



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 3J94
EMDB ID: : EMD-6204
Title : Structure of ATP-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 : 4.20 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

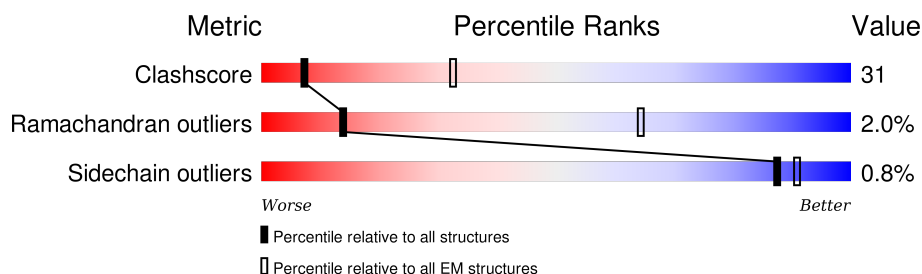
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	
1	B	747	
1	C	747	
1	D	747	
1	E	747	
1	F	747	

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	ATP	D	801	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21509 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.

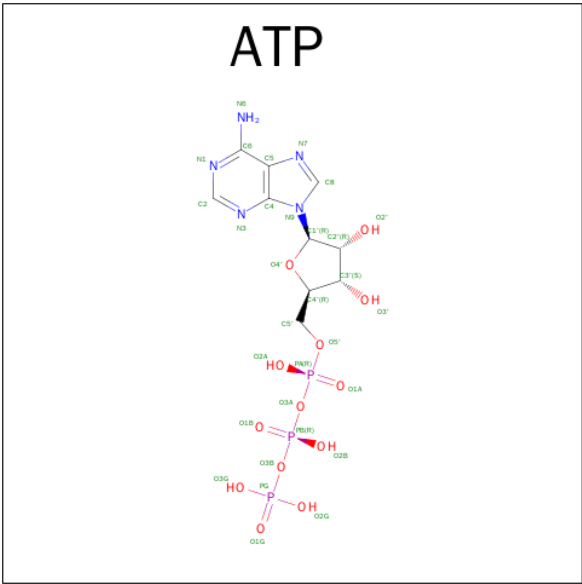
- Molecule 1 is a protein called Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	490	Total	C	N	O	S	0	0
			3559	2266	613	665	15		
1	B	484	Total	C	N	O	S	0	0
			3563	2264	618	665	16		
1	C	488	Total	C	N	O	S	0	0
			3573	2268	621	669	15		
1	D	485	Total	C	N	O	S	0	0
			3526	2244	603	663	16		
1	E	482	Total	C	N	O	S	0	0
			3529	2242	611	661	15		
1	F	466	Total	C	N	O	S	0	0
			3418	2164	598	640	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'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



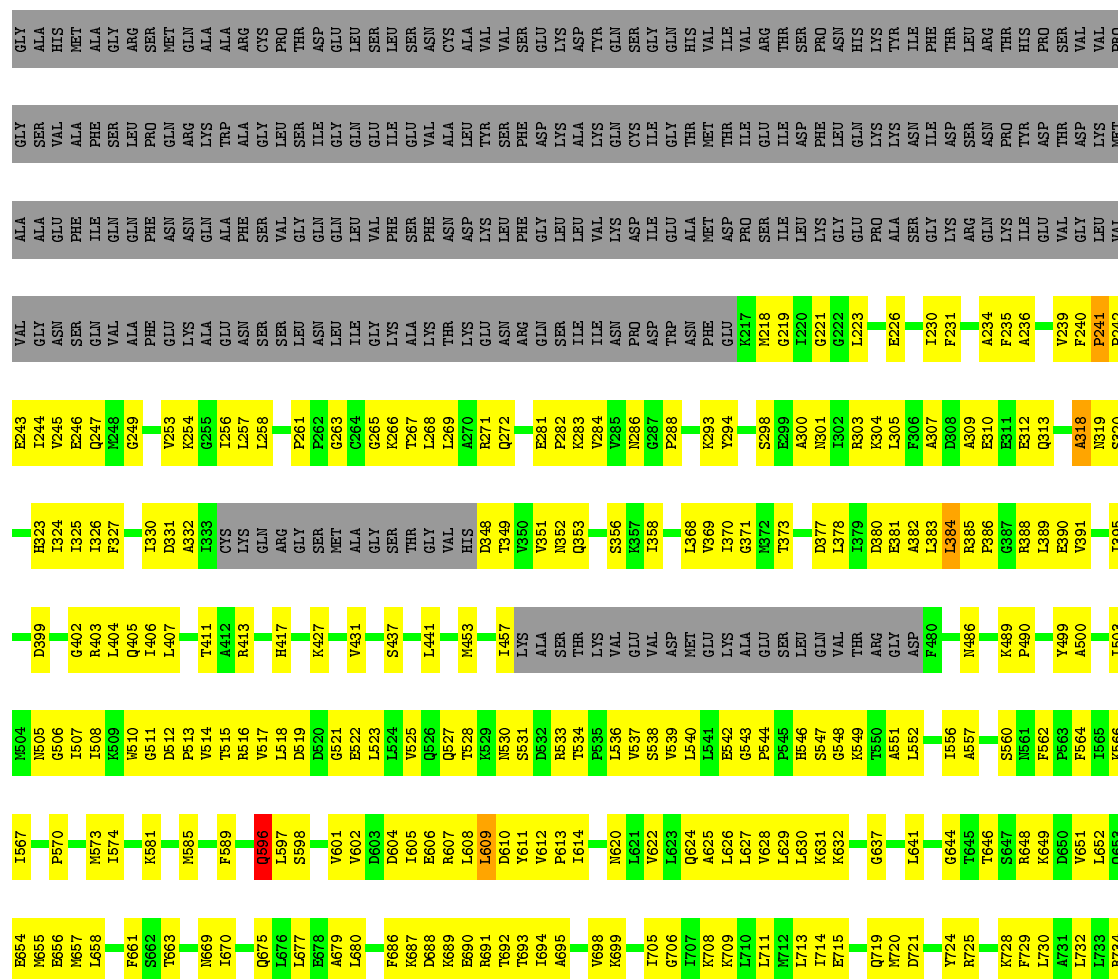
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	E	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	E	1	Total	C	N	O	P	0
			62	20	10	26	6	
2	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

GLY	ALA	GLY	ALA	VAL	E246	1322	Q402	P490		R448	PHE
ALA	SER	SER	GLU	GLY	Q247	H323	R403	A491	I574	K649	ASP
HIS	VAL	ASN	PHE	ASN	G248	1324	L404		G575		
MET	ALA	SER	ILE	GLN	G249	1325	Q405	D498	S576	E656	
GLY	SER	GLN	ILE	VAL		1326	L406	Y499	S577	M657	
ARG	LEU	PRO	GLN	VAL	K254	1327	L407		S578	L658	
			PHE	ALA	G255		H408	Y502	T579		
SER	PRO	GLN	ASN	PHE	I256	1330	R413	I503	A580	F661	
GLN	ARG	LYS	ASN	GLU	L257		M414	N504	K581	S662	
ALA	TRP	ALA	ALA	ILE	Y259			G506	I588	T663	
ALA	ALA	GLU	ASN	CYS	G265		L426	I507	F589	V667	
ARG	GLY	LEU	ASN	LYS	K266		K427	I508	D590	P668	
CYS	PRO	GLY	SER	GLN	T267		E428	R516	Y593	N669	
PRO	LEU	SER	VAL	ARG	L268		V431	V517	Q596	I670	
THR	ILE	LEU	GLY	ILE	L269		E432	L518	L597	Q675	
ASP	GLY	ASN	GLN	LEU	A270		F436	D519	S598	F686	
GLU	GLN	LEU	VAL	ILE	H271		S437	L523	C599	E690	
LEU	LEU	GLY	PHE	GLY	Q272		G438	L524	V600	R691	
SER	ILE	LYS	ALA	THR	I273		A439	V525	V601	T692	
LEU	GLY	ALA	LYS	GLY	E281		E440	Q526	V602	T693	
ALA	VAL	ASN	PHE	VAL	P282		L441	Q527	D603	I694	
CYS	LEU	LYS	ASP	THR	K283		L444	T528	E606	A695	
ALA	TYR	GLU	LYS	GLY	V284		V445	T529	R607	Q696	
VAL	SER	LEU	LEU	ASN			Q449	N530	L608	Q697	
VAL	PHE	GLY	PHE	ARG	P288			T534	L609	K697	
SER	ASP	GLY	GLY	GLN	E289			P535	D610	K699	
GLU	LYS	LEU	LEU	ILE	I290		A452		V611	G706	
LYS	ALA	VAL	VAL	ILE	L291		K453	S538	V612	I707	
ASP	ALA	LYS	LYS	ILE	E292		R454	V539	F613	L710	
TYR	GLN	LYS	ASN	PRO	K293		R455	L540	G615	L711	
GLN	ILE	GLY	TRP	ASP	G296		H456	L541	P616	M712	
ILE	THR	GLN	ILE	LEU	E297		I457	E542	R617	L713	
SER	SER	THR	ASP	LEU	S298		LYS	R543	F618	I714	
PRO	ASN	PRO	LEU	LYS	E299		ALA	S547	S619	E715	
ASN	HIS	HIS	GLN	GLY	A300		SER	G548	M620	M716	
HIS	LYS	TYR	ILE	GLY	N301		THR	K949	L621	S717	
LYS	TYR	ILE	ILE	ILE	I302		LYS	T550	V622	L718	
THR	THR	THR	ILE	THR	G219		VAL	A551	L623	Q719	
