



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:58 PM UTC

PDB ID : 7ML0 / pdb_00007ml0
EMDB ID : EMD-23904
Title : RNA polymerase II pre-initiation complex (PIC1)
Authors : Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on : 2021-04-27
Resolution : 3.00 Å(reported)
Based on initial model : 5OQJ

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
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

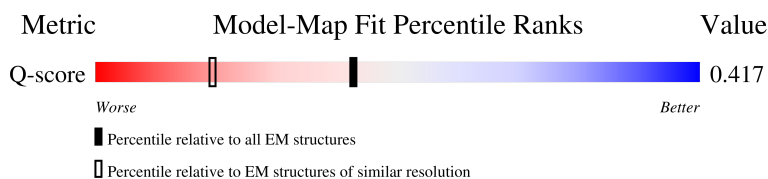
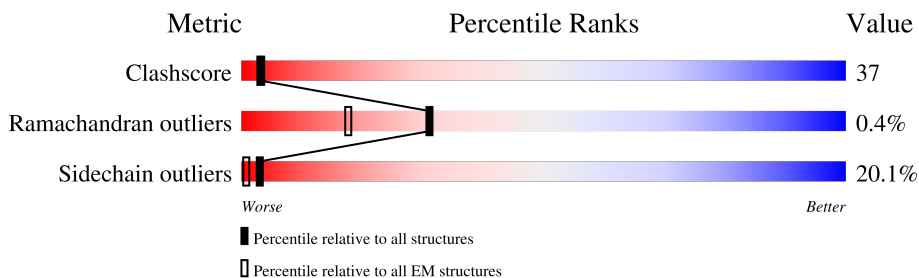
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	Q	735	
15	R	400	
16	W	482	
17	X	328	
18	O	240	
19	T	66	
20	N	66	
21	0	778	
22	1	541	
23	4	338	
24	6	461	
25	2	513	
26	5	72	
27	3	321	
28	7	843	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	SF4	0	801	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 64214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10996	6931	1926	2078	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1147	Total	C	N	O	S	0	0
			9132	5775	1602	1700	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 14 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 16 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

- Molecule 17 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	156	Total	C	N	O	S	0	0
			984	608	180	192	4		

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 19 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	66	Total	C	N	O	P	0	0
			1345	649	230	400	66		

- Molecule 20 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	66	Total	C	N	O	P	0	0
			1361	653	250	392	66		

- Molecule 21 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	753	Total	C	N	O	S	0	0
			6099	3886	1031	1144	38		

- Molecule 22 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1	367	Total	C	N	O	S	0	0
			2415	1538	439	431	7		

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 24 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

- Molecule 25 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	461	Total	C	N	O	S	0	0
			3020	1862	564	585	9		

- Molecule 26 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 27 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	137	Total	C	N	O	S	0	0
			890	552	164	166	8		

- Molecule 28 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	7	638	Total	C	N	O	S	0	0
			4478	2739	832	883	24		

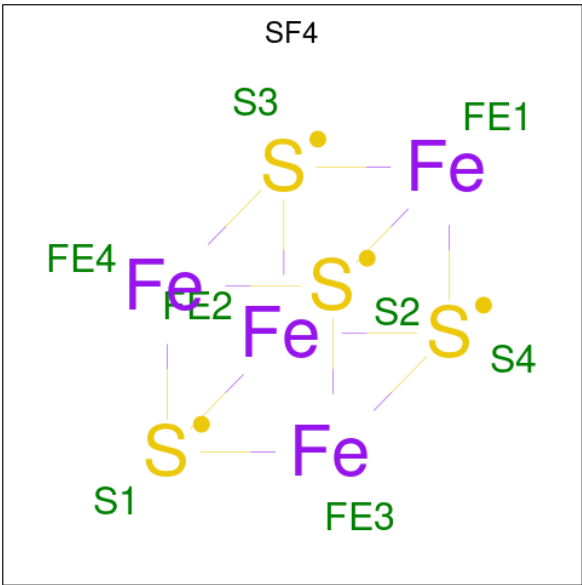
- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	A	2	Total	Zn	0
			2	2	
29	B	1	Total	Zn	0
			1	1	
29	C	1	Total	Zn	0
			1	1	
29	I	2	Total	Zn	0
			2	2	
29	J	1	Total	Zn	0
			1	1	
29	L	1	Total	Zn	0
			1	1	
29	M	1	Total	Zn	0
			1	1	
29	W	1	Total	Zn	0
			1	1	
29	4	1	Total	Zn	0
			1	1	
29	6	4	Total	Zn	0
			4	4	
29	3	2	Total	Zn	0
			2	2	

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Mg	0
			1	1	

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

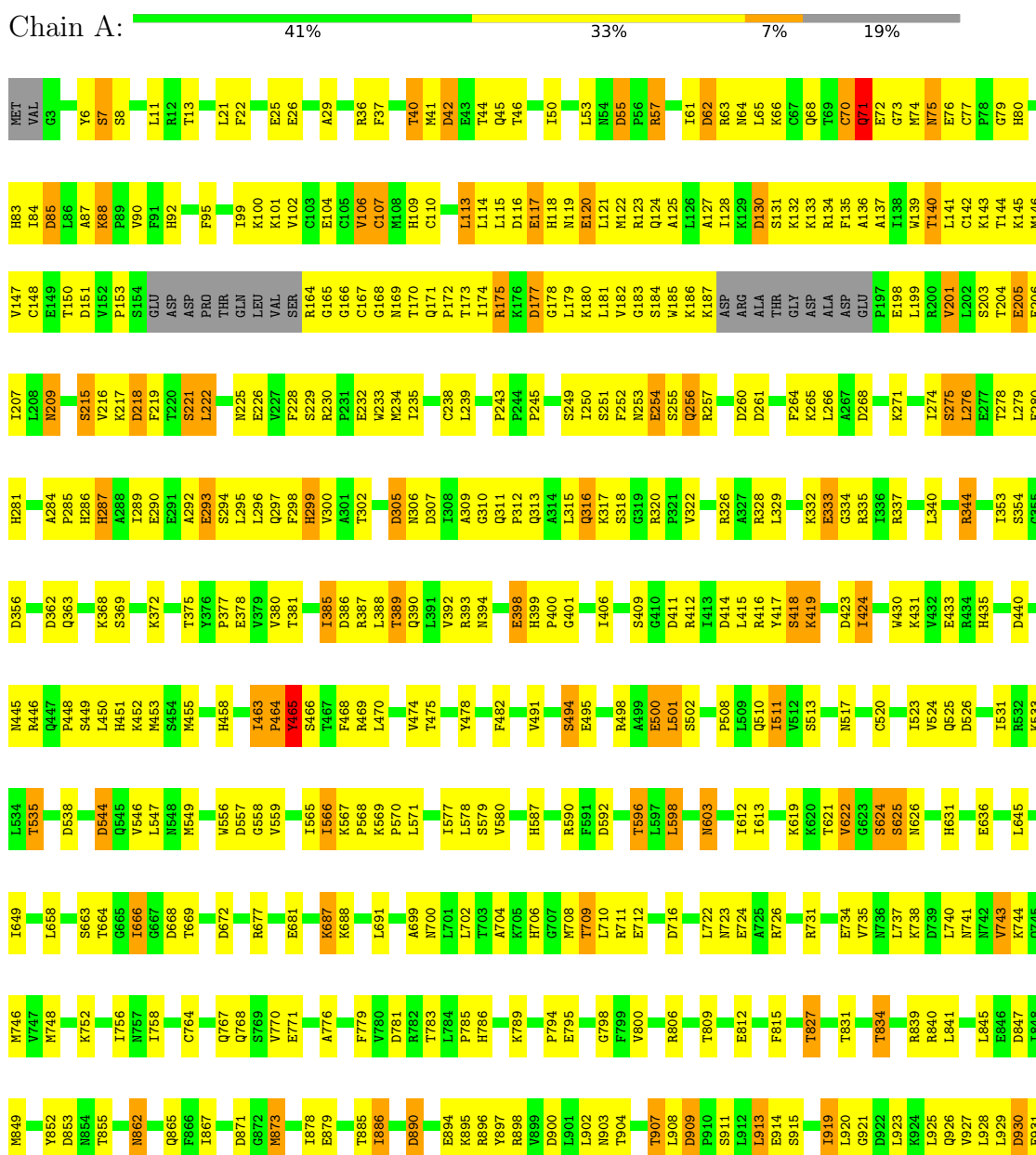


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
31	0	1	8	4	4	0

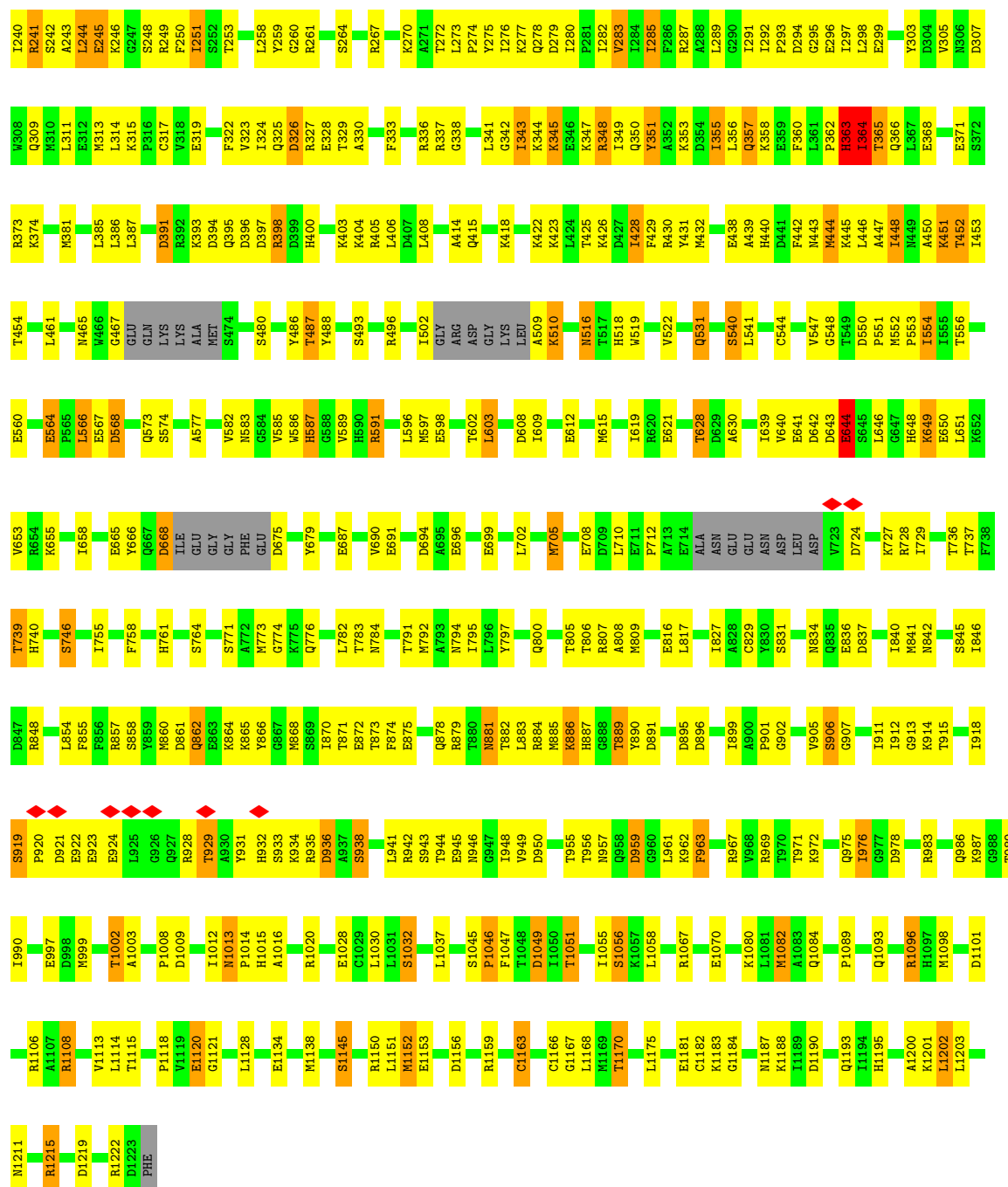
3 Residue-property plots

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-directed RNA polymerase subunit

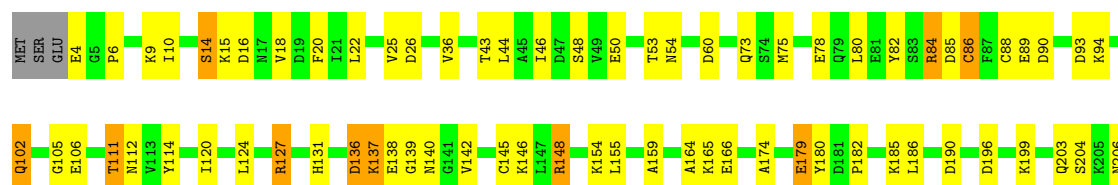




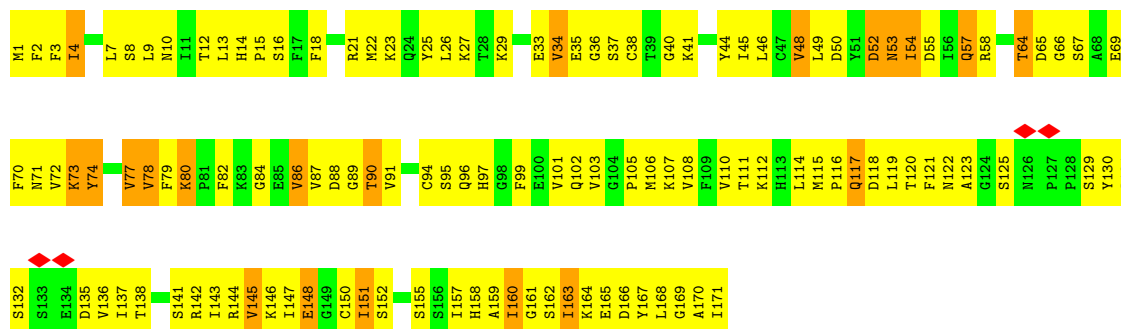


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 51% 27% 5% 18%

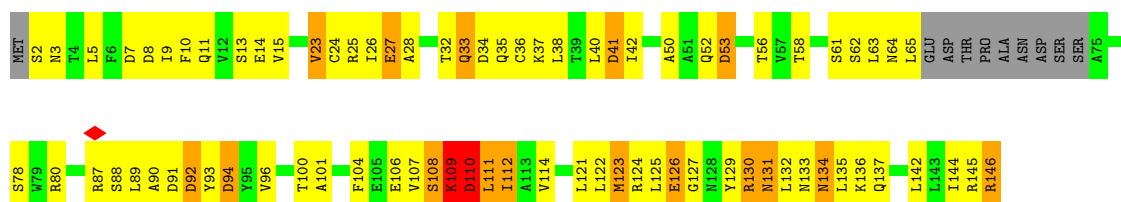


Chain G: 27% 60% 12%



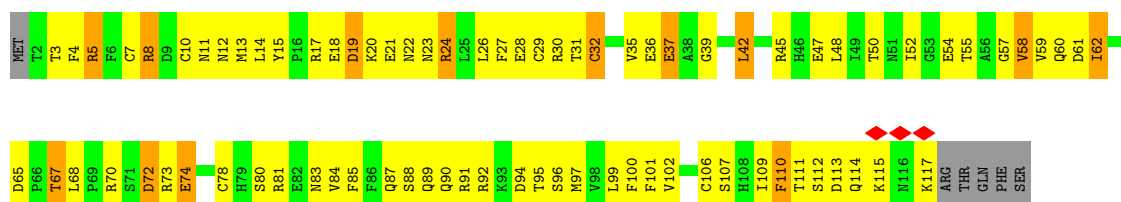
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 39% 42% 11% 7%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 29% 56% 11% 5%



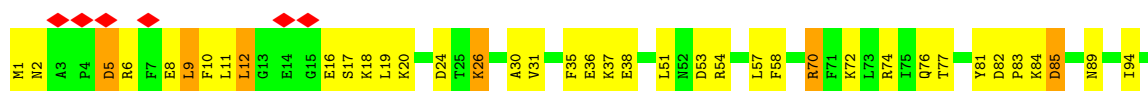
- Molecule 10: DNA-directed RNA polymerases II subunit RPABC5

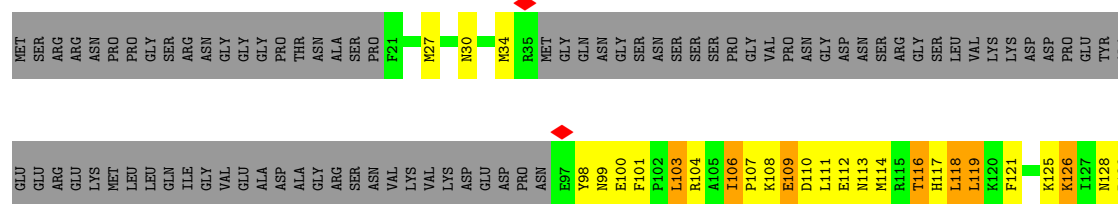
Chain J: 51% 33% 6% 7%

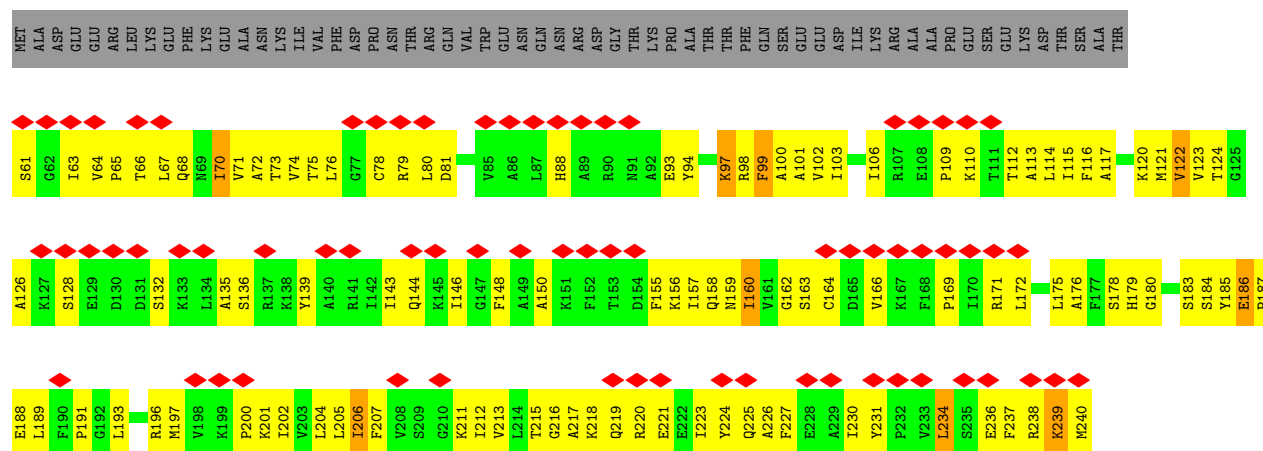


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

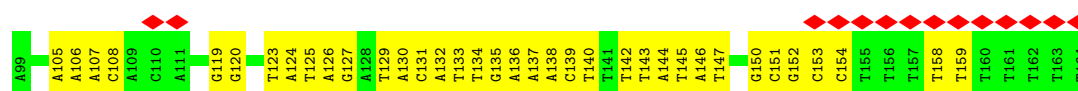
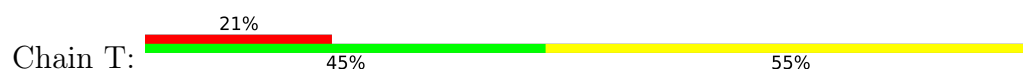
Chain K: 5% 58% 30% 5% 7%



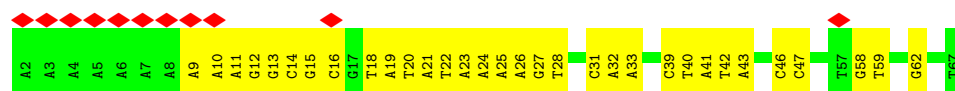




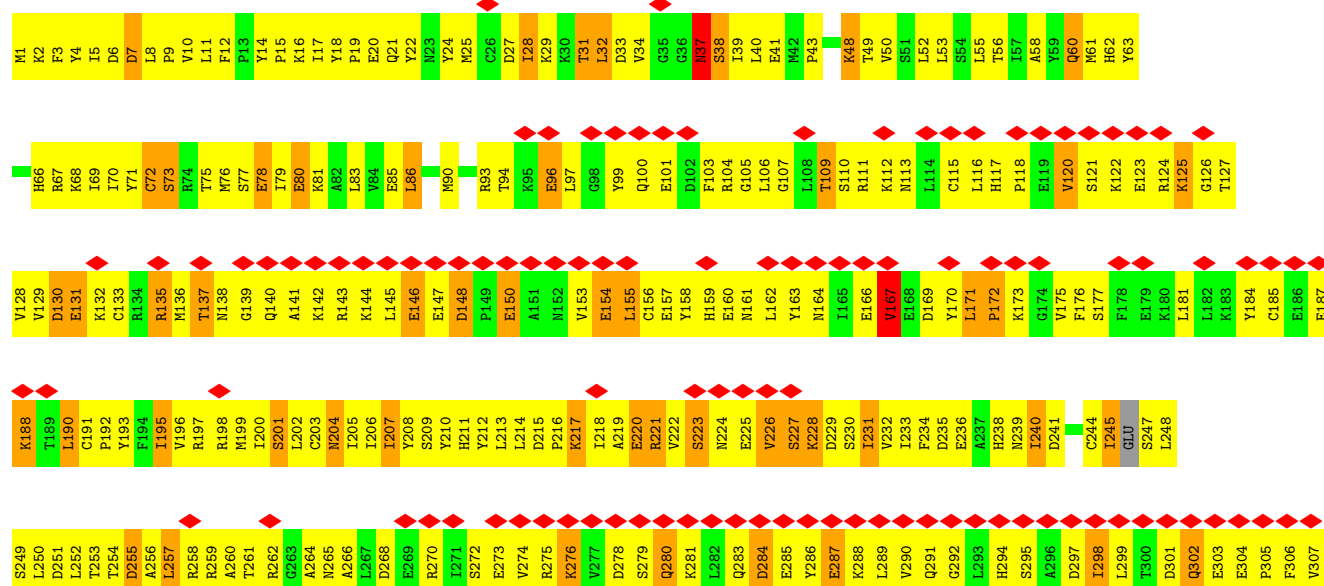
• Molecule 19: template strand DNA

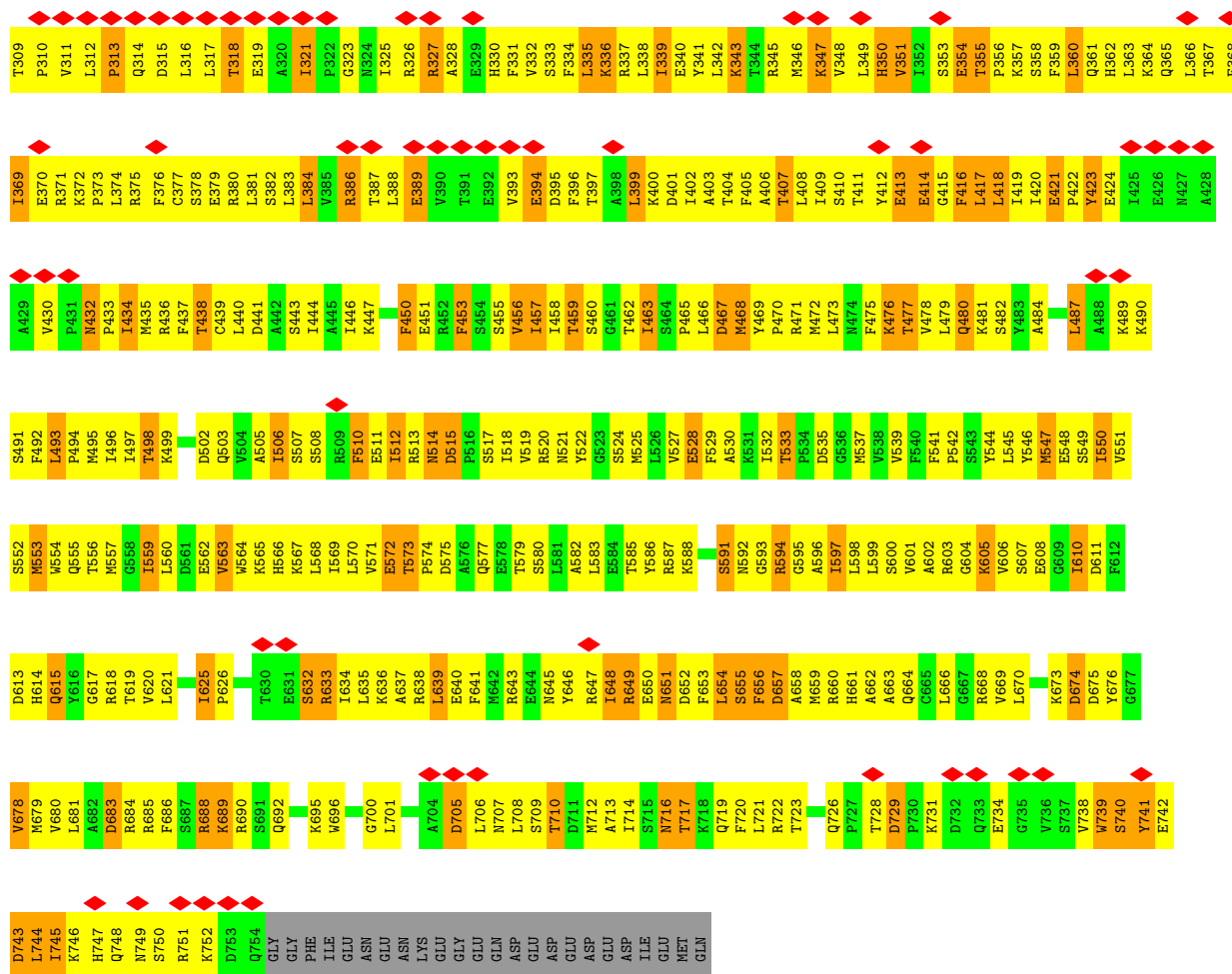


• Molecule 20: non-template strand DNA

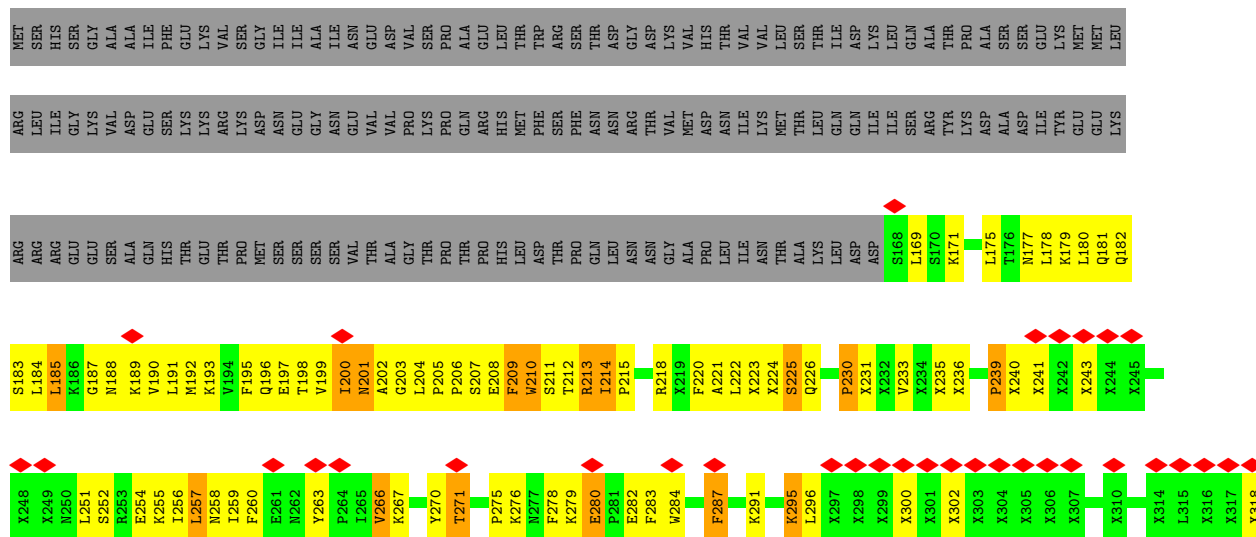
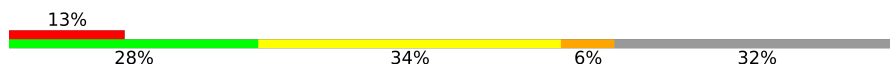


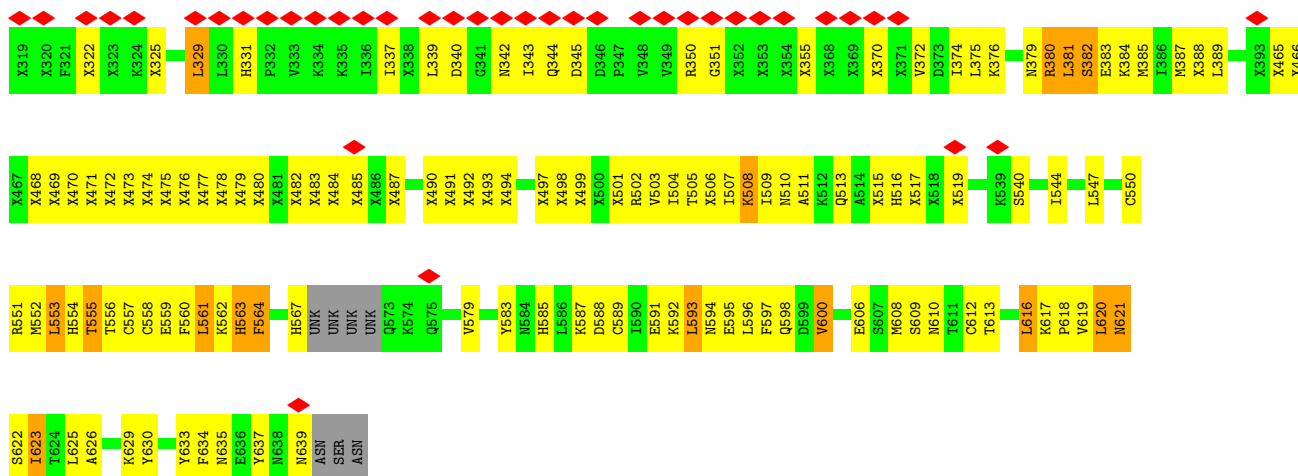
• Molecule 21: General transcription and DNA repair factor IIH helicase subunit XPD



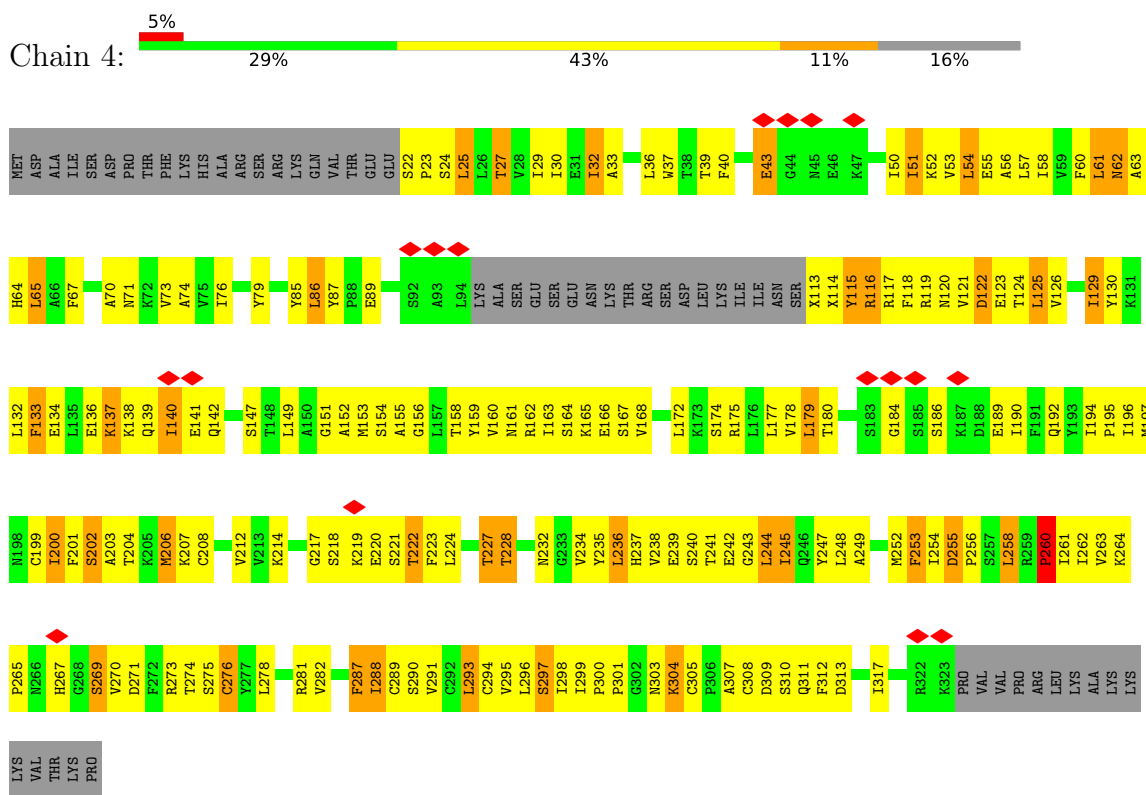


Chain 1:

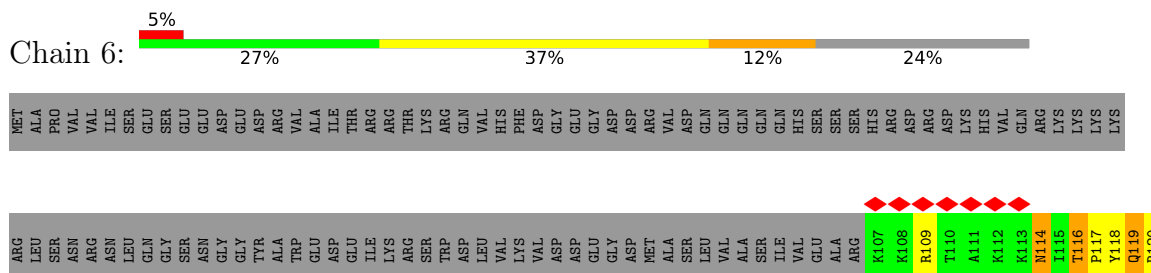


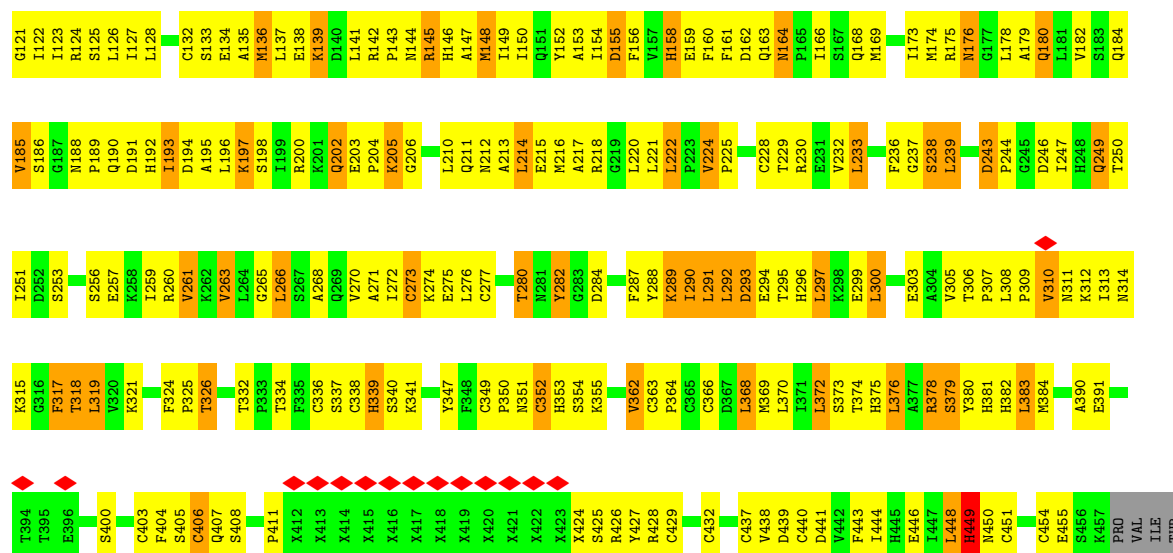


• Molecule 23: DNA-directed RNA polymerase II subunit RPB4

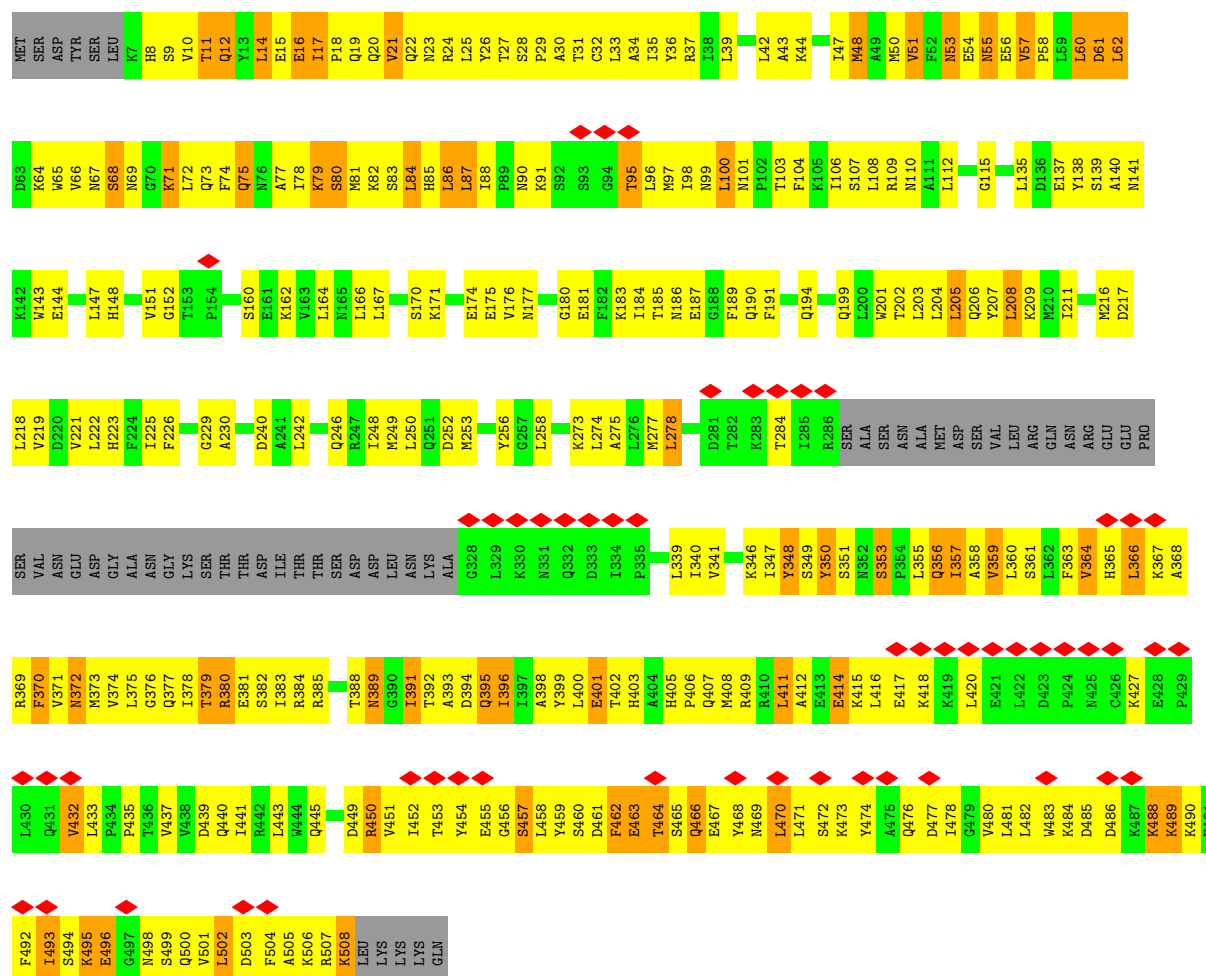


• Molecule 24: General transcription and DNA repair factor IIH subunit SSL1





• Molecule 25: RNA polymerase II transcription factor B subunit 2



• Molecule 26: General transcription and DNA repair factor IIH subunit TFB5

LYS	VAL	E715	S655	Q589	F529	H468	I408	R348
MET	GLY	H716	K656	A590	L530	D469	V409	N349
TYR	ASP	Y717	V657	C591	I531	D470	L410	P350
TYR	ALA	Y718	G658	Q592	G532	V471	C411	D351
LYS	ASP	S719	D659	F593	P533	V472	T412	L352
ASN	ASP	T720	T660	L594	K534	M474	S413	D353
ASN	ASN	K721	S661	I595	D475	D475	S414	I354
SER	SER	R722	S662	Q596	L535	F476	V415	D355
VAL	VAL	Q723	D663	Q597	Y536	L477	S416	L356
GLY	GLY	A724	D664	H598	E537	T478	V417	L357
ARG	ARG	F725	L664	E599	A538	M418	P358	K357
GLY	GLY	L726	P665	R600	N539	Q479	Q359	P358
SER	SER	V727	E666	R501	W540	R480	S359	P359
ASN	ASN	D728	A667	G602	M541	E481	T360	T360
GLY	GLY	Q729	T668	D603	E542	W482	Q361	Q361
HIS	HIS	Q730	K604	D603	L543	G483	I362	I362
LYS	LYS	Y731	L605	D604	S544	F484	R363	R363
ARG	ARG	A732	I606	I605	Q545	I485	P364	P364
PHE	PHE	F733	V607	V607	K546	I486	Y365	Y365
LYS	LYS	K734	F608	F608	G547	L487	Q366	Q366
SER	SER	V735	S609	S609	H548	C428	E367	E367
LYS	LYS	I736	D610	D610	I549	T429	K368	K368
ALA	ALA	T737	N611	N551	A550	L430	S369	S369
VAL	VAL	H738	G614	V552	Q553	Q431	L370	L370
ARG	ARG	L739	G678	Q553	C554	P432	S371	S371
GLY	GLY	H740	L615	V556	A555	E433	K372	K372
GLY	GLY	G741	Q616	W557	E556	N434	M373	M373
LEU	LEU	M742	E617	W558	V557	C435	F374	F374
SER	SER	E743	A684	A619	E557	A436	G375	G375
GLY	GLY	N744	Q685	L620	W558	N376	N376	N376
ALA	ALA	I745	Q686	K621	C559	G377	G377	G377
GLY	GLY	P746	L687	M622	P560	R378	R378	R378
GLY	GLY	N747	G688	G623	M561	A379	A379	A379
ASP	ASP	L748	R689	K624	T562	S440	S440	S440
MET	MET	A749	I690	P625	E564	N442	N442	N442
ALA	ALA	Y750	L691	F626	F565	K443	K443	K443
TYR	TYR	A751	R692	I627	H508	E444	E444	E444
GLY	GLY	S752	A693	Y628	A509	M445	M445	M445
P753	P753	R754	K694	T631	K510	F446	F446	F446
R754	R754	E755	R695	P632	L511	Q447	Q447	Q447
E755	E755	R756	R696	T631	G512	T448	T448	T448
R756	R756	E757	N697	P632	L451	E449	E449	E449
E757	E757	E758	D698	P632	G451	S450	S450	S450
E758	E758	L759	E699	P632	L452	G451	G451	G451
L759	L759	L760	G700	P632	V453	V453	V453	V453
L760	L760	Q761	F701	P632	S455	S455	S455	S455
Q761	Q761	E762	N702	P632	T456	T456	T456	T456
E762	E762	V763	A703	P632	Y457	Y457	Y457	Y457
V763	V763	L764	F704	P632	S458	S458	S458	S458
L764	L764	L765	F705	P632	M459	M459	M459	M459
L765	L765	K766	V706	P632	V395	V395	V395	V395
N767	N767	E768	S707	P632	G396	G396	G396	G396
E768	E768	E769	L708	P632	I397	I397	I397	I397
A770	A770	A770	V709	P632	T398	T398	T398	T398
ALA	ALA	GLY	S710	P632	L394	L394	L394	L394
GLY	GLY	ILE	K711	P632	V395	V395	V395	V395
D712	D712	GLY	T713	P632	G396	G396	G396	G396
T713	T713	GLY	D712	P632	I397	I397	I397	I397
F653	F653	GLY	T713	P632	T398	T398	T398	T398
L654	L654	GLY	Q714	P632	A399	A399	A399	A399
		GLY		P632	A400	A400	A400	A400
		GLY		P632	C401	C401	C401	C401
		GLY		P632	T402	T402	T402	T402
		GLY		P632	I403	I403	I403	I403
		GLY		P632	K404	K404	K404	K404
		GLY		P632	K405	K405	K405	K405
		GLY		P632	S406	S406	S406	S406
		GLY		P632	V407	V407	V407	V407

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137466	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0164	Depositor
Map size (Å)	545.89996, 469.58, 507.73996	wwPDB
Map dimensions	515, 443, 479	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.13	3/11191 (0.0%)	0.76	2/15127 (0.0%)
2	B	1.21	0/9311	0.76	3/12558 (0.0%)
3	C	1.23	0/2099	0.76	2/2845 (0.1%)
4	D	0.37	0/1262	0.54	0/1693
5	E	0.97	0/1780	0.69	0/2395
6	F	1.26	0/682	0.77	0/922
7	G	0.61	0/1368	0.59	0/1844
8	H	0.97	0/1107	0.75	0/1499
9	I	0.75	0/962	0.66	0/1295
10	J	1.39	0/541	0.84	0/727
11	K	1.18	0/922	0.72	0/1244
12	L	0.91	0/360	0.77	0/478
13	M	0.42	0/2204	0.56	0/2963
14	Q	0.43	0/1168	0.54	0/1579
15	R	0.31	0/1312	0.45	0/1777
16	W	0.24	0/1490	0.53	2/2014 (0.1%)
17	X	0.18	0/993	0.41	0/1357
18	O	0.21	0/1443	0.44	0/1942
19	T	0.33	0/1505	0.51	0/2319
20	N	0.37	0/1529	0.47	0/2359
21	0	0.39	0/6216	0.52	0/8392
22	1	0.38	0/1906	0.49	0/2558
23	4	0.56	0/2062	0.60	0/2805
24	6	0.53	0/2506	0.64	0/3402
25	2	0.42	0/3066	0.60	0/4082
26	5	0.46	0/502	0.74	0/677
27	3	0.28	0/902	0.48	0/1230
28	7	0.37	0/4552	0.70	7/6078 (0.1%)
All	All	0.82	3/64941 (0.0%)	0.65	16/88161 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	2
4	D	0	1
8	H	0	1
13	M	0	2
16	W	0	1
21	0	0	5
23	4	0	2
24	6	0	3
28	7	0	7
All	All	0	27

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	SER	C-N	-5.48	1.23	1.33
1	A	569	LYS	C-N	-5.17	1.27	1.33
1	A	1404	GLU	CA-CB	-5.03	1.37	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1013	ASN	CA-C-N	9.97	129.73	119.56
2	B	1013	ASN	C-N-CA	9.97	129.73	119.56
16	W	116	ASN	N-CA-C	6.34	116.83	108.07
28	7	333	ILE	N-CA-C	-5.97	106.67	112.29
1	A	71	GLN	N-CA-C	5.60	118.54	109.86
28	7	251	ILE	N-CA-C	-5.57	108.42	113.71
28	7	352	LEU	N-CA-C	5.53	117.16	109.31
16	W	117	SER	N-CA-C	5.23	117.39	111.11
3	C	89	GLU	CA-C-N	5.17	131.41	121.54
3	C	89	GLU	C-N-CA	5.17	131.41	121.54
2	B	363	HIS	N-CA-C	-5.15	99.83	110.80
28	7	348	ARG	N-CA-C	-5.13	106.71	112.87
1	A	465	TYR	N-CA-C	5.12	121.71	110.80
28	7	657	VAL	N-CA-C	-5.12	108.85	113.71
28	7	313	VAL	N-CA-C	-5.11	98.72	109.34
28	7	350	PRO	N-CA-C	-5.03	102.11	112.47

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	0	167	VAL	Peptide
21	0	171	LEU	Peptide
21	0	227	SER	Peptide
21	0	37	ASN	Peptide
21	0	740	SER	Peptide
23	4	255	ASP	Peptide
23	4	260	PRO	Peptide
24	6	372	LEU	Peptide
24	6	379	SER	Peptide
24	6	449	HIS	Peptide
28	7	165	SER	Peptide
28	7	228	LYS	Peptide
28	7	310	ILE	Peptide
28	7	312	ALA	Peptide
28	7	349	ASN	Peptide
28	7	350	PRO	Peptide
28	7	434	ASN	Peptide
1	A	465	TYR	Peptide
1	A	70	CYS	Peptide
1	A	71	GLN	Peptide
2	B	363	HIS	Peptide
2	B	644	GLU	Peptide
4	D	155	ARG	Peptide
8	H	109	LYS	Peptide
13	M	30	TYR	Peptide
13	M	31	PRO	Peptide
16	W	181	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10996	0	11079	535	0
2	B	9132	0	9146	402	0
3	C	2061	0	2029	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1253	0	1275	126	0
5	E	1744	0	1772	101	0
6	F	670	0	690	23	0
7	G	1340	0	1357	124	0
8	H	1089	0	1062	66	0
9	I	944	0	899	77	0
10	J	532	0	542	21	0
11	K	904	0	911	38	0
12	L	358	0	381	38	0
13	M	2175	0	2283	157	0
14	Q	1144	0	1034	84	0
15	R	1303	0	1110	98	0
16	W	1469	0	1432	124	0
17	X	984	0	722	53	0
18	O	1416	0	1493	105	0
19	T	1345	0	753	55	0
20	N	1361	0	749	48	0
21	0	6099	0	6160	690	0
22	1	2415	0	1887	234	0
23	4	2041	0	1954	194	0
24	6	2527	0	2322	227	0
25	2	3020	0	2613	375	0
26	5	498	0	506	129	0
27	3	890	0	680	57	0
28	7	4478	0	3928	670	0
29	3	2	0	0	0	0
29	4	1	0	0	0	0
29	6	4	0	0	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
29	M	1	0	0	0	0
29	W	1	0	0	0	0
30	A	1	0	0	0	0
31	0	8	0	0	3	0
All	All	64214	0	60769	4626	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 37.

