



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:42 AM UTC

PDB ID : 7QV9 / pdb_00007qv9
EMDB ID : EMD-14171
Title : CryoEM structure of bacterial transcription intermediate complex mediated by activator PspF
Authors : Ye, F.Z.; Zhang, X.D.
Deposited on : 2022-01-20
Resolution : 3.50 Å(reported)
Based on initial model : 5NSS

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

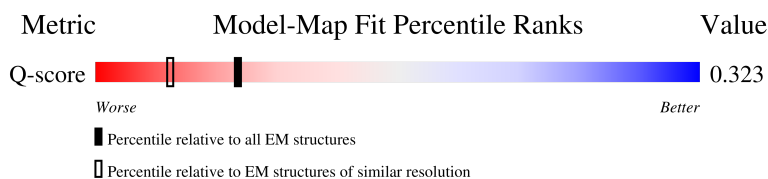
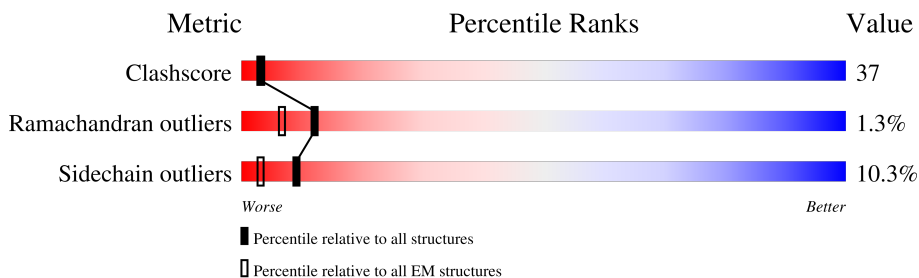
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



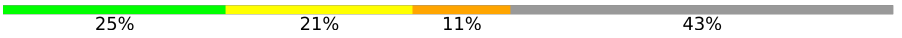
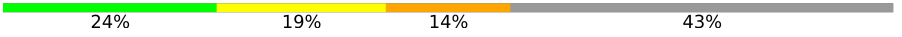
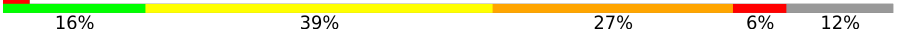
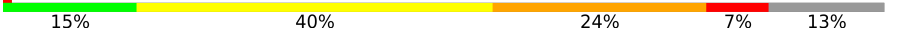
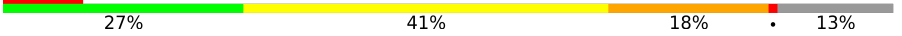
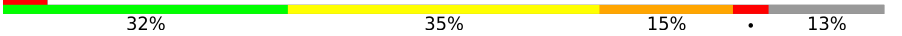
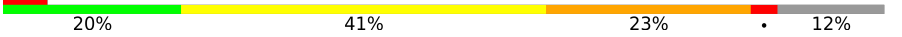
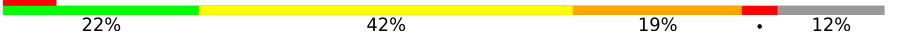
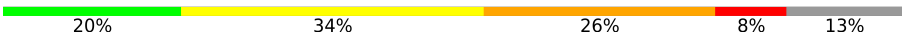
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	329	
1	B	329	
2	C	1342	
3	D	1407	

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Mol	Chain	Length	Quality of chain
4	E	91	
5	N	63	
6	T	63	
7	a	295	
7	b	295	
7	c	295	
7	d	295	
7	e	295	
7	f	295	
8	M	477	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ADP	a	601	-	-	X	-
9	ADP	e	601	-	-	X	-
9	ADP	f	601	-	X	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 41491 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	309	Total	C	N	O	S	0	0
			2322	1453	407	455	7		
1	B	223	Total	C	N	O	S	0	0
			1676	1045	294	332	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10125	6360	1761	1964	40		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0
			9634	6052	1730	1814	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	74	Total	C	N	O	S	0	0
			546	335	109	101	1		

- Molecule 5 is a DNA chain called Non-template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	36	Total	C	N	O	P	0	0
			738	349	137	216	36		

- Molecule 6 is a DNA chain called Template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	36	Total	C	N	O	P	0	0
			738	349	137	216	36		

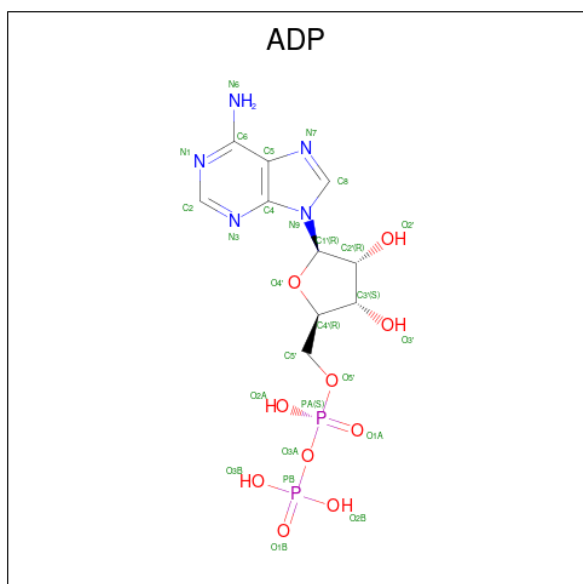
- Molecule 7 is a protein called Transcription activator PspF.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	259	Total	C	N	O	S	0	0
			2052	1301	361	380	10		
7	b	258	Total	C	N	O	S	0	0
			2052	1302	360	380	10		
7	c	256	Total	C	N	O	S	0	0
			2000	1270	349	372	9		
7	d	256	Total	C	N	O	S	0	0
			2041	1295	361	376	9		
7	f	259	Total	C	N	O	S	0	0
			2053	1304	358	381	10		
7	e	259	Total	C	N	O	S	0	0
			2062	1308	364	381	9		

- Molecule 8 is a protein called RNA polymerase sigma-54 factor.

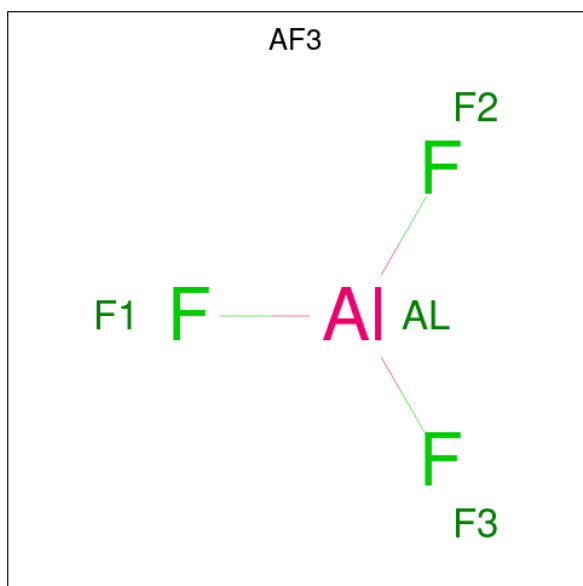
Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	417	Total	C	N	O	S	0	0
			3301	2071	572	646	12		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	f	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).

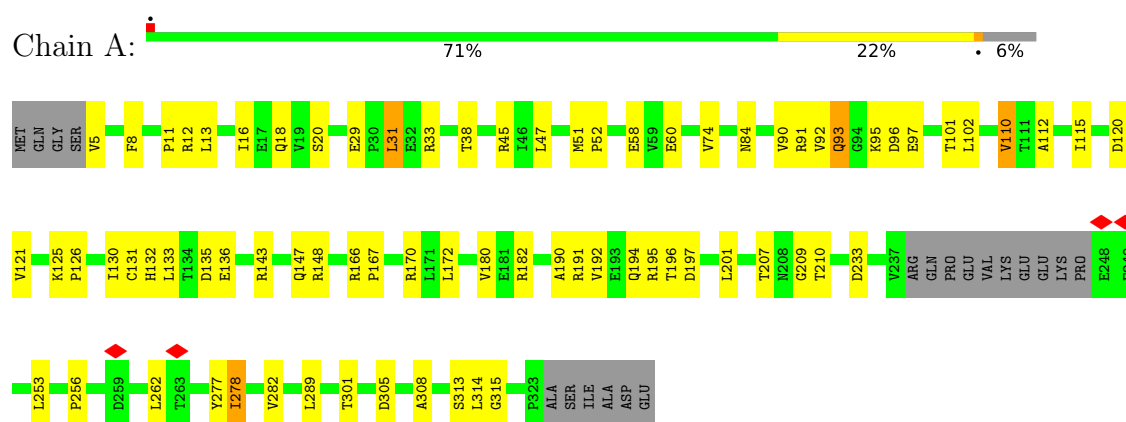


Mol	Chain	Residues	Atoms			AltConf
10	a	1	Total	Al	F	0
			4	1	3	
10	b	1	Total	Al	F	0
			4	1	3	
10	f	1	Total	Al	F	0
			4	1	3	
10	e	1	Total	Al	F	0
			4	1	3	

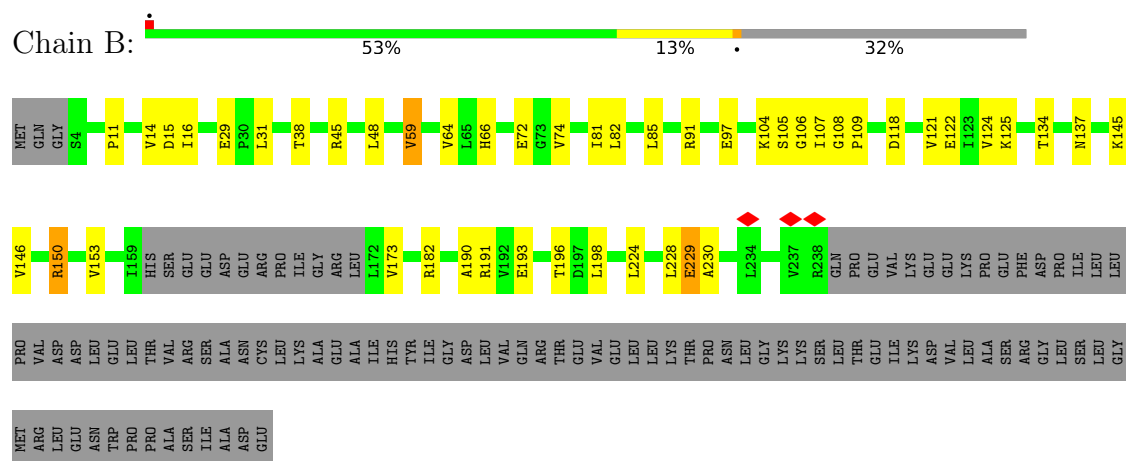
3 Residue-property plots

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.

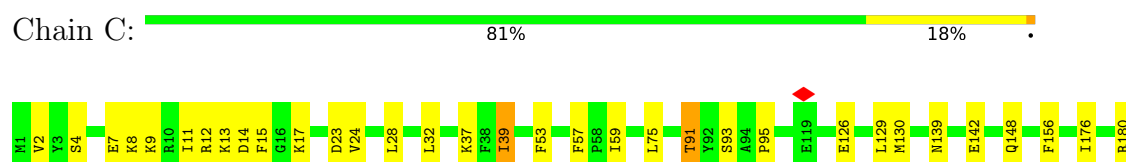
• Molecule 1: DNA-directed RNA polymerase subunit alpha

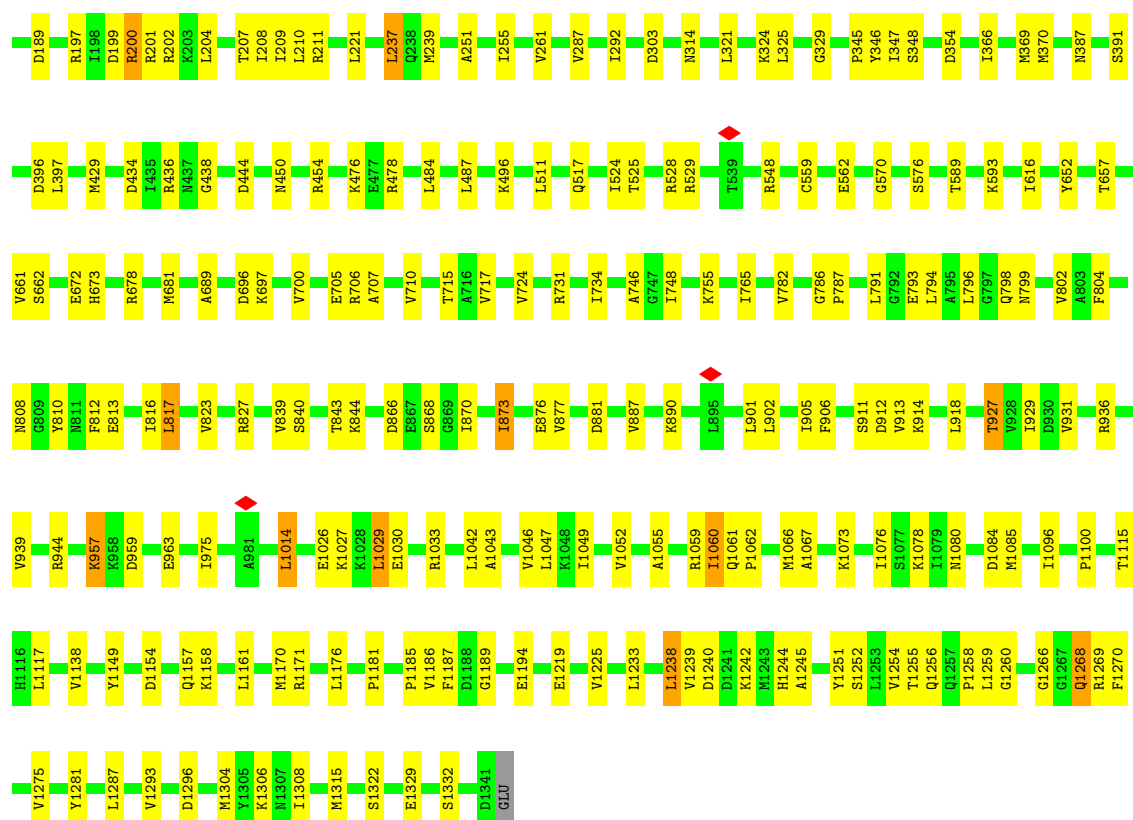


• Molecule 1: DNA-directed RNA polymerase subunit alpha

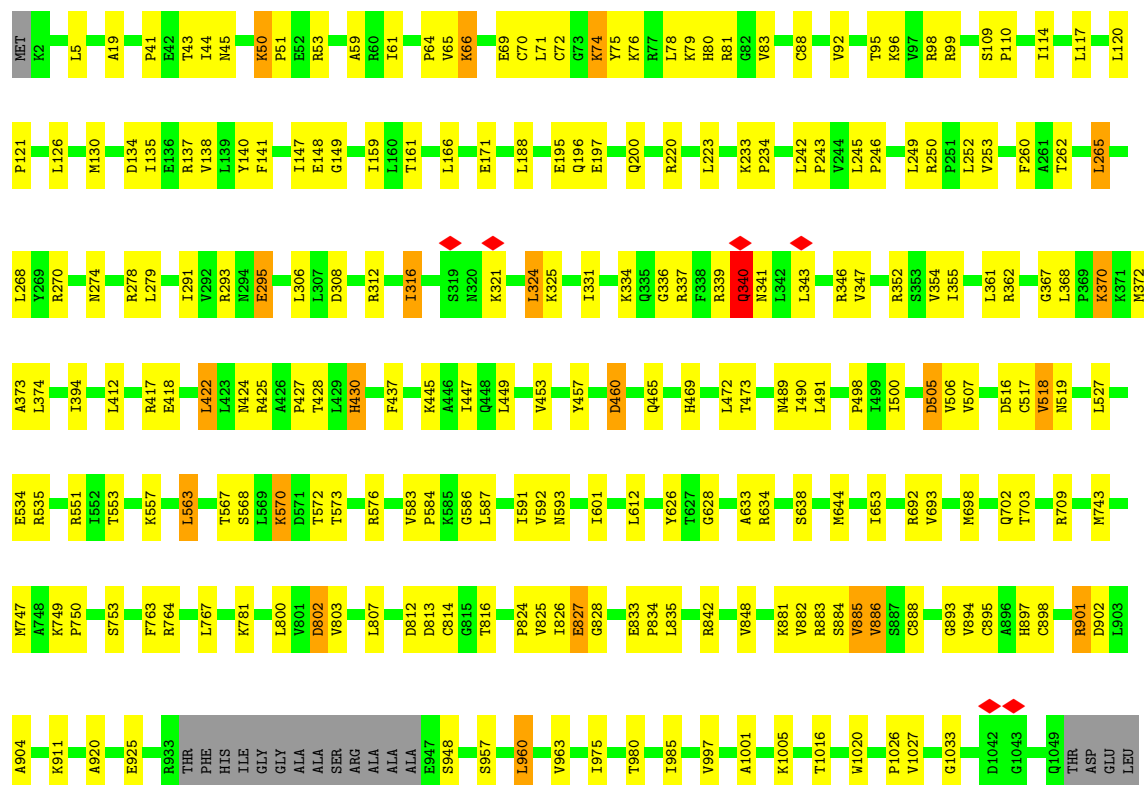
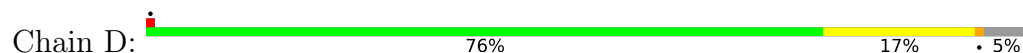


• Molecule 2: DNA-directed RNA polymerase subunit beta

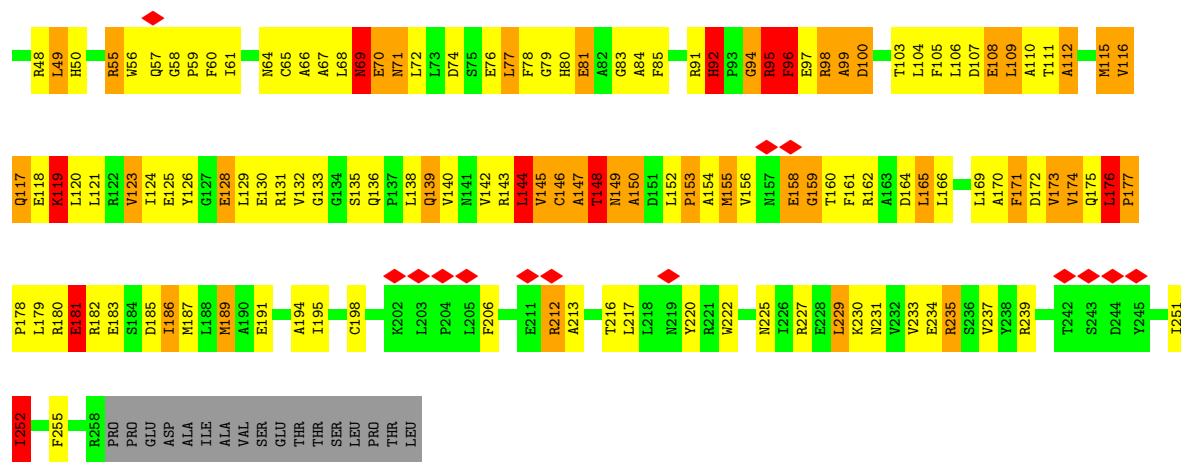




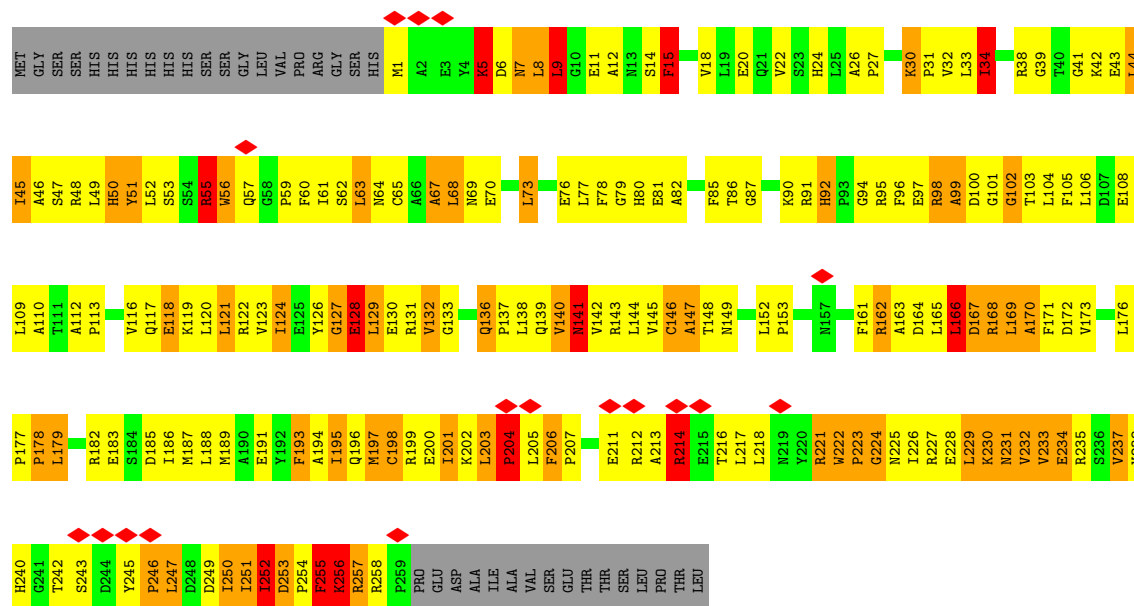
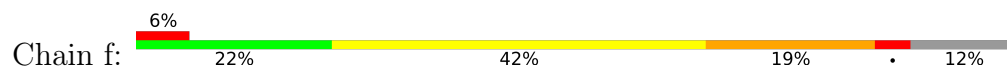
• Molecule 3: DNA-directed RNA polymerase subunit beta'



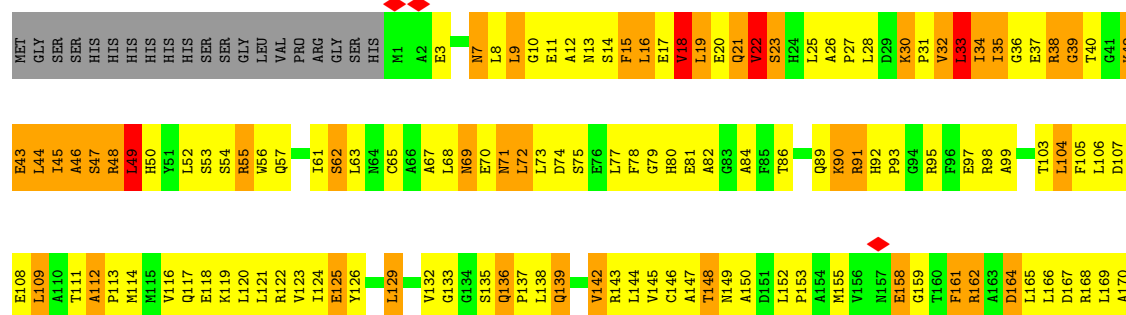
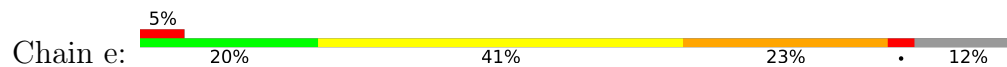


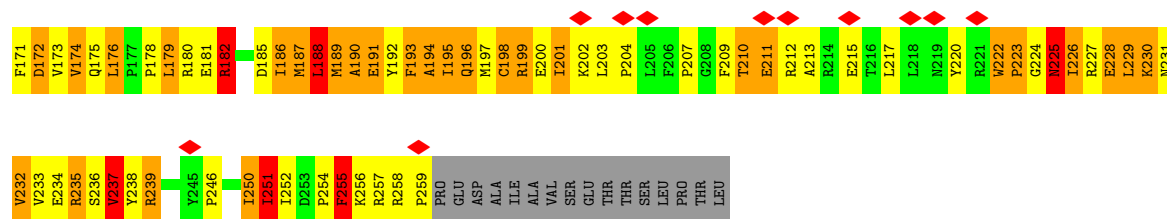


• Molecule 7: Transcription activator PspF



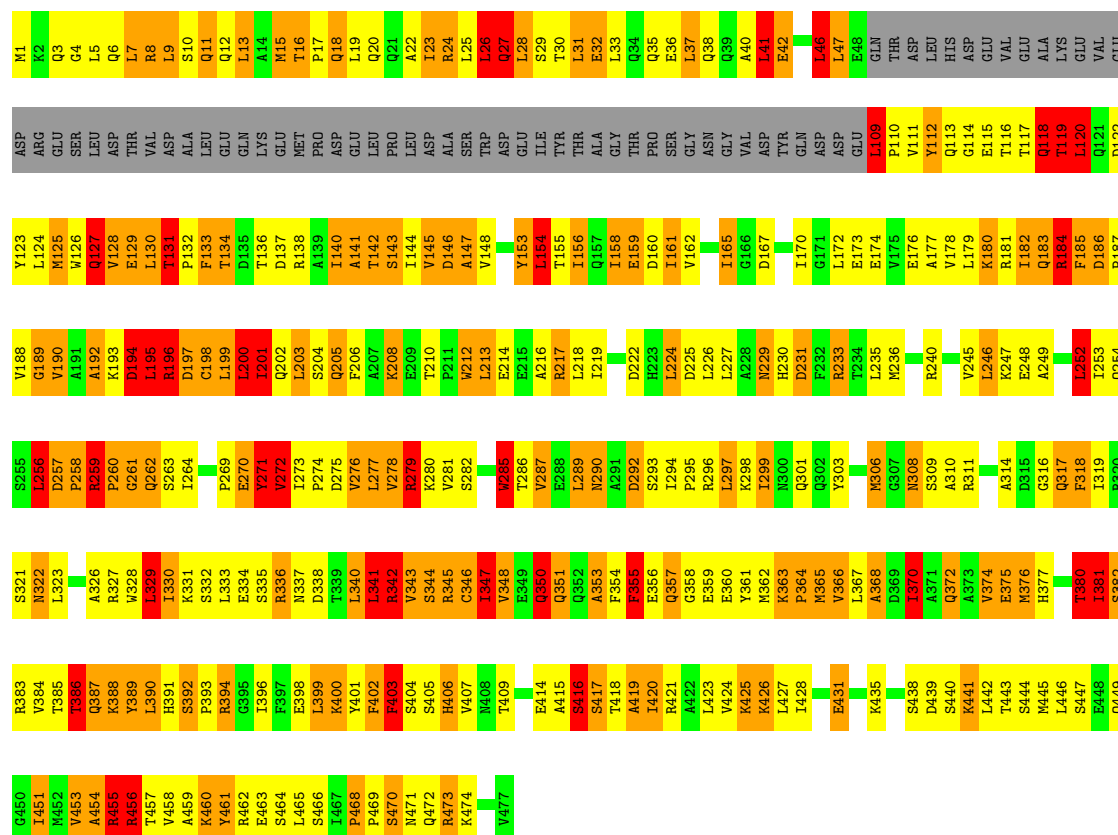
• Molecule 7: Transcription activator PspF





• Molecule 8: RNA polymerase sigma-54 factor

Chain M: 20% 34% 26% 8% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.302	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/2351	0.50	3/3202 (0.1%)
1	B	0.13	0/1693	0.39	0/2300
2	C	0.14	0/10283	0.41	0/13940
3	D	0.15	0/9768	0.46	0/13270
4	E	0.13	0/547	0.44	0/740
5	N	0.59	0/827	1.22	16/1274 (1.3%)
6	T	0.81	5/827 (0.6%)	1.27	15/1274 (1.2%)
7	a	2.38	106/2093 (5.1%)	2.12	127/2833 (4.5%)
7	b	2.36	124/2093 (5.9%)	2.28	154/2832 (5.4%)
7	c	1.56	47/2038 (2.3%)	1.78	73/2762 (2.6%)
7	d	1.55	50/2082 (2.4%)	1.73	72/2817 (2.6%)
7	e	2.02	78/2104 (3.7%)	2.03	105/2848 (3.7%)
7	f	2.10	91/2095 (4.3%)	2.05	114/2837 (4.0%)
8	M	2.38	200/3348 (6.0%)	2.44	257/4533 (5.7%)
All	All	1.30	701/42149 (1.7%)	1.36	936/57462 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	a	0	1
7	b	0	1
7	d	0	1
All	All	0	3

All (701) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	98	ARG	CZ-NH2	27.98	1.69	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	185	ASP	C-O	26.02	1.56	1.23
7	e	62	SER	C-O	22.84	1.50	1.23
7	b	143	ARG	CZ-NH1	22.67	1.64	1.32
7	a	48	ARG	CZ-NH1	19.70	1.60	1.32
7	e	23	SER	C-O	19.30	1.48	1.24
7	b	32	VAL	C-O	18.86	1.43	1.23
8	M	203	LEU	C-O	18.73	1.45	1.24
7	a	184	SER	C-O	18.69	1.47	1.24
7	a	98	ARG	CZ-NH1	18.35	1.58	1.32
7	e	62	SER	N-CA	18.24	1.68	1.46
7	f	149	ASN	CG-OD1	17.96	1.57	1.23
7	a	79	GLY	C-O	17.07	1.43	1.23
7	f	163	ALA	C-O	16.49	1.43	1.24
7	a	221	ARG	CA-C	16.48	1.74	1.52
7	b	239	ARG	C-O	16.31	1.44	1.24
7	e	173	VAL	N-CA	15.98	1.66	1.46
8	M	28	LEU	C-O	15.63	1.43	1.23
7	a	223	PRO	C-O	15.55	1.43	1.24
8	M	130	LEU	C-O	15.43	1.44	1.24
7	e	32	VAL	C-O	15.09	1.42	1.24
7	f	197	MET	C-O	15.06	1.42	1.24
7	f	179	LEU	C-O	15.03	1.41	1.24
7	b	178	PRO	N-CA	15.01	1.66	1.47
8	M	120	LEU	CA-C	-14.98	1.32	1.52
7	d	100	ASP	CG-OD1	14.66	1.53	1.25
7	b	32	VAL	CA-C	-14.44	1.35	1.52
8	M	120	LEU	C-O	14.38	1.42	1.24
7	b	190	ALA	CA-C	14.36	1.72	1.52
7	a	221	ARG	C-O	14.25	1.42	1.24
7	a	170	ALA	CA-C	-14.07	1.35	1.52
7	b	141	ASN	C-O	14.03	1.42	1.23
7	f	193	PHE	CG-CD2	13.93	1.68	1.38
8	M	153	TYR	CA-C	-13.80	1.36	1.52
7	b	256	LYS	CA-C	13.78	1.70	1.52
7	b	49	LEU	CA-CB	13.63	1.75	1.53
7	b	50	HIS	CA-CB	-13.50	1.32	1.53
7	f	222	TRP	C-O	13.50	1.41	1.24
8	M	190	VAL	C-O	13.43	1.38	1.23
7	f	255	PHE	CA-C	13.36	1.70	1.52
7	b	236	SER	C-O	13.34	1.39	1.24
7	d	99	ALA	CA-C	13.06	1.70	1.52
7	d	123	VAL	C-O	-13.00	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	197	MET	SD-CE	12.92	2.11	1.79
7	f	141	ASN	N-CA	12.88	1.62	1.46
7	a	172	ASP	C-O	-12.82	1.09	1.23
7	b	143	ARG	C-O	12.72	1.39	1.24
7	e	172	ASP	C-O	12.68	1.38	1.23
7	e	46	ALA	CA-C	12.60	1.69	1.52
7	e	55	ARG	CA-C	12.60	1.69	1.52
7	b	143	ARG	CZ-NH2	12.53	1.49	1.33
7	f	128	GLU	CD-OE1	12.46	1.49	1.25
7	e	32	VAL	CA-C	-12.44	1.36	1.52
7	f	146	CYS	C-O	12.24	1.39	1.23
7	b	190	ALA	C-O	12.23	1.39	1.24
7	b	49	LEU	N-CA	12.21	1.61	1.46
7	d	100	ASP	CG-OD2	12.19	1.48	1.25
7	b	237	VAL	CA-CB	12.18	1.68	1.54
7	a	182	ARG	CZ-NH1	12.00	1.49	1.32
7	f	141	ASN	CG-OD1	11.88	1.46	1.23
7	e	34	ILE	C-O	11.65	1.36	1.24
7	a	48	ARG	NE-CZ	11.64	1.45	1.33
7	b	121	LEU	N-CA	-11.60	1.31	1.46
7	b	188	LEU	CA-C	11.57	1.67	1.52
7	e	201	ILE	C-O	11.45	1.37	1.24
7	f	214	ARG	CZ-NH1	11.36	1.48	1.32
7	c	184	SER	C-O	11.15	1.35	1.24
7	b	70	GLU	CA-C	11.12	1.68	1.52
7	c	197	MET	CG-SD	11.09	2.08	1.80
8	M	183	GLN	CA-C	-11.07	1.38	1.52
7	e	187	MET	C-O	11.03	1.37	1.24
7	a	141	ASN	CG-ND2	11.03	1.56	1.33
7	a	174	VAL	CA-C	-10.95	1.39	1.52
7	f	193	PHE	CG-CD1	10.92	1.61	1.38
7	a	79	GLY	CA-C	10.79	1.64	1.52
7	a	80	HIS	CA-C	-10.69	1.39	1.52
8	M	326	ALA	N-CA	-10.66	1.33	1.46
7	a	222	TRP	CA-C	10.65	1.66	1.52
7	f	176	LEU	CA-CB	-10.63	1.34	1.53
7	c	230	LYS	C-O	10.60	1.36	1.24
8	M	262	GLN	C-O	10.59	1.36	1.24
7	b	141	ASN	CA-C	10.57	1.66	1.53
8	M	195	LEU	CA-C	-10.57	1.39	1.52
8	M	184	ARG	C-O	10.55	1.35	1.23
7	b	192	TYR	CG-CD2	10.53	1.61	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	51	TYR	C-O	10.51	1.37	1.24
7	a	186	ILE	C-O	10.44	1.35	1.24
7	d	159	GLY	N-CA	10.43	1.60	1.45
7	f	214	ARG	CD-NE	10.40	1.60	1.46
8	M	278	VAL	C-O	10.33	1.35	1.24
7	f	222	TRP	N-CA	10.32	1.60	1.46
7	e	39	GLY	C-O	10.31	1.38	1.23
7	d	158	GLU	C-O	10.27	1.37	1.24
8	M	125	MET	CA-CB	-10.26	1.36	1.53
7	a	141	ASN	CG-OD1	10.22	1.43	1.23
7	e	22	VAL	C-O	10.22	1.38	1.24
8	M	329	LEU	CA-C	-10.21	1.39	1.52
7	f	99	ALA	CA-CB	10.17	1.68	1.53
7	c	194	ALA	C-O	10.17	1.35	1.24
7	e	189	MET	CG-SD	10.13	2.06	1.80
8	M	354	PHE	CA-C	-10.13	1.39	1.52
7	a	173	VAL	C-O	10.11	1.37	1.24
8	M	456	ARG	CZ-NH1	10.10	1.46	1.32
8	M	262	GLN	CA-C	-10.07	1.39	1.52
7	b	184	SER	CA-C	-10.06	1.40	1.52
8	M	419	ALA	N-CA	-10.02	1.34	1.46
7	e	46	ALA	N-CA	10.00	1.58	1.46
8	M	41	LEU	CA-C	9.92	1.65	1.52
7	b	221	ARG	N-CA	9.91	1.59	1.46
8	M	133	PHE	CA-CB	9.91	1.70	1.53
7	b	70	GLU	CA-CB	9.87	1.69	1.53
8	M	126	TRP	CE2-CZ2	9.86	1.60	1.39
7	a	187	MET	N-CA	-9.84	1.34	1.46
7	b	69	ASN	CG-ND2	9.82	1.53	1.33
8	M	147	ALA	N-CA	-9.76	1.32	1.46
7	b	59	PRO	C-O	9.73	1.35	1.23
7	c	222	TRP	CA-C	-9.67	1.40	1.52
7	f	101	GLY	C-O	9.56	1.36	1.23
7	b	142	VAL	C-O	9.56	1.34	1.24
8	M	405	SER	CA-C	9.54	1.65	1.52
8	M	129	GLU	CA-CB	-9.50	1.38	1.53
7	b	218	LEU	CA-C	9.50	1.65	1.52
8	M	127	GLN	C-O	9.46	1.36	1.24
8	M	416	SER	CA-C	-9.43	1.40	1.52
7	d	171	PHE	C-O	9.43	1.34	1.24
8	M	117	THR	N-CA	9.43	1.56	1.45
7	e	44	LEU	CA-C	9.41	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	189	GLY	C-O	9.40	1.36	1.23
8	M	260	PRO	CA-C	9.39	1.65	1.52
7	b	235	ARG	CA-C	-9.33	1.41	1.52
7	e	194	ALA	C-O	9.30	1.35	1.24
7	a	79	GLY	N-CA	9.29	1.57	1.45
7	e	47	SER	CA-CB	9.26	1.68	1.53
7	e	255	PHE	N-CA	9.24	1.58	1.46
7	b	193	PHE	CG-CD1	9.24	1.58	1.38
8	M	276	VAL	CA-CB	-9.22	1.40	1.54
7	e	142	VAL	C-O	9.19	1.35	1.24
7	d	49	LEU	CA-C	9.17	1.65	1.52
7	c	222	TRP	N-CA	9.13	1.59	1.46
7	b	204	PRO	CA-C	9.11	1.65	1.52
8	M	249	ALA	CA-C	-9.11	1.41	1.52
8	M	389	TYR	C-O	9.09	1.35	1.24
7	f	231	ASN	CG-OD1	9.03	1.40	1.23
8	M	415	ALA	C-O	9.03	1.34	1.23
7	a	172	ASP	CA-C	-9.02	1.41	1.52
7	a	222	TRP	C-N	9.02	1.42	1.33
8	M	456	ARG	CZ-NH2	9.02	1.45	1.33
7	c	187	MET	C-O	9.00	1.34	1.24
7	b	177	PRO	C-O	8.99	1.34	1.24
7	f	79	GLY	C-O	-8.99	1.15	1.23
8	M	327	ARG	CA-C	-8.98	1.40	1.52
7	f	55	ARG	CA-C	8.91	1.64	1.52
7	a	100	ASP	C-O	8.89	1.34	1.23
7	b	32	VAL	CA-CB	8.88	1.70	1.55
8	M	128	VAL	CA-CB	-8.87	1.43	1.54
7	f	127	GLY	C-O	8.82	1.35	1.23
7	c	229	LEU	C-O	8.81	1.35	1.24
7	f	169	LEU	N-CA	8.81	1.56	1.46
7	b	227	ARG	CA-CB	8.78	1.67	1.53
7	f	92	HIS	CA-C	-8.74	1.43	1.52
8	M	380	THR	CA-CB	-8.74	1.39	1.53
7	d	45	ILE	N-CA	-8.69	1.34	1.46
8	M	386	THR	N-CA	8.68	1.56	1.45
7	c	253	ASP	C-O	-8.66	1.16	1.24
7	b	120	LEU	N-CA	8.64	1.56	1.46
7	a	224	GLY	C-O	8.61	1.35	1.23
7	c	255	PHE	N-CA	8.61	1.58	1.46
7	c	228	GLU	CA-C	8.56	1.64	1.52
7	f	92	HIS	C-O	-8.54	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	e	224	GLY	N-CA	8.54	1.57	1.45
7	a	198	CYS	CA-C	8.54	1.64	1.52
7	a	100	ASP	CA-CB	-8.52	1.40	1.53
7	a	183	GLU	C-O	8.51	1.33	1.23
7	e	34	ILE	CA-C	8.48	1.62	1.52
7	b	188	LEU	N-CA	-8.48	1.36	1.46
7	e	192	TYR	C-O	8.47	1.34	1.24
7	c	241	GLY	CA-C	8.46	1.63	1.51
8	M	356	GLU	C-O	8.44	1.33	1.24
7	b	60	PHE	N-CA	8.43	1.57	1.46
7	a	100	ASP	N-CA	-8.41	1.34	1.46
7	f	44	LEU	N-CA	-8.41	1.35	1.46
7	a	224	GLY	N-CA	8.40	1.57	1.45
8	M	120	LEU	CB-CG	8.39	1.70	1.53
7	b	143	ARG	N-CA	8.37	1.56	1.46
7	b	182	ARG	C-O	8.32	1.34	1.24
7	a	225	ASN	C-O	-8.27	1.15	1.24
7	a	34	ILE	C-O	-8.24	1.15	1.24
8	M	190	VAL	N-CA	-8.23	1.37	1.46
8	M	276	VAL	C-O	8.22	1.34	1.24
7	b	255	PHE	C-O	8.22	1.36	1.23
8	M	177	ALA	CA-C	8.21	1.63	1.52
8	M	473	ARG	N-CA	8.21	1.56	1.46
7	a	45	ILE	N-CA	-8.21	1.36	1.46
7	e	21	GLN	N-CA	-8.19	1.35	1.46
7	a	65	CYS	CA-C	8.18	1.64	1.52
8	M	260	PRO	C-O	8.18	1.34	1.24
7	a	190	ALA	N-CA	8.16	1.56	1.46
7	b	17	GLU	CA-C	8.11	1.63	1.52
7	a	65	CYS	CB-SG	8.10	2.08	1.81
6	T	9	DT	O3'-P	-8.06	1.49	1.61
8	M	344	SER	C-O	8.04	1.33	1.24
7	b	227	ARG	N-CA	-8.03	1.36	1.46
7	e	48	ARG	C-O	8.03	1.34	1.24
7	f	127	GLY	N-CA	8.02	1.56	1.45
7	e	44	LEU	CB-CG	8.01	1.69	1.53
7	b	227	ARG	C-O	8.00	1.33	1.24
7	a	222	TRP	N-CA	8.00	1.57	1.46
7	b	140	VAL	CA-C	7.99	1.61	1.52
7	f	214	ARG	NE-CZ	7.97	1.41	1.33
7	a	182	ARG	CA-C	7.95	1.63	1.52
7	f	127	GLY	CA-C	7.94	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	252	ILE	N-CA	-7.94	1.35	1.46
7	a	79	GLY	C-N	7.92	1.43	1.33
7	f	56	TRP	CA-C	7.91	1.63	1.52
7	a	226	ILE	C-O	7.91	1.33	1.24
7	e	235	ARG	CA-C	7.90	1.62	1.52
7	f	177	PRO	CA-C	7.89	1.59	1.52
8	M	262	GLN	N-CA	7.89	1.55	1.46
7	d	146	CYS	CA-C	-7.88	1.43	1.52
8	M	147	ALA	CA-CB	-7.83	1.41	1.53
7	f	222	TRP	CA-C	7.83	1.62	1.52
7	b	142	VAL	CA-C	7.82	1.63	1.52
7	f	56	TRP	CD2-CE3	7.81	1.52	1.40
8	M	381	ILE	CA-CB	-7.78	1.45	1.54
7	b	199	ARG	CA-C	7.77	1.63	1.52
7	a	196	GLN	C-O	7.75	1.32	1.24
7	e	161	PHE	CA-CB	7.74	1.66	1.53
7	f	163	ALA	CA-C	-7.74	1.43	1.52
7	c	241	GLY	C-O	7.72	1.34	1.23
8	M	348	VAL	CA-C	7.71	1.63	1.52
8	M	27	GLN	C-O	7.70	1.34	1.24
7	d	96	PHE	N-CA	7.66	1.56	1.46
7	b	243	SER	N-CA	7.65	1.55	1.46
7	a	169	LEU	N-CA	7.63	1.55	1.46
8	M	263	SER	N-CA	7.63	1.55	1.46
7	b	218	LEU	N-CA	-7.59	1.37	1.46
8	M	231	ASP	CA-C	-7.59	1.44	1.53
8	M	382	SER	CA-CB	-7.59	1.41	1.53
7	f	176	LEU	N-CA	7.58	1.56	1.45
8	M	262	GLN	C-N	7.58	1.43	1.33
7	a	213	ALA	C-O	7.57	1.33	1.24
8	M	177	ALA	N-CA	-7.57	1.37	1.46
7	f	99	ALA	CA-C	7.57	1.65	1.52
7	a	57	GLN	CA-CB	7.56	1.64	1.53
7	b	184	SER	C-O	7.56	1.34	1.23
8	M	399	LEU	CA-CB	-7.54	1.40	1.53
7	c	180	ARG	CA-C	7.53	1.62	1.52
7	f	230	LYS	CA-CB	-7.53	1.41	1.53
7	f	146	CYS	N-CA	-7.53	1.36	1.46
8	M	278	VAL	N-CA	7.52	1.56	1.46
8	M	296	ARG	CA-C	-7.48	1.44	1.52
7	b	255	PHE	CA-C	-7.48	1.43	1.52
7	b	216	THR	N-CA	-7.48	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	d	147	ALA	CA-C	7.47	1.62	1.52
7	a	191	GLU	N-CA	-7.47	1.37	1.46
7	e	254	PRO	CA-C	7.47	1.63	1.52
7	b	227	ARG	CA-C	-7.46	1.42	1.52
7	a	226	ILE	CA-CB	7.42	1.66	1.54
8	M	277	LEU	N-CA	7.40	1.55	1.46
7	b	254	PRO	N-CA	7.40	1.56	1.47
7	f	257	ARG	N-CA	7.40	1.55	1.46
7	f	98	ARG	CZ-NH2	-7.39	1.23	1.33
7	f	140	VAL	N-CA	7.38	1.55	1.46
7	e	234	GLU	N-CA	7.35	1.55	1.46
7	f	177	PRO	C-N	-7.34	1.24	1.33
7	a	185	ASP	CA-C	-7.33	1.43	1.52
7	f	198	CYS	C-O	7.33	1.32	1.24
7	b	192	TYR	C-O	7.32	1.32	1.24
7	a	99	ALA	CA-CB	7.30	1.62	1.52
7	a	188	LEU	N-CA	-7.30	1.37	1.46
7	a	99	ALA	N-CA	-7.30	1.37	1.46
7	e	198	CYS	C-O	7.29	1.33	1.24
7	a	185	ASP	C-N	7.26	1.42	1.33
7	f	44	LEU	C-O	7.26	1.32	1.23
8	M	198	CYS	CA-C	7.25	1.62	1.52
7	c	190	ALA	N-CA	-7.22	1.38	1.46
7	b	194	ALA	N-CA	-7.22	1.37	1.46
8	M	125	MET	SD-CE	7.20	1.97	1.79
7	f	255	PHE	C-O	7.19	1.33	1.24
7	e	21	GLN	CA-C	7.19	1.61	1.52
7	e	45	ILE	CA-CB	-7.18	1.45	1.54
6	T	9	DT	C4'-O4'	-7.17	1.31	1.45
7	c	242	THR	C-O	7.17	1.32	1.23
7	a	191	GLU	CA-C	7.16	1.62	1.52
8	M	350	GLN	CA-C	-7.14	1.43	1.52
7	f	169	LEU	C-O	7.12	1.31	1.24
7	c	167	ASP	CB-CG	7.11	1.69	1.52
8	M	230	HIS	C-O	7.10	1.32	1.23
7	a	99	ALA	CA-C	7.10	1.62	1.53
8	M	416	SER	N-CA	7.08	1.55	1.46
7	e	46	ALA	C-N	-7.06	1.24	1.33
7	d	146	CYS	N-CA	-7.04	1.36	1.45
8	M	249	ALA	N-CA	7.04	1.54	1.46
7	b	15	PHE	CA-C	7.04	1.62	1.52
7	a	258	ARG	CA-C	7.04	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	d	154	ALA	CA-C	-7.02	1.43	1.52
7	b	191	GLU	CA-C	-7.01	1.43	1.52
7	f	229	LEU	CA-C	-7.01	1.44	1.52
7	a	182	ARG	NE-CZ	6.99	1.40	1.33
7	a	188	LEU	CA-C	6.98	1.61	1.52
7	d	220	TYR	CA-C	-6.98	1.43	1.52
8	M	363	LYS	N-CA	6.96	1.56	1.46
7	d	154	ALA	N-CA	6.96	1.54	1.46
8	M	388	LYS	C-O	6.94	1.32	1.23
7	e	32	VAL	CA-CB	6.94	1.63	1.54
7	a	174	VAL	CA-CB	6.94	1.62	1.53
7	f	102	GLY	C-O	6.91	1.33	1.23
7	f	44	LEU	CA-CB	6.89	1.64	1.53
7	f	79	GLY	CA-C	-6.89	1.44	1.52
7	a	195	ILE	CA-C	6.87	1.61	1.52
8	M	208	LYS	N-CA	6.87	1.54	1.46
7	e	231	ASN	N-CA	-6.87	1.38	1.46
7	b	197	MET	C-O	6.85	1.32	1.24
7	b	239	ARG	CD-NE	6.84	1.55	1.46
7	b	32	VAL	N-CA	-6.82	1.38	1.46
7	e	187	MET	C-N	6.82	1.43	1.34
8	M	281	VAL	CA-C	6.81	1.59	1.53
7	a	65	CYS	CA-CB	6.79	1.64	1.53
8	M	345	ARG	N-CA	-6.79	1.38	1.46
7	a	183	GLU	N-CA	6.77	1.56	1.46
7	c	255	PHE	CA-CB	-6.75	1.42	1.53
8	M	402	PHE	N-CA	-6.75	1.38	1.46
7	a	170	ALA	C-O	6.75	1.32	1.24
7	d	97	GLU	C-O	6.74	1.32	1.24
7	b	235	ARG	CZ-NH2	6.73	1.42	1.33
7	a	182	ARG	CA-CB	-6.72	1.42	1.53
7	b	235	ARG	C-O	-6.71	1.16	1.24
7	a	45	ILE	CA-CB	-6.69	1.46	1.54
7	c	209	PHE	CA-C	-6.69	1.44	1.52
7	a	224	GLY	C-N	6.67	1.40	1.32
7	a	80	HIS	N-CA	6.66	1.54	1.45
7	b	60	PHE	CG-CD1	-6.66	1.24	1.38
8	M	458	VAL	CA-CB	-6.65	1.45	1.54
7	b	245	TYR	CA-C	6.64	1.61	1.52
8	M	344	SER	CA-C	-6.64	1.44	1.52
7	b	51	TYR	CA-C	6.60	1.61	1.52
7	f	230	LYS	C-O	6.59	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	364	PRO	CA-C	-6.58	1.45	1.52
8	M	403	PHE	N-CA	6.58	1.54	1.46
7	a	141	ASN	C-O	6.58	1.32	1.23
8	M	390	LEU	N-CA	6.56	1.54	1.46
8	M	459	ALA	CA-C	-6.55	1.44	1.52
7	d	109	LEU	CA-C	-6.55	1.43	1.52
7	c	228	GLU	C-O	6.55	1.31	1.24
8	M	285	TRP	CA-CB	-6.54	1.42	1.53
7	b	193	PHE	CG-CD2	6.54	1.52	1.38
8	M	270	GLU	N-CA	6.54	1.54	1.46
7	b	219	ASN	C-O	6.51	1.31	1.23
7	f	216	THR	CA-C	-6.51	1.44	1.52
8	M	145	VAL	CA-CB	-6.51	1.45	1.54
8	M	271	TYR	CA-CB	6.51	1.62	1.52
7	a	80	HIS	CG-ND1	6.50	1.45	1.38
8	M	440	SER	CA-C	6.50	1.61	1.52
7	b	239	ARG	CZ-NH2	6.50	1.41	1.33
8	M	197	ASP	N-CA	-6.50	1.38	1.46
7	b	245	TYR	C-N	6.49	1.41	1.33
7	e	195	ILE	N-CA	-6.49	1.38	1.46
7	b	177	PRO	N-CD	6.49	1.56	1.47
8	M	399	LEU	CA-C	-6.47	1.44	1.52
7	f	246	PRO	N-CA	-6.47	1.39	1.47
7	c	255	PHE	CG-CD2	6.46	1.52	1.38
7	f	45	ILE	CB-CG1	6.45	1.66	1.53
7	e	22	VAL	C-N	6.44	1.42	1.34
8	M	195	LEU	CB-CG	6.43	1.66	1.53
7	a	209	PHE	N-CA	-6.42	1.38	1.46
8	M	126	TRP	C-O	-6.42	1.15	1.24
8	M	317	GLN	CA-C	-6.41	1.44	1.52
8	M	314	ALA	N-CA	6.41	1.53	1.46
7	a	195	ILE	N-CA	-6.39	1.39	1.46
7	f	256	LYS	N-CA	6.39	1.54	1.46
7	b	235	ARG	CB-CG	6.38	1.71	1.52
7	f	205	LEU	CA-C	-6.38	1.45	1.52
8	M	42	GLU	C-O	-6.37	1.16	1.24
8	M	374	VAL	C-O	-6.37	1.16	1.24
7	b	140	VAL	C-O	6.36	1.31	1.24
7	b	61	ILE	C-O	6.36	1.30	1.24
7	d	14	SER	C-O	6.35	1.31	1.24
8	M	27	GLN	N-CA	-6.35	1.38	1.46
7	b	235	ARG	NE-CZ	6.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	180	ARG	CA-C	-6.34	1.43	1.52
8	M	399	LEU	N-CA	6.34	1.54	1.46
7	d	119	LYS	C-O	-6.32	1.16	1.24
7	b	182	ARG	CZ-NH1	6.29	1.41	1.32
8	M	347	ILE	C-N	-6.29	1.27	1.33
8	M	341	LEU	CA-CB	-6.28	1.43	1.53
8	M	190	VAL	CA-CB	-6.27	1.44	1.55
7	c	251	ILE	C-N	-6.27	1.26	1.33
8	M	42	GLU	CA-C	6.27	1.61	1.52
7	b	192	TYR	CG-CD1	6.27	1.52	1.39
8	M	258	PRO	C-O	6.26	1.30	1.23
7	b	236	SER	CA-CB	-6.25	1.43	1.53
7	f	213	ALA	C-O	6.24	1.31	1.24
7	b	254	PRO	C-O	6.23	1.32	1.24
7	f	201	ILE	C-O	6.23	1.31	1.24
7	f	127	GLY	C-N	6.23	1.42	1.33
7	e	161	PHE	C-O	6.23	1.31	1.24
7	d	99	ALA	C-O	6.21	1.31	1.24
7	f	176	LEU	C-O	6.21	1.32	1.24
8	M	438	SER	CA-C	6.21	1.61	1.53
7	b	245	TYR	N-CA	6.20	1.53	1.45
7	d	144	LEU	C-O	-6.20	1.16	1.23
7	e	180	ARG	N-CA	6.20	1.54	1.46
7	e	49	LEU	C-O	6.19	1.32	1.24
7	e	229	LEU	N-CA	6.19	1.53	1.46
8	M	454	ALA	CA-CB	-6.18	1.43	1.53
7	b	14	SER	N-CA	-6.18	1.38	1.46
8	M	402	PHE	C-O	6.18	1.31	1.24
8	M	319	ILE	N-CA	-6.16	1.38	1.46
7	d	108	GLU	N-CA	-6.14	1.38	1.46
7	e	149	ASN	CA-C	-6.14	1.44	1.52
7	c	236	SER	C-O	6.14	1.31	1.24
7	d	144	LEU	N-CA	6.14	1.53	1.46
7	e	192	TYR	CA-C	6.12	1.60	1.52
7	a	48	ARG	CA-C	-6.11	1.45	1.52
7	a	208	GLY	C-O	-6.11	1.17	1.24
8	M	199	LEU	N-CA	-6.11	1.38	1.46
7	b	218	LEU	CB-CG	6.11	1.65	1.53
7	f	201	ILE	CB-CG1	6.10	1.65	1.53
7	c	213	ALA	CA-CB	6.10	1.62	1.53
8	M	389	TYR	CG-CD1	6.10	1.52	1.39
7	e	236	SER	CA-C	6.09	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	222	TRP	CA-CB	-6.09	1.43	1.53
8	M	118	GLN	CA-C	6.09	1.60	1.52
8	M	257	ASP	C-O	-6.09	1.16	1.24
8	M	129	GLU	C-N	-6.09	1.26	1.33
7	a	198	CYS	C-O	6.08	1.31	1.24
8	M	453	VAL	CA-C	6.08	1.60	1.52
7	b	236	SER	CA-C	6.08	1.60	1.52
7	b	241	GLY	C-O	6.08	1.31	1.24
7	b	183	GLU	C-O	6.07	1.35	1.24
7	d	175	GLN	CD-OE1	6.07	1.35	1.23
7	f	251	ILE	N-CA	-6.07	1.39	1.46
8	M	133	PHE	N-CA	6.07	1.54	1.46
7	d	222	TRP	CA-C	6.06	1.60	1.52
8	M	376	MET	CA-C	6.05	1.61	1.53
8	M	27	GLN	CA-C	6.05	1.61	1.52
7	f	193	PHE	CE2-CZ	6.03	1.56	1.38
8	M	198	CYS	CB-SG	6.03	2.01	1.81
7	d	174	VAL	C-O	6.03	1.30	1.24
8	M	208	LYS	C-O	6.03	1.31	1.24
8	M	184	ARG	N-CA	6.03	1.55	1.46
8	M	258	PRO	N-CA	6.03	1.54	1.47
7	b	69	ASN	CB-CG	6.02	1.67	1.52
7	c	229	LEU	C-N	6.01	1.42	1.33
7	a	247	LEU	N-CA	6.00	1.53	1.46
7	b	215	GLU	C-O	6.00	1.31	1.24
8	M	126	TRP	CB-CG	6.00	1.68	1.50
7	e	39	GLY	N-CA	-5.99	1.36	1.45
8	M	46	LEU	CA-C	-5.99	1.44	1.52
8	M	417	SER	CA-C	-5.99	1.44	1.52
7	d	45	ILE	C-O	5.98	1.32	1.24
7	f	62	SER	N-CA	5.97	1.53	1.45
8	M	46	LEU	C-O	-5.97	1.14	1.23
8	M	146	ASP	CA-CB	-5.97	1.44	1.53
7	d	150	ALA	C-O	5.96	1.31	1.23
7	b	235	ARG	CD-NE	5.93	1.54	1.46
8	M	287	VAL	CA-C	5.91	1.59	1.52
7	a	94	GLY	N-CA	5.91	1.52	1.45
7	c	208	GLY	C-O	5.91	1.31	1.23
7	b	16	LEU	CA-C	-5.91	1.45	1.52
7	e	189	MET	CB-CG	5.91	1.70	1.52
8	M	406	HIS	CA-CB	5.91	1.62	1.53
7	b	33	LEU	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	179	LEU	CA-C	-5.90	1.44	1.52
7	f	255	PHE	CG-CD1	5.89	1.51	1.38
8	M	271	TYR	CB-CG	5.89	1.64	1.51
8	M	329	LEU	CA-CB	-5.89	1.44	1.53
7	b	58	GLY	N-CA	5.89	1.52	1.44
7	b	69	ASN	N-CA	5.88	1.53	1.46
8	M	351	GLN	C-O	5.88	1.31	1.23
8	M	202	GLN	CA-C	-5.88	1.44	1.52
8	M	350	GLN	N-CA	5.87	1.53	1.46
8	M	158	ILE	CB-CG1	5.87	1.65	1.53
7	c	218	LEU	N-CA	-5.86	1.38	1.46
7	a	184	SER	CB-OG	5.86	1.53	1.42
8	M	295	PRO	C-O	5.85	1.30	1.23
7	b	193	PHE	CA-C	5.85	1.60	1.52
6	T	6	DT	C4'-O4'	-5.85	1.33	1.45
7	c	217	LEU	N-CA	5.85	1.53	1.46
7	b	120	LEU	CA-CB	5.84	1.62	1.53
8	M	247	LYS	N-CA	-5.83	1.39	1.46
7	f	57	GLN	CD-OE1	5.82	1.34	1.23
8	M	214	GLU	N-CA	-5.81	1.39	1.46
8	M	271	TYR	CE2-CZ	5.81	1.52	1.38
7	e	193	PHE	C-O	5.81	1.30	1.24
8	M	28	LEU	CB-CG	5.80	1.65	1.53
7	a	183	GLU	CA-C	5.80	1.61	1.53
7	a	193	PHE	CG-CD1	5.80	1.51	1.38
7	f	178	PRO	N-CA	5.80	1.54	1.47
7	e	34	ILE	CB-CG1	5.79	1.65	1.53
7	b	215	GLU	CA-C	5.79	1.60	1.52
7	a	48	ARG	CA-CB	5.79	1.62	1.53
8	M	340	LEU	N-CA	-5.78	1.39	1.46
7	a	98	ARG	CA-CB	5.77	1.62	1.53
7	b	255	PHE	CA-CB	-5.77	1.44	1.53
8	M	258	PRO	N-CD	5.77	1.55	1.47
8	M	402	PHE	CA-CB	-5.75	1.44	1.53
7	a	13	ASN	CA-C	-5.75	1.45	1.52
7	a	186	ILE	CA-CB	-5.74	1.48	1.54
7	e	142	VAL	N-CA	5.74	1.53	1.46
7	d	176	LEU	CA-C	5.74	1.60	1.52
8	M	153	TYR	C-O	5.74	1.30	1.23
7	a	65	CYS	C-O	5.73	1.31	1.24
7	a	57	GLN	C-O	5.73	1.31	1.23
7	c	180	ARG	CD-NE	5.73	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	e	22	VAL	N-CA	-5.73	1.39	1.46
8	M	126	TRP	NE1-CE2	5.72	1.43	1.37
7	f	204	PRO	CA-C	5.72	1.60	1.52
8	M	40	ALA	C-N	-5.72	1.26	1.33
7	e	46	ALA	CA-CB	-5.71	1.44	1.53
7	b	235	ARG	CG-CD	5.71	1.69	1.52
7	b	139	GLN	CA-CB	5.70	1.62	1.53
7	e	55	ARG	CD-NE	-5.69	1.38	1.46
7	a	186	ILE	CA-C	5.69	1.59	1.52
7	b	182	ARG	CZ-NH2	5.69	1.40	1.33
8	M	133	PHE	CA-C	-5.68	1.45	1.52
8	M	180	LYS	CA-C	-5.68	1.44	1.52
8	M	426	LYS	CA-C	-5.67	1.45	1.52
7	d	181	GLU	C-O	-5.67	1.17	1.24
7	f	128	GLU	C-O	-5.66	1.17	1.23
7	e	223	PRO	N-CD	5.66	1.55	1.47
8	M	143	SER	CB-OG	5.65	1.53	1.42
7	d	96	PHE	CB-CG	-5.65	1.37	1.50
8	M	386	THR	CB-CG2	5.63	1.71	1.52
7	d	17	GLU	CA-C	-5.62	1.45	1.52
8	M	318	PHE	CG-CD1	5.61	1.50	1.38
7	e	222	TRP	CE3-CZ3	5.61	1.55	1.38
8	M	24	ARG	C-O	-5.60	1.16	1.24
7	e	254	PRO	C-N	5.59	1.41	1.33
8	M	40	ALA	CA-C	-5.59	1.45	1.52
7	e	147	ALA	CA-C	-5.58	1.45	1.52
8	M	321	SER	CA-C	5.58	1.60	1.52
8	M	404	SER	N-CA	5.57	1.52	1.45
8	M	346	CYS	C-O	-5.56	1.17	1.24
7	d	159	GLY	CA-C	5.55	1.59	1.51
8	M	195	LEU	N-CA	5.55	1.53	1.46
8	M	473	ARG	CA-CB	5.55	1.62	1.53
8	M	418	THR	CB-CG2	5.54	1.70	1.52
7	b	50	HIS	CA-C	-5.54	1.44	1.52
8	M	332	SER	C-N	-5.54	1.26	1.33
7	a	223	PRO	C-N	5.54	1.41	1.33
8	M	323	LEU	CA-CB	-5.54	1.44	1.53
8	M	316	GLY	C-O	5.53	1.30	1.23
7	f	197	MET	CA-CB	5.52	1.62	1.53
7	b	193	PHE	CE2-CZ	5.52	1.55	1.38
7	d	177	PRO	CA-C	-5.52	1.47	1.52
7	e	190	ALA	C-O	5.51	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	461	TYR	CA-C	5.50	1.60	1.52
7	a	188	LEU	CB-CG	5.50	1.64	1.53
7	f	179	LEU	CA-C	5.50	1.59	1.52
7	f	149	ASN	C-O	5.50	1.31	1.24
7	e	188	LEU	CA-C	5.50	1.60	1.52
8	M	454	ALA	C-O	5.50	1.30	1.24
7	d	252	ILE	CB-CG1	5.49	1.64	1.53
7	f	194	ALA	C-O	5.49	1.30	1.24
7	b	178	PRO	CG-CD	5.49	1.69	1.50
7	a	172	ASP	CA-CB	5.48	1.63	1.53
7	e	187	MET	N-CA	-5.48	1.39	1.46
7	c	180	ARG	NE-CZ	5.48	1.39	1.33
7	c	180	ARG	C-O	5.48	1.30	1.24
7	a	184	SER	C-N	5.47	1.41	1.33
7	c	195	ILE	C-O	5.47	1.30	1.24
7	a	226	ILE	N-CA	5.47	1.53	1.46
7	e	196	GLN	CD-OE1	5.45	1.33	1.23
7	c	167	ASP	CA-C	5.45	1.60	1.52
7	f	141	ASN	CB-CG	5.45	1.65	1.52
7	f	212	ARG	CD-NE	5.45	1.53	1.46
8	M	189	GLY	C-N	-5.44	1.26	1.33
8	M	195	LEU	C-O	5.44	1.30	1.23
8	M	27	GLN	CG-CD	5.43	1.65	1.52
8	M	298	LYS	CA-C	-5.43	1.45	1.52
7	a	172	ASP	N-CA	-5.43	1.39	1.46
7	e	148	THR	CA-CB	-5.42	1.42	1.54
7	b	47	SER	C-O	-5.42	1.17	1.24
7	b	57	GLN	CG-CD	5.42	1.65	1.52
7	e	62	SER	CB-OG	-5.42	1.31	1.42
8	M	356	GLU	CA-C	5.42	1.59	1.52
8	M	128	VAL	CA-C	-5.42	1.46	1.52
7	c	217	LEU	CA-C	-5.41	1.45	1.52
7	e	43	GLU	N-CA	-5.41	1.39	1.46
7	a	80	HIS	CA-CB	-5.41	1.44	1.53
7	b	178	PRO	CA-CB	5.40	1.61	1.53
7	e	49	LEU	CG-CD2	5.40	1.70	1.52
7	e	150	ALA	CA-CB	-5.40	1.45	1.53
7	a	199	ARG	CA-CB	5.39	1.61	1.53
7	c	209	PHE	CA-CB	-5.39	1.45	1.53
8	M	332	SER	CA-C	5.39	1.59	1.52
8	M	368	ALA	N-CA	-5.38	1.39	1.46
7	f	176	LEU	CG-CD1	5.38	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	f	176	LEU	C-N	5.38	1.39	1.33
7	d	191	GLU	CA-C	-5.38	1.45	1.52
7	a	225	ASN	CA-C	-5.37	1.46	1.53
7	c	252	ILE	CA-C	5.37	1.61	1.52
7	d	147	ALA	CA-CB	5.37	1.62	1.53
7	a	199	ARG	CZ-NH2	5.37	1.40	1.33
7	a	100	ASP	CA-C	5.36	1.59	1.52
7	b	236	SER	C-N	5.36	1.40	1.33
7	b	120	LEU	C-O	-5.35	1.17	1.24
8	M	127	GLN	CB-CG	-5.33	1.36	1.52
8	M	318	PHE	C-O	5.33	1.30	1.24
8	M	141	ALA	CA-C	-5.32	1.45	1.52
7	d	156	VAL	CA-C	5.31	1.60	1.52
7	a	13	ASN	CG-OD1	5.31	1.33	1.23
7	b	15	PHE	CG-CD2	5.31	1.50	1.38
7	b	139	GLN	CD-NE2	5.30	1.44	1.33
7	b	239	ARG	CA-C	-5.29	1.45	1.52
7	c	35	ILE	CA-C	-5.29	1.45	1.52
8	M	142	THR	CA-CB	-5.29	1.44	1.53
8	M	322	ASN	N-CA	-5.29	1.39	1.46
8	M	354	PHE	C-O	5.29	1.30	1.24
7	f	56	TRP	CZ2-CH2	5.28	1.47	1.37
7	b	179	LEU	CA-C	-5.28	1.46	1.52
7	a	199	ARG	N-CA	5.28	1.52	1.46
7	b	256	LYS	N-CA	-5.28	1.39	1.46
7	a	173	VAL	CB-CG1	5.28	1.70	1.52
7	d	109	LEU	N-CA	-5.27	1.39	1.46
7	f	92	HIS	CB-CG	5.26	1.57	1.50
7	e	193	PHE	CA-CB	5.26	1.61	1.53
8	M	161	ILE	N-CA	-5.25	1.39	1.46
8	M	203	LEU	C-N	5.25	1.40	1.33
7	c	193	PHE	C-O	5.25	1.30	1.24
7	b	202	LYS	CA-C	5.24	1.59	1.53
8	M	204	SER	CA-C	5.24	1.60	1.52
7	b	32	VAL	CB-CG2	5.23	1.69	1.52
7	f	195	ILE	N-CA	-5.23	1.40	1.46
6	T	7	DG	O3'-P	5.22	1.69	1.61
8	M	129	GLU	N-CA	5.21	1.52	1.46
7	f	229	LEU	CA-CB	-5.21	1.45	1.53
7	f	255	PHE	CG-CD2	-5.21	1.27	1.38
7	f	250	ILE	CA-CB	5.20	1.60	1.54
7	e	210	THR	C-O	5.20	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	120	LEU	CG-CD1	5.20	1.69	1.52
7	c	199	ARG	C-N	5.20	1.40	1.33
8	M	134	THR	N-CA	5.20	1.52	1.45
7	b	16	LEU	CB-CG	5.19	1.63	1.53
7	e	191	GLU	C-O	5.19	1.30	1.24
7	e	45	ILE	CB-CG1	-5.19	1.43	1.53
8	M	301	GLN	CA-C	-5.19	1.46	1.52
7	b	211	GLU	N-CA	5.19	1.52	1.46
7	f	176	LEU	CB-CG	5.19	1.63	1.53
7	d	44	LEU	C-N	-5.18	1.27	1.33
8	M	370	ILE	N-CA	-5.18	1.39	1.46
7	d	173	VAL	CA-C	-5.18	1.46	1.52
7	b	179	LEU	C-O	5.17	1.30	1.24
8	M	41	LEU	N-CA	-5.17	1.40	1.46
8	M	200	LEU	C-O	5.16	1.30	1.24
7	e	186	ILE	C-O	5.16	1.29	1.24
8	M	261	GLY	CA-C	5.16	1.59	1.51
8	M	212	TRP	CA-C	-5.15	1.45	1.53
8	M	341	LEU	CA-C	-5.15	1.46	1.52
7	a	222	TRP	CD2-CE2	-5.15	1.32	1.41
8	M	257	ASP	C-N	5.15	1.40	1.33
7	d	175	GLN	N-CA	-5.15	1.39	1.45
7	e	230	LYS	CE-NZ	5.14	1.64	1.49
7	b	246	PRO	CA-C	5.14	1.58	1.52
7	f	253	ASP	CA-C	5.14	1.58	1.52
8	M	263	SER	CB-OG	-5.14	1.31	1.42
7	c	246	PRO	CA-C	5.13	1.58	1.52
7	d	171	PHE	C-N	5.13	1.40	1.33
7	c	229	LEU	CA-C	-5.13	1.45	1.52
7	e	185	ASP	C-O	5.12	1.30	1.24
8	M	370	ILE	CA-CB	-5.12	1.47	1.54
8	M	126	TRP	CD2-CE2	-5.12	1.32	1.41
7	b	51	TYR	CG-CD1	5.12	1.50	1.39
7	d	158	GLU	C-N	5.11	1.41	1.33
7	e	161	PHE	CA-C	-5.11	1.46	1.52
6	T	7	DG	C4'-O4'	-5.11	1.35	1.45
8	M	129	GLU	CA-C	-5.10	1.46	1.52
8	M	263	SER	CA-C	-5.10	1.46	1.52
7	e	33	LEU	CG-CD2	5.10	1.69	1.52
8	M	35	GLN	CD-OE1	5.10	1.33	1.23
7	c	169	LEU	CA-C	5.09	1.61	1.52
8	M	282	SER	N-CA	5.08	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	182	ARG	N-CA	5.07	1.52	1.46
7	d	145	VAL	CA-CB	5.07	1.63	1.55
7	c	197	MET	CB-CG	5.07	1.67	1.52
7	f	222	TRP	CA-CB	5.07	1.61	1.53
8	M	415	ALA	C-N	5.07	1.40	1.33
7	f	212	ARG	NE-CZ	5.06	1.38	1.33
8	M	201	ILE	CB-CG1	5.06	1.63	1.53
8	M	414	GLU	C-O	5.06	1.30	1.23
7	d	156	VAL	N-CA	5.05	1.53	1.46
7	d	177	PRO	C-N	5.05	1.40	1.33
8	M	257	ASP	CA-C	5.05	1.59	1.52
8	M	35	GLN	CG-CD	5.05	1.64	1.52
7	b	239	ARG	C-N	5.04	1.40	1.33
8	M	381	ILE	CA-C	5.04	1.59	1.52
7	c	200	GLU	N-CA	5.04	1.52	1.46
7	b	120	LEU	CB-CG	5.03	1.63	1.53
8	M	323	LEU	C-O	5.03	1.30	1.24
7	d	48	ARG	CA-C	5.03	1.59	1.52
7	f	56	TRP	CZ3-CH2	5.03	1.53	1.40
7	f	258	ARG	N-CA	5.02	1.52	1.45
7	a	180	ARG	CZ-NH1	5.02	1.39	1.32
7	f	230	LYS	N-CA	-5.02	1.40	1.46
7	a	180	ARG	N-CA	5.02	1.52	1.46
7	d	149	ASN	N-CA	5.01	1.52	1.46
7	e	232	VAL	CA-CB	5.01	1.60	1.54
7	a	141	ASN	CA-C	5.00	1.59	1.53
7	b	205	LEU	C-O	5.00	1.29	1.23
7	f	212	ARG	CZ-NH2	5.00	1.40	1.33

