



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3J95
EMDB ID: : EMD-6205
Title : Structure of ADP-bound N-ethylmaleimide sensitive factor determined by single particle cryoelectron microscopy
Authors : Zhao, M.; Wu, S.; Cheng, Y.; Brunger, A.T.
Deposited on : 2014-12-05
Resolution : 7.60 Å(reported)
Based on PDB ID : 1NSF

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

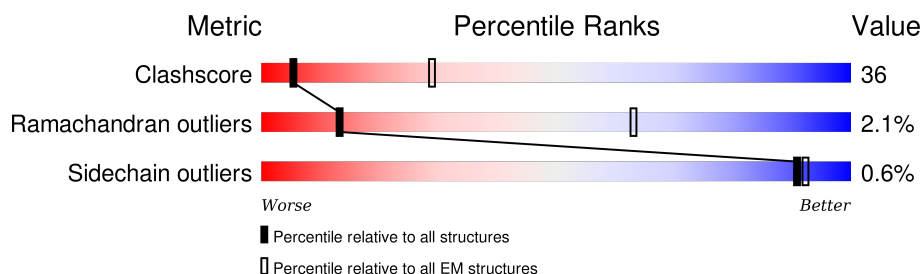
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	747	30% 32% . 35%
1	B	747	32% 31% . 36%
1	C	747	31% 33% . 35%
1	D	747	32% 31% . 36%
1	E	747	28% 35% . 35%
1	F	747	30% 32% .. 37%

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	B	801	-	-	X	-
2	ADP	D	801	-	-	X	-
2	ADP	E	801	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

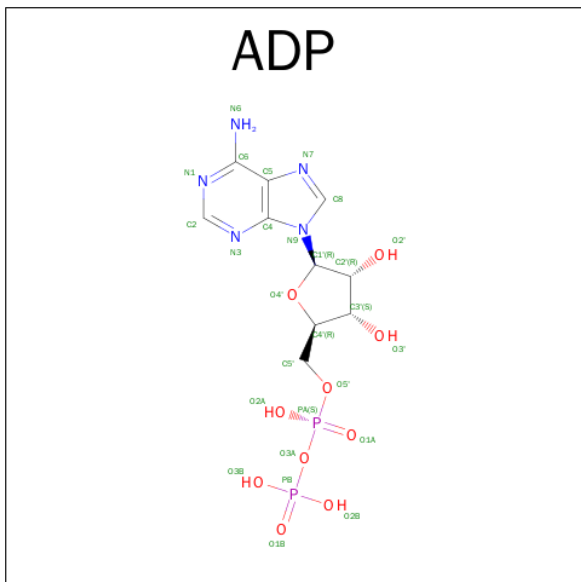
- Molecule 1 is a protein called Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	483	Total	C	N	O	S	0	0
			3513	2221	617	660	15		
1	B	481	Total	C	N	O	S	0	0
			3517	2230	611	660	16		
1	C	485	Total	C	N	O	S	0	0
			3535	2236	618	666	15		
1	D	479	Total	C	N	O	S	0	0
			3467	2203	594	654	16		
1	E	482	Total	C	N	O	S	0	0
			3516	2233	611	656	16		
1	F	473	Total	C	N	O	S	0	0
			3467	2197	609	645	16		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P18708
A	-1	ALA	-	EXPRESSION TAG	UNP P18708
A	0	HIS	-	EXPRESSION TAG	UNP P18708
B	-2	GLY	-	EXPRESSION TAG	UNP P18708
B	-1	ALA	-	EXPRESSION TAG	UNP P18708
B	0	HIS	-	EXPRESSION TAG	UNP P18708
C	-2	GLY	-	EXPRESSION TAG	UNP P18708
C	-1	ALA	-	EXPRESSION TAG	UNP P18708
C	0	HIS	-	EXPRESSION TAG	UNP P18708
D	-2	GLY	-	EXPRESSION TAG	UNP P18708
D	-1	ALA	-	EXPRESSION TAG	UNP P18708
D	0	HIS	-	EXPRESSION TAG	UNP P18708
E	-2	GLY	-	EXPRESSION TAG	UNP P18708
E	-1	ALA	-	EXPRESSION TAG	UNP P18708
E	0	HIS	-	EXPRESSION TAG	UNP P18708
F	-2	GLY	-	EXPRESSION TAG	UNP P18708
F	-1	ALA	-	EXPRESSION TAG	UNP P18708
F	0	HIS	-	EXPRESSION TAG	UNP P18708

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



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

GLY	ALA	GLY	P242	S320	V391	ALA	P535	Y611	L683
ALA	SER	ALA	E243	G321	I395	GLU	L536	V612	A695
HIS	VAL	GLU	I244	L322	T395	SER	W537	I613	K699
MET	ALA	SER	V245	H323	P398	LEU	S538	I614	I707
ALA	PHE	ILE	E246	H324	D399	GLN	V539	G615	L710
GLY	SER	GLN	Q247	I325	P399	VAL	L540	P616	L711
ARG	LEU	GLN	K248	I326	G402	THR	L541	S619	L713
SER	PRO	PHE	Q249	I330	H403	ARG	E542	N620	E715
MET	GLN	GLU	K254	ASP	L404	GLY	G543	L621	M716
GLN	ARG	LYS	G255	ALA	Q405	F479	P544	Q624	L717
ALA	TRP	ALA	I256	GLU	L481	F480	P545	S546	M718
ALA	ALA	PHE	L257	ILE	I406	L481	S547	A625	L714
ARG	GLY	SER	L258	LYS	H408	A482	G548	L626	E715
CYS	LEU	VAL	P261	GLN	I409	E485	R549	L627	M716
PRO	SER	GLY	P262	ARG	S421	T550	A551	V628	Q719
THR	LEU	THR	G263	GLY	A422	I488	L552	L629	Q719
GLU	ILE	GLN	C264	LEU	D423	K489	L552	L630	L728
LEU	GLN	LEU	T267	ILE	V424	P490	A553	K631	L732
SER	GLU	VAL	L268	GLY	D425	A491	A554	K632	G737
SER	GLU	PHE	L269	LYS	K427	F492	I556	R638	ALA
ASN	VAL	SER	THR	THR	E428	G493	P563	K639	SER
CYS	ALA	ASP	L270	GLY	V431	THR	I567	L640	PRO
ALA	LEU	LYS	E271	VAL	E432	GLN	S568	I642	LEU
VAL	TYR	LEU	Q272	R347	T433	E497	S569	I643	ASP
VAL	SER	SER	I273	D348	K434	D498	P570	G644	PHE
SER	PHE	GLY	E281	T349	H435	Y499	D571	S647	ASP
GLU	ASP	GLN	P282	V350	F436	I503	I574	K648	ALA
LYS	LYS	LEU	K283	V351	S437	I504	G575	K649	ALA
ASP	ALA	LEU	V284	N352	G438	M504	P576	V651	ALA
TYR	VAL	ILE	I285	Q353	E439	M505	S577	E654	ALA
GLN	LYS	ILE	E289	L354	E440	G506	E578	M655	ALA
SER	CYS	ASP	L291	S356	L441	I507	T579	E656	ALA
GLY	ILE	TRP	K292	K357	L444	I508	A580	M657	ALA
HIS	THR	ASN	K293	I358	L444	K509	K581	L658	ALA
VAL	MET	MET	G296	I367	Q449	M510	Q582	F661	ALA
ILE	THR	THR	E297	L368	S450	G511	P583	S662	ALA
VAL	ILE	GLU	K218	V369	T451	P513	Q583	T663	ALA
ARG	ILE	ILE	Q219	I370	A452	V514	I588	I664	ALA
THR	ILE	ASP	I220	G371	M453	T515	P589	T665	ALA
SER	LEU	LYS	G221	K372	H454	R516	Y593	I666	ALA
PRO	PHE	GLY	G222	R375	H455	L518	Q596	V667	ALA
ASN	LEU	GLU	L223	D377	F457	D520	L597	P668	ALA
HIS	LYS	PRO	D224	I378	LYS	L523	V600	M669	ALA
TYR	LYS	ALA	S228	I379	ALA	L524	D603	I670	ALA
ILE	ASN	GLY	D229	D380	SER	V525	L605	A671	ALA
PHE	ILE	LYS	I230	E381	THR	Q526	D604	T672	ALA
THR	ASP	ARG	F231	A382	LYS	Q527	I605	Q675	ALA
LEU	ASN	GLN	R232	L383	VAL	T528	B606	L676	ALA
ARG	PRO	LYS	Q313	R386	GLU	S531	R607	L677	ALA
THR	THR	ILE	R314	G387	VAL	D532	L608	E681	ALA
HIS	ASP	GLU	R315	R388	ASP	R533	L609	L682	ALA
PRO	THR	VAL	L316	R389	MET	R534	D610		ALA
SER	THR	GLY	G317	L389	GLU	T534			ALA
VAL	ASP	LEU	A318	P240	LYS				ALA
VAL	LYS	VAL	P241	E243	VAL				ALA
PRO	MET	VAL	E246	N319	VAL				ALA

• Molecule 1: Vesicle-fusing ATPase

Chain C:  31% 33% 35%

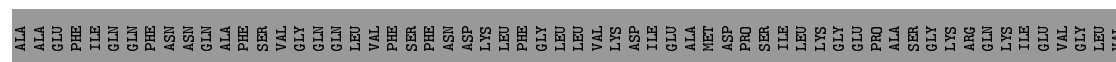
GLY	GLY	ALA	VAL	Q247
ALA	SER	ALA	GLY	P248
HIS	VAL	ALA	ASN	G249
MET	ALA	PHE	SER	E252
ALA	PHE	ILE	GLN	V253
GLY	LEU	GLN	VAL	K254
ARG	LEU	PHE	ALA	G255
SER	PRO	ARG	PHE	I256
MET	GLN	ASN	GLU	P261
GLN	ARG	LYS	LYS	P262
ALA	LYS	ALA	ALA	G263
TRP	ALA	ALA	GLU	G264
ALA	ARG	PHE	ASN	C264
CYS	GLY	SER	SER	G265
PRO	PRO	VAL	SER	L268
THR	SER	GLY	LEU	L269
THR	THR	THR	ILE	A270
GLY	GLY	GLN	GLY	K271
ILE	ILE	VAL	LYS	I273
SER	SER	PHE	ALA	E281
ASN	ASN	VAL	LYS	V284
ALA	ALA	ASP	GLY	V285
ALA	LEU	LYS	ASN	E289
VAL	TYR	LYS	GLN	I290
ASP	ALA	ASP	ILE	L291
LYS	LYS	LYS	ILE	N292
GLN	LYS	VAL	ASN	K293
GLY	LYS	ILE	TRP	E297
ASP	ALA	GLU	ASN	L305
THR	ALA	ASP	GLY	D308
VAL	VAL	PRO	K217	A309
ILE	ILE	SER	K218	E310
ARG	ILE	ILE	Q219	E311
ILE	ILE	ILE	I220	E312
ASP	ASP	PHE	F227	Q313
LEU	LEU	LEU		R314
ASN	ASN	GLY		G317
HIS	HIS	GLU	F231	A318
LYS	LYS	PRO	R232	S230
TYR	TYR	ALA	R233	N319
ILE	ILE	GLY	A234	G321
PHE	PHE	LYS	F235	L322
THR	THR	ARG	A236	H323
LEU	LEU	ASN	S237	I324
ARG	ARG	LYS	P241	I325
THR	THR	ILE	P242	I326
HIS	ASP	GLU	E243	D331
PRO	SER	VAL	I244	C334
SER	THR	GLY	V245	
VAL	LYS	LEU	E246	
VAL	MET	VAL		

K708	K709	L710	L711	L714	E715	M716	S717	L718	Q719	M720	D721	Y724	V725	L726	R727	K728	F729	A731	L732	L733	R734	G737	ALA	SER	PRO	LEU	ASP	PHE	ASP	LYS GLN ARG GLY SER MET ALA GLY SER THR GLY VAL H347 D348 T349 V350 V351 N352 L355 L358 N366 L367 L368 V369 I370 R375 P376 D377 L378 L379 SER LEU D380 E381 A382 L383 P386 G387 R388 L389 E390 V391 D399 R403 L404 L407 H408 L409 H410 T411 M414 L426	G511	D512	P513	V514	T515	R516	D519	D520	G521	E522	L523	F524	V525	Q526	T527	Y528	K529	N530	S531	D532	R533	L536	V537	S538	V539	L540	E541	E542	G543	P544	P545	A554	K555	L556	A557	E558	E559	S560	N561	F562	P563	F564	L565	C568	S569	P570	D571	B572	R573	L574
G575	F576	S577	E578	T579	A580	K581	C582	Q583	A584	I588	F589	D590	D591	A592	Y593	K594	S595	Q596	L597	S598	C599	V600	L601	D602	L603	D604	L605	E606	G607		L608	L609	D610	V611	V612	P613	L614	G615	P616	R617	M620	L621	Q624	L625	L626	L627	L628	L629	L630	K631	K632	A633	P634	P635	R638	L639	V703	W704	I705	G706	L707																			
L640	G644	T645	T646	S647	R648	K649	D650	V651	L652	Q653	B656	L657	L658	F661	S662	T663	T664	L665	H666	V667	P668	H669	L670	A671	T672	G673	G674	Q675	L676		L677	A679	L680	P681	L682	N685	F686	D688	R689	H690	R691	T692	T693	L694	A695	V698	K699	V703	W704	I705	G706	L707																												
K708	K709	L710	L711	L714	E715	M716	S717	L718	Q719	M720	D721	Y724	V725	L726	R727	K728	F729	A731	L732	L733	R734	G737	ALA	SER	PRO	LEU	ASP	PHE	ASP		N685	F686	D688	R689	H690	R691	T692	T693	L694	A695	V698	K699	V703	W704	I705	G706	L707																																	

• Molecule 1: Vesicle-fusing ATPase

Chain D:  32% 31% 36%

GLY	ALA	HIS	MET	ALA	GLY	ARG	SER	MET	GLN	ALA	ALA	ARG	CYS	PRO	THR	ASP	GLU	LEU	SER	ASN	CYS	ALA	VAL	VAL	SER	GLU	LYS	ASP	LYS	THR	GLN	VAL	ILE	VAL	ARG	THR	SER	PRO	ASN	HIS	LYS	TYR	ILE	PHE	THR	LEU	ARG	THR	HIS	PRO	SER	VAL	PRO		
GLY	SER	VAL	ALA	PHE	SER	LEU	PRO	GLN	ARG	LYS	TRP	ALA	GLY	GLY	LEU	GLN	ILE	ILE	GLU	SER	VAL	ALA	THR	LYS	PHE	GLY	LYS	LYS	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR			
ALA	ALA	PHE	GLN	ILE	GLN	GLN	PHE	ASN	ASN	ALA	ALA	PHE	SER	VAL	GLY	GLN	GLN	GLN	VAL	PHE	ASN	ASP	LYS	LYS	PHE	VAL	LEU	LEU	VAL	LYS	ASP	ASP	PRO	GLY	GLU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	
VAL	GLY	ASN	SER	GLN	VAL	ALA	PHE	GLU	LYS	ALA	GLU	ASN	SER	SER	SER	ASN	LYS	THR	LYS	THR	LYS	GLY	GLU	ASN	ASN	ARG	GLN	GLY	SER	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
V245	E246	Q247	M248	G249	V253	K254	G255	L256	L257	L258	V259	G260	P261	F262	G263	C264	C265	K266	L268	R271	E281	P282	V283	V284	V285	N286	E289	K293	S298	E299	A300	N301	L302	R303	K304	L305	F306	A307	D308	A309	E310	E311	E312	Q313	R314	A318	N319	S320	H323	I324					
I325	E326	F327	I330	D331	A332	L333	CYS	LYS	ARG	GLN	ARG	GLY	SER	MET	ALA	GLY	SER	THR	GLY	D348	T349	V350	V351	Q353	K357	L358	V361	L364	N365	L368	V369	I370	K371	M372	R375	F376	D377	L378	I379	D380	E381	A382	L383	P386	R387	R388	L389	V391							
I395	G396	L397	P398	D399	E400	K401	G402	L403	I405	I406	L407	T411	G416	H417	D427	S437	E440	L441	A448	M453	I457	LYS	ALA	SER	THR	LYS	VAL	GLU	VAL	ASP	MET	GLY	LYS	ALA	GLU	LYS	L541	E542	G543	P544	P545	H546	S547	G548	K549	T550	A551	L481	A482	M486					
K489	P490	ALA	PHE	GLY	THR	ASN	GLN	E497	Y502	I503	T507	M510	G511	D512	P513	F514	T515	R516	D519	E520	G521	E522	K523	L524	V525	Q526	T528	K529	H530	S531	T534	P535	L536	V537	S538	V539	L540	E541	E542	G543	P544	P545	H546	S547	G548	K549	T550	A551	L481	A482	M486				
A557	E558	E559	S560	N561	F562	P563	F564	I567	C568	S569	P570	M573	L574	G575	E578	K581	M585	F589	A592	Y593	K594	L597	S598	C599	V601	L536	V537	S538	V539	L540	E541	E542	G543	P544	P545	H546	S547	G548	K549	T550	A551	L481	A482	M486											
L630	M631	R632	P635	P636	G637	R638	R639	L640	L641	L642	L643	G644	R648	K649	D650	V651	L652	Q653	E654	M655	E656	M657	L658	M659	A660	F661	S662	T663	I670	Q675	V601	V602	D604	E606	R607	L608	L609	D610	P613	I614	F618	S619	M620	L621	V622	A695	V698	Q624	A625	L626	L627	I705	K708		



