



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 PM UTC

PDB ID : 3M6A / pdb_00003m6a
Title : Crystal structure of Bacillus subtilis Lon C-terminal domain
Authors : Duman, R.E.; Lowe, J.Y.
Deposited on : 2010-03-15
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

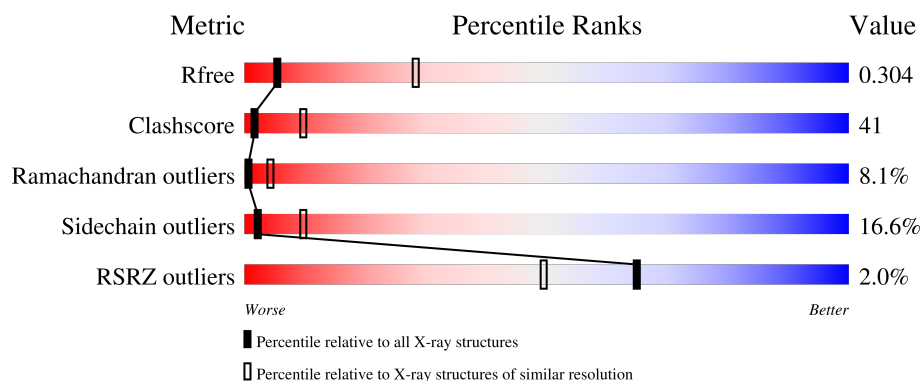
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	2% 37% 39% 14% 9%
1	B	543	3% 36% 40% 15% 9%
1	C	543	0% 34% 42% 14% 9%
1	D	543	2% 35% 41% 14% 9%
1	E	543	0% 36% 40% 13% 9%

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Mol	Chain	Length	Quality of chain
1	F	543	

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
2	ADP	D	783	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ATP-dependent protease La 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	B	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	C	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	D	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	E	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	F	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	ALA	SER	engineered mutation	UNP P37945
A	775	LEU	-	expression tag	UNP P37945
A	776	GLU	-	expression tag	UNP P37945
A	777	HIS	-	expression tag	UNP P37945
A	778	HIS	-	expression tag	UNP P37945
A	779	HIS	-	expression tag	UNP P37945
A	780	HIS	-	expression tag	UNP P37945
A	781	HIS	-	expression tag	UNP P37945
A	782	HIS	-	expression tag	UNP P37945
B	677	ALA	SER	engineered mutation	UNP P37945
B	775	LEU	-	expression tag	UNP P37945
B	776	GLU	-	expression tag	UNP P37945
B	777	HIS	-	expression tag	UNP P37945
B	778	HIS	-	expression tag	UNP P37945
B	779	HIS	-	expression tag	UNP P37945
B	780	HIS	-	expression tag	UNP P37945
B	781	HIS	-	expression tag	UNP P37945

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Chain	Residue	Modelled	Actual	Comment	Reference
B	782	HIS	-	expression tag	UNP P37945
C	677	ALA	SER	engineered mutation	UNP P37945
C	775	LEU	-	expression tag	UNP P37945
C	776	GLU	-	expression tag	UNP P37945
C	777	HIS	-	expression tag	UNP P37945
C	778	HIS	-	expression tag	UNP P37945
C	779	HIS	-	expression tag	UNP P37945
C	780	HIS	-	expression tag	UNP P37945
C	781	HIS	-	expression tag	UNP P37945
C	782	HIS	-	expression tag	UNP P37945
D	677	ALA	SER	engineered mutation	UNP P37945
D	775	LEU	-	expression tag	UNP P37945
D	776	GLU	-	expression tag	UNP P37945
D	777	HIS	-	expression tag	UNP P37945
D	778	HIS	-	expression tag	UNP P37945
D	779	HIS	-	expression tag	UNP P37945
D	780	HIS	-	expression tag	UNP P37945
D	781	HIS	-	expression tag	UNP P37945
D	782	HIS	-	expression tag	UNP P37945
E	677	ALA	SER	engineered mutation	UNP P37945
E	775	LEU	-	expression tag	UNP P37945
E	776	GLU	-	expression tag	UNP P37945
E	777	HIS	-	expression tag	UNP P37945
E	778	HIS	-	expression tag	UNP P37945
E	779	HIS	-	expression tag	UNP P37945
E	780	HIS	-	expression tag	UNP P37945
E	781	HIS	-	expression tag	UNP P37945
E	782	HIS	-	expression tag	UNP P37945
F	677	ALA	SER	engineered mutation	UNP P37945
F	775	LEU	-	expression tag	UNP P37945
F	776	GLU	-	expression tag	UNP P37945
F	777	HIS	-	expression tag	UNP P37945
F	778	HIS	-	expression tag	UNP P37945
F	779	HIS	-	expression tag	UNP P37945
F	780	HIS	-	expression tag	UNP P37945
F	781	HIS	-	expression tag	UNP P37945
F	782	HIS	-	expression tag	UNP P37945

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Chain A:

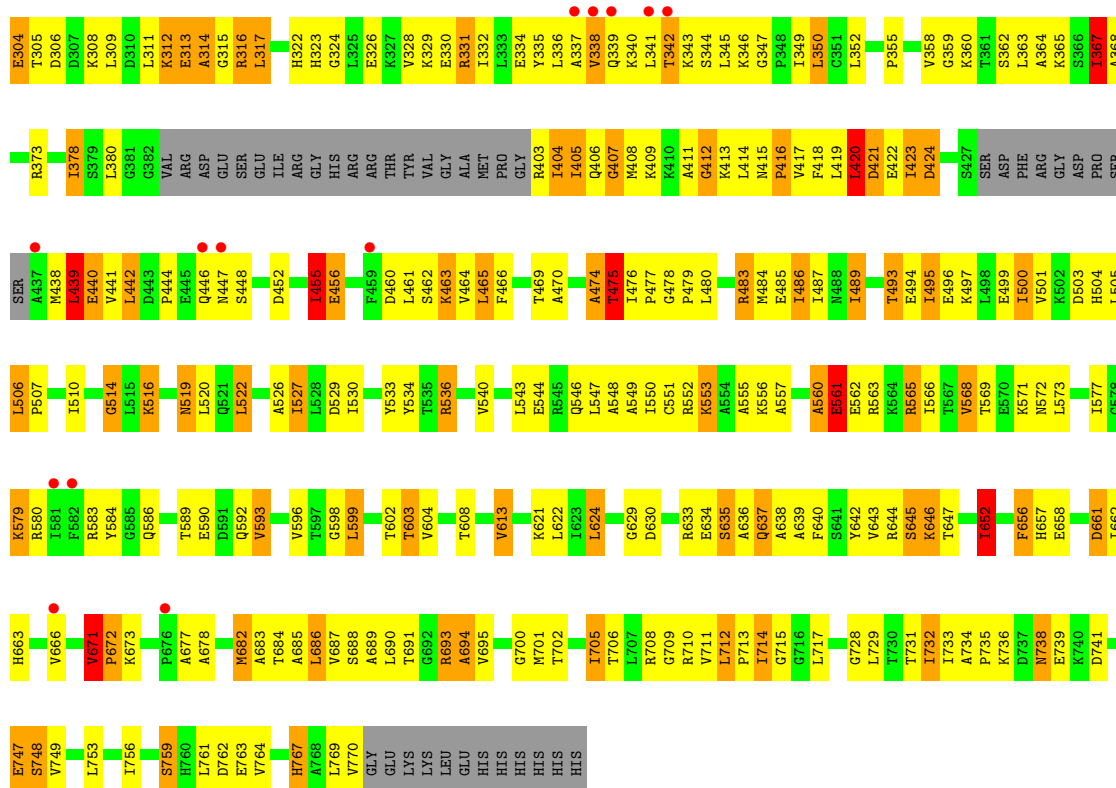
Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 2.00). The x-axis lists amino acids. The color scale at the top indicates conservation levels: 2% (red), 37% (green), 39% (yellow), 14% (orange), and 9% (grey).

Position	Conservation Level	Most Conserved Amino Acid(s)
1	37%	GLY
2	37%	ASP
3	37%	LYS
4	37%	GLU
5	37%	GLY
6	37%	LYS
7	37%	T246
8	37%	G247
9	37%	E248
10	37%	V249
11	37%	Q250
12	37%	T251
13	37%	L252
14	37%	E253
15	37%	K256
16	37%	L256
17	37%	E257
18	37%	E258
19	37%	A259
20	37%	G260
21	37%	M261
22	37%	P262
23	37%	D263
24	37%	K266
25	37%	E267
26	37%	T268
27	37%	A269
28	37%	L270
29	37%	K271
30	37%	E272
31	37%	L273
32	37%	N274
33	37%	R275
34	37%	Y276
35	37%	E277
36	37%	K278
37	37%	L279
38	37%	S280
39	37%	S281
40	37%	S282
41	37%	S283
42	37%	S286
43	37%	S287
44	37%	V288
45	37%	R289
46	37%	L290
47	37%	L293
48	37%	D294
49	37%	V295
50	37%	L296
51	37%	V297
52	37%	A298
53	37%	L299
54	37%	P300
55	37%	S301
56	37%	ASP
57	37%	T302
58	37%	L303
59	37%	L309
60	37%	D310
61	37%	L311
62	37%	E312
63	37%	E313
64	37%	A314
65	37%	G315
66	37%	R316
67	37%	L317
68	37%	H322
69	37%	ARG
70	37%	G324
71	37%	L325
72	37%	E326
73	37%	K327
74	37%	V328
75	37%	K329
76	37%	E330
77	37%	R331
78	37%	L332
79	37%	L333
80	37%	E334
81	37%	V335
82	37%	L336
83	37%	A337
84	37%	K338
85	37%	E339
86	37%	K340
87	37%	L341
88	37%	T342
89	37%	K343
90	37%	S344
91	37%	L345
92	37%	K346
93	37%	G347
94	37%	P348
95	37%	L349
96	37%	L350
97	37%	L352
98	37%	P355
99	37%	P356
100	37%	G357
101	37%	L420
102	37%	E421
103	37%	L423
104	37%	D424
105	37%	S427
106	37%	ASP
107	37%	PHE
108	37%	A364
109	37%	K365
110	37%	S366
111	37%	L367
112	37%	ASP
113	37%	R302
114	37%	L505
115	37%	L506
116	37%	P507
117	37%	I510
118	37%	G514
119	37%	L515
120	37%	K516
121	37%	N519
122	37%	L520
123	37%	Q521
124	37%	L522
125	37%	I527
126	37%	L528
127	37%	D529
128	37%	I530
129	37%	I531
130	37%	R532
131	37%	Y533
132	37%	Y534
133	37%	T535
134	37%	R536
135	37%	V540
136	37%	L543
137	37%	R544
138	37%	K545
139	37%	L547
140	37%	A548
141	37%	A549
142		

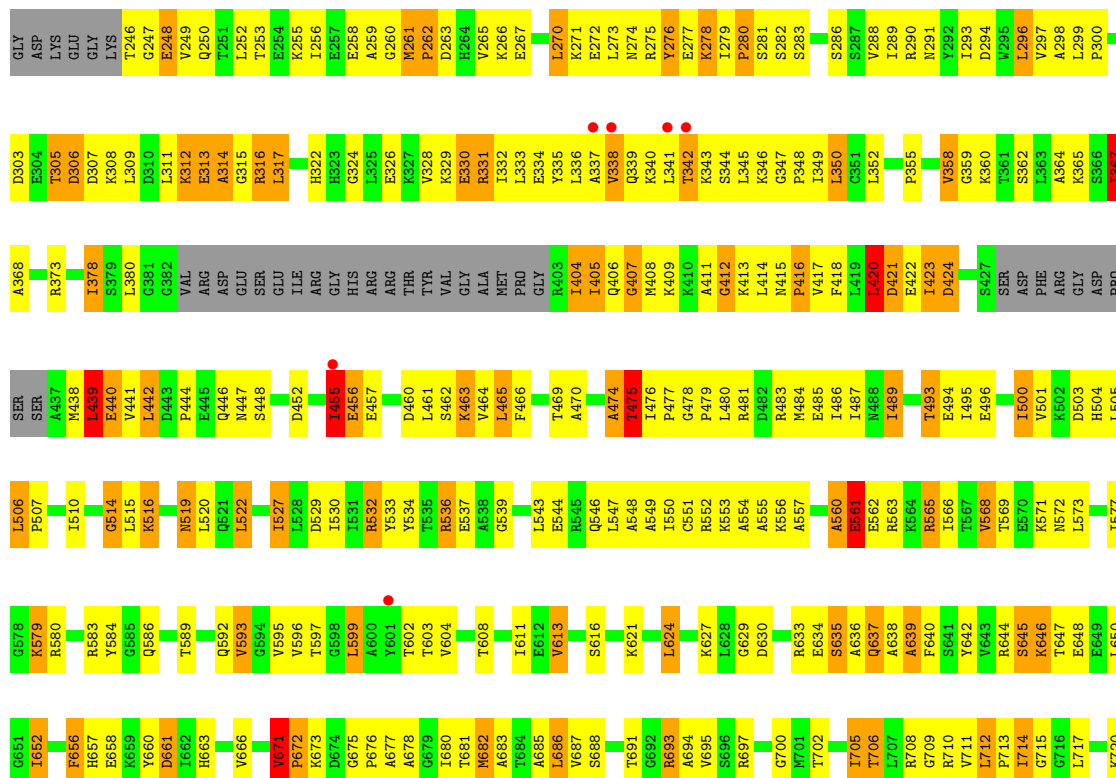
Chain B:

3% 36% 40% 15% 9%

Amino Acid	Percentage
GLY	3%
ASP	36%
LYS	40%
GLU	15%
GLY	9%
LYS	
T246	
G247	
V248	
V249	
Q250	
T251	
L252	
T253	
E254	
K255	
L256	
E257	
E258	
A259	
G260	
M261	
P262	
D263	
K266	
E267	
L270	
K271	
E272	
L273	
N274	
R275	
Y276	
E277	
K278	
T279	
P280	
S281	
S282	
S283	
S286	
S287	
V288	
T289	
R290	
T293	
D294	
W295	
L296	
V297	
A298	
L299	
P300	
W301	
T302	
T303	

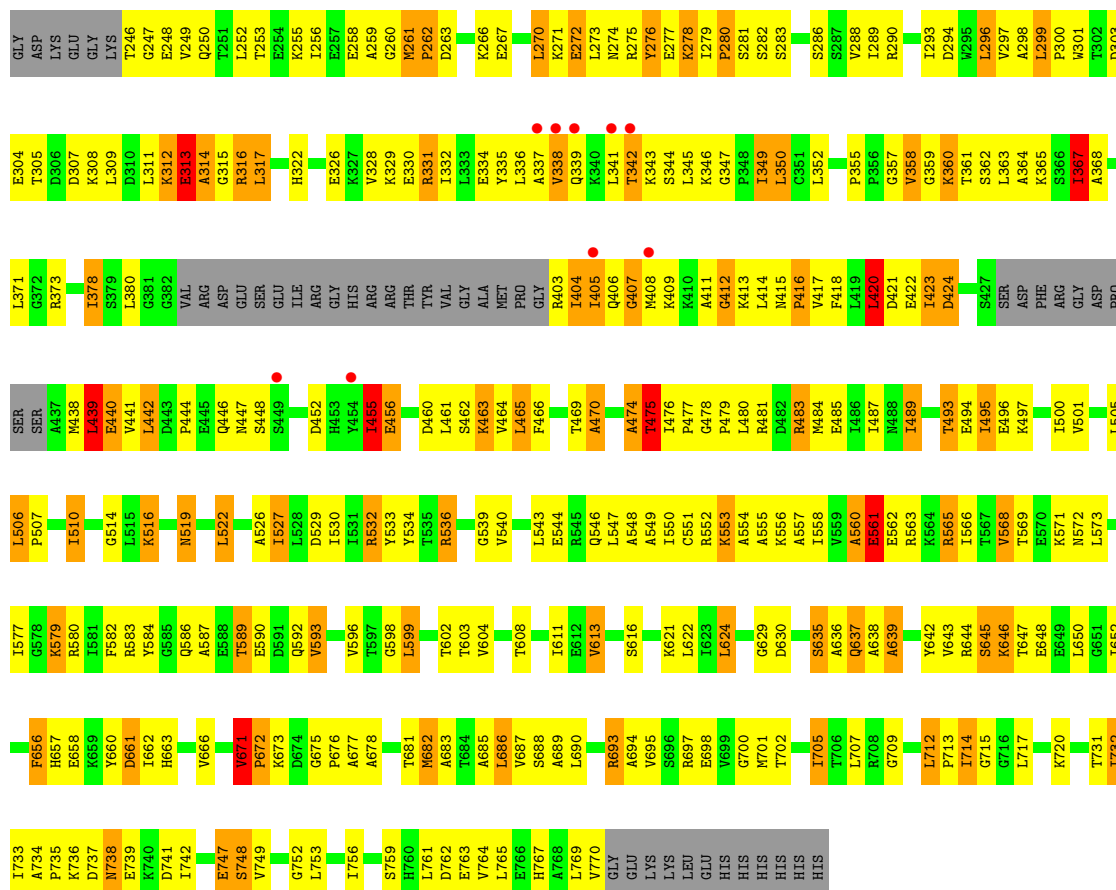


• Molecule 1: ATP-dependent protease La 1

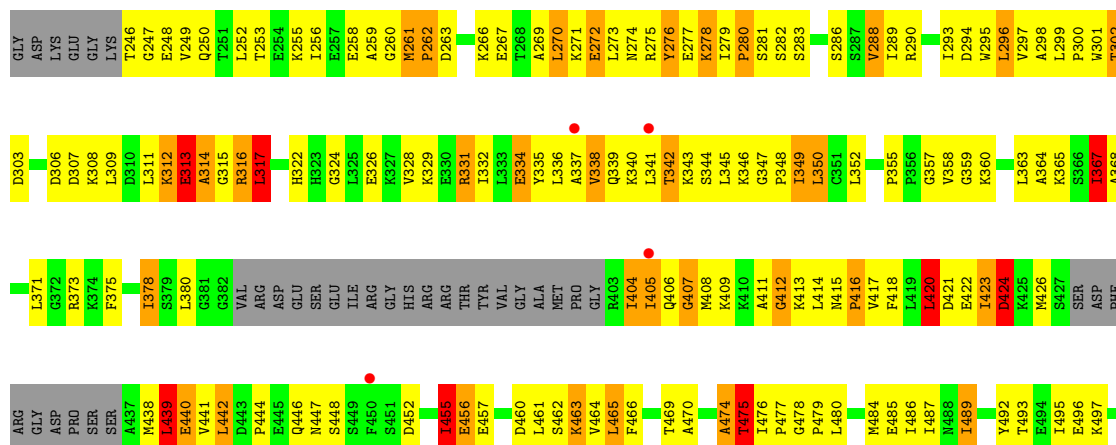


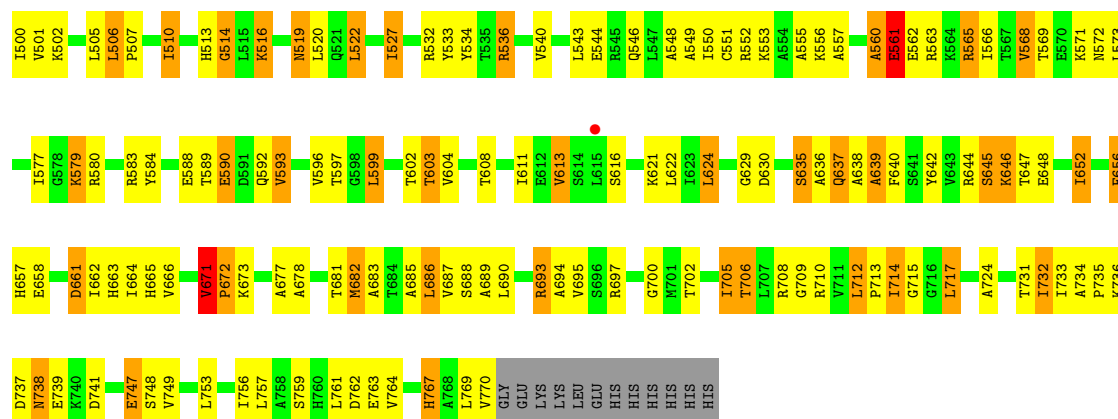


• Molecule 1: ATP-dependent protease La 1

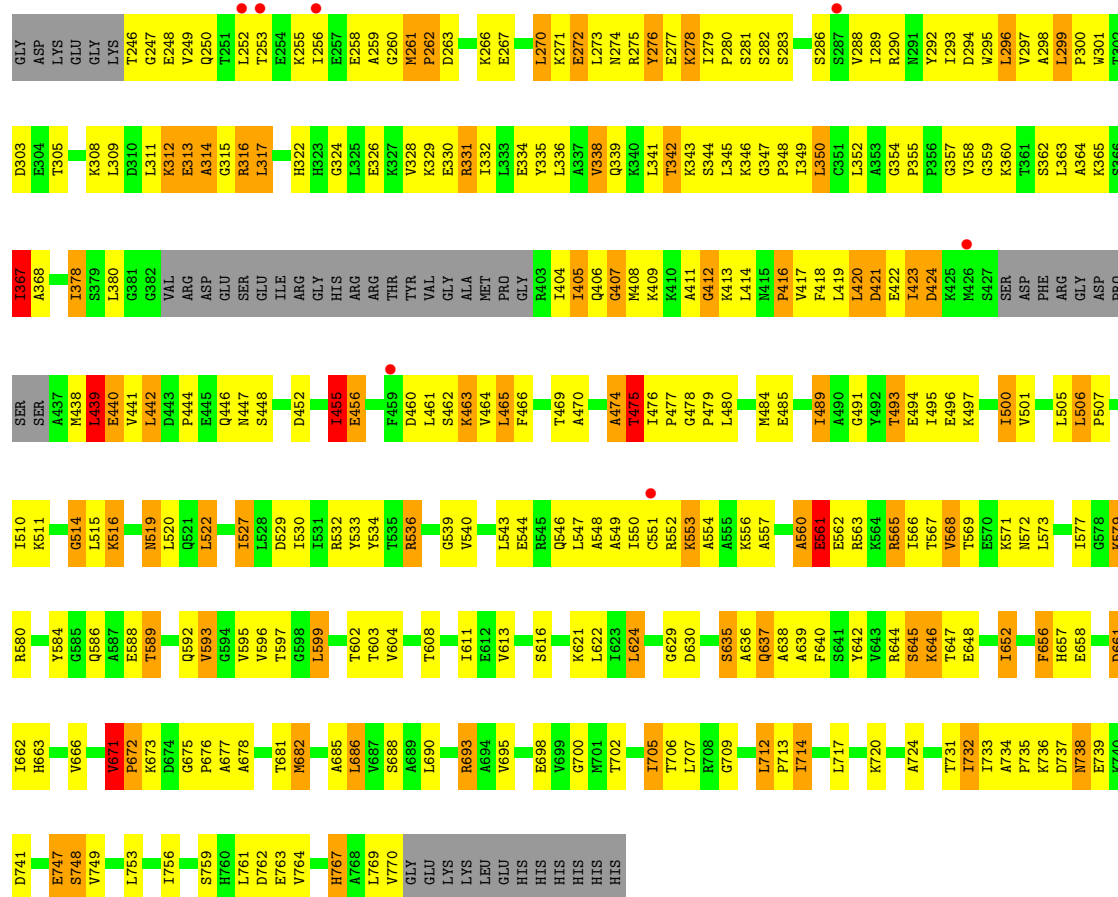


• Molecule 1: ATP-dependent protease La 1





• Molecule 1: ATP-dependent protease La 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.38Å 127.40Å 148.99Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	29.91 – 3.40 29.91 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.91-3.40) 99.5 (29.91-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_249)	Depositor
R, R_{free}	0.265 , 0.313 0.251 , 0.304	Depositor DCC
R_{free} test set	2607 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	117.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 213.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23196	wwPDB-VP
Average B, all atoms (Å ²)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.68	1/3892 (0.0%)	0.95	15/5246 (0.3%)
1	B	0.64	0/3892	0.93	11/5246 (0.2%)
1	C	0.61	0/3892	0.92	13/5246 (0.2%)
1	D	0.70	3/3892 (0.1%)	0.94	11/5246 (0.2%)
1	E	0.63	0/3892	0.95	15/5246 (0.3%)
1	F	0.59	0/3892	0.94	14/5246 (0.3%)
All	All	0.64	4/23352 (0.0%)	0.94	79/31476 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666	VAL	CA-CB	-7.76	1.47	1.54
1	D	470	ALA	CA-CB	-6.29	1.42	1.53
1	D	360	LYS	C-O	-5.89	1.17	1.24
1	D	358	VAL	CA-CB	-5.73	1.48	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	639	ALA	N-CA-C	-7.93	102.59	111.71
1	A	639	ALA	N-CA-C	-7.70	102.89	111.28
1	E	317	LEU	N-CA-C	-7.47	104.30	113.41
1	F	712	LEU	CA-C-N	7.45	127.45	119.78
1	F	712	LEU	C-N-CA	7.45	127.45	119.78
1	C	367	ILE	N-CA-C	-7.26	103.45	110.42
1	E	502	LYS	N-CA-C	7.12	118.69	111.07
1	D	317	LEU	N-CA-C	-7.03	105.23	113.88
1	C	639	ALA	N-CA-C	-6.69	104.02	111.71
1	D	712	LEU	CA-C-N	6.67	126.59	119.85
1	D	712	LEU	C-N-CA	6.67	126.59	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	671	VAL	CA-C-N	6.61	128.10	119.84
1	D	671	VAL	C-N-CA	6.61	128.10	119.84
1	E	671	VAL	CA-C-N	6.51	127.98	119.84
1	E	671	VAL	C-N-CA	6.51	127.98	119.84
1	B	317	LEU	N-CA-C	-6.48	105.51	113.41
1	A	671	VAL	CA-C-N	6.45	127.90	119.84
1	A	671	VAL	C-N-CA	6.45	127.90	119.84
1	A	317	LEU	N-CA-C	-6.39	105.61	113.41
1	E	712	LEU	CA-C-N	6.36	126.33	119.78
1	E	712	LEU	C-N-CA	6.36	126.33	119.78
1	B	712	LEU	CA-C-N	6.32	126.29	119.78
1	B	712	LEU	C-N-CA	6.32	126.29	119.78
1	B	639	ALA	N-CA-C	-6.26	104.52	111.71
1	C	724	ALA	N-CA-C	-6.22	104.39	112.23
1	F	317	LEU	N-CA-C	-6.22	105.82	113.41
1	A	367	ILE	N-CA-C	-6.16	104.34	110.62
1	F	639	ALA	N-CA-C	-6.00	104.82	111.71
1	D	367	ILE	N-CA-C	-5.97	104.69	110.42
1	A	724	ALA	N-CA-C	-5.94	104.75	112.23
1	E	630	ASP	N-CA-C	-5.93	105.88	113.23
1	C	317	LEU	N-CA-C	-5.91	106.20	113.41
1	F	367	ILE	N-CA-C	-5.89	104.77	110.42
1	E	724	ALA	N-CA-C	-5.84	104.88	112.23
1	A	404	ILE	N-CA-C	-5.83	103.81	111.09
1	D	639	ALA	N-CA-C	-5.79	105.05	111.71
1	E	404	ILE	N-CA-C	-5.75	104.51	112.50
1	C	630	ASP	N-CA-C	-5.75	106.11	113.23
1	C	278	LYS	N-CA-C	-5.73	105.38	112.38
1	C	712	LEU	CA-C-N	5.71	125.66	119.78
1	C	712	LEU	C-N-CA	5.71	125.66	119.78
1	F	589	THR	N-CA-C	5.70	117.94	108.99
1	B	278	LYS	N-CA-C	-5.69	105.44	112.38
1	B	671	VAL	CA-C-N	5.64	126.89	119.84
1	B	671	VAL	C-N-CA	5.64	126.89	119.84
1	F	278	LYS	N-CA-C	-5.62	105.53	112.38
1	A	278	LYS	N-CA-C	-5.61	105.53	112.38
1	D	278	LYS	N-CA-C	-5.61	105.53	112.38
1	E	367	ILE	N-CA-C	-5.59	104.91	110.62
1	B	486	ILE	N-CA-C	5.58	116.62	108.53
1	D	630	ASP	N-CA-C	-5.56	106.34	113.23
1	E	278	LYS	N-CA-C	-5.51	105.66	112.38
1	C	404	ILE	N-CA-C	-5.50	104.86	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	ILE	N-CA-C	5.49	116.89	108.71
1	C	486	ILE	N-CA-C	5.47	116.47	108.53
1	C	671	VAL	CA-C-N	5.44	126.64	119.84
1	C	671	VAL	C-N-CA	5.44	126.64	119.84
1	A	712	LEU	CA-C-N	5.42	125.36	119.78
1	A	712	LEU	C-N-CA	5.42	125.36	119.78
1	F	724	ALA	N-CA-C	-5.36	105.47	112.23
1	B	630	ASP	N-CA-C	-5.35	106.59	113.23
1	A	502	LYS	N-CA-C	5.32	117.16	111.36
1	A	630	ASP	N-CA-C	-5.30	106.66	113.23
1	F	630	ASP	N-CA-C	-5.29	106.67	113.23
1	F	491	GLY	N-CA-C	-5.29	104.25	112.45
1	B	367	ILE	N-CA-C	-5.27	105.24	110.62
1	B	404	ILE	N-CA-C	-5.27	104.38	111.44
1	E	486	ILE	N-CA-C	5.22	116.09	108.53
1	C	358	VAL	N-CA-C	-5.16	108.25	113.47
1	F	671	VAL	CA-C-N	5.14	126.26	119.84
1	F	671	VAL	C-N-CA	5.14	126.26	119.84
1	A	666	VAL	N-CA-C	5.11	113.21	108.15
1	E	334	GLU	N-CA-C	-5.09	105.17	111.33
1	D	404	ILE	N-CA-C	-5.08	104.74	111.09
1	A	666	VAL	CB-CA-C	-5.04	106.29	111.08
1	F	299	LEU	CA-C-N	5.02	125.23	120.31
1	F	299	LEU	C-N-CA	5.02	125.23	120.31
1	D	367	ILE	CB-CA-C	-5.01	105.56	111.97
1	E	510	ILE	CB-CA-C	-5.00	105.30	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3839	0	3968	320	0
1	B	3839	0	3968	356	0
1	C	3839	0	3968	343	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3839	0	3968	325	1
1	E	3839	0	3968	331	0
1	F	3839	0	3968	317	1
2	A	27	0	12	7	0
2	B	27	0	12	7	0
2	C	27	0	12	6	0
2	D	27	0	12	11	0
2	E	27	0	12	6	0
2	F	27	0	12	7	0
All	All	23196	0	23880	1951	1

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 41.