All (936) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	258	PRO	CB-CA-C	-22.59	82.32	111.46
7	b	143	ARG	NE-CZ-NH2	-19.91	101.29	119.20
7	a	98	ARG	NE-CZ-NH1	-18.50	103.00	121.50
7	a	48	ARG	NE-CZ-NH1	18.00	139.50	121.50
7	e	45	ILE	CB-CA-C	-17.89	88.60	112.04
5	N	-11	DA	O3'-P-O5'	-16.26	79.61	104.00
7	c	197	MET	CG-SD-CE	16.18	136.50	100.90
8	M	120	LEU	CD1-CG-CD2	-15.48	76.75	110.80
8	M	271	TYR	CB-CA-C	-14.70	93.21	111.43
8	M	262	GLN	O-C-N	14.64	137.64	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	235	ARG	CB-CA-C	-14.54	88.56	110.96
7	e	46	ALA	N-CA-C	14.03	127.84	111.71
8	M	279	ARG	N-CA-C	13.90	129.93	110.06
7	b	143	ARG	NH1-CZ-NH2	13.81	137.26	119.30
7	a	98	ARG	NH1-CZ-NH2	13.72	137.13	119.30
7	a	185	ASP	CA-C-N	-13.62	102.92	120.77
7	a	185	ASP	C-N-CA	-13.62	102.92	120.77
7	b	49	LEU	N-CA-CB	13.61	130.53	110.26
7	b	227	ARG	CG-CD-NE	-13.60	82.08	112.00
8	M	262	GLN	N-CA-C	-13.48	96.59	111.28
7	a	80	HIS	N-CA-C	13.34	128.84	108.96
7	d	96	PHE	N-CA-CB	13.26	130.02	110.26
7	e	62	SER	CA-C-O	-12.85	105.19	120.60
8	M	343	VAL	N-CA-C	12.79	123.67	110.62
7	e	180	ARG	N-CA-C	-12.65	97.23	113.17
8	M	195	LEU	CB-CA-C	-12.65	92.13	109.71
7	a	98	ARG	CA-C-O	12.64	133.72	120.70
7	a	223	PRO	CB-CA-C	-12.59	93.12	110.88
7	f	169	LEU	CA-C-O	12.58	134.40	118.54
8	M	257	ASP	CA-C-N	12.54	132.68	119.76
8	M	257	ASP	C-N-CA	12.54	132.68	119.76
7	a	185	ASP	O-C-N	12.38	137.45	122.48
7	b	235	ARG	NE-CZ-NH1	-12.38	109.12	121.50
7	b	79	GLY	O-C-N	-12.25	110.13	122.87
7	f	79	GLY	CA-C-O	-12.13	110.25	122.26
7	d	100	ASP	CB-CG-OD2	-12.10	90.56	118.40
8	M	203	LEU	O-C-N	12.02	134.45	122.07
7	f	222	TRP	CA-C-N	12.01	134.86	119.84
7	f	222	TRP	C-N-CA	12.01	134.86	119.84
7	e	252	ILE	N-CA-C	-11.96	97.97	111.00
7	a	48	ARG	CG-CD-NE	11.86	138.09	112.00
8	M	128	VAL	CA-CB-CG2	-11.86	90.24	110.40
7	b	32	VAL	CA-C-N	-11.79	104.31	122.81
7	b	32	VAL	C-N-CA	-11.79	104.31	122.81
7	e	46	ALA	CA-C-O	11.76	133.39	120.10
7	a	48	ARG	NE-CZ-NH2	-11.52	108.83	119.20
8	M	129	GLU	N-CA-C	11.47	123.79	111.28
7	e	189	MET	CB-CG-SD	11.43	147.00	112.70
7	b	235	ARG	NE-CZ-NH2	11.43	129.48	119.20
6	T	22	DG	C2'-C3'-O3'	11.41	128.62	111.50
7	b	59	PRO	N-CA-C	-11.33	90.86	111.03
8	M	158	ILE	CB-CA-C	-11.31	96.87	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	225	ASN	N-CA-C	11.12	122.97	111.07
7	f	79	GLY	N-CA-C	11.12	125.93	111.70
7	f	140	VAL	CB-CA-C	-11.04	90.87	111.30
8	M	384	VAL	CB-CA-C	-10.92	97.73	112.04
8	M	158	ILE	N-CA-C	10.91	121.75	110.62
7	f	163	ALA	N-CA-C	10.90	122.91	111.14
7	b	33	LEU	N-CA-C	10.83	127.04	109.72
7	a	98	ARG	N-CA-C	-10.81	99.46	111.14
7	d	176	LEU	CB-CG-CD1	-10.81	78.27	110.70
7	c	243	SER	N-CA-C	10.76	126.47	112.26
7	f	212	ARG	NE-CZ-NH2	10.75	128.87	119.20
8	M	259	ARG	CB-CG-CD	-10.74	86.60	111.30
7	a	183	GLU	CB-CA-C	-10.72	95.22	112.06
7	d	99	ALA	CA-C-N	-10.69	103.79	122.07
7	d	99	ALA	C-N-CA	-10.69	103.79	122.07
7	c	255	PHE	N-CA-C	10.68	125.90	113.19
7	a	186	ILE	N-CA-C	10.65	121.31	110.23
7	b	120	LEU	CA-C-O	10.60	132.73	121.07
7	e	49	LEU	CB-CG-CD1	-10.46	79.33	110.70
7	a	65	CYS	CA-CB-SG	-10.45	90.36	114.40
5	N	-11	DA	P-O3'-C3'	-10.44	104.54	120.20
7	e	228	GLU	N-CA-C	-10.28	101.50	114.56
7	a	173	VAL	CG1-CB-CG2	10.26	133.36	110.80
7	d	100	ASP	OD1-CG-OD2	10.16	147.29	122.90
8	M	196	ARG	N-CA-C	-10.10	89.29	110.80
7	f	140	VAL	N-CA-C	10.10	121.68	108.35
7	f	141	ASN	CA-CB-CG	-10.05	102.55	112.60
7	a	94	GLY	N-CA-C	-10.02	101.31	112.33
7	b	239	ARG	O-C-N	10.01	135.90	122.59
8	M	380	THR	CA-CB-OG1	-9.99	94.62	109.60
7	f	255	PHE	N-CA-C	9.99	132.07	110.80
7	f	149	ASN	CB-CG-ND2	-9.98	101.44	116.40
8	M	405	SER	N-CA-C	9.93	123.85	110.35
7	c	229	LEU	N-CA-C	-9.92	100.30	111.71
7	e	32	VAL	CB-CA-C	-9.87	95.11	111.29
7	e	48	ARG	N-CA-C	-9.86	101.04	112.87
7	b	194	ALA	N-CA-C	-9.85	100.54	111.28
7	f	193	PHE	CG-CD2-CE2	-9.82	104.01	120.70
7	f	45	ILE	CB-CA-C	-9.75	99.26	112.04
7	b	214	ARG	CB-CG-CD	-9.74	88.91	111.30
7	b	237	VAL	N-CA-C	9.68	119.71	110.42
7	e	55	ARG	CB-CG-CD	9.68	133.56	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	140	VAL	CG1-CB-CG2	-9.67	89.53	110.80
8	M	195	LEU	CD1-CG-CD2	-9.66	89.56	110.80
7	f	232	VAL	CB-CA-C	-9.63	99.41	112.02
6	T	6	DT	C5'-C4'-O4'	9.62	123.84	109.40
8	M	127	GLN	CA-C-N	-9.62	107.28	120.46
8	M	127	GLN	C-N-CA	-9.62	107.28	120.46
8	M	180	LYS	N-CA-C	-9.62	100.96	112.89
8	M	192	ALA	N-CA-C	9.60	121.74	111.28
8	M	451	ILE	N-CA-C	9.56	120.37	110.62
7	c	229	LEU	O-C-N	9.56	133.40	122.22
8	M	329	LEU	CB-CA-C	-9.54	94.63	110.85
7	f	203	LEU	CB-CG-CD1	-9.53	82.12	110.70
7	e	172	ASP	N-CA-CB	-9.49	94.15	111.13
7	e	182	ARG	NE-CZ-NH2	-9.48	110.67	119.20
8	M	120	LEU	N-CA-CB	9.46	126.48	110.49
7	f	169	LEU	CB-CG-CD2	-9.40	82.49	110.70
8	M	125	MET	CA-CB-CG	-9.39	95.32	114.10
7	b	40	THR	N-CA-C	9.39	125.88	113.30
7	f	253	ASP	CA-C-N	-9.35	108.15	119.84
7	f	253	ASP	C-N-CA	-9.35	108.15	119.84
7	b	227	ARG	N-CA-C	-9.33	100.05	111.33
8	M	133	PHE	CB-CA-C	-9.29	91.94	110.42
7	b	235	ARG	CD-NE-CZ	9.28	137.40	124.40
7	b	206	PHE	CA-C-N	9.28	128.97	118.85
7	b	206	PHE	C-N-CA	9.28	128.97	118.85
7	a	79	GLY	N-CA-C	-9.26	98.52	111.76
7	d	170	ALA	N-CA-C	-9.25	96.67	109.71
7	e	30	LYS	CA-C-N	9.24	129.31	119.89
7	e	30	LYS	C-N-CA	9.24	129.31	119.89
7	b	237	VAL	CB-CA-C	-9.21	100.18	111.97
7	b	237	VAL	CA-C-O	-9.20	111.42	121.17
8	M	271	TYR	N-CA-CB	-9.19	96.71	110.86
7	e	32	VAL	O-C-N	9.17	134.03	122.57
7	f	170	ALA	N-CA-C	9.16	124.01	113.02
8	M	384	VAL	CG1-CB-CG2	-9.12	90.73	110.80
8	M	287	VAL	N-CA-C	9.11	120.69	109.30
7	e	251	ILE	CB-CA-C	-9.11	103.02	113.22
8	M	354	PHE	CA-C-N	-9.08	108.64	120.44
8	M	354	PHE	C-N-CA	-9.08	108.64	120.44
7	c	232	VAL	N-CA-C	9.07	120.96	110.62
7	f	34	ILE	CA-C-O	9.02	131.70	120.97
8	M	329	LEU	CB-CG-CD2	9.01	137.73	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	185	ASP	N-CA-C	-9.00	102.45	113.97
7	e	172	ASP	CA-C-N	-8.99	105.79	121.97
7	e	172	ASP	C-N-CA	-8.99	105.79	121.97
7	a	217	LEU	CB-CA-C	-8.98	96.78	110.88
7	a	65	CYS	CA-C-O	8.96	130.93	120.00
7	c	229	LEU	CB-CG-CD1	-8.94	83.88	110.70
7	c	229	LEU	CB-CG-CD2	8.93	137.48	110.70
7	f	224	GLY	N-CA-C	-8.92	97.06	110.97
7	c	232	VAL	CB-CA-C	-8.91	100.37	112.04
7	f	197	MET	O-C-N	8.88	132.28	122.15
7	e	44	LEU	CD1-CG-CD2	-8.87	91.30	110.80
6	T	14	DC	P-O5'-C5'	-8.85	106.72	120.00
7	b	256	LYS	CB-CA-C	8.83	123.09	109.84
7	b	182	ARG	NE-CZ-NH2	-8.82	111.26	119.20
8	M	456	ARG	NE-CZ-NH1	-8.77	112.73	121.50
7	d	173	VAL	CB-CA-C	-8.76	98.90	111.34
7	e	182	ARG	CA-CB-CG	-8.71	96.68	114.10
7	b	236	SER	O-C-N	8.70	131.13	122.09
8	M	278	VAL	CA-C-O	-8.68	112.50	120.22
8	M	396	ILE	CB-CG1-CD1	-8.67	95.59	113.80
7	e	187	MET	CA-C-N	-8.66	107.15	120.31
7	e	187	MET	C-N-CA	-8.66	107.15	120.31
8	M	286	THR	N-CA-C	8.65	123.00	109.07
8	M	389	TYR	N-CA-CB	-8.65	95.78	110.83
7	d	45	ILE	CB-CG1-CD1	-8.64	95.65	113.80
7	b	14	SER	CA-C-N	-8.64	107.77	120.38
7	b	14	SER	C-N-CA	-8.64	107.77	120.38
8	M	125	MET	N-CA-C	8.63	120.76	111.36
7	f	166	LEU	N-CA-C	-8.62	101.89	111.28
7	b	51	TYR	CB-CA-C	8.60	126.54	110.63
7	b	142	VAL	N-CA-C	8.60	120.31	107.75
7	f	146	CYS	N-CA-C	-8.55	95.25	108.76
7	e	62	SER	N-CA-C	8.54	123.58	109.06
8	M	147	ALA	N-CA-CB	-8.53	100.80	110.35
8	M	417	SER	N-CA-C	-8.52	101.94	111.82
7	c	231	ASN	N-CA-C	-8.51	101.69	110.97
8	M	380	THR	CA-C-N	-8.51	108.53	120.53
8	M	380	THR	C-N-CA	-8.51	108.53	120.53
7	d	94	GLY	N-CA-C	8.50	121.55	111.35
7	b	225	ASN	N-CA-C	8.49	128.88	110.80
7	a	217	LEU	CB-CG-CD2	-8.44	85.38	110.70
7	b	49	LEU	CA-CB-CG	-8.42	86.84	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	255	PHE	CA-C-N	8.41	132.81	120.87
7	c	255	PHE	C-N-CA	8.41	132.81	120.87
8	M	190	VAL	N-CA-C	-8.40	94.96	108.90
8	M	143	SER	CA-CB-OG	-8.38	94.35	111.10
7	b	60	PHE	N-CA-C	-8.37	100.53	110.41
7	b	112	ALA	CA-C-N	8.36	128.30	120.03
7	b	112	ALA	C-N-CA	8.36	128.30	120.03
7	d	128	GLU	O-C-N	-8.35	113.15	123.01
8	M	345	ARG	N-CA-C	-8.35	102.13	111.14
7	b	51	TYR	CA-CB-CG	-8.33	98.91	113.90
8	M	119	THR	N-CA-C	8.33	129.94	113.29
7	f	255	PHE	N-CA-CB	-8.32	96.44	110.49
8	M	357	GLN	CA-C-N	-8.31	110.63	122.85
8	M	357	GLN	C-N-CA	-8.31	110.63	122.85
7	c	251	ILE	CA-C-O	8.29	131.15	120.78
7	b	184	SER	CA-C-O	-8.25	108.41	119.47
7	c	57	GLN	N-CA-C	8.25	120.27	111.28
7	a	205	LEU	CA-C-N	8.24	132.74	121.20
7	a	205	LEU	C-N-CA	8.24	132.74	121.20
7	a	63	LEU	N-CA-C	8.23	122.75	111.39
8	M	178	VAL	N-CA-C	-8.23	100.80	111.09
6	T	8	DA	C5'-C4'-O4'	8.22	121.72	109.40
7	b	202	LYS	N-CA-C	8.17	122.77	111.74
7	a	141	ASN	OD1-CG-ND2	8.17	130.77	122.60
7	a	225	ASN	CB-CA-C	-8.15	106.09	115.79
7	b	235	ARG	CB-CG-CD	8.13	130.00	111.30
7	b	233	VAL	N-CA-C	8.12	118.92	110.72
8	M	259	ARG	CA-C-N	8.11	129.98	119.84
8	M	259	ARG	C-N-CA	8.11	129.98	119.84
8	M	456	ARG	NH1-CZ-NH2	8.11	129.85	119.30
8	M	347	ILE	CB-CG1-CD1	-8.10	96.78	113.80
7	f	231	ASN	CA-CB-CG	-8.09	104.51	112.60
7	a	184	SER	CA-C-N	-8.09	108.84	122.11
7	a	184	SER	C-N-CA	-8.09	108.84	122.11
8	M	184	ARG	NE-CZ-NH1	-8.09	113.41	121.50
7	a	171	PHE	N-CA-C	-8.06	104.04	114.04
7	d	227	ARG	N-CA-C	8.05	121.07	111.33
7	d	144	LEU	CA-C-O	-8.04	111.88	120.80
7	b	70	GLU	CB-CA-C	8.03	124.07	110.74
7	e	34	ILE	CG1-CB-CG2	8.03	134.78	110.70
7	a	187	MET	CG-SD-CE	8.02	118.55	100.90
7	e	55	ARG	CA-CB-CG	-8.01	98.09	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	28	LEU	N-CA-C	-7.98	96.86	109.23
8	M	179	LEU	CD1-CG-CD2	-7.96	93.28	110.80
8	M	190	VAL	CA-CB-CG1	-7.96	96.88	110.40
8	M	394	ARG	N-CA-C	7.95	120.86	111.71
5	N	-18	DT	C5'-C4'-O4'	7.95	121.32	109.40
7	b	49	LEU	N-CA-C	-7.92	101.44	112.45
8	M	127	GLN	N-CA-C	-7.92	103.41	113.23
8	M	158	ILE	CG1-CB-CG2	7.92	134.46	110.70
7	b	59	PRO	CA-C-N	-7.91	109.42	121.53
7	b	59	PRO	C-N-CA	-7.91	109.42	121.53
7	e	46	ALA	O-C-N	-7.91	112.96	122.22
7	a	169	LEU	CD1-CG-CD2	-7.91	93.41	110.80
7	d	97	GLU	CA-C-O	-7.90	111.17	120.10
7	e	49	LEU	CD1-CG-CD2	7.88	128.15	110.80
7	b	33	LEU	CA-C-O	-7.88	112.21	121.11
7	a	48	ARG	CB-CG-CD	-7.87	93.20	111.30
7	f	167	ASP	N-CA-C	7.86	119.63	111.14
8	M	47	LEU	N-CA-CB	-7.86	97.63	110.59
7	c	228	GLU	N-CA-C	7.85	124.25	111.37
7	e	187	MET	CA-C-O	-7.84	112.11	120.42
7	b	182	ARG	NH1-CZ-NH2	7.81	129.45	119.30
7	b	222	TRP	CA-C-N	7.80	129.59	119.84
7	b	222	TRP	C-N-CA	7.80	129.59	119.84
1	A	191	ARG	N-CA-C	7.80	122.27	111.74
8	M	165	ILE	N-CA-C	7.78	118.55	110.62
7	e	182	ARG	NE-CZ-NH1	7.74	129.24	121.50
7	f	230	LYS	CA-C-N	-7.71	109.25	120.82
7	f	230	LYS	C-N-CA	-7.71	109.25	120.82
8	M	394	ARG	CA-CB-CG	-7.70	98.70	114.10
7	c	58	GLY	CA-C-N	7.69	129.46	119.84
7	c	58	GLY	C-N-CA	7.69	129.46	119.84
8	M	389	TYR	CA-C-N	-7.69	112.15	122.99
8	M	389	TYR	C-N-CA	-7.69	112.15	122.99
7	f	44	LEU	N-CA-C	-7.68	101.13	111.96
7	a	220	TYR	CA-C-N	-7.66	106.91	121.54
7	a	220	TYR	C-N-CA	-7.66	106.91	121.54
7	f	147	ALA	O-C-N	-7.65	114.91	123.48
8	M	348	VAL	CG1-CB-CG2	-7.64	94.00	110.80
7	a	182	ARG	NE-CZ-NH1	7.62	129.12	121.50
7	a	253	ASP	CA-C-N	7.62	127.50	119.05
7	a	253	ASP	C-N-CA	7.62	127.50	119.05
7	e	200	GLU	CA-C-O	-7.61	112.35	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	176	LEU	CA-C-N	-7.59	112.56	120.38
7	f	176	LEU	C-N-CA	-7.59	112.56	120.38
8	M	345	ARG	CB-CA-C	7.58	122.88	110.90
7	b	141	ASN	CA-C-N	7.57	133.16	123.10
7	b	141	ASN	C-N-CA	7.57	133.16	123.10
7	a	173	VAL	CB-CA-C	-7.56	100.32	110.98
7	f	45	ILE	N-CA-C	7.54	119.22	110.62
7	d	145	VAL	N-CA-CB	7.53	125.87	111.93
7	a	34	ILE	CB-CG1-CD1	-7.52	98.00	113.80
7	f	44	LEU	CA-C-N	-7.52	109.93	120.53
7	f	44	LEU	C-N-CA	-7.52	109.93	120.53
7	f	162	ARG	CA-C-N	-7.51	110.22	120.44
7	f	162	ARG	C-N-CA	-7.51	110.22	120.44
7	f	256	LYS	CA-C-O	-7.51	112.06	120.54
8	M	109	LEU	CA-C-N	7.50	129.22	119.84
8	M	109	LEU	C-N-CA	7.50	129.22	119.84
7	c	201	ILE	N-CA-C	7.50	121.43	112.80
8	M	396	ILE	CG1-CB-CG2	-7.50	88.21	110.70
7	c	256	LYS	N-CA-CB	-7.46	99.00	109.97
7	c	186	ILE	N-CA-C	-7.43	103.61	110.82
7	e	12	ALA	N-CA-C	7.42	119.37	111.28
7	a	99	ALA	CA-C-N	-7.41	111.13	122.09
7	a	99	ALA	C-N-CA	-7.41	111.13	122.09
8	M	41	LEU	N-CA-C	7.40	119.35	111.28
7	d	109	LEU	N-CA-C	-7.40	103.20	111.71
7	b	190	ALA	CA-C-O	7.39	131.08	120.51
7	d	100	ASP	CA-C-O	-7.39	112.49	121.36
7	c	56	TRP	N-CA-C	7.38	119.33	111.28
8	M	277	LEU	CA-C-O	-7.38	112.74	120.70
8	M	420	ILE	CB-CA-C	-7.37	100.31	112.26
7	f	67	ALA	N-CA-C	7.36	119.30	111.28
7	a	174	VAL	CA-CB-CG1	7.36	122.90	110.40
8	M	42	GLU	N-CA-C	7.35	120.22	111.33
7	b	257	ARG	N-CA-C	7.34	119.36	111.36
8	M	381	ILE	N-CA-C	7.34	118.98	110.62
7	b	256	LYS	N-CA-CB	-7.33	98.12	109.48
7	a	187	MET	N-CA-CB	-7.33	99.39	110.01
8	M	177	ALA	N-CA-C	7.33	118.95	110.97
7	f	121	LEU	N-CA-C	7.32	118.90	111.07
7	c	193	PHE	O-C-N	7.31	129.87	122.12
7	f	251	ILE	CB-CG1-CD1	7.30	129.13	113.80
7	d	25	LEU	N-CA-C	7.28	119.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	49	LEU	CB-CG-CD1	-7.28	88.86	110.70
8	M	27	GLN	CA-C-N	-7.26	110.31	122.29
8	M	27	GLN	C-N-CA	-7.26	110.31	122.29
8	M	41	LEU	CD1-CG-CD2	7.24	126.73	110.80
7	a	199	ARG	CA-CB-CG	7.24	128.57	114.10
7	d	252	ILE	CB-CG1-CD1	7.23	128.98	113.80
7	f	15	PHE	CD1-CE1-CZ	7.23	133.01	120.00
8	M	455	ARG	CA-C-N	-7.22	109.33	120.31
8	M	455	ARG	C-N-CA	-7.22	109.33	120.31
7	c	92	HIS	CA-C-N	7.22	127.06	119.05
7	c	92	HIS	C-N-CA	7.22	127.06	119.05
7	e	234	GLU	CB-CG-CD	7.21	124.86	112.60
7	e	188	LEU	N-CA-C	7.18	120.15	111.82
7	e	22	VAL	O-C-N	7.17	132.06	122.31
7	f	167	ASP	CA-C-O	-7.16	113.32	120.70
8	M	210	THR	N-CA-CB	7.16	120.24	110.14
8	M	117	THR	N-CA-C	7.16	121.05	110.46
7	d	252	ILE	CG1-CB-CG2	7.16	132.16	110.70
8	M	183	GLN	CA-C-O	-7.15	111.28	119.14
7	a	48	ARG	N-CA-CB	7.14	120.43	110.07
7	b	32	VAL	CA-CB-CG2	7.14	122.53	110.40
8	M	26	LEU	CB-CA-C	-7.14	98.50	110.56
7	a	98	ARG	CB-CG-CD	-7.12	94.92	111.30
8	M	333	LEU	CB-CA-C	-7.12	98.97	110.79
7	a	220	TYR	CG-CD2-CE2	-7.11	110.53	121.20
7	f	176	LEU	N-CA-CB	7.11	118.63	110.03
7	c	68	LEU	N-CA-C	7.09	120.50	110.50
8	M	269	PRO	CA-C-N	7.09	131.87	122.30
8	M	269	PRO	C-N-CA	7.09	131.87	122.30
7	a	168	ARG	CA-C-N	-7.08	109.41	122.09
7	a	168	ARG	C-N-CA	-7.08	109.41	122.09
8	M	140	ILE	N-CA-CB	-7.08	99.96	110.58
7	f	249	ASP	CB-CA-C	7.07	120.34	110.16
7	a	174	VAL	N-CA-C	-7.07	96.98	107.51
7	d	69	ASN	N-CA-C	7.07	118.98	111.28
7	b	12	ALA	N-CA-C	7.07	118.98	111.28
7	b	32	VAL	O-C-N	7.06	131.05	123.00
7	a	223	PRO	CA-C-O	-7.06	110.37	118.98
7	c	187	MET	O-C-N	7.05	129.33	122.07
6	T	8	DA	O3'-P-O5'	7.05	114.57	104.00
7	d	112	ALA	CA-C-N	7.02	126.78	119.76
7	d	112	ALA	C-N-CA	7.02	126.78	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	86	THR	N-CA-C	7.01	119.93	108.08
7	b	17	GLU	CA-C-O	6.98	127.95	120.55
7	b	227	ARG	NE-CZ-NH1	6.98	128.48	121.50
7	f	198	CYS	N-CA-C	-6.98	103.76	111.36
7	b	181	GLU	N-CA-C	6.97	121.54	112.89
8	M	38	GLN	CB-CA-C	-6.97	99.93	110.88
8	M	278	VAL	CB-CA-C	-6.97	102.46	110.41
7	f	257	ARG	CB-CG-CD	-6.96	95.28	111.30
7	b	215	GLU	N-CA-C	6.96	118.87	111.28
7	f	149	ASN	CA-C-O	-6.95	110.21	119.11
7	e	252	ILE	CB-CA-C	-6.95	102.92	112.24
8	M	357	GLN	N-CA-C	6.93	118.83	111.28
7	a	181	GLU	N-CA-C	6.91	122.78	111.37
7	e	33	LEU	CB-CA-C	6.89	124.86	109.56
7	b	15	PHE	N-CA-C	6.88	120.56	111.75
7	a	205	LEU	N-CA-C	6.88	119.70	108.55
7	b	140	VAL	N-CA-CB	-6.88	98.48	111.21
7	d	186	ILE	N-CA-C	6.88	117.58	110.36
8	M	125	MET	CB-CA-C	-6.87	99.17	110.85
7	a	224	GLY	O-C-N	6.87	131.63	122.70
7	b	205	LEU	N-CA-C	6.87	120.84	108.48
7	e	62	SER	CA-CB-OG	-6.86	97.37	111.10
7	d	153	PRO	CA-C-N	6.86	129.36	120.44
7	d	153	PRO	C-N-CA	6.86	129.36	120.44
7	b	124	ILE	N-CA-C	6.86	117.00	110.42
7	c	197	MET	CB-CG-SD	6.85	133.26	112.70
8	M	453	VAL	N-CA-C	6.85	117.61	110.62
7	a	48	ARG	CA-CB-CG	-6.84	100.41	114.10
8	M	342	ARG	N-CA-C	-6.83	103.52	110.97
6	T	9	DT	C5'-C4'-O4'	6.83	119.65	109.40
7	d	49	LEU	CA-C-O	6.83	127.78	119.38
7	b	68	LEU	CB-CG-CD2	-6.83	90.22	110.70
8	M	129	GLU	CB-CA-C	-6.82	99.46	110.79
7	e	251	ILE	CG1-CB-CG2	-6.82	90.25	110.70
8	M	401	TYR	N-CA-C	6.82	119.58	111.33
7	a	183	GLU	N-CA-C	6.81	120.78	111.17
7	b	203	LEU	N-CA-CB	-6.80	101.85	109.74
7	f	233	VAL	CA-CB-CG2	6.80	121.95	110.40
7	a	233	VAL	N-CA-C	6.78	116.90	110.53
7	a	196	GLN	CA-C-O	6.77	128.15	120.90
7	c	230	LYS	CG-CD-CE	6.77	126.87	111.30
8	M	297	LEU	CD1-CG-CD2	-6.77	95.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	385	THR	N-CA-C	6.76	121.13	112.34
7	f	230	LYS	CB-CG-CD	6.76	126.85	111.30
7	a	79	GLY	CA-C-O	-6.75	114.95	122.24
7	f	234	GLU	N-CA-C	6.74	121.52	113.16
8	M	260	PRO	CA-C-N	-6.74	108.20	121.41
8	M	260	PRO	C-N-CA	-6.74	108.20	121.41
7	e	48	ARG	CA-C-N	-6.73	109.36	121.14
7	e	48	ARG	C-N-CA	-6.73	109.36	121.14
7	f	168	ARG	N-CA-C	-6.73	102.12	111.81
7	f	233	VAL	CG1-CB-CG2	-6.72	96.02	110.80
7	f	30	LYS	CA-C-N	6.71	126.47	119.76
7	f	30	LYS	C-N-CA	6.71	126.47	119.76
7	b	51	TYR	CA-C-O	6.70	127.67	120.10
8	M	258	PRO	N-CA-CB	-6.70	97.35	103.31
8	M	183	GLN	O-C-N	6.70	131.47	122.49
8	M	398	GLU	CA-C-O	-6.70	113.77	121.47
8	M	289	LEU	N-CA-CB	-6.68	100.29	110.45
7	b	256	LYS	CA-C-N	6.68	129.78	120.29
7	b	256	LYS	C-N-CA	6.68	129.78	120.29
7	e	237	VAL	CB-CA-C	-6.68	103.00	112.22
7	f	140	VAL	CA-CB-CG2	6.67	121.75	110.40
7	a	9	LEU	N-CA-C	6.66	119.54	110.55
7	a	173	VAL	N-CA-C	6.66	118.64	108.71
7	a	195	ILE	N-CA-CB	-6.66	102.15	110.47
7	b	33	LEU	CB-CG-CD2	-6.66	90.73	110.70
7	f	169	LEU	CD1-CG-CD2	6.66	125.44	110.80
8	M	143	SER	N-CA-C	6.64	118.60	111.36
7	f	232	VAL	N-CA-CB	6.64	119.07	110.57
7	c	252	ILE	N-CA-CB	-6.64	98.40	110.95
7	b	238	TYR	N-CA-C	-6.63	104.06	111.28
7	a	187	MET	N-CA-C	-6.62	103.98	111.07
8	M	258	PRO	N-CD-CG	6.62	113.14	103.20
7	b	178	PRO	N-CA-CB	6.62	110.20	103.25
8	M	118	GLN	O-C-N	-6.62	113.79	122.59
8	M	332	SER	CA-C-O	6.61	127.58	120.24
8	M	47	LEU	CD1-CG-CD2	6.61	125.34	110.80
7	c	30	LYS	CA-C-N	6.60	128.09	119.84
7	c	30	LYS	C-N-CA	6.60	128.09	119.84
7	d	174	VAL	CA-C-O	6.59	128.08	121.09
8	M	344	SER	O-C-N	6.59	129.11	122.12
8	M	420	ILE	CA-CB-CG1	-6.59	99.19	110.40
8	M	38	GLN	N-CA-C	-6.58	104.02	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	189	MET	CG-SD-CE	-6.58	86.42	100.90
7	f	214	ARG	CB-CG-CD	6.58	126.43	111.30
8	M	190	VAL	N-CA-CB	-6.58	100.19	112.36
8	M	27	GLN	CA-C-O	6.56	127.24	119.56
7	b	245	TYR	CA-C-N	-6.55	114.03	120.52
7	b	245	TYR	C-N-CA	-6.55	114.03	120.52
7	f	127	GLY	N-CA-C	-6.55	97.65	113.18
7	a	203	LEU	CB-CG-CD1	-6.55	91.05	110.70
7	f	15	PHE	CE1-CZ-CE2	-6.55	108.21	120.00
7	e	173	VAL	CA-CB-CG2	-6.55	99.26	110.40
8	M	455	ARG	N-CA-CB	6.55	119.96	110.20
8	M	202	GLN	N-CA-CB	6.54	120.42	110.28
7	e	44	LEU	CB-CA-C	6.54	122.72	110.63
7	f	98	ARG	NE-CZ-NH1	6.53	128.03	121.50
8	M	327	ARG	N-CA-C	-6.52	104.25	111.82
7	e	34	ILE	CB-CG1-CD1	6.52	127.50	113.80
7	a	182	ARG	CA-C-O	-6.52	113.51	120.42
7	b	70	GLU	CA-C-O	6.51	128.22	120.92
7	c	7	ASN	N-CA-C	-6.50	104.35	113.20
7	c	182	ARG	N-CA-C	6.50	118.24	111.03
7	e	233	VAL	CA-C-O	-6.49	114.29	121.17
8	M	347	ILE	N-CA-C	6.49	116.63	110.53
8	M	127	GLN	CA-CB-CG	-6.49	101.13	114.10
7	d	124	ILE	N-CA-C	6.47	118.00	110.62
7	d	156	VAL	N-CA-C	6.47	121.21	111.89
7	b	239	ARG	NE-CZ-NH1	-6.47	115.03	121.50
7	e	18	VAL	CG1-CB-CG2	6.47	125.03	110.80
6	T	13	DG	O5'-P-OP2	6.46	127.38	108.00
7	a	200	GLU	CA-CB-CG	-6.46	101.18	114.10
7	a	57	GLN	N-CA-CB	6.46	119.18	110.59
7	d	220	TYR	CA-C-N	6.45	129.45	120.29
7	d	220	TYR	C-N-CA	6.45	129.45	120.29
7	b	16	LEU	CB-CG-CD1	6.45	130.04	110.70
7	a	45	ILE	N-CA-C	6.45	117.19	110.62
7	c	221	ARG	N-CA-C	6.45	120.72	112.34
7	a	13	ASN	CB-CG-ND2	-6.44	106.74	116.40
7	d	144	LEU	CB-CG-CD2	-6.44	91.38	110.70
7	f	163	ALA	CA-C-N	6.44	129.56	120.28
7	f	163	ALA	C-N-CA	6.44	129.56	120.28
8	M	222	ASP	CA-C-O	6.44	126.21	119.51
7	c	232	VAL	N-CA-CB	6.44	118.52	110.47
7	e	45	ILE	CG1-CB-CG2	-6.43	91.42	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	285	TRP	N-CA-C	6.43	119.79	110.28
7	f	193	PHE	CD1-CG-CD2	6.42	128.23	118.60
7	f	44	LEU	CD1-CG-CD2	-6.41	96.70	110.80
8	M	473	ARG	CD-NE-CZ	-6.41	115.43	124.40
7	b	226	ILE	CA-C-N	6.40	129.14	120.38
7	b	226	ILE	C-N-CA	6.40	129.14	120.38
7	d	44	LEU	CA-C-N	-6.39	110.16	120.64
7	d	44	LEU	C-N-CA	-6.39	110.16	120.64
7	a	226	ILE	CA-CB-CG2	6.39	121.36	110.50
7	e	235	ARG	CB-CA-C	6.38	121.70	110.85
8	M	184	ARG	NH1-CZ-NH2	6.38	127.59	119.30
7	c	34	ILE	CA-C-N	-6.37	114.63	123.10
7	c	34	ILE	C-N-CA	-6.37	114.63	123.10
8	M	402	PHE	CA-CB-CG	-6.36	107.44	113.80
8	M	287	VAL	N-CA-CB	-6.36	102.49	110.31
5	N	-27	DT	C2'-C3'-O3'	6.35	121.03	111.50
7	a	217	LEU	CD1-CG-CD2	6.35	124.77	110.80
7	a	99	ALA	CB-CA-C	6.34	119.68	111.50
7	e	209	PHE	N-CA-C	6.34	123.58	114.39
7	e	255	PHE	N-CA-CB	6.34	121.20	110.49
7	a	223	PRO	O-C-N	6.33	132.75	122.36
8	M	230	HIS	N-CA-C	-6.33	102.66	111.39
7	e	201	ILE	CB-CG1-CD1	6.32	127.08	113.80
7	a	13	ASN	CB-CG-OD1	6.32	133.44	120.80
7	b	249	ASP	CA-C-O	6.32	128.05	120.28
7	b	191	GLU	CA-CB-CG	-6.31	101.48	114.10
8	M	37	LEU	CB-CG-CD2	-6.31	91.77	110.70
8	M	263	SER	N-CA-CB	6.30	119.33	109.94
7	d	158	GLU	CA-C-N	6.29	133.75	121.41
7	d	158	GLU	C-N-CA	6.29	133.75	121.41
8	M	131	THR	CB-CA-C	6.28	118.22	108.61
7	a	184	SER	N-CA-C	-6.28	97.43	110.80
8	M	126	TRP	CG-CD1-NE1	-6.27	102.05	110.20
8	M	142	THR	OG1-CB-CG2	-6.27	96.77	109.30
5	N	-27	DT	C4'-C3'-O3'	-6.27	100.60	110.00
7	a	94	GLY	CA-C-O	6.26	130.38	122.24
6	T	13	DG	O5'-P-OP1	-6.26	90.23	109.00
7	b	142	VAL	CA-C-N	6.26	130.74	122.42
7	b	142	VAL	C-N-CA	6.26	130.74	122.42
7	f	149	ASN	CB-CG-OD1	6.26	133.31	120.80
7	b	239	ARG	NE-CZ-NH2	6.25	124.83	119.20
7	a	222	TRP	N-CA-C	6.25	123.62	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	-17	DT	C2'-C3'-O3'	-6.25	102.13	111.50
7	a	226	ILE	CG1-CB-CG2	-6.25	91.97	110.70
8	M	311	ARG	N-CA-C	6.24	120.63	112.89
8	M	461	TYR	N-CA-C	6.23	124.07	110.80
7	f	221	ARG	N-CA-C	-6.23	104.55	111.71
6	T	7	DG	C5'-C4'-O4'	6.23	118.74	109.40
6	T	9	DT	P-O3'-C3'	-6.22	110.86	120.20
7	f	62	SER	CA-C-O	6.22	129.17	121.89
8	M	131	THR	N-CA-C	-6.22	102.31	110.39
7	a	48	ARG	CB-CA-C	6.22	120.72	110.90
7	f	193	PHE	CB-CG-CD1	-6.22	110.13	120.70
8	M	473	ARG	N-CA-CB	6.22	119.64	110.56
7	d	175	GLN	CB-CA-C	6.20	122.48	109.65
7	f	15	PHE	N-CA-C	-6.20	104.98	112.54
8	M	258	PRO	CB-CG-CD	-6.20	86.27	106.10
7	b	143	ARG	CB-CA-C	-6.19	100.59	110.81
8	M	355	PHE	N-CA-C	6.19	117.69	111.07
8	M	372	GLN	N-CA-C	-6.18	105.22	112.89
7	f	140	VAL	CA-C-O	-6.18	114.29	120.90
7	b	218	LEU	O-C-N	-6.17	115.47	122.08
7	d	158	GLU	O-C-N	6.17	130.15	122.19
7	f	256	LYS	CB-CG-CD	6.17	125.48	111.30
7	e	162	ARG	N-CA-C	6.16	119.40	110.28
7	d	40	THR	N-CA-C	-6.16	101.85	110.35
7	b	255	PHE	CA-C-N	-6.16	112.25	121.05
7	b	255	PHE	C-N-CA	-6.16	112.25	121.05
7	a	170	ALA	O-C-N	6.15	130.62	123.30
8	M	343	VAL	CG1-CB-CG2	6.15	124.32	110.80
7	b	136	GLN	CA-C-N	6.14	127.52	119.84
7	b	136	GLN	C-N-CA	6.14	127.52	119.84
7	e	180	ARG	CB-CG-CD	6.14	125.42	111.30
7	a	65	CYS	CB-CA-C	6.14	121.71	110.11
8	M	128	VAL	CA-C-O	6.14	127.33	120.95
8	M	146	ASP	CB-CA-C	-6.13	100.61	110.79
8	M	470	SER	N-CA-C	6.13	117.63	111.07
7	d	222	TRP	CA-C-N	6.13	126.02	119.28
7	d	222	TRP	C-N-CA	6.13	126.02	119.28
8	M	189	GLY	CA-C-O	6.12	131.22	120.57
8	M	197	ASP	CA-C-N	-6.11	112.00	120.38
8	M	197	ASP	C-N-CA	-6.11	112.00	120.38
8	M	330	ILE	CA-CB-CG2	-6.11	100.11	110.50
7	a	188	LEU	CB-CG-CD2	6.11	129.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	218	LEU	CB-CG-CD2	6.11	129.02	110.70
8	M	403	PHE	N-CA-C	6.11	119.20	110.10
7	c	26	ALA	O-C-N	6.10	125.91	120.48
7	d	92	HIS	CA-C-N	6.10	125.50	118.85
7	d	92	HIS	C-N-CA	6.10	125.50	118.85
7	a	186	ILE	CA-C-O	6.09	127.75	121.41
7	d	97	GLU	N-CA-C	-6.09	104.70	111.71
7	a	212	ARG	CA-CB-CG	6.09	126.28	114.10
7	d	95	ARG	CA-C-N	-6.09	108.67	121.64
7	d	95	ARG	C-N-CA	-6.09	108.67	121.64
8	M	201	ILE	CB-CG1-CD1	6.07	126.54	113.80
8	M	290	ASN	N-CA-C	6.07	117.89	109.15
7	a	217	LEU	N-CA-C	6.06	117.55	111.07
7	b	141	ASN	O-C-N	6.06	130.02	122.63
7	b	143	ARG	N-CA-CB	-6.06	100.58	110.21
8	M	356	GLU	CA-C-O	6.05	126.93	120.70
8	M	252	LEU	O-C-N	6.04	128.29	122.07
7	b	59	PRO	CB-CA-C	-6.03	101.40	110.20
7	e	255	PHE	CB-CA-C	-6.03	98.42	110.42
8	M	297	LEU	CB-CG-CD1	-6.03	92.62	110.70
8	M	382	SER	CA-CB-OG	-6.03	99.05	111.10
7	c	199	ARG	CA-C-O	-6.03	114.03	120.42
7	f	178	PRO	N-CA-C	6.02	119.65	111.22
5	N	-11	DA	OP2-P-O3'	6.02	126.06	108.00
7	b	196	GLN	N-CA-C	-6.02	103.89	111.11
7	f	193	PHE	CE1-CZ-CE2	6.02	130.83	120.00
7	b	179	LEU	CB-CA-C	-6.01	100.62	110.85
8	M	333	LEU	CB-CG-CD1	-6.01	92.66	110.70
7	c	41	GLY	N-CA-C	6.01	123.66	115.30
7	c	198	CYS	N-CA-C	6.01	119.80	112.23
7	e	22	VAL	N-CA-C	-6.00	105.19	113.00
8	M	276	VAL	N-CA-CB	-6.00	101.39	112.43
7	e	44	LEU	CB-CG-CD2	6.00	128.69	110.70
7	a	186	ILE	O-C-N	5.97	128.41	121.96
7	b	255	PHE	O-C-N	5.97	131.09	122.13
8	M	456	ARG	CG-CD-NE	5.97	125.14	112.00
7	b	215	GLU	CA-C-O	5.97	126.87	120.55
7	a	221	ARG	CB-CA-C	5.96	122.27	110.42
7	e	201	ILE	O-C-N	5.95	130.01	122.57
7	f	5	LYS	N-CA-C	5.95	117.14	107.32
7	f	57	GLN	N-CA-C	-5.95	106.03	113.28
5	N	-22	DC	C2'-C3'-O3'	5.94	120.41	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	206	PHE	CA-C-N	5.94	125.81	119.28
7	f	206	PHE	C-N-CA	5.94	125.81	119.28
7	e	236	SER	N-CA-C	5.92	118.50	111.33
8	M	323	LEU	CB-CG-CD1	-5.92	92.94	110.70
7	a	188	LEU	CB-CA-C	5.91	120.06	110.96
8	M	407	VAL	CG1-CB-CG2	5.90	123.78	110.80
7	f	194	ALA	O-C-N	5.90	128.37	122.12
7	d	117	GLN	N-CA-C	-5.89	104.55	110.97
7	b	188	LEU	CB-CG-CD1	-5.89	93.03	110.70
7	c	257	ARG	N-CA-C	5.89	119.22	107.62
8	M	130	LEU	N-CA-C	5.89	119.22	112.57
7	d	48	ARG	NE-CZ-NH2	5.89	124.50	119.20
7	e	233	VAL	N-CA-CB	-5.89	103.66	110.55
8	M	219	ILE	CB-CA-C	-5.88	104.10	112.22
8	M	263	SER	CB-CA-C	-5.88	101.40	110.81
8	M	338	ASP	CB-CA-C	-5.88	101.65	110.88
7	c	218	LEU	CB-CA-C	5.87	119.98	109.29
7	a	48	ARG	NH1-CZ-NH2	-5.87	111.67	119.30
7	d	99	ALA	O-C-N	-5.87	114.78	122.59
8	M	416	SER	CA-C-N	-5.86	111.40	120.31
8	M	416	SER	C-N-CA	-5.86	111.40	120.31
7	b	140	VAL	CB-CA-C	-5.85	101.92	110.81
8	M	278	VAL	N-CA-CB	-5.85	104.74	112.34
7	b	177	PRO	CB-CA-C	-5.84	103.79	110.92
8	M	404	SER	N-CA-C	5.84	117.66	108.96
8	M	370	ILE	CB-CG1-CD1	-5.83	101.56	113.80
6	T	15	DA	C4'-C3'-O3'	-5.83	101.26	110.00
7	a	219	ASN	CB-CA-C	5.82	120.74	110.85
7	b	190	ALA	CA-C-N	-5.82	111.47	120.31
7	b	190	ALA	C-N-CA	-5.82	111.47	120.31
8	M	258	PRO	CA-C-O	-5.81	114.72	121.34
7	c	256	LYS	CA-C-N	-5.81	114.54	123.14
7	c	256	LYS	C-N-CA	-5.81	114.54	123.14
8	M	120	LEU	CA-C-O	-5.81	112.20	120.51
7	a	223	PRO	N-CA-CB	5.80	109.21	102.88
7	e	33	LEU	CA-CB-CG	-5.80	95.99	116.30
7	b	199	ARG	CA-CB-CG	5.80	125.70	114.10
7	c	252	ILE	N-CA-C	5.80	119.21	111.44
7	a	183	GLU	CG-CD-OE1	-5.78	105.10	118.40
7	b	240	HIS	N-CA-CB	5.78	118.62	110.12
7	c	169	LEU	CB-CG-CD1	5.78	128.04	110.70
7	f	98	ARG	NH1-CZ-NH2	-5.78	111.78	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	181	GLU	N-CA-C	5.78	118.52	111.82
8	M	297	LEU	N-CA-C	5.78	119.14	109.95
8	M	153	TYR	CA-C-N	-5.78	113.16	121.42
8	M	153	TYR	C-N-CA	-5.78	113.16	121.42
7	c	58	GLY	N-CA-C	5.77	124.11	112.34
7	c	199	ARG	N-CA-C	-5.77	105.07	111.36
7	d	96	PHE	CG-CD1-CE1	-5.77	110.89	120.70
8	M	158	ILE	CA-CB-CG2	-5.77	100.69	110.50
7	c	201	ILE	CA-CB-CG1	5.76	120.20	110.40
7	e	229	LEU	CB-CG-CD2	5.75	127.95	110.70
7	b	237	VAL	O-C-N	5.75	127.55	121.91
8	M	131	THR	CA-C-O	5.75	126.55	120.63
8	M	260	PRO	O-C-N	-5.73	114.91	122.64
8	M	179	LEU	CA-C-N	-5.72	111.12	121.14
8	M	179	LEU	C-N-CA	-5.72	111.12	121.14
7	b	14	SER	CA-C-O	-5.71	112.34	120.51
7	b	184	SER	N-CA-C	-5.71	105.58	113.18
7	e	23	SER	CA-C-O	-5.70	113.41	119.97
7	e	186	ILE	N-CA-C	-5.69	105.18	110.53
7	a	180	ARG	CB-CA-C	-5.69	101.30	110.74
7	a	62	SER	N-CA-C	5.69	117.28	111.14
8	M	37	LEU	CD1-CG-CD2	5.69	123.31	110.80
8	M	41	LEU	N-CA-CB	-5.68	101.77	110.12
7	d	148	THR	CA-C-O	-5.68	114.39	121.55
7	e	222	TRP	CA-C-N	-5.68	113.06	118.97
7	e	222	TRP	C-N-CA	-5.68	113.06	118.97
8	M	354	PHE	O-C-N	5.68	129.25	122.27
8	M	399	LEU	N-CA-C	5.67	118.40	111.82
7	f	167	ASP	O-C-N	-5.67	115.97	122.09
7	a	14	SER	N-CA-C	-5.67	105.10	111.28
7	f	99	ALA	CB-CA-C	5.67	120.61	110.81
7	d	171	PHE	O-C-N	5.66	128.14	122.08
8	M	180	LYS	CA-C-O	-5.66	112.29	119.31
7	a	183	GLU	CA-CB-CG	5.64	125.39	114.10
7	a	188	LEU	CA-CB-CG	-5.64	96.56	116.30
8	M	329	LEU	CA-C-O	-5.64	114.44	120.42
5	N	-27	DT	P-O5'-C5'	-5.64	111.55	120.00
7	b	177	PRO	CA-N-CD	5.64	119.89	112.00
7	d	177	PRO	O-C-N	5.64	128.11	121.46
7	b	202	LYS	CA-C-O	5.63	127.98	121.28
8	M	365	MET	N-CA-C	5.63	117.74	109.24
7	c	169	LEU	N-CA-CB	-5.62	102.80	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	212	ARG	NE-CZ-NH2	5.62	124.26	119.20
7	f	256	LYS	CG-CD-CE	5.62	124.23	111.30
7	e	55	ARG	CA-C-O	5.62	128.54	120.51
7	b	120	LEU	CA-CB-CG	-5.61	96.66	116.30
7	a	209	PHE	CA-C-O	5.61	126.42	120.36
7	e	210	THR	OG1-CB-CG2	5.61	120.52	109.30
7	a	217	LEU	O-C-N	5.59	127.83	122.07
7	e	32	VAL	CA-C-N	-5.59	113.06	122.29
7	e	32	VAL	C-N-CA	-5.59	113.06	122.29
7	e	33	LEU	CB-CG-CD1	-5.59	93.92	110.70
7	e	19	LEU	O-C-N	5.59	128.05	122.12
7	f	128	GLU	CA-CB-CG	5.58	125.26	114.10
5	N	-21	DG	C2'-C3'-O3'	5.57	119.86	111.50
7	a	61	ILE	N-CA-C	5.57	116.77	109.58
8	M	382	SER	CB-CA-C	-5.57	101.21	110.68
7	b	240	HIS	N-CA-C	-5.57	105.21	111.28
1	A	190	ALA	N-CA-C	5.57	116.72	108.60
7	e	230	LYS	CD-CE-NZ	5.56	129.70	111.90
7	a	193	PHE	CD1-CE1-CZ	-5.56	109.99	120.00
7	a	213	ALA	CA-C-N	-5.56	113.06	120.79
7	a	213	ALA	C-N-CA	-5.56	113.06	120.79
7	a	45	ILE	N-CA-CB	-5.55	102.99	110.54
7	e	239	ARG	N-CA-C	5.55	117.33	111.28
7	c	105	PHE	CA-C-N	-5.55	114.81	122.30
7	c	105	PHE	C-N-CA	-5.55	114.81	122.30
7	f	34	ILE	CB-CG1-CD1	5.55	125.45	113.80
7	f	176	LEU	CD1-CG-CD2	5.55	123.00	110.80
5	N	-27	DT	O5'-P-OP1	5.54	125.63	109.00
7	b	235	ARG	CA-CB-CG	-5.54	103.02	114.10
8	M	382	SER	N-CA-C	5.54	118.03	111.33
8	M	401	TYR	CB-CA-C	-5.53	101.28	110.68
7	a	213	ALA	CA-C-O	5.53	126.28	120.42
8	M	197	ASP	OD1-CG-OD2	5.52	136.16	122.90
7	c	40	THR	N-CA-C	5.52	117.59	108.49
7	b	68	LEU	CA-CB-CG	-5.51	97.00	116.30
7	c	142	VAL	CB-CA-C	-5.51	102.89	111.26
7	c	179	LEU	N-CA-C	-5.51	106.40	113.23
7	b	224	GLY	CA-C-N	5.50	132.04	121.54
7	b	224	GLY	C-N-CA	5.50	132.04	121.54
7	d	49	LEU	N-CA-C	5.49	119.24	112.54
7	e	230	LYS	N-CA-C	5.49	120.44	111.37
8	M	153	TYR	N-CA-C	-5.49	101.22	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	98	ARG	N-CA-C	-5.49	105.32	112.23
7	a	258	ARG	CB-CA-C	5.48	120.97	110.17
8	M	202	GLN	CA-CB-CG	-5.48	103.14	114.10
7	b	35	ILE	N-CA-C	5.47	115.74	107.75
7	b	196	GLN	O-C-N	5.47	127.78	122.09
7	d	154	ALA	N-CA-C	-5.47	105.22	111.07
7	b	236	SER	N-CA-CB	-5.47	101.80	109.94
7	c	254	PRO	CB-CA-C	5.47	119.69	111.44
7	f	213	ALA	O-C-N	5.47	127.70	122.07
7	b	144	LEU	N-CA-C	5.46	117.64	108.96
7	f	30	LYS	N-CA-C	5.46	115.88	109.60
8	M	146	ASP	CA-C-N	-5.46	114.48	122.06
8	M	146	ASP	C-N-CA	-5.46	114.48	122.06
8	M	261	GLY	CA-C-N	5.45	127.58	120.28
8	M	261	GLY	C-N-CA	5.45	127.58	120.28
7	d	109	LEU	CB-CG-CD1	5.44	127.03	110.70
8	M	363	LYS	N-CA-CB	5.44	117.81	110.14
7	f	197	MET	CA-CB-CG	5.44	124.98	114.10
8	M	400	LYS	CA-C-N	5.44	127.83	120.38
8	M	400	LYS	C-N-CA	5.44	127.83	120.38
8	M	399	LEU	CB-CA-C	-5.44	100.23	110.67
7	b	52	LEU	N-CA-C	5.43	118.71	112.57
7	b	69	ASN	CB-CG-ND2	5.43	124.55	116.40
7	e	32	VAL	N-CA-C	-5.43	98.04	109.34
5	N	-16	DT	C4'-C3'-O3'	-5.43	101.86	110.00
8	M	35	GLN	N-CA-C	-5.43	105.45	111.36
7	b	59	PRO	N-CD-CG	5.42	111.33	103.20
7	c	194	ALA	CA-C-N	-5.41	112.90	120.53
7	c	194	ALA	C-N-CA	-5.41	112.90	120.53
7	e	19	LEU	CA-C-N	5.41	132.12	121.58
7	e	19	LEU	C-N-CA	5.41	132.12	121.58
7	e	35	ILE	CB-CA-C	-5.41	102.44	110.33
8	M	154	LEU	CA-C-N	5.41	127.47	120.44
8	M	154	LEU	C-N-CA	5.41	127.47	120.44
7	e	147	ALA	CA-C-O	-5.40	114.11	120.60
8	M	276	VAL	CB-CA-C	-5.40	103.47	111.19
7	b	236	SER	CA-C-N	5.40	127.36	120.56
7	b	236	SER	C-N-CA	5.40	127.36	120.56
5	N	-26	DG	P-O5'-C5'	-5.39	111.91	120.00
6	T	17	DA	C4'-C3'-O3'	-5.39	101.92	110.00
8	M	317	GLN	N-CA-C	-5.38	105.49	111.36
7	f	34	ILE	CG1-CB-CG2	5.38	126.85	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	330	ILE	CB-CA-C	-5.38	102.47	111.29
8	M	285	TRP	CA-C-O	-5.38	115.13	121.16
7	f	201	ILE	CB-CG1-CD1	5.38	125.09	113.80
7	e	17	GLU	CA-CB-CG	-5.38	103.34	114.10
7	a	80	HIS	CB-CA-C	-5.37	98.90	111.09
7	b	227	ARG	CB-CA-C	5.36	119.80	110.68
7	a	222	TRP	CD2-CE3-CZ3	5.36	125.56	118.60
1	A	93	GLN	N-CA-C	5.36	116.92	109.31
7	d	220	TYR	O-C-N	5.35	129.42	122.89
7	b	242	THR	CA-C-N	5.35	132.19	121.81
7	b	242	THR	C-N-CA	5.35	132.19	121.81
8	M	260	PRO	CB-CA-C	-5.34	102.74	111.56
8	M	205	GLN	N-CA-C	5.34	116.78	111.07
7	a	217	LEU	N-CA-CB	-5.34	102.27	110.01
7	e	43	GLU	N-CA-C	-5.34	105.83	112.93
7	b	58	GLY	N-CA-C	5.33	118.69	112.23
7	e	33	LEU	N-CA-C	-5.33	100.96	109.23
7	f	255	PHE	CA-C-N	-5.33	114.67	122.19
7	f	255	PHE	C-N-CA	-5.33	114.67	122.19
7	c	256	LYS	CB-CA-C	-5.33	100.54	109.65
7	f	44	LEU	CB-CG-CD1	5.33	126.69	110.70
7	f	255	PHE	O-C-N	-5.33	115.50	122.59
7	b	121	LEU	N-CA-C	-5.33	103.11	110.35
8	M	146	ASP	N-CA-C	5.33	117.09	111.28
8	M	388	LYS	CB-CG-CD	-5.33	99.05	111.30
7	d	109	LEU	CB-CA-C	-5.32	100.78	110.63
8	M	142	THR	CA-CB-CG2	-5.32	101.46	110.50
7	e	142	VAL	N-CA-C	-5.31	100.81	108.89
7	d	99	ALA	CB-CA-C	5.31	120.99	110.42
7	e	187	MET	O-C-N	5.30	128.19	122.15
8	M	298	LYS	N-CA-C	-5.30	99.69	108.75
7	b	177	PRO	N-CA-CB	-5.29	97.94	103.08
7	b	197	MET	CB-CG-SD	-5.29	96.83	112.70
7	f	234	GLU	N-CA-CB	5.29	118.53	110.44
8	M	203	LEU	N-CA-CB	5.28	117.67	110.01
7	b	192	TYR	CB-CA-C	-5.27	102.57	110.90
7	b	193	PHE	CG-CD2-CE2	-5.27	111.74	120.70
7	c	220	TYR	CA-CB-CG	-5.27	104.41	113.90
7	a	173	VAL	O-C-N	5.27	128.51	122.93
8	M	155	THR	N-CA-C	5.27	116.71	111.07
7	c	28	LEU	CB-CG-CD2	5.26	126.49	110.70
7	d	96	PHE	CZ-CE2-CD2	-5.26	110.53	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	178	PRO	CB-CA-C	-5.26	103.27	111.22
7	b	142	VAL	CA-CB-CG1	5.26	119.34	110.40
8	M	203	LEU	CB-CA-C	-5.26	102.63	110.88
8	M	127	GLN	N-CA-CB	5.25	118.63	110.44
7	a	205	LEU	CD1-CG-CD2	5.25	122.34	110.80
7	a	221	ARG	N-CA-C	5.25	121.98	110.80
7	f	7	ASN	N-CA-C	5.24	115.76	108.00
7	b	50	HIS	N-CA-C	-5.24	106.03	112.90
7	e	173	VAL	CG1-CB-CG2	-5.24	99.27	110.80
8	M	278	VAL	CA-C-N	-5.24	114.08	122.62
8	M	278	VAL	C-N-CA	-5.24	114.08	122.62
8	M	153	TYR	CB-CA-C	-5.24	99.79	109.37
8	M	329	LEU	CB-CG-CD1	-5.24	95.00	110.70
7	a	169	LEU	CA-CB-CG	-5.23	97.98	116.30
8	M	194	ASP	CA-C-N	5.22	129.71	121.56
8	M	194	ASP	C-N-CA	5.22	129.71	121.56
7	c	175	GLN	N-CA-CB	5.22	118.69	110.23
8	M	392	SER	CA-C-N	5.22	126.37	119.84
8	M	392	SER	C-N-CA	5.22	126.37	119.84
7	d	49	LEU	N-CA-CB	-5.22	101.73	110.39
8	M	390	LEU	N-CA-C	-5.22	100.39	108.90
7	e	45	ILE	CA-C-N	-5.22	112.77	120.28
7	e	45	ILE	C-N-CA	-5.22	112.77	120.28
7	e	47	SER	N-CA-C	-5.21	105.51	111.14
8	M	376	MET	CB-CG-SD	-5.21	97.06	112.70
7	b	57	GLN	CA-C-N	-5.21	113.91	121.42
7	b	57	GLN	C-N-CA	-5.21	113.91	121.42
8	M	28	LEU	CB-CG-CD1	5.21	126.34	110.70
7	f	15	PHE	CA-CB-CG	5.21	119.01	113.80
8	M	120	LEU	N-CA-C	-5.21	99.70	110.80
7	c	182	ARG	NE-CZ-NH1	5.21	126.71	121.50
7	d	44	LEU	N-CA-C	-5.21	105.60	111.28
6	T	14	DC	C2'-C3'-O3'	5.21	119.31	111.50
7	f	162	ARG	CA-C-O	-5.20	115.47	121.19
6	T	10	DC	C5'-C4'-O4'	5.20	117.20	109.40
5	N	-16	DT	N1-C1'-C2'	5.20	121.30	113.50
8	M	200	LEU	CA-C-O	5.20	125.92	119.79
7	a	58	GLY	N-CA-C	-5.19	101.75	112.34
7	e	211	GLU	N-CA-C	5.19	121.86	110.80
8	M	353	ALA	CA-C-O	5.19	127.94	120.51
7	b	49	LEU	CA-C-N	-5.18	111.98	121.52
7	b	49	LEU	C-N-CA	-5.18	111.98	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	69	ASN	N-CA-C	5.18	117.22	110.53
8	M	337	ASN	N-CA-C	5.18	117.33	111.11
7	f	9	LEU	N-CA-C	5.17	116.92	111.28
7	e	252	ILE	CA-CB-CG2	5.17	119.30	110.50
7	e	142	VAL	CB-CA-C	5.17	119.27	110.95
7	a	45	ILE	CB-CA-C	5.17	119.12	112.14
7	a	222	TRP	CE3-CZ3-CH2	-5.17	114.38	121.10
7	b	33	LEU	CB-CG-CD1	-5.17	95.20	110.70
7	b	61	ILE	CB-CA-C	-5.16	103.00	111.51
8	M	345	ARG	NE-CZ-NH2	-5.16	114.56	119.20
7	d	17	GLU	O-C-N	5.15	127.58	122.12
7	e	35	ILE	N-CA-CB	-5.15	104.00	111.52
8	M	249	ALA	CB-CA-C	-5.15	102.24	110.79
8	M	402	PHE	N-CA-CB	-5.15	102.27	109.94
8	M	359	GLU	N-CA-CB	5.15	118.93	110.39
7	a	162	ARG	CA-C-N	5.15	127.43	120.38
7	a	162	ARG	C-N-CA	5.15	127.43	120.38
7	f	231	ASN	N-CA-C	5.15	119.86	111.37
8	M	285	TRP	CA-C-N	-5.14	115.90	123.00
8	M	285	TRP	C-N-CA	-5.14	115.90	123.00
7	b	218	LEU	CA-C-O	5.14	126.73	121.07
7	a	143	ARG	CB-CA-C	5.14	118.44	109.65
8	M	459	ALA	CB-CA-C	-5.14	102.81	110.88
8	M	299	ILE	CA-CB-CG2	5.14	119.23	110.50
7	a	226	ILE	CB-CA-C	5.13	119.54	112.05
7	d	44	LEU	CA-C-O	5.12	125.98	120.55
7	e	190	ALA	O-C-N	5.12	127.56	122.08
7	e	226	ILE	CA-C-N	-5.12	113.31	121.44
7	e	226	ILE	C-N-CA	-5.12	113.31	121.44
7	c	213	ALA	N-CA-C	-5.11	104.97	111.11
7	d	189	MET	O-C-N	5.11	127.33	122.07
7	b	16	LEU	CA-C-O	5.11	126.18	120.82
7	f	212	ARG	NE-CZ-NH1	-5.11	116.39	121.50
7	c	198	CYS	CA-CB-SG	-5.10	102.66	114.40
8	M	256	LEU	CA-CB-CG	5.10	134.15	116.30
8	M	145	VAL	CA-CB-CG1	-5.10	101.74	110.40
8	M	372	GLN	CB-CA-C	5.10	120.64	109.99
7	e	136	GLN	CA-C-N	5.09	126.21	119.84
7	e	136	GLN	C-N-CA	5.09	126.21	119.84
6	T	13	DG	C5'-C4'-O4'	5.09	117.04	109.40
7	b	212	ARG	NE-CZ-NH2	5.09	123.78	119.20
7	b	216	THR	CA-C-O	5.09	125.89	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	45	ILE	CA-CB-CG1	-5.09	101.75	110.40
7	c	212	ARG	CG-CD-NE	-5.09	100.81	112.00
7	b	120	LEU	CB-CG-CD1	5.08	125.95	110.70
8	M	348	VAL	CB-CA-C	-5.08	100.64	111.32
5	N	-26	DG	C4'-C3'-O3'	-5.08	102.38	110.00
7	f	214	ARG	NE-CZ-NH1	5.08	126.58	121.50
7	c	222	TRP	CB-CA-C	-5.08	100.16	110.17
7	f	44	LEU	CB-CA-C	5.07	119.85	110.88
7	e	35	ILE	CA-CB-CG2	5.07	119.11	110.50
5	N	-22	DC	N1-C1'-C2'	5.06	121.10	113.50
7	b	188	LEU	CB-CA-C	5.06	118.80	110.95
8	M	354	PHE	CZ-CE2-CD2	-5.06	110.89	120.00
7	e	250	ILE	CB-CA-C	5.06	118.22	111.19
7	c	187	MET	CG-SD-CE	5.06	112.03	100.90
7	b	49	LEU	CB-CA-C	5.06	119.67	110.11
8	M	180	LYS	CA-CB-CG	5.05	124.20	114.10
8	M	341	LEU	CA-C-O	-5.05	114.64	120.24
8	M	468	PRO	CA-C-N	5.05	126.15	119.84
8	M	468	PRO	C-N-CA	5.05	126.15	119.84
7	f	211	GLU	O-C-N	5.04	127.90	122.15
7	c	200	GLU	N-CA-CB	5.04	117.45	109.94
8	M	386	THR	N-CA-CB	5.04	117.42	110.17
7	f	127	GLY	CA-C-N	-5.04	114.64	122.09
7	f	127	GLY	C-N-CA	-5.04	114.64	122.09
7	d	144	LEU	CA-C-N	-5.03	114.69	122.69
7	d	144	LEU	C-N-CA	-5.03	114.69	122.69
8	M	201	ILE	CB-CA-C	-5.03	105.50	112.24
7	a	186	ILE	CA-C-N	5.03	126.98	120.44
7	a	186	ILE	C-N-CA	5.03	126.98	120.44
8	M	24	ARG	N-CA-CB	5.03	118.74	110.39
8	M	387	GLN	N-CA-C	5.03	121.51	110.80
7	d	146	CYS	N-CA-CB	-5.02	102.23	111.37
7	d	147	ALA	CB-CA-C	5.02	120.41	110.42
8	M	387	GLN	CA-CB-CG	5.02	124.14	114.10
7	a	202	LYS	N-CA-C	-5.02	106.03	113.40
7	b	30	LYS	CA-C-N	5.02	124.93	119.76
7	b	30	LYS	C-N-CA	5.02	124.93	119.76
7	a	253	ASP	N-CA-C	5.02	118.13	108.45
7	e	200	GLU	O-C-N	5.02	127.87	122.15
7	f	198	CYS	CB-CA-C	5.01	119.37	110.85
7	e	251	ILE	CA-CB-CG1	5.01	118.91	110.40
7	a	99	ALA	N-CA-C	-5.01	104.60	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	182	ARG	NE-CZ-NH2	-5.00	114.69	119.20
7	d	158	GLU	N-CA-C	5.00	118.22	112.57