[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	12830	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.52	3/3559 (0.1%)	0.95	11/4824 (0.2%)
1	B	0.47	0/3566	0.89	6/4834 (0.1%)
1	C	0.46	0/3584	0.87	5/4858 (0.1%)
1	D	0.43	0/3516	0.84	8/4775 (0.2%)
1	E	0.48	0/3566	0.93	8/4833 (0.2%)
1	F	0.49	0/3514	0.92	13/4759 (0.3%)
All	All	0.48	3/21305 (0.0%)	0.90	51/28883 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	E	0	1
1	F	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	PHE	CD1-CE1	-7.83	1.23	1.39
1	A	236	ALA	CA-CB	-5.78	1.40	1.52
1	A	235	PHE	CB-CG	-5.41	1.42	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	PHE	CB-CG-CD1	-10.55	113.42	120.80
1	C	677	LEU	CB-CG-CD2	-9.07	95.58	111.00
1	A	235	PHE	CB-CG-CD2	8.18	126.52	120.80
1	E	629	LEU	CB-CG-CD1	-8.14	97.16	111.00
1	C	322	LEU	CA-CB-CG	8.13	134.00	115.30
1	E	683	LEU	CB-CG-CD2	-7.94	97.50	111.00
1	E	305	LEU	CA-CB-CG	7.55	132.67	115.30
1	B	305	LEU	CA-CB-CG	7.52	132.60	115.30
1	F	305	LEU	CA-CB-CG	7.51	132.56	115.30
1	B	479	ASP	N-CA-C	-7.44	90.91	111.00
1	F	406	ILE	CG1-CB-CG2	-7.41	95.09	111.40
1	F	536	LEU	CA-CB-CG	7.37	132.25	115.30
1	E	552	LEU	CB-CG-CD2	-7.24	98.69	111.00
1	F	518	LEU	CB-CG-CD1	-7.05	99.02	111.00
1	A	322	LEU	CA-CB-CG	6.92	131.22	115.30
1	B	658	LEU	CB-CG-CD1	-6.69	99.63	111.00
1	A	641	LEU	CA-CB-CG	6.66	130.62	115.30
1	C	444	LEU	CA-CB-CG	6.59	130.45	115.30
1	F	683	LEU	CB-CG-CD2	-6.56	99.85	111.00
1	E	652	LEU	CB-CG-CD2	-6.29	100.30	111.00
1	D	395	ILE	CG1-CB-CG2	-6.28	97.58	111.40
1	F	397	LEU	C-N-CD	6.24	141.49	128.40
1	E	682	LEU	CA-CB-CG	-6.14	101.17	115.30
1	D	682	LEU	CA-CB-CG	-6.14	101.18	115.30
1	A	525	VAL	CG1-CB-CG2	6.09	120.65	110.90
1	F	525	VAL	CG1-CB-CG2	5.96	120.43	110.90
1	D	627	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	A	597	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	F	518	LEU	CB-CG-CD2	5.86	120.96	111.00
1	A	552	LEU	CA-CB-CG	5.78	128.58	115.30
1	D	397	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	216	GLU	N-CA-C	-5.64	95.76	111.00
1	E	522	GLU	CA-CB-CG	5.61	125.74	113.40
1	C	457	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	D	643	ILE	CB-CA-C	-5.54	100.52	111.60
1	A	683	LEU	CA-CB-CG	5.47	127.88	115.30
1	F	546	HIS	N-CA-CB	-5.38	100.91	110.60
1	D	404	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	407	LEU	CA-CB-CG	5.36	127.64	115.30
1	C	640	LEU	CA-CB-CG	5.34	127.59	115.30
1	F	455	ARG	N-CA-C	5.30	125.31	111.00
1	A	407	LEU	CA-CB-CG	5.30	127.48	115.30
1	F	640	LEU	CA-CB-CG	5.26	127.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	643	ILE	CG1-CB-CG2	-5.18	100.01	111.40
1	D	416	GLY	N-CA-C	-5.14	100.25	113.10
1	F	398	PRO	CA-N-CD	-5.07	104.40	111.50
1	B	609	LEU	CA-CB-CG	-5.05	103.68	115.30
1	B	610	ASP	N-CA-CB	-5.05	101.51	110.60
1	A	713	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	F	407	LEU	CA-CB-CG	5.03	126.87	115.30
1	E	407	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	B	438	GLY	Peptide
1	B	546	HIS	Mainchain
1	E	438	GLY	Peptide
1	F	438	GLY	Peptide
1	F	453	MET	Mainchain

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	3513	0	3416	260	0
1	B	3517	0	3436	261	0
1	C	3535	0	3431	278	0
1	D	3467	0	3351	250	0
1	E	3516	0	3424	286	0
1	F	3467	0	3409	263	0
2	B	27	0	10	11	0
2	C	27	0	12	8	0
2	D	27	0	9	11	0
2	E	27	0	10	9	0
All	All	21123	0	20508	1497	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 36.