All (4626) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.32	1.23
18:O:71:VAL:HA	18:O:123:VAL:O	1.40	1.17
18:O:106:ILE:O	18:O:110:LYS:HA	1.50	1.11
25:2:457:SER:HA	26:5:6:LYS:HA	1.33	1.07
24:6:403:CYS:SG	24:6:437:CYS:HB2	1.91	1.04
18:O:197:MET:O	18:O:201:LYS:HA	1.58	1.04
25:2:466:GLN:O	25:2:470:LEU:N	1.91	1.03
28:7:349:ASN:HD21	28:7:352:LEU:HB2	1.24	1.02
25:2:461:ASP:H	25:2:490:LYS:HG2	1.22	1.01
15:R:96:ARG:H	15:R:106:LEU:HA	1.25	0.99
16:W:101:LYS:HA	17:X:266:VAL:HG11	1.45	0.99
19:T:119:DG:N2	20:N:47:DC:O2	1.96	0.98
15:R:63:ARG:HD3	15:R:65:ASN:H	1.29	0.97
28:7:268:VAL:O	28:7:320:ASN:ND2	1.97	0.97
28:7:303:ARG:H	28:7:323:VAL:HG13	1.27	0.97
28:7:341:TYR:H	28:7:380:ARG:HA	1.31	0.96
13:M:215:ARG:HE	18:O:180:GLY:HA3	1.30	0.96
28:7:470:SER:OG	28:7:471:GLN:NE2	1.99	0.95
26:5:22:GLN:O	26:5:26:LYS:NZ	2.00	0.95
19:T:119:DG:N1	20:N:47:DC:N3	2.15	0.94
25:2:467:GLU:OE2	25:2:508:LYS:NZ	1.99	0.94
23:4:305:CYS:HB3	23:4:308:CYS:SG	2.08	0.93
9:I:59:VAL:HG23	9:I:61:ASP:H	1.33	0.92
21:0:139:GLY:HA3	21:0:304:GLU:HG2	1.50	0.92
1:A:1201:ALA:O	1:A:1205:LYS:NZ	2.04	0.91
22:1:188:ASN:HD22	22:1:191:LEU:HG	1.34	0.91
26:5:26:LYS:HD2	26:5:27:MET:HG2	1.53	0.90
2:B:242:SER:HG	2:B:363:HIS:HD1	0.95	0.90
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.04	0.90
24:6:120:ARG:HA	24:6:309:PRO:HG3	1.53	0.89
25:2:467:GLU:HA	25:2:471:LEU:HG	1.51	0.89
28:7:303:ARG:HB3	28:7:323:VAL:HG22	1.53	0.89
28:7:494:PRO:O	28:7:498:PHE:N	2.04	0.89
16:W:149:CYS:O	16:W:153:ASP:N	2.06	0.89
16:W:17:VAL:HG22	16:W:25:PHE:HB3	1.55	0.88
28:7:236:THR:H	28:7:313:VAL:H	0.89	0.88
24:6:338:CYS:SG	24:6:339:HIS:CE1	2.67	0.88
28:7:130:ARG:O	28:7:146:PHE:N	2.07	0.87
21:0:256:ALA:HA	21:0:259:ARG:HD3	1.57	0.87
26:5:50:VAL:O	26:5:54:LEU:N	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:175:ARG:NH2	24:6:203:GLU:O	2.07	0.87
28:7:104:PHE:O	28:7:528:ASN:ND2	2.06	0.86
28:7:489:GLU:HA	28:7:514:THR:HA	1.55	0.86
28:7:680:ARG:HH12	28:7:719:SER:HA	1.38	0.86
28:7:236:THR:N	28:7:313:VAL:H	1.73	0.86
19:T:120:DG:N2	20:N:46:DC:O2	2.06	0.86
28:7:207:GLU:O	28:7:211:ASN:N	2.09	0.86
28:7:356:LEU:HA	28:7:401:CYS:HB3	1.57	0.86
25:2:350:TYR:OH	28:7:133:TRP:O	1.93	0.86
17:X:274:LEU:HA	17:X:277:LYS:HB2	1.55	0.85
28:7:305:GLU:HB2	28:7:318:ILE:HG13	1.58	0.85
24:6:155:ASP:OD1	24:6:155:ASP:N	2.08	0.85
21:0:255:ASP:OD1	21:0:255:ASP:N	2.08	0.85
28:7:458:SER:O	28:7:462:ASN:ND2	2.09	0.85
2:B:343:ILE:O	2:B:345:LYS:NZ	2.10	0.85
28:7:767:ASN:HA	28:7:770:ALA:HB3	1.57	0.85
28:7:212:PHE:O	28:7:216:ALA:N	2.08	0.85
1:A:1329:THR:HG22	1:A:1331:SER:H	1.41	0.85
4:D:160:VAL:O	4:D:164:ILE:N	2.09	0.85
24:6:224:VAL:O	24:6:230:ARG:NH2	2.08	0.85
24:6:325:PRO:HB2	24:6:347:TYR:HB3	1.58	0.85
24:6:349:CYS:HB3	24:6:352:CYS:SG	2.17	0.85
26:5:43:ASN:OD1	26:5:45:SER:OG	1.95	0.85
23:4:113:UNK:H	23:4:119:ARG:HH21	1.24	0.84
23:4:289:CYS:SG	23:4:290:SER:N	2.50	0.84
25:2:459:TYR:OH	25:2:498:ASN:ND2	2.08	0.84
28:7:236:THR:H	28:7:313:VAL:N	1.74	0.84
1:A:1043:ASP:N	1:A:1043:ASP:OD1	2.06	0.84
5:E:32:GLN:NE2	5:E:36:GLU:OE2	2.10	0.84
22:1:196:GLN:O	22:1:200:ILE:N	2.10	0.84
21:0:705:ASP:N	21:0:705:ASP:OD1	2.10	0.84
28:7:304:GLU:OE1	28:7:320:ASN:ND2	2.10	0.84
28:7:269:LEU:HD13	28:7:304:GLU:HB3	1.57	0.84
21:0:571:VAL:HG11	22:1:375:LEU:HB3	1.58	0.83
1:A:767:GLN:NE2	1:A:768:GLN:O	2.08	0.83
28:7:340:GLU:OE1	28:7:380:ARG:NH2	2.11	0.83
25:2:364:VAL:HA	25:2:382:SER:HB3	1.60	0.83
24:6:144:ASN:OD1	24:6:147:ALA:N	2.10	0.83
28:7:561:MET:HE3	28:7:562:THR:H	1.44	0.83
3:C:148:ARG:HD3	10:J:65:PRO:HD3	1.59	0.83
21:0:375:ARG:NH1	21:0:410:SER:O	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:38:SER:HB3	21:0:479:LEU:H	1.43	0.83
2:B:879:ARG:HG3	2:B:885:MET:HE2	1.60	0.83
25:2:474:TYR:HA	25:2:477:ASP:HB2	1.60	0.83
9:I:10:CYS:SG	9:I:31:THR:OG1	2.36	0.83
25:2:498:ASN:O	25:2:501:VAL:N	2.11	0.83
21:0:633:ARG:H	21:0:633:ARG:HE	1.26	0.82
18:O:103:ILE:HA	18:O:113:ALA:O	1.79	0.82
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.19	0.82
26:5:48:GLU:O	26:5:52:HIS:N	2.11	0.82
28:7:574:ALA:O	28:7:576:LYS:NZ	2.13	0.82
21:0:232:VAL:HB	21:0:456:VAL:HA	1.60	0.82
1:A:179:LEU:HB3	1:A:297:GLN:HE21	1.42	0.82
14:Q:121:PHE:HB2	15:R:131:ASN:HB3	1.60	0.82
28:7:302:GLU:C	28:7:322:SER:H	1.88	0.82
1:A:219:PHE:HA	1:A:222:LEU:HB2	1.62	0.82
1:A:134:ARG:NH1	1:A:221:SER:O	2.13	0.82
1:A:913:LEU:HA	1:A:979:SER:H	1.44	0.82
9:I:52:ILE:O	9:I:90:GLN:NE2	2.13	0.82
28:7:388:CYS:SG	28:7:392:LYS:NZ	2.53	0.82
1:A:107:CYS:HB2	1:A:148:CYS:SG	2.20	0.81
5:E:36:GLU:N	5:E:36:GLU:OE1	2.12	0.81
8:H:92:ASP:O	8:H:145:ARG:NH1	2.13	0.81
25:2:73:GLN:O	25:2:77:ALA:N	2.13	0.81
26:5:51:LYS:HA	26:5:54:LEU:HB3	1.61	0.81
4:D:142:LYS:HA	4:D:145:MET:HB2	1.62	0.81
21:0:167:VAL:HG22	21:0:198:ARG:HD2	1.61	0.81
25:2:218:LEU:O	25:2:222:LEU:N	2.10	0.81
21:0:508:SER:H	21:0:685:ARG:HH22	1.25	0.81
24:6:169:MET:O	24:6:192:HIS:NE2	2.14	0.81
2:B:326:ASP:OD1	2:B:329:THR:N	2.11	0.81
21:0:109:THR:OG1	21:0:113:ASN:ND2	2.13	0.81
24:6:124:ARG:NH1	24:6:305:VAL:O	2.13	0.81
1:A:311:GLN:N	13:M:101:THR:O	2.13	0.81
21:0:568:LEU:H	21:0:596:ALA:HA	1.46	0.81
5:E:20:LYS:NZ	5:E:34:GLU:O	2.12	0.81
16:W:105:VAL:HA	16:W:108:ARG:HD2	1.62	0.80
25:2:415:LYS:NZ	28:7:166:ARG:O	2.13	0.80
21:0:651:ASN:OD1	21:0:651:ASN:N	2.12	0.80
24:6:294:GLU:H	24:6:294:GLU:CD	1.90	0.80
25:2:471:LEU:HA	25:2:474:TYR:HB3	1.64	0.80
28:7:324:GLU:OE1	28:7:328:LYS:NZ	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:225:LEU:N	28:7:310:ILE:O	2.12	0.80
28:7:354:ILE:HB	28:7:404:LYS:HA	1.64	0.80
16:W:127:CYS:SG	16:W:129:THR:OG1	2.38	0.80
28:7:407:VAL:HG22	28:7:484:PHE:HB3	1.62	0.80
2:B:363:HIS:O	2:B:365:THR:N	2.15	0.80
4:D:155:ARG:O	4:D:159:THR:OG1	1.99	0.80
15:R:65:ASN:O	15:R:67:GLN:NE2	2.15	0.80
16:W:174:ARG:HD3	17:X:255:ILE:HG23	1.61	0.80
21:0:490:LYS:NZ	21:0:492:PHE:O	2.13	0.80
26:5:56:ARG:O	26:5:60:LYS:N	2.13	0.80
27:3:138:GLU:O	27:3:142:GLN:N	2.15	0.80
28:7:754:ARG:O	28:7:758:GLU:N	2.13	0.80
7:G:106:MET:HE3	7:G:108:VAL:HG22	1.63	0.80
25:2:462:PHE:N	25:2:489:LYS:O	2.13	0.79
28:7:470:SER:O	28:7:474:MET:N	2.15	0.79
21:0:245:ILE:O	21:0:247:SER:N	2.15	0.79
23:4:273:ARG:HH22	24:6:372:LEU:HB3	1.45	0.79
28:7:383:ILE:HG13	28:7:531:ILE:HB	1.64	0.79
1:A:310:GLY:N	13:M:101:THR:OG1	2.12	0.79
28:7:543:LEU:O	28:7:546:LYS:N	2.15	0.79
2:B:428:ILE:HD11	2:B:448:ILE:HG13	1.64	0.79
2:B:1049:ASP:N	2:B:1049:ASP:OD1	2.13	0.79
5:E:67:GLU:OE1	5:E:68:SER:N	2.16	0.79
8:H:131:ASN:OD1	8:H:131:ASN:N	2.10	0.79
24:6:352:CYS:SG	24:6:354:SER:OG	2.41	0.79
27:3:129:THR:O	27:3:133:LEU:N	2.16	0.79
4:D:123:LEU:HD22	4:D:149:THR:HG21	1.64	0.78
7:G:150:CYS:HA	7:G:159:ALA:HA	1.66	0.78
24:6:444:ILE:HD11	24:6:451:CYS:HA	1.65	0.78
4:D:39:ASN:ND2	4:D:41:GLN:OE1	2.14	0.78
21:0:325:ILE:HG23	21:0:331:PHE:HB2	1.63	0.78
25:2:22:GLN:NE2	25:2:84:LEU:O	2.16	0.78
25:2:460:SER:OG	25:2:461:ASP:OD2	2.02	0.78
27:3:132:LYS:O	27:3:136:TYR:N	2.15	0.78
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.14	0.78
2:B:108:VAL:HG23	13:M:244:SER:HB2	1.66	0.78
22:1:479:UNK:O	22:1:483:UNK:N	2.17	0.78
25:2:346:LYS:HE2	25:2:375:LEU:HD12	1.65	0.78
28:7:469:ASP:OD1	28:7:469:ASP:N	2.13	0.78
1:A:1256:GLU:O	1:A:1260:LEU:N	2.15	0.78
4:D:197:SER:O	4:D:201:LYS:NZ	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:573:THR:OG1	28:7:574:ALA:N	2.08	0.78
27:3:78:VAL:O	27:3:82:VAL:N	2.14	0.78
28:7:428:CYS:SG	28:7:429:THR:N	2.55	0.78
4:D:139:LYS:HA	4:D:142:LYS:HB2	1.66	0.77
8:H:110:ASP:OD1	8:H:110:ASP:N	2.16	0.77
21:0:138:ASN:O	21:0:142:LYS:N	2.13	0.77
2:B:364:ILE:HD11	2:B:373:ARG:HB3	1.67	0.77
14:Q:374:VAL:HA	14:Q:388:PRO:HA	1.66	0.77
21:0:270:ARG:NH2	21:0:388:LEU:O	2.17	0.77
21:0:281:LYS:HA	21:0:284:ASP:HB3	1.65	0.77
22:1:553:LEU:O	22:1:556:THR:OG1	2.03	0.77
4:D:138:ASN:HB3	4:D:141:LEU:HD23	1.66	0.77
9:I:78:CYS:SG	9:I:80:SER:OG	2.42	0.77
24:6:451:CYS:SG	24:6:454:CYS:HB2	2.24	0.77
25:2:481:LEU:HA	25:2:493:ILE:HD13	1.65	0.77
25:2:62:LEU:HA	25:2:65:TRP:HD1	1.49	0.77
1:A:1269:GLU:OE1	1:A:1270:ASN:N	2.18	0.77
2:B:1002:THR:OG1	2:B:1003:ALA:N	2.18	0.77
12:L:31:CYS:SG	12:L:34:CYS:HB3	2.24	0.77
21:0:41:GLU:HB3	21:0:482:SER:HA	1.67	0.77
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.04	0.76
28:7:209:ILE:O	28:7:213:ILE:N	2.17	0.76
1:A:1199:ARG:O	1:A:1203:ASN:N	2.19	0.76
21:0:217:LYS:HE3	21:0:310:PRO:HA	1.65	0.76
21:0:332:VAL:O	21:0:336:LYS:NZ	2.18	0.76
25:2:368:ALA:HB3	25:2:375:LEU:HB3	1.68	0.76
14:Q:103:LEU:H	15:R:92:LEU:HA	1.49	0.76
23:4:239:GLU:OE1	23:4:241:THR:N	2.19	0.76
5:E:41:ASP:N	5:E:41:ASP:OD1	2.18	0.76
21:0:328:ALA:HA	21:0:331:PHE:HB3	1.66	0.76
21:0:343:LYS:O	21:0:347:LYS:NZ	2.17	0.76
28:7:384:ILE:HG12	28:7:535:LEU:HB2	1.67	0.76
8:H:109:LYS:O	8:H:111:LEU:N	2.19	0.76
1:A:42:ASP:OD2	1:A:46:THR:OG1	2.02	0.76
15:R:95:ILE:HA	15:R:106:LEU:HB2	1.68	0.76
28:7:609:SER:HB3	28:7:673:ILE:HB	1.66	0.76
28:7:766:LYS:O	28:7:770:ALA:N	2.18	0.76
2:B:496:ARG:NH2	2:B:540:SER:O	2.19	0.76
21:0:358:SER:O	21:0:361:GLN:NE2	2.17	0.76
16:W:15:PHE:O	16:W:19:GLY:N	2.19	0.75
23:4:288:ILE:HD11	23:4:293:LEU:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:540:TRP:CG	28:7:729:GLN:HE22	2.03	0.75
8:H:35:GLN:OE1	8:H:35:GLN:N	2.20	0.75
22:1:213:ARG:HH11	22:1:213:ARG:H	1.32	0.75
28:7:541:MET:O	28:7:545:GLN:NE2	2.18	0.75
15:R:62:GLU:OE2	15:R:66:ARG:NH2	2.20	0.75
25:2:392:THR:O	25:2:395:GLN:NE2	2.18	0.75
2:B:60:GLN:NE2	2:B:64:CYS:SG	2.60	0.75
14:Q:371:ASP:O	15:R:82:ARG:NH2	2.18	0.75
21:0:535:ASP:HB3	21:0:595:GLY:HA2	1.68	0.75
25:2:51:VAL:O	25:2:109:ARG:NH2	2.18	0.75
1:A:1232:ASN:ND2	1:A:1233:ASP:OD1	2.20	0.75
28:7:376:ASN:O	28:7:380:ARG:NH2	2.19	0.75
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	1.86	0.75
26:5:48:GLU:HA	26:5:51:LYS:HB2	1.68	0.75
28:7:471:GLN:HA	28:7:474:MET:HB2	1.69	0.75
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.20	0.75
21:0:112:LYS:NZ	21:0:123:GLU:O	2.19	0.75
21:0:748:GLN:O	21:0:752:LYS:N	2.20	0.75
25:2:246:GLN:O	25:2:250:LEU:N	2.17	0.75
8:H:94:ASP:OD1	8:H:94:ASP:N	2.14	0.75
7:G:50:ASP:OD1	7:G:53:ASN:ND2	2.20	0.74
25:2:498:ASN:OD1	25:2:502:LEU:N	2.20	0.74
28:7:164:ILE:O	28:7:166:ARG:N	2.20	0.74
22:1:510:ASN:O	22:1:513:GLN:NE2	2.21	0.74
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.20	0.74
13:M:250:MET:SD	13:M:254:THR:OG1	2.45	0.74
16:W:163:LYS:HA	16:W:166:LYS:HE2	1.69	0.74
19:T:120:DG:N1	20:N:46:DC:N3	2.29	0.74
21:0:265:ASN:HA	21:0:268:ASP:HB3	1.69	0.74
22:1:560:PHE:O	22:1:563:HIS:ND1	2.19	0.74
1:A:399:HIS:O	1:A:401:GLY:N	2.21	0.74
21:0:60:GLN:O	21:0:67:ARG:NH2	2.20	0.74
28:7:612:VAL:HA	28:7:615:LEU:HB3	1.69	0.74
28:7:751:ALA:O	28:7:756:ARG:NH2	2.19	0.74
2:B:444:MET:SD	2:B:444:MET:N	2.54	0.74
22:1:630:TYR:O	22:1:634:PHE:N	2.15	0.74
1:A:293:GLU:OE1	1:A:294:SER:N	2.20	0.74
21:0:5:ILE:O	21:0:29:LYS:NZ	2.20	0.74
25:2:473:LYS:NZ	25:2:473:LYS:O	2.20	0.74
26:5:10:VAL:N	26:5:40:LEU:O	2.20	0.74
12:L:47:ARG:HH12	12:L:49:LYS:HD3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:117:SER:HA	16:W:165:ASN:HB2	1.70	0.74
21:O:619:THR:HG22	21:O:678:VAL:HB	1.69	0.74
23:4:237:HIS:ND1	23:4:237:HIS:O	2.20	0.74
24:6:336:CYS:SG	24:6:337:SER:N	2.59	0.74
28:7:470:SER:HG	28:7:471:GLN:NE2	1.84	0.74
28:7:484:PHE:HE2	28:7:486:ILE:HG12	1.53	0.74
28:7:609:SER:HA	28:7:674:SER:H	1.53	0.74
24:6:351:ASN:ND2	24:6:366:CYS:SG	2.61	0.74
25:2:185:THR:O	25:2:189:PHE:N	2.17	0.74
23:4:269:SER:O	23:4:269:SER:OG	2.06	0.74
25:2:505:ALA:O	25:2:508:LYS:NZ	2.18	0.74
1:A:312:PRO:HB3	13:M:98:LYS:HA	1.68	0.73
21:O:253:THR:HG22	21:O:256:ALA:H	1.52	0.73
25:2:493:ILE:HG13	25:2:501:VAL:HG11	1.69	0.73
8:H:92:ASP:OD1	8:H:92:ASP:N	2.20	0.73
21:O:645:ASN:O	21:O:647:ARG:NH1	2.22	0.73
1:A:1199:ARG:NH1	1:A:1233:ASP:O	2.20	0.73
21:O:177:SER:O	21:O:181:LEU:N	2.17	0.73
27:3:135:THR:O	27:3:139:LEU:N	2.20	0.73
28:7:468:HIS:ND1	28:7:471:GLN:OE1	2.22	0.73
1:A:862:ASN:OD1	1:A:862:ASN:N	2.20	0.73
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.20	0.73
28:7:191:ASP:O	28:7:195:SER:N	2.17	0.73
2:B:650:GLU:OE1	2:B:651:LEU:N	2.18	0.73
21:O:220:GLU:HA	21:O:313:PRO:HB3	1.69	0.73
28:7:305:GLU:H	28:7:318:ILE:HG21	1.52	0.73
28:7:355:ASP:OD2	28:7:404:LYS:NZ	2.21	0.73
28:7:720:THR:HA	28:7:723:GLN:HB2	1.68	0.73
2:B:438:GLU:OE1	2:B:440:HIS:NE2	2.20	0.73
2:B:574:SER:OG	2:B:591:ARG:NH1	2.22	0.73
10:J:32:GLU:OE1	10:J:32:GLU:N	2.18	0.73
26:5:32:LEU:HB2	26:5:41:LEU:HB3	1.69	0.73
7:G:57:GLN:OE1	7:G:57:GLN:N	2.21	0.73
22:1:231:UNK:O	22:1:235:UNK:N	2.22	0.73
4:D:34:GLN:O	4:D:37:GLN:NE2	2.20	0.73
21:O:288:LYS:O	21:O:291:GLN:NE2	2.22	0.73
28:7:349:ASN:ND2	28:7:352:LEU:HB2	2.03	0.73
28:7:495:ALA:HA	28:7:498:PHE:HD1	1.53	0.73
1:A:903:ASN:OD1	1:A:904:THR:N	2.20	0.73
21:O:58:ALA:O	21:O:62:HIS:N	2.21	0.73
22:1:469:UNK:O	22:1:473:UNK:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:176:ASN:HA	24:6:206:GLY:HA3	1.71	0.73
25:2:205:LEU:O	25:2:209:LYS:N	2.20	0.73
28:7:595:ILE:HD13	28:7:624:LYS:HE2	1.70	0.73
2:B:705:MET:H	2:B:710:LEU:HD12	1.53	0.73
2:B:950:ASP:OD1	2:B:969:ARG:NH1	2.21	0.73
3:C:93:ASP:O	3:C:127:ARG:NH2	2.22	0.73
5:E:41:ASP:HA	5:E:44:ALA:HB3	1.70	0.73
13:M:208:ASN:O	13:M:212:ASN:ND2	2.21	0.73
21:0:220:GLU:O	21:0:314:GLN:NE2	2.20	0.73
25:2:160:SER:O	25:2:164:LEU:N	2.15	0.73
28:7:437:VAL:O	28:7:444:GLU:HB2	1.89	0.72
28:7:560:PRO:HA	28:7:711:LYS:HB2	1.69	0.72
23:4:62:ASN:HB3	23:4:118:PHE:HD2	1.54	0.72
25:2:462:PHE:N	25:2:489:LYS:HB3	2.04	0.72
28:7:563:ALA:O	28:7:567:GLN:N	2.22	0.72
1:A:130:ASP:OD1	1:A:133:LYS:N	2.16	0.72
1:A:316:GLN:NE2	13:M:94:THR:OG1	2.21	0.72
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.72	0.72
4:D:208:GLU:HA	4:D:211:LEU:HB2	1.71	0.72
25:2:365:HIS:HB3	25:2:385:ARG:HH22	1.53	0.72
26:5:17:LYS:HG3	26:5:40:LEU:HD11	1.70	0.72
28:7:327:LYS:O	28:7:331:GLN:NE2	2.21	0.72
22:1:490:UNK:O	22:1:492:UNK:N	2.22	0.72
23:4:151:GLY:O	23:4:154:SER:OG	2.05	0.72
3:C:86:CYS:HB3	3:C:88:CYS:SG	2.30	0.72
5:E:40:GLU:OE1	5:E:41:ASP:N	2.22	0.72
7:G:94:CYS:HA	7:G:99:PHE:HA	1.70	0.72
8:H:53:ASP:N	8:H:53:ASP:OD1	2.21	0.72
28:7:519:ARG:HH21	28:7:521:ASP:HB2	1.53	0.72
5:E:83:CYS:O	5:E:113:GLN:NE2	2.23	0.72
21:0:140:GLN:O	21:0:144:LYS:N	2.17	0.72
21:0:650:GLU:O	21:0:654:LEU:N	2.19	0.72
22:1:206:PRO:HA	22:1:209:PHE:HB3	1.71	0.72
24:6:221:LEU:O	24:6:230:ARG:NH1	2.22	0.72
21:0:337:ARG:HG2	21:0:367:THR:HG21	1.72	0.72
28:7:409:VAL:HA	28:7:486:ILE:HB	1.70	0.72
2:B:199:MET:N	2:B:199:MET:SD	2.57	0.72
7:G:7:LEU:HB2	7:G:74:TYR:CE1	2.25	0.72
21:0:357:LYS:HG3	21:0:360:LEU:HD22	1.70	0.72
28:7:383:ILE:HG12	28:7:512:GLY:HA3	1.70	0.72
2:B:864:LYS:N	2:B:872:GLU:OE1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:260:PRO:O	25:2:67:ASN:ND2	2.23	0.72
26:5:42:VAL:HG12	26:5:43:ASN:H	1.54	0.72
2:B:365:THR:OG1	2:B:366:GLN:N	2.21	0.72
18:O:72:ALA:O	18:O:122:VAL:HA	1.90	0.72
24:6:194:ASP:HA	24:6:197:LYS:HE3	1.70	0.72
1:A:1191:TRP:NE1	1:A:1256:GLU:OE2	2.23	0.71
21:0:157:GLU:O	21:0:161:ASN:ND2	2.22	0.71
21:0:396:PHE:HA	21:0:399:LEU:HG	1.72	0.71
21:0:744:LEU:HA	21:0:747:HIS:HB3	1.70	0.71
24:6:222:LEU:HA	24:6:230:ARG:HH12	1.54	0.71
28:7:305:GLU:HG3	28:7:323:VAL:HG11	1.72	0.71
13:M:96:ILE:HB	13:M:110:LEU:HD21	1.72	0.71
4:D:142:LYS:O	4:D:146:GLN:N	2.20	0.71
22:1:214:ILE:HG23	22:1:215:PRO:HD3	1.72	0.71
25:2:346:LYS:HZ3	25:2:376:GLY:H	1.38	0.71
27:3:37:ARG:O	27:3:56:TYR:OH	2.08	0.71
28:7:413:SER:O	28:7:416:SER:N	2.22	0.71
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.73	0.71
21:0:674:ASP:N	21:0:674:ASP:OD1	2.21	0.71
25:2:466:GLN:NE2	25:2:469:ASN:O	2.24	0.71
25:2:502:LEU:HD13	25:2:506:LYS:HZ1	1.52	0.71
28:7:574:ALA:HB3	28:7:576:LYS:HE3	1.73	0.71
1:A:890:ASP:N	1:A:890:ASP:OD1	2.21	0.71
2:B:486:TYR:HB3	2:B:1096:ARG:HH12	1.55	0.71
3:C:136:ASP:OD1	3:C:138:GLU:N	2.23	0.71
22:1:370:UNK:O	22:1:372:VAL:N	2.24	0.71
26:5:53:GLU:HA	26:5:56:ARG:HD2	1.70	0.71
28:7:206:ALA:O	28:7:210:ILE:N	2.17	0.71
1:A:834:THR:OG1	1:A:1076:ALA:O	2.09	0.71
4:D:33:PHE:HE2	7:G:80:LYS:HG2	1.56	0.71
4:D:183:LEU:HD12	4:D:195:ILE:HD11	1.72	0.71
23:4:311:GLN:NE2	23:4:312:PHE:O	2.23	0.71
2:B:248:SER:H	2:B:418:LYS:HE3	1.54	0.71
7:G:89:GLY:HA3	7:G:103:VAL:HG22	1.73	0.71
21:0:495:MET:HE1	21:0:717:THR:HG22	1.72	0.71
22:1:213:ARG:HH11	22:1:213:ARG:N	1.89	0.71
25:2:222:LEU:HD13	25:2:225:ILE:HD12	1.73	0.71
8:H:8:ASP:OD1	8:H:9:ILE:N	2.23	0.71
14:Q:337:GLU:OE2	14:Q:340:LYS:N	2.23	0.71
21:0:124:ARG:O	22:1:344:GLN:NE2	2.23	0.71
22:1:491:UNK:O	22:1:493:UNK:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:52:LYS:NZ	23:4:240:SER:O	2.23	0.71
25:2:384:ARG:O	25:2:388:THR:N	2.23	0.71
2:B:235:SER:HG	2:B:236:HIS:HD1	1.38	0.71
3:C:211:ASP:OD1	3:C:211:ASP:N	2.20	0.71
21:0:244:CYS:O	21:0:247:SER:OG	2.09	0.71
22:1:209:PHE:O	22:1:213:ARG:NH1	2.23	0.71
28:7:305:GLU:HB3	28:7:308:ASP:HB2	1.72	0.71
15:R:96:ARG:O	15:R:105:THR:OG1	2.02	0.71
25:2:455:GLU:HA	26:5:8:ALA:HA	1.71	0.71
28:7:267:ASP:O	28:7:348:ARG:NH2	2.24	0.71
9:I:7:CYS:SG	9:I:8:ARG:N	2.63	0.70
16:W:163:LYS:HE3	16:W:164:LYS:HG3	1.71	0.70
21:0:441:ASP:OD2	21:0:444:ILE:N	2.23	0.70
24:6:432:CYS:HB3	24:6:454:CYS:SG	2.31	0.70
25:2:369:ARG:HA	25:2:374:VAL:HG22	1.73	0.70
28:7:545:GLN:HB2	28:7:546:LYS:HZ1	1.55	0.70
1:A:985:ASP:OD1	1:A:985:ASP:N	2.22	0.70
2:B:889:THR:OG1	2:B:891:ASP:OD1	2.08	0.70
14:Q:339:ALA:O	14:Q:343:ARG:NH2	2.24	0.70
21:0:403:ALA:O	21:0:407:THR:OG1	2.08	0.70
22:1:619:VAL:HG12	22:1:623:ILE:HD13	1.71	0.70
24:6:406:CYS:SG	24:6:407:GLN:N	2.64	0.70
26:5:43:ASN:OD1	26:5:46:LYS:NZ	2.25	0.70
27:3:139:LEU:O	27:3:143:LEU:N	2.21	0.70
1:A:1166:ASP:CG	1:A:1239:ARG:HE	1.99	0.70
2:B:429:PHE:HA	2:B:432:MET:HE2	1.73	0.70
21:0:634:ILE:HG13	21:0:635:LEU:HD12	1.72	0.70
24:6:349:CYS:SG	24:6:352:CYS:N	2.65	0.70
25:2:20:GLN:OE1	25:2:20:GLN:N	2.24	0.70
25:2:396:ILE:HG23	25:2:400:LEU:HD12	1.73	0.70
1:A:980:ASP:N	1:A:980:ASP:OD1	2.23	0.70
1:A:433:GLU:OE2	2:B:1108:ARG:NH2	2.25	0.70
2:B:70:ILE:HG22	2:B:89:GLU:HB2	1.74	0.70
2:B:531:GLN:CD	2:B:531:GLN:H	1.95	0.70
18:O:73:THR:OG1	18:O:158:GLN:NE2	2.24	0.70
21:0:223:SER:H	21:0:226:VAL:HG22	1.56	0.70
24:6:243:ASP:N	24:6:243:ASP:OD1	2.21	0.70
2:B:106:ASP:OD1	2:B:108:VAL:N	2.21	0.70
7:G:7:LEU:HB2	7:G:74:TYR:HE1	1.56	0.70
15:R:66:ARG:NH1	15:R:215:VAL:O	2.24	0.70
21:0:211:HIS:O	21:0:215:ASP:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:254:THR:OG1	21:0:258:ARG:NH1	2.24	0.70
2:B:324:ILE:O	2:B:325:GLN:NE2	2.24	0.70
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.57	0.70
2:B:1181:GLU:OE2	2:B:1183:LYS:NZ	2.15	0.70
7:G:163:ILE:HD12	7:G:169:GLY:HA2	1.74	0.70
18:O:66:THR:H	18:O:164:CYS:HB3	1.55	0.70
18:O:70:ILE:HB	18:O:126:ALA:HB3	1.73	0.70
21:0:138:ASN:HB3	21:0:141:ALA:HB3	1.74	0.70
21:0:143:ARG:HA	21:0:146:GLU:HG2	1.72	0.70
25:2:478:ILE:O	25:2:500:GLN:NE2	2.25	0.70
26:5:20:ILE:HA	26:5:23:ILE:HD12	1.74	0.70
1:A:663:SER:OG	1:A:664:THR:N	2.23	0.70
1:A:1226:VAL:HG22	1:A:1240:CYS:HB2	1.73	0.70
4:D:203:SER:OG	4:D:205:ASP:OD1	2.09	0.70
8:H:62:SER:OG	8:H:63:LEU:N	2.23	0.70
21:0:600:SER:OG	21:0:601:VAL:N	2.22	0.70
1:A:394:ASN:ND2	1:A:398:GLU:OE2	2.25	0.70
1:A:406:ILE:HG12	1:A:412:ARG:HG3	1.74	0.70
2:B:866:TYR:HB2	2:B:870:ILE:HG13	1.74	0.70
21:0:393:VAL:O	21:0:397:THR:N	2.19	0.70
21:0:468:MET:O	21:0:472:MET:N	2.16	0.70
21:0:633:ARG:O	21:0:637:ALA:N	2.20	0.70
22:1:382:SER:HA	22:1:385:MET:HE3	1.71	0.70
28:7:460:VAL:O	28:7:500:ARG:NH1	2.22	0.70
1:A:909:ASP:OD2	1:A:911:SER:OG	2.08	0.70
3:C:78:GLU:OE1	3:C:78:GLU:N	2.20	0.70
12:L:33:GLU:OE2	12:L:53:HIS:ND1	2.25	0.70
28:7:556:GLU:OE1	28:7:723:GLN:NE2	2.25	0.70
28:7:559:CYS:O	28:7:711:LYS:N	2.21	0.70
1:A:1126:ALA:HA	1:A:1304:TRP:CD1	2.27	0.69
3:C:215:GLU:OE1	3:C:216:GLY:N	2.24	0.69
1:A:177:ASP:N	1:A:177:ASP:OD1	2.25	0.69
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.72	0.69
24:6:324:PHE:H	24:6:350:PRO:HG3	1.57	0.69
1:A:1198:ASP:OD1	1:A:1199:ARG:N	2.25	0.69
24:6:276:LEU:O	24:6:280:THR:OG1	2.09	0.69
28:7:469:ASP:HB3	28:7:472:LYS:HD3	1.74	0.69
28:7:570:LEU:HB2	28:7:571:ARG:HH12	1.55	0.69
1:A:26:GLU:OE2	2:B:1215:ARG:NH2	2.25	0.69
1:A:626:ASN:O	1:A:631:HIS:ND1	2.17	0.69
13:M:176:ILE:O	13:M:180:CYS:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:28:VAL:HG12	16:W:43:LEU:HD11	1.73	0.69
21:0:420:ILE:HG12	21:0:435:MET:HA	1.74	0.69
21:0:633:ARG:HA	21:0:636:LYS:HB2	1.73	0.69
24:6:381:HIS:HB2	24:6:449:HIS:CD2	2.27	0.69
1:A:215:SER:OG	1:A:218:ASP:N	2.25	0.69
22:1:372:VAL:HG22	22:1:376:LYS:HG3	1.73	0.69
25:2:61:ASP:N	25:2:61:ASP:OD1	2.24	0.69
2:B:649:LYS:NZ	2:B:736:THR:OG1	2.26	0.69
21:0:69:ILE:HG12	21:0:231:ILE:HD11	1.73	0.69
23:4:76:ILE:HG12	23:4:85:TYR:HA	1.72	0.69
2:B:106:ASP:OD1	2:B:107:GLY:N	2.25	0.69
11:K:5:ASP:OD1	11:K:5:ASP:N	2.26	0.69
16:W:97:ALA:HB1	17:X:268:LEU:HD22	1.74	0.69
21:0:400:LYS:O	21:0:404:THR:N	2.19	0.69
24:6:191:ASP:OD1	24:6:191:ASP:N	2.21	0.69
25:2:441:ILE:O	25:2:445:GLN:N	2.25	0.69
2:B:275:TYR:HB2	2:B:355:ILE:HD11	1.74	0.69
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.73	0.69
13:M:87:LEU:O	13:M:155:LYS:NZ	2.26	0.69
14:Q:375:LEU:N	14:Q:387:ILE:O	2.21	0.69
18:O:75:THR:HG23	18:O:120:LYS:HE2	1.75	0.69
24:6:424:UNK:O	24:6:426:ARG:N	2.26	0.69
28:7:680:ARG:HB3	28:7:722:ARG:HD2	1.73	0.69
28:7:764:LEU:O	28:7:768:GLU:N	2.26	0.69
5:E:68:SER:O	5:E:72:PHE:N	2.26	0.69
15:R:94:LYS:O	15:R:107:LEU:N	2.20	0.69
22:1:171:LYS:O	22:1:175:LEU:N	2.26	0.69
12:L:34:CYS:SG	12:L:36:SER:OG	2.45	0.69
16:W:69:ILE:HA	16:W:87:TYR:HA	1.74	0.69
17:X:224:LEU:O	17:X:229:LYS:N	2.26	0.69
17:X:277:LYS:HA	17:X:280:ASP:HB2	1.75	0.69
21:0:252:LEU:HD12	21:0:435:MET:HB2	1.74	0.69
21:0:582:ALA:O	21:0:585:THR:OG1	2.11	0.69
22:1:483:UNK:O	22:1:485:UNK:N	2.26	0.69
1:A:624:SER:O	1:A:624:SER:OG	2.10	0.68
1:A:1215:ARG:NH2	1:A:1273:LEU:O	2.25	0.68
23:4:290:SER:OG	23:4:291:VAL:N	2.26	0.68
24:6:293:ASP:OD2	24:6:296:HIS:ND1	2.16	0.68
16:W:6:ASP:OD2	16:W:10:LYS:NZ	2.26	0.68
16:W:140:LEU:HD13	16:W:147:PHE:HD1	1.59	0.68
20:N:39:DC:H3'	20:N:40:DT:H71	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:750:SER:OG	21:0:751:ARG:NH2	2.26	0.68
23:4:62:ASN:N	23:4:62:ASN:OD1	2.24	0.68
25:2:95:THR:OG1	25:2:96:LEU:N	2.26	0.68
1:A:930:ASP:O	1:A:934:LYS:N	2.21	0.68
14:Q:116:THR:N	14:Q:390:ASP:OD2	2.26	0.68
21:0:111:ARG:O	21:0:115:CYS:N	2.26	0.68
25:2:53:ASN:N	25:2:53:ASN:OD1	2.26	0.68
28:7:104:PHE:N	28:7:526:ASP:O	2.27	0.68
1:A:557:ASP:OD1	1:A:558:GLY:N	2.26	0.68
1:A:1115:SER:OG	1:A:1116:LEU:N	2.27	0.68
21:0:297:ASP:OD2	21:0:386:ARG:NH2	2.22	0.68
28:7:544:SER:OG	28:7:547:GLY:O	2.09	0.68
12:L:31:CYS:SG	12:L:34:CYS:N	2.66	0.68
16:W:182:ILE:O	16:W:186:LEU:N	2.26	0.68
21:0:374:LEU:HD21	21:0:409:ILE:HG23	1.76	0.68
24:6:403:CYS:SG	24:6:437:CYS:CB	2.76	0.68
28:7:476:PHE:O	28:7:480:ARG:N	2.26	0.68
19:T:142:DT:H1'	19:T:143:DT:H5'	1.76	0.68
21:0:332:VAL:HA	21:0:335:LEU:HD22	1.74	0.68
22:1:579:VAL:O	22:1:583:TYR:N	2.19	0.68
28:7:256:ILE:O	28:7:317:GLU:N	2.26	0.68
28:7:348:ARG:NH1	28:7:481:GLU:OE2	2.26	0.68
5:E:83:CYS:SG	5:E:84:ASP:N	2.67	0.68
7:G:112:LYS:HE2	7:G:117:GLN:HA	1.76	0.68
16:W:46:LEU:HB2	17:X:203:LYS:HB3	1.75	0.68
24:6:184:GLN:NE2	24:6:185:VAL:O	2.26	0.68
28:7:716:MET:O	28:7:720:THR:N	2.24	0.68
13:M:109:GLU:HA	13:M:112:LYS:HB2	1.75	0.68
1:A:128:ILE:HB	1:A:134:ARG:HG3	1.76	0.68
21:0:729:ASP:O	21:0:731:LYS:NZ	2.26	0.68
22:1:547:LEU:O	22:1:551:ARG:N	2.17	0.68
23:4:33:ALA:O	23:4:37:TRP:N	2.20	0.68
25:2:405:HIS:HA	25:2:408:MET:HB2	1.75	0.68
28:7:223:VAL:O	28:7:238:GLN:N	2.21	0.68
28:7:765:LEU:O	28:7:769:GLU:N	2.23	0.68
1:A:118:HIS:O	1:A:123:ARG:NH1	2.27	0.67
4:D:66:ARG:O	4:D:70:PHE:N	2.23	0.67
17:X:276:ARG:O	17:X:280:ASP:N	2.25	0.67
21:0:553:MET:O	21:0:556:THR:OG1	2.09	0.67
23:4:62:ASN:HB3	23:4:118:PHE:CD2	2.28	0.67
26:5:36:ASP:OD2	26:5:39:HIS:ND1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:550:ALA:HB3	28:7:691:LEU:HB3	1.76	0.67
3:C:73:GLN:HB3	3:C:131:HIS:H	1.59	0.67
4:D:214:LEU:HA	4:D:217:LEU:HB2	1.77	0.67
7:G:27:LYS:HE2	7:G:54:ILE:HD11	1.76	0.67
17:X:194:LYS:O	17:X:198:SER:N	2.28	0.67
25:2:437:VAL:O	25:2:441:ILE:N	2.22	0.67
1:A:1169:ILE:O	1:A:1173:HIS:ND1	2.25	0.67
7:G:138:THR:O	7:G:141:SER:OG	2.10	0.67
8:H:41:ASP:OD2	8:H:122:LEU:N	2.27	0.67
14:Q:141:ARG:NE	14:Q:348:TYR:O	2.23	0.67
16:W:190:ASP:HA	16:W:193:ARG:HG2	1.75	0.67
20:N:40:DT:H2'	20:N:41:DA:C8	2.29	0.67
21:0:744:LEU:O	21:0:748:GLN:N	2.26	0.67
22:1:594:ASN:O	22:1:598:GLN:N	2.26	0.67
28:7:568:GLU:OE2	28:7:571:ARG:NH2	2.27	0.67
28:7:719:SER:O	28:7:723:GLN:N	2.20	0.67
1:A:85:ASP:OD1	1:A:85:ASP:N	2.26	0.67
21:0:287:GLU:HA	21:0:290:VAL:HG12	1.75	0.67
22:1:256:ILE:O	22:1:260:PHE:N	2.27	0.67
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.76	0.67
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.75	0.67
1:A:926:GLN:O	1:A:926:GLN:NE2	2.27	0.67
2:B:20:ASP:OD1	2:B:21:GLU:N	2.28	0.67
4:D:139:LYS:O	4:D:143:ASN:N	2.27	0.67
21:0:261:THR:OG1	21:0:262:ARG:NH1	2.28	0.67
24:6:114:ASN:OD1	24:6:114:ASN:N	2.28	0.67
24:6:309:PRO:HB3	24:6:312:LYS:HZ2	1.59	0.67
26:5:17:LYS:O	26:5:21:LEU:N	2.21	0.67
28:7:436:ALA:HB1	28:7:444:GLU:HB3	1.75	0.67
2:B:282:ILE:HA	2:B:285:ILE:HG13	1.75	0.67
21:0:272:SER:O	21:0:275:ARG:NH2	2.27	0.67
28:7:448:THR:OG1	28:7:449:GLU:OE1	2.07	0.67
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.77	0.67
2:B:261:ARG:O	2:B:264:SER:OG	2.11	0.67
4:D:67:ARG:HG2	4:D:71:LYS:HE3	1.77	0.67
8:H:104:PHE:CE1	8:H:137:GLN:HG2	2.29	0.67
9:I:17:ARG:NH1	9:I:28:GLU:OE2	2.28	0.67
21:0:68:LYS:NZ	21:0:202:LEU:O	2.28	0.67
21:0:117:HIS:HB3	21:0:136:MET:HE1	1.77	0.67
21:0:120:VAL:HG22	21:0:132:LYS:HD2	1.75	0.67
21:0:284:ASP:O	21:0:288:LYS:N	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:443:SER:HB3	21:0:473:LEU:HA	1.76	0.67
24:6:369:MET:SD	24:6:370:LEU:N	2.67	0.67
25:2:110:ASN:O	25:2:115:GLY:N	2.28	0.67
6:F:140:ASP:OD1	6:F:141:GLY:N	2.26	0.67
18:O:67:LEU:HD11	18:O:220:ARG:HB3	1.77	0.67
25:2:9:SER:O	25:2:12:GLN:N	2.24	0.67
25:2:68:SER:OG	25:2:69:ASN:N	2.28	0.67
25:2:473:LYS:NZ	25:2:476:GLN:O	2.27	0.67
26:5:23:ILE:O	26:5:26:LYS:NZ	2.23	0.67
28:7:698:ASP:OD1	28:7:699:GLU:N	2.20	0.67
8:H:28:ALA:HB3	8:H:38:LEU:HB3	1.76	0.67
8:H:130:ARG:O	8:H:133:ASN:ND2	2.28	0.67
17:X:256:ASP:OD1	17:X:256:ASP:N	2.27	0.67
21:0:217:LYS:HB2	21:0:308:GLU:HB2	1.76	0.67
21:0:291:GLN:NE2	21:0:292:GLY:O	2.28	0.67
21:0:326:ARG:O	21:0:380:ARG:NH2	2.28	0.67
21:0:467:ASP:OD1	21:0:467:ASP:N	2.27	0.67
21:0:726:GLN:NE2	24:6:290:ILE:O	2.28	0.67
26:5:32:LEU:N	26:5:41:LEU:O	2.27	0.67
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.77	0.67
5:E:66:GLU:OE2	5:E:67:GLU:N	2.27	0.67
17:X:259:PHE:O	17:X:263:TRP:N	2.25	0.67
21:0:539:VAL:HG12	21:0:621:LEU:HD13	1.77	0.67
28:7:234:VAL:N	28:7:316:PHE:O	2.27	0.67
28:7:520:GLU:OE2	28:7:682:GLN:NE2	2.27	0.67
1:A:1151:GLU:OE2	9:I:45:ARG:NE	2.24	0.66
8:H:134:ASN:OD1	8:H:134:ASN:N	2.19	0.66
14:Q:386:MET:HA	14:Q:386:MET:HE2	1.77	0.66
17:X:220:THR:HA	17:X:223:GLN:HB2	1.77	0.66
21:0:341:TYR:OH	21:0:362:HIS:O	2.12	0.66
21:0:357:LYS:HA	21:0:360:LEU:HB3	1.77	0.66
25:2:356:GLN:HE21	25:2:403:HIS:HE1	1.44	0.66
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.76	0.66
10:J:28:ASP:N	10:J:28:ASP:OD1	2.27	0.66
10:J:29:GLU:OE1	10:J:29:GLU:N	2.28	0.66
25:2:72:LEU:HD23	25:2:72:LEU:H	1.60	0.66
25:2:166:LEU:O	25:2:170:SER:N	2.22	0.66
2:B:360:PHE:O	2:B:374:LYS:NZ	2.26	0.66
5:E:76:GLY:N	5:E:106:GLN:OE1	2.24	0.66
13:M:190:LYS:NZ	13:M:303:GLN:O	2.25	0.66
18:O:115:ILE:HG23	18:O:121:MET:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:471:ARG:HH12	21:0:646:TYR:HB3	1.60	0.66
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.77	0.66
3:C:196:ASP:OD1	3:C:199:LYS:N	2.28	0.66
5:E:6:GLU:HA	5:E:9:ILE:HD12	1.78	0.66
13:M:171:ILE:O	13:M:175:SER:N	2.27	0.66
16:W:141:ASN:OD1	16:W:141:ASN:N	2.28	0.66
21:0:28:ILE:O	21:0:32:LEU:N	2.27	0.66
21:0:210:TYR:O	21:0:214:LEU:N	2.29	0.66
23:4:275:SER:HA	23:4:282:VAL:HA	1.76	0.66
25:2:176:VAL:O	25:2:181:GLU:N	2.28	0.66
28:7:573:THR:HG1	28:7:574:ALA:H	1.38	0.66
28:7:656:LYS:NZ	28:7:659:ASP:OD2	2.29	0.66
1:A:1038:THR:OG1	1:A:1040:GLN:N	2.29	0.66
3:C:241:ASP:OD1	3:C:242:GLN:NE2	2.28	0.66
21:0:228:LYS:O	21:0:228:LYS:NZ	2.23	0.66
25:2:370:PHE:HA	28:7:121:LEU:H	1.60	0.66
28:7:392:LYS:HE3	28:7:513:LEU:HD13	1.76	0.66
28:7:500:ARG:O	28:7:504:THR:N	2.29	0.66
28:7:542:GLU:HA	28:7:545:GLN:HG2	1.76	0.66
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.31	0.66
7:G:94:CYS:SG	7:G:95:SER:N	2.68	0.66
21:0:641:PHE:O	21:0:645:ASN:ND2	2.19	0.66
24:6:400:SER:O	24:6:426:ARG:NH2	2.27	0.66
28:7:303:ARG:HB2	28:7:323:VAL:H	1.61	0.66
28:7:308:ASP:O	28:7:340:GLU:N	2.28	0.66
28:7:750:TYR:HA	28:7:755:GLU:HB3	1.77	0.66
2:B:57:TYR:OH	15:R:251:ARG:NE	2.24	0.66
2:B:87:LYS:HB3	2:B:137:TYR:HB3	1.77	0.66
21:0:192:PRO:HA	21:0:195:ILE:HB	1.75	0.66
1:A:1205:LYS:NZ	1:A:1205:LYS:H	1.94	0.66
2:B:942:ARG:HB2	2:B:945:GLU:HG3	1.76	0.66
4:D:144:THR:O	4:D:148:LEU:N	2.25	0.66
5:E:90:VAL:O	5:E:94:LYS:N	2.24	0.66
22:1:188:ASN:HD21	22:1:190:VAL:HB	1.60	0.66
22:1:503:VAL:O	22:1:507:ILE:N	2.28	0.66
23:4:155:ALA:O	23:4:158:THR:OG1	2.10	0.66
28:7:383:ILE:O	28:7:535:LEU:N	2.28	0.66
1:A:44:THR:OG1	1:A:46:THR:OG1	2.13	0.66
1:A:122:MET:HE2	1:A:141:LEU:HD12	1.77	0.66
2:B:955:THR:HG22	12:L:55:ILE:HA	1.76	0.66
4:D:71:LYS:HA	4:D:74:GLN:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:373:TYR:OH	15:R:72:ARG:NH1	2.28	0.66
17:X:195:LEU:HA	17:X:198:SER:HB3	1.78	0.66
1:A:254:GLU:OE1	2:B:935:ARG:NH1	2.27	0.66
4:D:25:ALA:HB2	7:G:84:GLY:HA3	1.77	0.66
22:1:254:GLU:O	22:1:258:ASN:N	2.20	0.66
21:0:572:GLU:OE1	21:0:579:THR:OG1	2.08	0.65
22:1:318:UNK:O	22:1:322:UNK:N	2.28	0.65
25:2:399:TYR:O	25:2:403:HIS:N	2.18	0.65
1:A:847:ASP:N	1:A:847:ASP:OD1	2.27	0.65
3:C:14:SER:OG	3:C:15:LYS:N	2.25	0.65
19:T:139:DC:H2'	19:T:140:DT:H6	1.62	0.65
25:2:71:LYS:O	25:2:75:GLN:NE2	2.27	0.65
28:7:313:VAL:O	28:7:314:HIS:C	2.37	0.65
1:A:182:VAL:HA	1:A:201:VAL:HA	1.77	0.65
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.77	0.65
8:H:110:ASP:OD2	8:H:130:ARG:NH2	2.29	0.65
13:M:201:LYS:NZ	20:N:18:DT:OP1	2.27	0.65
13:M:281:SER:HA	13:M:284:LEU:HD23	1.78	0.65
17:X:210:LEU:O	17:X:214:TRP:N	2.26	0.65
21:0:498:THR:HG22	21:0:499:LYS:HG3	1.78	0.65
25:2:367:LYS:HB2	25:2:375:LEU:HG	1.79	0.65
25:2:381:GLU:HA	25:2:384:ARG:NE	2.11	0.65
26:5:57:LEU:HA	26:5:60:LYS:HB2	1.78	0.65
28:7:543:LEU:O	28:7:546:LYS:NZ	2.29	0.65
1:A:203:SER:N	1:A:206:GLU:OE2	2.30	0.65
28:7:408:ILE:HG23	28:7:453:VAL:HB	1.79	0.65
2:B:573:GLN:OE1	2:B:573:GLN:N	2.30	0.65
4:D:194:LEU:HD21	7:G:167:TYR:HB2	1.77	0.65
6:F:77:ASP:OD1	6:F:77:ASP:N	2.21	0.65
21:0:275:ARG:HH22	21:0:276:LYS:HG3	1.61	0.65
25:2:252:ASP:O	25:2:256:TYR:N	2.21	0.65
28:7:411:CYS:SG	28:7:412:THR:N	2.70	0.65
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.79	0.65
5:E:63:ASN:OD1	5:E:77:SER:OG	2.14	0.65
9:I:73:ARG:O	9:I:83:ASN:ND2	2.30	0.65
15:R:94:LYS:HB2	15:R:107:LEU:HB3	1.78	0.65
17:X:204:GLY:HA2	17:X:244:VAL:H	1.61	0.65
28:7:249:SER:O	28:7:254:LEU:N	2.30	0.65
1:A:311:GLN:C	13:M:102:THR:HB	2.21	0.65
7:G:137:ILE:HG23	7:G:143:ILE:HD11	1.79	0.65
16:W:108:ARG:NH2	17:X:262:MET:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:117:ARG:HA	23:4:120:ASN:HD21	1.61	0.65
3:C:16:ASP:OD1	3:C:16:ASP:N	2.26	0.65
16:W:132:THR:H	16:W:135:GLU:HG3	1.61	0.65
24:6:142:ARG:HB2	24:6:143:PRO:HD3	1.79	0.65
25:2:456:GLY:HA2	25:2:495:LYS:HB2	1.79	0.65
28:7:501:VAL:HG23	28:7:505:ILE:HD11	1.79	0.65
28:7:628:TYR:O	28:7:631:THR:OG1	2.12	0.65
2:B:72:GLU:HA	2:B:87:LYS:HA	1.77	0.65
2:B:244:LEU:O	2:B:249:ARG:HA	1.97	0.65
2:B:326:ASP:OD1	2:B:328:GLU:N	2.30	0.65
16:W:20:PHE:HD1	17:X:255:ILE:HG21	1.62	0.65
21:0:215:ASP:HB3	21:0:218:ILE:HG12	1.79	0.65
21:0:247:SER:OG	21:0:248:LEU:N	2.21	0.65
24:6:238:SER:OG	24:6:239:LEU:N	2.28	0.65
28:7:331:GLN:C	28:7:334:ASP:H	2.05	0.65
28:7:357:LYS:HE2	28:7:430:LEU:HD12	1.79	0.65
28:7:477:LEU:O	28:7:482:TRP:NE1	2.28	0.65
28:7:673:ILE:HG23	28:7:708:LEU:HD12	1.77	0.65
4:D:173:HIS:N	4:D:176:GLU:OE2	2.28	0.65
8:H:64:ASN:OD1	8:H:65:LEU:N	2.30	0.65
13:M:41:GLY:HA2	13:M:56:LEU:HB2	1.79	0.65
25:2:504:PHE:O	25:2:508:LYS:N	2.30	0.65
1:A:508:PRO:O	1:A:511:ILE:HG13	1.96	0.64
5:E:155:ARG:NH1	5:E:194:GLU:OE2	2.29	0.64
23:4:304:LYS:H	23:4:311:GLN:HA	1.63	0.64
26:5:23:ILE:HD11	26:5:57:LEU:HD11	1.79	0.64
27:3:118:TYR:O	27:3:122:HIS:N	2.24	0.64
2:B:906:SER:OG	2:B:907:GLY:N	2.27	0.64
16:W:106:VAL:O	16:W:110:LYS:N	2.28	0.64
21:0:210:TYR:HB3	21:0:214:LEU:HD12	1.79	0.64
24:6:293:ASP:OD2	24:6:295:THR:OG1	2.10	0.64
7:G:91:VAL:HG23	7:G:143:ILE:HD13	1.79	0.64
21:0:141:ALA:O	21:0:145:LEU:N	2.30	0.64
22:1:583:TYR:O	22:1:587:LYS:N	2.18	0.64
28:7:303:ARG:N	28:7:323:VAL:HG13	2.07	0.64
28:7:546:LYS:N	28:7:546:LYS:HZ2	1.95	0.64
1:A:68:GLN:HB3	13:M:18:LEU:HD21	1.79	0.64
2:B:26:THR:OG1	2:B:708:GLU:OE1	2.14	0.64
3:C:9:LYS:NZ	3:C:10:ILE:O	2.27	0.64
4:D:167:LEU:O	4:D:170:THR:OG1	2.12	0.64
25:2:86:LEU:O	25:2:101:ASN:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:174:GLU:N	25:2:183:LYS:O	2.31	0.64
27:3:85:ARG:O	27:3:89:PHE:N	2.24	0.64
28:7:413:SER:N	28:7:416:SER:OG	2.28	0.64
28:7:608:PHE:HB2	28:7:672:GLN:HA	1.78	0.64
4:D:190:GLU:HA	7:G:167:TYR:CZ	2.32	0.64
5:E:6:GLU:N	5:E:6:GLU:OE1	2.30	0.64
13:M:191:GLU:O	13:M:194:SER:OG	2.11	0.64
21:0:607:SER:O	21:0:668:ARG:NH2	2.31	0.64
28:7:491:HIS:HB3	28:7:514:THR:HB	1.78	0.64
7:G:119:LEU:HB2	7:G:132:SER:HB3	1.80	0.64
21:0:278:ASP:HA	21:0:280:GLN:HE22	1.62	0.64
25:2:75:GLN:HA	25:2:78:ILE:HG12	1.80	0.64
28:7:608:PHE:O	28:7:673:ILE:N	2.31	0.64
1:A:494:SER:OG	1:A:495:GLU:N	2.30	0.64
2:B:936:ASP:OD2	2:B:938:SER:OG	2.15	0.64
2:B:972:LYS:HE3	2:B:1098:MET:HE3	1.79	0.64
12:L:41:SER:OG	12:L:44:ASP:OD1	2.14	0.64
21:0:572:GLU:OE1	21:0:573:THR:N	2.30	0.64
24:6:403:CYS:HB3	24:6:408:SER:H	1.60	0.64
25:2:372:ASN:N	25:2:372:ASN:OD1	2.29	0.64
28:7:340:GLU:HA	28:7:380:ARG:HB3	1.77	0.64
28:7:423:GLN:HG2	28:7:424:PHE:CZ	2.33	0.64
28:7:566:TYR:O	28:7:570:LEU:HG	1.98	0.64
1:A:292:ALA:HA	13:M:116:LYS:HZ3	1.63	0.64
2:B:70:ILE:HD11	14:Q:333:LYS:H	1.63	0.64
9:I:19:ASP:OD2	9:I:24:ARG:N	2.28	0.64
9:I:87:GLN:HE22	9:I:97:MET:HG2	1.63	0.64
21:0:302:GLN:HG2	21:0:303:GLU:HG3	1.79	0.64
21:0:315:ASP:OD1	21:0:316:LEU:N	2.31	0.64
26:5:49:PHE:O	26:5:53:GLU:HG2	1.98	0.64
1:A:121:LEU:O	1:A:125:ALA:N	2.31	0.64
1:A:317:LYS:HA	13:M:95:ARG:HG3	1.79	0.64
4:D:164:ILE:HA	4:D:167:LEU:HD12	1.79	0.64
8:H:110:ASP:O	8:H:129:TYR:N	2.31	0.64
13:M:286:ILE:HD11	13:M:291:ILE:HB	1.79	0.64
21:0:20:GLU:O	21:0:24:TYR:N	2.25	0.64
21:0:123:GLU:OE2	21:0:125:LYS:N	2.31	0.64
21:0:554:TRP:CD1	21:0:559:ILE:HG21	2.33	0.64
21:0:573:THR:OG1	21:0:575:ASP:OD1	2.12	0.64
25:2:349:SER:OG	25:2:373:MET:SD	2.55	0.64
2:B:71:LEU:O	2:B:88:TYR:N	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ILE:O	2:B:86:ARG:NH2	2.31	0.64
2:B:336:ARG:HH12	2:B:345:LYS:HD2	1.61	0.64
5:E:92:THR:O	5:E:95:THR:OG1	2.11	0.64
14:Q:337:GLU:OE1	14:Q:339:ALA:N	2.31	0.64
16:W:41:ASP:O	16:W:45:GLN:N	2.28	0.64
24:6:250:THR:O	24:6:253:SER:OG	2.15	0.64
25:2:502:LEU:O	25:2:506:LYS:NZ	2.24	0.64
28:7:489:GLU:N	28:7:513:LEU:O	2.31	0.64
1:A:72:GLU:HB3	13:M:20:ILE:HD11	1.80	0.63
21:0:185:CYS:HB3	21:0:190:LEU:HB2	1.80	0.63
21:0:413:GLU:HB2	21:0:414:GLU:HG3	1.80	0.63
21:0:625:ILE:HG21	21:0:685:ARG:HE	1.63	0.63
24:6:138:GLU:OE2	24:6:145:ARG:NE	2.31	0.63
22:1:190:VAL:HA	22:1:193:LYS:HB2	1.80	0.63
28:7:555:ALA:HB3	28:7:706:TYR:HA	1.80	0.63
28:7:610:ASP:H	28:7:674:SER:HB2	1.62	0.63
28:7:622:MET:O	28:7:624:LYS:NZ	2.26	0.63
2:B:398:ARG:HD3	2:B:509:ALA:HB2	1.79	0.63
9:I:113:ASP:OD1	9:I:114:GLN:N	2.32	0.63
18:O:101:ALA:HA	18:O:115:ILE:O	1.98	0.63
22:1:230:PRO:HD3	24:6:244:PRO:HA	1.79	0.63
25:2:56:GLU:OE1	25:2:56:GLU:N	2.30	0.63
25:2:454:TYR:HB3	25:2:492:PHE:CE1	2.33	0.63
2:B:241:ARG:HH21	2:B:251:ILE:HA	1.64	0.63
2:B:1012:ILE:HG13	2:B:1012:ILE:O	1.98	0.63
16:W:147:PHE:O	16:W:155:PRO:HA	1.97	0.63
21:0:270:ARG:HG3	21:0:388:LEU:HD13	1.79	0.63
25:2:75:GLN:NE2	25:2:75:GLN:H	1.96	0.63
28:7:567:GLN:HA	28:7:570:LEU:HD12	1.81	0.63
1:A:1240:CYS:SG	1:A:1241:ARG:N	2.72	0.63
5:E:55:ARG:HA	5:E:58:MET:HE2	1.81	0.63
2:B:294:ASP:OD1	2:B:295:GLY:N	2.32	0.63
14:Q:110:ASP:O	14:Q:114:MET:N	2.22	0.63
21:0:157:GLU:OE2	21:0:161:ASN:ND2	2.32	0.63
22:1:558:CYS:O	22:1:562:LYS:N	2.24	0.63
24:6:437:CYS:SG	24:6:438:VAL:N	2.72	0.63
25:2:462:PHE:H	25:2:489:LYS:HB3	1.63	0.63
25:2:488:LYS:HD2	25:2:490:LYS:HG3	1.81	0.63
26:5:55:ASN:O	26:5:59:SER:N	2.29	0.63
2:B:443:ASN:OD1	2:B:445:LYS:N	2.28	0.63
13:M:299:GLY:O	13:M:303:GLN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:119:DG:O6	20:N:47:DC:N4	2.26	0.63
21:O:199:MET:HA	21:O:202:LEU:HD13	1.80	0.63
23:4:223:PHE:O	23:4:227:THR:OG1	2.17	0.63
25:2:69:ASN:HA	25:2:71:LYS:HE3	1.81	0.63
25:2:249:MET:O	25:2:253:MET:N	2.27	0.63
25:2:505:ALA:C	25:2:508:LYS:H	2.05	0.63
28:7:491:HIS:CD2	28:7:492:VAL:H	2.15	0.63
28:7:727:VAL:HG13	28:7:732:ALA:HA	1.81	0.63
2:B:71:LEU:N	2:B:88:TYR:O	2.29	0.63
7:G:157:ILE:C	7:G:158:HIS:HD1	2.07	0.63
13:M:274:PRO:HD2	18:O:188:GLU:HG3	1.80	0.63
21:O:401:ASP:HA	21:O:404:THR:HB	1.80	0.63
22:1:207:SER:OG	22:1:208:GLU:OE1	2.13	0.63
27:3:88:VAL:O	27:3:92:PHE:N	2.32	0.63
28:7:423:GLN:HG2	28:7:424:PHE:CE1	2.34	0.63
28:7:487:LEU:HD11	28:7:501:VAL:HG21	1.81	0.63
15:R:70:LEU:HD12	15:R:71:VAL:H	1.63	0.63
15:R:124:LEU:HA	15:R:220:HIS:CE1	2.33	0.63
18:O:227:PHE:HA	18:O:230:ILE:HG22	1.81	0.63
21:O:148:ASP:N	21:O:148:ASP:OD1	2.32	0.63
21:O:341:TYR:CE2	21:O:366:LEU:HB2	2.34	0.63
21:O:625:ILE:HD12	21:O:626:PRO:HD2	1.79	0.63
26:5:51:LYS:O	26:5:55:ASN:N	2.31	0.63
2:B:101:MET:HB3	15:R:259:VAL:HG11	1.81	0.62
4:D:123:LEU:HG	4:D:124:GLU:N	2.14	0.62
13:M:204:GLY:O	13:M:208:ASN:ND2	2.32	0.62
18:O:171:ARG:NH1	18:O:236:GLU:O	2.31	0.62
23:4:24:SER:O	23:4:71:ASN:HB2	1.99	0.62
28:7:446:PHE:HZ	28:7:472:LYS:HB3	1.62	0.62
28:7:565:PHE:HD2	28:7:763:VAL:HG11	1.63	0.62
1:A:1225:PHE:HE1	1:A:1227:ILE:HG12	1.64	0.62
2:B:287:ARG:NH2	2:B:292:ILE:O	2.27	0.62
5:E:19:VAL:O	5:E:23:VAL:HG12	1.99	0.62
9:I:96:SER:OG	9:I:97:MET:N	2.31	0.62
21:O:221:ARG:HD3	21:O:221:ARG:H	1.64	0.62
28:7:637:MET:N	28:7:637:MET:SD	2.72	0.62
28:7:720:THR:O	28:7:724:ALA:N	2.32	0.62
28:7:729:GLN:O	28:7:729:GLN:NE2	2.32	0.62
1:A:143:LYS:HG3	1:A:144:THR:HG23	1.80	0.62
1:A:1107:VAL:HG12	1:A:1383:SER:HB3	1.80	0.62
2:B:344:LYS:O	2:B:348:ARG:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:258:GLU:O	17:X:262:MET:N	2.23	0.62
22:1:254:GLU:OE1	22:1:254:GLU:N	2.23	0.62
27:3:61:LYS:O	27:3:63:LEU:HD22	1.99	0.62
1:A:1264:GLU:O	1:A:1268:LEU:N	2.31	0.62
5:E:192:ARG:NH1	5:E:215:MET:OXT	2.31	0.62
13:M:185:VAL:HG11	13:M:187:ARG:HH21	1.65	0.62
16:W:152:CYS:HB3	16:W:154:GLU:HG3	1.81	0.62
21:0:592:ASN:OD1	21:0:593:GLY:N	2.31	0.62
21:0:637:ALA:HA	21:0:640:GLU:HG2	1.80	0.62
24:6:162:ASP:OD1	24:6:378:ARG:NH2	2.32	0.62
24:6:188:ASN:ND2	24:6:191:ASP:H	1.98	0.62
25:2:19:GLN:OE1	25:2:19:GLN:N	2.31	0.62
25:2:449:ASP:O	25:2:450:ARG:NE	2.32	0.62
25:2:483:TRP:CE2	25:2:485:ASP:HB2	2.34	0.62
28:7:331:GLN:HA	28:7:334:ASP:HA	1.81	0.62
1:A:84:ILE:O	1:A:239:LEU:N	2.32	0.62
1:A:399:HIS:O	1:A:435:HIS:ND1	2.30	0.62
1:A:1157:ASP:OD2	1:A:1160:SER:N	2.24	0.62
11:K:8:GLU:HA	11:K:11:LEU:O	1.99	0.62
13:M:305:THR:HG22	13:M:307:GLY:H	1.64	0.62
21:0:132:LYS:O	21:0:136:MET:N	2.28	0.62
21:0:142:LYS:NZ	21:0:146:GLU:OE1	2.30	0.62
21:0:345:ARG:HH11	21:0:345:ARG:HA	1.65	0.62
21:0:401:ASP:O	21:0:405:PHE:N	2.24	0.62
21:0:635:LEU:HD12	21:0:635:LEU:H	1.64	0.62
22:1:472:UNK:O	22:1:476:UNK:N	2.32	0.62
25:2:341:VAL:N	25:2:408:MET:SD	2.72	0.62
27:3:79:GLU:O	27:3:83:ASP:N	2.24	0.62
28:7:135:SER:O	28:7:140:ARG:N	2.32	0.62
28:7:439:THR:C	28:7:441:ASP:H	2.05	0.62
18:O:166:VAL:HG11	18:O:234:LEU:HD23	1.82	0.62
21:0:126:GLY:O	21:0:130:ASP:N	2.25	0.62
23:4:23:PRO:HG2	23:4:172:LEU:HD21	1.80	0.62
24:6:372:LEU:HD13	24:6:375:HIS:HE1	1.65	0.62
25:2:411:LEU:HA	25:2:414:GLU:HG2	1.82	0.62
28:7:596:GLN:OE1	28:7:600:ARG:NH2	2.33	0.62
28:7:608:PHE:N	28:7:671:ILE:O	2.33	0.62
1:A:131:SER:OG	1:A:132:LYS:N	2.32	0.62
1:A:137:ALA:O	1:A:140:THR:OG1	2.16	0.62
3:C:263:THR:OG1	3:C:264:GLN:OE1	2.10	0.62
7:G:35:GLU:HG3	7:G:48:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:373:TYR:HB3	15:R:70:LEU:HD11	1.82	0.62
21:0:341:TYR:O	21:0:345:ARG:HG2	2.00	0.62
24:6:197:LYS:HB3	24:6:200:ARG:HH21	1.63	0.62
25:2:346:LYS:NZ	25:2:347:ILE:HB	2.15	0.62
25:2:435:PRO:O	25:2:439:ASP:N	2.19	0.62
28:7:211:ASN:O	28:7:215:GLY:N	2.21	0.62
28:7:328:LYS:C	28:7:331:GLN:HE22	2.07	0.62
28:7:567:GLN:O	28:7:571:ARG:NH1	2.32	0.62
1:A:1171:GLN:HE22	1:A:1172:LEU:HD13	1.65	0.62
4:D:24:ALA:N	4:D:28:GLN:O	2.32	0.62
5:E:74:ASP:OD1	5:E:74:ASP:N	2.33	0.62
7:G:38:CYS:O	7:G:155:SER:HA	1.99	0.62
15:R:108:LEU:HD21	15:R:120:TYR:HB2	1.82	0.62
16:W:113:LEU:O	16:W:116:ASN:ND2	2.32	0.62
28:7:407:VAL:H	28:7:452:LEU:HD22	1.64	0.62
5:E:178:ILE:HG22	5:E:214:CYS:HA	1.81	0.62
6:F:140:ASP:OD1	6:F:142:SER:N	2.29	0.62
18:O:66:THR:O	18:O:68:GLN:NE2	2.32	0.62
21:0:155:LEU:HD23	21:0:157:GLU:HB2	1.82	0.62
22:1:492:UNK:O	22:1:494:UNK:N	2.26	0.62
26:5:57:LEU:O	26:5:61:ASN:N	2.33	0.62
28:7:574:ALA:O	28:7:576:LYS:N	2.32	0.62
2:B:921:ASP:OD1	2:B:921:ASP:N	2.30	0.62
4:D:64:VAL:O	4:D:67:ARG:N	2.33	0.62
7:G:52:ASP:OD1	7:G:52:ASP:N	2.23	0.62
21:0:651:ASN:HA	21:0:654:LEU:HB2	1.81	0.62
21:0:658:ALA:O	21:0:662:ALA:N	2.33	0.62
22:1:226:GLN:OE1	24:6:212:ASN:ND2	2.33	0.62
24:6:139:LYS:NZ	24:6:143:PRO:O	2.23	0.62
25:2:378:ILE:HD12	25:2:382:SER:HB2	1.80	0.62
2:B:98:THR:OG1	2:B:99:LYS:O	2.17	0.61
4:D:149:THR:O	4:D:152:SER:OG	2.12	0.61
13:M:283:TYR:HA	13:M:286:ILE:HG22	1.81	0.61
15:R:97:ILE:HB	15:R:104:ILE:HD12	1.81	0.61
15:R:302:TYR:O	15:R:306:LEU:N	2.28	0.61
16:W:127:CYS:SG	16:W:131:TYR:OH	2.57	0.61
21:0:75:THR:OG1	22:1:342:ASN:OD1	2.17	0.61
21:0:354:GLU:OE1	21:0:358:SER:OG	2.10	0.61
26:5:57:LEU:HA	26:5:60:LYS:HD2	1.82	0.61
3:C:124:LEU:O	3:C:127:ARG:NH1	2.33	0.61
9:I:5:ARG:HB2	9:I:14:LEU:HD12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:54:GLU:HB3	9:I:100:PHE:CZ	2.35	0.61
19:T:139:DC:H2'	19:T:140:DT:C6	2.35	0.61
21:0:104:ARG:HD2	21:0:173:LYS:HA	1.81	0.61
21:0:137:THR:O	21:0:137:THR:OG1	2.17	0.61
21:0:301:ASP:OD1	21:0:386:ARG:NH1	2.33	0.61
21:0:312:LEU:O	21:0:314:GLN:N	2.33	0.61
21:0:412:TYR:HB3	21:0:416:PHE:CE2	2.34	0.61
21:0:506:ILE:HG22	21:0:518:ILE:HD12	1.81	0.61
22:1:588:ASP:O	22:1:592:LYS:N	2.18	0.61
23:4:54:LEU:O	23:4:58:ILE:N	2.28	0.61
28:7:354:ILE:HG22	28:7:355:ASP:H	1.65	0.61
2:B:882:THR:HG22	2:B:934:LYS:HG3	1.82	0.61
4:D:208:GLU:HG2	4:D:212:LYS:HD3	1.81	0.61
6:F:147:SER:N	6:F:150:GLU:OE2	2.24	0.61
22:1:482:UNK:O	22:1:484:UNK:N	2.33	0.61
23:4:290:SER:O	23:4:293:LEU:N	2.34	0.61
28:7:222:LYS:O	28:7:241:ILE:N	2.27	0.61
28:7:331:GLN:HG3	28:7:529:PHE:CG	2.35	0.61
28:7:524:ILE:HD12	28:7:525:GLY:H	1.63	0.61
1:A:898:ARG:O	1:A:1029:ARG:NH2	2.31	0.61
4:D:157:GLN:O	4:D:161:GLY:N	2.19	0.61
7:G:115:MET:HG2	7:G:163:ILE:HG12	1.82	0.61
16:W:185:SER:HA	16:W:188:LYS:HB2	1.82	0.61
18:O:79:ARG:NH1	18:O:117:ALA:O	2.33	0.61
21:0:568:LEU:O	21:0:597:ILE:N	2.33	0.61
23:4:258:LEU:C	23:4:260:PRO:HD3	2.25	0.61
28:7:566:TYR:HA	28:7:569:TYR:HB3	1.82	0.61
18:O:169:PRO:HB2	18:O:239:LYS:HG2	1.82	0.61
21:0:285:GLU:HA	21:0:288:LYS:HB2	1.81	0.61
21:0:490:LYS:HZ1	21:0:493:LEU:HA	1.64	0.61
22:1:473:UNK:O	22:1:477:UNK:N	2.34	0.61
23:4:50:ILE:O	23:4:53:VAL:N	2.34	0.61
25:2:203:LEU:O	25:2:206:GLN:N	2.27	0.61
4:D:206:GLU:HA	4:D:209:ARG:HG2	1.83	0.61
14:Q:100:GLU:HA	15:R:95:ILE:H	1.66	0.61
21:0:615:GLN:N	21:0:615:GLN:OE1	2.33	0.61
21:0:636:LYS:NZ	21:0:650:GLU:OE2	2.33	0.61
21:0:681:LEU:HB3	21:0:686:PHE:CD2	2.35	0.61
22:1:260:PHE:HB3	22:1:267:LYS:HD3	1.83	0.61
28:7:457:TYR:O	28:7:461:ALA:N	2.32	0.61
21:0:384:LEU:O	21:0:387:THR:OG1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:460:SER:HB2	21:0:463:ILE:HG12	1.82	0.61
22:1:179:LYS:O	22:1:183:SER:N	2.26	0.61
22:1:476:UNK:O	22:1:480:UNK:N	2.33	0.61
24:6:134:GLU:CD	24:6:134:GLU:H	2.08	0.61
25:2:406:PRO:O	25:2:409:ARG:NH1	2.33	0.61
28:7:357:LYS:NZ	28:7:429:THR:OG1	2.34	0.61
8:H:7:ASP:OD1	8:H:8:ASP:N	2.33	0.61
14:Q:117:HIS:HD2	14:Q:393:TYR:HE2	1.47	0.61
18:O:216:GLY:HA2	20:N:22:DT:H4'	1.82	0.61
22:1:339:LEU:HD23	22:1:342:ASN:HD22	1.65	0.61
25:2:394:ASP:OD1	25:2:394:ASP:N	2.33	0.61
25:2:458:LEU:HD13	25:2:492:PHE:HD2	1.66	0.61
28:7:303:ARG:HD2	28:7:304:GLU:HG2	1.83	0.61
28:7:398:THR:OG1	28:7:399:ALA:N	2.32	0.61
28:7:517:LEU:HD12	28:7:518:VAL:H	1.66	0.61
28:7:676:HIS:O	28:7:679:SER:OG	2.19	0.61
1:A:117:GLU:OE1	1:A:118:HIS:N	2.34	0.61
2:B:296:GLU:O	2:B:299:GLU:N	2.32	0.61
16:W:176:MET:HA	16:W:179:ILE:HG12	1.83	0.61
20:N:9:DA:H1'	20:N:10:DA:H5'	1.83	0.61
20:N:26:DA:H1'	20:N:27:DG:H5'	1.82	0.61
24:6:379:SER:O	24:6:382:HIS:N	2.32	0.61
25:2:167:LEU:O	25:2:171:LYS:N	2.33	0.61
25:2:187:GLU:O	25:2:191:PHE:N	2.26	0.61
1:A:1147:THR:HG23	1:A:1197:LEU:HD23	1.82	0.61
1:A:1331:SER:OG	1:A:1334:ASP:OD2	2.16	0.61
17:X:260:VAL:HA	17:X:263:TRP:HB3	1.83	0.61
21:0:570:LEU:O	21:0:598:LEU:HD12	2.01	0.61
25:2:367:LYS:HG3	25:2:376:GLY:HA2	1.83	0.61
26:5:30:ILE:HG23	26:5:43:ASN:HB2	1.83	0.61
28:7:192:ASP:O	28:7:196:VAL:N	2.22	0.61
28:7:456:THR:HG23	28:7:459:MET:HE2	1.83	0.61
28:7:457:TYR:OH	28:7:488:ASP:O	2.17	0.61
3:C:240:VAL:O	3:C:243:VAL:N	2.35	0.60
7:G:148:GLU:N	7:G:160:ILE:O	2.34	0.60
21:0:484:ALA:HB2	21:0:695:LYS:HE3	1.82	0.60
21:0:563:VAL:HG22	21:0:569:ILE:HD11	1.82	0.60
22:1:222:LEU:HD13	24:6:216:MET:HG3	1.83	0.60
22:1:487:UNK:O	22:1:491:UNK:N	2.33	0.60
27:3:141:LYS:O	27:3:145:MET:N	2.33	0.60
28:7:467:SER:O	28:7:470:SER:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:683:GLU:OE1	28:7:722:ARG:NH1	2.34	0.60
7:G:164:LYS:HE3	27:3:49:LEU:HD12	1.83	0.60
13:M:186:ALA:H	13:M:237:THR:HG21	1.65	0.60
21:0:260:ALA:O	21:0:264:ALA:N	2.26	0.60
21:0:341:TYR:CZ	21:0:363:LEU:HA	2.36	0.60
23:4:201:PHE:O	23:4:204:THR:OG1	2.18	0.60
23:4:288:ILE:HD11	23:4:293:LEU:HD22	1.82	0.60
28:7:250:VAL:O	28:7:302:GLU:N	2.34	0.60
28:7:580:LEU:HA	28:7:583:MET:HG2	1.82	0.60
2:B:403:LYS:NZ	2:B:696:GLU:OE2	2.28	0.60
7:G:95:SER:OG	7:G:96:GLN:N	2.34	0.60
8:H:56:THR:OG1	8:H:146:ARG:NH1	2.34	0.60
9:I:60:GLN:OE1	9:I:60:GLN:N	2.30	0.60
18:O:68:GLN:NE2	18:O:163:SER:O	2.34	0.60
21:0:104:ARG:NH1	21:0:171:LEU:O	2.33	0.60
21:0:281:LYS:O	21:0:285:GLU:N	2.29	0.60
21:0:477:THR:OG1	21:0:478:VAL:N	2.33	0.60
25:2:473:LYS:HA	25:2:476:GLN:HB3	1.83	0.60
27:3:31:ASN:HD22	27:3:68:PHE:HA	1.65	0.60
28:7:310:ILE:HG23	28:7:376:ASN:HD21	1.65	0.60
28:7:682:GLN:O	28:7:686:ARG:N	2.32	0.60
21:0:99:TYR:OH	21:0:173:LYS:NZ	2.31	0.60
21:0:407:THR:O	21:0:411:THR:OG1	2.12	0.60
25:2:361:SER:HA	25:2:364:VAL:HG13	1.82	0.60
26:5:18:ALA:O	26:5:22:GLN:NE2	2.30	0.60
28:7:234:VAL:O	28:7:315:SER:HA	2.02	0.60
28:7:266:GLU:O	28:7:348:ARG:NE	2.34	0.60
28:7:439:THR:HB	28:7:442:ASN:H	1.66	0.60
1:A:706:HIS:CD2	1:A:1135:ARG:HH21	2.18	0.60
1:A:1205:LYS:H	1:A:1205:LYS:HZ3	1.49	0.60
2:B:235:SER:OG	2:B:236:HIS:ND1	2.27	0.60
16:W:126:ILE:H	16:W:126:ILE:HD12	1.66	0.60
19:T:150:DG:H2"	19:T:151:DC:C6	2.37	0.60
21:0:109:THR:O	21:0:212:TYR:OH	2.14	0.60
21:0:254:THR:HA	21:0:257:LEU:HB3	1.82	0.60
21:0:371:ARG:NE	21:0:410:SER:O	2.34	0.60
23:4:217:GLY:O	23:4:237:HIS:NE2	2.35	0.60
24:6:139:LYS:NZ	24:6:144:ASN:HB3	2.15	0.60
25:2:148:HIS:O	25:2:152:GLY:N	2.24	0.60
25:2:339:LEU:O	25:2:407:GLN:HB3	2.01	0.60
27:3:102:ASP:O	27:3:106:TYR:N	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:307:ASP:HB2	28:7:508:HIS:O	2.01	0.60
28:7:610:ASP:N	28:7:674:SER:HB2	2.16	0.60
1:A:146:MET:O	1:A:171:GLN:N	2.29	0.60
3:C:78:GLU:H	3:C:78:GLU:CD	2.04	0.60
21:0:262:ARG:O	21:0:266:ALA:N	2.22	0.60
22:1:621:ASN:OD1	22:1:621:ASN:N	2.34	0.60
28:7:194:ILE:O	28:7:198:ASP:N	2.34	0.60
28:7:412:THR:OG1	28:7:413:SER:N	2.31	0.60
1:A:372:LYS:HZ2	11:K:1:MET:HG2	1.65	0.60
2:B:739:THR:OG1	2:B:740:HIS:ND1	2.34	0.60
19:T:139:DC:O2	20:N:27:DG:N1	2.35	0.60
21:0:71:TYR:HB2	21:0:233:ILE:HD12	1.82	0.60
21:0:356:PRO:O	21:0:360:LEU:N	2.35	0.60
21:0:515:ASP:N	21:0:515:ASP:OD1	2.35	0.60
23:4:136:GLU:H	23:4:137:LYS:HZ3	1.50	0.60
23:4:189:GLU:O	23:4:192:GLN:NE2	2.33	0.60
24:6:175:ARG:O	24:6:178:LEU:N	2.34	0.60
2:B:950:ASP:OD2	2:B:967:ARG:NH2	2.33	0.60
12:L:51:CYS:C	12:L:53:HIS:H	2.08	0.60
15:R:108:LEU:HB2	15:R:117:PRO:N	2.17	0.60
22:1:236:UNK:O	22:1:240:UNK:N	2.34	0.60
25:2:194:GLN:O	25:2:199:GLN:N	2.35	0.60
28:7:342:ASP:OD1	28:7:342:ASP:N	2.35	0.60
1:A:278:THR:O	1:A:281:HIS:N	2.34	0.60
2:B:185:THR:HG23	2:B:188:ASP:HB2	1.84	0.60
4:D:211:LEU:HD22	4:D:214:LEU:HD22	1.84	0.60
13:M:272:LYS:HE2	18:O:191:PRO:HD3	1.84	0.60
17:X:256:ASP:HB2	17:X:259:PHE:HB2	1.83	0.60
18:O:185:TYR:CZ	18:O:187:PRO:HB3	2.36	0.60
21:0:618:ARG:NH1	21:0:676:TYR:O	2.34	0.60
24:6:253:SER:O	24:6:256:SER:OG	2.17	0.60
28:7:468:HIS:HA	28:7:471:GLN:HE22	1.67	0.60
2:B:975:GLN:O	2:B:990:ILE:HD12	2.02	0.60
7:G:163:ILE:HB	7:G:169:GLY:H	1.67	0.60
14:Q:369:ASN:HB3	14:Q:373:TYR:CE2	2.37	0.60
18:O:98:ARG:HH21	19:T:142:DT:H3'	1.67	0.60
22:1:180:LEU:HD21	22:1:220:PHE:HB3	1.83	0.60
25:2:346:LYS:HZ3	25:2:347:ILE:HB	1.66	0.60
25:2:493:ILE:HG22	25:2:494:SER:H	1.66	0.60
26:5:26:LYS:NZ	26:5:26:LYS:H	1.99	0.60
1:A:116:ASP:OD1	1:A:164:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:131:THR:OG1	14:Q:132:ASP:OD1	2.20	0.59
20:N:23:DA:H2'	20:N:24:DA:C8	2.37	0.59
21:0:83:LEU:HD13	21:0:177:SER:HA	1.84	0.59
21:0:105:GLY:H	21:0:175:VAL:HG12	1.67	0.59
21:0:331:PHE:CZ	21:0:335:LEU:HD21	2.38	0.59
22:1:198:THR:O	22:1:203:GLY:N	2.34	0.59
22:1:540:SER:O	22:1:544:ILE:N	2.33	0.59
25:2:502:LEU:HD22	25:2:506:LYS:HE3	1.84	0.59
28:7:486:ILE:HG23	28:7:511:LEU:HD23	1.84	0.59
2:B:363:HIS:CD2	2:B:364:ILE:H	2.20	0.59
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.32	0.59
11:K:12:LEU:HD13	11:K:18:LYS:HA	1.82	0.59
16:W:12:LEU:HA	16:W:15:PHE:CD2	2.37	0.59
17:X:269:PRO:HG2	17:X:274:LEU:HD13	1.83	0.59
17:X:272:ALA:HA	17:X:275:PRO:HD2	1.84	0.59
21:0:460:SER:H	21:0:463:ILE:HD11	1.67	0.59
21:0:669:VAL:HG13	21:0:670:LEU:HG	1.82	0.59
24:6:373:SER:O	24:6:376:LEU:N	2.34	0.59
28:7:262:VAL:C	28:7:347:HIS:HB3	2.27	0.59
28:7:302:GLU:HG2	28:7:329:ARG:HH22	1.67	0.59
1:A:88:LYS:NZ	1:A:205:GLU:OE1	2.19	0.59
1:A:926:GLN:NE2	1:A:930:ASP:OD1	2.35	0.59
7:G:158:HIS:CD2	16:W:138:GLN:HA	2.37	0.59
23:4:298:ILE:C	23:4:300:PRO:HD3	2.27	0.59
26:5:17:LYS:HZ1	26:5:34:GLU:HB3	1.67	0.59
28:7:330:CYS:O	28:7:334:ASP:N	2.34	0.59
28:7:556:GLU:HB2	28:7:733:PHE:CE1	2.37	0.59
1:A:965:GLN:O	1:A:968:GLN:N	2.35	0.59
1:A:1286:LYS:HB2	1:A:1304:TRP:CZ3	2.37	0.59
2:B:443:ASN:HB3	2:B:446:LEU:HG	1.84	0.59
4:D:211:LEU:HA	4:D:214:LEU:HB3	1.84	0.59
7:G:88:ASP:OD1	7:G:89:GLY:N	2.36	0.59
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.84	0.59
13:M:212:ASN:HD21	18:O:184:SER:HB2	1.67	0.59
21:0:327:ARG:HG2	21:0:330:HIS:H	1.66	0.59
21:0:649:ARG:HG2	21:0:652:ASP:CG	2.27	0.59
21:0:659:MET:HE3	21:0:689:LYS:HB3	1.85	0.59
21:0:675:ASP:OD1	21:0:676:TYR:N	2.33	0.59
22:1:551:ARG:NH1	24:6:336:CYS:H	2.01	0.59
25:2:450:ARG:HD2	25:2:451:VAL:HG13	1.83	0.59
27:3:32:PRO:HA	27:3:35:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:80:LYS:O	27:3:84:ILE:N	2.26	0.59
28:7:413:SER:O	28:7:417:VAL:HG23	2.01	0.59
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.67	0.59
25:2:412:ALA:O	25:2:416:LEU:HB2	2.03	0.59
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.83	0.59
5:E:104:ASN:ND2	5:E:104:ASN:O	2.34	0.59
5:E:124:VAL:O	5:E:126:SER:N	2.36	0.59
15:R:261:VAL:O	15:R:264:SER:OG	2.12	0.59
21:0:327:ARG:HB3	21:0:330:HIS:CD2	2.38	0.59
22:1:515:UNK:O	22:1:517:UNK:N	2.35	0.59
23:4:264:LYS:HE3	25:2:65:TRP:CZ3	2.38	0.59
24:6:150:ILE:HG21	24:6:200:ARG:HB2	1.85	0.59
25:2:356:GLN:HA	25:2:359:VAL:HB	1.84	0.59
27:3:108:LYS:O	27:3:112:GLU:N	2.30	0.59
28:7:378:ARG:O	28:7:380:ARG:NH2	2.30	0.59
28:7:605:ILE:HA	28:7:669:CYS:HB2	1.85	0.59
1:A:225:ASN:OD1	1:A:228:PHE:N	2.29	0.59
4:D:49:ALA:HB1	7:G:1:MET:HE3	1.84	0.59
5:E:39:LEU:O	5:E:42:PHE:HB3	2.03	0.59
13:M:243:CYS:SG	13:M:244:SER:N	2.74	0.59
19:T:151:DC:H2''	19:T:152:DG:C8	2.38	0.59
22:1:188:ASN:ND2	22:1:191:LEU:HG	2.12	0.59
22:1:381:LEU:HD22	22:1:385:MET:HE2	1.85	0.59
28:7:437:VAL:H	28:7:444:GLU:CD	2.11	0.59
1:A:902:LEU:HA	1:A:921:GLY:HA2	1.85	0.59
2:B:816:GLU:OE1	2:B:816:GLU:N	2.36	0.59
13:M:170:SER:O	13:M:174:ALA:N	2.36	0.59
21:0:158:TYR:HB2	21:0:191:CYS:SG	2.42	0.59
21:0:298:ILE:HD11	21:0:379:GLU:HB2	1.84	0.59
21:0:508:SER:H	21:0:685:ARG:NH2	1.97	0.59
22:1:633:TYR:O	22:1:637:TYR:N	2.28	0.59
25:2:222:LEU:HB3	25:2:226:PHE:HE2	1.68	0.59
25:2:480:VAL:HG11	25:2:500:GLN:HG3	1.84	0.59
27:3:34:CYS:HB3	27:3:61:LYS:HD2	1.84	0.59
28:7:255:ARG:C	28:7:316:PHE:HB2	2.27	0.59
28:7:398:THR:O	28:7:402:THR:OG1	2.19	0.59
1:A:101:LYS:HB3	1:A:135:PHE:HZ	1.68	0.59
1:A:118:HIS:C	1:A:123:ARG:HH11	2.10	0.59
5:E:143:ASN:OD1	5:E:146:HIS:ND1	2.31	0.59
13:M:235:ASN:OD1	13:M:235:ASN:N	2.36	0.59
20:N:24:DA:H2'	20:N:25:DA:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:103:PHE:CE2	21:0:204:ASN:HB2	2.38	0.59
21:0:158:TYR:HB3	21:0:190:LEU:HA	1.85	0.59
21:0:212:TYR:HA	21:0:218:ILE:HG13	1.85	0.59
21:0:507:SER:OG	21:0:508:SER:N	2.35	0.59
24:6:195:ALA:O	24:6:198:SER:OG	2.21	0.59
24:6:441:ASP:HA	24:6:444:ILE:HG22	1.85	0.59
25:2:463:GLU:OE1	25:2:508:LYS:NZ	2.36	0.59
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.35	0.59
2:B:568:ASP:N	2:B:568:ASP:OD1	2.33	0.59
8:H:26:ILE:N	8:H:40:LEU:O	2.32	0.59
21:0:29:LYS:HA	21:0:32:LEU:HB2	1.84	0.59
28:7:233:PHE:N	28:7:318:ILE:HG12	2.18	0.59
28:7:410:LEU:HA	28:7:455:SER:O	2.03	0.59
28:7:469:ASP:O	28:7:473:VAL:HG23	2.02	0.59
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.84	0.58
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.83	0.58
13:M:214:LEU:HA	13:M:217:LYS:HB2	1.85	0.58
21:0:77:SER:OG	21:0:81:LYS:NZ	2.36	0.58
21:0:643:ARG:HH11	21:0:650:GLU:HG3	1.68	0.58
25:2:79:LYS:O	25:2:83:SER:N	2.32	0.58
25:2:398:ALA:O	25:2:402:THR:N	2.36	0.58
28:7:471:GLN:HG3	28:7:474:MET:SD	2.43	0.58
1:A:806:ARG:HH21	2:B:729:ILE:HG13	1.68	0.58
1:A:1202:MET:O	1:A:1206:ASP:HA	2.03	0.58
13:M:162:THR:HB	13:M:209:ILE:HG21	1.85	0.58
14:Q:99:ASN:HB3	14:Q:101:PHE:CZ	2.38	0.58
21:0:116:LEU:N	31:0:801:SF4:S3	2.76	0.58
21:0:219:ALA:O	21:0:313:PRO:HB3	2.02	0.58
21:0:541:PHE:HE2	21:0:599:LEU:HB3	1.68	0.58
22:1:260:PHE:HD1	22:1:266:VAL:HG23	1.67	0.58
1:A:414:ASP:OD2	1:A:416:ARG:NH1	2.37	0.58
1:A:853:ASP:OD1	1:A:855:THR:OG1	2.14	0.58
11:K:24:ASP:OD2	11:K:74:ARG:NE	2.33	0.58
21:0:69:ILE:HB	21:0:205:ILE:HG13	1.84	0.58
21:0:557:MET:HB2	21:0:559:ILE:HG22	1.84	0.58
21:0:745:ILE:O	21:0:749:ASN:HB2	2.03	0.58
23:4:36:LEU:O	23:4:40:PHE:N	2.36	0.58
28:7:413:SER:O	28:7:417:VAL:N	2.30	0.58
2:B:97:VAL:HG12	15:R:252:ILE:HG21	1.85	0.58
2:B:878:GLN:O	2:B:882:THR:OG1	2.19	0.58
9:I:21:GLU:OE1	9:I:21:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:103:LEU:N	15:R:92:LEU:HA	2.17	0.58
17:X:170:GLU:N	17:X:179:LYS:O	2.36	0.58
22:1:210:TRP:O	22:1:213:ARG:N	2.36	0.58
25:2:219:VAL:O	25:2:223:HIS:N	2.31	0.58
25:2:461:ASP:OD1	25:2:490:LYS:HE2	2.04	0.58
1:A:275:SER:OG	1:A:276:LEU:N	2.36	0.58
1:A:840:ARG:NH1	1:A:1106:ASN:OD1	2.35	0.58
4:D:209:ARG:HG3	4:D:210:ILE:N	2.18	0.58
13:M:209:ILE:O	13:M:213:ILE:HG13	2.02	0.58
22:1:622:SER:O	22:1:626:ALA:N	2.29	0.58
25:2:184:ILE:O	25:2:389:ASN:ND2	2.37	0.58
28:7:322:SER:O	28:7:329:ARG:NH2	2.35	0.58
13:M:196:ILE:HG22	13:M:198:VAL:HG22	1.85	0.58
14:Q:139:LEU:HA	14:Q:351:VAL:O	2.04	0.58
21:0:117:HIS:N	31:0:801:SF4:S3	2.66	0.58
21:0:217:LYS:HZ2	21:0:217:LYS:H	1.51	0.58
21:0:334:PHE:HA	21:0:337:ARG:HE	1.68	0.58
21:0:517:SER:HA	21:0:520:ARG:NH2	2.19	0.58
21:0:583:LEU:HD21	21:0:610:ILE:HG21	1.84	0.58
21:0:632:SER:OG	21:0:633:ARG:N	2.31	0.58
23:4:30:ILE:HD13	23:4:179:LEU:HD13	1.85	0.58
23:4:162:ARG:NH2	24:6:407:GLN:O	2.37	0.58
24:6:246:ASP:OD1	24:6:247:ILE:N	2.35	0.58
25:2:340:ILE:N	25:2:348:TYR:O	2.37	0.58
28:7:670:LEU:HD21	28:7:690:ILE:HG21	1.85	0.58
1:A:40:THR:N	13:M:90:ASN:OD1	2.35	0.58
2:B:277:LYS:HG3	2:B:338:GLY:HA2	1.85	0.58
2:B:959:ASP:N	2:B:959:ASP:OD1	2.32	0.58
2:B:1013:ASN:CG	2:B:1014:PRO:HD2	2.28	0.58
4:D:189:ASP:OD1	7:G:167:TYR:OH	2.21	0.58
5:E:8:ASN:OD1	5:E:8:ASN:N	2.35	0.58
15:R:94:LYS:N	15:R:107:LEU:O	2.36	0.58
16:W:70:HIS:N	16:W:86:TYR:O	2.37	0.58
21:0:105:GLY:HA2	21:0:203:CYS:HB3	1.84	0.58
21:0:635:LEU:O	21:0:639:LEU:N	2.31	0.58
22:1:189:LYS:O	22:1:193:LYS:N	2.24	0.58
25:2:353:SER:HB2	25:2:356:GLN:HB3	1.84	0.58
2:B:739:THR:O	2:B:740:HIS:ND1	2.36	0.58
4:D:166:LEU:HD21	4:D:210:ILE:HG23	1.86	0.58
18:O:176:ALA:HB2	18:O:193:LEU:HD12	1.86	0.58
20:N:19:DA:H2''	20:N:20:DT:H5'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:394:GLU:OE1	21:0:395:ASP:N	2.32	0.58
22:1:339:LEU:HA	22:1:342:ASN:HD22	1.68	0.58
23:4:271:ASP:HB3	23:4:273:ARG:NH2	2.19	0.58
24:6:119:GLN:OE1	24:6:119:GLN:N	2.36	0.58
28:7:485:ILE:HD13	28:7:507:ALA:HB2	1.86	0.58
5:E:9:ILE:O	5:E:13:TRP:N	2.34	0.58
8:H:13:SER:N	8:H:27:GLU:O	2.36	0.58
9:I:113:ASP:OD1	9:I:115:LYS:N	2.37	0.58
15:R:277:PHE:H	15:R:279:LYS:HG2	1.68	0.58
16:W:171:LYS:HD2	17:X:259:PHE:CZ	2.39	0.58
21:0:421:GLU:OE1	21:0:422:PRO:HD2	2.02	0.58
23:4:192:GLN:OE1	23:4:192:GLN:N	2.37	0.58
24:6:236:PHE:O	24:6:266:LEU:HD23	2.03	0.58
25:2:16:GLU:OE1	25:2:17:ILE:N	2.37	0.58
25:2:474:TYR:O	25:2:478:ILE:HG13	2.03	0.58
26:5:16:ILE:HA	26:5:19:LEU:HD12	1.85	0.58
27:3:44:ASP:O	27:3:48:SER:N	2.35	0.58
28:7:441:ASP:OD1	28:7:442:ASN:N	2.36	0.58
28:7:470:SER:HG	28:7:471:GLN:HE21	1.40	0.58
2:B:451:LYS:HG3	13:M:138:ASP:HB3	1.85	0.58
4:D:193:THR:HB	7:G:167:TYR:HE2	1.67	0.58
7:G:14:HIS:HD1	7:G:16:SER:H	1.50	0.58
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.68	0.58
13:M:23:THR:HG23	13:M:32:PRO:HB3	1.86	0.58
21:0:198:ARG:O	21:0:201:SER:OG	2.22	0.58
21:0:258:ARG:HB3	21:0:262:ARG:HH22	1.69	0.58
25:2:175:GLU:CA	25:2:183:LYS:H	2.16	0.58
25:2:373:MET:SD	25:2:374:VAL:N	2.76	0.58
25:2:474:TYR:C	25:2:477:ASP:H	2.11	0.58
28:7:126:ASP:N	28:7:201:SER:O	2.37	0.58
28:7:302:GLU:N	28:7:322:SER:O	2.37	0.58
28:7:541:MET:HE3	28:7:542:GLU:OE2	2.03	0.58
28:7:584:ASN:HB3	28:7:587:LYS:HE3	1.85	0.58
1:A:186:LYS:NZ	1:A:187:LYS:O	2.37	0.57
20:N:13:DG:H2''	20:N:14:DC:H5	1.69	0.57
25:2:468:TYR:HA	25:2:472:SER:HB3	1.84	0.57
25:2:501:VAL:N	25:2:503:ASP:OD1	2.36	0.57
27:3:128:LYS:O	27:3:132:LYS:N	2.31	0.57
28:7:332:GLU:HG3	28:7:333:ILE:HG12	1.86	0.57
1:A:1209:MET:HE1	1:A:1236:LEU:HD22	1.86	0.57
4:D:190:GLU:O	4:D:194:LEU:N	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:LEU:HB3	7:G:86:VAL:HG21	1.84	0.57
7:G:165:GLU:H	7:G:168:LEU:HD12	1.68	0.57
14:Q:132:ASP:OD1	14:Q:132:ASP:N	2.38	0.57
19:T:108:DC:H42	20:N:58:DG:H22	1.51	0.57
21:0:210:TYR:OH	21:0:235:ASP:O	2.17	0.57
21:0:215:ASP:OD1	21:0:217:LYS:NZ	2.27	0.57
23:4:63:ALA:O	23:4:67:PHE:N	2.36	0.57
24:6:349:CYS:HB3	24:6:353:HIS:H	1.69	0.57
21:0:1:MET:HB2	21:0:12:PHE:HB3	1.86	0.57
21:0:16:LYS:HA	21:0:741:TYR:CD1	2.39	0.57
21:0:719:GLN:OE1	21:0:722:ARG:NH2	2.33	0.57
22:1:300:UNK:O	22:1:302:UNK:N	2.37	0.57
28:7:373:MET:HB2	28:7:380:ARG:O	2.04	0.57
28:7:670:LEU:O	28:7:706:TYR:N	2.37	0.57
1:A:309:ALA:HA	13:M:101:THR:HG21	1.85	0.57
2:B:72:GLU:CD	2:B:87:LYS:HB2	2.30	0.57
4:D:160:VAL:HA	4:D:163:VAL:HB	1.87	0.57
14:Q:101:PHE:HB3	14:Q:383:SER:HA	1.86	0.57
17:X:261:LYS:O	17:X:265:ASN:N	2.35	0.57
21:0:4:TYR:O	21:0:22:TYR:OH	2.23	0.57
21:0:71:TYR:O	21:0:207:ILE:HA	2.04	0.57
21:0:270:ARG:HE	21:0:388:LEU:HB3	1.68	0.57
21:0:610:ILE:HG23	22:1:337:ILE:HD12	1.85	0.57
28:7:355:ASP:HA	28:7:404:LYS:HD2	1.85	0.57
28:7:406:SER:O	28:7:483:GLY:N	2.37	0.57
28:7:409:VAL:H	28:7:454:VAL:HA	1.70	0.57
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.36	0.57
2:B:957:ASN:ND2	2:B:961:LEU:HB2	2.17	0.57
4:D:71:LYS:O	4:D:75:LYS:HG3	2.04	0.57
14:Q:384:PHE:HE2	15:R:95:ILE:HD11	1.69	0.57
14:Q:405:THR:O	14:Q:409:ALA:N	2.30	0.57
19:T:131:DC:H2"	19:T:132:DA:H8	1.69	0.57
21:0:39:ILE:HG22	21:0:458:ILE:HB	1.87	0.57
21:0:537:MET:N	21:0:586:TYR:OH	2.36	0.57
23:4:137:LYS:HG2	23:4:140:ILE:HG13	1.86	0.57
25:2:54:GLU:CD	25:2:109:ARG:HH22	2.13	0.57
25:2:480:VAL:O	25:2:493:ILE:HG23	2.05	0.57
27:3:9:ASN:HD22	27:3:9:ASN:N	2.02	0.57
28:7:412:THR:HG1	28:7:413:SER:N	2.02	0.57
28:7:475:ASP:OD1	28:7:475:ASP:N	2.35	0.57
28:7:672:GLN:OE1	28:7:673:ILE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:CD	2:B:1108:ARG:HH22	2.13	0.57
1:A:968:GLN:HA	1:A:973:ILE:HG12	1.86	0.57
4:D:119:ARG:HE	4:D:155:ARG:HH22	1.53	0.57
15:R:207:THR:OG1	15:R:207:THR:O	2.15	0.57
19:T:143:DT:H2"	19:T:144:DA:C8	2.40	0.57
21:0:340:GLU:HB3	27:3:73:PHE:HB3	1.86	0.57
24:6:439:ASP:O	24:6:443:PHE:N	2.37	0.57
28:7:354:ILE:HG13	28:7:405:LYS:O	2.04	0.57
28:7:501:VAL:HA	28:7:504:THR:HB	1.86	0.57
1:A:226:GLU:OE1	1:A:226:GLU:N	2.29	0.57
1:A:463:ILE:HD12	1:A:464:PRO:O	2.05	0.57
1:A:1166:ASP:HB3	1:A:1239:ARG:HH21	1.68	0.57
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.36	0.57
13:M:160:GLU:HB2	13:M:163:LEU:HG	1.86	0.57
14:Q:141:ARG:HA	14:Q:349:PRO:O	2.04	0.57
21:0:142:LYS:O	21:0:146:GLU:N	2.34	0.57
22:1:384:LYS:O	22:1:388:UNK:N	2.37	0.57
22:1:504:ILE:O	22:1:508:LYS:N	2.35	0.57
23:4:126:VAL:HA	23:4:129:ILE:HD13	1.86	0.57
25:2:140:ALA:O	25:2:144:GLU:N	2.38	0.57
25:2:353:SER:O	25:2:355:LEU:N	2.38	0.57
28:7:249:SER:C	28:7:254:LEU:H	2.12	0.57
28:7:490:VAL:N	28:7:514:THR:HG22	2.18	0.57
9:I:17:ARG:HH22	9:I:30:ARG:CZ	2.18	0.57
14:Q:30:ASN:O	14:Q:34:MET:N	2.38	0.57
21:0:190:LEU:HG	21:0:195:ILE:HD11	1.87	0.57
21:0:498:THR:HG23	21:0:684:ARG:HA	1.87	0.57
21:0:546:TYR:O	21:0:549:SER:OG	2.14	0.57
24:6:116:THR:OG1	24:6:119:GLN:N	2.26	0.57
25:2:381:GLU:HA	25:2:384:ARG:HE	1.69	0.57
26:5:28:SER:OG	26:5:29:ASP:N	2.35	0.57
28:7:138:ASP:O	28:7:175:ILE:N	2.38	0.57
1:A:55:ASP:CG	1:A:57:ARG:H	2.13	0.57
1:A:603:ASN:OD1	1:A:603:ASN:N	2.30	0.57
21:0:37:ASN:HD22	21:0:475:PHE:HD2	1.53	0.57
21:0:309:THR:O	21:0:309:THR:OG1	2.22	0.57
21:0:602:ALA:O	21:0:607:SER:OG	2.15	0.57
24:6:324:PHE:N	24:6:350:PRO:HG3	2.20	0.57
25:2:55:ASN:N	25:2:55:ASN:OD1	2.37	0.57
26:5:8:ALA:O	26:5:42:VAL:N	2.37	0.57
26:5:36:ASP:CG	26:5:39:HIS:HD1	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:117:ILE:O	27:3:121:ASP:N	2.29	0.57
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.36	0.57
7:G:46:LEU:HB2	7:G:77:VAL:HG22	1.86	0.57
7:G:55:ASP:HB3	7:G:73:LYS:HG3	1.87	0.57
13:M:241:ARG:O	13:M:245:HIS:ND1	2.38	0.57
14:Q:99:ASN:HB3	14:Q:101:PHE:CE2	2.40	0.57
15:R:62:GLU:OE1	15:R:63:ARG:N	2.38	0.57
22:1:192:MET:O	22:1:196:GLN:N	2.36	0.57
23:4:162:ARG:HD2	24:6:407:GLN:H	1.70	0.57
25:2:348:TYR:O	25:2:407:GLN:NE2	2.38	0.57
3:C:22:LEU:HD11	11:K:101:LEU:HD11	1.87	0.56
21:0:490:LYS:NZ	21:0:493:LEU:HA	2.20	0.56
21:0:499:LYS:O	21:0:709:SER:HA	2.05	0.56
22:1:226:GLN:OE1	24:6:179:ALA:N	2.25	0.56
25:2:465:SER:O	25:2:465:SER:OG	2.23	0.56
26:5:11:GLN:HA	26:5:38:THR:O	2.05	0.56
1:A:313:GLN:HB3	1:A:315:LEU:HD21	1.86	0.56
1:A:1325:THR:OG1	1:A:1326:ARG:N	2.33	0.56
18:O:94:TYR:HB2	18:O:102:VAL:HA	1.87	0.56
18:O:205:LEU:HB2	18:O:213:VAL:HB	1.86	0.56
21:0:295:SER:HA	21:0:298:ILE:HG22	1.86	0.56
21:0:326:ARG:C	21:0:380:ARG:HH21	2.13	0.56
24:6:176:ASN:N	24:6:205:LYS:O	2.36	0.56
25:2:240:ASP:O	25:2:242:LEU:N	2.39	0.56
1:A:556:TRP:O	11:K:26:LYS:NZ	2.37	0.56
1:A:1169:ILE:HA	1:A:1172:LEU:HB2	1.86	0.56
7:G:116:PRO:HD3	7:G:164:LYS:HA	1.86	0.56
7:G:125:SER:OG	7:G:129:SER:O	2.18	0.56
14:Q:108:LYS:O	14:Q:112:GLU:N	2.36	0.56
16:W:25:PHE:HA	16:W:57:LEU:HD21	1.87	0.56
16:W:173:ASN:O	16:W:177:ASP:N	2.37	0.56
20:N:22:DT:H2'	20:N:23:DA:C8	2.40	0.56
21:0:71:TYR:OH	21:0:235:ASP:OD2	2.22	0.56
21:0:328:ALA:O	21:0:332:VAL:N	2.24	0.56
22:1:380:ARG:HA	22:1:383:GLU:CD	2.31	0.56
24:6:179:ALA:HB2	24:6:212:ASN:HB3	1.86	0.56
24:6:372:LEU:H	24:6:375:HIS:CE1	2.24	0.56
27:3:46:ILE:HG13	27:3:55:PRO:HG3	1.87	0.56
28:7:331:GLN:HG3	28:7:529:PHE:CD2	2.40	0.56
28:7:565:PHE:HE2	28:7:763:VAL:HG21	1.70	0.56
28:7:682:GLN:HA	28:7:685:GLN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:PHE:CE1	1:A:1227:ILE:HG12	2.39	0.56
2:B:27:ALA:N	2:B:708:GLU:OE1	2.29	0.56
2:B:272:THR:O	2:B:272:THR:OG1	2.15	0.56
5:E:74:ASP:O	5:E:106:GLN:NE2	2.38	0.56
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.05	0.56
14:Q:103:LEU:O	15:R:92:LEU:HD23	2.05	0.56
16:W:140:LEU:HD13	16:W:147:PHE:CD1	2.40	0.56
21:0:163:TYR:HA	21:0:167:VAL:HG23	1.87	0.56
28:7:406:SER:HB2	28:7:482:TRP:CE3	2.41	0.56
28:7:671:ILE:HG12	28:7:706:TYR:HB2	1.87	0.56
1:A:109:HIS:HB2	1:A:167:CYS:SG	2.45	0.56
1:A:175:ARG:NH1	1:A:182:VAL:O	2.37	0.56
1:A:1328:TYR:OH	1:A:1351:GLU:OE1	2.18	0.56
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.40	0.56
7:G:151:ILE:HG12	16:W:134:LEU:HD13	1.88	0.56
17:X:170:GLU:H	17:X:179:LYS:H	1.53	0.56
19:T:123:DT:H2"	19:T:124:DA:N7	2.20	0.56
21:0:127:THR:O	21:0:131:GLU:N	2.38	0.56
21:0:346:MET:HB3	21:0:347:LYS:HZ2	1.70	0.56
21:0:362:HIS:HA	21:0:365:GLN:CD	2.31	0.56
21:0:374:LEU:HG	21:0:410:SER:HB2	1.87	0.56
24:6:349:CYS:HB3	24:6:353:HIS:N	2.20	0.56
25:2:147:LEU:O	25:2:151:VAL:N	2.30	0.56
2:B:444:MET:O	2:B:447:ALA:N	2.38	0.56
15:R:69:TRP:CE2	15:R:220:HIS:HB3	2.40	0.56
21:0:422:PRO:HG2	21:0:423:TYR:CZ	2.40	0.56
25:2:19:GLN:O	25:2:23:ASN:N	2.30	0.56
25:2:458:LEU:N	26:5:5:ARG:O	2.39	0.56
25:2:462:PHE:H	25:2:489:LYS:C	2.14	0.56
25:2:483:TRP:NE1	25:2:485:ASP:HB2	2.21	0.56
27:3:134:ARG:O	27:3:138:GLU:N	2.31	0.56
28:7:226:VAL:N	28:7:235:GLU:O	2.39	0.56
28:7:355:ASP:OD1	28:7:356:LEU:N	2.38	0.56
28:7:462:ASN:ND2	28:7:464:ARG:HD3	2.20	0.56
1:A:1168:GLU:O	1:A:1171:GLN:NE2	2.39	0.56
1:A:1205:LYS:O	1:A:1274:ARG:NH2	2.38	0.56
21:0:436:ARG:NH1	22:1:351:GLY:O	2.38	0.56
21:0:651:ASN:O	21:0:655:SER:OG	2.22	0.56
21:0:709:SER:HB3	21:0:712:MET:HE3	1.87	0.56
22:1:196:GLN:NE2	22:1:197:GLU:OE2	2.38	0.56
23:4:138:LYS:HA	23:4:141:GLU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:265:GLY:HA3	24:6:290:ILE:HG22	1.87	0.56
25:2:350:TYR:H	25:2:407:GLN:CD	2.14	0.56
25:2:465:SER:OG	25:2:469:ASN:OD1	2.17	0.56
27:3:136:TYR:O	27:3:140:ASN:N	2.30	0.56
28:7:324:GLU:C	28:7:328:LYS:HZ2	2.11	0.56
28:7:326:VAL:O	28:7:329:ARG:N	2.39	0.56
28:7:573:THR:HG23	28:7:576:LYS:HZ1	1.70	0.56
2:B:391:ASP:N	2:B:391:ASP:OD1	2.39	0.56
3:C:75:MET:O	3:C:246:ARG:NH2	2.29	0.56
4:D:119:ARG:HG2	4:D:155:ARG:HH12	1.71	0.56
4:D:214:LEU:O	4:D:218:GLU:N	2.39	0.56
16:W:165:ASN:OD1	16:W:169:GLN:NE2	2.39	0.56
17:X:189:PRO:HA	17:X:192:LEU:HB3	1.88	0.56
21:0:325:ILE:HG12	21:0:331:PHE:HA	1.86	0.56
25:2:273:LYS:O	25:2:277:MET:HG2	2.06	0.56
28:7:431:GLN:NE2	28:7:431:GLN:O	2.39	0.56
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.88	0.56
5:E:31:THR:OG1	5:E:34:GLU:OE1	2.20	0.56
7:G:137:ILE:HG12	7:G:170:ALA:HB2	1.87	0.56
16:W:141:ASN:CG	16:W:144:ARG:HB2	2.31	0.56
19:T:129:DT:H2"	19:T:130:DA:C8	2.41	0.56
23:4:203:ALA:O	23:4:207:LYS:N	2.39	0.56
28:7:558:TRP:HE1	28:7:735:VAL:HB	1.71	0.56
28:7:753:PRO:HB2	28:7:757:ARG:NH1	2.21	0.56
2:B:233:PRO:O	2:B:260:GLY:N	2.38	0.56
13:M:133:ILE:HA	13:M:136:LEU:HD12	1.88	0.56
21:0:649:ARG:HB2	21:0:651:ASN:OD1	2.05	0.56
21:0:683:ASP:OD1	21:0:686:PHE:N	2.39	0.56
25:2:346:LYS:HD2	25:2:376:GLY:O	2.06	0.56
28:7:421:ARG:O	28:7:426:GLN:NE2	2.35	0.56
1:A:113:LEU:HD23	1:A:114:LEU:N	2.21	0.55
1:A:1446:ASP:OD1	1:A:1447:GLU:N	2.40	0.55
2:B:918:ILE:HD12	2:B:928:ARG:CZ	2.37	0.55
13:M:166:LYS:O	13:M:167:SER:OG	2.23	0.55
13:M:259:THR:OG1	13:M:281:SER:OG	2.24	0.55
28:7:618:TYR:O	28:7:622:MET:N	2.40	0.55
1:A:61:ILE:HG22	1:A:62:ASP:H	1.71	0.55
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.36	0.55
1:A:840:ARG:NH1	1:A:1384:VAL:O	2.39	0.55
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.06	0.55
2:B:920:PRO:HB3	2:B:932:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:922:GLU:HB3	2:B:928:ARG:HH12	1.71	0.55
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.55
21:0:370:GLU:O	21:0:373:PRO:HD2	2.06	0.55
22:1:498:UNK:O	22:1:502:ARG:N	2.24	0.55
25:2:207:TYR:O	25:2:211:ILE:N	2.39	0.55
25:2:498:ASN:O	25:2:500:GLN:N	2.39	0.55
28:7:372:LYS:HE3	28:7:536:TYR:HB2	1.86	0.55
28:7:460:VAL:HG13	28:7:474:MET:HE2	1.88	0.55
1:A:115:LEU:HG	1:A:122:MET:HE3	1.87	0.55
1:A:271:LYS:NZ	13:M:92:LEU:O	2.40	0.55
1:A:1005:GLU:OE1	1:A:1009:ASN:ND2	2.39	0.55
13:M:30:TYR:HB3	13:M:32:PRO:HA	1.89	0.55
16:W:5:ILE:HD11	16:W:189:ILE:HG23	1.88	0.55
22:1:192:MET:O	22:1:196:GLN:HG3	2.06	0.55
22:1:284:TRP:HA	22:1:287:PHE:HD1	1.72	0.55
24:6:266:LEU:O	24:6:268:ALA:N	2.39	0.55
25:2:60:LEU:O	25:2:64:LYS:N	2.33	0.55
1:A:1159:ARG:O	1:A:1170:ILE:HG21	2.06	0.55
2:B:486:TYR:HA	2:B:1096:ARG:HH22	1.71	0.55
21:0:69:ILE:HG23	21:0:231:ILE:HG13	1.88	0.55
21:0:193:TYR:OH	21:0:197:ARG:NH2	2.40	0.55
21:0:318:THR:OG1	21:0:319:GLU:N	2.37	0.55
21:0:356:PRO:HG3	21:0:413:GLU:HA	1.89	0.55
22:1:466:UNK:O	22:1:468:UNK:N	2.40	0.55
23:4:305:CYS:O	23:4:307:ALA:N	2.39	0.55
28:7:759:LEU:O	28:7:763:VAL:N	2.32	0.55
1:A:55:ASP:OD1	1:A:57:ARG:N	2.40	0.55
1:A:70:CYS:SG	1:A:80:HIS:HE1	2.00	0.55
1:A:312:PRO:HA	13:M:99:GLY:H	1.71	0.55
1:A:1433:MET:HE2	1:A:1439:GLY:HA2	1.89	0.55
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.87	0.55
2:B:1166:CYS:O	2:B:1168:LEU:N	2.39	0.55
18:O:76:LEU:HD22	18:O:150:ALA:HB1	1.87	0.55
21:0:610:ILE:HD12	22:1:337:ILE:HG23	1.87	0.55
22:1:291:LYS:O	22:1:295:LYS:N	2.39	0.55
24:6:211:GLN:HE22	24:6:250:THR:HG21	1.70	0.55
25:2:62:LEU:HA	25:2:65:TRP:CD1	2.37	0.55
25:2:74:PHE:HB3	25:2:75:GLN:HE21	1.72	0.55
26:5:46:LYS:O	26:5:50:VAL:N	2.32	0.55
28:7:368:LYS:H	28:7:368:LYS:HD2	1.70	0.55
28:7:436:ALA:HA	28:7:444:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:528:ASN:O	28:7:532:GLY:N	2.40	0.55
