:LYS:HG2	12:4:243:ALA:HB1	2.02	0.41
12:4:227:ARG:O	12:4:230:ILE:N	2.53	0.41
12:4:624:SER:HB3	13:7:509:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:261:VAL:O	13:7:261:VAL:HG12	2.20	0.41
7:N:182:PHE:HB3	7:N:228:ILE:HD12	2.01	0.41
8:2:776:LEU:HD11	8:2:795:PHE:HD1	1.82	0.41
9:5:256:ASN:CG	9:5:257:ARG:H	2.29	0.41
9:5:380:PRO:HD3	9:5:486:ASN:ND2	2.36	0.41
10:6:40:TYR:CD2	10:6:57:VAL:HG12	2.55	0.41
11:3:550:ARG:O	11:3:552:ARG:N	2.51	0.41
11:3:597:VAL:HG12	11:3:598:GLU:N	2.36	0.41
12:4:375:LEU:N	12:4:375:LEU:HD23	2.35	0.41
12:4:486:LEU:O	12:4:488:GLY:HA2	2.20	0.41
12:4:513:ASP:N	12:4:514:PRO:CD	2.84	0.41
12:4:566:VAL:O	12:4:566:VAL:HG12	2.20	0.41
13:7:197:SER:O	13:7:198:LEU:HD23	2.20	0.41
13:7:446:GLU:OE1	13:7:488:ALA:HA	2.20	0.41
3:A:341:THR:O	3:A:344:ALA:N	2.46	0.41
8:2:661:ALA:CB	10:6:587:VAL:HG12	2.51	0.41
9:5:120:GLN:NE2	9:5:246:ARG:HB2	2.35	0.41
10:6:308:PRO:CG	10:6:312:VAL:HG21	2.50	0.41
11:3:142:VAL:HG12	11:3:151:VAL:HG13	2.02	0.41
11:3:394:VAL:HA	11:3:397:ASP:CG	2.45	0.41
13:7:372:ARG:HG3	13:7:464:GLN:OE1	2.20	0.41
3:A:536:GLU:HA	3:A:539:ALA:HB3	2.01	0.41
10:6:459:GLN:OE1	10:6:460:ARG:NH2	2.53	0.41
12:4:712:LEU:HA	12:4:715:ALA:HB3	2.01	0.41
13:7:164:ARG:HA	13:7:272:VAL:HA	2.02	0.41
4:H:149:PRO:O	4:H:151:LYS:NZ	2.47	0.41
5:L:164:LEU:O	5:L:168:ALA:HB2	2.21	0.41
6:M:172:GLN:CB	9:5:45:ASN:HA	2.50	0.41
10:6:306:ASP:OD1	10:6:320:GLN:N	2.54	0.41
10:6:634:GLU:OE1	10:6:634:GLU:N	2.44	0.41
11:3:34:LYS:O	11:3:38:ALA:N	2.54	0.41
11:3:136:PRO:O	13:7:294:SER:HB2	2.21	0.41
11:3:429:SER:O	11:3:431:ALA:N	2.49	0.41
12:4:282:MET:HE3	12:4:397:TYR:CD2	2.56	0.41
12:4:494:HIS:CE1	12:4:502:PHE:CA	3.04	0.41
3:A:24:ASN:OD1	3:A:25:TYR:N	2.50	0.41
3:A:219:PHE:CE1	3:A:233:LEU:HD21	2.56	0.41
4:H:93:LYS:HA	4:H:96:ARG:HB3	2.02	0.41
4:H:126:LEU:O	4:H:130:MET:N	2.45	0.41
7:N:145:ALA:HA	7:N:148:VAL:HG12	2.02	0.41
8:2:492:PRO:CD	8:2:498:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:762:ASN:OD1	8:2:762:ASN:N	2.54	0.41
9:5:459:MET:SD	9:5:511:PHE:HE1	2.44	0.41
9:5:516:ILE:HD12	9:5:516:ILE:N	2.35	0.41
10:6:149:VAL:HG13	10:6:159:ILE:H	1.85	0.41
10:6:559:TYR:CE2	10:6:564:VAL:HG22	2.56	0.41
11:3:471:LEU:HD23	11:3:606:PRO:HA	2.03	0.41
12:4:399:ALA:O	12:4:400:THR:HG23	2.20	0.41
12:4:492:LYS:HZ1	12:4:740:ILE:C	2.27	0.41
13:7:261:VAL:O	13:7:264:MET:HB2	2.21	0.41
13:7:280:LEU:HB3	13:7:295:GLU:O	2.21	0.41
13:7:340:LEU:HA	13:7:559:MET:HE1	2.01	0.41
3:A:330:GLU:O	8:2:258:THR:HG21	2.21	0.41
4:H:103:ILE:HG23	4:H:166:PHE:HB3	2.03	0.41
8:2:310:ILE:O	8:2:310:ILE:HG22	2.21	0.41
10:6:208:GLU:OE2	10:6:209:LEU:N	2.54	0.41
12:4:275:ARG:NH2	12:4:368:GLN:OE1	2.51	0.41
12:4:374:LEU:N	12:4:374:LEU:HD23	2.36	0.41
13:7:462:MET:CG	13:7:514:ARG:HB3	2.51	0.41
13:7:570:ASN:H	13:7:618:ARG:CZ	2.34	0.41
13:7:612:LEU:CD2	13:7:633:ALA:HB1	2.51	0.41
3:A:403:HIS:ND1	3:A:403:HIS:O	2.54	0.40
10:6:62:VAL:O	10:6:62:VAL:HG12	2.20	0.40
10:6:162:VAL:HA	10:6:164:GLN:OE1	2.21	0.40
11:3:62:LEU:HD12	11:3:63:LEU:CA	2.51	0.40
11:3:298:LEU:HD22	11:3:352:TYR:HB3	2.03	0.40
11:3:430:LYS:HA	13:7:409:SER:HA	2.03	0.40
12:4:732:TYR:O	12:4:735:GLN:NE2	2.54	0.40
3:A:54:GLY:O	3:A:57:GLY:N	2.50	0.40
4:H:192:LEU:HD13	4:H:195:GLN:NE2	2.35	0.40
8:2:568:VAL:HG12	8:2:569:CYS:N	2.36	0.40
8:2:636:GLU:O	8:2:639:LEU:N	2.54	0.40
9:5:70:GLU:C	9:5:73:VAL:HG22	2.47	0.40
9:5:136:LYS:O	9:5:139:CYS:N	2.47	0.40
10:6:544:ILE:O	10:6:547:LEU:HB3	2.20	0.40
11:3:116:ILE:HG12	11:3:117:TYR:H	1.86	0.40
12:4:672:TYR:HE2	13:7:573:ILE:HG22	1.86	0.40
13:7:349:ASP:OD1	13:7:350:VAL:N	2.54	0.40
13:7:459:HIS:CE1	13:7:514:ARG:HD3	2.55	0.40
13:7:459:HIS:HE1	13:7:514:ARG:HH11	1.69	0.40
3:A:106:VAL:O	3:A:106:VAL:HG12	2.22	0.40
3:A:128:PRO:O	3:A:132:THR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:151:LEU:HD23	6:M:170:TRP:CZ2	2.57	0.40
6:M:162:ARG:O	6:M:165:SER:OG	2.23	0.40
7:N:49:GLU:OE2	7:N:108:ARG:NH2	2.55	0.40
10:6:377:SER:O	10:6:379:ARG:NH1	2.55	0.40
13:7:49:THR:C	13:7:50:ILE:HD13	2.46	0.40
13:7:262:THR:CG2	13:7:263:ARG:N	2.84	0.40
13:7:379:LEU:HB2	13:7:486:ALA:O	2.21	0.40
13:7:477:THR:HG23	13:7:478:LEU:N	2.36	0.40
13:7:528:ASP:O	13:7:531:LEU:HG	2.21	0.40
3:A:18:ARG:C	3:A:19:ILE:HD12	2.45	0.40
3:A:70:LYS:HB3	3:A:93:VAL:HG23	2.02	0.40
3:A:517:VAL:HG22	3:A:518:GLY:H	1.85	0.40
5:L:92:TYR:OH	5:L:120:ILE:HG21	2.21	0.40
9:5:346:ILE:HD11	9:5:515:PHE:CZ	2.57	0.40
9:5:349:ALA:HB2	9:5:642:LEU:HD22	2.02	0.40
9:5:366:LEU:HD21	11:3:301:SER:HB2	2.03	0.40
9:5:480:SER:OG	9:5:481:VAL:N	2.54	0.40
10:6:551:ILE:N	10:6:551:ILE:HD12	2.36	0.40
11:3:238:TYR:C	11:3:239:ARG:HG2	2.46	0.40
11:3:314:CYS:HB2	11:3:334:ILE:HD13	2.04	0.40
12:4:503:ARG:CB	12:4:596:GLN:HE22	2.35	0.40
12:4:648:LEU:HD22	12:4:767:HIS:HA	2.04	0.40
13:7:400:ARG:HA	13:7:400:ARG:HD2	1.86	0.40
13:7:439:GLN:HE22	13:7:481:ARG:HH11	1.67	0.40
9:5:459:MET:HE2	9:5:460:GLU:HG2	2.04	0.40
10:6:409:ILE:HG22	10:6:411:THR:HG23	2.03	0.40
12:4:490:THR:HG21	12:4:702:PRO:CG	2.52	0.40
12:4:499:ARG:O	12:4:500:GLN:NE2	2.55	0.40
12:4:660:PHE:HA	12:4:663:ARG:HD3	2.04	0.40
13:7:446:GLU:N	13:7:487:ALA:O	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	515/575 (90%)	424 (82%)	88 (17%)	3 (1%)	21	59
4	H	193/202 (96%)	155 (80%)	36 (19%)	2 (1%)	12	47
5	L	175/203 (86%)	143 (82%)	32 (18%)	0	100	100
6	M	144/212 (68%)	115 (80%)	28 (19%)	1 (1%)	18	55
7	N	202/228 (89%)	169 (84%)	32 (16%)	1 (0%)	24	63
8	2	543/887 (61%)	453 (83%)	88 (16%)	2 (0%)	30	67
9	5	550/733 (75%)	429 (78%)	117 (21%)	4 (1%)	18	55
10	6	578/817 (71%)	461 (80%)	107 (18%)	10 (2%)	7	35
11	3	570/819 (70%)	461 (81%)	103 (18%)	6 (1%)	11	45
12	4	598/866 (69%)	482 (81%)	105 (18%)	11 (2%)	6	33
13	7	589/720 (82%)	498 (85%)	86 (15%)	5 (1%)	16	53
All	All	4657/6262 (74%)	3790 (81%)	822 (18%)	45 (1%)	15	47

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	2	512	THR
9	5	508	LEU
10	6	233	GLY
11	3	376	ALA
11	3	387	ARG
11	3	388	LEU
12	4	511	CYS
12	4	513	ASP
12	4	514	PRO
13	7	152	VAL
13	7	190	GLU
10	6	444	ALA
10	6	559	TYR
12	4	333	ASN
12	4	487	PHE
12	4	489	GLY
12	4	515	GLY
12	4	591	GLU
6	M	57	TRP
7	N	161	PRO