All (1497) 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:F:222:GLY:H	1:F:402:GLY:HA3	1.24	1.02
1:A:222:GLY:HA3	1:A:402:GLY:HA2	1.51	0.93
1:E:263:GLY:O	1:E:437:SER:HB2	1.71	0.89
1:D:448:ALA:HA	1:D:482:ALA:HB3	1.53	0.89
1:C:490:PRO:HA	1:C:491:ALA:HB3	1.53	0.88
1:F:538:SER:HB3	1:F:662:SER:H	1.40	0.86
1:F:545:PRO:HA	1:F:547:SER:H	1.39	0.85
1:F:256:ILE:HG13	1:F:370:ILE:HG22	1.58	0.84
1:E:686:PHE:HE1	1:E:714:ILE:HG23	1.43	0.84
1:C:670:ILE:HD13	1:C:675:GLN:HG2	1.58	0.84
1:A:549:LYS:NZ	1:A:647:SER:OG	2.10	0.83
1:F:538:SER:HG	1:F:661:PHE:HD1	1.24	0.83
1:E:490:PRO:HA	1:E:491:ALA:HB3	1.60	0.83
1:D:507:ILE:HA	2:D:801:ADP:N7	1.93	0.83
1:F:538:SER:H	1:F:662:SER:HB3	1.44	0.83
1:B:490:PRO:HA	1:B:491:ALA:HB3	1.60	0.83
1:C:256:ILE:HG13	1:C:370:ILE:HG22	1.59	0.83
1:C:687:LYS:N	1:C:690:GLU:OE2	2.12	0.82
1:B:508:ILE:H	2:B:801:ADP:HN61	1.23	0.82
1:A:285:VAL:HG13	1:A:326:ILE:HD11	1.61	0.82
1:E:526:GLN:NE2	1:F:719:GLN:O	2.12	0.81
1:E:527:GLN:O	1:E:531:SER:OG	1.97	0.81
1:B:589:PHE:HE1	1:B:600:VAL:HG11	1.45	0.81
1:A:510:TRP:HA	1:A:682:LEU:HD13	1.61	0.81
1:C:407:LEU:HD11	1:C:426:ILE:HG23	1.62	0.81
1:C:313:GLN:O	1:C:317:GLY:N	2.14	0.81
1:F:525:VAL:HG13	1:F:562:PHE:CE1	2.16	0.80
1:E:707:ILE:HD13	2:E:801:ADP:C8	2.17	0.80
1:F:536:LEU:HD11	1:F:634:PRO:HD3	1.62	0.80
1:B:386:PRO:HA	1:B:390:GLU:HA	1.64	0.80
1:D:527:GLN:HE22	1:E:715:GLU:C	1.83	0.80
1:D:406:ILE:HG22	1:D:441:LEU:HD22	1.61	0.80
1:F:386:PRO:HA	1:F:390:GLU:HA	1.62	0.80
1:E:587:LYS:NZ	1:E:587:LYS:O	2.15	0.79
1:A:713:LEU:HD21	1:A:732:LEU:HB3	1.64	0.79
1:E:534:THR:HG21	1:F:712:MET:HA	1.63	0.79
1:A:542:GLU:HG2	1:A:649:LYS:HD2	1.61	0.79
1:A:485:GLU:O	1:A:489:LYS:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:GLU:O	1:C:499:TYR:N	2.14	0.79
1:B:581:LYS:NZ	1:B:608:LEU:O	2.15	0.79
1:A:557:ALA:O	1:A:560:SER:OG	2.00	0.79
1:E:407:LEU:HD11	1:E:426:ILE:HG23	1.65	0.79
1:C:540:LEU:HB3	1:C:664:THR:HG22	1.63	0.79
1:F:570:PRO:HG2	1:F:604:ASP:HB2	1.65	0.78
1:F:564:PHE:O	1:F:598:SER:OG	2.00	0.78
1:F:517:VAL:HG13	1:F:665:ILE:HG21	1.66	0.78
1:E:680:LEU:HD13	1:E:694:ILE:HD13	1.66	0.78
1:F:222:GLY:N	1:F:402:GLY:HA3	1.97	0.78
1:E:386:PRO:HA	1:E:390:GLU:HA	1.63	0.78
1:A:397:LEU:HD13	1:A:435:ASN:HA	1.66	0.78
1:A:567:ILE:HG13	1:A:601:VAL:HB	1.66	0.77
1:E:706:GLY:O	1:E:710:LEU:N	2.16	0.77
1:E:685:ASN:HB3	1:E:718:LEU:HD11	1.67	0.77
1:D:626:LEU:HB3	1:D:657:MET:HE3	1.67	0.77
1:D:728:LYS:HE3	1:D:732:LEU:HD11	1.67	0.77
1:D:510:TRP:HE3	1:D:675:GLN:HG2	1.51	0.76
1:C:627:LEU:HD12	1:D:607:ARG:HH12	1.50	0.76
1:F:222:GLY:HA2	1:F:399:ASP:HB2	1.67	0.76
1:E:625:ALA:HA	1:F:574:ILE:HD11	1.67	0.76
1:B:627:LEU:HD21	1:B:657:MET:HG3	1.67	0.76
1:F:398:PRO:HG3	1:F:436:PHE:O	1.85	0.76
1:C:652:LEU:HD22	1:C:657:MET:HG2	1.67	0.76
1:D:502:TYR:O	2:D:801:ADP:O3'	2.03	0.76
1:B:300:ALA:O	1:B:304:LYS:HG2	1.86	0.76
1:C:578:GLU:HB3	1:C:621:LEU:HB3	1.68	0.76
1:C:718:LEU:O	1:C:725:ARG:NH1	2.19	0.75
1:A:351:VAL:O	1:A:355:LEU:HG	1.86	0.75
1:A:670:ILE:HG23	1:A:675:GLN:HB2	1.68	0.75
1:E:300:ALA:O	1:E:304:LYS:HG2	1.86	0.75
1:E:686:PHE:HB3	1:E:690:GLU:HB2	1.68	0.75
1:D:448:ALA:HA	1:D:482:ALA:CB	2.16	0.75
1:A:546:HIS:C	1:A:708:LYS:HB3	2.07	0.75
1:C:724:TYR:HD2	1:C:727:ARG:HH21	1.35	0.74
1:F:407:LEU:HD11	1:F:426:ILE:HG23	1.67	0.74
1:E:552:LEU:HD21	2:E:801:ADP:N6	1.99	0.74
1:F:589:PHE:HD2	1:F:629:LEU:HD13	1.52	0.74
1:C:691:ARG:HA	1:C:694:ILE:HD12	1.67	0.74
1:F:220:ILE:N	1:F:406:ILE:HD11	2.02	0.74
1:D:313:GLN:HE22	1:D:364:LEU:HA	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HA	1:A:252:HIS:CE1	2.21	0.74
1:E:563:PRO:HG2	1:E:595:SER:OG	1.87	0.74
1:C:711:LEU:O	1:C:715:GLU:HG2	1.88	0.74
1:B:540:LEU:HD23	1:B:661:PHE:CD1	2.23	0.74
1:C:544:PRO:O	1:C:547:SER:OG	2.06	0.74
1:C:690:GLU:HB2	1:C:726:VAL:HG21	1.69	0.74
1:C:318:ALA:O	1:C:319:ASN:ND2	2.21	0.74
1:C:386:PRO:HA	1:C:390:GLU:HA	1.70	0.74
1:F:300:ALA:O	1:F:304:LYS:HG2	1.87	0.73
1:A:236:ALA:HB1	1:B:453:MET:HB2	1.70	0.73
1:C:596:GLN:HA	1:C:638:ARG:HD3	1.71	0.73
1:B:524:LEU:HD21	1:B:663:THR:HG21	1.70	0.73
1:C:630:LEU:HD11	1:C:661:PHE:CE1	2.24	0.73
1:A:624:GLN:HG3	1:B:610:ASP:OD2	1.87	0.73
1:A:553:ALA:HA	1:A:556:ILE:HD12	1.69	0.73
1:F:535:PRO:HA	1:F:639:LYS:HG2	1.71	0.73
1:B:540:LEU:HD11	1:B:649:LYS:NZ	2.04	0.72
1:B:533:ARG:HG3	1:B:534:THR:H	1.53	0.72
1:C:508:ILE:HG13	1:C:510:TRP:HD1	1.53	0.72
1:B:407:LEU:HD11	1:B:426:ILE:HG23	1.71	0.72
1:D:352:ASN:HB3	1:E:288:PRO:HB2	1.70	0.72
1:E:311:GLU:OE1	1:E:314:ARG:NE	2.23	0.72
1:D:301:ASN:HA	1:D:304:LYS:HD3	1.70	0.72
1:E:585:MET:HA	1:E:588:ILE:HD12	1.69	0.72
1:C:513:PRO:O	1:C:516:ARG:HG2	1.89	0.72
1:B:508:ILE:N	2:B:801:ADP:HN61	1.88	0.72
1:E:653:GLN:HA	1:E:658:LEU:HB2	1.71	0.72
1:E:510:TRP:CD1	1:E:707:ILE:HD12	2.25	0.72
1:C:508:ILE:HD11	1:C:707:ILE:HD11	1.71	0.71
1:A:710:LEU:O	1:A:714:ILE:HG13	1.89	0.71
1:F:565:ILE:HG23	1:F:599:CYS:HB3	1.72	0.71
1:C:611:TYR:CE1	1:C:616:PRO:HB2	2.26	0.71
1:E:513:PRO:HA	1:E:516:ARG:HG2	1.70	0.71
1:D:605:ILE:HD11	1:D:644:GLY:HA3	1.72	0.71
1:F:634:PRO:HB2	1:F:638:ARG:HG3	1.73	0.71
1:F:569:SER:OG	1:F:571:ASP:OD2	2.05	0.71
1:D:528:THR:OG1	1:D:641:LEU:HD12	1.90	0.71
1:B:263:GLY:O	1:B:437:SER:HB3	1.91	0.71
1:D:230:ILE:HD11	1:D:256:ILE:HD13	1.72	0.71
1:E:236:ALA:HA	1:E:239:VAL:HG12	1.72	0.71
1:F:606:GLU:OE1	1:F:606:GLU:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:PRO:HA	1:D:390:GLU:HA	1.73	0.70
1:B:424:VAL:N	1:B:479:ASP:N	2.39	0.70
1:D:711:LEU:HA	1:D:714:ILE:HD12	1.73	0.70
1:B:656:GLU:OE1	1:C:648:ARG:NH2	2.24	0.70
1:A:221:GLY:HA3	1:A:406:ILE:HG13	1.74	0.70
1:B:303:ARG:HG3	1:B:357:LYS:HE2	1.73	0.70
1:F:510:TRP:CE3	1:F:675:GLN:HB3	2.25	0.70
1:E:603:ASP:OD2	1:E:645:THR:OG1	2.06	0.70
1:B:507:ILE:HA	2:B:801:ADP:N7	2.06	0.70
1:F:437:SER:OG	1:F:440:GLU:HG2	1.91	0.70
1:C:564:PHE:O	1:C:598:SER:OG	2.07	0.70
1:D:513:PRO:HA	1:D:516:ARG:HG2	1.70	0.70
1:A:326:ILE:HG22	1:A:370:ILE:HG12	1.73	0.70
1:F:303:ARG:HG3	1:F:357:LYS:HE2	1.74	0.70
1:E:604:ASP:HB3	1:E:607:ARG:HB3	1.73	0.70
1:C:262:PRO:HD2	1:C:594:LYS:HE2	1.73	0.70
1:E:514:VAL:HG13	2:E:801:ADP:HN61	1.55	0.70
1:A:309:ALA:HB1	1:A:367:ILE:HG21	1.74	0.70
1:F:721:ASP:HB2	1:F:724:TYR:HD1	1.57	0.70
1:C:669:ASN:OD1	1:C:706:GLY:HA2	1.90	0.70
1:D:348:ASP:O	1:D:352:ASN:ND2	2.25	0.70
1:A:669:ASN:HD22	1:A:706:GLY:HA2	1.57	0.70
1:F:510:TRP:HB3	1:F:679:ALA:HB2	1.74	0.70
1:E:538:SER:OG	1:E:661:PHE:HA	1.92	0.70
1:D:510:TRP:CE3	1:D:670:ILE:HG22	2.27	0.69
1:B:538:SER:HB3	1:B:661:PHE:HD2	1.57	0.69
1:F:224:ASP:O	1:F:228:SER:HB2	1.91	0.69
1:B:648:ARG:NH1	1:B:651:VAL:HG22	2.06	0.69
1:B:311:GLU:OE1	1:B:314:ARG:NE	2.23	0.69
1:F:311:GLU:OE1	1:F:314:ARG:NE	2.22	0.69
1:E:590:ASP:OD2	1:E:594:LYS:NZ	2.25	0.69
1:F:545:PRO:HA	1:F:547:SER:N	2.06	0.69
1:C:706:GLY:O	1:C:710:LEU:N	2.24	0.69
1:B:589:PHE:CE1	1:B:600:VAL:HG11	2.26	0.69
1:A:546:HIS:O	1:A:708:LYS:HB3	1.93	0.69
1:E:232:ARG:O	1:E:236:ALA:HB3	1.92	0.69
1:F:612:VAL:HG12	1:F:617:ARG:HB2	1.73	0.69
1:F:536:LEU:HD21	1:F:632:LYS:O	1.92	0.69
1:D:303:ARG:HD3	1:D:353:GLN:CG	2.22	0.69
1:F:222:GLY:HA3	1:F:399:ASP:H	1.57	0.69
1:E:303:ARG:HG3	1:E:357:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:ILE:HG22	1:B:672:THR:H	1.58	0.69
1:A:602:VAL:HG12	1:A:605:ILE:HG12	1.73	0.69
1:D:397:LEU:HD23	1:D:398:PRO:HD2	1.75	0.69
1:E:674:GLU:HA	1:E:677:LEU:HD12	1.75	0.69
1:A:565:ILE:HG13	1:A:599:CYS:HB3	1.74	0.69
1:E:652:LEU:CD2	1:E:657:MET:HB3	2.23	0.68
1:F:713:LEU:HD22	1:F:732:LEU:HB3	1.73	0.68
1:A:677:LEU:HD21	1:A:695:ALA:HA	1.75	0.68
1:D:548:GLY:HA2	2:D:801:ADP:C5'	2.23	0.68
1:F:546:HIS:CE1	1:F:709:LYS:HB3	2.28	0.68
1:E:536:LEU:HD12	1:E:640:LEU:O	1.94	0.68
1:C:533:ARG:HB2	1:D:715:GLU:OE1	1.92	0.68
1:E:652:LEU:HD23	1:E:657:MET:HB3	1.76	0.68
1:C:331:ASP:HA	1:C:379:ILE:HD11	1.76	0.68
1:A:521:GLY:O	1:A:525:VAL:HG23	1.95	0.67
1:E:237:SER:HA	1:F:453:MET:HG3	1.76	0.67
1:D:358:ILE:HD12	1:D:388:ARG:HB3	1.76	0.67
1:C:542:GLU:CB	1:C:649:LYS:HD3	2.24	0.67
1:D:527:GLN:HE21	1:E:715:GLU:HG3	1.59	0.67
1:C:649:LYS:HE2	1:C:658:LEU:HD13	1.77	0.67
1:A:564:PHE:CE1	1:A:566:LYS:HB2	2.29	0.67
1:B:358:ILE:HD12	1:B:388:ARG:HB3	1.77	0.67
1:B:649:LYS:HE3	1:B:658:LEU:HD11	1.76	0.67
1:B:542:GLU:HB3	1:B:649:LYS:HG3	1.77	0.67
1:F:236:ALA:HA	1:F:239:VAL:HG12	1.77	0.67
1:E:510:TRP:CD1	1:E:514:VAL:HG21	2.30	0.67
1:E:618:PHE:HZ	1:F:612:VAL:HG11	1.60	0.67
1:B:258:LEU:HB3	1:B:395:ILE:HD11	1.77	0.67
1:D:312:GLU:OE1	1:D:323:HIS:ND1	2.24	0.66
1:E:681:GLU:HA	1:E:691:ARG:HE	1.59	0.66
1:B:224:ASP:O	1:B:228:SER:HB2	1.95	0.66
1:E:624:GLN:NE2	1:F:610:ASP:OD1	2.29	0.66
1:A:531:SER:OG	1:B:715:GLU:OE1	2.14	0.66
1:D:263:GLY:O	1:D:437:SER:OG	2.12	0.66
1:E:671:ALA:HA	1:E:703:VAL:O	1.95	0.66
1:D:627:LEU:HD21	1:D:657:MET:HG3	1.77	0.66
1:B:528:THR:O	1:B:639:LYS:HD2	1.96	0.66
1:B:452:ALA:HA	1:B:455:ARG:NH2	2.10	0.66
1:B:538:SER:HB3	1:B:661:PHE:CD2	2.30	0.66
1:F:695:ALA:HB1	1:F:699:LYS:HE3	1.78	0.66
1:A:653:GLN:NE2	1:A:653:GLN:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:GLY:N	2:C:801:ADP:O2'	2.29	0.66
1:B:589:PHE:HE2	1:B:629:LEU:HB3	1.61	0.66
1:A:526:GLN:HE21	1:A:530:ASN:HD22	1.43	0.65
1:E:542:GLU:O	1:E:666:HIS:ND1	2.28	0.65
1:D:245:VAL:O	1:D:249:GLY:N	2.29	0.65
1:A:510:TRP:HB2	1:A:679:ALA:HA	1.78	0.65
1:D:234:ALA:HA	1:D:253:VAL:HG11	1.78	0.65
1:E:245:VAL:O	1:E:249:GLY:N	2.28	0.65
1:E:592:ALA:HB1	1:E:640:LEU:HD22	1.77	0.65
1:E:437:SER:OG	1:E:440:GLU:HG2	1.96	0.65
1:E:625:ALA:O	1:E:629:LEU:HG	1.97	0.65
1:A:687:LYS:N	1:A:690:GLU:OE1	2.29	0.65
1:E:640:LEU:HD12	1:E:641:LEU:N	2.12	0.65
1:D:284:VAL:HG23	1:D:324:ILE:O	1.97	0.65
1:D:404:LEU:HA	1:D:407:LEU:HD12	1.78	0.65
1:D:573:MET:SD	1:D:581:LYS:HD3	2.36	0.65
1:F:358:ILE:HD12	1:F:388:ARG:HB3	1.77	0.65
1:D:695:ALA:HB1	1:D:699:LYS:HE3	1.79	0.65
1:A:707:ILE:HA	1:A:710:LEU:HB2	1.79	0.64
1:A:628:VAL:HG11	1:B:571:ASP:HA	1.79	0.64
1:F:510:TRP:HB2	1:F:675:GLN:O	1.97	0.64
1:C:261:PRO:HB2	1:C:594:LYS:HG3	1.77	0.64
1:A:256:ILE:HG13	1:A:370:ILE:HG22	1.80	0.64
1:D:620:ASN:O	1:D:624:GLN:HG2	1.96	0.64
1:E:509:LYS:HD2	1:E:515:THR:HG22	1.79	0.64
1:B:548:GLY:HA3	2:B:801:ADP:H2	1.63	0.64
1:B:404:LEU:HG	1:B:426:ILE:HG22	1.80	0.64
1:F:438:GLY:O	1:F:441:LEU:N	2.30	0.64
1:B:624:GLN:NE2	1:C:610:ASP:O	2.30	0.64
1:F:570:PRO:HG2	1:F:604:ASP:CB	2.28	0.64
1:F:546:HIS:CD2	1:F:546:HIS:H	2.15	0.64
1:E:502:TYR:OH	1:E:569:SER:OG	2.15	0.64
1:D:319:ASN:HB3	1:D:320:SER:HB2	1.79	0.64
1:C:358:ILE:CB	1:C:388:ARG:HG3	2.26	0.64
1:F:570:PRO:HA	1:F:573:MET:HE2	1.78	0.64
1:A:223:LEU:HD12	1:A:227:PHE:HB2	1.80	0.64
1:E:710:LEU:O	1:E:714:ILE:HG13	1.97	0.64
1:E:224:ASP:O	1:E:228:SER:HB2	1.98	0.64
1:E:358:ILE:HD12	1:E:388:ARG:HB3	1.79	0.64
1:E:505:ASN:HB2	2:E:801:ADP:O3'	1.98	0.64
1:A:617:ARG:HH11	1:A:617:ARG:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ARG:HG3	1:B:534:THR:HG23	1.79	0.64
1:C:711:LEU:HA	1:C:714:ILE:HD12	1.80	0.64
1:F:307:ALA:O	1:F:311:GLU:HG2	1.98	0.64
1:F:538:SER:O	1:F:663:THR:HG22	1.98	0.63
1:B:540:LEU:HD11	1:B:649:LYS:HZ3	1.60	0.63
1:B:307:ALA:O	1:B:311:GLU:HG2	1.98	0.63
1:B:713:LEU:HD22	1:B:732:LEU:HB3	1.79	0.63
1:A:232:ARG:O	1:A:236:ALA:HB2	1.97	0.63
1:C:311:GLU:HA	1:C:314:ARG:HG2	1.81	0.63
1:B:628:VAL:HG13	1:C:571:ASP:OD1	1.97	0.63
1:A:544:PRO:HG2	1:A:669:ASN:OD1	1.98	0.63
1:D:256:ILE:HG22	1:D:391:VAL:HG12	1.80	0.63
1:A:258:LEU:HA	1:A:393:MET:O	1.98	0.63
1:E:602:VAL:O	1:E:644:GLY:HA2	1.98	0.63
1:A:687:LYS:HB2	1:A:690:GLU:HG3	1.81	0.63
1:F:562:PHE:CD1	1:F:599:CYS:HB2	2.34	0.63
1:F:635:PRO:O	1:F:638:ARG:HG2	1.98	0.63
1:D:404:LEU:HD11	1:D:427:LYS:HE3	1.81	0.63
1:D:604:ASP:HB3	1:D:607:ARG:CB	2.28	0.63
1:D:256:ILE:O	1:D:370:ILE:HA	1.99	0.63
1:A:313:GLN:NE2	1:A:365:ASN:O	2.32	0.63
1:E:307:ALA:O	1:E:311:GLU:HG2	1.98	0.63
1:B:570:PRO:HD3	1:B:603:ASP:HB3	1.81	0.63
1:C:383:LEU:HD22	1:C:388:ARG:HD2	1.80	0.63
1:C:511:GLY:HA3	1:C:513:PRO:HD2	1.78	0.62
1:F:546:HIS:O	1:F:546:HIS:ND1	2.32	0.62
1:D:503:ILE:HA	2:D:801:ADP:O2'	1.99	0.62
1:E:550:THR:HA	1:E:645:THR:HG21	1.81	0.62
1:E:686:PHE:CE1	1:E:714:ILE:HG23	2.31	0.62
1:A:563:PRO:HD2	1:A:597:LEU:HD22	1.81	0.62
1:D:521:GLY:O	1:D:525:VAL:HG23	1.98	0.62
1:D:548:GLY:HA2	2:D:801:ADP:H5'1	1.80	0.62
1:F:268:LEU:HD21	1:F:438:GLY:HA3	1.80	0.62
1:C:285:VAL:HG13	1:C:326:ILE:HD11	1.81	0.62
1:B:589:PHE:CE2	1:B:629:LEU:HB3	2.34	0.62
1:A:508:ILE:HG13	1:A:508:ILE:O	2.00	0.62
1:C:621:LEU:HD11	1:D:575:GLY:HA2	1.82	0.62
1:F:404:LEU:O	1:F:408:HIS:HB2	1.99	0.62
1:D:599:CYS:SG	1:D:641:LEU:HD22	2.39	0.62
1:F:436:PHE:HD2	1:F:444:LEU:HD11	1.64	0.62
1:F:550:THR:HA	1:F:645:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:THR:HB	2:C:801:ADP:PA	2.39	0.62
1:E:380:ASP:OD1	1:E:382:ALA:N	2.33	0.62
1:F:380:ASP:OD1	1:F:382:ALA:N	2.33	0.62
1:B:326:ILE:HG22	1:B:370:ILE:HG13	1.82	0.62
1:E:326:ILE:HG22	1:E:370:ILE:HG13	1.82	0.62
1:A:231:PHE:CD1	1:A:235:PHE:HE2	2.17	0.61
1:E:705:ILE:HG13	1:E:709:LYS:HG3	1.81	0.61
1:B:527:GLN:HB2	1:C:719:GLN:HG3	1.82	0.61
1:C:624:GLN:O	1:C:628:VAL:HG23	2.00	0.61
1:A:720:MET:O	1:A:725:ARG:NE	2.23	0.61
1:E:532:ASP:OD2	1:E:533:ARG:N	2.32	0.61
1:D:554:ALA:O	1:D:558:GLU:HG2	2.00	0.61
1:D:286:ASN:HB2	1:D:327:PHE:HD1	1.65	0.61
1:C:728:LYS:O	1:C:732:LEU:HG	2.00	0.61
1:B:542:GLU:HG3	1:B:666:HIS:CE1	2.35	0.61
1:B:245:VAL:O	1:B:249:GLY:N	2.32	0.61
1:C:670:ILE:HG22	1:C:672:THR:H	1.65	0.61
1:F:546:HIS:CE1	1:F:709:LYS:CB	2.84	0.61
1:D:606:GLU:O	1:D:610:ASP:N	2.33	0.61
1:C:542:GLU:HB3	1:C:649:LYS:HD3	1.81	0.61
1:D:507:ILE:HA	2:D:801:ADP:C8	2.36	0.61
1:E:581:LYS:NZ	1:E:610:ASP:OD1	2.30	0.61
1:C:334:CYS:HA	1:C:351:VAL:HG22	1.81	0.61
1:D:261:PRO:HG2	1:D:264:CYS:HB2	1.82	0.61
1:F:566:LYS:HD2	1:F:567:ILE:N	2.16	0.61
1:B:380:ASP:OD1	1:B:382:ALA:N	2.33	0.61
1:B:625:ALA:O	1:B:629:LEU:HG	2.01	0.60
1:E:513:PRO:O	1:E:517:VAL:HG23	2.01	0.60
1:B:437:SER:OG	1:B:440:GLU:HG2	2.00	0.60
1:D:513:PRO:HB3	1:D:516:ARG:HE	1.65	0.60
1:D:656:GLU:OE1	1:E:613:PRO:HB3	2.01	0.60
1:C:579:THR:O	1:C:583:GLN:HG2	2.01	0.60
1:F:650:ASP:O	1:F:653:GLN:HG3	2.01	0.60
1:A:408:HIS:HA	1:A:426:ILE:HD12	1.83	0.60
1:A:223:LEU:CD1	1:A:227:PHE:HB2	2.32	0.60
1:F:326:ILE:HG22	1:F:370:ILE:HG13	1.83	0.60
1:C:407:LEU:CD1	1:C:426:ILE:HG23	2.31	0.60
1:B:421:SER:HB3	1:B:424:VAL:HG23	1.83	0.60
1:D:246:GLU:O	1:E:413:ARG:NH1	2.30	0.60
1:D:249:GLY:HA3	1:E:413:ARG:NH1	2.16	0.60
1:A:299:GLU:HG2	1:A:353:GLN:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:SER:OG	1:A:640:LEU:HD12	2.01	0.60
1:B:563:PRO:HD2	1:B:597:LEU:HB2	1.82	0.60
1:C:399:ASP:O	1:C:403:ARG:N	2.29	0.60
1:F:715:GLU:O	1:F:719:GLN:HG2	2.00	0.60
1:C:677:LEU:HD11	1:C:698:VAL:HG21	1.84	0.60
1:D:512:ASP:O	1:D:515:THR:OG1	2.18	0.60
1:A:677:LEU:HG	1:A:695:ALA:HB2	1.83	0.60
1:C:375:ARG:HH12	1:C:378:LEU:HG	1.65	0.60
1:C:577:SER:O	1:C:580:ALA:N	2.33	0.60
1:C:247:GLN:HA	1:D:417:HIS:CD2	2.36	0.60
1:E:514:VAL:HG13	2:E:801:ADP:N6	2.17	0.60
1:E:544:PRO:O	1:E:547:SER:HB3	2.01	0.60
1:A:510:TRP:CB	1:A:679:ALA:HA	2.31	0.60
1:F:508:ILE:HD11	1:F:510:TRP:HD1	1.67	0.60
1:A:565:ILE:HA	1:A:599:CYS:O	2.02	0.60
1:F:268:LEU:CD2	1:F:439:ALA:H	2.15	0.60
1:C:254:LYS:O	1:C:368:LEU:HA	2.02	0.60
1:C:540:LEU:HD12	1:C:644:GLY:O	2.01	0.60
1:C:606:GLU:HB2	1:C:648:ARG:HD2	1.82	0.60
1:A:582:CYS:SG	1:A:621:LEU:HG	2.42	0.60
1:E:247:GLN:HA	1:F:417:HIS:ND1	2.17	0.60
1:F:521:GLY:O	1:F:525:VAL:HG23	2.02	0.60
1:B:540:LEU:HA	1:B:644:GLY:O	2.02	0.60
1:B:513:PRO:HD2	1:B:670:ILE:HD11	1.83	0.60
1:C:236:ALA:HB1	1:D:453:MET:HB3	1.84	0.60
1:A:270:ALA:O	1:A:273:ILE:HG22	2.01	0.60
1:A:508:ILE:HB	1:A:682:LEU:HB3	1.83	0.60
1:D:407:LEU:HG	1:D:441:LEU:HD11	1.83	0.60
1:A:236:ALA:HB1	1:B:450:SER:HA	1.82	0.60
1:B:407:LEU:CD1	1:B:426:ILE:HG23	2.31	0.60
1:C:590:ASP:HA	1:C:593:TYR:CD2	2.37	0.60
1:E:508:ILE:HD11	1:E:707:ILE:HD11	1.84	0.59
1:B:541:LEU:HD11	1:B:549:LYS:HA	1.83	0.59
1:E:404:LEU:O	1:E:408:HIS:HB2	2.02	0.59
1:B:510:TRP:HZ3	1:B:670:ILE:HD12	1.67	0.59
1:F:449:GLN:O	1:F:453:MET:HG2	2.01	0.59
1:D:527:GLN:NE2	1:E:715:GLU:HG3	2.17	0.59
1:C:695:ALA:HB1	1:C:699:LYS:HE3	1.84	0.59
1:B:383:LEU:O	1:B:389:LEU:HB2	2.02	0.59
1:D:585:MET:O	1:D:589:PHE:HD2	1.84	0.59
1:D:312:GLU:CG	1:D:313:GLN:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:628:VAL:O	1:E:632:LYS:N	2.36	0.59
1:D:299:GLU:OE1	1:D:350:VAL:HG13	2.02	0.59
1:A:571:ASP:HA	1:A:574:ILE:HG23	1.85	0.59
1:B:539:VAL:HG21	1:B:665:ILE:HD12	1.84	0.59
1:D:652:LEU:HB3	1:D:658:LEU:HB2	1.83	0.59
1:A:686:PHE:O	1:A:691:ARG:NH2	2.36	0.59
1:A:694:ILE:O	1:A:698:VAL:HG13	2.02	0.59
1:C:606:GLU:HG2	1:C:607:ARG:N	2.18	0.59