28:7:616:GLN:HE22	28:7:626:PHE:HD1	1.54	0.55
4:D:33:PHE:CE2	7:G:80:LYS:HG2	2.39	0.55
4:D:208:GLU:O	4:D:212:LYS:N	2.29	0.55
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.89	0.55
16:W:12:LEU:HD22	16:W:185:SER:HB2	1.88	0.55
17:X:216:GLN:HG3	17:X:219:GLU:HB3	1.88	0.55
17:X:262:MET:SD	17:X:265:ASN:ND2	2.80	0.55
21:0:301:ASP:HB2	21:0:305:PRO:HG3	1.89	0.55
21:0:498:THR:HB	21:0:707:ASN:HA	1.87	0.55
22:1:210:TRP:CE3	22:1:210:TRP:HA	2.41	0.55
23:4:52:LYS:NZ	23:4:242:GLU:O	2.34	0.55
23:4:79:TYR:CD2	23:4:132:LEU:HD11	2.41	0.55
24:6:257:GLU:HB2	24:6:259:ILE:HG12	1.88	0.55
24:6:379:SER:O	24:6:381:HIS:N	2.39	0.55
25:2:504:PHE:HD1	25:2:507:ARG:HB2	1.72	0.55
28:7:437:VAL:HG12	28:7:454:VAL:HG13	1.87	0.55
28:7:540:TRP:HB3	28:7:731:TYR:CZ	2.41	0.55
28:7:596:GLN:NE2	28:7:747:ASN:OD1	2.39	0.55
7:G:132:SER:OG	7:G:135:ASP:O	2.17	0.55
17:X:271:PHE:O	17:X:273:GLU:N	2.40	0.55
21:0:2:LYS:HD2	21:0:97:LEU:HD11	1.88	0.55
21:0:686:PHE:HA	21:0:689:LYS:HB2	1.88	0.55
22:1:178:LEU:HD12	22:1:182:GLN:HE22	1.71	0.55
22:1:192:MET:HA	22:1:195:PHE:HB3	1.87	0.55
25:2:226:PHE:O	25:2:230:ALA:N	2.39	0.55
1:A:795:GLU:OE1	1:A:795:GLU:N	2.32	0.55
2:B:396:ASP:OD1	2:B:397:ASP:N	2.40	0.55
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.20	0.55
8:H:14:GLU:OE1	8:H:15:VAL:N	2.40	0.55
13:M:215:ARG:NE	18:O:180:GLY:HA3	2.12	0.55
13:M:250:MET:O	13:M:254:THR:N	2.34	0.55
14:Q:101:PHE:CZ	14:Q:382:GLY:HA3	2.41	0.55
15:R:258:THR:HG23	15:R:261:VAL:HG22	1.87	0.55
16:W:143:ASP:OD1	16:W:143:ASP:N	2.32	0.55
21:0:355:THR:HA	21:0:417:LEU:HG	1.89	0.55
21:0:462:THR:O	21:0:462:THR:OG1	2.25	0.55
21:0:521:ASN:O	21:0:524:SER:OG	2.21	0.55
21:0:683:ASP:HB3	21:0:686:PHE:CE2	2.42	0.55
25:2:218:LEU:HA	25:2:221:VAL:HB	1.88	0.55
28:7:136:PRO:O	28:7:139:GLY:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:554:CYS:HB2	28:7:733:PHE:HA	1.89	0.55
1:A:1134:ILE:O	1:A:1137:ALA:N	2.40	0.55
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.72	0.55
1:A:1199:ARG:NH2	1:A:1231:ASP:O	2.40	0.55
15:R:299:ILE:O	15:R:303:LEU:N	2.35	0.55
16:W:12:LEU:HD11	16:W:182:ILE:HG23	1.89	0.55
17:X:257:GLU:O	17:X:261:LYS:N	2.27	0.55
21:0:156:CYS:SG	21:0:191:CYS:SG	3.05	0.55
22:1:465:UNK:O	22:1:470:UNK:N	2.40	0.55
24:6:116:THR:HG1	24:6:119:GLN:H	1.51	0.55
24:6:126:LEU:HD11	24:6:233:LEU:HB3	1.89	0.55
25:2:380:ARG:NH1	25:2:440:GLN:O	2.40	0.55
26:5:19:LEU:O	26:5:23:ILE:HG13	2.07	0.55
28:7:431:GLN:NE2	28:7:434:ASN:H	2.05	0.55
28:7:494:PRO:HD2	28:7:497:MET:HG2	1.89	0.55
2:B:41:LYS:O	2:B:45:SER:HB3	2.06	0.55
18:O:188:GLU:O	18:O:189:LEU:HD13	2.07	0.55
21:0:493:LEU:O	21:0:679:MET:N	2.36	0.55
21:0:544:TYR:OH	21:0:574:PRO:HD3	2.07	0.55
21:0:647:ARG:C	21:0:649:ARG:HH21	2.15	0.55
22:1:475:UNK:O	22:1:479:UNK:N	2.40	0.55
23:4:192:GLN:O	23:4:195:PRO:HD2	2.07	0.55
25:2:96:LEU:HB3	25:2:98:ILE:HD11	1.88	0.55
28:7:340:GLU:HG3	28:7:379:ALA:O	2.07	0.55
28:7:593:PHE:HD1	28:7:745:ILE:HD11	1.71	0.55
2:B:831:SER:O	2:B:831:SER:OG	2.25	0.54
17:X:216:GLN:OE1	17:X:219:GLU:N	2.39	0.54
21:0:70:ILE:HG13	21:0:206:ILE:HD11	1.89	0.54
21:0:107:GLY:HA3	21:0:207:ILE:HG12	1.88	0.54
21:0:364:LYS:HG3	21:0:368:PHE:HA	1.88	0.54
25:2:496:GLU:OE1	25:2:496:GLU:N	2.39	0.54
1:A:1209:MET:HB2	1:A:1228:TRP:CD1	2.41	0.54
2:B:358:LYS:O	2:B:366:GLN:NE2	2.26	0.54
2:B:868:MET:HG3	13:M:182:ARG:O	2.07	0.54
4:D:189:ASP:HA	4:D:192:LYS:HE3	1.90	0.54
17:X:199:GLN:HA	17:X:202:PHE:HD2	1.71	0.54
18:O:202:ILE:HD12	18:O:223:ILE:HD13	1.89	0.54
21:0:666:LEU:HB3	21:0:679:MET:HE3	1.89	0.54
22:1:221:ALA:O	22:1:225:SER:OG	2.16	0.54
22:1:340:ASP:HA	22:1:343:ILE:HG12	1.88	0.54
22:1:550:CYS:HA	22:1:553:LEU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ASP:OD1	1:A:1296:GLY:HA3	2.06	0.54
13:M:109:GLU:O	13:M:113:ALA:N	2.39	0.54
15:R:126:LYS:O	15:R:220:HIS:ND1	2.40	0.54
18:O:169:PRO:O	18:O:239:LYS:N	2.41	0.54
21:0:377:CYS:SG	21:0:378:SER:N	2.80	0.54
21:0:477:THR:OG1	21:0:480:GLN:OE1	2.16	0.54
22:1:275:PRO:HG2	22:1:276:LYS:HD2	1.89	0.54
23:4:114:UNK:C	23:4:116:ARG:H	2.21	0.54
24:6:186:SER:HB2	24:6:192:HIS:HE1	1.72	0.54
28:7:410:LEU:HD23	28:7:457:TYR:N	2.22	0.54
2:B:705:MET:H	2:B:710:LEU:CD1	2.20	0.54
2:B:861:ASP:OD1	2:B:862:GLN:N	2.37	0.54
2:B:896:ASP:N	2:B:896:ASP:OD1	2.33	0.54
13:M:152:GLU:O	13:M:155:LYS:N	2.41	0.54
13:M:194:SER:HB3	15:R:270:MET:HA	1.89	0.54
15:R:96:ARG:N	15:R:106:LEU:HA	2.09	0.54
16:W:171:LYS:O	16:W:175:LEU:N	2.30	0.54
18:O:143:ILE:HA	18:O:146:ILE:HD12	1.89	0.54
19:T:145:DT:H2''	19:T:146:DA:O4'	2.08	0.54
21:0:105:GLY:HA3	21:0:205:ILE:HG22	1.89	0.54
21:0:195:ILE:O	21:0:199:MET:HB2	2.07	0.54
22:1:184:LEU:C	22:1:187:GLY:H	2.16	0.54
23:4:27:THR:O	23:4:27:THR:OG1	2.21	0.54
23:4:162:ARG:HB2	24:6:406:CYS:HB2	1.89	0.54
23:4:287:PHE:HB3	24:6:319:LEU:HD21	1.89	0.54
25:2:17:ILE:HG13	25:2:21:VAL:HG21	1.88	0.54
28:7:558:TRP:HB3	28:7:711:LYS:HE2	1.89	0.54
28:7:561:MET:HE1	28:7:584:ASN:HA	1.89	0.54
28:7:578:MET:HE3	28:7:579:LEU:HA	1.90	0.54
13:M:305:THR:HG22	13:M:307:GLY:N	2.23	0.54
13:M:305:THR:OG1	19:T:151:DC:OP1	2.20	0.54
14:Q:100:GLU:HA	15:R:95:ILE:N	2.21	0.54
14:Q:380:ASP:OD1	14:Q:380:ASP:N	2.40	0.54
21:0:239:ASN:HA	21:0:660:ARG:NH1	2.23	0.54
23:4:24:SER:OG	23:4:25:LEU:N	2.40	0.54
25:2:454:TYR:CE1	25:2:482:LEU:HB3	2.42	0.54
28:7:269:LEU:HD12	28:7:348:ARG:HD2	1.88	0.54
28:7:495:ALA:HA	28:7:498:PHE:CD1	2.38	0.54
1:A:226:GLU:HA	1:A:230:ARG:HD3	1.89	0.54
1:A:386:ASP:OD1	1:A:387:ARG:N	2.40	0.54
1:A:982:THR:OG1	1:A:985:ASP:OD1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:HG	2:B:236:HIS:CE1	2.26	0.54
2:B:328:GLU:N	2:B:328:GLU:OE1	2.40	0.54
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.07	0.54
8:H:108:SER:OG	8:H:109:LYS:N	2.40	0.54
21:0:12:PHE:HE1	21:0:14:TYR:HB3	1.73	0.54
22:1:188:ASN:OD1	22:1:189:LYS:N	2.40	0.54
25:2:47:ILE:O	25:2:51:VAL:HG23	2.08	0.54
25:2:84:LEU:HD11	25:2:86:LEU:HD23	1.89	0.54
25:2:176:VAL:O	25:2:180:GLY:N	2.40	0.54
28:7:303:ARG:HA	28:7:321:GLU:N	2.22	0.54
28:7:376:ASN:H	28:7:380:ARG:NH1	2.05	0.54
28:7:766:LYS:HA	28:7:769:GLU:CD	2.32	0.54
1:A:318:SER:C	13:M:95:ARG:HH21	2.16	0.54
1:A:645:LEU:O	1:A:649:ILE:HG12	2.06	0.54
1:A:1009:ASN:O	1:A:1012:ARG:HB2	2.07	0.54
2:B:39:ARG:HD2	2:B:665:GLU:OE1	2.08	0.54
2:B:278:GLN:N	2:B:278:GLN:OE1	2.40	0.54
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.89	0.54
11:K:36:GLU:OE2	11:K:70:ARG:NH1	2.36	0.54
21:0:689:LYS:HA	21:0:692:GLN:HE22	1.73	0.54
23:4:192:GLN:C	23:4:195:PRO:HD2	2.32	0.54
23:4:249:ALA:O	23:4:253:PHE:HB2	2.08	0.54
26:5:46:LYS:C	26:5:49:PHE:HB3	2.33	0.54
28:7:329:ARG:O	28:7:333:ILE:N	2.37	0.54
28:7:331:GLN:OE1	28:7:332:GLU:N	2.40	0.54
28:7:360:THR:OG1	28:7:361:GLN:N	2.40	0.54
28:7:754:ARG:HD2	28:7:757:ARG:HB2	1.89	0.54
1:A:464:PRO:HA	11:K:2:ASN:HB2	1.90	0.54
5:E:91:LYS:O	5:E:95:THR:HG23	2.07	0.54
7:G:125:SER:OG	7:G:129:SER:N	2.38	0.54
12:L:51:CYS:O	12:L:53:HIS:N	2.37	0.54
16:W:124:CYS:HB3	16:W:127:CYS:SG	2.47	0.54
18:O:106:ILE:HD11	18:O:135:ALA:HB1	1.90	0.54
18:O:116:PHE:CD2	20:N:26:DA:H5'	2.43	0.54
21:0:424:GLU:OE1	21:0:432:ASN:ND2	2.39	0.54
23:4:158:THR:OG1	23:4:159:TYR:N	2.40	0.54
24:6:160:PHE:O	24:6:164:ASN:ND2	2.32	0.54
24:6:440:CYS:O	24:6:444:ILE:N	2.30	0.54
28:7:309:ASP:CG	28:7:337:VAL:HB	2.33	0.54
1:A:217:LYS:O	1:A:221:SER:OG	2.25	0.54
1:A:1341:ILE:HD13	1:A:1380:GLY:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:179:ILE:HA	16:W:183:ILE:HG12	1.90	0.54
19:T:137:DA:H2''	19:T:138:DA:C8	2.43	0.54
21:0:71:TYR:HA	21:0:233:ILE:HB	1.89	0.54
21:0:537:MET:HE3	21:0:597:ILE:HD11	1.90	0.54
23:4:118:PHE:H	23:4:118:PHE:HD1	1.56	0.54
25:2:439:ASP:O	25:2:443:LEU:N	2.26	0.54
26:5:7:GLY:HA3	26:5:41:LEU:HD21	1.88	0.54
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.89	0.54
2:B:644:GLU:HB2	2:B:648:HIS:O	2.07	0.54
7:G:34:VAL:O	7:G:37:SER:OG	2.24	0.54
8:H:104:PHE:HZ	8:H:137:GLN:H	1.56	0.54
12:L:47:ARG:HH22	12:L:49:LYS:HA	1.73	0.54
21:0:223:SER:HB2	21:0:226:VAL:HG13	1.88	0.54
21:0:432:ASN:N	21:0:432:ASN:OD1	2.38	0.54
21:0:587:ARG:O	21:0:591:SER:OG	2.24	0.54
24:6:188:ASN:HD21	24:6:190:GLN:HB3	1.73	0.54
26:5:21:LEU:O	26:5:25:ALA:N	2.41	0.54
28:7:366:GLN:O	28:7:369:SER:OG	2.22	0.54
28:7:468:HIS:HA	28:7:471:GLN:NE2	2.22	0.54
28:7:753:PRO:HB2	28:7:757:ARG:HH12	1.73	0.54
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.08	0.53
2:B:283:VAL:O	2:B:287:ARG:HG3	2.08	0.53
21:0:236:GLU:HA	21:0:460:SER:HA	1.90	0.53
22:1:255:LYS:O	22:1:259:ILE:N	2.40	0.53
22:1:376:LYS:HB3	22:1:380:ARG:HH12	1.73	0.53
22:1:547:LEU:HA	22:1:550:CYS:SG	2.48	0.53
23:4:61:LEU:H	23:4:61:LEU:HD22	1.74	0.53
25:2:43:ALA:O	25:2:47:ILE:HG12	2.08	0.53
25:2:81:MET:HB2	25:2:86:LEU:HD11	1.90	0.53
25:2:99:ASN:N	25:2:99:ASN:OD1	2.40	0.53
1:A:394:ASN:HB3	1:A:398:GLU:CG	2.38	0.53
1:A:1452:LYS:HB3	1:A:1452:LYS:HZ3	1.74	0.53
4:D:39:ASN:HD21	4:D:41:GLN:HB2	1.72	0.53
4:D:187:THR:OG1	4:D:190:GLU:N	2.41	0.53
8:H:132:LEU:O	8:H:134:ASN:N	2.41	0.53
16:W:164:LYS:O	16:W:168:LYS:HD2	2.09	0.53
17:X:189:PRO:O	17:X:193:LEU:N	2.40	0.53
21:0:48:LYS:NZ	21:0:236:GLU:OE2	2.41	0.53
21:0:285:GLU:O	21:0:289:LEU:N	2.41	0.53
21:0:438:THR:OG1	21:0:439:CYS:O	2.24	0.53
21:0:469:TYR:HB2	21:0:470:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:85:TYR:OH	24:6:405:SER:O	2.26	0.53
24:6:271:ALA:O	24:6:275:GLU:N	2.30	0.53
25:2:488:LYS:HZ1	25:2:490:LYS:HD2	1.74	0.53
28:7:413:SER:H	28:7:416:SER:HG	1.54	0.53
1:A:332:LYS:HD2	1:A:337:ARG:HH22	1.72	0.53
13:M:24:CYS:HB2	13:M:45:CYS:HB2	1.90	0.53
21:0:69:ILE:N	21:0:204:ASN:O	2.41	0.53
21:0:605:LYS:HE3	21:0:605:LYS:H	1.74	0.53
21:0:739:TRP:NE1	21:0:748:GLN:OE1	2.26	0.53
24:6:256:SER:OG	24:6:257:GLU:OE2	2.27	0.53
28:7:331:GLN:CD	28:7:331:GLN:N	2.66	0.53
28:7:573:THR:HG23	28:7:576:LYS:NZ	2.23	0.53
28:7:577:ARG:NH1	28:7:714:GLN:OE1	2.41	0.53
28:7:754:ARG:NH2	28:7:761:GLN:OE1	2.31	0.53
1:A:418:SER:O	1:A:418:SER:OG	2.26	0.53
1:A:1277:GLU:O	1:A:1279:ILE:HG12	2.08	0.53
2:B:275:TYR:O	2:B:276:ILE:HD13	2.08	0.53
4:D:53:SER:O	4:D:56:ARG:HB3	2.09	0.53
4:D:59:ILE:HG23	4:D:63:LEU:HD21	1.91	0.53
17:X:273:GLU:O	17:X:277:LYS:N	2.41	0.53
18:O:215:THR:OG1	20:N:22:DT:O4'	2.25	0.53
21:0:140:GLN:NE2	21:0:386:ARG:O	2.33	0.53
23:4:79:TYR:HB3	23:4:132:LEU:HD21	1.91	0.53
26:5:28:SER:C	26:5:30:ILE:H	2.17	0.53
1:A:254:GLU:O	1:A:257:ARG:NH2	2.40	0.53
1:A:1214:GLU:HA	1:A:1217:LYS:HB2	1.91	0.53
1:A:1328:TYR:CG	1:A:1329:THR:N	2.77	0.53
2:B:248:SER:HB3	2:B:250:PHE:CE1	2.42	0.53
2:B:1128:LEU:HD22	2:B:1128:LEU:N	2.24	0.53
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.44	0.53
15:R:71:VAL:HG22	15:R:222:CYS:HB2	1.91	0.53
16:W:19:GLY:HA2	17:X:252:LEU:HD12	1.89	0.53
18:O:163:SER:HA	18:O:212:ILE:O	2.08	0.53
19:T:152:DG:H2''	19:T:153:DC:C5	2.44	0.53
21:0:11:LEU:HD23	21:0:93:ARG:HG3	1.90	0.53
21:0:141:ALA:HA	21:0:144:LYS:HB2	1.89	0.53
21:0:238:HIS:N	21:0:460:SER:OG	2.40	0.53
21:0:447:LYS:O	21:0:451:GLU:N	2.36	0.53
21:0:533:THR:O	21:0:567:LYS:NZ	2.37	0.53
21:0:562:GLU:O	21:0:565:LYS:HB3	2.09	0.53
21:0:657:ASP:HA	21:0:660:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:166:GLU:O	23:4:168:VAL:N	2.42	0.53
23:4:297:SER:C	23:4:299:ILE:H	2.15	0.53
25:2:471:LEU:HD22	25:2:504:PHE:CG	2.43	0.53
25:2:488:LYS:C	25:2:490:LYS:H	2.16	0.53
26:5:18:ALA:O	26:5:22:GLN:N	2.26	0.53
28:7:305:GLU:HB3	28:7:308:ASP:CB	2.39	0.53
28:7:403:ILE:O	28:7:405:LYS:HG2	2.09	0.53
28:7:423:GLN:HG3	28:7:423:GLN:O	2.09	0.53
28:7:446:PHE:CE1	28:7:447:GLN:HG3	2.43	0.53
28:7:473:VAL:HG12	28:7:477:LEU:HD13	1.91	0.53
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	1.90	0.53
1:A:279:LEU:HB3	1:A:289:ILE:CD1	2.38	0.53
1:A:746:MET:HE1	2:B:1015:HIS:HA	1.89	0.53
2:B:999:MET:HE3	2:B:1008:PRO:HG2	1.91	0.53
7:G:144:ARG:HB2	7:G:171:ILE:HD11	1.90	0.53
21:0:5:ILE:HD11	21:0:10:VAL:HG21	1.90	0.53
21:0:286:TYR:HB3	21:0:326:ARG:NH1	2.23	0.53
23:4:190:ILE:HA	23:4:192:GLN:HE22	1.74	0.53
28:7:363:ARG:HB3	28:7:365:TYR:CE2	2.43	0.53
28:7:668:THR:O	28:7:668:THR:OG1	2.26	0.53
1:A:951:GLU:OE2	1:A:952:ALA:N	2.40	0.53
2:B:922:GLU:HB3	2:B:928:ARG:NH1	2.23	0.53
3:C:136:ASP:OD1	3:C:137:LYS:N	2.42	0.53
8:H:58:THR:O	8:H:142:LEU:HD12	2.08	0.53
15:R:119:GLU:N	15:R:119:GLU:OE1	2.41	0.53
16:W:159:ASP:OD1	16:W:160:ASP:N	2.40	0.53
21:0:261:THR:HG22	21:0:339:ILE:HG12	1.90	0.53
24:6:153:ALA:O	24:6:156:PHE:HB3	2.09	0.53
25:2:478:ILE:HB	25:2:500:GLN:NE2	2.24	0.53
27:3:19:ASP:OD1	27:3:20:ARG:N	2.42	0.53
28:7:103:ASP:N	28:7:530:LEU:HD22	2.23	0.53
28:7:303:ARG:CB	28:7:323:VAL:H	2.21	0.53
28:7:364:PRO:HD2	28:7:365:TYR:CZ	2.43	0.53
28:7:601:ARG:NH2	28:7:603:ASP:HB2	2.23	0.53
1:A:1156:PRO:HA	1:A:1190:PRO:HB2	1.91	0.53
7:G:8:SER:HA	7:G:73:LYS:HA	1.90	0.53
16:W:18:ARG:HD2	17:X:247:ASN:CB	2.39	0.53
18:O:200:PRO:HG3	18:O:225:GLN:HB2	1.90	0.53
21:0:37:ASN:HA	21:0:456:VAL:HG13	1.89	0.53
21:0:103:PHE:HE1	21:0:205:ILE:HG22	1.73	0.53
21:0:143:ARG:O	21:0:147:GLU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:264:ALA:O	21:0:268:ASP:N	2.33	0.53
21:0:749:ASN:HA	21:0:752:LYS:HB3	1.89	0.53
23:4:87:TYR:O	23:4:89:GLU:N	2.42	0.53
26:5:16:ILE:HD11	26:5:54:LEU:HD11	1.90	0.53
26:5:22:GLN:HA	26:5:25:ALA:CB	2.39	0.53
27:3:82:VAL:O	27:3:86:LYS:N	2.25	0.53
28:7:213:ILE:O	28:7:217:THR:N	2.42	0.53
28:7:352:LEU:N	28:7:404:LYS:O	2.41	0.53
28:7:356:LEU:HD23	28:7:401:CYS:HB3	1.90	0.53
28:7:565:PHE:CE2	28:7:763:VAL:HG21	2.44	0.53
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.09	0.53
2:B:315:LYS:HE3	9:I:4:PHE:CE2	2.44	0.53
13:M:121:LYS:HB2	13:M:123:ASP:HB2	1.91	0.53
18:O:159:ASN:ND2	20:N:22:DT:O2	2.41	0.53
19:T:134:DT:H2''	19:T:135:DG:C8	2.44	0.53
21:0:1:MET:HG2	21:0:742:GLU:HG2	1.91	0.53
21:0:150:GLU:HG2	21:0:153:VAL:HG23	1.90	0.53
21:0:499:LYS:NZ	21:0:707:ASN:OD1	2.40	0.53
22:1:257:LEU:HA	22:1:260:PHE:HB2	1.91	0.53
23:4:56:ALA:HB1	23:4:245:ILE:HG23	1.90	0.53
24:6:173:ILE:HG13	24:6:180:GLN:HG3	1.90	0.53
28:7:484:PHE:CE2	28:7:486:ILE:HG12	2.40	0.53
28:7:709:VAL:HG12	28:7:716:MET:HG2	1.91	0.53
1:A:840:ARG:NH1	1:A:1385:THR:HG22	2.24	0.53
2:B:891:ASP:OD1	2:B:891:ASP:N	2.41	0.53
2:B:1159:ARG:HG2	2:B:1159:ARG:HH11	1.74	0.53
5:E:67:GLU:O	5:E:70:SER:OG	2.13	0.53
13:M:22:LEU:O	13:M:32:PRO:HG3	2.09	0.53
13:M:272:LYS:HA	13:M:272:LYS:HE3	1.90	0.53
15:R:110:GLU:HA	15:R:117:PRO:HA	1.90	0.53
21:0:274:VAL:HG11	21:0:388:LEU:HD22	1.91	0.53
23:4:236:LEU:HB2	23:4:238:VAL:HG13	1.91	0.53
28:7:328:LYS:O	28:7:332:GLU:HB3	2.09	0.53
28:7:345:ASN:ND2	28:7:378:ARG:HH11	2.08	0.53
28:7:480:ARG:NH2	28:7:481:GLU:O	2.41	0.53
1:A:394:ASN:N	1:A:394:ASN:OD1	2.41	0.52
1:A:1230:GLU:N	1:A:1233:ASP:OD2	2.35	0.52
8:H:34:ASP:N	8:H:35:GLN:OE1	2.42	0.52
16:W:73:ARG:HA	16:W:83:GLU:HA	1.91	0.52
16:W:122:TYR:CZ	16:W:158:GLU:HG3	2.44	0.52
19:T:126:DA:H2''	19:T:127:DG:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:350:HIS:C	21:0:422:PRO:HD3	2.34	0.52
21:0:418:LEU:HA	21:0:437:PHE:HA	1.91	0.52
21:0:743:ASP:O	21:0:747:HIS:N	2.33	0.52
23:4:242:GLU:OE2	23:4:243:GLY:N	2.42	0.52
25:2:139:SER:O	25:2:143:TRP:N	2.24	0.52
27:3:30:VAL:HB	27:3:35:TYR:HA	1.92	0.52
28:7:519:ARG:NE	28:7:521:ASP:O	2.42	0.52
1:A:315:LEU:O	13:M:94:THR:HG23	2.09	0.52
2:B:104:GLU:OE2	2:B:120:ARG:NH1	2.29	0.52
2:B:293:PRO:O	2:B:296:GLU:N	2.34	0.52
14:Q:126:LYS:HZ3	14:Q:126:LYS:H	1.56	0.52
21:0:9:PRO:HD2	21:0:62:HIS:HD2	1.74	0.52
21:0:68:LYS:HE2	21:0:204:ASN:HA	1.89	0.52
22:1:235:UNK:O	22:1:239:PRO:HD2	2.09	0.52
22:1:236:UNK:HA	22:1:239:PRO:HG2	1.90	0.52
22:1:251:LEU:HD22	22:1:255:LYS:HE3	1.91	0.52
23:4:130:TYR:O	23:4:134:GLU:HG2	2.10	0.52
25:2:498:ASN:HA	25:2:501:VAL:HB	1.91	0.52
27:3:104:VAL:O	27:3:108:LYS:N	2.36	0.52
1:A:7:SER:OG	2:B:1193:GLN:OE1	2.26	0.52
1:A:557:ASP:OD1	1:A:559:VAL:N	2.43	0.52
4:D:51:ASN:OD1	4:D:54:GLU:HB3	2.09	0.52
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.44	0.52
7:G:166:ASP:O	7:G:168:LEU:HG	2.09	0.52
8:H:112:ILE:HG23	8:H:132:LEU:HD12	1.91	0.52
13:M:167:SER:C	13:M:169:GLU:H	2.17	0.52
15:R:318:LEU:O	15:R:322:THR:N	2.41	0.52
18:O:71:VAL:HB	18:O:159:ASN:HB3	1.91	0.52
21:0:7:ASP:O	21:0:62:HIS:NE2	2.42	0.52
21:0:355:THR:O	21:0:358:SER:OG	2.28	0.52
21:0:506:ILE:HD12	21:0:522:TYR:HE1	1.74	0.52
21:0:571:VAL:HG21	22:1:375:LEU:HD22	1.90	0.52
21:0:594:ARG:HB2	21:0:594:ARG:CZ	2.37	0.52
21:0:605:LYS:HZ1	21:0:605:LYS:N	2.06	0.52
23:4:214:LYS:HE3	23:4:237:HIS:CD2	2.44	0.52
24:6:116:THR:OG1	24:6:119:GLN:OE1	2.26	0.52
25:2:103:THR:OG1	25:2:104:PHE:N	2.40	0.52
28:7:325:VAL:HG13	28:7:329:ARG:NE	2.24	0.52
28:7:411:CYS:SG	28:7:417:VAL:HG22	2.49	0.52
28:7:455:SER:HB3	28:7:459:MET:HE1	1.91	0.52
28:7:580:LEU:H	28:7:580:LEU:HD12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ARG:NH1	1:A:734:GLU:OE1	2.42	0.52
2:B:283:VAL:HG21	2:B:317:CYS:O	2.09	0.52
15:R:277:PHE:H	15:R:279:LYS:HE2	1.75	0.52
18:O:73:THR:HA	18:O:121:MET:O	2.09	0.52
19:T:124:DA:H1'	19:T:125:DT:H5'	1.91	0.52
28:7:208:SER:O	28:7:212:PHE:N	2.27	0.52
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.90	0.52
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.92	0.52
1:A:716:ASP:OD1	1:A:716:ASP:N	2.42	0.52
1:A:1203:ASN:HA	1:A:1206:ASP:CG	2.35	0.52
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.57	0.52
2:B:395:GLN:HG2	2:B:396:ASP:N	2.25	0.52
2:B:881:ASN:OD1	2:B:881:ASN:N	2.36	0.52
4:D:190:GLU:OE2	7:G:144:ARG:NH1	2.43	0.52
7:G:165:GLU:OE1	7:G:165:GLU:N	2.43	0.52
13:M:214:LEU:O	13:M:218:SER:OG	2.21	0.52
21:0:254:THR:HB	21:0:346:MET:SD	2.49	0.52
21:0:302:GLN:OE1	21:0:303:GLU:N	2.43	0.52
22:1:474:UNK:O	22:1:478:UNK:N	2.42	0.52
22:1:517:UNK:O	22:1:519:UNK:N	2.43	0.52
23:4:129:ILE:O	23:4:133:PHE:HB2	2.10	0.52
25:2:25:LEU:HA	25:2:219:VAL:HG22	1.91	0.52
28:7:325:VAL:O	28:7:329:ARG:N	2.39	0.52
28:7:325:VAL:O	28:7:329:ARG:HG3	2.10	0.52
28:7:408:ILE:HD11	28:7:482:TRP:CE2	2.45	0.52
28:7:548:HIS:CE1	28:7:551:ASN:HB2	2.44	0.52
28:7:598:HIS:O	28:7:602:GLY:N	2.43	0.52
1:A:380:VAL:HG23	1:A:430:TRP:O	2.09	0.52
1:A:886:ILE:HD11	1:A:950:GLY:HA2	1.92	0.52
1:A:928:LEU:O	1:A:931:GLU:N	2.43	0.52
9:I:94:ASP:OD1	9:I:94:ASP:N	2.40	0.52
13:M:157:CYS:O	13:M:159:ASP:N	2.38	0.52
14:Q:366:GLU:HB3	14:Q:392:VAL:HG13	1.91	0.52
18:O:128:SER:HB2	18:O:220:ARG:HH12	1.75	0.52
21:0:27:ASP:O	21:0:31:THR:OG1	2.28	0.52
21:0:310:PRO:HB3	21:0:404:THR:HG23	1.90	0.52
22:1:189:LYS:O	22:1:192:MET:HG3	2.10	0.52
25:2:186:ASN:O	25:2:190:GLN:N	2.29	0.52
25:2:275:ALA:O	25:2:278:LEU:HB3	2.09	0.52
25:2:361:SER:O	25:2:364:VAL:N	2.31	0.52
2:B:329:THR:O	2:B:333:PHE:N	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:MET:HE1	2:B:615:MET:HB2	1.92	0.52
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.90	0.52
5:E:123:LEU:O	5:E:126:SER:OG	2.18	0.52
13:M:169:GLU:O	13:M:173:ALA:N	2.42	0.52
14:Q:139:LEU:HB3	15:R:212:THR:HG21	1.92	0.52
21:0:422:PRO:HG2	21:0:423:TYR:CE2	2.45	0.52
21:0:555:GLN:HA	21:0:560:LEU:HD22	1.92	0.52
22:1:606:GLU:O	22:1:610:ASN:N	2.30	0.52
23:4:54:LEU:O	23:4:58:ILE:HG12	2.10	0.52
28:7:266:GLU:O	28:7:269:LEU:N	2.42	0.52
28:7:266:GLU:C	28:7:348:ARG:HE	2.18	0.52
28:7:354:ILE:HD11	28:7:407:VAL:HG23	1.92	0.52
28:7:383:ILE:H	28:7:535:LEU:HD13	1.75	0.52
28:7:558:TRP:HE3	28:7:711:LYS:HD3	1.74	0.52
28:7:583:MET:N	28:7:583:MET:SD	2.83	0.52
1:A:25:GLU:OE1	1:A:25:GLU:N	2.27	0.52
1:A:1364:ASN:OD1	1:A:1365:TYR:N	2.42	0.52
2:B:708:GLU:O	2:B:710:LEU:N	2.42	0.52
2:B:862:GLN:HB2	2:B:963:PHE:HB2	1.92	0.52
2:B:1082:MET:HG3	2:B:1082:MET:O	2.10	0.52
3:C:214:ASN:O	3:C:214:ASN:ND2	2.35	0.52
14:Q:109:GLU:OE1	14:Q:109:GLU:N	2.42	0.52
17:X:193:LEU:HB3	17:X:194:LYS:NZ	2.25	0.52
18:O:74:VAL:HG21	18:O:136:SER:HB3	1.92	0.52
20:N:19:DA:H2'	20:N:20:DT:C6	2.45	0.52
21:0:160:GLU:O	21:0:164:ASN:ND2	2.43	0.52
25:2:67:ASN:OD1	25:2:68:SER:N	2.43	0.52
25:2:369:ARG:HB2	28:7:118:PHE:O	2.10	0.52
28:7:668:THR:O	28:7:670:LEU:HG	2.09	0.52
2:B:333:PHE:C	2:B:333:PHE:CD2	2.88	0.52
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.10	0.52
13:M:43:VAL:HG23	13:M:52:LEU:HB2	1.92	0.52
13:M:61:SER:HA	13:M:64:ARG:HB2	1.92	0.52
18:O:144:GLN:NE2	18:O:150:ALA:O	2.39	0.52
18:O:231:TYR:HA	18:O:234:LEU:HD22	1.92	0.52
21:0:1:MET:N	21:0:12:PHE:O	2.39	0.52
21:0:52:LEU:O	21:0:56:THR:HG23	2.10	0.52
21:0:286:TYR:OH	21:0:328:ALA:N	2.43	0.52
21:0:564:TRP:HZ3	22:1:385:MET:HE1	1.74	0.52
22:1:625:LEU:O	22:1:629:LYS:N	2.28	0.52
24:6:163:GLN:OE1	24:6:163:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:668:THR:HB	28:7:694:LYS:HZ1	1.75	0.52
1:A:251:SER:HA	1:A:257:ARG:HA	1.92	0.52
16:W:183:ILE:HA	16:W:186:LEU:HD12	1.92	0.52
21:0:25:MET:HA	21:0:28:ILE:HG23	1.91	0.52
21:0:37:ASN:ND2	21:0:476:LYS:O	2.43	0.52
21:0:125:LYS:HD2	21:0:127:THR:HG23	1.92	0.52
21:0:250:LEU:HD13	22:1:350:ARG:NH1	2.25	0.52
21:0:346:MET:HB3	21:0:347:LYS:NZ	2.25	0.52
23:4:239:GLU:OE1	23:4:240:SER:N	2.42	0.52
24:6:451:CYS:O	24:6:455:GLU:N	2.42	0.52
25:2:451:VAL:HB	26:5:51:LYS:HZ3	1.75	0.52
28:7:392:LYS:NZ	28:7:513:LEU:HB3	2.25	0.52
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.91	0.51
2:B:315:LYS:HE3	9:I:4:PHE:HE2	1.75	0.51
2:B:746:SER:O	2:B:746:SER:OG	2.26	0.51
5:E:191:LYS:N	5:E:194:GLU:OE1	2.41	0.51
11:K:17:SER:H	11:K:20:LYS:NZ	2.08	0.51
13:M:153:ALA:HB3	13:M:175:SER:HB2	1.92	0.51
14:Q:141:ARG:HB3	14:Q:348:TYR:HB3	1.91	0.51
21:0:196:VAL:O	21:0:200:ILE:N	2.42	0.51
21:0:393:VAL:O	21:0:396:PHE:N	2.43	0.51
22:1:199:VAL:HG21	22:1:206:PRO:HG3	1.92	0.51
24:6:145:ARG:NH1	24:6:237:GLY:O	2.36	0.51
25:2:455:GLU:HG3	26:5:8:ALA:HB2	1.91	0.51
26:5:5:ARG:NH1	26:5:32:LEU:HB3	2.25	0.51
27:3:97:ASP:O	27:3:101:GLY:N	2.28	0.51
28:7:576:LYS:HA	28:7:579:LEU:HD21	1.91	0.51
28:7:672:GLN:O	28:7:708:LEU:N	2.43	0.51
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.45	0.51
2:B:230:ALA:C	2:B:232:SER:H	2.18	0.51
2:B:363:HIS:CG	2:B:364:ILE:H	2.27	0.51
2:B:902:GLY:O	12:L:65:VAL:HG11	2.10	0.51
5:E:75:MET:HA	5:E:106:GLN:HE22	1.75	0.51
12:L:47:ARG:NH2	12:L:49:LYS:HA	2.25	0.51
13:M:157:CYS:SG	13:M:158:HIS:N	2.76	0.51
13:M:206:THR:HA	13:M:209:ILE:HD11	1.91	0.51
13:M:208:ASN:ND2	18:O:186:GLU:OE2	2.44	0.51
16:W:91:TYR:CD2	16:W:92:PRO:HD3	2.45	0.51
16:W:182:ILE:HG22	16:W:186:LEU:HG	1.91	0.51
21:0:136:MET:HA	21:0:155:LEU:HA	1.92	0.51
21:0:651:ASN:O	21:0:655:SER:N	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:6:390:ALA:N	24:6:428:ARG:O	2.39	0.51
25:2:453:THR:OG1	26:5:51:LYS:NZ	2.32	0.51
25:2:474:TYR:O	25:2:478:ILE:N	2.44	0.51
25:2:488:LYS:HE2	26:5:35:LEU:HB3	1.92	0.51
25:2:502:LEU:N	25:2:503:ASP:OD1	2.43	0.51
28:7:347:HIS:C	28:7:349:ASN:H	2.18	0.51
28:7:353:ASP:HB3	28:7:451:GLY:HA2	1.90	0.51
28:7:468:HIS:O	28:7:471:GLN:N	2.43	0.51
2:B:134:LYS:HD2	15:R:275:SER:HB2	1.91	0.51
5:E:46:TYR:O	5:E:54:GLN:HG2	2.10	0.51
13:M:187:ARG:HA	13:M:241:ARG:HH22	1.75	0.51
14:Q:384:PHE:CE2	15:R:95:ILE:HD11	2.45	0.51
15:R:130:GLU:O	15:R:132:GLU:HG3	2.11	0.51
16:W:160:ASP:HB3	16:W:164:LYS:HD2	1.93	0.51
17:X:262:MET:HA	17:X:265:ASN:HB2	1.91	0.51
19:T:131:DC:H2"	19:T:132:DA:C8	2.46	0.51
21:0:286:TYR:O	21:0:290:VAL:N	2.33	0.51
21:0:443:SER:HA	21:0:446:ILE:HB	1.92	0.51
21:0:572:GLU:HB2	21:0:600:SER:HA	1.92	0.51
22:1:593:LEU:HA	22:1:596:LEU:HD12	1.90	0.51
24:6:156:PHE:O	24:6:160:PHE:N	2.31	0.51
24:6:287:PHE:HA	24:6:289:LYS:HE2	1.91	0.51
26:5:24:ASP:O	26:5:27:MET:N	2.43	0.51
28:7:413:SER:C	28:7:417:VAL:HG23	2.34	0.51
28:7:469:ASP:O	28:7:472:LYS:HB2	2.10	0.51
1:A:1155:ASP:HB2	1:A:1162:VAL:HG22	1.92	0.51
2:B:230:ALA:O	2:B:261:ARG:NH1	2.44	0.51
2:B:393:LYS:HZ1	2:B:621:GLU:CD	2.18	0.51
5:E:55:ARG:O	5:E:58:MET:N	2.38	0.51
5:E:124:VAL:O	5:E:126:SER:OG	2.27	0.51
7:G:119:LEU:HD21	7:G:130:TYR:HB3	1.92	0.51
18:O:204:LEU:HD22	18:O:230:ILE:HG21	1.91	0.51
20:N:12:DG:C5	20:N:13:DG:C5	2.98	0.51
23:4:156:GLY:O	23:4:160:VAL:N	2.36	0.51
25:2:454:TYR:CD1	25:2:482:LEU:HB3	2.44	0.51
28:7:491:HIS:CD2	28:7:492:VAL:HG23	2.46	0.51
28:7:520:GLU:HG3	28:7:681:ARG:NE	2.25	0.51
1:A:36:ARG:HH21	1:A:37:PHE:HZ	1.58	0.51
2:B:22:SER:O	2:B:22:SER:OG	2.29	0.51
2:B:336:ARG:HB2	2:B:337:ARG:HD3	1.93	0.51
13:M:117:ASN:N	13:M:117:ASN:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:15:PHE:HD1	16:W:18:ARG:HH11	1.58	0.51
21:0:643:ARG:NE	21:0:649:ARG:HA	2.26	0.51
22:1:213:ARG:H	22:1:213:ARG:NH1	2.06	0.51
23:4:113:UNK:O	23:4:119:ARG:NE	2.43	0.51
24:6:273:CYS:HA	24:6:276:LEU:HB3	1.92	0.51
25:2:32:CYS:O	25:2:35:ILE:HG12	2.10	0.51
25:2:459:TYR:CZ	25:2:501:VAL:HG12	2.45	0.51
28:7:383:ILE:HD11	28:7:527:LEU:HB2	1.91	0.51
1:A:448:PRO:O	1:A:449:SER:OG	2.27	0.51
2:B:258:LEU:HD12	2:B:259:TYR:H	1.74	0.51
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.45	0.51
6:F:103:MET:SD	7:G:15:PRO:HG2	2.50	0.51
10:J:3:VAL:H	10:J:53:HIS:CE1	2.29	0.51
13:M:148:ASP:O	13:M:152:GLU:N	2.40	0.51
14:Q:126:LYS:H	14:Q:126:LYS:CE	2.24	0.51
16:W:144:ARG:NH1	16:W:147:PHE:O	2.43	0.51
21:0:234:PHE:N	21:0:457:ILE:O	2.40	0.51
21:0:552:SER:O	21:0:556:THR:HG23	2.09	0.51
23:4:129:ILE:HG12	23:4:130:TYR:N	2.26	0.51
25:2:377:GLN:O	25:2:382:SER:OG	2.25	0.51
26:5:64:ASN:HA	28:7:721:LYS:NZ	2.26	0.51
28:7:164:ILE:N	28:7:172:GLU:H	2.07	0.51
28:7:335:TYR:O	28:7:337:VAL:HG22	2.11	0.51
28:7:640:LEU:HA	28:7:643:PHE:CD2	2.45	0.51
1:A:115:LEU:HD11	1:A:141:LEU:HB3	1.91	0.51
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.29	0.51
1:A:1256:GLU:O	1:A:1259:MET:N	2.44	0.51
2:B:357:GLN:NE2	2:B:358:LYS:HG3	2.26	0.51
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.44	0.51
12:L:27:LEU:O	12:L:39:SER:HA	2.11	0.51
12:L:28:LYS:HZ3	12:L:37:LYS:HZ1	1.59	0.51
21:0:220:GLU:HA	21:0:313:PRO:CB	2.40	0.51
22:1:635:ASN:O	22:1:639:ASN:N	2.34	0.51
24:6:349:CYS:SG	24:6:351:ASN:N	2.82	0.51
24:6:390:ALA:O	24:6:428:ARG:N	2.33	0.51
25:2:451:VAL:HB	26:5:51:LYS:NZ	2.26	0.51
25:2:461:ASP:N	25:2:490:LYS:HG2	2.07	0.51
28:7:104:PHE:H	28:7:529:PHE:H	1.59	0.51
28:7:130:ARG:O	28:7:145:SER:N	2.44	0.51
28:7:266:GLU:O	28:7:348:ARG:NH2	2.44	0.51
28:7:409:VAL:HG22	28:7:486:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.51	0.51
1:A:150:THR:HA	1:A:165:GLY:O	2.11	0.51
2:B:241:ARG:NH2	2:B:251:ILE:HA	2.25	0.51
16:W:123:MET:HE2	16:W:130:LYS:HZ2	1.75	0.51
24:6:137:LEU:HD21	24:6:204:PRO:HD2	1.93	0.51
24:6:145:ARG:O	24:6:149:ILE:HG12	2.10	0.51
25:2:177:ASN:C	25:2:180:GLY:H	2.19	0.51
25:2:216:MET:O	25:2:218:LEU:HD23	2.11	0.51
26:5:30:ILE:HG23	26:5:43:ASN:CB	2.40	0.51
27:3:25:ASP:OD1	27:3:25:ASP:N	2.44	0.51
28:7:543:LEU:C	28:7:545:GLN:N	2.69	0.51
1:A:107:CYS:SG	1:A:109:HIS:N	2.72	0.51
1:A:711:ARG:NE	9:I:97:MET:HG3	2.26	0.51
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.51
5:E:27:GLY:O	5:E:65:THR:OG1	2.22	0.51
18:O:74:VAL:HG22	18:O:155:PHE:HD2	1.76	0.51
21:0:106:LEU:HD21	21:0:176:PHE:N	2.26	0.51
21:0:171:LEU:HD13	21:0:184:TYR:HE1	1.75	0.51
21:0:234:PHE:HB2	21:0:458:ILE:HA	1.93	0.51
21:0:382:SER:O	21:0:386:ARG:HB3	2.11	0.51
21:0:690:ARG:NH2	21:0:701:LEU:O	2.44	0.51
22:1:550:CYS:O	22:1:554:HIS:N	2.26	0.51
22:1:597:PHE:CE2	22:1:620:LEU:HD12	2.46	0.51
23:4:117:ARG:HG3	23:4:118:PHE:CD1	2.46	0.51
25:2:86:LEU:HD12	25:2:87:LEU:N	2.26	0.51
25:2:458:LEU:HD13	25:2:492:PHE:CD2	2.46	0.51
25:2:466:GLN:O	25:2:467:GLU:C	2.54	0.51
28:7:439:THR:N	28:7:442:ASN:O	2.44	0.51
28:7:460:VAL:O	28:7:500:ARG:HD2	2.11	0.51
28:7:718:TYR:O	28:7:722:ARG:N	2.39	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.46	0.51
2:B:400:HIS:NE2	2:B:699:GLU:OE2	2.37	0.51
4:D:206:GLU:O	4:D:210:ILE:HG12	2.11	0.51
6:F:72:LYS:HD2	6:F:72:LYS:O	2.11	0.51
7:G:142:ARG:C	7:G:143:ILE:HD12	2.36	0.51
13:M:158:HIS:ND1	13:M:158:HIS:O	2.44	0.51
18:O:68:GLN:HE21	18:O:163:SER:H	1.56	0.51
18:O:171:ARG:N	18:O:237:PHE:O	2.35	0.51
21:0:351:VAL:HB	21:0:421:GLU:HG2	1.92	0.51
25:2:77:ALA:O	25:2:80:SER:OG	2.21	0.51
25:2:495:LYS:HD3	26:5:6:LYS:NZ	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5:9:LEU:HD12	26:5:10:VAL:N	2.26	0.51
28:7:256:ILE:O	28:7:258:SER:N	2.44	0.51
28:7:544:SER:C	28:7:546:LYS:N	2.65	0.51
28:7:555:ALA:O	28:7:707:SER:N	2.44	0.51
28:7:572:GLU:OE1	28:7:576:LYS:NZ	2.44	0.51
28:7:584:ASN:ND2	28:7:586:THR:OG1	2.34	0.51
1:A:1198:ASP:OD2	1:A:1201:ALA:N	2.32	0.50
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.41	0.50
14:Q:139:LEU:HD11	14:Q:350:TRP:HB3	1.92	0.50
21:0:112:LYS:HD3	21:0:129:VAL:HG21	1.93	0.50
21:0:280:GLN:O	21:0:284:ASP:N	2.29	0.50
22:1:196:GLN:O	22:1:199:VAL:N	2.41	0.50
22:1:201:ASN:N	22:1:201:ASN:OD1	2.43	0.50
23:4:39:THR:O	23:4:43:GLU:N	2.31	0.50
23:4:156:GLY:O	23:4:160:VAL:HG23	2.10	0.50
25:2:18:PRO:HB2	25:2:20:GLN:OE1	2.11	0.50
25:2:225:ILE:O	25:2:229:GLY:N	2.42	0.50
1:A:116:ASP:O	1:A:119:ASN:N	2.40	0.50
1:A:119:ASN:OD1	1:A:121:LEU:N	2.44	0.50
1:A:150:THR:HA	1:A:166:GLY:HA2	1.93	0.50
2:B:642:ASP:HA	2:B:649:LYS:HA	1.93	0.50
15:R:73:LEU:HB2	15:R:77:LEU:HB3	1.94	0.50
15:R:224:VAL:HG12	15:R:226:PRO:HD3	1.92	0.50
21:0:286:TYR:CZ	21:0:327:ARG:HA	2.46	0.50
21:0:570:LEU:O	21:0:599:LEU:HD12	2.11	0.50
21:0:714:ILE:O	21:0:717:THR:HG23	2.11	0.50
23:4:116:ARG:O	23:4:120:ASN:ND2	2.44	0.50
24:6:391:GLU:HA	24:6:427:TYR:HA	1.92	0.50
25:2:11:THR:O	25:2:15:GLU:HG3	2.11	0.50
25:2:474:TYR:HA	25:2:477:ASP:CB	2.38	0.50
28:7:355:ASP:CG	28:7:404:LYS:HZ2	2.16	0.50
1:A:1211:GLN:HG2	1:A:1212:VAL:N	2.26	0.50
2:B:280:ILE:HD12	2:B:280:ILE:N	2.26	0.50
2:B:1084:GLN:NE2	3:C:190:ASP:O	2.32	0.50
8:H:11:GLN:OE1	8:H:52:GLN:HG3	2.12	0.50
13:M:103:ASP:O	13:M:107:THR:HG23	2.11	0.50
13:M:259:THR:HB	13:M:284:LEU:HD21	1.93	0.50
16:W:91:TYR:HD2	16:W:92:PRO:HD3	1.76	0.50
21:0:726:GLN:O	21:0:728:THR:N	2.42	0.50
22:1:497:UNK:O	22:1:501:UNK:N	2.44	0.50
26:5:16:ILE:O	26:5:19:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:557:VAL:O	28:7:709:VAL:HG23	2.11	0.50
28:7:663:ASP:OD1	28:7:663:ASP:N	2.45	0.50
1:A:900:ASP:OD1	1:A:900:ASP:N	2.43	0.50
1:A:1230:GLU:OE1	1:A:1231:ASP:N	2.45	0.50
1:A:1266:THR:OG1	1:A:1267:MET:N	2.44	0.50
5:E:38:PRO:HD2	5:E:41:ASP:OD2	2.11	0.50
13:M:130:PHE:HB3	13:M:151:LYS:HE2	1.92	0.50
14:Q:125:LYS:HB3	14:Q:128:ASN:HB2	1.94	0.50
15:R:69:TRP:NE1	15:R:219:CYS:SG	2.75	0.50
21:0:689:LYS:HD3	21:0:689:LYS:N	2.26	0.50
22:1:193:LYS:HA	22:1:196:GLN:HE21	1.76	0.50
22:1:597:PHE:CE1	22:1:613:THR:HG22	2.46	0.50
25:2:30:ALA:O	25:2:34:ALA:N	2.33	0.50
26:5:62:ILE:C	26:5:64:ASN:H	2.20	0.50
28:7:326:VAL:HG23	28:7:329:ARG:HH21	1.76	0.50
28:7:490:VAL:H	28:7:514:THR:HG22	1.77	0.50
28:7:717:TYR:O	28:7:720:THR:OG1	2.22	0.50
1:A:120:GLU:HA	1:A:123:ARG:CZ	2.42	0.50
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.11	0.50
2:B:516:ASN:OD1	2:B:516:ASN:N	2.38	0.50
7:G:87:VAL:N	7:G:145:VAL:O	2.29	0.50
18:O:156:LYS:HD3	18:O:158:GLN:HE22	1.76	0.50
21:0:223:SER:O	21:0:227:SER:N	2.44	0.50
21:0:745:ILE:HG13	21:0:746:LYS:N	2.27	0.50
28:7:387:PRO:HG3	28:7:692:ARG:HD2	1.94	0.50
1:A:42:ASP:CG	1:A:44:THR:H	2.20	0.50
1:A:284:ALA:HB1	1:A:286:HIS:CD2	2.46	0.50
1:A:566:ILE:HG13	8:H:96:VAL:HG12	1.93	0.50
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.45	0.50
2:B:1168:LEU:O	2:B:1170:THR:N	2.44	0.50
19:T:151:DC:C4	19:T:152:DG:O6	2.65	0.50
21:0:77:SER:O	21:0:80:GLU:HG2	2.11	0.50
21:0:167:VAL:HA	21:0:198:ARG:CZ	2.42	0.50
21:0:420:ILE:HA	21:0:434:ILE:O	2.12	0.50
21:0:554:TRP:HB3	21:0:560:LEU:HD13	1.93	0.50
21:0:639:LEU:HD23	21:0:650:GLU:HG2	1.92	0.50
24:6:141:LEU:HB2	24:6:145:ARG:HA	1.94	0.50
24:6:363:CYS:HB3	24:6:368:LEU:H	1.75	0.50
25:2:21:VAL:O	25:2:24:ARG:HB2	2.12	0.50
25:2:57:VAL:HG22	25:2:58:PRO:HD2	1.93	0.50
25:2:482:LEU:HG	25:2:493:ILE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5:17:LYS:O	26:5:21:LEU:HG	2.11	0.50
28:7:553:GLN:HB2	28:7:704:PHE:HD2	1.76	0.50
28:7:570:LEU:HB2	28:7:571:ARG:NH1	2.26	0.50
1:A:1146:VAL:HG22	1:A:1197:LEU:HB3	1.94	0.50
2:B:450:ALA:O	2:B:452:THR:N	2.45	0.50
7:G:97:HIS:O	7:G:111:THR:HG23	2.12	0.50
14:Q:118:LEU:HD22	14:Q:119:LEU:H	1.75	0.50
19:T:108:DC:H41	28:7:466:ARG:NH2	2.10	0.50
25:2:137:GLU:O	25:2:141:ASN:N	2.25	0.50
25:2:457:SER:HA	26:5:6:LYS:CA	2.23	0.50
25:2:461:ASP:OD2	26:5:3:ARG:NH1	2.44	0.50
25:2:473:LYS:HZ1	25:2:477:ASP:CG	2.15	0.50
28:7:673:ILE:HA	28:7:708:LEU:HB2	1.93	0.50
1:A:453:MET:HE3	1:A:513:SER:HB2	1.93	0.50
2:B:327:ARG:HH21	2:B:353:LYS:HE3	1.77	0.50
2:B:348:ARG:NH1	2:B:348:ARG:HB2	2.27	0.50
4:D:154:PHE:CZ	4:D:163:VAL:HG21	2.47	0.50
6:F:89:GLU:O	6:F:93:ILE:HG12	2.11	0.50
7:G:86:VAL:HA	7:G:146:LYS:HA	1.93	0.50
13:M:309:ILE:O	13:M:313:TYR:N	2.42	0.50
13:M:319:HIS:C	13:M:321:ASP:H	2.20	0.50
16:W:102:VAL:O	16:W:106:VAL:HG23	2.12	0.50
21:0:126:GLY:HA2	21:0:129:VAL:HB	1.93	0.50
21:0:280:GLN:CD	21:0:280:GLN:H	2.18	0.50
23:4:85:TYR:CZ	24:6:407:GLN:HG3	2.46	0.50
23:4:244:LEU:O	23:4:247:TYR:N	2.45	0.50
24:6:141:LEU:HB3	24:6:148:MET:HG3	1.93	0.50
24:6:175:ARG:CZ	24:6:202:GLN:HE22	2.25	0.50
25:2:74:PHE:CD1	25:2:78:ILE:HD13	2.47	0.50
25:2:467:GLU:HG2	25:2:505:ALA:HA	1.93	0.50
26:5:12:CYS:O	26:5:38:THR:HA	2.12	0.50
27:3:51:PRO:HG3	27:3:64:ARG:HG2	1.94	0.50
28:7:305:GLU:O	28:7:308:ASP:HB2	2.12	0.50
1:A:61:ILE:HA	1:A:74:MET:HG3	1.92	0.50
1:A:517:ASN:O	1:A:517:ASN:ND2	2.41	0.50
2:B:929:THR:O	2:B:932:HIS:NE2	2.45	0.50
2:B:1134:GLU:OE1	2:B:1134:GLU:N	2.43	0.50
3:C:18:VAL:O	3:C:231:ASN:ND2	2.45	0.50
16:W:19:GLY:O	17:X:252:LEU:HB2	2.12	0.50
21:0:378:SER:O	21:0:382:SER:N	2.39	0.50
22:1:380:ARG:HB3	22:1:380:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:510:ASN:OD1	22:1:513:GLN:NE2	2.45	0.50
28:7:385:VAL:HG12	28:7:534:LYS:HB2	1.93	0.50
28:7:556:GLU:HB2	28:7:733:PHE:CZ	2.46	0.50
2:B:451:LYS:HE2	13:M:138:ASP:CG	2.37	0.49
4:D:140:ASP:HA	4:D:143:ASN:HB2	1.93	0.49
6:F:110:ASP:OD1	6:F:110:ASP:N	2.36	0.49
16:W:174:ARG:NH2	16:W:177:ASP:OD2	2.45	0.49
21:0:367:THR:O	21:0:369:ILE:HG12	2.11	0.49
21:0:396:PHE:HD1	21:0:399:LEU:HG	1.76	0.49
21:0:610:ILE:O	21:0:668:ARG:NH1	2.42	0.49
21:0:692:GLN:OE1	21:0:692:GLN:N	2.45	0.49
23:4:262:ILE:O	23:4:264:LYS:NZ	2.35	0.49
25:2:494:SER:OG	25:2:496:GLU:OE2	2.20	0.49
28:7:478:THR:HG22	28:7:504:THR:HG23	1.93	0.49
28:7:486:ILE:HA	28:7:511:LEU:HB3	1.94	0.49
28:7:590:ALA:O	28:7:594:LEU:HG	2.12	0.49
1:A:849:MET:HE3	1:A:1063:MET:SD	2.52	0.49
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.94	0.49
4:D:138:ASN:O	4:D:142:LYS:N	2.41	0.49
5:E:41:ASP:O	5:E:45:LYS:HB2	2.12	0.49
7:G:29:LYS:O	7:G:33:GLU:HG2	2.12	0.49
7:G:64:THR:C	7:G:66:GLY:H	2.19	0.49
11:K:9:LEU:HA	11:K:37:LYS:HD2	1.95	0.49
21:0:7:ASP:HB3	21:0:8:LEU:HD12	1.94	0.49
21:0:330:HIS:O	21:0:333:SER:OG	2.30	0.49
22:1:198:THR:HB	22:1:204:LEU:HB2	1.93	0.49
23:4:139:GLN:CD	23:4:140:ILE:HG12	2.36	0.49
24:6:282:TYR:O	24:6:284:ASP:N	2.42	0.49
25:2:217:ASP:O	25:2:221:VAL:N	2.44	0.49
25:2:481:LEU:HD22	25:2:484:LYS:HB3	1.94	0.49
28:7:354:ILE:HG12	28:7:452:LEU:HD11	1.93	0.49
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.12	0.49
3:C:166:GLU:OE2	12:L:70:ARG:NH2	2.38	0.49
5:E:101:GLN:HB2	5:E:127:ILE:HD12	1.94	0.49
7:G:164:LYS:HD2	27:3:50:GLY:HA3	1.93	0.49
13:M:40:GLU:OE1	13:M:40:GLU:N	2.45	0.49
14:Q:141:ARG:CZ	14:Q:350:TRP:HE1	2.25	0.49
17:X:200:VAL:HG22	17:X:201:THR:HG23	1.95	0.49
21:0:120:VAL:HG11	21:0:129:VAL:HA	1.93	0.49
21:0:275:ARG:O	21:0:279:SER:HB2	2.12	0.49
21:0:719:GLN:HA	21:0:722:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:303:ASN:HA	23:4:312:PHE:H	1.76	0.49
24:6:155:ASP:HA	24:6:158:HIS:CE1	2.47	0.49
25:2:36:TYR:OH	25:2:44:LYS:O	2.23	0.49
26:5:15:SER:OG	28:7:561:MET:O	2.31	0.49
28:7:445:MET:HB2	28:7:448:THR:HG21	1.93	0.49
28:7:520:GLU:H	28:7:520:GLU:CD	2.19	0.49
1:A:332:LYS:C	1:A:333:GLU:HG2	2.38	0.49
1:A:423:ASP:OD1	1:A:424:ILE:N	2.45	0.49
1:A:1161:THR:H	1:A:1167:GLU:CD	2.19	0.49
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.94	0.49
2:B:244:LEU:HD22	2:B:245:GLU:N	2.28	0.49
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.48	0.49
3:C:102:GLN:HG3	3:C:154:LYS:HG2	1.94	0.49
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.93	0.49
19:T:108:DC:N4	20:N:58:DG:H22	2.09	0.49
21:0:495:MET:HE2	21:0:716:ASN:HB2	1.94	0.49
23:4:57:LEU:O	23:4:61:LEU:HD22	2.11	0.49
25:2:135:LEU:C	25:2:138:TYR:H	2.20	0.49
2:B:347:LYS:HA	2:B:350:GLN:HB3	1.95	0.49
12:L:47:ARG:NH2	12:L:48:CYS:O	2.46	0.49
16:W:24:SER:HA	16:W:27:LEU:HD13	1.93	0.49
20:N:27:DG:H2"	20:N:28:DT:OP2	2.12	0.49
21:0:103:PHE:CZ	21:0:204:ASN:HB2	2.48	0.49
22:1:502:ARG:O	22:1:505:THR:OG1	2.24	0.49
23:4:163:ILE:O	23:4:167:SER:N	2.46	0.49
23:4:218:SER:HA	23:4:237:HIS:CE1	2.48	0.49
23:4:243:GLY:O	23:4:245:ILE:HG12	2.12	0.49
24:6:116:THR:N	24:6:117:PRO:HA	2.27	0.49
24:6:149:ILE:O	24:6:153:ALA:N	2.43	0.49
24:6:294:GLU:CD	24:6:294:GLU:N	2.67	0.49
25:2:87:LEU:HA	25:2:100:LEU:HA	1.92	0.49
28:7:101:PRO:C	28:7:328:LYS:HA	2.38	0.49
28:7:309:ASP:OD1	28:7:309:ASP:N	2.44	0.49
1:A:55:ASP:OD2	1:A:57:ARG:NE	2.40	0.49
1:A:175:ARG:HH22	1:A:184:SER:CB	2.26	0.49
1:A:271:LYS:O	1:A:274:ILE:N	2.46	0.49
1:A:928:LEU:O	1:A:929:LEU:C	2.55	0.49
1:A:1169:ILE:HA	1:A:1172:LEU:CB	2.43	0.49
2:B:68:THR:HG22	2:B:91:SER:HA	1.94	0.49
3:C:174:ALA:HB3	3:C:233:GLU:HG2	1.95	0.49
4:D:154:PHE:HZ	4:D:163:VAL:HG21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:PRO:HB2	5:E:69:ILE:HD13	1.94	0.49
19:T:152:DG:H2'	19:T:152:DG:OP2	2.12	0.49
21:0:133:CYS:O	21:0:136:MET:HB2	2.13	0.49
21:0:371:ARG:HG2	21:0:375:ARG:HH22	1.77	0.49
22:1:551:ARG:O	22:1:555:THR:OG1	2.27	0.49
23:4:70:ALA:HB2	23:4:117:ARG:HH12	1.77	0.49
25:2:360:LEU:HD21	25:2:399:TYR:OH	2.12	0.49
25:2:485:ASP:HB3	25:2:488:LYS:HB2	1.95	0.49
26:5:5:ARG:HD2	26:5:32:LEU:HD13	1.94	0.49
28:7:341:TYR:CG	28:7:509:ALA:HB2	2.48	0.49
28:7:362:ILE:HG13	28:7:366:GLN:HB2	1.93	0.49
28:7:364:PRO:HG2	28:7:546:LYS:CB	2.42	0.49
28:7:418:MET:C	28:7:420:TRP:H	2.21	0.49
28:7:556:GLU:CD	28:7:723:GLN:HE21	2.20	0.49
1:A:852:TYR:OH	6:F:89:GLU:OE2	2.22	0.49
2:B:319:GLU:HG2	9:I:15:TYR:OH	2.12	0.49
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.95	0.49
2:B:628:THR:O	2:B:628:THR:OG1	2.29	0.49
8:H:5:LEU:HD21	8:H:61:SER:HB3	1.95	0.49
13:M:166:LYS:HD2	13:M:202:GLU:OE2	2.12	0.49
18:O:72:ALA:HA	18:O:157:ILE:HA	1.95	0.49
21:0:230:SER:O	21:0:455:SER:OG	2.30	0.49
22:1:492:UNK:C	22:1:494:UNK:H	2.20	0.49
23:4:118:PHE:CD1	23:4:118:PHE:N	2.81	0.49
23:4:161:ASN:HA	23:4:164:SER:HB3	1.93	0.49
24:6:403:CYS:SG	24:6:404:PHE:N	2.85	0.49
25:2:467:GLU:CA	25:2:471:LEU:HG	2.33	0.49
28:7:517:LEU:HD12	28:7:518:VAL:N	2.28	0.49
28:7:540:TRP:CD1	28:7:729:GLN:HE22	2.29	0.49
28:7:725:PHE:HA	28:7:728:ASP:HB2	1.94	0.49
1:A:372:LYS:NZ	11:K:1:MET:HG2	2.26	0.49
1:A:965:GLN:N	1:A:965:GLN:OE1	2.45	0.49
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.13	0.49
2:B:874:PHE:HD2	2:B:962:LYS:HE2	1.77	0.49
2:B:914:LYS:HB3	2:B:914:LYS:HE2	1.63	0.49
4:D:162:ALA:HA	4:D:165:GLN:HB2	1.95	0.49
14:Q:110:ASP:OD1	14:Q:110:ASP:N	2.44	0.49
21:0:53:LEU:HD13	21:0:86:LEU:HB2	1.94	0.49
21:0:66:HIS:NE2	21:0:229:ASP:O	2.46	0.49
21:0:239:ASN:HA	21:0:660:ARG:HH11	1.77	0.49
21:0:363:LEU:HD21	21:0:369:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:573:THR:HG23	21:0:579:THR:OG1	2.12	0.49
21:0:605:LYS:HG3	22:1:339:LEU:HD22	1.95	0.49
22:1:499:UNK:O	22:1:503:VAL:HG23	2.13	0.49
22:1:592:LYS:O	22:1:596:LEU:N	2.31	0.49
24:6:134:GLU:OE1	24:6:206:GLY:N	2.46	0.49
24:6:210:LEU:O	24:6:214:LEU:HD22	2.12	0.49
25:2:412:ALA:HA	25:2:416:LEU:HD13	1.95	0.49
28:7:736:ILE:HD13	28:7:739:LEU:HD13	1.95	0.49
1:A:278:THR:O	1:A:280:GLU:N	2.45	0.49
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.94	0.49
1:A:386:ASP:OD1	1:A:386:ASP:N	2.40	0.49
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.94	0.49
4:D:128:VAL:HA	4:D:131:GLU:HB3	1.95	0.49
5:E:147:HIS:ND1	5:E:148:GLU:N	2.61	0.49
18:O:88:HIS:HB2	18:O:146:ILE:HG12	1.94	0.49
21:0:493:LEU:HD13	21:0:495:MET:HE3	1.93	0.49
22:1:196:GLN:HB2	22:1:200:ILE:HB	1.93	0.49
23:4:25:LEU:HB3	23:4:174:SER:HB3	1.95	0.49
24:6:214:LEU:HD22	24:6:214:LEU:H	1.78	0.49
26:5:26:LYS:H	26:5:26:LYS:HZ3	1.58	0.49
28:7:234:VAL:C	28:7:315:SER:HA	2.38	0.49
28:7:354:ILE:HD12	28:7:405:LYS:H	1.78	0.49
28:7:581:TYR:CE1	28:7:710:SER:HB2	2.48	0.49
1:A:316:GLN:N	1:A:320:ARG:O	2.42	0.49
1:A:849:MET:HB2	1:A:1063:MET:SD	2.53	0.49
1:A:914:GLU:HG2	1:A:979:SER:O	2.13	0.49
1:A:1422:ARG:NH2	2:B:1222:ARG:HH21	2.11	0.49
2:B:784:ASN:HB3	10:J:63:TYR:OH	2.13	0.49
2:B:889:THR:OG1	2:B:890:TYR:N	2.45	0.49
2:B:905:VAL:HG23	2:B:941:LEU:HD22	1.93	0.49
3:C:179:GLU:HG3	3:C:180:TYR:N	2.25	0.49
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.95	0.49
4:D:166:LEU:HD11	4:D:210:ILE:HD12	1.95	0.49
5:E:91:LYS:HA	5:E:94:LYS:HB2	1.95	0.49
9:I:7:CYS:O	9:I:11:ASN:HA	2.13	0.49
15:R:107:LEU:HD13	15:R:119:GLU:HG3	1.95	0.49
15:R:315:LEU:O	15:R:319:LYS:N	2.29	0.49
18:O:99:PHE:HZ	20:N:25:DA:H2	1.61	0.49
21:0:111:ARG:HG3	21:0:193:TYR:CE1	2.48	0.49
21:0:156:CYS:C	21:0:158:TYR:H	2.19	0.49
21:0:264:ALA:HB1	21:0:336:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:530:ALA:O	21:0:567:LYS:HE3	2.13	0.49
21:0:535:ASP:OD1	21:0:535:ASP:N	2.44	0.49
22:1:263:TYR:O	22:1:266:VAL:N	2.44	0.49
23:4:32:ILE:HG13	23:4:79:TYR:HA	1.93	0.49
23:4:51:ILE:HD12	23:4:52:LYS:N	2.27	0.49
25:2:20:GLN:O	25:2:24:ARG:N	2.39	0.49
28:7:326:VAL:HG23	28:7:329:ARG:NH2	2.27	0.49
28:7:439:THR:C	28:7:441:ASP:N	2.71	0.49
28:7:710:SER:O	28:7:713:THR:OG1	2.23	0.49
1:A:173:THR:O	1:A:183:GLY:HA2	2.13	0.48
2:B:486:TYR:CA	2:B:1096:ARG:HH22	2.26	0.48
8:H:50:ALA:N	8:H:53:ASP:OD2	2.27	0.48
8:H:90:ALA:HA	8:H:93:TYR:HD1	1.77	0.48
16:W:112:ASP:HB3	16:W:168:LYS:HE2	1.93	0.48
17:X:170:GLU:N	17:X:179:LYS:H	2.10	0.48
18:O:76:LEU:HD12	18:O:80:LEU:HD11	1.95	0.48
19:T:146:DA:H2'	19:T:147:DT:O4'	2.12	0.48
21:0:294:HIS:NE2	21:0:297:ASP:HB2	2.28	0.48
21:0:740:SER:HB3	21:0:744:LEU:HD22	1.94	0.48
25:2:380:ARG:HH12	25:2:440:GLN:C	2.21	0.48
25:2:466:GLN:HB3	25:2:470:LEU:HD23	1.95	0.48
28:7:458:SER:HA	28:7:461:ALA:HB3	1.95	0.48
28:7:604:LYS:HD3	28:7:650:ASN:HB3	1.94	0.48
28:7:762:GLU:O	28:7:765:LEU:HG	2.13	0.48
1:A:95:PHE:O	1:A:99:ILE:N	2.46	0.48
2:B:598:GLU:O	2:B:602:THR:HG23	2.13	0.48
5:E:99:HIS:HE1	5:E:103:LYS:HG3	1.78	0.48
5:E:162:ARG:CZ	5:E:162:ARG:HB3	2.43	0.48
21:0:111:ARG:HG3	21:0:193:TYR:CZ	2.48	0.48
23:4:115:TYR:C	23:4:117:ARG:H	2.20	0.48
26:5:20:ILE:O	26:5:23:ILE:HB	2.13	0.48
28:7:113:PHE:O	28:7:115:SER:N	2.45	0.48
28:7:624:LYS:HB2	28:7:653:PHE:CE1	2.47	0.48
28:7:754:ARG:HD2	28:7:757:ARG:HE	1.78	0.48
1:A:66:LYS:HA	1:A:72:GLU:HA	1.94	0.48
1:A:873:MET:HE3	1:A:1056:SER:HB2	1.95	0.48
1:A:925:LEU:O	1:A:928:LEU:N	2.46	0.48
2:B:37:PHE:CE2	2:B:41:LYS:HD2	2.49	0.48
2:B:248:SER:N	2:B:418:LYS:HE3	2.27	0.48
2:B:1009:ASP:OD2	10:J:9:SER:OG	2.30	0.48
4:D:56:ARG:HH22	4:D:57:LEU:HG	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:14:HIS:ND1	7:G:16:SER:OG	2.45	0.48
13:M:38:PHE:HZ	13:M:58:ASP:HA	1.78	0.48
20:N:20:DT:H2"	20:N:21:DA:N7	2.27	0.48
21:0:111:ARG:HB3	21:0:129:VAL:HG12	1.95	0.48
21:0:158:TYR:O	21:0:162:LEU:N	2.29	0.48
21:0:643:ARG:HD2	21:0:650:GLU:HG3	1.94	0.48
25:2:175:GLU:N	25:2:183:LYS:H	2.11	0.48
25:2:353:SER:O	25:2:356:GLN:N	2.46	0.48
27:3:47:PHE:HB3	27:3:65:LYS:HB2	1.95	0.48
28:7:228:LYS:O	28:7:231:ARG:N	2.46	0.48
28:7:325:VAL:HG13	28:7:329:ARG:HE	1.78	0.48
4:D:210:ILE:O	4:D:214:LEU:N	2.40	0.48
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.94	0.48
16:W:115:LYS:HB3	16:W:164:LYS:HD3	1.94	0.48
21:0:161:ASN:HA	21:0:164:ASN:CG	2.37	0.48
21:0:380:ARG:HH11	21:0:383:LEU:HD11	1.77	0.48
22:1:295:LYS:HB3	22:1:295:LYS:HZ3	1.78	0.48
22:1:558:CYS:HA	22:1:561:LEU:HD23	1.96	0.48
23:4:275:SER:HB2	23:4:281:ARG:C	2.39	0.48
24:6:222:LEU:O	24:6:230:ARG:NH2	2.28	0.48
24:6:253:SER:O	24:6:257:GLU:HG2	2.14	0.48
25:2:405:HIS:CE1	25:2:409:ARG:HG2	2.48	0.48
25:2:498:ASN:CG	25:2:501:VAL:HB	2.38	0.48
28:7:103:ASP:C	28:7:529:PHE:HB2	2.38	0.48
28:7:393:THR:O	28:7:397:ILE:HG12	2.12	0.48
28:7:408:ILE:HD11	28:7:482:TRP:CZ2	2.49	0.48
28:7:498:PHE:HE1	28:7:499:ARG:HH21	1.60	0.48
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.48	0.48
1:A:579:SER:OG	1:A:612:ILE:HG13	2.13	0.48
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.94	0.48
1:A:1448:GLU:O	1:A:1451:VAL:HG13	2.13	0.48
2:B:519:TRP:CD1	2:B:519:TRP:C	2.92	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.95	0.48
2:B:1152:MET:HE1	2:B:1195:HIS:HB3	1.95	0.48
4:D:128:VAL:O	4:D:131:GLU:HB3	2.14	0.48
4:D:217:LEU:O	4:D:219:THR:HG23	2.14	0.48
7:G:121:PHE:CZ	7:G:123:ALA:HA	2.49	0.48
21:0:468:MET:HA	21:0:471:ARG:HB2	1.94	0.48
21:0:608:GLU:C	21:0:668:ARG:HH22	2.21	0.48
23:4:117:ARG:NH1	25:2:37:ARG:HH22	2.12	0.48
24:6:338:CYS:C	24:6:339:HIS:HD1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:368:LYS:HG2	28:7:369:SER:H	1.77	0.48
28:7:540:TRP:HE1	28:7:692:ARG:NH1	2.12	0.48
28:7:701:PHE:CE1	28:7:703:ALA:HB2	2.48	0.48
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.94	0.48
1:A:1132:LYS:HD3	1:A:1284:MET:HE1	1.96	0.48
5:E:136:ASN:HD21	5:E:138:ALA:HB3	1.79	0.48
7:G:90:THR:HG22	7:G:141:SER:C	2.39	0.48
14:Q:130:VAL:HA	14:Q:133:PHE:HB2	1.94	0.48
15:R:73:LEU:HA	15:R:224:VAL:HB	1.95	0.48
16:W:132:THR:HG22	16:W:135:GLU:HG2	1.96	0.48
22:1:224:UNK:C	22:1:226:GLN:H	2.27	0.48
22:1:551:ARG:HE	22:1:616:LEU:HD11	1.78	0.48
22:1:620:LEU:HA	22:1:623:ILE:HD11	1.96	0.48
25:2:66:VAL:HG12	25:2:67:ASN:O	2.13	0.48
28:7:342:ASP:OD2	28:7:345:ASN:HB3	2.14	0.48
28:7:565:PHE:CE1	28:7:585:PRO:HD3	2.48	0.48
28:7:613:TYR:H	28:7:613:TYR:HD2	1.54	0.48
1:A:416:ARG:HH21	13:M:37:ARG:CZ	2.27	0.48
1:A:959:ASN:O	1:A:963:ILE:HG13	2.14	0.48
1:A:1147:THR:HA	1:A:1197:LEU:HA	1.95	0.48
5:E:12:LEU:HD21	5:E:58:MET:HE1	1.96	0.48
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.49	0.48
17:X:144:VAL:O	17:X:148:LEU:N	2.45	0.48
20:N:42:DT:H2"	20:N:43:DA:C8	2.49	0.48
21:0:232:VAL:N	21:0:455:SER:O	2.44	0.48
21:0:546:TYR:CZ	21:0:550:ILE:HD11	2.48	0.48
21:0:636:LYS:HA	21:0:639:LEU:HB2	1.95	0.48
22:1:585:HIS:O	22:1:589:CYS:N	2.35	0.48
23:4:217:GLY:HA3	23:4:219:LYS:NZ	2.29	0.48
23:4:235:TYR:C	23:4:236:LEU:HD23	2.39	0.48
23:4:305:CYS:C	23:4:307:ALA:H	2.21	0.48
25:2:62:LEU:O	25:2:65:TRP:HB2	2.13	0.48
25:2:174:GLU:H	25:2:185:THR:H	1.61	0.48
26:5:24:ASP:HA	26:5:27:MET:C	2.38	0.48
26:5:24:ASP:C	26:5:27:MET:H	2.20	0.48
26:5:55:ASN:O	26:5:58:LEU:HG	2.14	0.48
28:7:302:GLU:CG	28:7:329:ARG:HH22	2.26	0.48
28:7:309:ASP:CB	28:7:337:VAL:HB	2.44	0.48
28:7:375:GLY:HA3	28:7:380:ARG:HD2	1.95	0.48
28:7:403:ILE:O	28:7:405:LYS:NZ	2.42	0.48
28:7:439:THR:O	28:7:441:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:483:GLY:HA2	28:7:508:HIS:HB2	1.94	0.48
2:B:486:TYR:HB3	2:B:1096:ARG:NH1	2.25	0.48
2:B:739:THR:O	2:B:740:HIS:CG	2.66	0.48
2:B:841:MET:HG2	2:B:842:ASN:H	1.79	0.48
4:D:120:GLU:OE1	4:D:120:GLU:N	2.44	0.48
11:K:11:LEU:O	11:K:12:LEU:C	2.57	0.48
15:R:68:VAL:HG22	15:R:218:VAL:HA	1.95	0.48
16:W:127:CYS:HB3	16:W:151:LEU:HD22	1.96	0.48
18:O:136:SER:HA	18:O:139:TYR:HD2	1.77	0.48
21:0:66:HIS:CD2	21:0:230:SER:HA	2.49	0.48
21:0:270:ARG:O	21:0:273:GLU:HG2	2.12	0.48
21:0:395:ASP:OD1	21:0:396:PHE:N	2.45	0.48
21:0:422:PRO:HA	21:0:433:PRO:HB3	1.95	0.48
22:1:257:LEU:HA	22:1:260:PHE:CD2	2.48	0.48
22:1:623:ILE:HA	22:1:626:ALA:HB3	1.96	0.48
23:4:184:GLY:C	23:4:186:SER:H	2.22	0.48
23:4:288:ILE:HA	23:4:294:CYS:O	2.12	0.48
25:2:454:TYR:N	26:5:9:LEU:O	2.28	0.48
28:7:493:VAL:HG12	28:7:498:PHE:HB2	1.95	0.48
1:A:167:CYS:O	1:A:169:ASN:N	2.47	0.48
1:A:1255:GLU:OE1	1:A:1256:GLU:N	2.47	0.48
2:B:865:LYS:HD3	2:B:868:MET:SD	2.54	0.48
2:B:868:MET:HG2	13:M:149:CYS:SG	2.53	0.48
5:E:83:CYS:C	5:E:113:GLN:HE22	2.22	0.48
7:G:148:GLU:OE2	7:G:162:SER:OG	2.20	0.48
9:I:37:GLU:OE1	9:I:39:GLY:N	2.47	0.48
18:O:71:VAL:HG12	18:O:122:VAL:HG12	1.96	0.48
21:0:1:MET:O	21:0:12:PHE:N	2.47	0.48
21:0:4:TYR:HA	21:0:8:LEU:O	2.14	0.48
21:0:43:PRO:HG3	21:0:696:TRP:CD1	2.48	0.48
21:0:334:PHE:CD1	21:0:369:ILE:HG23	2.48	0.48
23:4:260:PRO:HD2	23:4:261:ILE:HG22	1.96	0.48
26:5:30:ILE:HD12	26:5:46:LYS:HG3	1.96	0.48
28:7:302:GLU:HG3	28:7:322:SER:HB2	1.96	0.48
28:7:655:SER:OG	28:7:656:LYS:N	2.47	0.48
1:A:544:ASP:OD1	1:A:544:ASP:N	2.40	0.48
2:B:289:LEU:HD22	2:B:371:GLU:HB3	1.96	0.48
7:G:4:ILE:HG13	7:G:77:VAL:HG12	1.96	0.48
12:L:26:THR:OG1	12:L:40:LEU:O	2.19	0.48
21:0:67:ARG:O	21:0:204:ASN:HB3	2.14	0.48
21:0:517:SER:HA	21:0:520:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:199:VAL:C	22:1:202:ALA:H	2.22	0.48
22:1:231:UNK:HA	22:1:385:MET:SD	2.53	0.48
22:1:263:TYR:O	22:1:266:VAL:HG22	2.13	0.48
24:6:403:CYS:CB	24:6:408:SER:H	2.27	0.48
28:7:443:LYS:H	28:7:443:LYS:HG3	1.35	0.48
1:A:672:ASP:OD1	1:A:672:ASP:N	2.47	0.47
1:A:913:LEU:HD12	1:A:915:SER:H	1.79	0.47
1:A:923:LEU:HD12	1:A:923:LEU:HA	1.58	0.47
2:B:241:ARG:NH2	2:B:243:ALA:HB2	2.28	0.47
3:C:240:VAL:O	3:C:241:ASP:C	2.57	0.47
5:E:46:TYR:CD1	5:E:58:MET:HG3	2.49	0.47
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.61	0.47
5:E:67:GLU:OE1	5:E:68:SER:OG	2.31	0.47
5:E:122:LYS:O	5:E:125:PRO:HD2	2.14	0.47
8:H:14:GLU:HG3	8:H:27:GLU:HB2	1.96	0.47
15:R:127:LYS:HA	15:R:220:HIS:ND1	2.28	0.47
18:O:160:ILE:HD12	18:O:220:ARG:N	2.29	0.47
21:0:71:TYR:HD1	21:0:207:ILE:HG22	1.78	0.47
21:0:106:LEU:HD11	21:0:176:PHE:HB2	1.96	0.47
21:0:156:CYS:HB2	21:0:158:TYR:CD2	2.49	0.47
21:0:169:ASP:OD1	21:0:170:TYR:N	2.40	0.47
21:0:688:ARG:H	21:0:688:ARG:HG2	1.46	0.47
26:5:10:VAL:O	26:5:40:LEU:N	2.47	0.47
27:3:133:LEU:O	27:3:137:GLU:N	2.29	0.47
28:7:234:VAL:H	28:7:316:PHE:N	2.12	0.47
28:7:320:ASN:HD21	28:7:348:ARG:CZ	2.27	0.47
28:7:540:TRP:HE1	28:7:692:ARG:HH12	1.62	0.47
1:A:335:ARG:NH2	2:B:1114:LEU:HD21	2.30	0.47
1:A:625:SER:OG	1:A:626:ASN:N	2.45	0.47
2:B:94:LYS:HD2	2:B:96:TYR:CZ	2.50	0.47
2:B:294:ASP:HA	2:B:297:ILE:HB	1.97	0.47
2:B:343:ILE:HA	2:B:348:ARG:HH22	1.79	0.47
2:B:356:LEU:O	2:B:360:PHE:HB3	2.14	0.47
2:B:848:ARG:NH1	10:J:8:PHE:O	2.46	0.47
4:D:193:THR:HB	7:G:167:TYR:CE2	2.48	0.47
9:I:110:PHE:N	9:I:110:PHE:CD1	2.82	0.47
11:K:35:PHE:N	11:K:35:PHE:CD1	2.81	0.47
15:R:126:LYS:HB3	15:R:221:GLU:HB3	1.97	0.47
19:T:105:DA:C2	19:T:106:DA:C5	3.02	0.47
19:T:126:DA:H2"	19:T:127:DG:H8	1.79	0.47
21:0:110:SER:HB3	22:1:345:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:133:CYS:HA	21:0:136:MET:SD	2.54	0.47
28:7:104:PHE:N	28:7:529:PHE:H	2.11	0.47
28:7:347:HIS:C	28:7:349:ASN:N	2.69	0.47
28:7:407:VAL:CG2	28:7:484:PHE:HB3	2.41	0.47
28:7:598:HIS:HA	28:7:601:ARG:CZ	2.44	0.47
28:7:601:ARG:HH22	28:7:603:ASP:HB2	1.79	0.47
1:A:95:PHE:O	1:A:99:ILE:HG13	2.14	0.47
2:B:978:ASP:O	2:B:989:THR:HA	2.14	0.47
7:G:9:LEU:N	7:G:72:VAL:O	2.47	0.47
14:Q:359:ASN:N	14:Q:359:ASN:OD1	2.46	0.47
14:Q:378:VAL:HB	15:R:67:GLN:H	1.80	0.47
18:O:63:ILE:HD13	18:O:166:VAL:HA	1.95	0.47
18:O:81:ASP:HB3	18:O:148:PHE:HZ	1.79	0.47
21:0:75:THR:HG23	21:0:78:GLU:H	1.78	0.47
21:0:241:ASP:OD1	21:0:241:ASP:N	2.46	0.47
22:1:208:GLU:H	22:1:208:GLU:CD	2.16	0.47
22:1:260:PHE:HB3	22:1:267:LYS:HB2	1.96	0.47
22:1:491:UNK:C	22:1:493:UNK:N	2.77	0.47
22:1:591:GLU:O	22:1:595:GLU:N	2.29	0.47
23:4:217:GLY:O	23:4:219:LYS:N	2.47	0.47
23:4:304:LYS:HG3	23:4:309:ASP:HA	1.95	0.47
28:7:440:SER:C	28:7:443:LYS:HG2	2.40	0.47
1:A:106:VAL:HG22	1:A:113:LEU:HA	1.95	0.47
1:A:1188:GLN:HE22	1:A:1225:PHE:HB2	1.80	0.47
2:B:487:THR:OG1	2:B:488:TYR:N	2.47	0.47
7:G:91:VAL:HA	7:G:101:VAL:HA	1.95	0.47
7:G:148:GLU:HG2	7:G:161:GLY:HA2	1.96	0.47
8:H:23:VAL:HA	8:H:42:ILE:O	2.15	0.47
13:M:164:LYS:HE2	19:T:138:DA:H3'	1.95	0.47
21:0:236:GLU:N	21:0:459:THR:O	2.47	0.47
21:0:544:TYR:OH	21:0:573:THR:HA	2.15	0.47
22:1:210:TRP:O	22:1:212:THR:N	2.48	0.47
22:1:259:ILE:HG23	22:1:263:TYR:HD2	1.78	0.47
23:4:162:ARG:HE	24:6:407:GLN:C	2.22	0.47
25:2:452:ILE:HB	26:5:11:GLN:CD	2.40	0.47
26:5:22:GLN:HA	26:5:25:ALA:HB3	1.96	0.47
28:7:246:LEU:C	28:7:248:ASP:H	2.22	0.47
28:7:335:TYR:HB3	28:7:337:VAL:HG13	1.95	0.47
28:7:409:VAL:C	28:7:410:LEU:HD12	2.40	0.47
28:7:526:ASP:C	28:7:528:ASN:H	2.21	0.47
28:7:568:GLU:HA	28:7:571:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.96	0.47
1:A:1436:ILE:O	1:A:1437:GLY:C	2.58	0.47
2:B:195:CYS:SG	2:B:783:THR:OG1	2.43	0.47
2:B:668:ASP:N	2:B:668:ASP:OD1	2.47	0.47
4:D:162:ALA:O	4:D:166:LEU:N	2.39	0.47
11:K:17:SER:H	11:K:20:LYS:HZ2	1.63	0.47
12:L:31:CYS:HB3	12:L:35:SER:H	1.79	0.47
20:N:11:DA:H1'	20:N:12:DG:C8	2.50	0.47
21:O:248:LEU:HA	21:O:248:LEU:HD13	1.71	0.47
24:6:374:THR:O	24:6:378:ARG:N	2.46	0.47
25:2:395:GLN:NE2	25:2:395:GLN:H	2.12	0.47
26:5:8:ALA:HB3	26:5:42:VAL:C	2.39	0.47
28:7:430:LEU:HG	28:7:431:GLN:N	2.30	0.47
1:A:1163:ILE:HA	1:A:1163:ILE:HD13	1.77	0.47
3:C:241:ASP:OD1	3:C:242:GLN:N	2.47	0.47
9:I:31:THR:OG1	9:I:32:CYS:N	2.46	0.47
13:M:126:VAL:HG22	13:M:158:HIS:CE1	2.50	0.47
13:M:269:ILE:H	13:M:269:ILE:HD12	1.77	0.47
16:W:46:LEU:HD22	17:X:203:LYS:HD2	1.95	0.47
21:O:240:ILE:HA	21:O:240:ILE:HD12	1.63	0.47
21:O:250:LEU:HD13	22:1:350:ARG:CZ	2.44	0.47
21:O:301:ASP:HB3	21:O:304:GLU:HB2	1.96	0.47
21:O:361:GLN:O	21:O:365:GLN:N	2.42	0.47
21:O:424:GLU:H	21:O:432:ASN:ND2	2.12	0.47
21:O:659:MET:HA	21:O:662:ALA:HB3	1.97	0.47
25:2:81:MET:O	25:2:85:HIS:N	2.47	0.47
28:7:236:THR:O	28:7:313:VAL:N	2.47	0.47
28:7:526:ASP:HB2	28:7:528:ASN:ND2	2.29	0.47
28:7:534:LYS:HZ2	28:7:537:GLU:N	2.12	0.47
28:7:563:ALA:HA	28:7:566:TYR:HB3	1.96	0.47
28:7:698:ASP:OD1	28:7:699:GLU:HG2	2.15	0.47
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.79	0.47
1:A:390:GLN:OE1	1:A:393:ARG:NH1	2.47	0.47
1:A:709:THR:OG1	1:A:710:LEU:N	2.48	0.47
1:A:993:LEU:HD13	1:A:1046:LEU:HD22	1.96	0.47
1:A:1048:ASN:O	1:A:1051:ALA:N	2.48	0.47
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.54	0.47
1:A:1256:GLU:H	1:A:1256:GLU:CD	2.23	0.47
2:B:70:ILE:O	14:Q:332:LEU:HB2	2.15	0.47
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.78	0.47
2:B:1202:LEU:HD23	2:B:1202:LEU:HA	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.97	0.47
4:D:141:LEU:O	4:D:144:THR:HG23	2.14	0.47
9:I:8:ARG:C	9:I:10:CYS:H	2.22	0.47
11:K:9:LEU:HA	11:K:9:LEU:HD22	1.72	0.47
11:K:77:THR:OG1	11:K:81:TYR:O	2.26	0.47
21:0:63:TYR:O	21:0:67:ARG:NH2	2.47	0.47
21:0:112:LYS:HZ3	21:0:124:ARG:HA	1.79	0.47
21:0:140:GLN:NE2	21:0:389:GLU:H	2.13	0.47
21:0:354:GLU:OE1	21:0:359:PHE:N	2.48	0.47
21:0:499:LYS:HB3	21:0:503:GLN:C	2.39	0.47
21:0:514:ASN:OD1	21:0:514:ASN:N	2.48	0.47
21:0:583:LEU:HD23	22:1:337:ILE:HG21	1.96	0.47
22:1:551:ARG:HH11	24:6:340:SER:HA	1.80	0.47
23:4:153:MET:HE1	23:4:196:ILE:HG23	1.95	0.47
24:6:132:CYS:HB2	24:6:175:ARG:HG2	1.97	0.47
24:6:139:LYS:HZ1	24:6:144:ASN:HB3	1.78	0.47
25:2:10:VAL:O	25:2:14:LEU:HD22	2.15	0.47
25:2:24:ARG:O	25:2:27:THR:HG22	2.15	0.47
25:2:90:ASN:HB3	25:2:97:MET:HB2	1.95	0.47
26:5:43:ASN:C	26:5:47:VAL:HG13	2.40	0.47
28:7:226:VAL:CA	28:7:235:GLU:H	2.28	0.47
28:7:303:ARG:HA	28:7:321:GLU:H	1.78	0.47
28:7:428:CYS:HG	28:7:429:THR:H	1.61	0.47
28:7:585:PRO:O	28:7:588:PHE:HD1	1.97	0.47
2:B:101:MET:HB2	2:B:110:HIS:O	2.15	0.47
4:D:147:TYR:CD1	4:D:147:TYR:C	2.92	0.47
13:M:199:LYS:C	13:M:201:LYS:H	2.22	0.47
14:Q:98:TYR:HB3	15:R:97:ILE:O	2.15	0.47
21:0:643:ARG:NH1	21:0:650:GLU:H	2.13	0.47
25:2:108:LEU:O	25:2:112:LEU:N	2.41	0.47
25:2:346:LYS:HB2	25:2:377:GLN:NE2	2.30	0.47
25:2:365:HIS:NE2	25:2:377:GLN:O	2.47	0.47
26:5:5:ARG:HD3	26:5:6:LYS:C	2.40	0.47
26:5:26:LYS:CD	26:5:27:MET:HG2	2.36	0.47
28:7:357:LYS:NZ	28:7:357:LYS:HB2	2.30	0.47
28:7:393:THR:O	28:7:397:ILE:N	2.46	0.47
28:7:593:PHE:HB2	28:7:745:ILE:HG13	1.96	0.47
1:A:121:LEU:HA	1:A:124:GLN:HB3	1.97	0.47
1:A:500:GLU:OE1	2:B:1145:SER:OG	2.25	0.47
4:D:25:ALA:C	4:D:27:LEU:H	2.23	0.47
7:G:145:VAL:HG13	7:G:163:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:32:THR:OG1	8:H:33:GLN:N	2.47	0.47
15:R:125:THR:HB	15:R:221:GLU:HG3	1.97	0.47
16:W:8:ILE:O	16:W:12:LEU:N	2.31	0.47
21:0:518:ILE:O	21:0:522:TYR:N	2.45	0.47
21:0:606:VAL:O	21:0:610:ILE:HG12	2.15	0.47
21:0:626:PRO:HG2	21:0:658:ALA:HB1	1.97	0.47
22:1:224:UNK:O	22:1:226:GLN:N	2.46	0.47
22:1:280:GLU:HA	22:1:284:TRP:CD1	2.50	0.47
24:6:150:ILE:HD12	24:6:200:ARG:HA	1.97	0.47
24:6:314:ASN:HB3	24:6:317:PHE:HZ	1.79	0.47
25:2:18:PRO:HB2	25:2:20:GLN:HE22	1.80	0.47
25:2:473:LYS:HD2	25:2:476:GLN:OE1	2.14	0.47
25:2:482:LEU:N	25:2:492:PHE:O	2.32	0.47
25:2:490:LYS:NZ	26:5:33:GLU:OE2	2.25	0.47
28:7:304:GLU:HG3	28:7:508:HIS:HE1	1.80	0.47
28:7:407:VAL:HA	28:7:484:PHE:O	2.15	0.47
28:7:558:TRP:C	28:7:711:LYS:HG2	2.39	0.47
1:A:708:MET:HB2	1:A:712:GLU:HB2	1.97	0.47
2:B:25:ILE:HA	2:B:655:LYS:HE3	1.96	0.47
2:B:98:THR:OG1	2:B:99:LYS:N	2.48	0.47
7:G:96:GLN:HG2	7:G:97:HIS:ND1	2.30	0.47
14:Q:98:TYR:HA	15:R:97:ILE:HG12	1.96	0.47
16:W:173:ASN:HA	16:W:176:MET:HB2	1.95	0.47
21:0:306:PHE:CZ	21:0:393:VAL:HG13	2.50	0.47
21:0:383:LEU:HD12	21:0:384:LEU:HD23	1.97	0.47
21:0:681:LEU:HD23	21:0:686:PHE:CG	2.50	0.47
21:0:716:ASN:OD1	21:0:716:ASN:N	2.49	0.47
22:1:239:PRO:O	22:1:241:UNK:N	2.48	0.47
23:4:166:GLU:CD	23:4:166:GLU:C	2.83	0.47
25:2:72:LEU:HA	25:2:75:GLN:OE1	2.15	0.47
28:7:302:GLU:HG3	28:7:322:SER:CB	2.45	0.47
28:7:562:THR:HG21	28:7:585:PRO:HG2	1.97	0.47
28:7:683:GLU:HB3	28:7:722:ARG:HH22	1.80	0.47
1:A:295:LEU:O	1:A:298:PHE:N	2.46	0.46
1:A:1106:ASN:O	1:A:1107:VAL:C	2.57	0.46
1:A:1223:ASP:OD1	1:A:1224:LEU:N	2.48	0.46
7:G:10:ASN:HA	7:G:70:PHE:O	2.14	0.46
8:H:80:ARG:HG2	11:K:57:LEU:HD13	1.96	0.46
9:I:29:CYS:O	9:I:31:THR:N	2.48	0.46
16:W:149:CYS:SG	16:W:152:CYS:N	2.85	0.46
20:N:20:DT:O3'	20:N:21:DA:C8	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:72:CYS:SG	21:0:210:TYR:HA	2.55	0.46
21:0:138:ASN:HB3	21:0:141:ALA:CB	2.44	0.46
21:0:144:LYS:O	21:0:153:VAL:HG21	2.15	0.46
21:0:353:SER:HA	21:0:419:ILE:HA	1.97	0.46
21:0:605:LYS:H	21:0:605:LYS:CE	2.28	0.46
22:1:178:LEU:O	22:1:182:GLN:N	2.25	0.46
23:4:122:ASP:O	23:4:126:VAL:HG23	2.14	0.46
23:4:137:LYS:N	23:4:140:ILE:HG13	2.31	0.46
24:6:119:GLN:O	24:6:309:PRO:HG3	2.15	0.46
24:6:175:ARG:HH21	24:6:204:PRO:C	2.24	0.46
24:6:192:HIS:O	24:6:196:LEU:HD12	2.15	0.46
24:6:293:ASP:O	24:6:296:HIS:HB2	2.15	0.46
25:2:350:TYR:O	25:2:372:ASN:HB2	2.15	0.46
25:2:408:MET:O	25:2:411:LEU:HB3	2.14	0.46
28:7:440:SER:HB3	28:7:467:SER:OG	2.14	0.46
1:A:178:GLY:HA3	13:M:106:PHE:CE2	2.51	0.46
1:A:1212:VAL:O	1:A:1216:ILE:HG12	2.16	0.46
2:B:279:ASP:OD1	2:B:279:ASP:N	2.47	0.46
2:B:422:LYS:O	2:B:425:THR:N	2.48	0.46
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.98	0.46
2:B:836:GLU:O	2:B:837:ASP:HB2	2.15	0.46
4:D:156:ASP:O	4:D:158:GLU:N	2.48	0.46
8:H:36:CYS:HA	8:H:126:GLU:O	2.15	0.46
9:I:72:ASP:O	9:I:81:ARG:HB3	2.15	0.46
14:Q:377:SER:O	14:Q:384:PHE:HD1	1.99	0.46
15:R:70:LEU:HD12	15:R:71:VAL:N	2.29	0.46
16:W:135:GLU:O	16:W:139:LEU:N	2.43	0.46
16:W:140:LEU:HD22	16:W:147:PHE:HE1	1.80	0.46
22:1:251:LEU:O	22:1:255:LYS:HG2	2.16	0.46
22:1:260:PHE:CD1	22:1:266:VAL:HG23	2.48	0.46
24:6:134:GLU:HA	24:6:137:LEU:HD12	1.96	0.46
25:2:24:ARG:O	25:2:24:ARG:NH1	2.49	0.46
25:2:50:MET:HE3	25:2:50:MET:HB2	1.75	0.46
26:5:19:LEU:HB3	26:5:57:LEU:HD13	1.98	0.46
28:7:341:TYR:N	28:7:379:ALA:O	2.48	0.46
28:7:413:SER:OG	28:7:416:SER:N	2.48	0.46
28:7:576:LYS:H	28:7:576:LYS:HG3	1.27	0.46
1:A:260:ASP:OD2	1:A:328:ARG:NH2	2.48	0.46
1:A:566:ILE:O	1:A:567:LYS:C	2.59	0.46
1:A:965:GLN:O	1:A:966:ASN:C	2.56	0.46
2:B:87:LYS:O	2:B:137:TYR:N	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:PHE:CZ	9:I:30:ARG:HB3	2.50	0.46
7:G:101:VAL:O	7:G:108:VAL:N	2.48	0.46
9:I:21:GLU:N	9:I:21:GLU:CD	2.73	0.46
11:K:89:ASN:OD1	11:K:89:ASN:N	2.47	0.46
12:L:53:HIS:CD2	12:L:55:ILE:H	2.34	0.46
21:O:371:ARG:NE	21:O:375:ARG:HH12	2.13	0.46
21:O:393:VAL:HG12	21:O:397:THR:HG23	1.98	0.46
21:O:585:THR:O	21:O:588:LYS:N	2.48	0.46
21:O:720:PHE:HD2	21:O:721:LEU:HD22	1.80	0.46
23:4:299:ILE:N	23:4:300:PRO:HD3	2.30	0.46
24:6:141:LEU:HA	24:6:142:ARG:NH1	2.30	0.46
25:2:346:LYS:HG3	25:2:347:ILE:O	2.15	0.46
28:7:469:ASP:HA	28:7:472:LYS:HB2	1.96	0.46
28:7:495:ALA:O	28:7:499:ARG:HD2	2.15	0.46
28:7:610:ASP:OD2	28:7:675:SER:HA	2.15	0.46
28:7:690:ILE:HG22	28:7:691:LEU:HD23	1.96	0.46
1:A:332:LYS:HD2	1:A:337:ARG:NH2	2.30	0.46
1:A:1116:LEU:HD12	1:A:1117:THR:N	2.30	0.46
1:A:1168:GLU:C	1:A:1171:GLN:HE21	2.24	0.46
2:B:450:ALA:C	2:B:452:THR:H	2.24	0.46
2:B:694:ASP:C	2:B:694:ASP:OD1	2.58	0.46
2:B:807:ARG:H	2:B:1045:SER:HG	1.61	0.46
2:B:1120:GLU:HG3	2:B:1121:GLY:N	2.28	0.46
4:D:152:SER:C	4:D:153:ARG:HD3	2.41	0.46
4:D:158:GLU:HA	4:D:161:GLY:HA3	1.97	0.46
7:G:165:GLU:HG3	27:3:51:PRO:HD3	1.96	0.46
13:M:130:PHE:HA	13:M:133:ILE:HG12	1.96	0.46
14:Q:375:LEU:HA	14:Q:375:LEU:HD13	1.56	0.46
15:R:125:THR:OG1	15:R:223:GLN:N	2.48	0.46
21:O:283:GLN:O	21:O:286:TYR:HB2	2.15	0.46
24:6:148:MET:HE3	24:6:152:TYR:HE1	1.80	0.46
24:6:251:ILE:HG12	24:6:276:LEU:HD13	1.97	0.46
24:6:332:THR:C	24:6:334:THR:H	2.24	0.46
28:7:582:ILE:O	28:7:587:LYS:NZ	2.37	0.46
28:7:614:ALA:HA	28:7:617:GLU:CD	2.40	0.46
1:A:287:HIS:HA	1:A:290:GLU:OE1	2.16	0.46
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.15	0.46
1:A:704:ALA:HB1	1:A:708:MET:O	2.15	0.46
1:A:1255:GLU:HB3	1:A:1258:HIS:NE2	2.30	0.46
3:C:226:ASP:N	3:C:226:ASP:OD1	2.49	0.46
9:I:74:GLU:HB3	9:I:81:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:338:LEU:O	21:0:342:LEU:HG	2.15	0.46
21:0:405:PHE:O	21:0:409:ILE:HG22	2.15	0.46
21:0:423:TYR:HA	21:0:432:ASN:C	2.40	0.46
21:0:565:LYS:HG2	21:0:566:HIS:ND1	2.30	0.46
21:0:613:ASP:O	21:0:617:GLY:N	2.44	0.46
21:0:722:ARG:HD2	24:6:292:LEU:HA	1.97	0.46
22:1:267:LYS:O	22:1:271:THR:OG1	2.33	0.46
23:4:244:LEU:H	23:4:244:LEU:HG	1.36	0.46
24:6:175:ARG:HB2	24:6:176:ASN:ND2	2.30	0.46
25:2:208:LEU:HG	25:2:209:LYS:N	2.30	0.46
25:2:347:ILE:O	25:2:373:MET:HE1	2.15	0.46
25:2:460:SER:O	26:5:3:ARG:HD3	2.15	0.46
28:7:324:GLU:O	28:7:327:LYS:HE2	2.16	0.46
28:7:363:ARG:O	28:7:365:TYR:N	2.47	0.46
28:7:542:GLU:O	28:7:545:GLN:HG2	2.15	0.46
28:7:578:MET:O	28:7:581:TYR:HB3	2.15	0.46
28:7:754:ARG:HA	28:7:757:ARG:HB2	1.97	0.46
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.72	0.46
2:B:73:GLN:O	2:B:86:ARG:N	2.49	0.46
2:B:87:LYS:N	2:B:137:TYR:O	2.46	0.46
2:B:431:TYR:HE1	2:B:442:PHE:CE2	2.33	0.46
5:E:98:ILE:HG13	5:E:99:HIS:N	2.30	0.46
7:G:1:MET:SD	7:G:2:PHE:N	2.89	0.46
7:G:22:MET:HA	7:G:25:TYR:CD1	2.50	0.46
9:I:13:MET:HE3	9:I:13:MET:HB2	1.70	0.46
13:M:249:PRO:O	13:M:252:VAL:HG13	2.14	0.46
13:M:287:LEU:HD13	13:M:287:LEU:HA	1.80	0.46
14:Q:106:ILE:HD12	14:Q:385:THR:HB	1.97	0.46
15:R:97:ILE:HB	15:R:104:ILE:HG23	1.98	0.46
19:T:151:DC:H2'	19:T:151:DC:OP2	2.15	0.46
20:N:19:DA:H2'	20:N:20:DT:H6	1.80	0.46
21:0:76:MET:SD	21:0:77:SER:N	2.89	0.46
21:0:705:ASP:O	21:0:708:LEU:HG	2.16	0.46
22:1:197:GLU:HA	22:1:201:ASN:OD1	2.15	0.46
22:1:507:ILE:O	22:1:510:ASN:N	2.46	0.46
25:2:39:LEU:O	25:2:44:LYS:HE3	2.16	0.46
25:2:398:ALA:HA	25:2:401:GLU:HB2	1.98	0.46
26:5:46:LYS:O	26:5:49:PHE:HB3	2.16	0.46
26:5:56:ARG:HB3	26:5:60:LYS:HE2	1.98	0.46
28:7:357:LYS:HE3	28:7:401:CYS:SG	2.56	0.46
28:7:495:ALA:HB1	28:7:499:ARG:NE	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:681:ARG:H	28:7:681:ARG:HG2	1.50	0.46
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.43	0.46
1:A:1025:ARG:HD3	1:A:1025:ARG:HA	1.70	0.46
2:B:773:MET:O	2:B:776:GLN:HG2	2.15	0.46
2:B:806:THR:HG22	2:B:808:ALA:H	1.80	0.46
2:B:883:LEU:HD12	2:B:884:ARG:H	1.81	0.46
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.98	0.46
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.59	0.46
7:G:1:MET:HG3	7:G:3:PHE:CE1	2.51	0.46
7:G:163:ILE:HB	7:G:169:GLY:N	2.31	0.46
13:M:149:CYS:O	13:M:153:ALA:N	2.36	0.46
16:W:12:LEU:O	16:W:16:VAL:HG12	2.15	0.46
16:W:60:ARG:HH12	17:X:264:GLU:HG2	1.81	0.46
17:X:271:PHE:O	17:X:274:LEU:N	2.31	0.46
21:0:256:ALA:HA	21:0:259:ARG:HH11	1.80	0.46
21:0:430:VAL:HG23	21:0:432:ASN:OD1	2.15	0.46
21:0:709:SER:OG	21:0:710:THR:N	2.49	0.46
22:1:370:UNK:C	22:1:372:VAL:N	2.79	0.46
23:4:199:CYS:O	23:4:202:SER:OG	2.29	0.46
25:2:162:LYS:O	25:2:166:LEU:N	2.36	0.46
27:3:72:ILE:HB	27:3:73:PHE:CE2	2.50	0.46
27:3:105:GLU:O	27:3:109:TYR:N	2.26	0.46
28:7:519:ARG:O	28:7:681:ARG:NH2	2.49	0.46
28:7:534:LYS:NZ	28:7:537:GLU:HG3	2.31	0.46
28:7:704:PHE:HB2	28:7:706:TYR:OH	2.16	0.46
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.70	0.46
1:A:770:VAL:HG12	1:A:771:GLU:HG3	1.96	0.46
1:A:885:THR:HG23	1:A:1024:SER:HB3	1.97	0.46
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.31	0.46
1:A:1149:ALA:HB1	9:I:47:GLU:H	1.81	0.46
2:B:282:ILE:O	2:B:285:ILE:N	2.49	0.46
2:B:816:GLU:O	2:B:817:LEU:HD23	2.16	0.46
3:C:182:PRO:HD2	3:C:210:GLU:OE2	2.16	0.46
3:C:226:ASP:O	3:C:227:THR:OG1	2.32	0.46
6:F:92:ARG:O	6:F:96:THR:HG23	2.16	0.46
8:H:25:ARG:NE	8:H:41:ASP:OD1	2.42	0.46
21:0:20:GLU:H	21:0:20:GLU:CD	2.23	0.46
21:0:69:ILE:HA	21:0:231:ILE:HG12	1.98	0.46
21:0:192:PRO:CA	21:0:195:ILE:HB	2.46	0.46
22:1:200:ILE:HG22	22:1:201:ASN:OD1	2.16	0.46
22:1:209:PHE:O	22:1:213:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:241:UNK:O	22:1:243:UNK:N	2.49	0.46
23:4:57:LEU:O	23:4:60:PHE:N	2.49	0.46
23:4:57:LEU:O	23:4:58:ILE:C	2.59	0.46
24:6:190:GLN:HA	24:6:193:ILE:HB	1.98	0.46
24:6:296:HIS:HA	24:6:299:GLU:OE2	2.16	0.46
25:2:461:ASP:HB2	26:5:3:ARG:NH1	2.31	0.46
26:5:24:ASP:CG	26:5:31:VAL:HG23	2.40	0.46
26:5:56:ARG:HB3	26:5:60:LYS:HZ1	1.81	0.46
27:3:28:PHE:O	27:3:29:LEU:HD23	2.16	0.46
27:3:36:HIS:HB3	27:3:56:TYR:CE1	2.50	0.46
28:7:482:TRP:O	28:7:508:HIS:N	2.35	0.46
28:7:579:LEU:HD12	28:7:767:ASN:ND2	2.31	0.46
1:A:120:GLU:O	1:A:123:ARG:HB2	2.16	0.46
1:A:1215:ARG:HD3	1:A:1218:GLN:OE1	2.16	0.46
1:A:1354:ASN:O	1:A:1358:SER:HB3	2.15	0.46
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.56	0.46
2:B:450:ALA:C	2:B:452:THR:N	2.74	0.46
8:H:24:CYS:O	8:H:41:ASP:HA	2.16	0.46
8:H:87:ARG:CZ	8:H:87:ARG:HA	2.46	0.46
9:I:8:ARG:NH1	9:I:8:ARG:HB2	2.31	0.46
16:W:140:LEU:HD12	16:W:140:LEU:HA	1.71	0.46
21:0:118:PRO:C	21:0:122:LYS:HZ3	2.23	0.46
21:0:471:ARG:NH1	21:0:646:TYR:HB3	2.30	0.46
21:0:656:PHE:CE1	21:0:660:ARG:HD3	2.51	0.46
21:0:657:ASP:O	21:0:661:HIS:ND1	2.29	0.46
22:1:562:LYS:HD2	22:1:562:LYS:HA	1.79	0.46
23:4:137:LYS:O	23:4:141:GLU:HG3	2.16	0.46
23:4:263:VAL:C	23:4:265:PRO:HD3	2.41	0.46
23:4:287:PHE:CG	24:6:319:LEU:HD11	2.51	0.46
24:6:273:CYS:HB2	24:6:288:TYR:HE1	1.81	0.46
24:6:449:HIS:ND1	24:6:449:HIS:N	2.64	0.46
25:2:18:PRO:O	25:2:22:GLN:HG3	2.16	0.46
25:2:462:PHE:HZ	25:2:505:ALA:CB	2.28	0.46
25:2:502:LEU:HD13	25:2:506:LYS:NZ	2.28	0.46
26:5:30:ILE:HA	26:5:43:ASN:HD22	1.80	0.46
28:7:364:PRO:HG2	28:7:546:LYS:HB3	1.97	0.46
1:A:113:LEU:HD23	1:A:114:LEU:H	1.81	0.46
2:B:342:GLY:O	2:B:348:ARG:NH2	2.49	0.46
4:D:163:VAL:HG12	4:D:167:LEU:HD11	1.97	0.46
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.31	0.46
9:I:70:ARG:HD3	9:I:70:ARG:HA	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:110:ASP:OD1	14:Q:111:LEU:N	2.47	0.46
15:R:80:LYS:C	15:R:81:TRP:CD1	2.94	0.46
21:0:48:LYS:HE3	21:0:48:LYS:HB2	1.76	0.46
21:0:86:LEU:HD21	21:0:175:VAL:HG11	1.98	0.46
21:0:489:LYS:NZ	21:0:728:THR:O	2.49	0.46
22:1:205:PRO:HB2	22:1:208:GLU:OE1	2.15	0.46
22:1:339:LEU:HA	22:1:342:ASN:ND2	2.31	0.46
24:6:293:ASP:OD2	24:6:296:HIS:N	2.48	0.46
24:6:372:LEU:HD13	24:6:375:HIS:CE1	2.48	0.46
25:2:29:PRO:HB3	25:2:107:SER:O	2.16	0.46
25:2:363:PHE:HD1	25:2:378:ILE:HD13	1.81	0.46
25:2:470:LEU:HG	25:2:471:LEU:N	2.30	0.46
28:7:234:VAL:H	28:7:316:PHE:C	2.24	0.46
28:7:309:ASP:HA	28:7:339:GLU:HA	1.97	0.46
28:7:341:TYR:N	28:7:380:ARG:HA	2.14	0.46
28:7:540:TRP:HD1	28:7:731:TYR:OH	1.99	0.46
1:A:100:LYS:O	1:A:104:GLU:HG3	2.15	0.45
1:A:549:MET:HE2	1:A:577:ILE:HG21	1.98	0.45
1:A:915:SER:O	1:A:919:ILE:HG12	2.16	0.45
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.16	0.45
1:A:1258:HIS:CD2	1:A:1258:HIS:H	2.33	0.45
2:B:705:MET:N	2:B:710:LEU:HD12	2.28	0.45
2:B:1181:GLU:OE2	2:B:1183:LYS:HB3	2.16	0.45
3:C:251:LEU:HA	3:C:251:LEU:HD12	1.61	0.45
5:E:118:PRO:HA	5:E:121:MET:CB	2.46	0.45
7:G:7:LEU:O	7:G:74:TYR:HD1	1.97	0.45
7:G:142:ARG:O	7:G:171:ILE:N	2.47	0.45
13:M:259:THR:HG21	13:M:285:ASN:HD21	1.81	0.45
14:Q:350:TRP:O	14:Q:363:GLY:N	2.48	0.45
17:X:141:PRO:HA	17:X:178:PHE:H	1.81	0.45
18:O:94:TYR:CG	18:O:102:VAL:HG22	2.51	0.45
21:0:15:PRO:O	21:0:741:TYR:HB3	2.16	0.45
21:0:321:ILE:HG13	21:0:323:GLY:N	2.30	0.45
21:0:419:ILE:O	21:0:436:ARG:N	2.49	0.45
21:0:510:PHE:CG	21:0:511:GLU:N	2.84	0.45
24:6:137:LEU:HG	24:6:204:PRO:HG2	1.97	0.45
25:2:91:LYS:HA	25:2:95:THR:O	2.16	0.45
28:7:484:PHE:CZ	28:7:511:LEU:HB2	2.51	0.45
28:7:572:GLU:CD	28:7:573:THR:H	2.19	0.45
1:A:362:ASP:N	1:A:362:ASP:OD1	2.48	0.45
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:GLU:HB3	2:B:646:LEU:N	2.30	0.45
3:C:217:ASP:N	3:C:217:ASP:OD1	2.46	0.45
9:I:90:GLN:O	9:I:92:ARG:N	2.50	0.45
12:L:60:ARG:HG3	12:L:61:THR:N	2.29	0.45
15:R:73:LEU:HB3	15:R:224:VAL:HG21	1.98	0.45
15:R:80:LYS:HB3	15:R:81:TRP:HD1	1.80	0.45
16:W:109:LEU:HA	16:W:112:ASP:HB2	1.98	0.45
16:W:115:LYS:O	16:W:164:LYS:HB3	2.16	0.45
18:O:67:LEU:HD11	18:O:220:ARG:HD3	1.98	0.45
21:O:3:PHE:O	21:O:10:VAL:HG23	2.16	0.45
21:O:167:VAL:HA	21:O:198:ARG:NE	2.32	0.45
21:O:318:THR:HG23	21:O:376:PHE:CE1	2.51	0.45
21:O:495:MET:N	21:O:679:MET:O	2.46	0.45
22:1:389:LEU:HD21	24:6:243:ASP:O	2.17	0.45
22:1:511:ALA:HB2	23:4:264:LYS:HD2	1.98	0.45
23:4:137:LYS:HG3	23:4:139:GLN:HG3	1.98	0.45
24:6:154:ILE:HG23	24:6:193:ILE:HD12	1.98	0.45
25:2:74:PHE:HD1	25:2:78:ILE:HD13	1.81	0.45
25:2:366:LEU:HD13	25:2:369:ARG:HG3	1.97	0.45
26:5:34:GLU:HA	26:5:40:LEU:CD2	2.45	0.45
28:7:323:VAL:HG12	28:7:326:VAL:HG21	1.98	0.45
28:7:526:ASP:O	28:7:528:ASN:N	2.49	0.45
1:A:230:ARG:HG2	1:A:233:TRP:CH2	2.51	0.45
1:A:668:ASP:HB3	1:A:743:VAL:HG12	1.97	0.45
4:D:139:LYS:HA	4:D:142:LYS:HD3	1.98	0.45
13:M:157:CYS:HB3	13:M:210:MET:HE1	1.98	0.45
16:W:126:ILE:HD13	16:W:154:GLU:HB3	1.98	0.45
19:T:132:DA:H1'	19:T:133:DT:H5'	1.99	0.45
21:O:60:GLN:NE2	21:O:67:ARG:O	2.48	0.45
21:O:227:SER:HB2	21:O:453:PHE:HE2	1.81	0.45
21:O:351:VAL:N	21:O:422:PRO:HD3	2.31	0.45
24:6:173:ILE:HG12	24:6:180:GLN:O	2.16	0.45
25:2:366:LEU:CD1	25:2:369:ARG:HG3	2.46	0.45