SER	ASP	SER	ASP	SER	G220		GLU	L552	Q624	M720	
PRO	PHE	PRO	LEU	PRO	G221		VAL		L626	D721	
ASN	LEU	ASN	GLY	ASN	D224		ASP	K555	L627		
HIS	LEU	HIS	GLU	GLN			MET	I556	V628	Y724	
LYS	LYS	LYS	PRO	LYS	S228		GLU		L629	R725	
TYR	ASN	ASN	ALA	ASN	E310		LYS	E559	L630		
ILE	ASN	ILE	SER	ILE	E311		GLU	S560	K631	K728	
PHE	ILE	PHE	GLY	LYS	E312		SER	N561	R632		
THR	ASP	THR	ARG	LYS	Q313		LEU	P562	R638	L732	
LEU	SER	LEU	GLN	ARG	A236		GLN	P563	K639	G737	
ARG	ASN	ASN	LYS	LYS	V239		VAL	K566		ALA	
THR	TYR	THR	ILE	ILE	P240		THR	I567		SER	
HIS	ASP	HIS	GLY	GLY	P241		ARG	K567		PRO	
PRO	THR	PRO	VAL	VAL	P242		GLY	C568	I643	ASP	
SER	THR	SER	GLY	GLY	P243		LEU	S569	Q644		
VAL	ASP	VAL	LEU	LEU	E243		LEU	P570	S647		
LYS	LYS	LYS	VAL	VAL	I244		ASP	D571			
PRO	MET		VAL		V245		K489				

● Molecule 1: Vesicle-fusing ATPase



GLY	ALA	GLY	ALA	VAL	V245		GLY	ALA	GLY	ALA	VAL
ALA	SER	SER	GLU	GLY	E246		ALA	ALA	GLY	ALA	VAL
HIS	VAL	ASN	PHE	ASN	Q247		GLU	GLU	GLY	ALA	VAL
MET	ALA	SER	ILE	GLN	M248		ILE	ASN	GLY	ALA	VAL
GLY	SER	GLN	GLN	VAL	G249		ALA	LYS	TRP	ALA	VAL
ARG	LEU	PRO	GLN	ALA	K254		ALA	ALA	ALA	ALA	VAL
			PHE	PHE	G255		ASN	PHE	SER	ALA	VAL
SER	PRO	GLN	ASN	GLY	I256		GLY	SER	GLY	ALA	VAL
GLN	ARG	LYS	ASN	ALA	L257		LEU	VAL	LEU	ALA	VAL
ALA	LYS	ALA	GLU	ALA	G263		ILE	GLN	GLY	ALA	VAL
ALA	TRP	ALA	ASN	SER			GLY	LEU	LEU	ALA	VAL
ALA	ALA	SER	SER	THR	T267		ILE	GLY	GLY	ALA	VAL
ALA	GLY	LEU	LEU	ASP	A270		GLY	ILE	ILE	ALA	VAL
GLN	ILE	ILE	GLN	GLY	Q271		VAL	PHE	GLY	ALA	VAL
LEU	GLN	LEU	VAL	GLY	Q272		VAL	SER	GLY	ALA	VAL
LEU	GLN	ILE	VAL	GLY	I273		VAL	PHE	VAL	ALA	VAL
SER	GLU	GLY	VAL	GLY	V284		VAL	ASN	GLY	ALA	VAL
LEU	LEU	ILE	VAL	GLY	V285		VAL	PHE	GLY	ALA	VAL
GLY	GLY	GLY	VAL	GLY			VAL	ASN	GLY	ALA	VAL
LEU	GLN	LEU	VAL	GLY	E289		VAL	LEU	LEU	ALA	VAL
SER	ILE	ILE	VAL	GLY	L290		VAL	LYS	TYR	ALA	VAL
THR	LYS	ILE	VAL	GLY	L291		VAL	ASP	LEU	ALA	VAL
LYS	GLY	ILE	VAL	GLY	E292		VAL	LYS	TYR	ALA	VAL
ASN	ASN	ASN	PHE	ASN	K293		VAL	LEU	TYR	ALA	VAL
GLY	GLY	GLN	GLY	GLY	Y294		VAL	GLY	SER	ALA	VAL
LEU	LYS	SER	GLY	GLY	V295		VAL	LEU	ASP	ALA	VAL
ALA	ALA	ILE	VAL	VAL	G296		VAL	LEU	ASP	ALA	VAL
ASP	LYS	ILE	VAL	VAL	E297		VAL	LYS	ASP	ALA	VAL
TYR	GLY	ILE	VAL	VAL	S298		VAL	VAL	ASP	ALA	VAL
GLN	ASN	ASN	ASP	ASN	E299		VAL	LYS	ASP	ALA	VAL
ILE	PRO	PRO	ILE	PRO	A300		VAL	GLY	ASP	ALA	VAL
GLY	ASP	ASP	ILE	ASP	N301		VAL	ILE	ASP	ALA	VAL
GLY	TRP	TRP	GLY	TRP			VAL	GLY	ASP	ALA	VAL
ALA	ASN	ASN	GLY	ASN	L305		VAL	MET	ASP	ALA	VAL
VAL	PHE	PHE	MET	VAL			VAL	ASP	ASP	ALA	VAL
GLY	GLY	GLY	THR	GLY	P217		VAL	PRO	THR	ALA	VAL
ILE	ILE	ILE	ILE	ILE	M218		VAL	SER	ILE	ALA	VAL
ARG	GLY	GLY	GLY	GLY	G219		VAL	GLY	GLY	ALA	VAL
THR	ILE	ILE	ILE	ILE	E310		VAL	ILE	ILE	ALA	VAL
SER	ASP	SER	ASP	SER	E311		VAL	LYS	ASP	ALA	VAL
PRO	PRO	PRO	PHE	PRO	E312		VAL	LEU	PHE	ALA	VAL
ASN	ASN	ASN	LEU	ASN	Q313		VAL	GLN	LEU	ALA	VAL
HIS	LYS	HIS	GLN	GLY	R314		VAL	PRO	GLY	ALA	VAL
LYS	ASN	LYS	ALA	GLY	R315		VAL	LYS	ILE	ALA	VAL
TYR	ASN	TYR	SER	GLY	L316		VAL	ASN	ILE	ALA	VAL
ILE	ILE	ILE	ILE	LYS	A318		VAL	ILE	ILE	ALA	VAL
PHE	ASP	PHE	THR	LYS	N319		VAL	ASP	ASP	ALA	VAL
THR	THR	THR	ARG	S320	G321		VAL	SER	THR	ALA	VAL
LEU	ASN	LEU	GLN	G322	I322		VAL	GLY	ASP	ALA	VAL
ARG	ASN	ARG	LYS	H323	L322		VAL	LEU	LEU	ALA	VAL
THR	PRO	THR	LYS	R323			VAL	THR	VAL	ALA	VAL