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Mol	Chain	Res	Type
8	2	314	CYS
10	6	310	SER
10	6	395	SER
12	4	474	GLU
12	4	488	GLY
12	4	599	SER
13	7	281	MET
13	7	289	ILE
3	A	24	ASN
3	A	528	ARG
9	5	575	GLU
10	6	105	TYR
3	A	353	PHE
10	6	112	PRO
10	6	113	THR
11	3	242	PRO
11	3	471	LEU
4	H	100	GLY
11	3	372	GLY
4	H	149	PRO
10	6	177	PRO
13	7	383	PRO
9	5	189	PRO
9	5	507	ILE
10	6	215	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	
3	A	451/501 (90%)	435 (96%)	16 (4%)	32	53
4	H	170/176 (97%)	159 (94%)	11 (6%)	15	37
5	L	166/184 (90%)	156 (94%)	10 (6%)	17	39
6	M	138/188 (73%)	128 (93%)	10 (7%)	13	35
7	N	185/205 (90%)	177 (96%)	8 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2	492/781 (63%)	462 (94%)	30 (6%)	17	39
9	5	486/630 (77%)	458 (94%)	28 (6%)	18	40
10	6	494/718 (69%)	464 (94%)	30 (6%)	17	39
11	3	500/699 (72%)	467 (93%)	33 (7%)	15	37
12	4	531/759 (70%)	504 (95%)	27 (5%)	21	43
13	7	482/630 (76%)	432 (90%)	50 (10%)	7	22
All	All	4095/5471 (75%)	3842 (94%)	253 (6%)	18	38

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	17	LYS
3	A	45	MET
3	A	49	VAL
3	A	107	CYS
3	A	115	VAL
3	A	136	ASP
3	A	258	LEU
3	A	261	ILE
3	A	300	THR
3	A	310	SER
3	A	341	THR
3	A	350	ARG
3	A	377	SER
3	A	490	THR
3	A	516	LEU
3	A	519	ILE
4	H	25	THR
4	H	41	ILE
4	H	47	GLU
4	H	49	VAL
4	H	67	LEU
4	H	81	LEU
4	H	89	CYS
4	H	92	ILE
4	H	107	ILE
4	H	129	TYR
4	H	144	THR
5	L	2	ASP
5	L	15	ILE

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Mol	Chain	Res	Type
5	L	17	ILE
5	L	89	CYS
5	L	94	VAL
5	L	115	THR
5	L	120	ILE
5	L	159	ILE
5	L	163	SER
5	L	185	SER
6	M	59	ILE
6	M	85	CYS
6	M	89	THR
6	M	90	THR
6	M	92	ILE
6	M	109	THR
6	M	116	VAL
6	M	168	ILE
6	M	170	TRP
6	M	174	THR
7	N	51	CYS
7	N	70	VAL
7	N	109	LEU
7	N	114	THR
7	N	133	LEU
7	N	173	VAL
7	N	181	VAL
7	N	197	ASP
8	2	217	VAL
8	2	265	GLU
8	2	279	LEU
8	2	293	THR
8	2	300	THR
8	2	314	CYS
8	2	315	VAL
8	2	357	ASN
8	2	361	ILE
8	2	411	LEU
8	2	422	THR
8	2	425	ILE
8	2	470	ILE
8	2	484	LEU
8	2	499	ARG
8	2	512	THR

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Mol	Chain	Res	Type
8	2	532	THR
8	2	534	GLN
8	2	539	VAL
8	2	546	ARG
8	2	587	GLU
8	2	603	THR
8	2	635	SER
8	2	639	LEU
8	2	664	VAL
8	2	696	LEU
8	2	715	ILE
8	2	736	SER
8	2	751	SER
8	2	794	THR
9	5	59	LEU
9	5	91	LEU
9	5	105	ILE
9	5	106	THR
9	5	123	LEU
9	5	130	THR
9	5	192	CYS
9	5	219	PHE
9	5	226	GLU
9	5	249	CYS
9	5	250	GLU
9	5	253	VAL
9	5	285	VAL
9	5	297	VAL
9	5	328	ILE
9	5	336	LEU
9	5	339	SER
9	5	346	ILE
9	5	353	MET
9	5	399	VAL
9	5	420	GLN
9	5	441	ILE
9	5	452	ARG
9	5	463	THR
9	5	501	ILE
9	5	503	PHE
9	5	510	ARG
9	5	609	VAL

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Mol	Chain	Res	Type
10	6	41	THR
10	6	58	SER
10	6	113	THR
10	6	120	LEU
10	6	121	THR
10	6	135	VAL
10	6	177	PRO
10	6	187	LEU
10	6	196	ASP
10	6	222	LEU
10	6	230	VAL
10	6	231	GLN
10	6	236	TYR
10	6	313	THR
10	6	341	ASN
10	6	370	LYS
10	6	378	LEU
10	6	387	VAL
10	6	389	ASP
10	6	391	SER
10	6	394	LYS
10	6	403	ASP
10	6	429	GLU
10	6	485	LEU
10	6	492	LEU
10	6	496	ASN
10	6	514	LEU
10	6	524	LEU
10	6	531	GLU
10	6	560	THR
11	3	20	LEU
11	3	25	ASP
11	3	29	TYR
11	3	63	LEU
11	3	73	PHE
11	3	97	VAL
11	3	113	LEU
11	3	124	VAL
11	3	139	VAL
11	3	141	SER
11	3	173	THR
11	3	196	LEU

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Mol	Chain	Res	Type
11	3	210	LEU
11	3	219	ASP
11	3	221	ASP
11	3	226	CYS
11	3	232	VAL
11	3	245	ARG
11	3	341	ASP
11	3	346	LYS
11	3	348	GLN
11	3	350	LEU
11	3	354	LEU
11	3	373	LEU
11	3	385	GLU
11	3	387	ARG
11	3	437	LEU
11	3	459	THR
11	3	466	LEU
11	3	478	PHE
11	3	504	ASN
11	3	631	VAL
11	3	642	LEU
12	4	159	VAL
12	4	176	ILE
12	4	230	ILE
12	4	241	ASP
12	4	244	ILE
12	4	259	HIS
12	4	302	MET
12	4	329	THR
12	4	332	THR
12	4	372	ASN
12	4	378	HIS
12	4	392	THR
12	4	393	VAL
12	4	404	THR
12	4	411	VAL
12	4	422	VAL
12	4	493	LYS
12	4	496	THR
12	4	500	GLN
12	4	502	PHE
12	4	507	HIS

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Mol	Chain	Res	Type
12	4	575	ILE
12	4	590	HIS
12	4	669	VAL
12	4	712	LEU
12	4	753	ASN
12	4	757	LEU
13	7	48	ILE
13	7	70	CYS
13	7	79	ASP
13	7	80	VAL
13	7	150	ARG
13	7	160	LEU
13	7	166	ILE
13	7	168	THR
13	7	171	THR
13	7	173	VAL
13	7	246	VAL
13	7	248	HIS
13	7	253	MET
13	7	262	THR
13	7	264	MET
13	7	283	THR
13	7	285	PHE
13	7	293	LEU
13	7	298	LEU
13	7	327	LEU
13	7	329	GLN
13	7	358	LEU
13	7	367	ASP
13	7	380	MET
13	7	382	ASP
13	7	385	VAL
13	7	387	LYS
13	7	388	SER
13	7	423	LEU
13	7	424	THR
13	7	467	ILE
13	7	474	ILE
13	7	476	THR
13	7	482	VAL
13	7	484	ILE
13	7	501	VAL

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Mol	Chain	Res	Type
13	7	537	ILE
13	7	551	VAL
13	7	555	ASP
13	7	565	LEU
13	7	573	ILE
13	7	575	ASP
13	7	577	LEU
13	7	606	LEU
13	7	610	LEU
13	7	611	ARG
13	7	612	LEU
13	7	614	THR
13	7	623	ASP
13	7	644	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	290	HIS
3	A	325	HIS
4	H	75	GLN
4	H	182	HIS
4	H	195	GLN
4	H	200	HIS
5	L	27	HIS
5	L	97	GLN
5	L	166	HIS
6	M	53	ASN
6	M	98	HIS
6	M	131	HIS
6	M	166	GLN
7	N	36	GLN
7	N	69	GLN
7	N	72	HIS
7	N	76	GLN
7	N	153	HIS
7	N	164	GLN
7	N	223	ASN
8	2	210	GLN
8	2	288	ASN
8	2	436	GLN
8	2	503	ASN

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Mol	Chain	Res	Type
8	2	591	GLN
8	2	659	GLN
8	2	694	GLN
8	2	699	GLN
9	5	21	GLN
9	5	24	GLN
9	5	45	ASN
9	5	60	ASN
9	5	120	GLN
9	5	128	ASN
9	5	134	GLN
9	5	176	ASN
9	5	193	ASN
9	5	196	GLN
9	5	239	HIS
9	5	423	ASN
9	5	541	ASN
9	5	635	HIS
10	6	181	ASN
10	6	337	ASN
10	6	383	ASN
10	6	550	ASN
10	6	645	ASN
11	3	47	ASN
11	3	55	ASN
11	3	288	ASN
11	3	310	GLN
11	3	326	ASN
11	3	348	GLN
11	3	490	GLN
11	3	622	HIS
12	4	204	HIS
12	4	212	ASN
12	4	260	GLN
12	4	333	ASN
12	4	337	ASN
12	4	423	HIS
12	4	485	GLN
12	4	523	GLN
12	4	596	GLN
12	4	625	GLN
12	4	710	GLN

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Mol	Chain	Res	Type
12	4	728	GLN
12	4	735	GLN
12	4	746	HIS
13	7	45	GLN
13	7	105	HIS
13	7	147	HIS
13	7	301	HIS
13	7	389	GLN
13	7	439	GLN
13	7	479	ASN
13	7	536	HIS
13	7	541	HIS
13	7	557	ASN
13	7	564	ASN
13	7	605	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
15	ATP	6	902	-	32,33,33	1.38	5 (15%)	48,52,52	1.91	11 (22%)
14	ADP	5	801	-	28,29,29	1.39	4 (14%)	43,45,45	2.08	12 (27%)
14	ADP	6	901	-	28,29,29	1.42	4 (14%)	43,45,45	1.80	9 (20%)
15	ATP	4	901	-	32,33,33	1.37	5 (15%)	48,52,52	1.78	13 (27%)
15	ATP	3	901	-	32,33,33	1.32	4 (12%)	48,52,52	1.77	9 (18%)
15	ATP	7	801	-	32,33,33	1.27	4 (12%)	48,52,52	2.01	10 (20%)