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	a	162	ARG	Mainchain
7	b	219	ASN	Mainchain
7	d	92	HIS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2322	0	2308	54	0
1	B	1676	0	1676	28	0
2	C	10125	0	9829	160	0
3	D	9634	0	9244	165	0
4	E	546	0	548	3	0
5	N	738	0	404	71	0
6	T	738	0	404	44	0
7	a	2052	0	2048	454	0
7	b	2052	0	2048	472	0
7	c	2000	0	1969	363	0
7	d	2041	0	2038	297	0
7	e	2062	0	2059	353	0
7	f	2053	0	2044	367	0
8	M	3301	0	3331	512	0
9	a	27	0	12	11	0
9	b	27	0	12	5	0
9	c	27	0	12	7	0
9	e	27	0	12	12	0
9	f	27	0	12	19	0
10	a	4	0	0	0	0
10	b	4	0	0	0	0
10	e	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	f	4	0	0	1	0
All	All	41491	0	40010	3035	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 (3035) 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)
7:b:49:LEU:CA	7:b:49:LEU:CB	1.75	1.62
7:a:221:ARG:C	7:a:221:ARG:CA	1.74	1.59
7:e:62:SER:N	7:e:62:SER:CA	1.68	1.55
7:a:98:ARG:CZ	7:a:98:ARG:NH2	1.69	1.53
7:a:179:LEU:CD2	7:a:226:ILE:HD13	1.37	1.52
7:d:85:PHE:CB	8:M:1:MET:HE1	1.40	1.51
7:d:68:LEU:HD22	7:d:72:LEU:CD2	1.39	1.49
7:f:103:THR:HG22	7:f:143:ARG:CB	1.41	1.45
7:c:32:VAL:HG22	7:c:145:VAL:CG1	1.47	1.45
7:c:104:LEU:HD11	7:c:142:VAL:CG2	1.45	1.44
7:e:189:MET:SD	7:e:189:MET:CG	2.06	1.43
7:a:216:THR:HG21	7:a:250:ILE:CD1	1.50	1.42
7:a:65:CYS:SG	7:a:65:CYS:CB	2.08	1.42
7:c:197:MET:SD	7:c:197:MET:CG	2.08	1.42
6:T:31:DG:H3'	8:M:233:ARG:NH2	1.34	1.41
7:a:96:PHE:CD2	7:a:123:VAL:HG11	1.55	1.40
7:c:104:LEU:CD1	7:c:142:VAL:HG22	1.52	1.38
7:c:197:MET:SD	7:c:197:MET:CE	2.11	1.38
5:N:-8:DT:H5''	7:b:90:LYS:CE	1.51	1.37
7:d:78:PHE:CD2	7:d:129:LEU:HD11	1.59	1.37
7:f:103:THR:CG2	7:f:143:ARG:HB3	1.55	1.37
7:c:61:ILE:CG2	7:c:99:ALA:HB2	1.54	1.34
7:e:44:LEU:CD1	9:e:601:ADP:H2'	1.54	1.34
7:b:80:HIS:HB3	7:b:132:VAL:CG2	1.57	1.34
7:b:8:LEU:HD11	7:b:19:LEU:CD2	1.57	1.34
7:a:216:THR:CG2	7:a:250:ILE:HD11	1.55	1.33
7:a:193:PHE:CE2	7:a:229:LEU:HD11	1.63	1.33
7:b:77:LEU:HD11	7:b:96:PHE:CE1	1.62	1.33
7:a:72:LEU:CD1	8:M:7:LEU:HD21	1.57	1.32
7:c:152:LEU:CG	7:c:166:LEU:HD12	1.59	1.31
7:c:8:LEU:HD21	7:c:15:PHE:CZ	1.65	1.29
7:a:240:HIS:ND1	7:a:247:LEU:HB3	1.46	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:182:ARG:CG	7:d:185:ASP:HB2	1.66	1.26
7:b:121:LEU:O	7:b:122:ARG:HG2	1.28	1.26
7:c:99:ALA:CB	7:c:104:LEU:HD23	1.65	1.26
5:N:-27:DT:H73	8:M:455:ARG:NH2	1.47	1.26
7:a:179:LEU:HD21	7:a:226:ILE:CD1	1.65	1.25
7:b:195:ILE:HA	7:b:206:PHE:CZ	1.72	1.25
7:d:41:GLY:HA3	7:d:176:LEU:CD2	1.65	1.23
7:a:42:LYS:HD3	9:a:601:ADP:O3B	1.37	1.22
7:a:193:PHE:CD2	7:a:229:LEU:HD11	1.73	1.22
8:M:195:LEU:HD11	8:M:199:LEU:CD1	1.69	1.22
7:d:78:PHE:CZ	7:d:119:LYS:HG2	1.72	1.21
7:f:15:PHE:CD2	7:f:182:ARG:HD2	1.75	1.21
8:M:153:TYR:CD1	8:M:192:ALA:HB3	1.73	1.21
7:c:8:LEU:HD11	7:c:15:PHE:CZ	1.75	1.20
7:e:104:LEU:HD21	7:e:144:LEU:CD2	1.69	1.20
7:e:146:CYS:SG	7:e:169:LEU:HD13	1.80	1.20
7:d:85:PHE:HB3	8:M:1:MET:CE	1.71	1.20
2:C:843:THR:HB	8:M:271:TYR:CE1	1.76	1.19
7:f:34:ILE:HB	7:f:147:ALA:CB	1.73	1.19
8:M:182:ILE:HG23	8:M:185:PHE:CD2	1.76	1.19
7:a:96:PHE:CE2	7:a:123:VAL:HG11	1.77	1.19
7:f:226:ILE:HG21	9:f:601:ADP:C8	1.76	1.19
7:f:238:TYR:CD2	7:e:28:LEU:HD11	1.78	1.17
7:e:61:ILE:CD1	7:e:98:ARG:HG2	1.73	1.17
5:N:-13:DC:C2	8:M:15:MET:HE2	1.79	1.17
7:b:197:MET:CG	7:b:237:VAL:HG11	1.74	1.16
7:d:68:LEU:CD2	7:d:72:LEU:HD23	1.73	1.16
7:a:193:PHE:CD2	7:a:229:LEU:CD1	2.28	1.16
8:M:182:ILE:HG23	8:M:185:PHE:CE2	1.80	1.16
1:A:305:ASP:OD2	8:M:180:LYS:HE2	1.46	1.16
7:a:180:ARG:NH1	7:a:221:ARG:HD3	1.60	1.15
7:d:85:PHE:CB	8:M:1:MET:CE	2.24	1.15
7:f:63:LEU:HD11	7:f:106:LEU:CD2	1.77	1.15
7:f:85:PHE:CE2	8:M:5:LEU:HD22	1.82	1.14
7:b:8:LEU:CD1	7:b:19:LEU:HD22	1.75	1.14
7:d:155:MET:HB3	7:d:160:THR:OG1	1.48	1.14
7:f:65:CYS:SG	7:f:109:LEU:HA	1.87	1.14
7:a:22:VAL:HG22	7:a:49:LEU:HD21	1.17	1.14
7:e:26:ALA:HB1	7:e:53:SER:CA	1.77	1.14
7:e:104:LEU:CD2	7:e:144:LEU:HD23	1.77	1.14
7:b:49:LEU:CA	7:b:49:LEU:CG	2.25	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:32:VAL:CG2	7:c:145:VAL:HG11	1.77	1.14
7:b:62:SER:HB3	7:b:105:PHE:HB3	1.26	1.14
7:b:30:LYS:HB2	7:b:171:PHE:CE2	1.82	1.13
7:e:26:ALA:HB1	7:e:53:SER:CB	1.79	1.13
6:T:12:DT:H6	8:M:23:ILE:HD13	0.97	1.13
5:N:-13:DC:C2'	8:M:15:MET:CE	2.26	1.12
7:b:152:LEU:HB3	7:b:166:LEU:CD1	1.78	1.13
2:C:844:LYS:HB2	8:M:272:VAL:HG13	1.21	1.12
6:T:12:DT:C6	8:M:23:ILE:HD13	1.84	1.12
7:c:61:ILE:CG2	7:c:99:ALA:CB	2.27	1.12
7:d:153:PRO:HD3	7:e:255:PHE:CE2	1.83	1.12
7:e:32:VAL:HG21	7:e:143:ARG:NH2	1.65	1.12
7:e:124:ILE:HG12	7:e:144:LEU:HD12	1.19	1.12
7:c:104:LEU:HD13	7:c:144:LEU:HB3	1.20	1.11
8:M:278:VAL:HG12	8:M:287:VAL:HG22	1.31	1.11
7:a:91:ARG:HD3	7:a:131:ARG:NH1	1.66	1.11
7:c:152:LEU:HG	7:c:166:LEU:HD12	1.15	1.11
7:a:252:ILE:HG22	7:a:253:ASP:OD1	1.50	1.11
7:b:198:CYS:SG	7:b:206:PHE:CZ	2.43	1.11
7:f:32:VAL:HG23	7:f:172:ASP:O	1.47	1.11
7:b:191:GLU:O	7:b:195:ILE:HG12	1.51	1.10
1:A:166:ARG:HE	1:A:172:LEU:CD1	1.63	1.10
7:f:82:ALA:HB2	7:f:90:LYS:CA	1.80	1.10
7:e:179:LEU:HD13	7:e:225:ASN:O	1.51	1.10
3:D:69:GLU:HG2	3:D:76:LYS:HB2	1.14	1.10
7:a:66:ALA:CB	7:f:118:GLU:HG3	1.81	1.10
7:a:178:PRO:HG2	7:a:181:GLU:HG3	1.26	1.10
7:d:123:VAL:HG23	7:d:128:GLU:O	1.52	1.09
7:d:112:ALA:HB1	7:d:116:VAL:HG11	1.21	1.09
7:d:182:ARG:HD3	7:d:185:ASP:CB	1.80	1.09
1:A:166:ARG:HE	1:A:172:LEU:HD11	1.17	1.09
7:d:153:PRO:HD3	7:e:255:PHE:HE2	0.94	1.09
5:N:-13:DC:H2'	8:M:15:MET:HE1	1.32	1.09
7:b:195:ILE:HA	7:b:206:PHE:CE1	1.86	1.09
7:d:108:GLU:HB3	7:d:111:THR:HG23	1.17	1.09
7:d:176:LEU:HD12	7:d:177:PRO:HD2	1.29	1.09
7:e:86:THR:HG22	8:M:4:GLY:O	1.52	1.09
7:a:91:ARG:HD3	7:a:131:ARG:HH12	1.14	1.08
7:b:32:VAL:CG1	7:b:145:VAL:HG12	1.84	1.08
7:e:61:ILE:HD12	7:e:98:ARG:HG2	1.13	1.08
7:b:77:LEU:CD1	7:b:96:PHE:CD1	2.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:197:MET:HG2	7:b:237:VAL:HG11	1.23	1.08
7:c:99:ALA:HB3	7:c:104:LEU:HD23	1.30	1.08
7:e:39:GLY:HA2	9:e:601:ADP:O2A	1.52	1.08
5:N:-13:DC:C2	8:M:15:MET:CE	2.37	1.07
7:d:78:PHE:CD2	7:d:129:LEU:CD1	2.35	1.07
7:b:152:LEU:HB3	7:b:166:LEU:HD11	1.33	1.07
7:a:111:THR:HG21	7:f:162:ARG:HH22	1.18	1.07
7:f:226:ILE:HG21	9:f:601:ADP:N9	1.67	1.07
8:M:285:TRP:CH2	8:M:355:PHE:HB2	1.88	1.07
7:a:78:PHE:CD1	7:a:129:LEU:HD12	1.90	1.07
7:b:62:SER:CB	7:b:105:PHE:HB3	1.84	1.06
7:b:109:LEU:HD22	7:b:146:CYS:SG	1.94	1.06
7:e:44:LEU:HD11	9:e:601:ADP:H2'	1.20	1.06
7:a:33:LEU:HD12	7:a:34:ILE:N	1.70	1.06
7:d:182:ARG:HH12	7:d:189:MET:CE	1.68	1.06
7:b:49:LEU:CB	7:b:49:LEU:HA	1.77	1.06
7:b:77:LEU:HD11	7:b:96:PHE:CD1	1.90	1.06
7:a:9:LEU:HD23	7:a:9:LEU:H	1.18	1.06
7:f:34:ILE:HB	7:f:147:ALA:HB2	1.28	1.06
7:c:104:LEU:CD2	7:c:142:VAL:HG21	1.84	1.06
7:a:205:LEU:HD12	7:a:206:PHE:H	1.03	1.05
7:d:68:LEU:CD2	7:d:72:LEU:CD2	2.31	1.05
7:d:85:PHE:HB2	8:M:1:MET:HE1	1.11	1.05
7:e:26:ALA:HB1	7:e:53:SER:HB3	1.32	1.05
5:N:-14:DG:H2''	5:N:-13:DC:O5'	1.55	1.05
7:a:63:LEU:HD13	7:a:106:LEU:HD22	1.31	1.05
7:f:50:HIS:CE1	7:f:60:PHE:HB2	1.90	1.05
7:d:112:ALA:HB1	7:d:116:VAL:CG1	1.84	1.05
7:f:235:ARG:NH1	7:f:251:ILE:CG2	2.20	1.05
7:b:187:MET:HE3	7:b:187:MET:HA	1.38	1.05
7:f:235:ARG:NH1	7:f:251:ILE:HG22	1.71	1.05
7:e:44:LEU:HD11	9:e:601:ADP:C2'	1.85	1.05
7:a:72:LEU:HD11	8:M:7:LEU:HD21	1.31	1.04
7:a:111:THR:HG21	7:f:162:ARG:NH2	1.71	1.04
7:f:214:ARG:O	7:f:218:LEU:HG	1.55	1.04
7:c:152:LEU:CD2	7:c:166:LEU:HD12	1.86	1.04
7:a:210:THR:HG21	7:a:248:ASP:HB3	1.39	1.04
7:e:44:LEU:HD12	9:e:601:ADP:H2'	1.40	1.04
8:M:123:TYR:HE1	8:M:186:ASP:HB3	1.18	1.04
7:f:69:ASN:HB2	7:e:74:ASP:OD2	1.56	1.04
7:b:80:HIS:HB3	7:b:132:VAL:HG22	1.05	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:41:GLY:HA3	7:d:176:LEU:HD22	1.08	1.04
7:b:30:LYS:HB2	7:b:171:PHE:HE2	0.91	1.03
7:b:127:GLY:O	7:b:139:GLN:HA	1.55	1.03
7:d:68:LEU:HD13	7:d:72:LEU:HG	1.06	1.03
7:e:109:LEU:CD1	7:e:161:PHE:CE2	2.41	1.03
7:b:207:PRO:HB2	7:b:246:PRO:HA	1.06	1.03
5:N:-8:DT:H5''	7:b:90:LYS:HE3	1.36	1.03
7:a:66:ALA:HB1	7:f:118:GLU:HG3	1.07	1.03
7:b:63:LEU:CD2	7:b:106:LEU:HD23	1.88	1.03
7:d:182:ARG:HD3	7:d:185:ASP:HB3	1.41	1.03
7:d:182:ARG:CD	7:d:185:ASP:HB2	1.89	1.03
2:C:843:THR:HB	8:M:271:TYR:HE1	1.02	1.02
7:c:8:LEU:CD2	7:c:15:PHE:CZ	2.43	1.02
7:d:41:GLY:CA	7:d:176:LEU:HD22	1.88	1.02
8:M:390:LEU:O	8:M:390:LEU:HD23	1.58	1.02
5:N:-8:DT:C5'	7:b:90:LYS:CE	2.38	1.02
7:c:33:LEU:HG	7:c:35:ILE:HD11	1.03	1.02
7:d:41:GLY:CA	7:d:176:LEU:CD2	2.36	1.02
7:d:153:PRO:CD	7:e:255:PHE:HE2	1.72	1.02
7:c:8:LEU:HD22	7:c:44:LEU:CD2	1.88	1.02
7:f:187:MET:SD	7:f:218:LEU:HD21	1.99	1.02
6:T:12:DT:C6	8:M:23:ILE:CD1	2.43	1.02
7:a:193:PHE:HD2	7:a:229:LEU:CD1	1.69	1.02
1:A:315:GLY:HA3	8:M:132:PRO:HG2	1.42	1.01
5:N:-13:DC:H2'	8:M:15:MET:CE	1.89	1.01
7:a:179:LEU:CD2	7:a:226:ILE:CD1	2.32	1.01
8:M:131:THR:HG21	8:M:133:PHE:CZ	1.94	1.01
7:b:48:ARG:O	7:b:52:LEU:HD12	1.60	1.01
7:c:226:ILE:H	7:c:226:ILE:HD12	1.21	1.01
7:f:15:PHE:CE2	7:f:182:ARG:HD2	1.94	1.01
7:e:109:LEU:HD11	7:e:161:PHE:CZ	1.95	1.01
7:b:143:ARG:HG2	7:b:143:ARG:HH11	1.25	1.01
7:c:35:ILE:HD13	7:c:173:VAL:HG23	1.40	1.01
7:c:104:LEU:HD21	7:c:142:VAL:HG21	1.07	1.01
8:M:258:PRO:O	8:M:258:PRO:HG2	1.58	1.01
5:N:-13:DC:C2'	8:M:15:MET:HE1	1.87	1.00
8:M:153:TYR:HD1	8:M:192:ALA:HB3	0.87	1.00
7:c:8:LEU:HG	7:c:15:PHE:CE2	1.96	1.00
7:c:32:VAL:H	7:c:145:VAL:HG12	1.23	1.00
7:c:114:MET:HB3	7:d:67:ALA:HB1	1.41	1.00
7:e:45:ILE:CD1	7:e:176:LEU:HD11	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:-8:DT:H5''	7:b:90:LYS:HE2	1.42	1.00
7:a:179:LEU:HD22	7:a:226:ILE:HD13	1.39	1.00
7:c:224:GLY:HA3	7:c:228:GLU:HB2	1.40	1.00
7:b:30:LYS:CB	7:b:171:PHE:HE2	1.73	1.00
7:b:247:LEU:HD21	7:b:250:ILE:HD11	1.41	1.00
7:f:15:PHE:CE2	7:f:182:ARG:CD	2.45	1.00
2:C:1259:LEU:HD21	8:M:115:GLU:HG2	1.40	1.00
7:c:8:LEU:HG	7:c:15:PHE:HE2	1.26	1.00
7:c:32:VAL:HG22	7:c:145:VAL:CB	1.92	1.00
7:d:68:LEU:CD1	7:d:72:LEU:HG	1.90	1.00
7:a:64:ASN:HB3	7:a:67:ALA:HB3	1.40	0.99
7:b:38:ARG:HD2	7:b:224:GLY:HA3	1.00	0.99
7:f:12:ALA:HB2	7:f:185:ASP:CG	1.86	0.99
7:b:59:PRO:HD2	7:b:102:GLY:HA3	1.42	0.99
7:e:213:ALA:O	7:e:217:LEU:HG	1.61	0.99
7:b:25:LEU:CD2	7:c:238:TYR:CE2	2.45	0.99
7:c:99:ALA:HB1	7:c:104:LEU:HD23	1.44	0.99
7:d:104:LEU:HD13	7:d:142:VAL:HG11	1.00	0.99
7:b:201:ILE:HG23	7:b:203:LEU:HD23	1.42	0.99
8:M:195:LEU:CD1	8:M:199:LEU:HD11	1.92	0.99
7:f:63:LEU:HD11	7:f:106:LEU:HD23	0.99	0.99
7:c:55:ARG:HA	7:c:143:ARG:NH1	1.78	0.99
6:T:31:DG:C3'	8:M:233:ARG:NH2	2.25	0.99
7:f:50:HIS:ND1	7:f:60:PHE:CD1	2.30	0.99
7:a:66:ALA:HB1	7:f:118:GLU:CG	1.93	0.98
7:a:119:LYS:HE3	7:b:67:ALA:HA	1.45	0.98
7:d:40:THR:HG22	7:d:225:ASN:HB2	1.41	0.98
7:a:96:PHE:HZ	7:a:120:LEU:HD11	1.26	0.98
7:b:12:ALA:HB3	7:b:15:PHE:H	1.24	0.98
7:b:38:ARG:CD	7:b:224:GLY:HA3	1.93	0.98
7:d:104:LEU:HD13	7:d:142:VAL:CG1	1.93	0.98
7:b:65:CYS:SG	7:b:112:ALA:HB2	2.03	0.98
6:T:12:DT:H6	8:M:23:ILE:CD1	1.75	0.98
8:M:258:PRO:O	8:M:258:PRO:CG	2.05	0.98
1:A:166:ARG:NE	1:A:172:LEU:HD11	1.78	0.98
7:a:19:LEU:HD22	7:a:48:ARG:NH1	1.77	0.98
7:c:35:ILE:HD13	7:c:173:VAL:CG2	1.92	0.98
7:f:196:GLN:HA	7:f:199:ARG:CD	1.93	0.98
7:c:61:ILE:HG21	7:c:99:ALA:CB	1.90	0.98
7:f:63:LEU:CD1	7:f:106:LEU:HD23	1.94	0.98
7:a:179:LEU:HD23	7:a:225:ASN:C	1.89	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:82:ALA:HB2	7:f:90:LYS:HA	1.00	0.97
7:a:8:LEU:HG	7:a:15:PHE:HZ	1.29	0.97
7:e:63:LEU:HD23	7:e:95:ARG:CD	1.93	0.97
7:e:81:GLU:HG2	7:e:91:ARG:NH2	1.78	0.97
7:a:64:ASN:HB3	7:a:67:ALA:CB	1.94	0.97
7:d:182:ARG:HH12	7:d:189:MET:HE2	1.28	0.97
7:b:168:ARG:NH1	7:c:227:ARG:HH12	1.61	0.97
7:b:195:ILE:CA	7:b:206:PHE:CZ	2.48	0.97
7:d:104:LEU:CD1	7:d:142:VAL:HG11	1.93	0.97
8:M:195:LEU:HD11	8:M:199:LEU:HD11	0.99	0.97
7:a:19:LEU:HD22	7:a:48:ARG:HH11	1.27	0.97
7:b:121:LEU:O	7:b:122:ARG:CG	2.11	0.97
8:M:279:ARG:HH21	8:M:279:ARG:HG3	1.28	0.97
6:T:23:DT:OP2	8:M:457:THR:HG21	1.63	0.97
5:N:-13:DC:N1	8:M:15:MET:HE1	1.80	0.96
8:M:154:LEU:HD11	8:M:193:LYS:HB2	1.44	0.96
8:M:278:VAL:HG23	8:M:278:VAL:O	1.65	0.96
7:b:80:HIS:CB	7:b:132:VAL:CG2	2.43	0.96
7:c:8:LEU:HD21	7:c:15:PHE:HZ	1.21	0.96
7:a:205:LEU:HD12	7:a:206:PHE:N	1.79	0.96
7:a:221:ARG:C	7:a:221:ARG:HA	1.91	0.96
7:b:8:LEU:CD1	7:b:19:LEU:CD2	2.39	0.96
7:f:82:ALA:CB	7:f:90:LYS:HA	1.94	0.96
7:f:226:ILE:HG13	9:f:601:ADP:N7	1.80	0.96
8:M:123:TYR:CE1	8:M:186:ASP:HB3	1.99	0.96
7:a:66:ALA:O	7:f:119:LYS:HE2	1.65	0.96
7:c:8:LEU:CG	7:c:15:PHE:CE2	2.49	0.96
7:c:61:ILE:HG21	7:c:99:ALA:HB2	0.96	0.96
7:d:83:GLY:HA3	7:e:89:GLN:HE22	1.28	0.96
7:d:182:ARG:NH1	7:d:189:MET:CE	2.28	0.96
7:d:85:PHE:HB3	8:M:1:MET:HE1	1.26	0.96
8:M:182:ILE:HD13	8:M:185:PHE:HE2	1.31	0.96
7:c:33:LEU:CG	7:c:35:ILE:HD11	1.96	0.95
7:d:176:LEU:CD1	7:d:177:PRO:HD2	1.96	0.95
7:b:38:ARG:HD2	7:b:224:GLY:CA	1.95	0.95
7:c:8:LEU:HD22	7:c:44:LEU:HD21	1.49	0.95
7:b:34:ILE:HG21	7:b:42:LYS:HG3	1.48	0.95
7:a:193:PHE:HE2	7:a:229:LEU:HD11	1.29	0.95
7:b:63:LEU:HD21	7:b:106:LEU:HD23	1.48	0.95
7:d:98:ARG:HB2	7:d:98:ARG:NH2	1.81	0.95
7:e:44:LEU:CD1	9:e:601:ADP:C2'	2.43	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:8:LEU:CD1	7:c:15:PHE:CZ	2.49	0.95
7:a:226:ILE:HG21	9:a:601:ADP:C4	2.00	0.95
7:c:39:GLY:HA2	9:c:400:ADP:O1A	1.65	0.95
8:M:197:ASP:O	8:M:201:ILE:HD13	1.64	0.95
7:d:108:GLU:HB3	7:d:111:THR:CG2	1.96	0.95
7:a:92:HIS:HE1	7:f:133:GLY:O	1.50	0.94
7:f:105:PHE:HA	7:f:145:VAL:O	1.65	0.94
7:d:182:ARG:HG2	7:d:185:ASP:HB2	1.46	0.94
8:M:158:ILE:CG2	8:M:158:ILE:O	2.13	0.94
8:M:196:ARG:HG3	8:M:197:ASP:N	1.82	0.94
7:a:86:THR:CG2	8:M:8:ARG:HB2	1.97	0.94
7:b:33:LEU:CD1	7:b:146:CYS:HB3	1.97	0.94
5:N:-13:DC:N1	8:M:15:MET:CE	2.31	0.94
3:D:69:GLU:HG2	3:D:76:LYS:CB	1.98	0.94
7:a:72:LEU:HD13	8:M:7:LEU:HD21	1.47	0.94
7:d:78:PHE:HD2	7:d:129:LEU:HD21	1.33	0.94
7:f:103:THR:HG22	7:f:143:ARG:CG	1.98	0.94
7:a:78:PHE:O	7:a:94:GLY:HA3	1.67	0.94
7:e:31:PRO:O	7:e:171:PHE:HB3	1.68	0.94
7:e:189:MET:HE1	7:e:226:ILE:HG12	1.49	0.93
5:N:-8:DT:C5'	7:b:90:LYS:HE2	1.95	0.93
7:b:207:PRO:HB2	7:b:246:PRO:CA	1.97	0.93
7:f:196:GLN:O	7:f:199:ARG:HG2	1.67	0.93
7:e:63:LEU:HD23	7:e:95:ARG:HD2	1.49	0.93
7:a:96:PHE:CZ	7:a:120:LEU:HD11	2.03	0.93
7:b:25:LEU:HD23	7:c:238:TYR:CE2	2.01	0.93
7:c:49:LEU:HD12	7:c:105:PHE:HZ	1.30	0.93
7:a:96:PHE:CD2	7:a:123:VAL:CG1	2.50	0.93
8:M:274:PRO:HB3	8:M:391:HIS:HB2	1.51	0.93
7:b:8:LEU:HD11	7:b:19:LEU:HD22	0.96	0.93
7:b:247:LEU:CD2	7:b:250:ILE:HD11	1.98	0.93
6:T:31:DG:C3'	8:M:233:ARG:HH22	1.80	0.93
7:b:197:MET:HG2	7:b:237:VAL:CG1	1.98	0.93
7:a:193:PHE:CE2	7:a:229:LEU:CD1	2.48	0.93
7:c:32:VAL:N	7:c:145:VAL:HG12	1.84	0.93
7:e:109:LEU:HD13	7:e:161:PHE:HE2	1.32	0.93
8:M:182:ILE:HD13	8:M:185:PHE:CE2	2.03	0.93
7:f:238:TYR:CE2	7:e:28:LEU:HD11	2.04	0.92
2:C:905:ILE:HD11	8:M:224:LEU:HD11	1.50	0.92
7:b:63:LEU:HB2	7:b:95:ARG:NH2	1.85	0.92
7:b:31:PRO:HB2	7:b:170:ALA:H	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:24:HIS:HB2	7:e:238:TYR:OH	1.69	0.92
7:e:91:ARG:HH21	7:e:91:ARG:HG3	1.33	0.92
8:M:259:ARG:HH11	8:M:259:ARG:HG3	1.29	0.92
7:b:222:TRP:HZ3	7:b:229:LEU:HA	1.35	0.92
5:N:-13:DC:O2	8:M:15:MET:HE2	1.70	0.92
5:N:-27:DT:H73	8:M:455:ARG:HH22	1.18	0.92
7:d:116:VAL:O	7:d:120:LEU:HD23	1.69	0.92
7:b:32:VAL:HG13	7:b:145:VAL:HG12	1.50	0.92
7:c:230:LYS:HA	7:c:233:VAL:CG1	1.99	0.92
7:f:179:LEU:HD11	7:f:186:ILE:CD1	1.99	0.92
7:f:226:ILE:CG2	9:f:601:ADP:H1'	2.00	0.92
2:C:843:THR:CB	8:M:271:TYR:HE1	1.83	0.91
7:c:61:ILE:HG22	7:c:99:ALA:CB	1.97	0.91
7:f:47:SER:O	7:f:51:TYR:CE1	2.23	0.91
7:e:26:ALA:CB	7:e:53:SER:HB3	1.99	0.91
7:e:45:ILE:HD11	7:e:176:LEU:HD11	1.49	0.91
5:N:-27:DT:H73	8:M:455:ARG:CZ	1.99	0.91
7:c:9:LEU:HD12	7:c:189:MET:CE	2.00	0.91
7:c:35:ILE:CD1	7:c:173:VAL:HG23	2.00	0.91
7:d:61:ILE:HD11	7:d:95:ARG:CZ	2.00	0.91
7:f:65:CYS:HB3	7:f:112:ALA:HB2	1.53	0.91
7:e:26:ALA:HB1	7:e:53:SER:N	1.85	0.91
7:e:63:LEU:HB3	7:e:95:ARG:HH21	1.34	0.91
7:a:96:PHE:CG	7:a:123:VAL:HG11	2.06	0.91
7:c:32:VAL:CG2	7:c:145:VAL:CG1	2.43	0.91
7:d:108:GLU:CB	7:d:111:THR:HG23	2.00	0.91
7:a:63:LEU:HD13	7:a:106:LEU:CD2	1.99	0.91
7:a:118:GLU:O	7:a:121:LEU:HB2	1.68	0.91
7:e:90:LYS:H	7:e:90:LYS:HD3	1.33	0.91
7:d:78:PHE:HD2	7:d:129:LEU:CD2	1.83	0.91
7:a:70:GLU:HA	7:a:73:LEU:HD23	1.49	0.91
7:f:15:PHE:HD2	7:f:182:ARG:HD2	1.36	0.91
7:b:50:HIS:HD2	7:b:51:TYR:CD1	1.89	0.91
7:d:80:HIS:NE2	8:M:1:MET:SD	2.44	0.91
7:f:5:LYS:HZ3	7:f:5:LYS:HB2	1.36	0.91
7:c:33:LEU:HG	7:c:35:ILE:CD1	1.97	0.90
7:e:187:MET:O	7:e:190:ALA:HB3	1.71	0.90
7:c:99:ALA:CB	7:c:104:LEU:CD2	2.49	0.90
7:f:34:ILE:CB	7:f:147:ALA:HB2	2.00	0.90
2:C:1306:LYS:HA	8:M:130:LEU:HD21	1.53	0.90
7:c:8:LEU:HD21	7:c:15:PHE:CE2	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:187:MET:O	7:c:190:ALA:HB3	1.70	0.90
8:M:195:LEU:CD1	8:M:199:LEU:CD1	2.48	0.90
7:b:117:GLN:NE2	7:b:161:PHE:HD1	1.67	0.90
7:f:33:LEU:HB3	7:f:173:VAL:HG12	1.53	0.90
7:e:105:PHE:HA	7:e:145:VAL:CG2	2.00	0.90
7:b:79:GLY:O	7:b:131:ARG:HB3	1.72	0.90
7:e:146:CYS:SG	7:e:169:LEU:CD1	2.58	0.90
8:M:131:THR:CG2	8:M:133:PHE:CZ	2.55	0.90
8:M:213:LEU:HD12	8:M:217:ARG:NH2	1.86	0.90
8:M:276:VAL:HB	8:M:390:LEU:HB2	1.52	0.90
5:N:-27:DT:C7	8:M:455:ARG:NH1	2.35	0.90
7:c:152:LEU:HD23	7:c:166:LEU:CD1	2.02	0.90
7:d:182:ARG:NH1	7:d:189:MET:HE2	1.86	0.90
7:f:34:ILE:HB	7:f:147:ALA:HB1	1.54	0.90
7:a:55:ARG:HH21	7:a:55:ARG:HG3	1.36	0.89
7:c:104:LEU:CD1	7:c:144:LEU:HB3	2.02	0.89
7:b:247:LEU:HD21	7:b:250:ILE:CD1	2.03	0.89
7:e:109:LEU:CD1	7:e:161:PHE:HE2	1.82	0.89
8:M:153:TYR:HD1	8:M:192:ALA:CB	1.82	0.89
7:a:179:LEU:HD21	7:a:226:ILE:HD13	0.91	0.89
7:d:182:ARG:CD	7:d:185:ASP:CB	2.47	0.89
7:a:205:LEU:CD1	7:a:206:PHE:H	1.86	0.89
7:c:114:MET:HE2	7:d:65:CYS:SG	2.11	0.89
7:e:30:LYS:NZ	7:e:171:PHE:HE2	1.71	0.89
8:M:46:LEU:HD11	8:M:322:ASN:HB3	1.55	0.89
8:M:118:GLN:O	8:M:122:ASP:HB2	1.73	0.89
7:a:8:LEU:HG	7:a:15:PHE:CZ	2.06	0.89
7:a:8:LEU:CG	7:a:15:PHE:HZ	1.85	0.89
7:b:46:ALA:HB2	7:b:105:PHE:HE2	1.38	0.89
5:N:-27:DT:C7	8:M:455:ARG:CZ	2.51	0.89
7:b:48:ARG:O	7:b:52:LEU:CD1	2.21	0.89
7:c:8:LEU:CD2	7:c:15:PHE:HZ	1.85	0.89
7:d:99:ALA:HB3	7:d:104:LEU:HD11	1.55	0.89
7:a:180:ARG:HH12	7:a:221:ARG:HD3	1.30	0.88
7:b:30:LYS:CB	7:b:171:PHE:CE2	2.52	0.88
7:b:194:ALA:C	7:b:206:PHE:HZ	1.82	0.88
7:e:30:LYS:HZ3	7:e:171:PHE:HE2	0.93	0.88
7:c:9:LEU:HD12	7:c:189:MET:HE2	1.51	0.88
7:c:104:LEU:HD21	7:c:142:VAL:CG2	2.00	0.88
7:d:98:ARG:HB2	7:d:98:ARG:HH21	1.37	0.88
7:e:81:GLU:HG2	7:e:91:ARG:HH22	1.33	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:173:VAL:HG23	7:d:173:VAL:O	1.74	0.88
7:f:255:PHE:CZ	7:e:153:PRO:HD3	2.09	0.88
9:f:601:ADP:O2A	9:f:601:ADP:O2B	1.90	0.88
7:b:36:GLY:O	7:b:149:ASN:HA	1.74	0.88
7:c:230:LYS:O	7:c:233:VAL:HG13	1.72	0.88
7:b:77:LEU:CD1	7:b:96:PHE:CE1	2.51	0.88
7:f:61:ILE:O	7:f:104:LEU:HD12	1.72	0.88
7:f:226:ILE:CG2	9:f:601:ADP:C8	2.57	0.88
7:c:37:GLU:O	7:c:40:THR:HG22	1.73	0.88
7:c:152:LEU:CG	7:c:166:LEU:CD1	2.51	0.88
7:a:38:ARG:HH21	7:f:164:ASP:HB3	1.38	0.87
7:b:222:TRP:CZ3	7:b:229:LEU:HA	2.10	0.87
6:T:12:DT:H72	8:M:22:ALA:O	1.75	0.87
8:M:200:LEU:HD13	8:M:200:LEU:C	1.99	0.87
6:T:31:DG:H3'	8:M:233:ARG:HH22	1.05	0.87
7:a:178:PRO:HG2	7:a:181:GLU:CG	2.03	0.87
8:M:336:ARG:NH1	8:M:388:LYS:NZ	2.22	0.87
8:M:343:VAL:O	8:M:347:ILE:HG22	1.72	0.87
7:b:195:ILE:HA	7:b:206:PHE:HZ	1.34	0.87
7:d:40:THR:HA	7:d:225:ASN:HB3	1.57	0.87
7:f:179:LEU:HD11	7:f:186:ILE:HD13	1.56	0.87
7:d:68:LEU:HD13	7:d:72:LEU:CG	2.01	0.87
7:d:128:GLU:HA	7:d:138:LEU:O	1.74	0.87
7:d:182:ARG:CG	7:d:185:ASP:CB	2.52	0.87
8:M:455:ARG:HD2	8:M:455:ARG:C	1.99	0.87
7:a:222:TRP:CE3	7:a:228:GLU:CG	2.58	0.87
7:b:80:HIS:CB	7:b:132:VAL:HG22	2.01	0.87
7:c:32:VAL:H	7:c:145:VAL:CG1	1.88	0.87
7:d:182:ARG:HD3	7:d:185:ASP:HB2	1.51	0.87
7:e:121:LEU:HD21	7:e:168:ARG:HH21	1.38	0.87
5:N:-11:DA:H1'	5:N:-10:DG:O4'	1.75	0.86
7:a:222:TRP:CZ3	7:a:228:GLU:HG3	2.09	0.86
8:M:154:LEU:HD11	8:M:193:LYS:CB	2.04	0.86
7:c:8:LEU:CD2	7:c:15:PHE:CE2	2.58	0.86
7:a:240:HIS:ND1	7:a:247:LEU:CB	2.37	0.86
7:a:130:GLU:OE2	7:a:130:GLU:N	2.08	0.86
7:a:222:TRP:HE3	7:a:228:GLU:CG	1.88	0.86
7:e:62:SER:N	7:e:62:SER:HA	1.90	0.86
7:a:240:HIS:CE1	7:a:247:LEU:HB3	2.11	0.86
7:b:197:MET:CG	7:b:237:VAL:CG1	2.54	0.86
7:f:5:LYS:O	7:f:5:LYS:NZ	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:96:PHE:CE2	7:a:123:VAL:CG1	2.57	0.86
7:a:204:PRO:HG2	7:a:205:LEU:H	1.40	0.86
7:e:86:THR:CG2	8:M:4:GLY:O	2.22	0.86
7:b:25:LEU:HG	7:c:238:TYR:OH	1.75	0.86
7:b:77:LEU:HD11	7:b:96:PHE:HE1	1.39	0.86
7:b:194:ALA:C	7:b:206:PHE:CZ	2.53	0.86
7:c:152:LEU:HG	7:c:166:LEU:CD1	2.03	0.86
7:d:10:GLY:HA3	7:d:15:PHE:CD2	2.10	0.86
7:d:41:GLY:N	7:d:176:LEU:HD21	1.91	0.86
8:M:392:SER:HB2	8:M:393:PRO:HD2	1.57	0.86
7:d:176:LEU:HD12	7:d:177:PRO:CD	2.05	0.85
7:f:20:GLU:O	7:f:24:HIS:HD2	1.59	0.85
7:f:59:PRO:O	7:f:102:GLY:HA3	1.76	0.85
8:M:18:GLN:HE22	8:M:328:TRP:NE1	1.73	0.85
8:M:26:LEU:HB3	8:M:336:ARG:HG2	1.56	0.85
7:d:50:HIS:CD2	7:d:60:PHE:HB2	2.11	0.85
7:b:207:PRO:CB	7:b:246:PRO:HA	2.01	0.85
7:e:61:ILE:HD12	7:e:98:ARG:CG	2.04	0.85
8:M:158:ILE:O	8:M:158:ILE:HG22	1.67	0.85
7:a:86:THR:HG21	8:M:8:ARG:HB2	1.59	0.85
8:M:141:ALA:O	8:M:145:VAL:HG12	1.76	0.85
7:d:78:PHE:CZ	7:d:119:LYS:CG	2.58	0.85
7:a:180:ARG:NH1	7:a:221:ARG:CD	2.40	0.85
7:c:60:PHE:HA	7:c:103:THR:O	1.75	0.85
7:c:99:ALA:HB1	7:c:104:LEU:CD2	2.07	0.85
7:a:108:GLU:OE2	7:f:121:LEU:HD11	1.77	0.85
7:b:195:ILE:CA	7:b:206:PHE:HZ	1.86	0.85
7:e:33:LEU:HD12	7:e:34:ILE:N	1.91	0.85
7:b:63:LEU:HD23	7:b:63:LEU:O	1.77	0.84
5:N:-27:DT:C7	8:M:455:ARG:NH2	2.36	0.84
7:a:99:ALA:O	7:a:142:VAL:HB	1.77	0.84
7:a:120:LEU:HG	7:a:124:ILE:HD11	1.57	0.84
7:a:250:ILE:H	7:a:250:ILE:HD13	1.42	0.84
7:b:62:SER:HB3	7:b:105:PHE:CB	2.05	0.84
7:b:234:GLU:O	7:b:237:VAL:HG12	1.77	0.84
7:a:65:CYS:SG	7:a:65:CYS:CA	2.65	0.84
7:d:78:PHE:CE2	7:d:129:LEU:HD11	2.13	0.84
5:N:-27:DT:C5	8:M:455:ARG:NH1	2.45	0.84
7:b:197:MET:HG3	7:b:237:VAL:HG11	1.58	0.84
7:e:43:GLU:OE1	7:e:105:PHE:CE2	2.29	0.84
7:d:78:PHE:HD2	7:d:129:LEU:HD11	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:26:ALA:O	7:f:53:SER:HA	1.77	0.84
7:c:32:VAL:HG22	7:c:145:VAL:HG11	0.86	0.84
7:c:164:ASP:OD1	7:c:164:ASP:N	2.11	0.84
7:a:96:PHE:CZ	7:a:120:LEU:CD1	2.60	0.84
7:c:32:VAL:CG2	7:c:145:VAL:CB	2.56	0.84
7:c:152:LEU:HD23	7:c:166:LEU:CG	2.07	0.84
7:f:196:GLN:OE1	7:f:199:ARG:HD3	1.77	0.84
8:M:357:GLN:HB3	8:M:361:TYR:HB2	1.59	0.84
7:f:226:ILE:HG21	9:f:601:ADP:C1'	2.08	0.84
7:a:22:VAL:CG2	7:a:49:LEU:HD21	2.05	0.83
7:b:240:HIS:CE1	7:b:242:THR:HG23	2.12	0.83
7:c:152:LEU:HD23	7:c:166:LEU:HG	1.58	0.83
7:e:18:VAL:O	7:e:22:VAL:HG12	1.78	0.83
7:b:109:LEU:CD2	7:b:146:CYS:SG	2.65	0.83
7:d:179:LEU:C	7:d:179:LEU:HD13	2.02	0.83
7:d:182:ARG:NH1	7:d:189:MET:HE3	1.94	0.83
2:C:1258:PRO:HG2	3:D:346:ARG:HB3	1.60	0.83
7:a:211:GLU:CD	7:a:212:ARG:H	1.86	0.83
7:b:140:VAL:HG23	7:b:140:VAL:O	1.79	0.83
7:c:55:ARG:HA	7:c:143:ARG:HH12	1.42	0.83
7:d:121:LEU:HD12	7:d:121:LEU:O	1.79	0.83
8:M:358:GLY:HA2	8:M:394:ARG:HH12	1.43	0.83
7:a:34:ILE:HB	7:a:147:ALA:HB1	1.58	0.83
7:f:68:LEU:HD23	7:f:68:LEU:O	1.77	0.83
7:f:238:TYR:HD2	7:e:28:LEU:HD11	1.43	0.83
7:e:179:LEU:CD1	7:e:225:ASN:O	2.25	0.83
7:f:30:LYS:HB2	7:f:171:PHE:CE2	2.14	0.83
7:e:8:LEU:HD13	7:e:48:ARG:NH1	1.93	0.83
7:e:22:VAL:HA	7:e:25:LEU:HD12	1.61	0.83
7:d:161:PHE:HD2	7:d:166:LEU:HB2	1.43	0.83
7:e:223:PRO:HD2	7:e:228:GLU:OE1	1.77	0.83
7:e:105:PHE:HE1	7:e:107:ASP:HB2	1.39	0.83
7:a:22:VAL:HG22	7:a:49:LEU:CD2	2.04	0.83
7:b:143:ARG:HG2	7:b:143:ARG:NH1	1.94	0.83
7:b:226:ILE:HG21	9:b:601:ADP:C8	2.13	0.83
7:d:83:GLY:HA3	7:e:89:GLN:NE2	1.94	0.83
7:f:12:ALA:HB2	7:f:185:ASP:OD2	1.78	0.83
2:C:844:LYS:CB	8:M:272:VAL:HG13	2.09	0.82
7:a:65:CYS:SG	7:a:65:CYS:HA	2.19	0.82
7:b:168:ARG:HH12	7:c:227:ARG:HH12	1.22	0.82
7:e:74:ASP:HB2	7:e:119:LYS:NZ	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:-11:DA:H2''	5:N:-10:DG:C8	2.13	0.82
7:c:121:LEU:CD2	7:c:162:ARG:HD3	2.08	0.82
7:d:68:LEU:HD22	7:d:72:LEU:HD21	1.59	0.82
7:d:179:LEU:HD13	7:d:179:LEU:O	1.79	0.82
2:C:1254:VAL:HB	8:M:111:VAL:HB	1.60	0.82
7:b:143:ARG:NH1	7:b:143:ARG:CG	2.42	0.82
7:d:78:PHE:CD2	7:d:129:LEU:HD21	2.13	0.82
7:f:179:LEU:CD1	7:f:186:ILE:HD11	2.08	0.82
7:a:240:HIS:HE1	7:a:247:LEU:N	1.76	0.82
7:b:25:LEU:HD21	7:c:238:TYR:CE2	2.15	0.82
7:b:42:LYS:HD3	7:b:147:ALA:HB1	1.59	0.82
7:a:92:HIS:CE1	7:f:133:GLY:O	2.32	0.82
7:a:129:LEU:O	7:a:138:LEU:HD21	1.78	0.82
7:d:117:GLN:HB3	7:d:165:LEU:HD23	1.59	0.82
7:f:197:MET:HG2	7:f:237:VAL:HG11	1.61	0.82
8:M:259:ARG:HG3	8:M:259:ARG:NH1	1.90	0.82
7:a:78:PHE:CD1	7:a:129:LEU:CD1	2.63	0.82
7:a:251:ILE:H	7:a:251:ILE:HD13	1.44	0.82
7:e:63:LEU:HB3	7:e:95:ARG:NH2	1.95	0.82
7:b:210:THR:HG23	7:b:247:LEU:O	1.77	0.82
7:e:78:PHE:HE1	7:e:123:VAL:CG2	1.93	0.82
8:M:41:LEU:O	8:M:41:LEU:HD12	1.79	0.82
7:a:42:LYS:CD	9:a:601:ADP:O3B	2.23	0.81
7:b:65:CYS:SG	7:b:112:ALA:CB	2.68	0.81
7:a:96:PHE:HZ	7:a:120:LEU:CD1	1.93	0.81
7:b:195:ILE:HD13	7:b:206:PHE:CZ	2.16	0.81
7:c:49:LEU:HD12	7:c:105:PHE:CZ	2.14	0.81
7:a:221:ARG:O	7:a:221:ARG:HD2	1.79	0.81
7:b:152:LEU:CB	7:b:166:LEU:HD11	2.10	0.81
7:c:99:ALA:HB3	7:c:104:LEU:CD2	2.10	0.81
7:c:136:GLN:NE2	7:c:136:GLN:H	1.78	0.81
7:f:197:MET:HG2	7:f:237:VAL:CG1	2.10	0.81
8:M:420:ILE:CD1	8:M:451:ILE:HG21	2.10	0.81
7:b:14:SER:O	7:b:18:VAL:HG23	1.81	0.81
7:f:226:ILE:HG21	9:f:601:ADP:H1'	1.60	0.81
7:e:124:ILE:CG1	7:e:144:LEU:HD12	2.06	0.81
8:M:182:ILE:CG2	8:M:185:PHE:CD2	2.62	0.81
2:C:870:ILE:HG12	2:C:944:ARG:HH22	1.45	0.81
7:d:112:ALA:CB	7:d:116:VAL:HG11	2.07	0.81
7:c:21:GLN:NE2	7:c:174:VAL:HG22	1.95	0.81
7:f:196:GLN:HA	7:f:199:ARG:HD3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:222:TRP:N	7:f:223:PRO:CD	2.42	0.81
8:M:25:LEU:O	8:M:25:LEU:HD13	1.80	0.81
7:b:117:GLN:NE2	7:b:161:PHE:CD1	2.49	0.81
7:c:106:LEU:O	7:c:109:LEU:HD21	1.80	0.81
5:N:-8:DT:H5"	7:b:90:LYS:NZ	1.96	0.81
7:c:8:LEU:CG	7:c:15:PHE:CZ	2.64	0.81
8:M:420:ILE:HD11	8:M:451:ILE:CG2	2.11	0.81
7:f:12:ALA:HB2	7:f:185:ASP:OD1	1.79	0.80
7:b:195:ILE:HD13	7:b:206:PHE:CE1	2.16	0.80
7:b:198:CYS:SG	7:b:206:PHE:CE1	2.71	0.80
8:M:213:LEU:HD12	8:M:217:ARG:HH21	1.45	0.80
8:M:370:ILE:HD13	8:M:381:ILE:HD13	1.63	0.80
3:D:69:GLU:CG	3:D:76:LYS:HB2	2.07	0.80
7:e:105:PHE:CE1	7:e:107:ASP:HB2	2.16	0.80
7:f:47:SER:O	7:f:51:TYR:CD1	2.35	0.80
7:f:49:LEU:O	7:f:49:LEU:HD23	1.81	0.80
7:f:201:ILE:HG21	7:e:28:LEU:HD21	1.62	0.80
7:a:72:LEU:CD1	8:M:7:LEU:CD2	2.51	0.80
7:c:114:MET:CE	7:d:65:CYS:SG	2.69	0.80
7:f:15:PHE:HE2	7:f:182:ARG:HD3	1.44	0.80
7:e:90:LYS:HD3	7:e:90:LYS:N	1.95	0.80
8:M:390:LEU:O	8:M:390:LEU:CD2	2.29	0.80
1:A:305:ASP:CG	8:M:180:LYS:HE2	2.07	0.80
5:N:-12:DC:N3	8:M:20:GLN:NE2	2.29	0.80
7:a:43:GLU:HG2	7:f:126:TYR:OH	1.81	0.79
7:b:46:ALA:CB	7:b:105:PHE:CE2	2.65	0.79
7:b:249:ASP:O	7:b:250:ILE:HD13	1.82	0.79
7:c:152:LEU:CD2	7:c:166:LEU:CD1	2.60	0.79
8:M:158:ILE:HD11	8:M:193:LYS:CD	2.13	0.79
7:a:20:GLU:O	7:a:24:HIS:HD2	1.64	0.79
7:b:187:MET:HE2	7:b:214:ARG:NH1	1.95	0.79
7:e:22:VAL:HA	7:e:25:LEU:CD1	2.13	0.79
7:e:109:LEU:HD11	7:e:161:PHE:CE2	2.12	0.79
8:M:19:LEU:HD23	8:M:19:LEU:O	1.81	0.79
8:M:258:PRO:O	8:M:259:ARG:CB	2.27	0.79
7:a:34:ILE:HB	7:a:147:ALA:CB	2.12	0.79
7:a:256:LYS:HA	7:a:256:LYS:HE3	1.62	0.79
7:b:239:ARG:HH11	7:b:239:ARG:HG2	1.46	0.79
7:c:230:LYS:HA	7:c:233:VAL:HG12	1.62	0.79
7:d:61:ILE:HD13	7:d:95:ARG:HD2	1.64	0.79
7:f:20:GLU:O	7:f:24:HIS:CD2	2.35	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:844:LYS:HB2	8:M:272:VAL:CG1	2.09	0.79
7:a:175:GLN:OE1	7:a:175:GLN:N	2.16	0.79
7:d:68:LEU:HD22	7:d:72:LEU:HD23	0.79	0.79
7:d:79:GLY:HA3	7:d:92:HIS:HD2	1.48	0.79
7:a:38:ARG:HH11	7:a:224:GLY:HA2	1.47	0.79
7:b:12:ALA:HB3	7:b:15:PHE:N	1.97	0.79
7:c:165:LEU:O	7:c:165:LEU:HD23	1.81	0.79
7:d:121:LEU:HD22	7:d:165:LEU:CA	2.12	0.79
7:f:227:ARG:HH12	7:e:168:ARG:CZ	1.95	0.79
8:M:13:LEU:O	8:M:13:LEU:HD13	1.82	0.79
7:d:100:ASP:OD1	7:d:140:VAL:HB	1.83	0.79
7:f:5:LYS:HB2	7:f:5:LYS:NZ	1.98	0.79
7:f:61:ILE:CD1	7:f:98:ARG:HH21	1.94	0.79
7:f:94:GLY:O	7:f:98:ARG:HG3	1.83	0.79
8:M:153:TYR:CD1	8:M:192:ALA:CB	2.63	0.79
8:M:196:ARG:HG3	8:M:197:ASP:H	1.45	0.79
7:a:210:THR:OG1	7:a:248:ASP:HA	1.83	0.79
7:c:222:TRP:CZ3	7:c:229:LEU:HA	2.17	0.79
7:b:81:GLU:HG3	7:b:131:ARG:HD2	1.64	0.79
7:b:34:ILE:CG2	7:b:42:LYS:HG3	2.13	0.78
7:d:121:LEU:HD22	7:d:165:LEU:HA	1.64	0.78
7:f:235:ARG:HH11	7:f:251:ILE:CG2	1.93	0.78
7:e:104:LEU:HD21	7:e:144:LEU:HD23	0.84	0.78
7:b:31:PRO:O	7:b:170:ALA:HA	1.83	0.78
7:d:179:LEU:HB2	7:d:225:ASN:HA	1.64	0.78
8:M:420:ILE:HD11	8:M:451:ILE:HG21	1.64	0.78
7:a:55:ARG:C	7:a:57:GLN:H	1.88	0.78
7:e:45:ILE:HD11	7:e:176:LEU:CD1	2.12	0.78
7:c:8:LEU:HB2	7:c:44:LEU:HD21	1.66	0.78
7:c:114:MET:HB3	7:d:67:ALA:CB	2.13	0.78
7:d:161:PHE:CD2	7:d:166:LEU:HB2	2.18	0.78
8:M:11:GLN:OE1	8:M:11:GLN:HA	1.84	0.78
7:c:8:LEU:CG	7:c:15:PHE:HE2	1.94	0.78
7:a:193:PHE:CD2	7:a:229:LEU:HD12	2.19	0.78
7:e:33:LEU:HD12	7:e:34:ILE:H	1.46	0.78
5:N:-13:DC:C1'	8:M:15:MET:CE	2.60	0.78
7:f:73:LEU:HD11	7:f:116:VAL:HG22	1.63	0.78
7:e:45:ILE:HD13	7:e:176:LEU:HD11	1.64	0.78
7:a:30:LYS:N	7:a:30:LYS:HD2	1.98	0.78
7:b:187:MET:HA	7:b:187:MET:CE	2.14	0.78
7:a:34:ILE:HD12	7:a:147:ALA:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:213:LEU:CD1	8:M:217:ARG:HH21	1.97	0.77
8:M:336:ARG:HH11	8:M:388:LYS:HZ1	1.31	0.77
8:M:367:LEU:CD2	8:M:403:PHE:CE2	2.66	0.77
7:a:86:THR:CG2	7:f:86:THR:OG1	2.32	0.77
7:c:114:MET:CB	7:d:67:ALA:HB1	2.12	0.77
7:f:34:ILE:CG1	7:f:147:ALA:HB2	2.14	0.77
2:C:1252:SER:HA	8:M:114:GLY:O	1.83	0.77
7:b:13:ASN:H	7:b:16:LEU:HD13	1.48	0.77
7:f:238:TYR:CD2	7:e:28:LEU:CD1	2.64	0.77
7:e:63:LEU:HD23	7:e:95:ARG:HD3	1.65	0.77
7:b:63:LEU:HD22	7:b:106:LEU:HD23	1.64	0.77
7:a:179:LEU:HD23	7:a:225:ASN:CA	2.14	0.77
7:a:235:ARG:NH2	7:a:254:PRO:HD3	2.00	0.77
7:c:8:LEU:HD13	7:c:44:LEU:HD13	1.66	0.77
7:d:165:LEU:O	7:d:165:LEU:HD12	1.84	0.77
7:e:61:ILE:HD12	7:e:98:ARG:HH21	1.49	0.77
7:a:89:GLN:N	7:a:89:GLN:OE1	2.16	0.77
7:b:47:SER:O	7:b:51:TYR:HB2	1.85	0.77
7:b:63:LEU:HD21	7:b:106:LEU:CD2	2.15	0.77
2:C:804:PHE:HB3	2:C:1100:PRO:HB3	1.65	0.77
7:a:78:PHE:O	7:a:94:GLY:CA	2.33	0.77
7:e:61:ILE:CD1	7:e:98:ARG:HH21	1.98	0.77
8:M:285:TRP:HH2	8:M:355:PHE:HB2	1.47	0.77
6:T:6:DT:H2'	6:T:7:DG:C8	2.21	0.76
7:a:77:LEU:O	7:a:94:GLY:HA3	1.85	0.76
7:b:205:LEU:HD23	7:b:206:PHE:O	1.84	0.76
7:c:255:PHE:N	7:c:255:PHE:CD1	2.53	0.76
7:e:129:LEU:O	7:e:129:LEU:HD13	1.85	0.76
7:b:80:HIS:HB3	7:b:132:VAL:HG23	1.61	0.76
7:b:25:LEU:HD21	7:c:238:TYR:CZ	2.21	0.76
7:d:78:PHE:CE2	7:d:129:LEU:CD1	2.67	0.76
7:d:128:GLU:OE1	7:d:128:GLU:N	2.17	0.76
8:M:197:ASP:OD1	8:M:198:CYS:N	2.18	0.76
7:a:105:PHE:HA	7:a:145:VAL:O	1.84	0.76
7:b:222:TRP:HZ3	7:b:229:LEU:CA	1.97	0.76
7:f:69:ASN:CB	7:e:74:ASP:OD2	2.33	0.76
7:e:42:LYS:HB2	7:e:42:LYS:NZ	2.01	0.76
8:M:200:LEU:HD13	8:M:200:LEU:O	1.86	0.76
7:a:200:GLU:O	7:a:200:GLU:HG2	1.84	0.76
7:c:5:LYS:HB3	7:c:48:ARG:NH1	2.01	0.76
7:f:47:SER:O	7:f:51:TYR:HE1	1.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:179:LEU:HB2	7:e:225:ASN:HB3	1.68	0.76
8:M:158:ILE:HD11	8:M:193:LYS:HD3	1.68	0.76
8:M:279:ARG:HG3	8:M:279:ARG:NH2	1.97	0.76
7:a:11:GLU:H	7:a:11:GLU:CD	1.94	0.76
7:b:46:ALA:CB	7:b:105:PHE:HE2	1.99	0.76
7:d:99:ALA:CB	7:d:104:LEU:HD11	2.16	0.76
7:f:81:GLU:HA	7:f:91:ARG:HA	1.67	0.76
7:e:61:ILE:C	7:e:62:SER:CA	2.57	0.76
8:M:351:GLN:NE2	8:M:362:MET:HG3	1.99	0.76
8:M:360:GLU:OE2	8:M:423:LEU:HA	1.86	0.76
5:N:-13:DC:C1'	8:M:15:MET:HE1	2.15	0.76
7:b:42:LYS:CD	7:b:147:ALA:HB1	2.15	0.76
7:f:6:ASP:O	7:f:8:LEU:HD22	1.86	0.76
7:f:30:LYS:HB3	7:f:171:PHE:CD2	2.20	0.76
7:c:31:PRO:HA	7:c:145:VAL:HG12	1.68	0.75
8:M:196:ARG:CG	8:M:197:ASP:N	2.49	0.75
7:b:69:ASN:OD1	7:b:71:ASN:HB2	1.85	0.75
7:d:182:ARG:HH12	7:d:189:MET:HE3	1.51	0.75
7:e:36:GLY:CA	7:e:42:LYS:HE3	2.16	0.75
7:b:49:LEU:CA	7:b:49:LEU:HG	2.13	0.75
7:e:109:LEU:HD13	7:e:109:LEU:O	1.87	0.75
7:a:37:GLU:CB	7:a:225:ASN:HD21	1.98	0.75
7:a:106:LEU:N	7:a:106:LEU:HD23	2.02	0.75
7:a:222:TRP:CE3	7:a:228:GLU:HG3	2.21	0.75
7:b:240:HIS:CE1	7:b:242:THR:CG2	2.69	0.75
7:f:85:PHE:CD2	8:M:5:LEU:HD22	2.22	0.75
7:f:179:LEU:CG	7:f:186:ILE:HD11	2.17	0.75
7:f:222:TRP:N	7:f:223:PRO:HD2	2.00	0.75
7:c:82:ALA:HB3	7:c:131:ARG:HD3	1.68	0.75
1:A:315:GLY:CA	8:M:132:PRO:HG2	2.16	0.75
5:N:-13:DC:C2'	8:M:15:MET:HE3	2.16	0.75
7:c:104:LEU:CD1	7:c:142:VAL:CG2	2.31	0.75
7:e:189:MET:CG	7:e:189:MET:CE	2.65	0.75
8:M:9:LEU:HD22	8:M:9:LEU:N	2.02	0.75
8:M:357:GLN:CB	8:M:361:TYR:HB2	2.16	0.75
7:b:48:ARG:O	7:b:48:ARG:HG3	1.87	0.75
7:c:187:MET:HA	7:c:187:MET:HE3	1.69	0.75
7:f:65:CYS:SG	7:f:109:LEU:CA	2.72	0.75
7:e:42:LYS:HB3	9:e:601:ADP:O1B	1.87	0.75
8:M:193:LYS:O	8:M:194:ASP:HB3	1.86	0.75
7:e:81:GLU:CG	7:e:91:ARG:HH22	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:-10:DG:H2'	5:N:-9:DA:C8	2.21	0.74
7:a:95:ARG:HH12	7:a:98:ARG:HH22	1.35	0.74
7:a:252:ILE:CG2	7:a:253:ASP:OD1	2.31	0.74
7:b:36:GLY:O	7:b:149:ASN:CB	2.35	0.74
7:d:85:PHE:HB3	8:M:1:MET:HE3	1.69	0.74
7:e:71:ASN:C	7:e:73:LEU:H	1.95	0.74
3:D:41:PRO:O	3:D:270:ARG:NH1	2.20	0.74
7:a:20:GLU:O	7:a:24:HIS:CD2	2.40	0.74
7:b:50:HIS:CD2	7:b:51:TYR:CD1	2.74	0.74
7:b:76:GLU:O	7:b:95:ARG:HB2	1.87	0.74
7:f:30:LYS:HB2	7:f:171:PHE:HE2	1.50	0.74
8:M:28:LEU:HD13	8:M:33:LEU:HB2	1.68	0.74
8:M:461:TYR:O	8:M:465:LEU:HG	1.86	0.74
7:b:152:LEU:HB3	7:b:166:LEU:HD12	1.66	0.74
7:d:64:ASN:CB	7:d:106:LEU:HD13	2.16	0.74
8:M:357:GLN:HB3	8:M:361:TYR:CB	2.17	0.74
5:N:-27:DT:H71	8:M:455:ARG:NH1	2.01	0.74
7:b:195:ILE:N	7:b:206:PHE:CZ	2.56	0.74
8:M:190:VAL:O	8:M:190:VAL:HG12	1.86	0.74
7:b:198:CYS:SG	7:b:206:PHE:CE2	2.81	0.74
7:f:30:LYS:CB	7:f:171:PHE:CD2	2.70	0.74
7:a:24:HIS:HB3	7:b:238:TYR:OH	1.87	0.74
7:c:61:ILE:HG22	7:c:99:ALA:HB1	1.70	0.74
5:N:-27:DT:C7	8:M:455:ARG:HH12	1.97	0.74
7:a:179:LEU:HD21	7:a:226:ILE:HA	1.70	0.74
7:a:222:TRP:HE3	7:a:228:GLU:HG2	1.51	0.74
7:e:21:GLN:OE1	7:e:174:VAL:HG22	1.87	0.74
7:a:12:ALA:O	7:a:13:ASN:HB2	1.87	0.73
7:a:55:ARG:HG3	7:a:55:ARG:NH2	1.98	0.73
7:a:180:ARG:HH11	7:a:221:ARG:HD3	1.51	0.73
7:a:59:PRO:HD2	7:a:102:GLY:CA	2.18	0.73
7:c:63:LEU:HB3	7:c:106:LEU:CD1	2.19	0.73
7:f:196:GLN:HA	7:f:199:ARG:HD2	1.68	0.73
7:f:201:ILE:CG2	7:e:28:LEU:CD2	2.66	0.73
7:b:194:ALA:O	7:b:206:PHE:HZ	1.70	0.73
7:c:8:LEU:HD11	7:c:15:PHE:HZ	1.51	0.73
7:d:55:ARG:H	7:d:55:ARG:HD3	1.52	0.73
7:d:85:PHE:HB2	8:M:1:MET:CE	2.05	0.73
7:f:179:LEU:CD1	7:f:186:ILE:CD1	2.66	0.73
7:e:55:ARG:O	7:e:55:ARG:HG3	1.88	0.73
8:M:28:LEU:CD1	8:M:33:LEU:HB2	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:118:GLN:HA	8:M:118:GLN:HE21	1.54	0.73
2:C:914:LYS:HG2	8:M:262:GLN:HE21	1.50	0.73
7:a:73:LEU:HD22	7:a:116:VAL:CG2	2.18	0.73
7:b:12:ALA:CB	7:b:15:PHE:H	2.01	0.73
7:b:77:LEU:CD1	7:b:96:PHE:HD1	1.99	0.73
7:f:165:LEU:O	7:f:169:LEU:HB2	1.87	0.73
7:e:77:LEU:HD21	7:e:120:LEU:HB3	1.70	0.73
8:M:133:PHE:HB3	8:M:137:ASP:HB2	1.68	0.73
8:M:303:TYR:CD1	8:M:306:MET:SD	2.82	0.73
7:a:119:LYS:CE	7:b:67:ALA:HA	2.17	0.73
7:c:121:LEU:HD23	7:c:162:ARG:CD	2.18	0.73
7:e:195:ILE:HA	7:e:198:CYS:SG	2.29	0.73
7:e:47:SER:C	7:e:49:LEU:H	1.96	0.73
7:f:201:ILE:CG2	7:e:28:LEU:HD21	2.18	0.73
7:f:250:ILE:HG22	7:f:252:ILE:HG12	1.69	0.73
7:d:169:LEU:HD23	7:d:169:LEU:C	2.14	0.73
7:a:8:LEU:HD12	9:a:601:ADP:N6	2.02	0.72
7:a:59:PRO:HD2	7:a:102:GLY:N	2.04	0.72
7:c:70:GLU:CD	7:c:70:GLU:H	1.95	0.72
7:e:32:VAL:CG2	7:e:143:ARG:NH2	2.49	0.72
6:T:12:DT:H71	8:M:22:ALA:HB1	1.71	0.72
7:c:32:VAL:CG2	7:c:145:VAL:HB	2.18	0.72
7:c:138:LEU:HD22	7:c:138:LEU:N	2.04	0.72
7:d:24:HIS:CB	7:e:238:TYR:OH	2.36	0.72
2:C:843:THR:CB	8:M:271:TYR:CE1	2.63	0.72
7:c:8:LEU:HD22	7:c:44:LEU:HD22	1.72	0.72
7:d:166:LEU:HD23	7:d:166:LEU:C	2.14	0.72
7:f:30:LYS:HB3	7:f:171:PHE:HD2	1.53	0.72
7:e:120:LEU:C	7:e:120:LEU:HD12	2.14	0.72
8:M:195:LEU:HG	8:M:196:ARG:N	2.02	0.72
7:c:63:LEU:HB3	7:c:106:LEU:HD12	1.71	0.72
7:c:63:LEU:HD13	7:c:63:LEU:C	2.14	0.72
7:f:117:GLN:HE22	7:f:161:PHE:HA	1.53	0.72
7:a:91:ARG:CD	7:a:131:ARG:HH12	1.98	0.72
7:b:36:GLY:O	7:b:149:ASN:CA	2.37	0.72
7:c:44:LEU:HD23	7:c:44:LEU:C	2.15	0.72
8:M:27:GLN:O	8:M:27:GLN:HG3	1.89	0.72
5:N:-27:DT:C7	8:M:455:ARG:HH22	1.99	0.72
7:d:171:PHE:O	7:e:235:ARG:HD3	1.88	0.72
7:f:30:LYS:CB	7:f:171:PHE:CE2	2.72	0.72
7:f:50:HIS:CE1	7:f:60:PHE:CB	2.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:121:LEU:HD23	7:e:121:LEU:C	2.14	0.72
7:a:80:HIS:HA	7:a:131:ARG:HB2	1.69	0.72
7:a:19:LEU:CD2	7:a:48:ARG:HH11	2.02	0.72
7:d:32:VAL:HG21	7:d:143:ARG:HH11	1.52	0.72
7:e:175:GLN:OE1	7:e:175:GLN:N	2.22	0.72
7:a:37:GLU:HB2	7:a:225:ASN:HD21	1.54	0.72
7:b:182:ARG:O	7:b:183:GLU:HG2	1.89	0.72
8:M:409:THR:HG22	8:M:451:ILE:HA	1.70	0.72
7:a:213:ALA:O	7:a:214:ARG:C	2.32	0.72
7:c:26:ALA:CB	7:c:52:LEU:HG	2.19	0.72
7:d:78:PHE:HD2	7:d:129:LEU:CD1	1.90	0.72
7:f:9:LEU:HD22	7:f:9:LEU:N	2.05	0.72
7:f:39:GLY:O	7:f:226:ILE:HB	1.90	0.72
8:M:367:LEU:HD23	8:M:403:PHE:CE2	2.24	0.72
7:f:238:TYR:CE2	7:e:28:LEU:CD1	2.72	0.71
8:M:173:GLU:OE1	8:M:173:GLU:N	2.19	0.71
7:c:144:LEU:C	7:c:144:LEU:HD22	2.15	0.71
7:f:103:THR:CG2	7:f:143:ARG:CG	2.64	0.71
8:M:423:LEU:CD1	8:M:446:LEU:HD21	2.20	0.71
7:b:25:LEU:CD2	7:c:238:TYR:CZ	2.73	0.71
7:b:148:THR:HG21	7:b:152:LEU:HD21	1.72	0.71
7:f:129:LEU:HD12	7:f:129:LEU:C	2.16	0.71
7:e:42:LYS:HB2	7:e:42:LYS:HZ2	1.52	0.71
7:e:164:ASP:OD1	7:e:164:ASP:N	2.24	0.71
7:a:38:ARG:NH2	7:f:164:ASP:HB3	2.04	0.71
7:a:222:TRP:CE3	7:a:228:GLU:HB3	2.26	0.71
8:M:367:LEU:CD2	8:M:403:PHE:CD2	2.72	0.71
6:T:14:DC:O3'	8:M:11:GLN:NE2	2.23	0.71
7:f:9:LEU:HD22	7:f:9:LEU:H	1.55	0.71
7:f:141:ASN:OD1	7:f:141:ASN:N	2.22	0.71
7:e:129:LEU:HD22	7:e:129:LEU:C	2.15	0.71
7:b:63:LEU:HB2	7:b:95:ARG:HH22	1.56	0.71
7:d:64:ASN:HB3	7:d:106:LEU:HD13	1.73	0.71
7:f:226:ILE:HG13	9:f:601:ADP:C8	2.25	0.71
8:M:357:GLN:HB3	8:M:361:TYR:CD2	2.26	0.71
7:a:40:THR:HG22	7:a:42:LYS:HD2	1.71	0.71
7:a:85:PHE:HB2	8:M:8:ARG:O	1.90	0.71
7:c:104:LEU:HD13	7:c:144:LEU:CB	2.10	0.71
7:c:224:GLY:CA	7:c:228:GLU:HB2	2.20	0.71
7:d:10:GLY:HA3	7:d:15:PHE:CG	2.26	0.71
7:f:65:CYS:HB3	7:f:112:ALA:CB	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:26:ALA:CB	7:e:53:SER:N	2.53	0.71
8:M:342:ARG:HB3	8:M:342:ARG:HH11	1.56	0.71
3:D:334:LYS:HA	3:D:339:ARG:HH21	1.56	0.71
6:T:15:DA:P	8:M:11:GLN:NE2	2.63	0.71
7:a:180:ARG:HH11	7:a:221:ARG:CD	2.03	0.71
8:M:154:LEU:HD12	8:M:193:LYS:HA	1.71	0.71
8:M:453:VAL:O	8:M:454:ALA:HB3	1.90	0.71
7:a:86:THR:HG22	7:f:86:THR:OG1	1.91	0.70
7:b:166:LEU:HD23	7:b:166:LEU:C	2.16	0.70
7:c:255:PHE:N	7:c:255:PHE:HD1	1.87	0.70
7:f:34:ILE:HG12	7:f:146:CYS:O	1.91	0.70
7:f:81:GLU:CG	7:f:131:ARG:HD2	2.21	0.70
7:e:30:LYS:HB3	7:e:31:PRO:HD2	1.72	0.70
7:a:119:LYS:HG3	7:b:67:ALA:CB	2.21	0.70
7:d:162:ARG:HB3	7:d:165:LEU:HB3	1.71	0.70
7:e:8:LEU:HD13	7:e:48:ARG:HH11	1.56	0.70
7:a:77:LEU:O	7:a:94:GLY:CA	2.38	0.70
7:a:252:ILE:HD12	7:a:252:ILE:N	2.06	0.70
7:d:85:PHE:CG	8:M:1:MET:HE1	2.25	0.70
7:f:34:ILE:O	7:f:147:ALA:HB1	1.91	0.70
7:e:136:GLN:OE1	7:e:137:PRO:HD3	1.92	0.70
1:A:166:ARG:CD	1:A:172:LEU:HD11	2.20	0.70
7:a:9:LEU:HD23	7:a:9:LEU:N	2.02	0.70
8:M:381:ILE:HG22	8:M:382:SER:N	2.05	0.70
8:M:451:ILE:HG22	8:M:453:VAL:HG13	1.71	0.70
3:D:824:PRO:HB3	3:D:834:PRO:HA	1.73	0.70
7:a:178:PRO:CG	7:a:181:GLU:HG3	2.13	0.70
7:c:106:LEU:O	7:c:109:LEU:CD2	2.39	0.70
7:d:61:ILE:HD11	7:d:95:ARG:NH1	2.05	0.70
8:M:358:GLY:CA	8:M:394:ARG:HH12	2.05	0.70
7:a:72:LEU:HD11	8:M:7:LEU:CD2	2.18	0.70
7:c:138:LEU:HD22	7:c:138:LEU:H	1.55	0.70
7:c:152:LEU:HB3	7:c:166:LEU:HD11	1.74	0.70
8:M:274:PRO:CB	8:M:391:HIS:HB2	2.22	0.70
1:A:102:LEU:HD13	1:A:115:ILE:HG12	1.74	0.70
5:N:-11:DA:C8	5:N:-10:DG:C5	2.80	0.70
7:a:64:ASN:ND2	7:a:67:ALA:HB2	2.06	0.70
7:c:114:MET:HG2	7:d:67:ALA:HB2	1.72	0.70
7:c:121:LEU:HD23	7:c:162:ARG:HD3	1.70	0.70
7:e:50:HIS:HB2	7:e:103:THR:OG1	1.91	0.70
7:a:138:LEU:N	7:a:138:LEU:HD23	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:251:ILE:H	7:a:251:ILE:CD1	2.05	0.70
7:d:10:GLY:CA	7:d:15:PHE:CD2	2.74	0.70
7:d:79:GLY:HA3	7:d:92:HIS:CD2	2.26	0.70
8:M:37:LEU:HD11	8:M:297:LEU:HD21	1.72	0.70
7:f:120:LEU:HD13	7:f:124:ILE:HD12	1.73	0.70
7:e:47:SER:C	7:e:49:LEU:N	2.43	0.70
8:M:278:VAL:O	8:M:278:VAL:CG2	2.39	0.70
7:c:64:ASN:HA	7:c:107:ASP:HB2	1.74	0.69
7:a:210:THR:HG21	7:a:248:ASP:CB	2.20	0.69
7:c:32:VAL:O	7:c:145:VAL:HB	1.91	0.69
7:d:155:MET:HB3	7:d:160:THR:HG1	1.56	0.69
7:e:38:ARG:O	7:e:38:ARG:HG2	1.91	0.69
7:e:106:LEU:HB2	7:e:145:VAL:O	1.92	0.69
7:a:66:ALA:O	7:f:119:LYS:CE	2.39	0.69
7:e:109:LEU:HD11	7:e:161:PHE:HZ	1.53	0.69
7:c:26:ALA:HB2	7:c:52:LEU:HG	1.73	0.69
7:e:188:LEU:O	7:e:191:GLU:HG3	1.92	0.69
7:a:179:LEU:CD2	7:a:225:ASN:C	2.65	0.69
7:b:195:ILE:CD1	7:b:206:PHE:CE1	2.76	0.69
8:M:336:ARG:NH1	8:M:388:LYS:HZ1	1.88	0.69
7:a:33:LEU:HD12	7:a:33:LEU:C	2.16	0.69
7:a:33:LEU:HD12	7:a:34:ILE:H	1.50	0.69
8:M:303:TYR:HD1	8:M:306:MET:SD	2.15	0.69
8:M:336:ARG:HH12	8:M:388:LYS:HZ2	1.41	0.69
1:A:47:LEU:HD23	1:A:51:MET:HE3	1.72	0.69
7:e:118:GLU:OE1	7:e:162:ARG:HD2	1.93	0.69
8:M:41:LEU:HD12	8:M:41:LEU:C	2.18	0.69
5:N:-12:DC:H2"	5:N:-11:DA:H5"	1.74	0.69
7:b:140:VAL:O	7:b:140:VAL:CG2	2.39	0.69
7:f:34:ILE:HG22	7:f:42:LYS:HG3	1.75	0.69
7:f:179:LEU:HG	7:f:186:ILE:HD11	1.75	0.69
8:M:33:LEU:HD23	8:M:33:LEU:C	2.18	0.69
8:M:428:ILE:O	8:M:431:GLU:HG3	1.93	0.69
7:b:152:LEU:HD12	7:b:166:LEU:HD12	1.72	0.69
7:b:194:ALA:O	7:b:206:PHE:CZ	2.46	0.69
7:c:144:LEU:O	7:c:144:LEU:HD13	1.93	0.69
8:M:119:THR:HG22	8:M:122:ASP:OD2	1.93	0.69
8:M:278:VAL:CG2	8:M:392:SER:HB3	2.23	0.69
7:c:41:GLY:O	7:c:45:ILE:HG12	1.92	0.69
7:c:144:LEU:HD22	7:c:144:LEU:O	1.93	0.69
7:f:130:GLU:OE1	7:f:130:GLU:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:187:MET:HA	7:f:187:MET:HE3	1.75	0.69
6:T:13:DG:OP2	8:M:377:HIS:HB2	1.93	0.68
7:b:31:PRO:HA	7:b:144:LEU:O	1.93	0.68
7:f:226:ILE:CG2	9:f:601:ADP:C1'	2.70	0.68
7:c:8:LEU:CD2	7:c:44:LEU:HD21	2.23	0.68
7:c:35:ILE:HD13	7:c:173:VAL:HG22	1.76	0.68
7:d:79:GLY:CA	7:d:92:HIS:HD2	2.05	0.68
8:M:355:PHE:O	8:M:394:ARG:HD3	1.92	0.68
7:f:12:ALA:CB	7:f:185:ASP:OD2	2.40	0.68
7:f:80:HIS:CE1	7:f:92:HIS:CB	2.75	0.68
7:a:33:LEU:O	7:a:173:VAL:HG13	1.94	0.68
7:f:50:HIS:HE1	7:f:60:PHE:HB2	1.55	0.68
7:e:171:PHE:HD1	7:e:172:ASP:HB2	1.57	0.68
2:C:715:THR:HG22	2:C:786:GLY:H	1.57	0.68
7:b:92:HIS:CG	7:b:93:PRO:HD2	2.28	0.68
7:c:64:ASN:O	7:c:68:LEU:HD23	1.94	0.68
7:d:117:GLN:HB3	7:d:165:LEU:CD2	2.23	0.68
7:d:179:LEU:HD23	7:d:225:ASN:OD1	1.93	0.68
7:d:153:PRO:CD	7:e:255:PHE:CE2	2.60	0.68
7:f:34:ILE:CB	7:f:147:ALA:CB	2.59	0.68
7:f:38:ARG:O	7:f:38:ARG:HD3	1.94	0.68
7:f:226:ILE:HG22	9:f:601:ADP:H1'	1.74	0.68
8:M:336:ARG:NH1	8:M:388:LYS:HZ2	1.92	0.68
7:b:46:ALA:HB2	7:b:105:PHE:CE2	2.24	0.68
7:f:61:ILE:HD13	7:f:98:ARG:NH2	2.09	0.68
7:e:179:LEU:CB	7:e:225:ASN:HB3	2.23	0.68
1:A:91:ARG:NH2	1:A:209:GLY:O	2.24	0.68
6:T:10:DC:H2''	6:T:11:DG:C8	2.28	0.68
7:a:251:ILE:HD13	7:a:251:ILE:N	2.08	0.68
7:b:240:HIS:CE1	7:b:242:THR:O	2.47	0.68
8:M:357:GLN:HB3	8:M:361:TYR:CG	2.28	0.68
7:a:16:LEU:HD23	7:a:16:LEU:C	2.19	0.67
7:a:171:PHE:HE2	7:b:234:GLU:HG2	1.58	0.67
7:b:63:LEU:HD23	7:b:63:LEU:C	2.18	0.67
7:c:8:LEU:HD13	7:c:44:LEU:CD1	2.24	0.67
7:f:6:ASP:O	7:f:8:LEU:CD2	2.42	0.67
7:f:85:PHE:CE2	8:M:5:LEU:CD2	2.71	0.67
7:f:255:PHE:CE1	7:e:153:PRO:HD3	2.29	0.67
7:e:222:TRP:CH2	7:e:229:LEU:HD12	2.29	0.67
8:M:113:GLN:OE1	8:M:113:GLN:HA	1.94	0.67
7:c:22:VAL:HG13	7:c:49:LEU:CD2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:159:GLY:C	7:e:161:PHE:H	2.02	0.67
3:D:886:VAL:HB	3:D:1258:ARG:HG3	1.77	0.67
7:b:204:PRO:HG2	7:b:205:LEU:H	1.58	0.67
8:M:367:LEU:HD23	8:M:403:PHE:CD2	2.29	0.67
5:N:-13:DC:H2"	8:M:15:MET:CE	2.19	0.67
7:a:16:LEU:HD23	7:a:16:LEU:O	1.94	0.67
7:a:35:ILE:HG12	7:a:173:VAL:HG11	1.75	0.67
7:b:50:HIS:CD2	7:b:51:TYR:CE1	2.82	0.67
7:e:61:ILE:HD13	7:e:98:ARG:HG2	1.70	0.67
7:a:11:GLU:OE1	7:a:11:GLU:N	2.27	0.67
7:a:73:LEU:C	7:a:75:SER:H	2.03	0.67
7:f:233:VAL:HG13	7:f:234:GLU:HG3	1.76	0.67
8:M:19:LEU:HD23	8:M:19:LEU:C	2.19	0.67
1:B:48:LEU:HD11	3:D:534:GLU:HG3	1.75	0.67
7:b:124:ILE:HD12	7:b:124:ILE:N	2.10	0.67
7:b:195:ILE:N	7:b:206:PHE:HZ	1.89	0.67
7:d:32:VAL:CG2	7:d:143:ARG:HH11	2.07	0.67
7:b:109:LEU:HB2	7:b:146:CYS:SG	2.34	0.67
7:f:65:CYS:CB	7:f:112:ALA:HB2	2.22	0.67
7:e:16:LEU:HD23	7:e:16:LEU:C	2.20	0.67
7:b:86:THR:HA	8:M:12:GLN:HG2	1.77	0.67
7:e:26:ALA:CB	7:e:53:SER:CA	2.65	0.67
7:a:210:THR:HG23	7:a:247:LEU:O	1.95	0.67
8:M:245:VAL:O	8:M:248:GLU:HG2	1.94	0.67
7:d:182:ARG:HG3	7:d:185:ASP:HB2	1.70	0.67
7:e:8:LEU:CD1	7:e:48:ARG:HH11	2.07	0.67
7:e:26:ALA:CA	7:e:53:SER:HB3	2.24	0.67
7:e:33:LEU:HB2	7:e:146:CYS:HB2	1.75	0.67
2:C:4:SER:HB3	2:C:7:GLU:HB3	1.76	0.66