1:B:548:GLY:HA3	2:B:801:ADP:C2	2.37	0.59
1:B:404:LEU:O	1:B:408:HIS:HB2	2.02	0.59
1:B:670:ILE:HD13	1:B:675:GLN:HB3	1.85	0.59
1:A:382:ALA:O	1:A:385:ARG:HG2	2.03	0.59
1:D:593:TYR:O	1:D:638:ARG:HG2	2.01	0.59
1:C:551:ALA:HB2	2:C:801:ADP:H3'	1.84	0.59
1:D:604:ASP:HB3	1:D:607:ARG:HB3	1.84	0.59
1:C:624:GLN:NE2	1:D:610:ASP:HB2	2.18	0.59
1:F:606:GLU:OE2	1:F:647:SER:HB2	2.02	0.59
1:B:695:ALA:HB1	1:B:699:LYS:HE3	1.85	0.59
1:A:307:ALA:O	1:A:310:GLU:HG3	2.03	0.59
1:E:449:GLN:O	1:E:453:MET:HG2	2.03	0.59
1:E:527:GLN:NE2	1:F:716:MET:HG2	2.18	0.58
1:A:624:GLN:OE1	1:B:607:ARG:NH1	2.36	0.58
1:B:284:VAL:HG23	1:B:324:ILE:O	2.03	0.58
1:E:648:ARG:NE	1:E:650:ASP:OD1	2.34	0.58
1:E:697:GLN:HG3	1:E:730:LEU:HD11	1.83	0.58
1:C:669:ASN:CG	1:C:706:GLY:HA2	2.24	0.58
1:F:562:PHE:HB2	1:F:565:ILE:HG12	1.84	0.58
1:A:671:ALA:HA	1:A:703:VAL:O	2.03	0.58
1:B:261:PRO:HG2	1:B:264:CYS:HB2	1.84	0.58
1:C:404:LEU:O	1:C:408:HIS:HB2	2.03	0.58
1:B:571:ASP:OD2	1:B:571:ASP:N	2.35	0.58
1:E:383:LEU:O	1:E:389:LEU:HB2	2.02	0.58
1:A:597:LEU:HD23	1:A:597:LEU:C	2.23	0.58
1:F:549:LYS:HE2	1:F:645:THR:HB	1.86	0.58
1:C:527:GLN:HB2	1:D:719:GLN:HG3	1.84	0.58
1:D:519:ASP:O	1:D:523:LEU:HG	2.03	0.58
1:C:694:ILE:O	1:C:698:VAL:HG22	2.04	0.58
1:E:284:VAL:HG23	1:E:324:ILE:O	2.03	0.58
1:B:533:ARG:HD2	1:C:711:LEU:HD13	1.86	0.58
1:B:526:GLN:HE21	1:C:719:GLN:HB3	1.68	0.58
1:C:540:LEU:HB2	1:C:661:PHE:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLN:O	1:B:453:MET:HG3	2.03	0.58
1:D:528:THR:HG22	1:D:597:LEU:HD11	1.85	0.58
1:D:513:PRO:O	1:D:516:ARG:HG2	2.03	0.58
1:C:653:GLN:HG3	1:C:658:LEU:HD23	1.86	0.58
1:F:513:PRO:O	1:F:517:VAL:HG23	2.03	0.58
1:F:407:LEU:CD1	1:F:426:ILE:HG23	2.33	0.58
1:F:383:LEU:O	1:F:389:LEU:HB2	2.02	0.58
1:B:236:ALA:HA	1:B:239:VAL:HG12	1.86	0.58
1:A:222:GLY:H	1:A:405:GLN:HB3	1.68	0.58
1:C:658:LEU:HD11	1:C:664:THR:HG21	1.85	0.58
1:C:436:PHE:HB3	1:C:440:GLU:OE1	2.04	0.58
1:F:410:HIS:O	1:F:414:MET:HG2	2.02	0.58
1:E:407:LEU:CD1	1:E:426:ILE:HG23	2.32	0.58
1:E:236:ALA:HA	1:E:239:VAL:CG1	2.33	0.58
1:E:502:TYR:CZ	1:E:567:ILE:HG21	2.38	0.58
1:A:411:THR:OG1	1:A:426:ILE:HD11	2.03	0.58
1:E:548:GLY:HA2	2:E:801:ADP:O5'	2.04	0.58
1:A:678:GLU:O	1:A:681:GLU:HG2	2.03	0.58
1:C:614:ILE:C	1:C:616:PRO:HA	2.24	0.58
1:E:624:GLN:HA	1:E:624:GLN:OE1	2.02	0.58
1:A:690:GLU:O	1:A:694:ILE:HG13	2.04	0.57
1:F:602:VAL:N	1:F:643:ILE:O	2.23	0.57
1:D:711:LEU:O	1:D:715:GLU:HG2	2.04	0.57
1:D:383:LEU:O	1:D:389:LEU:HB2	2.03	0.57
1:E:693:THR:O	1:E:697:GLN:NE2	2.20	0.57
1:B:236:ALA:O	1:B:239:VAL:HG12	2.04	0.57
1:D:380:ASP:OD1	1:D:382:ALA:N	2.36	0.57
1:F:284:VAL:HG23	1:F:324:ILE:O	2.03	0.57
1:D:527:GLN:OE1	1:E:716:MET:HA	2.04	0.57
1:E:296:GLY:H	1:E:297:GLU:CB	2.18	0.57
1:B:549:LYS:NZ	1:B:647:SER:HA	2.19	0.57
1:C:688:ASP:OD1	1:C:691:ARG:NH2	2.25	0.57
1:B:670:ILE:HG21	1:B:675:GLN:OE1	2.04	0.57
1:B:395:ILE:HD12	1:B:395:ILE:H	1.69	0.57
1:A:539:VAL:HG23	1:A:665:ILE:HD13	1.85	0.57
1:A:539:VAL:HG13	1:A:643:ILE:HA	1.87	0.57
1:D:524:LEU:O	1:D:527:GLN:HB3	2.04	0.57
1:D:625:ALA:O	1:D:629:LEU:HG	2.05	0.57
1:D:651:VAL:O	1:D:655:MET:HG2	2.03	0.57
1:C:508:ILE:HG13	1:C:510:TRP:CD1	2.37	0.57
1:A:672:THR:OG1	1:A:675:GLN:OE1	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ILE:HD11	1:B:644:GLY:HA3	1.87	0.57
1:B:620:ASN:HD21	1:B:624:GLN:HE21	1.51	0.57
1:C:509:LYS:O	1:C:682:LEU:HD12	2.04	0.57
1:C:449:GLN:O	1:C:453:MET:HG2	2.04	0.57
1:E:640:LEU:HD12	1:E:641:LEU:H	1.68	0.57
1:A:598:SER:O	1:A:640:LEU:HA	2.05	0.57
1:B:552:LEU:O	1:B:556:ILE:HG13	2.04	0.57
1:F:222:GLY:CA	1:F:399:ASP:HB2	2.33	0.57
1:A:257:LEU:HG	1:A:389:LEU:HD12	1.87	0.57
1:E:354:LEU:O	1:E:358:ILE:HG12	2.05	0.57
1:F:554:ALA:O	1:F:558:GLU:HG3	2.05	0.57
1:A:267:THR:OG1	1:A:328:ASP:OD2	2.21	0.57
1:F:354:LEU:O	1:F:358:ILE:HG12	2.05	0.57
1:C:375:ARG:NH2	1:C:377:ASP:OD1	2.38	0.57
1:B:593:TYR:O	1:B:638:ARG:NE	2.38	0.57
1:D:267:THR:HA	1:D:372:MET:SD	2.45	0.57
1:E:721:ASP:O	1:E:725:ARG:HG3	2.05	0.57
1:F:653:GLN:HB3	1:F:658:LEU:HD23	1.87	0.57
1:D:543:GLY:N	1:D:549:LYS:HD3	2.19	0.57
1:D:551:ALA:HB3	2:D:801:ADP:N3	2.20	0.57
1:F:604:ASP:HB3	1:F:607:ARG:HB2	1.85	0.57
1:B:510:TRP:CZ3	1:B:670:ILE:HD12	2.40	0.57
1:D:648:ARG:HG3	1:D:651:VAL:HG23	1.87	0.57
1:D:303:ARG:HD3	1:D:353:GLN:HG3	1.87	0.57
1:B:578:GLU:HG3	1:B:619:SER:HB2	1.86	0.57
1:C:677:LEU:HD11	1:C:698:VAL:CG2	2.34	0.56
1:A:546:HIS:ND1	1:A:709:LYS:HE3	2.20	0.56
1:E:652:LEU:HD22	1:E:658:LEU:HD13	1.86	0.56
1:D:528:THR:CB	1:D:641:LEU:HD12	2.34	0.56
1:C:613:PRO:HD3	1:C:648:ARG:HH22	1.70	0.56
1:B:221:GLY:HA3	1:B:406:ILE:CD1	2.35	0.56
1:C:536:LEU:HD12	1:C:640:LEU:HB3	1.87	0.56
1:F:245:VAL:O	1:F:249:GLY:N	2.36	0.56
1:E:713:LEU:HD22	1:E:732:LEU:HD13	1.87	0.56
1:A:549:LYS:HB3	1:A:667:VAL:HG21	1.86	0.56
1:F:508:ILE:CD1	1:F:510:TRP:HD1	2.18	0.56
1:B:354:LEU:O	1:B:358:ILE:HG12	2.06	0.56
1:D:284:VAL:HB	1:D:325:ILE:HA	1.86	0.56
1:E:242:PRO:HD2	1:E:243:GLU:H	1.70	0.56
1:B:242:PRO:HD2	1:B:243:GLU:H	1.70	0.56
1:B:546:HIS:O	1:B:547:SER:OG	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:LEU:CD1	1:A:710:LEU:HD11	2.36	0.56
1:D:312:GLU:HG2	1:D:313:GLN:H	1.67	0.56
1:F:635:PRO:HD2	1:F:638:ARG:HD2	1.86	0.56
1:C:542:GLU:HG2	1:C:666:HIS:HA	1.88	0.56
1:D:312:GLU:CG	1:D:313:GLN:N	2.69	0.56
1:D:680:LEU:HB2	1:D:691:ARG:HH21	1.69	0.56
1:E:550:THR:HB	2:E:801:ADP:O1A	2.05	0.56
1:C:688:ASP:O	1:C:692:THR:HG23	2.05	0.56
1:F:296:GLY:H	1:F:297:GLU:CB	2.18	0.56
1:A:407:LEU:HD12	1:A:426:ILE:HG23	1.87	0.56
1:C:281:GLU:CB	1:C:324:ILE:HD13	2.36	0.56
1:F:518:LEU:H	1:F:518:LEU:HD12	1.70	0.56
1:E:267:THR:HA	1:E:372:MET:SD	2.44	0.56
1:B:296:GLY:H	1:B:297:GLU:CB	2.18	0.56
1:D:686:PHE:HB2	1:D:691:ARG:HG2	1.87	0.56
1:B:654:GLU:O	1:C:613:PRO:HG3	2.05	0.56
1:F:546:HIS:CE1	1:F:706:GLY:N	2.74	0.56
1:E:573:MET:SD	1:E:581:LYS:HG2	2.45	0.56
1:D:242:PRO:HD2	1:D:243:GLU:H	1.69	0.56
1:D:687:LYS:O	1:D:691:ARG:HG3	2.06	0.56
1:A:683:LEU:HD12	1:A:714:ILE:HD13	1.87	0.56
1:D:657:MET:HG2	1:D:661:PHE:CE2	2.41	0.56
1:A:513:PRO:O	1:A:517:VAL:HG23	2.05	0.56
1:F:261:PRO:HG2	1:F:264:CYS:HB2	1.87	0.56
1:A:536:LEU:HD23	1:A:633:ALA:HA	1.88	0.56
1:A:688:ASP:OD1	1:A:689:LYS:N	2.39	0.56
1:A:293:LYS:O	1:A:294:TYR:CG	2.59	0.56
1:A:231:PHE:CE1	1:A:235:PHE:HE2	2.24	0.55
1:E:551:ALA:HB2	2:E:801:ADP:H3'	1.88	0.55
1:B:596:GLN:HA	1:B:638:ARG:HG2	1.87	0.55
1:B:582:CYS:SG	1:C:574:ILE:HG22	2.46	0.55
1:E:549:LYS:HA	1:E:552:LEU:HD12	1.87	0.55
1:B:571:ASP:O	1:B:574:ILE:HG13	2.05	0.55
1:B:270:ALA:O	1:B:273:ILE:HG22	2.06	0.55
1:B:621:LEU:HD11	1:C:575:GLY:HA2	1.87	0.55
1:F:538:SER:OG	1:F:661:PHE:HD1	1.86	0.55
1:C:686:PHE:CE1	1:C:714:ILE:HG23	2.42	0.55
1:A:383:LEU:O	1:A:389:LEU:HB2	2.06	0.55
1:F:404:LEU:HG	1:F:426:ILE:HG22	1.88	0.55
1:E:264:CYS:SG	1:E:395:ILE:HG21	2.46	0.55
1:E:510:TRP:HB2	1:E:679:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ILE:O	2:B:801:ADP:N6	2.40	0.55
1:A:726:VAL:O	1:A:730:LEU:HG	2.05	0.55
1:E:587:LYS:HZ3	1:E:587:LYS:C	2.07	0.55
1:D:632:LYS:NZ	1:E:571:ASP:HB3	2.21	0.55
1:A:683:LEU:HB3	1:A:685:ASN:ND2	2.21	0.55
1:A:521:GLY:HA2	1:A:524:LEU:HD12	1.88	0.55
1:C:589:PHE:CD2	1:C:629:LEU:HD13	2.42	0.55
1:F:503:ILE:HG22	1:F:506:GLY:H	1.71	0.55
1:A:678:GLU:O	1:A:682:LEU:HD12	2.07	0.55
1:F:437:SER:O	1:F:440:GLU:HB2	2.06	0.55
1:D:681:GLU:HG2	1:D:691:ARG:NH1	2.22	0.55
1:C:531:SER:OG	1:D:715:GLU:OE1	2.25	0.55
1:D:257:LEU:HB2	1:D:389:LEU:HD13	1.88	0.55
1:E:270:ALA:O	1:E:273:ILE:HG22	2.06	0.55
1:F:544:PRO:O	1:F:547:SER:OG	2.25	0.55
1:C:616:PRO:HG2	1:D:614:ILE:HD13	1.88	0.55
1:E:232:ARG:O	1:E:236:ALA:CB	2.54	0.55
1:A:531:SER:O	1:A:639:LYS:HE2	2.07	0.55
1:A:231:PHE:CD1	1:A:235:PHE:CE2	2.95	0.55
1:E:437:SER:O	1:E:440:GLU:HB2	2.07	0.55
1:A:352:ASN:HA	1:A:355:LEU:HD12	1.89	0.55
1:C:347:HIS:O	1:C:350:VAL:HG22	2.06	0.55
1:A:540:LEU:HD11	1:A:646:THR:HG22	1.88	0.55
1:F:605:ILE:HD11	1:F:644:GLY:HA3	1.88	0.55
1:A:300:ALA:HA	1:A:303:ARG:HG2	1.89	0.55
1:A:222:GLY:O	1:A:224:ASP:N	2.40	0.55
1:D:534:THR:OG1	1:E:715:GLU:HG2	2.07	0.55
1:E:674:GLU:O	1:E:677:LEU:HB2	2.06	0.55
1:B:289:GLU:O	1:B:291:LEU:N	2.32	0.55
1:B:533:ARG:HG3	1:B:534:THR:N	2.21	0.54
1:C:546:HIS:HB2	1:C:709:LYS:HB2	1.89	0.54
1:E:673:GLY:HA3	1:E:698:VAL:HB	1.88	0.54
1:D:528:THR:OG1	1:D:537:VAL:HG21	2.07	0.54
1:C:375:ARG:NH1	1:C:378:LEU:HG	2.21	0.54
1:F:559:GLU:OE1	1:F:559:GLU:HA	2.07	0.54
1:B:508:ILE:H	2:B:801:ADP:N6	2.01	0.54
1:B:508:ILE:HD13	1:B:683:LEU:HD21	1.88	0.54
1:C:555:LYS:HA	1:C:558:GLU:OE1	2.06	0.54
1:F:512:ASP:OD1	1:F:513:PRO:HD3	2.08	0.54
1:F:397:LEU:CB	1:F:398:PRO:CD	2.86	0.54
1:A:627:LEU:HD13	1:B:607:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ALA:O	1:A:629:LEU:HG	2.08	0.54
1:A:242:PRO:HD2	1:A:243:GLU:CD	2.28	0.54
1:A:286:ASN:HB2	1:A:327:PHE:CB	2.38	0.54
1:A:315:ARG:HG2	1:A:316:LEU:CD1	2.37	0.54
1:F:436:PHE:HB3	1:F:440:GLU:CB	2.37	0.54
1:E:595:SER:HB3	1:E:598:SER:HB3	1.89	0.54
1:E:310:GLU:OE2	1:E:357:LYS:NZ	2.40	0.54
1:D:512:ASP:N	1:D:513:PRO:CD	2.71	0.54
1:F:612:VAL:CG1	1:F:617:ARG:HB2	2.38	0.54
1:F:411:THR:O	1:F:414:MET:HB2	2.07	0.54
1:C:284:VAL:HG11	1:C:305:LEU:HD11	1.89	0.54
1:A:535:PRO:HB3	1:B:504:MET:SD	2.47	0.54
1:A:437:SER:OG	1:A:440:GLU:HG2	2.07	0.54
1:F:548:GLY:HA3	1:F:707:ILE:CG2	2.38	0.54
1:F:223:LEU:HD21	1:F:397:LEU:O	2.06	0.54
1:D:677:LEU:O	1:D:691:ARG:NH2	2.40	0.54
1:C:577:SER:O	1:C:579:THR:N	2.40	0.54
1:A:724:TYR:HD1	1:A:727:ARG:HH12	1.54	0.54
1:A:227:PHE:CE2	1:A:231:PHE:HD1	2.26	0.54
1:D:657:MET:HG2	1:D:661:PHE:HE2	1.73	0.54
1:A:563:PRO:HG2	1:A:597:LEU:O	2.08	0.54
1:E:510:TRP:HB2	1:E:679:ALA:HB2	1.88	0.54
1:E:705:ILE:HD13	1:E:710:LEU:HD13	1.89	0.54
1:A:683:LEU:HD11	1:A:711:LEU:HD23	1.89	0.54
1:A:355:LEU:HB3	1:A:388:ARG:NH1	2.23	0.54
1:D:686:PHE:CE1	1:D:714:ILE:HG23	2.42	0.54
1:F:686:PHE:HE1	1:F:714:ILE:HG23	1.73	0.54
1:D:670:ILE:HG12	1:D:705:ILE:O	2.08	0.54
1:D:310:GLU:O	1:D:313:GLN:NE2	2.40	0.54
1:C:728:LYS:HE3	1:C:732:LEU:HD21	1.90	0.54
1:A:235:PHE:CE1	1:A:277:LEU:CB	2.90	0.54
1:E:516:ARG:O	1:E:519:ASP:OD1	2.25	0.54
1:F:546:HIS:CE1	1:F:706:GLY:H	2.26	0.54
1:B:315:ARG:HG3	1:B:316:LEU:HD12	1.90	0.54
1:F:267:THR:HA	1:F:372:MET:SD	2.48	0.54
1:C:245:VAL:O	1:C:249:GLY:N	2.36	0.54
1:C:546:HIS:CB	1:C:709:LYS:HB2	2.38	0.54
1:C:677:LEU:HD21	1:C:695:ALA:CB	2.38	0.54
1:B:479:ASP:O	1:B:482:ALA:N	2.41	0.54
1:E:662:SER:HA	1:F:709:LYS:NZ	2.23	0.54
1:A:611:TYR:HD1	1:A:618:PHE:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:PHE:HE1	1:C:714:ILE:HG23	1.73	0.53
1:F:562:PHE:HE2	1:F:597:LEU:HD12	1.73	0.53
1:A:716:MET:HG2	1:A:732:LEU:HD11	1.88	0.53
1:B:576:PHE:HB2	1:B:581:LYS:HG3	1.90	0.53
1:B:648:ARG:HG3	1:B:651:VAL:HG23	1.90	0.53
1:A:227:PHE:CE1	1:A:273:ILE:HD13	2.44	0.53
1:C:521:GLY:HA3	1:C:556:ILE:HD13	1.91	0.53
1:B:569:SER:HA	1:B:603:ASP:HB3	1.88	0.53
1:C:540:LEU:HD23	1:C:649:LYS:HE3	1.90	0.53
1:F:582:CYS:SG	1:F:586:LYS:HE3	2.48	0.53
1:A:548:GLY:N	1:A:708:LYS:HB2	2.22	0.53
1:C:591:ASP:O	1:C:594:LYS:HB3	2.08	0.53
1:A:264:CYS:SG	1:A:265:GLY:N	2.80	0.53
1:B:267:THR:HA	1:B:372:MET:SD	2.47	0.53
1:B:527:GLN:NE2	1:C:716:MET:SD	2.77	0.53
1:F:510:TRP:HZ3	1:F:675:GLN:NE2	2.06	0.53
1:F:310:GLU:OE2	1:F:357:LYS:NZ	2.41	0.53
1:C:308:ASP:OD1	1:C:309:ALA:N	2.41	0.53
1:E:664:THR:C	1:E:665:ILE:HD13	2.29	0.53
1:A:406:ILE:O	1:A:409:ILE:HG22	2.07	0.53
1:C:256:ILE:HA	1:C:391:VAL:HG13	1.90	0.53
1:C:227:PHE:O	1:C:231:PHE:HB2	2.09	0.53
1:F:315:ARG:HG3	1:F:316:LEU:HD12	1.90	0.53
1:F:522:GLU:OE2	1:F:526:GLN:HG2	2.08	0.53
1:C:690:GLU:CB	1:C:726:VAL:HG21	2.38	0.53
1:C:570:PRO:HG2	1:C:604:ASP:HB2	1.91	0.53
1:D:265:GLY:O	1:D:268:LEU:HG	2.09	0.53
1:C:708:LYS:HA	1:C:711:LEU:HG	1.90	0.53
1:D:527:GLN:NE2	1:E:716:MET:HA	2.24	0.53
1:B:310:GLU:OE2	1:B:357:LYS:NZ	2.40	0.53
1:F:721:ASP:HB2	1:F:724:TYR:CD1	2.42	0.53
1:F:450:SER:O	1:F:453:MET:HB2	2.09	0.53
1:C:444:LEU:HD12	1:C:445:VAL:HG23	1.91	0.53
1:A:536:LEU:HD23	1:A:634:PRO:HD3	1.90	0.53
1:C:410:HIS:O	1:C:414:MET:HG2	2.09	0.53
1:D:618:PHE:CE2	1:E:614:ILE:HD12	2.43	0.53
1:C:508:ILE:O	2:C:801:ADP:N6	2.42	0.53
1:F:263:GLY:O	1:F:437:SER:HB3	2.08	0.53
1:E:604:ASP:O	1:E:608:LEU:N	2.38	0.53
1:F:242:PRO:HD2	1:F:243:GLU:H	1.72	0.53
1:C:611:TYR:HE1	1:C:616:PRO:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:O	1:A:246:GLU:HG2	2.09	0.53
1:A:306:PHE:CD1	1:A:357:LYS:HB3	2.43	0.53
1:D:375:ARG:NH2	1:D:377:ASP:OD2	2.42	0.53
1:F:436:PHE:CD2	1:F:444:LEU:HD11	2.44	0.52
1:F:503:ILE:HD11	1:F:551:ALA:HA	1.90	0.52
1:C:242:PRO:HD2	1:C:243:GLU:H	1.73	0.52
1:F:440:GLU:O	1:F:444:LEU:HG	2.09	0.52
1:D:560:SER:HB2	1:D:562:PHE:CD1	2.45	0.52
1:D:523:LEU:HD13	1:E:720:MET:SD	2.49	0.52
1:F:515:THR:HA	1:F:518:LEU:CD1	2.39	0.52
1:F:260:GLY:N	1:F:266:LYS:HD3	2.25	0.52
1:B:589:PHE:HD2	1:B:629:LEU:HD22	1.74	0.52
1:A:706:GLY:O	1:A:710:LEU:N	2.43	0.52
1:D:604:ASP:HB3	1:D:607:ARG:HB2	1.91	0.52
1:C:612:VAL:HG12	1:C:617:ARG:HB3	1.91	0.52
1:C:377:ASP:OD2	1:C:377:ASP:N	2.36	0.52
1:E:696:GLN:HB3	1:E:697:GLN:NE2	2.24	0.52
1:D:731:ALA:HA	1:D:734:ARG:NH1	2.23	0.52
1:B:576:PHE:HB3	1:B:580:ALA:HB3	1.90	0.52
1:E:684:GLY:HA2	1:E:691:ARG:NH2	2.25	0.52
1:D:628:VAL:HG13	1:E:571:ASP:OD1	2.08	0.52
1:A:286:ASN:HB2	1:A:327:PHE:HB3	1.91	0.52
1:C:490:PRO:HB2	1:C:492:PHE:N	2.25	0.52
1:F:529:LYS:HG3	1:F:597:LEU:HD11	1.90	0.52
1:C:681:GLU:HG3	1:C:691:ARG:HD2	1.91	0.52
1:D:686:PHE:HB3	1:D:690:GLU:HG3	1.91	0.52
1:F:617:ARG:HG3	1:F:617:ARG:HH11	1.74	0.52
1:F:270:ALA:O	1:F:273:ILE:HG22	2.09	0.52
1:C:510:TRP:CZ3	1:C:670:ILE:HD12	2.45	0.52
1:F:593:TYR:O	1:F:638:ARG:HD3	2.10	0.52
1:C:613:PRO:HD3	1:C:648:ARG:NH2	2.24	0.52
1:A:263:GLY:C	1:A:437:SER:HB3	2.30	0.52
1:E:315:ARG:HG3	1:E:316:LEU:HD12	1.90	0.52
1:C:715:GLU:HA	1:C:715:GLU:OE1	2.09	0.52
1:F:517:VAL:HG21	1:F:667:VAL:HG21	1.91	0.52
1:F:268:LEU:HD23	1:F:439:ALA:H	1.75	0.52
1:C:388:ARG:NH1	1:C:388:ARG:HB2	2.24	0.52
1:D:627:LEU:HD13	1:E:607:ARG:HH12	1.74	0.52
1:D:313:GLN:OE1	1:D:365:ASN:O	2.28	0.52
1:D:686:PHE:HE1	1:D:714:ILE:HG23	1.75	0.52
1:A:673:GLY:O	1:A:677:LEU:HD22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:HA3	1:A:402:GLY:CA	2.32	0.52
1:C:611:TYR:CZ	1:C:651:VAL:HG11	2.45	0.52
1:F:236:ALA:HA	1:F:239:VAL:CG1	2.39	0.52
1:A:568:CYS:O	1:A:603:ASP:HB3	2.10	0.52
1:C:256:ILE:HG22	1:C:391:VAL:HG11	1.92	0.52
1:F:525:VAL:HG13	1:F:562:PHE:HE1	1.73	0.52
1:F:635:PRO:HB2	1:F:638:ARG:NH1	2.25	0.52
1:A:398:PRO:HG3	1:A:436:PHE:O	2.09	0.51
1:D:567:ILE:HG23	1:D:601:VAL:HB	1.92	0.51
1:A:548:GLY:CA	1:A:708:LYS:HB2	2.39	0.51
1:D:531:SER:HG	1:D:534:THR:HG1	1.56	0.51
1:A:611:TYR:CE2	1:A:651:VAL:HG11	2.44	0.51
1:A:258:LEU:O	1:A:372:MET:HA	2.10	0.51
1:A:300:ALA:O	1:A:304:LYS:HG3	2.10	0.51
1:E:327:PHE:CZ	1:E:369:VAL:HG21	2.45	0.51
1:A:549:LYS:HE3	1:A:646:THR:C	2.31	0.51
1:A:683:LEU:HB3	1:A:685:ASN:HD22	1.73	0.51
1:D:527:GLN:HA	1:E:719:GLN:HG3	1.92	0.51
1:D:690:GLU:O	1:D:693:THR:OG1	2.23	0.51
1:B:728:LYS:HE3	1:B:732:LEU:HD21	1.91	0.51
1:B:406:ILE:H	1:B:406:ILE:HD12	1.74	0.51
1:D:592:ALA:HB1	1:D:640:LEU:HD13	1.93	0.51
1:A:231:PHE:CE2	1:A:235:PHE:HD2	2.29	0.51
1:C:256:ILE:O	1:C:370:ILE:HA	2.10	0.51
1:D:527:GLN:NE2	1:E:715:GLU:O	2.40	0.51
1:A:255:GLY:HA3	1:A:389:LEU:HD13	1.91	0.51
1:A:503:ILE:HG22	1:A:506:GLY:H	1.75	0.51
1:A:222:GLY:H	1:A:405:GLN:CB	2.23	0.51
1:D:254:LYS:O	1:D:368:LEU:HA	2.10	0.51
1:E:717:SER:OG	1:E:729:PHE:HB2	2.11	0.51
1:C:445:VAL:HG12	1:C:449:GLN:HE22	1.75	0.51
1:C:231:PHE:O	1:C:235:PHE:HB2	2.11	0.51
1:D:522:GLU:OE2	1:D:556:ILE:HA	2.10	0.51
1:E:527:GLN:CD	1:F:716:MET:HG2	2.31	0.51
1:A:681:GLU:HA	1:A:691:ARG:CZ	2.41	0.51
1:F:508:ILE:C	1:F:509:LYS:HD3	2.30	0.51
1:B:221:GLY:HA3	1:B:406:ILE:HD11	1.92	0.51
1:D:531:SER:OG	1:D:534:THR:OG1	2.27	0.51
1:D:298:SER:O	1:D:301:ASN:HB3	2.10	0.51
1:C:547:SER:HB2	1:C:549:LYS:HG3	1.93	0.51
1:C:510:TRP:HB2	1:C:679:ALA:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:LEU:CD1	1:E:607:ARG:HH12	2.24	0.51
1:C:688:ASP:HA	1:C:691:ARG:NH1	2.26	0.51
1:C:270:ALA:O	1:C:273:ILE:HG22	2.11	0.51
1:A:550:THR:HG23	1:A:603:ASP:OD1	2.11	0.51
1:C:285:VAL:HA	1:C:326:ILE:HG13	1.93	0.51
1:C:499:TYR:HB3	1:C:558:GLU:OE2	2.11	0.51
1:B:421:SER:HG	1:B:479:ASP:N	2.08	0.51
1:D:260:GLY:HA3	1:D:266:LYS:HD3	1.92	0.51
1:A:235:PHE:N	1:A:235:PHE:CD1	2.71	0.50
1:C:542:GLU:HB2	1:C:649:LYS:HD3	1.91	0.50
1:F:303:ARG:CG	1:F:357:LYS:HE2	2.41	0.50
1:A:527:GLN:HB2	1:B:719:GLN:HG3	1.93	0.50
1:D:570:PRO:HA	1:D:573:MET:HB3	1.93	0.50
1:F:428:GLU:O	1:F:432:GLU:HG2	2.11	0.50
1:B:507:ILE:HA	2:B:801:ADP:C5	2.45	0.50
1:F:265:GLY:CA	1:F:437:SER:HB2	2.41	0.50