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
15	ATP	6	902	-	-	5/22/38/38	0/3/3/3
14	ADP	5	801	-	-	2/16/32/32	0/3/3/3
14	ADP	6	901	-	-	2/16/32/32	0/3/3/3
15	ATP	4	901	-	-	5/22/38/38	0/3/3/3
15	ATP	3	901	-	-	4/22/38/38	0/3/3/3
15	ATP	7	801	-	-	4/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	901	ATP	C5-C4	4.82	1.47	1.39
14	5	801	ADP	C5-C4	4.76	1.47	1.39
15	6	902	ATP	C5-C4	4.57	1.47	1.39
15	3	901	ATP	C5-C4	4.48	1.47	1.39
15	7	801	ATP	C5-C4	4.42	1.47	1.39
14	6	901	ADP	PB-O1B	3.47	1.61	1.50
14	6	901	ADP	PA-O1A	3.30	1.62	1.50
14	5	801	ADP	C5-C6	2.89	1.49	1.41
15	6	902	ATP	C5-C6	2.74	1.48	1.41
14	6	901	ADP	PA-O3A	2.52	1.62	1.59
15	7	801	ATP	C5-C6	2.51	1.48	1.41
15	3	901	ATP	C5-N7	-2.51	1.34	1.39
15	4	901	ATP	C8-N7	2.49	1.36	1.31
15	4	901	ATP	C5-C6	2.47	1.47	1.41
15	7	801	ATP	C5-N7	-2.44	1.34	1.39
14	5	801	ADP	C8-N7	2.44	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	6	902	ATP	C8-N7	2.33	1.36	1.31
15	6	902	ATP	C5-N7	-2.33	1.34	1.39
15	3	901	ATP	C5-C6	2.30	1.47	1.41
15	6	902	ATP	PB-O3A	2.27	1.61	1.59
15	4	901	ATP	C4-N9	-2.25	1.33	1.37
14	5	801	ADP	C5-N7	-2.15	1.35	1.39
14	6	901	ADP	C5-N7	-2.10	1.35	1.39
15	4	901	ATP	C5-N7	-2.10	1.35	1.39
15	3	901	ATP	C8-N7	2.04	1.35	1.31
15	7	801	ATP	C8-N7	2.03	1.35	1.31

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	801	ADP	C5-C4-N3	-6.84	117.29	126.72
15	7	801	ATP	C5-C4-N3	-6.59	117.65	126.72
15	6	902	ATP	C5-C4-N3	-6.22	118.15	126.72
15	3	901	ATP	C5-C4-N3	-5.73	118.83	126.72
15	7	801	ATP	N3-C4-N9	5.51	136.54	127.17
14	5	801	ADP	N3-C4-N9	5.51	136.54	127.17
14	6	901	ADP	C5-C4-N3	-5.24	119.50	126.72
15	4	901	ATP	C5-C4-N3	-4.97	119.88	126.72
15	3	901	ATP	N3-C4-N9	4.93	135.55	127.17
15	6	902	ATP	N3-C4-N9	4.86	135.44	127.17
14	6	901	ADP	N3-C2-N1	-4.71	121.45	128.58
14	6	901	ADP	N3-C4-N9	4.55	134.91	127.17
14	5	801	ADP	C2-N3-C4	4.30	122.33	111.83
15	7	801	ATP	C2-N3-C4	4.13	121.93	111.83
15	4	901	ATP	C4-C5-N7	-4.03	105.97	110.58
15	6	902	ATP	C2-N3-C4	3.92	121.40	111.83
14	6	901	ADP	C2-N3-C4	3.69	120.85	111.83
14	6	901	ADP	C5-N7-C8	3.64	109.17	103.45
14	5	801	ADP	C4-C5-N7	-3.64	106.42	110.58
15	6	902	ATP	C4-C5-N7	-3.63	106.43	110.58
15	4	901	ATP	N3-C4-N9	3.51	133.13	127.17
14	5	801	ADP	N3-C2-N1	-3.50	123.29	128.58
15	3	901	ATP	C2-N3-C4	3.45	120.26	111.83
15	7	801	ATP	C2'-C1'-N9	-3.41	104.82	113.30
15	4	901	ATP	C2-N3-C4	3.41	120.16	111.83
15	4	901	ATP	N3-C2-N1	-3.35	123.51	128.58
15	7	801	ATP	C4-C5-N7	-3.23	106.89	110.58
15	7	801	ATP	N3-C2-N1	-3.21	123.73	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	6	902	ATP	N3-C2-N1	-3.20	123.73	128.58
14	5	801	ADP	C5-N7-C8	3.00	108.17	103.45
15	6	902	ATP	C3'-C2'-C1'	2.99	107.12	101.46
15	3	901	ATP	N3-C2-N1	-2.95	124.11	128.58
15	3	901	ATP	C4-N9-C8	2.92	108.81	105.74
15	7	801	ATP	C4-N9-C8	2.84	108.72	105.74
15	3	901	ATP	C4-C5-N7	-2.79	107.39	110.58
14	5	801	ADP	C4-N9-C8	2.78	108.66	105.74
15	6	902	ATP	C5-N7-C8	2.73	107.73	103.45
15	4	901	ATP	C4-N9-C8	2.67	108.54	105.74
15	4	901	ATP	C5-N7-C8	2.66	107.63	103.45
15	7	801	ATP	C5-N7-C8	2.65	107.61	103.45
15	4	901	ATP	C6-C5-N7	2.63	137.15	132.09
15	6	902	ATP	C4-N9-C8	2.47	108.33	105.74
14	6	901	ADP	C4-C5-N7	-2.40	107.83	110.58
15	3	901	ATP	C2'-C1'-N9	-2.39	107.36	113.30
14	5	801	ADP	N9-C8-N7	-2.35	110.61	113.94
15	6	902	ATP	O2A-PA-O3A	-2.31	101.04	107.27
14	6	901	ADP	PA-O5'-C5'	-2.29	108.25	121.35
15	4	901	ATP	C2-N1-C6	2.26	122.44	118.73
15	4	901	ATP	O2A-PA-O5'	2.24	117.70	107.57
15	3	901	ATP	C5-N7-C8	2.23	106.96	103.45
14	5	801	ADP	O3A-PA-O1A	-2.23	104.01	110.70
15	7	801	ATP	C2'-C3'-C4'	2.22	106.89	102.61
15	4	901	ATP	O2A-PA-O1A	2.21	122.75	112.44
15	6	902	ATP	C2'-C1'-N9	-2.19	107.87	113.30
14	5	801	ADP	O2A-PA-O1A	2.18	122.60	112.44
15	3	901	ATP	C3'-C2'-C1'	2.17	105.56	101.46
14	5	801	ADP	O3B-PB-O2B	2.15	115.86	107.80
15	6	902	ATP	C6-C5-N7	2.14	136.22	132.09
15	4	901	ATP	N9-C8-N7	-2.13	110.91	113.94
14	5	801	ADP	C6-C5-N7	2.13	136.19	132.09
15	4	901	ATP	PA-O5'-C5'	2.10	133.36	121.35
15	7	801	ATP	N9-C8-N7	-2.09	110.98	113.94
14	6	901	ADP	C2-N1-C6	2.05	122.09	118.73
14	6	901	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	6	902	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
15	6	902	ATP	C5'-O5'-PA-O2A
15	6	902	ATP	C5'-O5'-PA-O3A
15	3	901	ATP	C5'-O5'-PA-O1A
15	3	901	ATP	C5'-O5'-PA-O2A
15	3	901	ATP	C5'-O5'-PA-O3A
15	4	901	ATP	C5'-O5'-PA-O2A
15	4	901	ATP	C5'-O5'-PA-O3A
15	7	801	ATP	C5'-O5'-PA-O1A
15	7	801	ATP	C5'-O5'-PA-O2A
15	7	801	ATP	C5'-O5'-PA-O3A
14	6	901	ADP	C2'-C1'-N9-C8
14	5	801	ADP	C2'-C1'-N9-C4
14	6	901	ADP	C2'-C1'-N9-C4
15	6	902	ATP	C4'-C5'-O5'-PA
14	5	801	ADP	C2'-C1'-N9-C8
15	4	901	ATP	C5'-O5'-PA-O1A
15	3	901	ATP	C4'-C5'-O5'-PA
15	4	901	ATP	C4'-C5'-O5'-PA
15	7	801	ATP	C4'-C5'-O5'-PA
15	4	901	ATP	O4'-C4'-C5'-O5'
15	6	902	ATP	O4'-C4'-C5'-O5'

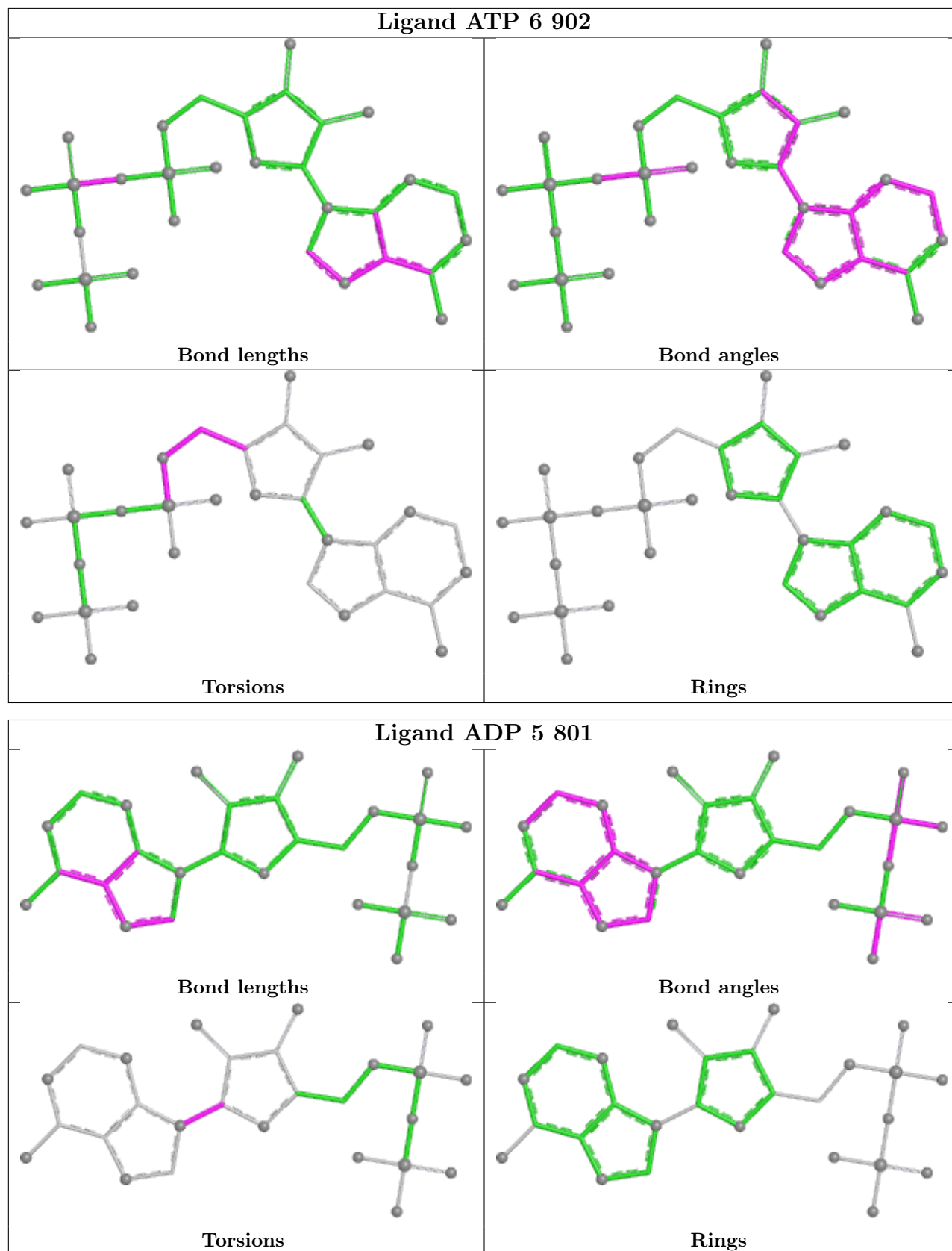
There are no ring outliers.