All (1951) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:ARG:HG3	1:E:338:VAL:HG21	1.31	1.08
1:F:493:THR:HG21	1:F:748:SER:HB2	1.26	1.08
1:C:350:LEU:H	1:C:350:LEU:HD12	1.18	1.02
1:B:337:ALA:CB	1:F:556:LYS:HA	1.89	1.02
1:A:501:VAL:HG11	1:A:527:ILE:HD13	1.39	1.01
1:F:501:VAL:HG11	1:F:527:ILE:HD13	1.42	0.97
1:B:350:LEU:HD12	1:B:350:LEU:H	1.28	0.96
1:B:501:VAL:HG11	1:B:527:ILE:HD13	1.48	0.95
1:D:501:VAL:HG11	1:D:527:ILE:HD13	1.49	0.95
1:F:586:GLN:HG2	1:F:698:GLU:HG2	1.46	0.93
1:C:569:THR:HG23	1:C:571:LYS:H	1.33	0.93
1:A:350:LEU:H	1:A:350:LEU:HD12	1.31	0.93
1:A:378:ILE:O	1:A:378:ILE:HG12	1.69	0.93
1:A:596:VAL:HG22	1:A:695:VAL:HG21	1.48	0.92
1:E:671:VAL:HG22	1:E:672:PRO:HD2	1.51	0.91
1:F:671:VAL:HG22	1:F:672:PRO:HD2	1.49	0.91
1:B:493:THR:HG21	1:B:748:SER:HB2	1.50	0.91
1:B:378:ILE:HG12	1:B:378:ILE:O	1.69	0.91
1:E:501:VAL:HG11	1:E:527:ILE:HD13	1.51	0.91
1:E:350:LEU:H	1:E:350:LEU:HD12	1.32	0.91
1:F:586:GLN:HE21	1:F:698:GLU:HA	1.38	0.89
1:E:536:ARG:HH11	1:E:536:ARG:HG3	1.35	0.89
1:D:350:LEU:H	1:D:350:LEU:HD12	1.36	0.88
1:C:501:VAL:HG11	1:C:527:ILE:HD13	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:ILE:HG23	1:D:418:PHE:CE2	2.08	0.88
1:C:536:ARG:HH11	1:C:536:ARG:HG3	1.37	0.88
1:C:671:VAL:HG22	1:C:672:PRO:HD2	1.55	0.88
1:A:569:THR:HG23	1:A:571:LYS:H	1.37	0.88
1:C:337:ALA:CB	1:E:556:LYS:HA	2.03	0.87
1:B:536:ARG:HH11	1:B:536:ARG:HG3	1.40	0.87
1:C:596:VAL:HG22	1:C:695:VAL:HG21	1.56	0.87
1:D:359:GLY:HA2	2:D:783:ADP:C5'	2.04	0.87
1:F:569:THR:HG23	1:F:571:LYS:H	1.37	0.87
1:D:688:SER:HB2	1:D:769:LEU:HD21	1.55	0.87
1:E:569:THR:HG23	1:E:571:LYS:H	1.39	0.87
1:A:536:ARG:HH11	1:A:536:ARG:HG3	1.40	0.86
1:D:671:VAL:HG22	1:D:672:PRO:HD2	1.57	0.86
1:B:569:THR:HG23	1:B:571:LYS:H	1.39	0.86
1:D:378:ILE:O	1:D:378:ILE:HG12	1.74	0.86
1:D:536:ARG:HG3	1:D:536:ARG:HH11	1.39	0.86
1:D:493:THR:HG21	1:D:748:SER:HB2	1.58	0.85
1:E:688:SER:HB2	1:E:769:LEU:HD21	1.56	0.85
1:F:536:ARG:HH11	1:F:536:ARG:HG3	1.42	0.85
1:F:596:VAL:HG22	1:F:695:VAL:HG21	1.58	0.85
1:E:378:ILE:O	1:E:378:ILE:HG12	1.77	0.84
1:B:522:LEU:HD12	1:B:527:ILE:HG12	1.60	0.84
1:D:596:VAL:HG22	1:D:695:VAL:HG21	1.60	0.84
1:A:671:VAL:HG22	1:A:672:PRO:HD2	1.60	0.83
1:D:569:THR:HG23	1:D:571:LYS:H	1.40	0.83
1:C:688:SER:HB2	1:C:769:LEU:HD21	1.59	0.83
1:E:596:VAL:HG22	1:E:695:VAL:HG21	1.60	0.83
1:F:516:LYS:HA	1:F:516:LYS:NZ	1.93	0.83
1:F:360:LYS:HD2	1:F:469:THR:HG23	1.60	0.83
1:B:733:ILE:HG21	1:B:764:VAL:HG13	1.58	0.82
1:A:733:ILE:HG21	1:A:764:VAL:HG13	1.62	0.82
1:A:456:GLU:CD	1:C:291:ASN:HD21	1.88	0.81
1:D:733:ILE:HG21	1:D:764:VAL:HG13	1.62	0.81
1:F:378:ILE:O	1:F:378:ILE:HG12	1.80	0.81
1:B:516:LYS:O	1:B:519:ASN:HB2	1.80	0.81
1:C:536:ARG:HH11	1:C:536:ARG:CG	1.93	0.81
1:A:411:ALA:O	1:A:413:LYS:N	2.14	0.81
1:F:404:ILE:HG23	1:F:418:PHE:CE2	2.16	0.81
1:F:688:SER:HB2	1:F:769:LEU:HD21	1.63	0.81
1:C:501:VAL:HA	1:C:505:LEU:HB2	1.62	0.81
1:F:516:LYS:O	1:F:519:ASN:HB2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:HD12	1:A:527:ILE:HG12	1.60	0.80
1:C:522:LEU:HB3	1:C:568:VAL:HG13	1.62	0.80
1:F:522:LEU:HB3	1:F:568:VAL:HG13	1.64	0.80
1:F:733:ILE:HG21	1:F:764:VAL:HG13	1.63	0.80
1:E:439:LEU:H	1:E:439:LEU:HD22	1.44	0.79
1:F:522:LEU:HD12	1:F:527:ILE:HG12	1.65	0.79
1:D:536:ARG:HH11	1:D:536:ARG:CG	1.96	0.79
1:F:506:LEU:HD21	1:F:522:LEU:HD21	1.65	0.79
1:A:337:ALA:CB	1:C:556:LYS:HA	2.12	0.79
1:C:404:ILE:HG23	1:C:418:PHE:CE2	2.17	0.79
1:C:439:LEU:HD22	1:C:439:LEU:H	1.47	0.79
1:C:506:LEU:HD21	1:C:522:LEU:HD21	1.65	0.79
1:D:522:LEU:HD12	1:D:527:ILE:HG12	1.65	0.79
1:E:536:ARG:HH11	1:E:536:ARG:CG	1.96	0.79
1:F:411:ALA:O	1:F:413:LYS:N	2.17	0.78
1:C:337:ALA:HB1	1:E:556:LYS:HA	1.64	0.78
1:A:338:VAL:HG21	1:C:552:ARG:HG3	1.63	0.78
1:A:536:ARG:HH11	1:A:536:ARG:CG	1.97	0.78
1:B:501:VAL:HA	1:B:505:LEU:HB2	1.65	0.78
1:E:404:ILE:HG23	1:E:418:PHE:CE2	2.19	0.78
1:B:337:ALA:HB1	1:F:556:LYS:HA	1.63	0.78
1:B:536:ARG:HH11	1:B:536:ARG:CG	1.96	0.78
1:B:688:SER:HB2	1:B:769:LEU:HD21	1.64	0.78
1:E:414:LEU:O	1:E:416:PRO:HD3	1.83	0.78
1:E:583:ARG:HD3	1:E:588:GLU:CD	2.08	0.78
1:F:359:GLY:HA2	2:F:783:ADP:O5'	1.84	0.78
1:E:411:ALA:O	1:E:413:LYS:N	2.18	0.77
1:D:411:ALA:O	1:D:413:LYS:N	2.18	0.77
1:B:282:SER:HB2	1:E:276:TYR:OH	1.82	0.77
1:B:671:VAL:HG22	1:B:672:PRO:HD2	1.66	0.77
1:E:584:TYR:O	1:E:584:TYR:CD1	2.37	0.77
1:B:411:ALA:O	1:B:413:LYS:N	2.17	0.77
1:C:414:LEU:O	1:C:416:PRO:HD3	1.85	0.77
1:D:522:LEU:HB3	1:D:568:VAL:HG13	1.65	0.77
1:A:404:ILE:HG23	1:A:418:PHE:CE2	2.20	0.76
1:C:270:LEU:HD21	1:C:296:LEU:HD22	1.66	0.76
1:D:359:GLY:HA2	2:D:783:ADP:O5'	1.85	0.76
1:B:596:VAL:HG22	1:B:695:VAL:HG21	1.66	0.76
1:A:272:GLU:HB3	1:C:248:GLU:OE1	1.85	0.76
1:B:303:ASP:O	1:B:304:GLU:HB2	1.86	0.76
1:B:506:LEU:HB3	1:B:507:PRO:HD3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ALA:O	1:C:413:LYS:N	2.18	0.75
1:A:273:LEU:HD11	1:C:290:ARG:HH12	1.50	0.75
1:B:439:LEU:H	1:B:439:LEU:HD22	1.51	0.75
1:B:506:LEU:HD21	1:B:522:LEU:HD21	1.68	0.75
1:E:516:LYS:O	1:E:519:ASN:HB2	1.86	0.75
1:B:274:ASN:C	1:B:276:TYR:H	1.94	0.75
1:D:359:GLY:HA2	2:D:783:ADP:H5'2	1.69	0.75
1:E:733:ILE:HG21	1:E:764:VAL:HG13	1.67	0.75
1:D:439:LEU:HD22	1:D:439:LEU:H	1.50	0.75
1:A:408:MET:H	1:A:408:MET:HE2	1.51	0.75
1:A:439:LEU:HD22	1:A:439:LEU:H	1.51	0.74
1:C:733:ILE:HG21	1:C:764:VAL:HG13	1.68	0.74
1:F:350:LEU:H	1:F:350:LEU:HD12	1.51	0.74
1:F:439:LEU:HD22	1:F:439:LEU:H	1.53	0.74
1:D:505:LEU:HD22	1:D:544:GLU:HG3	1.70	0.74
1:E:274:ASN:C	1:E:276:TYR:H	1.96	0.74
1:F:536:ARG:HH11	1:F:536:ARG:CG	1.99	0.74
1:C:493:THR:HG21	1:C:748:SER:HB2	1.70	0.74
1:E:270:LEU:HD21	1:E:296:LEU:HD22	1.70	0.74
1:B:359:GLY:HA2	2:B:783:ADP:O5'	1.88	0.74
1:D:274:ASN:C	1:D:276:TYR:H	1.96	0.74
1:E:738:ASN:O	1:E:741:ASP:HB2	1.88	0.74
1:A:505:LEU:HD22	1:A:544:GLU:HG3	1.68	0.73
1:C:516:LYS:HA	1:C:516:LYS:NZ	2.02	0.73
1:C:522:LEU:HD12	1:C:527:ILE:HG12	1.70	0.73
1:F:274:ASN:C	1:F:276:TYR:H	1.96	0.73
1:A:688:SER:HB2	1:A:769:LEU:HD21	1.69	0.73
1:A:270:LEU:HD21	1:A:296:LEU:HD22	1.70	0.73
1:A:516:LYS:O	1:A:519:ASN:HB2	1.89	0.73
1:D:404:ILE:HG23	1:D:418:PHE:HE2	1.53	0.73
1:E:506:LEU:HD21	1:E:522:LEU:HD21	1.70	0.73
1:C:602:THR:HG22	1:C:604:VAL:H	1.54	0.72
1:D:738:ASN:O	1:D:741:ASP:HB2	1.89	0.72
1:F:501:VAL:CG1	1:F:527:ILE:HD13	2.19	0.72
1:A:501:VAL:CG1	1:A:527:ILE:HD13	2.17	0.72
1:C:274:ASN:C	1:C:276:TYR:H	1.97	0.72
1:F:516:LYS:HA	1:F:516:LYS:CE	2.19	0.72
1:A:522:LEU:HB3	1:A:568:VAL:HG13	1.72	0.72
1:A:274:ASN:C	1:A:276:TYR:H	1.96	0.72
1:F:493:THR:HG21	1:F:748:SER:CB	2.15	0.72
1:B:347:GLY:HA3	1:B:444:PRO:HG3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:LEU:HD22	1:B:420:LEU:H	1.54	0.72
1:B:404:ILE:HG23	1:B:418:PHE:CE2	2.25	0.72
1:C:332:ILE:HD12	1:C:367:ILE:HD11	1.72	0.72
1:C:359:GLY:HA2	2:C:783:ADP:O5'	1.90	0.72
1:D:270:LEU:HD21	1:D:296:LEU:HD22	1.71	0.71
1:E:501:VAL:HA	1:E:505:LEU:HB2	1.72	0.71
1:F:270:LEU:HD21	1:F:296:LEU:HD22	1.71	0.71
1:A:677:ALA:HA	1:A:714:ILE:HD11	1.72	0.71
1:D:677:ALA:HA	1:D:714:ILE:HD11	1.72	0.71
1:B:501:VAL:CG1	1:B:527:ILE:HD13	2.20	0.71
1:C:677:ALA:HA	1:C:714:ILE:HD11	1.72	0.71
1:D:586:GLN:HA	1:D:586:GLN:OE1	1.90	0.71
1:A:559:VAL:HG21	1:D:337:ALA:HB1	1.72	0.71
1:F:347:GLY:HA3	1:F:444:PRO:HG3	1.71	0.71
1:C:506:LEU:HB3	1:C:507:PRO:HD3	1.72	0.71
1:D:347:GLY:HA3	1:D:444:PRO:HG3	1.71	0.71
1:D:501:VAL:HA	1:D:505:LEU:HB2	1.71	0.71
1:E:300:PRO:HB2	1:E:414:LEU:HB3	1.71	0.71
1:F:408:MET:H	1:F:408:MET:HE2	1.55	0.71
1:F:506:LEU:HB3	1:F:507:PRO:HD3	1.71	0.71
1:B:505:LEU:HD22	1:B:544:GLU:HG3	1.72	0.71
1:C:267:GLU:HA	1:C:270:LEU:HD12	1.73	0.70
1:D:506:LEU:HD21	1:D:522:LEU:HD21	1.72	0.70
1:E:506:LEU:HB3	1:E:507:PRO:HD3	1.72	0.70
1:E:352:LEU:HD22	1:E:489:ILE:HD11	1.73	0.70
1:A:271:LYS:HA	1:A:274:ASN:HB3	1.74	0.70
1:E:522:LEU:HD12	1:E:527:ILE:HG12	1.73	0.70
1:B:267:GLU:HA	1:B:270:LEU:HD12	1.72	0.70
1:B:602:THR:HG22	1:B:604:VAL:H	1.56	0.70
1:C:378:ILE:O	1:C:378:ILE:HG12	1.92	0.70
1:E:271:LYS:HA	1:E:274:ASN:HB3	1.72	0.70
1:D:506:LEU:HB3	1:D:507:PRO:HD3	1.74	0.70
1:D:602:THR:HG22	1:D:604:VAL:H	1.56	0.70
1:C:505:LEU:HD22	1:C:544:GLU:HG3	1.74	0.70
1:F:271:LYS:HA	1:F:274:ASN:HB3	1.73	0.70
1:A:347:GLY:HA3	1:A:444:PRO:HG3	1.73	0.70
1:D:271:LYS:HA	1:D:274:ASN:HB3	1.74	0.70
1:D:420:LEU:HD22	1:D:420:LEU:H	1.57	0.70
1:A:337:ALA:HB1	1:C:556:LYS:HA	1.71	0.70
1:D:702:THR:O	1:D:735:PRO:HD3	1.90	0.70
1:B:569:THR:H	1:B:572:ASN:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LYS:HA	1:C:274:ASN:HB3	1.74	0.70
1:C:347:GLY:HA3	1:C:444:PRO:HG3	1.73	0.70
1:F:441:VAL:HG13	1:F:442:LEU:HG	1.73	0.70
1:F:671:VAL:CG2	1:F:672:PRO:HD2	2.22	0.70
1:C:350:LEU:HD12	1:C:350:LEU:N	1.98	0.69
1:D:266:LYS:HG3	1:D:267:GLU:N	2.07	0.69
1:C:349:ILE:HD12	1:C:349:ILE:O	1.92	0.69
1:C:516:LYS:O	1:C:519:ASN:HB2	1.92	0.69
1:C:737:ASP:HB3	1:E:583:ARG:HH12	1.57	0.69
1:F:501:VAL:HA	1:F:505:LEU:HB2	1.73	0.69
1:B:338:VAL:HG21	1:F:552:ARG:HG3	1.74	0.69
1:A:441:VAL:HG13	1:A:442:LEU:HG	1.75	0.69
1:B:271:LYS:HA	1:B:274:ASN:HB3	1.74	0.69
1:B:421:ASP:O	1:B:469:THR:HB	1.92	0.69
1:A:506:LEU:HD12	1:A:510:ILE:HG12	1.74	0.69
1:B:677:ALA:HA	1:B:714:ILE:HD11	1.72	0.69
1:F:267:GLU:HA	1:F:270:LEU:HD12	1.75	0.69
1:B:516:LYS:NZ	1:B:516:LYS:HA	2.08	0.69
1:C:266:LYS:HG3	1:C:267:GLU:N	2.08	0.69
1:D:464:VAL:O	1:D:466:PHE:HD1	1.76	0.69
1:D:516:LYS:HA	1:D:516:LYS:NZ	2.07	0.69
1:E:347:GLY:HA3	1:E:444:PRO:HG3	1.73	0.69
1:E:408:MET:HE2	1:E:408:MET:H	1.56	0.69
1:F:464:VAL:O	1:F:466:PHE:HD1	1.76	0.69
1:D:414:LEU:O	1:D:416:PRO:HD3	1.93	0.69
1:D:421:ASP:O	1:D:469:THR:HB	1.92	0.69
1:B:408:MET:H	1:B:408:MET:HE2	1.58	0.69
1:B:464:VAL:O	1:B:466:PHE:HD1	1.76	0.69
1:B:522:LEU:HB3	1:B:568:VAL:HG13	1.73	0.68
1:D:532:ARG:HG2	1:D:584:TYR:CE2	2.28	0.68
1:A:501:VAL:HA	1:A:505:LEU:HB2	1.74	0.68
1:B:556:LYS:HA	1:E:337:ALA:HB1	1.75	0.68
1:C:256:ILE:HD11	1:C:293:ILE:HD11	1.76	0.68
1:E:516:LYS:HA	1:E:516:LYS:NZ	2.08	0.68
1:F:424:ASP:HB2	1:F:475:THR:HG23	1.76	0.68
1:F:266:LYS:HG3	1:F:267:GLU:N	2.08	0.68
1:F:295:TRP:CZ3	1:F:405:ILE:HG21	2.28	0.68
1:B:337:ALA:HB3	1:F:556:LYS:HA	1.75	0.68
1:E:335:TYR:HE2	1:E:465:LEU:HD21	1.57	0.68
1:E:420:LEU:HD22	1:E:420:LEU:H	1.58	0.68
1:A:516:LYS:HA	1:A:516:LYS:NZ	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:LEU:HD12	1:C:510:ILE:HG12	1.76	0.68
1:E:505:LEU:HD22	1:E:544:GLU:HG3	1.75	0.68
1:E:421:ASP:O	1:E:469:THR:HB	1.94	0.67
1:E:646:LYS:H	1:E:646:LYS:HD2	1.58	0.67
1:E:702:THR:O	1:E:735:PRO:HD3	1.94	0.67
1:F:738:ASN:O	1:F:741:ASP:HB2	1.94	0.67
1:A:464:VAL:O	1:A:466:PHE:HD1	1.76	0.67
1:D:300:PRO:HB3	1:D:412:GLY:C	2.20	0.67
1:F:420:LEU:H	1:F:420:LEU:HD22	1.58	0.67
1:F:506:LEU:HD12	1:F:510:ILE:HG12	1.77	0.67
1:A:267:GLU:HA	1:A:270:LEU:HD12	1.75	0.67
1:A:420:LEU:HD21	1:A:466:PHE:HD2	1.59	0.67
1:F:505:LEU:HD22	1:F:544:GLU:HG3	1.77	0.67
1:A:266:LYS:HG3	1:A:267:GLU:N	2.09	0.67
1:C:317:LEU:HD23	1:C:317:LEU:O	1.94	0.67
1:B:506:LEU:C	1:B:506:LEU:HD12	2.20	0.67
1:B:556:LYS:HA	1:E:337:ALA:CB	2.24	0.67
1:C:423:ILE:CD1	1:C:484:MET:HE1	2.24	0.67
1:B:270:LEU:HD21	1:B:296:LEU:HD22	1.75	0.67
1:E:464:VAL:O	1:E:466:PHE:HD1	1.77	0.67
1:B:702:THR:O	1:B:735:PRO:HD3	1.94	0.67
1:E:267:GLU:HA	1:E:270:LEU:HD12	1.77	0.67
1:E:671:VAL:CG2	1:E:672:PRO:HD2	2.23	0.67
1:D:441:VAL:HG13	1:D:442:LEU:HG	1.76	0.67
1:B:315:GLY:C	1:B:316:ARG:HD2	2.20	0.66
1:C:408:MET:H	1:C:408:MET:HE2	1.59	0.66
1:D:267:GLU:HA	1:D:270:LEU:HD12	1.76	0.66
1:D:501:VAL:CG1	1:D:527:ILE:HD13	2.24	0.66
1:A:315:GLY:C	1:A:316:ARG:HD2	2.20	0.66
1:A:506:LEU:HB3	1:A:507:PRO:HD3	1.75	0.66
1:C:424:ASP:HB2	1:C:475:THR:HG23	1.77	0.66
1:C:702:THR:O	1:C:735:PRO:HD3	1.95	0.66
1:E:441:VAL:HG13	1:E:442:LEU:HG	1.78	0.66
1:A:702:THR:O	1:A:735:PRO:HD3	1.96	0.66
1:F:702:THR:O	1:F:735:PRO:HD3	1.96	0.66
1:B:266:LYS:HG3	1:B:267:GLU:N	2.09	0.66
1:E:266:LYS:HG3	1:E:267:GLU:N	2.09	0.66
1:F:421:ASP:O	1:F:469:THR:HB	1.96	0.66
2:C:783:ADP:O1A	2:C:783:ADP:O1B	2.14	0.66
1:D:646:LYS:H	1:D:646:LYS:HD2	1.60	0.66
1:B:414:LEU:O	1:B:416:PRO:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLU:HG2	1:C:260:GLY:H	1.60	0.66
1:C:501:VAL:CG1	1:C:527:ILE:HD13	2.26	0.66
1:D:315:GLY:C	1:D:316:ARG:HD2	2.21	0.66
1:D:569:THR:H	1:D:572:ASN:HB2	1.61	0.66
1:F:677:ALA:HA	1:F:714:ILE:HD11	1.78	0.66
1:D:505:LEU:CD2	1:D:544:GLU:HG3	2.25	0.66
1:E:506:LEU:HD12	1:E:510:ILE:HG12	1.76	0.66
1:D:424:ASP:HB2	1:D:475:THR:HG23	1.77	0.65
1:E:315:GLY:C	1:E:316:ARG:HD2	2.22	0.65
1:C:315:GLY:C	1:C:316:ARG:HD2	2.21	0.65
1:F:474:ALA:O	1:F:476:ILE:N	2.29	0.65
1:A:252:LEU:O	1:A:256:ILE:HG13	1.97	0.65
1:A:258:GLU:HG2	1:A:260:GLY:H	1.61	0.65
1:A:644:ARG:HD2	1:C:616:SER:OG	1.96	0.65
1:B:345:LEU:HD23	1:B:346:LYS:N	2.12	0.65
1:E:345:LEU:HD11	1:E:465:LEU:HD22	1.78	0.65
1:E:474:ALA:O	1:E:476:ILE:N	2.28	0.65
1:E:522:LEU:HB3	1:E:568:VAL:HG13	1.77	0.65
1:E:677:ALA:HA	1:E:714:ILE:HD11	1.77	0.65
1:A:602:THR:HG22	1:A:604:VAL:H	1.61	0.65
1:C:335:TYR:HE2	1:C:465:LEU:HD21	1.61	0.65
1:F:292:TYR:CZ	1:F:455:ILE:HA	2.31	0.65
1:F:646:LYS:H	1:F:646:LYS:HD2	1.61	0.65
1:C:474:ALA:O	1:C:476:ILE:N	2.30	0.65
1:F:300:PRO:HB2	1:F:414:LEU:HB3	1.79	0.65
1:F:579:LYS:HE2	1:F:579:LYS:O	1.96	0.65
1:A:421:ASP:O	1:A:469:THR:HB	1.96	0.65
1:C:420:LEU:HD21	1:C:466:PHE:HD2	1.61	0.65
1:A:300:PRO:HG3	1:A:412:GLY:C	2.22	0.65
1:A:579:LYS:HE2	1:A:579:LYS:O	1.96	0.65
1:F:352:LEU:HD22	1:F:489:ILE:HD11	1.77	0.65
1:A:332:ILE:HD12	1:A:367:ILE:HD11	1.79	0.65
1:B:352:LEU:HD22	1:B:489:ILE:HD11	1.79	0.65
1:C:464:VAL:O	1:C:466:PHE:HD1	1.80	0.65
1:E:349:ILE:HD12	1:E:349:ILE:O	1.97	0.65
1:F:252:LEU:O	1:F:256:ILE:HG13	1.97	0.65
1:B:299:LEU:HD12	1:B:301:TRP:HE1	1.62	0.64
1:C:362:SER:HB2	2:C:783:ADP:H5'1	1.78	0.64
1:A:424:ASP:HB2	1:A:475:THR:HG23	1.77	0.64
1:C:646:LYS:H	1:C:646:LYS:HD2	1.61	0.64
1:A:414:LEU:O	1:A:416:PRO:HD3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:LEU:H	1:C:599:LEU:HD22	1.62	0.64
1:E:252:LEU:O	1:E:256:ILE:HG13	1.98	0.64
1:F:315:GLY:C	1:F:316:ARG:HD2	2.23	0.64
1:F:345:LEU:HD11	1:F:465:LEU:HD22	1.79	0.64
1:A:477:PRO:HB2	1:A:480:LEU:HD23	1.79	0.64
1:A:506:LEU:HD21	1:A:522:LEU:HD21	1.78	0.64
1:C:644:ARG:HE	1:C:657:HIS:CG	2.16	0.64
1:D:252:LEU:O	1:D:256:ILE:HG13	1.98	0.64
1:F:569:THR:H	1:F:572:ASN:HB2	1.62	0.64
1:B:258:GLU:HG2	1:B:259:ALA:N	2.13	0.64
1:D:256:ILE:HD11	1:D:293:ILE:HD11	1.79	0.64
1:B:252:LEU:O	1:B:256:ILE:HG13	1.98	0.64
1:B:258:GLU:HG2	1:B:260:GLY:H	1.62	0.64
1:E:644:ARG:HE	1:E:657:HIS:CG	2.16	0.64
1:F:414:LEU:O	1:F:416:PRO:HD3	1.97	0.64
1:F:644:ARG:HE	1:F:657:HIS:CG	2.15	0.64
1:A:646:LYS:H	1:A:646:LYS:HD2	1.62	0.64
1:B:267:GLU:O	1:B:270:LEU:HB2	1.98	0.64
1:B:424:ASP:HB2	1:B:475:THR:HG23	1.79	0.64
1:E:588:GLU:HG2	1:E:589:THR:N	2.13	0.64
1:E:569:THR:H	1:E:572:ASN:HB2	1.62	0.64
1:F:258:GLU:HG2	1:F:260:GLY:H	1.61	0.64
1:B:493:THR:HG21	1:B:748:SER:CB	2.27	0.64
1:C:267:GLU:O	1:C:270:LEU:HB2	1.97	0.64
1:C:360:LYS:HD2	1:C:469:THR:HG23	1.80	0.64
1:B:644:ARG:HE	1:B:657:HIS:CG	2.16	0.63
1:C:671:VAL:CG2	1:C:672:PRO:HD2	2.26	0.63
1:D:258:GLU:HG2	1:D:260:GLY:H	1.61	0.63
1:D:345:LEU:HD11	1:D:465:LEU:HD22	1.79	0.63
1:D:506:LEU:HD12	1:D:510:ILE:HG12	1.79	0.63
1:E:258:GLU:HG2	1:E:260:GLY:H	1.62	0.63
1:E:253:THR:HA	1:E:256:ILE:HD12	1.79	0.63
1:E:256:ILE:HD11	1:E:293:ILE:HD11	1.80	0.63
1:E:249:VAL:HG12	1:E:278:LYS:HG2	1.81	0.63
1:E:501:VAL:CG1	1:E:527:ILE:HD13	2.26	0.63
1:A:644:ARG:HE	1:A:657:HIS:CG	2.16	0.63
1:B:296:LEU:HA	1:B:299:LEU:HD21	1.79	0.63
1:B:583:ARG:NH1	1:E:737:ASP:OD1	2.31	0.63
1:A:423:ILE:CD1	1:A:484:MET:HE1	2.27	0.63
1:A:493:THR:HG21	1:A:748:SER:HB2	1.81	0.63
1:E:424:ASP:HB2	1:E:475:THR:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLY:O	1:A:413:LYS:HG2	1.98	0.63
1:B:412:GLY:O	1:B:413:LYS:HG2	1.99	0.63
1:B:444:PRO:HA	1:B:447:ASN:HD21	1.64	0.63
1:C:420:LEU:H	1:C:420:LEU:HD22	1.64	0.63
1:C:506:LEU:HD12	1:C:506:LEU:C	2.24	0.63
1:F:253:THR:HA	1:F:256:ILE:HD12	1.81	0.63
1:F:550:ILE:O	1:F:551:CYS:C	2.42	0.63
1:A:444:PRO:HA	1:A:447:ASN:HD21	1.64	0.63
1:B:493:THR:CG2	1:B:748:SER:HB2	2.25	0.63
1:E:412:GLY:O	1:E:413:LYS:HG2	1.99	0.63
1:C:421:ASP:O	1:C:469:THR:HB	1.98	0.63
1:F:256:ILE:HD11	1:F:293:ILE:HD11	1.80	0.63
1:F:412:GLY:O	1:F:413:LYS:HG2	1.98	0.63
1:A:256:ILE:HD11	1:A:293:ILE:HD11	1.81	0.62
1:C:258:GLU:HG2	1:C:259:ALA:N	2.14	0.62
1:C:350:LEU:H	1:C:350:LEU:CD1	1.98	0.62
1:C:584:TYR:C	1:C:584:TYR:CD1	2.76	0.62
1:A:317:LEU:O	1:A:317:LEU:HD23	1.99	0.62
1:A:253:THR:HA	1:A:256:ILE:HD12	1.80	0.62
1:A:360:LYS:HD2	1:A:469:THR:HG23	1.80	0.62
1:A:345:LEU:HD11	1:A:465:LEU:HD22	1.82	0.62
1:B:332:ILE:HD12	1:B:367:ILE:HD11	1.80	0.62
1:D:332:ILE:HD12	1:D:367:ILE:HD11	1.80	0.62
1:F:477:PRO:HB2	1:F:480:LEU:HD23	1.82	0.62
1:A:738:ASN:O	1:A:741:ASP:HB2	2.00	0.62
1:C:252:LEU:O	1:C:256:ILE:HG13	1.99	0.62
1:C:345:LEU:HD23	1:C:346:LYS:N	2.15	0.62
1:E:477:PRO:HB2	1:E:480:LEU:HD23	1.81	0.62
1:A:352:LEU:HD22	1:A:489:ILE:HD11	1.81	0.62
1:B:277:GLU:HB3	1:B:279:ILE:O	1.99	0.62
1:B:299:LEU:CD1	1:B:301:TRP:HE1	2.12	0.62
1:D:412:GLY:O	1:D:413:LYS:HG2	1.99	0.62
1:F:423:ILE:CD1	1:F:484:MET:HE1	2.29	0.62
1:D:249:VAL:HG12	1:D:278:LYS:HG2	1.81	0.62
1:D:345:LEU:HD23	1:D:346:LYS:N	2.15	0.62
1:F:613:VAL:HA	1:F:663:HIS:O	2.00	0.62
1:C:253:THR:HA	1:C:256:ILE:HD12	1.82	0.62
1:A:569:THR:H	1:A:572:ASN:HB2	1.64	0.61
1:A:734:ALA:HB1	1:A:735:PRO:HD2	1.82	0.61
1:B:256:ILE:HD11	1:B:293:ILE:HD11	1.82	0.61
1:D:258:GLU:HG2	1:D:259:ALA:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:602:THR:HG22	1:F:604:VAL:H	1.64	0.61
1:A:506:LEU:HD12	1:A:506:LEU:C	2.24	0.61
1:B:474:ALA:O	1:B:476:ILE:N	2.33	0.61
1:C:412:GLY:O	1:C:413:LYS:HG2	1.99	0.61
1:D:671:VAL:CG2	1:D:672:PRO:HD2	2.28	0.61
1:E:734:ALA:HB1	1:E:735:PRO:HD2	1.82	0.61
1:F:444:PRO:HA	1:F:447:ASN:HD21	1.66	0.61
1:B:360:LYS:HD2	1:B:469:THR:HG23	1.82	0.61
1:B:646:LYS:H	1:B:646:LYS:HD2	1.64	0.61
1:D:644:ARG:HE	1:D:657:HIS:CG	2.17	0.61
1:F:368:ALA:HB2	1:F:417:VAL:HG21	1.82	0.61
1:A:258:GLU:HG2	1:A:259:ALA:N	2.14	0.61
1:B:441:VAL:HG13	1:B:442:LEU:HG	1.81	0.61
1:B:253:THR:HA	1:B:256:ILE:HD12	1.80	0.61
1:C:249:VAL:HG12	1:C:278:LYS:HG2	1.81	0.61
1:D:277:GLU:HB3	1:D:279:ILE:O	2.01	0.61
1:F:516:LYS:HA	1:F:516:LYS:HZ1	1.65	0.61
1:C:686:LEU:O	1:C:686:LEU:HD22	2.01	0.61
1:A:474:ALA:O	1:A:476:ILE:N	2.33	0.61
1:D:565:ARG:HG2	1:D:566:ILE:N	2.14	0.61
1:E:444:PRO:HA	1:E:447:ASN:HD21	1.66	0.61
1:B:506:LEU:HD12	1:B:510:ILE:HG12	1.81	0.61
1:E:438:MET:O	1:E:439:LEU:C	2.44	0.61
1:A:249:VAL:HG12	1:A:278:LYS:HG2	1.82	0.61
1:B:565:ARG:HG2	1:B:566:ILE:N	2.14	0.61
1:C:277:GLU:HB3	1:C:279:ILE:O	2.01	0.61
1:E:533:TYR:HB3	1:E:580:ARG:HD2	1.83	0.61
1:B:613:VAL:HA	1:B:663:HIS:O	2.01	0.61
1:C:345:LEU:HD11	1:C:465:LEU:HD22	1.82	0.61
1:E:602:THR:HG22	1:E:604:VAL:H	1.64	0.61
1:D:253:THR:HA	1:D:256:ILE:HD12	1.81	0.60
1:D:474:ALA:O	1:D:476:ILE:N	2.34	0.60
1:E:258:GLU:HG2	1:E:259:ALA:N	2.15	0.60
1:F:258:GLU:HG2	1:F:259:ALA:N	2.14	0.60
1:F:345:LEU:HD23	1:F:346:LYS:N	2.16	0.60
1:F:540:VAL:HG23	2:F:783:ADP:H1'	1.82	0.60
1:D:349:ILE:O	1:D:349:ILE:HD12	2.01	0.60
1:D:636:ALA:C	1:D:638:ALA:H	2.08	0.60
1:F:277:GLU:HB3	1:F:279:ILE:O	2.02	0.60
1:A:560:ALA:O	1:A:562:GLU:HG3	2.01	0.60
1:B:261:MET:H	1:B:262:PRO:HD3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LYS:N	2:B:783:ADP:O1B	2.34	0.60
1:C:477:PRO:HB2	1:C:480:LEU:HD23	1.82	0.60
1:C:738:ASN:O	1:C:741:ASP:HB2	2.00	0.60
1:D:560:ALA:O	1:D:562:GLU:HG3	2.01	0.60
1:F:249:VAL:HG12	1:F:278:LYS:HG2	1.82	0.60
1:C:579:LYS:HE2	1:C:579:LYS:O	2.01	0.60
1:D:361:THR:HB	2:D:783:ADP:O1A	2.01	0.60
1:B:345:LEU:HD11	1:B:465:LEU:HD22	1.82	0.60
1:B:738:ASN:O	1:B:741:ASP:HB2	2.00	0.60
1:D:444:PRO:HA	1:D:447:ASN:HD21	1.67	0.60
1:F:565:ARG:HG2	1:F:566:ILE:N	2.16	0.60
1:F:586:GLN:N	1:F:586:GLN:OE1	2.34	0.60
1:B:359:GLY:HA2	2:B:783:ADP:C5'	2.31	0.60
1:B:560:ALA:O	1:B:562:GLU:HG3	2.02	0.60
1:D:260:GLY:O	1:D:261:MET:HB2	2.02	0.60
1:D:335:TYR:HE2	1:D:465:LEU:HD21	1.65	0.60
1:F:261:MET:H	1:F:262:PRO:HD3	1.67	0.60
1:A:345:LEU:HD23	1:A:346:LYS:N	2.16	0.60
1:B:260:GLY:O	1:B:261:MET:HB2	2.02	0.60
1:D:261:MET:N	1:D:262:PRO:HD3	2.17	0.60
1:F:357:GLY:O	1:F:539:GLY:CA	2.49	0.60
1:C:444:PRO:HA	1:C:447:ASN:HD21	1.66	0.60
1:C:469:THR:HG22	1:C:470:ALA:N	2.17	0.60
1:F:380:LEU:HB2	1:F:422:GLU:O	2.02	0.60
1:A:642:TYR:CD2	1:A:761:LEU:HD12	2.37	0.60
1:A:565:ARG:HG2	1:A:566:ILE:N	2.16	0.59
1:D:357:GLY:O	1:D:540:VAL:N	2.33	0.59
1:A:267:GLU:O	1:A:270:LEU:HB2	2.02	0.59
1:A:420:LEU:H	1:A:420:LEU:HD22	1.66	0.59
1:C:441:VAL:HG13	1:C:442:LEU:HG	1.83	0.59
1:E:345:LEU:HD23	1:E:346:LYS:N	2.17	0.59
1:E:548:ALA:O	1:E:549:ALA:C	2.45	0.59
1:F:357:GLY:N	2:F:783:ADP:O2B	2.35	0.59
1:A:277:GLU:HB3	1:A:279:ILE:O	2.01	0.59
1:C:380:LEU:HB2	1:C:422:GLU:O	2.02	0.59
1:C:496:GLU:O	1:C:500:ILE:HG13	2.03	0.59
1:C:602:THR:HG21	1:C:604:VAL:HG22	1.83	0.59
1:E:416:PRO:HD2	1:E:464:VAL:HG13	1.84	0.59
1:A:261:MET:N	1:A:262:PRO:HD3	2.17	0.59
1:B:267:GLU:HA	1:B:270:LEU:CG	2.32	0.59
1:E:261:MET:H	1:E:262:PRO:HD3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:MET:N	1:F:262:PRO:HD3	2.18	0.59
1:F:328:VAL:O	1:F:332:ILE:HG12	2.02	0.59
1:A:341:LEU:HB3	1:C:514:GLY:O	2.03	0.59
1:B:249:VAL:HG12	1:B:278:LYS:HG2	1.82	0.59
1:B:380:LEU:HD12	1:B:423:ILE:HG23	1.83	0.59
1:C:516:LYS:HA	1:C:516:LYS:CE	2.33	0.59
1:E:261:MET:N	1:E:262:PRO:HD3	2.17	0.59
1:F:267:GLU:O	1:F:270:LEU:HB2	2.03	0.59
1:B:267:GLU:HA	1:B:270:LEU:CD1	2.33	0.59
1:D:261:MET:H	1:D:262:PRO:HD3	1.66	0.59
1:D:357:GLY:O	1:D:539:GLY:CA	2.51	0.59
1:A:335:TYR:HE2	1:A:465:LEU:HD21	1.67	0.59
1:B:261:MET:N	1:B:262:PRO:HD3	2.17	0.59
1:D:357:GLY:N	2:D:783:ADP:O1B	2.34	0.59
1:D:408:MET:H	1:D:408:MET:HE2	1.68	0.59
1:E:420:LEU:HD21	1:E:466:PHE:HD2	1.68	0.59
1:A:300:PRO:HB2	1:A:414:LEU:HB3	1.85	0.59
1:C:260:GLY:O	1:C:261:MET:HB2	2.03	0.59
1:C:569:THR:H	1:C:572:ASN:HB2	1.67	0.59
1:B:404:ILE:O	1:B:405:ILE:C	2.45	0.58
1:C:506:LEU:CD2	1:C:522:LEU:HD21	2.32	0.58
1:C:533:TYR:HB3	1:C:580:ARG:HD2	1.84	0.58
1:E:277:GLU:HB3	1:E:279:ILE:O	2.03	0.58
1:D:352:LEU:HD22	1:D:489:ILE:HD11	1.83	0.58
1:B:276:TYR:CZ	1:F:246:THR:HB	2.38	0.58
1:B:349:ILE:HD12	1:B:349:ILE:O	2.03	0.58
1:C:261:MET:N	1:C:262:PRO:HD3	2.18	0.58
1:C:565:ARG:HG2	1:C:566:ILE:N	2.16	0.58
1:E:380:LEU:HB2	1:E:422:GLU:O	2.03	0.58
1:B:747:GLU:H	1:B:747:GLU:CD	2.10	0.58
1:D:420:LEU:HD21	1:D:466:PHE:HD2	1.68	0.58
1:E:589:THR:O	1:E:697:ARG:HD2	2.04	0.58
1:F:335:TYR:HE2	1:F:465:LEU:HD21	1.67	0.58
1:A:261:MET:H	1:A:262:PRO:HD3	1.66	0.58
1:A:461:LEU:O	1:A:464:VAL:HG23	2.04	0.58
1:B:593:VAL:HB	1:E:708:ARG:NH2	2.18	0.58
1:E:506:LEU:HD12	1:E:506:LEU:C	2.28	0.58
1:A:636:ALA:C	1:A:638:ALA:H	2.10	0.58
1:C:336:LEU:O	1:C:339:GLN:N	2.37	0.58
1:C:602:THR:CG2	1:C:604:VAL:HG22	2.33	0.58
1:E:317:LEU:HD23	1:E:317:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:VAL:CG2	1:A:672:PRO:HD2	2.33	0.58
1:C:516:LYS:HA	1:C:516:LYS:HZ3	1.67	0.58
1:D:438:MET:O	1:D:439:LEU:C	2.47	0.58
1:E:590:GLU:HA	1:E:697:ARG:CD	2.33	0.58
1:F:506:LEU:CD2	1:F:522:LEU:HD21	2.33	0.58
1:A:267:GLU:HA	1:A:270:LEU:CG	2.34	0.58
1:B:438:MET:O	1:B:439:LEU:C	2.45	0.58
1:D:477:PRO:HB2	1:D:480:LEU:HD23	1.85	0.58
1:E:613:VAL:HG23	1:E:685:ALA:HB1	1.86	0.58
1:A:260:GLY:O	1:A:261:MET:HB2	2.03	0.58
1:B:316:ARG:HD2	1:B:316:ARG:N	2.19	0.58
1:B:341:LEU:HD13	1:F:514:GLY:O	2.04	0.58
1:B:477:PRO:HB2	1:B:480:LEU:HD23	1.86	0.58
1:C:267:GLU:HA	1:C:270:LEU:CG	2.33	0.58
1:F:260:GLY:O	1:F:261:MET:HB2	2.03	0.58
1:C:261:MET:H	1:C:262:PRO:HD3	1.68	0.58
1:C:438:MET:O	1:C:439:LEU:C	2.46	0.58
1:E:260:GLY:O	1:E:261:MET:HB2	2.02	0.58
1:E:700:GLY:O	1:E:732:ILE:HA	2.04	0.58
1:C:705:ILE:HD11	1:C:761:LEU:HD21	1.86	0.57
1:A:747:GLU:CD	1:A:747:GLU:H	2.12	0.57
1:B:336:LEU:O	1:B:339:GLN:N	2.37	0.57
1:C:557:ALA:HB3	1:C:566:ILE:HD11	1.87	0.57
1:D:267:GLU:O	1:D:270:LEU:HB2	2.03	0.57
1:D:368:ALA:HB2	1:D:417:VAL:HG21	1.84	0.57
1:F:294:ASP:HA	1:F:297:VAL:HG23	1.86	0.57
1:B:335:TYR:HE2	1:B:465:LEU:HD21	1.68	0.57
1:B:439:LEU:O	1:B:441:VAL:N	2.37	0.57
1:A:420:LEU:HD21	1:A:466:PHE:CD2	2.40	0.57
1:A:438:MET:O	1:A:439:LEU:C	2.46	0.57
1:B:636:ALA:C	1:B:638:ALA:H	2.12	0.57
1:E:439:LEU:O	1:E:441:VAL:N	2.38	0.57
1:B:536:ARG:CG	1:B:536:ARG:NH1	2.65	0.57
1:F:420:LEU:HD21	1:F:466:PHE:HD2	1.70	0.57
1:F:461:LEU:O	1:F:464:VAL:HG23	2.05	0.57
1:D:250:GLN:HA	1:D:253:THR:OG1	2.05	0.57
1:D:267:GLU:HA	1:D:270:LEU:CG	2.34	0.57
1:E:613:VAL:HA	1:E:663:HIS:O	2.03	0.57
1:A:316:ARG:HD2	1:A:316:ARG:N	2.19	0.57
1:B:250:GLN:HA	1:B:253:THR:OG1	2.05	0.57
1:B:586:GLN:HE22	1:B:729:LEU:HA	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:ALA:HB1	1:B:735:PRO:HD2	1.87	0.57
1:E:497:LYS:HG2	1:E:540:VAL:HG12	1.86	0.57
1:F:493:THR:O	1:F:494:GLU:C	2.48	0.57
1:B:276:TYR:OH	1:F:247:GLY:N	2.37	0.57
1:B:317:LEU:HD23	1:B:317:LEU:O	2.04	0.57
1:C:267:GLU:HA	1:C:270:LEU:CD1	2.34	0.57
1:E:262:PRO:HD2	1:E:301:TRP:CB	2.35	0.57
1:F:247:GLY:C	1:F:249:VAL:H	2.13	0.57
1:A:439:LEU:O	1:A:441:VAL:N	2.38	0.57
1:C:506:LEU:HD21	1:C:522:LEU:CD2	2.34	0.57
1:C:636:ALA:C	1:C:638:ALA:H	2.12	0.57
1:D:274:ASN:C	1:D:276:TYR:N	2.63	0.57
1:A:404:ILE:O	1:A:405:ILE:C	2.47	0.56
1:B:548:ALA:O	1:B:549:ALA:C	2.47	0.56
1:C:406:GLN:O	1:C:407:GLY:C	2.48	0.56
1:C:734:ALA:HB1	1:C:735:PRO:HD2	1.86	0.56
1:D:516:LYS:HA	1:D:516:LYS:HZ1	1.69	0.56
1:E:250:GLN:HA	1:E:253:THR:OG1	2.05	0.56
1:E:350:LEU:HD12	1:E:350:LEU:N	2.07	0.56
1:E:747:GLU:H	1:E:747:GLU:CD	2.13	0.56
1:A:406:GLN:O	1:A:407:GLY:C	2.48	0.56
1:B:409:LYS:C	1:B:411:ALA:H	2.13	0.56
1:D:602:THR:HG21	1:D:604:VAL:HG22	1.87	0.56
1:E:423:ILE:CD1	1:E:484:MET:HE1	2.35	0.56
1:E:565:ARG:HG2	1:E:566:ILE:N	2.20	0.56
1:F:332:ILE:HD12	1:F:367:ILE:HD11	1.86	0.56
1:A:274:ASN:C	1:A:276:TYR:N	2.64	0.56
1:B:350:LEU:HD23	1:B:487:ILE:HD11	1.87	0.56
1:B:414:LEU:C	1:B:416:PRO:HD3	2.30	0.56
1:C:250:GLN:HA	1:C:253:THR:OG1	2.05	0.56
1:D:548:ALA:O	1:D:549:ALA:C	2.49	0.56
1:B:290:ARG:O	1:B:293:ILE:HG22	2.05	0.56
1:B:294:ASP:HA	1:B:297:VAL:HG23	1.88	0.56
1:C:294:ASP:HA	1:C:297:VAL:HG23	1.87	0.56
1:D:469:THR:O	1:D:470:ALA:HB2	2.05	0.56
1:D:596:VAL:HG23	1:D:685:ALA:HB2	1.87	0.56
1:A:414:LEU:C	1:A:416:PRO:HD3	2.31	0.56
1:D:362:SER:CB	2:D:783:ADP:H5'1	2.35	0.56
1:E:267:GLU:O	1:E:270:LEU:HB2	2.04	0.56
1:F:438:MET:O	1:F:439:LEU:C	2.48	0.56
1:F:586:GLN:HG2	1:F:698:GLU:CG	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:VAL:CG2	1:D:337:ALA:HB1	2.35	0.56
1:C:656:PHE:C	1:C:658:GLU:H	2.13	0.56
1:E:404:ILE:O	1:E:405:ILE:C	2.49	0.56
1:F:602:THR:HG21	1:F:604:VAL:HG22	1.86	0.56
1:A:294:ASP:HA	1:A:297:VAL:HG23	1.88	0.56
1:A:557:ALA:HB3	1:A:566:ILE:HD11	1.88	0.56
1:C:352:LEU:HD22	1:C:489:ILE:HD11	1.86	0.56
1:E:294:ASP:HA	1:E:297:VAL:HG23	1.88	0.56
1:F:267:GLU:HA	1:F:270:LEU:CG	2.36	0.56
1:F:602:THR:CG2	1:F:604:VAL:HG22	2.36	0.56
1:B:700:GLY:O	1:B:732:ILE:HA	2.06	0.56
1:C:439:LEU:O	1:C:441:VAL:N	2.39	0.56
1:F:250:GLN:HA	1:F:253:THR:OG1	2.04	0.56
1:A:350:LEU:HD12	1:A:350:LEU:N	2.11	0.56
1:D:380:LEU:HB2	1:D:422:GLU:O	2.05	0.56
1:E:247:GLY:C	1:E:249:VAL:H	2.14	0.56
1:E:274:ASN:C	1:E:276:TYR:N	2.64	0.56
1:E:316:ARG:HD2	1:E:316:ARG:N	2.21	0.56
1:E:579:LYS:HE2	1:E:579:LYS:O	2.06	0.56
1:F:560:ALA:O	1:F:562:GLU:HG3	2.05	0.56
1:A:250:GLN:HA	1:A:253:THR:OG1	2.05	0.56
1:D:404:ILE:O	1:D:405:ILE:C	2.49	0.56
1:F:406:GLN:O	1:F:407:GLY:C	2.49	0.56
1:F:506:LEU:HD12	1:F:506:LEU:C	2.30	0.56
1:A:328:VAL:O	1:A:332:ILE:HG12	2.05	0.55
1:A:336:LEU:O	1:A:339:GLN:N	2.39	0.55
1:B:756:ILE:HG13	1:B:767:HIS:CD2	2.41	0.55
1:C:290:ARG:O	1:C:293:ILE:HG22	2.06	0.55
1:C:747:GLU:CD	1:C:747:GLU:H	2.13	0.55
1:D:316:ARG:HD2	1:D:316:ARG:N	2.20	0.55
1:E:267:GLU:HA	1:E:270:LEU:CG	2.37	0.55
1:F:267:GLU:HA	1:F:270:LEU:CD1	2.36	0.55
1:B:247:GLY:C	1:B:249:VAL:H	2.14	0.55
1:D:328:VAL:O	1:D:332:ILE:HG12	2.05	0.55
1:F:593:VAL:HG13	1:F:693:ARG:O	2.06	0.55
1:A:756:ILE:HG13	1:A:767:HIS:CD2	2.42	0.55
1:B:420:LEU:HD21	1:B:466:PHE:HD2	1.71	0.55
1:D:534:TYR:N	1:D:534:TYR:CD1	2.74	0.55
1:D:550:ILE:O	1:D:551:CYS:C	2.47	0.55
1:B:579:LYS:HE2	1:B:579:LYS:O	2.05	0.55
2:B:783:ADP:O2A	2:B:783:ADP:O4'	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:579:LYS:O	1:D:579:LYS:HE2	2.05	0.55
1:D:613:VAL:HA	1:D:663:HIS:O	2.05	0.55
1:A:469:THR:HG22	1:A:470:ALA:N	2.21	0.55
1:B:317:LEU:HD23	1:B:317:LEU:C	2.32	0.55
1:C:316:ARG:HD2	1:C:316:ARG:N	2.20	0.55
1:C:548:ALA:O	1:C:549:ALA:C	2.46	0.55