28:7:340:GLU:CD	28:7:378:ARG:H	2.24	0.45
28:7:341:TYR:HE2	28:7:403:ILE:HG21	1.81	0.45
28:7:404:LYS:O	28:7:405:LYS:HD3	2.17	0.45
28:7:564:GLU:N	28:7:564:GLU:OE1	2.49	0.45
28:7:628:TYR:CZ	28:7:631:THR:HG23	2.51	0.45
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.62	0.45
1:A:982:THR:HG23	1:A:985:ASP:OD2	2.17	0.45
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:GLY:O	2:B:351:TYR:OH	2.28	0.45
2:B:343:ILE:C	2:B:348:ARG:HH12	2.24	0.45
2:B:860:MET:HG2	2:B:861:ASP:N	2.30	0.45
4:D:205:ASP:OD1	4:D:206:GLU:N	2.45	0.45
5:E:93:MET:HG2	5:E:123:LEU:HD23	1.98	0.45
10:J:31:ASP:OD1	10:J:31:ASP:N	2.45	0.45
13:M:270:ALA:O	13:M:277:ILE:HG21	2.17	0.45
13:M:273:SER:HA	18:O:188:GLU:HA	1.98	0.45
14:Q:387:ILE:HD13	14:Q:387:ILE:HA	1.85	0.45
18:O:171:ARG:CZ	18:O:237:PHE:HA	2.47	0.45
19:T:124:DA:P	19:T:124:DA:H8	2.40	0.45
23:4:154:SER:O	23:4:158:THR:HG23	2.17	0.45
23:4:297:SER:OG	23:4:298:ILE:N	2.45	0.45
24:6:338:CYS:HB3	24:6:364:PRO:HG3	1.97	0.45
25:2:96:LEU:HD23	25:2:96:LEU:HA	1.64	0.45
25:2:203:LEU:O	25:2:204:LEU:C	2.59	0.45
25:2:348:TYR:C	25:2:407:GLN:HE22	2.24	0.45
25:2:395:GLN:H	25:2:395:GLN:CD	2.24	0.45
25:2:449:ASP:O	25:2:451:VAL:HG22	2.16	0.45
28:7:640:LEU:HA	28:7:643:PHE:HD2	1.80	0.45
1:A:907:THR:OG1	1:A:908:LEU:N	2.50	0.45
1:A:1062:GLU:OE1	6:F:88:TYR:OH	2.34	0.45
9:I:17:ARG:N	9:I:26:LEU:O	2.39	0.45
12:L:28:LYS:HZ3	12:L:37:LYS:NZ	2.14	0.45
12:L:47:ARG:NH1	12:L:49:LYS:HD3	2.27	0.45
20:N:14:DC:C4	20:N:15:DG:C6	3.05	0.45
21:0:542:PRO:HD2	21:0:546:TYR:CD2	2.51	0.45
21:0:656:PHE:O	21:0:660:ARG:N	2.43	0.45
22:1:195:PHE:O	22:1:198:THR:OG1	2.29	0.45
22:1:278:PHE:HA	22:1:279:LYS:HZ2	1.81	0.45
23:4:122:ASP:O	23:4:125:LEU:N	2.50	0.45
23:4:288:ILE:HG13	23:4:293:LEU:HD13	1.98	0.45
25:2:380:ARG:O	25:2:383:ILE:HG12	2.17	0.45
26:5:24:ASP:CG	26:5:31:VAL:H	2.24	0.45
28:7:368:LYS:HG2	28:7:369:SER:N	2.31	0.45
28:7:431:GLN:HG2	28:7:433:GLU:H	1.82	0.45
28:7:440:SER:HB3	28:7:467:SER:CB	2.46	0.45
1:A:401:GLY:H	1:A:435:HIS:HD1	1.65	0.45
1:A:416:ARG:HG3	1:A:417:TYR:CD2	2.51	0.45
1:A:702:LEU:HD12	1:A:702:LEU:HA	1.70	0.45
2:B:106:ASP:OD1	2:B:108:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:TYR:CE2	2:B:270:LYS:HD2	2.51	0.45
2:B:327:ARG:O	2:B:330:ALA:HB3	2.16	0.45
2:B:710:LEU:HD23	2:B:710:LEU:HA	1.77	0.45
13:M:142:LEU:HD23	13:M:143:PRO:HD2	1.98	0.45
18:O:113:ALA:HB2	18:O:123:VAL:HG22	1.98	0.45
21:0:2:LYS:HA	21:0:10:VAL:O	2.17	0.45
21:0:12:PHE:HD1	21:0:14:TYR:H	1.65	0.45
21:0:71:TYR:CD1	21:0:207:ILE:HG22	2.51	0.45
23:4:222:THR:OG1	23:4:223:PHE:N	2.49	0.45
23:4:238:VAL:HG23	23:4:239:GLU:O	2.15	0.45
24:6:363:CYS:N	24:6:368:LEU:O	2.49	0.45
25:2:393:ALA:HB1	25:2:396:ILE:HB	1.99	0.45
25:2:432:VAL:HA	25:2:433:LEU:HA	1.66	0.45
28:7:107:ASP:O	28:7:517:LEU:HD22	2.15	0.45
28:7:545:GLN:NE2	28:7:545:GLN:N	2.65	0.45
1:A:184:SER:HA	1:A:198:GLU:O	2.15	0.45
1:A:378:GLU:O	1:A:431:LYS:HA	2.16	0.45
1:A:385:ILE:O	1:A:389:THR:OG1	2.27	0.45
1:A:1206:ASP:OD1	1:A:1207:LEU:N	2.50	0.45
2:B:291:ILE:HD12	2:B:291:ILE:N	2.32	0.45
2:B:548:GLY:HA3	2:B:630:ALA:HB2	1.99	0.45
3:C:206:ASN:C	3:C:208:GLU:H	2.24	0.45
4:D:184:ALA:HB3	7:G:144:ARG:NH2	2.31	0.45
8:H:89:LEU:HD12	8:H:90:ALA:H	1.82	0.45
9:I:101:PHE:CE1	9:I:112:SER:HB3	2.51	0.45
18:O:200:PRO:HG2	18:O:226:ALA:HB2	1.99	0.45
19:T:152:DG:H2"	19:T:153:DC:C6	2.51	0.45
21:0:19:PRO:HA	21:0:739:TRP:CE3	2.52	0.45
21:0:223:SER:O	21:0:227:SER:OG	2.33	0.45
21:0:351:VAL:HA	21:0:420:ILE:O	2.16	0.45
21:0:603:ARG:NH2	21:0:626:PRO:HB2	2.32	0.45
24:6:443:PHE:O	24:6:446:GLU:N	2.46	0.45
25:2:371:VAL:HG23	28:7:121:LEU:C	2.42	0.45
25:2:459:TYR:HH	25:2:501:VAL:C	2.25	0.45
25:2:460:SER:HA	25:2:490:LYS:HB3	1.99	0.45
25:2:488:LYS:C	25:2:490:LYS:N	2.74	0.45
28:7:446:PHE:CD1	28:7:473:VAL:HG13	2.52	0.45
28:7:587:LYS:HE2	28:7:587:LYS:HB3	1.54	0.45
28:7:711:LYS:HA	28:7:711:LYS:HD2	1.65	0.45
28:7:745:ILE:HB	28:7:748:LEU:HD11	1.97	0.45
1:A:700:ASN:CG	9:I:115:LYS:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:PHE:CD2	1:A:1224:LEU:HD12	2.52	0.45
1:A:1309:ASP:OD1	1:A:1310:GLY:N	2.49	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.81	0.45
4:D:119:ARG:HA	4:D:122:GLU:HG2	1.98	0.45
4:D:173:HIS:HB3	4:D:176:GLU:CD	2.42	0.45
7:G:57:GLN:HG2	7:G:58:ARG:N	2.32	0.45
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.98	0.45
13:M:84:ASN:O	13:M:88:ASP:N	2.36	0.45
13:M:163:LEU:O	13:M:164:LYS:C	2.60	0.45
21:O:123:GLU:CD	21:O:128:VAL:HB	2.42	0.45
21:O:223:SER:H	21:O:226:VAL:CG2	2.26	0.45
21:O:465:PRO:HB2	21:O:467:ASP:OD1	2.17	0.45
21:O:605:LYS:HG2	21:O:606:VAL:N	2.31	0.45
22:1:259:ILE:HG23	22:1:263:TYR:CD2	2.52	0.45
22:1:259:ILE:O	22:1:263:TYR:N	2.43	0.45
23:4:120:ASN:O	23:4:121:VAL:C	2.60	0.45
23:4:271:ASP:OD2	23:4:273:ARG:NH1	2.50	0.45
24:6:127:ILE:HD13	24:6:127:ILE:HA	1.79	0.45
25:2:465:SER:O	25:2:469:ASN:HB2	2.15	0.45
25:2:466:GLN:HB3	25:2:470:LEU:CD2	2.47	0.45
26:5:2:ALA:N	26:5:3:ARG:HE	2.15	0.45
28:7:392:LYS:HZ1	28:7:513:LEU:HB3	1.81	0.45
28:7:406:SER:OG	28:7:480:ARG:NH2	2.50	0.45
28:7:572:GLU:OE1	28:7:573:THR:N	2.29	0.45
1:A:7:SER:OG	1:A:8:SER:N	2.48	0.45
1:A:139:TRP:O	1:A:143:LYS:HB3	2.17	0.45
1:A:524:VAL:HG13	1:A:524:VAL:O	2.16	0.45
1:A:1116:LEU:O	1:A:1308:THR:HB	2.16	0.45
1:A:1204:ASP:OD2	1:A:1205:LYS:HG3	2.17	0.45
1:A:1450:LEU:HD23	1:A:1450:LEU:HA	1.55	0.45
2:B:68:THR:HA	2:B:90:ILE:O	2.17	0.45
2:B:343:ILE:H	2:B:343:ILE:HG13	1.49	0.45
2:B:1030:LEU:HD12	2:B:1030:LEU:HA	1.71	0.45
3:C:82:TYR:O	3:C:85:ASP:N	2.37	0.45
3:C:105:GLY:HA2	3:C:111:THR:HG21	1.98	0.45
5:E:156:LEU:HB2	5:E:195:VAL:O	2.17	0.45
6:F:128:LYS:NZ	6:F:151:LEU:O	2.50	0.45
7:G:111:THR:HB	7:G:114:LEU:HD13	1.98	0.45
9:I:102:VAL:HG22	9:I:109:ILE:HG13	1.98	0.45
10:J:2:ILE:O	10:J:3:VAL:C	2.60	0.45
13:M:273:SER:OG	18:O:188:GLU:O	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:342:LEU:HB2	14:Q:343:ARG:HH22	1.81	0.45
15:R:63:ARG:CZ	15:R:66:ARG:HG2	2.47	0.45
16:W:163:LYS:HB3	16:W:163:LYS:HE2	1.74	0.45
21:O:124:ARG:HA	21:O:124:ARG:HH11	1.80	0.45
21:O:124:ARG:HD2	22:1:344:GLN:HE21	1.82	0.45
21:O:162:LEU:O	21:O:166:GLU:HB2	2.16	0.45
21:O:545:LEU:HA	21:O:548:GLU:HB2	1.99	0.45
22:1:188:ASN:ND2	22:1:191:LEU:H	2.14	0.45
22:1:597:PHE:O	22:1:600:VAL:HB	2.16	0.45
23:4:177:LEU:HD12	23:4:178:VAL:H	1.82	0.45
24:6:270:VAL:HG12	24:6:272:ILE:HG22	1.98	0.45
24:6:272:ILE:O	24:6:276:LEU:N	2.44	0.45
24:6:296:HIS:O	24:6:300:LEU:HG	2.17	0.45
24:6:318:THR:OG1	24:6:319:LEU:N	2.50	0.45
25:2:357:ILE:HG13	25:2:358:ALA:H	1.81	0.45
25:2:462:PHE:HD1	25:2:462:PHE:HA	1.63	0.45
28:7:318:ILE:HD13	28:7:318:ILE:HA	1.81	0.45
1:A:173:THR:O	1:A:175:ARG:NH2	2.49	0.45
1:A:317:LYS:HD3	13:M:93:SER:HB2	1.99	0.45
1:A:538:ASP:HB3	8:H:23:VAL:HG13	1.99	0.45
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.45
1:A:988:LEU:HD13	1:A:988:LEU:HA	1.68	0.45
2:B:919:SER:OG	2:B:922:GLU:N	2.50	0.45
4:D:156:ASP:O	4:D:159:THR:HG23	2.17	0.45
5:E:69:ILE:H	5:E:69:ILE:HG12	1.45	0.45
8:H:124:ARG:NH2	8:H:126:GLU:OE1	2.50	0.45
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.47	0.45
16:W:12:LEU:HD11	16:W:182:ILE:HA	1.99	0.45
18:O:98:ARG:NE	19:T:142:DT:OP1	2.47	0.45
21:O:68:LYS:NZ	21:O:225:GLU:OE2	2.50	0.45
21:O:97:LEU:O	21:O:100:GLN:NE2	2.50	0.45
21:O:185:CYS:SG	21:O:192:PRO:HB3	2.56	0.45
21:O:250:LEU:O	21:O:436:ARG:HD2	2.17	0.45
21:O:327:ARG:NH2	27:3:115:ASP:HA	2.32	0.45
21:O:657:ASP:OD1	21:O:658:ALA:N	2.50	0.45
23:4:113:UNK:H	23:4:119:ARG:NH2	2.04	0.45
24:6:326:THR:O	24:6:347:TYR:HA	2.16	0.45
25:2:274:LEU:H	25:2:274:LEU:HG	1.45	0.45
25:2:454:TYR:HB2	26:5:9:LEU:HB3	1.98	0.45
25:2:467:GLU:OE2	25:2:508:LYS:HG3	2.17	0.45
28:7:266:GLU:O	28:7:267:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:331:GLN:CD	28:7:331:GLN:H	2.24	0.45
28:7:596:GLN:NE2	28:7:745:ILE:HG23	2.31	0.45
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.69	0.44
2:B:104:GLU:N	2:B:108:VAL:O	2.48	0.44
3:C:25:VAL:HG22	3:C:26:ASP:H	1.82	0.44
6:F:116:ASP:OD2	6:F:119:ARG:HG3	2.17	0.44
13:M:261:LYS:O	13:M:264:LYS:HE2	2.17	0.44
14:Q:365:TYR:CE2	14:Q:367:ALA:HB2	2.52	0.44
18:O:143:ILE:HD13	18:O:146:ILE:HD12	1.99	0.44
18:O:175:LEU:O	18:O:179:HIS:HB2	2.17	0.44
21:O:75:THR:OG1	21:O:76:MET:N	2.50	0.44
21:O:176:PHE:O	21:O:181:LEU:HB2	2.17	0.44
21:O:594:ARG:NH1	21:O:595:GLY:O	2.49	0.44
22:1:181:GLN:C	22:1:185:LEU:HD22	2.42	0.44
22:1:556:THR:O	22:1:557:CYS:C	2.59	0.44
23:4:234:VAL:HG12	23:4:263:VAL:HG13	1.98	0.44
25:2:10:VAL:HG11	25:2:201:TRP:CE3	2.52	0.44
25:2:17:ILE:HD12	25:2:17:ILE:HA	1.67	0.44
25:2:75:GLN:H	25:2:75:GLN:HE21	1.63	0.44
25:2:498:ASN:OD1	25:2:502:LEU:HB2	2.17	0.44
28:7:413:SER:OG	28:7:415:VAL:HB	2.16	0.44
28:7:475:ASP:O	28:7:478:THR:OG1	2.34	0.44
28:7:541:MET:C	28:7:545:GLN:NE2	2.75	0.44
1:A:465:TYR:CD1	1:A:465:TYR:N	2.83	0.44
2:B:293:PRO:O	2:B:294:ASP:C	2.60	0.44
2:B:368:GLU:HB2	14:Q:340:LYS:NZ	2.33	0.44
4:D:148:LEU:O	4:D:152:SER:HB3	2.17	0.44
4:D:175:PHE:HD1	7:G:1:MET:HE2	1.82	0.44
8:H:87:ARG:HA	8:H:87:ARG:NE	2.32	0.44
13:M:59:THR:HA	13:M:62:GLU:OE2	2.17	0.44
15:R:69:TRP:NE1	15:R:220:HIS:HB3	2.32	0.44
17:X:207:CYS:O	17:X:211:LYS:HE3	2.17	0.44
21:O:69:ILE:O	21:O:206:ILE:HG12	2.17	0.44
22:1:608:MET:O	22:1:612:CYS:N	2.48	0.44
25:2:222:LEU:HA	25:2:225:ILE:HD12	1.99	0.44
28:7:313:VAL:O	28:7:315:SER:N	2.50	0.44
1:A:83:HIS:HD2	1:A:238:CYS:SG	2.40	0.44
1:A:340:LEU:HA	1:A:340:LEU:HD23	1.74	0.44
1:A:699:ALA:HB1	9:I:114:GLN:HG2	1.99	0.44
1:A:740:LEU:HD23	1:A:740:LEU:HA	1.76	0.44
1:A:1171:GLN:CD	1:A:1172:LEU:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:ARG:NH1	1:A:1234:GLU:HA	2.32	0.44
1:A:1289:ARG:O	1:A:1291:VAL:HG13	2.17	0.44
1:A:1452:LYS:HB3	1:A:1452:LYS:NZ	2.32	0.44
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.16	0.44
2:B:408:LEU:HD23	2:B:408:LEU:HA	1.75	0.44
2:B:924:GLU:HA	2:B:928:ARG:HB3	1.99	0.44
4:D:207:LEU:HD23	4:D:211:LEU:HG	2.00	0.44
12:L:49:LYS:C	12:L:51:CYS:H	2.25	0.44
21:0:158:TYR:HA	21:0:161:ASN:HD21	1.82	0.44
21:0:171:LEU:HD13	21:0:184:TYR:CE1	2.51	0.44
21:0:411:THR:HB	21:0:412:TYR:CD2	2.53	0.44
21:0:512:ILE:HB	21:0:513:ARG:CZ	2.47	0.44
21:0:564:TRP:CE2	21:0:569:ILE:HD13	2.51	0.44
21:0:649:ARG:O	21:0:652:ASP:HB2	2.18	0.44
23:4:61:LEU:O	23:4:64:HIS:N	2.50	0.44
23:4:206:MET:HE3	23:4:206:MET:HB2	1.70	0.44
23:4:262:ILE:H	23:4:262:ILE:HG13	1.57	0.44
25:2:22:GLN:HE22	25:2:84:LEU:C	2.21	0.44
26:5:32:LEU:HD12	26:5:41:LEU:HG	1.99	0.44
27:3:27:LYS:O	27:3:40:GLU:HG3	2.18	0.44
28:7:227:ILE:N	28:7:311:ASP:HB2	2.32	0.44
28:7:235:GLU:CA	28:7:313:VAL:HG22	2.46	0.44
28:7:329:ARG:HA	28:7:332:GLU:HG2	1.99	0.44
28:7:753:PRO:O	28:7:757:ARG:N	2.50	0.44
1:A:62:ASP:C	1:A:64:ASN:N	2.75	0.44
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.51	0.44
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.18	0.44
2:B:30:SER:O	2:B:33:VAL:N	2.50	0.44
2:B:426:LYS:O	2:B:430:ARG:HG3	2.16	0.44
2:B:582:VAL:HG12	2:B:583:ASN:OD1	2.16	0.44
4:D:140:ASP:O	4:D:143:ASN:HB2	2.17	0.44
6:F:138:LEU:HA	6:F:138:LEU:HD13	1.66	0.44
9:I:59:VAL:HG23	9:I:61:ASP:N	2.16	0.44
11:K:53:ASP:OD1	11:K:54:ARG:N	2.51	0.44
13:M:211:LYS:NZ	18:O:185:TYR:O	2.49	0.44
14:Q:119:LEU:HD11	14:Q:121:PHE:CE2	2.52	0.44
15:R:93:GLY:O	15:R:94:LYS:HG3	2.17	0.44
16:W:148:LEU:HA	16:W:148:LEU:HD23	1.87	0.44
21:0:10:VAL:O	21:0:12:PHE:N	2.51	0.44
21:0:135:ARG:HD3	21:0:154:GLU:OE1	2.17	0.44
21:0:331:PHE:CE2	21:0:335:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:341:TYR:CE2	21:0:363:LEU:HD12	2.53	0.44
21:0:529:PHE:O	21:0:533:THR:HG23	2.17	0.44
24:6:174:MET:SD	24:6:213:ALA:HB2	2.56	0.44
25:2:58:PRO:HG2	25:2:61:ASP:CG	2.42	0.44
25:2:455:GLU:CG	26:5:44:PRO:HG3	2.47	0.44
25:2:498:ASN:O	25:2:499:SER:C	2.61	0.44
26:5:66:MET:H	28:7:721:LYS:HE3	1.83	0.44
28:7:311:ASP:OD1	28:7:311:ASP:N	2.49	0.44
28:7:408:ILE:HA	28:7:453:VAL:O	2.17	0.44
28:7:664:LEU:C	28:7:666:GLU:H	2.26	0.44
1:A:6:TYR:CD1	1:A:6:TYR:C	2.96	0.44
1:A:250:ILE:HD12	1:A:250:ILE:N	2.33	0.44
1:A:306:ASN:ND2	1:A:322:VAL:H	2.16	0.44
1:A:1111:MET:HB3	1:A:1111:MET:HE2	1.64	0.44
1:A:1237:ILE:HA	1:A:1237:ILE:HD13	1.60	0.44
2:B:26:THR:N	2:B:29:ASP:OD2	2.31	0.44
4:D:167:LEU:O	4:D:170:THR:N	2.50	0.44
5:E:86:PRO:HB3	5:E:114:ASN:OD1	2.17	0.44
7:G:26:LEU:HD23	7:G:26:LEU:HA	1.70	0.44
7:G:102:GLN:HA	7:G:107:LYS:HA	1.98	0.44
7:G:129:SER:HB3	7:G:137:ILE:O	2.18	0.44
8:H:10:PHE:HB3	8:H:28:ALA:HB1	2.00	0.44
11:K:9:LEU:O	11:K:9:LEU:HD13	2.17	0.44
13:M:121:LYS:C	13:M:123:ASP:H	2.26	0.44
13:M:160:GLU:O	13:M:164:LYS:N	2.44	0.44
13:M:171:ILE:H	13:M:171:ILE:HG12	1.61	0.44
13:M:274:PRO:O	13:M:277:ILE:HG13	2.17	0.44
16:W:191:ASP:OD1	16:W:191:ASP:N	2.50	0.44
18:O:61:SER:HA	18:O:231:TYR:CD1	2.52	0.44
18:O:97:LYS:H	18:O:97:LYS:HG2	1.32	0.44
18:O:211:LYS:HG3	19:T:147:DT:H5'	1.98	0.44
19:T:140:DT:O2	19:T:140:DT:H2'	2.17	0.44
21:0:310:PRO:CB	21:0:404:THR:HG23	2.48	0.44
21:0:348:VAL:O	21:0:422:PRO:HB3	2.17	0.44
21:0:643:ARG:CZ	21:0:649:ARG:HA	2.47	0.44
21:0:653:PHE:O	21:0:657:ASP:HB3	2.17	0.44
21:0:708:LEU:HA	21:0:712:MET:SD	2.57	0.44
23:4:137:LYS:HG2	23:4:140:ILE:CG1	2.48	0.44
23:4:221:SER:OG	23:4:224:LEU:HG	2.18	0.44
24:6:150:ILE:O	24:6:154:ILE:HG12	2.17	0.44
25:2:464:THR:HG22	25:2:465:SER:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:478:ILE:HD13	25:2:500:GLN:CD	2.43	0.44
28:7:225:LEU:N	28:7:309:ASP:HB2	2.33	0.44
28:7:310:ILE:HG12	28:7:338:LEU:HB3	1.99	0.44
28:7:528:ASN:HA	28:7:532:GLY:O	2.18	0.44
28:7:546:LYS:HA	28:7:546:LYS:HD3	1.78	0.44
1:A:372:LYS:HE3	11:K:1:MET:HB3	1.99	0.44
1:A:849:MET:HE2	1:A:1061:GLY:HA2	2.00	0.44
1:A:896:ARG:O	1:A:1029:ARG:HG2	2.18	0.44
1:A:982:THR:O	1:A:985:ASP:N	2.50	0.44
4:D:212:LYS:HA	4:D:212:LYS:HD2	1.66	0.44
11:K:18:LYS:O	11:K:19:LEU:HD23	2.17	0.44
12:L:38:LEU:HD22	12:L:38:LEU:HA	1.68	0.44
14:Q:350:TRP:N	14:Q:350:TRP:CD1	2.85	0.44
16:W:31:ALA:HB3	16:W:43:LEU:HD12	2.00	0.44
16:W:97:ALA:O	16:W:101:LYS:N	2.37	0.44
18:O:73:THR:HG23	18:O:122:VAL:HG13	1.98	0.44
18:O:159:ASN:ND2	20:N:22:DT:H1'	2.32	0.44
20:N:13:DG:H2''	20:N:14:DC:C5	2.51	0.44
20:N:15:DG:H2''	20:N:16:DC:C5	2.52	0.44
21:0:633:ARG:H	21:0:633:ARG:NE	2.05	0.44
22:1:597:PHE:HA	22:1:600:VAL:HB	1.99	0.44
23:4:197:MET:HA	23:4:200:ILE:HG13	2.00	0.44
23:4:255:ASP:O	23:4:256:PRO:C	2.61	0.44
23:4:313:ASP:O	23:4:317:ILE:N	2.34	0.44
25:2:256:TYR:C	25:2:258:LEU:H	2.25	0.44
26:5:14:PRO:HG3	26:5:37:ASP:HB2	2.00	0.44
28:7:583:MET:HG3	28:7:763:VAL:HG13	2.00	0.44
28:7:733:PHE:CE2	28:7:735:VAL:HG12	2.53	0.44
1:A:1172:LEU:HB3	1:A:1173:HIS:CE1	2.53	0.44
2:B:245:GLU:O	2:B:246:LYS:HG2	2.18	0.44
2:B:278:GLN:OE1	2:B:337:ARG:HB3	2.17	0.44
2:B:425:THR:O	2:B:426:LYS:C	2.59	0.44
2:B:591:ARG:HE	2:B:591:ARG:HB3	1.47	0.44
2:B:841:MET:SD	2:B:846:ILE:HD11	2.56	0.44
3:C:145:CYS:SG	3:C:146:LYS:N	2.91	0.44
4:D:24:ALA:N	4:D:28:GLN:HB2	2.32	0.44
7:G:12:THR:O	7:G:12:THR:OG1	2.36	0.44
8:H:89:LEU:C	8:H:91:ASP:H	2.26	0.44
8:H:111:LEU:HA	8:H:111:LEU:HD13	1.69	0.44
11:K:54:ARG:HD3	11:K:54:ARG:HA	1.76	0.44
16:W:20:PHE:CD1	17:X:255:ILE:HG13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:101:ALA:HB2	18:O:116:PHE:CD2	2.52	0.44
18:O:193:LEU:HD22	18:O:206:ILE:HD12	2.00	0.44
18:O:218:LYS:NZ	20:N:23:DA:H4'	2.32	0.44
19:T:158:DT:H2''	19:T:159:DT:OP2	2.18	0.44
21:O:69:ILE:HD12	21:O:205:ILE:HB	1.98	0.44
21:O:124:ARG:CD	22:1:344:GLN:HE21	2.30	0.44
21:O:355:THR:HG22	21:O:417:LEU:HD11	1.99	0.44
21:O:450:PHE:CE2	21:O:475:PHE:HB2	2.52	0.44
23:4:304:LYS:HA	23:4:310:SER:H	1.83	0.44
25:2:405:HIS:CE1	25:2:409:ARG:HA	2.53	0.44
25:2:466:GLN:CB	25:2:470:LEU:HB3	2.47	0.44
28:7:372:LYS:HD3	28:7:535:LEU:HB3	2.00	0.44
28:7:383:ILE:HD12	28:7:532:GLY:O	2.18	0.44
28:7:624:LYS:HB2	28:7:653:PHE:HE1	1.82	0.44
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.63	0.44
1:A:781:ASP:OD2	9:I:91:ARG:NH2	2.51	0.44
4:D:39:ASN:CG	4:D:41:GLN:H	2.26	0.44
5:E:48:ASP:OD2	5:E:52:ARG:HB2	2.18	0.44
5:E:151:PRO:O	5:E:153:HIS:ND1	2.50	0.44
12:L:44:ASP:OD1	12:L:44:ASP:N	2.51	0.44
13:M:195:LEU:HD22	13:M:195:LEU:HA	1.79	0.44
14:Q:126:LYS:H	14:Q:126:LYS:NZ	2.15	0.44
15:R:70:LEU:O	15:R:222:CYS:N	2.40	0.44
16:W:183:ILE:HG13	16:W:184:ASP:N	2.32	0.44
18:O:180:GLY:HA2	18:O:183:SER:O	2.18	0.44
21:O:213:LEU:HD23	21:O:234:PHE:HE1	1.83	0.44
23:4:214:LYS:HE3	23:4:237:HIS:NE2	2.33	0.44
23:4:244:LEU:HD13	23:4:248:LEU:HD21	2.00	0.44
24:6:123:ILE:O	24:6:228:CYS:HA	2.18	0.44
24:6:232:VAL:HB	24:6:261:VAL:HG13	1.99	0.44
25:2:502:LEU:HA	25:2:502:LEU:HD23	1.53	0.44
26:5:34:GLU:HA	26:5:40:LEU:HD23	1.98	0.44
28:7:252:GLY:C	28:7:255:ARG:H	2.26	0.44
28:7:269:LEU:C	28:7:318:ILE:HG22	2.43	0.44
1:A:218:ASP:O	1:A:221:SER:OG	2.23	0.44
1:A:261:ASP:O	1:A:264:PHE:N	2.51	0.44
3:C:164:ALA:C	3:C:166:GLU:N	2.75	0.44
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.52	0.44
5:E:136:ASN:ND2	5:E:138:ALA:HB3	2.33	0.44
5:E:186:LEU:HA	5:E:186:LEU:HD23	1.69	0.44
7:G:79:PHE:CD2	7:G:105:PRO:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.53	0.44
12:L:47:ARG:HD2	12:L:52:GLY:HA2	1.99	0.44
15:R:103:LYS:H	15:R:103:LYS:HG2	1.60	0.44
18:O:171:ARG:HG3	18:O:239:LYS:HB2	1.99	0.44
20:N:12:DG:C6	20:N:13:DG:C6	3.06	0.44
21:O:307:VAL:HG13	21:O:400:LYS:HB2	1.99	0.44
21:O:460:SER:H	21:O:463:ILE:CD1	2.30	0.44
23:4:147:SER:C	23:4:149:LEU:H	2.25	0.44
24:6:291:LEU:HD12	24:6:293:ASP:O	2.17	0.44
25:2:346:LYS:HD2	25:2:347:ILE:H	1.82	0.44
28:7:232:TYR:C	28:7:318:ILE:HB	2.43	0.44
28:7:302:GLU:HG3	28:7:322:SER:OG	2.18	0.44
28:7:557:VAL:HA	28:7:736:ILE:O	2.17	0.44
28:7:766:LYS:O	28:7:769:GLU:HB2	2.18	0.44
1:A:412:ARG:HB3	13:M:51:VAL:CG1	2.48	0.43
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.51	0.43
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.30	0.43
2:B:404:LYS:O	2:B:405:ARG:NH1	2.43	0.43
2:B:414:ALA:O	2:B:415:GLN:C	2.61	0.43
3:C:18:VAL:HG22	3:C:20:PHE:HD1	1.82	0.43
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.61	0.43
5:E:88:VAL:O	5:E:117:THR:HG23	2.17	0.43
5:E:99:HIS:HA	5:E:102:GLU:OE1	2.18	0.43
14:Q:142:LYS:C	14:Q:348:TYR:HD2	2.25	0.43
16:W:123:MET:HB2	16:W:130:LYS:HD3	2.00	0.43
21:O:620:VAL:O	21:O:680:VAL:HG22	2.17	0.43
21:O:639:LEU:O	21:O:643:ARG:N	2.26	0.43
22:1:295:LYS:HZ3	22:1:296:LEU:HG	1.82	0.43
23:4:228:THR:O	23:4:232:ASN:N	2.51	0.43
24:6:178:LEU:HA	24:6:178:LEU:HD12	1.74	0.43
24:6:429:CYS:HB3	24:6:432:CYS:SG	2.58	0.43
25:2:69:ASN:N	25:2:69:ASN:OD1	2.51	0.43
25:2:460:SER:CB	26:5:3:ARG:HH11	2.31	0.43
25:2:480:VAL:HG13	25:2:500:GLN:HE21	1.83	0.43
28:7:372:LYS:HB3	28:7:535:LEU:HD23	2.00	0.43
28:7:572:GLU:HB3	28:7:577:ARG:HG3	2.00	0.43
28:7:596:GLN:HE22	28:7:747:ASN:HD21	1.66	0.43
1:A:74:MET:HE3	1:A:74:MET:HB3	1.94	0.43
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.53	0.43
1:A:587:HIS:CD2	1:A:969:GLN:HG3	2.54	0.43
1:A:964:ILE:HA	1:A:964:ILE:HD13	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:O	2:B:232:SER:N	2.51	0.43
2:B:309:GLN:H	2:B:309:GLN:HG2	1.58	0.43
2:B:702:LEU:HA	2:B:702:LEU:HD12	1.70	0.43
3:C:164:ALA:O	3:C:166:GLU:N	2.52	0.43
7:G:40:GLY:CA	7:G:152:SER:HB2	2.48	0.43
7:G:64:THR:OG1	7:G:65:ASP:N	2.51	0.43
8:H:38:LEU:HD12	8:H:38:LEU:HA	1.78	0.43
13:M:210:MET:HE3	13:M:213:ILE:HB	1.99	0.43
14:Q:100:GLU:CD	15:R:94:LYS:HB3	2.43	0.43
21:0:125:LYS:HA	22:1:344:GLN:HE22	1.83	0.43
21:0:158:TYR:HA	21:0:161:ASN:ND2	2.33	0.43
21:0:197:ARG:HA	21:0:200:ILE:HG12	1.99	0.43
21:0:270:ARG:HA	21:0:273:GLU:CD	2.42	0.43
21:0:505:ALA:HB1	21:0:684:ARG:HB3	2.00	0.43
21:0:547:MET:O	21:0:551:VAL:HG23	2.17	0.43
21:0:604:GLY:O	21:0:607:SER:OG	2.36	0.43
22:1:213:ARG:N	22:1:213:ARG:HD3	2.29	0.43
22:1:506:UNK:C	22:1:507:ILE:HD13	2.48	0.43
22:1:508:LYS:HG3	22:1:509:ILE:N	2.30	0.43
24:6:139:LYS:HD3	24:6:139:LYS:HA	1.62	0.43
25:2:218:LEU:HB3	25:2:222:LEU:HD23	2.00	0.43
28:7:223:VAL:O	28:7:310:ILE:HB	2.18	0.43
28:7:446:PHE:O	28:7:447:GLN:NE2	2.39	0.43
28:7:541:MET:HB3	28:7:542:GLU:OE2	2.18	0.43
28:7:563:ALA:HA	28:7:566:TYR:CB	2.47	0.43
28:7:607:VAL:HG13	28:7:671:ILE:HB	2.00	0.43
1:A:568:PRO:HB2	3:C:221:TYR:CE2	2.53	0.43
1:A:738:LYS:HE2	1:A:738:LYS:HB3	1.76	0.43
1:A:1042:PHE:O	1:A:1045:VAL:N	2.50	0.43
1:A:1378:GLN:H	1:A:1378:GLN:HG2	1.71	0.43
2:B:235:SER:O	2:B:236:HIS:ND1	2.52	0.43
2:B:241:ARG:CZ	2:B:251:ILE:HG23	2.48	0.43
3:C:6:PRO:HB2	11:K:101:LEU:HD13	1.99	0.43
5:E:64:PRO:HB2	5:E:69:ILE:CD1	2.49	0.43
8:H:37:LYS:HA	8:H:37:LYS:HD3	1.50	0.43
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.00	0.43
12:L:29:TYR:HD1	12:L:57:LEU:O	2.01	0.43
13:M:39:SER:OG	13:M:40:GLU:OE1	2.35	0.43
13:M:123:ASP:HA	13:M:126:VAL:CG2	2.48	0.43
13:M:157:CYS:C	13:M:159:ASP:H	2.24	0.43
15:R:66:ARG:HD2	15:R:215:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:65:PRO:HA	18:O:164:CYS:SG	2.58	0.43
18:O:202:ILE:CD1	18:O:217:ALA:HB2	2.48	0.43
21:O:211:HIS:HB3	21:O:215:ASP:HB2	2.00	0.43
21:O:307:VAL:HG22	21:O:400:LYS:HE3	1.99	0.43
21:O:372:LYS:HB3	21:O:373:PRO:HD3	2.01	0.43
21:O:643:ARG:HD2	21:O:650:GLU:N	2.33	0.43
21:O:657:ASP:O	21:O:660:ARG:HB3	2.19	0.43
22:1:192:MET:HE2	22:1:192:MET:HB2	1.86	0.43
22:1:389:LEU:HD23	22:1:389:LEU:HA	1.84	0.43
22:1:564:PHE:HA	22:1:567:HIS:O	2.18	0.43
23:4:125:LEU:O	23:4:129:ILE:HG23	2.19	0.43
24:6:290:ILE:O	24:6:290:ILE:HG13	2.17	0.43
25:2:56:GLU:HG3	25:2:97:MET:HB3	2.00	0.43
25:2:364:VAL:HB	25:2:378:ILE:HB	2.00	0.43
25:2:468:TYR:OH	25:2:490:LYS:N	2.51	0.43
26:5:37:ASP:CG	26:5:38:THR:HG23	2.43	0.43
28:7:225:LEU:O	28:7:311:ASP:HA	2.17	0.43
28:7:310:ILE:HD12	28:7:376:ASN:HD21	1.83	0.43
28:7:358:PRO:O	28:7:360:THR:N	2.51	0.43
1:A:711:ARG:HE	9:I:97:MET:HG3	1.83	0.43
1:A:776:ALA:O	1:A:783:THR:HG22	2.18	0.43
1:A:902:LEU:HD22	1:A:926:GLN:HG2	2.01	0.43
1:A:960:ILE:O	1:A:961:ARG:C	2.61	0.43
2:B:439:ALA:O	15:R:280:VAL:HG21	2.17	0.43
5:E:106:GLN:O	5:E:130:ALA:HA	2.19	0.43
7:G:116:PRO:HA	7:G:164:LYS:HG2	1.99	0.43
12:L:36:SER:O	12:L:38:LEU:HD23	2.17	0.43
14:Q:106:ILE:HG13	14:Q:107:PRO:HD2	1.99	0.43
15:R:71:VAL:HA	15:R:222:CYS:O	2.17	0.43
16:W:71:LYS:O	16:W:73:ARG:N	2.51	0.43
21:O:278:ASP:HA	21:O:280:GLN:NE2	2.28	0.43
21:O:298:ILE:HG23	21:O:299:LEU:HG	1.99	0.43
21:O:634:ILE:HG13	21:O:635:LEU:H	1.82	0.43
22:1:279:LYS:HA	22:1:283:PHE:HB2	2.01	0.43
24:6:133:SER:H	24:6:136:MET:HG3	1.83	0.43
25:2:347:ILE:HG22	25:2:373:MET:HE1	1.99	0.43
25:2:382:SER:O	25:2:385:ARG:HD3	2.19	0.43
25:2:462:PHE:CZ	25:2:505:ALA:HB1	2.52	0.43
26:5:65:PRO:C	26:5:67:ASP:N	2.75	0.43
28:7:716:MET:O	28:7:720:THR:HG23	2.18	0.43
1:A:305:ASP:OD1	1:A:305:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LEU:HD12	1:A:1017:LEU:HA	1.71	0.43
1:A:1026:LEU:HA	1:A:1026:LEU:HD23	1.61	0.43
1:A:1390:ASN:HD21	1:A:1402:PHE:HB3	1.84	0.43
2:B:259:TYR:O	2:B:267:ARG:HA	2.19	0.43
2:B:1046:PRO:HB2	2:B:1047:PHE:CD2	2.54	0.43
5:E:48:ASP:OD1	5:E:52:ARG:N	2.37	0.43
7:G:131:GLN:HG3	7:G:136:VAL:HG23	2.00	0.43
9:I:60:GLN:HG2	9:I:61:ASP:OD1	2.19	0.43
13:M:190:LYS:C	15:R:270:MET:HG2	2.43	0.43
15:R:220:HIS:CE1	15:R:221:GLU:O	2.72	0.43
21:O:3:PHE:O	21:O:9:PRO:HA	2.17	0.43
21:O:21:GLN:O	21:O:24:TYR:HB3	2.17	0.43
21:O:128:VAL:HA	21:O:131:GLU:HB3	1.99	0.43
21:O:142:LYS:HA	21:O:145:LEU:HB3	2.00	0.43
21:O:492:PHE:HZ	21:O:700:GLY:HA3	1.84	0.43
21:O:493:LEU:HD23	21:O:494:PRO:HD2	1.99	0.43
25:2:208:LEU:C	25:2:211:ILE:H	2.26	0.43
26:5:24:ASP:O	26:5:28:SER:N	2.52	0.43
26:5:55:ASN:O	26:5:59:SER:OG	2.28	0.43
28:7:680:ARG:HD2	28:7:722:ARG:HD2	1.99	0.43
1:A:115:LEU:HD21	1:A:142:CYS:HA	2.00	0.43
1:A:531:ILE:O	1:A:535:THR:OG1	2.35	0.43
1:A:666:ILE:O	1:A:669:THR:N	2.36	0.43
1:A:722:LEU:HD11	1:A:794:PRO:HB3	2.01	0.43
1:A:840:ARG:HH12	1:A:1385:THR:HG22	1.81	0.43
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.99	0.43
9:I:55:THR:O	9:I:58:VAL:HG12	2.19	0.43
10:J:6:ARG:H	10:J:6:ARG:HG2	1.40	0.43
10:J:24:LEU:HD22	10:J:30:LEU:HD12	2.01	0.43
15:R:137:GLU:HA	15:R:211:LYS:O	2.18	0.43
18:O:74:VAL:HG22	18:O:155:PHE:CD2	2.54	0.43
18:O:175:LEU:O	18:O:179:HIS:N	2.45	0.43
19:T:136:DA:H2'	19:T:137:DA:C8	2.54	0.43
19:T:142:DT:H5'	19:T:142:DT:H6	1.83	0.43
21:O:37:ASN:HB2	21:O:477:THR:HA	2.00	0.43
21:O:58:ALA:O	21:O:61:MET:N	2.51	0.43
21:O:117:HIS:CD2	21:O:156:CYS:HA	2.54	0.43
23:4:271:ASP:C	23:4:273:ARG:HD3	2.43	0.43
25:2:74:PHE:HB3	25:2:75:GLN:NE2	2.32	0.43
25:2:379:THR:O	25:2:383:ILE:HG23	2.18	0.43
28:7:102:ALA:O	28:7:530:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:323:VAL:HA	28:7:326:VAL:HB	2.00	0.43
28:7:519:ARG:HG3	28:7:522:ASP:CG	2.43	0.43
28:7:548:HIS:NE2	28:7:551:ASN:HB2	2.34	0.43
28:7:599:GLU:HA	28:7:602:GLY:HA2	2.00	0.43
28:7:680:ARG:HD2	28:7:722:ARG:HH11	1.82	0.43
28:7:690:ILE:O	28:7:694:LYS:HG3	2.18	0.43
1:A:135:PHE:HB2	1:A:222:LEU:O	2.19	0.43
1:A:332:LYS:C	1:A:334:GLY:H	2.26	0.43
1:A:1144:LYS:HE2	1:A:1144:LYS:HB2	1.86	0.43
2:B:510:LYS:HA	2:B:510:LYS:HD2	1.37	0.43
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.19	0.43
2:B:596:LEU:HD12	2:B:596:LEU:HA	1.73	0.43
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.01	0.43
9:I:14:LEU:HB3	9:I:27:PHE:HB3	2.00	0.43
13:M:109:GLU:C	13:M:112:LYS:H	2.27	0.43
16:W:123:MET:HG3	16:W:130:LYS:NZ	2.34	0.43
16:W:172:LEU:O	16:W:176:MET:N	2.44	0.43
17:X:187:HIS:N	17:X:214:TRP:HB2	2.33	0.43
21:O:48:LYS:HD3	21:O:49:THR:N	2.33	0.43
21:O:161:ASN:HA	21:O:164:ASN:OD1	2.19	0.43
21:O:423:TYR:HA	21:O:432:ASN:O	2.18	0.43
22:1:492:UNK:C	22:1:494:UNK:N	2.79	0.43
23:4:86:LEU:HD12	23:4:125:LEU:HD12	1.99	0.43
25:2:174:GLU:H	25:2:185:THR:N	2.16	0.43
25:2:468:TYR:HE1	25:2:489:LYS:HA	1.82	0.43
28:7:309:ASP:HB3	28:7:337:VAL:HB	2.01	0.43
28:7:398:THR:O	28:7:402:THR:N	2.51	0.43
28:7:490:VAL:HG12	28:7:493:VAL:HB	2.01	0.43
28:7:675:SER:HB3	28:7:683:GLU:OE1	2.18	0.43
1:A:127:ALA:O	1:A:128:ILE:C	2.61	0.43
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.75	0.43
1:A:265:LYS:HD2	1:A:265:LYS:HA	1.65	0.43
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.48	0.43
1:A:596:THR:C	1:A:598:LEU:N	2.75	0.43
1:A:1124:HIS:ND1	1:A:1130:GLN:OE1	2.49	0.43
2:B:552:MET:HB2	2:B:553:PRO:HD3	1.99	0.43
2:B:794:ASN:ND2	2:B:855:PHE:HD1	2.17	0.43
2:B:901:PRO:HA	2:B:949:VAL:HG12	2.00	0.43
4:D:176:GLU:H	4:D:176:GLU:HG3	1.66	0.43
9:I:52:ILE:C	9:I:54:GLU:H	2.26	0.43
9:I:60:GLN:H	9:I:60:GLN:CD	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:27:MET:HE3	14:Q:27:MET:HB3	1.93	0.43
14:Q:103:LEU:H	15:R:92:LEU:CA	2.25	0.43
21:0:106:LEU:HA	21:0:106:LEU:HD23	1.62	0.43
21:0:331:PHE:CE1	21:0:335:LEU:HD11	2.54	0.43
21:0:347:LYS:HZ2	21:0:347:LYS:N	2.15	0.43
21:0:499:LYS:HE3	21:0:499:LYS:HB2	1.71	0.43
25:2:485:ASP:O	25:2:488:LYS:HB2	2.18	0.43
26:5:15:SER:HA	28:7:563:ALA:HB2	2.01	0.43
1:A:71:GLN:HB3	1:A:72:GLU:H	1.67	0.43
1:A:148:CYS:HB2	1:A:171:GLN:HE21	1.84	0.43
1:A:253:ASN:C	1:A:255:SER:H	2.26	0.43
1:A:356:ASP:OD2	1:A:469:ARG:NH1	2.50	0.43
1:A:908:LEU:HA	1:A:908:LEU:HD12	1.76	0.43
1:A:966:ASN:OD1	1:A:966:ASN:N	2.50	0.43
2:B:1138:MET:HA	2:B:1138:MET:HE2	2.00	0.43
3:C:22:LEU:HD12	3:C:22:LEU:HA	1.82	0.43
3:C:206:ASN:O	3:C:208:GLU:N	2.52	0.43
4:D:56:ARG:HD3	4:D:148:LEU:O	2.18	0.43
4:D:67:ARG:HA	4:D:133:THR:HG21	2.00	0.43
4:D:145:MET:HA	4:D:148:LEU:HB2	2.01	0.43
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.54	0.43
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.48	0.43
13:M:167:SER:C	13:M:169:GLU:N	2.77	0.43
16:W:8:ILE:HA	16:W:11:ASN:HB2	2.01	0.43
16:W:134:LEU:HD23	16:W:134:LEU:HA	1.63	0.43
16:W:185:SER:O	16:W:189:ILE:HG13	2.19	0.43
21:0:96:GLU:OE1	21:0:97:LEU:HG	2.18	0.43
21:0:144:LYS:HB3	21:0:153:VAL:HG22	2.01	0.43
21:0:249:SER:OG	21:0:436:ARG:NH1	2.52	0.43
21:0:270:ARG:O	21:0:274:VAL:HG22	2.19	0.43
21:0:371:ARG:NH2	21:0:411:THR:O	2.50	0.43
21:0:542:PRO:HD2	21:0:546:TYR:CE2	2.53	0.43
23:4:303:ASN:HB3	23:4:311:GLN:OE1	2.19	0.43
24:6:141:LEU:HB3	24:6:148:MET:SD	2.58	0.43
26:5:53:GLU:HA	26:5:56:ARG:HH21	1.84	0.43
28:7:354:ILE:CD1	28:7:405:LYS:H	2.31	0.43
28:7:439:THR:OG1	28:7:442:ASN:HB2	2.19	0.43
28:7:485:ILE:HG12	28:7:505:ILE:HG21	2.01	0.43
28:7:524:ILE:H	28:7:524:ILE:HG13	1.48	0.43
28:7:672:GLN:OE1	28:7:674:SER:N	2.52	0.43
28:7:754:ARG:NH2	28:7:757:ARG:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HA	1:A:305:ASP:O	2.18	0.43
1:A:313:GLN:H	13:M:99:GLY:HA3	1.84	0.43
1:A:368:LYS:HE3	1:A:368:LYS:HB2	1.81	0.43
1:A:1348:LEU:HD12	1:A:1348:LEU:HA	1.76	0.43
2:B:363:HIS:CG	2:B:364:ILE:N	2.87	0.43
2:B:386:LEU:HA	2:B:386:LEU:HD23	1.63	0.43
2:B:883:LEU:HD12	2:B:884:ARG:N	2.33	0.43
2:B:1101:ASP:N	2:B:1101:ASP:OD1	2.49	0.43
2:B:1128:LEU:HD22	2:B:1128:LEU:H	1.83	0.43
5:E:31:THR:OG1	5:E:34:GLU:HB3	2.18	0.43
7:G:151:ILE:N	7:G:158:HIS:O	2.52	0.43
13:M:214:LEU:O	13:M:218:SER:N	2.52	0.43
14:Q:347:PHE:CD1	14:Q:347:PHE:N	2.87	0.43
14:Q:372:SER:C	14:Q:373:TYR:CD2	2.97	0.43
18:O:202:ILE:HD11	18:O:217:ALA:HB2	2.00	0.43
21:O:28:ILE:HD11	21:O:55:LEU:HD22	2.01	0.43
21:O:457:ILE:HA	21:O:457:ILE:HD13	1.57	0.43
21:O:506:ILE:HA	21:O:518:ILE:HD12	2.01	0.43
21:O:524:SER:O	21:O:525:MET:C	2.62	0.43
22:1:556:THR:HB	22:1:560:PHE:HE1	1.83	0.43
24:6:142:ARG:NE	24:6:142:ARG:HA	2.34	0.43
24:6:314:ASN:HB3	24:6:317:PHE:CZ	2.53	0.43
28:7:431:GLN:HE21	28:7:433:GLU:H	1.66	0.43
28:7:439:THR:HB	28:7:441:ASP:OD1	2.18	0.43
28:7:500:ARG:O	28:7:504:THR:OG1	2.33	0.43
28:7:760:LEU:HA	28:7:763:VAL:HB	2.01	0.43
1:A:344:ARG:CZ	2:B:1120:GLU:HB2	2.48	0.42
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.66	0.42
1:A:920:LEU:HD23	1:A:920:LEU:HA	1.88	0.42
2:B:615:MET:HB3	2:B:615:MET:HE2	1.72	0.42
2:B:641:GLU:C	2:B:643:ASP:H	2.26	0.42
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.62	0.42
4:D:55:ALA:HA	4:D:58:VAL:HG12	2.00	0.42
7:G:112:LYS:HD3	7:G:119:LEU:O	2.19	0.42
7:G:146:LYS:HE2	7:G:148:GLU:OE1	2.19	0.42
8:H:64:ASN:O	8:H:65:LEU:HD23	2.18	0.42
13:M:238:TYR:N	13:M:238:TYR:CD1	2.86	0.42
14:Q:337:GLU:CD	14:Q:340:LYS:H	2.19	0.42
21:O:40:LEU:HA	21:O:40:LEU:HD23	1.69	0.42
21:O:112:LYS:HA	21:O:129:VAL:HG11	2.01	0.42
21:O:195:ILE:O	21:O:199:MET:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:388:LEU:HA	21:0:388:LEU:HD23	1.81	0.42
21:0:408:LEU:HD22	21:0:412:TYR:HE2	1.83	0.42
21:0:502:ASP:OD1	21:0:502:ASP:N	2.51	0.42
21:0:571:VAL:HG12	22:1:379:ASN:HD21	1.84	0.42
21:0:656:PHE:CG	21:0:657:ASP:N	2.84	0.42
22:1:552:MET:O	22:1:556:THR:HG23	2.19	0.42
24:6:362:VAL:HG12	24:6:363:CYS:H	1.84	0.42
25:2:17:ILE:CG2	25:2:21:VAL:HB	2.49	0.42
25:2:21:VAL:HA	25:2:24:ARG:HB2	2.01	0.42
25:2:356:GLN:O	25:2:360:LEU:N	2.44	0.42
25:2:363:PHE:CE2	25:2:396:ILE:HD11	2.53	0.42
25:2:398:ALA:O	25:2:402:THR:OG1	2.22	0.42
25:2:462:PHE:H	25:2:489:LYS:CB	2.28	0.42
28:7:426:GLN:C	28:7:428:CYS:H	2.27	0.42
1:A:77:CYS:SG	1:A:79:GLY:N	2.82	0.42
1:A:148:CYS:HB2	1:A:171:GLN:NE2	2.33	0.42
2:B:72:GLU:HB2	2:B:87:LYS:HG3	1.99	0.42
2:B:422:LYS:O	2:B:423:LYS:C	2.61	0.42
2:B:453:ILE:O	2:B:454:THR:C	2.61	0.42
2:B:829:CYS:SG	2:B:1013:ASN:ND2	2.92	0.42
2:B:1082:MET:HE2	2:B:1082:MET:HB2	1.59	0.42
4:D:56:ARG:HB2	4:D:148:LEU:HD13	2.01	0.42
9:I:19:ASP:OD1	9:I:22:ASN:N	2.52	0.42
10:J:50:ILE:HA	10:J:50:ILE:HD13	1.85	0.42
13:M:167:SER:OG	13:M:202:GLU:OE1	2.27	0.42
13:M:267:LYS:HB3	13:M:268:GLU:OE1	2.19	0.42
15:R:263:MET:HE3	15:R:263:MET:HB3	1.89	0.42
16:W:31:ALA:HA	16:W:34:PHE:CE2	2.55	0.42
16:W:90:LYS:HG3	16:W:93:HIS:HB2	2.00	0.42
18:O:112:THR:O	18:O:124:THR:HG22	2.19	0.42
19:T:132:DA:H1'	19:T:133:DT:C5'	2.48	0.42
21:0:316:LEU:C	21:0:317:LEU:HD12	2.44	0.42
21:0:446:ILE:HD13	21:0:446:ILE:HA	1.92	0.42
22:1:619:VAL:O	22:1:620:LEU:C	2.62	0.42
24:6:135:ALA:O	24:6:145:ARG:HD2	2.19	0.42
24:6:403:CYS:HB3	24:6:406:CYS:SG	2.59	0.42
25:2:381:GLU:O	25:2:384:ARG:HG3	2.20	0.42
26:5:38:THR:O	26:5:39:HIS:CG	2.72	0.42
27:3:114:GLU:O	27:3:118:TYR:N	2.23	0.42
28:7:256:ILE:N	28:7:316:PHE:HB2	2.34	0.42
28:7:309:ASP:HA	28:7:338:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:7:329:ARG:O	28:7:333:ILE:HG12	2.19	0.42
28:7:371:SER:HA	28:7:374:PHE:CE2	2.54	0.42
28:7:494:PRO:C	28:7:498:PHE:HB3	2.44	0.42
28:7:676:HIS:O	28:7:680:ARG:HD3	2.19	0.42
28:7:715:GLU:CD	28:7:715:GLU:N	2.77	0.42
1:A:238:CYS:SG	1:A:239:LEU:N	2.93	0.42
1:A:984:LYS:O	1:A:988:LEU:HB2	2.18	0.42
2:B:345:LYS:HD3	2:B:345:LYS:HA	1.80	0.42
2:B:429:PHE:CD1	14:Q:332:LEU:HD13	2.55	0.42
4:D:27:LEU:HD21	4:D:175:PHE:HB3	2.01	0.42
9:I:99:LEU:HD23	9:I:99:LEU:HA	1.76	0.42
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.75	0.42
16:W:102:VAL:O	16:W:105:VAL:HG22	2.19	0.42
20:N:18:DT:H2'	20:N:19:DA:C8	2.53	0.42
21:O:571:VAL:HG12	22:1:379:ASN:ND2	2.33	0.42
21:O:708:LEU:HB3	21:O:712:MET:HG3	2.01	0.42
24:6:148:MET:HE3	24:6:148:MET:HB3	1.80	0.42
24:6:448:LEU:O	24:6:448:LEU:HD13	2.18	0.42
25:2:358:ALA:O	25:2:361:SER:OG	2.18	0.42
26:5:54:LEU:HD12	26:5:57:LEU:HD12	2.01	0.42
28:7:269:LEU:HD12	28:7:481:GLU:OE1	2.18	0.42
28:7:465:ASN:OD1	28:7:465:ASN:N	2.52	0.42
28:7:477:LEU:H	28:7:477:LEU:HD12	1.84	0.42
28:7:540:TRP:CD1	28:7:729:GLN:NE2	2.88	0.42
28:7:568:GLU:C	28:7:571:ARG:H	2.28	0.42
28:7:598:HIS:HA	28:7:601:ARG:NH2	2.33	0.42
28:7:601:ARG:HH21	28:7:603:ASP:H	1.68	0.42
1:A:305:ASP:OD1	1:A:307:ASP:N	2.36	0.42
1:A:596:THR:O	1:A:598:LEU:N	2.53	0.42
1:A:1230:GLU:HB3	1:A:1232:ASN:ND2	2.35	0.42
1:A:1255:GLU:O	1:A:1258:HIS:HD2	2.02	0.42
2:B:381:MET:HE3	2:B:381:MET:HB2	1.47	0.42
2:B:644:GLU:HG3	2:B:646:LEU:HG	2.01	0.42
2:B:708:GLU:C	2:B:710:LEU:H	2.28	0.42
2:B:865:LYS:HG2	2:B:871:THR:HG23	2.02	0.42
2:B:955:THR:HG21	12:L:55:ILE:HG12	2.00	0.42
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.50	0.42
2:B:1200:ALA:O	2:B:1203:LEU:N	2.53	0.42
3:C:137:LYS:HB3	3:C:137:LYS:HE3	1.76	0.42
4:D:46:GLU:OE2	4:D:174:PRO:HG3	2.19	0.42
5:E:35:VAL:HG12	5:E:36:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:ASP:O	7:G:67:SER:N	2.52	0.42
12:L:42:ARG:NH1	12:L:42:ARG:HB2	2.34	0.42
12:L:49:LYS:H	12:L:49:LYS:HG2	1.66	0.42
13:M:45:CYS:SG	13:M:47:LEU:HB2	2.59	0.42
13:M:185:VAL:HG12	13:M:187:ARG:HE	1.83	0.42
14:Q:381:ASP:OD1	14:Q:381:ASP:N	2.50	0.42
15:R:123:GLU:HB2	15:R:225:MET:SD	2.59	0.42
16:W:34:PHE:CZ	17:X:201:THR:HA	2.55	0.42
16:W:167:GLU:HB3	16:W:171:LYS:HE2	2.00	0.42
20:N:32:DA:H2"	20:N:33:DA:C8	2.54	0.42
21:0:286:TYR:HA	21:0:289:LEU:HD12	2.01	0.42
21:0:370:GLU:C	21:0:373:PRO:HD2	2.45	0.42
22:1:182:GLN:HA	22:1:185:LEU:HB2	2.02	0.42
22:1:222:LEU:HD13	24:6:216:MET:HA	2.02	0.42
23:4:27:THR:HA	23:4:74:ALA:O	2.19	0.42
26:5:32:LEU:HB2	26:5:41:LEU:CB	2.44	0.42
28:7:269:LEU:HB3	28:7:304:GLU:OE1	2.19	0.42
28:7:469:ASP:HA	28:7:472:LYS:CG	2.49	0.42
28:7:704:PHE:HB2	28:7:706:TYR:CZ	2.53	0.42
1:A:252:PHE:HB3	1:A:256:GLN:O	2.20	0.42
1:A:281:HIS:O	1:A:281:HIS:ND1	2.44	0.42
1:A:1295:THR:OG1	1:A:1297:GLU:OE2	2.37	0.42
2:B:230:ALA:C	2:B:232:SER:N	2.77	0.42
2:B:586:TRP:HD1	2:B:587:HIS:H	1.68	0.42
2:B:883:LEU:HB2	2:B:931:TYR:CE2	2.54	0.42
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.50	0.42
8:H:111:LEU:HA	8:H:127:GLY:O	2.19	0.42
14:Q:365:TYR:CD1	14:Q:366:GLU:N	2.86	0.42
15:R:80:LYS:C	15:R:81:TRP:HD1	2.27	0.42
16:W:60:ARG:HA	16:W:63:SER:OG	2.19	0.42
18:O:65:PRO:HG3	18:O:227:PHE:CG	2.55	0.42
20:N:42:DT:H2"	20:N:43:DA:N7	2.34	0.42
21:0:52:LEU:HD23	21:0:52:LEU:HA	1.74	0.42
21:0:73:SER:HB2	21:0:78:GLU:HB3	2.01	0.42
21:0:311:VAL:HG13	21:0:312:LEU:O	2.20	0.42
21:0:360:LEU:HD23	21:0:361:GLN:H	1.83	0.42
21:0:364:LYS:HA	21:0:367:THR:O	2.19	0.42
21:0:377:CYS:O	21:0:381:LEU:N	2.31	0.42
21:0:656:PHE:HE1	21:0:660:ARG:HD3	1.84	0.42
22:1:325:UNK:O	22:1:329:LEU:HB2	2.18	0.42
22:1:620:LEU:O	22:1:623:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:130:TYR:HA	23:4:133:PHE:HB2	2.01	0.42
24:6:246:ASP:OD1	24:6:249:GLN:N	2.46	0.42
24:6:260:ARG:NH1	24:6:282:TYR:OH	2.52	0.42
24:6:266:LEU:HD22	24:6:266:LEU:HA	1.80	0.42
25:2:71:LYS:HD2	25:2:72:LEU:N	2.34	0.42
25:2:468:TYR:HA	25:2:472:SER:CB	2.48	0.42
25:2:496:GLU:N	25:2:496:GLU:CD	2.77	0.42
26:5:33:GLU:HB3	26:5:35:LEU:CD2	2.49	0.42
27:3:122:HIS:O	27:3:124:ILE:N	2.53	0.42
28:7:521:ASP:HB3	28:7:523:LYS:HE3	2.00	0.42
28:7:680:ARG:HH12	28:7:719:SER:CA	2.19	0.42
28:7:753:PRO:HA	28:7:756:ARG:CG	2.50	0.42
1:A:170:THR:HG23	1:A:185:TRP:HD1	1.83	0.42
1:A:677:ARG:O	1:A:681:GLU:HG2	2.20	0.42
1:A:878:ILE:HG23	1:A:878:ILE:HD12	1.73	0.42
1:A:1155:ASP:CG	1:A:1161:THR:HA	2.44	0.42
1:A:1220:PHE:O	1:A:1221:LYS:HE3	2.19	0.42
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.83	0.42
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.28	0.42
2:B:314:LEU:HD23	2:B:314:LEU:HA	1.84	0.42
2:B:886:LYS:NZ	2:B:938:SER:OG	2.52	0.42
2:B:1175:LEU:H	2:B:1175:LEU:HD23	1.85	0.42
3:C:43:THR:HG22	3:C:44:LEU:N	2.34	0.42
3:C:206:ASN:C	3:C:208:GLU:N	2.77	0.42
5:E:205:SER:O	5:E:207:ARG:N	2.49	0.42
12:L:42:ARG:HG2	12:L:43:THR:HG23	2.02	0.42
13:M:284:LEU:HG	13:M:285:ASN:N	2.34	0.42
13:M:314:LYS:HE2	13:M:314:LYS:HB2	1.70	0.42
15:R:268:MET:N	15:R:268:MET:HE2	2.35	0.42
16:W:21:TYR:HB3	16:W:25:PHE:CD2	2.55	0.42
18:O:238:ARG:HE	18:O:240:MET:HG2	1.85	0.42
19:T:152:DG:C4	19:T:153:DC:C2	3.07	0.42
21:0:18:TYR:HB2	21:0:21:GLN:HG3	2.02	0.42
21:0:345:ARG:HE	21:0:362:HIS:CE1	2.38	0.42
21:0:361:GLN:O	21:0:365:GLN:HG3	2.19	0.42
21:0:466:LEU:HD12	21:0:466:LEU:H	1.84	0.42
22:1:198:THR:OG1	22:1:199:VAL:HG23	2.19	0.42
24:6:353:HIS:O	24:6:353:HIS:ND1	2.47	0.42
25:2:205:LEU:HA	25:2:208:LEU:HD23	2.01	0.42
25:2:452:ILE:HD13	25:2:452:ILE:HA	1.95	0.42
26:5:12:CYS:SG	26:5:39:HIS:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5:19:LEU:O	26:5:23:ILE:N	2.45	0.42
26:5:51:LYS:HA	26:5:54:LEU:CB	2.40	0.42
27:3:31:ASN:O	27:3:35:TYR:N	2.44	0.42
27:3:47:PHE:CB	27:3:65:LYS:HB2	2.50	0.42
28:7:539:ASN:HA	28:7:540:TRP:CE3	2.54	0.42
28:7:579:LEU:H	28:7:579:LEU:HG	1.49	0.42
28:7:589:GLN:HA	28:7:748:LEU:HD13	2.01	0.42
1:A:250:ILE:HG23	13:M:62:GLU:HB2	2.01	0.42
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.89	0.42
1:A:377:PRO:HB3	1:A:433:GLU:HG2	2.02	0.42
1:A:411:ASP:OD2	13:M:50:LEU:HD11	2.19	0.42
1:A:934:LYS:HD2	1:A:938:LYS:HE2	2.01	0.42
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	2.01	0.42
1:A:1212:VAL:O	1:A:1215:ARG:HB3	2.19	0.42
2:B:67:SER:OG	2:B:92:PHE:O	2.35	0.42
2:B:425:THR:OG1	2:B:426:LYS:N	2.52	0.42
2:B:442:PHE:CD2	15:R:278:LEU:HD12	2.54	0.42
3:C:262:LEU:HA	3:C:262:LEU:HD12	1.69	0.42
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.84	0.42
18:O:100:ALA:HB3	20:N:26:DA:H4'	2.01	0.42
18:O:162:GLY:O	18:O:213:VAL:HA	2.20	0.42
19:T:105:DA:C2	20:N:62:DG:C2	3.08	0.42
21:O:86:LEU:O	21:O:90:MET:N	2.31	0.42
21:O:380:ARG:NH1	21:O:383:LEU:HD11	2.35	0.42
21:O:663:ALA:O	21:O:666:LEU:N	2.53	0.42
22:1:372:VAL:O	22:1:376:LYS:N	2.40	0.42
22:1:506:UNK:O	22:1:507:ILE:HD13	2.20	0.42
23:4:115:TYR:O	23:4:117:ARG:N	2.51	0.42
23:4:204:THR:O	23:4:207:LYS:N	2.50	0.42
23:4:252:MET:HE2	23:4:252:MET:HB2	1.62	0.42
23:4:273:ARG:HG3	24:6:373:SER:OG	2.19	0.42
24:6:293:ASP:OD1	24:6:295:THR:HG23	2.20	0.42
24:6:336:CYS:HB3	24:6:341:LYS:N	2.35	0.42
25:2:405:HIS:NE2	25:2:409:ARG:HA	2.35	0.42
25:2:483:TRP:CZ2	25:2:485:ASP:HB2	2.54	0.42
26:5:57:LEU:H	26:5:57:LEU:HG	1.49	0.42
28:7:484:PHE:HD1	28:7:509:ALA:HB3	1.85	0.42
28:7:598:HIS:CD2	28:7:605:ILE:HG12	2.54	0.42
28:7:711:LYS:O	28:7:713:THR:HG23	2.19	0.42
1:A:565:ILE:C	1:A:566:ILE:HG12	2.43	0.42
1:A:1043:ASP:O	1:A:1047:SER:OG	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:GLU:O	2:B:297:ILE:C	2.61	0.42
2:B:313:MET:HB3	2:B:313:MET:HE2	1.61	0.42
2:B:531:GLN:OE1	2:B:531:GLN:N	2.45	0.42
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.01	0.42
2:B:1163:CYS:HB2	2:B:1182:CYS:HB2	2.02	0.42
7:G:23:LYS:HE2	7:G:23:LYS:HB2	1.80	0.42
7:G:129:SER:HB3	7:G:138:THR:HA	2.02	0.42
9:I:12:ASN:ND2	9:I:31:THR:HG21	2.34	0.42
13:M:104:MET:HA	13:M:107:THR:OG1	2.19	0.42
16:W:58:ILE:HD13	16:W:61:LEU:HD12	2.01	0.42
16:W:99:LYS:NZ	16:W:193:ARG:HH22	2.18	0.42
16:W:177:ASP:O	16:W:181:PRO:HG2	2.19	0.42
21:0:133:CYS:HB2	31:0:801:SF4:S4	2.60	0.42
21:0:171:LEU:HB3	21:0:172:PRO:HD2	2.02	0.42
21:0:208:TYR:HE1	21:0:213:LEU:HB2	1.85	0.42
21:0:224:ASN:HB3	21:0:228:LYS:HB2	2.01	0.42
21:0:288:LYS:O	21:0:294:HIS:HB2	2.20	0.42
21:0:440:LEU:HD22	21:0:638:ARG:HA	2.01	0.42
24:6:197:LYS:HA	24:6:200:ARG:HB3	2.02	0.42
24:6:224:VAL:HG22	24:6:225:PRO:HD2	2.02	0.42
24:6:300:LEU:HA	24:6:303:GLU:CD	2.44	0.42
24:6:373:SER:O	24:6:374:THR:C	2.63	0.42
25:2:221:VAL:O	25:2:225:ILE:HG13	2.19	0.42
25:2:380:ARG:HA	25:2:380:ARG:HE	1.85	0.42
25:2:418:LYS:HZ2	25:2:420:LEU:HD23	1.84	0.42
25:2:454:TYR:CD1	25:2:482:LEU:HD13	2.55	0.42
25:2:458:LEU:HD22	26:5:41:LEU:HD13	2.01	0.42
26:5:26:LYS:HZ2	26:5:26:LYS:HG3	1.07	0.42
26:5:33:GLU:CD	26:5:35:LEU:HD23	2.45	0.42
28:7:530:LEU:HD12	28:7:530:LEU:HA	1.93	0.42
1:A:121:LEU:HD23	1:A:124:GLN:OE1	2.20	0.42
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.55	0.42
1:A:613:ILE:HD12	1:A:613:ILE:HG23	1.80	0.42
1:A:951:GLU:HG3	1:A:954:TRP:NE1	2.35	0.42
1:A:1128:GLN:O	1:A:1132:LYS:HG2	2.20	0.42
1:A:1268:LEU:HA	1:A:1268:LEU:HD23	1.59	0.42
1:A:1393:ASN:OD1	1:A:1393:ASN:N	2.45	0.42
2:B:345:LYS:O	2:B:348:ARG:HB3	2.20	0.42
2:B:465:ASN:O	2:B:467:GLY:N	2.53	0.42
2:B:566:LEU:HD12	2:B:566:LEU:HA	1.61	0.42
2:B:997:GLU:OE1	2:B:997:GLU:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.53	0.42
3:C:136:ASP:OD2	3:C:139:GLY:N	2.53	0.42
4:D:46:GLU:HG3	4:D:47:LEU:O	2.20	0.42
4:D:158:GLU:O	4:D:162:ALA:N	2.27	0.42
4:D:185:CYS:HB3	4:D:211:LEU:HD21	2.00	0.42
5:E:99:HIS:HD1	5:E:99:HIS:C	2.27	0.42
6:F:133:VAL:HG23	6:F:146:TRP:O	2.20	0.42
7:G:116:PRO:CD	7:G:164:LYS:HA	2.50	0.42
11:K:83:PRO:O	11:K:85:ASP:N	2.52	0.42
16:W:11:ASN:HA	16:W:14:LYS:HD2	2.02	0.42
16:W:41:ASP:O	16:W:45:GLN:HG2	2.19	0.42
16:W:122:TYR:CE1	16:W:147:PHE:HE2	2.38	0.42
21:0:198:ARG:HG3	21:0:199:MET:N	2.35	0.42
21:0:311:VAL:HG21	21:0:316:LEU:O	2.19	0.42
21:0:545:LEU:HD23	22:1:355:UNK:O	2.20	0.42
22:1:337:ILE:O	22:1:339:LEU:N	2.53	0.42
22:1:510:ASN:C	22:1:513:GLN:HE21	2.27	0.42
23:4:287:PHE:HD1	23:4:287:PHE:HA	1.66	0.42
24:6:136:MET:HA	24:6:145:ARG:CD	2.50	0.42
24:6:215:GLU:CD	24:6:218:ARG:HE	2.28	0.42
24:6:432:CYS:N	24:6:454:CYS:SG	2.93	0.42
27:3:40:GLU:HA	27:3:43:VAL:HB	2.01	0.42
28:7:101:PRO:O	28:7:328:LYS:HA	2.19	0.42
28:7:542:GLU:CA	28:7:545:GLN:HG2	2.48	0.42
28:7:697:ASN:OD1	28:7:697:ASN:N	2.53	0.42
1:A:1209:MET:HE3	1:A:1231:ASP:HA	2.01	0.42
2:B:362:PRO:C	2:B:363:HIS:O	2.60	0.42
2:B:486:TYR:CB	2:B:1096:ARG:HH22	2.33	0.42
2:B:564:GLU:H	2:B:564:GLU:HG2	1.44	0.42
3:C:142:VAL:HG11	10:J:5:VAL:HG13	2.02	0.42
3:C:228:PHE:CD1	3:C:228:PHE:N	2.88	0.42
5:E:140:LEU:HA	5:E:140:LEU:HD23	1.78	0.42
7:G:118:ASP:OD1	7:G:118:ASP:N	2.50	0.42
9:I:95:THR:HG22	9:I:96:SER:O	2.19	0.42
9:I:107:SER:O	9:I:107:SER:OG	2.31	0.42
10:J:32:GLU:C	10:J:34:THR:N	2.78	0.42
13:M:29:VAL:HG22	13:M:30:TYR:HB2	2.02	0.42
13:M:210:MET:SD	13:M:213:ILE:HD12	2.59	0.42
21:0:76:MET:O	21:0:79:ILE:HB	2.20	0.42
21:0:283:GLN:O	21:0:287:GLU:N	2.45	0.42
21:0:496:ILE:HD13	21:0:681:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:497:ILE:HD11	21:0:713:ALA:HB2	2.01	0.42
21:0:512:ILE:O	21:0:513:ARG:NH2	2.53	0.42
21:0:721:LEU:HA	21:0:721:LEU:HD13	1.77	0.42
23:4:159:TYR:OH	23:4:163:ILE:HD11	2.20	0.42
23:4:228:THR:HG21	23:4:235:TYR:HB2	2.01	0.42
23:4:262:ILE:HB	23:4:264:LYS:NZ	2.34	0.42
23:4:287:PHE:HB2	23:4:296:LEU:O	2.19	0.42
23:4:287:PHE:O	23:4:296:LEU:N	2.51	0.42
24:6:158:HIS:O	24:6:159:GLU:C	2.62	0.42
24:6:451:CYS:SG	24:6:454:CYS:N	2.76	0.42
25:2:31:THR:O	25:2:35:ILE:HG23	2.20	0.42
25:2:391:ILE:HG23	25:2:392:THR:O	2.20	0.42
27:3:15:ILE:HD11	27:3:56:TYR:CE1	2.54	0.42
28:7:269:LEU:CG	28:7:348:ARG:HD2	2.50	0.42
28:7:352:LEU:O	28:7:354:ILE:N	2.45	0.42
28:7:477:LEU:HG	28:7:482:TRP:HZ2	1.85	0.42
28:7:491:HIS:NE2	28:7:492:VAL:HG23	2.34	0.42
28:7:540:TRP:CD2	28:7:540:TRP:N	2.85	0.42
28:7:613:TYR:CD2	28:7:613:TYR:N	2.80	0.42
1:A:66:LYS:HG2	1:A:72:GLU:HG2	2.02	0.41
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.55	0.41
1:A:411:ASP:CG	13:M:50:LEU:HD11	2.45	0.41
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.55	0.41
1:A:806:ARG:HE	2:B:728:ARG:HA	1.84	0.41
1:A:1198:ASP:CG	1:A:1201:ALA:H	2.23	0.41
1:A:1239:ARG:NH1	1:A:1239:ARG:HB2	2.34	0.41
1:A:1339:LEU:HD11	5:E:147:HIS:CD2	2.55	0.41
2:B:173:MET:HE3	2:B:173:MET:HB2	1.86	0.41
2:B:176:SER:O	2:B:177:LYS:C	2.63	0.41
2:B:783:THR:H	2:B:783:THR:HG1	1.53	0.41
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.83	0.41
4:D:59:ILE:HG21	4:D:145:MET:SD	2.60	0.41
4:D:157:GLN:O	4:D:160:VAL:HG23	2.20	0.41
6:F:111:LEU:O	6:F:113:GLY:N	2.50	0.41
7:G:90:THR:HG22	7:G:141:SER:O	2.20	0.41
13:M:187:ARG:HA	13:M:241:ARG:NH2	2.35	0.41
13:M:187:ARG:HD3	13:M:241:ARG:NH2	2.35	0.41
13:M:267:LYS:HD3	13:M:267:LYS:HA	1.75	0.41
15:R:63:ARG:HD2	15:R:66:ARG:CZ	2.50	0.41
18:O:106:ILE:HG13	18:O:109:PRO:O	2.20	0.41
18:O:139:TYR:O	18:O:143:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:479:LEU:HD11	21:0:481:LYS:NZ	2.35	0.41
23:4:29:ILE:O	23:4:179:LEU:HD12	2.20	0.41
23:4:40:PHE:HA	23:4:43:GLU:CD	2.44	0.41
23:4:54:LEU:HD12	23:4:55:GLU:N	2.35	0.41
23:4:113:UNK:O	23:4:119:ARG:HB2	2.20	0.41
24:6:122:ILE:HD13	24:6:122:ILE:HA	1.89	0.41
24:6:125:SER:OG	24:6:229:THR:O	2.29	0.41
24:6:154:ILE:HD13	24:6:196:LEU:HD13	2.02	0.41
24:6:310:VAL:HG13	24:6:311:ASN:H	1.85	0.41
25:2:353:SER:CB	25:2:356:GLN:HB3	2.50	0.41
26:5:23:ILE:C	26:5:26:LYS:HZ3	2.20	0.41
28:7:312:ALA:HA	28:7:315:SER:OG	2.20	0.41
28:7:457:TYR:O	28:7:460:VAL:N	2.52	0.41
28:7:725:PHE:CA	28:7:728:ASP:HB2	2.49	0.41
1:A:217:LYS:HD2	1:A:217:LYS:HA	1.65	0.41
1:A:1148:ILE:O	9:I:48:LEU:HB2	2.20	0.41
1:A:1205:LYS:HZ3	1:A:1205:LYS:N	2.17	0.41
2:B:518:HIS:HB3	2:B:522:VAL:HG22	2.02	0.41
2:B:643:ASP:OD1	2:B:644:GLU:N	2.52	0.41
2:B:794:ASN:HD21	2:B:855:PHE:HD1	1.68	0.41
3:C:186:LEU:HA	3:C:186:LEU:HD23	1.79	0.41
5:E:14:ARG:O	5:E:17:ARG:N	2.53	0.41
9:I:61:ASP:O	9:I:62:ILE:C	2.64	0.41
11:K:30:ALA:HB2	11:K:76:GLN:HG3	2.01	0.41
14:Q:113:ASN:O	15:R:138:GLN:HA	2.19	0.41
15:R:267:GLY:C	15:R:268:MET:HE2	2.46	0.41
16:W:149:CYS:O	16:W:152:CYS:N	2.53	0.41
16:W:163:LYS:O	16:W:167:GLU:N	2.44	0.41
18:O:219:GLN:HB3	18:O:221:GLU:OE1	2.21	0.41
18:O:220:ARG:HB2	18:O:224:TYR:CZ	2.55	0.41
19:T:130:DA:H2"	19:T:131:DC:H6	1.86	0.41
21:0:492:PHE:CE2	21:0:494:PRO:HD3	2.55	0.41
23:4:161:ASN:OD1	23:4:165:LYS:HE2	2.19	0.41
23:4:222:THR:O	23:4:223:PHE:C	2.63	0.41
25:2:36:TYR:OH	25:2:48:MET:SD	2.78	0.41
25:2:408:MET:HB3	25:2:411:LEU:HD22	2.01	0.41
26:5:12:CYS:H	26:5:38:THR:C	2.28	0.41
28:7:446:PHE:CE1	28:7:473:VAL:HG22	2.55	0.41
28:7:539:ASN:O	28:7:549:ILE:HD11	2.19	0.41
28:7:757:ARG:O	28:7:760:LEU:HG	2.20	0.41
1:A:894:GLU:O	1:A:898:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:LEU:HD13	2:B:246:LYS:H	1.85	0.41
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.85	0.41
2:B:1051:THR:O	2:B:1055:ILE:HG13	2.21	0.41
3:C:82:TYR:HB3	3:C:84:ARG:HD3	2.02	0.41
4:D:41:GLN:N	4:D:41:GLN:CD	2.78	0.41
4:D:56:ARG:NH2	4:D:57:LEU:HG	2.36	0.41
11:K:82:ASP:O	11:K:83:PRO:C	2.64	0.41
11:K:83:PRO:C	11:K:85:ASP:N	2.76	0.41
15:R:98:ASN:O	15:R:104:ILE:HD13	2.20	0.41
21:0:423:TYR:HB3	21:0:430:VAL:O	2.21	0.41
22:1:617:LYS:O	22:1:620:LEU:HB3	2.20	0.41
23:4:295:VAL:C	23:4:296:LEU:HD12	2.45	0.41
24:6:161:PHE:CD2	24:6:189:PRO:HG3	2.55	0.41
24:6:347:TYR:O	24:6:355:LYS:HA	2.20	0.41
25:2:43:ALA:O	25:2:44:LYS:C	2.63	0.41
25:2:248:ILE:O	25:2:252:ASP:N	2.34	0.41
25:2:473:LYS:O	25:2:477:ASP:CG	2.63	0.41
28:7:249:SER:C	28:7:254:LEU:N	2.76	0.41
28:7:617:GLU:OE2	28:7:766:LYS:NZ	2.49	0.41
1:A:151:ASP:CG	1:A:153:PRO:HD3	2.45	0.41
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.01	0.41
1:A:389:THR:H	1:A:389:THR:HG1	1.58	0.41
1:A:723:ASN:OD1	1:A:726:ARG:NH2	2.52	0.41
1:A:1114:PRO:O	1:A:1311:VAL:HG23	2.21	0.41
1:A:1285:MET:HB3	1:A:1285:MET:HE2	1.77	0.41
2:B:276:ILE:HG21	2:B:280:ILE:HD11	2.02	0.41
2:B:357:GLN:HE21	2:B:357:GLN:HB3	1.58	0.41
2:B:431:TYR:CD1	2:B:431:TYR:C	2.96	0.41
2:B:923:GLU:H	2:B:928:ARG:NH1	2.19	0.41
2:B:1032:SER:HB2	2:B:1089:PRO:HG2	2.03	0.41
4:D:198:LEU:HD23	4:D:198:LEU:HA	1.79	0.41
6:F:92:ARG:O	6:F:92:ARG:HG3	2.20	0.41
6:F:146:TRP:CD1	6:F:146:TRP:N	2.86	0.41
13:M:193:GLN:HA	13:M:196:ILE:O	2.20	0.41
16:W:135:GLU:HG2	16:W:135:GLU:H	1.45	0.41
17:X:194:LYS:HA	17:X:194:LYS:HD3	1.82	0.41
20:N:31:DC:H2"	20:N:32:DA:C8	2.55	0.41
21:0:570:LEU:HD13	21:0:586:TYR:HD1	1.85	0.41
22:1:278:PHE:N	22:1:282:GLU:OE1	2.53	0.41
22:1:471:UNK:O	22:1:475:UNK:N	2.53	0.41
22:1:504:ILE:C	22:1:507:ILE:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:4:120:ASN:O	23:4:124:THR:OG1	2.35	0.41
23:4:126:VAL:O	23:4:129:ILE:HG12	2.21	0.41
23:4:287:PHE:CD1	24:6:321:LYS:HA	2.55	0.41
26:5:28:SER:O	26:5:30:ILE:HG12	2.20	0.41
26:5:33:GLU:HB3	26:5:35:LEU:HD23	2.02	0.41
26:5:53:GLU:O	26:5:56:ARG:HB2	2.20	0.41
28:7:470:SER:OG	28:7:471:GLN:N	2.53	0.41
28:7:471:GLN:NE2	28:7:471:GLN:H	2.18	0.41
1:A:55:ASP:OD1	1:A:55:ASP:C	2.63	0.41
1:A:65:LEU:HA	13:M:18:LEU:O	2.21	0.41
1:A:501:LEU:HD12	1:A:501:LEU:HA	1.70	0.41
1:A:687:LYS:H	1:A:687:LYS:HG2	1.65	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.03	0.41
1:A:1127:ASP:O	1:A:1128:GLN:C	2.63	0.41
1:A:1188:GLN:NE2	1:A:1225:PHE:HB2	2.35	0.41
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.35	0.41
2:B:425:THR:O	2:B:428:ILE:N	2.53	0.41
2:B:541:LEU:HD23	2:B:541:LEU:HA	1.68	0.41
4:D:175:PHE:CE1	7:G:1:MET:HG2	2.55	0.41
5:E:55:ARG:O	5:E:57:MET:N	2.53	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.54	0.41
6:F:110:ASP:O	6:F:112:GLU:N	2.54	0.41
11:K:18:LYS:C	11:K:19:LEU:HD23	2.46	0.41
12:L:32:ALA:HB3	12:L:53:HIS:NE2	2.36	0.41
14:Q:371:ASP:N	14:Q:371:ASP:OD1	2.39	0.41
21:0:29:LYS:HB2	21:0:55:LEU:HD11	2.02	0.41
21:0:334:PHE:HA	21:0:337:ARG:NE	2.34	0.41
21:0:648:ILE:N	21:0:649:ARG:HH21	2.17	0.41
21:0:685:ARG:HB3	21:0:689:LYS:NZ	2.36	0.41
22:1:222:LEU:O	22:1:223:UNK:C	2.68	0.41
22:1:252:SER:O	22:1:256:ILE:HG12	2.21	0.41
22:1:556:THR:O	22:1:559:GLU:N	2.54	0.41
22:1:617:LYS:O	22:1:618:PRO:C	2.63	0.41
23:4:175:ARG:HA	23:4:208:CYS:SG	2.60	0.41
23:4:271:ASP:O	23:4:273:ARG:HD3	2.20	0.41
23:4:276:CYS:SG	23:4:278:LEU:HB3	2.60	0.41
24:6:152:TYR:CD1	24:6:297:LEU:HD21	2.56	0.41
28:7:489:GLU:OE1	28:7:515:ALA:N	2.53	0.41
28:7:597:TYR:CZ	28:7:601:ARG:HD3	2.56	0.41
28:7:619:ALA:HA	28:7:653:PHE:CZ	2.55	0.41
28:7:716:MET:HE3	28:7:716:MET:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:CA	1:A:72:GLU:HA	2.49	0.41
1:A:1012:ARG:HA	1:A:1012:ARG:NE	2.36	0.41
2:B:679:TYR:OH	2:B:687:GLU:OE2	2.26	0.41
4:D:188:ALA:HB1	4:D:207:LEU:HD13	2.01	0.41
5:E:29:PHE:O	5:E:30:ILE:HD12	2.20	0.41
7:G:9:LEU:O	7:G:71:ASN:HA	2.20	0.41
13:M:272:LYS:HE2	18:O:191:PRO:HG3	2.02	0.41
14:Q:121:PHE:HD1	14:Q:361:TRP:CE3	2.38	0.41
16:W:144:ARG:HH22	16:W:146:GLU:CB	2.34	0.41
17:X:211:LYS:HE2	17:X:211:LYS:HB3	1.86	0.41
18:O:186:GLU:O	18:O:188:GLU:N	2.53	0.41
21:0:162:LEU:HD12	21:0:195:ILE:HG13	2.03	0.41
21:0:216:PRO:HB2	21:0:311:VAL:O	2.20	0.41
21:0:251:ASP:N	21:0:436:ARG:HH11	2.18	0.41
21:0:525:MET:HA	21:0:528:GLU:OE2	2.20	0.41
21:0:557:MET:HE2	21:0:557:MET:HB3	1.99	0.41
22:1:562:LYS:NZ	24:6:352:CYS:HA	2.35	0.41
23:4:65:LEU:HD13	23:4:65:LEU:HA	1.71	0.41
25:2:26:TYR:CG	25:2:104:PHE:HB2	2.55	0.41
26:5:23:ILE:HD11	26:5:54:LEU:HA	2.02	0.41
28:7:236:THR:N	28:7:313:VAL:HG13	2.36	0.41
28:7:412:THR:HG1	28:7:413:SER:H	1.68	0.41
28:7:486:ILE:HA	28:7:511:LEU:CB	2.50	0.41
28:7:718:TYR:HD1	28:7:718:TYR:H	1.67	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.56	0.41
1:A:1002:GLY:O	1:A:1008:GLN:NE2	2.54	0.41
1:A:1153:TYR:CD1	9:I:42:LEU:HA	2.56	0.41
1:A:1280:GLU:OE1	1:A:1280:GLU:N	2.54	0.41
2:B:101:MET:HE2	2:B:169:ARG:HH22	1.85	0.41
2:B:129:PHE:HA	2:B:165:VAL:O	2.20	0.41
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.50	0.41
2:B:274:PRO:O	2:B:276:ILE:HG12	2.20	0.41
2:B:547:VAL:HG22	2:B:612:GLU:OE2	2.20	0.41
2:B:554:ILE:H	2:B:554:ILE:HG12	1.47	0.41
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.02	0.41
3:C:25:VAL:HG22	3:C:26:ASP:N	2.36	0.41
5:E:42:PHE:O	5:E:46:TYR:N	2.49	0.41
9:I:85:PHE:HB3	9:I:101:PHE:CD2	2.56	0.41
14:Q:358:TYR:N	14:Q:358:TYR:CD1	2.89	0.41
18:O:65:PRO:HG2	18:O:224:TYR:HA	2.01	0.41
19:T:153:DC:C2	19:T:154:DC:N4	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:0:184:TYR:O	21:0:188:LYS:HE2	2.21	0.41
21:0:185:CYS:HA	21:0:190:LEU:HD23	2.03	0.41
21:0:315:ASP:CG	21:0:316:LEU:N	2.79	0.41
21:0:476:LYS:NZ	21:0:477:THR:O	2.54	0.41
21:0:522:TYR:HD1	21:0:522:TYR:HA	1.69	0.41
22:1:183:SER:OG	22:1:184:LEU:N	2.52	0.41
22:1:556:THR:OG1	22:1:557:CYS:N	2.54	0.41
23:4:76:ILE:HD11	23:4:85:TYR:CZ	2.56	0.41
23:4:114:UNK:O	23:4:116:ARG:N	2.54	0.41
24:6:121:GLY:O	24:6:307:PRO:HB3	2.21	0.41
24:6:126:LEU:O	24:6:169:MET:HA	2.20	0.41
24:6:217:ALA:O	24:6:220:LEU:N	2.53	0.41
24:6:272:ILE:HG23	24:6:273:CYS:N	2.35	0.41
25:2:48:MET:HA	25:2:51:VAL:HB	2.03	0.41
25:2:406:PRO:HA	25:2:409:ARG:CZ	2.50	0.41
26:5:28:SER:C	26:5:30:ILE:N	2.77	0.41
28:7:224:LYS:C	28:7:309:ASP:HB2	2.45	0.41
28:7:303:ARG:HB2	28:7:322:SER:N	2.35	0.41
28:7:354:ILE:O	28:7:404:LYS:HG3	2.21	0.41
28:7:383:ILE:HB	28:7:532:GLY:O	2.21	0.41
28:7:392:LYS:HD2	28:7:513:LEU:HD22	2.01	0.41
28:7:413:SER:C	28:7:415:VAL:N	2.75	0.41
28:7:420:TRP:CD1	28:7:420:TRP:N	2.89	0.41
28:7:431:GLN:HG2	28:7:433:GLU:OE2	2.20	0.41
28:7:754:ARG:HB2	28:7:757:ARG:HH21	1.86	0.41
1:A:264:PHE:CE1	13:M:92:LEU:HD13	2.55	0.41
1:A:1140:HIS:NE2	1:A:1272:THR:HB	2.35	0.41
2:B:134:LYS:HB2	15:R:277:PHE:CD1	2.55	0.41
2:B:176:SER:O	2:B:178:ASN:N	2.54	0.41
2:B:797:TYR:CE1	2:B:854:LEU:HG	2.56	0.41
2:B:933:SER:HB2	2:B:934:LYS:NZ	2.36	0.41
5:E:23:VAL:HG23	5:E:28:TYR:CD2	2.56	0.41
5:E:176:PRO:O	5:E:212:ARG:HA	2.21	0.41
7:G:64:THR:O	7:G:66:GLY:N	2.54	0.41
7:G:142:ARG:CB	7:G:171:ILE:HB	2.51	0.41
8:H:145:ARG:HE	8:H:146:ARG:NH1	2.19	0.41
9:I:62:ILE:HD12	9:I:62:ILE:HA	1.67	0.41
11:K:94:ILE:HD13	11:K:94:ILE:HA	1.83	0.41
12:L:30:ILE:HG22	12:L:31:CYS:O	2.20	0.41
13:M:58:ASP:OD1	13:M:61:SER:N	2.52	0.41
13:M:129:ALA:O	13:M:133:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:134:HIS:O	14:Q:135:LEU:HD22	2.20	0.41
15:R:68:VAL:O	15:R:69:TRP:HD1	2.04	0.41
16:W:30:ASP:OD1	16:W:30:ASP:N	2.51	0.41
16:W:180:GLN:H	16:W:180:GLN:HG2	1.49	0.41
21:0:136:MET:HA	21:0:154:GLU:O	2.20	0.41
21:0:223:SER:O	21:0:226:VAL:HG22	2.21	0.41
21:0:274:VAL:O	21:0:278:ASP:N	2.54	0.41
21:0:367:THR:HG22	21:0:369:ILE:HD11	2.02	0.41
23:4:137:LYS:H	23:4:140:ILE:HG13	1.85	0.41
24:6:263:VAL:HG13	24:6:277:CYS:SG	2.61	0.41
25:2:42:LEU:HD13	25:2:42:LEU:HA	1.76	0.41
25:2:84:LEU:HD11	25:2:86:LEU:HB3	2.02	0.41
25:2:348:TYR:CD1	25:2:348:TYR:N	2.89	0.41
25:2:449:ASP:C	25:2:450:ARG:HG3	2.46	0.41
25:2:478:ILE:HB	25:2:500:GLN:CD	2.46	0.41
26:5:56:ARG:O	26:5:60:LYS:NZ	2.38	0.41
27:3:32:PRO:HA	27:3:35:TYR:CZ	2.55	0.41
28:7:320:ASN:HD21	28:7:348:ARG:NH1	2.18	0.41
28:7:325:VAL:HA	28:7:328:LYS:HG3	2.03	0.41
28:7:426:GLN:C	28:7:428:CYS:N	2.77	0.41
28:7:519:ARG:NH2	28:7:521:ASP:HB2	2.28	0.41
28:7:570:LEU:HG	28:7:570:LEU:H	1.65	0.41
28:7:608:PHE:HE1	28:7:670:LEU:HB3	1.86	0.41
28:7:663:ASP:OD1	28:7:689:ARG:HD3	2.20	0.41
1:A:205:GLU:O	1:A:209:ASN:HB3	2.21	0.41
1:A:388:LEU:O	1:A:392:VAL:HG23	2.21	0.41
1:A:419:LYS:H	1:A:419:LYS:HG3	1.49	0.41
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.36	0.41
1:A:896:ARG:HD2	1:A:897:TYR:CE2	2.56	0.41
1:A:959:ASN:OD1	1:A:962:ARG:HB2	2.20	0.41
1:A:973:ILE:HD13	1:A:973:ILE:HA	1.71	0.41
1:A:1094:VAL:HG12	1:A:1113:THR:HG21	2.02	0.41
1:A:1197:LEU:H	1:A:1197:LEU:HG	1.70	0.41
1:A:1209:MET:H	1:A:1209:MET:HG2	1.49	0.41
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.21	0.41
1:A:1286:LYS:HD3	1:A:1304:TRP:CH2	2.56	0.41
2:B:26:THR:HG23	2:B:28:GLU:H	1.86	0.41
2:B:186:GLU:O	2:B:189:LEU:N	2.54	0.41
2:B:666:TYR:C	2:B:668:ASP:H	2.29	0.41
2:B:805:THR:HG22	2:B:809:MET:HE1	2.02	0.41
2:B:911:ILE:HG22	2:B:912:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASN:OD1	3:C:112:ASN:N	2.51	0.41
4:D:51:ASN:HA	4:D:182:SER:OG	2.20	0.41
4:D:137:ASN:OD1	4:D:137:ASN:N	2.53	0.41
5:E:69:ILE:HG22	5:E:73:PRO:HA	2.03	0.41
5:E:135:PHE:HB3	5:E:140:LEU:HD11	2.03	0.41
7:G:40:GLY:HA2	7:G:152:SER:HB2	2.03	0.41
7:G:90:THR:HA	7:G:141:SER:O	2.21	0.41
7:G:151:ILE:HD13	7:G:151:ILE:HA	1.72	0.41
7:G:160:ILE:HD13	7:G:160:ILE:HA	1.62	0.41
8:H:63:LEU:HB3	8:H:89:LEU:HB3	2.03	0.41
8:H:146:ARG:HE	8:H:146:ARG:HB3	1.64	0.41
9:I:24:ARG:CZ	9:I:26:LEU:HD21	2.51	0.41
9:I:35:VAL:HG12	9:I:36:GLU:N	2.36	0.41
12:L:53:HIS:NE2	12:L:55:ILE:HB	2.35	0.41
13:M:111:ASN:OD1	13:M:111:ASN:N	2.54	0.41
13:M:217:LYS:HB3	13:M:217:LYS:HE3	1.78	0.41
13:M:285:ASN:O	13:M:289:PHE:HD1	2.04	0.41
15:R:124:LEU:HD23	15:R:220:HIS:NE2	2.36	0.41
16:W:17:VAL:C	16:W:21:TYR:HB2	2.45	0.41
16:W:97:ALA:O	16:W:101:LYS:HG3	2.21	0.41
16:W:119:PRO:HB3	16:W:161:SER:HB3	2.03	0.41
16:W:133:GLN:HA	16:W:133:GLN:NE2	2.36	0.41
18:O:81:ASP:HB3	18:O:148:PHE:CZ	2.55	0.41
19:T:130:DA:H8	19:T:130:DA:OP2	2.04	0.41
19:T:135:DG:OP2	19:T:135:DG:H2'	2.21	0.41
21:O:125:LYS:O	21:O:129:VAL:HG23	2.21	0.41
21:O:250:LEU:C	21:O:436:ARG:HH11	2.29	0.41
21:O:371:ARG:NH2	21:O:410:SER:O	2.54	0.41
21:O:487:LEU:HG	21:O:491:SER:OG	2.20	0.41
21:O:490:LYS:O	21:O:491:SER:OG	2.29	0.41
21:O:505:ALA:HB1	21:O:684:ARG:HD2	2.03	0.41
21:O:524:SER:O	21:O:527:VAL:HG12	2.20	0.41
21:O:577:GLN:O	21:O:580:SER:OG	2.28	0.41
21:O:610:ILE:HD11	22:1:339:LEU:HD21	2.03	0.41
21:O:719:GLN:O	21:O:723:THR:HG23	2.20	0.41
21:O:726:GLN:O	21:O:728:THR:HG23	2.21	0.41
21:O:731:LYS:HA	21:O:734:GLU:CD	2.45	0.41
22:1:270:TYR:HD2	22:1:283:PHE:CZ	2.39	0.41
22:1:466:UNK:C	22:1:468:UNK:N	2.84	0.41
22:1:561:LEU:HG	22:1:562:LYS:N	2.36	0.41
22:1:597:PHE:CE1	22:1:613:THR:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:616:LEU:HD13	22:1:616:LEU:HA	1.87	0.41
23:4:51:ILE:HA	23:4:54:LEU:HD21	2.03	0.41
23:4:192:GLN:N	23:4:192:GLN:CD	2.77	0.41
23:4:301:PRO:HB2	23:4:303:ASN:OD1	2.21	0.41
24:6:120:ARG:HA	24:6:309:PRO:CG	2.37	0.41
24:6:169:MET:O	24:6:185:VAL:HA	2.20	0.41
24:6:191:ASP:HA	24:6:194:ASP:OD2	2.20	0.41
24:6:380:TYR:O	24:6:383:LEU:N	2.54	0.41
25:2:12:GLN:N	25:2:12:GLN:CD	2.79	0.41
25:2:203:LEU:O	25:2:205:LEU:N	2.54	0.41
25:2:347:ILE:HG12	25:2:376:GLY:O	2.21	0.41
25:2:449:ASP:O	25:2:451:VAL:N	2.54	0.41
25:2:462:PHE:HB2	25:2:489:LYS:HA	2.03	0.41
25:2:466:GLN:O	25:2:468:TYR:N	2.53	0.41
25:2:478:ILE:HB	25:2:500:GLN:HE22	1.85	0.41
25:2:495:LYS:NZ	25:2:496:GLU:HA	2.36	0.41
26:5:5:ARG:HD3	26:5:6:LYS:O	2.21	0.41
26:5:24:ASP:OD1	26:5:30:ILE:HB	2.20	0.41
26:5:66:MET:N	28:7:721:LYS:HE3	2.36	0.41
28:7:228:LYS:O	28:7:229:HIS:C	2.64	0.41
28:7:266:GLU:O	28:7:348:ARG:CZ	2.68	0.41
28:7:320:ASN:ND2	28:7:348:ARG:CZ	2.84	0.41
28:7:446:PHE:CD1	28:7:473:VAL:HG22	2.56	0.41
28:7:483:GLY:O	28:7:509:ALA:N	2.54	0.41
28:7:484:PHE:HA	28:7:509:ALA:O	2.21	0.41
28:7:489:GLU:O	28:7:491:HIS:HD2	2.04	0.41
28:7:550:ALA:HA	28:7:701:PHE:CE2	2.56	0.41
28:7:581:TYR:HD2	28:7:582:ILE:HD13	1.86	0.41
28:7:620:LEU:HD23	28:7:620:LEU:HA	1.86	0.41
28:7:631:THR:O	28:7:636:ARG:NH2	2.29	0.41
28:7:656:LYS:NZ	28:7:656:LYS:HA	2.35	0.41
28:7:716:MET:HA	28:7:719:SER:HB3	2.03	0.41
1:A:276:LEU:O	1:A:276:LEU:HG	2.20	0.41
1:A:531:ILE:HG21	1:A:531:ILE:HD13	1.84	0.41
1:A:567:LYS:HA	1:A:568:PRO:HA	1.88	0.41
1:A:568:PRO:HD3	8:H:94:ASP:O	2.20	0.41
2:B:293:PRO:HG2	2:B:296:GLU:HG3	2.02	0.41
2:B:307:ASP:C	2:B:307:ASP:OD1	2.64	0.41
2:B:658:ILE:HD12	2:B:658:ILE:HG23	1.82	0.41
2:B:976:ILE:O	2:B:990:ILE:O	2.39	0.41
2:B:1058:LEU:HA	2:B:1058:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:GLU:CD	3:C:208:GLU:C	2.89	0.41
3:C:227:THR:OG1	3:C:227:THR:O	2.37	0.41
4:D:199:ASN:OD1	4:D:200:ASN:N	2.53	0.41
5:E:123:LEU:HA	5:E:123:LEU:HD12	1.84	0.41
7:G:44:TYR:O	7:G:78:VAL:HA	2.21	0.41
9:I:113:ASP:O	9:I:117:LYS:HE3	2.21	0.41
11:K:6:ARG:HE	11:K:9:LEU:HB2	1.86	0.41
11:K:12:LEU:HD22	11:K:18:LYS:N	2.36	0.41
15:R:124:LEU:HA	15:R:124:LEU:HD23	1.98	0.41
18:O:172:LEU:HD23	18:O:172:LEU:HA	1.89	0.41
19:T:138:DA:H2''	19:T:139:DC:H5''	2.03	0.41
19:T:142:DT:H5'	19:T:142:DT:C6	2.56	0.41
21:O:118:PRO:HA	21:O:121:SER:HB2	2.02	0.41
21:O:661:HIS:O	21:O:664:GLN:HB3	2.21	0.41
22:1:169:LEU:HA	22:1:218:ARG:NH1	2.35	0.41
22:1:177:ASN:O	22:1:178:LEU:C	2.64	0.41
23:4:224:LEU:O	23:4:228:THR:HG22	2.21	0.41
23:4:287:PHE:CB	24:6:319:LEU:HD21	2.50	0.41
24:6:132:CYS:SG	24:6:173:ILE:HB	2.61	0.41
25:2:24:ARG:HH11	25:2:24:ARG:HA	1.86	0.41
25:2:90:ASN:N	25:2:97:MET:O	2.54	0.41
25:2:222:LEU:HD12	25:2:226:PHE:CZ	2.56	0.41
25:2:361:SER:C	25:2:363:PHE:N	2.79	0.41
25:2:460:SER:HA	25:2:490:LYS:CB	2.50	0.41
25:2:461:ASP:CG	25:2:490:LYS:HE2	2.46	0.41
27:3:36:HIS:HE1	27:3:59:CYS:CB	2.34	0.41
28:7:144:GLU:O	28:7:147:SER:N	2.40	0.41
28:7:406:SER:HB2	28:7:482:TRP:HE3	1.84	0.41
28:7:461:ALA:HA	28:7:500:ARG:HD2	2.02	0.41
28:7:564:GLU:HA	28:7:567:GLN:CD	2.46	0.41
28:7:598:HIS:NE2	28:7:669:CYS:HB3	2.36	0.41
28:7:718:TYR:CD1	28:7:718:TYR:N	2.89	0.41
1:A:133:LYS:HA	1:A:136:ALA:HB3	2.03	0.40
1:A:268:ASP:O	1:A:299:HIS:HD2	2.03	0.40
1:A:533:LYS:HE2	1:A:533:LYS:HB3	1.76	0.40
1:A:746:MET:HE3	2:B:1015:HIS:CD2	2.56	0.40
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.51	0.40
2:B:125:SER:HB3	2:B:171:PRO:HA	2.03	0.40
2:B:405:ARG:O	2:B:406:LEU:HD23	2.21	0.40
4:D:124:GLU:O	4:D:128:VAL:HG23	2.21	0.40
5:E:66:GLU:CD	5:E:67:GLU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:112:LYS:O	7:G:115:MET:N	2.54	0.40
8:H:15:VAL:HG22	8:H:26:ILE:HD12	2.03	0.40
9:I:57:GLY:O	9:I:59:VAL:HG13	2.21	0.40
10:J:51:LEU:O	10:J:51:LEU:HG	2.20	0.40
12:L:50:ASP:OD1	12:L:50:ASP:N	2.55	0.40
13:M:171:ILE:O	13:M:174:ALA:N	2.54	0.40
13:M:272:LYS:HE2	18:O:191:PRO:CD	2.51	0.40
13:M:300:GLN:O	15:R:271:ARG:HD2	2.20	0.40
14:Q:399:ASN:HB3	14:Q:402:ALA:HB2	2.02	0.40
16:W:18:ARG:HD3	16:W:26:VAL:HG21	2.03	0.40
19:T:144:DA:O3'	19:T:145:DT:H3'	2.21	0.40
21:O:27:ASP:OD1	21:O:27:ASP:N	2.51	0.40
21:O:291:GLN:NE2	21:O:294:HIS:HB2	2.36	0.40
21:O:308:GLU:N	21:O:308:GLU:OE1	2.54	0.40
22:1:597:PHE:HE2	22:1:620:LEU:HD12	1.86	0.40
23:4:76:ILE:HD11	23:4:85:TYR:CE2	2.55	0.40
23:4:87:TYR:C	23:4:89:GLU:H	2.29	0.40
23:4:149:LEU:O	23:4:152:ALA:HB3	2.21	0.40
24:6:152:TYR:CG	24:6:297:LEU:HD21	2.56	0.40
24:6:287:PHE:N	24:6:287:PHE:CD1	2.86	0.40
25:2:222:LEU:HD12	25:2:226:PHE:CE2	2.56	0.40
25:2:468:TYR:CE1	25:2:489:LYS:HA	2.56	0.40
25:2:476:GLN:O	25:2:476:GLN:HG2	2.21	0.40
27:3:30:VAL:HG12	27:3:36:HIS:O	2.21	0.40
28:7:578:MET:HG3	28:7:579:LEU:HD23	2.03	0.40
28:7:599:GLU:C	28:7:602:GLY:H	2.29	0.40
28:7:699:GLU:N	28:7:699:GLU:CD	2.80	0.40
28:7:705:PHE:CG	28:7:706:TYR:N	2.89	0.40
1:A:184:SER:OG	1:A:199:LEU:HG	2.21	0.40
1:A:253:ASN:O	1:A:255:SER:N	2.52	0.40
1:A:315:LEU:HA	1:A:315:LEU:HD23	1.84	0.40
1:A:565:ILE:O	1:A:570:PRO:HA	2.21	0.40
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.21	0.40
2:B:432:MET:HE2	2:B:432:MET:HB3	2.00	0.40
4:D:54:GLU:OE1	4:D:55:ALA:N	2.54	0.40
4:D:175:PHE:CD1	7:G:1:MET:HE2	2.57	0.40
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.36	0.40
5:E:157:SER:C	5:E:159:ASP:N	2.77	0.40
14:Q:130:VAL:HG12	14:Q:133:PHE:HB2	2.02	0.40
14:Q:378:VAL:O	15:R:66:ARG:HB3	2.20	0.40
16:W:99:LYS:HZ3	16:W:193:ARG:NH2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:174:ARG:O	16:W:177:ASP:HB2	2.21	0.40
21:0:323:GLY:HA2	27:3:107:ASN:HA	2.03	0.40
21:0:562:GLU:OE2	21:0:565:LYS:HD2	2.21	0.40
21:0:610:ILE:HD12	22:1:337:ILE:CG2	2.52	0.40
21:0:654:LEU:HD13	21:0:654:LEU:HA	1.88	0.40
23:4:202:SER:HB3	24:6:448:LEU:HB3	2.02	0.40
23:4:262:ILE:HB	23:4:264:LYS:HZ2	1.86	0.40
23:4:264:LYS:HA	23:4:264:LYS:HD3	1.81	0.40
26:5:20:ILE:HA	26:5:23:ILE:CD1	2.47	0.40
28:7:269:LEU:CD1	28:7:348:ARG:HD2	2.50	0.40
28:7:471:GLN:HA	28:7:474:MET:CB	2.45	0.40
1:A:73:GLY:C	1:A:75:ASN:N	2.77	0.40
1:A:285:PRO:O	1:A:287:HIS:N	2.54	0.40
1:A:578:LEU:HA	1:A:578:LEU:HD12	1.79	0.40
1:A:1217:LYS:HE2	1:A:1228:TRP:HZ3	1.87	0.40
2:B:552:MET:HE3	2:B:552:MET:HB3	1.81	0.40
2:B:708:GLU:O	2:B:712:PRO:HD2	2.22	0.40
4:D:27:LEU:HD22	4:D:173:HIS:CE1	2.56	0.40
4:D:29:LEU:HD22	7:G:82:PHE:CZ	2.56	0.40
5:E:23:VAL:HG23	5:E:28:TYR:HD2	1.86	0.40
9:I:90:GLN:HE21	9:I:90:GLN:HB2	1.50	0.40
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.40
10:J:1:MET:HE2	10:J:1:MET:HB3	1.79	0.40
13:M:191:GLU:O	15:R:268:MET:HB3	2.21	0.40
14:Q:129:PRO:HG2	14:Q:132:ASP:OD1	2.21	0.40
15:R:80:LYS:HB3	15:R:81:TRP:CD1	2.57	0.40
19:T:107:DA:H2	20:N:59:DT:O2	2.05	0.40
19:T:135:DG:OP2	19:T:135:DG:H8	2.03	0.40
21:0:1:MET:HE3	21:0:742:GLU:H	1.86	0.40
21:0:159:HIS:ND1	21:0:162:LEU:HD22	2.36	0.40
21:0:185:CYS:O	21:0:190:LEU:N	2.43	0.40
21:0:357:LYS:O	21:0:360:LEU:HB3	2.22	0.40
21:0:415:GLY:C	21:0:416:PHE:CG	2.99	0.40
21:0:611:ASP:HA	21:0:668:ARG:HB3	2.04	0.40
21:0:618:ARG:NH1	21:0:675:ASP:OD1	2.55	0.40
22:1:212:THR:HB	22:1:213:ARG:CZ	2.52	0.40
22:1:259:ILE:HG22	22:1:266:VAL:HG21	2.03	0.40
22:1:619:VAL:C	22:1:622:SER:HG	2.23	0.40
23:4:159:TYR:O	23:4:162:ARG:HB3	2.22	0.40
24:6:403:CYS:SG	24:6:406:CYS:N	2.94	0.40
24:6:449:HIS:O	24:6:450:ASN:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:462:PHE:CE2	25:2:467:GLU:HB3	2.56	0.40
25:2:481:LEU:HD13	25:2:483:TRP:C	2.46	0.40
27:3:88:VAL:O	27:3:90:ASN:N	2.54	0.40
28:7:302:GLU:HG2	28:7:329:ARG:NH2	2.33	0.40
28:7:462:ASN:H	28:7:500:ARG:NH1	2.19	0.40
28:7:553:GLN:HB2	28:7:704:PHE:CD2	2.55	0.40
28:7:558:TRP:HB3	28:7:711:LYS:CD	2.52	0.40
1:A:95:PHE:HB3	1:A:234:MET:SD	2.62	0.40
1:A:688:LYS:HA	1:A:688:LYS:HD2	1.90	0.40
1:A:827:THR:O	1:A:831:THR:HG23	2.21	0.40
2:B:773:MET:O	2:B:774:GLY:C	2.65	0.40
2:B:807:ARG:HA	2:B:807:ARG:HD2	1.85	0.40
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.54	0.40
4:D:150:ASN:O	7:G:142:ARG:NH2	2.54	0.40
4:D:209:ARG:HG3	4:D:210:ILE:H	1.85	0.40
4:D:211:LEU:HA	4:D:211:LEU:HD23	1.92	0.40
5:E:46:TYR:HD1	5:E:57:MET:SD	2.45	0.40
5:E:170:LEU:HD23	5:E:170:LEU:HA	1.79	0.40
5:E:179:GLN:O	5:E:182:ASP:HB3	2.21	0.40
8:H:2:SER:HA	8:H:62:SER:HB3	2.02	0.40
8:H:101:ALA:HB3	8:H:137:GLN:HA	2.03	0.40
18:O:99:PHE:CZ	20:N:25:DA:H2	2.40	0.40
20:N:20:DT:H3'	20:N:20:DT:OP2	2.21	0.40
21:0:372:LYS:HA	21:0:375:ARG:HH21	1.87	0.40
21:0:495:MET:O	21:0:496:ILE:HD13	2.21	0.40
22:1:278:PHE:O	22:1:283:PHE:N	2.55	0.40
22:1:284:TRP:HA	22:1:287:PHE:CD1	2.55	0.40
22:1:560:PHE:C	22:1:563:HIS:HD1	2.28	0.40
23:4:273:ARG:NH2	24:6:372:LEU:HB3	2.23	0.40
23:4:305:CYS:C	23:4:307:ALA:N	2.79	0.40
24:6:313:ILE:O	24:6:315:LYS:NZ	2.47	0.40
25:2:201:TRP:O	25:2:202:THR:C	2.65	0.40
26:5:56:ARG:HB3	26:5:60:LYS:NZ	2.36	0.40
27:3:37:ARG:NH1	27:3:37:ARG:HB3	2.35	0.40
28:7:164:ILE:H	28:7:172:GLU:H	1.69	0.40
28:7:222:LYS:CA	28:7:240:ASP:H	2.34	0.40
28:7:223:VAL:C	28:7:310:ILE:HB	2.47	0.40
28:7:459:MET:HE3	28:7:459:MET:HB3	1.88	0.40
28:7:598:HIS:HE1	28:7:706:TYR:CZ	2.38	0.40
28:7:754:ARG:NH1	28:7:757:ARG:HB3	2.36	0.40
1:A:526:ASP:CG	2:B:1013:ASN:HD21	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	2.03	0.40
1:A:786:HIS:NE2	2:B:705:MET:HE2	2.37	0.40
1:A:879:GLU:O	1:A:955:PRO:HA	2.22	0.40
1:A:1154:TYR:OH	9:I:18:GLU:HG3	2.22	0.40
1:A:1434:ALA:O	1:A:1436:ILE:N	2.53	0.40
2:B:73:GLN:N	2:B:86:ARG:O	2.34	0.40
2:B:172:ILE:HA	2:B:172:ILE:HD13	1.83	0.40
2:B:311:LEU:HA	2:B:311:LEU:HD23	1.82	0.40
2:B:641:GLU:C	2:B:643:ASP:N	2.80	0.40
2:B:948:ILE:HG22	2:B:949:VAL:O	2.22	0.40
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.40
4:D:27:LEU:HD23	4:D:27:LEU:HA	1.77	0.40
7:G:36:GLY:N	7:G:45:ILE:O	2.52	0.40
9:I:22:ASN:HB3	9:I:24:ARG:HE	1.86	0.40
9:I:74:GLU:HA	9:I:80:SER:O	2.22	0.40
10:J:36:LEU:HD11	10:J:51:LEU:HB2	2.04	0.40
13:M:56:LEU:HA	13:M:56:LEU:HD12	1.61	0.40
15:R:255:LEU:HD12	15:R:255:LEU:HA	1.79	0.40
16:W:7:ASP:O	16:W:11:ASN:HB2	2.21	0.40
18:O:211:LYS:HD3	18:O:211:LYS:HA	1.97	0.40
20:N:24:DA:H8	20:N:24:DA:O5'	2.05	0.40
20:N:27:DG:C2	20:N:28:DT:C2	3.10	0.40
21:O:249:SER:OG	22:1:351:GLY:HA2	2.21	0.40
21:O:402:ILE:O	21:O:406:ALA:N	2.31	0.40
21:O:471:ARG:HH22	21:O:647:ARG:N	2.19	0.40
21:O:493:LEU:HB3	21:O:678:VAL:HG22	2.03	0.40
21:O:517:SER:HA	21:O:520:ARG:CZ	2.51	0.40
21:O:519:VAL:HA	21:O:522:TYR:HB2	2.03	0.40
22:1:213:ARG:HH11	22:1:213:ARG:HB2	1.86	0.40
25:2:82:LYS:C	25:2:85:HIS:H	2.29	0.40
25:2:467:GLU:OE2	25:2:508:LYS:HA	2.20	0.40
28:7:352:LEU:O	28:7:404:LYS:HG3	2.20	0.40
28:7:712:ASP:N	28:7:716:MET:HE1	2.36	0.40
28:7:750:TYR:HD2	28:7:755:GLU:C	2.30	0.40
28:7:755:GLU:HA	28:7:758:GLU:CD	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1386/1733 (80%)	1206 (87%)	174 (13%)	6 (0%)	30	65
2	B	1133/1224 (93%)	1030 (91%)	100 (9%)	3 (0%)	36	70
3	C	260/318 (82%)	229 (88%)	31 (12%)	0	100	100
4	D	153/221 (69%)	131 (86%)	21 (14%)	1 (1%)	18	53
5	E	211/215 (98%)	190 (90%)	21 (10%)	0	100	100
6	F	81/155 (52%)	75 (93%)	6 (7%)	0	100	100
7	G	169/171 (99%)	145 (86%)	24 (14%)	0	100	100
8	H	132/146 (90%)	106 (80%)	25 (19%)	1 (1%)	16	50
9	I	114/122 (93%)	85 (75%)	29 (25%)	0	100	100
10	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	3	18
11	K	110/120 (92%)	98 (89%)	12 (11%)	0	100	100
12	L	43/70 (61%)	32 (74%)	11 (26%)	0	100	100
13	M	273/345 (79%)	225 (82%)	48 (18%)	0	100	100
14	Q	140/735 (19%)	117 (84%)	23 (16%)	0	100	100
15	R	176/400 (44%)	150 (85%)	26 (15%)	0	100	100
16	W	189/482 (39%)	170 (90%)	18 (10%)	1 (0%)	24	60
17	X	152/328 (46%)	131 (86%)	19 (12%)	2 (1%)	9	38
18	O	178/240 (74%)	169 (95%)	9 (5%)	0	100	100
21	0	749/778 (96%)	631 (84%)	116 (16%)	2 (0%)	36	70
22	1	257/541 (48%)	223 (87%)	30 (12%)	4 (2%)	7	34
23	4	279/338 (82%)	202 (72%)	76 (27%)	1 (0%)	30	65
24	6	336/461 (73%)	263 (78%)	71 (21%)	2 (1%)	21	56
25	2	457/513 (89%)	345 (76%)	111 (24%)	1 (0%)	43	76
26	5	64/72 (89%)	46 (72%)	18 (28%)	0	100	100
27	3	135/321 (42%)	121 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	7	634/843 (75%)	448 (71%)	184 (29%)	2 (0%)	36	70
All	All	7874/10962 (72%)	6624 (84%)	1222 (16%)	28 (0%)	31	65