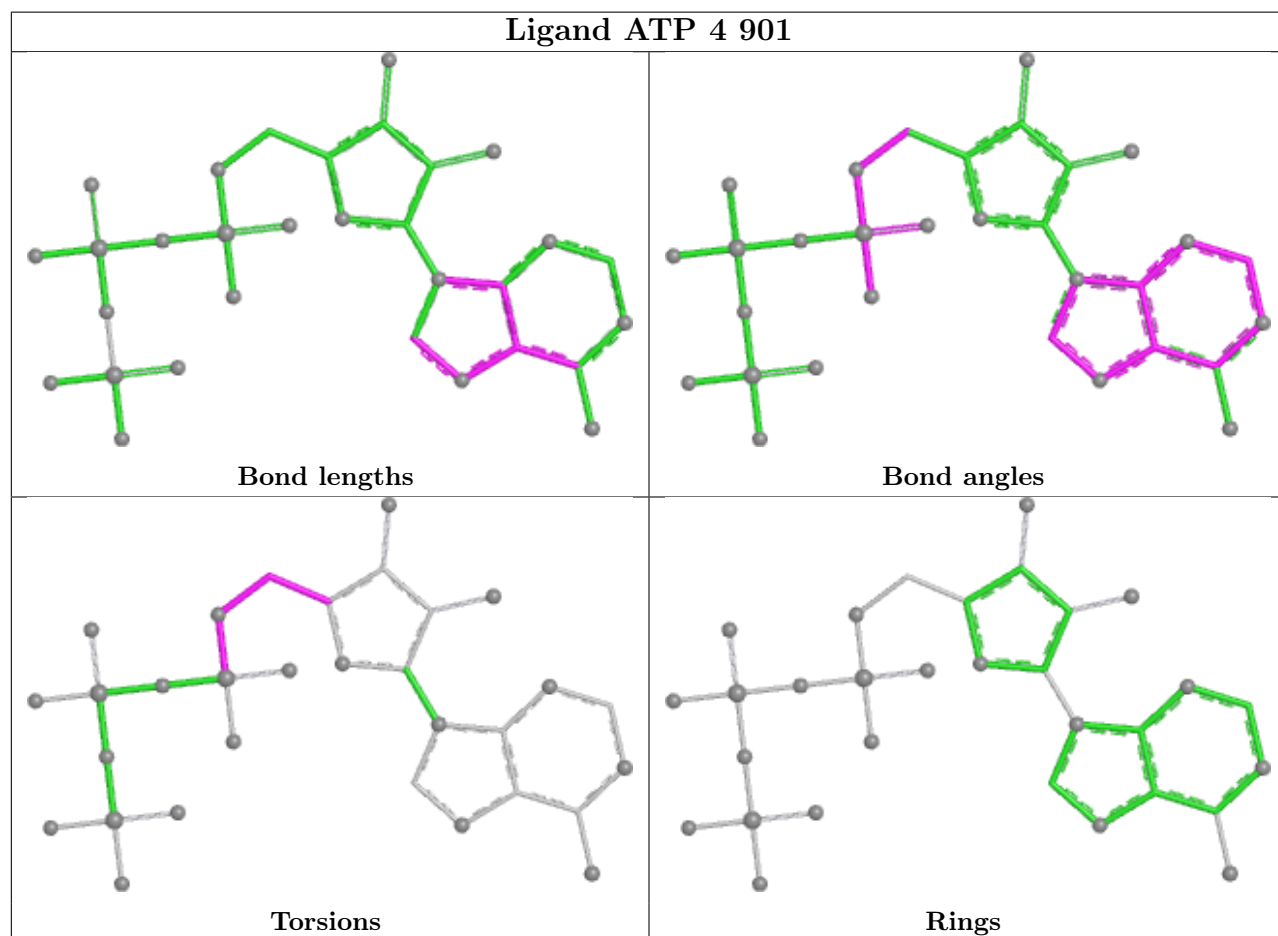
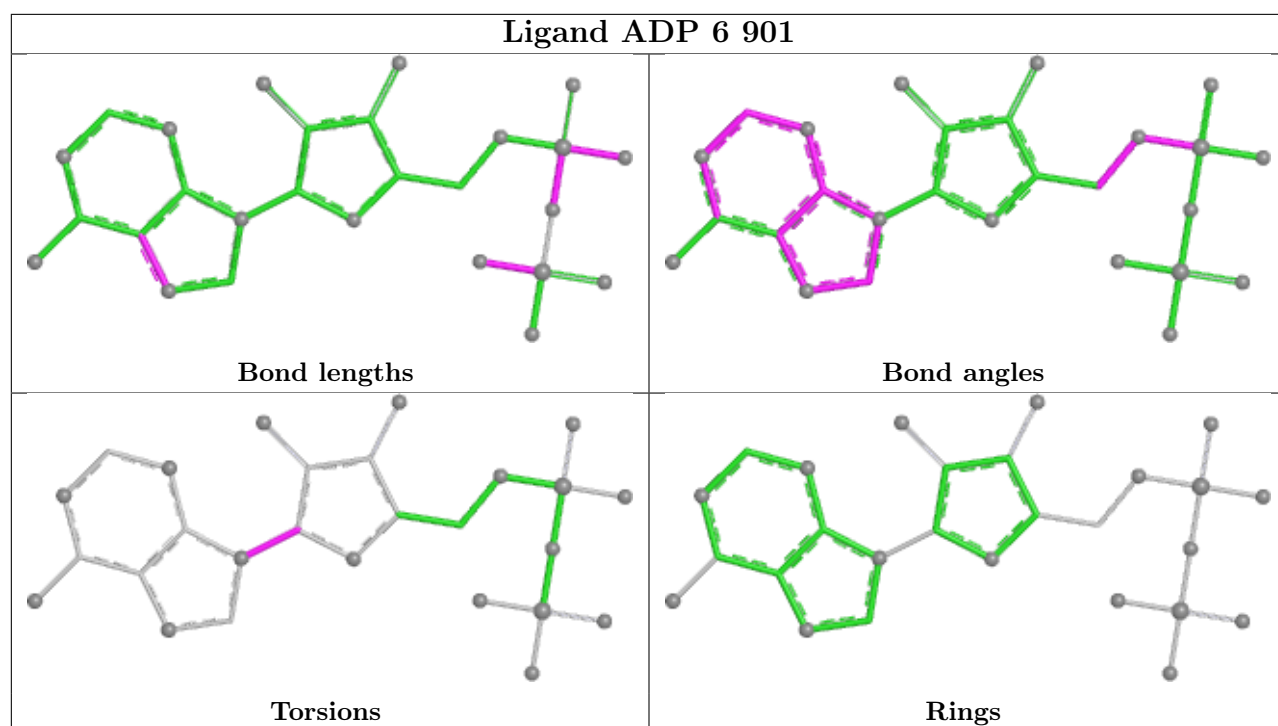
6 monomers are involved in 39 short contacts:

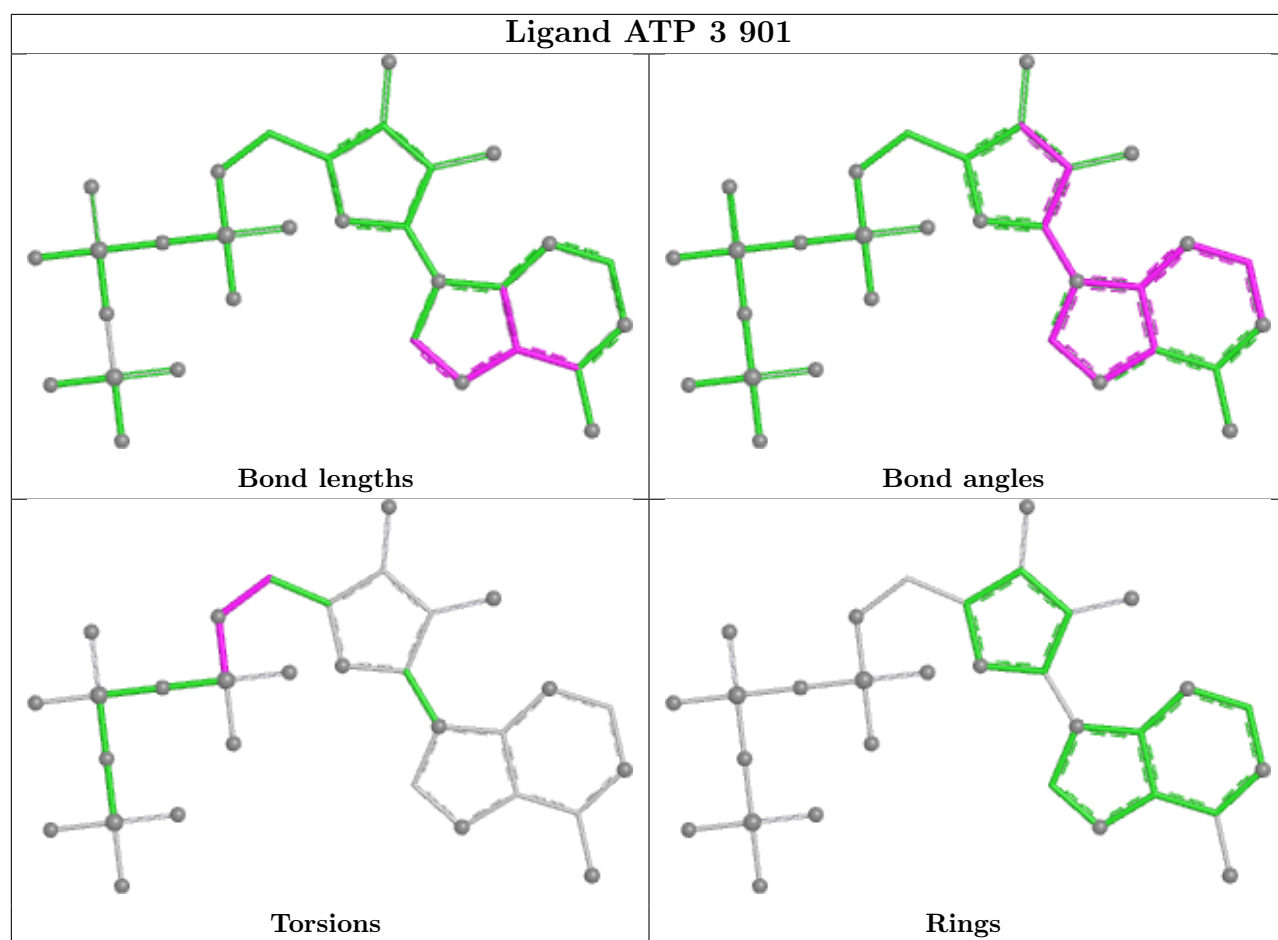
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	6	902	ATP	6	0
14	5	801	ADP	5	0
14	6	901	ADP	5	0
15	4	901	ATP	5	0
15	3	901	ATP	7	0
15	7	801	ATP	11	0