1:D:350:LEU:HD12	1:D:350:LEU:N	2.14	0.55
1:D:439:LEU:O	1:D:441:VAL:N	2.39	0.55
1:A:357:GLY:N	2:A:783:ADP:O2B	2.26	0.55
1:B:516:LYS:HA	1:B:516:LYS:CE	2.36	0.55
1:C:274:ASN:C	1:C:276:TYR:N	2.65	0.55
1:C:414:LEU:C	1:C:416:PRO:HD3	2.31	0.55
1:A:267:GLU:HA	1:A:270:LEU:CD1	2.36	0.55
1:D:290:ARG:O	1:D:293:ILE:HG22	2.06	0.55
1:D:406:GLN:O	1:D:407:GLY:C	2.50	0.55
1:E:290:ARG:O	1:E:293:ILE:HG22	2.06	0.55
1:F:317:LEU:O	1:F:317:LEU:HD23	2.07	0.55
1:F:596:VAL:HG23	1:F:685:ALA:HB2	1.87	0.55
1:A:380:LEU:HB2	1:A:422:GLU:O	2.06	0.55
1:B:355:PRO:O	1:B:358:VAL:HG22	2.07	0.55
1:C:613:VAL:HA	1:C:663:HIS:O	2.07	0.55
1:D:313:GLU:O	1:D:314:ALA:C	2.50	0.55
1:D:336:LEU:O	1:D:339:GLN:N	2.39	0.55
1:D:635:SER:O	1:D:638:ALA:HB3	2.07	0.55
1:E:624:LEU:H	1:E:624:LEU:HD12	1.72	0.55
2:A:783:ADP:O4'	2:A:783:ADP:O2A	2.24	0.55
1:C:378:ILE:HD13	1:C:420:LEU:CD1	2.37	0.55
1:F:316:ARG:HD2	1:F:316:ARG:N	2.21	0.55
1:F:349:ILE:HD12	1:F:349:ILE:O	2.06	0.55
1:F:404:ILE:O	1:F:405:ILE:C	2.50	0.55
1:F:734:ALA:HB1	1:F:735:PRO:HD2	1.88	0.55
1:B:599:LEU:HD22	1:B:599:LEU:H	1.71	0.54
1:C:313:GLU:O	1:C:314:ALA:C	2.50	0.54
1:C:317:LEU:HD23	1:C:317:LEU:C	2.31	0.54
1:D:461:LEU:O	1:D:464:VAL:HG23	2.07	0.54
1:E:756:ILE:HG13	1:E:767:HIS:CD2	2.42	0.54
1:B:328:VAL:O	1:B:332:ILE:HG12	2.07	0.54
1:C:270:LEU:HD21	1:C:296:LEU:CD2	2.37	0.54
1:D:573:LEU:HG	1:D:577:ILE:HD11	1.88	0.54
1:E:378:ILE:HD13	1:E:420:LEU:CD1	2.37	0.54
1:E:380:LEU:HD12	1:E:423:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLU:O	1:A:314:ALA:C	2.49	0.54
1:C:247:GLY:C	1:C:249:VAL:H	2.15	0.54
1:D:602:THR:CG2	1:D:604:VAL:HG22	2.38	0.54
1:D:700:GLY:O	1:D:732:ILE:HA	2.08	0.54
1:F:557:ALA:HB3	1:F:566:ILE:HD11	1.89	0.54
1:F:569:THR:CG2	1:F:572:ASN:H	2.20	0.54
1:C:277:GLU:C	1:C:279:ILE:N	2.63	0.54
1:C:560:ALA:O	1:C:562:GLU:HG3	2.07	0.54
1:D:362:SER:HB3	2:D:783:ADP:H5'1	1.89	0.54
1:D:516:LYS:O	1:D:519:ASN:HB2	2.07	0.54
1:E:360:LYS:HD2	1:E:469:THR:HG23	1.89	0.54
1:A:273:LEU:HD13	1:A:289:ILE:HD12	1.90	0.54
1:B:282:SER:HA	1:B:286:SER:HB3	1.89	0.54
1:B:408:MET:HE2	1:B:408:MET:N	2.23	0.54
1:B:708:ARG:HD3	1:F:613:VAL:O	2.07	0.54
1:D:247:GLY:C	1:D:249:VAL:H	2.15	0.54
1:D:267:GLU:HA	1:D:270:LEU:CD1	2.37	0.54
1:D:579:LYS:H	1:D:579:LYS:NZ	2.05	0.54
1:D:739:GLU:C	1:D:741:ASP:H	2.15	0.54
1:E:282:SER:HA	1:E:286:SER:HB3	1.90	0.54
1:F:290:ARG:O	1:F:293:ILE:HG22	2.07	0.54
1:F:522:LEU:HB3	1:F:568:VAL:CG1	2.36	0.54
1:A:700:GLY:O	1:A:732:ILE:HA	2.07	0.54
1:B:550:ILE:O	1:B:551:CYS:C	2.49	0.54
1:C:420:LEU:HD21	1:C:466:PHE:CD2	2.41	0.54
1:C:536:ARG:CG	1:C:536:ARG:NH1	2.62	0.54
1:D:294:ASP:HA	1:D:297:VAL:HG23	1.90	0.54
1:F:455:ILE:O	1:F:456:GLU:C	2.51	0.54
1:C:569:THR:CG2	1:C:572:ASN:H	2.21	0.54
1:D:516:LYS:HA	1:D:516:LYS:CE	2.37	0.54
1:F:548:ALA:O	1:F:549:ALA:C	2.51	0.54
1:A:583:ARG:NH1	1:D:737:ASP:HB3	2.22	0.54
1:A:613:VAL:HA	1:A:663:HIS:O	2.08	0.54
1:B:347:GLY:CA	1:B:444:PRO:HG3	2.38	0.54
1:B:350:LEU:HD12	1:B:350:LEU:N	2.10	0.54
1:E:267:GLU:HA	1:E:270:LEU:CD1	2.38	0.54
1:B:469:THR:HG22	1:B:470:ALA:N	2.23	0.54
1:C:282:SER:HA	1:C:286:SER:HB3	1.90	0.54
1:E:424:ASP:N	1:E:424:ASP:OD1	2.41	0.54
1:C:338:VAL:HG21	1:E:552:ARG:HG3	1.90	0.53
1:D:317:LEU:C	1:D:317:LEU:HD23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:PRO:HD2	1:D:464:VAL:HG13	1.89	0.53
1:D:536:ARG:HG3	1:D:536:ARG:NH1	2.16	0.53
1:D:599:LEU:HD22	1:D:599:LEU:H	1.73	0.53
1:E:332:ILE:HD12	1:E:367:ILE:HD11	1.89	0.53
1:E:560:ALA:O	1:E:562:GLU:HG3	2.08	0.53
1:F:510:ILE:HG22	1:F:515:LEU:O	2.08	0.53
1:A:540:VAL:CG2	2:A:783:ADP:C8	2.90	0.53
1:B:277:GLU:C	1:B:279:ILE:N	2.62	0.53
1:E:506:LEU:CD2	1:E:522:LEU:HD21	2.37	0.53
1:F:516:LYS:HA	1:F:516:LYS:HE2	1.90	0.53
1:A:282:SER:HA	1:A:286:SER:HB3	1.90	0.53
1:C:700:GLY:O	1:C:732:ILE:HA	2.07	0.53
1:D:277:GLU:C	1:D:279:ILE:N	2.63	0.53
1:E:492:TYR:OH	2:E:783:ADP:N6	2.41	0.53
1:C:368:ALA:HB2	1:C:417:VAL:HG21	1.90	0.53
1:C:506:LEU:O	1:C:507:PRO:C	2.49	0.53
1:C:599:LEU:HD22	1:C:599:LEU:N	2.23	0.53
1:C:644:ARG:NE	1:C:657:HIS:CG	2.77	0.53
1:D:590:GLU:HA	1:D:697:ARG:CD	2.38	0.53
1:E:455:ILE:O	1:E:456:GLU:C	2.51	0.53
1:A:705:ILE:HD11	1:A:761:LEU:HD21	1.91	0.53
1:B:300:PRO:HB2	1:B:414:LEU:HB3	1.90	0.53
1:B:305:THR:HB	1:B:415:ASN:HD22	1.74	0.53
1:D:329:LYS:C	1:D:331:ARG:N	2.63	0.53
1:D:536:ARG:CG	1:D:536:ARG:NH1	2.64	0.53
1:E:461:LEU:O	1:E:464:VAL:HG23	2.09	0.53
1:E:534:TYR:N	1:E:534:TYR:CD1	2.77	0.53
1:F:362:SER:HB2	2:F:783:ADP:H5'1	1.89	0.53
1:A:247:GLY:C	1:A:249:VAL:H	2.14	0.53
1:A:347:GLY:CA	1:A:444:PRO:HG3	2.39	0.53
1:C:550:ILE:O	1:C:551:CYS:C	2.51	0.53
1:D:317:LEU:HD23	1:D:317:LEU:O	2.09	0.53
1:E:602:THR:C	1:E:604:VAL:H	2.16	0.53
1:F:347:GLY:CA	1:F:444:PRO:HG3	2.37	0.53
1:A:304:GLU:O	1:A:305:THR:C	2.50	0.53
1:A:408:MET:HE2	1:A:408:MET:N	2.22	0.53
1:B:557:ALA:HB3	1:B:566:ILE:HD11	1.90	0.53
1:E:611:ILE:HD12	1:E:681:THR:CG2	2.39	0.53
1:F:644:ARG:NE	1:F:657:HIS:CG	2.77	0.53
1:A:380:LEU:HD12	1:A:423:ILE:HG23	1.91	0.53
1:B:380:LEU:HB2	1:B:422:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ILE:O	1:C:405:ILE:C	2.51	0.53
1:D:533:TYR:HB3	1:D:580:ARG:HD2	1.91	0.53
1:E:307:ASP:HB3	1:E:309:LEU:HD21	1.91	0.53
1:E:569:THR:CG2	1:E:572:ASN:H	2.22	0.53
1:F:331:ARG:HH22	1:F:485:GLU:CD	2.17	0.53
1:A:277:GLU:C	1:A:279:ILE:N	2.63	0.53
1:A:329:LYS:C	1:A:331:ARG:N	2.65	0.53
1:B:656:PHE:C	1:B:658:GLU:H	2.16	0.53
1:E:599:LEU:HD22	1:E:599:LEU:H	1.74	0.53
1:E:636:ALA:C	1:E:638:ALA:H	2.17	0.53
1:F:439:LEU:O	1:F:441:VAL:N	2.41	0.53
1:A:635:SER:O	1:A:638:ALA:HB3	2.09	0.53
1:B:276:TYR:CE2	1:F:246:THR:HG21	2.43	0.53
1:B:404:ILE:HG23	1:B:418:PHE:HE2	1.73	0.53
1:B:406:GLN:O	1:B:407:GLY:C	2.51	0.53
1:D:656:PHE:C	1:D:658:GLU:H	2.16	0.53
1:E:328:VAL:O	1:E:332:ILE:HG12	2.09	0.53
1:E:406:GLN:O	1:E:407:GLY:C	2.51	0.53
1:F:334:GLU:O	1:F:338:VAL:HB	2.09	0.53
1:B:644:ARG:NE	1:B:657:HIS:CG	2.77	0.52
1:B:671:VAL:CG2	1:B:672:PRO:HD2	2.37	0.52
1:E:506:LEU:HD21	1:E:522:LEU:CD2	2.38	0.52
1:E:593:VAL:HG13	1:E:693:ARG:O	2.08	0.52
1:F:506:LEU:HD21	1:F:522:LEU:CD2	2.37	0.52
1:B:739:GLU:C	1:B:741:ASP:H	2.17	0.52
1:C:313:GLU:O	1:C:315:GLY:N	2.43	0.52
1:D:497:LYS:HG2	1:D:540:VAL:HG12	1.91	0.52
1:D:734:ALA:HB1	1:D:735:PRO:HD2	1.91	0.52
1:F:274:ASN:C	1:F:276:TYR:N	2.64	0.52
1:F:282:SER:HA	1:F:286:SER:HB3	1.90	0.52
1:F:739:GLU:C	1:F:741:ASP:H	2.17	0.52
1:A:313:GLU:O	1:A:315:GLY:N	2.42	0.52
1:E:277:GLU:C	1:E:279:ILE:N	2.64	0.52
1:E:536:ARG:CG	1:E:536:ARG:NH1	2.64	0.52
1:A:644:ARG:HB3	1:C:616:SER:HB2	1.92	0.52
1:B:336:LEU:HA	1:B:339:GLN:HB3	1.92	0.52
1:E:469:THR:HG22	1:E:470:ALA:N	2.25	0.52
1:F:277:GLU:C	1:F:279:ILE:N	2.63	0.52
1:A:317:LEU:HD23	1:A:317:LEU:C	2.34	0.52
1:B:359:GLY:O	1:B:360:LYS:C	2.52	0.52
1:D:529:ASP:O	1:D:530:ILE:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:LEU:CD2	1:E:544:GLU:HG3	2.37	0.52
1:E:739:GLU:C	1:E:741:ASP:H	2.17	0.52
1:A:644:ARG:NE	1:A:657:HIS:CG	2.77	0.52
1:B:461:LEU:O	1:B:464:VAL:HG23	2.10	0.52
1:B:635:SER:O	1:B:638:ALA:HB3	2.10	0.52
1:C:347:GLY:CA	1:C:444:PRO:HG3	2.40	0.52
1:E:336:LEU:O	1:E:339:GLN:N	2.43	0.52
1:E:414:LEU:C	1:E:416:PRO:HD3	2.33	0.52
1:B:313:GLU:O	1:B:314:ALA:C	2.52	0.52
1:F:378:ILE:HD13	1:F:420:LEU:CD1	2.39	0.52
1:F:448:SER:O	1:F:460:ASP:HA	2.08	0.52
1:F:469:THR:HG22	1:F:470:ALA:N	2.24	0.52
1:A:290:ARG:O	1:A:293:ILE:HG22	2.10	0.52
1:A:469:THR:O	1:A:470:ALA:HB2	2.09	0.52
1:B:448:SER:O	1:B:460:ASP:HA	2.10	0.52
1:D:378:ILE:HD13	1:D:420:LEU:CD1	2.40	0.52
1:E:364:ALA:O	1:E:365:LYS:C	2.53	0.52
1:E:602:THR:C	1:E:604:VAL:N	2.67	0.52
1:F:313:GLU:O	1:F:314:ALA:C	2.53	0.52
1:C:328:VAL:O	1:C:332:ILE:HG12	2.10	0.52
1:E:313:GLU:O	1:E:314:ALA:C	2.51	0.52
1:E:516:LYS:HA	1:E:516:LYS:CE	2.40	0.52
1:E:656:PHE:C	1:E:658:GLU:H	2.17	0.52
1:D:347:GLY:CA	1:D:444:PRO:HG3	2.38	0.52
1:D:569:THR:CG2	1:D:572:ASN:H	2.22	0.52
1:E:496:GLU:O	1:E:500:ILE:HG13	2.10	0.52
1:F:599:LEU:H	1:F:599:LEU:HD22	1.75	0.52
1:F:611:ILE:HD12	1:F:681:THR:CG2	2.39	0.52
1:F:686:LEU:O	1:F:686:LEU:HD22	2.10	0.52
1:F:714:ILE:HB	1:F:735:PRO:HG2	1.91	0.52
1:A:656:PHE:C	1:A:658:GLU:H	2.17	0.51
1:B:331:ARG:HH22	1:B:485:GLU:CD	2.17	0.51
1:B:455:ILE:O	1:B:456:GLU:C	2.53	0.51
1:B:569:THR:HG22	1:B:572:ASN:OD1	2.10	0.51
1:B:706:THR:OG1	1:B:710:ARG:HB2	2.10	0.51
1:C:506:LEU:HB3	1:C:507:PRO:CD	2.40	0.51
1:C:522:LEU:HB3	1:C:568:VAL:CG1	2.36	0.51
1:D:414:LEU:C	1:D:416:PRO:HD3	2.35	0.51
1:D:455:ILE:O	1:D:456:GLU:C	2.54	0.51
1:D:557:ALA:HB3	1:D:566:ILE:HD11	1.92	0.51
1:D:613:VAL:HG23	1:D:685:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:LEU:HD23	1:E:317:LEU:C	2.34	0.51
1:F:656:PHE:C	1:F:658:GLU:H	2.17	0.51
1:A:572:ASN:O	1:A:573:LEU:C	2.53	0.51
1:A:602:THR:HG21	1:A:604:VAL:HG22	1.90	0.51
1:A:624:LEU:H	1:A:624:LEU:HD12	1.74	0.51
1:B:599:LEU:HD21	1:B:700:GLY:C	2.35	0.51
1:D:522:LEU:HB3	1:D:568:VAL:CG1	2.39	0.51
1:E:329:LYS:C	1:E:331:ARG:N	2.68	0.51
1:F:329:LYS:C	1:F:331:ARG:N	2.67	0.51
1:A:308:LYS:O	1:A:309:LEU:HD23	2.11	0.51
1:A:516:LYS:HA	1:A:516:LYS:CE	2.41	0.51
1:A:714:ILE:HG23	1:A:715:GLY:N	2.24	0.51
1:B:506:LEU:HD12	1:B:506:LEU:O	2.10	0.51
1:C:329:LYS:C	1:C:331:ARG:N	2.64	0.51
1:E:273:LEU:HD13	1:E:289:ILE:HD12	1.92	0.51
1:F:362:SER:HB2	2:F:783:ADP:C5'	2.40	0.51
1:A:331:ARG:HH22	1:A:485:GLU:CD	2.18	0.51
1:A:569:THR:CG2	1:A:572:ASN:H	2.22	0.51
1:B:624:LEU:H	1:B:624:LEU:HD12	1.75	0.51
1:D:282:SER:HA	1:D:286:SER:HB3	1.91	0.51
1:B:380:LEU:HD12	1:B:423:ILE:CG2	2.40	0.51
1:C:334:GLU:O	1:C:338:VAL:HB	2.11	0.51
1:C:624:LEU:HD12	1:C:624:LEU:H	1.76	0.51
1:D:273:LEU:HD13	1:D:289:ILE:HD12	1.92	0.51
1:E:331:ARG:HH22	1:E:485:GLU:CD	2.17	0.51
1:F:533:TYR:HB3	1:F:580:ARG:HD2	1.92	0.51
1:F:569:THR:HG22	1:F:572:ASN:OD1	2.11	0.51
1:A:409:LYS:C	1:A:411:ALA:H	2.17	0.51
1:A:448:SER:O	1:A:460:ASP:HA	2.11	0.51
1:A:462:SER:HB2	1:A:463:LYS:HD2	1.93	0.51
1:A:533:TYR:HB3	1:A:580:ARG:HD2	1.92	0.51
1:C:331:ARG:HH22	1:C:485:GLU:CD	2.18	0.51
1:C:448:SER:O	1:C:460:ASP:HA	2.11	0.51
1:D:308:LYS:O	1:D:309:LEU:HD23	2.11	0.51
1:D:420:LEU:HD21	1:D:466:PHE:CD2	2.46	0.51
1:E:262:PRO:CD	1:E:301:TRP:HB2	2.40	0.51
1:F:273:LEU:HD13	1:F:289:ILE:HD12	1.93	0.51
1:A:322:HIS:CE1	1:A:363:LEU:HD23	2.46	0.51
1:A:438:MET:O	1:A:440:GLU:N	2.44	0.51
1:E:569:THR:HG22	1:E:572:ASN:OD1	2.11	0.51
1:A:286:SER:O	1:A:290:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD23	1:A:487:ILE:HD11	1.92	0.51
1:B:305:THR:HB	1:B:415:ASN:ND2	2.25	0.51
1:C:308:LYS:O	1:C:309:LEU:HD23	2.11	0.51
1:C:404:ILE:HG23	1:C:418:PHE:HE2	1.71	0.51
1:D:300:PRO:O	1:D:301:TRP:CD2	2.64	0.51
1:D:331:ARG:HH22	1:D:485:GLU:CD	2.18	0.51
1:D:438:MET:O	1:D:440:GLU:N	2.44	0.51
2:D:783:ADP:O2A	2:D:783:ADP:C4'	2.59	0.51
1:E:420:LEU:HD21	1:E:466:PHE:CD2	2.45	0.51
1:E:584:TYR:O	1:E:584:TYR:HD1	1.91	0.51
1:A:599:LEU:HD22	1:A:599:LEU:H	1.76	0.51
1:B:368:ALA:HB2	1:B:417:VAL:HG21	1.92	0.51
1:B:506:LEU:HD21	1:B:522:LEU:CD2	2.40	0.51
1:C:656:PHE:C	1:C:658:GLU:N	2.68	0.51
1:D:644:ARG:NE	1:D:657:HIS:CG	2.78	0.51
1:E:347:GLY:CA	1:E:444:PRO:HG3	2.40	0.51
1:E:602:THR:HG22	1:E:603:THR:N	2.26	0.51
1:F:438:MET:O	1:F:440:GLU:N	2.44	0.51
1:F:497:LYS:HG2	1:F:540:VAL:HG12	1.92	0.51
1:A:311:LEU:O	1:A:312:LYS:C	2.54	0.51
1:A:334:GLU:O	1:A:338:VAL:HB	2.11	0.51
1:B:273:LEU:HD13	1:B:289:ILE:HD12	1.93	0.51
1:B:286:SER:O	1:B:290:ARG:HB2	2.11	0.51
1:C:336:LEU:HA	1:C:339:GLN:HB3	1.93	0.51
1:C:337:ALA:HB3	1:E:556:LYS:HA	1.92	0.51
1:D:611:ILE:HD12	1:D:681:THR:CG2	2.41	0.51
1:E:644:ARG:NE	1:E:657:HIS:CG	2.78	0.51
1:F:409:LYS:C	1:F:411:ALA:H	2.18	0.51
1:F:586:GLN:NE2	1:F:698:GLU:HA	2.16	0.51
1:F:624:LEU:HD12	1:F:624:LEU:H	1.75	0.51
1:F:700:GLY:O	1:F:732:ILE:HA	2.10	0.51
1:F:705:ILE:HD11	1:F:761:LEU:HD21	1.92	0.51
1:B:274:ASN:O	1:B:276:TYR:N	2.43	0.50
1:B:329:LYS:C	1:B:331:ARG:N	2.66	0.50
1:B:506:LEU:CD2	1:B:522:LEU:HD21	2.38	0.50
1:E:557:ALA:HB3	1:E:566:ILE:HD11	1.93	0.50
1:F:423:ILE:HD12	1:F:484:MET:HE1	1.92	0.50
1:B:322:HIS:CE1	1:B:363:LEU:HD23	2.46	0.50
1:B:621:LYS:O	1:B:661:ASP:OD1	2.29	0.50
1:D:313:GLU:O	1:D:315:GLY:N	2.44	0.50
1:D:448:SER:O	1:D:460:ASP:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:ARG:HG2	1:D:584:TYR:CD2	2.46	0.50
1:D:536:ARG:HH11	1:D:536:ARG:CB	2.25	0.50
1:E:573:LEU:HG	1:E:577:ILE:HD11	1.93	0.50
1:C:736:LYS:C	1:C:738:ASN:H	2.17	0.50
1:D:656:PHE:C	1:D:658:GLU:N	2.70	0.50
1:F:549:ALA:HA	1:F:552:ARG:NH2	2.26	0.50
1:C:536:ARG:HH11	1:C:536:ARG:CB	2.24	0.50
1:D:496:GLU:O	1:D:497:LYS:C	2.55	0.50
1:D:589:THR:O	1:D:697:ARG:HD2	2.12	0.50
1:D:624:LEU:H	1:D:624:LEU:HD12	1.76	0.50
1:F:286:SER:O	1:F:290:ARG:HB2	2.12	0.50
1:F:636:ALA:C	1:F:638:ALA:H	2.19	0.50
1:B:274:ASN:C	1:B:276:TYR:N	2.62	0.50
1:B:299:LEU:HD12	1:B:299:LEU:O	2.11	0.50
1:B:311:LEU:O	1:B:312:LYS:C	2.54	0.50
1:C:300:PRO:HG3	1:C:412:GLY:HA2	1.94	0.50
1:C:455:ILE:O	1:C:456:GLU:C	2.54	0.50
1:D:462:SER:HB2	1:D:463:LYS:HD2	1.94	0.50
1:D:686:LEU:O	1:D:686:LEU:HD22	2.11	0.50
1:D:747:GLU:H	1:D:747:GLU:CD	2.18	0.50
1:E:448:SER:O	1:E:460:ASP:HA	2.12	0.50
1:F:546:GLN:OE1	1:F:577:ILE:HB	2.11	0.50
1:A:329:LYS:O	1:A:331:ARG:N	2.44	0.50
1:A:637:GLN:HG2	1:A:637:GLN:O	2.11	0.50
1:B:438:MET:O	1:B:440:GLU:N	2.45	0.50
1:C:439:LEU:H	1:C:439:LEU:CD2	2.20	0.50
1:A:455:ILE:O	1:A:456:GLU:C	2.53	0.50
1:A:534:TYR:N	1:A:534:TYR:CD1	2.80	0.50
1:D:593:VAL:HG13	1:D:693:ARG:O	2.12	0.50
1:E:438:MET:O	1:E:440:GLU:N	2.43	0.50
1:A:424:ASP:HB2	1:A:475:THR:CG2	2.42	0.50
1:A:562:GLU:O	1:A:563:ARG:C	2.55	0.50
1:B:334:GLU:O	1:B:338:VAL:HB	2.11	0.50
1:C:350:LEU:HD23	1:C:487:ILE:HD11	1.93	0.50
1:E:733:ILE:HA	1:E:756:ILE:O	2.12	0.50
1:A:579:LYS:HE2	1:A:579:LYS:C	2.37	0.50
1:A:602:THR:CG2	1:A:604:VAL:HG22	2.42	0.50
1:C:424:ASP:HB2	1:C:475:THR:CG2	2.42	0.50
1:C:461:LEU:O	1:C:464:VAL:HG23	2.11	0.50
1:D:714:ILE:HG23	1:D:715:GLY:N	2.25	0.50
1:E:311:LEU:O	1:E:312:LYS:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:THR:O	1:E:470:ALA:HB2	2.11	0.50
1:F:414:LEU:C	1:F:416:PRO:HD3	2.37	0.50
1:F:424:ASP:HB2	1:F:475:THR:CG2	2.42	0.50
1:A:732:ILE:HG21	1:A:753:LEU:HD13	1.94	0.49
1:B:364:ALA:O	1:B:365:LYS:C	2.55	0.49
1:C:362:SER:CB	2:C:783:ADP:H5'	2.41	0.49
1:C:438:MET:O	1:C:440:GLU:N	2.45	0.49
1:C:593:VAL:O	1:C:595:VAL:HG23	2.11	0.49
1:D:506:LEU:O	1:D:507:PRO:C	2.55	0.49
1:E:439:LEU:H	1:E:439:LEU:CD2	2.19	0.49
1:B:596:VAL:HG23	1:B:685:ALA:HB2	1.93	0.49
1:B:687:VAL:O	1:B:691:THR:HG23	2.12	0.49
1:C:439:LEU:O	1:C:440:GLU:C	2.55	0.49
1:C:702:THR:O	1:C:702:THR:CG2	2.60	0.49
1:D:569:THR:HG23	1:D:572:ASN:H	1.78	0.49
1:E:409:LYS:C	1:E:411:ALA:H	2.19	0.49
1:F:336:LEU:O	1:F:339:GLN:N	2.45	0.49
1:F:412:GLY:C	1:F:413:LYS:HG2	2.37	0.49
1:B:462:SER:HB2	1:B:463:LYS:HD2	1.95	0.49
1:D:424:ASP:HB2	1:D:475:THR:CG2	2.41	0.49
1:E:313:GLU:O	1:E:315:GLY:N	2.44	0.49
1:E:359:GLY:HA2	2:E:783:ADP:C5'	2.42	0.49
1:E:407:GLY:HA3	1:E:418:PHE:CZ	2.47	0.49
1:A:520:LEU:HA	1:A:566:ILE:O	2.12	0.49
1:B:299:LEU:HD13	1:B:301:TRP:CZ2	2.47	0.49
1:F:404:ILE:HG23	1:F:418:PHE:HE2	1.70	0.49
1:A:686:LEU:O	1:A:686:LEU:HD22	2.12	0.49
1:C:506:LEU:HD12	1:C:506:LEU:O	2.13	0.49
1:D:359:GLY:CA	2:D:783:ADP:O5'	2.58	0.49
1:D:439:LEU:O	1:D:440:GLU:C	2.55	0.49
1:E:255:LYS:NZ	1:E:255:LYS:HB3	2.28	0.49
1:F:404:ILE:HG22	1:F:408:MET:HE1	1.94	0.49
1:A:464:VAL:O	1:A:466:PHE:CD1	2.63	0.49
1:A:493:THR:O	1:A:494:GLU:C	2.54	0.49
1:B:414:LEU:C	1:B:414:LEU:HD12	2.37	0.49
1:D:602:THR:C	1:D:604:VAL:N	2.71	0.49
1:D:637:GLN:HG2	1:D:637:GLN:O	2.11	0.49
1:D:742:ILE:O	1:D:742:ILE:HG22	2.13	0.49
1:E:637:GLN:O	1:E:637:GLN:HG2	2.12	0.49
1:A:506:LEU:HD21	1:A:522:LEU:CD2	2.42	0.49
1:A:550:ILE:O	1:A:551:CYS:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:LYS:C	1:A:738:ASN:H	2.20	0.49
1:B:313:GLU:O	1:B:315:GLY:N	2.46	0.49
1:D:364:ALA:O	1:D:365:LYS:C	2.56	0.49
1:F:308:LYS:O	1:F:309:LEU:HD23	2.12	0.49
1:A:404:ILE:HG23	1:A:418:PHE:HE2	1.72	0.49
1:A:596:VAL:HG23	1:A:685:ALA:HB2	1.94	0.49
1:A:734:ALA:HB1	1:A:735:PRO:CD	2.42	0.49
1:B:378:ILE:HD13	1:B:420:LEU:CD1	2.43	0.49
1:B:533:TYR:HB3	1:B:580:ARG:HD2	1.94	0.49
1:B:602:THR:HG21	1:B:604:VAL:HG22	1.94	0.49
1:D:286:SER:O	1:D:290:ARG:HB2	2.12	0.49
1:E:286:SER:O	1:E:290:ARG:HB2	2.13	0.49
1:E:734:ALA:HB1	1:E:735:PRO:CD	2.42	0.49
1:C:602:THR:C	1:C:604:VAL:N	2.70	0.49
1:E:736:LYS:C	1:E:738:ASN:H	2.19	0.49
1:F:246:THR:HG23	1:F:250:GLN:NE2	2.28	0.49
1:F:255:LYS:HB3	1:F:255:LYS:NZ	2.28	0.49
1:A:407:GLY:HA3	1:A:418:PHE:CZ	2.48	0.49
1:A:656:PHE:C	1:A:658:GLU:N	2.71	0.49
1:A:708:ARG:NH2	1:C:593:VAL:HB	2.27	0.49
1:B:496:GLU:O	1:B:497:LYS:C	2.54	0.49
1:B:562:GLU:O	1:B:563:ARG:C	2.56	0.49
1:C:298:ALA:O	1:C:299:LEU:C	2.55	0.49
1:C:584:TYR:HD1	1:C:584:TYR:O	1.95	0.49
1:D:705:ILE:HD11	1:D:761:LEU:HD21	1.94	0.49
1:E:562:GLU:O	1:E:563:ARG:C	2.56	0.49
1:A:548:ALA:O	1:A:549:ALA:C	2.54	0.48
1:B:439:LEU:O	1:B:440:GLU:C	2.55	0.48
1:B:573:LEU:HG	1:B:577:ILE:HD11	1.95	0.48
1:F:317:LEU:HD23	1:F:317:LEU:C	2.38	0.48
1:A:336:LEU:HA	1:A:339:GLN:HB3	1.95	0.48
1:B:705:ILE:HD11	1:B:761:LEU:HD21	1.95	0.48
1:C:409:LYS:C	1:C:411:ALA:H	2.21	0.48
1:C:423:ILE:HD12	1:C:484:MET:HE1	1.93	0.48
1:C:756:ILE:HG13	1:C:767:HIS:CD2	2.48	0.48
1:D:255:LYS:NZ	1:D:255:LYS:HB3	2.28	0.48
1:D:423:ILE:CD1	1:D:484:MET:HE1	2.43	0.48
1:F:551:CYS:O	1:F:554:ALA:HB3	2.13	0.48
1:A:298:ALA:O	1:A:299:LEU:C	2.54	0.48
1:B:444:PRO:HA	1:B:447:ASN:ND2	2.28	0.48
1:B:714:ILE:HB	1:B:735:PRO:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:VAL:HG13	1:C:547:LEU:HD11	1.95	0.48
1:C:635:SER:O	1:C:638:ALA:HB3	2.13	0.48
1:D:506:LEU:HD12	1:D:506:LEU:C	2.38	0.48
1:D:656:PHE:CE2	1:D:690:LEU:HD11	2.48	0.48
1:E:262:PRO:HG3	1:E:302:THR:OG1	2.13	0.48
1:E:602:THR:HG21	1:E:604:VAL:HG22	1.95	0.48
1:A:439:LEU:O	1:A:440:GLU:C	2.55	0.48
1:A:602:THR:C	1:A:604:VAL:H	2.21	0.48
1:C:536:ARG:HG3	1:C:536:ARG:NH1	2.16	0.48
1:F:313:GLU:O	1:F:315:GLY:N	2.47	0.48
1:F:579:LYS:HE2	1:F:579:LYS:C	2.38	0.48
1:A:506:LEU:CD2	1:A:522:LEU:HD21	2.44	0.48
1:A:599:LEU:O	1:A:720:LYS:HE2	2.13	0.48
1:B:642:TYR:CE1	1:B:709:GLY:HA3	2.48	0.48
1:B:736:LYS:C	1:B:738:ASN:H	2.20	0.48
1:C:642:TYR:CD2	1:C:761:LEU:HD12	2.49	0.48
1:E:686:LEU:O	1:E:686:LEU:HD22	2.14	0.48
1:A:349:ILE:HD12	1:A:349:ILE:O	2.14	0.48
1:A:496:GLU:O	1:A:497:LYS:C	2.56	0.48
1:A:621:LYS:O	1:A:661:ASP:OD1	2.31	0.48
1:B:350:LEU:H	1:B:350:LEU:CD1	2.10	0.48
1:C:260:GLY:O	1:C:261:MET:HE3	2.13	0.48
1:C:705:ILE:HD11	1:C:761:LEU:CD2	2.44	0.48
1:D:409:LYS:C	1:D:411:ALA:H	2.20	0.48
1:E:424:ASP:HB2	1:E:475:THR:CG2	2.42	0.48
1:F:656:PHE:CG	1:F:657:HIS:N	2.80	0.48
1:A:412:GLY:C	1:A:413:LYS:HG2	2.37	0.48
1:B:423:ILE:CD1	1:B:484:MET:HE1	2.43	0.48
1:C:462:SER:HB2	1:C:463:LYS:HD2	1.94	0.48
1:C:562:GLU:O	1:C:563:ARG:C	2.56	0.48
1:E:262:PRO:HD2	1:E:301:TRP:HB3	1.94	0.48
1:E:516:LYS:HA	1:E:516:LYS:HZ1	1.77	0.48
1:E:656:PHE:CG	1:E:657:HIS:N	2.82	0.48
1:F:407:GLY:HA3	1:F:418:PHE:CZ	2.49	0.48
1:F:756:ILE:HG13	1:F:767:HIS:CD2	2.49	0.48
1:A:739:GLU:C	1:A:741:ASP:H	2.21	0.48
1:B:296:LEU:HD23	1:B:299:LEU:HD11	1.95	0.48
1:B:536:ARG:HH11	1:B:536:ARG:CB	2.27	0.48
1:C:273:LEU:HD13	1:C:289:ILE:HD12	1.95	0.48
1:C:493:THR:O	1:C:494:GLU:C	2.57	0.48
1:C:712:LEU:HB3	1:C:713:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:LEU:O	1:E:440:GLU:C	2.57	0.48
1:E:462:SER:HB2	1:E:463:LYS:HD2	1.95	0.48
1:E:590:GLU:HA	1:E:697:ARG:HD3	1.96	0.48
1:F:547:LEU:HA	1:F:547:LEU:HD23	1.75	0.48
1:F:642:TYR:CE1	1:F:709:GLY:HA3	2.49	0.48
1:C:412:GLY:C	1:C:413:LYS:HG2	2.39	0.48
1:E:579:LYS:NZ	1:E:579:LYS:H	2.12	0.48
1:E:635:SER:O	1:E:638:ALA:HB3	2.14	0.48
1:F:336:LEU:HA	1:F:339:GLN:HB3	1.95	0.48
1:B:493:THR:O	1:B:494:GLU:C	2.57	0.48
1:B:526:ALA:O	1:B:530:ILE:HG13	2.14	0.48
1:B:552:ARG:O	1:B:553:LYS:C	2.57	0.48
1:C:286:SER:O	1:C:290:ARG:HB2	2.14	0.48
1:D:311:LEU:O	1:D:312:LYS:C	2.57	0.48
1:E:270:LEU:HD21	1:E:296:LEU:CD2	2.43	0.48
1:E:334:GLU:O	1:E:338:VAL:HB	2.14	0.48
1:E:357:GLY:H	2:E:783:ADP:PB	2.37	0.48
1:E:359:GLY:O	1:E:360:LYS:C	2.55	0.48
1:F:621:LYS:O	1:F:661:ASP:OD1	2.32	0.48
1:A:350:LEU:H	1:A:350:LEU:CD1	2.07	0.47
1:A:424:ASP:OD1	1:A:424:ASP:N	2.45	0.47
1:B:246:THR:HG23	1:B:250:GLN:NE2	2.29	0.47
1:C:656:PHE:CG	1:C:657:HIS:N	2.82	0.47
1:D:678:ALA:O	1:D:682:MET:HG2	2.14	0.47
1:F:536:ARG:HG3	1:F:536:ARG:NH1	2.21	0.47
1:F:656:PHE:C	1:F:658:GLU:N	2.71	0.47
1:F:747:GLU:CD	1:F:747:GLU:H	2.20	0.47
1:A:747:GLU:CD	1:A:747:GLU:N	2.72	0.47
1:C:255:LYS:HB3	1:C:255:LYS:NZ	2.28	0.47
1:C:329:LYS:O	1:C:331:ARG:N	2.47	0.47
1:D:336:LEU:HA	1:D:339:GLN:HB3	1.96	0.47
1:E:416:PRO:HG2	1:E:464:VAL:HG13	1.96	0.47
1:F:362:SER:CB	2:F:783:ADP:H5'2	2.44	0.47
1:F:420:LEU:HD21	1:F:466:PHE:CD2	2.47	0.47
1:F:439:LEU:O	1:F:440:GLU:C	2.57	0.47
1:F:642:TYR:CD2	1:F:761:LEU:HD12	2.49	0.47
1:B:536:ARG:HG3	1:B:536:ARG:NH1	2.18	0.47
1:C:613:VAL:HG23	1:C:685:ALA:HB1	1.95	0.47
1:C:636:ALA:O	1:C:638:ALA:N	2.45	0.47
1:C:733:ILE:HA	1:C:756:ILE:O	2.15	0.47
1:C:734:ALA:HB1	1:C:735:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LYS:C	1:D:331:ARG:H	2.22	0.47
1:D:360:LYS:HD2	1:D:469:THR:HG23	1.95	0.47
1:E:276:TYR:CD1	1:E:277:GLU:N	2.83	0.47
1:E:404:ILE:HG22	1:E:408:MET:HE1	1.96	0.47
1:F:411:ALA:O	1:F:412:GLY:C	2.57	0.47
1:A:602:THR:C	1:A:604:VAL:N	2.72	0.47
1:B:424:ASP:HB2	1:B:475:THR:CG2	2.43	0.47
1:C:534:TYR:N	1:C:534:TYR:CD1	2.81	0.47
1:C:569:THR:HG23	1:C:571:LYS:N	2.16	0.47
1:D:411:ALA:O	1:D:412:GLY:C	2.57	0.47
1:E:300:PRO:HG3	1:E:412:GLY:C	2.40	0.47
1:E:546:GLN:O	1:E:549:ALA:HB3	2.15	0.47
1:E:717:LEU:O	1:E:717:LEU:HD22	2.14	0.47
1:A:329:LYS:C	1:A:331:ARG:H	2.22	0.47
1:B:579:LYS:HE2	1:B:579:LYS:C	2.40	0.47
1:B:656:PHE:C	1:B:658:GLU:N	2.70	0.47
1:D:329:LYS:O	1:D:330:GLU:C	2.57	0.47
1:D:604:VAL:HG23	1:D:604:VAL:O	2.12	0.47
1:E:336:LEU:HA	1:E:339:GLN:HB3	1.95	0.47
1:E:550:ILE:O	1:E:551:CYS:C	2.58	0.47
1:F:546:GLN:O	1:F:549:ALA:HB3	2.14	0.47
1:A:478:GLY:N	1:A:479:PRO:HD2	2.30	0.47
1:C:407:GLY:HA3	1:C:418:PHE:CZ	2.49	0.47
1:C:423:ILE:HD11	1:C:484:MET:HE1	1.95	0.47
1:C:546:GLN:O	1:C:549:ALA:HB3	2.15	0.47
1:C:733:ILE:CD1	1:C:768:ALA:HB2	2.45	0.47
1:D:464:VAL:O	1:D:466:PHE:CD1	2.64	0.47
1:E:656:PHE:C	1:E:658:GLU:N	2.70	0.47
1:F:536:ARG:CG	1:F:536:ARG:NH1	2.67	0.47
1:F:562:GLU:O	1:F:563:ARG:C	2.58	0.47
1:F:599:LEU:HD22	1:F:599:LEU:N	2.29	0.47
1:A:246:THR:HG23	1:A:250:GLN:NE2	2.29	0.47
1:A:270:LEU:HD21	1:A:296:LEU:CD2	2.44	0.47
1:A:452:ASP:O	1:A:455:ILE:HG22	2.15	0.47
1:A:647:THR:HG22	1:A:648:GLU:N	2.30	0.47
1:B:255:LYS:NZ	1:B:255:LYS:HB3	2.30	0.47
1:C:469:THR:O	1:C:470:ALA:HB2	2.15	0.47
1:C:572:ASN:O	1:C:573:LEU:C	2.57	0.47
1:C:611:ILE:HD12	1:C:681:THR:CG2	2.45	0.47
1:D:334:GLU:O	1:D:338:VAL:HB	2.15	0.47
1:D:562:GLU:O	1:D:563:ARG:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ALA:O	1:E:299:LEU:C	2.57	0.47
1:E:308:LYS:O	1:E:309:LEU:HD23	2.14	0.47
1:E:705:ILE:HD11	1:E:761:LEU:HD21	1.96	0.47
1:E:705:ILE:HD12	1:E:705:ILE:HA	1.61	0.47
1:F:462:SER:HB2	1:F:463:LYS:HD2	1.95	0.47
1:F:493:THR:CG2	1:F:748:SER:HB2	2.20	0.47
1:F:613:VAL:HG23	1:F:685:ALA:HB1	1.97	0.47
1:F:645:SER:O	1:F:647:THR:N	2.47	0.47
1:A:423:ILE:HD11	1:A:484:MET:HE1	1.96	0.47
1:B:452:ASP:O	1:B:455:ILE:HG22	2.15	0.47
1:B:584:TYR:CE2	1:B:728:GLY:HA3	2.49	0.47
1:B:656:PHE:CG	1:B:657:HIS:N	2.83	0.47
1:C:311:LEU:O	1:C:312:LYS:C	2.56	0.47
1:C:520:LEU:HA	1:C:566:ILE:O	2.15	0.47
1:D:506:LEU:HD21	1:D:522:LEU:CD2	2.42	0.47
1:D:602:THR:C	1:D:604:VAL:H	2.23	0.47
1:F:534:TYR:CD2	1:F:577:ILE:HD12	2.50	0.47
1:A:506:LEU:HD12	1:A:506:LEU:O	2.15	0.47
1:A:656:PHE:CG	1:A:657:HIS:N	2.82	0.47
1:A:680:ILE:HG22	1:A:705:ILE:HD13	1.97	0.47
1:B:255:LYS:O	1:B:258:GLU:HB3	2.15	0.47
1:B:260:GLY:O	1:B:261:MET:CB	2.63	0.47
1:B:276:TYR:CD1	1:B:277:GLU:N	2.83	0.47
1:B:282:SER:HB2	1:E:276:TYR:HH	1.80	0.47
1:B:569:THR:CG2	1:B:572:ASN:H	2.27	0.47
1:C:712:LEU:HB3	1:C:713:PRO:HD2	1.97	0.47
1:C:747:GLU:CD	1:C:747:GLU:N	2.73	0.47
1:E:274:ASN:O	1:E:276:TYR:N	2.44	0.47
1:F:496:GLU:O	1:F:497:LYS:C	2.58	0.47
1:F:656:PHE:CE2	1:F:690:LEU:HD11	2.50	0.47
1:A:255:LYS:NZ	1:A:255:LYS:HB3	2.29	0.47
1:A:645:SER:O	1:A:647:THR:N	2.48	0.47
1:B:579:LYS:NZ	1:B:579:LYS:H	2.13	0.47
1:B:732:ILE:O	1:B:732:ILE:HD13	2.15	0.47
1:D:579:LYS:HE2	1:D:579:LYS:C	2.39	0.47
1:E:621:LYS:O	1:E:661:ASP:OD1	2.33	0.47
1:E:645:SER:O	1:E:647:THR:N	2.48	0.47
1:A:255:LYS:O	1:A:258:GLU:HB3	2.16	0.46
2:A:783:ADP:O4'	2:A:783:ADP:PA	2.71	0.46
1:B:636:ALA:O	1:B:638:ALA:N	2.46	0.46
1:C:732:ILE:HG21	1:C:753:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:PRO:O	1:D:358:VAL:HG22	2.15	0.46
1:D:444:PRO:HA	1:D:447:ASN:ND2	2.30	0.46
1:D:702:THR:O	1:D:702:THR:HG23	2.16	0.46
1:E:411:ALA:O	1:E:412:GLY:C	2.58	0.46
1:F:540:VAL:CG2	2:F:783:ADP:H1'	2.45	0.46
1:F:593:VAL:O	1:F:595:VAL:HG23	2.15	0.46
1:F:712:LEU:HB3	1:F:713:PRO:HD2	1.97	0.46
1:A:586:GLN:NE2	1:A:728:GLY:O	2.49	0.46
1:B:341:LEU:O	1:B:343:LYS:N	2.48	0.46
1:B:534:TYR:N	1:B:534:TYR:CD1	2.82	0.46
1:C:307:ASP:HB3	1:C:309:LEU:HD21	1.97	0.46
1:C:341:LEU:O	1:C:343:LYS:N	2.48	0.46
1:D:246:THR:HG23	1:D:250:GLN:NE2	2.30	0.46
1:E:341:LEU:O	1:E:343:LYS:N	2.48	0.46
1:E:404:ILE:HG23	1:E:418:PHE:HE2	1.72	0.46
1:E:412:GLY:C	1:E:413:LYS:HG2	2.39	0.46
1:F:260:GLY:O	1:F:261:MET:CB	2.63	0.46
1:F:360:LYS:CD	1:F:469:THR:HG23	2.41	0.46
1:F:496:GLU:O	1:F:500:ILE:HG13	2.14	0.46
1:A:411:ALA:O	1:A:412:GLY:C	2.58	0.46
1:B:678:ALA:O	1:B:682:MET:HG2	2.15	0.46
1:B:747:GLU:CD	1:B:747:GLU:N	2.73	0.46
1:C:380:LEU:HD12	1:C:423:ILE:CG2	2.46	0.46
1:C:444:PRO:HA	1:C:447:ASN:ND2	2.30	0.46
1:C:714:ILE:HG23	1:C:715:GLY:N	2.29	0.46
1:D:266:LYS:HG3	1:D:267:GLU:H	1.78	0.46
1:E:246:THR:HG23	1:E:250:GLN:NE2	2.30	0.46
1:E:307:ASP:O	1:E:309:LEU:HG	2.16	0.46
1:E:423:ILE:C	1:E:424:ASP:OD1	2.58	0.46
1:E:732:ILE:HG21	1:E:753:LEU:HD13	1.96	0.46
1:F:329:LYS:O	1:F:331:ARG:N	2.48	0.46
1:F:329:LYS:O	1:F:330:GLU:C	2.58	0.46
1:A:439:LEU:H	1:A:439:LEU:CD2	2.25	0.46
1:A:444:PRO:HA	1:A:447:ASN:ND2	2.28	0.46
1:A:536:ARG:HH11	1:A:536:ARG:CB	2.28	0.46
1:B:412:GLY:C	1:B:413:LYS:HG2	2.39	0.46
1:B:439:LEU:H	1:B:439:LEU:CD2	2.26	0.46
1:C:579:LYS:NZ	1:C:579:LYS:H	2.14	0.46
1:D:569:THR:HG22	1:D:572:ASN:OD1	2.15	0.46
1:D:636:ALA:O	1:D:638:ALA:N	2.40	0.46
1:A:380:LEU:HD12	1:A:423:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:TYR:CE1	1:A:709:GLY:HA3	2.50	0.46
1:B:424:ASP:N	1:B:424:ASP:OD1	2.49	0.46
1:B:637:GLN:O	1:B:637:GLN:HG2	2.15	0.46
1:C:529:ASP:O	1:C:530:ILE:C	2.58	0.46
1:D:478:GLY:N	1:D:479:PRO:HD2	2.31	0.46
1:E:260:GLY:O	1:E:261:MET:CB	2.63	0.46
1:F:352:LEU:HB3	1:F:360:LYS:HG2	1.96	0.46
1:F:637:GLN:HG2	1:F:637:GLN:O	2.16	0.46
1:F:734:ALA:HB1	1:F:735:PRO:CD	2.46	0.46
1:A:274:ASN:O	1:A:276:TYR:N	2.46	0.46
1:C:329:LYS:C	1:C:331:ARG:H	2.22	0.46
1:C:536:ARG:NH1	1:C:536:ARG:CB	2.79	0.46
1:C:596:VAL:HG23	1:C:685:ALA:HB2	1.97	0.46
1:E:368:ALA:HB2	1:E:417:VAL:HG21	1.97	0.46
1:E:478:GLY:N	1:E:479:PRO:HD2	2.30	0.46
1:F:444:PRO:HA	1:F:447:ASN:ND2	2.29	0.46
1:F:569:THR:HG23	1:F:572:ASN:H	1.79	0.46
1:A:359:GLY:O	1:A:360:LYS:C	2.59	0.46
1:A:506:LEU:O	1:A:507:PRO:C	2.58	0.46
1:A:569:THR:HG22	1:A:572:ASN:OD1	2.16	0.46
1:B:710:ARG:HH21	1:B:710:ARG:HG2	1.81	0.46
1:B:734:ALA:HB1	1:B:735:PRO:CD	2.45	0.46
2:B:783:ADP:N3	2:B:783:ADP:H2'	2.30	0.46
1:C:246:THR:HG23	1:C:250:GLN:NE2	2.30	0.46
1:C:579:LYS:HE2	1:C:579:LYS:C	2.40	0.46
1:C:645:SER:O	1:C:647:THR:N	2.49	0.46
1:E:322:HIS:CE1	1:E:363:LEU:HD23	2.51	0.46
1:E:444:PRO:HA	1:E:447:ASN:ND2	2.30	0.46
1:E:579:LYS:HE2	1:E:579:LYS:C	2.41	0.46
1:F:322:HIS:CE1	1:F:363:LEU:HD23	2.50	0.46
1:A:260:GLY:O	1:A:261:MET:CB	2.64	0.46
1:A:505:LEU:CD2	1:A:544:GLU:HG3	2.44	0.46
1:A:604:VAL:O	1:A:604:VAL:HG23	2.16	0.46
1:C:266:LYS:HG3	1:C:267:GLU:H	1.80	0.46
1:C:364:ALA:O	1:C:365:LYS:C	2.58	0.46
1:C:602:THR:C	1:C:604:VAL:H	2.22	0.46
1:D:407:GLY:HA3	1:D:418:PHE:CZ	2.50	0.46
1:D:412:GLY:C	1:D:413:LYS:HG2	2.39	0.46
1:D:656:PHE:CG	1:D:657:HIS:N	2.84	0.46
1:E:355:PRO:O	1:E:358:VAL:HG22	2.15	0.46
1:E:506:LEU:HD12	1:E:506:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:642:TYR:CE1	1:E:709:GLY:HA3	2.51	0.46
1:A:414:LEU:C	1:A:414:LEU:HD12	2.41	0.46
1:A:456:GLU:OE2	1:C:291:ASN:ND2	2.49	0.46
1:A:636:ALA:O	1:A:638:ALA:N	2.43	0.46
1:B:290:ARG:HH12	1:E:273:LEU:HD21	1.80	0.46
1:C:260:GLY:O	1:C:261:MET:CB	2.64	0.46
1:C:510:ILE:HG22	1:C:515:LEU:O	2.15	0.46
1:C:569:THR:HG22	1:C:572:ASN:OD1	2.16	0.46
1:D:329:LYS:O	1:D:331:ARG:N	2.48	0.46