HIS	TYR	HIS	ILE	F240	I324		VAL	ASP	GLY	ALA	VAL
PRO	ASP	PRO	GLY	P241	I325		VAL	THR	GLY	ALA	VAL
SER	THR	SER	VAL	P242	I326		VAL	ASP	LEU	ALA	VAL
VAL	ASP	VAL	LYS	E243	F327		VAL	LYS	VAL	ALA	VAL
LYS	MET		VAL				VAL				





M712	L713	L714	L715	M716	S717	L718	L719	R720	D721	Y724	R725	K728	L732	L733	R734	G737	ALA	SER	PRO	LEU	ASP	PHE	ASP																																						
I639	I640	I641	I642	I643	G644	T645	T646	S647	R648	R649	D650	Q653	E654	M655	E656	M657	L658	F661	S662	T663	T664	I665	H666	V667	P668	M669	I670	G673	E674	Q675	L676	L677	E678	E681	L682	L683	G684	M685	P686	E690	I694	A695	V698	K699	W704	I707	K708	K709	L710	L711											
K566	I567	C568	S569	P570	D571	K572	M573	I574		S577	E578	T579	A580	K581	Q582	Q583	K586	F589	Y593	L597	S598	C599	V600	V601	V602	D603	D604	I605	E606	R607	L608	L609	D610	D611	V612	P613	I614	G615	P616	R617	F618	S619	N620	Q624	V628	L629	K632	A633	P634	P635	R638										
Y499		Y502	I503	Y504	M505	G506	I507	I508	K509	M510	G511	D512	F513	V514	T515	R516	V517	L518	G521	E522	L523	L524	V525	Q526	Q527	T528	K529	N530	P535	L536	Y537	S538	V539	L540	L541	E542	G543	P544	P545	H546	S547	G548	K549	T550	A551	L552	A553	A554	K555	I556	A557	E558	E559	S560	F564	I565					
V431	E432		S437	C438	A439	E440	L441	E442		V445	R446		A452	M453	R454	R455		LYS	ALA	SER	THR	LYS	VAL	GLU	VAL	ASP	MET	LYS	ALA	GLU	GLU	GLU	GLU	GLU	THR	ARG	GLY	ASP	PHE	LEU	ALA	ALA	LYS	PRO	LYS	VAL	THR	ASN	GLN	E497	D498										
ARG	GLY	SER	MET	ALA	GLY	SER	THR	GLY	VAL	R3347	V350	V351	L354	M453	R454	R455	I358	D359	N365	R366	T367	L368	V369	I370	GLU	VAL	ASP	MET	LYS	GLU	N374	R375	P376	D377	L378	L379	D380	R385	P386	G387	R388	L389	E390	V391	S392	M393	L397	P398	L404	Q405	L406	P407	I409	H408	GLY	THR	ASN	GLN	E428	L429	A430
VAL	P242	E243	I244	V245		G249	I256	L257	L258	Y259	P261		A270		I273		E281	P282	K283	V284		K293		G296	E297		K304	L305	F306	A307	D308	A309	E310	E311	E312	Q313	R314	R315	L316	G317	A318	N319	S320	G321	L322	H323	I324	I325	F327	I330	ASP	ALA	ILE	CYS	LYS	F239	F240	P241			

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	50781	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 ($e^-/\text{\AA}^2$)	26.4	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: ATP

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	0.37	0/3612	0.81	4/4904 (0.1%)
1	B	0.37	0/3615	0.77	1/4898 (0.0%)
1	C	0.38	0/3625	0.77	3/4915 (0.1%)
1	D	0.36	0/3577	0.77	3/4856 (0.1%)
1	E	0.35	0/3580	0.79	2/4854 (0.0%)
1	F	0.39	0/3467	0.82	3/4697 (0.1%)
All	All	0.37	0/21476	0.79	16/29124 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	8

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	223	LEU	CA-CB-CG	6.62	130.52	115.30
1	F	536	LEU	CA-CB-CG	6.52	130.31	115.30
1	F	518	LEU	CA-CB-CG	6.32	129.84	115.30
1	C	385	ARG	NE-CZ-NH2	6.20	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	609	LEU	CA-CB-CG	6.07	129.27	115.30
1	D	596	GLN	CA-CB-CG	5.93	126.44	113.40
1	A	641	LEU	CA-CB-CG	5.91	128.89	115.30
1	C	384	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	419	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	305	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	322	LEU	CA-CB-CG	5.52	128.00	115.30
1	F	378	LEU	CA-CB-CG	5.50	127.95	115.30