1:F:658:LEU:HA	1:F:661:PHE:HD2	1.75	0.50
1:C:525:VAL:HG13	1:C:562:PHE:CZ	2.46	0.50
1:D:260:GLY:N	1:D:266:LYS:HD3	2.26	0.50
1:B:348:ASP:O	1:B:352:ASN:ND2	2.45	0.50
1:B:570:PRO:HG3	1:B:608:LEU:HD23	1.93	0.50
1:D:310:GLU:O	1:D:313:GLN:HG2	2.12	0.50
1:C:261:PRO:CB	1:C:594:LYS:HG3	2.41	0.50
1:D:325:ILE:O	1:D:369:VAL:HA	2.12	0.50
1:B:428:GLU:O	1:B:432:GLU:HG2	2.12	0.50
1:A:222:GLY:H	1:A:405:GLN:CG	2.25	0.50
1:A:270:ALA:HA	1:A:273:ILE:HG22	1.93	0.50
1:C:511:GLY:CA	1:C:513:PRO:HD2	2.41	0.50
1:A:411:THR:HG21	1:A:426:ILE:HD11	1.93	0.50
1:B:549:LYS:HZ3	1:B:647:SER:HA	1.76	0.50
1:A:687:LYS:NZ	1:A:722:PRO:HB3	2.26	0.50
1:E:404:LEU:HG	1:E:426:ILE:HG22	1.94	0.50
1:E:627:LEU:HD13	1:F:607:ARG:CZ	2.42	0.50
1:E:586:LYS:NZ	1:F:574:ILE:O	2.36	0.50
1:B:627:LEU:CD2	1:B:657:MET:HG3	2.40	0.50
1:E:261:PRO:HB3	1:E:594:LYS:HE2	1.93	0.50
1:C:584:ALA:O	1:C:588:ILE:HG13	2.11	0.50
1:B:606:GLU:N	1:B:606:GLU:OE1	2.45	0.50
1:F:268:LEU:HD12	1:F:269:LEU:N	2.27	0.50
1:D:543:GLY:H	1:D:549:LYS:HD3	1.76	0.50
1:A:510:TRP:HB2	1:A:679:ALA:CA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:GLN:HG3	1:D:314:ARG:N	2.27	0.50
1:C:331:ASP:HA	1:C:379:ILE:CD1	2.42	0.50
1:D:236:ALA:HB1	1:E:453:MET:HG3	1.93	0.50
1:A:428:GLU:O	1:A:431:VAL:HG12	2.12	0.50
1:C:730:LEU:O	1:C:734:ARG:HG3	2.12	0.50
1:B:423:ASP:HB2	1:B:479:ASP:N	2.27	0.50
1:E:612:VAL:HG11	1:E:617:ARG:HH21	1.76	0.50
1:A:399:ASP:O	1:A:403:ARG:N	2.22	0.50
1:C:511:GLY:C	1:C:513:PRO:HD2	2.33	0.49
1:E:684:GLY:HA2	1:E:691:ARG:HH21	1.77	0.49
1:C:614:ILE:O	1:C:616:PRO:HA	2.12	0.49
1:D:330:ILE:HD12	1:D:331:ASP:N	2.27	0.49
1:E:553:ALA:HA	1:E:556:ILE:HD12	1.94	0.49
1:C:568:CYS:HB2	1:C:602:VAL:HA	1.93	0.49
1:C:707:ILE:HD12	1:C:710:LEU:HD23	1.94	0.49
1:B:516:ARG:O	1:B:519:ASP:OD1	2.30	0.49
1:B:631:LYS:NZ	1:C:604:ASP:OD2	2.38	0.49
1:B:303:ARG:CG	1:B:357:LYS:HE2	2.41	0.49
1:A:509:LYS:HD2	1:A:509:LYS:N	2.26	0.49
1:A:326:ILE:HG22	1:A:370:ILE:CG1	2.39	0.49
1:E:563:PRO:HD2	1:E:597:LEU:O	2.11	0.49
1:B:648:ARG:HH11	1:B:651:VAL:HG22	1.75	0.49
1:F:514:VAL:O	1:F:518:LEU:HD12	2.12	0.49
1:E:233:ARG:HG2	1:F:454:ASN:HB2	1.94	0.49
1:B:626:LEU:O	1:B:630:LEU:HG	2.11	0.49
1:E:510:TRP:CE2	1:E:707:ILE:HB	2.47	0.49
1:A:261:PRO:HD2	1:A:396:GLY:HA2	1.94	0.49
1:E:519:ASP:O	1:E:522:GLU:HB2	2.13	0.49
1:D:681:GLU:HG2	1:D:691:ARG:CZ	2.42	0.49
1:C:612:VAL:CG1	1:C:617:ARG:HB3	2.41	0.49
1:E:540:LEU:HD12	1:E:644:GLY:O	2.13	0.49
1:F:544:PRO:HD2	1:F:669:ASN:OD1	2.13	0.49
1:C:513:PRO:HA	1:C:516:ARG:HG2	1.94	0.49
1:C:513:PRO:HD3	1:C:675:GLN:NE2	2.28	0.49
1:D:548:GLY:HA2	2:D:801:ADP:H5'2	1.91	0.49
1:E:303:ARG:CG	1:E:357:LYS:HE2	2.41	0.49
1:B:455:ARG:NH2	1:B:481:LEU:CB	2.75	0.49
1:B:256:ILE:O	1:B:370:ILE:HA	2.13	0.49
1:D:628:VAL:O	1:D:632:LYS:N	2.46	0.49
1:F:261:PRO:HB3	1:F:594:LYS:CB	2.43	0.49
1:D:402:GLY:HA2	1:D:405:GLN:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:LEU:HD11	1:E:663:THR:HG21	1.94	0.49
1:D:527:GLN:HE22	1:E:716:MET:HA	1.78	0.49
1:B:436:PHE:HB3	1:B:440:GLU:CB	2.42	0.49
1:E:590:ASP:O	1:E:593:TYR:HB2	2.13	0.49
1:C:322:LEU:HD22	1:C:366:ASN:O	2.13	0.49
1:D:268:LEU:HA	1:D:271:ARG:CD	2.43	0.49
1:C:703:VAL:O	1:C:704:TRP:HD1	1.95	0.49
1:C:428:GLU:O	1:C:432:GLU:HG2	2.12	0.49
1:E:221:GLY:HA3	1:E:406:ILE:HD12	1.94	0.49
1:A:222:GLY:H	1:A:405:GLN:HG2	1.76	0.49
1:E:653:GLN:OE1	1:E:658:LEU:HD23	2.12	0.49
1:F:510:TRP:HA	1:F:678:GLU:HG3	1.95	0.49
1:D:581:LYS:O	1:D:585:MET:HG2	2.13	0.49
1:A:313:GLN:OE1	1:A:317:GLY:HA2	2.13	0.49
1:A:509:LYS:HG2	1:A:515:THR:OG1	2.12	0.49
1:C:671:ALA:HA	1:C:703:VAL:O	2.13	0.49
1:E:313:GLN:O	1:E:317:GLY:N	2.45	0.49
1:C:512:ASP:N	1:C:513:PRO:CD	2.76	0.49
1:D:602:VAL:O	1:D:644:GLY:HA2	2.13	0.49
1:F:236:ALA:O	1:F:239:VAL:HG12	2.13	0.49
1:D:589:PHE:CE2	1:D:629:LEU:HD13	2.48	0.49
1:C:325:ILE:HG13	1:C:369:VAL:HG23	1.93	0.49
1:E:672:THR:OG1	1:E:675:GLN:HB2	2.13	0.49
1:E:428:GLU:O	1:E:432:GLU:HG2	2.12	0.49
1:C:540:LEU:HD11	1:C:646:THR:HG22	1.94	0.49
1:C:604:ASP:H	1:C:645:THR:HG1	1.58	0.49
1:D:242:PRO:HD2	1:D:243:GLU:N	2.28	0.49
1:B:352:ASN:HA	1:B:355:LEU:HD12	1.95	0.49
1:B:313:GLN:O	1:B:317:GLY:N	2.45	0.49
1:D:539:VAL:HG13	1:D:643:ILE:HG13	1.94	0.49
1:A:283:LYS:HA	1:A:324:ILE:O	2.13	0.49
1:C:352:ASN:HD22	1:D:289:GLU:CB	2.26	0.49
1:A:652:LEU:HA	1:A:655:MET:SD	2.53	0.49
1:C:560:SER:HB2	1:C:562:PHE:CE1	2.48	0.49
1:D:540:LEU:HD12	1:D:661:PHE:CE1	2.48	0.49
1:F:223:LEU:O	1:F:227:PHE:HB3	2.13	0.49
1:C:573:MET:HB3	1:C:576:PHE:CD2	2.48	0.49
1:D:241:PRO:HA	1:D:242:PRO:HA	1.66	0.49
1:D:424:VAL:HG21	1:D:480:PHE:HA	1.93	0.49
1:D:486:ASN:O	1:D:490:PRO:HD3	2.13	0.49
1:F:313:GLN:O	1:F:317:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:ILE:O	1:F:370:ILE:HA	2.13	0.48
1:C:691:ARG:HB2	1:C:691:ARG:HH11	1.76	0.48
1:B:437:SER:O	1:B:440:GLU:HB2	2.13	0.48
1:F:677:LEU:O	1:F:681:GLU:HG3	2.13	0.48
1:D:284:VAL:HG21	1:D:325:ILE:HG22	1.95	0.48
1:B:222:GLY:HA3	1:B:399:ASP:HB2	1.95	0.48
1:B:406:ILE:HB	1:B:441:LEU:HD13	1.95	0.48
1:F:526:GLN:O	1:F:530:ASN:HB2	2.11	0.48
1:C:404:LEU:HG	1:C:426:ILE:HG22	1.95	0.48
1:F:436:PHE:N	1:F:436:PHE:CD1	2.80	0.48
1:E:254:LYS:O	1:E:368:LEU:HA	2.13	0.48
1:E:256:ILE:O	1:E:370:ILE:HA	2.13	0.48
1:E:689:LYS:O	1:E:692:THR:OG1	2.25	0.48
1:D:721:ASP:O	1:D:725:ARG:HG3	2.13	0.48
1:B:281:GLU:N	1:B:282:PRO:HA	2.28	0.48
1:E:714:ILE:O	1:E:718:LEU:HG	2.13	0.48
1:B:541:LEU:O	1:B:541:LEU:HD12	2.13	0.48
1:A:508:ILE:HD12	1:A:682:LEU:HB2	1.96	0.48
1:C:497:GLU:OE1	1:C:498:ASP:N	2.46	0.48
1:D:264:CYS:SG	1:D:395:ILE:HG21	2.53	0.48
1:F:566:LYS:HD2	1:F:567:ILE:H	1.77	0.48
1:A:517:VAL:HG13	1:A:665:ILE:CG2	2.43	0.48
1:D:260:GLY:CA	1:D:266:LYS:HD3	2.43	0.48
1:E:596:GLN:O	1:E:638:ARG:HA	2.13	0.48
1:C:322:LEU:HD12	1:C:324:ILE:HD11	1.95	0.48
1:F:552:LEU:O	1:F:556:ILE:HG13	2.14	0.48
1:C:237:SER:OG	1:C:252:HIS:ND1	2.44	0.48
1:A:567:ILE:HG13	1:A:601:VAL:CB	2.41	0.48
1:D:694:ILE:O	1:D:698:VAL:HG22	2.13	0.48
1:B:236:ALA:HA	1:B:239:VAL:CG1	2.43	0.48
1:A:436:PHE:CD2	1:A:444:LEU:HD11	2.48	0.48
1:B:485:GLU:O	1:B:490:PRO:HD3	2.13	0.48
1:C:596:GLN:HA	1:C:638:ARG:CD	2.41	0.48
1:F:720:MET:HB3	1:F:724:TYR:HB2	1.95	0.48
1:A:428:GLU:O	1:A:432:GLU:HG2	2.14	0.48
1:E:281:GLU:N	1:E:282:PRO:HA	2.27	0.48
1:B:246:GLU:HG2	1:B:247:GLN:N	2.28	0.48
1:C:326:ILE:HB	1:C:370:ILE:HD11	1.95	0.48
1:A:690:GLU:HB3	1:A:726:VAL:HG22	1.95	0.48
1:C:604:ASP:N	1:C:645:THR:OG1	2.43	0.48
1:B:452:ALA:HA	1:B:455:ARG:CZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:438:GLY:O	1:F:441:LEU:HB2	2.13	0.48
1:E:289:GLU:O	1:E:291:LEU:N	2.32	0.48
1:C:289:GLU:O	1:C:291:LEU:N	2.34	0.48
1:E:705:ILE:HD12	1:E:713:LEU:HD12	1.96	0.48
1:E:627:LEU:HG	1:E:657:MET:HE1	1.96	0.48
1:B:307:ALA:HA	1:B:310:GLU:HG2	1.96	0.48
1:C:311:GLU:O	1:C:314:ARG:HG2	2.14	0.48
1:D:331:ASP:HA	1:D:379:ILE:HD11	1.96	0.48
1:C:589:PHE:CE1	1:C:600:VAL:HG11	2.49	0.48
1:F:281:GLU:N	1:F:282:PRO:HA	2.28	0.48
1:F:570:PRO:CG	1:F:604:ASP:HB2	2.41	0.48
1:E:562:PHE:CD1	1:E:597:LEU:HG	2.49	0.48
1:B:479:ASP:O	1:B:480:PHE:C	2.51	0.48
1:A:499:TYR:OH	1:A:565:ILE:HB	2.14	0.48
1:A:677:LEU:HG	1:A:695:ALA:CB	2.43	0.48
1:E:257:LEU:HG	1:E:371:GLY:O	2.14	0.48
1:A:407:LEU:CD1	1:A:426:ILE:HG23	2.44	0.48
1:F:257:LEU:HG	1:F:371:GLY:O	2.14	0.48
1:E:286:ASN:OD1	1:E:327:PHE:HD1	1.97	0.48
1:E:352:ASN:HA	1:E:355:LEU:HD12	1.96	0.48
1:E:508:ILE:HD13	1:E:683:LEU:HD21	1.95	0.47
1:A:543:GLY:O	1:A:647:SER:HA	2.14	0.47
1:F:629:LEU:O	1:F:632:LYS:HB3	2.14	0.47
1:B:670:ILE:HG21	1:B:675:GLN:HB2	1.96	0.47
1:A:517:VAL:HG13	1:A:665:ILE:HG21	1.96	0.47
1:A:241:PRO:HA	1:A:242:PRO:HA	1.39	0.47
1:B:230:ILE:HD11	1:B:391:VAL:HG11	1.96	0.47
1:A:540:LEU:HD12	1:A:644:GLY:O	2.14	0.47
1:B:438:GLY:O	1:B:441:LEU:N	2.42	0.47
1:A:398:PRO:HD2	1:A:434:LYS:O	2.14	0.47
1:B:428:GLU:O	1:B:431:VAL:HG12	2.14	0.47
1:D:578:GLU:OE1	1:D:621:LEU:HD13	2.14	0.47
1:F:609:LEU:HD13	1:F:655:MET:CE	2.43	0.47
1:C:538:SER:OG	1:C:662:SER:N	2.38	0.47
1:D:627:LEU:CD2	1:D:657:MET:HG3	2.45	0.47
1:D:670:ILE:HD11	1:D:705:ILE:CG2	2.44	0.47
1:A:388:ARG:O	1:A:389:LEU:HD22	2.14	0.47
1:C:576:PHE:HB3	1:C:580:ALA:HB3	1.96	0.47
1:D:593:TYR:OH	1:D:632:LYS:HD2	2.14	0.47
1:A:242:PRO:O	1:A:246:GLU:OE1	2.32	0.47
1:D:268:LEU:HA	1:D:271:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:428:GLU:O	1:E:431:VAL:HG12	2.14	0.47
1:F:327:PHE:CB	1:F:330:ILE:HG22	2.44	0.47
1:A:650:ASP:OD1	1:A:650:ASP:N	2.46	0.47
1:E:440:GLU:O	1:E:444:LEU:HG	2.14	0.47
1:F:525:VAL:HG11	1:F:560:SER:CB	2.45	0.47
1:F:510:TRP:CB	1:F:679:ALA:HB2	2.43	0.47
1:D:397:LEU:HD23	1:D:398:PRO:CD	2.42	0.47
1:E:677:LEU:HD11	1:E:695:ALA:HA	1.95	0.47
1:F:710:LEU:O	1:F:714:ILE:HG13	2.14	0.47
1:F:579:THR:O	1:F:583:GLN:HG2	2.14	0.47
1:C:513:PRO:HD3	1:C:675:GLN:HE22	1.80	0.47
1:D:527:GLN:HE22	1:E:716:MET:N	2.13	0.47
1:C:666:HIS:CE1	1:C:668:PRO:HB3	2.49	0.47
1:D:310:GLU:O	1:D:313:GLN:CG	2.63	0.47
1:A:237:SER:OG	1:A:252:HIS:HA	2.14	0.47
1:B:540:LEU:HD11	1:B:649:LYS:HZ2	1.79	0.47
1:C:609:LEU:O	1:C:610:ASP:HB2	2.13	0.47
1:E:508:ILE:HG13	1:E:510:TRP:HB3	1.95	0.47
1:E:705:ILE:CD1	1:E:713:LEU:HD12	2.45	0.47
1:D:652:LEU:HD13	1:D:657:MET:HB3	1.95	0.47
1:D:510:TRP:CE3	1:D:675:GLN:HG2	2.40	0.47
1:C:721:ASP:O	1:C:725:ARG:HG3	2.13	0.47
1:B:540:LEU:O	1:B:540:LEU:HD12	2.15	0.47
1:D:303:ARG:HH11	1:D:357:LYS:CE	2.28	0.47
1:E:612:VAL:HG22	1:E:613:PRO:HD2	1.97	0.47
1:C:536:LEU:CD1	1:C:640:LEU:HB3	2.44	0.47
1:B:241:PRO:HA	1:B:242:PRO:HA	1.58	0.47
1:F:428:GLU:O	1:F:431:VAL:HG12	2.15	0.47
1:D:564:PHE:HB3	1:D:598:SER:HB3	1.97	0.47
1:B:503:ILE:HG22	1:B:506:GLY:H	1.79	0.47
1:C:510:TRP:CD2	1:C:707:ILE:HD13	2.50	0.47
1:E:531:SER:HB3	1:E:534:THR:O	2.14	0.47
1:A:683:LEU:HD13	1:A:685:ASN:HD22	1.79	0.47
1:E:311:GLU:O	1:E:314:ARG:HG2	2.15	0.47
1:A:617:ARG:NH1	1:A:617:ARG:HG3	2.28	0.47
1:F:548:GLY:HA3	1:F:707:ILE:HG22	1.95	0.47
1:E:289:GLU:C	1:E:291:LEU:H	2.17	0.47
1:D:281:GLU:N	1:D:282:PRO:HA	2.30	0.47
1:E:526:GLN:HA	1:E:529:LYS:HG2	1.96	0.47
1:F:535:PRO:HB2	1:F:536:LEU:HD13	1.97	0.47
1:F:311:GLU:O	1:F:314:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LEU:HG	1:D:371:GLY:O	2.14	0.47
1:C:428:GLU:O	1:C:431:VAL:HG12	2.15	0.47
1:D:247:GLN:HA	1:E:417:HIS:CE1	2.50	0.47
1:E:272:GLN:HA	1:E:272:GLN:OE1	2.15	0.47
1:B:272:GLN:OE1	1:B:272:GLN:HA	2.15	0.47
1:E:549:LYS:O	1:E:552:LEU:HB2	2.15	0.47
1:B:533:ARG:CG	1:B:534:THR:H	2.18	0.47
1:B:523:LEU:HA	1:B:526:GLN:HG2	1.96	0.47
1:B:527:GLN:HA	1:C:719:GLN:CD	2.36	0.47
1:C:355:LEU:O	1:C:388:ARG:NH2	2.40	0.47
1:B:237:SER:HA	1:C:453:MET:HG3	1.97	0.47
1:B:640:LEU:CD2	1:B:642:ILE:HG13	2.45	0.47
1:B:402:GLY:O	1:B:406:ILE:HD12	2.15	0.47
1:E:233:ARG:CG	1:F:454:ASN:HB2	2.45	0.47
1:C:490:PRO:HA	1:C:491:ALA:CB	2.29	0.47
1:C:550:THR:HB	2:C:801:ADP:O2A	2.15	0.47
1:D:536:LEU:HD21	1:D:630:LEU:O	2.15	0.47
1:C:582:CYS:SG	1:C:621:LEU:HG	2.55	0.47
1:E:697:GLN:HG3	1:E:730:LEU:CD1	2.45	0.47
1:D:654:GLU:HB3	1:E:614:ILE:HD11	1.96	0.47
1:D:688:ASP:O	1:D:692:THR:HG23	2.14	0.47
1:B:710:LEU:O	1:B:714:ILE:HG13	2.15	0.47
1:C:540:LEU:HD22	1:C:661:PHE:CD2	2.50	0.46
1:E:307:ALA:HA	1:E:310:GLU:HG2	1.96	0.46
1:E:540:LEU:HD12	1:E:541:LEU:N	2.30	0.46
1:B:503:ILE:HG12	1:B:551:ALA:HA	1.96	0.46
1:B:319:ASN:HB3	1:B:320:SER:HB2	1.97	0.46
1:A:222:GLY:N	1:A:405:GLN:HB3	2.31	0.46
1:D:407:LEU:O	1:D:411:THR:HG23	2.14	0.46
1:F:307:ALA:HA	1:F:310:GLU:HG2	1.96	0.46
1:B:513:PRO:CD	1:B:670:ILE:HD11	2.44	0.46
1:B:257:LEU:HG	1:B:371:GLY:O	2.15	0.46
1:D:286:ASN:HB2	1:D:327:PHE:CD1	2.47	0.46
1:A:263:GLY:CA	1:A:264:CYS:HB2	2.45	0.46
1:C:670:ILE:HD13	1:C:675:GLN:CG	2.38	0.46
1:D:527:GLN:CD	1:E:716:MET:HA	2.36	0.46
1:C:657:MET:HE3	1:C:661:PHE:CZ	2.50	0.46
1:C:721:ASP:HB2	1:C:724:TYR:CD1	2.50	0.46
1:E:564:PHE:HB3	1:E:595:SER:HB2	1.97	0.46
1:B:542:GLU:CD	1:B:649:LYS:HD3	2.35	0.46
1:D:528:THR:HG21	1:D:641:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLY:C	1:B:437:SER:HB3	2.35	0.46
1:B:311:GLU:O	1:B:314:ARG:HG2	2.15	0.46
1:D:589:PHE:CD2	1:D:629:LEU:HD13	2.50	0.46
1:A:347:HIS:N	1:A:348:ASP:HA	2.31	0.46
1:F:557:ALA:HB2	1:F:601:VAL:HG21	1.98	0.46
1:B:614:ILE:O	1:B:616:PRO:HA	2.14	0.46
1:B:568:CYS:SG	1:B:588:ILE:HD12	2.56	0.46
1:B:499:TYR:HA	1:B:502:TYR:CE2	2.49	0.46
1:B:523:LEU:O	1:B:526:GLN:HG2	2.14	0.46
1:F:223:LEU:HD23	1:F:223:LEU:N	2.31	0.46
1:B:512:ASP:N	1:B:513:PRO:CD	2.78	0.46
1:B:578:GLU:CG	1:B:619:SER:HB2	2.45	0.46
1:B:438:GLY:O	1:B:441:LEU:HB2	2.15	0.46
1:F:261:PRO:O	1:F:264:CYS:HB2	2.15	0.46
1:E:683:LEU:HB3	1:E:685:ASN:OD1	2.16	0.46
1:E:713:LEU:HD23	1:E:713:LEU:HA	1.75	0.46
1:C:510:TRP:NE1	1:C:514:VAL:HG21	2.30	0.46
1:C:546:HIS:HA	1:C:708:LYS:HE2	1.98	0.46
1:C:717:SER:OG	1:C:725:ARG:O	2.30	0.46
1:C:612:VAL:CG2	1:C:613:PRO:HD2	2.46	0.46
1:B:513:PRO:O	1:B:517:VAL:HG23	2.15	0.46
1:A:258:LEU:HD12	1:A:258:LEU:O	2.15	0.46
1:D:609:LEU:O	1:D:610:ASP:OD1	2.34	0.46
1:C:436:PHE:CD1	1:C:436:PHE:N	2.82	0.46
1:A:322:LEU:HD12	1:A:323:HIS:H	1.80	0.46
1:A:231:PHE:CE1	1:A:235:PHE:CE2	3.04	0.46
1:F:653:GLN:HA	1:F:658:LEU:HB3	1.97	0.46
1:C:510:TRP:HA	1:C:679:ALA:HA	1.98	0.46
1:D:550:THR:HG23	2:D:801:ADP:PA	2.56	0.46
1:B:576:PHE:HB2	1:B:581:LYS:CG	2.46	0.46
1:D:510:TRP:CB	1:D:679:ALA:HB2	2.46	0.46
1:F:571:ASP:HA	1:F:574:ILE:HB	1.97	0.46
1:F:268:LEU:HA	1:F:271:ARG:HG2	1.98	0.46
1:A:403:ARG:O	1:A:407:LEU:HG	2.15	0.46
1:D:453:MET:O	1:D:457:ILE:HG13	2.16	0.46
1:B:222:GLY:N	1:B:402:GLY:HA3	2.31	0.46
1:F:230:ILE:HD11	1:F:391:VAL:HG11	1.97	0.46
1:E:451:THR:HB	1:E:481:LEU:CB	2.45	0.46
1:E:397:LEU:HG	1:E:398:PRO:HD2	1.96	0.46
1:E:261:PRO:HG2	1:E:264:CYS:HB2	1.96	0.46
1:E:593:TYR:CD2	1:E:635:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ASP:OD1	1:C:382:ALA:N	2.44	0.46
1:C:539:VAL:HG23	1:C:663:THR:HG23	1.96	0.46
1:E:490:PRO:HA	1:E:491:ALA:CB	2.34	0.46
1:E:527:GLN:HA	1:F:719:GLN:HG3	1.96	0.46
1:C:674:GLU:O	1:C:677:LEU:HB2	2.16	0.46
1:E:261:PRO:HB3	1:E:594:LYS:CE	2.46	0.46
1:B:325:ILE:HG13	1:B:369:VAL:HB	1.98	0.46
1:C:233:ARG:CZ	1:C:233:ARG:HB2	2.45	0.46
1:A:628:VAL:CG1	1:B:571:ASP:HA	2.45	0.46
1:F:261:PRO:HD2	1:F:264:CYS:SG	2.56	0.46
1:D:627:LEU:HA	1:D:627:LEU:HD23	1.68	0.46
1:D:635:PRO:O	1:D:638:ARG:HB2	2.15	0.46
1:E:327:PHE:CE2	1:E:369:VAL:HG21	2.50	0.46
1:D:636:GLN:NE2	1:E:504:MET:SD	2.82	0.46
1:F:694:ILE:O	1:F:698:VAL:HG22	2.17	0.46
1:A:709:LYS:HA	1:A:709:LYS:HE2	1.97	0.45
1:F:589:PHE:CD2	1:F:629:LEU:HD22	2.50	0.45
1:A:624:GLN:HA	1:A:624:GLN:OE1	2.16	0.45
1:B:436:PHE:N	1:B:436:PHE:CD1	2.83	0.45
1:B:440:GLU:O	1:B:444:LEU:HG	2.16	0.45
1:E:648:ARG:NE	1:E:651:VAL:HG13	2.32	0.45
1:B:507:ILE:HG13	1:B:555:LYS:HD3	1.97	0.45
1:F:712:MET:O	1:F:716:MET:HG3	2.15	0.45
1:A:510:TRP:O	1:A:678:GLU:HB3	2.17	0.45
1:A:627:LEU:O	1:A:631:LYS:NZ	2.49	0.45
1:D:686:PHE:HB2	1:D:691:ARG:CG	2.46	0.45
1:B:707:ILE:O	1:B:711:LEU:HG	2.15	0.45
1:E:218:MET:HA	1:E:219:GLY:HA2	1.74	0.45
1:E:319:ASN:HB3	1:E:320:SER:HB2	1.97	0.45
1:E:508:ILE:HD11	1:E:707:ILE:CD1	2.46	0.45
1:B:527:GLN:CB	1:C:719:GLN:HG3	2.45	0.45
1:A:620:ASN:ND2	1:B:610:ASP:OD1	2.49	0.45
1:F:502:TYR:CD2	1:F:503:ILE:HG13	2.51	0.45
1:E:611:TYR:CE1	1:E:616:PRO:HB2	2.51	0.45
1:A:261:PRO:CG	1:A:397:LEU:H	2.30	0.45
1:E:586:LYS:NZ	1:F:575:GLY:HA3	2.32	0.45
1:F:510:TRP:HB3	1:F:679:ALA:CB	2.43	0.45
1:F:307:ALA:O	1:F:310:GLU:HG2	2.17	0.45
1:D:318:ALA:O	1:D:319:ASN:ND2	2.49	0.45
1:A:721:ASP:O	1:A:725:ARG:HG3	2.16	0.45
1:D:564:PHE:HD2	1:D:598:SER:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLN:HA	1:E:417:HIS:ND1	2.31	0.45
1:D:399:ASP:HB3	1:D:401:LYS:HG2	1.98	0.45
1:D:327:PHE:HB2	1:D:330:ILE:CG2	2.47	0.45
1:F:686:PHE:CE1	1:F:714:ILE:HG23	2.50	0.45
1:F:241:PRO:HA	1:F:242:PRO:HA	1.63	0.45
1:C:352:ASN:ND2	1:D:289:GLU:H	2.14	0.45
1:C:562:PHE:O	1:C:565:ILE:HD11	2.17	0.45
1:E:627:LEU:HG	1:E:657:MET:CE	2.46	0.45
1:B:307:ALA:O	1:B:310:GLU:HG2	2.16	0.45
1:F:510:TRP:CE2	1:F:670:ILE:HG12	2.52	0.45
1:F:670:ILE:O	1:F:704:TRP:HA	2.16	0.45
1:C:247:GLN:HA	1:D:417:HIS:NE2	2.31	0.45
1:E:325:ILE:HG13	1:E:369:VAL:HB	1.97	0.45
1:F:319:ASN:HB3	1:F:320:SER:HB2	1.97	0.45
1:C:320:SER:O	1:C:320:SER:OG	2.31	0.45
1:F:612:VAL:HG13	1:F:614:ILE:O	2.17	0.45
1:A:612:VAL:HG12	1:A:617:ARG:HB2	1.99	0.45
1:A:315:ARG:O	1:A:316:LEU:HD12	2.17	0.45
1:C:550:THR:H	2:C:801:ADP:PB	2.40	0.45
1:B:539:VAL:HA	1:B:663:THR:O	2.16	0.45
1:F:632:LYS:HD2	1:F:633:ALA:H	1.81	0.45
1:A:713:LEU:CD2	1:A:732:LEU:HB3	2.42	0.45
1:C:236:ALA:HB1	1:D:453:MET:CB	2.47	0.45
1:C:593:TYR:CE2	1:C:632:LYS:NZ	2.84	0.45
1:A:220:ILE:HG22	1:A:221:GLY:N	2.32	0.45
1:E:732:LEU:HD23	1:E:732:LEU:HA	1.71	0.45