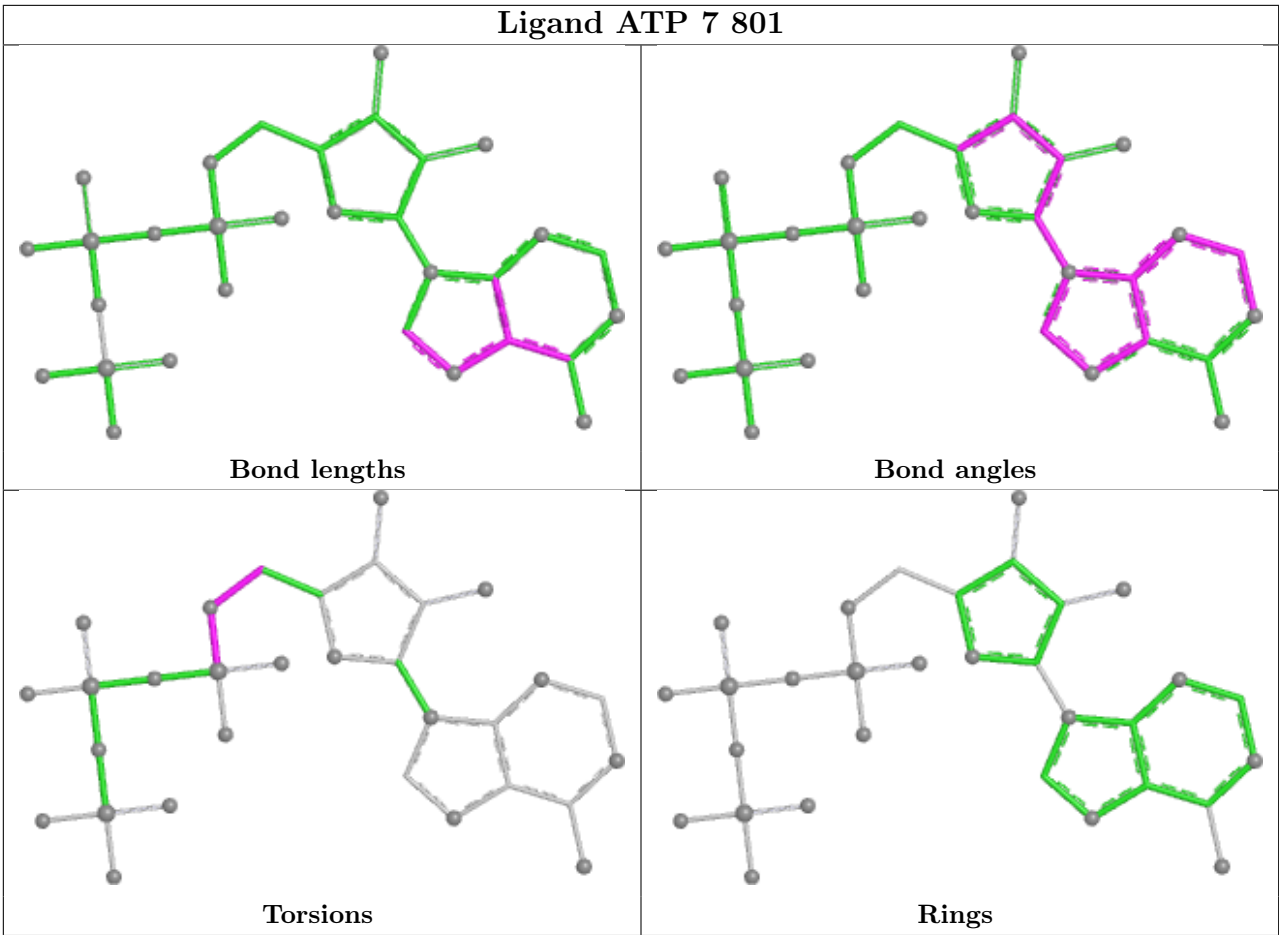
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	5	2
8	2	1
12	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	405:GLY	C	408:SER	N	5.55
1	2	435:LYS	C	436:GLN	N	4.80
1	5	507:ILE	C	508:LEU	N	1.04

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	491:LYS	C	492:LYS	N	0.72

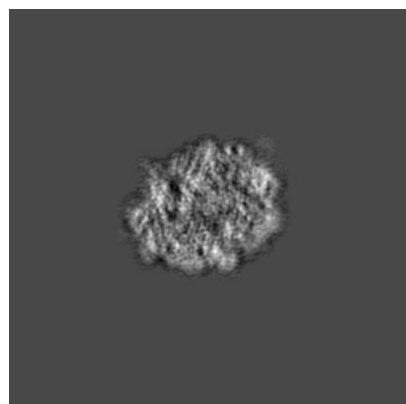
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4788. These allow visual inspection of the internal detail of the map and identification of artifacts.

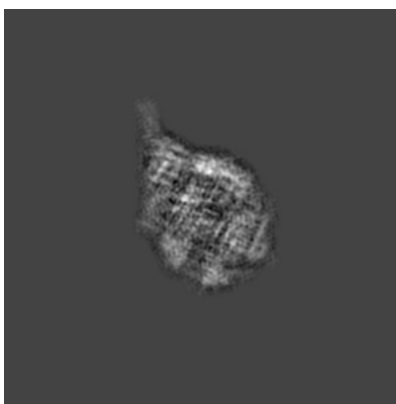
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

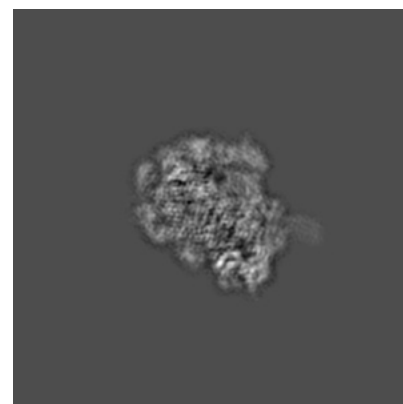
6.1.1 Primary map



X

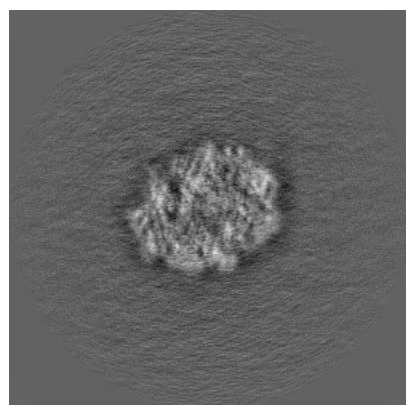


Y

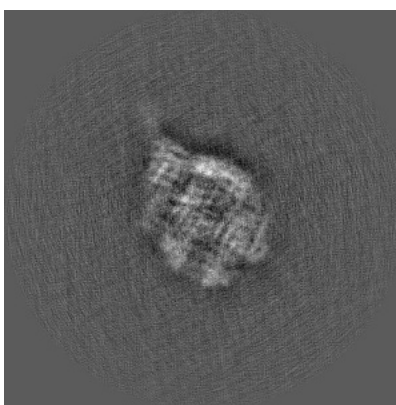


Z

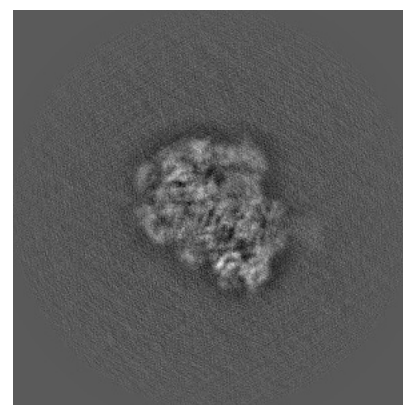
6.1.2 Raw map



X



Y

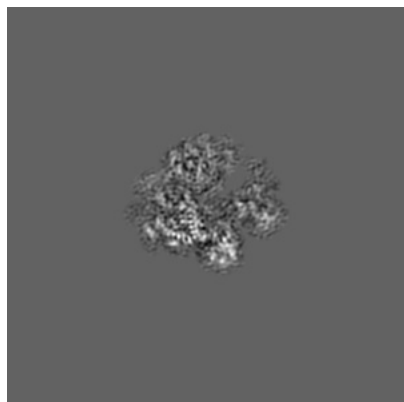


Z

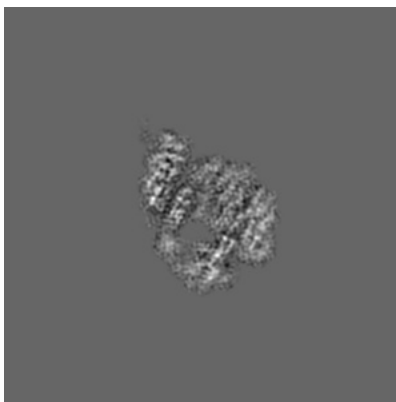
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

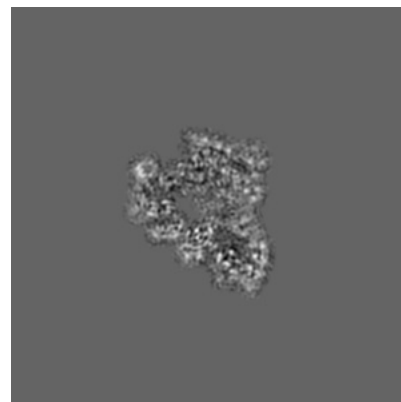
6.2.1 Primary map



X Index: 192

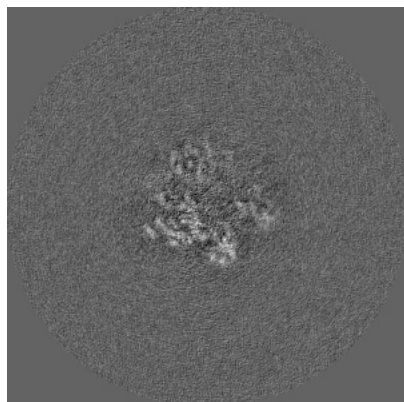


Y Index: 192

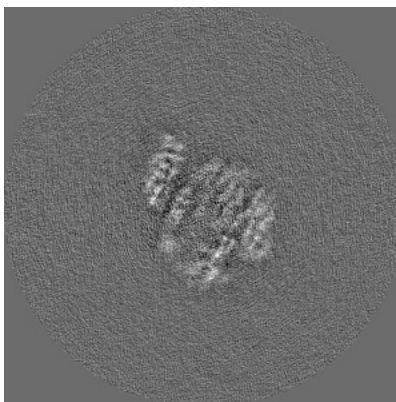


Z Index: 192

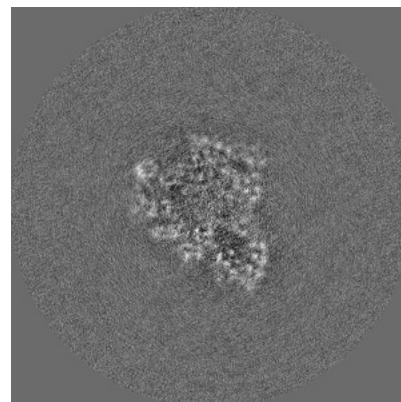
6.2.2 Raw map



X Index: 192



Y Index: 192

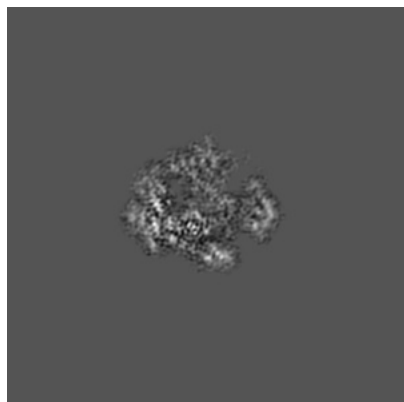


Z Index: 192

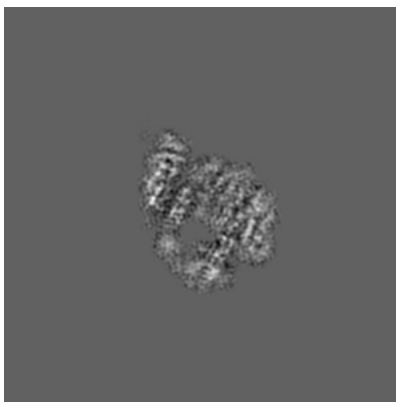
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