7:a:179:LEU:HD23	7:a:225:ASN:HA	1.77	0.66
7:b:29:ASP:HA	7:b:143:ARG:HD3	1.77	0.66
7:c:192:TYR:O	7:c:195:ILE:HG12	1.95	0.66
8:M:9:LEU:HD22	8:M:9:LEU:H	1.60	0.66
8:M:273:ILE:HG13	8:M:273:ILE:O	1.94	0.66
8:M:421:ARG:CG	8:M:465:LEU:HD21	2.25	0.66
5:N:-13:DC:C6	8:M:15:MET:HE1	2.30	0.66
7:c:35:ILE:N	7:c:35:ILE:HD12	2.10	0.66
7:d:8:LEU:HD23	7:d:44:LEU:HD11	1.76	0.66
8:M:25:LEU:HD13	8:M:25:LEU:C	2.20	0.66
7:a:46:ALA:HB2	7:a:105:PHE:CE1	2.30	0.66
7:a:211:GLU:CD	7:a:212:ARG:N	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:226:ILE:HD12	7:c:226:ILE:N	2.05	0.66
8:M:370:ILE:HD13	8:M:381:ILE:CD1	2.26	0.66
7:b:3:GLU:N	7:b:3:GLU:OE2	2.27	0.66
7:b:92:HIS:CD2	7:b:93:PRO:HD2	2.31	0.66
7:c:42:LYS:HB2	9:c:400:ADP:O2B	1.96	0.66
2:C:870:ILE:HD12	2:C:931:VAL:HG21	1.78	0.66
7:b:234:GLU:O	7:b:237:VAL:CG1	2.42	0.66
7:c:166:LEU:HD23	7:c:166:LEU:C	2.20	0.66
7:f:61:ILE:CD1	7:f:98:ARG:NH2	2.58	0.66
7:f:77:LEU:O	7:f:96:PHE:HD2	1.79	0.66
7:f:81:GLU:HG3	7:f:131:ARG:CD	2.26	0.66
7:e:8:LEU:CD1	7:e:48:ARG:NH1	2.58	0.66
7:e:106:LEU:HD12	7:e:144:LEU:HD22	1.76	0.66
7:a:55:ARG:O	7:a:57:GLN:N	2.27	0.66
7:a:73:LEU:HD22	7:a:116:VAL:HG22	1.77	0.66
7:a:85:PHE:CD2	8:M:7:LEU:HD13	2.31	0.66
7:b:72:LEU:HD22	7:b:72:LEU:N	2.11	0.66
7:b:139:GLN:NE2	7:b:139:GLN:H	1.92	0.66
7:c:68:LEU:HD22	7:c:68:LEU:N	2.10	0.66
7:a:119:LYS:HE2	7:b:67:ALA:O	1.95	0.66
7:b:129:LEU:HD23	7:b:129:LEU:H	1.61	0.66
7:f:187:MET:SD	7:f:218:LEU:CD2	2.82	0.66
7:e:71:ASN:O	7:e:73:LEU:N	2.28	0.66
7:a:169:LEU:C	7:a:169:LEU:HD12	2.20	0.66
7:c:26:ALA:N	7:c:27:PRO:HD2	2.11	0.66
7:e:178:PRO:O	7:e:181:GLU:HB3	1.95	0.66
8:M:203:LEU:HD21	8:M:256:LEU:HD11	1.77	0.66
7:a:117:GLN:O	7:a:165:LEU:HD12	1.94	0.66
7:d:180:ARG:HG3	7:d:181:GLU:OE1	1.96	0.66
7:e:34:ILE:O	7:e:148:THR:HG22	1.96	0.66
7:e:63:LEU:HD12	7:e:63:LEU:C	2.21	0.66
7:e:225:ASN:HD22	7:e:225:ASN:N	1.94	0.66
2:C:1259:LEU:HD21	8:M:115:GLU:CG	2.20	0.65
7:b:36:GLY:O	7:b:149:ASN:HB2	1.96	0.65
7:b:124:ILE:HD12	7:b:124:ILE:H	1.62	0.65
7:d:76:GLU:OE1	7:d:76:GLU:HA	1.96	0.65
8:M:138:ARG:O	8:M:142:THR:HG23	1.96	0.65
8:M:140:ILE:HD11	8:M:170:ILE:HD12	1.77	0.65
3:D:460:ASP:OD1	3:D:460:ASP:N	2.27	0.65
7:a:37:GLU:HB2	7:a:225:ASN:ND2	2.11	0.65
7:a:252:ILE:HD12	7:a:252:ILE:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:46:ALA:HB1	7:b:105:PHE:CD2	2.31	0.65
7:b:91:ARG:NH2	7:b:91:ARG:HG2	2.11	0.65
7:f:61:ILE:HG12	7:f:98:ARG:HH21	1.60	0.65
3:D:50:LYS:HB2	3:D:71:LEU:HD11	1.77	0.65
7:a:72:LEU:HD13	8:M:7:LEU:CD2	2.20	0.65
7:b:15:PHE:HA	7:b:18:VAL:HG23	1.77	0.65
7:d:41:GLY:H	7:d:176:LEU:HD21	1.61	0.65
7:e:105:PHE:HA	7:e:145:VAL:HG22	1.76	0.65
8:M:18:GLN:HE22	8:M:328:TRP:HE1	1.44	0.65
1:A:167:PRO:HD2	1:A:170:ARG:NH2	2.11	0.65
7:e:72:LEU:CD1	8:M:3:GLN:HE21	2.09	0.65
7:e:189:MET:CE	7:e:226:ILE:HG12	2.24	0.65
3:D:885:VAL:HG23	3:D:894:VAL:HG21	1.78	0.65
6:T:32:DT:OP2	8:M:233:ARG:NH2	2.23	0.65
7:b:79:GLY:CA	7:b:92:HIS:HD2	2.08	0.65
7:f:61:ILE:CG1	7:f:98:ARG:HH21	2.09	0.65
7:f:235:ARG:HH12	7:f:251:ILE:HG22	1.61	0.65
7:b:33:LEU:HD12	7:b:146:CYS:HB3	1.76	0.65
7:d:112:ALA:CB	7:d:116:VAL:CG1	2.68	0.65
7:d:121:LEU:HD22	7:d:165:LEU:N	2.12	0.65
7:d:173:VAL:O	7:d:173:VAL:CG2	2.43	0.65
7:e:7:ASN:H	7:e:7:ASN:HD22	1.44	0.65
2:C:823:VAL:HA	2:C:1060:ILE:HD11	1.79	0.65
2:C:843:THR:HB	8:M:271:TYR:CD1	2.30	0.65
3:D:551:ARG:HA	3:D:568:SER:O	1.96	0.65
7:a:33:LEU:O	7:a:173:VAL:CG1	2.45	0.65
7:a:78:PHE:CG	7:a:129:LEU:HD12	2.32	0.65
7:a:96:PHE:CE2	7:a:120:LEU:HD12	2.31	0.65
7:b:33:LEU:HD12	7:b:146:CYS:O	1.97	0.65
7:c:63:LEU:O	7:c:106:LEU:HA	1.97	0.65
7:f:32:VAL:HG11	7:f:49:LEU:HD11	1.78	0.65
8:M:158:ILE:CD1	8:M:193:LYS:HE2	2.27	0.65
7:a:179:LEU:CD2	7:a:226:ILE:HA	2.27	0.65
7:b:32:VAL:HG11	7:b:145:VAL:HG12	1.77	0.65
7:d:41:GLY:N	7:d:176:LEU:CD2	2.55	0.65
7:e:179:LEU:HD13	7:e:225:ASN:C	2.21	0.65
1:A:38:THR:HB	1:B:45:ARG:HD2	1.77	0.65
7:c:8:LEU:HB2	7:c:44:LEU:HD11	1.79	0.65
1:A:45:ARG:NH1	1:B:38:THR:OG1	2.30	0.64
5:N:-16:DT:OP2	8:M:400:LYS:NZ	2.29	0.64
7:b:63:LEU:CB	7:b:95:ARG:NH2	2.59	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:69:ASN:HB2	7:c:72:LEU:HD12	1.78	0.64
7:f:43:GLU:HG2	7:e:126:TYR:CZ	2.32	0.64
7:e:113:PRO:HD2	7:e:116:VAL:HG21	1.80	0.64
7:b:226:ILE:HG21	9:b:601:ADP:H8	1.63	0.64
7:d:182:ARG:HG3	7:d:185:ASP:OD2	1.96	0.64
7:f:188:LEU:N	7:f:188:LEU:HD12	2.13	0.64
7:e:32:VAL:HG21	7:e:143:ARG:HH21	1.56	0.64
7:e:61:ILE:CD1	7:e:98:ARG:NH2	2.60	0.64
1:A:166:ARG:NE	1:A:172:LEU:CD1	2.43	0.64
7:a:104:LEU:O	7:a:145:VAL:HG13	1.96	0.64
7:e:63:LEU:HD12	7:e:63:LEU:O	1.96	0.64
8:M:235:LEU:HD12	8:M:246:LEU:CD1	2.27	0.64
7:a:229:LEU:O	7:a:233:VAL:HB	1.97	0.64
7:b:196:GLN:OE1	7:b:196:GLN:HA	1.96	0.64
7:c:165:LEU:HD23	7:c:165:LEU:C	2.23	0.64
7:c:230:LYS:CA	7:c:233:VAL:HG12	2.27	0.64
7:d:78:PHE:HB3	7:d:131:ARG:HA	1.79	0.64
7:d:78:PHE:CE1	7:d:119:LYS:HG2	2.31	0.64
8:M:182:ILE:HG23	8:M:185:PHE:HD2	1.52	0.64
7:b:92:HIS:CG	7:b:93:PRO:CD	2.81	0.64
7:f:234:GLU:HA	7:f:237:VAL:HG12	1.80	0.64
7:a:34:ILE:HD12	7:a:147:ALA:CB	2.28	0.64
7:b:53:SER:O	7:b:56:TRP:HB3	1.97	0.64
7:e:35:ILE:O	7:e:175:GLN:HA	1.98	0.64
7:e:176:LEU:HD22	7:e:176:LEU:N	2.13	0.64
8:M:147:ALA:HB1	8:M:156:ILE:HD12	1.78	0.64
8:M:276:VAL:HG12	8:M:277:LEU:N	2.12	0.64
8:M:308:ASN:N	8:M:308:ASN:OD1	2.27	0.64
7:a:26:ALA:N	7:a:27:PRO:CD	2.61	0.64
7:b:129:LEU:HD23	7:b:129:LEU:O	1.98	0.64
8:M:154:LEU:CD1	8:M:193:LYS:CB	2.76	0.64
8:M:259:ARG:HH11	8:M:259:ARG:CG	2.08	0.64
7:f:196:GLN:O	7:f:199:ARG:CG	2.45	0.64
7:e:121:LEU:HD21	7:e:168:ARG:NH2	2.12	0.64
8:M:336:ARG:HH11	8:M:388:LYS:NZ	1.91	0.64
5:N:-26:DG:OP2	8:M:462:ARG:NH2	2.28	0.64
7:a:213:ALA:O	7:a:217:LEU:HG	1.98	0.64
7:d:10:GLY:N	7:d:15:PHE:CE2	2.66	0.64
7:d:194:ALA:HB1	7:d:206:PHE:CE1	2.33	0.64
7:b:72:LEU:HD21	8:M:7:LEU:HD12	1.79	0.63
7:d:40:THR:HA	7:d:225:ASN:CB	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:201:ILE:HG22	7:e:28:LEU:CD2	2.28	0.63
7:e:104:LEU:HD23	7:e:104:LEU:O	1.98	0.63
8:M:421:ARG:HG3	8:M:465:LEU:HD21	1.80	0.63
7:a:50:HIS:C	7:a:52:LEU:H	2.06	0.63
7:c:193:PHE:HZ	7:c:226:ILE:CG2	2.11	0.63
7:f:61:ILE:HG22	7:f:99:ALA:HB2	1.80	0.63
8:M:176:GLU:OE1	8:M:176:GLU:HA	1.96	0.63
7:b:125:GLU:OE1	7:b:125:GLU:HA	1.98	0.63
7:b:201:ILE:CG2	7:b:203:LEU:HD23	2.23	0.63
7:c:250:ILE:C	7:c:251:ILE:HG13	2.23	0.63
7:e:91:ARG:NH2	7:e:91:ARG:HG3	2.09	0.63
7:a:254:PRO:HB2	7:f:173:VAL:HG22	1.80	0.63
7:b:240:HIS:HE1	7:b:242:THR:O	1.81	0.63
7:c:54:SER:C	7:c:143:ARG:HH22	2.05	0.63
7:e:63:LEU:CB	7:e:95:ARG:HH21	2.06	0.63
8:M:260:PRO:HG2	8:M:261:GLY:H	1.63	0.63
7:b:91:ARG:HG2	7:b:91:ARG:HH21	1.63	0.63
7:b:139:GLN:H	7:b:139:GLN:CD	2.06	0.63
7:c:104:LEU:CG	7:c:142:VAL:CG2	2.76	0.63
7:f:124:ILE:HD13	7:f:144:LEU:CD2	2.28	0.63
8:M:132:PRO:O	8:M:133:PHE:CD1	2.52	0.63
8:M:292:ASP:OD1	8:M:292:ASP:N	2.28	0.63
7:a:31:PRO:HB2	7:a:169:LEU:O	1.99	0.63
7:a:252:ILE:C	7:a:253:ASP:OD1	2.41	0.63
7:c:136:GLN:H	7:c:136:GLN:HE21	1.45	0.63
8:M:428:ILE:O	8:M:431:GLU:CG	2.47	0.63
2:C:1061:GLN:NE2	2:C:1240:ASP:OD1	2.31	0.63
7:b:26:ALA:HB3	7:b:27:PRO:HD3	1.81	0.63
7:b:60:PHE:CG	7:b:60:PHE:O	2.47	0.63
7:d:106:LEU:O	7:d:147:ALA:HB3	1.99	0.63
7:f:80:HIS:CE1	7:f:92:HIS:HB2	2.33	0.63
8:M:196:ARG:HD2	8:M:196:ARG:C	2.24	0.63
7:c:55:ARG:HA	7:c:143:ARG:CZ	2.27	0.63
7:a:8:LEU:CD1	7:a:15:PHE:HZ	2.12	0.63
7:a:166:LEU:O	7:a:166:LEU:HD13	1.97	0.63
7:b:73:LEU:HD22	7:b:119:LYS:HG2	1.81	0.63
7:b:240:HIS:HE1	7:b:242:THR:C	2.07	0.63
7:a:16:LEU:O	7:a:20:GLU:HG2	1.99	0.62
7:a:153:PRO:HD3	7:b:255:PHE:HE2	1.64	0.62
7:b:193:PHE:CD2	7:b:230:LYS:HA	2.34	0.62
7:c:22:VAL:HG13	7:c:49:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:-13:DC:H2''	8:M:15:MET:HE3	1.80	0.62
7:c:9:LEU:HB2	7:c:189:MET:HE3	1.81	0.62
7:c:225:ASN:HB2	7:c:226:ILE:HD12	1.81	0.62
7:f:103:THR:CG2	7:f:143:ARG:CB	2.34	0.62
7:e:32:VAL:HG21	7:e:143:ARG:HH22	1.62	0.62
7:e:72:LEU:H	7:e:72:LEU:HD22	1.63	0.62
8:M:156:ILE:CD1	8:M:156:ILE:H	2.12	0.62
7:a:20:GLU:HA	7:a:20:GLU:OE2	1.98	0.62
7:a:64:ASN:HB3	7:a:67:ALA:HB2	1.79	0.62
7:a:193:PHE:HD2	7:a:229:LEU:HD12	1.53	0.62
7:b:89:GLN:CD	7:b:89:GLN:H	2.06	0.62
7:f:108:GLU:OE1	7:f:108:GLU:HA	1.98	0.62
8:M:199:LEU:CD2	8:M:256:LEU:HD12	2.29	0.62
7:a:222:TRP:HZ3	7:a:228:GLU:HG3	1.63	0.62
7:b:228:GLU:HA	7:b:228:GLU:OE2	2.00	0.62
7:c:73:LEU:HD23	7:c:113:PRO:CD	2.29	0.62
7:c:152:LEU:HB3	7:c:166:LEU:CD1	2.29	0.62
7:f:136:GLN:HB2	7:f:137:PRO:HD2	1.80	0.62
2:C:902:LEU:HD11	8:M:195:LEU:HD22	1.80	0.62
3:D:583:VAL:HG21	3:D:592:VAL:HG11	1.82	0.62
7:b:169:LEU:HD23	7:b:169:LEU:C	2.24	0.62
7:c:73:LEU:HD23	7:c:113:PRO:HD2	1.81	0.62
7:c:152:LEU:HD11	7:c:161:PHE:CD2	2.35	0.62
7:d:179:LEU:CB	7:d:225:ASN:HA	2.28	0.62
8:M:367:LEU:HD21	8:M:403:PHE:CD2	2.34	0.62
7:a:9:LEU:H	7:a:9:LEU:CD2	2.00	0.62
7:d:68:LEU:HD22	7:d:72:LEU:CG	2.26	0.62
8:M:199:LEU:HD23	8:M:256:LEU:HD12	1.80	0.62
7:a:180:ARG:HG2	7:a:181:GLU:H	1.64	0.62
7:a:240:HIS:CE1	7:a:247:LEU:CB	2.80	0.62
7:b:80:HIS:H	7:b:92:HIS:CD2	2.16	0.62
3:D:814:CYS:CB	3:D:895:CYS:SG	2.87	0.62
7:a:38:ARG:NH1	7:a:224:GLY:HA2	2.12	0.62
7:b:211:GLU:H	7:b:211:GLU:CD	2.08	0.62
7:d:85:PHE:HE2	7:d:133:GLY:HA2	1.64	0.62
8:M:28:LEU:HD13	8:M:33:LEU:CB	2.30	0.62
8:M:275:ASP:O	8:M:290:ASN:HB2	2.00	0.62
5:N:-11:DA:C2'	5:N:-10:DG:C8	2.81	0.62
7:a:19:LEU:CD2	7:a:48:ARG:NH1	2.58	0.62
7:d:108:GLU:CB	7:d:111:THR:CG2	2.68	0.62
7:e:124:ILE:HG23	7:e:124:ILE:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:334:GLU:OE1	8:M:334:GLU:HA	1.99	0.62
3:D:250:ARG:HD3	3:D:265:LEU:HD12	1.82	0.61
7:b:53:SER:OG	7:b:55:ARG:HG2	1.99	0.61
8:M:208:LYS:HD2	8:M:208:LYS:N	2.14	0.61
1:A:125:LYS:HG2	1:A:125:LYS:O	1.98	0.61
3:D:957:SER:H	3:D:985:ILE:H	1.48	0.61
7:a:46:ALA:CB	7:a:105:PHE:CE1	2.83	0.61
7:d:106:LEU:N	7:d:145:VAL:O	2.33	0.61
7:d:179:LEU:CG	7:d:225:ASN:HA	2.30	0.61
7:e:106:LEU:CD1	7:e:144:LEU:HD22	2.30	0.61
2:C:1269:ARG:HH11	3:D:340:GLN:HB3	1.65	0.61
7:b:194:ALA:HB1	7:b:206:PHE:HE2	1.65	0.61
7:d:169:LEU:HD23	7:d:169:LEU:O	2.01	0.61
7:f:87:GLY:HA3	7:e:86:THR:HA	1.82	0.61
7:e:82:ALA:HB2	7:e:91:ARG:N	2.16	0.61
3:D:527:LEU:HD23	3:D:535:ARG:HE	1.63	0.61
6:T:15:DA:P	8:M:11:GLN:HE21	2.22	0.61
7:b:77:LEU:HD13	7:b:96:PHE:HD1	1.64	0.61
7:c:98:ARG:HB2	7:c:98:ARG:NH1	2.15	0.61
7:d:68:LEU:CD1	7:d:76:GLU:HB2	2.30	0.61
7:d:125:GLU:HB2	7:d:126:TYR:HD1	1.65	0.61
7:f:80:HIS:CE1	7:f:92:HIS:CG	2.88	0.61
7:b:80:HIS:CB	7:b:132:VAL:HG23	2.24	0.61
7:b:212:ARG:HD3	7:b:248:ASP:O	1.99	0.61
7:b:152:LEU:CB	7:b:166:LEU:CD1	2.68	0.61
7:e:61:ILE:HD11	7:e:98:ARG:NH2	2.16	0.61
7:e:125:GLU:OE1	7:e:125:GLU:HA	1.99	0.61
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.34	0.61
7:b:204:PRO:HG2	7:b:205:LEU:N	2.16	0.61
7:f:63:LEU:CD1	7:f:106:LEU:CD2	2.68	0.61
1:A:93:GLN:OE1	1:A:93:GLN:HA	2.01	0.61
4:E:26:ARG:HE	4:E:30:MET:HE3	1.64	0.61
7:c:108:GLU:OE1	7:c:108:GLU:HA	2.00	0.61
7:c:152:LEU:CB	7:c:166:LEU:HD12	2.29	0.61
7:f:226:ILE:CB	9:f:601:ADP:C8	2.84	0.61
2:C:1254:VAL:HG12	2:C:1255:THR:HG23	1.82	0.61
7:a:82:ALA:HB2	7:a:91:ARG:N	2.16	0.61
7:a:85:PHE:HD1	7:a:86:THR:O	1.84	0.61
7:a:240:HIS:CE1	7:a:247:LEU:N	2.64	0.61
7:b:80:HIS:HA	7:b:131:ARG:HB3	1.83	0.61
7:f:8:LEU:HG	7:f:48:ARG:HH11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:ARG:NH1	2:C:370:MET:SD	2.74	0.61
7:a:222:TRP:CE3	7:a:228:GLU:CB	2.83	0.61
7:a:228:GLU:OE1	7:a:228:GLU:HA	2.01	0.61
7:b:40:THR:O	7:b:40:THR:HG22	2.00	0.61
7:b:62:SER:HB2	7:b:105:PHE:HB3	1.80	0.61
7:c:153:PRO:HG3	7:d:255:PHE:CE2	2.36	0.61
8:M:31:LEU:C	8:M:31:LEU:HD13	2.25	0.61
7:c:5:LYS:CB	7:c:48:ARG:NH1	2.64	0.60
2:C:975:ILE:HG12	2:C:1014:LEU:HD23	1.82	0.60
2:C:1251:TYR:O	8:M:116:THR:HG23	2.01	0.60
6:T:7:DG:H2"	6:T:8:DA:C8	2.35	0.60
7:a:95:ARG:HH11	7:a:95:ARG:CG	2.15	0.60
7:b:15:PHE:HA	7:b:18:VAL:CG2	2.32	0.60
7:e:136:GLN:OE1	7:e:136:GLN:HA	2.01	0.60
2:C:528:ARG:NH1	2:C:576:SER:O	2.34	0.60
7:a:72:LEU:O	7:a:72:LEU:HG	2.00	0.60
7:a:78:PHE:C	7:a:94:GLY:HA3	2.25	0.60
7:a:96:PHE:CE2	7:a:123:VAL:HG21	2.36	0.60
7:c:32:VAL:HG23	7:c:145:VAL:HB	1.82	0.60
7:f:222:TRP:CH2	7:f:229:LEU:HD12	2.36	0.60
8:M:351:GLN:HE21	8:M:362:MET:HG3	1.65	0.60
2:C:843:THR:HG22	8:M:270:GLU:HA	1.82	0.60
2:C:868:SER:H	2:C:944:ARG:HE	1.49	0.60
3:D:506:VAL:HG13	3:D:628:GLY:HA3	1.83	0.60
7:a:179:LEU:HD11	7:a:226:ILE:HD11	1.82	0.60
7:c:34:ILE:C	7:c:35:ILE:HD12	2.26	0.60
7:c:234:GLU:O	7:c:237:VAL:HB	2.02	0.60
7:e:7:ASN:H	7:e:7:ASN:ND2	1.99	0.60
7:e:33:LEU:HD23	7:e:170:ALA:HB2	1.83	0.60
7:e:118:GLU:HA	7:e:118:GLU:OE2	2.01	0.60
2:C:197:ARG:NH1	2:C:201:ARG:O	2.35	0.60
7:a:16:LEU:HD23	7:a:20:GLU:HG2	1.83	0.60
7:a:95:ARG:HH12	7:a:98:ARG:NH2	1.98	0.60
7:a:113:PRO:HG2	7:a:116:VAL:HB	1.83	0.60
7:a:222:TRP:CH2	7:a:229:LEU:HA	2.37	0.60
7:a:226:ILE:CG2	9:a:601:ADP:C4	2.81	0.60
7:d:183:GLU:OE1	7:d:183:GLU:HA	2.00	0.60
8:M:200:LEU:C	8:M:200:LEU:CD1	2.73	0.60
3:D:78:LEU:HB2	8:M:146:ASP:OD2	2.01	0.60
7:c:13:ASN:HA	7:c:16:LEU:HB2	1.84	0.60
7:f:9:LEU:HD23	9:f:601:ADP:C2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:191:GLU:OE1	7:f:191:GLU:HA	2.02	0.60
7:e:74:ASP:HB2	7:e:119:LYS:HZ2	1.64	0.60
3:D:653:ILE:HG23	3:D:692:ARG:HH11	1.65	0.60
7:a:75:SER:O	7:a:79:GLY:HA2	2.02	0.60
7:a:85:PHE:HB3	7:b:72:LEU:HD11	1.83	0.60
7:f:9:LEU:H	7:f:9:LEU:CD2	2.14	0.60
7:a:250:ILE:CD1	7:a:250:ILE:H	2.14	0.60
7:c:121:LEU:HD21	7:c:162:ARG:HD3	1.82	0.60
7:d:81:GLU:HB2	7:d:133:GLY:HA3	1.84	0.60
7:f:94:GLY:O	7:f:98:ARG:N	2.35	0.60
8:M:165:ILE:HG21	8:M:170:ILE:HG13	1.83	0.60
1:A:166:ARG:HE	1:A:172:LEU:HD12	1.62	0.60
1:B:106:GLY:HA3	1:B:137:ASN:HA	1.84	0.60
2:C:902:LEU:CD1	8:M:195:LEU:HD22	2.32	0.60
7:c:43:GLU:OE1	7:c:43:GLU:HA	2.01	0.60
7:f:99:ALA:HB1	7:f:142:VAL:HG23	1.83	0.60
7:e:72:LEU:HD22	7:e:72:LEU:N	2.16	0.60
7:e:226:ILE:HG22	7:e:226:ILE:O	2.02	0.60
8:M:224:LEU:HD13	8:M:224:LEU:O	2.02	0.60
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.83	0.60
6:T:6:DT:C2'	6:T:7:DG:C8	2.85	0.60
7:a:162:ARG:HB3	7:a:164:ASP:OD1	2.01	0.60
7:b:197:MET:HG3	7:b:237:VAL:CG1	2.29	0.60
7:c:224:GLY:C	7:c:228:GLU:HB3	2.27	0.60
7:e:174:VAL:O	7:e:174:VAL:HG12	2.00	0.60
7:c:26:ALA:HB1	7:c:52:LEU:CB	2.31	0.59
7:c:121:LEU:HD22	7:c:164:ASP:HB2	1.84	0.59
7:c:227:ARG:HB2	9:c:400:ADP:H5'2	1.82	0.59
7:d:182:ARG:HG3	7:d:185:ASP:CG	2.27	0.59
8:M:158:ILE:O	8:M:158:ILE:HG23	2.00	0.59
8:M:423:LEU:HD11	8:M:446:LEU:HD21	1.83	0.59
2:C:1259:LEU:HD11	8:M:115:GLU:CD	2.27	0.59
7:a:153:PRO:HD3	7:b:255:PHE:CE2	2.38	0.59
7:b:176:LEU:HD22	7:b:176:LEU:N	2.17	0.59
7:b:222:TRP:CH2	7:b:229:LEU:HD12	2.37	0.59
7:f:164:ASP:OD1	7:f:164:ASP:N	2.35	0.59
3:D:1262:ARG:NH2	3:D:1312:ALA:O	2.35	0.59
6:T:14:DC:OP2	8:M:377:HIS:CD2	2.55	0.59
7:a:34:ILE:CD1	7:a:147:ALA:HB2	2.31	0.59
7:f:201:ILE:HG21	7:e:28:LEU:CD2	2.31	0.59
8:M:258:PRO:O	8:M:259:ARG:HB2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:55:ARG:C	7:a:57:GLN:N	2.56	0.59
7:b:33:LEU:HB3	7:b:173:VAL:HG12	1.84	0.59
7:b:86:THR:C	7:b:88:ALA:H	2.11	0.59
7:c:76:GLU:OE1	7:c:76:GLU:HA	2.01	0.59
7:d:144:LEU:HD23	7:d:146:CYS:SG	2.42	0.59
7:d:164:ASP:OD1	7:d:164:ASP:N	2.36	0.59
8:M:158:ILE:HD12	8:M:193:LYS:HE2	1.85	0.59
8:M:260:PRO:HG2	8:M:261:GLY:N	2.17	0.59
1:A:166:ARG:HD2	1:A:172:LEU:HD11	1.85	0.59
7:f:166:LEU:HD12	7:f:166:LEU:O	2.03	0.59
7:e:7:ASN:HD22	7:e:7:ASN:N	1.99	0.59
7:e:65:CYS:SG	7:e:112:ALA:HA	2.42	0.59
3:D:339:ARG:O	3:D:341:ASN:N	2.33	0.59
7:a:56:TRP:C	7:a:56:TRP:HE3	2.10	0.59
7:b:117:GLN:CD	7:b:161:PHE:CD1	2.80	0.59
7:c:119:LYS:HE3	7:c:130:GLU:HG2	1.85	0.59
7:c:156:VAL:HG23	7:c:161:PHE:O	2.03	0.59
7:d:35:ILE:HG22	7:d:35:ILE:O	2.02	0.59
7:e:72:LEU:HD13	8:M:3:GLN:HE21	1.67	0.59
5:N:-9:DA:H2'	5:N:-8:DT:H71	1.85	0.59
7:a:97:GLU:OE1	7:a:131:ARG:NH2	2.26	0.59
7:a:142:VAL:O	7:a:142:VAL:HG13	2.03	0.59
7:b:120:LEU:O	7:b:121:LEU:C	2.42	0.59
7:d:55:ARG:H	7:d:55:ARG:CD	2.14	0.59
7:f:61:ILE:CG2	7:f:99:ALA:HB2	2.33	0.59
7:f:203:LEU:HD22	7:f:204:PRO:HD2	1.83	0.59
8:M:182:ILE:HG22	8:M:182:ILE:O	2.03	0.59
7:b:156:VAL:HG13	7:b:163:ALA:HB2	1.84	0.59
7:d:182:ARG:HG3	7:d:185:ASP:CB	2.31	0.59
7:f:32:VAL:HG11	7:f:49:LEU:CD1	2.31	0.59
7:e:113:PRO:HD2	7:e:116:VAL:CG2	2.31	0.59
3:D:43:THR:HG21	3:D:270:ARG:HH22	1.66	0.59
3:D:430:HIS:HB3	3:D:925:GLU:HG3	1.85	0.59
7:a:96:PHE:CE2	7:a:123:VAL:CB	2.85	0.59
7:b:73:LEU:CD2	7:b:119:LYS:HG2	2.33	0.59
7:f:81:GLU:HG3	7:f:131:ARG:HD2	1.84	0.59
7:f:103:THR:HG22	7:f:143:ARG:HB3	0.66	0.59
7:f:142:VAL:HG13	7:f:142:VAL:O	2.03	0.59
8:M:358:GLY:HA2	8:M:394:ARG:NH1	2.16	0.59
3:D:45:ASN:ND2	3:D:50:LYS:O	2.35	0.59
3:D:885:VAL:HG22	3:D:1258:ARG:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:64:ASN:HD22	7:a:67:ALA:HB2	1.65	0.59
7:a:96:PHE:CZ	7:a:120:LEU:HD12	2.37	0.59
7:a:201:ILE:O	7:a:202:LYS:HB2	2.03	0.59
7:b:25:LEU:HD11	7:b:172:ASP:OD2	2.03	0.59
7:b:98:ARG:O	7:b:98:ARG:HG2	2.02	0.59
7:b:113:PRO:O	7:b:117:GLN:HG3	2.02	0.59
7:d:179:LEU:C	7:d:179:LEU:CD1	2.75	0.59
2:C:13:LYS:NZ	2:C:1149:TYR:O	2.35	0.58
3:D:279:LEU:HD13	3:D:295:GLU:HB3	1.85	0.58
7:b:212:ARG:HG3	7:b:213:ALA:N	2.18	0.58
7:f:34:ILE:CG2	7:f:42:LYS:HG3	2.33	0.58
7:f:50:HIS:CE1	7:f:60:PHE:CD1	2.91	0.58
8:M:156:ILE:H	8:M:156:ILE:HD13	1.67	0.58
7:a:254:PRO:HB2	7:f:173:VAL:CG2	2.34	0.58
7:d:128:GLU:CA	7:d:138:LEU:O	2.49	0.58
7:e:227:ARG:HG3	9:e:601:ADP:H5'2	1.85	0.58
7:a:78:PHE:HA	7:a:129:LEU:HD11	1.84	0.58
7:a:126:TYR:OH	7:b:43:GLU:HG2	2.03	0.58
7:a:222:TRP:CZ3	7:a:228:GLU:C	2.81	0.58
7:b:171:PHE:O	7:c:235:ARG:NE	2.36	0.58
7:f:227:ARG:HD2	7:e:167:ASP:HB3	1.86	0.58
8:M:111:VAL:HG22	8:M:111:VAL:O	2.04	0.58
8:M:193:LYS:O	8:M:193:LYS:HG3	2.03	0.58
1:A:95:LYS:NZ	1:A:120:ASP:OD2	2.36	0.58
2:C:876:GLU:HG3	2:C:927:THR:HB	1.85	0.58
5:N:-8:DT:H4'	7:b:90:LYS:HE2	1.85	0.58
6:T:0:DC:H2''	6:T:1:DA:C8	2.38	0.58
7:e:74:ASP:HB2	7:e:119:LYS:HZ3	1.65	0.58
3:D:1156:LEU:HD22	3:D:1208:ASP:HB3	1.84	0.58
5:N:-12:DC:H2'	8:M:17:PRO:HD3	1.83	0.58
2:C:887:VAL:HB	2:C:913:VAL:HB	1.84	0.58
5:N:-11:DA:H2''	5:N:-10:DG:H8	1.65	0.58
7:c:187:MET:HA	7:c:187:MET:CE	2.34	0.58
7:d:78:PHE:CD2	7:d:129:LEU:CD2	2.75	0.58
2:C:142:GLU:OE1	2:C:517:GLN:NE2	2.36	0.58
2:C:706:ARG:NH2	2:C:791:LEU:O	2.37	0.58
3:D:586:GLY:HA3	3:D:612:LEU:HD11	1.85	0.58
6:T:12:DT:C7	8:M:22:ALA:O	2.48	0.58
7:d:68:LEU:CD2	7:d:72:LEU:HD21	2.24	0.58
7:f:198:CYS:O	7:f:203:LEU:HB2	2.04	0.58
7:b:61:ILE:HD11	7:b:99:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:173:VAL:HG22	7:c:254:PRO:HB2	1.84	0.58
7:b:234:GLU:C	7:b:237:VAL:HG12	2.27	0.58
2:C:148:GLN:OE1	2:C:454:ARG:NH1	2.37	0.58
7:b:211:GLU:OE2	7:b:211:GLU:N	2.21	0.58
7:c:138:LEU:H	7:c:138:LEU:CD2	2.16	0.58
7:c:197:MET:HB2	7:c:234:GLU:HG2	1.85	0.58
7:d:84:ALA:HB2	7:e:90:LYS:HE2	1.85	0.58
8:M:455:ARG:C	8:M:455:ARG:CD	2.76	0.58
7:a:26:ALA:N	7:a:27:PRO:HD2	2.19	0.58
7:a:56:TRP:CZ3	7:a:57:GLN:HB3	2.39	0.58
7:a:89:GLN:O	7:a:90:LYS:HG2	2.04	0.58
7:e:37:GLU:OE1	7:e:37:GLU:HA	2.04	0.58
1:A:18:GLN:NE2	1:A:20:SER:O	2.37	0.57
7:c:114:MET:HE1	7:d:65:CYS:SG	2.44	0.57
7:c:170:ALA:O	7:d:235:ARG:CD	2.51	0.57
7:a:253:ASP:OD1	7:a:253:ASP:N	2.35	0.57
7:b:49:LEU:HD11	7:b:145:VAL:HG11	1.85	0.57
7:d:74:ASP:OD1	7:d:132:VAL:HG21	2.04	0.57
1:A:195:ARG:HD3	1:A:196:THR:HG22	1.87	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.86	0.57
7:b:121:LEU:O	7:b:122:ARG:CB	2.52	0.57
7:c:141:ASN:HD22	7:c:141:ASN:N	2.00	0.57
7:f:50:HIS:C	7:f:50:HIS:CD2	2.82	0.57
7:a:256:LYS:HD2	7:a:256:LYS:N	2.19	0.57
8:M:423:LEU:HD12	8:M:446:LEU:HD21	1.86	0.57
2:C:1154:ASP:OD1	2:C:1157:GLN:NE2	2.36	0.57
7:b:77:LEU:HD13	7:b:96:PHE:CD1	2.34	0.57
7:b:124:ILE:H	7:b:124:ILE:CD1	2.17	0.57
7:c:8:LEU:HA	9:c:400:ADP:N6	2.19	0.57
7:d:78:PHE:CE2	7:d:129:LEU:HD13	2.38	0.57
7:f:129:LEU:HD12	7:f:129:LEU:O	2.04	0.57
7:f:182:ARG:HE	7:f:185:ASP:HB2	1.69	0.57
8:M:355:PHE:H	8:M:355:PHE:HD1	1.53	0.57
1:A:45:ARG:NH2	2:C:1084:ASP:OD1	2.37	0.57
7:a:138:LEU:HD23	7:a:138:LEU:H	1.70	0.57
7:d:50:HIS:CB	7:d:60:PHE:CD1	2.88	0.57
7:d:130:GLU:HA	7:d:130:GLU:OE2	2.05	0.57
7:d:165:LEU:HD12	7:d:165:LEU:C	2.30	0.57
7:f:235:ARG:NH1	7:f:251:ILE:HG21	2.13	0.57
7:e:25:LEU:HB2	7:e:49:LEU:HD21	1.86	0.57
7:e:70:GLU:HA	7:e:70:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:9:LEU:HD12	9:b:601:ADP:C2	2.40	0.57
7:c:123:VAL:HG13	7:c:129:LEU:HG	1.85	0.57
7:d:179:LEU:HG	7:d:225:ASN:HA	1.87	0.57
8:M:330:ILE:O	8:M:330:ILE:HG22	2.02	0.57
2:C:661:VAL:HG21	2:C:1186:VAL:HG11	1.86	0.57
2:C:901:LEU:HD11	8:M:224:LEU:HD11	1.87	0.57
1:A:101:THR:HG22	1:A:143:ARG:HG2	1.86	0.57
1:B:191:ARG:NH2	1:B:193:GLU:O	2.38	0.57
3:D:884:SER:HA	3:D:898:CYS:HB2	1.87	0.57
7:d:40:THR:CA	7:d:225:ASN:HB3	2.32	0.57
7:f:51:TYR:CD1	7:f:51:TYR:N	2.72	0.57
7:e:72:LEU:H	7:e:72:LEU:CD2	2.18	0.57
8:M:364:PRO:HB3	8:M:416:SER:HA	1.86	0.57
2:C:303:ASP:HA	2:C:329:GLY:HA2	1.86	0.57
7:a:46:ALA:HB1	7:a:105:PHE:CD1	2.39	0.57
7:b:46:ALA:HB1	7:b:105:PHE:HD2	1.69	0.57
7:b:111:THR:O	7:b:112:ALA:C	2.47	0.57
7:d:33:LEU:HD21	7:d:35:ILE:HD11	1.87	0.57
7:f:222:TRP:N	7:f:223:PRO:HD3	2.19	0.57
7:d:78:PHE:HD2	7:d:129:LEU:CG	2.18	0.56
7:d:176:LEU:CD1	7:d:177:PRO:CD	2.75	0.56
7:f:45:ILE:O	7:f:49:LEU:HB2	2.05	0.56
8:M:131:THR:HG23	8:M:133:PHE:CZ	2.39	0.56
7:b:201:ILE:HD12	7:b:201:ILE:O	2.05	0.56
7:f:255:PHE:HZ	7:e:152:LEU:HB2	1.69	0.56
1:B:64:VAL:HG12	1:B:66:HIS:H	1.70	0.56
2:C:802:VAL:HG12	2:C:1096:ILE:HB	1.87	0.56
7:a:63:LEU:HD12	7:a:104:LEU:HG	1.87	0.56
7:a:252:ILE:H	7:a:252:ILE:CD1	2.18	0.56
7:c:41:GLY:O	7:c:45:ILE:CG1	2.54	0.56
7:c:58:GLY:HA3	7:c:102:GLY:HA2	1.87	0.56
7:c:230:LYS:O	7:c:233:VAL:CG1	2.47	0.56
7:d:50:HIS:ND1	7:d:103:THR:HG22	2.21	0.56
7:d:158:GLU:HG3	7:d:160:THR:HG23	1.86	0.56
7:d:158:GLU:HG3	7:d:158:GLU:O	2.06	0.56
7:f:1:MET:HB3	7:f:56:TRP:CD1	2.40	0.56
7:f:43:GLU:OE1	7:f:43:GLU:HA	2.06	0.56
1:B:11:PRO:HA	1:B:29:GLU:HG2	1.87	0.56
2:C:657:THR:HB	2:C:1187:PHE:HB2	1.87	0.56
7:b:168:ARG:CZ	7:c:227:ARG:HH12	2.18	0.56
7:f:26:ALA:CB	7:f:52:LEU:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:34:ILE:HG13	7:f:147:ALA:HB2	1.87	0.56
7:f:235:ARG:HH11	7:f:251:ILE:HG21	1.69	0.56
7:b:59:PRO:HD2	7:b:102:GLY:CA	2.26	0.56
7:c:121:LEU:C	7:c:121:LEU:HD12	2.30	0.56
7:c:175:GLN:O	7:c:176:LEU:HD23	2.05	0.56
7:d:61:ILE:CD1	7:d:95:ARG:NH1	2.67	0.56
7:f:227:ARG:HH12	7:e:168:ARG:NH1	2.03	0.56
8:M:182:ILE:HG23	8:M:185:PHE:HE2	1.61	0.56
8:M:386:THR:O	8:M:388:LYS:HG2	2.06	0.56
3:D:553:THR:HG22	3:D:567:THR:HG22	1.87	0.56
7:b:31:PRO:HB2	7:b:170:ALA:N	2.12	0.56
7:d:28:LEU:HD12	7:d:28:LEU:O	2.05	0.56
8:M:342:ARG:HH22	8:M:376:MET:HE2	1.70	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.69	0.56
7:b:131:ARG:HH22	7:b:138:LEU:HD13	1.70	0.56
7:e:33:LEU:CD1	7:e:34:ILE:N	2.66	0.56
8:M:420:ILE:CD1	8:M:451:ILE:CG2	2.78	0.56
3:D:980:THR:OG1	3:D:997:VAL:O	2.24	0.56
7:c:8:LEU:CD1	7:c:15:PHE:CE2	2.87	0.56
7:d:68:LEU:HD12	7:d:76:GLU:HB2	1.87	0.56
7:d:148:THR:OG1	7:d:149:ASN:N	2.39	0.56
7:e:26:ALA:HB1	7:e:53:SER:HA	1.81	0.56
7:e:36:GLY:C	7:e:42:LYS:HE3	2.30	0.56
7:e:78:PHE:CE1	7:e:123:VAL:CG2	2.83	0.56
7:e:103:THR:HG22	7:e:143:ARG:HB3	1.88	0.56
8:M:18:GLN:NE2	8:M:328:TRP:NE1	2.51	0.56
8:M:329:LEU:O	8:M:329:LEU:HD13	2.06	0.56
3:D:355:ILE:HD12	3:D:449:LEU:HB2	1.88	0.56
3:D:901:ARG:HD2	3:D:902:ASP:H	1.71	0.56
7:a:178:PRO:HB2	7:a:180:ARG:HD3	1.88	0.56
7:c:32:VAL:N	7:c:145:VAL:CG1	2.59	0.56
7:d:121:LEU:HD12	7:d:121:LEU:C	2.30	0.56
7:f:197:MET:HG2	7:f:237:VAL:HG13	1.85	0.56
1:A:12:ARG:H	1:A:29:GLU:HB2	1.70	0.56
2:C:17:LYS:NZ	2:C:1194:GLU:OE2	2.38	0.56
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.87	0.56
7:a:104:LEU:O	7:a:145:VAL:CG1	2.52	0.56
7:a:111:THR:CG2	7:f:162:ARG:NH2	2.57	0.56
7:a:179:LEU:HD23	7:a:225:ASN:O	2.04	0.56
7:d:164:ASP:HB2	7:e:227:ARG:NH2	2.21	0.56
8:M:203:LEU:CD2	8:M:256:LEU:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:351:GLN:NE2	8:M:362:MET:CG	2.68	0.56
6:T:12:DT:C7	8:M:22:ALA:C	2.79	0.55
7:a:73:LEU:C	7:a:75:SER:N	2.64	0.55
7:b:61:ILE:O	7:b:61:ILE:HG13	2.04	0.55
7:b:165:LEU:HD12	7:b:165:LEU:O	2.06	0.55
7:c:8:LEU:HA	7:c:44:LEU:HD11	1.87	0.55
7:c:37:GLU:HB2	7:c:40:THR:HG21	1.88	0.55
7:c:152:LEU:CB	7:c:166:LEU:CD1	2.83	0.55
7:c:230:LYS:CA	7:c:233:VAL:CG1	2.77	0.55
2:C:906:PHE:HZ	8:M:199:LEU:HD21	1.70	0.55
7:a:119:LYS:HG3	7:b:67:ALA:HB1	1.88	0.55
7:a:197:MET:HB2	7:a:234:GLU:CD	2.32	0.55
7:b:25:LEU:HD23	7:c:238:TYR:HE2	1.69	0.55
7:d:74:ASP:OD1	7:d:132:VAL:CG2	2.53	0.55
7:e:120:LEU:HD12	7:e:120:LEU:O	2.06	0.55
8:M:278:VAL:HG21	8:M:392:SER:HB3	1.88	0.55
8:M:355:PHE:CD1	8:M:355:PHE:N	2.74	0.55
3:D:141:PHE:O	3:D:293:ARG:NH2	2.40	0.55
7:b:54:SER:C	7:b:56:TRP:H	2.15	0.55
7:b:186:ILE:O	7:b:190:ALA:HB3	2.06	0.55
7:c:8:LEU:CB	7:c:44:LEU:HD11	2.36	0.55
7:e:155:MET:HA	7:e:158:GLU:HG3	1.88	0.55
7:e:222:TRP:CZ3	7:e:229:LEU:HD12	2.41	0.55
8:M:360:GLU:OE2	8:M:423:LEU:HD23	2.06	0.55
8:M:424:VAL:HG13	8:M:428:ILE:HD11	1.88	0.55
2:C:1275:VAL:HG23	2:C:1287:LEU:HD11	1.87	0.55
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.88	0.55
6:T:21:DC:H2'	6:T:22:DG:C8	2.41	0.55
7:a:59:PRO:HD2	7:a:102:GLY:HA3	1.89	0.55
7:c:37:GLU:C	7:c:40:THR:HG22	2.31	0.55
7:d:180:ARG:CG	7:d:181:GLU:OE1	2.55	0.55
7:e:191:GLU:O	7:e:195:ILE:HG13	2.06	0.55
8:M:154:LEU:CD1	8:M:193:LYS:HB2	2.27	0.55
6:T:31:DG:C2'	8:M:233:ARG:HH22	2.19	0.55
7:a:129:LEU:O	7:a:129:LEU:HD23	2.05	0.55
7:d:125:GLU:OE1	7:e:227:ARG:NH1	2.39	0.55
8:M:427:LEU:O	8:M:427:LEU:HD12	2.07	0.55
6:T:12:DT:C7	8:M:22:ALA:HB1	2.35	0.55
7:a:210:THR:OG1	7:a:248:ASP:CA	2.55	0.55
7:b:136:GLN:OE1	7:b:136:GLN:N	2.40	0.55
7:b:166:LEU:HD23	7:b:166:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:15:PHE:CD2	7:f:182:ARG:CD	2.66	0.55
7:f:230:LYS:O	7:f:231:ASN:C	2.47	0.55
7:e:22:VAL:O	7:e:25:LEU:HB2	2.06	0.55
7:a:24:HIS:C	7:b:238:TYR:OH	2.49	0.55
7:a:126:TYR:N	7:a:126:TYR:CD1	2.73	0.55
7:a:217:LEU:HB2	7:a:218:LEU:HD23	1.87	0.55
7:e:31:PRO:HB2	7:e:171:PHE:HB2	1.89	0.55
7:e:121:LEU:HD23	7:e:121:LEU:O	2.06	0.55
7:e:152:LEU:HB2	7:e:153:PRO:HD3	1.88	0.55
8:M:423:LEU:O	8:M:426:LYS:HG3	2.07	0.55
3:D:64:PRO:O	3:D:98:ARG:NH1	2.40	0.55
6:T:6:DT:H2''	6:T:7:DG:C5'	2.37	0.55
6:T:13:DG:H2''	6:T:14:DC:C6	2.42	0.55
7:a:176:LEU:HD23	7:a:176:LEU:N	2.21	0.55
7:a:193:PHE:HE2	7:a:229:LEU:CD1	2.06	0.55
7:b:173:VAL:HG23	7:b:173:VAL:O	2.06	0.55
7:c:121:LEU:HD23	7:c:162:ARG:HD2	1.89	0.55
7:c:179:LEU:HD11	7:c:222:TRP:HB3	1.89	0.55
7:f:227:ARG:CD	7:e:167:ASP:HB3	2.36	0.55
8:M:276:VAL:C	8:M:277:LEU:HD22	2.31	0.55
2:C:911:SER:HB3	8:M:259:ARG:CZ	2.36	0.55
7:a:211:GLU:N	7:a:211:GLU:OE2	2.40	0.55
7:b:125:GLU:HG3	7:b:168:ARG:HH21	1.72	0.55
7:c:22:VAL:CG1	7:c:49:LEU:HD23	2.37	0.55
7:c:170:ALA:O	7:d:235:ARG:HD3	2.07	0.55
7:e:73:LEU:HD21	7:e:116:VAL:HG22	1.89	0.55
7:e:78:PHE:CE1	7:e:123:VAL:HG21	2.42	0.55
2:C:840:SER:HB2	2:C:1047:LEU:HB3	1.89	0.55
3:D:644:MET:O	3:D:764:ARG:NH1	2.40	0.55
7:e:104:LEU:CD2	7:e:144:LEU:HA	2.37	0.55
7:e:113:PRO:HB2	7:e:116:VAL:HG23	1.88	0.55
8:M:197:ASP:O	8:M:201:ILE:CD1	2.48	0.55
2:C:877:VAL:HG23	2:C:881:ASP:HB2	1.88	0.54
7:b:46:ALA:CB	7:b:105:PHE:CD2	2.90	0.54
7:c:114:MET:HG2	7:d:67:ALA:CB	2.35	0.54
7:c:165:LEU:CD2	7:c:169:LEU:HD21	2.37	0.54
7:d:116:VAL:O	7:d:120:LEU:CD2	2.50	0.54
7:f:50:HIS:CG	7:f:60:PHE:CD1	2.95	0.54
7:e:78:PHE:HZ	7:e:119:LYS:O	1.90	0.54
7:e:210:THR:O	7:e:212:ARG:N	2.40	0.54
8:M:144:ILE:HG22	8:M:145:VAL:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:303:TYR:HA	8:M:306:MET:SD	2.47	0.54
1:A:308:ALA:HA	1:A:313:SER:H	1.71	0.54
7:a:152:LEU:N	7:a:153:PRO:HD2	2.22	0.54
7:b:179:LEU:HD12	7:b:226:ILE:HD13	1.89	0.54
7:d:7:ASN:HD22	7:d:7:ASN:N	2.05	0.54
7:f:226:ILE:HG21	9:f:601:ADP:C4	2.40	0.54
8:M:212:TRP:NE1	8:M:248:GLU:OE2	2.40	0.54
8:M:235:LEU:CD1	8:M:246:LEU:CD1	2.85	0.54
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.88	0.54
5:N:-21:DG:H2''	5:N:-20:DA:C8	2.42	0.54
7:a:197:MET:HB2	7:a:234:GLU:OE1	2.07	0.54
7:a:250:ILE:HD13	7:a:250:ILE:N	2.15	0.54
7:b:91:ARG:HH21	7:b:91:ARG:CG	2.20	0.54
2:C:548:ARG:HB2	2:C:570:GLY:HA3	1.88	0.54
5:N:-13:DC:C1'	8:M:15:MET:HE2	2.32	0.54
5:N:-8:DT:C4'	7:b:90:LYS:HE2	2.36	0.54
7:a:49:LEU:HD23	7:a:49:LEU:N	2.21	0.54
7:b:63:LEU:CD2	7:b:106:LEU:CD2	2.75	0.54
7:b:114:MET:SD	7:b:160:THR:O	2.65	0.54
7:b:130:GLU:N	7:b:130:GLU:OE2	2.40	0.54
7:c:104:LEU:N	7:c:104:LEU:HD12	2.22	0.54
7:c:131:ARG:HH11	7:c:138:LEU:HD21	1.72	0.54
7:d:161:PHE:CD2	7:d:166:LEU:HD12	2.42	0.54
8:M:18:GLN:HE21	8:M:18:GLN:C	2.15	0.54
7:c:26:ALA:HB1	7:c:52:LEU:HB3	1.89	0.54
7:c:118:GLU:HB2	7:c:162:ARG:HE	1.71	0.54
7:f:152:LEU:HB3	7:f:166:LEU:HD22	1.90	0.54
7:f:253:ASP:C	7:f:253:ASP:OD1	2.51	0.54
7:e:32:VAL:O	7:e:145:VAL:HA	2.06	0.54
7:e:179:LEU:O	7:e:182:ARG:HB2	2.07	0.54
8:M:280:LYS:HD3	8:M:285:TRP:CE3	2.42	0.54
7:a:64:ASN:CB	7:a:67:ALA:CB	2.80	0.54
7:c:47:SER:HB2	7:c:51:TYR:CE2	2.43	0.54
7:e:201:ILE:CD1	7:e:203:LEU:HD22	2.37	0.54
7:e:210:THR:O	7:e:210:THR:HG22	2.08	0.54
7:a:24:HIS:C	7:b:238:TYR:HH	2.16	0.54
7:a:34:ILE:CG1	7:a:147:ALA:HB2	2.37	0.54
7:a:56:TRP:C	7:a:56:TRP:CE3	2.85	0.54
7:a:129:LEU:O	7:a:138:LEU:CD2	2.52	0.54
7:c:114:MET:CG	7:d:67:ALA:CB	2.86	0.54
7:c:193:PHE:HZ	7:c:226:ILE:HG22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:189:MET:HE1	7:f:226:ILE:HD12	1.90	0.54
7:f:221:ARG:C	7:f:223:PRO:HD3	2.33	0.54
7:f:245:TYR:HB2	7:f:246:PRO:HD2	1.89	0.54
7:e:43:GLU:OE1	7:e:105:PHE:CD2	2.60	0.54
8:M:256:LEU:O	8:M:257:ASP:C	2.49	0.54
8:M:275:ASP:N	8:M:389:TYR:O	2.32	0.54
1:B:190:ALA:O	1:B:198:LEU:HB2	2.08	0.54
3:D:422:LEU:HG	3:D:469:HIS:HB2	1.88	0.54
6:T:15:DA:OP1	8:M:11:GLN:NE2	2.41	0.54
7:f:81:GLU:CG	7:f:131:ARG:CD	2.84	0.54
7:e:104:LEU:O	7:e:145:VAL:HG22	2.08	0.54
8:M:120:LEU:O	8:M:123:TYR:HB3	2.07	0.54
2:C:180:ARG:HH22	2:C:396:ASP:HB3	1.73	0.54
2:C:901:LEU:HD11	8:M:224:LEU:CD1	2.38	0.54
7:a:171:PHE:CE2	7:b:234:GLU:HG2	2.40	0.54
7:b:162:ARG:HH12	7:c:67:ALA:HA	1.73	0.54
7:e:44:LEU:HD11	9:e:601:ADP:C3'	2.38	0.54
2:C:251:ALA:HB1	2:C:255:ILE:HG13	1.89	0.54
3:D:43:THR:HG23	3:D:270:ARG:HH12	1.72	0.54
7:a:171:PHE:CD1	7:a:171:PHE:C	2.85	0.54
7:a:192:TYR:CD1	7:a:192:TYR:C	2.86	0.54
7:c:179:LEU:HD23	7:c:225:ASN:HB3	1.89	0.54
7:c:255:PHE:HD1	7:c:255:PHE:H	1.56	0.54
7:d:155:MET:CB	7:d:160:THR:OG1	2.40	0.54
8:M:285:TRP:CZ2	8:M:355:PHE:HB2	2.41	0.54
7:b:122:ARG:H	7:b:124:ILE:HD11	1.72	0.53
7:c:152:LEU:HD11	7:c:161:PHE:CE2	2.42	0.53
1:A:192:VAL:HG13	1:A:192:VAL:O	2.07	0.53
2:C:32:LEU:HA	2:C:130:MET:HE1	1.90	0.53
7:b:238:TYR:O	7:b:239:ARG:C	2.49	0.53
7:c:63:LEU:O	7:c:107:ASP:N	2.39	0.53
7:c:99:ALA:HB1	7:c:104:LEU:CG	2.38	0.53
7:f:203:LEU:CD2	7:f:204:PRO:HD2	2.38	0.53
8:M:195:LEU:CD1	8:M:199:LEU:HD12	2.36	0.53
2:C:11:ILE:HG21	2:C:1158:LYS:HE2	1.89	0.53
2:C:724:VAL:HG22	2:C:734:ILE:HG12	1.90	0.53
2:C:957:LYS:HE3	2:C:1029:LEU:HD11	1.91	0.53
3:D:41:PRO:HB2	3:D:270:ARG:HG3	1.90	0.53
7:a:216:THR:HG21	7:a:250:ILE:HD11	0.66	0.53
7:b:11:GLU:HG3	7:b:11:GLU:O	2.08	0.53
7:f:26:ALA:O	7:f:53:SER:CA	2.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:85:PHE:CZ	8:M:5:LEU:HD22	2.40	0.53
8:M:28:LEU:CD1	8:M:33:LEU:CB	2.86	0.53
2:C:12:ARG:NH1	2:C:705:GLU:OE2	2.42	0.53
2:C:1244:HIS:NE2	2:C:1266:GLY:O	2.40	0.53
3:D:331:ILE:HA	3:D:337:ARG:H	1.73	0.53
7:c:224:GLY:HA3	7:c:228:GLU:CB	2.28	0.53
7:d:40:THR:HG22	7:d:225:ASN:CB	2.28	0.53
7:f:255:PHE:CE1	7:e:153:PRO:CD	2.90	0.53
7:e:73:LEU:CD2	7:e:116:VAL:HG22	2.39	0.53
8:M:342:ARG:HH11	8:M:342:ARG:CB	2.20	0.53
8:M:428:ILE:HG23	8:M:473:ARG:NH1	2.23	0.53
8:M:455:ARG:HD2	8:M:456:ARG:N	2.23	0.53
1:A:301:THR:HG21	8:M:174:GLU:HG2	1.90	0.53
7:a:73:LEU:O	7:a:75:SER:N	2.42	0.53
3:D:490:ILE:HD13	3:D:500:ILE:HD13	1.89	0.53
3:D:576:ARG:NH1	3:D:593:ASN:OD1	2.42	0.53
6:T:31:DG:P	8:M:233:ARG:HH12	2.31	0.53
7:b:143:ARG:NH1	7:b:143:ARG:HG3	2.24	0.53
7:b:220:TYR:HB3	7:b:222:TRP:CD1	2.43	0.53
7:b:222:TRP:CH2	7:b:229:LEU:CD1	2.92	0.53
7:f:24:HIS:O	7:f:27:PRO:HG2	2.08	0.53
7:f:103:THR:CG2	7:f:143:ARG:HG2	2.38	0.53
7:f:222:TRP:CH2	7:f:229:LEU:HA	2.43	0.53
3:D:1145:PHE:HB3	3:D:1309:ILE:HD12	1.91	0.53
5:N:-13:DC:C2	8:M:15:MET:SD	3.01	0.53
7:a:156:VAL:HG13	7:a:163:ALA:HA	1.91	0.53
7:c:25:LEU:C	7:c:25:LEU:HD12	2.34	0.53
7:c:35:ILE:HA	7:c:148:THR:O	2.09	0.53
7:c:193:PHE:CZ	7:c:226:ILE:HG22	2.44	0.53
8:M:46:LEU:HD11	8:M:322:ASN:CB	2.33	0.53
7:a:205:LEU:CD1	7:a:206:PHE:N	2.57	0.53
7:c:153:PRO:HG2	7:d:255:PHE:CD2	2.44	0.53
7:f:164:ASP:HA	7:f:167:ASP:HB2	1.90	0.53
8:M:176:GLU:O	8:M:180:LYS:HG3	2.08	0.53
8:M:182:ILE:CG2	8:M:185:PHE:HD2	2.14	0.53
1:A:60:GLU:HB3	1:A:170:ARG:HG3	1.90	0.53
5:N:-13:DC:H2'	8:M:15:MET:HE3	1.82	0.53
7:a:35:ILE:HG12	7:a:173:VAL:CG1	2.39	0.53
7:b:42:LYS:HB3	7:b:42:LYS:NZ	2.24	0.53
7:b:43:GLU:HA	7:b:43:GLU:OE1	2.09	0.53
7:b:122:ARG:HB2	7:b:122:ARG:CZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:165:LEU:HD23	7:c:169:LEU:HD21	1.90	0.53
7:d:8:LEU:HD23	7:d:44:LEU:CD1	2.39	0.53
7:f:188:LEU:CD1	7:f:188:LEU:H	2.22	0.53
7:e:62:SER:CB	7:e:105:PHE:HB3	2.39	0.53
7:e:171:PHE:C	7:e:171:PHE:CD1	2.86	0.53
7:a:96:PHE:CZ	7:a:123:VAL:HG11	2.37	0.53
7:a:222:TRP:CZ3	7:a:228:GLU:CG	2.84	0.53
7:f:68:LEU:HD23	7:f:68:LEU:C	2.34	0.53
7:f:224:GLY:O	7:f:228:GLU:HB3	2.09	0.53
1:A:45:ARG:HH11	1:B:38:THR:HG1	1.56	0.52
2:C:211:ARG:NH1	2:C:354:ASP:OD2	2.42	0.52
7:c:8:LEU:CD1	7:c:15:PHE:HZ	2.06	0.52
7:c:32:VAL:H	7:c:145:VAL:CB	2.21	0.52
7:d:230:LYS:HG2	7:d:234:GLU:OE1	2.09	0.52
7:f:140:VAL:O	7:f:140:VAL:HG23	2.07	0.52
7:e:91:ARG:HH21	7:e:91:ARG:CG	2.12	0.52
8:M:119:THR:CG2	8:M:122:ASP:OD2	2.57	0.52
8:M:275:ASP:HB2	8:M:389:TYR:O	2.09	0.52
8:M:364:PRO:HB2	8:M:406:HIS:HB3	1.91	0.52
2:C:931:VAL:HG12	2:C:1052:VAL:HG22	1.90	0.52
5:N:-15:DT:C5	8:M:383:ARG:NH2	2.77	0.52
7:a:8:LEU:CG	7:a:15:PHE:CZ	2.75	0.52
7:a:171:PHE:HE2	7:b:234:GLU:CG	2.22	0.52
7:a:211:GLU:OE1	7:a:212:ARG:HB2	2.09	0.52
7:b:48:ARG:HG3	7:b:52:LEU:HD11	1.90	0.52
7:c:8:LEU:CB	7:c:44:LEU:HD21	2.38	0.52
7:c:59:PRO:HD2	7:c:101:GLY:O	2.09	0.52
7:f:26:ALA:N	7:f:27:PRO:HD2	2.23	0.52
7:f:80:HIS:H	7:f:92:HIS:HB3	1.73	0.52
2:C:525:THR:OG1	2:C:562:GLU:OE2	2.28	0.52
2:C:1060:ILE:HD13	2:C:1060:ILE:H	1.73	0.52
3:D:1314:LEU:HA	3:D:1322:ALA:HB1	1.91	0.52
7:a:78:PHE:CD1	7:a:78:PHE:N	2.73	0.52
7:c:76:GLU:O	7:c:94:GLY:HA3	2.08	0.52
7:f:15:PHE:CE2	7:f:182:ARG:NH2	2.76	0.52
8:M:357:GLN:CB	8:M:361:TYR:CB	2.81	0.52
6:T:13:DG:OP2	8:M:377:HIS:CB	2.57	0.52
7:a:64:ASN:CB	7:a:67:ALA:HB2	2.39	0.52
7:b:42:LYS:HB3	7:b:42:LYS:HZ3	1.71	0.52
7:b:44:LEU:O	7:b:47:SER:OG	2.22	0.52
7:d:26:ALA:N	7:d:27:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:104:LEU:O	7:d:145:VAL:N	2.39	0.52
7:f:227:ARG:NH1	7:e:168:ARG:NH1	2.57	0.52
8:M:468:PRO:HB2	8:M:469:PRO:HD2	1.91	0.52
1:A:96:ASP:HB3	1:A:148:ARG:HH11	1.75	0.52
7:a:165:LEU:HD23	7:a:165:LEU:C	2.35	0.52
7:c:42:LYS:HE3	9:c:400:ADP:O2B	2.10	0.52
7:c:68:LEU:N	7:c:68:LEU:CD2	2.73	0.52
7:c:153:PRO:CG	7:d:255:PHE:CD2	2.93	0.52
7:e:78:PHE:HE1	7:e:123:VAL:HG21	1.70	0.52
3:D:1230:THR:HG22	3:D:1257:VAL:HG11	1.92	0.52
7:a:86:THR:CB	8:M:8:ARG:HB2	2.39	0.52
7:a:103:THR:HG21	7:a:143:ARG:HD3	1.92	0.52
7:a:179:LEU:HD11	7:a:226:ILE:CD1	2.40	0.52
7:a:256:LYS:HA	7:a:256:LYS:CE	2.36	0.52
7:b:249:ASP:C	7:b:250:ILE:HD13	2.34	0.52
7:c:114:MET:CB	7:d:67:ALA:CB	2.82	0.52
7:d:40:THR:HA	7:d:225:ASN:HD22	1.74	0.52
7:f:195:ILE:HA	7:f:198:CYS:SG	2.50	0.52
8:M:439:ASP:OD1	8:M:462:ARG:HD3	2.10	0.52
7:a:42:LYS:HB2	9:a:601:ADP:O3B	2.08	0.52
7:a:188:LEU:O	7:a:188:LEU:HD22	2.09	0.52
7:b:59:PRO:O	7:b:59:PRO:CD	2.57	0.52
7:c:157:ASN:HD22	7:c:157:ASN:N	2.06	0.52
9:f:601:ADP:N3	9:f:601:ADP:O2'	2.34	0.52
8:M:425:LYS:NZ	8:M:425:LYS:CB	2.73	0.52
2:C:929:ILE:HD11	2:C:1055:ALA:HB2	1.92	0.52
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.92	0.52
7:c:106:LEU:HD22	7:c:106:LEU:N	2.24	0.52
7:d:150:ALA:O	7:d:152:LEU:HD23	2.09	0.52
7:d:153:PRO:CG	7:e:255:PHE:CE2	2.93	0.52
7:f:97:GLU:OE1	7:f:131:ARG:NH2	2.42	0.52
7:f:168:ARG:HG3	7:f:168:ARG:O	2.09	0.52
7:f:255:PHE:CZ	7:e:152:LEU:HB2	2.45	0.52
7:e:191:GLU:O	7:e:194:ALA:HB3	2.09	0.52
8:M:213:LEU:CD1	8:M:217:ARG:NH2	2.58	0.52
8:M:308:ASN:C	8:M:310:ALA:H	2.17	0.52
1:B:108:GLY:HA2	1:B:134:THR:HG22	1.92	0.52
7:b:42:LYS:NZ	7:b:42:LYS:CB	2.73	0.52
7:d:61:ILE:CD1	7:d:95:ARG:HD2	2.38	0.52
7:e:35:ILE:HA	7:e:148:THR:CG2	2.39	0.52
8:M:158:ILE:HG13	8:M:193:LYS:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD13	1:B:173:VAL:HG22	1.92	0.52
2:C:4:SER:O	2:C:8:LYS:N	2.40	0.52
7:a:138:LEU:N	7:a:138:LEU:CD2	2.73	0.52
7:b:81:GLU:HG3	7:b:131:ARG:CD	2.38	0.52
7:b:138:LEU:HD23	7:b:138:LEU:H	1.75	0.52
7:c:6:ASP:C	7:c:8:LEU:H	2.17	0.52
7:c:152:LEU:N	7:c:153:PRO:CD	2.73	0.52
7:d:231:ASN:HD22	7:d:231:ASN:N	2.07	0.52
7:d:231:ASN:O	7:d:235:ARG:HB2	2.10	0.52
7:e:179:LEU:N	7:e:225:ASN:OD1	2.35	0.52
8:M:258:PRO:O	8:M:259:ARG:HB3	2.09	0.52
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.92	0.51
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.92	0.51
3:D:370:LYS:HA	3:D:373:ALA:HB3	1.92	0.51
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.92	0.51
7:a:61:ILE:HG21	7:a:95:ARG:HG2	1.92	0.51
7:a:204:PRO:HG2	7:a:205:LEU:N	2.17	0.51
7:b:28:LEU:HD13	7:c:197:MET:HE3	1.91	0.51
7:b:129:LEU:H	7:b:129:LEU:CD2	2.23	0.51
7:c:14:SER:O	7:c:18:VAL:HG23	2.10	0.51
7:d:8:LEU:N	7:d:8:LEU:CD1	2.73	0.51
7:f:235:ARG:HH11	7:f:251:ILE:HB	1.73	0.51
7:e:36:GLY:HA3	7:e:42:LYS:HE3	1.91	0.51
8:M:453:VAL:O	8:M:454:ALA:CB	2.55	0.51
1:B:91:ARG:NH2	1:B:122:GLU:OE1	2.42	0.51
2:C:678:ARG:NH1	2:C:681:MET:SD	2.83	0.51
7:a:152:LEU:N	7:a:153:PRO:CD	2.73	0.51
7:b:72:LEU:N	7:b:72:LEU:CD2	2.73	0.51
7:b:103:THR:HG22	7:b:143:ARG:CG	2.40	0.51
7:c:46:ALA:HA	7:c:105:PHE:CZ	2.45	0.51
7:f:49:LEU:HD23	7:f:49:LEU:C	2.34	0.51
7:e:34:ILE:HG22	7:e:35:ILE:N	2.23	0.51
8:M:13:LEU:N	8:M:13:LEU:CD1	2.73	0.51
8:M:165:ILE:HG22	8:M:167:ASP:H	1.75	0.51
7:a:32:VAL:CG2	7:a:172:ASP:O	2.58	0.51
7:a:178:PRO:HD2	7:a:181:GLU:OE1	2.10	0.51
7:b:195:ILE:HA	7:b:206:PHE:HE1	1.64	0.51
7:d:158:GLU:OE2	7:d:160:THR:HG21	2.10	0.51
7:f:26:ALA:CB	7:f:52:LEU:CB	2.89	0.51
7:e:182:ARG:HH22	7:e:226:ILE:HD11	1.76	0.51
8:M:29:SER:O	8:M:33:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:939:VAL:HG21	2:C:1047:LEU:HD11	1.91	0.51
7:a:250:ILE:CD1	7:a:250:ILE:N	2.73	0.51
7:b:200:GLU:OE1	7:b:200:GLU:HA	2.10	0.51
7:d:70:GLU:OE1	7:d:70:GLU:N	2.43	0.51
8:M:109:LEU:N	8:M:109:LEU:CD1	2.73	0.51
8:M:131:THR:CG2	8:M:133:PHE:CE2	2.93	0.51
2:C:700:VAL:HG13	2:C:1117:LEU:HD23	1.92	0.51
3:D:1177:ILE:HD11	3:D:1187:GLU:HA	1.91	0.51
7:c:238:TYR:C	7:c:238:TYR:CD1	2.88	0.51
7:f:61:ILE:O	7:f:61:ILE:HG23	2.10	0.51
2:C:237:LEU:HD21	2:C:292:ILE:HD11	1.93	0.51
3:D:425:ARG:HB2	3:D:457:TYR:HD1	1.74	0.51
7:c:104:LEU:HB2	7:c:144:LEU:CB	2.41	0.51
7:f:206:PHE:CD1	7:f:207:PRO:HD2	2.45	0.51
7:e:42:LYS:NZ	7:e:42:LYS:CB	2.73	0.51
7:e:176:LEU:N	7:e:176:LEU:CD2	2.73	0.51
8:M:158:ILE:HD11	8:M:193:LYS:CE	2.40	0.51
2:C:866:ASP:HB3	2:C:944:ARG:NH2	2.25	0.51
3:D:827:GLU:OE1	3:D:828:GLY:N	2.44	0.51
7:a:33:LEU:O	7:a:173:VAL:HA	2.11	0.51
7:a:169:LEU:HD12	7:a:170:ALA:N	2.25	0.51
7:c:235:ARG:O	7:c:239:ARG:HG2	2.10	0.51
7:f:50:HIS:CE1	7:f:60:PHE:CG	2.98	0.51
8:M:9:LEU:N	8:M:9:LEU:CD2	2.73	0.51
8:M:444:SER:O	8:M:447:SER:OG	2.27	0.51
7:a:175:GLN:H	7:a:175:GLN:CD	2.16	0.51
7:c:104:LEU:HD12	7:c:143:ARG:C	2.36	0.51
7:d:64:ASN:HB3	7:d:106:LEU:CD1	2.40	0.51
7:f:5:LYS:NZ	7:f:5:LYS:CB	2.73	0.51
7:e:136:GLN:HB3	7:e:137:PRO:CD	2.40	0.51
1:B:191:ARG:HB3	1:B:196:THR:HA	1.93	0.51
2:C:12:ARG:HA	2:C:1181:PRO:HB2	1.93	0.51
3:D:1033:GLY:HA3	3:D:1082:ASP:HA	1.93	0.51
7:a:37:GLU:CB	7:a:225:ASN:ND2	2.68	0.51
7:a:255:PHE:CE1	7:f:153:PRO:HD3	2.46	0.51
7:b:33:LEU:HD13	7:b:146:CYS:HB3	1.91	0.51
7:c:64:ASN:HD22	7:c:107:ASP:HB2	1.76	0.51
7:c:239:ARG:HG3	7:c:251:ILE:HD11	1.93	0.51
7:e:199:ARG:HB3	7:e:199:ARG:CZ	2.40	0.51
8:M:343:VAL:O	8:M:347:ILE:CG2	2.52	0.51
5:N:-8:DT:C5'	7:b:90:LYS:NZ	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:57:GLN:OE1	7:b:57:GLN:HA	2.10	0.51
7:b:61:ILE:CD1	7:b:99:ALA:HB2	2.40	0.51
7:b:131:ARG:O	7:b:132:VAL:C	2.54	0.51
7:d:10:GLY:N	7:d:15:PHE:CD2	2.78	0.51
7:d:118:GLU:HA	7:d:118:GLU:OE2	2.11	0.51
7:f:51:TYR:H	7:f:51:TYR:HD1	1.58	0.51
7:f:196:GLN:C	7:f:199:ARG:HG2	2.36	0.51
7:e:207:PRO:CG	7:e:246:PRO:HA	2.41	0.51
1:A:58:GLU:HG3	1:A:172:LEU:HG	1.93	0.50
1:A:253:LEU:HB3	1:A:278:ILE:HD12	1.92	0.50
1:A:256:PRO:HA	1:A:277:TYR:HB3	1.92	0.50
2:C:798:GLN:HG2	2:C:827:ARG:HE	1.76	0.50
3:D:885:VAL:CG2	3:D:894:VAL:HG21	2.41	0.50
7:a:109:LEU:HD22	7:a:146:CYS:SG	2.51	0.50
7:a:178:PRO:HB2	7:a:180:ARG:CD	2.41	0.50
7:b:222:TRP:HH2	7:b:229:LEU:HD12	1.76	0.50
7:c:142:VAL:HG13	7:c:142:VAL:O	2.11	0.50
7:d:68:LEU:HB3	7:d:72:LEU:HB3	1.91	0.50
7:d:115:MET:SD	7:d:115:MET:C	2.94	0.50
7:f:226:ILE:CG1	9:f:601:ADP:C8	2.94	0.50
7:e:124:ILE:HG12	7:e:144:LEU:CD1	2.13	0.50
2:C:91:THR:HB	2:C:139:ASN:H	1.75	0.50
7:f:11:GLU:HG3	7:f:11:GLU:O	2.12	0.50
7:f:188:LEU:N	7:f:188:LEU:CD1	2.73	0.50
7:e:42:LYS:N	9:e:601:ADP:O1A	2.43	0.50
8:M:423:LEU:HD13	8:M:423:LEU:C	2.34	0.50
3:D:425:ARG:HG3	3:D:427:PRO:HD2	1.92	0.50
7:a:71:ASN:O	7:a:71:ASN:ND2	2.43	0.50
7:a:96:PHE:CG	7:a:123:VAL:CG1	2.89	0.50
7:a:240:HIS:CE1	7:a:247:LEU:CA	2.95	0.50
7:c:138:LEU:N	7:c:138:LEU:CD2	2.73	0.50
7:c:156:VAL:HG21	7:c:163:ALA:HA	1.93	0.50
7:d:125:GLU:HB2	7:d:126:TYR:CD1	2.46	0.50
7:d:174:VAL:O	7:d:174:VAL:HG13	2.09	0.50
7:e:20:GLU:OE1	7:e:20:GLU:HA	2.11	0.50
7:e:108:GLU:OE1	7:e:108:GLU:HA	2.11	0.50
2:C:1256:GLN:HB2	2:C:1296:ASP:HB2	1.92	0.50
7:a:5:LYS:N	7:a:5:LYS:HD2	2.25	0.50
7:a:252:ILE:N	7:a:252:ILE:CD1	2.73	0.50
8:M:360:GLU:OE2	8:M:423:LEU:CA	2.58	0.50
3:D:842:ARG:NH2	3:D:884:SER:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:178:PRO:HB2	7:a:180:ARG:HE	1.75	0.50
7:e:136:GLN:HB3	7:e:137:PRO:HD2	1.94	0.50
7:b:193:PHE:CE2	7:b:230:LYS:HB2	2.46	0.50
7:c:9:LEU:O	7:c:15:PHE:CD2	2.65	0.50
8:M:280:LYS:H	8:M:285:TRP:HB3	1.77	0.50
8:M:374:VAL:HG23	8:M:376:MET:H	1.75	0.50
8:M:441:LYS:O	8:M:444:SER:OG	2.24	0.50
7:a:85:PHE:CD1	7:a:85:PHE:C	2.90	0.50
7:b:15:PHE:CD1	7:b:182:ARG:NH1	2.80	0.50
7:b:179:LEU:O	7:b:180:ARG:C	2.55	0.50
7:c:29:ASP:HB2	7:c:143:ARG:HD3	1.93	0.50
7:c:32:VAL:CG2	7:c:145:VAL:HG21	2.41	0.50
7:d:129:LEU:N	7:d:138:LEU:O	2.45	0.50
7:d:153:PRO:HG3	7:e:255:PHE:CE2	2.46	0.50
8:M:259:ARG:NH1	8:M:259:ARG:CG	2.66	0.50
8:M:276:VAL:HB	8:M:390:LEU:CB	2.35	0.50
3:D:270:ARG:O	3:D:274:ASN:ND2	2.44	0.50
3:D:519:ASN:HD21	3:D:709:ARG:HH11	1.60	0.50
3:D:591:ILE:HG23	3:D:592:VAL:HG13	1.93	0.50
7:a:25:LEU:HD23	7:b:238:TYR:CZ	2.47	0.50
7:b:26:ALA:N	7:b:27:PRO:CD	2.74	0.50
7:d:109:LEU:HD21	7:d:169:LEU:CD1	2.42	0.50
7:d:126:TYR:CD1	7:d:126:TYR:N	2.78	0.50
7:e:11:GLU:O	7:e:16:LEU:HD12	2.11	0.50
8:M:260:PRO:O	8:M:261:GLY:C	2.54	0.50
1:B:74:VAL:HG11	1:B:81:ILE:HD11	1.93	0.50
2:C:239:MET:HE2	2:C:287:VAL:HG11	1.93	0.50
2:C:1239:VAL:HG23	3:D:354:VAL:HG21	1.93	0.50
6:T:15:DA:H2"	6:T:16:DA:C8	2.47	0.50
7:a:155:MET:HG2	7:a:160:THR:HB	1.93	0.50
7:b:69:ASN:OD1	7:b:71:ASN:N	2.42	0.50
7:b:247:LEU:HD22	7:b:250:ILE:HD11	1.90	0.50
7:c:110:ALA:HB2	7:c:148:THR:HG21	1.94	0.50
7:c:179:LEU:CD2	7:c:225:ASN:HB3	2.40	0.50
7:d:43:GLU:HG3	7:d:43:GLU:O	2.11	0.50
7:f:30:LYS:HB2	7:f:171:PHE:CD2	2.41	0.50
7:f:136:GLN:NE2	7:f:136:GLN:N	2.60	0.50
1:A:97:GLU:HA	1:A:147:GLN:HG2	1.94	0.49
6:T:23:DT:H2"	6:T:24:DG:H8	1.77	0.49
7:a:57:GLN:O	7:a:58:GLY:O	2.29	0.49
7:a:187:MET:HE1	7:a:217:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:203:LEU:CD2	7:b:203:LEU:N	2.75	0.49
7:d:96:PHE:N	7:d:96:PHE:CD1	2.80	0.49
7:e:48:ARG:O	7:e:52:LEU:HG	2.12	0.49
7:e:105:PHE:HA	7:e:145:VAL:HG23	1.90	0.49
8:M:33:LEU:C	8:M:33:LEU:CD2	2.85	0.49
8:M:390:LEU:O	8:M:390:LEU:CG	2.60	0.49
3:D:833:GLU:OE1	3:D:1242:ARG:NH1	2.43	0.49
5:N:-11:DA:C8	5:N:-10:DG:C4	2.99	0.49
7:a:25:LEU:C	7:a:27:PRO:HD2	2.37	0.49
7:a:180:ARG:HG2	7:a:181:GLU:N	2.27	0.49
7:b:194:ALA:CB	7:b:206:PHE:HE2	2.25	0.49
7:c:14:SER:O	7:c:17:GLU:HG2	2.12	0.49
7:c:165:LEU:C	7:c:165:LEU:CD2	2.85	0.49
7:d:50:HIS:HB2	7:d:60:PHE:CD1	2.48	0.49
7:f:45:ILE:O	7:f:45:ILE:CG2	2.60	0.49
8:M:159:GLU:OE1	8:M:160:ASP:N	2.45	0.49
8:M:471:ASN:N	8:M:471:ASN:OD1	2.43	0.49
1:A:135:ASP:OD1	1:A:136:GLU:N	2.45	0.49
3:D:1143:ASP:HA	3:D:1148:ARG:HD3	1.95	0.49
7:c:104:LEU:O	7:c:144:LEU:HA	2.12	0.49
7:f:15:PHE:HE2	7:f:182:ARG:HH21	1.60	0.49
7:e:61:ILE:C	7:e:62:SER:HA	2.32	0.49
8:M:449:GLN:OE1	8:M:449:GLN:HA	2.12	0.49
7:a:50:HIS:C	7:a:52:LEU:N	2.70	0.49
7:a:63:LEU:O	7:a:63:LEU:HD22	2.13	0.49
7:a:81:GLU:OE1	7:a:134:GLY:HA2	2.13	0.49