1	D	384	LEU	CA-CB-CG	5.47	127.89	115.30
1	E	305	LEU	CA-CB-CG	5.37	127.66	115.30
1	C	322	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	385	ARG	NE-CZ-NH2	5.26	122.93	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	A	261	PRO	Peptide
1	B	438	GLY	Peptide
1	B	546	HIS	Sidechain
1	C	530	ASN	Sidechain
1	D	596	GLN	Sidechain
1	E	438	GLY	Peptide
1	F	438	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3559	0	3451	224	0
1	B	3563	0	3497	215	0
1	C	3573	0	3487	212	0
1	D	3526	0	3429	251	0
1	E	3529	0	3439	263	0
1	F	3418	0	3332	228	0
2	A	62	0	23	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	62	0	21	11	0
2	C	62	0	22	9	0
2	D	62	0	20	18	0
2	E	62	0	17	9	0
2	F	31	0	9	5	0
All	All	21509	0	20747	1292	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 31.

All (1292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ASN:HB2	2:A:801:ATP:H1'	1.39	1.01
1:C:257:LEU:HB2	1:C:389:LEU:HD13	1.56	0.87
1:B:526:GLN:HE21	1:C:719:GLN:HB3	1.39	0.85
1:B:386:PRO:HA	1:B:390:GLU:HA	1.58	0.84
1:A:705:ILE:HD13	1:A:710:LEU:HD12	1.59	0.84
1:D:386:PRO:HA	1:D:390:GLU:HA	1.58	0.84
1:E:604:ASP:HB3	1:E:607:ARG:HB3	1.60	0.84
1:F:545:PRO:HA	1:F:547:SER:H	1.42	0.83
1:F:538:SER:HB3	1:F:662:SER:H	1.42	0.83
1:F:569:SER:OG	1:F:571:ASP:OD2	1.97	0.83
1:A:490:PRO:HA	1:A:491:ALA:HB3	1.59	0.82
1:F:535:PRO:HA	1:F:639:LYS:HG2	1.60	0.82
1:E:624:GLN:NE2	1:F:610:ASP:OD1	2.12	0.82
1:E:490:PRO:HA	1:E:491:ALA:HB3	1.62	0.82
1:B:303:ARG:HG3	1:B:357:LYS:HE2	1.60	0.82
1:D:301:ASN:HA	1:D:304:LYS:HD3	1.61	0.82
1:A:331:ASP:HA	1:A:379:ILE:HD11	1.61	0.81
1:C:691:ARG:HA	1:C:694:ILE:HD12	1.61	0.81
1:A:305:LEU:HD23	1:A:325:ILE:HG21	1.61	0.81
1:C:497:GLU:O	1:C:499:TYR:N	2.13	0.81
1:F:358:ILE:HD12	1:F:388:ARG:HB3	1.63	0.80
1:C:724:TYR:HD2	1:C:727:ARG:HH21	1.30	0.80
1:C:490:PRO:HA	1:C:491:ALA:HB3	1.64	0.80
1:C:540:LEU:HB3	1:C:664:THR:HG22	1.60	0.80
1:E:593:TYR:O	1:E:638:ARG:NH1	2.15	0.80
1:E:528:THR:HG22	1:E:537:VAL:HG21	1.63	0.79
1:D:312:GLU:OE1	1:D:323:HIS:ND1	2.16	0.79
1:D:606:GLU:HA	1:D:609:LEU:HG	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:ASN:HD21	1:E:617:ARG:HG2	1.48	0.79
1:C:687:LYS:N	1:C:690:GLU:OE2	2.14	0.79
1:D:508:ILE:H	2:D:801:ATP:HN61	1.28	0.78
1:C:697:GLN:HG3	1:C:730:LEU:HD11	1.65	0.78
1:E:653:GLN:HA	1:E:658:LEU:HB2	1.64	0.78
1:D:627:LEU:HD21	1:D:657:MET:HG3	1.64	0.78
1:B:407:LEU:HD11	1:B:426:ILE:HG23	1.66	0.78
1:A:672:THR:OG1	1:A:675:GLN:OE1	2.02	0.78
1:A:238:ARG:HA	1:A:252:HIS:CE1	2.18	0.77
1:D:546:HIS:HB3	1:D:708:LYS:HB3	1.65	0.77
1:D:605:ILE:HD11	1:D:644:GLY:HA3	1.65	0.77
1:F:564:PHE:O	1:F:598:SER:OG	2.00	0.77
1:B:490:PRO:HA	1:B:491:ALA:HB3	1.64	0.77
1:C:544:PRO:O	1:C:547:SER:OG	2.02	0.77
1:B:388:ARG:NH1	2:C:802:ATP:O3G	2.16	0.77
1:D:670:ILE:HD11	1:D:705:ILE:HG23	1.67	0.76
1:E:606:GLU:OE2	1:E:646:THR:OG1	2.03	0.76
1:B:540:LEU:HD23	1:B:661:PHE:CD1	2.21	0.76
1:F:606:GLU:OE1	1:F:606:GLU:N	2.17	0.76
1:E:527:GLN:O	1:E:531:SER:OG	2.02	0.76
1:D:549:LYS:NZ	2:D:801:ATP:O1G	2.16	0.76
1:C:564:PHE:O	1:C:598:SER:OG	2.04	0.76
1:A:264:CYS:SG	1:A:265:GLY:N	2.59	0.76
1:E:693:THR:O	1:E:697:GLN:NE2	2.14	0.76
1:C:313:GLN:O	1:C:317:GLY:N	2.19	0.75
1:C:627:LEU:HD12	1:D:607:ARG:HH12	1.51	0.75