1:D:350:LEU:HD23	1:D:487:ILE:HD11	1.97	0.46
1:D:367:ILE:HG22	1:D:368:ALA:N	2.28	0.46
1:D:739:GLU:C	1:D:741:ASP:N	2.73	0.46
1:E:714:ILE:HG23	1:E:715:GLY:N	2.30	0.46
1:F:534:TYR:N	1:F:534:TYR:CD1	2.84	0.46
1:F:622:LEU:HB2	1:F:662:ILE:HG12	1.98	0.46
1:F:739:GLU:C	1:F:741:ASP:N	2.74	0.46
1:A:341:LEU:O	1:A:343:LYS:N	2.49	0.46
1:A:423:ILE:HD12	1:A:484:MET:HE1	1.98	0.46
2:A:783:ADP:O1B	2:A:783:ADP:O1A	2.34	0.46
1:B:506:LEU:C	1:B:506:LEU:CD1	2.88	0.46
1:C:411:ALA:O	1:C:412:GLY:C	2.59	0.46
1:C:546:GLN:OE1	1:C:577:ILE:HB	2.15	0.46
1:D:307:ASP:HB3	1:D:309:LEU:HD21	1.98	0.46
1:D:645:SER:O	1:D:647:THR:N	2.48	0.46
1:D:733:ILE:HA	1:D:756:ILE:O	2.16	0.46
1:F:380:LEU:HD12	1:F:423:ILE:HG23	1.97	0.46
1:A:364:ALA:O	1:A:365:LYS:C	2.56	0.45
1:A:378:ILE:HD13	1:A:420:LEU:CD1	2.45	0.45
1:A:496:GLU:O	1:A:500:ILE:HG13	2.16	0.45
1:B:276:TYR:CE2	1:F:246:THR:CG2	3.00	0.45
1:D:341:LEU:O	1:D:343:LYS:N	2.49	0.45
1:D:572:ASN:O	1:D:573:LEU:C	2.59	0.45
1:A:680:ILE:HG22	1:A:705:ILE:CD1	2.46	0.45
1:B:497:LYS:HG2	1:B:540:VAL:HG12	1.99	0.45
1:C:469:THR:HG22	1:C:470:ALA:H	1.81	0.45
1:D:260:GLY:O	1:D:261:MET:CB	2.63	0.45
1:D:350:LEU:HA	1:D:485:GLU:O	2.16	0.45
1:D:489:ILE:H	1:D:489:ILE:HG12	1.58	0.45
1:F:255:LYS:O	1:F:258:GLU:HB3	2.16	0.45
1:F:675:GLY:N	1:F:676:PRO:CD	2.79	0.45
1:A:589:THR:O	1:A:590:GLU:CD	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ALA:O	1:B:412:GLY:C	2.59	0.45
1:B:478:GLY:N	1:B:479:PRO:HD2	2.31	0.45
1:B:604:VAL:O	1:B:604:VAL:HG23	2.15	0.45
1:B:711:VAL:N	1:B:759:SER:O	2.47	0.45
1:D:452:ASP:O	1:D:455:ILE:HG22	2.17	0.45
1:F:260:GLY:O	1:F:261:MET:HE3	2.16	0.45
1:B:276:TYR:OH	1:F:247:GLY:CA	2.64	0.45
1:B:602:THR:C	1:B:604:VAL:N	2.74	0.45
1:B:645:SER:O	1:B:647:THR:N	2.49	0.45
1:C:380:LEU:HD12	1:C:423:ILE:HG23	1.98	0.45
1:D:357:GLY:H	2:D:783:ADP:PB	2.39	0.45
1:D:481:ARG:O	1:D:481:ARG:HG2	2.16	0.45
1:A:329:LYS:O	1:A:330:GLU:C	2.59	0.45
1:B:308:LYS:O	1:B:309:LEU:HD23	2.17	0.45
1:B:373:ARG:NE	1:B:415:ASN:OD1	2.50	0.45
1:B:505:LEU:CD2	1:B:544:GLU:HG3	2.45	0.45
1:C:341:LEU:HB3	1:E:514:GLY:O	2.17	0.45
1:C:555:ALA:O	1:C:556:LYS:C	2.57	0.45
1:C:714:ILE:HB	1:C:735:PRO:HG2	1.98	0.45
1:D:260:GLY:O	1:D:261:MET:HE3	2.16	0.45
1:D:555:ALA:O	1:D:556:LYS:C	2.58	0.45
1:E:642:TYR:CD2	1:E:761:LEU:HD12	2.52	0.45
1:E:706:THR:OG1	1:E:710:ARG:HB2	2.15	0.45
1:F:597:THR:O	1:F:700:GLY:HA2	2.16	0.45
1:F:635:SER:O	1:F:638:ALA:HB3	2.16	0.45
1:A:276:TYR:CD1	1:A:277:GLU:N	2.84	0.45
1:B:294:ASP:C	1:B:296:LEU:N	2.72	0.45
1:B:441:VAL:O	1:B:441:VAL:HG22	2.16	0.45
1:B:572:ASN:O	1:B:573:LEU:C	2.60	0.45
1:C:274:ASN:O	1:C:276:TYR:N	2.48	0.45
1:C:276:TYR:CD1	1:C:277:GLU:N	2.84	0.45
1:D:276:TYR:CD1	1:D:277:GLU:N	2.85	0.45
1:E:423:ILE:HD12	1:E:484:MET:HE1	1.97	0.45
1:F:292:TYR:OH	1:F:455:ILE:HA	2.17	0.45
1:F:300:PRO:C	1:F:301:TRP:CG	2.94	0.45
1:B:260:GLY:O	1:B:261:MET:HE3	2.17	0.45
1:B:560:ALA:O	1:B:562:GLU:N	2.50	0.45
1:B:560:ALA:O	1:B:561:GLU:C	2.59	0.45
1:B:636:ALA:HB2	1:B:682:MET:HE1	1.99	0.45
1:C:255:LYS:O	1:C:258:GLU:HB3	2.16	0.45
1:C:714:ILE:HD12	1:C:714:ILE:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ALA:O	1:D:299:LEU:C	2.59	0.45
1:D:621:LYS:O	1:D:661:ASP:OD1	2.35	0.45
1:E:452:ASP:O	1:E:455:ILE:HG22	2.17	0.45
1:E:647:THR:HG22	1:E:648:GLU:N	2.32	0.45
1:F:276:TYR:CD1	1:F:277:GLU:N	2.84	0.45
1:F:295:TRP:HZ3	1:F:405:ILE:HG21	1.81	0.45
1:A:493:THR:HG21	1:A:748:SER:CB	2.46	0.45
1:B:464:VAL:O	1:B:466:PHE:CD1	2.63	0.45
1:B:495:ILE:HD13	1:B:495:ILE:HA	1.78	0.45
1:C:373:ARG:NE	1:C:415:ASN:OD1	2.50	0.45
1:C:424:ASP:OD1	1:C:424:ASP:N	2.50	0.45
1:D:423:ILE:HG21	1:D:423:ILE:HD13	1.62	0.45
1:D:424:ASP:N	1:D:424:ASP:OD1	2.50	0.45
1:D:552:ARG:O	1:D:553:LYS:C	2.60	0.45
1:D:598:GLY:HA2	1:D:701:MET:O	2.17	0.45
1:A:280:PRO:HB2	1:A:281:SER:H	1.67	0.45
1:A:294:ASP:C	1:A:296:LEU:N	2.72	0.45
1:B:613:VAL:HG23	1:B:685:ALA:HB1	1.99	0.45
1:D:298:ALA:O	1:D:299:LEU:O	2.35	0.45
1:D:506:LEU:CD2	1:D:522:LEU:HD21	2.44	0.45
1:D:599:LEU:HD22	1:D:599:LEU:N	2.32	0.45
1:D:736:LYS:C	1:D:738:ASN:H	2.24	0.45
1:F:266:LYS:HG3	1:F:267:GLU:H	1.81	0.45
1:F:602:THR:C	1:F:604:VAL:H	2.25	0.45
1:F:736:LYS:C	1:F:738:ASN:H	2.25	0.45
1:A:536:ARG:CG	1:A:536:ARG:NH1	2.65	0.45
1:A:569:THR:HG23	1:A:571:LYS:N	2.19	0.45
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.38	0.45
1:B:599:LEU:HD22	1:B:599:LEU:N	2.31	0.45
1:B:714:ILE:HG23	1:B:715:GLY:N	2.31	0.45
1:C:616:SER:O	1:C:661:ASP:N	2.50	0.45
1:C:647:THR:HG22	1:C:648:GLU:N	2.31	0.45
1:E:260:GLY:O	1:E:261:MET:HE3	2.17	0.45
1:E:599:LEU:HD21	1:E:700:GLY:C	2.42	0.45
1:E:747:GLU:CD	1:E:747:GLU:N	2.74	0.45
1:F:419:LEU:O	1:F:421:ASP:N	2.50	0.45
1:F:732:ILE:HD13	1:F:732:ILE:O	2.17	0.45
1:A:260:GLY:O	1:A:261:MET:HE3	2.16	0.44
1:B:266:LYS:HG3	1:B:267:GLU:H	1.82	0.44
1:E:712:LEU:HB3	1:E:713:PRO:HD2	1.99	0.44
1:F:364:ALA:O	1:F:365:LYS:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:478:GLY:N	1:F:479:PRO:HD2	2.31	0.44
1:F:505:LEU:HA	1:F:505:LEU:HD23	1.38	0.44
1:B:296:LEU:O	1:B:299:LEU:HD11	2.16	0.44
1:C:265:VAL:O	1:C:457:GLU:OE1	2.35	0.44
1:C:322:HIS:HA	2:C:783:ADP:N1	2.32	0.44
1:C:478:GLY:N	1:C:479:PRO:HD2	2.31	0.44
1:D:274:ASN:O	1:D:276:TYR:N	2.45	0.44
1:D:616:SER:O	1:D:661:ASP:N	2.49	0.44
1:D:732:ILE:HG21	1:D:753:LEU:HD13	1.99	0.44
1:E:536:ARG:HH11	1:E:536:ARG:CB	2.30	0.44
1:E:546:GLN:OE1	1:E:577:ILE:HB	2.17	0.44
1:F:294:ASP:C	1:F:296:LEU:N	2.73	0.44
1:F:359:GLY:O	1:F:360:LYS:C	2.60	0.44
1:F:380:LEU:HD12	1:F:423:ILE:CG2	2.47	0.44
1:F:732:ILE:HG21	1:F:753:LEU:HD13	1.99	0.44
1:B:267:GLU:HA	1:B:270:LEU:HG	1.98	0.44
1:B:569:THR:HG23	1:B:571:LYS:N	2.21	0.44
1:C:346:LYS:HG3	1:C:348:PRO:HD2	1.99	0.44
1:C:416:PRO:HD2	1:C:464:VAL:HG13	1.99	0.44
1:D:359:GLY:O	1:D:360:LYS:C	2.60	0.44
1:D:362:SER:HB3	2:D:783:ADP:C5'	2.47	0.44
1:D:599:LEU:O	1:D:720:LYS:HE2	2.17	0.44
1:D:714:ILE:HB	1:D:735:PRO:HG2	2.00	0.44
1:E:710:ARG:HH21	1:E:710:ARG:HG2	1.82	0.44
1:F:452:ASP:O	1:F:455:ILE:HG22	2.17	0.44
1:F:520:LEU:HA	1:F:566:ILE:O	2.17	0.44
1:B:280:PRO:HB2	1:B:281:SER:H	1.67	0.44
1:B:350:LEU:HA	1:B:485:GLU:O	2.18	0.44
1:B:407:GLY:HA3	1:B:418:PHE:CZ	2.52	0.44
1:B:420:LEU:HD21	1:B:466:PHE:CD2	2.50	0.44
1:B:520:LEU:HA	1:B:566:ILE:O	2.17	0.44
1:B:683:ALA:O	1:B:684:THR:C	2.61	0.44
1:C:423:ILE:HG21	1:C:423:ILE:HD13	1.76	0.44
1:C:621:LYS:O	1:C:661:ASP:OD1	2.35	0.44
1:C:637:GLN:HA	1:C:640:PHE:HB3	1.99	0.44
1:D:590:GLU:HA	1:D:697:ARG:HD3	1.99	0.44
1:F:550:ILE:C	1:F:552:ARG:N	2.75	0.44
1:A:495:ILE:HD13	1:A:495:ILE:HA	1.82	0.44
1:A:497:LYS:HG2	1:A:540:VAL:HG12	2.00	0.44
1:A:546:GLN:O	1:A:549:ALA:HB3	2.17	0.44
1:B:299:LEU:O	1:B:301:TRP:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:TYR:CD2	1:B:761:LEU:HD12	2.53	0.44
1:C:267:GLU:HG3	1:C:270:LEU:HD12	1.99	0.44
1:C:569:THR:HG23	1:C:572:ASN:H	1.82	0.44
1:E:506:LEU:HB3	1:E:507:PRO:CD	2.45	0.44
1:E:506:LEU:O	1:E:507:PRO:C	2.58	0.44
1:E:569:THR:HG23	1:E:571:LYS:N	2.21	0.44
1:F:368:ALA:CB	1:F:417:VAL:HG21	2.47	0.44
1:A:579:LYS:H	1:A:579:LYS:NZ	2.16	0.44
1:C:283:SER:N	1:C:286:SER:HB3	2.33	0.44
1:C:342:THR:HG22	1:C:344:SER:O	2.18	0.44
2:E:783:ADP:H5'2	2:E:783:ADP:C8	2.53	0.44
1:F:705:ILE:HD11	1:F:761:LEU:CD2	2.47	0.44
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.45	0.44
1:B:262:PRO:HG2	1:B:302:THR:OG1	2.17	0.44
1:B:522:LEU:HB3	1:B:568:VAL:CG1	2.43	0.44
1:C:739:GLU:C	1:C:741:ASP:H	2.24	0.44
1:E:329:LYS:C	1:E:331:ARG:H	2.25	0.44
1:E:455:ILE:O	1:E:455:ILE:HG23	2.18	0.44
1:E:597:THR:O	1:E:700:GLY:HA2	2.17	0.44
1:E:604:VAL:O	1:E:604:VAL:HG23	2.17	0.44
1:B:294:ASP:O	1:B:295:TRP:C	2.60	0.44
1:B:480:LEU:O	1:B:483:ARG:N	2.50	0.44
1:D:342:THR:HG22	1:D:344:SER:O	2.17	0.44
1:D:586:GLN:HG3	1:D:698:GLU:HG2	2.00	0.44
1:E:255:LYS:O	1:E:258:GLU:HB3	2.18	0.44
1:E:295:TRP:O	1:E:299:LEU:HG	2.18	0.44
1:A:569:THR:HG23	1:A:572:ASN:H	1.82	0.44
1:A:675:GLY:N	1:A:676:PRO:CD	2.81	0.44
1:A:711:VAL:N	1:A:759:SER:O	2.47	0.44
1:C:532:ARG:HG2	1:C:584:TYR:CE2	2.53	0.44
1:C:675:GLY:N	1:C:676:PRO:CD	2.81	0.44
1:D:255:LYS:O	1:D:258:GLU:HB3	2.17	0.44
1:D:441:VAL:HG22	1:D:441:VAL:O	2.17	0.44
1:E:300:PRO:HG3	1:E:413:LYS:N	2.32	0.44
1:F:477:PRO:O	1:F:478:GLY:C	2.61	0.44
1:F:579:LYS:NZ	1:F:579:LYS:H	2.15	0.44
1:A:267:GLU:HA	1:A:270:LEU:HG	1.99	0.43
1:A:271:LYS:CA	1:A:274:ASN:HB3	2.46	0.43
1:A:493:THR:CG2	1:A:748:SER:HB2	2.47	0.43
1:B:329:LYS:C	1:B:331:ARG:H	2.26	0.43
1:B:477:PRO:C	1:B:479:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:GLN:O	1:B:549:ALA:HB3	2.18	0.43
1:C:333:LEU:HD23	1:C:336:LEU:HD12	2.00	0.43
1:D:506:LEU:HD12	1:D:510:ILE:CG1	2.48	0.43
1:D:643:VAL:O	1:D:644:ARG:C	2.61	0.43
1:D:756:ILE:HG13	1:D:767:HIS:CD2	2.54	0.43
1:E:294:ASP:C	1:E:296:LEU:N	2.75	0.43
1:E:569:THR:HG23	1:E:572:ASN:H	1.82	0.43
1:E:739:GLU:C	1:E:741:ASP:N	2.76	0.43
1:F:311:LEU:O	1:F:312:LYS:C	2.60	0.43
1:F:346:LYS:HG3	1:F:348:PRO:HD2	2.00	0.43
1:A:357:GLY:H	2:A:783:ADP:PB	2.38	0.43
1:A:469:THR:HG22	1:A:470:ALA:H	1.83	0.43
1:B:335:TYR:CD2	1:B:335:TYR:O	2.71	0.43
1:B:345:LEU:HD23	1:B:345:LEU:C	2.43	0.43
1:B:739:GLU:C	1:B:741:ASP:N	2.75	0.43
1:C:260:GLY:C	1:C:261:MET:HE3	2.43	0.43
1:C:557:ALA:CB	1:C:566:ILE:HD11	2.48	0.43
1:D:712:LEU:HB3	1:D:713:PRO:CD	2.47	0.43
1:E:367:ILE:O	1:E:371:LEU:HD13	2.17	0.43
1:E:637:GLN:HA	1:E:640:PHE:HB3	2.00	0.43
1:F:298:ALA:O	1:F:299:LEU:C	2.61	0.43
1:B:514:GLY:O	1:E:341:LEU:HD13	2.17	0.43
1:C:329:LYS:O	1:C:330:GLU:C	2.62	0.43
1:C:350:LEU:HA	1:C:485:GLU:O	2.18	0.43
1:C:642:TYR:CE1	1:C:709:GLY:HA3	2.52	0.43
1:E:350:LEU:H	1:E:350:LEU:CD1	2.09	0.43
1:F:506:LEU:O	1:F:507:PRO:C	2.59	0.43
1:F:584:TYR:CD1	1:F:584:TYR:C	2.95	0.43
1:A:536:ARG:CB	1:A:536:ARG:NH1	2.82	0.43
1:B:656:PHE:C	1:B:656:PHE:CD2	2.96	0.43
1:C:452:ASP:O	1:C:455:ILE:HG22	2.18	0.43
1:C:637:GLN:O	1:C:637:GLN:HG2	2.18	0.43
1:D:584:TYR:CD1	1:D:584:TYR:C	2.96	0.43
1:E:602:THR:CG2	1:E:604:VAL:HG22	2.49	0.43
1:E:616:SER:O	1:E:661:ASP:N	2.52	0.43
1:F:455:ILE:O	1:F:455:ILE:HG23	2.18	0.43
1:A:260:GLY:C	1:A:261:MET:HE3	2.44	0.43
1:A:350:LEU:HA	1:A:485:GLU:O	2.19	0.43
1:C:589:THR:O	1:C:697:ARG:NE	2.52	0.43
1:D:322:HIS:CE1	1:D:363:LEU:HD23	2.53	0.43
1:D:439:LEU:H	1:D:439:LEU:CD2	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:THR:HG22	1:E:344:SER:O	2.18	0.43
1:E:639:ALA:HB1	1:E:683:ALA:HB2	2.00	0.43
1:F:439:LEU:H	1:F:439:LEU:CD2	2.26	0.43
1:A:455:ILE:O	1:A:455:ILE:HG23	2.18	0.43
1:A:714:ILE:HB	1:A:735:PRO:HG2	2.00	0.43
1:B:602:THR:HG22	1:B:603:THR:N	2.33	0.43
1:B:613:VAL:O	1:E:708:ARG:HD3	2.17	0.43
1:B:735:PRO:O	1:B:738:ASN:HB2	2.18	0.43
1:C:270:LEU:CD2	1:C:296:LEU:HD22	2.44	0.43
1:C:693:ARG:O	1:C:694:ALA:HB2	2.19	0.43
1:C:752:GLY:O	1:C:753:LEU:HD23	2.19	0.43
1:D:546:GLN:O	1:D:549:ALA:HB3	2.18	0.43
1:E:732:ILE:O	1:E:732:ILE:HD13	2.19	0.43
2:E:783:ADP:C5'	2:E:783:ADP:C8	3.01	0.43
1:A:656:PHE:C	1:A:656:PHE:CD2	2.96	0.43
1:B:267:GLU:HG3	1:B:270:LEU:HD12	2.01	0.43
1:B:299:LEU:CD1	1:B:301:TRP:NE1	2.82	0.43
1:B:362:SER:HB3	2:B:783:ADP:H5'2	2.01	0.43
1:C:474:ALA:O	1:C:475:THR:C	2.61	0.43
1:E:300:PRO:HB2	1:E:414:LEU:CB	2.46	0.43
1:F:357:GLY:O	1:F:539:GLY:HA2	2.18	0.43
1:A:423:ILE:C	1:A:424:ASP:OD1	2.62	0.43
1:A:477:PRO:O	1:A:478:GLY:C	2.61	0.43
1:B:416:PRO:HD2	1:B:464:VAL:HG13	2.01	0.43
1:C:338:VAL:HG23	1:E:555:ALA:HB3	2.00	0.43
1:C:732:ILE:HD13	1:C:732:ILE:O	2.18	0.43
1:D:293:ILE:O	1:D:297:VAL:HG23	2.19	0.43
1:E:602:THR:O	1:E:604:VAL:N	2.52	0.43
1:E:611:ILE:HG23	1:E:665:HIS:O	2.19	0.43
1:A:477:PRO:C	1:A:479:PRO:HD2	2.44	0.43
1:A:599:LEU:HD22	1:A:599:LEU:N	2.32	0.43
1:B:409:LYS:C	1:B:411:ALA:N	2.74	0.43
1:B:602:THR:CG2	1:B:604:VAL:HG22	2.48	0.43
1:C:378:ILE:HD13	1:C:420:LEU:HD12	1.99	0.43
1:D:300:PRO:C	1:D:301:TRP:CG	2.96	0.43
1:D:332:ILE:CG2	1:D:367:ILE:HD11	2.49	0.43
1:D:647:THR:HG22	1:D:648:GLU:N	2.34	0.43
1:E:416:PRO:CD	1:E:464:VAL:HG13	2.49	0.43
1:E:687:VAL:C	1:E:689:ALA:N	2.76	0.43
1:F:274:ASN:O	1:F:276:TYR:N	2.46	0.43
1:F:350:LEU:HA	1:F:485:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:C	1:A:274:ASN:OD1	2.62	0.43
1:A:283:SER:N	1:A:286:SER:HB3	2.34	0.43
1:A:476:ILE:HG21	1:A:481:ARG:HB2	2.00	0.43
1:B:569:THR:HG22	1:B:572:ASN:CG	2.44	0.43
1:E:269:ALA:CB	1:E:457:GLU:OE1	2.67	0.43
1:E:474:ALA:O	1:E:475:THR:C	2.61	0.43
1:F:409:LYS:C	1:F:411:ALA:N	2.77	0.43
1:F:712:LEU:HB3	1:F:713:PRO:CD	2.48	0.43
1:A:333:LEU:HD23	1:A:336:LEU:HD12	2.01	0.42
1:A:656:PHE:CD2	1:A:657:HIS:N	2.87	0.42
1:B:273:LEU:O	1:B:276:TYR:HB2	2.19	0.42
1:B:301:TRP:O	1:B:414:LEU:HD21	2.19	0.42
1:B:339:GLN:O	1:B:340:LYS:C	2.62	0.42
1:B:529:ASP:O	1:B:530:ILE:C	2.62	0.42
1:B:593:VAL:HG13	1:B:693:ARG:O	2.19	0.42
1:B:622:LEU:HB2	1:B:662:ILE:HG12	2.01	0.42
1:B:637:GLN:HA	1:B:640:PHE:HB3	2.01	0.42
1:B:686:LEU:HD22	1:B:686:LEU:O	2.19	0.42
1:B:687:VAL:C	1:B:689:ALA:N	2.77	0.42
1:B:733:ILE:HA	1:B:756:ILE:O	2.19	0.42
1:C:633:ARG:O	1:C:634:GLU:C	2.62	0.42
1:D:267:GLU:HA	1:D:270:LEU:HG	2.00	0.42
1:D:642:TYR:CE1	1:D:709:GLY:HA3	2.54	0.42
1:E:373:ARG:NE	1:E:415:ASN:OD1	2.52	0.42
1:E:489:ILE:H	1:E:489:ILE:HG12	1.65	0.42
1:E:572:ASN:O	1:E:573:LEU:C	2.61	0.42
1:F:569:THR:HG23	1:F:571:LYS:N	2.19	0.42
1:F:622:LEU:HB2	1:F:662:ILE:CG1	2.49	0.42
1:F:678:ALA:O	1:F:682:MET:HG2	2.19	0.42
1:A:546:GLN:OE1	1:A:577:ILE:HB	2.19	0.42
1:B:260:GLY:C	1:B:261:MET:HE3	2.44	0.42
1:B:277:GLU:OE1	1:F:246:THR:N	2.52	0.42
1:B:293:ILE:O	1:B:297:VAL:HG23	2.19	0.42
1:B:546:GLN:OE1	1:B:577:ILE:HB	2.20	0.42
1:B:647:THR:HG23	1:B:652:ILE:HG23	2.00	0.42
1:C:408:MET:HE2	1:C:408:MET:N	2.29	0.42
1:C:505:LEU:HA	1:C:505:LEU:HD23	1.43	0.42
1:C:505:LEU:CD2	1:C:544:GLU:HG3	2.47	0.42
1:C:569:THR:HG22	1:C:572:ASN:CG	2.45	0.42
1:D:403:ARG:O	1:D:403:ARG:CG	2.67	0.42
1:E:513:HIS:O	1:E:514:GLY:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:656:PHE:CD2	1:E:657:HIS:N	2.87	0.42
1:F:260:GLY:C	1:F:261:MET:HE3	2.43	0.42
1:F:464:VAL:CG1	1:F:466:PHE:CE1	3.02	0.42
1:A:342:THR:HG22	1:A:344:SER:O	2.20	0.42
1:B:290:ARG:NH1	1:E:273:LEU:HD21	2.34	0.42
1:B:455:ILE:O	1:B:455:ILE:HG23	2.19	0.42
1:B:712:LEU:HB3	1:B:713:PRO:HD2	2.01	0.42
1:C:346:LYS:HZ1	1:E:513:HIS:CE1	2.36	0.42
1:C:464:VAL:O	1:C:466:PHE:CD1	2.68	0.42
1:C:597:THR:O	1:C:700:GLY:HA2	2.19	0.42
1:D:256:ILE:CD1	1:D:293:ILE:HD11	2.48	0.42
1:D:439:LEU:HD13	1:D:480:LEU:HD13	2.00	0.42
1:D:712:LEU:HB3	1:D:713:PRO:HD2	2.01	0.42
1:E:346:LYS:HG3	1:E:348:PRO:HD2	2.01	0.42
1:F:602:THR:C	1:F:604:VAL:N	2.75	0.42
1:F:647:THR:HG22	1:F:648:GLU:N	2.34	0.42
1:A:373:ARG:NE	1:A:415:ASN:OD1	2.52	0.42
1:A:456:GLU:O	1:A:457:GLU:HB2	2.20	0.42
1:A:593:VAL:HG13	1:A:693:ARG:O	2.19	0.42
1:B:359:GLY:HA2	2:B:783:ADP:H5'2	2.01	0.42
1:B:569:THR:HG23	1:B:572:ASN:H	1.84	0.42
1:C:455:ILE:O	1:C:455:ILE:HG23	2.18	0.42
1:C:506:LEU:C	1:C:506:LEU:CD1	2.91	0.42
1:C:636:ALA:C	1:C:638:ALA:N	2.77	0.42
1:C:646:LYS:H	1:C:646:LYS:CD	2.32	0.42
1:D:270:LEU:HD21	1:D:296:LEU:CD2	2.45	0.42
1:D:536:ARG:NH1	1:D:536:ARG:CB	2.82	0.42
1:F:474:ALA:O	1:F:475:THR:C	2.62	0.42
1:A:409:LYS:C	1:A:411:ALA:N	2.77	0.42
1:B:283:SER:N	1:B:286:SER:HB3	2.34	0.42
1:B:477:PRO:O	1:B:478:GLY:C	2.62	0.42
1:C:305:THR:O	1:C:306:ASP:C	2.62	0.42
1:C:305:THR:O	1:C:307:ASP:N	2.52	0.42
1:E:299:LEU:O	1:E:301:TRP:CE2	2.73	0.42
1:E:596:VAL:HG23	1:E:685:ALA:HB2	2.00	0.42
1:F:247:GLY:C	1:F:249:VAL:N	2.78	0.42
1:F:378:ILE:HD13	1:F:420:LEU:HD12	2.02	0.42
1:F:440:GLU:HG3	1:F:446:GLN:OE1	2.19	0.42
1:A:522:LEU:HB3	1:A:568:VAL:CG1	2.45	0.42
1:A:561:GLU:O	1:A:562:GLU:HB2	2.19	0.42
1:A:733:ILE:HA	1:A:756:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:THR:C	1:B:604:VAL:H	2.27	0.42
1:B:656:PHE:CD2	1:B:657:HIS:N	2.88	0.42
1:C:279:ILE:HA	1:C:280:PRO:HA	1.86	0.42
1:C:536:ARG:NH1	1:C:536:ARG:HB2	2.34	0.42
1:C:627:LYS:O	1:C:627:LYS:HG3	2.20	0.42
1:E:365:LYS:HG3	1:E:375:PHE:CZ	2.55	0.42
1:E:505:LEU:HD23	1:E:505:LEU:HA	1.38	0.42
1:E:561:GLU:O	1:E:562:GLU:HB2	2.19	0.42
1:E:599:LEU:HD22	1:E:599:LEU:N	2.34	0.42
1:E:714:ILE:HB	1:E:735:PRO:HG2	2.00	0.42
1:F:283:SER:N	1:F:286:SER:HB3	2.35	0.42
1:F:342:THR:HG22	1:F:344:SER:O	2.20	0.42
1:F:529:ASP:O	1:F:530:ILE:C	2.63	0.42
1:F:599:LEU:O	1:F:720:LYS:HE2	2.20	0.42
1:A:262:PRO:HD2	1:A:301:TRP:HB3	2.01	0.42
1:A:266:LYS:HG3	1:A:267:GLU:H	1.82	0.42
1:A:529:ASP:O	1:A:530:ILE:C	2.61	0.42
1:B:460:ASP:O	1:B:461:LEU:HD23	2.18	0.42
1:C:271:LYS:CA	1:C:274:ASN:HB3	2.48	0.42
1:D:279:ILE:HA	1:D:280:PRO:HA	1.86	0.42
1:D:283:SER:N	1:D:286:SER:HB3	2.34	0.42
1:E:622:LEU:HB2	1:E:662:ILE:HG12	2.02	0.42
1:F:256:ILE:CD1	1:F:293:ILE:HD11	2.49	0.42
1:F:299:LEU:HA	1:F:300:PRO:HD3	1.69	0.42
1:F:705:ILE:HD12	1:F:705:ILE:HA	1.74	0.42
1:A:480:LEU:O	1:A:483:ARG:N	2.53	0.42
1:B:271:LYS:CA	1:B:274:ASN:HB3	2.46	0.42
1:B:329:LYS:O	1:B:331:ARG:N	2.53	0.42
1:B:503:ASP:C	1:B:504:HIS:ND1	2.78	0.42
1:C:706:THR:OG1	1:C:710:ARG:HB2	2.19	0.42
1:D:469:THR:HG22	1:D:470:ALA:N	2.34	0.42
1:D:477:PRO:C	1:D:479:PRO:HD2	2.45	0.42
1:D:747:GLU:CD	1:D:747:GLU:N	2.78	0.42
1:E:569:THR:HG22	1:E:572:ASN:CG	2.45	0.42
1:F:329:LYS:C	1:F:331:ARG:H	2.27	0.42
1:F:354:GLY:O	1:F:355:PRO:C	2.61	0.42
1:A:573:LEU:HD12	1:A:573:LEU:HA	1.93	0.42
1:B:561:GLU:O	1:B:562:GLU:HB2	2.18	0.42
1:C:335:TYR:CD2	1:C:335:TYR:O	2.73	0.42
1:C:503:ASP:C	1:C:504:HIS:ND1	2.78	0.42
1:C:593:VAL:HG13	1:C:693:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:PHE:C	1:C:656:PHE:CD2	2.98	0.42
1:D:294:ASP:C	1:D:296:LEU:N	2.76	0.42
1:D:345:LEU:HD23	1:D:345:LEU:C	2.44	0.42
1:D:357:GLY:C	1:D:539:GLY:HA3	2.45	0.42
1:D:705:ILE:HD11	1:D:761:LEU:CD2	2.50	0.42
1:E:283:SER:N	1:E:286:SER:HB3	2.34	0.42
1:F:274:ASN:C	1:F:274:ASN:OD1	2.62	0.42
1:F:599:LEU:HD21	1:F:700:GLY:C	2.45	0.42
1:A:441:VAL:O	1:A:441:VAL:HG22	2.19	0.42
1:A:611:ILE:HD12	1:A:681:THR:CG2	2.50	0.42
1:B:272:GLU:C	1:B:274:ASN:H	2.27	0.42
1:B:289:ILE:O	1:B:290:ARG:C	2.62	0.42
1:B:342:THR:HG22	1:B:344:SER:O	2.20	0.42
1:B:486:ILE:CG2	1:B:487:ILE:N	2.82	0.42
1:C:293:ILE:O	1:C:297:VAL:HG23	2.18	0.42
1:D:505:LEU:HD23	1:D:505:LEU:HA	1.37	0.42
1:E:589:THR:O	1:E:697:ARG:CD	2.68	0.42
1:F:293:ILE:O	1:F:297:VAL:HG23	2.20	0.42
1:A:293:ILE:O	1:A:297:VAL:HG23	2.20	0.41
1:A:300:PRO:HG3	1:A:412:GLY:HA2	2.02	0.41
1:A:516:LYS:HA	1:A:516:LYS:HZ1	1.82	0.41
1:A:547:LEU:HA	1:A:547:LEU:HD23	1.78	0.41
1:A:746:PRO:O	1:A:747:GLU:C	2.63	0.41
1:B:329:LYS:O	1:B:330:GLU:C	2.63	0.41
1:B:732:ILE:HG21	1:B:753:LEU:HD13	2.02	0.41
1:C:329:LYS:O	1:C:332:ILE:N	2.41	0.41
1:C:355:PRO:O	1:C:358:VAL:HG22	2.20	0.41
1:C:477:PRO:C	1:C:479:PRO:HD2	2.45	0.41
1:C:680:ILE:HG22	1:C:705:ILE:HD13	2.02	0.41
1:D:368:ALA:CB	1:D:417:VAL:HG21	2.48	0.41
1:D:495:ILE:HD13	1:D:495:ILE:HA	1.87	0.41
1:D:573:LEU:CG	1:D:577:ILE:HD11	2.50	0.41
1:D:702:THR:O	1:D:702:THR:CG2	2.65	0.41
1:F:267:GLU:HA	1:F:270:LEU:HG	2.02	0.41
1:F:341:LEU:O	1:F:343:LYS:N	2.53	0.41
1:F:519:ASN:HD22	1:F:519:ASN:HA	1.53	0.41
1:F:536:ARG:HH11	1:F:536:ARG:CB	2.32	0.41
1:F:737:ASP:OD2	1:F:737:ASP:N	2.53	0.41
1:B:705:ILE:HA	1:B:705:ILE:HD12	1.75	0.41
1:C:656:PHE:CD2	1:C:657:HIS:N	2.88	0.41
1:D:496:GLU:O	1:D:500:ILE:HG13	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:THR:HG22	1:D:572:ASN:CG	2.45	0.41
1:D:734:ALA:HB1	1:D:735:PRO:CD	2.51	0.41
1:F:572:ASN:O	1:F:573:LEU:C	2.62	0.41
1:A:336:LEU:CD2	1:A:371:LEU:HD11	2.51	0.41
1:A:622:LEU:HB2	1:A:662:ILE:HG12	2.03	0.41
1:A:739:GLU:C	1:A:741:ASP:N	2.78	0.41
1:B:506:LEU:O	1:B:507:PRO:C	2.62	0.41
1:B:693:ARG:O	1:B:694:ALA:HB2	2.19	0.41
1:B:705:ILE:HD11	1:B:761:LEU:CD2	2.49	0.41
1:D:547:LEU:HD23	1:D:547:LEU:HA	1.79	0.41
1:D:558:ILE:H	1:D:558:ILE:HG12	1.65	0.41
1:D:675:GLY:N	1:D:676:PRO:CD	2.83	0.41
1:E:350:LEU:HD23	1:E:487:ILE:HD11	2.02	0.41
1:E:656:PHE:C	1:E:656:PHE:CD2	2.97	0.41
1:E:736:LYS:HA	1:E:757:LEU:HB3	2.03	0.41
1:F:414:LEU:C	1:F:414:LEU:HD12	2.45	0.41
1:F:423:ILE:HD13	1:F:423:ILE:HG21	1.78	0.41
1:A:355:PRO:O	1:A:358:VAL:HG22	2.20	0.41
1:A:710:ARG:HG2	1:A:710:ARG:HH21	1.85	0.41
1:B:633:ARG:O	1:B:634:GLU:C	2.63	0.41
1:C:339:GLN:O	1:C:340:LYS:C	2.62	0.41
1:C:440:GLU:HG3	1:C:446:GLN:OE1	2.20	0.41
1:C:506:LEU:HD12	1:C:510:ILE:CG1	2.49	0.41
1:D:272:GLU:C	1:D:274:ASN:H	2.28	0.41
1:D:455:ILE:O	1:D:455:ILE:HG23	2.19	0.41
1:D:622:LEU:HB2	1:D:662:ILE:HG12	2.02	0.41
1:D:636:ALA:C	1:D:638:ALA:N	2.73	0.41
1:D:707:LEU:HD23	1:D:707:LEU:HA	1.92	0.41
1:E:329:LYS:O	1:E:331:ARG:N	2.54	0.41
1:F:424:ASP:OD1	1:F:424:ASP:N	2.53	0.41
1:A:417:VAL:HG22	1:A:465:LEU:HB3	2.02	0.41
1:B:352:LEU:CD2	1:B:489:ILE:HD11	2.50	0.41
1:B:419:LEU:O	1:B:421:ASP:N	2.53	0.41
1:B:636:ALA:C	1:B:638:ALA:N	2.76	0.41
1:C:267:GLU:HA	1:C:270:LEU:HB2	2.02	0.41
1:C:551:CYS:O	1:C:554:ALA:HB3	2.20	0.41
1:D:474:ALA:O	1:D:476:ILE:O	2.38	0.41
1:E:262:PRO:HD2	1:E:301:TRP:HB2	2.03	0.41
1:E:266:LYS:HG3	1:E:267:GLU:H	1.81	0.41
1:A:735:PRO:O	1:A:738:ASN:HB2	2.19	0.41
1:B:423:ILE:C	1:B:424:ASP:OD1	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:GLU:HA	1:C:270:LEU:HG	2.01	0.41
1:C:584:TYR:CD1	1:C:584:TYR:O	2.73	0.41
1:D:534:TYR:C	1:D:582:PHE:HE2	2.29	0.41
1:E:352:LEU:CD2	1:E:489:ILE:HD11	2.47	0.41
1:E:464:VAL:O	1:E:466:PHE:CD1	2.64	0.41
1:E:536:ARG:HG3	1:E:536:ARG:NH1	2.14	0.41
1:E:555:ALA:O	1:E:556:LYS:C	2.61	0.41
1:E:573:LEU:CG	1:E:577:ILE:HD11	2.51	0.41
1:E:717:LEU:HD23	1:E:717:LEU:HA	1.87	0.41
1:A:288:VAL:C	1:A:290:ARG:N	2.78	0.41
1:A:712:LEU:HB3	1:A:713:PRO:HD2	2.03	0.41
1:A:736:LYS:HA	1:A:757:LEU:HB3	2.03	0.41
1:B:276:TYR:HD1	1:B:277:GLU:N	2.17	0.41
1:C:349:ILE:HD12	1:C:349:ILE:C	2.45	0.41
1:C:359:GLY:O	1:C:360:LYS:C	2.62	0.41
1:C:476:ILE:HG21	1:C:481:ARG:HB2	2.02	0.41
1:C:477:PRO:O	1:C:478:GLY:C	2.63	0.41
1:C:569:THR:HG22	1:C:572:ASN:H	1.86	0.41
1:C:599:LEU:O	1:C:720:LYS:HE2	2.21	0.41
1:D:367:ILE:O	1:D:371:LEU:HD13	2.21	0.41
1:D:460:ASP:O	1:D:461:LEU:HD23	2.20	0.41
1:D:639:ALA:HB1	1:D:683:ALA:HA	2.03	0.41
1:E:260:GLY:C	1:E:261:MET:HE3	2.45	0.41
1:E:273:LEU:O	1:E:276:TYR:HB2	2.20	0.41
1:E:678:ALA:O	1:E:682:MET:HG2	2.20	0.41
1:F:637:GLN:HA	1:F:640:PHE:HB3	2.02	0.41
1:A:551:CYS:O	1:A:554:ALA:HB3	2.21	0.41
1:A:586:GLN:CD	1:A:586:GLN:N	2.77	0.41
1:B:341:LEU:HB3	1:F:514:GLY:O	2.20	0.41
1:B:644:ARG:C	1:F:616:SER:HG	2.28	0.41
1:C:678:ALA:O	1:C:682:MET:HG2	2.21	0.41
1:D:506:LEU:HB3	1:D:507:PRO:CD	2.48	0.41
1:E:409:LYS:C	1:E:411:ALA:N	2.78	0.41
1:F:552:ARG:O	1:F:553:LYS:C	2.63	0.41
1:F:567:THR:O	1:F:567:THR:HG22	2.21	0.41
1:F:569:THR:HG22	1:F:572:ASN:CG	2.45	0.41
1:A:272:GLU:C	1:A:274:ASN:H	2.29	0.41
1:A:294:ASP:O	1:A:295:TRP:C	2.62	0.41
1:A:304:GLU:O	1:A:304:GLU:HG2	2.20	0.41
1:A:339:GLN:O	1:A:340:LYS:C	2.63	0.41
1:A:560:ALA:O	1:A:561:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:SER:O	1:A:661:ASP:N	2.54	0.41
1:A:761:LEU:HD23	1:A:761:LEU:HA	1.83	0.41
1:B:247:GLY:C	1:B:249:VAL:N	2.79	0.41
1:B:274:ASN:C	1:B:274:ASN:OD1	2.64	0.41
1:B:305:THR:CG2	1:B:306:ASP:N	2.83	0.41
1:B:332:ILE:CG2	1:B:367:ILE:HD11	2.51	0.41
1:B:440:GLU:HG3	1:B:446:GLN:OE1	2.21	0.41
1:B:478:GLY:N	1:B:479:PRO:CD	2.84	0.41
1:B:489:ILE:H	1:B:489:ILE:HG12	1.49	0.41
1:B:499:GLU:O	1:B:500:ILE:C	2.63	0.41
1:B:598:GLY:HA2	1:B:701:MET:O	2.21	0.41
1:B:761:LEU:HD23	1:B:761:LEU:HA	1.95	0.41
1:C:307:ASP:CG	1:C:373:ARG:NH2	2.78	0.41
1:C:469:THR:CG2	1:C:470:ALA:N	2.82	0.41
1:C:602:THR:HG22	1:C:603:THR:N	2.35	0.41
1:C:711:VAL:N	1:C:759:SER:O	2.51	0.41
1:D:336:LEU:O	1:D:337:ALA:C	2.63	0.41
1:D:409:LYS:C	1:D:411:ALA:N	2.79	0.41
1:D:642:TYR:CD2	1:D:761:LEU:HD12	2.56	0.41
1:D:650:LEU:HD11	1:D:765:LEU:HD13	2.03	0.41
1:D:687:VAL:C	1:D:689:ALA:N	2.79	0.41
1:E:271:LYS:CA	1:E:274:ASN:HB3	2.45	0.41
1:E:288:VAL:C	1:E:290:ARG:N	2.78	0.41
1:E:359:GLY:HA2	2:E:783:ADP:H5'1	2.03	0.41
1:E:408:MET:HE2	1:E:408:MET:N	2.29	0.41
1:E:520:LEU:HA	1:E:566:ILE:O	2.21	0.41
1:E:693:ARG:HB3	1:E:694:ALA:H	1.73	0.41
1:E:705:ILE:HD11	1:E:761:LEU:CD2	2.51	0.41
1:F:271:LYS:CA	1:F:274:ASN:HB3	2.46	0.41
1:F:561:GLU:O	1:F:562:GLU:HB2	2.21	0.41
1:F:656:PHE:CD2	1:F:657:HIS:N	2.89	0.41
1:F:707:LEU:HD23	1:F:707:LEU:HA	1.90	0.41
1:A:247:GLY:C	1:A:249:VAL:N	2.79	0.41
1:A:403:ARG:N	1:A:405:ILE:HG13	2.36	0.41
1:A:536:ARG:HG3	1:A:536:ARG:NH1	2.20	0.41
1:A:536:ARG:NH1	1:A:536:ARG:HB2	2.36	0.41
1:B:622:LEU:HB2	1:B:662:ILE:CG1	2.51	0.41
1:C:276:TYR:HD1	1:C:277:GLU:N	2.19	0.41
1:C:409:LYS:C	1:C:411:ALA:N	2.79	0.41
1:C:710:ARG:HG2	1:C:710:ARG:HH21	1.86	0.41
1:C:761:LEU:O	1:C:762:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ARG:O	1:D:403:ARG:HG2	2.21	0.41
1:D:493:THR:O	1:D:494:GLU:C	2.62	0.41
1:D:551:CYS:O	1:D:554:ALA:HB3	2.21	0.41
1:D:752:GLY:O	1:D:753:LEU:HD23	2.21	0.41
1:E:267:GLU:HA	1:E:270:LEU:HG	2.01	0.41
1:E:272:GLU:C	1:E:274:ASN:H	2.29	0.41
1:E:279:ILE:HA	1:E:280:PRO:HA	1.87	0.41
1:A:557:ALA:CB	1:A:566:ILE:HD11	2.50	0.40
1:B:656:PHE:CE2	1:B:690:LEU:HD11	2.56	0.40
1:C:256:ILE:CD1	1:C:293:ILE:HD11	2.46	0.40
1:C:274:ASN:C	1:C:274:ASN:OD1	2.64	0.40
1:C:639:ALA:HB1	1:C:683:ALA:HA	2.04	0.40
1:D:648:GLU:C	1:D:650:LEU:H	2.29	0.40
1:E:536:ARG:NH2	1:E:583:ARG:O	2.47	0.40
1:F:272:GLU:C	1:F:274:ASN:H	2.29	0.40
1:F:367:ILE:HG22	1:F:368:ALA:N	2.35	0.40
1:F:557:ALA:CB	1:F:566:ILE:HD11	2.50	0.40
1:F:656:PHE:C	1:F:656:PHE:CD2	2.99	0.40
1:A:341:LEU:HD13	1:C:514:GLY:O	2.21	0.40
1:A:359:GLY:HA2	2:A:783:ADP:O5'	2.21	0.40
1:A:678:ALA:O	1:A:682:MET:HG2	2.21	0.40
1:B:423:ILE:HD12	1:B:484:MET:HE1	2.02	0.40
1:B:536:ARG:NH1	1:B:536:ARG:CB	2.84	0.40
1:C:345:LEU:HD23	1:C:345:LEU:C	2.46	0.40
1:C:586:GLN:HB3	1:C:697:ARG:HE	1.86	0.40
1:C:708:ARG:NH2	1:E:593:VAL:HB	2.36	0.40
1:D:331:ARG:NH1	1:D:485:GLU:OE1	2.46	0.40
1:D:373:ARG:NE	1:D:415:ASN:OD1	2.54	0.40
1:D:693:ARG:O	1:D:694:ALA:HB2	2.21	0.40
1:E:560:ALA:O	1:E:561:GLU:C	2.65	0.40
1:F:349:ILE:O	1:F:484:MET:HB2	2.21	0.40
1:F:474:ALA:C	1:F:476:ILE:N	2.78	0.40
1:A:270:LEU:CD2	1:A:296:LEU:HD22	2.48	0.40
1:A:714:ILE:HD12	1:A:714:ILE:HA	1.79	0.40
1:B:367:ILE:HG22	1:B:368:ALA:N	2.36	0.40
1:B:547:LEU:HD23	1:B:547:LEU:HA	1.76	0.40
1:B:645:SER:HA	1:F:616:SER:HA	2.03	0.40
1:C:533:TYR:CB	1:C:580:ARG:HD2	2.50	0.40
1:C:537:GLU:HG3	1:C:539:GLY:O	2.22	0.40
1:C:687:VAL:O	1:C:691:THR:HG23	2.21	0.40
1:D:267:GLU:HG3	1:D:270:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ASN:C	1:D:274:ASN:OD1	2.64	0.40
1:D:307:ASP:O	1:D:309:LEU:HG	2.21	0.40
1:D:308:LYS:C	1:D:309:LEU:HD23	2.46	0.40
1:D:440:GLU:HG3	1:D:446:GLN:OE1	2.21	0.40
1:D:534:TYR:CD2	1:D:577:ILE:HD12	2.56	0.40
1:D:646:LYS:H	1:D:646:LYS:CD	2.31	0.40
1:E:274:ASN:C	1:E:274:ASN:OD1	2.64	0.40
1:E:656:PHE:CE2	1:E:690:LEU:HD11	2.56	0.40
1:F:355:PRO:O	1:F:358:VAL:HG22	2.21	0.40
1:A:262:PRO:HD2	1:A:301:TRP:CB	2.52	0.40
1:A:478:GLY:N	1:A:479:PRO:CD	2.84	0.40
1:A:569:THR:HG22	1:A:572:ASN:CG	2.47	0.40
1:B:464:VAL:CG1	1:B:466:PHE:CE1	3.04	0.40
1:B:474:ALA:O	1:B:475:THR:C	2.65	0.40
1:C:561:GLU:O	1:C:562:GLU:HB2	2.20	0.40
1:D:260:GLY:C	1:D:261:MET:HE3	2.46	0.40
1:D:483:ARG:HB3	1:D:483:ARG:NH2	2.37	0.40
1:D:526:ALA:O	1:D:530:ILE:HG13	2.21	0.40
1:E:267:GLU:HG3	1:E:270:LEU:HD12	2.03	0.40
1:E:339:GLN:O	1:E:340:LYS:C	2.63	0.40
1:E:423:ILE:HA	1:E:426:MET:HE2	2.02	0.40
1:E:478:GLY:N	1:E:479:PRO:CD	2.85	0.40
1:F:477:PRO:C	1:F:479:PRO:HD2	2.47	0.40
1:A:302:THR:O	1:A:303:ASP:O	2.40	0.40
1:A:408:MET:O	1:A:411:ALA:N	2.50	0.40
1:A:510:ILE:HG22	1:A:515:LEU:O	2.21	0.40
1:B:305:THR:HG22	1:B:306:ASP:N	2.36	0.40
1:B:403:ARG:N	1:B:405:ILE:HG13	2.36	0.40
1:B:555:ALA:O	1:B:556:LYS:C	2.65	0.40
1:B:643:VAL:O	1:B:644:ARG:C	2.65	0.40
1:C:362:SER:HB2	2:C:783:ADP:C5'	2.49	0.40
1:C:493:THR:CG2	1:C:748:SER:HB2	2.47	0.40
1:C:648:GLU:C	1:C:650:LEU:H	2.29	0.40
1:D:550:ILE:C	1:D:552:ARG:N	2.78	0.40
1:D:560:ALA:O	1:D:561:GLU:C	2.65	0.40
1:D:561:GLU:O	1:D:562:GLU:HB2	2.21	0.40
1:E:440:GLU:HG3	1:E:446:GLN:OE1	2.20	0.40
1:E:611:ILE:HD12	1:E:681:THR:HG22	2.02	0.40
1:E:613:VAL:HG13	1:E:664:ILE:HG12	2.02	0.40
1:E:622:LEU:HB2	1:E:662:ILE:CG1	2.51	0.40
1:F:276:TYR:HD1	1:F:277:GLU:N	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:ALA:O	1:F:511:LYS:NZ[2_646]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	490/543 (90%)	350 (71%)	97 (20%)	43 (9%)	0	3
1	B	490/543 (90%)	354 (72%)	94 (19%)	42 (9%)	0	4
1	C	490/543 (90%)	347 (71%)	104 (21%)	39 (8%)	1	4
1	D	490/543 (90%)	350 (71%)	102 (21%)	38 (8%)	1	4
1	E	490/543 (90%)	350 (71%)	102 (21%)	38 (8%)	1	4
1	F	490/543 (90%)	352 (72%)	99 (20%)	39 (8%)	1	4
All	All	2940/3258 (90%)	2103 (72%)	598 (20%)	239 (8%)	1	4