7:a:178:PRO:HB2	7:a:180:ARG:NE	2.27	0.49
7:c:157:ASN:N	7:c:157:ASN:ND2	2.60	0.49
7:c:225:ASN:N	7:c:225:ASN:ND2	2.60	0.49
7:d:99:ALA:CB	7:d:104:LEU:CD1	2.88	0.49
7:f:63:LEU:CD1	7:f:63:LEU:C	2.85	0.49
7:f:98:ARG:NH1	7:e:135:SER:O	2.45	0.49
7:f:187:MET:HA	7:f:187:MET:CE	2.42	0.49
8:M:158:ILE:HD11	8:M:193:LYS:HE2	1.95	0.49
8:M:390:LEU:HD23	8:M:390:LEU:C	2.31	0.49
1:A:110:VAL:HG12	1:A:132:HIS:HA	1.93	0.49
7:a:16:LEU:C	7:a:16:LEU:CD2	2.85	0.49
7:a:187:MET:HE1	7:a:217:LEU:HD12	1.95	0.49
7:b:194:ALA:C	7:b:206:PHE:CE2	2.90	0.49
7:d:65:CYS:HA	7:d:107:ASP:HB3	1.93	0.49
7:f:103:THR:HG21	7:f:143:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:109:LEU:HD23	7:f:148:THR:HB	1.95	0.49
7:e:63:LEU:C	7:e:63:LEU:CD1	2.85	0.49
8:M:125:MET:O	8:M:129:GLU:HG2	2.12	0.49
8:M:425:LYS:HB3	8:M:425:LYS:HZ3	1.78	0.49
8:M:427:LEU:HG	8:M:442:LEU:HD21	1.93	0.49
2:C:9:LYS:HE2	2:C:1171:ARG:HH12	1.77	0.49
4:E:44:ASP:OD1	4:E:45:LYS:N	2.45	0.49
7:b:152:LEU:O	7:b:156:VAL:HG23	2.12	0.49
7:b:166:LEU:C	7:b:166:LEU:CD2	2.86	0.49
7:f:34:ILE:HG22	7:f:42:LYS:CG	2.40	0.49
7:f:38:ARG:CD	7:f:224:GLY:HA2	2.42	0.49
7:f:44:LEU:O	7:f:45:ILE:C	2.55	0.49
7:f:63:LEU:C	7:f:63:LEU:HD12	2.37	0.49
7:e:43:GLU:OE1	7:e:43:GLU:HA	2.13	0.49
8:M:119:THR:HG22	8:M:122:ASP:CG	2.38	0.49
8:M:197:ASP:C	8:M:201:ILE:HD13	2.33	0.49
2:C:93:SER:HA	2:C:129:LEU:H	1.78	0.49
2:C:202:ARG:HH21	2:C:369:MET:HA	1.78	0.49
3:D:505:ASP:OD1	3:D:505:ASP:N	2.44	0.49
7:a:55:ARG:NH2	7:a:101:GLY:O	2.45	0.49
7:b:7:ASN:OD1	7:b:7:ASN:N	2.45	0.49
7:b:226:ILE:CG2	9:b:601:ADP:C8	2.92	0.49
7:d:239:ARG:HD2	7:d:251:ILE:HD11	1.93	0.49
8:M:158:ILE:CD1	8:M:193:LYS:CD	2.87	0.49
8:M:416:SER:O	8:M:417:SER:C	2.53	0.49
2:C:314:ASN:OD1	2:C:348:SER:OG	2.29	0.49
2:C:1329:GLU:HA	3:D:245:LEU:HD21	1.94	0.49
3:D:1261:LEU:HD23	3:D:1306:LEU:HB3	1.95	0.49
7:a:180:ARG:O	7:a:183:GLU:HG2	2.13	0.49
7:a:235:ARG:HH21	7:a:254:PRO:HD3	1.73	0.49
7:b:55:ARG:C	7:b:57:GLN:N	2.70	0.49
7:c:152:LEU:HB3	7:c:153:PRO:HD3	1.93	0.49
7:d:7:ASN:N	7:d:7:ASN:ND2	2.60	0.49
7:f:170:ALA:O	7:f:173:VAL:HG13	2.13	0.49
8:M:380:THR:HG22	8:M:381:ILE:N	2.27	0.49
7:b:10:GLY:O	7:b:16:LEU:HD11	2.13	0.49
7:d:20:GLU:OE1	7:d:20:GLU:HA	2.13	0.49
7:f:122:ARG:O	7:f:122:ARG:HD3	2.13	0.49
7:e:21:GLN:C	7:e:23:SER:H	2.19	0.49
8:M:27:GLN:HA	8:M:383:ARG:O	2.13	0.49
8:M:347:ILE:HD11	8:M:402:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:367:LEU:O	8:M:368:ALA:C	2.54	0.49
2:C:673:HIS:ND1	3:D:763:PHE:O	2.36	0.49
2:C:717:VAL:HG12	2:C:782:VAL:HG12	1.94	0.49
5:N:-27:DT:H71	8:M:455:ARG:CZ	2.37	0.49
7:b:25:LEU:HG	7:c:238:TYR:CZ	2.48	0.49
7:b:49:LEU:C	7:b:49:LEU:HD12	2.38	0.49
7:b:103:THR:HA	7:b:143:ARG:HB3	1.94	0.49
7:b:222:TRP:CZ3	7:b:229:LEU:CA	2.83	0.49
7:c:166:LEU:C	7:c:166:LEU:CD2	2.86	0.49
7:f:120:LEU:C	7:f:120:LEU:HD12	2.38	0.49
7:f:201:ILE:HG22	7:e:28:LEU:HD23	1.93	0.49
7:e:117:GLN:CD	7:e:165:LEU:HD23	2.38	0.49
5:N:-25:DG:N7	8:M:456:ARG:NH1	2.59	0.48
7:a:37:GLU:HB3	7:a:225:ASN:HD21	1.73	0.48
7:b:105:PHE:HE1	7:b:107:ASP:HB2	1.78	0.48
7:c:131:ARG:HG2	7:c:133:GLY:H	1.78	0.48
7:e:104:LEU:HD23	7:e:144:LEU:HA	1.95	0.48
2:C:53:PHE:O	2:C:57:PHE:HB2	2.13	0.48
3:D:140:TYR:OH	3:D:312:ARG:NE	2.46	0.48
6:T:12:DT:C7	8:M:22:ALA:CB	2.91	0.48
7:a:217:LEU:N	7:a:217:LEU:HD23	2.14	0.48
7:b:122:ARG:CB	7:b:122:ARG:NH1	2.75	0.48
7:b:210:THR:HG21	7:b:248:ASP:HA	1.95	0.48
7:c:104:LEU:HB2	7:c:144:LEU:HB3	1.95	0.48
7:c:193:PHE:CZ	7:c:226:ILE:CG2	2.96	0.48
7:d:112:ALA:HB1	7:d:116:VAL:HG12	1.85	0.48
7:f:5:LYS:HZ2	7:f:5:LYS:C	2.09	0.48
7:f:235:ARG:NH1	7:f:251:ILE:HB	2.28	0.48
7:e:80:HIS:HB2	7:e:132:VAL:CG1	2.44	0.48
8:M:19:LEU:C	8:M:19:LEU:CD2	2.85	0.48
8:M:145:VAL:HG13	8:M:146:ASP:N	2.28	0.48
2:C:804:PHE:HE2	2:C:1115:THR:HG21	1.77	0.48
3:D:253:VAL:HG21	8:M:112:TYR:CD1	2.47	0.48
7:a:55:ARG:O	7:a:55:ARG:HG2	2.13	0.48
7:c:108:GLU:HB3	7:c:111:THR:CG2	2.44	0.48
7:f:61:ILE:HG23	7:f:104:LEU:CD1	2.43	0.48
7:e:26:ALA:HB3	7:e:27:PRO:HD3	1.95	0.48
8:M:206:PHE:HE1	8:M:213:LEU:HD21	1.78	0.48
7:a:128:GLU:O	7:a:128:GLU:HG2	2.11	0.48
7:b:201:ILE:HG12	7:b:238:TYR:HD1	1.78	0.48
7:f:46:ALA:HB1	7:f:105:PHE:CD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:196:GLN:OE1	7:f:199:ARG:CD	2.54	0.48
7:e:120:LEU:C	7:e:120:LEU:CD1	2.86	0.48
8:M:236:MET:HE2	8:M:246:LEU:HD22	1.95	0.48
2:C:1254:VAL:HB	8:M:111:VAL:CB	2.37	0.48
7:a:34:ILE:HB	7:a:147:ALA:HB2	1.96	0.48
7:a:165:LEU:C	7:a:165:LEU:CD2	2.86	0.48
7:d:103:THR:HA	7:d:142:VAL:HG13	1.94	0.48
7:d:128:GLU:HA	7:d:139:GLN:HA	1.96	0.48
7:d:229:LEU:HD13	7:d:229:LEU:C	2.38	0.48
7:f:30:LYS:HG3	7:f:171:PHE:CE2	2.49	0.48
8:M:347:ILE:HG21	8:M:347:ILE:HD13	1.56	0.48
8:M:360:GLU:OE2	8:M:426:LYS:HD3	2.13	0.48
2:C:1062:PRO:HA	2:C:1076:ILE:HB	1.96	0.48
2:C:1080:ASN:HB3	2:C:1085:MET:HE2	1.95	0.48
3:D:65:VAL:HG22	3:D:66:LYS:H	1.78	0.48
7:a:179:LEU:CD1	7:a:226:ILE:CD1	2.91	0.48
7:a:185:ASP:O	7:a:189:MET:CE	2.62	0.48
7:c:118:GLU:HB2	7:c:162:ARG:NE	2.29	0.48
7:d:69:ASN:OD1	7:d:69:ASN:N	2.46	0.48
7:f:140:VAL:O	7:f:140:VAL:CG2	2.61	0.48
7:f:235:ARG:NH1	7:f:251:ILE:CB	2.75	0.48
7:e:109:LEU:CD1	7:e:161:PHE:CZ	2.74	0.48
3:D:233:LYS:HG3	3:D:234:PRO:HD2	1.96	0.48
7:a:182:ARG:HB3	7:a:185:ASP:HB2	1.96	0.48
7:c:232:VAL:HG13	7:c:251:ILE:O	2.13	0.48
7:d:81:GLU:O	7:d:91:ARG:HA	2.14	0.48
7:f:34:ILE:O	7:f:147:ALA:CB	2.62	0.48
7:f:99:ALA:CB	7:f:142:VAL:HG23	2.42	0.48
7:e:34:ILE:HG23	7:e:174:VAL:O	2.12	0.48
7:e:145:VAL:O	7:e:145:VAL:HG23	2.13	0.48
8:M:192:ALA:HB2	8:M:198:CYS:HB2	1.96	0.48
8:M:271:TYR:CD1	8:M:271:TYR:N	2.80	0.48
7:a:166:LEU:HD13	7:a:166:LEU:C	2.39	0.48
7:b:73:LEU:HD11	7:b:116:VAL:HG22	1.96	0.48
7:b:79:GLY:O	7:b:131:ARG:CB	2.54	0.48
7:f:124:ILE:HD13	7:f:144:LEU:HD21	1.96	0.48
7:f:234:GLU:HA	7:f:237:VAL:CG1	2.44	0.48
8:M:336:ARG:HH12	8:M:388:LYS:NZ	2.00	0.48
8:M:392:SER:CB	8:M:393:PRO:HD2	2.29	0.48
8:M:427:LEU:HD12	8:M:427:LEU:C	2.39	0.48
3:D:362:ARG:NH1	3:D:626:TYR:OH	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:33:LEU:HD21	7:a:152:LEU:HD12	1.96	0.48
7:b:8:LEU:CD1	7:b:19:LEU:HD21	2.40	0.48
7:b:65:CYS:SG	7:b:112:ALA:HB1	2.53	0.48
7:b:203:LEU:N	7:b:203:LEU:HD22	2.29	0.48
7:c:243:SER:O	7:c:243:SER:OG	2.32	0.48
7:d:126:TYR:HB2	7:d:128:GLU:OE1	2.12	0.48
7:f:188:LEU:HD12	7:f:188:LEU:H	1.79	0.48
7:e:121:LEU:C	7:e:121:LEU:CD2	2.85	0.48
8:M:120:LEU:O	8:M:123:TYR:N	2.46	0.48
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.47	0.48
2:C:1242:LYS:HG3	3:D:465:GLN:HE21	1.79	0.48
7:a:155:MET:CG	7:a:160:THR:HB	2.44	0.48
7:b:72:LEU:CD2	8:M:7:LEU:HD12	2.42	0.48
7:d:66:ALA:HB2	7:d:111:THR:OG1	2.14	0.48
7:f:164:ASP:O	7:f:168:ARG:N	2.46	0.48
7:e:26:ALA:O	7:e:53:SER:HB2	2.13	0.48
7:e:223:PRO:HD2	7:e:228:GLU:CD	2.38	0.48
8:M:278:VAL:CG2	8:M:392:SER:CB	2.91	0.48
8:M:285:TRP:CD1	8:M:285:TRP:H	2.28	0.48
8:M:317:GLN:O	8:M:317:GLN:HG2	2.14	0.48
1:B:107:ILE:HG13	1:B:109:PRO:HD2	1.95	0.47
2:C:23:ASP:OD1	2:C:24:VAL:N	2.48	0.47
3:D:557:LYS:HA	3:D:563:LEU:HA	1.96	0.47
7:b:53:SER:OG	7:b:55:ARG:CG	2.62	0.47
7:c:104:LEU:HD12	7:c:104:LEU:H	1.79	0.47
7:d:98:ARG:HB2	7:d:98:ARG:CZ	2.42	0.47
7:d:148:THR:OG1	7:d:152:LEU:HD21	2.14	0.47
7:f:222:TRP:CZ3	7:f:229:LEU:HA	2.48	0.47
7:f:226:ILE:HG22	9:f:601:ADP:O4'	2.14	0.47
7:e:56:TRP:HE3	7:e:56:TRP:O	1.97	0.47
7:e:117:GLN:HG2	7:e:165:LEU:CD2	2.44	0.47
7:e:159:GLY:C	7:e:161:PHE:N	2.70	0.47
8:M:18:GLN:NE2	8:M:328:TRP:CE2	2.82	0.47
8:M:346:CYS:O	8:M:350:GLN:NE2	2.47	0.47
3:D:1005:LYS:NZ	3:D:1016:THR:O	2.48	0.47
5:N:-8:DT:C4'	7:b:90:LYS:NZ	2.77	0.47
7:a:179:LEU:HD21	7:a:226:ILE:HD12	1.81	0.47
7:b:8:LEU:HD11	7:b:19:LEU:HD23	1.80	0.47
7:b:32:VAL:C	7:b:170:ALA:HB2	2.39	0.47
7:b:42:LYS:HD2	7:b:147:ALA:HB1	1.95	0.47
7:c:224:GLY:C	7:c:228:GLU:CB	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:55:ARG:CD	7:d:55:ARG:N	2.75	0.47
7:d:118:GLU:HG3	7:e:67:ALA:HB2	1.97	0.47
7:d:121:LEU:HB2	7:d:165:LEU:HB2	1.96	0.47
7:f:5:LYS:O	7:f:5:LYS:HD3	2.14	0.47
7:e:62:SER:OG	7:e:105:PHE:HB3	2.13	0.47
3:D:507:VAL:HG22	3:D:601:ILE:HD11	1.94	0.47
7:b:119:LYS:HA	7:b:119:LYS:HE3	1.96	0.47
7:c:8:LEU:CA	7:c:44:LEU:HD11	2.44	0.47
7:f:26:ALA:HB1	7:f:52:LEU:HB2	1.95	0.47
7:e:226:ILE:HD12	7:e:226:ILE:N	2.29	0.47
8:M:162:VAL:HG21	8:M:172:LEU:HD23	1.96	0.47
2:C:387:ASN:HA	2:C:391:SER:HB3	1.96	0.47
7:a:31:PRO:O	7:a:171:PHE:HB3	2.14	0.47
7:a:226:ILE:HG21	9:a:601:ADP:C5	2.46	0.47
7:b:157:ASN:HD22	7:b:157:ASN:N	2.11	0.47
7:b:212:ARG:HG3	7:b:213:ALA:H	1.78	0.47
7:c:33:LEU:HA	7:c:146:CYS:O	2.13	0.47
7:c:115:MET:SD	7:c:116:VAL:HG23	2.54	0.47
7:d:50:HIS:CG	7:d:60:PHE:CD1	3.02	0.47
8:M:428:ILE:HG12	8:M:442:LEU:HD11	1.97	0.47
2:C:765:ILE:HG22	2:C:787:PRO:HG2	1.96	0.47
3:D:19:ALA:HA	3:D:1343:GLU:HA	1.96	0.47
7:b:3:GLU:N	7:b:3:GLU:CD	2.73	0.47
7:b:26:ALA:HB1	7:b:52:LEU:HB2	1.95	0.47
7:c:136:GLN:O	7:c:136:GLN:HG2	2.13	0.47
7:d:71:ASN:HD22	7:d:71:ASN:H	1.62	0.47
7:d:128:GLU:CB	7:d:139:GLN:HG2	2.45	0.47
7:d:166:LEU:C	7:d:166:LEU:CD2	2.85	0.47
7:f:45:ILE:O	7:f:45:ILE:HG22	2.14	0.47
7:f:232:VAL:O	7:f:232:VAL:HG12	2.03	0.47
8:M:420:ILE:HD13	8:M:451:ILE:HG21	1.91	0.47
3:D:948:SER:OG	3:D:1020:TRP:O	2.30	0.47
7:d:25:LEU:HD21	7:d:172:ASP:OD2	2.15	0.47
7:d:169:LEU:C	7:d:169:LEU:CD2	2.85	0.47
7:d:171:PHE:CD2	7:d:172:ASP:HB2	2.49	0.47
7:e:30:LYS:NZ	7:e:171:PHE:CE2	2.54	0.47
8:M:329:LEU:HD13	8:M:329:LEU:C	2.40	0.47
1:B:191:ARG:HA	1:B:198:LEU:HD23	1.96	0.47
2:C:1225:VAL:HA	3:D:638:SER:HB2	1.96	0.47
3:D:79:LYS:O	3:D:81:ARG:NH2	2.48	0.47
3:D:812:ASP:O	3:D:897:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:32:VAL:HG22	7:a:172:ASP:O	2.15	0.47
7:a:56:TRP:HZ3	7:a:57:GLN:HB3	1.77	0.47
7:a:122:ARG:HD3	7:b:64:ASN:HB2	1.97	0.47
7:b:89:GLN:OE1	7:b:89:GLN:N	2.48	0.47
7:b:131:ARG:NH2	7:b:138:LEU:HD22	2.29	0.47
7:b:226:ILE:C	7:b:228:GLU:N	2.69	0.47
7:b:234:GLU:HA	7:b:237:VAL:HG12	1.96	0.47
7:d:55:ARG:HD3	7:d:55:ARG:O	2.15	0.47
7:d:213:ALA:O	7:d:217:LEU:HG	2.15	0.47
7:f:77:LEU:HD13	7:f:119:LYS:HB3	1.96	0.47
7:f:152:LEU:HD12	7:f:166:LEU:HD13	1.97	0.47
7:e:109:LEU:HD13	7:e:109:LEU:C	2.39	0.47
7:e:225:ASN:N	7:e:225:ASN:ND2	2.61	0.47
8:M:198:CYS:O	8:M:199:LEU:C	2.53	0.47
8:M:216:ALA:HA	8:M:253:ILE:HD11	1.95	0.47
8:M:358:GLY:HA2	8:M:394:ARG:HH22	1.79	0.47
8:M:425:LYS:CB	8:M:425:LYS:HZ3	2.27	0.47
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.95	0.47
2:C:817:LEU:HD21	2:C:1078:LYS:HD3	1.97	0.47
7:a:71:ASN:ND2	7:a:71:ASN:C	2.73	0.47
7:b:217:LEU:HD21	7:b:250:ILE:HG21	1.97	0.47
7:c:32:VAL:CG2	7:c:145:VAL:CG2	2.93	0.47
7:f:8:LEU:HG	7:f:48:ARG:NH1	2.29	0.47
7:f:22:VAL:HG13	7:f:49:LEU:HG	1.96	0.47
7:f:232:VAL:HG13	7:f:251:ILE:O	2.15	0.47
8:M:131:THR:HG21	8:M:133:PHE:HZ	1.67	0.47
2:C:14:ASP:OD1	2:C:15:PHE:N	2.47	0.47
2:C:1281:TYR:HE1	3:D:489:ASN:HD21	1.62	0.47
7:a:11:GLU:O	7:a:13:ASN:N	2.46	0.47
7:f:235:ARG:HH11	7:f:251:ILE:CB	2.27	0.47
7:e:61:ILE:HG22	7:e:99:ALA:HB2	1.97	0.47
8:M:290:ASN:HB3	8:M:293:SER:HB3	1.96	0.47
2:C:156:PHE:HE1	2:C:450:ASN:HB3	1.80	0.47
2:C:696:ASP:OD2	2:C:799:ASN:ND2	2.42	0.47
2:C:890:LYS:N	2:C:912:ASP:O	2.45	0.47
3:D:96:LYS:O	3:D:99:ARG:HG2	2.15	0.47
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.97	0.47
7:a:176:LEU:N	7:a:176:LEU:CD2	2.78	0.47
7:b:49:LEU:CA	7:b:49:LEU:CD1	2.92	0.47
7:c:153:PRO:CG	7:d:255:PHE:CE2	2.97	0.47
7:c:230:LYS:HA	7:c:233:VAL:HG11	1.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:144:LEU:CD2	7:d:146:CYS:SG	3.03	0.47
7:f:69:ASN:CA	7:e:74:ASP:OD2	2.63	0.47
7:e:37:GLU:O	7:e:40:THR:OG1	2.29	0.47
7:e:220:TYR:HE2	7:e:228:GLU:OE1	1.98	0.47
8:M:464:SER:C	8:M:466:SER:H	2.22	0.47
2:C:210:LEU:HD21	2:C:429:MET:HE1	1.97	0.46
2:C:873:ILE:H	2:C:873:ILE:HD13	1.80	0.46
5:N:-8:DT:H5''	7:b:90:LYS:HZ1	1.79	0.46
6:T:11:DG:H5''	6:T:11:DG:H8	1.79	0.46
7:a:25:LEU:CD2	7:b:238:TYR:CE2	2.98	0.46
7:a:220:TYR:HE2	7:a:228:GLU:HG2	1.79	0.46
7:a:240:HIS:HE1	7:a:247:LEU:CA	2.29	0.46
7:b:68:LEU:HD23	7:b:68:LEU:HA	1.26	0.46
7:b:129:LEU:HD22	7:b:140:VAL:HG13	1.96	0.46
7:d:41:GLY:CA	7:d:176:LEU:HD21	2.22	0.46
7:d:92:HIS:NE2	7:d:94:GLY:HA2	2.29	0.46
7:f:63:LEU:HD11	7:f:106:LEU:HA	1.97	0.46
7:f:65:CYS:SG	7:f:109:LEU:CB	3.03	0.46
8:M:216:ALA:CB	8:M:252:LEU:HD12	2.45	0.46
8:M:318:PHE:C	8:M:318:PHE:CD1	2.93	0.46
1:B:97:GLU:HA	1:B:146:VAL:O	2.16	0.46
3:D:196:GLN:HE21	3:D:200:GLN:HE21	1.61	0.46
7:a:85:PHE:CE2	8:M:7:LEU:HD13	2.50	0.46
7:b:32:VAL:HG13	7:b:145:VAL:HA	1.97	0.46
7:b:194:ALA:CB	7:b:206:PHE:CE2	2.98	0.46
7:e:166:LEU:HD12	7:e:166:LEU:O	2.14	0.46
8:M:46:LEU:HD12	8:M:46:LEU:H	1.80	0.46
8:M:133:PHE:HB3	8:M:137:ASP:CB	2.41	0.46
2:C:1270:PHE:HB3	3:D:343:LEU:O	2.15	0.46
6:T:12:DT:H72	8:M:22:ALA:C	2.40	0.46
7:a:124:ILE:HD12	7:a:124:ILE:H	1.79	0.46
7:a:179:LEU:CD1	7:a:226:ILE:HD11	2.45	0.46
7:b:61:ILE:CG1	7:b:99:ALA:HB2	2.45	0.46
7:b:197:MET:CE	7:b:238:TYR:HB2	2.45	0.46
7:b:210:THR:O	7:b:213:ALA:HB3	2.15	0.46
7:c:33:LEU:HD12	7:c:34:ILE:N	2.31	0.46
7:c:225:ASN:HD22	7:c:225:ASN:H	1.62	0.46
7:f:80:HIS:CE1	7:f:92:HIS:CD2	3.03	0.46
3:D:1249:ASN:OD1	3:D:1250:ASP:N	2.48	0.46
7:a:39:GLY:O	7:a:225:ASN:HB2	2.16	0.46
7:a:111:THR:O	7:a:111:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:179:LEU:CD2	7:a:226:ILE:N	2.78	0.46
7:b:25:LEU:CD2	7:b:28:LEU:HD12	2.46	0.46
7:b:72:LEU:HD21	8:M:7:LEU:HB2	1.98	0.46
7:b:129:LEU:CD2	7:b:129:LEU:N	2.78	0.46
7:c:8:LEU:CD2	7:c:44:LEU:CD2	2.78	0.46
7:c:114:MET:SD	7:d:67:ALA:HA	2.56	0.46
7:c:233:VAL:O	7:c:237:VAL:HG23	2.15	0.46
7:e:8:LEU:HD13	7:e:48:ARG:HH12	1.79	0.46
7:e:35:ILE:HA	7:e:148:THR:HG22	1.96	0.46
7:e:176:LEU:CD2	7:e:176:LEU:H	2.28	0.46
2:C:207:THR:OG1	2:C:354:ASP:OD2	2.31	0.46
7:a:202:LYS:HD2	7:a:202:LYS:HA	1.59	0.46
7:b:79:GLY:HA2	7:b:92:HIS:CD2	2.51	0.46
8:M:424:VAL:O	8:M:428:ILE:HG13	2.16	0.46
2:C:844:LYS:CB	8:M:272:VAL:CG1	2.83	0.46
3:D:1250:ASP:HA	3:D:1253:ILE:HD12	1.98	0.46
5:N:-21:DG:H2''	5:N:-20:DA:H8	1.80	0.46
7:a:179:LEU:HB2	7:a:225:ASN:HA	1.97	0.46
7:b:123:VAL:O	7:b:123:VAL:HG12	2.14	0.46
7:c:144:LEU:HD13	7:c:144:LEU:H	1.79	0.46
7:d:110:ALA:HB1	7:d:155:MET:HE3	1.98	0.46
7:e:80:HIS:HA	7:e:132:VAL:HG12	1.98	0.46
3:D:43:THR:CG2	3:D:270:ARG:HH22	2.29	0.46
7:b:29:ASP:CA	7:b:143:ARG:HD3	2.45	0.46
7:b:108:GLU:HA	7:b:108:GLU:OE2	2.16	0.46
7:c:63:LEU:C	7:c:63:LEU:CD1	2.85	0.46
7:d:105:PHE:HA	7:d:145:VAL:O	2.16	0.46
7:d:126:TYR:HD1	7:d:126:TYR:N	2.14	0.46
7:d:181:GLU:OE1	7:d:181:GLU:N	2.49	0.46
7:f:106:LEU:O	7:f:146:CYS:HA	2.15	0.46
7:f:193:PHE:O	7:f:234:GLU:OE2	2.34	0.46
8:M:33:LEU:HD23	8:M:33:LEU:O	2.14	0.46
7:a:245:TYR:HB2	7:a:246:PRO:HD2	1.98	0.46
7:b:11:GLU:HA	7:b:11:GLU:OE2	2.16	0.46
7:c:229:LEU:O	7:c:233:VAL:HG12	2.15	0.46
7:f:197:MET:O	7:f:200:GLU:HB3	2.15	0.46
7:f:223:PRO:HG2	7:f:228:GLU:OE2	2.15	0.46
7:e:193:PHE:CE2	7:e:230:LYS:HB2	2.51	0.46
8:M:190:VAL:O	8:M:190:VAL:CG1	2.41	0.46
8:M:229:ASN:HA	8:M:472:GLN:HE22	1.80	0.46
3:D:885:VAL:HG13	3:D:886:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:38:ARG:NH2	7:f:164:ASP:HA	2.31	0.46
7:a:61:ILE:HG12	7:a:99:ALA:HB2	1.97	0.46
7:a:80:HIS:CE1	7:a:92:HIS:HB3	2.51	0.46
7:a:180:ARG:HH11	7:a:221:ARG:HD2	1.79	0.46
7:b:121:LEU:C	7:b:122:ARG:HG2	2.27	0.46
7:c:167:ASP:HB3	7:d:231:ASN:OD1	2.16	0.46
7:d:45:ILE:H	7:d:45:ILE:HG12	1.38	0.46
7:d:179:LEU:HB2	7:d:225:ASN:CA	2.39	0.46
7:f:26:ALA:HB1	7:f:52:LEU:CB	2.45	0.46
7:f:63:LEU:CD1	7:f:106:LEU:HA	2.46	0.46
8:M:299:ILE:HD12	8:M:299:ILE:HA	1.53	0.46
8:M:343:VAL:O	8:M:343:VAL:CG1	2.57	0.46
8:M:343:VAL:O	8:M:343:VAL:HG13	2.15	0.46
8:M:357:GLN:HA	8:M:357:GLN:OE1	2.15	0.46
1:B:124:VAL:HG13	1:B:125:LYS:HG2	1.98	0.46
7:a:8:LEU:CD1	7:a:15:PHE:CZ	2.96	0.46
7:c:34:ILE:CA	7:c:35:ILE:HD12	2.46	0.46
7:d:55:ARG:HD3	7:d:55:ARG:N	2.19	0.46
8:M:18:GLN:NE2	8:M:18:GLN:C	2.73	0.46
5:N:-11:DA:C4	5:N:-10:DG:C4	3.04	0.45
7:b:25:LEU:HG	7:c:238:TYR:HH	1.79	0.45
7:c:144:LEU:C	7:c:144:LEU:CD2	2.87	0.45
7:f:152:LEU:CD1	7:f:166:LEU:HD13	2.45	0.45
7:f:207:PRO:HG3	7:f:243:SER:HA	1.98	0.45
1:A:12:ARG:HB2	1:A:29:GLU:HG3	1.98	0.45
3:D:246:PRO:HD2	3:D:249:LEU:HD12	1.97	0.45
7:a:69:ASN:HD22	7:a:72:LEU:HB3	1.81	0.45
7:a:180:ARG:HD3	7:a:180:ARG:H	1.80	0.45
7:b:35:ILE:HA	7:b:148:THR:O	2.15	0.45
7:b:79:GLY:CA	7:b:92:HIS:CD2	2.94	0.45
7:b:161:PHE:HE2	7:b:166:LEU:HB2	1.81	0.45
7:d:128:GLU:HB3	7:d:139:GLN:HG2	1.98	0.45
7:f:113:PRO:HD2	7:f:116:VAL:HG21	1.98	0.45
7:f:182:ARG:NH1	7:f:189:MET:SD	2.84	0.45
8:M:252:LEU:O	8:M:252:LEU:HD22	2.16	0.45
2:C:1308:ILE:HG13	3:D:472:LEU:HD23	1.99	0.45
5:N:-12:DC:C2'	8:M:17:PRO:HD3	2.47	0.45
7:b:240:HIS:CE1	7:b:242:THR:C	2.90	0.45
7:c:95:ARG:HD2	7:c:95:ARG:N	2.31	0.45
7:f:78:PHE:HD1	7:f:129:LEU:HD13	1.82	0.45
7:f:122:ARG:C	7:f:122:ARG:CD	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:40:THR:O	7:e:40:THR:HG22	2.16	0.45
7:e:63:LEU:CD2	7:e:95:ARG:HD2	2.34	0.45
8:M:25:LEU:C	8:M:25:LEU:CD1	2.89	0.45
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.99	0.45
7:a:30:LYS:N	7:a:30:LYS:CD	2.73	0.45
7:a:119:LYS:HG3	7:b:67:ALA:CA	2.46	0.45
7:d:239:ARG:HD2	7:d:251:ILE:HG13	1.97	0.45
7:f:14:SER:O	7:f:18:VAL:HG22	2.16	0.45
7:f:64:ASN:HB3	7:f:67:ALA:HB3	1.98	0.45
7:e:36:GLY:N	7:e:42:LYS:HE3	2.30	0.45
7:e:84:ALA:HB1	7:e:133:GLY:HA3	1.99	0.45
7:e:201:ILE:HD12	7:e:203:LEU:HD22	1.99	0.45
8:M:32:GLU:OE2	8:M:36:GLU:OE2	2.34	0.45
1:A:305:ASP:OD2	8:M:180:LYS:CE	2.39	0.45
7:b:55:ARG:HB2	7:b:101:GLY:O	2.17	0.45
7:b:84:ALA:O	7:b:88:ALA:HB3	2.16	0.45
7:b:152:LEU:HD22	7:b:152:LEU:N	2.31	0.45
7:c:44:LEU:HD23	7:c:44:LEU:O	2.17	0.45
7:c:193:PHE:CD2	7:c:229:LEU:HD22	2.51	0.45
7:d:31:PRO:O	7:d:171:PHE:HB3	2.15	0.45
7:d:233:VAL:O	7:d:237:VAL:HG23	2.16	0.45
8:M:308:ASN:C	8:M:310:ALA:N	2.73	0.45
2:C:1268:GLN:CD	2:C:1269:ARG:H	2.25	0.45
7:a:34:ILE:CB	7:a:147:ALA:HB2	2.47	0.45
7:f:15:PHE:CZ	7:f:182:ARG:NH2	2.85	0.45
7:f:179:LEU:CG	7:f:186:ILE:CD1	2.92	0.45
7:e:129:LEU:C	7:e:129:LEU:CD2	2.86	0.45
8:M:226:LEU:HB3	8:M:235:LEU:HD23	1.98	0.45
8:M:279:ARG:HD2	8:M:279:ARG:C	2.40	0.45
7:a:85:PHE:CD1	7:a:86:THR:O	2.67	0.45
7:b:13:ASN:HA	7:b:16:LEU:HD22	1.99	0.45
7:b:78:PHE:N	7:b:78:PHE:CD1	2.83	0.45
7:b:122:ARG:HB2	7:b:122:ARG:NH1	2.32	0.45
7:b:197:MET:O	7:b:201:ILE:HG22	2.17	0.45
7:c:119:LYS:HD2	7:c:119:LYS:HA	1.82	0.45
7:d:186:ILE:HG13	7:d:187:MET:N	2.31	0.45
7:f:152:LEU:N	7:f:153:PRO:CD	2.80	0.45
7:e:34:ILE:CG2	7:e:35:ILE:N	2.78	0.45
8:M:186:ASP:HA	8:M:187:PRO:HA	1.80	0.45
8:M:257:ASP:HA	8:M:258:PRO:HD2	1.47	0.45
8:M:285:TRP:CD1	8:M:285:TRP:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:278:ARG:HA	8:M:42:GLU:HB2	1.98	0.45
3:D:975:ILE:HD12	3:D:1001:ALA:HB3	1.98	0.45
7:c:63:LEU:HD13	7:c:64:ASN:N	2.32	0.45
7:e:175:GLN:N	7:e:175:GLN:CD	2.73	0.45
1:A:233:ASP:OD1	1:A:233:ASP:N	2.47	0.45
2:C:731:ARG:HH12	2:C:959:ASP:HB3	1.81	0.45
3:D:69:GLU:CG	3:D:76:LYS:CB	2.83	0.45
7:a:95:ARG:HG3	7:a:95:ARG:NH1	2.32	0.45
7:c:100:ASP:HB3	7:c:140:VAL:HG21	1.99	0.45
7:d:50:HIS:CG	7:d:60:PHE:HD1	2.35	0.45
7:e:39:GLY:HA2	9:e:601:ADP:PA	2.56	0.45
7:e:90:LYS:N	7:e:90:LYS:CD	2.73	0.45
8:M:142:THR:O	8:M:146:ASP:HB2	2.17	0.45
3:D:270:ARG:CZ	3:D:270:ARG:HB2	2.47	0.45
7:a:64:ASN:CG	7:a:67:ALA:HB2	2.42	0.45
7:a:78:PHE:O	7:a:94:GLY:N	2.49	0.45
7:a:179:LEU:CD2	7:a:226:ILE:CA	2.93	0.45
7:a:226:ILE:HG21	9:a:601:ADP:N9	2.29	0.45
7:a:229:LEU:HD12	7:a:229:LEU:C	2.42	0.45
7:c:100:ASP:HA	7:c:142:VAL:HG23	1.99	0.45
7:d:80:HIS:CD2	8:M:1:MET:SD	3.10	0.45
7:f:105:PHE:O	7:f:105:PHE:CG	2.70	0.45
7:e:139:GLN:NE2	7:e:139:GLN:C	2.75	0.45
7:e:178:PRO:O	7:e:181:GLU:CB	2.64	0.45
7:e:186:ILE:O	7:e:190:ALA:HB2	2.17	0.45
7:e:193:PHE:CD2	7:e:230:LYS:HA	2.52	0.45
8:M:119:THR:HG23	8:M:119:THR:O	2.16	0.45
8:M:195:LEU:O	8:M:195:LEU:CG	2.55	0.45
2:C:672:GLU:HB2	3:D:767:LEU:HB3	1.98	0.44
3:D:134:ASP:HB3	3:D:159:ILE:HD11	1.99	0.44
7:a:6:ASP:O	7:a:8:LEU:N	2.49	0.44
7:a:8:LEU:HD11	7:a:15:PHE:CZ	2.52	0.44
7:b:125:GLU:HG2	7:b:168:ARG:HD3	1.99	0.44
7:b:222:TRP:HZ3	7:b:229:LEU:N	2.14	0.44
7:b:239:ARG:HA	7:b:239:ARG:HD3	1.61	0.44
7:c:41:GLY:O	7:c:45:ILE:HB	2.17	0.44
7:c:114:MET:CG	7:d:67:ALA:HB2	2.42	0.44
7:d:231:ASN:N	7:d:231:ASN:ND2	2.65	0.44
7:f:7:ASN:HB3	7:f:8:LEU:H	1.60	0.44
7:e:257:ARG:HD2	7:e:257:ARG:N	2.31	0.44
8:M:184:ARG:HH11	8:M:184:ARG:HD3	1.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:442:LEU:O	8:M:443:THR:C	2.58	0.44
2:C:816:ILE:HD12	2:C:1066:MET:HB3	2.00	0.44
7:a:96:PHE:CE2	7:a:120:LEU:CD1	2.93	0.44
7:b:86:THR:C	7:b:88:ALA:N	2.75	0.44
7:b:152:LEU:N	7:b:153:PRO:CD	2.81	0.44
7:c:70:GLU:OE1	7:c:70:GLU:N	2.51	0.44
7:c:225:ASN:O	7:c:229:LEU:HB3	2.17	0.44
7:d:64:ASN:HB2	7:d:106:LEU:HD13	1.99	0.44
7:f:50:HIS:ND1	7:f:60:PHE:CG	2.82	0.44
8:M:357:GLN:HB2	8:M:361:TYR:HB2	1.96	0.44
1:A:110:VAL:HG22	1:A:130:ILE:HD12	1.99	0.44
1:A:166:ARG:HH12	2:C:876:GLU:CD	2.26	0.44
5:N:0:DG:C2	6:T:1:DA:C2	3.05	0.44
7:a:229:LEU:O	7:a:233:VAL:CB	2.63	0.44
7:b:48:ARG:HG3	7:b:52:LEU:CD1	2.47	0.44
7:c:31:PRO:CA	7:c:145:VAL:HG12	2.45	0.44
7:f:77:LEU:O	7:f:96:PHE:CD2	2.64	0.44
1:B:229:GLU:OE1	1:B:230:ALA:N	2.51	0.44
3:D:137:ARG:HH12	3:D:159:ILE:HG21	1.83	0.44
3:D:491:LEU:HA	3:D:498:PRO:HA	1.99	0.44
3:D:803:VAL:HB	3:D:1309:ILE:HG23	1.99	0.44
3:D:1027:VAL:O	3:D:1120:THR:OG1	2.33	0.44
7:a:63:LEU:C	7:a:63:LEU:CD2	2.90	0.44
7:a:105:PHE:CD2	7:a:105:PHE:O	2.71	0.44
7:b:20:GLU:HA	7:b:20:GLU:OE1	2.18	0.44
7:b:197:MET:HE2	7:b:237:VAL:HG13	1.99	0.44
7:f:105:PHE:O	7:f:105:PHE:CD2	2.70	0.44
7:e:56:TRP:O	7:e:56:TRP:CE3	2.70	0.44
7:e:179:LEU:HB3	7:e:225:ASN:HB3	2.00	0.44
8:M:156:ILE:HD13	8:M:156:ILE:N	2.32	0.44
3:D:197:GLU:OE2	3:D:220:ARG:NH2	2.38	0.44
3:D:316:ILE:HD13	3:D:316:ILE:H	1.82	0.44
7:a:96:PHE:HE2	7:a:120:LEU:HD12	1.79	0.44
7:b:61:ILE:HG12	7:b:99:ALA:HB2	1.99	0.44
7:d:34:ILE:HG12	7:d:174:VAL:HG13	1.98	0.44
7:d:109:LEU:HD21	7:d:169:LEU:HD13	1.98	0.44
7:e:112:ALA:HB1	7:e:117:GLN:HG3	2.00	0.44
7:e:239:ARG:HG3	7:e:251:ILE:HD11	1.98	0.44
8:M:23:ILE:HD12	8:M:23:ILE:HA	1.76	0.44
8:M:355:PHE:O	8:M:394:ARG:CD	2.62	0.44
8:M:460:LYS:O	8:M:463:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:HIS:HB3	3:D:83:VAL:HG12	2.00	0.44
3:D:516:ASP:OD1	3:D:516:ASP:N	2.49	0.44
7:a:34:ILE:HA	7:a:174:VAL:O	2.18	0.44
7:a:197:MET:SD	7:a:234:GLU:HG3	2.57	0.44
7:b:19:LEU:HD11	7:b:48:ARG:HD2	2.00	0.44
7:b:50:HIS:CD2	7:b:50:HIS:C	2.86	0.44
7:b:152:LEU:HB2	7:c:255:PHE:HE2	1.83	0.44
7:c:57:GLN:OE1	7:c:57:GLN:HA	2.17	0.44
7:c:144:LEU:H	7:c:144:LEU:CD1	2.30	0.44
7:f:55:ARG:NH2	7:f:143:ARG:HB2	2.33	0.44
7:f:195:ILE:HA	7:f:198:CYS:HG	1.83	0.44
7:e:8:LEU:HA	7:e:8:LEU:HD23	1.47	0.44
7:e:63:LEU:HD11	7:e:106:LEU:CD2	2.47	0.44
8:M:128:VAL:HG22	8:M:182:ILE:CD1	2.47	0.44
8:M:446:LEU:CD1	8:M:453:VAL:HG21	2.47	0.44
1:A:282:VAL:HG13	1:A:314:LEU:HA	2.00	0.44
2:C:59:ILE:HG23	2:C:476:LYS:HG2	2.00	0.44
2:C:366:ILE:HD11	2:C:370:MET:HE2	2.00	0.44
2:C:1296:ASP:OD2	2:C:1322:SER:N	2.49	0.44
7:a:25:LEU:HD21	7:b:238:TYR:CE2	2.53	0.44
7:b:59:PRO:HG2	7:b:99:ALA:HA	1.99	0.44
7:b:210:THR:CG2	7:b:248:ASP:HA	2.48	0.44
7:b:239:ARG:HG2	7:b:239:ARG:NH1	2.24	0.44
7:b:240:HIS:CE1	7:b:242:THR:HG22	2.49	0.44
7:c:39:GLY:HA2	9:c:400:ADP:PA	2.55	0.44
7:d:146:CYS:SG	7:d:169:LEU:HD11	2.58	0.44
7:d:152:LEU:N	7:d:153:PRO:CD	2.81	0.44
7:d:239:ARG:HD2	7:d:251:ILE:CD1	2.46	0.44
7:e:48:ARG:HE	7:e:52:LEU:HD11	1.82	0.44
7:e:117:GLN:OE1	7:e:165:LEU:HD23	2.18	0.44
8:M:8:ARG:HA	8:M:8:ARG:HD3	1.68	0.44
1:A:51:MET:SD	1:A:52:PRO:HD2	2.57	0.44
3:D:572:THR:OG1	3:D:573:THR:N	2.51	0.44
7:a:43:GLU:CG	7:f:126:TYR:OH	2.59	0.44
7:a:115:MET:H	7:a:115:MET:HG2	1.44	0.44
7:b:117:GLN:OE1	7:b:161:PHE:HA	2.18	0.44
7:c:60:PHE:O	7:c:60:PHE:CG	2.70	0.44
7:c:166:LEU:HD23	7:c:166:LEU:O	2.17	0.44
7:d:71:ASN:HD22	7:d:71:ASN:N	2.16	0.44
7:e:21:GLN:C	7:e:23:SER:N	2.72	0.44
8:M:345:ARG:O	8:M:348:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:364:PRO:HB2	8:M:406:HIS:CB	2.48	0.44
1:A:180:VAL:HA	1:A:207:THR:HA	2.00	0.44
2:C:1219:GLU:OE1	3:D:634:ARG:NH1	2.51	0.44
3:D:1208:ASP:O	3:D:1224:ARG:NH2	2.48	0.44
7:a:55:ARG:HH21	7:a:55:ARG:CG	2.14	0.44
7:a:59:PRO:CD	7:a:102:GLY:HA3	2.48	0.44
7:c:118:GLU:CD	7:c:118:GLU:C	2.86	0.44
7:d:28:LEU:HD13	7:d:30:LYS:HB2	2.00	0.44
7:d:166:LEU:HD23	7:d:166:LEU:O	2.17	0.44
7:f:179:LEU:HD21	7:f:186:ILE:CD1	2.48	0.44
8:M:289:LEU:HD11	8:M:341:LEU:HB2	1.99	0.44
2:C:148:GLN:HB2	2:C:511:LEU:HD21	2.00	0.43
2:C:1138:VAL:HG22	2:C:1170:MET:HE2	2.00	0.43
2:C:1293:VAL:HG13	2:C:1304:MET:HG2	1.99	0.43
3:D:518:VAL:HG23	3:D:519:ASN:H	1.83	0.43
7:a:34:ILE:CB	7:a:147:ALA:CB	2.91	0.43
7:a:57:GLN:C	7:a:58:GLY:O	2.57	0.43
7:a:83:GLY:H	7:a:88:ALA:HB1	1.83	0.43
7:b:131:ARG:NH2	7:b:138:LEU:CD2	2.81	0.43
7:b:255:PHE:O	7:b:256:LYS:C	2.61	0.43
7:f:34:ILE:O	7:f:148:THR:N	2.51	0.43
7:f:240:HIS:CD2	7:f:247:LEU:HA	2.53	0.43
8:M:260:PRO:CG	8:M:261:GLY:N	2.80	0.43
8:M:274:PRO:CB	8:M:391:HIS:CB	2.94	0.43
1:A:91:ARG:CZ	1:A:210:THR:O	2.65	0.43
1:B:82:LEU:HB3	1:B:173:VAL:HG13	1.98	0.43
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.53	0.43
2:C:1245:ALA:HB2	3:D:372:MET:HG3	2.01	0.43
2:C:1329:GLU:O	2:C:1332:SER:OG	2.33	0.43
3:D:361:LEU:HD21	3:D:367:GLY:N	2.32	0.43
5:N:-11:DA:C6	5:N:-10:DG:C2	3.05	0.43
6:T:6:DT:H2''	6:T:7:DG:H5'	2.00	0.43
6:T:14:DC:OP2	8:M:377:HIS:HD2	2.01	0.43
7:a:30:LYS:HE3	7:b:200:GLU:OE2	2.18	0.43
7:a:188:LEU:O	7:a:188:LEU:CD2	2.66	0.43
7:b:185:ASP:OD1	7:b:185:ASP:N	2.33	0.43
7:c:18:VAL:O	7:c:22:VAL:HG23	2.17	0.43
7:c:152:LEU:HD11	7:c:161:PHE:CG	2.53	0.43
7:c:170:ALA:O	7:d:235:ARG:HD2	2.17	0.43
7:c:175:GLN:C	7:c:176:LEU:HD23	2.44	0.43
7:c:225:ASN:N	7:c:225:ASN:HD22	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:126:TYR:HB3	7:f:128:GLU:OE2	2.18	0.43
7:f:132:VAL:O	7:f:132:VAL:HG12	2.17	0.43
8:M:394:ARG:HD3	8:M:394:ARG:HH11	1.69	0.43
2:C:12:ARG:NH2	2:C:793:GLU:OE1	2.52	0.43
2:C:1254:VAL:HG23	8:M:111:VAL:HG23	1.98	0.43
3:D:66:LYS:O	3:D:95:THR:OG1	2.33	0.43
7:a:38:ARG:NH2	7:f:164:ASP:CB	2.78	0.43
7:a:96:PHE:HE2	7:a:123:VAL:HG21	1.82	0.43
7:a:166:LEU:C	7:a:166:LEU:CD1	2.91	0.43
7:f:34:ILE:CB	7:f:147:ALA:HB1	2.38	0.43
2:C:199:ASP:HB2	2:C:201:ARG:HE	1.84	0.43
3:D:417:ARG:NH1	3:D:418:GLU:OE2	2.51	0.43
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.99	0.43
7:a:186:ILE:H	7:a:186:ILE:HG12	1.62	0.43
7:b:97:GLU:CD	7:b:97:GLU:C	2.86	0.43
7:b:176:LEU:HA	7:b:177:PRO:HD3	1.91	0.43
7:b:247:LEU:HD21	7:b:250:ILE:HD13	1.96	0.43
7:f:47:SER:O	7:f:51:TYR:HD1	1.93	0.43
7:f:80:HIS:NE2	7:f:92:HIS:HB2	2.32	0.43
7:e:32:VAL:CG2	7:e:143:ARG:HH21	2.24	0.43
8:M:365:MET:HE1	8:M:370:ILE:HB	2.00	0.43
8:M:424:VAL:CG1	8:M:428:ILE:HD11	2.48	0.43
2:C:1238:LEU:HD13	2:C:1240:ASP:HB2	2.00	0.43
3:D:70:CYS:CB	3:D:88:CYS:SG	3.07	0.43
3:D:72:CYS:CB	3:D:88:CYS:HB3	2.49	0.43
3:D:807:LEU:HD12	3:D:893:GLY:HA2	2.01	0.43
6:T:22:DG:H2'	6:T:23:DT:H71	1.99	0.43
7:a:25:LEU:HD22	7:a:28:LEU:HD12	1.99	0.43
7:a:45:ILE:O	7:a:46:ALA:C	2.59	0.43
7:a:95:ARG:CG	7:a:95:ARG:NH1	2.73	0.43
7:a:178:PRO:CG	7:a:181:GLU:CD	2.92	0.43
7:b:35:ILE:O	7:b:176:LEU:HD23	2.18	0.43
7:b:80:HIS:N	7:b:92:HIS:CD2	2.85	0.43
7:b:179:LEU:HD23	7:b:179:LEU:C	2.44	0.43
7:c:26:ALA:CB	7:c:52:LEU:CG	2.94	0.43
7:d:212:ARG:O	7:d:216:THR:HG23	2.18	0.43
8:M:147:ALA:CB	8:M:156:ILE:HD12	2.47	0.43
8:M:335:SER:O	8:M:336:ARG:C	2.62	0.43
8:M:350:GLN:H	8:M:350:GLN:HG2	1.30	0.43
2:C:95:PRO:HA	2:C:126:GLU:HG2	2.01	0.43
2:C:434:ASP:O	2:C:438:GLY:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:-17:DT:OP2	8:M:367:LEU:HD12	2.17	0.43
7:a:187:MET:HA	7:a:187:MET:HE3	2.01	0.43
7:b:65:CYS:HG	7:b:112:ALA:CB	2.29	0.43
7:c:37:GLU:CD	7:c:178:PRO:HB3	2.44	0.43
7:f:70:GLU:O	7:f:73:LEU:HB2	2.18	0.43
7:a:82:ALA:HB2	7:a:90:LYS:C	2.44	0.43
7:a:178:PRO:HD2	7:a:181:GLU:CD	2.43	0.43
7:b:15:PHE:HB2	7:b:182:ARG:CZ	2.48	0.43
7:c:12:ALA:C	7:c:14:SER:H	2.26	0.43
7:d:119:LYS:HE3	7:d:130:GLU:HB3	2.00	0.43
7:e:15:PHE:O	7:e:19:LEU:HD23	2.19	0.43
7:e:61:ILE:O	7:e:62:SER:HA	2.18	0.43
7:e:201:ILE:HD11	7:e:203:LEU:HD22	1.99	0.43
8:M:47:LEU:HD11	8:M:297:LEU:HB3	2.00	0.43
2:C:478:ARG:NH1	2:C:478:ARG:O	2.52	0.43
2:C:689:ALA:HB2	2:C:1233:LEU:HD12	2.00	0.43
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.53	0.43
3:D:130:MET:HE2	3:D:134:ASP:HB3	2.00	0.43
6:T:32:DT:H2"	6:T:33:DC:C5	2.53	0.43
7:a:61:ILE:CG1	7:a:99:ALA:HB2	2.49	0.43
7:c:60:PHE:CA	7:c:103:THR:O	2.58	0.43
7:d:252:ILE:H	7:d:252:ILE:HG12	1.59	0.43
7:f:85:PHE:CE1	8:M:5:LEU:HD13	2.54	0.43
9:f:601:ADP:O3B	10:f:602:AF3:F3	2.27	0.43
7:e:9:LEU:HB3	7:e:10:GLY:H	1.73	0.43
8:M:41:LEU:C	8:M:41:LEU:CD1	2.89	0.43
8:M:46:LEU:HB3	8:M:303:TYR:HB2	2.01	0.43
8:M:360:GLU:O	8:M:419:ALA:HB1	2.19	0.43
8:M:399:LEU:HD23	8:M:399:LEU:HA	1.82	0.43
7:a:43:GLU:HG2	7:f:126:TYR:CZ	2.54	0.43
7:a:204:PRO:CG	7:a:205:LEU:N	2.79	0.43
7:b:89:GLN:CD	7:b:89:GLN:N	2.73	0.43
7:b:136:GLN:H	7:b:136:GLN:CD	2.26	0.43
7:b:175:GLN:OE1	7:b:175:GLN:HA	2.19	0.43
7:c:5:LYS:HB3	7:c:48:ARG:HH11	1.80	0.43
7:c:108:GLU:HB3	7:c:111:THR:HG23	2.01	0.43
7:c:257:ARG:HE	7:c:257:ARG:HB3	1.65	0.43
7:f:193:PHE:HB3	7:f:234:GLU:OE2	2.18	0.43
7:e:44:LEU:HD11	9:e:601:ADP:H3'	2.01	0.43
7:e:250:ILE:HD13	7:e:250:ILE:HA	1.89	0.43
2:C:823:VAL:HG12	2:C:1059:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:839:VAL:HB	2:C:1046:VAL:HG13	2.01	0.43
3:D:368:LEU:HD22	3:D:373:ALA:HB2	2.00	0.43
3:D:807:LEU:HD11	3:D:894:VAL:HG23	2.00	0.43
5:N:-11:DA:C5	5:N:-10:DG:C2	3.06	0.43
9:a:601:ADP:H3'	9:a:601:ADP:PA	2.58	0.43
7:b:31:PRO:C	7:b:170:ALA:HA	2.43	0.43
7:b:60:PHE:O	7:b:61:ILE:C	2.59	0.43
7:b:109:LEU:CB	7:b:146:CYS:SG	3.05	0.43
7:b:122:ARG:HB3	7:b:122:ARG:HH11	1.84	0.43
7:b:210:THR:OG1	7:b:212:ARG:CG	2.67	0.43
7:b:222:TRP:HA	7:b:223:PRO:HD2	1.74	0.43
7:e:152:LEU:N	7:e:153:PRO:CD	2.82	0.43
8:M:277:LEU:N	8:M:277:LEU:HD22	2.34	0.43
8:M:345:ARG:O	8:M:348:VAL:CG1	2.67	0.43
1:A:33:ARG:NH2	1:A:197:ASP:O	2.47	0.42
3:D:148:GLU:HG3	3:D:149:GLY:H	1.84	0.42
3:D:1026:PRO:HA	3:D:1120:THR:HG21	2.01	0.42
7:a:34:ILE:HD13	7:a:34:ILE:HG21	1.33	0.42
7:a:173:VAL:HG21	7:b:254:PRO:O	2.19	0.42
7:b:29:ASP:O	7:b:143:ARG:CD	2.67	0.42
7:b:38:ARG:O	7:b:38:ARG:HG2	2.18	0.42
7:b:194:ALA:HB1	7:b:206:PHE:CE2	2.50	0.42
7:b:201:ILE:O	7:b:201:ILE:CG1	2.67	0.42
7:b:248:ASP:OD1	7:b:248:ASP:N	2.48	0.42
7:c:37:GLU:HB2	7:c:40:THR:CG2	2.48	0.42
7:c:44:LEU:CD2	7:c:44:LEU:C	2.85	0.42
7:c:96:PHE:CE1	7:c:129:LEU:HD21	2.54	0.42
7:f:108:GLU:HG3	7:f:108:GLU:O	2.19	0.42
7:e:258:ARG:N	7:e:259:PRO:HD2	2.34	0.42
8:M:308:ASN:O	8:M:310:ALA:N	2.52	0.42
1:B:59:VAL:HG11	1:B:85:LEU:HD13	2.00	0.42
2:C:1306:LYS:HA	8:M:130:LEU:CD2	2.37	0.42
3:D:126:LEU:O	3:D:220:ARG:NH1	2.53	0.42
7:a:189:MET:O	7:a:190:ALA:C	2.62	0.42
7:b:124:ILE:HG22	7:b:144:LEU:CD1	2.49	0.42
7:c:63:LEU:HD13	7:c:64:ASN:C	2.44	0.42
7:c:183:GLU:HG3	7:c:183:GLU:O	2.19	0.42
7:e:81:GLU:CD	7:e:91:ARG:HH22	2.27	0.42
8:M:224:LEU:HD13	8:M:224:LEU:C	2.44	0.42
8:M:348:VAL:O	8:M:348:VAL:CG2	2.57	0.42
3:D:960:LEU:HD13	3:D:963:VAL:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:-16:DT:P	8:M:400:LYS:HZ3	2.42	0.42
7:b:145:VAL:HG23	7:b:145:VAL:O	2.19	0.42
7:d:195:ILE:HA	7:d:198:CYS:SG	2.60	0.42
7:f:18:VAL:O	7:f:22:VAL:HG23	2.19	0.42
7:e:78:PHE:CZ	7:e:119:LYS:O	2.71	0.42
8:M:15:MET:C	8:M:16:THR:CG2	2.92	0.42
1:A:180:VAL:HG22	1:A:207:THR:HG22	2.01	0.42
1:B:104:LYS:HG2	1:B:105:SER:H	1.84	0.42
5:N:-8:DT:C4'	7:b:90:LYS:CE	2.94	0.42
7:a:86:THR:HB	8:M:8:ARG:HB2	2.00	0.42
7:a:195:ILE:HA	7:a:198:CYS:HB3	2.01	0.42
7:b:124:ILE:HG22	7:b:144:LEU:HD12	2.01	0.42
7:b:195:ILE:HD12	7:b:206:PHE:CE1	2.54	0.42
7:b:239:ARG:HH11	7:b:239:ARG:CG	2.22	0.42
7:c:179:LEU:HG	7:c:225:ASN:HA	2.01	0.42
7:f:76:GLU:O	7:f:95:ARG:HG2	2.19	0.42
7:e:72:LEU:N	7:e:72:LEU:CD2	2.80	0.42
7:e:75:SER:O	7:e:79:GLY:HA2	2.19	0.42
8:M:460:LYS:HZ2	8:M:460:LYS:HG2	1.75	0.42
3:D:65:VAL:HA	3:D:98:ARG:HH11	1.85	0.42
5:N:-18:DT:H3'	8:M:366:VAL:CG1	2.49	0.42
7:a:7:ASN:N	7:a:7:ASN:OD1	2.52	0.42
7:a:105:PHE:O	7:a:105:PHE:CG	2.70	0.42
7:b:104:LEU:O	7:b:145:VAL:HG22	2.18	0.42
7:c:117:GLN:O	7:c:165:LEU:HD12	2.19	0.42
7:f:217:LEU:HD12	7:f:218:LEU:HD23	2.01	0.42
7:e:33:LEU:HD13	7:e:146:CYS:HB2	2.01	0.42
7:e:62:SER:HB2	7:e:105:PHE:HB3	2.00	0.42
7:e:189:MET:CE	7:e:226:ILE:CG1	2.97	0.42
8:M:125:MET:O	8:M:128:VAL:N	2.52	0.42
8:M:134:THR:OG1	8:M:137:ASP:OD1	2.37	0.42
1:A:74:VAL:HG12	1:A:133:LEU:HD22	2.00	0.42
3:D:339:ARG:NE	3:D:339:ARG:HA	2.35	0.42
3:D:802:ASP:OD2	3:D:1348:LYS:NZ	2.52	0.42
3:D:813:ASP:OD1	3:D:883:ARG:NH1	2.41	0.42
7:a:73:LEU:C	7:a:73:LEU:HD12	2.44	0.42
7:a:119:LYS:HG3	7:b:67:ALA:HA	2.00	0.42
7:b:32:VAL:O	7:b:145:VAL:HA	2.19	0.42
7:b:42:LYS:HD3	7:b:147:ALA:CB	2.40	0.42
7:b:73:LEU:HD11	7:b:116:VAL:CG2	2.50	0.42
7:b:130:GLU:O	7:b:130:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:99:ALA:HB1	7:d:104:LEU:CD1	2.50	0.42
7:d:186:ILE:HG13	7:d:187:MET:H	1.85	0.42
7:e:197:MET:HG3	7:e:237:VAL:HG11	2.01	0.42
8:M:129:GLU:OE1	8:M:129:GLU:HA	2.20	0.42
2:C:1067:ALA:HA	2:C:1073:LYS:HA	2.01	0.42
2:C:1315:MET:HB2	3:D:473:THR:HG21	2.02	0.42
3:D:824:PRO:HG3	3:D:835:LEU:HB2	2.02	0.42
5:N:-11:DA:C5	5:N:-10:DG:C4	3.08	0.42
7:a:180:ARG:HD3	7:a:180:ARG:N	2.34	0.42
7:b:55:ARG:C	7:b:57:GLN:H	2.27	0.42
7:b:172:ASP:OD1	7:b:173:VAL:N	2.53	0.42
7:c:26:ALA:HB1	7:c:52:LEU:HG	2.01	0.42
7:c:35:ILE:HD11	7:c:173:VAL:HG23	1.91	0.42
7:c:141:ASN:HD22	7:c:141:ASN:H	1.66	0.42
7:c:217:LEU:HD22	7:c:217:LEU:HA	1.87	0.42
7:d:177:PRO:HA	7:d:178:PRO:HD3	1.92	0.42
7:f:30:LYS:CG	7:f:171:PHE:CE2	3.03	0.42
7:f:50:HIS:CD2	7:f:50:HIS:O	2.73	0.42
7:f:64:ASN:HB3	7:f:67:ALA:CB	2.50	0.42
8:M:197:ASP:N	8:M:197:ASP:OD1	2.50	0.42
8:M:245:VAL:O	8:M:248:GLU:CG	2.65	0.42
2:C:525:THR:O	2:C:529:ARG:HG3	2.19	0.42
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.02	0.42
2:C:765:ILE:HA	2:C:787:PRO:HG3	2.01	0.42
3:D:437:PHE:HZ	3:D:453:VAL:HG11	1.85	0.42
7:a:96:PHE:CZ	7:a:123:VAL:CG1	3.00	0.42
7:a:245:TYR:CD1	7:a:245:TYR:C	2.97	0.42
7:b:25:LEU:CG	7:c:238:TYR:CZ	3.03	0.42
7:b:257:ARG:H	7:b:257:ARG:HG2	1.53	0.42
7:c:33:LEU:HD12	7:c:34:ILE:H	1.83	0.42
7:c:98:ARG:HB2	7:c:98:ARG:HH11	1.82	0.42
7:f:104:LEU:O	7:f:144:LEU:HD12	2.19	0.42
7:f:130:GLU:H	7:f:130:GLU:CD	2.23	0.42
7:f:136:GLN:NE2	7:f:136:GLN:H	2.16	0.42
7:f:187:MET:HE2	7:f:214:ARG:HH21	1.85	0.42
7:f:235:ARG:HD2	7:f:251:ILE:HG21	2.02	0.42
7:a:95:ARG:NH1	7:a:98:ARG:NH2	2.65	0.42
7:a:178:PRO:CG	7:a:181:GLU:CG	2.84	0.42
7:b:131:ARG:HH22	7:b:138:LEU:HD22	1.84	0.42
7:b:136:GLN:HA	7:b:137:PRO:HD3	1.68	0.42
7:b:157:ASN:N	7:b:157:ASN:ND2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:204:PRO:CG	7:b:205:LEU:N	2.83	0.42
7:b:236:SER:O	7:b:239:ARG:HB3	2.20	0.42
7:c:229:LEU:O	7:c:233:VAL:N	2.50	0.42
7:d:28:LEU:HD12	7:d:28:LEU:C	2.44	0.42
7:e:35:ILE:CD1	7:e:148:THR:HG21	2.50	0.42
8:M:355:PHE:HD1	8:M:355:PHE:N	2.14	0.42
3:D:147:ILE:HA	3:D:188:LEU:HD21	2.02	0.42
6:T:23:DT:H2"	6:T:24:DG:C8	2.53	0.42
7:d:15:PHE:O	7:d:18:VAL:HG22	2.19	0.42
7:f:9:LEU:HD23	9:f:601:ADP:H2	1.85	0.42
7:f:26:ALA:HB1	7:f:52:LEU:C	2.45	0.42
7:f:31:PRO:HB3	7:f:144:LEU:HB3	2.02	0.42
7:f:127:GLY:O	7:f:139:GLN:HA	2.20	0.42
8:M:124:LEU:CD1	8:M:145:VAL:HG23	2.50	0.42
8:M:165:ILE:HG22	8:M:167:ASP:N	2.35	0.42
8:M:279:ARG:HD2	8:M:279:ARG:O	2.20	0.42
1:A:180:VAL:C	1:A:182:ARG:H	2.28	0.41
2:C:321:LEU:HG	2:C:325:LEU:HD23	2.02	0.41
3:D:698:MET:O	3:D:702:GLN:N	2.52	0.41
7:a:96:PHE:CE2	7:a:123:VAL:CG2	3.02	0.41
7:a:109:LEU:O	7:a:109:LEU:HD12	2.20	0.41
7:a:185:ASP:O	7:a:189:MET:HE3	2.20	0.41
7:b:33:LEU:HD13	7:b:169:LEU:HD21	2.02	0.41
7:b:201:ILE:O	7:b:201:ILE:CD1	2.68	0.41
7:c:41:GLY:O	7:c:45:ILE:CB	2.68	0.41
7:c:152:LEU:N	7:c:153:PRO:HD2	2.35	0.41
7:d:40:THR:O	7:d:42:LYS:N	2.53	0.41
7:f:130:GLU:O	7:f:130:GLU:HG2	2.20	0.41
8:M:375:GLU:CD	8:M:375:GLU:H	2.28	0.41
8:M:421:ARG:HG2	8:M:465:LEU:HD21	2.01	0.41
2:C:345:PRO:C	2:C:347:ILE:H	2.29	0.41
3:D:1115:ILE:HD12	3:D:1115:ILE:HA	1.97	0.41
5:N:-27:DT:OP1	8:M:470:SER:OG	2.35	0.41
7:a:74:ASP:OD1	7:a:119:LYS:HD3	2.20	0.41
7:a:104:LEU:HD12	7:a:104:LEU:HA	1.77	0.41
7:a:167:ASP:OD1	7:a:167:ASP:N	2.53	0.41
7:a:228:GLU:O	7:a:232:VAL:HB	2.19	0.41
7:b:19:LEU:CD1	7:b:48:ARG:HD2	2.50	0.41
7:b:120:LEU:HA	7:b:120:LEU:HD23	1.47	0.41
7:b:129:LEU:CD2	7:b:138:LEU:O	2.67	0.41
7:c:8:LEU:CD2	7:c:15:PHE:HE2	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:7:ASN:HB2	7:d:8:LEU:HD13	2.02	0.41
7:d:49:LEU:HA	7:d:49:LEU:HD23	1.81	0.41
7:f:55:ARG:HH21	7:f:143:ARG:HB2	1.85	0.41
7:f:124:ILE:HD13	7:f:144:LEU:HD22	2.01	0.41
7:f:128:GLU:OE2	7:f:128:GLU:N	2.53	0.41
7:e:91:ARG:NH2	7:e:91:ARG:CG	2.73	0.41
8:M:127:GLN:O	8:M:128:VAL:C	2.61	0.41
8:M:180:LYS:HA	8:M:183:GLN:HB2	2.02	0.41
1:A:84:ASN:ND2	1:A:131:CYS:SG	2.93	0.41
1:B:118:ASP:HB2	1:B:121:VAL:HB	2.02	0.41
1:B:150:ARG:O	1:B:150:ARG:NE	2.46	0.41
2:C:1260:GLY:HA2	3:D:346:ARG:HG2	2.01	0.41
3:D:253:VAL:HG11	8:M:112:TYR:CG	2.55	0.41
3:D:394:ILE:HD11	8:M:130:LEU:O	2.20	0.41
7:b:33:LEU:HD23	7:b:173:VAL:HG12	2.02	0.41
7:b:210:THR:OG1	7:b:212:ARG:HG3	2.20	0.41
7:d:60:PHE:CD2	7:d:60:PHE:O	2.73	0.41
7:f:77:LEU:CD1	7:f:119:LYS:HB3	2.50	0.41
7:e:30:LYS:HB3	7:e:31:PRO:CD	2.45	0.41
7:e:45:ILE:HB	7:e:46:ALA:H	1.71	0.41
8:M:154:LEU:HD12	8:M:193:LYS:CA	2.46	0.41
8:M:195:LEU:HD11	8:M:199:LEU:HD12	1.81	0.41
8:M:199:LEU:HD22	8:M:256:LEU:HD12	2.01	0.41
3:D:252:LEU:HB3	3:D:260:PHE:HB3	2.02	0.41
3:D:816:THR:HG21	3:D:888:CYS:HA	2.01	0.41
3:D:1178:THR:N	3:D:1179:PRO:HD3	2.35	0.41
7:b:232:VAL:O	7:b:236:SER:HB2	2.20	0.41
7:c:224:GLY:O	7:c:228:GLU:HB3	2.21	0.41
7:f:197:MET:CG	7:f:237:VAL:HG11	2.39	0.41
7:e:3:GLU:HA	7:e:3:GLU:OE2	2.20	0.41
7:e:35:ILE:HD13	7:e:148:THR:CG2	2.49	0.41
7:e:202:LYS:HA	7:e:202:LYS:HD3	1.79	0.41
8:M:165:ILE:HG21	8:M:170:ILE:CG1	2.48	0.41
1:B:15:ASP:N	1:B:15:ASP:OD1	2.53	0.41
3:D:135:ILE:HA	3:D:138:VAL:HG12	2.02	0.41
3:D:374:LEU:HB2	3:D:412:LEU:HD22	2.03	0.41
7:a:32:VAL:HG23	7:a:172:ASP:O	2.21	0.41
7:b:49:LEU:HG	7:b:49:LEU:N	2.34	0.41
7:b:65:CYS:SG	7:b:65:CYS:O	2.78	0.41
7:b:119:LYS:O	7:b:120:LEU:C	2.63	0.41
7:b:195:ILE:O	7:b:196:GLN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:225:ASN:O	7:c:229:LEU:CB	2.68	0.41
7:f:232:VAL:O	7:f:233:VAL:C	2.63	0.41
7:e:71:ASN:C	7:e:73:LEU:N	2.60	0.41
8:M:420:ILE:HD11	8:M:451:ILE:HG23	2.00	0.41
3:D:51:PRO:HD2	3:D:71:LEU:HD13	2.02	0.41
7:a:151:ASP:HB2	7:a:153:PRO:HD2	2.02	0.41
7:a:180:ARG:CD	7:a:180:ARG:H	2.34	0.41
7:b:29:ASP:OD1	7:b:143:ARG:HD3	2.21	0.41
7:b:50:HIS:ND1	7:b:103:THR:OG1	2.37	0.41
7:b:81:GLU:OE1	7:b:132:VAL:O	2.39	0.41
7:b:197:MET:CE	7:b:237:VAL:HG13	2.51	0.41
1:B:104:LYS:HE2	1:B:104:LYS:HB3	1.86	0.41
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.03	0.41
3:D:114:ILE:HD13	3:D:308:ASP:HB2	2.02	0.41
3:D:336:GLY:O	3:D:339:ARG:HB2	2.20	0.41
7:a:30:LYS:HE3	7:b:200:GLU:HG3	2.01	0.41
7:b:15:PHE:HD1	7:b:182:ARG:NH1	2.18	0.41
7:b:236:SER:OG	7:b:250:ILE:HG23	2.21	0.41
7:c:69:ASN:HB2	7:c:72:LEU:CD1	2.48	0.41
7:c:100:ASP:HB3	7:c:140:VAL:HG11	2.01	0.41
7:f:117:GLN:NE2	7:f:161:PHE:HA	2.28	0.41
7:e:197:MET:CG	7:e:237:VAL:HG11	2.51	0.41
8:M:15:MET:HE3	8:M:15:MET:HB3	1.86	0.41
3:D:570:LYS:HE2	3:D:570:LYS:HB3	1.97	0.41
3:D:1177:ILE:HG12	3:D:1179:PRO:HD3	2.02	0.41
7:a:225:ASN:O	7:a:226:ILE:C	2.63	0.41
7:b:176:LEU:N	7:b:176:LEU:CD2	2.84	0.41
7:b:211:GLU:CD	7:b:211:GLU:N	2.76	0.41
7:c:224:GLY:CA	7:c:228:GLU:CB	2.93	0.41
7:c:226:ILE:H	7:c:226:ILE:CD1	1.96	0.41
7:f:164:ASP:O	7:f:167:ASP:N	2.53	0.41
7:e:114:MET:O	7:e:118:GLU:HG2	2.21	0.41
7:e:129:LEU:O	7:e:129:LEU:HD22	2.20	0.41
7:e:132:VAL:O	7:e:132:VAL:HG13	2.20	0.41
1:B:11:PRO:HB3	1:B:31:LEU:HD21	2.01	0.41
2:C:28:LEU:HD21	2:C:524:ILE:HG13	2.03	0.41
2:C:39:ILE:HG21	2:C:75:LEU:HD22	2.02	0.41
3:D:253:VAL:HG11	8:M:112:TYR:CB	2.51	0.41
3:D:291:ILE:HG12	8:M:303:TYR:CE1	2.56	0.41
3:D:749:LYS:HA	3:D:753:SER:O	2.21	0.41
5:N:-6:DA:H2"	5:N:-5:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:117:GLN:HG2	7:a:165:LEU:HD13	2.03	0.41
7:a:221:ARG:C	7:a:221:ARG:HD2	2.45	0.41
7:b:189:MET:HE1	9:b:601:ADP:C6	2.56	0.41
7:c:8:LEU:HD11	7:c:15:PHE:CE2	2.41	0.41
7:c:15:PHE:O	7:c:19:LEU:HG	2.21	0.41
7:c:26:ALA:N	7:c:27:PRO:CD	2.82	0.41
7:c:152:LEU:CD2	7:c:166:LEU:CG	2.89	0.41
7:d:42:LYS:O	7:d:44:LEU:N	2.54	0.41
7:d:77:LEU:O	7:d:95:ARG:N	2.54	0.41
7:f:47:SER:C	7:f:51:TYR:HE1	2.28	0.41
7:f:82:ALA:HB2	7:f:90:LYS:C	2.42	0.41
7:f:87:GLY:CA	7:e:86:THR:HA	2.49	0.41
7:e:89:GLN:HE21	7:e:89:GLN:HB2	1.69	0.41
7:e:98:ARG:HG2	7:e:98:ARG:HH21	1.86	0.41
7:e:203:LEU:HA	7:e:204:PRO:HD3	1.88	0.41
8:M:156:ILE:CD1	8:M:156:ILE:N	2.83	0.41
8:M:344:SER:O	8:M:347:ILE:HG23	2.21	0.41
8:M:424:VAL:HG13	8:M:428:ILE:CD1	2.51	0.41
2:C:346:TYR:OH	2:C:436:ARG:NH2	2.54	0.41
3:D:59:ALA:C	3:D:61:ILE:H	2.29	0.41
3:D:74:LYS:HE3	3:D:75:TYR:CE2	2.56	0.41
3:D:252:LEU:HA	3:D:262:THR:HG22	2.04	0.41
3:D:352:ARG:NE	3:D:465:GLN:OE1	2.54	0.41
7:a:206:PHE:HA	7:a:207:PRO:HD3	1.76	0.41
7:b:225:ASN:O	7:b:227:ARG:N	2.55	0.41
7:b:234:GLU:CA	7:b:237:VAL:HG12	2.51	0.41
7:c:66:ALA:HB2	7:c:111:THR:HG21	2.03	0.41
7:c:77:LEU:N	7:c:77:LEU:CD1	2.84	0.41
7:c:104:LEU:HB2	7:c:144:LEU:HB2	2.03	0.41
7:d:38:ARG:O	7:d:38:ARG:HG2	2.20	0.41
7:d:125:GLU:H	7:d:125:GLU:HG3	1.65	0.41
7:d:152:LEU:N	7:d:153:PRO:HD2	2.36	0.41
7:f:227:ARG:HH22	7:e:168:ARG:HH12	1.68	0.41
7:e:196:GLN:OE1	7:e:196:GLN:HA	2.17	0.41
2:C:1042:LEU:HD13	2:C:1049:ILE:HG13	2.03	0.40
7:c:69:ASN:CB	7:c:72:LEU:HD12	2.48	0.40
7:f:256:LYS:HD2	7:f:256:LYS:C	2.46	0.40
7:e:22:VAL:HA	7:e:25:LEU:CG	2.50	0.40
7:e:26:ALA:CB	7:e:53:SER:HA	2.43	0.40
7:e:212:ARG:HA	7:e:215:GLU:OE1	2.21	0.40
7:e:256:LYS:HD2	7:e:256:LYS:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:185:PHE:HD1	8:M:185:PHE:HA	1.74	0.40
1:B:191:ARG:HB3	1:B:196:THR:HG22	2.03	0.40
2:C:199:ASP:HA	2:C:200:ARG:HH21	1.85	0.40
7:a:111:THR:CG2	7:f:162:ARG:HH22	2.09	0.40
7:a:178:PRO:CB	7:a:180:ARG:HE	2.34	0.40
7:c:26:ALA:HB1	7:c:52:LEU:CG	2.50	0.40
7:c:35:ILE:CD1	7:c:35:ILE:N	2.78	0.40
7:c:37:GLU:O	7:c:40:THR:CG2	2.56	0.40
7:d:58:GLY:HA2	7:d:59:PRO:HD3	1.87	0.40
7:f:99:ALA:O	7:f:100:ASP:C	2.63	0.40
7:f:191:GLU:OE2	7:f:195:ILE:HD11	2.20	0.40
7:e:117:GLN:OE1	7:e:161:PHE:CE2	2.74	0.40
8:M:306:MET:HG3	8:M:306:MET:O	2.21	0.40
1:A:11:PRO:HG3	1:A:31:LEU:HD23	2.03	0.40
2:C:707:ALA:HA	2:C:710:VAL:HG22	2.03	0.40
2:C:746:ALA:HB2	2:C:963:GLU:HG3	2.02	0.40
5:N:-11:DA:C5	5:N:-10:DG:N3	2.89	0.40
6:T:8:DA:H2''	6:T:9:DT:O5'	2.22	0.40
7:a:35:ILE:HD13	7:a:148:THR:HG22	2.03	0.40
7:a:41:GLY:HA2	9:a:601:ADP:H8	1.87	0.40
7:c:42:LYS:HE3	9:c:400:ADP:PB	2.62	0.40
7:c:100:ASP:HA	7:c:142:VAL:CG2	2.50	0.40
7:c:194:ALA:O	7:c:198:CYS:SG	2.67	0.40
8:M:124:LEU:HD12	8:M:145:VAL:HG23	2.02	0.40
1:A:308:ALA:HB1	8:M:181:ARG:CB	2.52	0.40
2:C:444:ASP:O	2:C:450:ASN:ND2	2.42	0.40
3:D:195:GLU:H	3:D:195:GLU:HG3	1.76	0.40
3:D:963:VAL:HG22	3:D:980:THR:HG22	2.03	0.40
4:E:29:GLN:HA	4:E:32:VAL:HG12	2.04	0.40
7:a:41:GLY:HA2	9:a:601:ADP:C8	2.57	0.40
7:a:119:LYS:HE2	7:b:67:ALA:C	2.47	0.40
7:a:185:ASP:O	7:a:189:MET:HE2	2.21	0.40
7:b:95:ARG:HD3	7:b:95:ARG:HA	1.47	0.40
7:b:212:ARG:HE	7:b:212:ARG:HB2	1.60	0.40
7:e:37:GLU:HB2	7:e:40:THR:OG1	2.21	0.40
7:e:48:ARG:HG2	7:e:52:LEU:HD11	2.02	0.40
7:e:178:PRO:O	7:e:181:GLU:N	2.51	0.40
8:M:28:LEU:HD12	8:M:28:LEU:O	2.20	0.40
8:M:442:LEU:O	8:M:445:MET:N	2.55	0.40
3:D:109:SER:HA	3:D:110:PRO:HD3	1.98	0.40
7:a:173:VAL:HG23	7:b:254:PRO:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:199:ARG:HE	7:a:199:ARG:HA	1.87	0.40
7:b:50:HIS:O	7:b:50:HIS:CG	2.71	0.40
7:b:77:LEU:O	7:b:95:ARG:HB3	2.21	0.40
7:c:5:LYS:CD	7:c:5:LYS:C	2.95	0.40
7:f:178:PRO:HA	7:f:225:ASN:ND2	2.36	0.40
7:e:65:CYS:HA	7:e:68:LEU:HD12	2.03	0.40
7:e:92:HIS:HA	7:e:93:PRO:HD3	1.90	0.40
8:M:367:LEU:HD21	8:M:403:PHE:CE2	2.53	0.40
8:M:424:VAL:CG1	8:M:428:ILE:CD1	2.99	0.40
8:M:439:ASP:O	8:M:442:LEU:HB2	2.22	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	305/329 (93%)	282 (92%)	22 (7%)	1 (0%)	36	67
1	B	219/329 (67%)	203 (93%)	16 (7%)	0	100	100
2	C	1339/1342 (100%)	1264 (94%)	75 (6%)	0	100	100
3	D	1322/1407 (94%)	1226 (93%)	93 (7%)	3 (0%)	43	74
4	E	72/91 (79%)	70 (97%)	2 (3%)	0	100	100
7	a	257/295 (87%)	200 (78%)	43 (17%)	14 (5%)	1	14
7	b	256/295 (87%)	216 (84%)	27 (10%)	13 (5%)	1	15
7	c	254/295 (86%)	221 (87%)	31 (12%)	2 (1%)	16	49
7	d	254/295 (86%)	226 (89%)	23 (9%)	5 (2%)	6	32
7	e	257/295 (87%)	217 (84%)	30 (12%)	10 (4%)	2	20
7	f	257/295 (87%)	225 (88%)	22 (9%)	10 (4%)	2	20
8	M	413/477 (87%)	360 (87%)	42 (10%)	11 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5205/5745 (91%)	4710 (90%)	426 (8%)	69 (1%)	12	39