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
1	A	525	GLN
2	B	364	ILE
8	H	110	ASP
10	J	6	ARG
22	1	516	HIS
24	6	411	PRO
24	6	425	SER
1	A	958	VAL
2	B	363	HIS
22	1	225	SER
22	1	230	PRO
25	2	68	SER
28	7	574	ALA
17	X	272	ALA
23	4	115	TYR
17	X	271	PHE
1	A	464	PRO
1	A	957	PRO
16	W	181	PRO
28	7	575	ARG
4	D	157	GLN
22	1	239	PRO
2	B	1046	PRO
10	J	5	VAL
21	0	313	PRO
1	A	168	GLY
21	0	172	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1221/1520 (80%)	1010 (83%)	211 (17%)	2	10
2	B	995/1061 (94%)	847 (85%)	148 (15%)	3	15
3	C	230/274 (84%)	197 (86%)	33 (14%)	3	16
4	D	139/200 (70%)	110 (79%)	29 (21%)	1	7
5	E	195/197 (99%)	159 (82%)	36 (18%)	1	9
6	F	73/137 (53%)	60 (82%)	13 (18%)	2	10
7	G	152/152 (100%)	122 (80%)	30 (20%)	1	8
8	H	119/128 (93%)	92 (77%)	27 (23%)	1	5
9	I	110/116 (95%)	88 (80%)	22 (20%)	1	7
10	J	60/65 (92%)	48 (80%)	12 (20%)	1	7
11	K	97/102 (95%)	86 (89%)	11 (11%)	5	24
12	L	40/57 (70%)	29 (72%)	11 (28%)	0	2
13	M	245/299 (82%)	192 (78%)	53 (22%)	1	6
14	Q	109/641 (17%)	84 (77%)	25 (23%)	1	5
15	R	107/363 (30%)	74 (69%)	33 (31%)	0	1
16	W	155/429 (36%)	121 (78%)	34 (22%)	1	5
17	X	62/295 (21%)	51 (82%)	11 (18%)	2	10
18	O	152/205 (74%)	135 (89%)	17 (11%)	6	24
21	0	685/707 (97%)	527 (77%)	158 (23%)	1	5
22	1	170/396 (43%)	135 (79%)	35 (21%)	1	7
23	4	198/298 (66%)	149 (75%)	49 (25%)	1	4
24	6	247/406 (61%)	183 (74%)	64 (26%)	0	3
25	2	259/468 (55%)	189 (73%)	70 (27%)	0	2
26	5	53/66 (80%)	37 (70%)	16 (30%)	0	1
27	3	63/303 (21%)	51 (81%)	12 (19%)	1	8
28	7	417/737 (57%)	299 (72%)	118 (28%)	0	2
All	All	6353/9622 (66%)	5075 (80%)	1278 (20%)	3	7