1:F:257:LEU:HB2	1:F:389:LEU:HD13	1.67	0.75
1:F:565:ILE:HG23	1:F:599:CYS:HB3	1.67	0.75
1:E:286:ASN:ND2	1:E:326:ILE:O	2.19	0.75
1:F:507:ILE:HG13	1:F:555:LYS:HE2	1.67	0.75
1:B:538:SER:HB3	1:B:661:PHE:HD2	1.52	0.75
1:C:438:GLY:HA3	2:C:802:ATP:HN61	1.50	0.74
1:D:624:GLN:OE1	1:E:607:ARG:NH1	2.21	0.74
1:E:593:TYR:OH	1:E:632:LYS:NZ	2.17	0.74
1:D:548:GLY:HA3	2:D:801:ATP:H2	1.51	0.74
1:A:267:THR:OG1	1:A:328:ASP:OD2	2.05	0.74
1:D:256:ILE:HG13	1:D:370:ILE:HG22	1.70	0.74
1:B:385:ARG:NH2	2:C:802:ATP:O3B	2.21	0.74
1:E:268:LEU:HD23	2:E:802:ATP:H3'	1.67	0.74
1:F:634:PRO:HB2	1:F:638:ARG:HG3	1.70	0.74
1:A:527:GLN:HB2	1:B:719:GLN:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:PRO:HA	1:C:390:GLU:HA	1.70	0.74
1:C:496:GLN:O	1:C:498:ASP:N	2.20	0.73
1:C:318:ALA:O	1:C:319:ASN:ND2	2.21	0.73
1:B:720:MET:HG3	1:B:728:LYS:HG3	1.69	0.73
1:F:546:HIS:CE1	1:F:709:LYS:HB2	2.24	0.73
1:B:596:GLN:HA	1:B:638:ARG:HG2	1.71	0.73
1:A:246:GLU:O	1:B:413:ARG:NH2	2.18	0.73
1:B:385:ARG:NE	2:C:802:ATP:O3G	2.20	0.72
1:D:230:ILE:HD11	1:D:256:ILE:HD13	1.70	0.72
1:D:711:LEU:HA	1:D:714:ILE:HD12	1.70	0.72
1:A:353:GLN:HA	1:B:288:PRO:HG3	1.71	0.72
1:D:533:ARG:HD2	1:E:505:ASN:HD21	1.53	0.72
1:A:485:GLU:O	1:A:489:LYS:N	2.23	0.72
1:F:570:PRO:HG2	1:F:604:ASP:HB2	1.71	0.72
1:A:502:TYR:HE2	1:A:567:ILE:HG21	1.54	0.72
1:E:596:GLN:HA	1:E:638:ARG:HG2	1.71	0.71
1:C:256:ILE:HG13	1:C:370:ILE:HG22	1.71	0.71
1:A:497:GLU:O	1:A:499:TYR:N	2.23	0.71
1:C:711:LEU:HA	1:C:714:ILE:HD12	1.72	0.71
1:F:526:GLN:NE2	1:F:530:ASN:OD1	2.23	0.71
1:C:399:ASP:O	1:C:403:ARG:N	2.24	0.71
1:B:559:GLU:O	1:B:561:ASN:ND2	2.24	0.71
1:E:300:ALA:O	1:E:304:LYS:HG2	1.90	0.71
1:E:235:PHE:O	1:E:239:VAL:HG13	1.91	0.71
1:A:525:VAL:HG13	1:A:562:PHE:CZ	2.25	0.70
1:C:616:PRO:HG2	1:D:614:ILE:HD13	1.71	0.70
1:F:570:PRO:HA	1:F:573:MET:HE2	1.72	0.70
1:B:624:GLN:NE2	1:C:610:ASP:O	2.23	0.70
1:F:538:SER:H	1:F:662:SER:HB2	1.56	0.70
1:E:452:ALA:O	1:E:456:HIS:ND1	2.23	0.70
1:B:540:LEU:HD11	1:B:649:LYS:NZ	2.07	0.70
1:F:234:ALA:HB2	1:F:256:ILE:HG21	1.72	0.70
1:C:513:PRO:O	1:C:516:ARG:HG2	1.92	0.70
1:E:553:ALA:HA	1:E:556:ILE:HD12	1.74	0.69
1:E:670:ILE:HD12	1:E:670:ILE:H	1.57	0.69
1:E:652:LEU:HD23	1:E:657:MET:HB3	1.72	0.69
1:E:587:LYS:HZ1	1:E:591:ASP:CG	1.94	0.69
1:F:452:ALA:O	1:F:456:HIS:ND1	2.23	0.69
1:C:690:GLU:HB2	1:C:726:VAL:HG21	1.74	0.69
1:D:510:TRP:CD2	1:D:670:ILE:HG22	2.27	0.69
1:A:247:GLN:O	1:B:413:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:587:LYS:NZ	1:E:587:LYS:O	2.25	0.69
1:F:236:ALA:HA	1:F:239:VAL:HG12	1.73	0.69
1:C:718:LEU:O	1:C:725:ARG:NH1	2.25	0.69
1:F:721:ASP:HB2	1:F:724:TYR:HD1	1.57	0.69
1:D:399:ASP:O	1:D:403:ARG:N	2.25	0.69
1:D:330:ILE:HD11	1:D:373:THR:HB	1.75	0.69
1:E:720:MET:HG3	1:E:728:LYS:HE3	1.74	0.69
1:D:513:PRO:HA	1:D:516:ARG:HG2	1.75	0.68
1:B:718:LEU:HD12	1:B:725:ARG:HD3	1.75	0.68
1:F:670:ILE:HG23	1:F:675:GLN:HB2	1.75	0.68
1:E:596:GLN:O	1:E:639:LYS:N	2.25	0.68
1:A:624:GLN:NE2	1:B:610:ASP:OD1	2.20	0.68
1:A:553:ALA:HA	1:A:556:ILE:HD12	1.75	0.68
1:B:686:PHE:O	1:B:691:ARG:NH1	2.26	0.68
1:B:549:LYS:HZ2	1:B:647:SER:HA	1.58	0.68
1:A:309:ALA:HB1	1:A:367:ILE:HG21	1.76	0.67
1:C:624:GLN:NE2	1:D:610:ASP:HB2	2.09	0.67
1:A:454:ASN:HA	1:A:457:ILE:HD12	1.75	0.67