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	a	12	ALA
7	a	56	TRP
7	a	121	LEU
7	b	81	GLU
7	b	93	PRO
7	b	225	ASN
7	b	226	ILE
7	f	183	GLU
7	e	72	LEU
7	e	211	GLU
8	M	194	ASP
8	M	196	ARG
8	M	353	ALA
7	a	5	LYS
7	a	7	ASN
7	a	74	ASP
7	a	184	SER
7	b	223	PRO
7	d	41	GLY
7	f	110	ALA
7	f	255	PHE
8	M	189	GLY
7	a	2	ALA
7	a	51	TYR
7	a	126	TYR
7	b	66	ALA
7	b	170	ALA
7	d	43	GLU
7	d	135	SER
7	f	223	PRO
7	e	54	SER
7	e	71	ASN
8	M	112	TYR
8	M	120	LEU
8	M	309	SER
3	D	886	VAL
7	a	166	LEU

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Mol	Chain	Res	Type
7	b	55	ARG
7	b	137	PRO
7	d	77	LEU
7	d	159	GLY
7	f	132	VAL
7	e	112	ALA
7	e	125	GLU
3	D	340	GLN
7	b	178	PRO
7	b	254	PRO
7	f	73	LEU
7	e	69	ASN
7	e	182	ARG
8	M	10	SER
8	M	110	PRO
1	A	194	GLN
7	a	127	GLY
7	b	9	LEU
7	c	251	ILE
7	f	254	PRO
7	e	14	SER
7	e	111	THR
8	M	264	ILE
7	a	145	VAL
7	b	204	PRO
7	f	204	PRO
7	a	204	PRO
7	c	204	PRO
7	f	252	ILE
8	M	272	VAL
3	D	750	PRO
7	f	41	GLY