1:E:538:SER:OG	1:E:662:SER:N	2.47	0.45
1:D:303:ARG:HH11	1:D:357:LYS:HE3	1.82	0.45
1:D:542:GLU:OE2	1:D:649:LYS:HD2	2.17	0.45
1:E:713:LEU:CD2	1:E:732:LEU:HD13	2.47	0.45
1:E:714:ILE:HG12	1:E:729:PHE:HE1	1.82	0.45
1:D:550:THR:HG23	2:D:801:ADP:O2A	2.16	0.45
1:B:519:ASP:O	1:B:523:LEU:HG	2.17	0.45
1:A:508:ILE:CD1	1:A:683:LEU:HG	2.47	0.45
1:F:297:GLU:O	1:F:300:ALA:HB3	2.17	0.45
1:E:726:VAL:O	1:E:730:LEU:HG	2.17	0.45
1:B:545:PRO:O	1:B:546:HIS:HB2	2.17	0.45
1:B:503:ILE:HD11	1:B:554:ALA:HB3	1.99	0.45
1:D:218:MET:HA	1:D:219:GLY:HA2	1.77	0.45
1:A:646:THR:HG21	1:A:652:LEU:HD22	1.99	0.44
1:E:297:GLU:O	1:E:300:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:ASP:N	1:E:513:PRO:CD	2.79	0.44
1:E:236:ALA:CA	1:E:239:VAL:HG12	2.44	0.44
1:F:441:LEU:O	1:F:445:VAL:HG23	2.16	0.44
1:D:424:VAL:CG2	1:D:480:PHE:HA	2.46	0.44
1:D:564:PHE:HB3	1:D:598:SER:CB	2.46	0.44
1:E:230:ILE:HD11	1:E:391:VAL:HG11	1.98	0.44
1:E:436:PHE:CD1	1:E:436:PHE:N	2.85	0.44
1:D:312:GLU:HG3	1:D:313:GLN:N	2.32	0.44
1:F:549:LYS:HE3	1:F:646:THR:C	2.38	0.44
1:F:325:ILE:HG13	1:F:369:VAL:HB	1.98	0.44
1:D:231:PHE:HA	1:D:235:PHE:CD2	2.53	0.44
1:C:555:LYS:O	1:C:559:GLU:HG2	2.18	0.44
1:E:307:ALA:O	1:E:310:GLU:HG2	2.16	0.44
1:E:573:MET:O	1:E:576:PHE:HB2	2.16	0.44
1:E:246:GLU:HG2	1:E:247:GLN:N	2.33	0.44
1:F:289:GLU:O	1:F:291:LEU:N	2.35	0.44
1:E:506:GLY:O	1:E:508:ILE:N	2.49	0.44
1:F:525:VAL:HG11	1:F:560:SER:HB2	1.99	0.44
1:D:626:LEU:O	1:D:630:LEU:HG	2.18	0.44
1:B:436:PHE:HB3	1:B:440:GLU:HB2	1.99	0.44
1:F:602:VAL:O	1:F:644:GLY:HA2	2.17	0.44
1:C:355:LEU:HA	1:C:388:ARG:NE	2.31	0.44
1:A:220:ILE:HD11	1:A:227:PHE:CZ	2.53	0.44
1:B:297:GLU:O	1:B:300:ALA:HB3	2.17	0.44
1:A:355:LEU:HD22	1:A:388:ARG:NH1	2.32	0.44
1:A:236:ALA:CB	1:B:453:MET:HB2	2.43	0.44
1:F:546:HIS:CE1	1:F:709:LYS:HB2	2.51	0.44
1:D:300:ALA:O	1:D:303:ARG:HB3	2.18	0.44
1:D:573:MET:SD	1:D:608:LEU:HD22	2.58	0.44
1:E:721:ASP:HB2	1:E:724:TYR:CD2	2.52	0.44
1:F:240:PHE:HA	1:F:241:PRO:HD3	1.82	0.44
1:C:546:HIS:O	1:C:708:LYS:HG2	2.17	0.44
1:D:655:MET:O	1:D:656:GLU:HB2	2.18	0.44
1:B:284:VAL:O	1:B:326:ILE:HG12	2.18	0.44
1:E:586:LYS:NZ	1:F:574:ILE:HG23	2.32	0.44
1:E:696:GLN:OE1	1:E:696:GLN:HA	2.18	0.44
1:B:536:LEU:HD12	1:B:640:LEU:O	2.18	0.44
1:B:240:PHE:HA	1:B:241:PRO:HD3	1.88	0.44
1:D:361:VAL:CB	1:E:285:VAL:HG21	2.48	0.44
1:F:593:TYR:O	1:F:638:ARG:CD	2.66	0.44
1:D:510:TRP:HB3	1:D:679:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:LEU:HD22	1:F:395:ILE:HG23	1.99	0.44
1:B:503:ILE:HD11	1:B:551:ALA:O	2.17	0.44
1:F:443:GLY:O	1:F:446:ARG:HB3	2.18	0.44
1:D:546:HIS:HB3	1:D:708:LYS:CB	2.47	0.44
1:F:272:GLN:OE1	1:F:272:GLN:HA	2.16	0.44
1:C:514:VAL:HG11	2:C:801:ADP:N6	2.33	0.44
1:C:726:VAL:H	1:C:726:VAL:HG23	1.62	0.44
1:A:508:ILE:HD11	1:A:683:LEU:HG	2.00	0.44
1:B:531:SER:HA	1:B:639:LYS:HD3	1.99	0.44
1:A:526:GLN:NE2	1:A:530:ASN:HD22	2.13	0.44
1:B:289:GLU:C	1:B:291:LEU:H	2.16	0.44
1:B:533:ARG:HH21	1:C:685:ASN:HD21	1.65	0.43
1:F:436:PHE:HB3	1:F:440:GLU:HB2	1.98	0.43
1:B:510:TRP:CE2	1:B:514:VAL:CG2	3.01	0.43
1:B:221:GLY:HA3	1:B:406:ILE:HD12	2.00	0.43
1:E:250:CYS:SG	1:F:446:ARG:HA	2.58	0.43
1:B:548:GLY:HA2	2:B:801:ADP:O1A	2.18	0.43
1:B:507:ILE:CG1	1:B:555:LYS:HD3	2.48	0.43
1:F:536:LEU:HD11	1:F:633:ALA:HA	2.00	0.43
1:A:397:LEU:CD1	1:A:435:ASN:HA	2.43	0.43
1:A:564:PHE:CZ	1:A:566:LYS:HB2	2.53	0.43
1:E:242:PRO:HD2	1:E:243:GLU:N	2.33	0.43
1:F:352:ASN:HA	1:F:355:LEU:HD12	1.99	0.43
1:C:519:ASP:O	1:C:523:LEU:HG	2.18	0.43
1:B:375:ARG:NH2	1:B:377:ASP:OD2	2.50	0.43
1:C:220:ILE:HD11	1:C:272:GLN:HG3	1.99	0.43
1:A:402:GLY:O	1:A:406:ILE:HD12	2.18	0.43
1:B:533:ARG:HD2	1:C:711:LEU:CD1	2.48	0.43
1:B:542:GLU:OE1	1:B:649:LYS:HD3	2.18	0.43
1:D:690:GLU:O	1:D:694:ILE:HG13	2.18	0.43
1:E:248:MET:HA	1:F:449:GLN:OE1	2.18	0.43
1:A:611:TYR:HA	1:A:617:ARG:O	2.19	0.43
1:A:300:ALA:O	1:A:303:ARG:HG2	2.17	0.43
1:B:612:VAL:HG13	1:B:614:ILE:O	2.17	0.43
1:C:218:MET:HA	1:C:219:GLY:HA2	1.75	0.43
1:C:676:LEU:O	1:C:679:ALA:HB3	2.18	0.43
1:F:589:PHE:O	1:F:593:TYR:CD1	2.71	0.43
1:B:499:TYR:HA	1:B:502:TYR:CD2	2.53	0.43
1:C:265:GLY:O	1:C:268:LEU:HG	2.18	0.43
1:F:657:MET:SD	1:F:661:PHE:CE2	3.11	0.43
1:C:510:TRP:CG	1:C:707:ILE:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:VAL:CG2	1:B:665:ILE:HD12	2.47	0.43
1:C:540:LEU:HD22	1:C:661:PHE:CE2	2.53	0.43
1:A:357:LYS:HE3	1:A:357:LYS:HA	2.00	0.43
1:A:593:TYR:HB3	1:A:635:PRO:HD3	2.00	0.43
1:A:410:HIS:NE2	1:A:442:GLU:HG2	2.33	0.43
1:C:547:SER:O	1:C:707:ILE:HG22	2.19	0.43
1:B:490:PRO:HA	1:B:491:ALA:CB	2.34	0.43
1:B:541:LEU:HA	1:B:665:ILE:O	2.19	0.43
1:C:319:ASN:HA	1:C:320:SER:HA	1.88	0.43
1:B:254:LYS:O	1:B:368:LEU:HA	2.18	0.43
1:D:240:PHE:HA	1:D:241:PRO:HD3	1.79	0.43
1:E:221:GLY:HA3	1:E:406:ILE:CD1	2.49	0.43
1:A:322:LEU:HD13	1:A:366:ASN:O	2.18	0.43
1:E:375:ARG:NH2	1:E:377:ASP:OD2	2.51	0.43
1:D:538:SER:OG	1:D:661:PHE:HA	2.18	0.43
1:B:510:TRP:CE2	1:B:514:VAL:HG22	2.53	0.43
1:B:670:ILE:HG22	1:B:672:THR:N	2.30	0.43
1:E:406:ILE:HB	1:E:441:LEU:HD13	2.00	0.43
1:A:573:MET:HA	1:A:576:PHE:CD2	2.54	0.43
1:F:265:GLY:HA3	1:F:437:SER:HB2	1.99	0.43
1:C:677:LEU:O	1:C:681:GLU:OE1	2.35	0.43
1:D:227:PHE:O	1:D:230:ILE:HG22	2.19	0.43
1:A:632:LYS:HE3	1:A:633:ALA:O	2.19	0.43
1:C:526:GLN:OE1	1:C:530:ASN:ND2	2.51	0.43
1:A:676:LEU:O	1:A:679:ALA:HB3	2.19	0.43
1:C:521:GLY:O	1:C:525:VAL:HG23	2.18	0.43
1:E:658:LEU:HD12	1:E:658:LEU:HA	1.61	0.43
1:C:596:GLN:O	1:C:638:ARG:HA	2.19	0.43
1:F:510:TRP:HB3	1:F:679:ALA:CA	2.49	0.43
1:F:257:LEU:HB2	1:F:389:LEU:HD13	2.00	0.43
1:A:299:GLU:OE1	1:A:303:ARG:NH2	2.48	0.43
1:A:659:ASN:HD21	1:B:545:PRO:HB2	1.84	0.43
1:E:352:ASN:CB	1:F:288:PRO:HG2	2.49	0.43
1:F:320:SER:O	1:F:320:SER:OG	2.36	0.43
1:B:609:LEU:HA	1:B:609:LEU:HD23	1.67	0.43
1:E:549:LYS:HE2	1:E:645:THR:HB	2.00	0.43
1:C:635:PRO:HB2	1:C:638:ARG:NH1	2.33	0.43
1:D:303:ARG:HG3	1:D:357:LYS:HG3	2.00	0.43
1:F:677:LEU:HD21	1:F:695:ALA:HA	2.01	0.43
1:C:576:PHE:HB2	1:C:581:LYS:HE3	2.00	0.43
1:E:676:LEU:HD22	1:E:703:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:LEU:CB	1:F:398:PRO:HD3	2.49	0.42
1:A:313:GLN:NE2	1:A:365:ASN:OD1	2.52	0.42
1:B:232:ARG:O	1:B:236:ALA:HB3	2.19	0.42
1:B:536:LEU:HD22	1:B:632:LYS:O	2.19	0.42
1:A:315:ARG:HG2	1:A:316:LEU:HD12	2.00	0.42
1:F:270:ALA:HA	1:F:273:ILE:HG22	1.99	0.42
1:A:227:PHE:CE2	1:A:231:PHE:CD1	3.07	0.42
1:F:254:LYS:O	1:F:368:LEU:HA	2.18	0.42
1:C:554:ALA:O	1:C:558:GLU:OE1	2.37	0.42
1:F:395:ILE:HD12	1:F:395:ILE:N	2.34	0.42
1:E:388:ARG:O	1:E:389:LEU:HD23	2.20	0.42
1:B:406:ILE:O	1:B:409:ILE:HG22	2.20	0.42
1:C:324:ILE:HD12	1:C:324:ILE:N	2.34	0.42
1:D:377:ASP:OD1	1:D:378:LEU:N	2.52	0.42
1:E:253:VAL:HA	1:F:446:ARG:HH21	1.83	0.42
1:E:377:ASP:OD1	1:E:378:LEU:N	2.53	0.42
1:C:656:GLU:OE1	1:D:613:PRO:HD3	2.19	0.42
1:B:541:LEU:HD13	1:B:667:VAL:HG21	2.01	0.42
1:B:526:GLN:NE2	1:C:719:GLN:HB3	2.33	0.42
1:A:713:LEU:HD23	1:A:713:LEU:HA	1.69	0.42
1:E:605:ILE:HA	1:E:608:LEU:HB3	2.01	0.42
1:B:257:LEU:HB2	1:B:389:LEU:HD13	2.01	0.42
1:A:242:PRO:HD2	1:A:243:GLU:OE1	2.19	0.42
1:B:377:ASP:OD1	1:B:378:LEU:N	2.53	0.42
1:A:380:ASP:OD1	1:A:381:GLU:N	2.52	0.42
1:B:543:GLY:O	1:B:549:LYS:NZ	2.50	0.42
1:A:708:LYS:O	1:A:711:LEU:HB2	2.19	0.42
1:D:407:LEU:HA	1:D:441:LEU:HD21	2.01	0.42
1:D:539:VAL:HG23	1:D:663:THR:HG23	2.01	0.42
1:B:579:THR:O	1:B:583:GLN:HG2	2.20	0.42
1:B:677:LEU:O	1:B:681:GLU:HG3	2.19	0.42
1:B:520:ASP:OD2	1:B:665:ILE:HG12	2.20	0.42
1:B:548:GLY:CA	2:B:801:ADP:H2	2.31	0.42
1:F:597:LEU:HA	1:F:639:LYS:O	2.19	0.42
1:C:499:TYR:OH	1:C:565:ILE:HB	2.20	0.42
1:F:401:LYS:O	1:F:404:LEU:HB3	2.19	0.42
1:C:688:ASP:HA	1:C:691:ARG:CZ	2.49	0.42
1:B:531:SER:CB	1:B:639:LYS:HD3	2.49	0.42
1:F:388:ARG:O	1:F:389:LEU:HD23	2.19	0.42
1:B:620:ASN:ND2	1:B:624:GLN:HE21	2.16	0.42
1:C:682:LEU:N	1:C:682:LEU:HD23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:VAL:O	1:C:449:GLN:OE1	2.38	0.42
1:B:242:PRO:CD	1:B:243:GLU:H	2.32	0.42
1:B:621:LEU:HD21	1:C:575:GLY:HA2	2.01	0.42
1:C:528:THR:O	1:C:639:LYS:HD3	2.19	0.42
1:A:219:GLY:O	1:A:220:ILE:HG13	2.20	0.42
1:A:706:GLY:O	1:A:709:LYS:HB3	2.20	0.42
1:E:691:ARG:HA	1:E:694:ILE:HD12	2.02	0.42
1:E:607:ARG:HD3	1:E:607:ARG:HA	1.88	0.42
1:C:386:PRO:HG2	1:D:440:GLU:OE1	2.20	0.42
1:A:624:GLN:HG3	1:B:610:ASP:CG	2.37	0.42
1:F:721:ASP:O	1:F:725:ARG:HG3	2.19	0.42
1:E:632:LYS:HE3	1:E:632:LYS:HB3	1.87	0.42
1:D:331:ASP:CA	1:D:379:ILE:HD11	2.50	0.42
1:B:593:TYR:OH	1:B:632:LYS:HG2	2.19	0.42
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.89	0.42
1:C:498:ASP:O	1:C:500:ALA:N	2.53	0.42
1:C:560:SER:HB2	1:C:562:PHE:CZ	2.55	0.42
1:D:626:LEU:HD23	1:D:626:LEU:HA	1.72	0.42
1:D:304:LYS:HA	1:D:307:ALA:HB3	2.02	0.42
1:C:604:ASP:HB3	1:C:607:ARG:HB3	2.02	0.42
1:D:608:LEU:O	1:D:622:VAL:HG11	2.20	0.42
1:E:612:VAL:CG2	1:E:613:PRO:HD2	2.49	0.42
1:C:349:THR:O	1:C:352:ASN:HB3	2.20	0.42
1:F:609:LEU:HD13	1:F:655:MET:HE2	2.01	0.42
1:B:347:HIS:O	1:B:350:VAL:HG22	2.20	0.42
1:C:707:ILE:O	1:C:711:LEU:HG	2.19	0.42
1:B:569:SER:OG	1:B:571:ASP:OD2	2.34	0.42
1:F:221:GLY:N	1:F:406:ILE:HD13	2.35	0.42
1:E:236:ALA:O	1:E:239:VAL:HG12	2.20	0.42
1:B:395:ILE:N	1:B:395:ILE:HD12	2.34	0.42
1:D:236:ALA:HA	1:D:239:VAL:HG12	2.01	0.42
1:E:242:PRO:CD	1:E:243:GLU:H	2.31	0.42
1:A:377:ASP:OD2	1:A:378:LEU:HD23	2.20	0.42
1:F:653:GLN:CB	1:F:658:LEU:HD23	2.50	0.42
1:F:284:VAL:O	1:F:326:ILE:HG12	2.19	0.42
1:E:547:SER:OG	1:E:549:LYS:HG2	2.19	0.42
1:F:589:PHE:CD2	1:F:629:LEU:HD13	2.43	0.42
1:C:603:ASP:HA	1:C:645:THR:OG1	2.20	0.42
1:D:388:ARG:O	1:D:389:LEU:HD23	2.20	0.42
1:B:388:ARG:O	1:B:389:LEU:HD23	2.20	0.42
1:F:232:ARG:O	1:F:236:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ILE:HG12	1:B:368:LEU:HD11	2.01	0.42
1:B:502:TYR:CE2	1:B:567:ILE:HD13	2.54	0.42
1:A:256:ILE:CG1	1:A:370:ILE:HG22	2.47	0.42
1:A:627:LEU:HA	1:A:627:LEU:HD23	1.94	0.42
1:E:536:LEU:HD22	1:E:634:PRO:HD3	2.02	0.42
1:E:319:ASN:HA	1:E:320:SER:HA	1.90	0.42
1:B:323:HIS:HB2	1:B:367:ILE:HG22	2.02	0.42
1:B:712:MET:O	1:B:716:MET:HG3	2.19	0.42
1:B:398:PRO:HG2	1:B:434:LYS:O	2.19	0.42
1:E:530:ASN:O	1:E:639:LYS:HE3	2.19	0.42
1:E:547:SER:N	2:E:801:ADP:O2B	2.53	0.41
1:A:534:THR:HG23	1:B:715:GLU:HG3	2.01	0.41
1:E:270:ALA:HA	1:E:273:ILE:HG22	2.02	0.41
1:A:315:ARG:C	1:A:316:LEU:HD12	2.40	0.41
1:E:260:GLY:HA3	1:E:266:LYS:HD3	2.01	0.41
1:F:324:ILE:HG12	1:F:368:LEU:HD11	2.01	0.41
1:E:510:TRP:HA	1:E:679:ALA:HA	2.01	0.41
1:C:510:TRP:HB2	1:C:679:ALA:HB2	2.03	0.41
1:A:285:VAL:HG13	1:A:326:ILE:CD1	2.43	0.41
1:C:653:GLN:HA	1:C:658:LEU:HB3	2.02	0.41
1:D:560:SER:HB2	1:D:562:PHE:CE1	2.55	0.41
1:E:593:TYR:CE1	1:E:632:LYS:NZ	2.88	0.41
1:A:566:LYS:HA	1:A:566:LYS:HD3	1.79	0.41
1:A:718:LEU:O	1:A:725:ARG:NE	2.54	0.41
1:C:284:VAL:HB	1:C:325:ILE:HA	2.01	0.41
1:F:451:THR:O	1:F:454:ASN:HB3	2.20	0.41
1:E:406:ILE:O	1:E:409:ILE:HG22	2.20	0.41
1:A:254:LYS:O	1:A:368:LEU:HA	2.20	0.41
1:F:658:LEU:O	1:F:658:LEU:HD12	2.21	0.41
1:A:396:GLY:O	1:A:397:LEU:HB2	2.20	0.41
1:C:318:ALA:C	1:C:319:ASN:HD22	2.21	0.41
1:D:710:LEU:HG	1:D:714:ILE:HD11	2.02	0.41
1:A:499:TYR:CE2	1:A:565:ILE:HB	2.55	0.41
1:D:620:ASN:OD1	1:E:617:ARG:NH1	2.53	0.41
1:E:540:LEU:HD12	1:E:541:LEU:H	1.84	0.41
1:D:659:ASN:HD21	1:E:545:PRO:HB3	1.85	0.41
1:B:268:LEU:HD12	1:B:269:LEU:N	2.35	0.41
1:F:542:GLU:OE1	1:F:666:HIS:HB2	2.19	0.41
1:C:690:GLU:HB2	1:C:726:VAL:CG2	2.44	0.41
1:A:498:ASP:OD2	1:A:567:ILE:HD13	2.21	0.41
1:C:638:ARG:HH11	1:C:638:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:LEU:HD12	1:D:594:LYS:O	2.20	0.41
1:B:715:GLU:O	1:B:719:GLN:HG2	2.21	0.41
1:E:324:ILE:HG12	1:E:368:LEU:HD11	2.01	0.41
1:F:609:LEU:HD23	1:F:609:LEU:HA	1.86	0.41
1:D:544:PRO:O	1:D:547:SER:HB3	2.21	0.41
1:D:223:LEU:HD23	1:D:223:LEU:O	2.20	0.41
1:E:682:LEU:HD23	1:E:682:LEU:HA	1.72	0.41
1:E:440:GLU:OE2	1:E:492:PHE:HA	2.20	0.41
1:E:669:ASN:ND2	1:E:706:GLY:N	2.69	0.41
1:E:705:ILE:CG1	1:E:709:LYS:HG3	2.49	0.41
1:C:507:ILE:HG23	2:C:801:ADP:C6	2.56	0.41
1:C:687:LYS:HB2	1:C:690:GLU:OE1	2.21	0.41
1:F:560:SER:HB2	1:F:562:PHE:CD1	2.54	0.41
1:E:587:LYS:HZ1	1:E:591:ASP:CG	2.24	0.41
1:E:676:LEU:O	1:E:680:LEU:HG	2.21	0.41
1:C:331:ASP:CA	1:C:379:ILE:HD11	2.47	0.41
1:A:407:LEU:O	1:A:411:THR:HG23	2.21	0.41
1:A:411:THR:CG2	1:A:426:ILE:HD11	2.50	0.41
1:D:231:PHE:O	1:D:235:PHE:HB2	2.20	0.41
1:F:525:VAL:CG1	1:F:560:SER:HB2	2.51	0.41
1:A:560:SER:O	1:A:561:ASN:OD1	2.39	0.41
1:D:312:GLU:CD	1:D:323:HIS:ND1	2.74	0.41
1:A:236:ALA:HA	1:B:453:MET:HB3	2.03	0.41
1:F:508:ILE:CD1	1:F:510:TRP:CD1	3.02	0.41
1:E:257:LEU:HB2	1:E:389:LEU:HD13	2.02	0.41
1:F:502:TYR:HD2	1:F:503:ILE:HG13	1.85	0.41
1:A:549:LYS:HG3	1:A:550:THR:N	2.35	0.41
1:A:683:LEU:HD13	1:A:685:ASN:ND2	2.36	0.41
1:C:498:ASP:O	1:C:501:SER:N	2.45	0.41
1:C:691:ARG:HB2	1:C:691:ARG:NH1	2.35	0.41
1:A:233:ARG:O	1:A:236:ALA:HB3	2.20	0.41
1:C:595:SER:O	1:C:638:ARG:HD2	2.20	0.41
1:B:648:ARG:HG3	1:B:651:VAL:CG2	2.51	0.41
1:B:621:LEU:HD11	1:C:575:GLY:H	1.86	0.41
1:F:323:HIS:HB2	1:F:367:ILE:HG22	2.02	0.41
1:F:377:ASP:OD1	1:F:378:LEU:N	2.53	0.41
1:F:512:ASP:N	1:F:513:PRO:CD	2.84	0.41
1:E:564:PHE:CB	1:E:595:SER:HB2	2.50	0.41
1:B:218:MET:HA	1:B:219:GLY:HA2	1.70	0.41
1:A:219:GLY:O	1:A:272:GLN:HG2	2.21	0.41
1:B:488:ILE:O	1:B:490:PRO:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:LYS:HD3	1:D:597:LEU:CD2	2.51	0.41
1:E:620:ASN:O	1:E:624:GLN:HG2	2.21	0.41
1:D:569:SER:HA	1:D:570:PRO:HD3	1.90	0.41
1:D:331:ASP:O	1:D:332:ALA:HB3	2.20	0.41
1:A:636:GLN:HA	1:A:637:GLY:HA2	1.49	0.41
1:F:671:ALA:HA	1:F:703:VAL:O	2.21	0.41
1:E:655:MET:C	1:E:656:GLU:HG3	2.41	0.41
1:A:262:PRO:CG	1:A:374:ASN:OD1	2.69	0.41
1:C:263:GLY:C	1:C:437:SER:HB3	2.41	0.41
1:A:538:SER:O	1:A:662:SER:HB2	2.20	0.41
1:A:693:THR:O	1:A:697:GLN:OE1	2.38	0.41
1:A:284:VAL:O	1:A:326:ILE:HG13	2.21	0.41
1:A:676:LEU:HD23	1:A:698:VAL:HG11	2.03	0.41
1:F:525:VAL:HG11	1:F:560:SER:HA	2.03	0.41
1:E:673:GLY:O	1:E:676:LEU:HB3	2.20	0.41
1:D:309:ALA:HA	1:D:312:GLU:OE2	2.20	0.41
1:E:513:PRO:HA	1:E:516:ARG:CG	2.46	0.41
1:E:258:LEU:HB3	1:E:395:ILE:HD11	2.02	0.41
1:A:564:PHE:HE1	1:A:566:LYS:HB2	1.83	0.41
1:E:569:SER:HA	1:E:570:PRO:HD3	1.95	0.41
1:E:284:VAL:O	1:E:326:ILE:HG12	2.20	0.41
1:B:242:PRO:HD2	1:B:243:GLU:N	2.34	0.41
1:F:289:GLU:C	1:F:291:LEU:H	2.21	0.41
1:A:239:VAL:O	1:A:240:PHE:C	2.57	0.41
1:B:516:ARG:O	1:B:520:ASP:HB2	2.22	0.40
1:C:627:LEU:O	1:C:631:LYS:HG3	2.21	0.40
1:D:331:ASP:HA	1:D:379:ILE:CD1	2.51	0.40
1:C:411:THR:O	1:C:414:MET:HB2	2.20	0.40
1:C:242:PRO:HD2	1:C:243:GLU:N	2.36	0.40
1:E:323:HIS:HB2	1:E:367:ILE:HG22	2.02	0.40
1:A:375:ARG:HA	1:A:376:PRO:HD2	1.97	0.40
1:C:626:LEU:HA	1:C:626:LEU:HD23	1.85	0.40
1:A:215:PHE:N	1:A:231:PHE:CZ	2.89	0.40
1:B:549:LYS:HB2	2:B:801:ADP:O1B	2.20	0.40
1:F:562:PHE:H	1:F:565:ILE:HD11	1.87	0.40
1:E:532:ASP:OD2	1:E:533:ARG:HG2	2.20	0.40
1:E:721:ASP:HB2	1:E:724:TYR:HD2	1.87	0.40
1:A:259:TYR:HB2	1:A:373:THR:O	2.21	0.40
1:C:633:ALA:HA	1:C:634:PRO:HD3	1.90	0.40
1:D:527:GLN:O	1:D:527:GLN:HG3	2.20	0.40
1:F:375:ARG:NH2	1:F:377:ASP:OD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:656:GLU:HG2	1:F:648:ARG:NH2	2.36	0.40
1:F:544:PRO:HA	1:F:545:PRO:HD3	1.98	0.40
1:B:534:THR:HA	1:B:535:PRO:HD3	1.98	0.40
1:C:709:LYS:HD2	1:C:709:LYS:HA	1.93	0.40
1:A:716:MET:HG2	1:A:732:LEU:CD1	2.52	0.40
1:E:513:PRO:O	1:E:516:ARG:HG2	2.22	0.40
1:A:653:GLN:HB2	1:A:658:LEU:HD23	2.04	0.40
1:B:326:ILE:HG22	1:B:370:ILE:CG1	2.51	0.40
1:D:258:LEU:HD11	1:D:372:MET:HG2	2.04	0.40
1:F:588:ILE:O	1:F:591:ASP:HB2	2.21	0.40
1:C:675:GLN:O	1:C:678:GLU:HB3	2.21	0.40
1:D:549:LYS:HE2	2:D:801:ADP:O1B	2.22	0.40
1:E:698:VAL:O	1:E:701:LYS:HB2	2.22	0.40
1:C:677:LEU:HD21	1:C:695:ALA:HA	2.03	0.40
1:D:562:PHE:CD2	1:D:597:LEU:HG	2.56	0.40
1:F:605:ILE:N	1:F:606:GLU:OE1	2.54	0.40
1:E:640:LEU:HG	1:E:642:ILE:CD1	2.51	0.40
1:E:641:LEU:HD12	1:E:641:LEU:O	2.22	0.40
1:B:531:SER:CA	1:B:639:LYS:HD3	2.52	0.40
1:D:319:ASN:HA	1:D:320:SER:HA	1.86	0.40
1:C:620:ASN:O	1:C:624:GLN:HG2	2.21	0.40
1:A:436:PHE:HA	1:A:440:GLU:OE2	2.22	0.40
1:F:309:ALA:HA	1:F:312:GLU:OE1	2.22	0.40
1:E:643:ILE:N	1:E:643:ILE:HD12	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	475/747 (64%)	443 (93%)	20 (4%)	12 (2%)	7 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	473/747 (63%)	429 (91%)	32 (7%)	12 (2%)	7	46
1	C	477/747 (64%)	450 (94%)	18 (4%)	9 (2%)	10	52
1	D	471/747 (63%)	439 (93%)	27 (6%)	5 (1%)	17	63
1	E	474/747 (64%)	441 (93%)	22 (5%)	11 (2%)	8	48
1	F	465/747 (62%)	428 (92%)	26 (6%)	11 (2%)	7	47
All	All	2835/4482 (63%)	2630 (93%)	145 (5%)	60 (2%)	13	50