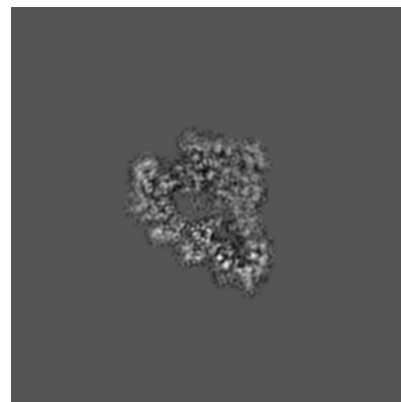
6.3.1 Primary map



X Index: 200

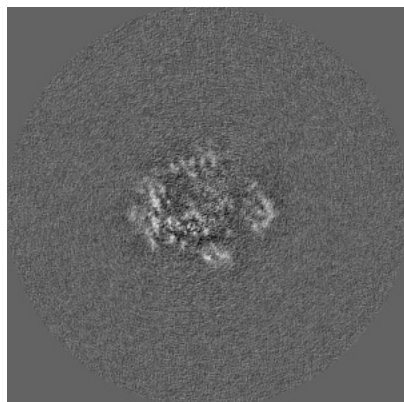


Y Index: 193

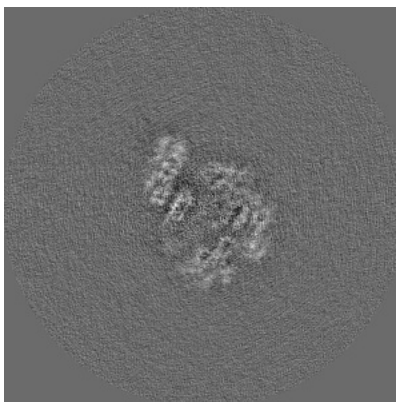


Z Index: 195

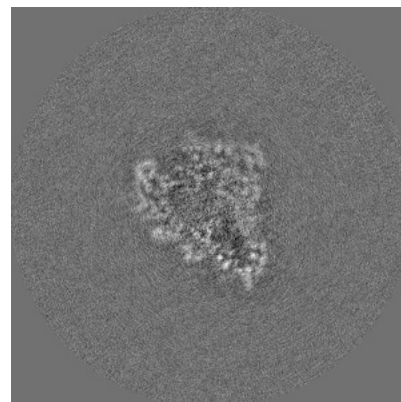
6.3.2 Raw map



X Index: 199



Y Index: 189

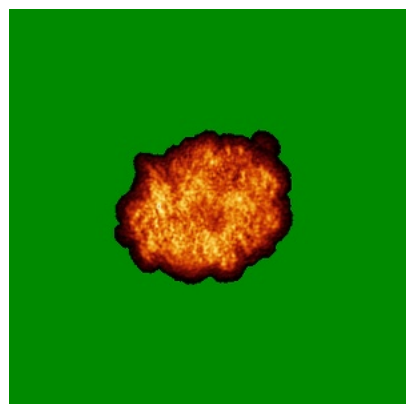


Z Index: 195

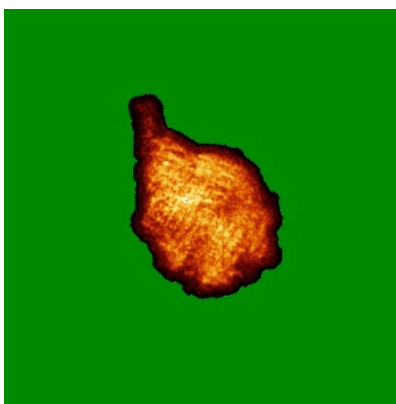
The images above show the largest variance slices of the map in three orthogonal directions.

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

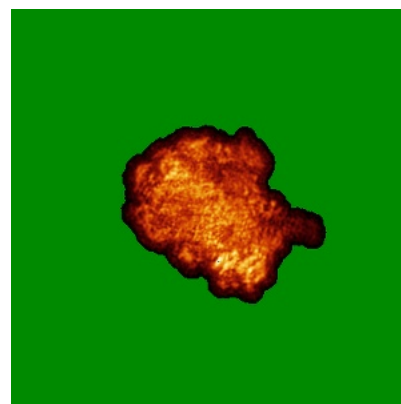
6.4.1 Primary map



X

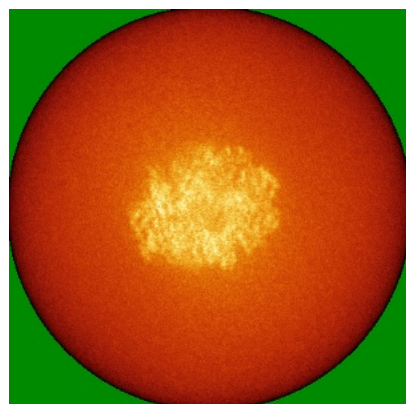


Y

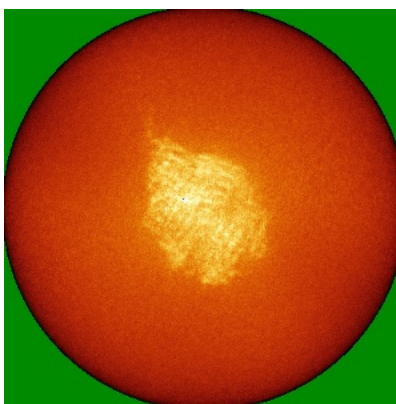


Z

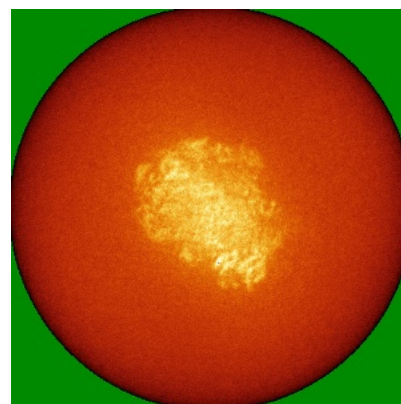
6.4.2 Raw map



X



Y

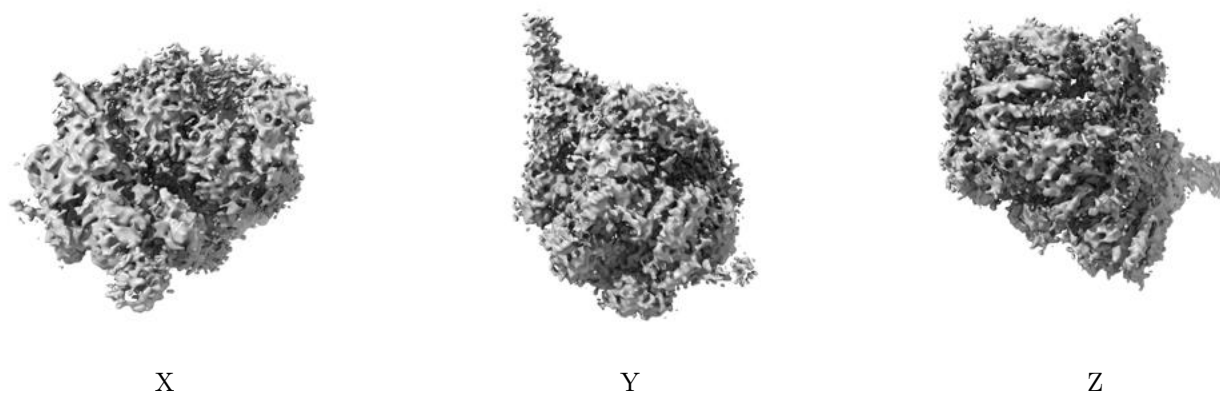


Z

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.

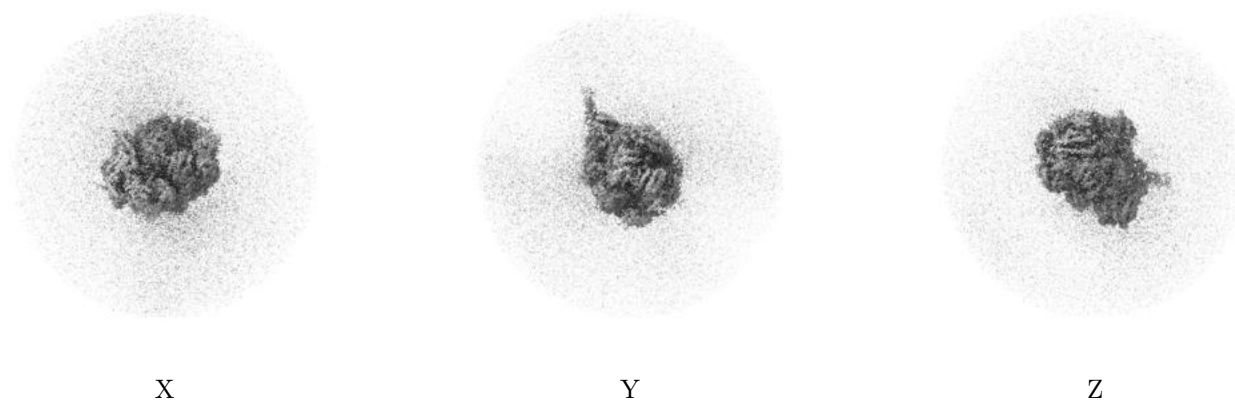
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. 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.