1:E:502:TYR:HH	1:E:569:SER:HG	1.42	0.67
1:C:527:GLN:HB2	1:D:719:GLN:HG3	1.76	0.67
1:B:311:GLU:OE1	1:B:314:ARG:NE	2.25	0.67
1:D:240:PHE:HD2	1:D:244:ILE:HG21	1.60	0.67
1:B:551:ALA:HB2	2:B:801:ATP:H3'	1.75	0.67
1:D:527:GLN:HE21	1:E:715:GLU:HG3	1.59	0.67
1:A:678:GLU:O	1:A:682:LEU:HD12	1.95	0.67
1:F:259:TYR:HE1	1:F:379:ILE:HD13	1.59	0.67
1:A:326:ILE:HG22	1:A:370:ILE:HG12	1.75	0.66
1:C:604:ASP:N	1:C:645:THR:OG1	2.24	0.66
1:D:527:GLN:HE22	1:E:716:MET:HA	1.61	0.66
1:C:385:ARG:HD2	1:D:263:GLY:CA	2.25	0.66
1:A:687:LYS:N	1:A:690:GLU:OE1	2.27	0.66
1:E:625:ALA:HA	1:F:574:ILE:HD11	1.77	0.66
1:B:548:GLY:HA3	2:B:801:ATP:H2	1.61	0.66
1:D:528:THR:OG1	1:D:641:LEU:HD12	1.96	0.66
1:E:670:ILE:HG22	1:E:672:THR:H	1.61	0.66
1:E:380:ASP:OD1	1:E:382:ALA:N	2.28	0.66
1:E:399:ASP:O	1:E:403:ARG:N	2.24	0.66
1:A:685:ASN:ND2	1:A:714:ILE:HD13	2.11	0.66
1:D:646:THR:HG21	1:D:652:LEU:HD23	1.78	0.66
1:F:545:PRO:HA	1:F:547:SER:N	2.11	0.66
1:E:530:ASN:O	1:E:639:LYS:NZ	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:O	1:A:389:LEU:HB2	1.96	0.66
1:B:656:GLU:HG3	1:C:613:PRO:HG3	1.77	0.66
1:E:652:LEU:HD21	1:E:661:PHE:HE1	1.61	0.66
1:C:604:ASP:H	1:C:645:THR:HG1	1.44	0.66
1:E:538:SER:OG	1:E:662:SER:N	2.23	0.66
1:E:436:PHE:HB3	1:E:440:GLU:HB2	1.77	0.65
1:B:540:LEU:HD11	1:B:649:LYS:HZ3	1.59	0.65
1:B:538:SER:HB3	1:B:661:PHE:CD2	2.31	0.65
1:F:546:HIS:CD2	1:F:709:LYS:HG3	2.31	0.65
1:A:602:VAL:HG12	1:A:605:ILE:HG12	1.77	0.65
1:C:542:GLU:HG3	1:C:649:LYS:HE2	1.78	0.65
1:E:603:ASP:OD2	1:E:645:THR:OG1	2.09	0.65
1:C:426:ILE:HD12	1:C:427:LYS:H	1.62	0.65
1:A:710:LEU:O	1:A:714:ILE:HG13	1.96	0.65
1:C:656:GLU:OE2	1:D:648:ARG:NH1	2.30	0.65
1:F:546:HIS:NE2	1:F:709:LYS:HB2	2.11	0.65
1:A:353:GLN:HE21	1:A:357:LYS:HG2	1.61	0.65
1:F:686:PHE:HB3	1:F:690:GLU:HB3	1.78	0.65
1:C:533:ARG:O	1:D:505:ASN:ND2	2.30	0.65
1:E:232:ARG:HE	1:F:454:ASN:HA	1.61	0.64
1:B:399:ASP:O	1:B:403:ARG:N	2.27	0.64
1:E:319:ASN:HB2	1:E:320:SER:OG	1.97	0.64
1:E:513:PRO:HA	1:E:516:ARG:HG2	1.79	0.64
1:F:653:GLN:HB3	1:F:658:LEU:HD23	1.79	0.64
1:A:256:ILE:HG13	1:A:370:ILE:HG22	1.79	0.64
1:D:651:VAL:O	1:D:655:MET:HG2	1.97	0.64
1:F:550:THR:HA	1:F:645:THR:HG21	1.79	0.64
1:F:406:ILE:HB	1:F:441:LEU:HD22	1.79	0.64
1:E:585:MET:HG3	1:E:589:PHE:CZ	2.32	0.64
1:E:604:ASP:O	1:E:608:LEU:N	2.29	0.64
1:D:319:ASN:HB3	1:D:320:SER:HB2	1.79	0.64
1:C:546:HIS:HA	1:C:708:LYS:HD3	1.80	0.64
1:F:536:LEU:HD11	1:F:634:PRO:HD3	1.78	0.64
1:E:689:LYS:O	1:E:692:THR:OG1	2.13	0.64
1:A:617:ARG:HH11	1:A:617:ARG:HG3	1.63	0.64
1:C:381:GLU:OE1	1:C:381:GLU:N	2.31	0.64
1:B:300:ALA:O	1:B:304:LYS:HG2	1.97	0.64
1:C:438:GLY:HA3	2:C:802:ATP:N6	2.12	0.64
1:B:315:ARG:HG3	1:B:316:LEU:HD12	1.78	0.64
1:C:540:LEU:HB2	1:C:661:PHE:CD2	2.33	0.64
1:A:351:VAL:O	1:A:355:LEU:HG	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ASN:HD22	1:A:714:ILE:HG21	1.62	0.64
1:F:437:SER:O	1:F:440:GLU:HB2	1.98	0.64
1:E:327:PHE:HB3	1:E:330:ILE:HG22	1.80	0.64
1:A:319:ASN:OD1	1:A:320:SER:N	2.31	0.64
1:E:264:CYS:SG	1:E:266:LYS:HG3	2.38	0.64
1:E:510:TRP:CZ3	1:E:670:ILE:HG13	2.32	0.64
1:F:259:TYR:CE1	1:F:376:PRO:HA	2.33	0.64
1:C:231:PHE:O	1:C:235:PHE:HB2	1.98	0.63
1:E:606:GLU:OE2	1:E:648:ARG:N	2.26	0.63
1:A:285:VAL:HG13	1:A:326:ILE:HD11	1.80	0.63