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	293	LYS
1	A	294	TYR
1	A	318	ALA
1	A	320	SER
1	A	333	ILE
1	B	283	LYS
1	B	297	GLU
1	B	318	ALA
1	B	439	ALA
1	B	489	LYS
1	C	297	GLU
1	C	318	ALA
1	C	498	ASP
1	C	578	GLU
1	D	283	LYS
1	D	318	ALA
1	D	489	LYS
1	E	283	LYS
1	E	297	GLU
1	E	318	ALA
1	E	439	ALA
1	E	489	LYS
1	F	283	LYS
1	F	297	GLU
1	F	318	ALA
1	F	397	LEU
1	F	439	ALA
1	F	489	LYS
1	A	264	CYS

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Mol	Chain	Res	Type
1	A	397	LEU
1	C	293	LYS
1	C	499	TYR
1	E	507	ILE
1	A	241	PRO
1	B	241	PRO
1	B	293	LYS
1	B	502	TYR
1	C	241	PRO
1	C	610	ASP
1	D	293	LYS
1	E	241	PRO
1	E	293	LYS
1	F	241	PRO
1	F	293	LYS
1	A	242	PRO
1	F	398	PRO
1	B	490	PRO
1	B	546	HIS
1	D	241	PRO
1	E	438	GLY
1	B	438	GLY
1	E	490	PRO
1	F	438	GLY
1	A	398	PRO
1	B	668	PRO
1	E	668	PRO
1	F	684	GLY
1	C	490	PRO
1	A	668	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	344/638 (54%)	343 (100%)	1 (0%)	94 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	349/638 (55%)	346 (99%)	3 (1%)	84	93
1	C	347/638 (54%)	346 (100%)	1 (0%)	94	96
1	D	340/638 (53%)	339 (100%)	1 (0%)	94	96
1	E	345/638 (54%)	342 (99%)	3 (1%)	84	93
1	F	345/638 (54%)	342 (99%)	3 (1%)	84	93
All	All	2070/3828 (54%)	2058 (99%)	12 (1%)	91	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	B	305	LEU
1	B	322	LEU
1	B	651	VAL
1	C	305	LEU
1	D	305	LEU
1	E	305	LEU
1	E	322	LEU
1	E	327	PHE
1	F	305	LEU
1	F	322	LEU
1	F	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	530	ASN
1	A	596	GLN
1	A	685	ASN
1	B	352	ASN
1	B	526	GLN
1	B	620	ASN
1	C	319	ASN
1	C	352	ASN
1	C	675	GLN
1	D	313	GLN
1	D	319	ASN
1	D	352	ASN
1	D	527	GLN