5.3.2 Protein sidechains [i](#)

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	249/286 (87%)	236 (95%)	13 (5%)	21	47
1	B	180/286 (63%)	169 (94%)	11 (6%)	17	43
2	C	1047/1157 (90%)	1009 (96%)	38 (4%)	31	57
3	D	913/1168 (78%)	865 (95%)	48 (5%)	20	47
4	E	53/75 (71%)	53 (100%)	0	100	100
7	a	219/252 (87%)	154 (70%)	65 (30%)	0	2
7	b	219/252 (87%)	178 (81%)	41 (19%)	1	9
7	c	208/252 (82%)	181 (87%)	27 (13%)	4	21
7	d	218/252 (86%)	189 (87%)	29 (13%)	4	20
7	e	220/252 (87%)	185 (84%)	35 (16%)	2	14
7	f	219/252 (87%)	192 (88%)	27 (12%)	4	22
8	M	367/423 (87%)	276 (75%)	91 (25%)	1	4
All	All	4112/4907 (84%)	3687 (90%)	425 (10%)	9	28

All (425) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	8	PHE
1	A	13	LEU
1	A	16	ILE
1	A	31	LEU
1	A	90	VAL
1	A	92	VAL
1	A	110	VAL
1	A	121	VAL
1	A	201	LEU
1	A	262	LEU
1	A	278	ILE
1	A	289	LEU
1	B	14	VAL
1	B	16	ILE
1	B	59	VAL
1	B	72	GLU
1	B	145	LYS
1	B	150	ARG
1	B	153	VAL
1	B	182	ARG
1	B	224	LEU

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Mol	Chain	Res	Type
1	B	228	LEU
1	B	229	GLU
2	C	2	VAL
2	C	37	LYS
2	C	39	ILE
2	C	91	THR
2	C	176	ILE
2	C	189	ASP
2	C	200	ARG
2	C	204	LEU
2	C	208	ILE
2	C	209	ILE
2	C	221	LEU
2	C	237	LEU
2	C	261	VAL
2	C	324	LYS
2	C	397	LEU
2	C	484	LEU
2	C	487	LEU
2	C	496	LYS
2	C	589	THR
2	C	593	LYS
2	C	697	LYS
2	C	748	ILE
2	C	755	LYS
2	C	796	LEU
2	C	817	LEU
2	C	873	ILE
2	C	918	LEU
2	C	927	THR
2	C	957	LYS
2	C	1014	LEU
2	C	1026	GLU
2	C	1027	LYS
2	C	1029	LEU
2	C	1060	ILE
2	C	1161	LEU
2	C	1176	LEU
2	C	1238	LEU
2	C	1268	GLN
3	D	5	LEU
3	D	44	ILE

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Mol	Chain	Res	Type
3	D	50	LYS
3	D	53	ARG
3	D	66	LYS
3	D	74	LYS
3	D	92	VAL
3	D	117	LEU
3	D	161	THR
3	D	166	LEU
3	D	171	GLU
3	D	223	LEU
3	D	265	LEU
3	D	295	GLU
3	D	316	ILE
3	D	321	LYS
3	D	324	LEU
3	D	325	LYS
3	D	340	GLN
3	D	347	VAL
3	D	370	LYS
3	D	422	LEU
3	D	424	ASN
3	D	428	THR
3	D	430	HIS
3	D	445	LYS
3	D	447	ILE
3	D	460	ASP
3	D	505	ASP
3	D	517	CYS
3	D	518	VAL
3	D	563	LEU
3	D	570	LYS
3	D	703	THR
3	D	747	MET
3	D	781	LYS
3	D	802	ASP
3	D	825	VAL
3	D	826	ILE
3	D	827	GLU
3	D	848	VAL
3	D	881	LYS
3	D	885	VAL
3	D	901	ARG

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Mol	Chain	Res	Type
3	D	911	LYS
3	D	960	LEU
3	D	1247	LYS
3	D	1266	ILE
7	a	3	GLU
7	a	4	TYR
7	a	5	LYS
7	a	9	LEU
7	a	11	GLU
7	a	22	VAL
7	a	28	LEU
7	a	30	LYS
7	a	32	VAL
7	a	33	LEU
7	a	38	ARG
7	a	42	LYS
7	a	44	LEU
7	a	49	LEU
7	a	52	LEU
7	a	54	SER
7	a	55	ARG
7	a	56	TRP
7	a	63	LEU
7	a	70	GLU
7	a	86	THR
7	a	89	GLN
7	a	91	ARG
7	a	95	ARG
7	a	98	ARG
7	a	103	THR
7	a	104	LEU
7	a	106	LEU
7	a	107	ASP
7	a	114	MET
7	a	115	MET
7	a	117	GLN
7	a	118	GLU
7	a	119	LYS
7	a	126	TYR
7	a	128	GLU
7	a	129	LEU
7	a	132	VAL

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Mol	Chain	Res	Type
7	a	138	LEU
7	a	140	VAL
7	a	143	ARG
7	a	144	LEU
7	a	145	VAL
7	a	149	ASN
7	a	155	MET
7	a	161	PHE
7	a	166	LEU
7	a	171	PHE
7	a	173	VAL
7	a	175	GLN
7	a	176	LEU
7	a	179	LEU
7	a	180	ARG
7	a	185	ASP
7	a	188	LEU
7	a	196	GLN
7	a	199	ARG
7	a	203	LEU
7	a	225	ASN
7	a	226	ILE
7	a	234	GLU
7	a	250	ILE
7	a	251	ILE
7	a	252	ILE
7	a	253	ASP
7	b	7	ASN
7	b	17	GLU
7	b	32	VAL
7	b	40	THR
7	b	42	LYS
7	b	47	SER
7	b	48	ARG
7	b	50	HIS
7	b	52	LEU
7	b	53	SER
7	b	57	GLN
7	b	62	SER
7	b	63	LEU
7	b	74	ASP
7	b	76	GLU

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Mol	Chain	Res	Type
7	b	77	LEU
7	b	81	GLU
7	b	89	GLN
7	b	91	ARG
7	b	95	ARG
7	b	111	THR
7	b	124	ILE
7	b	129	LEU
7	b	139	GLN
7	b	142	VAL
7	b	143	ARG
7	b	179	LEU
7	b	185	ASP
7	b	200	GLU
7	b	201	ILE
7	b	202	LYS
7	b	204	PRO
7	b	211	GLU
7	b	225	ASN
7	b	227	ARG
7	b	235	ARG
7	b	236	SER
7	b	239	ARG
7	b	240	HIS
7	b	256	LYS
7	b	257	ARG
7	c	5	LYS
7	c	28	LEU
7	c	29	ASP
7	c	56	TRP
7	c	70	GLU
7	c	104	LEU
7	c	111	THR
7	c	121	LEU
7	c	130	GLU
7	c	136	GLN
7	c	138	LEU
7	c	141	ASN
7	c	144	LEU
7	c	148	THR
7	c	156	VAL
7	c	164	ASP

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Mol	Chain	Res	Type
7	c	180	ARG
7	c	217	LEU
7	c	225	ASN
7	c	226	ILE
7	c	227	ARG
7	c	229	LEU
7	c	233	VAL
7	c	236	SER
7	c	250	ILE
7	c	251	ILE
7	c	255	PHE
7	d	7	ASN
7	d	8	LEU
7	d	33	LEU
7	d	43	GLU
7	d	45	ILE
7	d	55	ARG
7	d	56	TRP
7	d	57	GLN
7	d	69	ASN
7	d	70	GLU
7	d	71	ASN
7	d	81	GLU
7	d	95	ARG
7	d	96	PHE
7	d	98	ARG
7	d	115	MET
7	d	116	VAL
7	d	119	LYS
7	d	136	GLN
7	d	139	GLN
7	d	144	LEU
7	d	148	THR
7	d	155	MET
7	d	165	LEU
7	d	176	LEU
7	d	181	GLU
7	d	229	LEU
7	d	235	ARG
7	d	252	ILE
7	f	5	LYS
7	f	8	LEU

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Mol	Chain	Res	Type
7	f	9	LEU
7	f	15	PHE
7	f	34	ILE
7	f	50	HIS
7	f	51	TYR
7	f	55	ARG
7	f	63	LEU
7	f	68	LEU
7	f	118	GLU
7	f	123	VAL
7	f	124	ILE
7	f	128	GLU
7	f	129	LEU
7	f	136	GLN
7	f	138	LEU
7	f	141	ASN
7	f	166	LEU
7	f	202	LYS
7	f	214	ARG
7	f	237	VAL
7	f	242	THR
7	f	247	LEU
7	f	252	ILE
7	f	256	LYS
7	f	257	ARG
7	e	7	ASN
7	e	9	LEU
7	e	13	ASN
7	e	15	PHE
7	e	16	LEU
7	e	18	VAL
7	e	22	VAL
7	e	33	LEU
7	e	38	ARG
7	e	42	LYS
7	e	49	LEU
7	e	57	GLN
7	e	69	ASN
7	e	90	LYS
7	e	91	ARG
7	e	97	GLU
7	e	104	LEU

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Mol	Chain	Res	Type
7	e	109	LEU
7	e	122	ARG
7	e	129	LEU
7	e	138	LEU
7	e	139	GLN
7	e	142	VAL
7	e	158	GLU
7	e	164	ASP
7	e	174	VAL
7	e	176	LEU
7	e	179	LEU
7	e	188	LEU
7	e	199	ARG
7	e	225	ASN
7	e	232	VAL
7	e	237	VAL
7	e	251	ILE
7	e	255	PHE
8	M	6	GLN
8	M	7	LEU
8	M	8	ARG
8	M	9	LEU
8	M	11	GLN
8	M	13	LEU
8	M	15	MET
8	M	16	THR
8	M	18	GLN
8	M	23	ILE
8	M	24	ARG
8	M	26	LEU
8	M	27	GLN
8	M	30	THR
8	M	31	LEU
8	M	32	GLU
8	M	41	LEU
8	M	46	LEU
8	M	109	LEU
8	M	118	GLN
8	M	119	THR
8	M	127	GLN
8	M	131	THR
8	M	136	THR

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Mol	Chain	Res	Type
8	M	143	SER
8	M	148	VAL
8	M	154	LEU
8	M	156	ILE
8	M	159	GLU
8	M	161	ILE
8	M	182	ILE
8	M	184	ARG
8	M	185	PHE
8	M	186	ASP
8	M	188	VAL
8	M	195	LEU
8	M	196	ARG
8	M	200	LEU
8	M	201	ILE
8	M	205	GLN
8	M	213	LEU
8	M	217	ARG
8	M	218	LEU
8	M	224	LEU
8	M	225	ASP
8	M	227	LEU
8	M	229	ASN
8	M	231	ASP
8	M	233	ARG
8	M	240	ARG
8	M	246	LEU
8	M	252	LEU
8	M	254	GLN
8	M	256	LEU
8	M	259	ARG
8	M	271	TYR
8	M	272	VAL
8	M	279	ARG
8	M	285	TRP
8	M	292	ASP
8	M	294	ILE
8	M	306	MET
8	M	308	ASN
8	M	329	LEU
8	M	331	LYS
8	M	336	ARG

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Mol	Chain	Res	Type
8	M	340	LEU
8	M	341	LEU
8	M	342	ARG
8	M	347	ILE
8	M	350	GLN
8	M	355	PHE
8	M	363	LYS
8	M	366	VAL
8	M	370	ILE
8	M	372	GLN
8	M	375	GLU
8	M	380	THR
8	M	381	ILE
8	M	386	THR
8	M	387	GLN
8	M	403	PHE
8	M	416	SER
8	M	425	LYS
8	M	431	GLU
8	M	435	LYS
8	M	441	LYS
8	M	455	ARG
8	M	456	ARG
8	M	460	LYS
8	M	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	B	147	GLN
2	C	513	GLN
2	C	554	HIS
2	C	580	GLN
2	C	761	GLN
2	C	1013	GLN
2	C	1061	GLN
3	D	45	ASN
3	D	200	GLN
3	D	209	ASN
3	D	232	ASN
3	D	294	ASN

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Mol	Chain	Res	Type
3	D	594	GLN
3	D	875	ASN
3	D	1259	GLN
4	E	15	ASN
4	E	31	GLN
7	a	21	GLN
7	a	24	HIS
7	a	92	HIS
7	a	117	GLN
7	a	196	GLN
7	a	225	ASN
7	a	231	ASN
7	b	92	HIS
7	b	139	GLN
7	b	157	ASN
7	b	225	ASN
7	c	13	ASN
7	c	64	ASN
7	c	136	GLN
7	c	141	ASN
7	c	157	ASN
7	c	225	ASN
7	d	7	ASN
7	d	92	HIS
7	f	7	ASN
7	f	13	ASN
7	f	24	HIS
7	f	80	HIS
7	f	117	GLN
7	f	136	GLN
7	f	157	ASN
7	e	7	ASN
7	e	13	ASN
7	e	89	GLN
7	e	139	GLN
7	e	149	ASN
8	M	3	GLN
8	M	11	GLN
8	M	18	GLN
8	M	27	GLN
8	M	118	GLN
8	M	127	GLN

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Mol	Chain	Res	Type
8	M	157	GLN
8	M	205	GLN
8	M	262	GLN
8	M	265	GLN
8	M	324	GLN
8	M	377	HIS
8	M	387	GLN
8	M	432	ASN
8	M	472	GLN

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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	ADP	b	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
10	AF3	e	602	-	0,3,3	-	-	-		
10	AF3	f	602	-	0,3,3	-	-	-		
10	AF3	b	602	-	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	f	601	-	28,29,29	3.36	17 (60%)	43,45,45	4.70	34 (79%)
9	ADP	a	601	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
10	AF3	a	602	-	0,3,3	-	-	-	-	-
9	ADP	c	400	-	28,29,29	1.42	4 (14%)	43,45,45	1.83	9 (20%)
9	ADP	e	601	-	28,29,29	2.39	8 (28%)	43,45,45	2.79	25 (58%)

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
9	ADP	b	601	-	-	5/16/32/32	0/3/3/3
9	ADP	f	601	-	-	5/16/32/32	0/3/3/3
9	ADP	a	601	-	-	3/16/32/32	0/3/3/3
9	ADP	c	400	-	-	1/16/32/32	0/3/3/3
9	ADP	e	601	-	-	1/16/32/32	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	601	ADP	C5-C4	7.58	1.52	1.39
9	f	601	ADP	O2'-C2'	7.13	1.60	1.43
9	f	601	ADP	PA-O1A	5.82	1.71	1.50
9	f	601	ADP	C8-N9	-5.35	1.28	1.37
9	f	601	ADP	O4'-C1'	5.07	1.53	1.42
9	e	601	ADP	PA-O1A	-4.95	1.33	1.50
9	b	601	ADP	C5-C4	4.78	1.47	1.39
9	c	400	ADP	C5-C4	4.77	1.47	1.39
9	f	601	ADP	C4-N9	-4.70	1.27	1.37
9	a	601	ADP	C5-C4	4.60	1.47	1.39
9	f	601	ADP	C5'-C4'	4.46	1.65	1.51
9	f	601	ADP	C2'-C3'	4.42	1.65	1.53
9	f	601	ADP	C2'-C1'	-4.28	1.40	1.53
9	e	601	ADP	C5-C6	4.03	1.52	1.41
9	f	601	ADP	C5-N7	-3.91	1.32	1.39
9	e	601	ADP	PA-O3A	-3.73	1.55	1.59
9	f	601	ADP	PB-O2B	3.40	1.67	1.54
9	f	601	ADP	C5-C4	3.28	1.44	1.39
9	e	601	ADP	C2-N3	3.13	1.39	1.33
9	f	601	ADP	O4'-C4'	3.03	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	601	ADP	C5-C6	3.00	1.49	1.41
9	f	601	ADP	PA-O2A	2.95	1.69	1.55
9	c	400	ADP	C5-C6	2.79	1.48	1.41
9	a	601	ADP	C5-C6	2.77	1.48	1.41
9	e	601	ADP	C4-N9	-2.76	1.31	1.37
9	b	601	ADP	C5-C6	2.76	1.48	1.41
9	f	601	ADP	C3'-C4'	-2.70	1.46	1.53
9	f	601	ADP	C6-N1	-2.60	1.28	1.35
9	f	601	ADP	C4-N3	2.53	1.39	1.34
9	e	601	ADP	C6-N1	-2.53	1.28	1.35
9	b	601	ADP	C8-N7	2.36	1.36	1.31
9	a	601	ADP	C8-N7	2.34	1.36	1.31
9	c	400	ADP	C8-N7	2.29	1.36	1.31
9	c	400	ADP	C5-N7	-2.25	1.35	1.39
9	b	601	ADP	C5-N7	-2.22	1.35	1.39
9	a	601	ADP	C5-N7	-2.19	1.35	1.39
9	e	601	ADP	O4'-C4'	-2.12	1.40	1.45

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	f	601	ADP	O4'-C1'-N9	15.90	138.63	108.09
9	f	601	ADP	O3A-PA-O1A	-7.02	89.58	110.70
9	f	601	ADP	C5'-C4'-C3'	-6.74	90.95	115.21
9	f	601	ADP	O4'-C4'-C5'	6.71	130.81	109.33
9	f	601	ADP	O2A-PA-O1A	6.59	143.08	112.44
9	f	601	ADP	O3B-PB-O2B	6.28	131.34	107.80
9	f	601	ADP	N3-C4-N9	6.22	137.74	127.17
9	b	601	ADP	C5-C4-N3	-5.83	118.69	126.72
9	a	601	ADP	C5-C4-N3	-5.83	118.69	126.72
9	c	400	ADP	C5-C4-N3	-5.81	118.71	126.72
9	e	601	ADP	O5'-PA-O1A	5.53	130.86	108.94
9	f	601	ADP	O3'-C3'-C2'	5.53	129.55	111.82
9	f	601	ADP	O2A-PA-O3A	-5.51	92.39	107.27
9	f	601	ADP	O5'-PA-O1A	5.46	130.58	108.94
9	f	601	ADP	C4-N9-C8	5.21	111.21	105.74
9	f	601	ADP	C5-C4-N9	-5.14	100.21	105.81
9	e	601	ADP	C5-C4-N3	-5.12	119.67	126.72
9	f	601	ADP	O3B-PB-O3A	-4.99	87.92	104.64
9	f	601	ADP	O4'-C4'-C3'	-4.74	95.75	105.15
9	f	601	ADP	O2A-PA-O5'	-4.72	86.18	107.57
9	f	601	ADP	C2'-C1'-N9	-4.72	101.58	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e	601	ADP	C4-C5-N7	-4.69	105.22	110.58
9	f	601	ADP	C6-C5-C4	-4.63	110.85	117.18
9	b	601	ADP	N3-C4-N9	4.62	135.03	127.17
9	c	400	ADP	N3-C4-N9	4.61	135.01	127.17
9	a	601	ADP	N3-C4-N9	4.53	134.87	127.17
9	e	601	ADP	O5'-C5'-C4'	4.38	123.92	108.99
9	f	601	ADP	N6-C6-N1	-4.37	108.63	118.38
9	e	601	ADP	C4'-O4'-C1'	4.37	119.11	109.47
9	f	601	ADP	O2'-C2'-C1'	-4.31	95.27	110.10
9	e	601	ADP	C5'-C4'-C3'	-4.12	100.40	115.21
9	e	601	ADP	O2B-PB-O3A	-4.07	90.98	104.64
9	f	601	ADP	C4'-O4'-C1'	-3.96	100.73	109.47
9	e	601	ADP	O4'-C4'-C5'	-3.86	96.97	109.33
9	e	601	ADP	O3B-PB-O1B	3.83	125.75	110.83
9	e	601	ADP	C3'-C2'-C1'	3.73	108.52	101.46
9	b	601	ADP	C2-N3-C4	3.71	120.90	111.83
9	c	400	ADP	C2-N3-C4	3.70	120.86	111.83
9	a	601	ADP	C2-N3-C4	3.66	120.76	111.83
9	e	601	ADP	O2A-PA-O5'	-3.60	91.26	107.57
9	e	601	ADP	O3'-C3'-C2'	3.55	123.21	111.82
9	e	601	ADP	O3B-PB-O2B	-3.55	94.49	107.80
9	b	601	ADP	C4-C5-N7	-3.49	106.59	110.58
9	a	601	ADP	C4-C5-N7	-3.48	106.60	110.58
9	c	400	ADP	C4-C5-N7	-3.47	106.61	110.58
9	f	601	ADP	O4'-C1'-C2'	3.46	114.03	106.62
9	e	601	ADP	N3-C4-N9	3.45	133.04	127.17
9	f	601	ADP	PA-O5'-C5'	-3.44	101.66	121.35
9	f	601	ADP	C5-C4-N3	-3.43	121.99	126.72
9	b	601	ADP	N3-C2-N1	-3.22	123.70	128.58
9	c	400	ADP	N3-C2-N1	-3.21	123.72	128.58
9	a	601	ADP	N3-C2-N1	-3.15	123.81	128.58
9	e	601	ADP	C2'-C1'-N9	3.12	121.05	113.30
9	f	601	ADP	C2'-C3'-C4'	3.01	108.42	102.61
9	e	601	ADP	C6-C5-N7	3.00	137.88	132.09
9	f	601	ADP	C3'-C2'-C1'	-3.00	95.78	101.46
9	f	601	ADP	C4-C5-N7	2.84	113.83	110.58
9	f	601	ADP	C5-N7-C8	-2.82	99.01	103.45
9	f	601	ADP	N3-C2-N1	-2.74	124.44	128.58
9	e	601	ADP	O3'-C3'-C4'	2.65	118.69	111.08
9	b	601	ADP	C4-N9-C8	2.64	108.51	105.74
9	e	601	ADP	O2'-C2'-C1'	2.61	119.10	110.10
9	c	400	ADP	C4-N9-C8	2.57	108.43	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	601	ADP	C5-N7-C8	2.56	107.47	103.45
9	f	601	ADP	O2B-PB-O1B	2.56	120.81	110.83
9	c	400	ADP	C5-N7-C8	2.55	107.46	103.45
9	f	601	ADP	O2B-PB-O3A	-2.55	96.09	104.64
9	a	601	ADP	C5-N7-C8	2.50	107.38	103.45
9	e	601	ADP	C5-N7-C8	2.49	107.37	103.45
9	a	601	ADP	C3'-C2'-C1'	2.48	106.16	101.46
9	a	601	ADP	C4-N9-C8	2.48	108.34	105.74
9	f	601	ADP	C2-N3-C4	2.42	117.75	111.83
9	b	601	ADP	C3'-C2'-C1'	2.40	106.01	101.46
9	e	601	ADP	O3A-PA-O1A	-2.39	103.50	110.70
9	f	601	ADP	O3'-C3'-C4'	-2.38	104.25	111.08
9	e	601	ADP	N6-C6-N1	-2.37	113.10	118.38
9	f	601	ADP	O3B-PB-O1B	-2.36	101.62	110.83
9	e	601	ADP	C2-N1-C6	2.36	122.60	118.73
9	c	400	ADP	C3'-C2'-C1'	2.35	105.92	101.46
9	e	601	ADP	O4'-C1'-C2'	-2.34	101.62	106.62
9	f	601	ADP	C5-C6-N1	2.33	123.42	117.51
9	e	601	ADP	O2B-PB-O1B	2.32	119.86	110.83
9	b	601	ADP	C6-C5-N7	2.11	136.15	132.09
9	e	601	ADP	C4-N9-C8	2.10	107.95	105.74
9	c	400	ADP	C6-C5-N7	2.10	136.15	132.09
9	a	601	ADP	C6-C5-N7	2.05	136.03	132.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	b	601	ADP	C5'-O5'-PA-O2A
9	b	601	ADP	C5'-O5'-PA-O3A
9	c	400	ADP	C5'-O5'-PA-O1A
9	f	601	ADP	C5'-O5'-PA-O2A
9	f	601	ADP	C5'-O5'-PA-O3A
9	f	601	ADP	C3'-C4'-C5'-O5'
9	f	601	ADP	O4'-C4'-C5'-O5'
9	e	601	ADP	O4'-C4'-C5'-O5'
9	b	601	ADP	O4'-C4'-C5'-O5'
9	a	601	ADP	O4'-C4'-C5'-O5'
9	b	601	ADP	C5'-O5'-PA-O1A
9	f	601	ADP	C5'-O5'-PA-O1A
9	a	601	ADP	PB-O3A-PA-O2A
9	b	601	ADP	C3'-C4'-C5'-O5'