1:F:674:GLU:O	1:F:678:GLU:HG2	1.98	0.63
1:F:536:LEU:HD21	1:F:632:LYS:O	1.98	0.63
1:C:385:ARG:HH21	1:D:263:GLY:HA2	1.63	0.63
1:D:266:LYS:N	2:D:802:ATP:O1B	2.30	0.63
1:B:303:ARG:HB2	1:B:353:GLN:NE2	2.13	0.63
1:C:614:ILE:C	1:C:616:PRO:HA	2.19	0.63
1:D:631:LYS:NZ	2:E:801:ATP:O2G	2.26	0.63
1:D:507:ILE:HA	2:D:801:ATP:N7	2.13	0.63
1:D:543:GLY:H	1:D:549:LYS:HD3	1.64	0.63
1:E:526:GLN:NE2	1:F:719:GLN:O	2.31	0.63
1:B:505:ASN:HB2	2:B:801:ATP:H1'	1.81	0.63
1:E:310:GLU:OE2	1:E:357:LYS:NZ	2.31	0.63
1:D:240:PHE:HB3	1:D:244:ILE:HD13	1.80	0.62
1:C:385:ARG:NH2	1:D:263:GLY:HA2	2.14	0.62
1:E:672:THR:OG1	1:E:675:GLN:HB2	1.99	0.62
1:D:404:LEU:HA	1:D:407:LEU:HD12	1.81	0.62
1:E:680:LEU:HB3	1:E:686:PHE:CZ	2.34	0.62
1:D:652:LEU:HB3	1:D:658:LEU:HB2	1.80	0.62
1:D:242:PRO:HD2	1:D:243:GLU:OE1	2.00	0.62
1:D:380:ASP:OD1	1:D:382:ALA:N	2.32	0.62
1:A:557:ALA:O	1:A:560:SER:OG	2.13	0.62
1:C:618:PHE:HE2	1:D:614:ILE:HD11	1.63	0.62
1:D:695:ALA:HB1	1:D:699:LYS:HE3	1.80	0.62
1:F:546:HIS:O	1:F:546:HIS:ND1	2.33	0.62
1:F:695:ALA:HB1	1:F:699:LYS:HE3	1.81	0.62
1:F:385:ARG:HH22	1:F:388:ARG:NH2	1.98	0.62
1:A:527:GLN:NE2	1:B:715:GLU:OE2	2.32	0.62
1:A:653:GLN:NE2	1:A:653:GLN:O	2.33	0.62
1:B:323:HIS:HB2	1:B:367:ILE:HG22	1.82	0.62
1:E:508:ILE:HB	1:E:682:LEU:HD13	1.82	0.62
1:E:618:PHE:HZ	1:F:612:VAL:HG11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:ALA:HA	1:E:310:GLU:HG2	1.82	0.62
1:B:508:ILE:O	2:B:801:ATP:N6	2.32	0.62
1:E:315:ARG:HG3	1:E:316:LEU:HD12	1.80	0.62
1:E:532:ASP:OD2	1:E:533:ARG:N	2.33	0.61
1:C:638:ARG:HH11	1:C:638:ARG:HG3	1.65	0.61
1:F:566:LYS:HD2	1:F:567:ILE:N	2.15	0.61
1:D:548:GLY:HA3	2:D:801:ATP:C2	2.34	0.61
1:D:257:LEU:HB2	1:D:389:LEU:HD13	1.81	0.61
1:E:705:ILE:HD13	1:E:710:LEU:HD13	1.81	0.61
1:D:680:LEU:HB2	1:D:691:ARG:HH21	1.65	0.61
1:F:518:LEU:HD21	1:F:555:LYS:HD2	1.83	0.61
1:E:527:GLN:NE2	1:F:716:MET:HG2	2.15	0.61
1:E:399:ASP:OD1	1:E:400:GLU:N	2.32	0.61
1:A:231:PHE:CE1	1:A:235:PHE:HE2	2.19	0.61
1:F:554:ALA:O	1:F:558:GLU:HG3	2.00	0.61
1:C:688:ASP:HA	1:C:691:ARG:NH1	2.15	0.61
1:D:551:ALA:HB2	2:D:801:ATP:H3'	1.82	0.61
1:F:539:VAL:HB	1:F:643:ILE:HG12	1.81	0.61
1:B:326:ILE:HG22	1:B:370:ILE:HG13	1.83	0.61
1:A:441:LEU:HD23	1:A:444:LEU:HD12	1.83	0.61
1:F:284:VAL:HG11	1:F:305:LEU:HD11	1.83	0.60
1:C:688:ASP:O	1:C:692:THR:HG23	2.00	0.60
1:A:386:PRO:HA	1:A:390:GLU:HA	1.82	0.60
1:B:670:ILE:HG23	1:B:675:GLN:HB2	1.82	0.60
1:C:618:PHE:CE2	1:D:614:ILE:HD11	2.36	0.60
1:A:445:VAL:O	1:A:449:GLN:HG2	2.02	0.60
1:E:311:GLU:OE1	1:E:314:ARG:NE	2.26	0.60
1:D:381:GLU:N	1:D:381:GLU:OE1	2.31	0.60
1:E:595:SER:HB3	1:E:598:SER:HB3	1.83	0.60
1:E:428:GLU:O	1:E:432:GLU:HG2	2.02	0.60
1:F:544:PRO:O	1:F:547:SER:OG	2.19	0.60
1:F:240:PHE:HD2	1:F:244:ILE:HG21	1.66	0.60
1:C:728:LYS:HE3	1:C:732:LEU:HD21	1.84	0.60
1:D:256:ILE:HG22	1:D:391:VAL:HG12	1.83	0.60
1:A:536:LEU:HD23	1:A:633:ALA:HA	1.83	0.60
1:D:686:PHE:HE1	1:D:714:ILE:HG23	1.66	0.60
1:B:713:LEU:HD22	1:B:732:LEU:HB3	1.83	0.60
1:F:602:VAL:N	1:F:643:ILE:O	2.24	0.60
1:F:442:GLU:O	1:F:446:ARG:HG3	2.01	0.60
1:E:415:ARG:HA	1:E:420:LEU:HD11	1.83	0.60
1:E:527:GLN:HE22	1:F:716:MET:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:LEU:HD22	1:C:657:MET:HG2	1.84	0.60