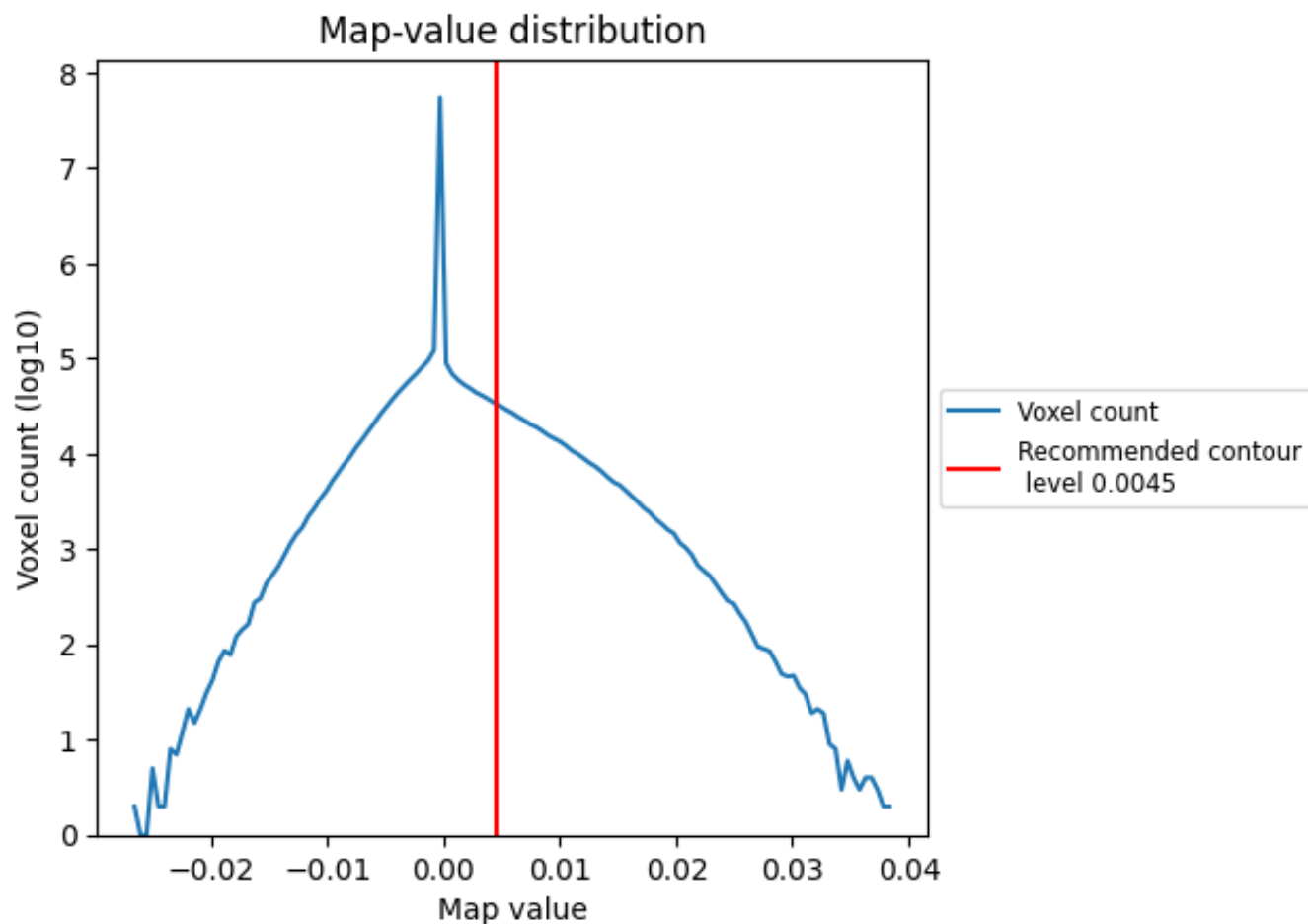
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

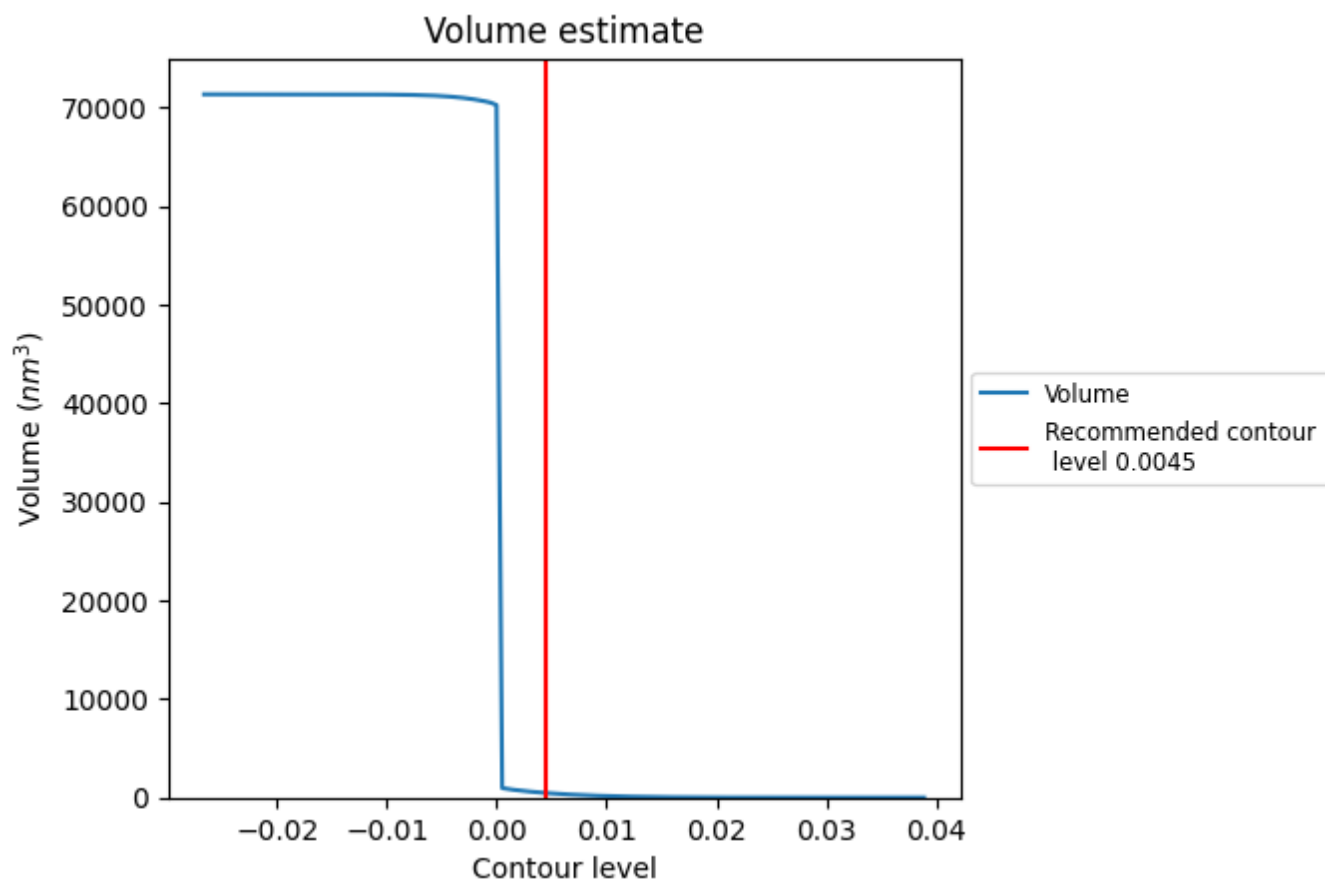
This section contains the results of statistical analysis of the map.

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.

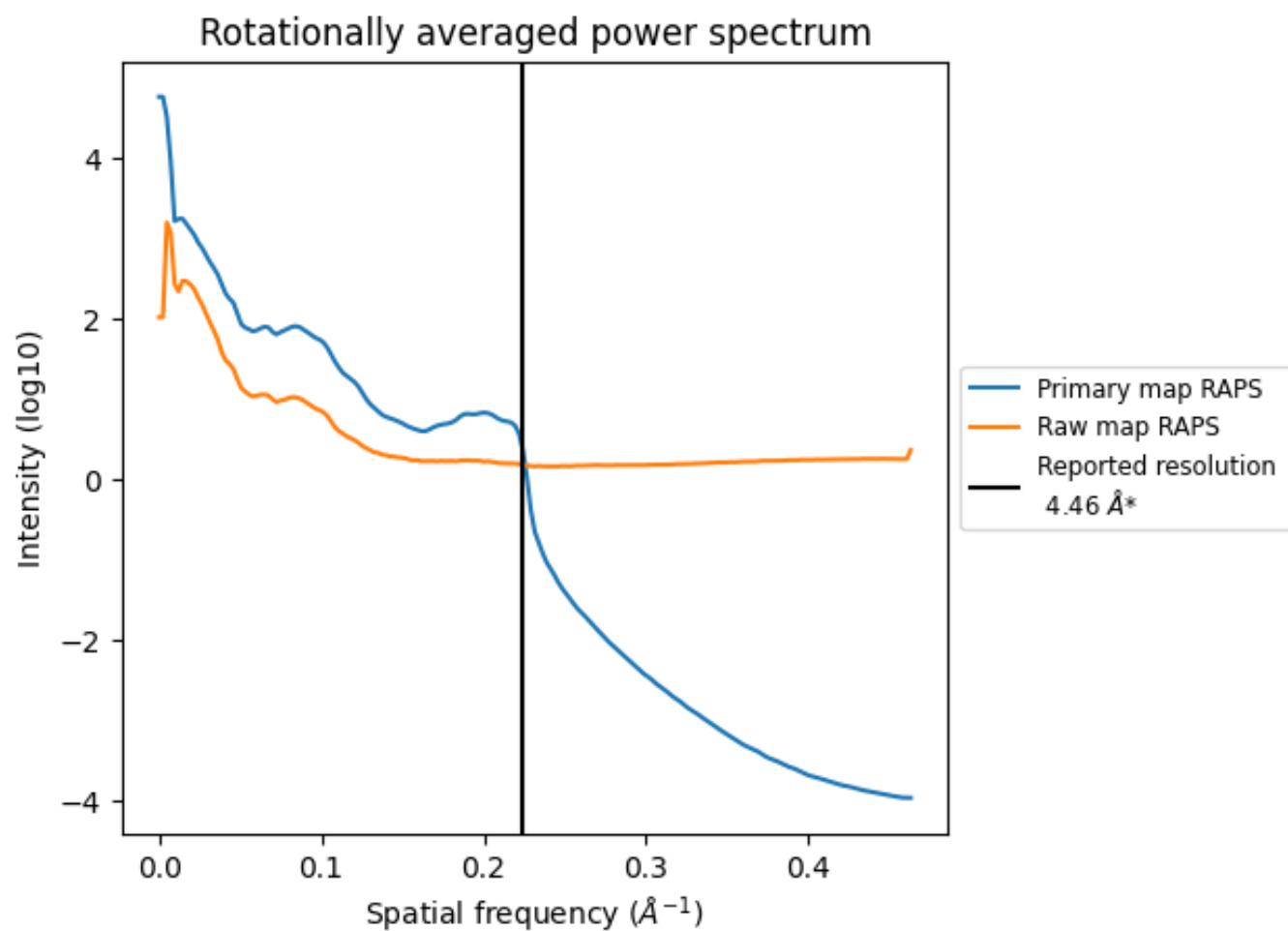
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 463 nm³; this corresponds to an approximate mass of 418 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 ⓘ