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Mol	Chain	Res	Type
1	E	675	GLN
1	F	546	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	B	801	-	24,29,29	1.07	2 (8%)	23,45,45	1.45	4 (17%)
2	ADP	C	801	-	24,29,29	1.27	2 (8%)	23,45,45	2.37	5 (21%)
2	ADP	D	801	-	24,29,29	1.06	2 (8%)	23,45,45	2.79	6 (26%)
2	ADP	E	801	-	24,29,29	1.28	3 (12%)	23,45,45	1.86	8 (34%)

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	B	801	-	-	0/12/32/32	0/3/3/3
2	ADP	C	801	-	-	0/12/32/32	0/3/3/3
2	ADP	D	801	-	-	0/12/32/32	0/3/3/3
2	ADP	E	801	-	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	ADP	C2-N3	2.11	1.35	1.32
2	C	801	ADP	O4'-C1'	2.36	1.44	1.41
2	B	801	ADP	O4'-C1'	2.44	1.44	1.41
2	E	801	ADP	O4'-C1'	2.46	1.44	1.41
2	E	801	ADP	C2-N3	2.50	1.36	1.32
2	D	801	ADP	C5-C4	2.54	1.46	1.40
2	B	801	ADP	C5-C4	3.03	1.47	1.40
2	E	801	ADP	C5-C4	3.68	1.48	1.40
2	C	801	ADP	C5-C4	4.29	1.50	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ADP	N3-C2-N1	-11.41	119.91	128.87
2	C	801	ADP	N3-C2-N1	-7.18	123.23	128.87
2	C	801	ADP	C1'-N9-C4	-5.35	120.83	126.81
2	B	801	ADP	N3-C2-N1	-4.33	125.47	128.87
2	D	801	ADP	C1'-N9-C4	-2.80	123.68	126.81
2	E	801	ADP	O4'-C1'-N9	-2.65	103.10	108.11
2	D	801	ADP	O2'-C2'-C1'	-2.63	103.38	111.61
2	D	801	ADP	C2'-C1'-N9	-2.61	106.48	113.47
2	E	801	ADP	N3-C2-N1	-2.58	126.84	128.87
2	C	801	ADP	O2'-C2'-C3'	-2.23	104.64	111.86
2	B	801	ADP	C1'-N9-C4	-2.13	124.43	126.81
2	D	801	ADP	O2A-PA-O5'	-2.08	98.30	108.24
2	E	801	ADP	O5'-C5'-C4'	2.04	116.45	109.09
2	C	801	ADP	C2-N1-C6	2.19	122.67	118.77
2	B	801	ADP	C4'-O4'-C1'	2.22	111.99	109.64
2	D	801	ADP	C2-N1-C6	2.25	122.78	118.77
2	B	801	ADP	O5'-C5'-C4'	2.25	117.21	109.09
2	E	801	ADP	O4'-C4'-C5'	2.40	117.88	109.29
2	E	801	ADP	C2'-C1'-N9	2.60	120.42	113.47
2	E	801	ADP	C2'-C3'-C4'	2.77	108.30	102.64
2	E	801	ADP	C1'-N9-C4	3.36	130.55	126.81
2	E	801	ADP	N6-C6-N1	3.70	124.72	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ADP	C4'-O4'-C1'	4.06	113.94	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ADP	11	0
2	C	801	ADP	8	0
2	D	801	ADP	11	0
2	E	801	ADP	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.