All (239) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	TYR
1	A	288	VAL
1	A	303	ASP
1	A	304	GLU
1	A	314	ALA
1	A	407	GLY
1	A	412	GLY
1	A	424	ASP
1	A	439	LEU
1	A	440	GLU
1	A	455	ILE
1	A	475	THR

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Mol	Chain	Res	Type
1	A	560	ALA
1	A	646	LYS
1	A	693	ARG
1	B	276	TYR
1	B	288	VAL
1	B	314	ALA
1	B	405	ILE
1	B	407	GLY
1	B	412	GLY
1	B	424	ASP
1	B	439	LEU
1	B	440	GLU
1	B	455	ILE
1	B	475	THR
1	B	560	ALA
1	B	646	LYS
1	B	693	ARG
1	C	276	TYR
1	C	288	VAL
1	C	306	ASP
1	C	314	ALA
1	C	407	GLY
1	C	412	GLY
1	C	424	ASP
1	C	439	LEU
1	C	440	GLU
1	C	455	ILE
1	C	475	THR
1	C	646	LYS
1	C	693	ARG
1	D	276	TYR
1	D	288	VAL
1	D	314	ALA
1	D	407	GLY
1	D	412	GLY
1	D	424	ASP
1	D	439	LEU
1	D	440	GLU
1	D	455	ILE
1	D	475	THR
1	D	560	ALA
1	D	646	LYS