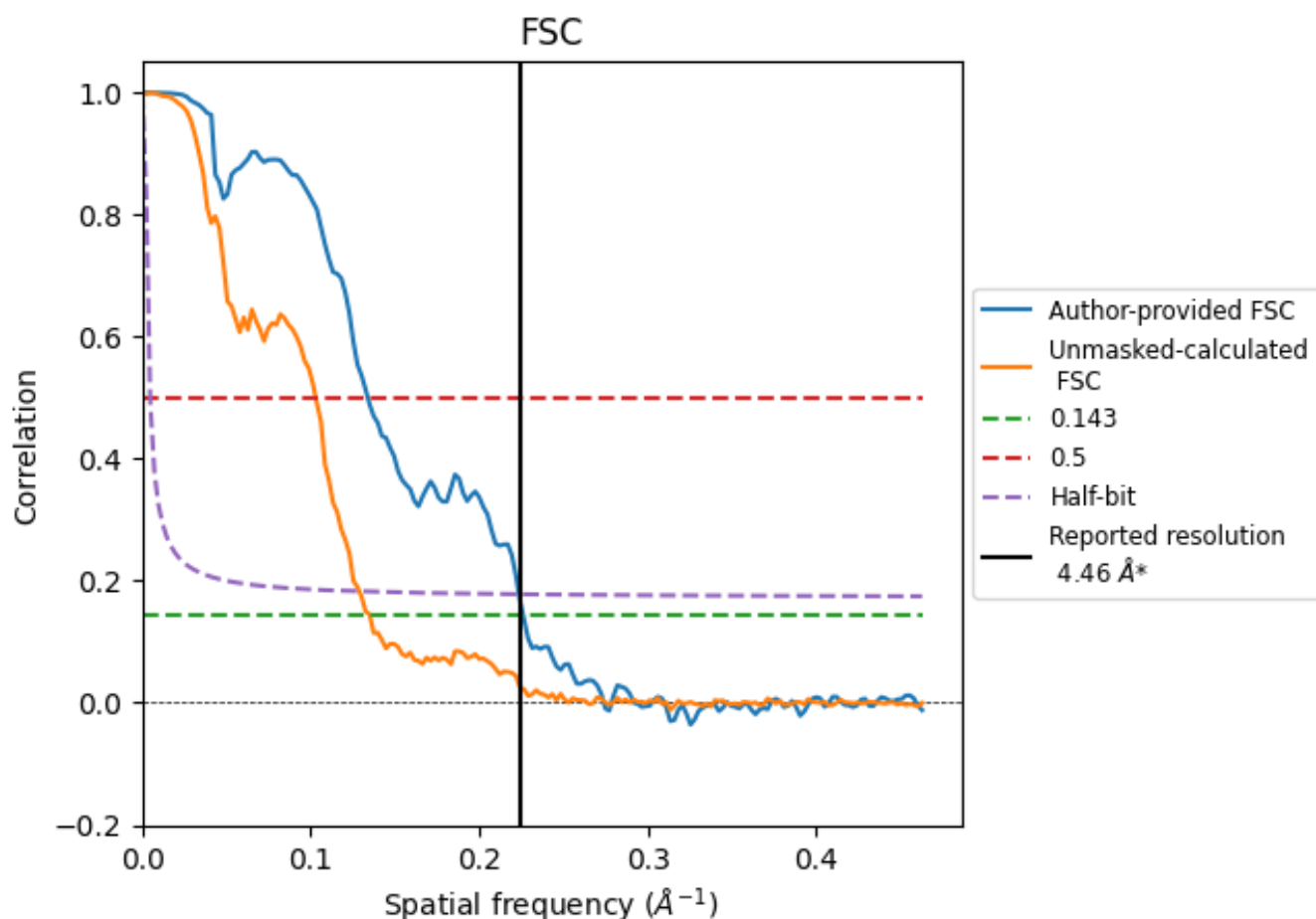


*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

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 0.224 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

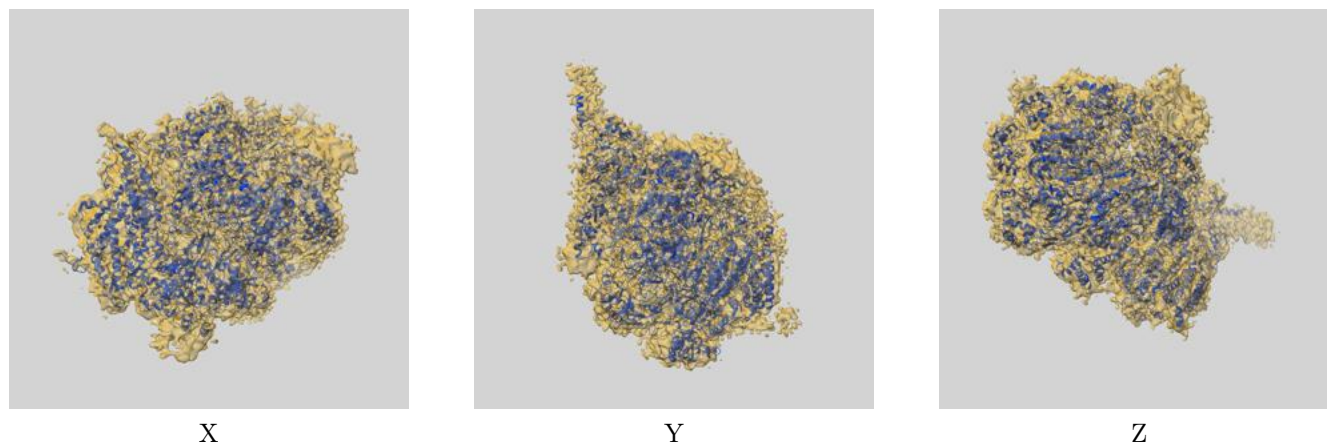
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.46	-	-
Author-provided FSC curve	4.42	7.46	4.47
Unmasked-calculated*	7.40	9.71	7.76

*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 7.40 differs from the reported value 4.46 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4788 and PDB model 6RAZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



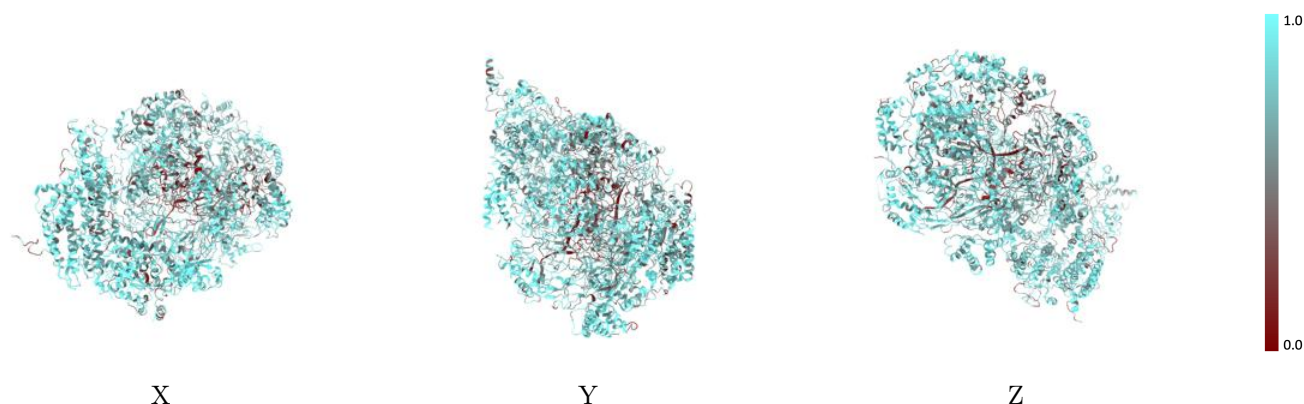
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



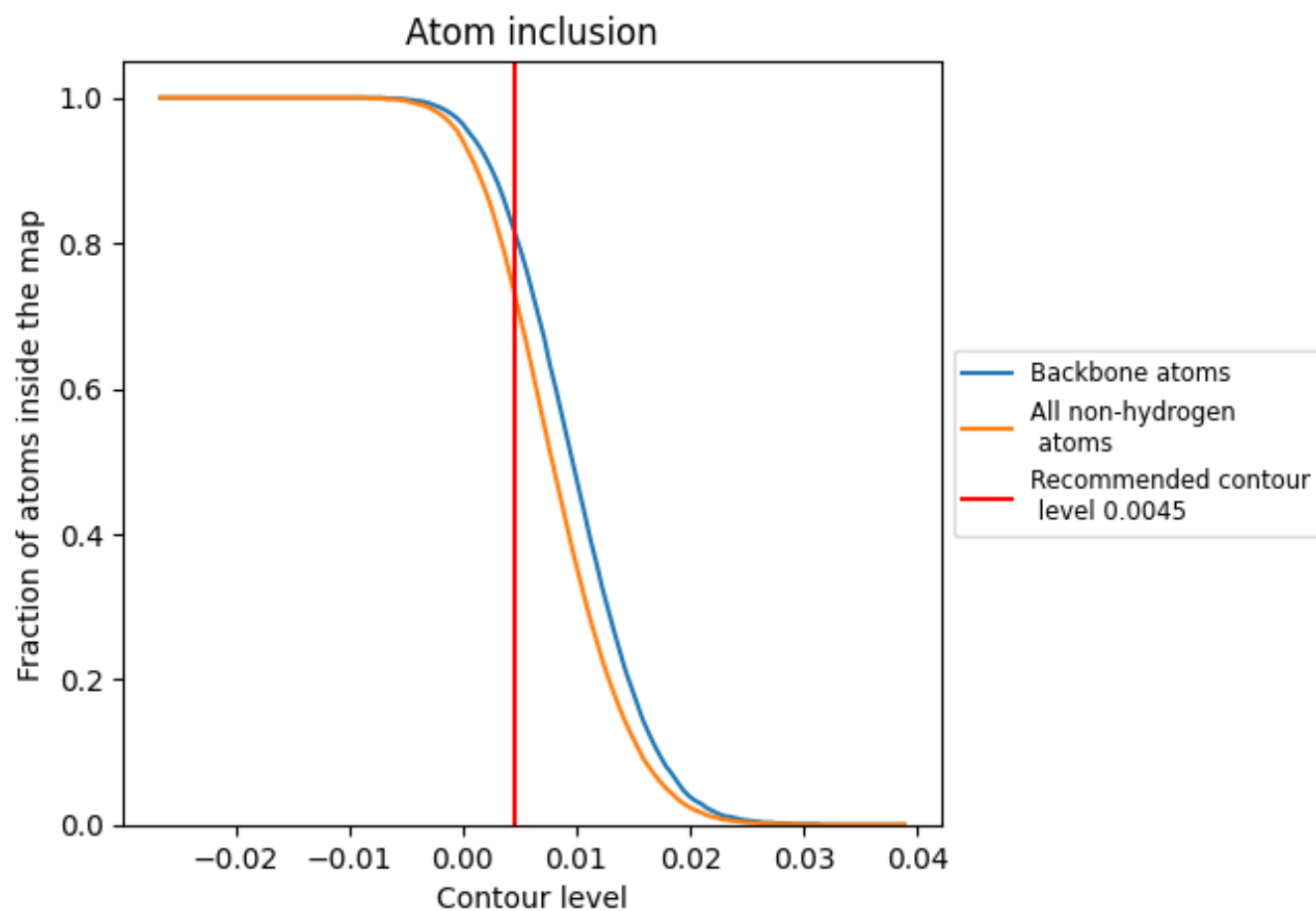
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0045).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.2460
2	 0.7080	 0.2360
3	 0.7460	 0.2630
4	 0.7370	 0.2460
5	 0.6750	 0.2360
6	 0.6970	 0.2250
7	 0.7640	 0.2680
A	 0.8020	 0.2700
H	 0.7370	 0.1920
L	 0.8360	 0.2760
M	 0.7710	 0.2610
N	 0.7960	 0.2460
X	 0.2660	 0.0990
Y	 0.1950	 0.1090