All (1278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	13	THR
1	A	22	PHE
1	A	40	THR
1	A	41	MET
1	A	42	ASP
1	A	45	GLN
1	A	50	ILE
1	A	53	LEU
1	A	55	ASP
1	A	57	ARG
1	A	62	ASP
1	A	63	ARG
1	A	71	GLN
1	A	75	ASN
1	A	76	GLU
1	A	85	ASP
1	A	88	LYS
1	A	90	VAL
1	A	92	HIS
1	A	102	VAL
1	A	106	VAL
1	A	107	CYS
1	A	113	LEU
1	A	117	GLU
1	A	120	GLU
1	A	130	ASP
1	A	140	THR
1	A	145	LYS
1	A	147	VAL
1	A	174	ILE
1	A	175	ARG
1	A	177	ASP
1	A	180	LYS
1	A	201	VAL
1	A	204	THR
1	A	205	GLU
1	A	207	ILE
1	A	209	ASN
1	A	215	SER
1	A	218	ASP
1	A	221	SER

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Mol	Chain	Res	Type
1	A	222	LEU
1	A	232	GLU
1	A	235	ILE
1	A	249	SER
1	A	254	GLU
1	A	256	GLN
1	A	275	SER
1	A	276	LEU
1	A	287	HIS
1	A	293	GLU
1	A	296	LEU
1	A	299	HIS
1	A	300	VAL
1	A	305	ASP
1	A	316	GLN
1	A	329	LEU
1	A	333	GLU
1	A	344	ARG
1	A	363	GLN
1	A	369	SER
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	398	GLU
1	A	409	SER
1	A	415	LEU
1	A	418	SER
1	A	419	LYS
1	A	424	ILE
1	A	446	ARG
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	463	ILE
1	A	465	TYR
1	A	466	SER
1	A	470	LEU
1	A	474	VAL
1	A	475	THR
1	A	494	SER
1	A	500	GLU