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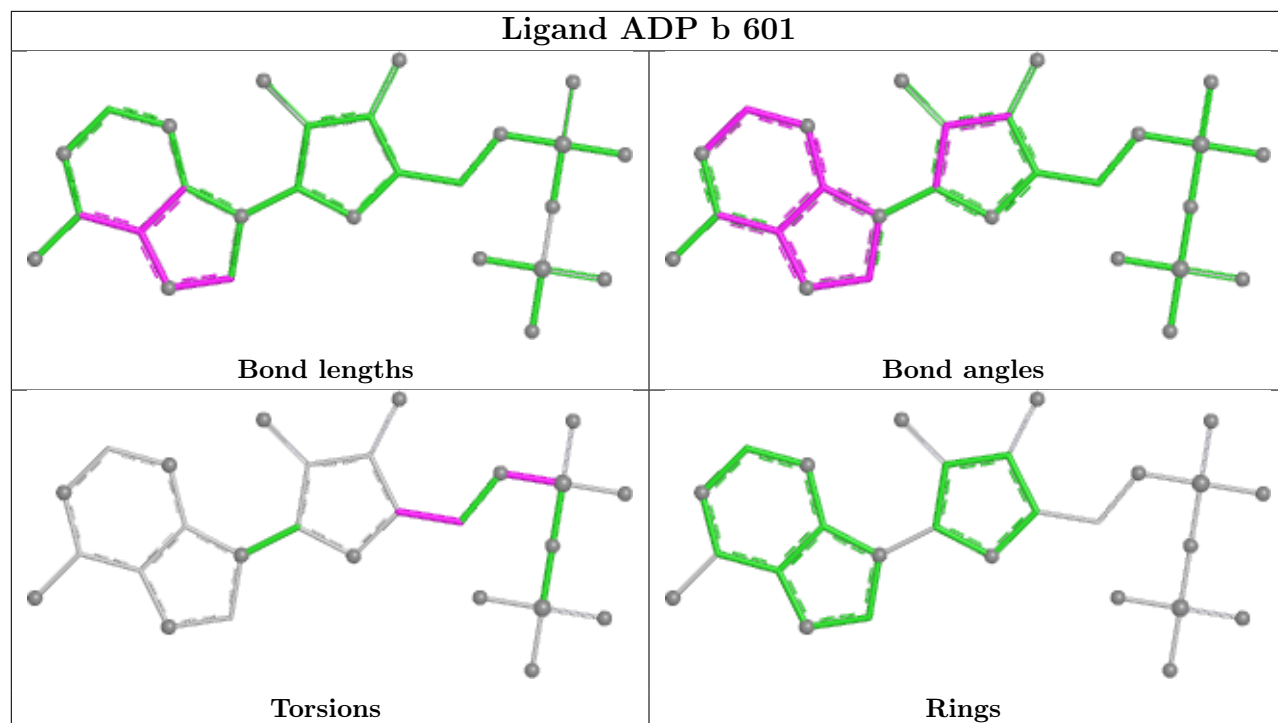
Mol	Chain	Res	Type	Atoms
9	a	601	ADP	C4'-C5'-O5'-PA

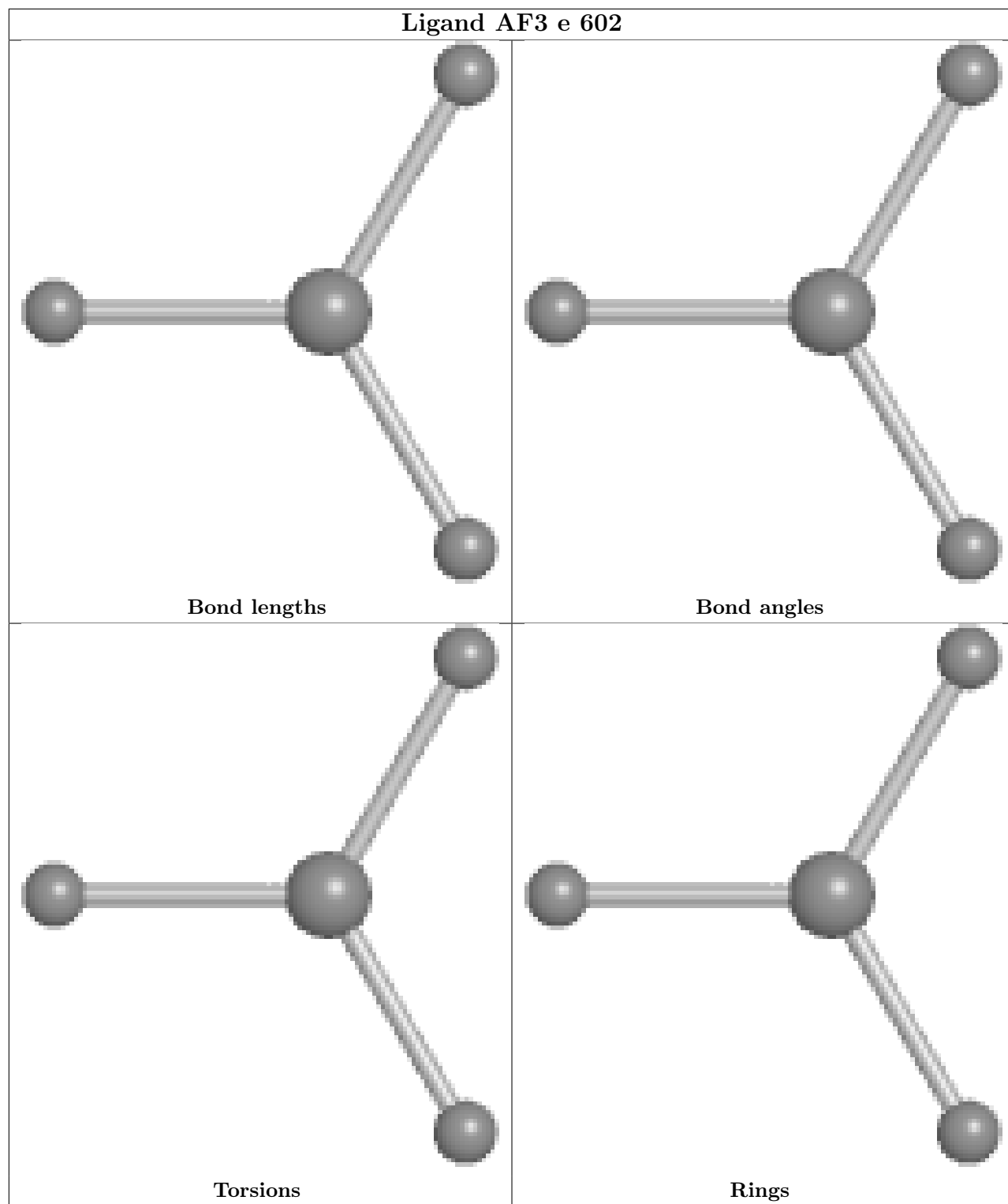
There are no ring outliers.

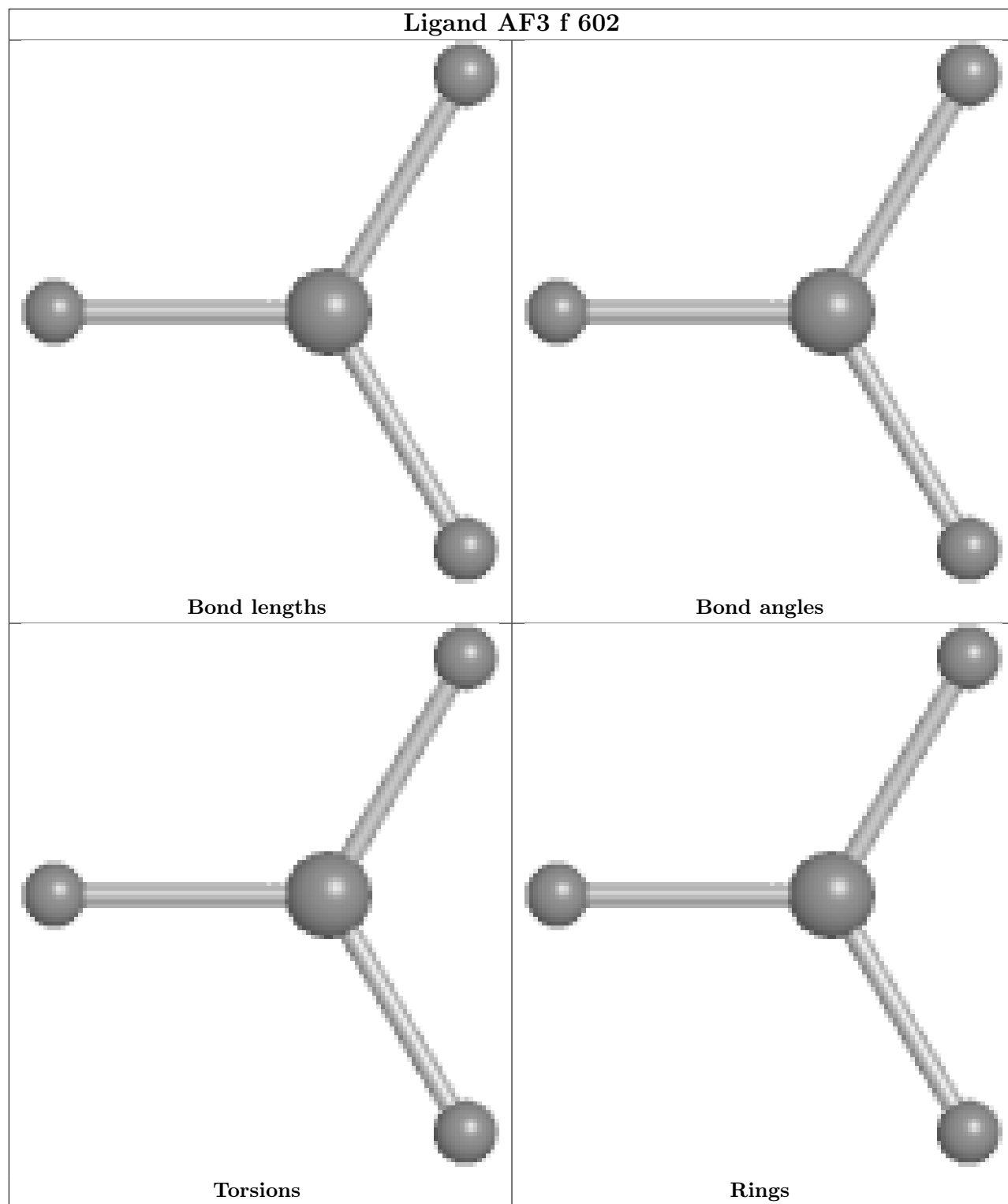
6 monomers are involved in 54 short contacts:

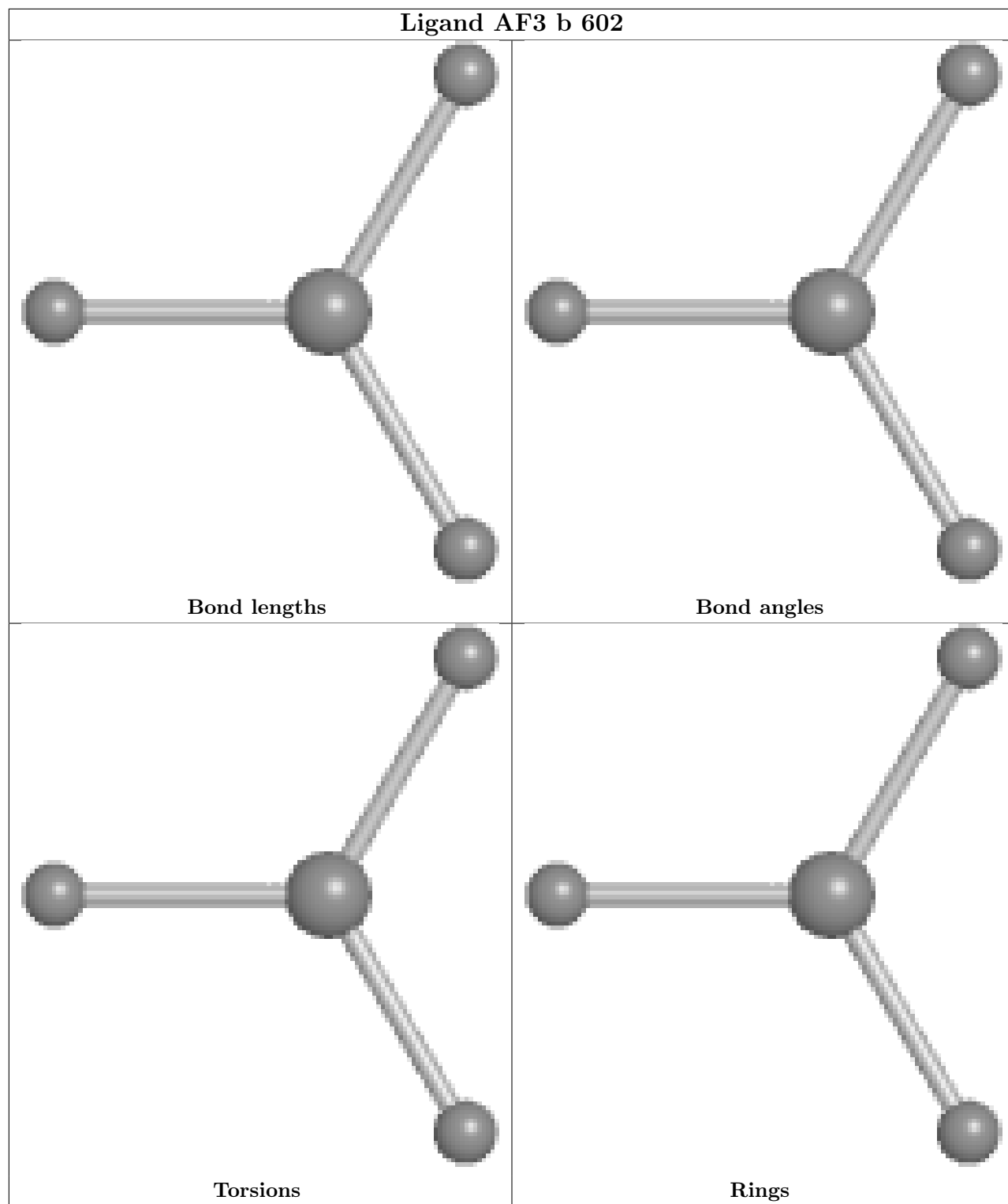
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	b	601	ADP	5	0
10	f	602	AF3	1	0
9	f	601	ADP	19	0
9	a	601	ADP	11	0
9	c	400	ADP	7	0
9	e	601	ADP	12	0

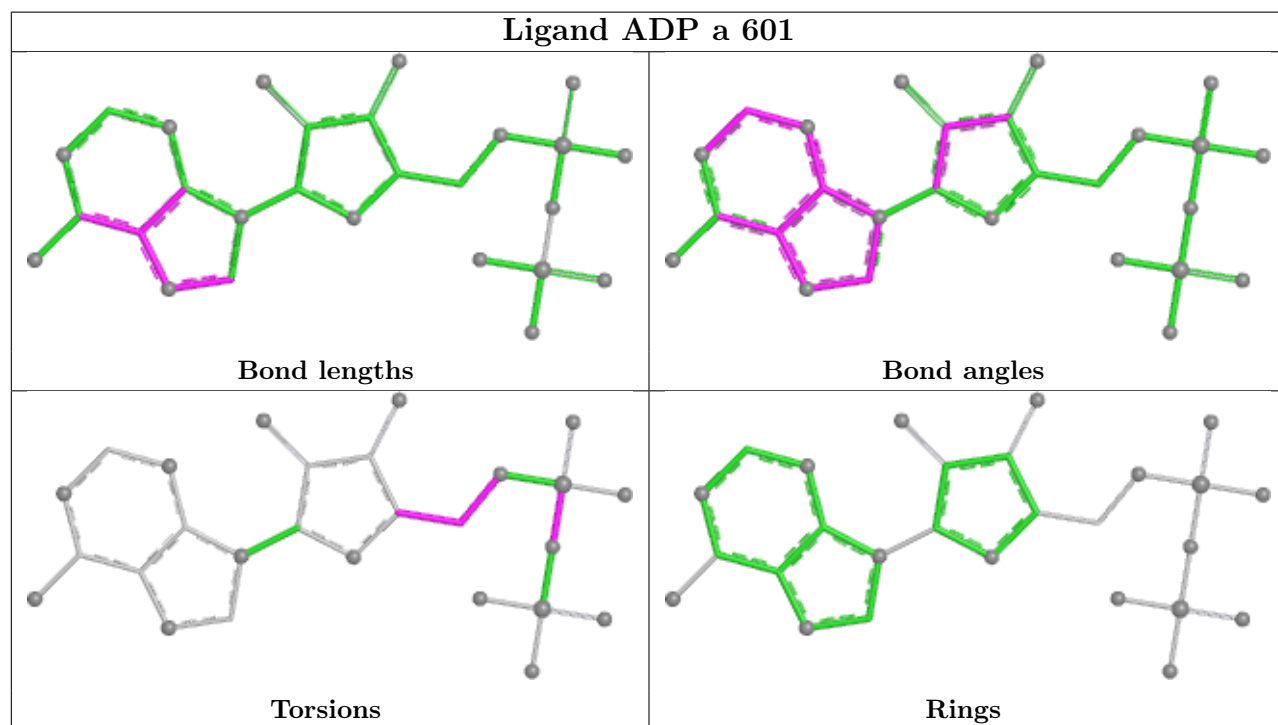
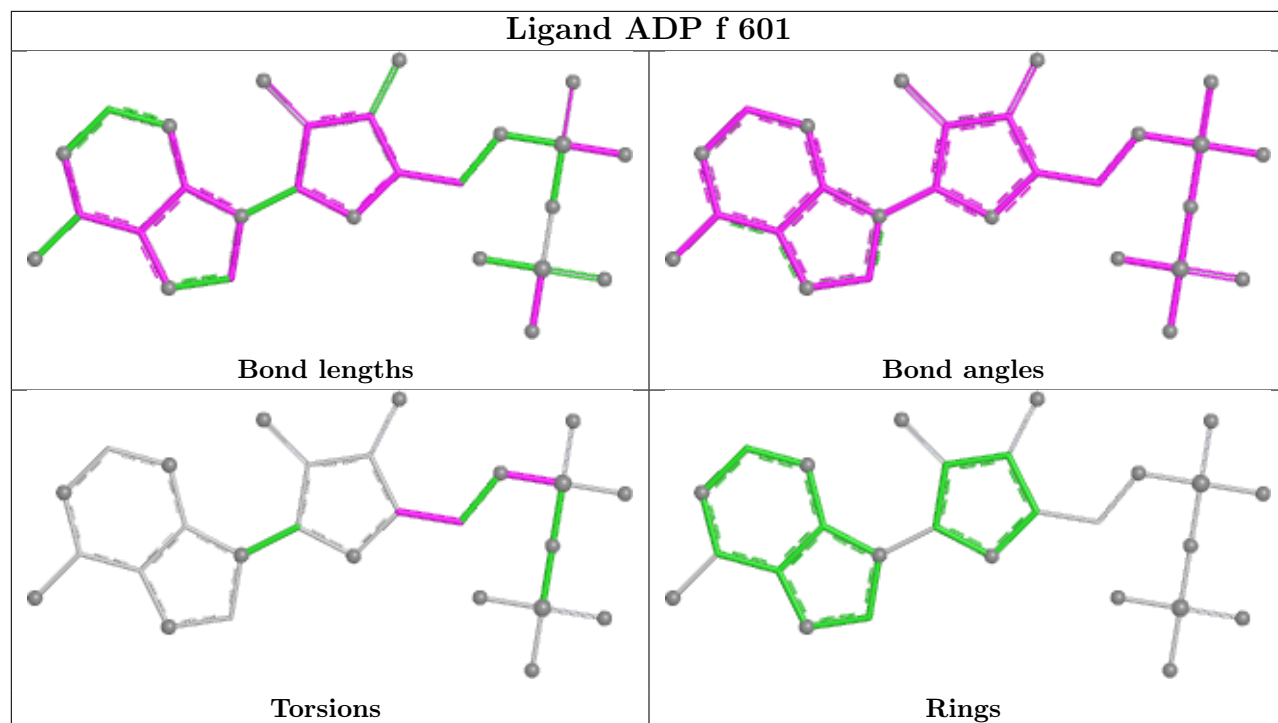
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

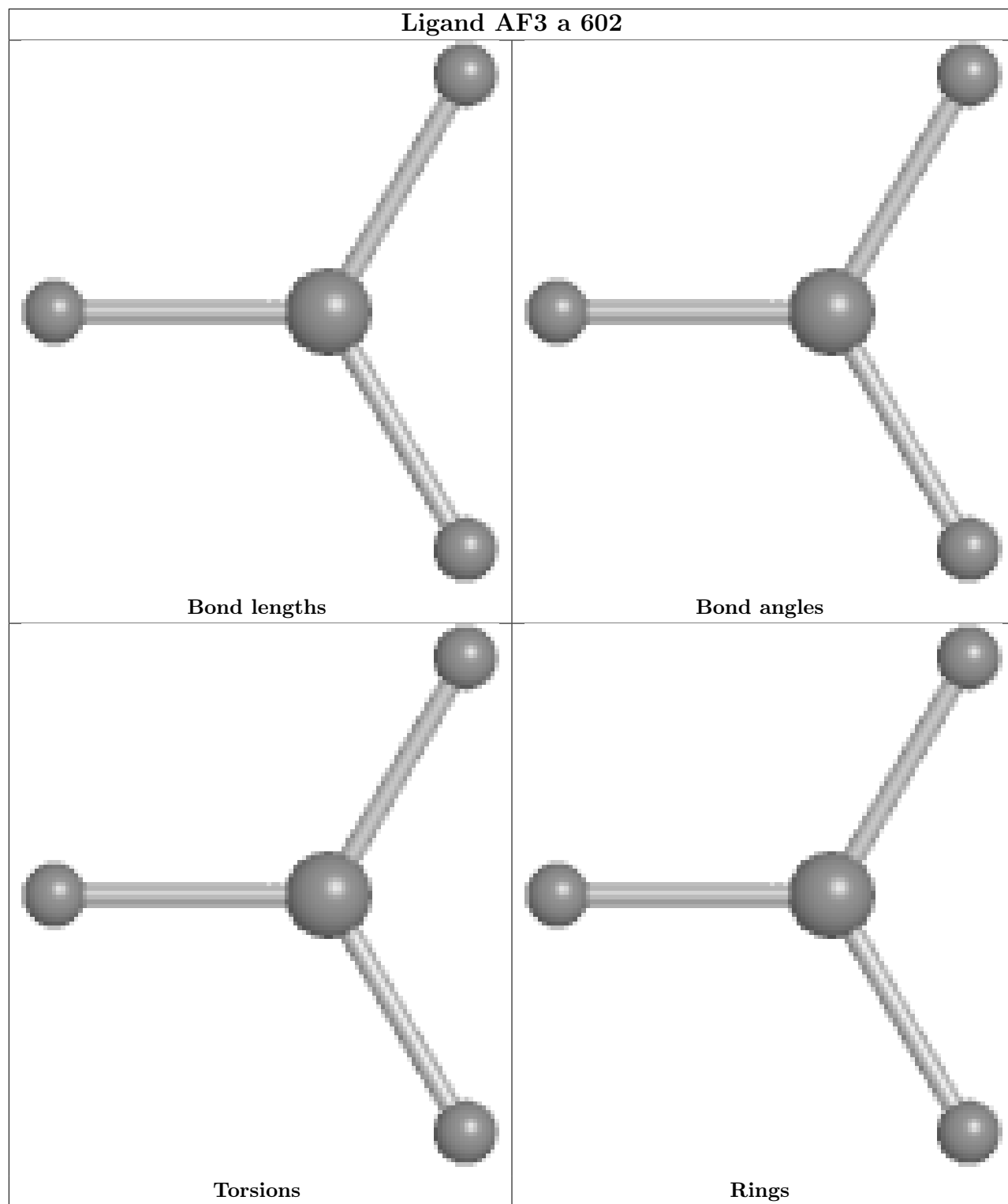


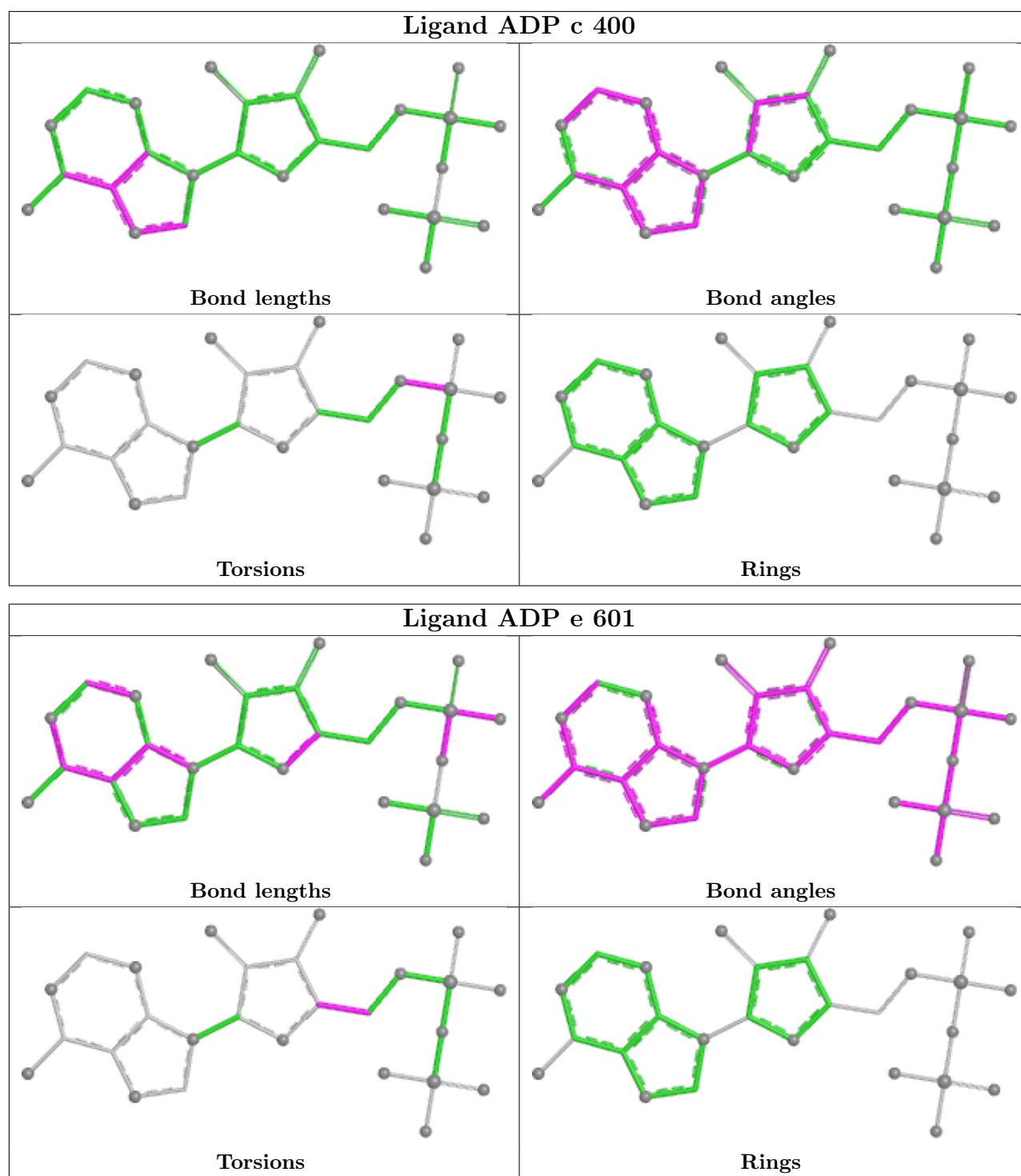












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

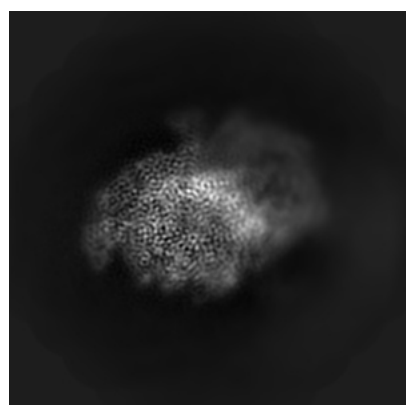
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14171. These allow visual inspection of the internal detail of the map and identification of artifacts.

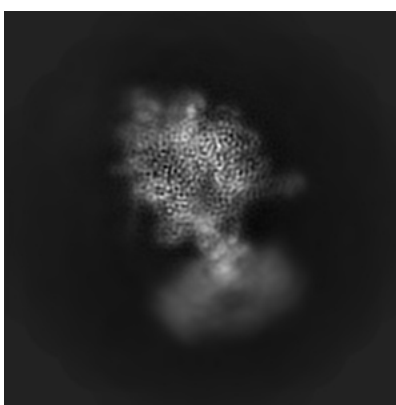
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

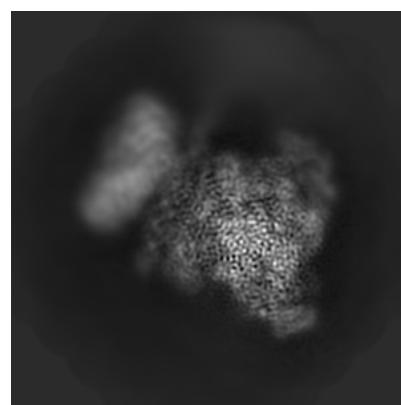
6.1.1 Primary map



X



Y

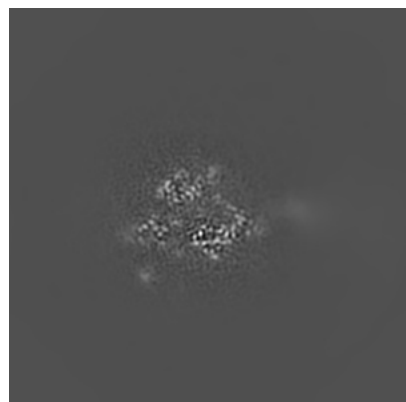


Z

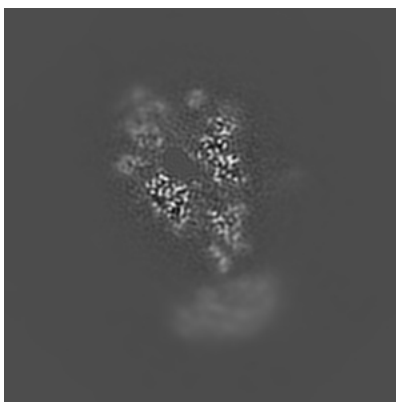
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

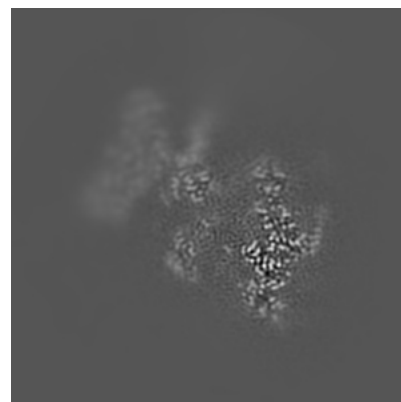
6.2.1 Primary map



X Index: 140



Y Index: 140

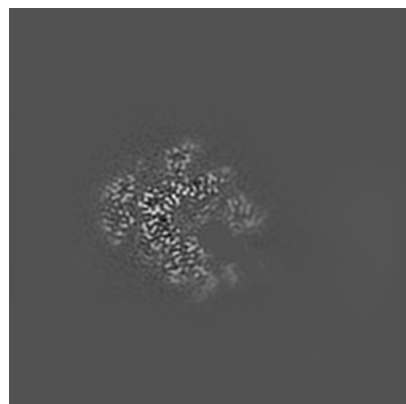


Z Index: 140

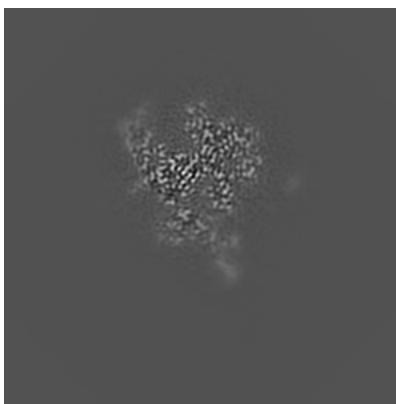
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

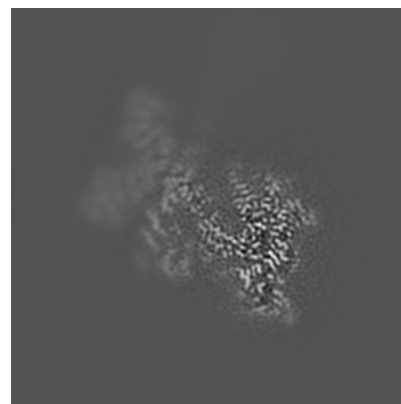
6.3.1 Primary map



X Index: 173



Y Index: 111

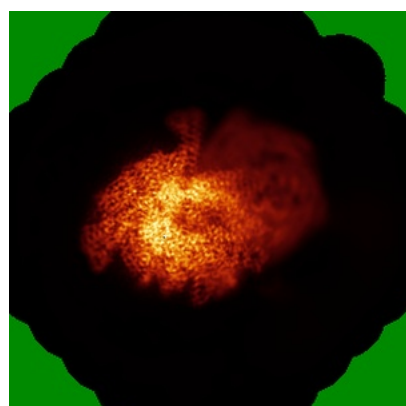


Z Index: 149

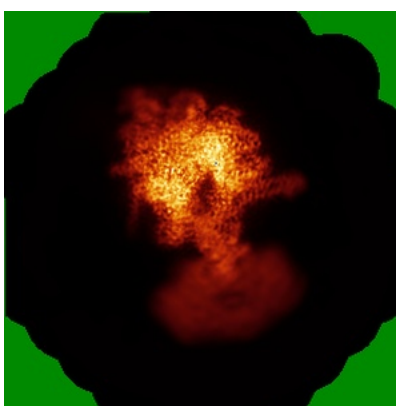
The images above show the largest variance slices of the map in three orthogonal directions.

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

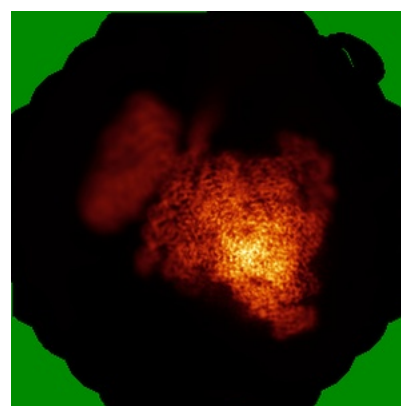
6.4.1 Primary map



X



Y

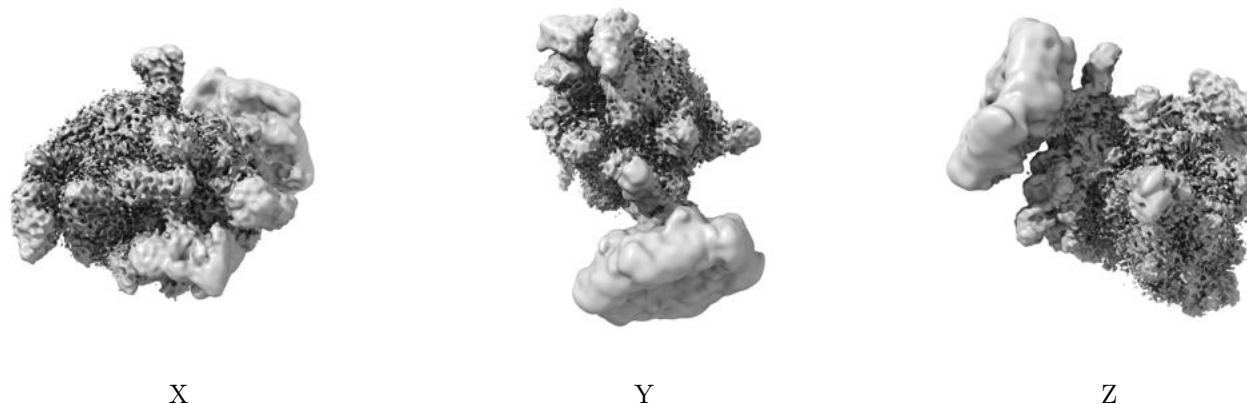


Z

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 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

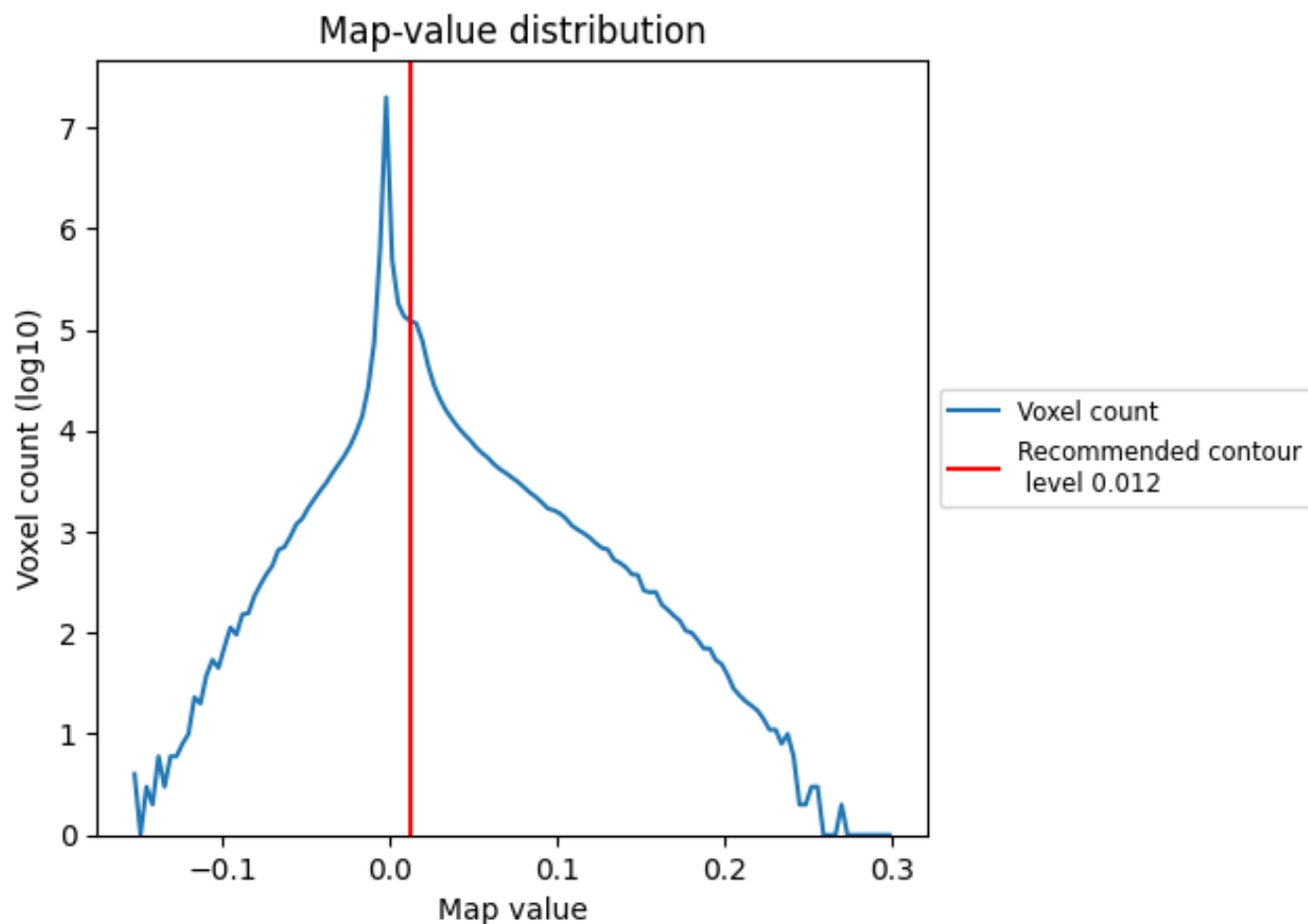
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

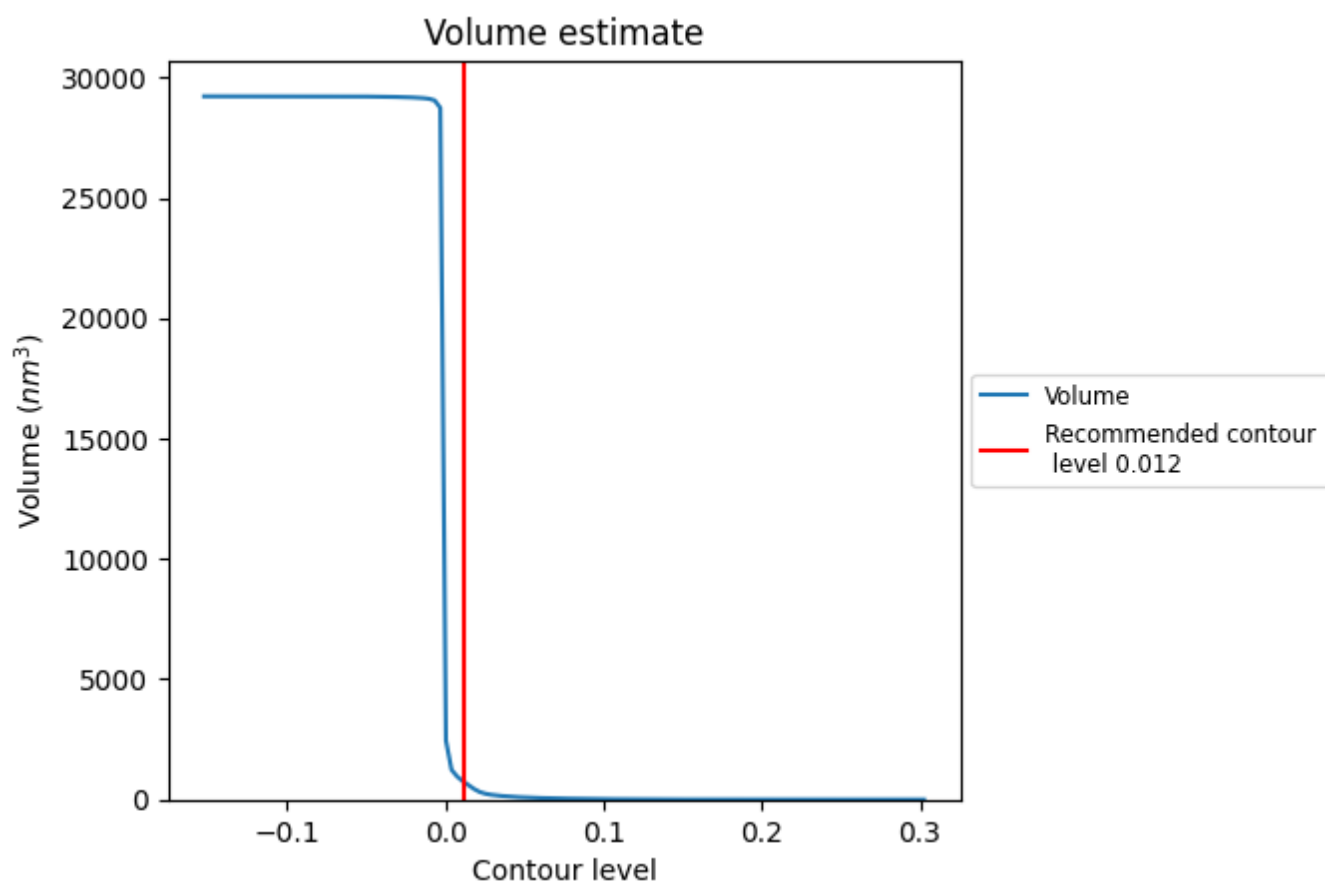
This section contains the results of statistical analysis of the map.

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.

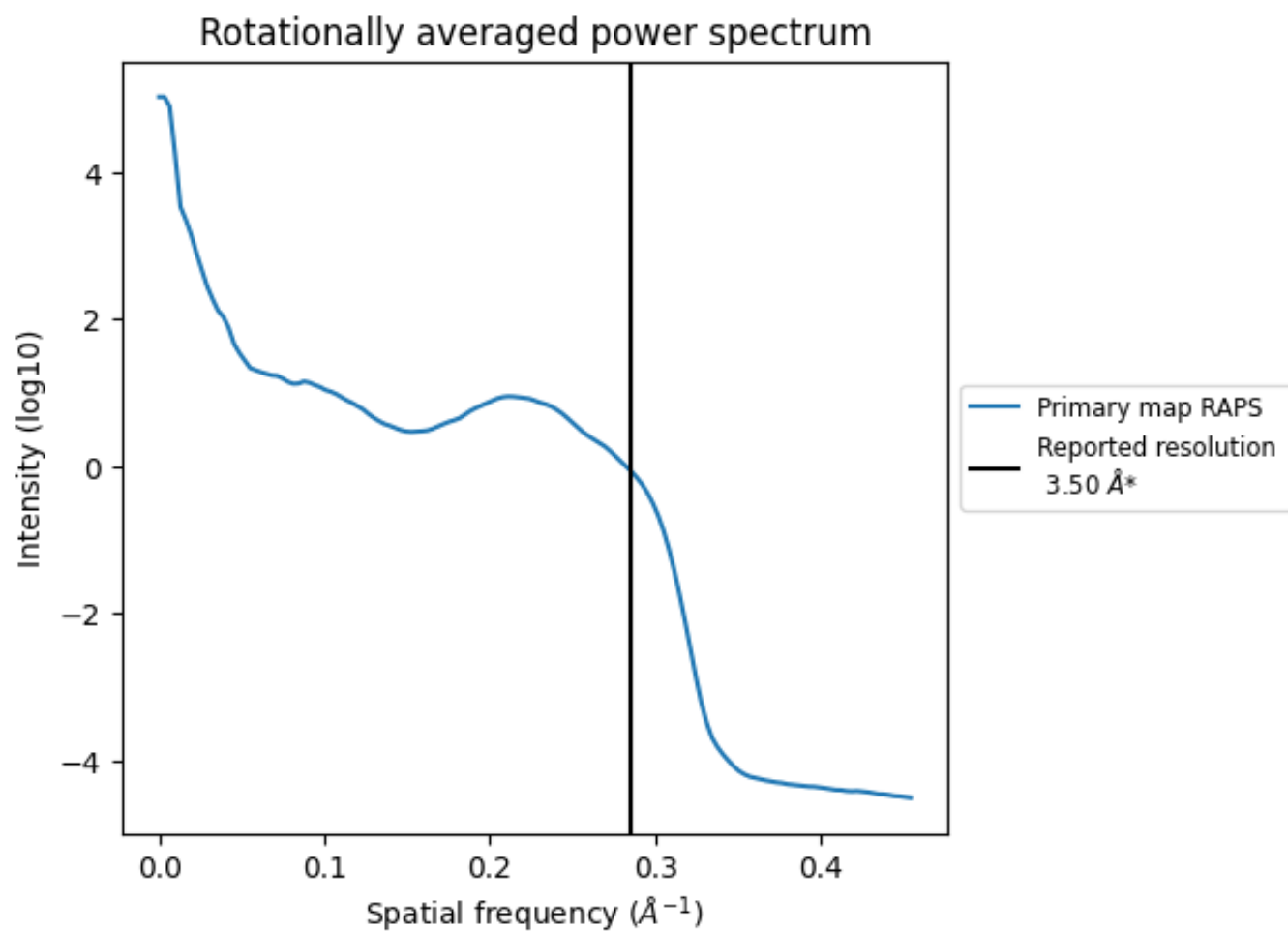
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 723 nm^3 ; this corresponds to an approximate mass of 653 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

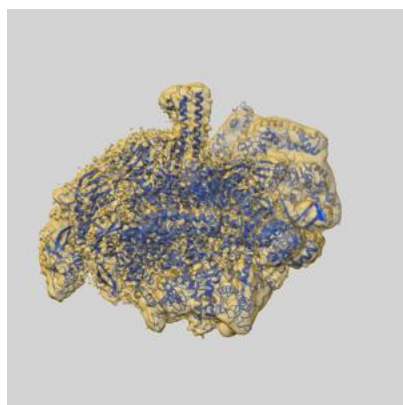
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

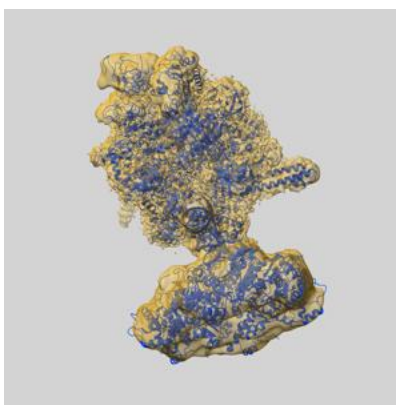
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14171 and PDB model 7QV9. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

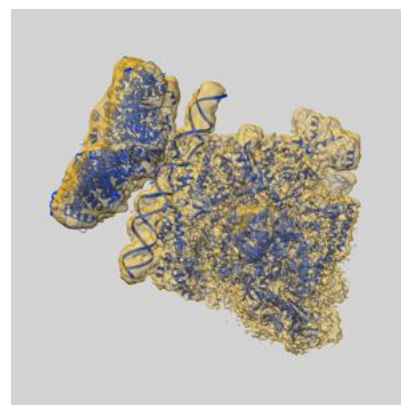
9.1 Map-model overlay [i](#)



X



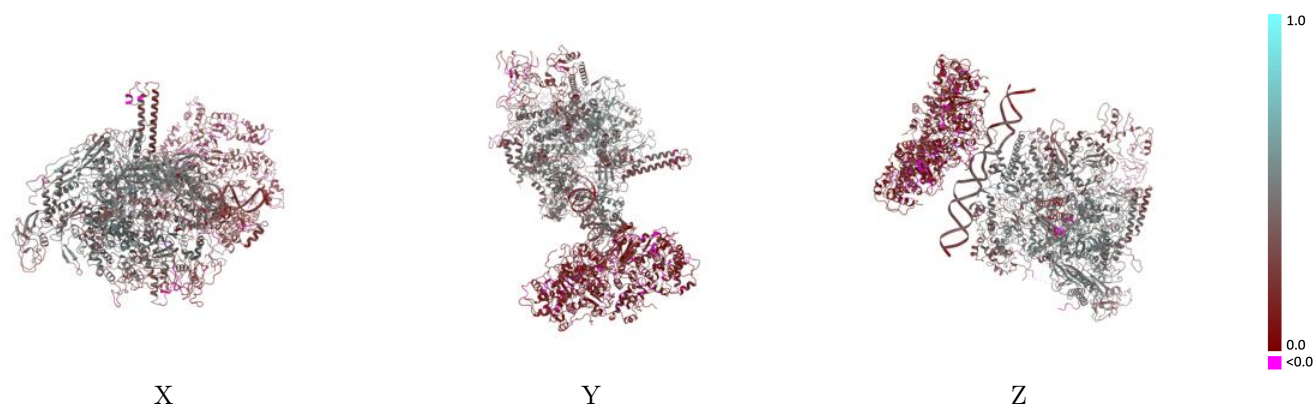
Y



Z

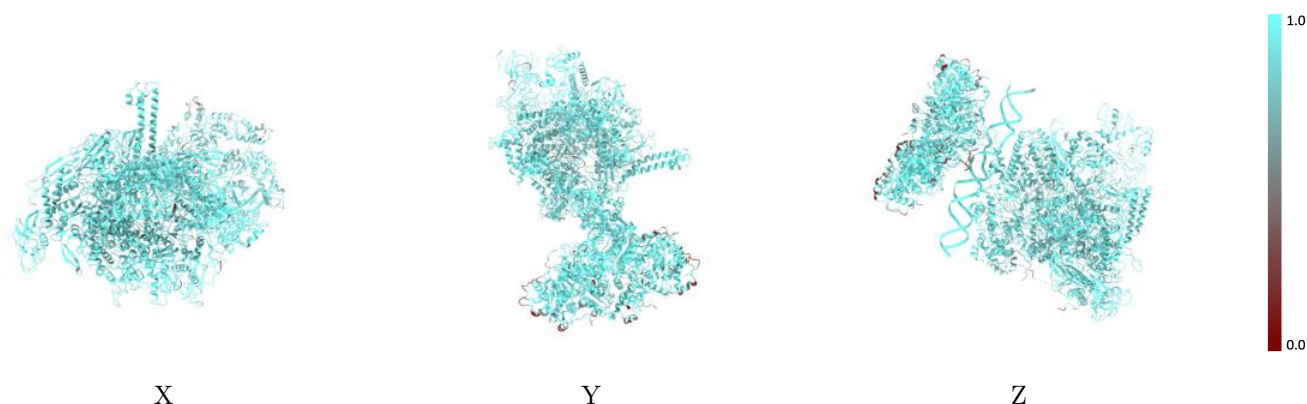
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



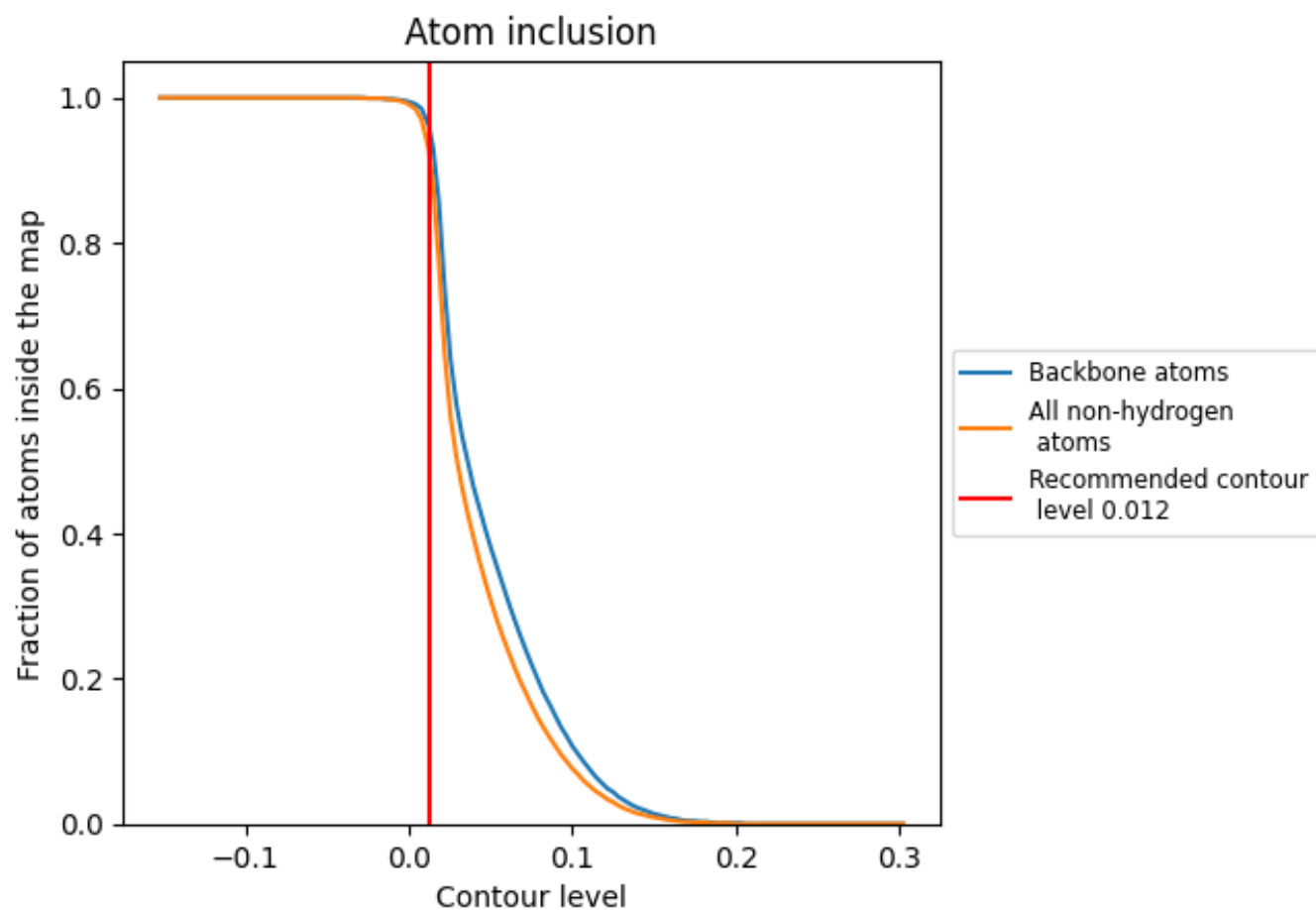
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9290	0.3230
A	0.8950	0.3980
B	0.9260	0.3830
C	0.9410	0.4200
D	0.9290	0.3910
E	0.9490	0.4320
M	0.9590	0.4280
N	0.9860	0.3110
T	0.9770	0.3090
a	0.9170	0.1500
b	0.9390	0.1620
c	0.8730	0.1240
d	0.9080	0.1270
e	0.9290	0.1350
f	0.9020	0.1310