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Mol	Chain	Res	Type
1	D	693	ARG
1	E	276	TYR
1	E	288	VAL
1	E	314	ALA
1	E	407	GLY
1	E	412	GLY
1	E	424	ASP
1	E	439	LEU
1	E	440	GLU
1	E	455	ILE
1	E	475	THR
1	E	560	ALA
1	E	646	LYS
1	E	693	ARG
1	F	276	TYR
1	F	288	VAL
1	F	314	ALA
1	F	407	GLY
1	F	412	GLY
1	F	424	ASP
1	F	439	LEU
1	F	440	GLU
1	F	455	ILE
1	F	475	THR
1	F	560	ALA
1	F	646	LYS
1	F	693	ARG
1	A	275	ARG
1	A	281	SER
1	A	313	GLU
1	A	405	ILE
1	A	474	ALA
1	A	514	GLY
1	A	603	THR
1	A	629	GLY
1	A	645	SER
1	B	275	ARG
1	B	281	SER
1	B	304	GLU
1	B	313	GLU
1	B	420	LEU
1	B	474	ALA

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Mol	Chain	Res	Type
1	B	514	GLY
1	B	629	GLY
1	B	645	SER
1	C	275	ARG
1	C	281	SER
1	C	313	GLU
1	C	405	ILE
1	C	474	ALA
1	C	514	GLY
1	C	560	ALA
1	C	629	GLY
1	C	645	SER
1	D	275	ARG
1	D	281	SER
1	D	313	GLU
1	D	405	ILE
1	D	474	ALA
1	D	514	GLY
1	D	587	ALA
1	D	629	GLY
1	D	645	SER
1	E	275	ARG
1	E	281	SER
1	E	313	GLU
1	E	405	ILE
1	E	474	ALA
1	E	514	GLY
1	E	629	GLY
1	F	275	ARG
1	F	281	SER
1	F	303	ASP
1	F	313	GLU
1	F	405	ILE
1	F	420	LEU
1	F	514	GLY
1	F	629	GLY
1	F	645	SER
1	A	262	PRO
1	A	342	THR
1	A	416	PRO
1	A	420	LEU
1	A	456	GLU