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Mol	Chain	Res	Type
1	A	501	LEU
1	A	502	SER
1	A	510	GLN
1	A	511	ILE
1	A	535	THR
1	A	544	ASP
1	A	546	VAL
1	A	566	ILE
1	A	571	LEU
1	A	580	VAL
1	A	596	THR
1	A	598	LEU
1	A	603	ASN
1	A	619	LYS
1	A	622	VAL
1	A	624	SER
1	A	625	SER
1	A	658	LEU
1	A	666	ILE
1	A	687	LYS
1	A	691	LEU
1	A	709	THR
1	A	724	GLU
1	A	735	VAL
1	A	743	VAL
1	A	752	LYS
1	A	756	ILE
1	A	758	ILE
1	A	764	CYS
1	A	827	THR
1	A	834	THR
1	A	839	ARG
1	A	845	LEU
1	A	862	ASN
1	A	865	GLN
1	A	867	ILE
1	A	873	MET
1	A	886	ILE
1	A	890	ASP
1	A	895	LYS
1	A	907	THR
1	A	909	ASP

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Mol	Chain	Res	Type
1	A	913	LEU
1	A	919	ILE
1	A	930	ASP
1	A	934	LYS
1	A	948	VAL
1	A	965	GLN
1	A	974	ASP
1	A	977	LYS
1	A	979	SER
1	A	980	ASP
1	A	982	THR
1	A	985	ASP
1	A	988	LEU
1	A	1005	GLU
1	A	1022	LEU
1	A	1028	THR
1	A	1038	THR
1	A	1040	GLN
1	A	1043	ASP
1	A	1048	ASN
1	A	1074	GLU
1	A	1093	LYS
1	A	1095	THR
1	A	1098	VAL
1	A	1102	LYS
1	A	1116	LEU
1	A	1120	LEU
1	A	1121	GLU
1	A	1127	ASP
1	A	1130	GLN
1	A	1145	SER
1	A	1146	VAL
1	A	1163	ILE
1	A	1168	GLU
1	A	1170	ILE
1	A	1187	GLN
1	A	1194	ARG
1	A	1195	LEU
1	A	1197	LEU
1	A	1204	ASP
1	A	1205	LYS
1	A	1208	THR