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Mol	Chain	Res	Type
1	A	637	GLN
1	B	262	PRO
1	B	303	ASP
1	B	342	THR
1	B	456	GLU
1	B	561	GLU
1	B	637	GLN
1	B	672	PRO
1	C	262	PRO
1	C	342	THR
1	C	416	PRO
1	C	456	GLU
1	C	672	PRO
1	D	262	PRO
1	D	299	LEU
1	D	342	THR
1	D	416	PRO
1	D	456	GLU
1	D	561	GLU
1	D	603	THR
1	D	637	GLN
1	D	672	PRO
1	E	262	PRO
1	E	306	ASP
1	E	342	THR
1	E	416	PRO
1	E	456	GLU
1	E	637	GLN
1	E	645	SER
1	E	672	PRO
1	F	262	PRO
1	F	342	THR
1	F	416	PRO
1	F	456	GLU
1	F	474	ALA
1	F	603	THR
1	F	672	PRO
1	A	280	PRO
1	A	305	THR
1	A	330	GLU
1	A	561	GLU
1	A	672	PRO

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Mol	Chain	Res	Type
1	B	280	PRO
1	B	416	PRO
1	B	694	ALA
1	C	280	PRO
1	C	420	LEU
1	C	561	GLU
1	C	637	GLN
1	D	280	PRO
1	E	280	PRO
1	E	420	LEU
1	E	603	THR
1	F	280	PRO
1	F	421	ASP
1	F	637	GLN
1	A	248	GLU
1	A	272	GLU
1	A	591	ASP
1	B	248	GLU
1	B	270	LEU
1	B	272	GLU
1	B	323	HIS
1	B	603	THR
1	C	248	GLU
1	C	270	LEU
1	C	272	GLU
1	C	421	ASP
1	D	248	GLU
1	D	270	LEU
1	D	272	GLU
1	D	304	GLU
1	D	420	LEU
1	E	248	GLU
1	E	270	LEU
1	E	561	GLU
1	F	248	GLU
1	F	270	LEU
1	F	272	GLU
1	F	561	GLU
1	A	261	MET
1	A	270	LEU
1	A	421	ASP
1	B	261	MET

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Mol	Chain	Res	Type
1	B	421	ASP
1	C	261	MET
1	C	330	GLU
1	D	261	MET
1	E	261	MET
1	E	272	GLU
1	F	261	MET
1	C	324	GLY
1	E	324	GLY
1	F	652	ILE
1	B	324	GLY
1	B	652	ILE
1	F	324	GLY
1	C	652	ILE
1	A	324	GLY
1	A	652	ILE
1	E	652	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	415/454 (91%)	348 (84%)	67 (16%)	2	10
1	B	415/454 (91%)	347 (84%)	68 (16%)	2	10
1	C	415/454 (91%)	345 (83%)	70 (17%)	2	9
1	D	415/454 (91%)	344 (83%)	71 (17%)	2	9
1	E	415/454 (91%)	344 (83%)	71 (17%)	2	9
1	F	415/454 (91%)	349 (84%)	66 (16%)	2	10
All	All	2490/2724 (91%)	2077 (83%)	413 (17%)	2	10

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	ASP

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Mol	Chain	Res	Type
1	A	296	LEU
1	A	312	LYS
1	A	313	GLU
1	A	316	ARG
1	A	326	GLU
1	A	331	ARG
1	A	338	VAL
1	A	349	ILE
1	A	350	LEU
1	A	367	ILE
1	A	378	ILE
1	A	420	LEU
1	A	423	ILE
1	A	439	LEU
1	A	442	LEU
1	A	455	ILE
1	A	463	LYS
1	A	465	LEU
1	A	475	THR
1	A	489	ILE
1	A	493	THR
1	A	495	ILE
1	A	500	ILE
1	A	506	LEU
1	A	516	LYS
1	A	519	ASN
1	A	522	LEU
1	A	527	ILE
1	A	532	ARG
1	A	534	TYR
1	A	536	ARG
1	A	543	LEU
1	A	553	LYS
1	A	561	GLU
1	A	565	ARG
1	A	568	VAL
1	A	579	LYS
1	A	590	GLU
1	A	592	GLN
1	A	593	VAL
1	A	599	LEU
1	A	608	THR

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Mol	Chain	Res	Type
1	A	613	VAL
1	A	624	LEU
1	A	635	SER
1	A	652	ILE
1	A	656	PHE
1	A	661	ASP
1	A	666	VAL
1	A	671	VAL
1	A	673	LYS
1	A	682	MET
1	A	686	LEU
1	A	705	ILE
1	A	714	ILE
1	A	717	LEU
1	A	731	THR
1	A	732	ILE
1	A	738	ASN
1	A	747	GLU
1	A	748	SER
1	A	749	VAL
1	A	759	SER
1	A	762	ASP
1	A	763	GLU
1	A	770	VAL
1	B	263	ASP
1	B	296	LEU
1	B	299	LEU
1	B	302	THR
1	B	312	LYS
1	B	316	ARG
1	B	326	GLU
1	B	331	ARG
1	B	338	VAL
1	B	350	LEU
1	B	367	ILE
1	B	378	ILE
1	B	420	LEU
1	B	423	ILE
1	B	439	LEU
1	B	442	LEU
1	B	455	ILE
1	B	463	LYS

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Mol	Chain	Res	Type
1	B	465	LEU
1	B	475	THR
1	B	483	ARG
1	B	489	ILE
1	B	493	THR
1	B	495	ILE
1	B	500	ILE
1	B	506	LEU
1	B	516	LYS
1	B	519	ASN
1	B	522	LEU
1	B	527	ILE
1	B	536	ARG
1	B	543	LEU
1	B	553	LYS
1	B	561	GLU
1	B	565	ARG
1	B	568	VAL
1	B	579	LYS
1	B	589	THR
1	B	590	GLU
1	B	592	GLN
1	B	593	VAL
1	B	599	LEU
1	B	608	THR
1	B	613	VAL
1	B	624	LEU
1	B	635	SER
1	B	652	ILE
1	B	656	PHE
1	B	661	ASP
1	B	666	VAL
1	B	671	VAL
1	B	673	LYS
1	B	682	MET
1	B	686	LEU
1	B	705	ILE
1	B	714	ILE
1	B	717	LEU
1	B	731	THR
1	B	732	ILE
1	B	738	ASN

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Mol	Chain	Res	Type
1	B	747	GLU
1	B	748	SER
1	B	749	VAL
1	B	759	SER
1	B	762	ASP
1	B	763	GLU
1	B	767	HIS
1	B	770	VAL
1	C	263	ASP
1	C	296	LEU
1	C	303	ASP
1	C	305	THR
1	C	312	LYS
1	C	316	ARG
1	C	326	GLU
1	C	331	ARG
1	C	338	VAL
1	C	350	LEU
1	C	367	ILE
1	C	378	ILE
1	C	420	LEU
1	C	423	ILE
1	C	439	LEU
1	C	442	LEU
1	C	455	ILE
1	C	463	LYS
1	C	465	LEU
1	C	475	THR
1	C	483	ARG
1	C	489	ILE
1	C	493	THR
1	C	495	ILE
1	C	500	ILE
1	C	506	LEU
1	C	516	LYS
1	C	519	ASN
1	C	522	LEU
1	C	527	ILE
1	C	532	ARG
1	C	536	ARG
1	C	543	LEU
1	C	553	LYS

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Mol	Chain	Res	Type
1	C	561	GLU
1	C	565	ARG
1	C	568	VAL
1	C	579	LYS
1	C	583	ARG
1	C	592	GLN
1	C	593	VAL
1	C	599	LEU
1	C	608	THR
1	C	613	VAL
1	C	624	LEU
1	C	635	SER
1	C	652	ILE
1	C	656	PHE
1	C	660	TYR
1	C	661	ASP
1	C	666	VAL
1	C	671	VAL
1	C	673	LYS
1	C	682	MET
1	C	686	LEU
1	C	705	ILE
1	C	706	THR
1	C	714	ILE
1	C	717	LEU
1	C	731	THR
1	C	732	ILE
1	C	738	ASN
1	C	747	GLU
1	C	748	SER
1	C	749	VAL
1	C	759	SER
1	C	762	ASP
1	C	763	GLU
1	C	767	HIS
1	C	770	VAL
1	D	263	ASP
1	D	296	LEU
1	D	303	ASP
1	D	305	THR
1	D	312	LYS
1	D	313	GLU

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Mol	Chain	Res	Type
1	D	316	ARG
1	D	326	GLU
1	D	331	ARG
1	D	338	VAL
1	D	349	ILE
1	D	350	LEU
1	D	367	ILE
1	D	378	ILE
1	D	420	LEU
1	D	423	ILE
1	D	439	LEU
1	D	442	LEU
1	D	455	ILE
1	D	463	LYS
1	D	465	LEU
1	D	475	THR
1	D	483	ARG
1	D	489	ILE
1	D	493	THR
1	D	495	ILE
1	D	506	LEU
1	D	510	ILE
1	D	516	LYS
1	D	519	ASN
1	D	522	LEU
1	D	527	ILE
1	D	532	ARG
1	D	536	ARG
1	D	543	LEU
1	D	553	LYS
1	D	561	GLU
1	D	565	ARG
1	D	568	VAL
1	D	579	LYS
1	D	583	ARG
1	D	589	THR
1	D	592	GLN
1	D	593	VAL
1	D	599	LEU
1	D	608	THR
1	D	613	VAL
1	D	624	LEU

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Mol	Chain	Res	Type
1	D	635	SER
1	D	652	ILE
1	D	656	PHE
1	D	660	TYR
1	D	661	ASP
1	D	666	VAL
1	D	671	VAL
1	D	673	LYS
1	D	682	MET
1	D	686	LEU
1	D	705	ILE
1	D	714	ILE
1	D	717	LEU
1	D	731	THR
1	D	732	ILE
1	D	738	ASN
1	D	747	GLU
1	D	748	SER
1	D	749	VAL
1	D	759	SER
1	D	762	ASP
1	D	763	GLU
1	D	770	VAL
1	E	263	ASP
1	E	296	LEU
1	E	302	THR
1	E	303	ASP
1	E	312	LYS
1	E	313	GLU
1	E	316	ARG
1	E	317	LEU
1	E	326	GLU
1	E	331	ARG
1	E	338	VAL
1	E	349	ILE
1	E	350	LEU
1	E	367	ILE
1	E	378	ILE
1	E	420	LEU
1	E	423	ILE
1	E	424	ASP
1	E	439	LEU

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Mol	Chain	Res	Type
1	E	442	LEU
1	E	455	ILE
1	E	463	LYS
1	E	465	LEU
1	E	475	THR
1	E	489	ILE
1	E	493	THR
1	E	495	ILE
1	E	506	LEU
1	E	516	LYS
1	E	519	ASN
1	E	522	LEU
1	E	527	ILE
1	E	532	ARG
1	E	536	ARG
1	E	543	LEU
1	E	553	LYS
1	E	561	GLU
1	E	565	ARG
1	E	568	VAL
1	E	579	LYS
1	E	590	GLU
1	E	592	GLN
1	E	593	VAL
1	E	599	LEU
1	E	608	THR
1	E	613	VAL
1	E	624	LEU
1	E	635	SER
1	E	652	ILE
1	E	656	PHE
1	E	661	ASP
1	E	666	VAL
1	E	671	VAL
1	E	673	LYS
1	E	682	MET
1	E	686	LEU
1	E	705	ILE
1	E	706	THR
1	E	714	ILE
1	E	717	LEU
1	E	731	THR

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Mol	Chain	Res	Type
1	E	732	ILE
1	E	738	ASN
1	E	747	GLU
1	E	748	SER
1	E	749	VAL
1	E	759	SER
1	E	762	ASP
1	E	763	GLU
1	E	767	HIS
1	E	770	VAL
1	F	263	ASP
1	F	296	LEU
1	F	305	THR
1	F	312	LYS
1	F	316	ARG
1	F	326	GLU
1	F	331	ARG
1	F	338	VAL
1	F	350	LEU
1	F	367	ILE
1	F	378	ILE
1	F	423	ILE
1	F	439	LEU
1	F	442	LEU
1	F	455	ILE
1	F	463	LYS
1	F	465	LEU
1	F	475	THR
1	F	489	ILE
1	F	493	THR
1	F	495	ILE
1	F	500	ILE
1	F	506	LEU
1	F	516	LYS
1	F	519	ASN
1	F	522	LEU
1	F	527	ILE
1	F	532	ARG
1	F	536	ARG
1	F	543	LEU
1	F	553	LYS
1	F	561	GLU

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Mol	Chain	Res	Type
1	F	565	ARG
1	F	568	VAL
1	F	579	LYS
1	F	588	GLU
1	F	589	THR
1	F	592	GLN
1	F	593	VAL
1	F	599	LEU
1	F	608	THR
1	F	624	LEU
1	F	635	SER
1	F	652	ILE
1	F	656	PHE
1	F	661	ASP
1	F	666	VAL
1	F	671	VAL
1	F	673	LYS
1	F	682	MET
1	F	686	LEU
1	F	705	ILE
1	F	706	THR
1	F	714	ILE
1	F	717	LEU
1	F	731	THR
1	F	732	ILE
1	F	738	ASN
1	F	747	GLU
1	F	748	SER
1	F	749	VAL
1	F	759	SER
1	F	762	ASP
1	F	763	GLU
1	F	767	HIS
1	F	770	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	446	GLN
1	A	767	HIS
1	B	250	GLN

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Continued from previous page...

Mol	Chain	Res	Type
1	B	446	GLN
1	B	586	GLN
1	B	767	HIS
1	C	250	GLN
1	C	291	ASN
1	C	446	GLN
1	C	586	GLN
1	C	767	HIS
1	D	250	GLN
1	D	446	GLN
1	D	767	HIS
1	E	250	GLN
1	E	446	GLN
1	E	767	HIS
1	F	250	GLN
1	F	767	HIS

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	E	783	-	28,29,29	1.55	4 (14%)	43,45,45	2.57	15 (34%)
2	ADP	F	783	-	28,29,29	1.43	4 (14%)	43,45,45	2.24	14 (32%)
2	ADP	C	783	-	28,29,29	1.60	4 (14%)	43,45,45	2.44	16 (37%)
2	ADP	D	783	-	28,29,29	1.75	5 (17%)	43,45,45	2.19	14 (32%)
2	ADP	A	783	-	28,29,29	1.69	4 (14%)	43,45,45	2.40	15 (34%)
2	ADP	B	783	-	28,29,29	1.38	3 (10%)	43,45,45	2.15	10 (23%)

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
2	ADP	E	783	-	-	8/16/32/32	0/3/3/3
2	ADP	F	783	-	-	6/16/32/32	0/3/3/3
2	ADP	C	783	-	-	6/16/32/32	0/3/3/3
2	ADP	D	783	-	-	6/16/32/32	0/3/3/3
2	ADP	A	783	-	-	5/16/32/32	0/3/3/3
2	ADP	B	783	-	-	5/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	783	ADP	C5-C4	6.22	1.50	1.39
2	C	783	ADP	C5-C4	5.76	1.49	1.39
2	D	783	ADP	C5-C4	5.30	1.48	1.39
2	E	783	ADP	C5-C4	5.09	1.48	1.39
2	F	783	ADP	C5-C4	4.68	1.47	1.39
2	B	783	ADP	C5-C4	4.27	1.46	1.39
2	D	783	ADP	C5-N7	-3.67	1.32	1.39
2	E	783	ADP	C5-C6	3.50	1.50	1.41
2	A	783	ADP	C5-C6	3.18	1.49	1.41
2	D	783	ADP	C8-N7	3.05	1.37	1.31
2	A	783	ADP	C8-N7	2.95	1.37	1.31
2	C	783	ADP	C5-C6	2.91	1.49	1.41
2	D	783	ADP	PA-O3A	2.90	1.62	1.59
2	F	783	ADP	C5-N7	-2.79	1.34	1.39
2	C	783	ADP	C5-N7	-2.79	1.34	1.39
2	B	783	ADP	C5-N7	-2.74	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	783	ADP	C8-N7	2.74	1.36	1.31
2	F	783	ADP	C5-C6	2.51	1.48	1.41
2	C	783	ADP	C8-N7	2.48	1.36	1.31
2	B	783	ADP	C8-N7	2.45	1.36	1.31
2	A	783	ADP	C5-N7	-2.44	1.34	1.39
2	F	783	ADP	C8-N7	2.22	1.35	1.31
2	D	783	ADP	PB-O3B	-2.18	1.46	1.54
2	E	783	ADP	C5-N7	-2.05	1.35	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	783	ADP	C5-C4-N3	-8.99	114.34	126.72
2	A	783	ADP	C5-C4-N3	-8.67	114.78	126.72
2	C	783	ADP	C5-C4-N3	-7.77	116.01	126.72
2	D	783	ADP	C5-C4-N3	-7.54	116.33	126.72
2	B	783	ADP	C5-C4-N3	-7.00	117.08	126.72
2	F	783	ADP	C5-C4-N3	-6.78	117.38	126.72
2	E	783	ADP	C4-C5-N7	-5.89	103.85	110.58
2	A	783	ADP	N3-C4-N9	5.69	136.85	127.17
2	E	783	ADP	N3-C4-N9	5.63	136.74	127.17
2	C	783	ADP	N3-C4-N9	5.43	136.41	127.17
2	B	783	ADP	N3-C4-N9	5.42	136.39	127.17
2	A	783	ADP	C4-C5-N7	-5.29	104.53	110.58
2	F	783	ADP	N3-C4-N9	5.05	135.75	127.17
2	D	783	ADP	N3-C4-N9	4.61	135.00	127.17
2	E	783	ADP	C2-N3-C4	4.59	123.05	111.83
2	C	783	ADP	C4-C5-N7	-4.15	105.83	110.58
2	D	783	ADP	C4-C5-N7	-4.15	105.83	110.58
2	F	783	ADP	O2'-C2'-C1'	-4.07	96.08	110.10
2	B	783	ADP	C2-N3-C4	4.04	121.70	111.83
2	C	783	ADP	O4'-C1'-C2'	-3.95	98.17	106.62
2	F	783	ADP	C2-N3-C4	3.94	121.45	111.83
2	C	783	ADP	C2-N3-C4	3.81	121.14	111.83
2	B	783	ADP	O2'-C2'-C1'	-3.65	97.52	110.10
2	F	783	ADP	O4'-C1'-C2'	-3.63	98.85	106.62
2	A	783	ADP	C2-N3-C4	3.63	120.69	111.83
2	D	783	ADP	C2-N3-C4	3.61	120.64	111.83
2	F	783	ADP	C2'-C3'-C4'	-3.60	95.65	102.61
2	E	783	ADP	C5-N7-C8	3.59	109.09	103.45
2	F	783	ADP	C4-C5-N7	-3.47	106.62	110.58
2	B	783	ADP	N3-C2-N1	-3.41	123.42	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	783	ADP	C4-C5-N7	-3.36	106.74	110.58
2	C	783	ADP	O3B-PB-O2B	3.28	120.09	107.80
2	C	783	ADP	C2'-C3'-C4'	-3.26	96.31	102.61
2	C	783	ADP	O2'-C2'-C1'	-3.24	98.94	110.10
2	C	783	ADP	C4-N9-C1'	3.12	133.93	126.63
2	C	783	ADP	O2A-PA-O1A	3.10	126.84	112.44
2	D	783	ADP	O3B-PB-O3A	-3.07	94.35	104.64
2	A	783	ADP	C5-N7-C8	3.07	108.27	103.45
2	F	783	ADP	N3-C2-N1	-3.05	123.96	128.58
2	A	783	ADP	C6-C5-C4	3.00	121.28	117.18
2	C	783	ADP	C1'-N9-C8	-2.99	120.46	127.09
2	A	783	ADP	C4-N9-C1'	2.99	133.62	126.63
2	D	783	ADP	C2'-C1'-N9	-2.91	106.07	113.30
2	A	783	ADP	C1'-N9-C8	-2.89	120.67	127.09
2	E	783	ADP	C5-C4-N9	2.84	108.91	105.81
2	C	783	ADP	O5'-C5'-C4'	-2.84	99.34	108.99
2	E	783	ADP	O5'-C5'-C4'	-2.77	99.57	108.99
2	A	783	ADP	O3A-PB-O1B	-2.69	96.90	111.04
2	E	783	ADP	O4'-C4'-C5'	-2.66	100.80	109.33
2	D	783	ADP	N3-C2-N1	-2.65	124.57	128.58
2	B	783	ADP	O2'-C2'-C3'	-2.64	103.37	111.82
2	D	783	ADP	C5-C4-N9	2.62	108.67	105.81
2	D	783	ADP	C2-N1-C6	2.62	123.03	118.73
2	B	783	ADP	C5-N7-C8	2.59	107.52	103.45
2	E	783	ADP	O2A-PA-O1A	2.56	124.36	112.44
2	D	783	ADP	C4-N9-C1'	2.55	132.59	126.63
2	B	783	ADP	O3A-PB-O1B	-2.54	97.66	111.04
2	A	783	ADP	O2'-C2'-C1'	-2.53	101.39	110.10
2	F	783	ADP	O3B-PB-O2B	2.51	117.20	107.80
2	E	783	ADP	O3B-PB-O2B	2.50	117.19	107.80
2	C	783	ADP	N3-C2-N1	-2.50	124.80	128.58
2	E	783	ADP	O2B-PB-O3A	-2.48	96.33	104.64
2	F	783	ADP	O2'-C2'-C3'	-2.46	103.93	111.82
2	C	783	ADP	C5-N7-C8	2.45	107.30	103.45
2	F	783	ADP	C5-N7-C8	2.40	107.22	103.45
2	F	783	ADP	O5'-C5'-C4'	-2.39	100.86	108.99
2	D	783	ADP	C5-N7-C8	2.37	107.18	103.45
2	D	783	ADP	C6-C5-C4	2.35	120.39	117.18
2	A	783	ADP	O2B-PB-O3A	2.35	112.51	104.64
2	A	783	ADP	C5-C4-N9	2.34	108.36	105.81
2	C	783	ADP	C6-C5-C4	2.29	120.31	117.18
2	D	783	ADP	O5'-C5'-C4'	2.25	116.67	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	783	ADP	O2A-PA-O1A	2.24	122.87	112.44
2	A	783	ADP	O2A-PA-O1A	2.24	122.86	112.44
2	E	783	ADP	C6-C5-N7	2.19	136.31	132.09
2	C	783	ADP	O2'-C2'-C3'	-2.18	104.82	111.82
2	E	783	ADP	O5'-PA-O1A	-2.15	100.40	108.94
2	A	783	ADP	O3B-PB-O1B	2.15	119.21	110.83
2	E	783	ADP	PA-O5'-C5'	-2.14	109.11	121.35
2	E	783	ADP	N3-C2-N1	-2.12	125.37	128.58
2	A	783	ADP	O3B-PB-O3A	-2.11	97.56	104.64
2	B	783	ADP	C4-N9-C8	2.10	107.94	105.74
2	D	783	ADP	O3B-PB-O2B	2.04	115.44	107.80
2	F	783	ADP	C1'-N9-C8	-2.00	122.65	127.09

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	783	ADP	C4'-C5'-O5'-PA
2	A	783	ADP	O4'-C4'-C5'-O5'
2	A	783	ADP	C3'-C4'-C5'-O5'
2	A	783	ADP	C2'-C1'-N9-C8
2	A	783	ADP	C2'-C1'-N9-C4
2	B	783	ADP	C4'-C5'-O5'-PA
2	B	783	ADP	O4'-C4'-C5'-O5'
2	C	783	ADP	C5'-O5'-PA-O2A
2	C	783	ADP	O4'-C4'-C5'-O5'
2	D	783	ADP	PA-O3A-PB-O3B
2	D	783	ADP	C4'-C5'-O5'-PA
2	E	783	ADP	C5'-O5'-PA-O1A
2	E	783	ADP	C5'-O5'-PA-O2A
2	E	783	ADP	C5'-O5'-PA-O3A
2	F	783	ADP	O4'-C4'-C5'-O5'
2	B	783	ADP	C3'-C4'-C5'-O5'
2	C	783	ADP	C3'-C4'-C5'-O5'
2	F	783	ADP	C3'-C4'-C5'-O5'
2	E	783	ADP	O4'-C4'-C5'-O5'
2	E	783	ADP	C3'-C4'-C5'-O5'
2	B	783	ADP	C2'-C1'-N9-C4
2	C	783	ADP	C2'-C1'-N9-C4
2	E	783	ADP	C2'-C1'-N9-C4
2	C	783	ADP	C4'-C5'-O5'-PA
2	C	783	ADP	C2'-C1'-N9-C8

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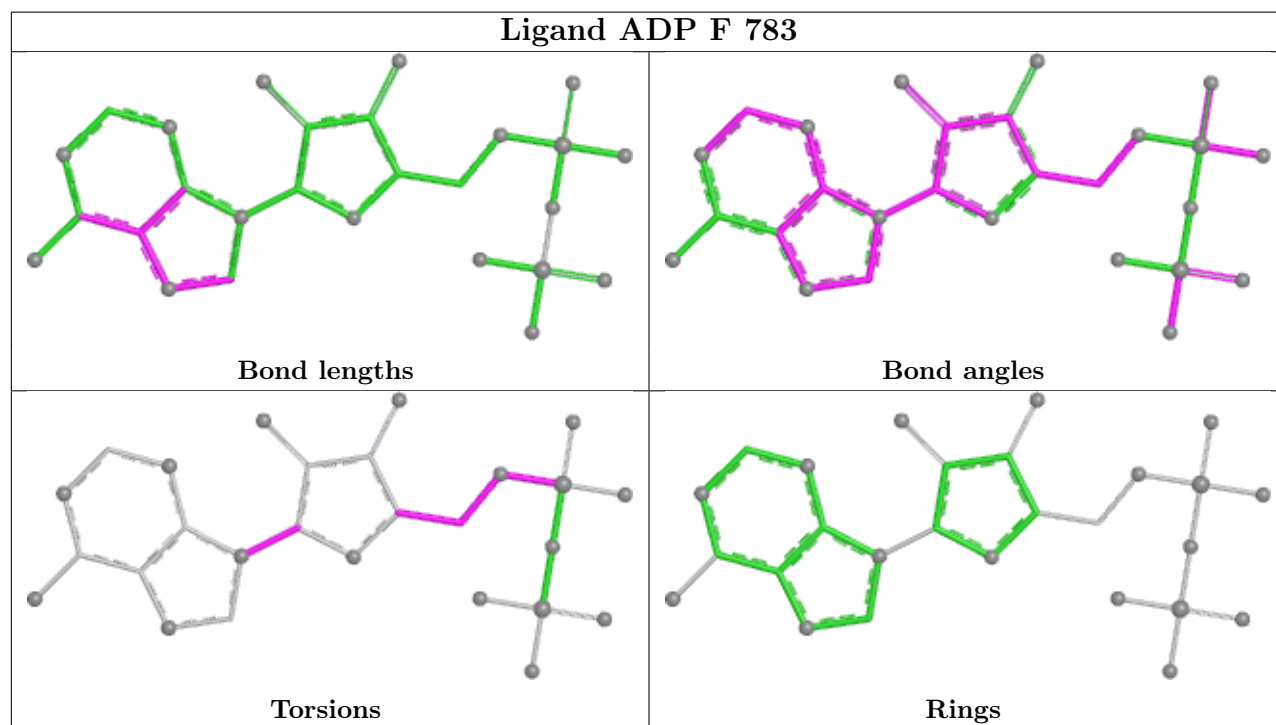
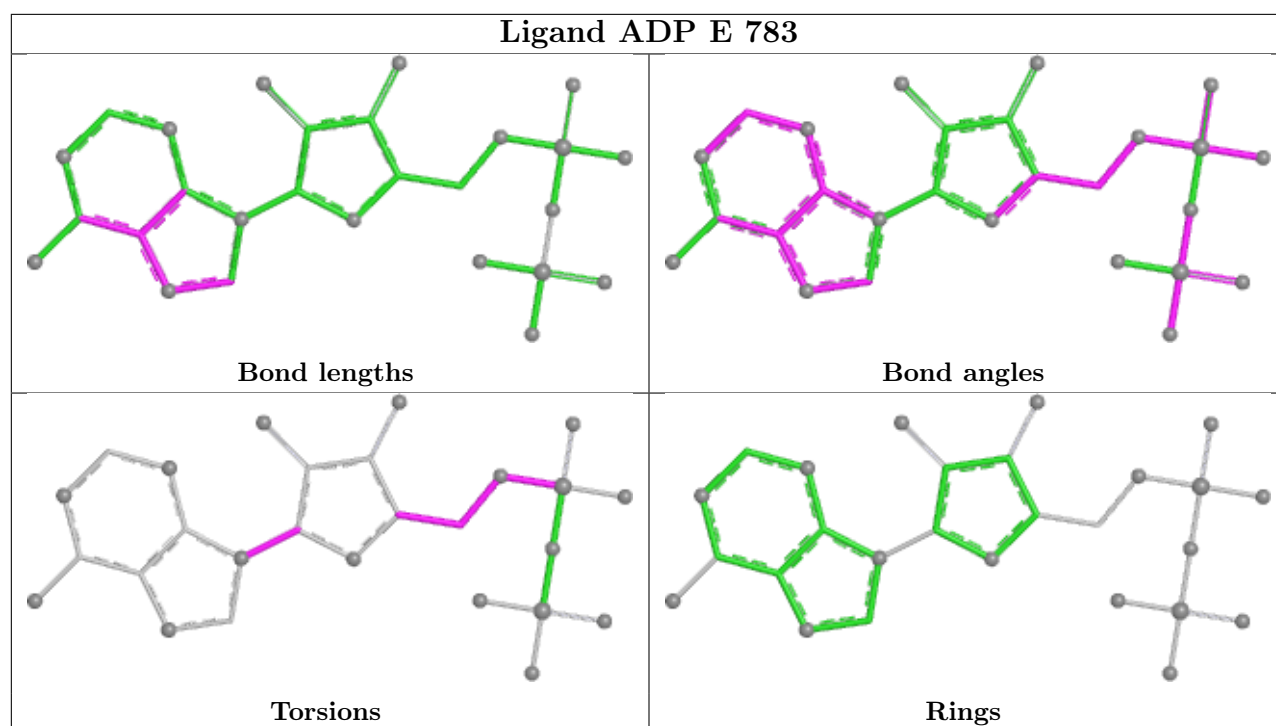
Mol	Chain	Res	Type	Atoms
2	F	783	ADP	C2'-C1'-N9-C4
2	D	783	ADP	C3'-C4'-C5'-O5'
2	F	783	ADP	C4'-C5'-O5'-PA
2	E	783	ADP	C4'-C5'-O5'-PA
2	B	783	ADP	C2'-C1'-N9-C8
2	E	783	ADP	C2'-C1'-N9-C8
2	F	783	ADP	C2'-C1'-N9-C8
2	F	783	ADP	C5'-O5'-PA-O2A
2	D	783	ADP	O4'-C4'-C5'-O5'
2	D	783	ADP	C2'-C1'-N9-C8
2	D	783	ADP	C2'-C1'-N9-C4

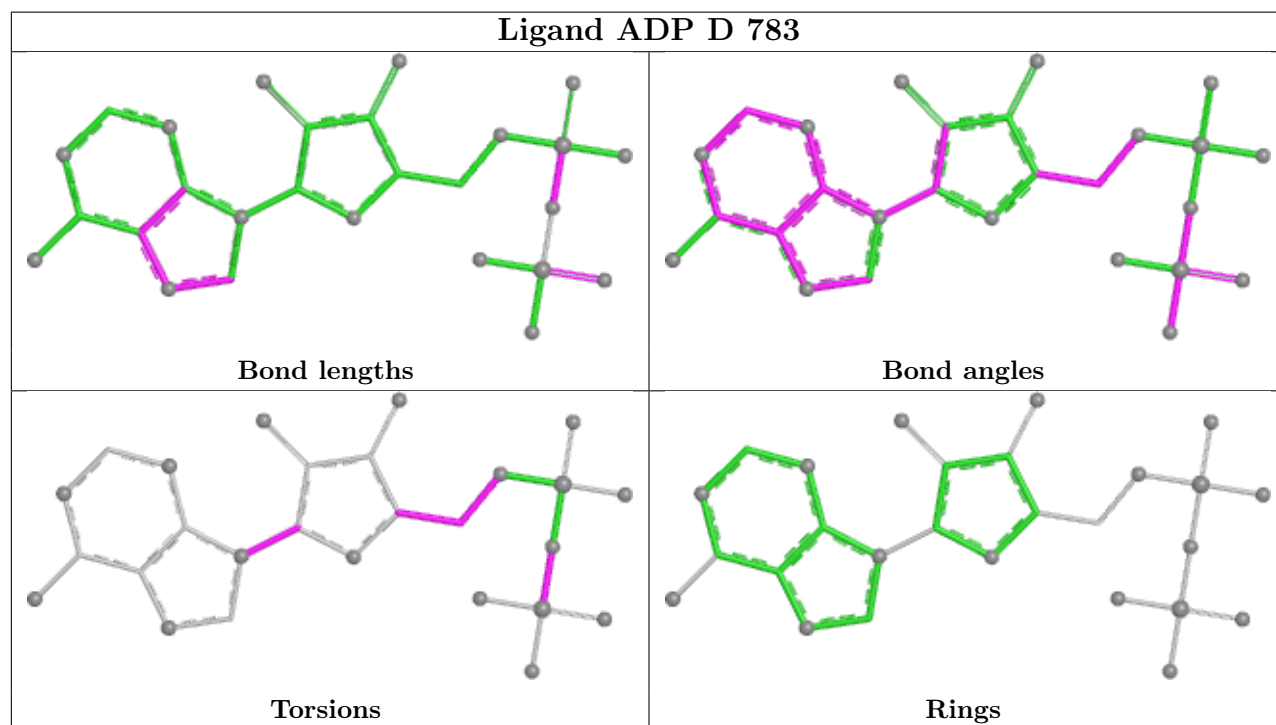
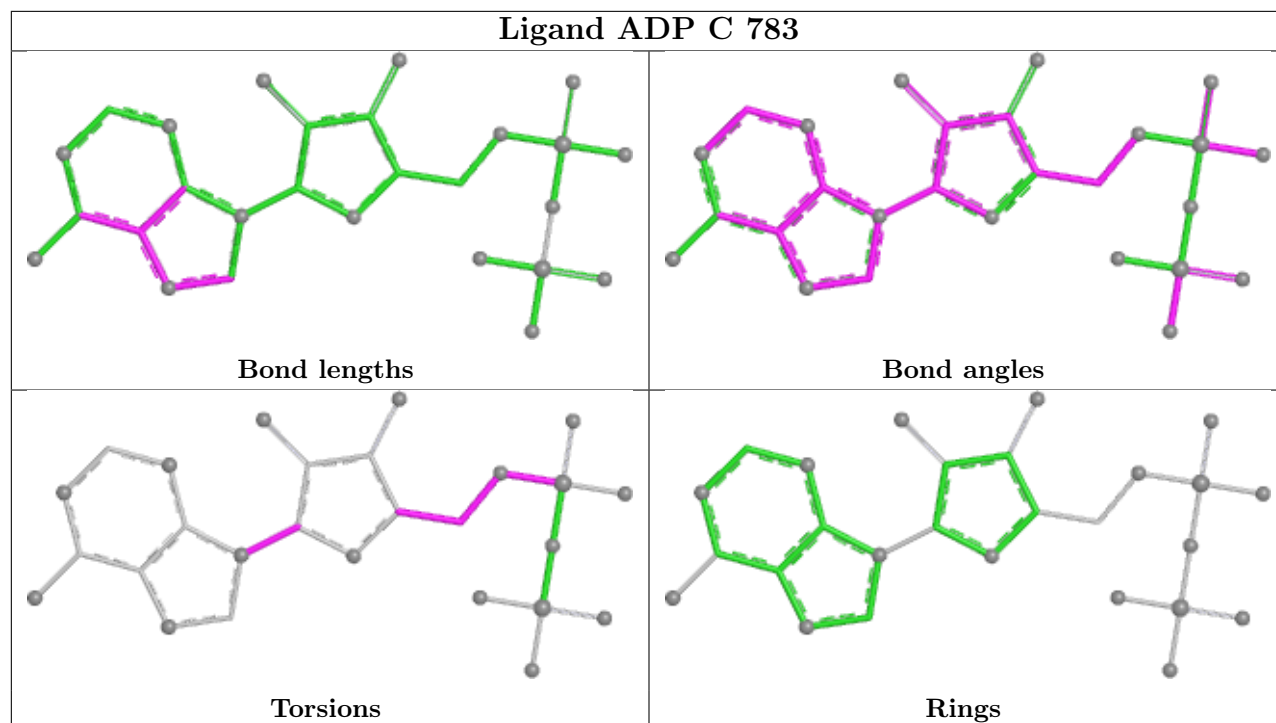
There are no ring outliers.

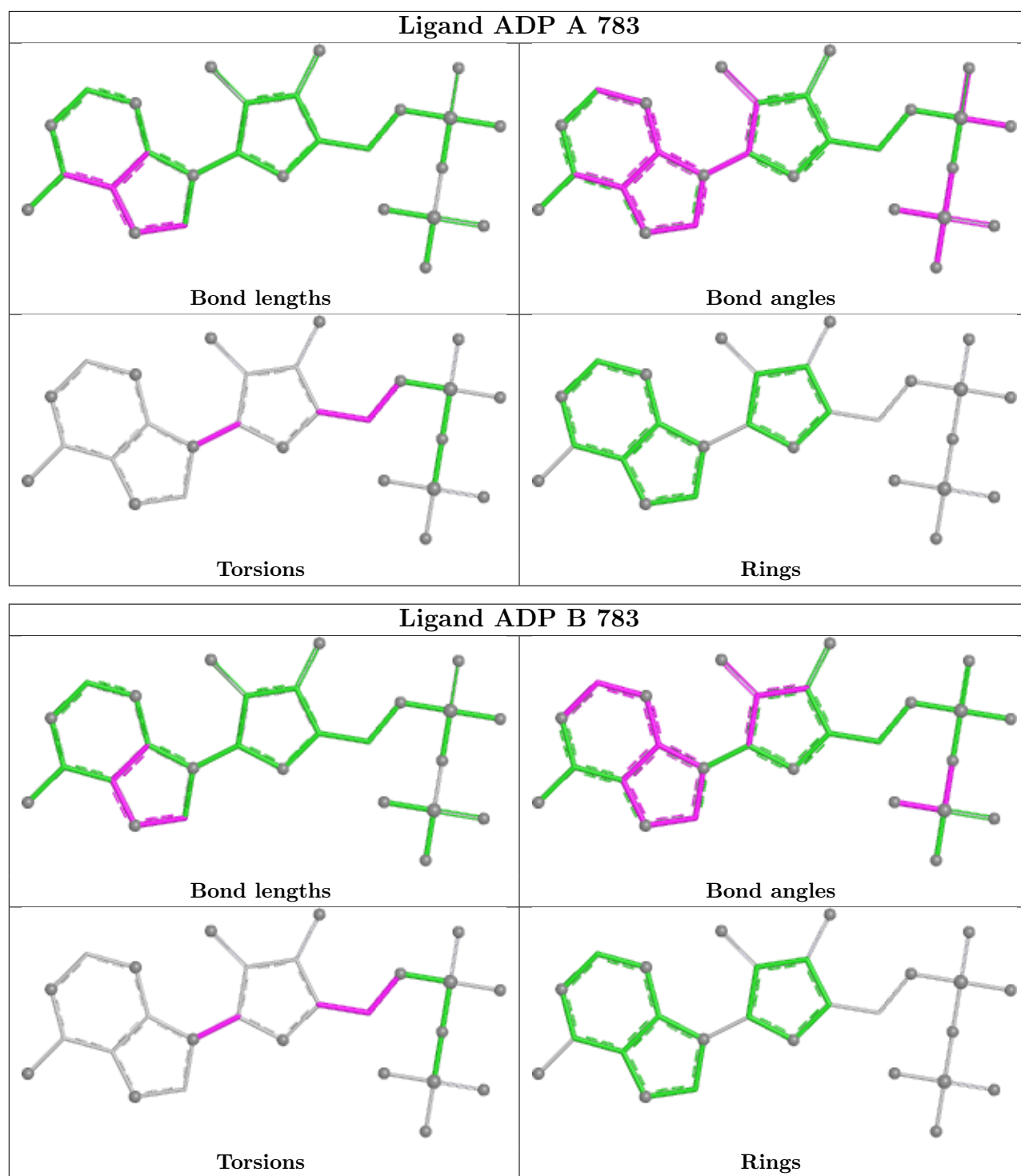
6 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	783	ADP	6	0
2	F	783	ADP	7	0
2	C	783	ADP	6	0
2	D	783	ADP	11	0
2	A	783	ADP	7	0
2	B	783	ADP	7	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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/543 (91%)	-0.13	13 (2%) 57 42	69, 145, 461, 643	0
1	B	496/543 (91%)	-0.05	19 (3%) 44 31	75, 143, 456, 637	0
1	C	496/543 (91%)	-0.25	6 (1%) 76 63	71, 145, 458, 683	0
1	D	496/543 (91%)	-0.18	9 (1%) 67 53	65, 144, 463, 696	0
1	E	496/543 (91%)	-0.16	5 (1%) 79 66	75, 146, 466, 682	0
1	F	496/543 (91%)	-0.23	7 (1%) 73 59	78, 148, 457, 672	0
All	All	2976/3258 (91%)	-0.17	59 (1%) 65 49	65, 145, 464, 696	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	ALA	5.7
1	C	337	ALA	5.2
1	A	337	ALA	5.0
1	B	341	LEU	4.5
1	B	337	ALA	4.5
1	A	338	VAL	4.3
1	B	342	THR	4.0
1	B	338	VAL	3.6
1	D	341	LEU	3.4
1	C	455	ILE	3.3
1	B	437	ALA	3.2
1	B	282	SER	3.1
1	A	341	LEU	3.1
1	C	341	LEU	3.1
1	D	405	ILE	3.0
1	F	256	ILE	3.0
1	F	252	LEU	3.0
1	E	337	ALA	2.9
1	A	249	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	253	THR	2.8
1	A	639	ALA	2.7
1	D	342	THR	2.7
1	D	338	VAL	2.7
1	D	449	SER	2.6
1	A	301	TRP	2.5
1	D	408	MET	2.5
1	A	459	PHE	2.5
1	F	253	THR	2.5
1	F	459	PHE	2.5
1	E	615	LEU	2.5
1	E	341	LEU	2.4
1	D	454	TYR	2.4
1	B	666	VAL	2.4
1	B	582	PHE	2.4
1	D	339	GLN	2.4
1	C	601	TYR	2.3
1	B	446	GLN	2.3
1	B	581	ILE	2.2
1	B	301	TRP	2.2
1	F	551	CYS	2.2
1	E	405	ILE	2.2
1	A	268	THR	2.2
1	B	339	GLN	2.2
1	B	253	THR	2.2
1	B	676	PRO	2.2
1	A	293	ILE	2.1
1	B	300	PRO	2.1
1	A	270	LEU	2.1
1	A	746	PRO	2.1
1	B	286	SER	2.1
1	B	459	PHE	2.1
1	C	342	THR	2.1
1	F	426	MET	2.1
1	B	447	ASN	2.0
1	E	450	PHE	2.0
1	C	338	VAL	2.0
1	F	287	SER	2.0
1	B	274	ASN	2.0
1	A	450	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

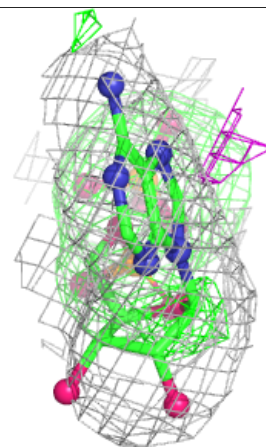
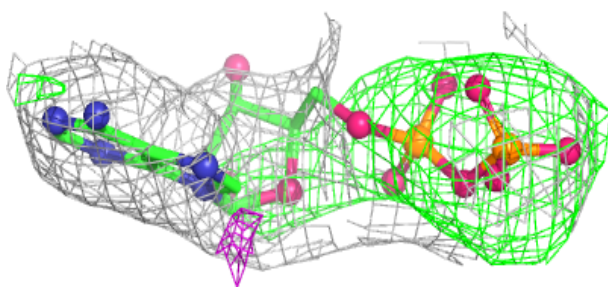
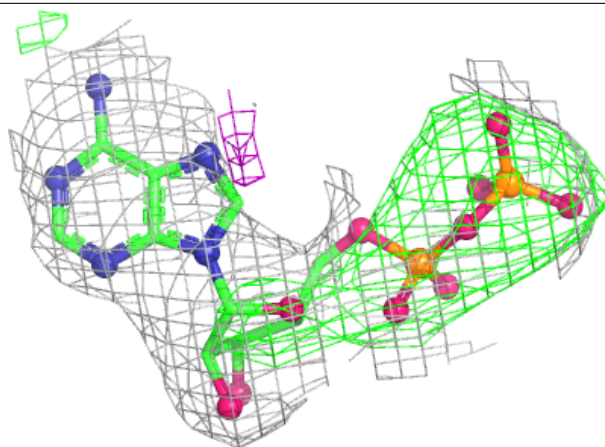
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	D	783	27/27	0.86	0.20	30,142,369,458	0
2	ADP	B	783	27/27	0.94	0.09	73,123,341,499	0
2	ADP	C	783	27/27	0.96	0.10	57,125,341,462	0
2	ADP	A	783	27/27	0.96	0.07	55,104,341,499	0
2	ADP	E	783	27/27	0.96	0.07	53,114,341,491	0
2	ADP	F	783	27/27	0.96	0.07	57,123,341,482	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

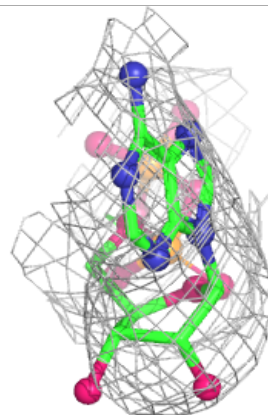
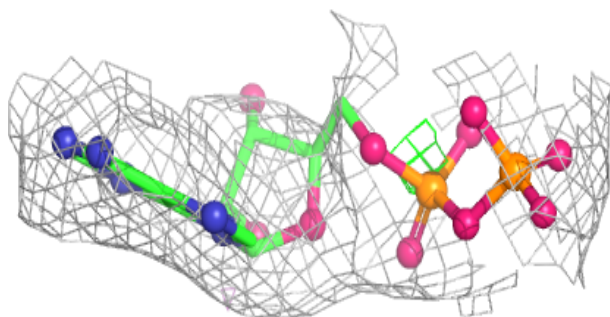
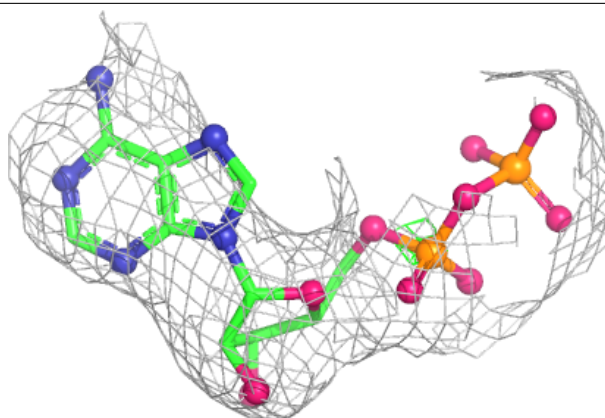
Electron density around ADP D 783:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



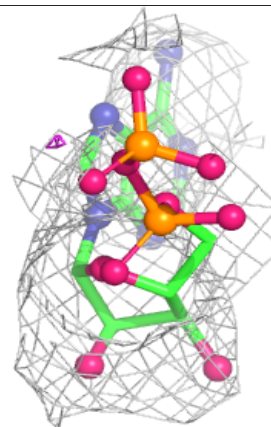
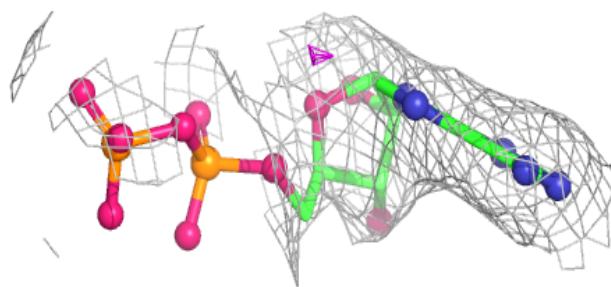
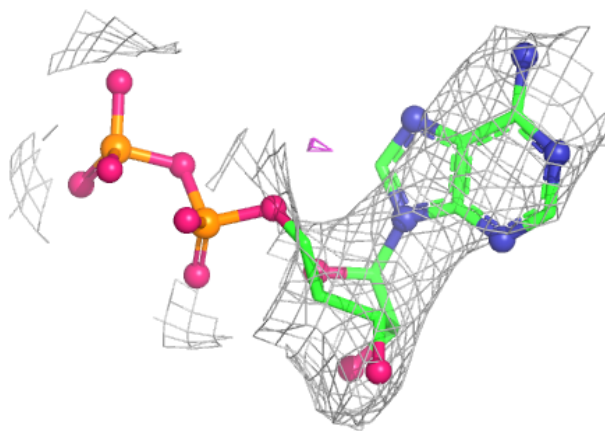
Electron density around ADP B 783:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



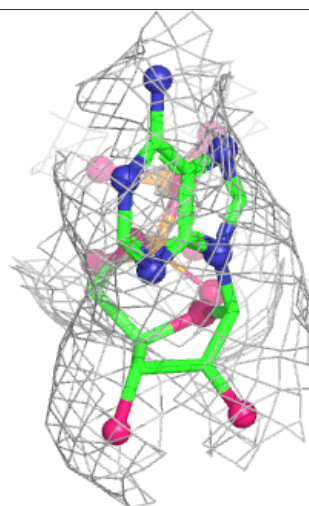
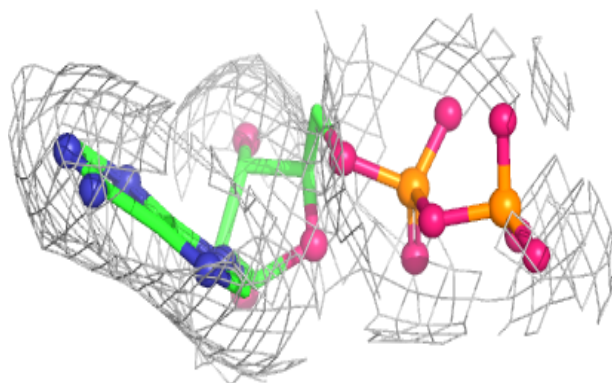
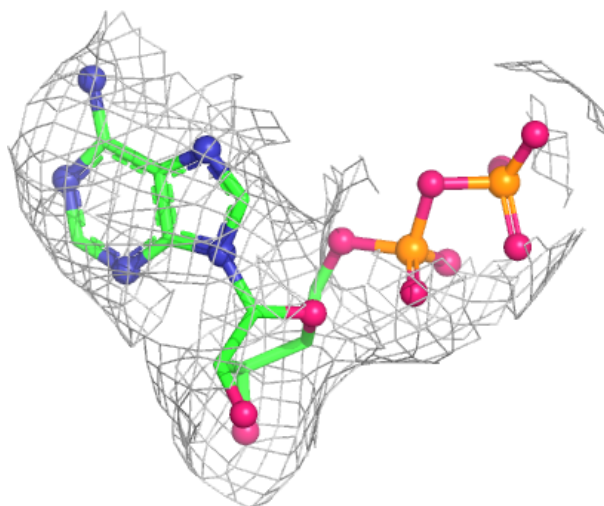
Electron density around ADP C 783:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



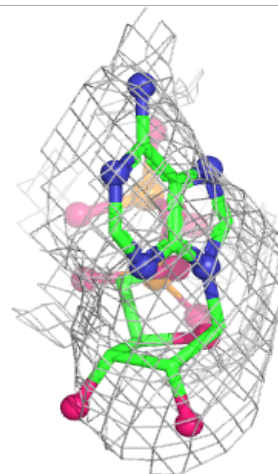
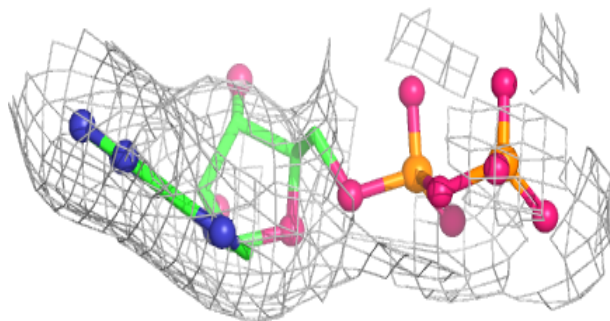
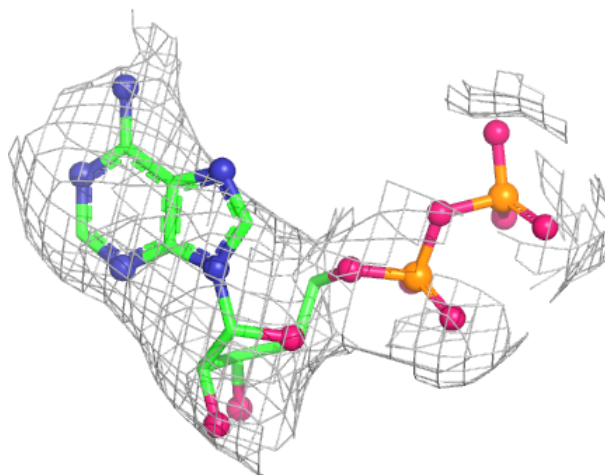
Electron density around ADP A 783:

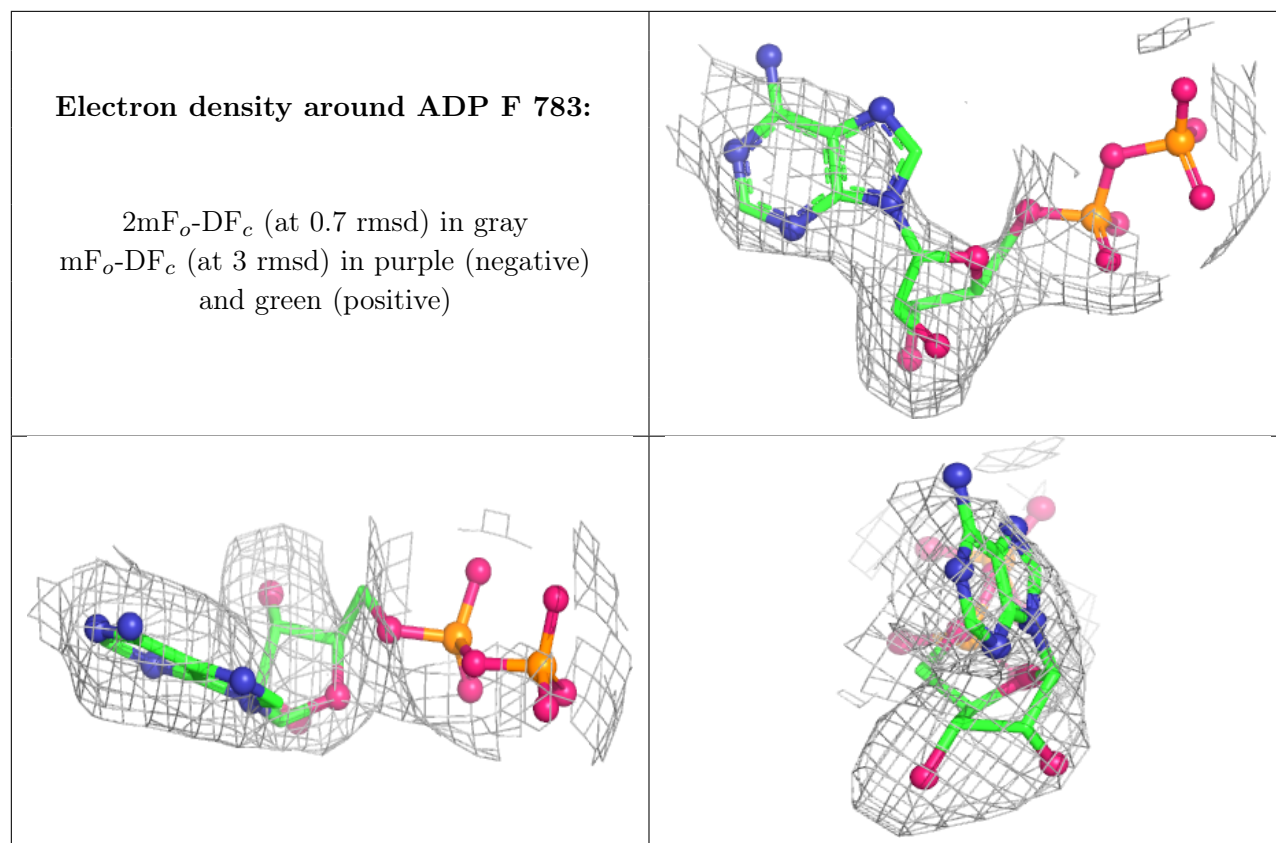
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP E 783:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.