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Mol	Chain	Res	Type
1	A	1209	MET
1	A	1211	GLN
1	A	1214	GLU
1	A	1230	GLU
1	A	1232	ASN
1	A	1235	LYS
1	A	1237	ILE
1	A	1239	ARG
1	A	1240	CYS
1	A	1243	VAL
1	A	1255	GLU
1	A	1256	GLU
1	A	1258	HIS
1	A	1260	LEU
1	A	1263	ILE
1	A	1266	THR
1	A	1269	GLU
1	A	1272	THR
1	A	1280	GLU
1	A	1281	ARG
1	A	1297	GLU
1	A	1301	GLU
1	A	1308	THR
1	A	1318	THR
1	A	1325	THR
1	A	1327	ILE
1	A	1335	ILE
1	A	1350	LYS
1	A	1359	ASP
1	A	1361	SER
1	A	1372	VAL
1	A	1378	GLN
1	A	1404	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1408	ILE
1	A	1417	GLU
1	A	1418	LEU
1	A	1424	VAL
1	A	1436	ILE
1	A	1445	ILE
1	A	1452	LYS

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Mol	Chain	Res	Type
2	B	21	GLU
2	B	22	SER
2	B	30	SER
2	B	50	SER
2	B	55	VAL
2	B	58	THR
2	B	69	LEU
2	B	74	LEU
2	B	86	ARG
2	B	89	GLU
2	B	97	VAL
2	B	98	THR
2	B	101	MET
2	B	105	SER
2	B	137	TYR
2	B	164	LYS
2	B	178	ASN
2	B	183	GLU
2	B	185	THR
2	B	193	LYS
2	B	199	MET
2	B	205	ILE
2	B	211	VAL
2	B	217	ARG
2	B	222	ILE
2	B	235	SER
2	B	239	GLU
2	B	240	ILE
2	B	241	ARG
2	B	244	LEU
2	B	245	GLU
2	B	251	ILE
2	B	253	THR
2	B	273	LEU
2	B	283	VAL
2	B	285	ILE
2	B	298	LEU
2	B	303	TYR
2	B	305	VAL
2	B	323	VAL
2	B	326	ASP
2	B	341	LEU

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Mol	Chain	Res	Type
2	B	343	ILE
2	B	345	LYS
2	B	348	ARG
2	B	349	ILE
2	B	351	TYR
2	B	355	ILE
2	B	357	GLN
2	B	364	ILE
2	B	365	THR
2	B	387	LEU
2	B	391	ASP
2	B	398	ARG
2	B	428	ILE
2	B	444	MET
2	B	448	ILE
2	B	451	LYS
2	B	452	THR
2	B	461	LEU
2	B	480	SER
2	B	487	THR
2	B	493	SER
2	B	502	ILE
2	B	510	LYS
2	B	516	ASN
2	B	531	GLN
2	B	540	SER
2	B	544	CYS
2	B	554	ILE
2	B	556	THR
2	B	560	GLU
2	B	564	GLU
2	B	566	LEU
2	B	567	GLU
2	B	568	ASP
2	B	587	HIS
2	B	591	ARG
2	B	603	LEU
2	B	608	ASP
2	B	619	ILE
2	B	628	THR
2	B	644	GLU
2	B	649	LYS

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Mol	Chain	Res	Type
2	B	653	VAL
2	B	668	ASP
2	B	675	ASP
2	B	690	VAL
2	B	705	MET
2	B	737	THR
2	B	739	THR
2	B	746	SER
2	B	755	ILE
2	B	764	SER
2	B	771	SER
2	B	791	THR
2	B	792	MET
2	B	795	ILE
2	B	827	ILE
2	B	845	SER
2	B	858	SER
2	B	862	GLN
2	B	873	THR
2	B	881	ASN
2	B	886	LYS
2	B	887	HIS
2	B	889	THR
2	B	895	ASP
2	B	899	ILE
2	B	906	SER
2	B	919	SER
2	B	929	THR
2	B	936	ASP
2	B	938	SER
2	B	943	SER
2	B	944	THR
2	B	946	ASN
2	B	956	THR
2	B	959	ASP
2	B	963	PHE
2	B	971	THR
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	1002	THR
2	B	1032	SER

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Mol	Chain	Res	Type
2	B	1049	ASP
2	B	1051	THR
2	B	1056	SER
2	B	1070	GLU
2	B	1080	LYS
2	B	1082	MET
2	B	1093	GLN
2	B	1096	ARG
2	B	1108	ARG
2	B	1113	VAL
2	B	1115	THR
2	B	1120	GLU
2	B	1145	SER
2	B	1151	LEU
2	B	1152	MET
2	B	1163	CYS
2	B	1170	THR
2	B	1201	LYS
2	B	1202	LEU
2	B	1211	ASN
2	B	1215	ARG
2	B	1219	ASP
3	C	4	GLU
3	C	14	SER
3	C	36	VAL
3	C	48	SER
3	C	50	GLU
3	C	53	THR
3	C	84	ARG
3	C	86	CYS
3	C	90	ASP
3	C	94	LYS
3	C	102	GLN
3	C	106	GLU
3	C	111	THR
3	C	127	ARG
3	C	136	ASP
3	C	137	LYS
3	C	148	ARG
3	C	155	LEU
3	C	165	LYS
3	C	179	GLU

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Mol	Chain	Res	Type
3	C	203	GLN
3	C	204	SER
3	C	207	CYS
3	C	214	ASN
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	237	SER
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	262	LEU
3	C	264	GLN
4	D	34	GLN
4	D	43	GLU
4	D	52	LEU
4	D	54	GLU
4	D	59	ILE
4	D	63	LEU
4	D	75	LYS
4	D	119	ARG
4	D	121	LYS
4	D	123	LEU
4	D	131	GLU
4	D	140	ASP
4	D	141	LEU
4	D	144	THR
4	D	147	TYR
4	D	157	GLN
4	D	160	VAL
4	D	167	LEU
4	D	170	THR
4	D	177	VAL
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	202	ILE
4	D	206	GLU
4	D	212	LYS
4	D	214	LEU
4	D	216	ASN
4	D	220	LEU

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Mol	Chain	Res	Type
5	E	6	GLU
5	E	8	ASN
5	E	12	LEU
5	E	30	ILE
5	E	33	GLU
5	E	35	VAL
5	E	37	LEU
5	E	40	GLU
5	E	41	ASP
5	E	45	LYS
5	E	50	MET
5	E	54	GLN
5	E	56	LYS
5	E	58	MET
5	E	66	GLU
5	E	67	GLU
5	E	69	ILE
5	E	77	SER
5	E	78	LEU
5	E	81	GLU
5	E	83	CYS
5	E	90	VAL
5	E	92	THR
5	E	93	MET
5	E	107	THR
5	E	113	GLN
5	E	126	SER
5	E	131	THR
5	E	156	LEU
5	E	157	SER
5	E	162	ARG
5	E	164	LEU
5	E	180	ARG
5	E	182	ASP
5	E	203	GLU
5	E	204	THR
6	F	72	LYS
6	F	77	ASP
6	F	82	THR
6	F	85	MET
6	F	102	SER
6	F	104	ASN

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Mol	Chain	Res	Type
6	F	111	LEU
6	F	133	VAL
6	F	138	LEU
6	F	148	VAL
6	F	149	GLU
6	F	150	GLU
6	F	153	VAL
7	G	4	ILE
7	G	13	LEU
7	G	21	ARG
7	G	34	VAL
7	G	41	LYS
7	G	48	VAL
7	G	49	LEU
7	G	52	ASP
7	G	53	ASN
7	G	54	ILE
7	G	57	GLN
7	G	64	THR
7	G	69	GLU
7	G	73	LYS
7	G	74	TYR
7	G	77	VAL
7	G	78	VAL
7	G	80	LYS
7	G	86	VAL
7	G	90	THR
7	G	110	VAL
7	G	117	GLN
7	G	120	THR
7	G	122	ASN
7	G	145	VAL
7	G	147	ILE
7	G	148	GLU
7	G	151	ILE
7	G	160	ILE
7	G	163	ILE
8	H	3	ASN
8	H	23	VAL
8	H	27	GLU
8	H	33	GLN
8	H	41	ASP

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Mol	Chain	Res	Type
8	H	53	ASP
8	H	78	SER
8	H	88	SER
8	H	92	ASP
8	H	94	ASP
8	H	100	THR
8	H	106	GLU
8	H	107	VAL
8	H	108	SER
8	H	109	LYS
8	H	110	ASP
8	H	111	LEU
8	H	112	ILE
8	H	114	VAL
8	H	123	MET
8	H	126	GLU
8	H	130	ARG
8	H	131	ASN
8	H	134	ASN
8	H	135	LEU
8	H	144	ILE
8	H	146	ARG
9	I	3	THR
9	I	5	ARG
9	I	8	ARG
9	I	19	ASP
9	I	20	LYS
9	I	23	ASN
9	I	24	ARG
9	I	32	CYS
9	I	37	GLU
9	I	42	LEU
9	I	50	THR
9	I	58	VAL
9	I	62	ILE
9	I	67	THR
9	I	72	ASP
9	I	74	GLU
9	I	84	VAL
9	I	88	SER
9	I	89	GLN
9	I	106	CYS

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Mol	Chain	Res	Type
9	I	110	PHE
9	I	111	THR
10	J	2	ILE
10	J	5	VAL
10	J	6	ARG
10	J	7	CYS
10	J	14	VAL
10	J	17	LYS
10	J	23	ASN
10	J	28	ASP
10	J	29	GLU
10	J	52	THR
10	J	59	LYS
10	J	64	ASN
11	K	5	ASP
11	K	9	LEU
11	K	10	PHE
11	K	12	LEU
11	K	16	GLU
11	K	26	LYS
11	K	31	VAL
11	K	70	ARG
11	K	72	LYS
11	K	85	ASP
11	K	103	THR
12	L	33	GLU
12	L	34	CYS
12	L	35	SER
12	L	38	LEU
12	L	40	LEU
12	L	46	VAL
12	L	50	ASP
12	L	60	ARG
12	L	63	ARG
12	L	65	VAL
12	L	66	GLN
13	M	17	ASN
13	M	19	ASN
13	M	29	VAL
13	M	30	TYR
13	M	44	VAL
13	M	47	LEU

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Mol	Chain	Res	Type
13	M	51	VAL
13	M	52	LEU
13	M	56	LEU
13	M	62	GLU
13	M	86	LEU
13	M	87	LEU
13	M	94	THR
13	M	96	ILE
13	M	100	GLU
13	M	104	MET
13	M	110	LEU
13	M	111	ASN
13	M	118	VAL
13	M	141	GLU
13	M	142	LEU
13	M	171	ILE
13	M	176	ILE
13	M	177	LEU
13	M	181	ARG
13	M	193	GLN
13	M	195	LEU
13	M	197	HIS
13	M	198	VAL
13	M	199	LYS
13	M	200	THR
13	M	201	LYS
13	M	202	GLU
13	M	209	ILE
13	M	214	LEU
13	M	215	ARG
13	M	234	GLN
13	M	235	ASN
13	M	236	LEU
13	M	237	THR
13	M	252	VAL
13	M	253	THR
13	M	272	LYS
13	M	273	SER
13	M	275	ILE
13	M	276	THR
13	M	284	LEU
13	M	304	VAL

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Mol	Chain	Res	Type
13	M	308	THR
13	M	315	ILE
13	M	317	TYR
13	M	322	LYS
13	M	323	LEU
14	Q	103	LEU
14	Q	104	ARG
14	Q	106	ILE
14	Q	109	GLU
14	Q	116	THR
14	Q	118	LEU
14	Q	119	LEU
14	Q	126	LYS
14	Q	130	VAL
14	Q	132	ASP
14	Q	134	HIS
14	Q	135	LEU
14	Q	332	LEU
14	Q	336	ASP
14	Q	343	ARG
14	Q	346	GLU
14	Q	347	PHE
14	Q	358	TYR
14	Q	359	ASN
14	Q	375	LEU
14	Q	376	LEU
14	Q	381	ASP
14	Q	385	THR
14	Q	392	VAL
14	Q	396	THR
15	R	62	GLU
15	R	63	ARG
15	R	68	VAL
15	R	73	LEU
15	R	77	LEU
15	R	80	LYS
15	R	92	LEU
15	R	94	LYS
15	R	96	ARG
15	R	98	ASN
15	R	106	LEU
15	R	108	LEU

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Mol	Chain	Res	Type
15	R	126	LYS
15	R	128	VAL
15	R	129	VAL
15	R	131	ASN
15	R	136	THR
15	R	207	THR
15	R	212	THR
15	R	221	GLU
15	R	224	VAL
15	R	250	GLU
15	R	253	THR
15	R	254	THR
15	R	256	ASP
15	R	258	THR
15	R	259	VAL
15	R	262	THR
15	R	268	MET
15	R	269	SER
15	R	273	ASP
15	R	275	SER
15	R	280	VAL
16	W	5	ILE
16	W	6	ASP
16	W	16	VAL
16	W	17	VAL
16	W	30	ASP
16	W	36	SER
16	W	40	GLU
16	W	43	LEU
16	W	57	LEU
16	W	91	TYR
16	W	103	HIS
16	W	105	VAL
16	W	109	LEU
16	W	111	ASP
16	W	115	LYS
16	W	120	ASN
16	W	133	GLN
16	W	135	GLU
16	W	137	VAL
16	W	141	ASN
16	W	143	ASP

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Mol	Chain	Res	Type
16	W	145	THR
16	W	149	CYS
16	W	166	LYS
16	W	168	LYS
16	W	169	GLN
16	W	171	LYS
16	W	173	ASN
16	W	174	ARG
16	W	176	MET
16	W	178	GLN
16	W	180	GLN
16	W	183	ILE
16	W	185	SER
17	X	192	LEU
17	X	193	LEU
17	X	209	ASP
17	X	216	GLN
17	X	217	CYS
17	X	220	THR
17	X	256	ASP
17	X	261	LYS
17	X	273	GLU
17	X	278	LEU
17	X	280	ASP
18	O	64	VAL
18	O	70	ILE
18	O	78	CYS
18	O	93	GLU
18	O	97	LYS
18	O	99	PHE
18	O	114	LEU
18	O	122	VAL
18	O	132	SER
18	O	160	ILE
18	O	178	SER
18	O	186	GLU
18	O	196	ARG
18	O	206	ILE
18	O	207	PHE
18	O	234	LEU
18	O	239	LYS
21	0	6	ASP

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Mol	Chain	Res	Type
21	0	7	ASP
21	0	17	ILE
21	0	28	ILE
21	0	31	THR
21	0	32	LEU
21	0	33	ASP
21	0	34	VAL
21	0	37	ASN
21	0	38	SER
21	0	48	LYS
21	0	50	VAL
21	0	60	GLN
21	0	72	CYS
21	0	73	SER
21	0	78	GLU
21	0	80	GLU
21	0	85	GLU
21	0	86	LEU
21	0	94	THR
21	0	96	GLU
21	0	101	GLU
21	0	109	THR
21	0	120	VAL
21	0	125	LYS
21	0	130	ASP
21	0	131	GLU
21	0	135	ARG
21	0	137	THR
21	0	146	GLU
21	0	148	ASP
21	0	150	GLU
21	0	154	GLU
21	0	155	LEU
21	0	167	VAL
21	0	187	GLU
21	0	188	LYS
21	0	190	LEU
21	0	195	ILE
21	0	201	SER
21	0	204	ASN
21	0	207	ILE
21	0	209	SER

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Mol	Chain	Res	Type
21	0	217	LYS
21	0	220	GLU
21	0	221	ARG
21	0	222	VAL
21	0	223	SER
21	0	226	VAL
21	0	228	LYS
21	0	231	ILE
21	0	240	ILE
21	0	245	ILE
21	0	255	ASP
21	0	257	LEU
21	0	276	LYS
21	0	280	GLN
21	0	284	ASP
21	0	287	GLU
21	0	298	ILE
21	0	302	GLN
21	0	308	GLU
21	0	318	THR
21	0	321	ILE
21	0	327	ARG
21	0	335	LEU
21	0	336	LYS
21	0	339	ILE
21	0	343	LYS
21	0	347	LYS
21	0	349	LEU
21	0	350	HIS
21	0	351	VAL
21	0	354	GLU
21	0	355	THR
21	0	360	LEU
21	0	369	ILE
21	0	384	LEU
21	0	386	ARG
21	0	389	GLU
21	0	394	GLU
21	0	399	LEU
21	0	407	THR
21	0	413	GLU
21	0	414	GLU

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Mol	Chain	Res	Type
21	0	416	PHE
21	0	417	LEU
21	0	418	LEU
21	0	421	GLU
21	0	423	TYR
21	0	432	ASN
21	0	434	ILE
21	0	438	THR
21	0	450	PHE
21	0	453	PHE
21	0	456	VAL
21	0	457	ILE
21	0	459	THR
21	0	463	ILE
21	0	467	ASP
21	0	468	MET
21	0	476	LYS
21	0	477	THR
21	0	480	GLN
21	0	487	LEU
21	0	493	LEU
21	0	498	THR
21	0	506	ILE
21	0	510	PHE
21	0	512	ILE
21	0	514	ASN
21	0	515	ASP
21	0	528	GLU
21	0	532	ILE
21	0	533	THR
21	0	547	MET
21	0	550	ILE
21	0	553	MET
21	0	559	ILE
21	0	563	VAL
21	0	572	GLU
21	0	573	THR
21	0	591	SER
21	0	594	ARG
21	0	597	ILE
21	0	605	LYS
21	0	610	ILE

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Mol	Chain	Res	Type
21	0	614	HIS
21	0	615	GLN
21	0	625	ILE
21	0	632	SER
21	0	633	ARG
21	0	639	LEU
21	0	648	ILE
21	0	649	ARG
21	0	651	ASN
21	0	654	LEU
21	0	655	SER
21	0	656	PHE
21	0	657	ASP
21	0	673	LYS
21	0	674	ASP
21	0	678	VAL
21	0	683	ASP
21	0	688	ARG
21	0	689	LYS
21	0	705	ASP
21	0	706	LEU
21	0	710	THR
21	0	716	ASN
21	0	717	THR
21	0	729	ASP
21	0	738	VAL
21	0	739	TRP
21	0	741	TYR
21	0	743	ASP
21	0	744	LEU
21	0	745	ILE
22	1	185	LEU
22	1	200	ILE
22	1	201	ASN
22	1	209	PHE
22	1	210	TRP
22	1	211	SER
22	1	213	ARG
22	1	214	ILE
22	1	233	VAL
22	1	257	LEU
22	1	266	VAL

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Mol	Chain	Res	Type
22	1	271	THR
22	1	280	GLU
22	1	287	PHE
22	1	295	LYS
22	1	329	LEU
22	1	331	HIS
22	1	374	ILE
22	1	380	ARG
22	1	381	LEU
22	1	382	SER
22	1	387	MET
22	1	508	LYS
22	1	553	LEU
22	1	555	THR
22	1	561	LEU
22	1	563	HIS
22	1	564	PHE
22	1	593	LEU
22	1	600	VAL
22	1	609	SER
22	1	616	LEU
22	1	620	LEU
22	1	621	ASN
22	1	623	ILE
23	4	22	SER
23	4	25	LEU
23	4	27	THR
23	4	32	ILE
23	4	43	GLU
23	4	51	ILE
23	4	54	LEU
23	4	61	LEU
23	4	62	ASN
23	4	65	LEU
23	4	73	VAL
23	4	86	LEU
23	4	116	ARG
23	4	122	ASP
23	4	123	GLU
23	4	125	LEU
23	4	129	ILE
23	4	133	PHE

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Mol	Chain	Res	Type
23	4	137	LYS
23	4	140	ILE
23	4	142	GLN
23	4	179	LEU
23	4	180	THR
23	4	194	ILE
23	4	200	ILE
23	4	202	SER
23	4	206	MET
23	4	212	VAL
23	4	220	GLU
23	4	222	THR
23	4	227	THR
23	4	228	THR
23	4	236	LEU
23	4	244	LEU
23	4	245	ILE
23	4	253	PHE
23	4	254	ILE
23	4	258	LEU
23	4	260	PRO
23	4	267	HIS
23	4	269	SER
23	4	270	VAL
23	4	274	THR
23	4	276	CYS
23	4	287	PHE
23	4	288	ILE
23	4	293	LEU
23	4	297	SER
23	4	304	LYS
24	6	109	ARG
24	6	114	ASN
24	6	116	THR
24	6	118	TYR
24	6	119	GLN
24	6	128	LEU
24	6	136	MET
24	6	139	LYS
24	6	145	ARG
24	6	146	HIS
24	6	148	MET

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Mol	Chain	Res	Type
24	6	155	ASP
24	6	158	HIS
24	6	164	ASN
24	6	166	ILE
24	6	168	GLN
24	6	176	ASN
24	6	180	GLN
24	6	182	VAL
24	6	185	VAL
24	6	193	ILE
24	6	197	LYS
24	6	202	GLN
24	6	205	LYS
24	6	214	LEU
24	6	222	LEU
24	6	224	VAL
24	6	233	LEU
24	6	238	SER
24	6	239	LEU
24	6	243	ASP
24	6	249	GLN
24	6	261	VAL
24	6	263	VAL
24	6	266	LEU
24	6	273	CYS
24	6	274	LYS
24	6	280	THR
24	6	282	TYR
24	6	289	LYS
24	6	290	ILE
24	6	291	LEU
24	6	292	LEU
24	6	293	ASP
24	6	297	LEU
24	6	300	LEU
24	6	306	THR
24	6	308	LEU
24	6	310	VAL
24	6	317	PHE
24	6	318	THR
24	6	319	LEU
24	6	326	THR

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Mol	Chain	Res	Type
24	6	339	HIS
24	6	352	CYS
24	6	362	VAL
24	6	368	LEU
24	6	376	LEU
24	6	378	ARG
24	6	383	LEU
24	6	384	MET
24	6	406	CYS
24	6	448	LEU
24	6	449	HIS
25	2	8	HIS
25	2	11	THR
25	2	12	GLN
25	2	14	LEU
25	2	16	GLU
25	2	17	ILE
25	2	21	VAL
25	2	28	SER
25	2	33	LEU
25	2	48	MET
25	2	51	VAL
25	2	53	ASN
25	2	55	ASN
25	2	57	VAL
25	2	60	LEU
25	2	61	ASP
25	2	62	LEU
25	2	71	LYS
25	2	75	GLN
25	2	79	LYS
25	2	80	SER
25	2	84	LEU
25	2	86	LEU
25	2	87	LEU
25	2	88	ILE
25	2	95	THR
25	2	100	LEU
25	2	106	ILE
25	2	205	LEU
25	2	208	LEU
25	2	278	LEU

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Mol	Chain	Res	Type
25	2	284	THR
25	2	348	TYR
25	2	350	TYR
25	2	351	SER
25	2	353	SER
25	2	356	GLN
25	2	357	ILE
25	2	359	VAL
25	2	364	VAL
25	2	366	LEU
25	2	370	PHE
25	2	372	ASN
25	2	379	THR
25	2	380	ARG
25	2	389	ASN
25	2	391	ILE
25	2	395	GLN
25	2	396	ILE
25	2	401	GLU
25	2	411	LEU
25	2	414	GLU
25	2	417	GLU
25	2	427	LYS
25	2	432	VAL
25	2	450	ARG
25	2	457	SER
25	2	462	PHE
25	2	463	GLU
25	2	464	THR
25	2	466	GLN
25	2	470	LEU
25	2	486	ASP
25	2	488	LYS
25	2	489	LYS
25	2	493	ILE
25	2	495	LYS
25	2	496	GLU
25	2	502	LEU
25	2	508	LYS
26	5	9	LEU
26	5	11	GLN
26	5	13	ASP

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Mol	Chain	Res	Type
26	5	22	GLN
26	5	24	ASP
26	5	26	LYS
26	5	29	ASP
26	5	33	GLU
26	5	42	VAL
26	5	46	LYS
26	5	47	VAL
26	5	50	VAL
26	5	52	HIS
26	5	57	LEU
26	5	58	LEU
26	5	60	LYS
27	3	9	ASN
27	3	10	LYS
27	3	25	ASP
27	3	30	VAL
27	3	41	SER
27	3	44	ASP
27	3	45	ARG
27	3	49	LEU
27	3	53	GLN
27	3	64	ARG
27	3	71	GLN
27	3	73	PHE
28	7	269	LEU
28	7	302	GLU
28	7	304	GLU
28	7	309	ASP
28	7	314	HIS
28	7	315	SER
28	7	316	PHE
28	7	318	ILE
28	7	320	ASN
28	7	322	SER
28	7	331	GLN
28	7	332	GLU
28	7	342	ASP
28	7	343	PHE
28	7	344	ARG
28	7	352	LEU
28	7	357	LYS

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Mol	Chain	Res	Type
28	7	360	THR
28	7	362	ILE
28	7	365	TYR
28	7	368	LYS
28	7	378	ARG
28	7	384	ILE
28	7	393	THR
28	7	398	THR
28	7	402	THR
28	7	412	THR
28	7	419	GLN
28	7	425	LEU
28	7	428	CYS
28	7	431	GLN
28	7	435	CYS
28	7	437	VAL
28	7	439	THR
28	7	442	ASN
28	7	443	LYS
28	7	444	GLU
28	7	446	PHE
28	7	447	GLN
28	7	453	VAL
28	7	454	VAL
28	7	456	THR
28	7	457	TYR
28	7	459	MET
28	7	460	VAL
28	7	464	ARG
28	7	469	ASP
28	7	473	VAL
28	7	475	ASP
28	7	485	ILE
28	7	487	LEU
28	7	490	VAL
28	7	497	MET
28	7	498	PHE
28	7	499	ARG
28	7	500	ARG
28	7	501	VAL
28	7	505	ILE
28	7	511	LEU

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Mol	Chain	Res	Type
28	7	517	LEU
28	7	518	VAL
28	7	520	GLU
28	7	524	ILE
28	7	527	LEU
28	7	530	LEU
28	7	531	ILE
28	7	534	LYS
28	7	541	MET
28	7	543	LEU
28	7	545	GLN
28	7	546	LYS
28	7	549	ILE
28	7	552	VAL
28	7	559	CYS
28	7	562	THR
28	7	565	PHE
28	7	569	TYR
28	7	571	ARG
28	7	573	THR
28	7	576	LYS
28	7	578	MET
28	7	579	LEU
28	7	584	ASN
28	7	586	THR
28	7	601	ARG
28	7	607	VAL
28	7	613	TYR
28	7	622	MET
28	7	627	ILE
28	7	637	MET
28	7	647	ASP
28	7	652	ILE
28	7	656	LYS
28	7	659	ASP
28	7	666	GLU
28	7	668	THR
28	7	676	HIS
28	7	681	ARG
28	7	682	GLN
28	7	692	ARG
28	7	695	ARG

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Mol	Chain	Res	Type
28	7	697	ASN
28	7	699	GLU
28	7	709	VAL
28	7	712	ASP
28	7	717	TYR
28	7	719	SER
28	7	728	ASP
28	7	729	GLN
28	7	735	VAL
28	7	736	ILE
28	7	740	HIS
28	7	742	MET
28	7	743	GLU
28	7	747	ASN
28	7	760	LEU
28	7	761	GLN
28	7	767	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	297	GLN
1	A	299	HIS
1	A	363	GLN
1	A	399	HIS
1	A	742	ASN
1	A	1171	GLN
1	A	1188	GLN
1	A	1232	ASN
2	B	60	GLN
2	B	325	GLN
2	B	770	GLN
2	B	1205	GLN
3	C	203	GLN
3	C	231	ASN
4	D	39	ASN
4	D	41	GLN
4	D	143	ASN
4	D	216	ASN
5	E	114	ASN
6	F	104	ASN

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Mol	Chain	Res	Type
7	G	24	GLN
8	H	128	ASN
9	I	90	GLN
13	M	212	ASN
13	M	285	ASN
14	Q	113	ASN
14	Q	117	HIS
17	X	251	ASN
17	X	270	GLN
18	O	68	GLN
18	O	95	ASN
18	O	158	GLN
21	0	164	ASN
21	0	330	HIS
21	0	555	GLN
22	1	188	ASN
22	1	513	GLN
23	4	120	ASN
24	6	176	ASN
24	6	227	HIS
24	6	302	ASN
24	6	382	HIS
25	2	75	GLN
25	2	403	HIS
25	2	500	GLN
27	3	31	ASN
27	3	71	GLN
28	7	331	GLN
28	7	345	ASN
28	7	431	GLN
28	7	471	GLN
28	7	528	ASN
28	7	545	GLN
28	7	553	GLN
28	7	596	GLN
28	7	598	HIS
28	7	611	ASN
28	7	646	ASN
28	7	729	GLN
28	7	747	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
31	SF4	0	801	21	0,12,12	-	-	-		

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
31	SF4	0	801	21	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	801	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	86.50
1	1	519:UNK	C	537:GLU	N	13.64
1	1	355:UNK	C	368:UNK	N	9.80

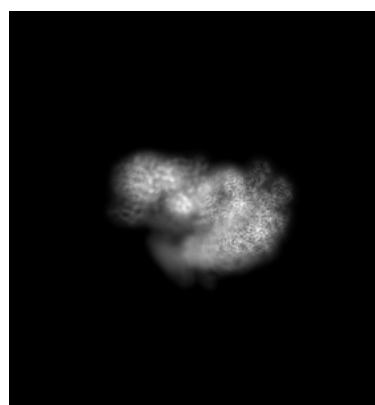
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23904. These allow visual inspection of the internal detail of the map and identification of artifacts.

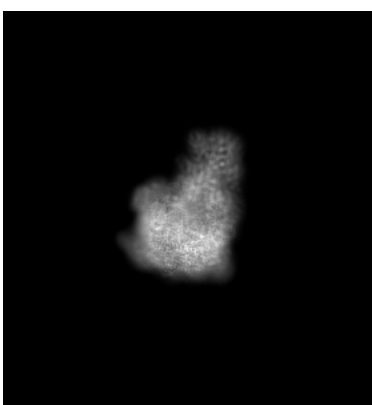
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

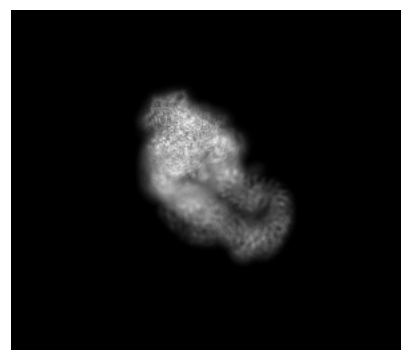
6.1.1 Primary map



X



Y

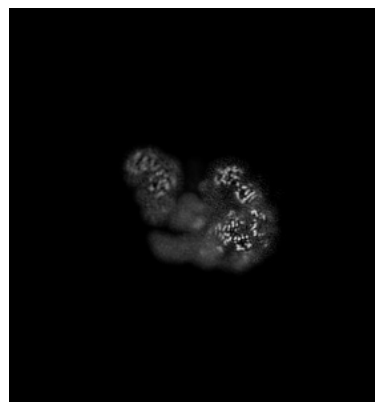


Z

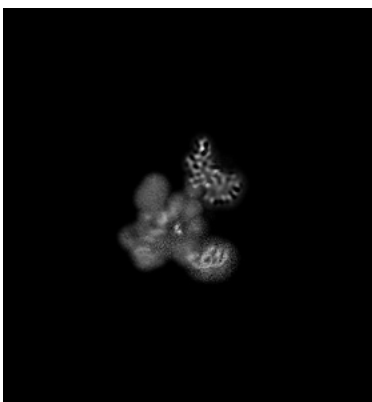
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 257



Y Index: 221

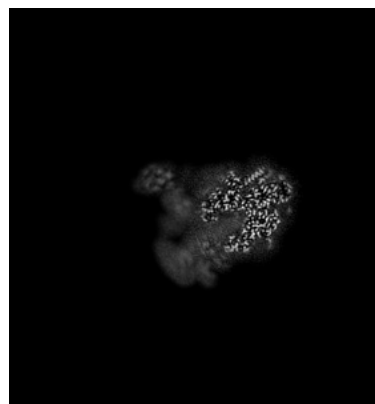


Z Index: 239

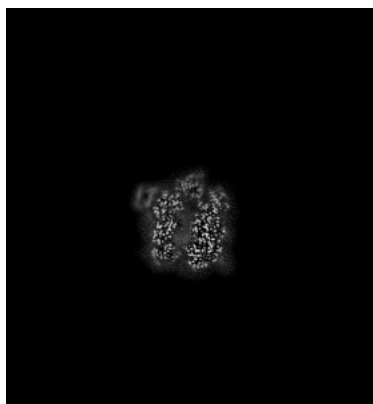
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

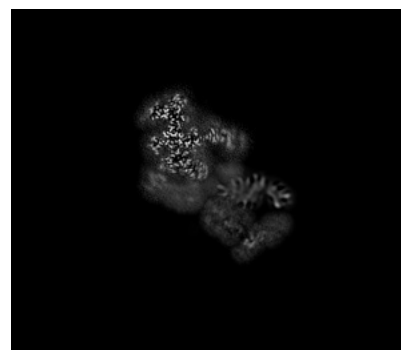
6.3.1 Primary map



X Index: 215



Y Index: 273

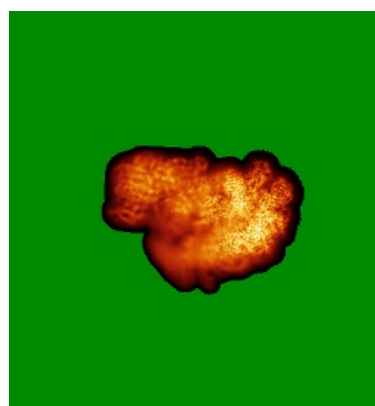


Z Index: 248

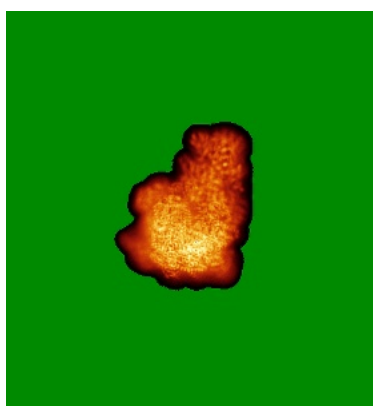
The images above show the largest variance slices of the map in three orthogonal directions.

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

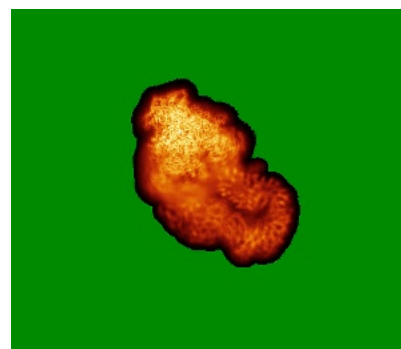
6.4.1 Primary map



X



Y

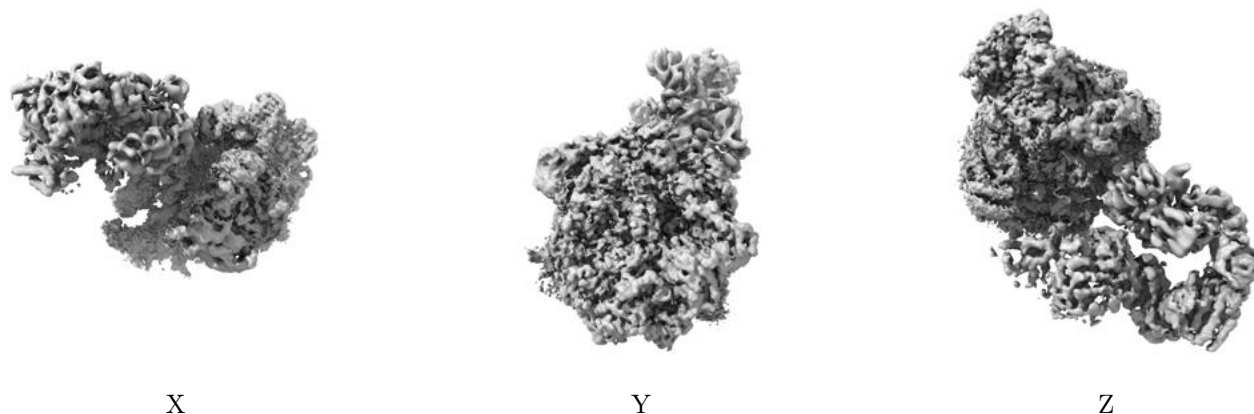


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0164. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

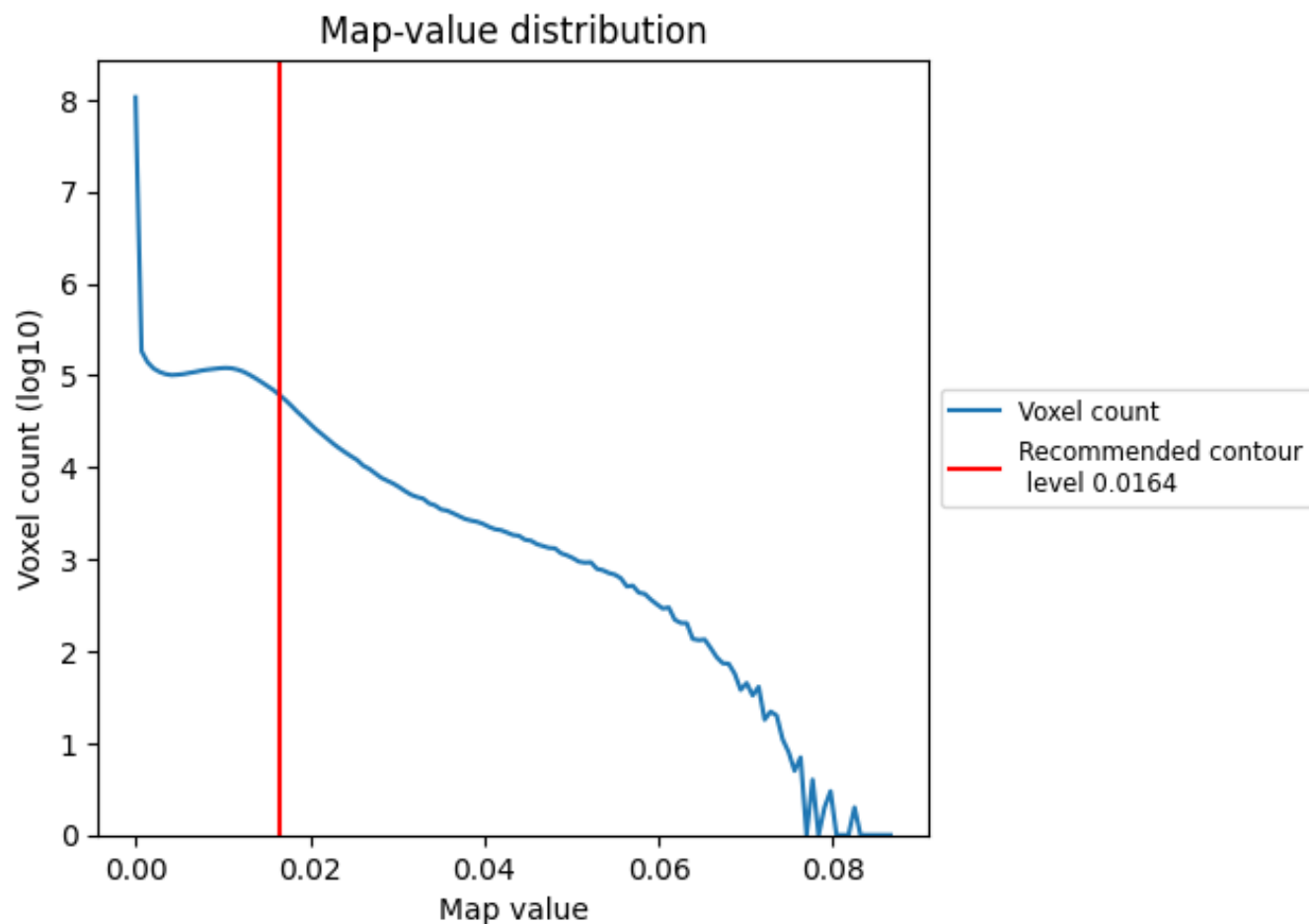
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

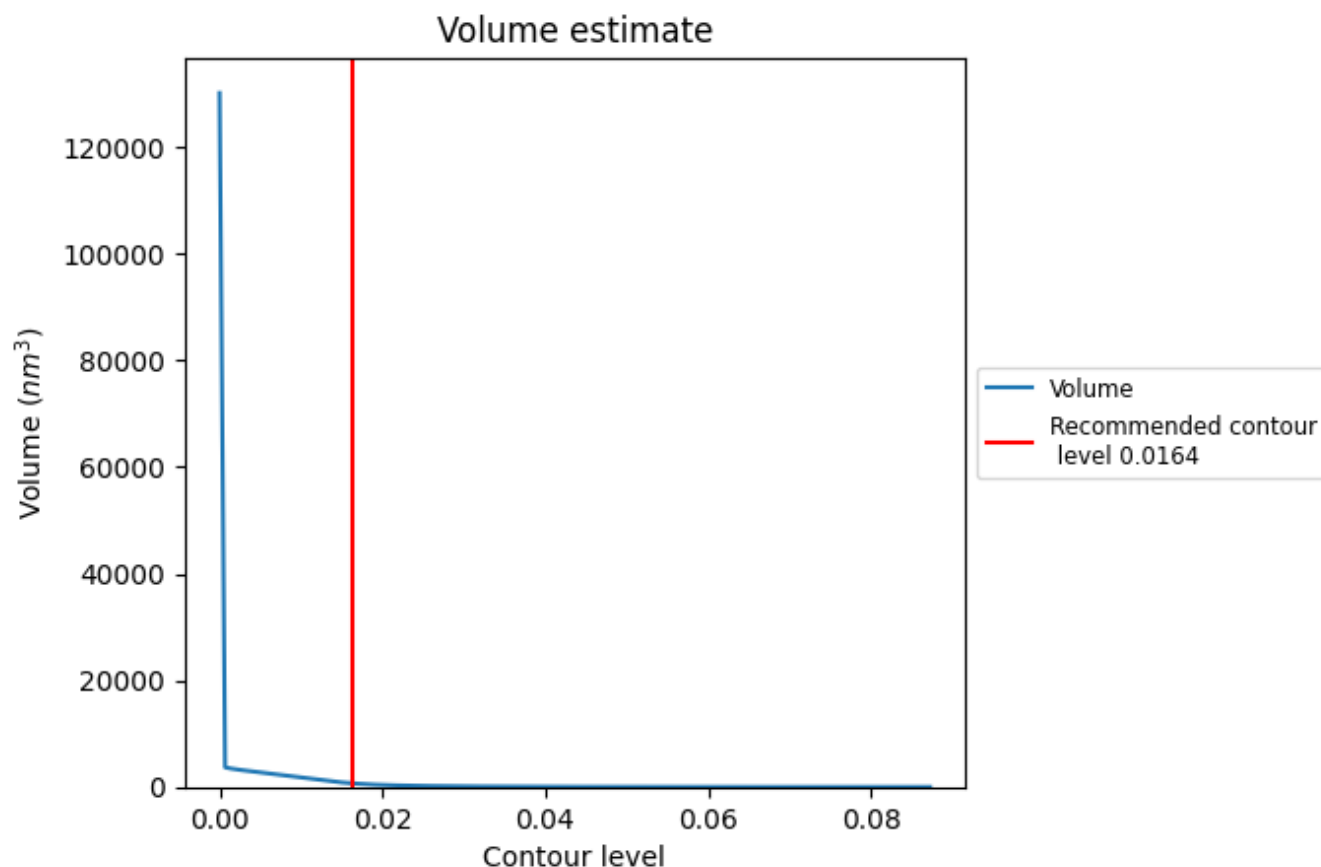
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 672 nm³; this corresponds to an approximate mass of 607 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.

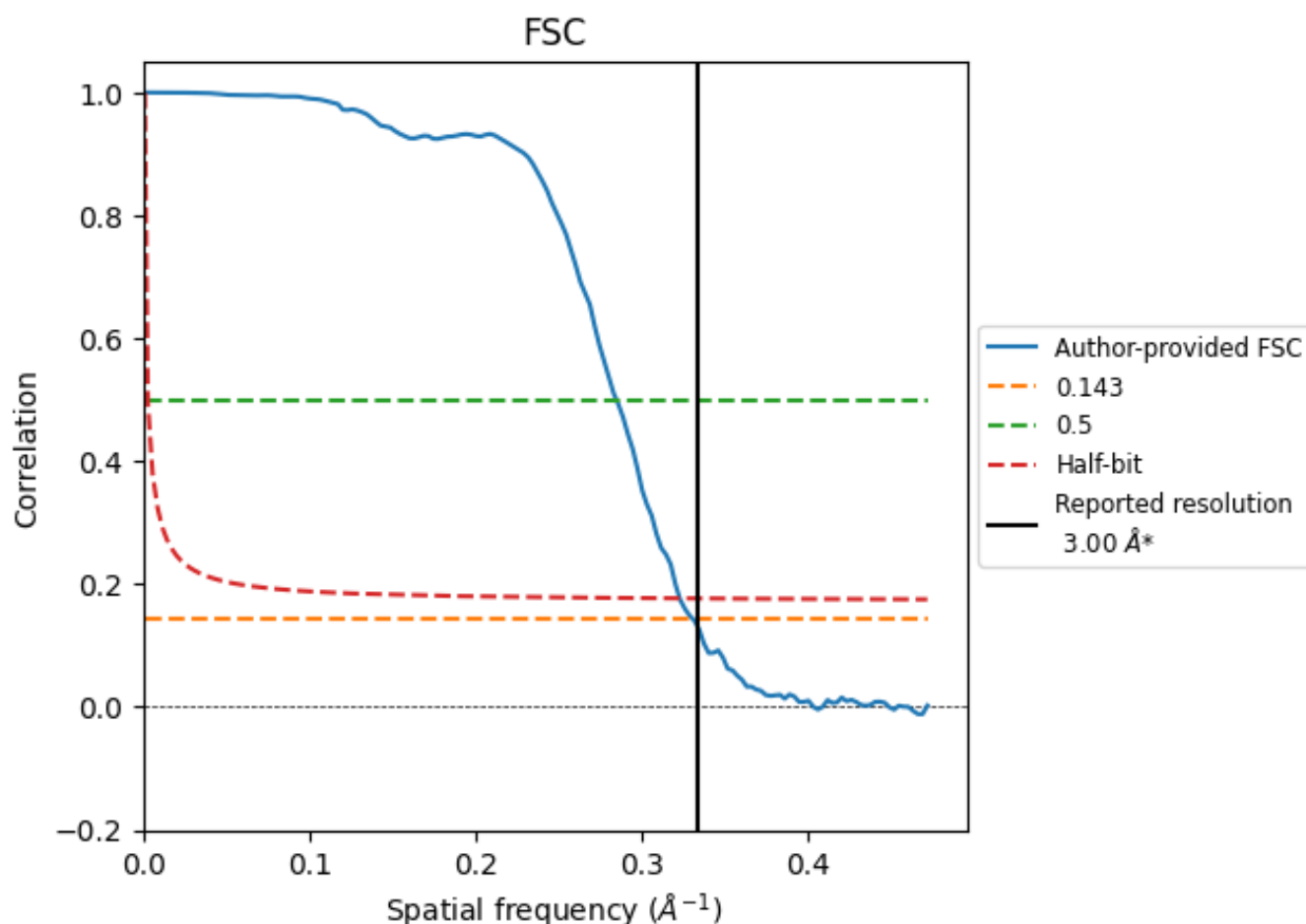
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

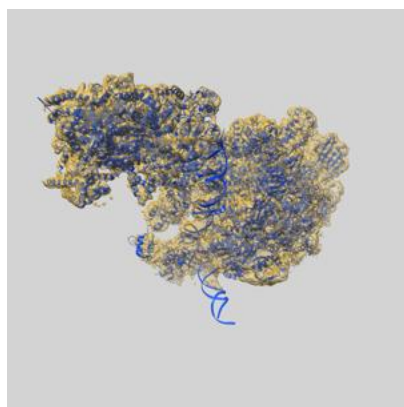
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.51	3.10
Unmasked-calculated*	-	-	-

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

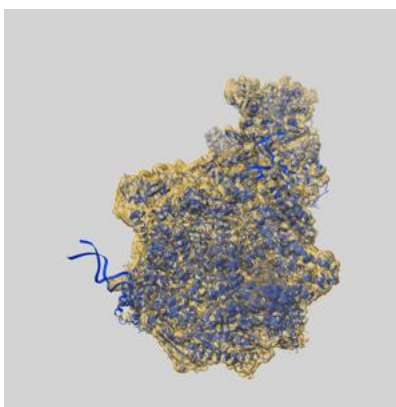
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23904 and PDB model 7ML0. Per-residue inclusion information can be found in section 3 on page 11.

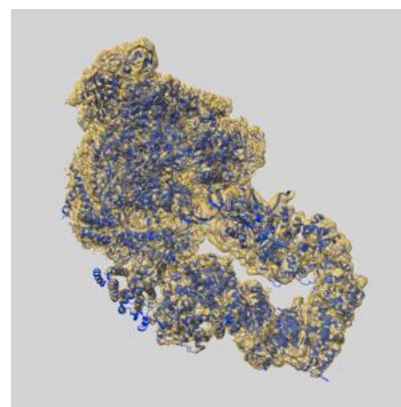
9.1 Map-model overlay [i](#)



X



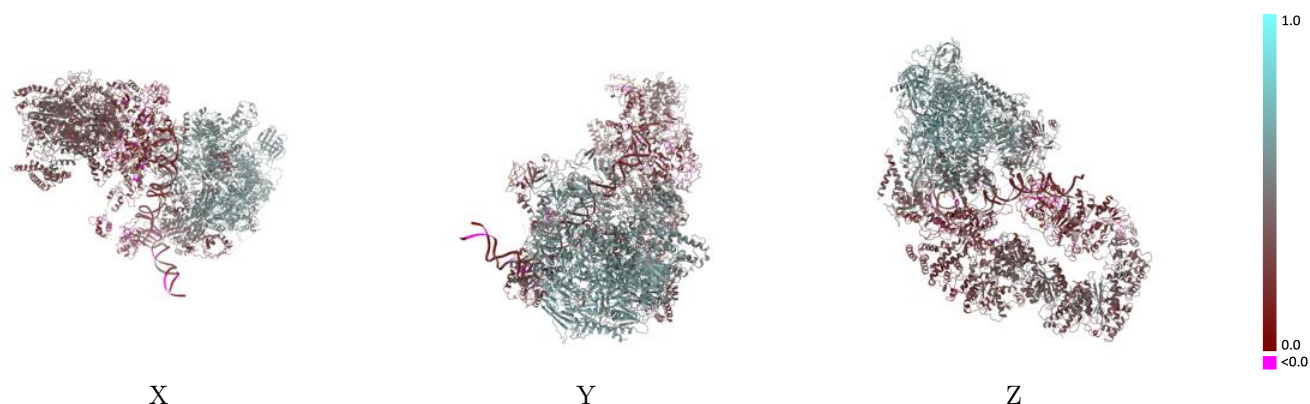
Y



Z

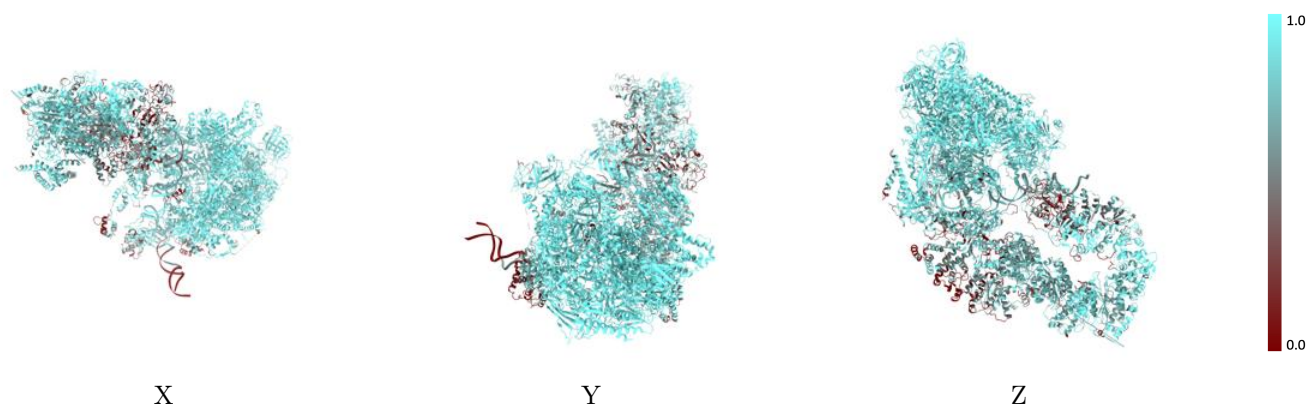
The images above show the 3D surface view of the map at the recommended contour level 0.0164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



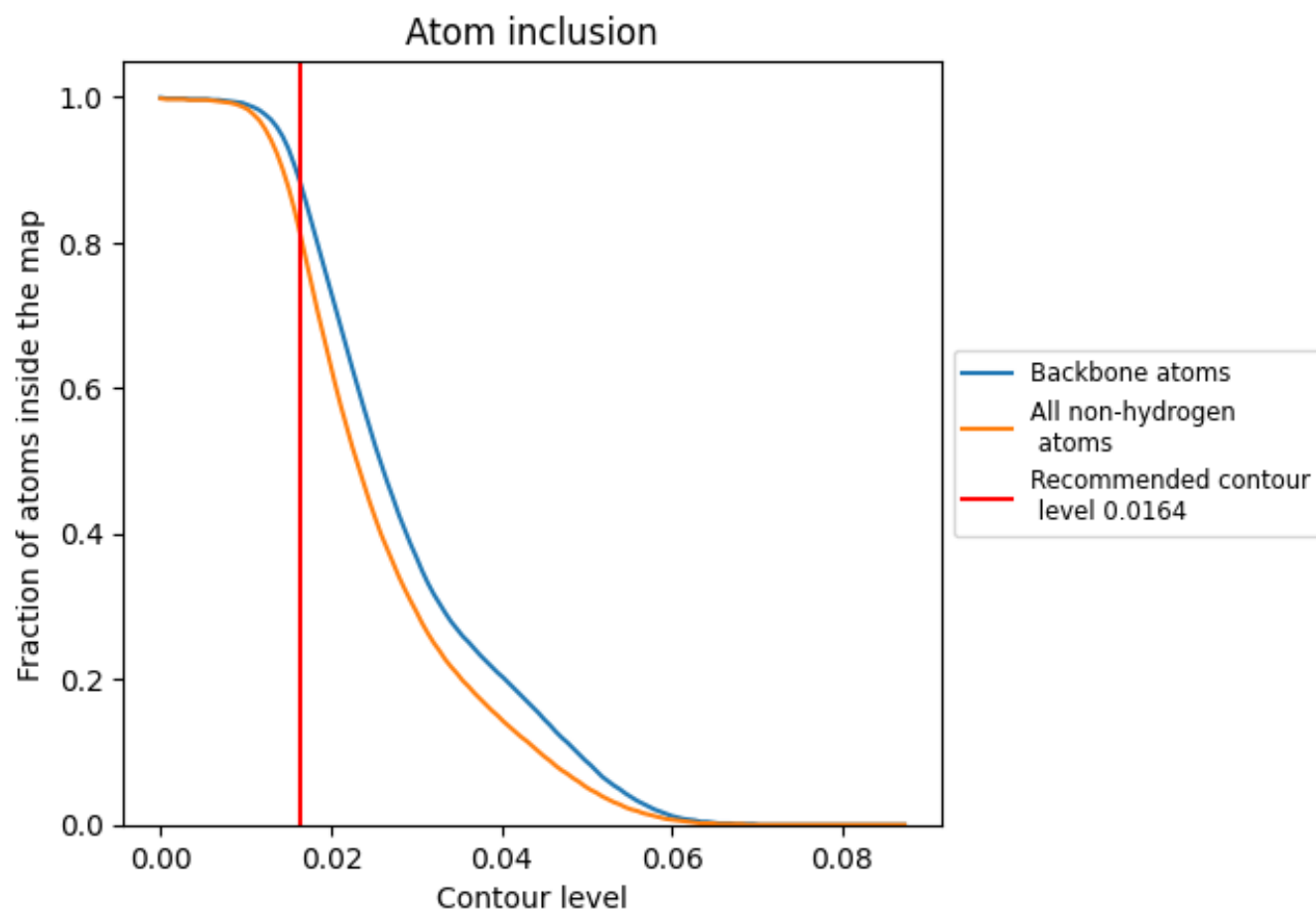
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0164).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.0164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8110	 0.4170
0	 0.5870	 0.3220
1	 0.6460	 0.3280
2	 0.7520	 0.3140
3	 0.4590	 0.2560
4	 0.7880	 0.3870
5	 0.6420	 0.2530
6	 0.8190	 0.4040
7	 0.5220	 0.2200
A	 0.9760	 0.5500
B	 0.9760	 0.5650
C	 0.9800	 0.5840
D	 0.8240	 0.3720
E	 0.9650	 0.5270
F	 0.9880	 0.5850
G	 0.9270	 0.4510
H	 0.9570	 0.5370
I	 0.9290	 0.4960
J	 0.9880	 0.5880
K	 0.9270	 0.5450
L	 0.9830	 0.5410
M	 0.6340	 0.3970
N	 0.6520	 0.1870
O	 0.5260	 0.1790
Q	 0.9140	 0.3960
R	 0.8380	 0.3200
T	 0.6510	 0.1850
W	 0.8850	 0.2360
X	 0.7130	 0.2050