1:C:240:PHE:HD2	1:C:244:ILE:HG21	1.65	0.60
1:D:548:GLY:HA2	2:D:801:ATP:H5'1	1.82	0.59
1:D:564:PHE:HD2	1:D:598:SER:HB2	1.67	0.59
1:D:284:VAL:HG23	1:D:324:ILE:O	2.02	0.59
1:F:538:SER:HG	1:F:661:PHE:HD1	1.50	0.59
1:A:521:GLY:O	1:A:525:VAL:HG23	2.01	0.59
1:B:621:LEU:HD11	1:C:575:GLY:HA2	1.84	0.59
1:B:546:HIS:O	1:B:547:SER:OG	2.10	0.59
1:D:538:SER:OG	1:D:661:PHE:HA	2.02	0.59
1:F:236:ALA:HB1	1:F:240:PHE:CZ	2.38	0.59
1:B:256:ILE:HG13	1:B:370:ILE:HG22	1.82	0.59
1:D:628:VAL:HG11	1:E:574:ILE:HG21	1.84	0.59
1:F:658:LEU:HA	1:F:661:PHE:HD2	1.68	0.59
1:E:630:LEU:HD22	1:E:660:ALA:HB1	1.84	0.59
1:B:380:ASP:OD1	1:B:382:ALA:N	2.33	0.59
1:C:577:SER:O	1:C:580:ALA:N	2.34	0.59
1:D:573:MET:SD	1:D:581:LYS:HD3	2.43	0.59
1:D:518:LEU:HD21	1:D:552:LEU:HD22	1.83	0.59
1:A:521:GLY:HA2	1:A:524:LEU:HD12	1.83	0.59
1:C:245:VAL:O	1:C:249:GLY:N	2.35	0.59
1:B:498:ASP:OD1	1:B:499:TYR:N	2.35	0.59
1:C:658:LEU:HD11	1:C:664:THR:HG21	1.84	0.59
1:D:548:GLY:H	2:D:801:ATP:PB	2.25	0.59
1:C:538:SER:OG	1:C:662:SER:N	2.32	0.59
1:E:640:LEU:HD12	1:E:641:LEU:N	2.18	0.59
1:D:528:THR:OG1	1:D:537:VAL:HG21	2.02	0.59
1:B:449:GLN:O	1:B:453:MET:HG2	2.03	0.59
1:A:502:TYR:CE2	1:A:567:ILE:HG21	2.36	0.58
1:E:299:GLU:OE2	1:E:353:GLN:HB2	2.02	0.58
1:E:513:PRO:O	1:E:517:VAL:HG23	2.03	0.58
1:E:235:PHE:HZ	1:E:273:ILE:HG12	1.66	0.58
1:A:255:GLY:HA3	1:A:389:LEU:HD13	1.85	0.58
1:E:680:LEU:HD22	1:E:686:PHE:HE2	1.68	0.58
1:F:612:VAL:CG1	1:F:617:ARG:HB2	2.33	0.58
1:A:240:PHE:HB3	1:A:244:ILE:HD11	1.84	0.58
1:C:589:PHE:CD2	1:C:629:LEU:HD13	2.38	0.58
1:D:521:GLY:O	1:D:525:VAL:HG23	2.04	0.58
1:A:407:LEU:O	1:A:411:THR:HG23	2.02	0.58
1:E:536:LEU:HD22	1:E:634:PRO:HD3	1.85	0.58
1:C:611:TYR:CE1	1:C:616:PRO:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:655:MET:O	1:D:656:GLU:HB2	2.02	0.58
1:C:381:GLU:O	1:C:384:LEU:HG	2.02	0.58
1:D:531:SER:HG	1:D:534:THR:HG1	1.52	0.58
1:B:571:ASP:OD2	1:B:571:ASP:N	2.36	0.58
1:D:688:ASP:OD1	1:D:689:LYS:N	2.36	0.58
1:B:436:PHE:HB3	1:B:440:GLU:HB2	1.85	0.58
1:D:606:GLU:O	1:D:610:ASP:N	2.37	0.58
1:A:605:ILE:HD11	1:A:644:GLY:HA3	1.86	0.58
1:F:327:PHE:CE2	1:F:330:ILE:HA	2.39	0.58
1:F:508:ILE:HD13	1:F:510:TRP:HD1	1.68	0.58
1:F:650:ASP:O	1:F:653:GLN:HG3	2.04	0.58
1:A:628:VAL:HG11	1:B:571:ASP:HA	1.85	0.58
1:C:331:ASP:HA	1:C:379:ILE:HD11	1.85	0.58
1:C:586:LYS:NZ	1:D:574:ILE:O	2.29	0.58
1:D:234:ALA:HA	1:D:253:VAL:HG11	1.85	0.58
1:D:348:ASP:O	1:D:352:ASN:ND2	2.36	0.58
1:C:377:ASP:OD2	1:C:377:ASP:N	2.37	0.58
1:E:536:LEU:HD12	1:E:640:LEU:O	2.03	0.58
1:D:309:ALA:HA	1:D:312:GLU:OE2	2.03	0.58
1:D:539:VAL:HG23	1:D:663:THR:HG23	1.84	0.58
1:F:307:ALA:O	1:F:311:GLU:HG2	2.03	0.58
1:E:374:ASN:ND2	2:E:802:ATP:O1G	2.36	0.58
1:E:307:ALA:O	1:E:311:GLU:HG2	2.04	0.58
1:E:540:LEU:HD11	1:E:646:THR:HG22	1.85	0.57
1:C:324:ILE:HG23	1:C:368:LEU:HD22	1.84	0.57
1:F:535:PRO:HB2	1:F:536:LEU:HD13	1.85	0.57
1:A:726:VAL:O	1:A:730:LEU:HG	2.03	0.57
1:A:713:LEU:HD21	1:A:732:LEU:HB3	1.85	0.57
1:F:386:PRO:HA	1:F:390:GLU:HA	1.86	0.57
1:A:507:ILE:HD12	1:A:555:LYS:HG2	1.86	0.57
1:C:383:LEU:O	1:C:389:LEU:HB2	2.04	0.57
1:E:624:GLN:OE1	1:E:624:GLN:HA	2.03	0.57
1:E:525:VAL:O	1:E:528:THR:OG1	2.15	0.57
1:A:536:LEU:HD23	1:A:634:PRO:HD3	1.86	0.57
1:B:540:LEU:HA	1:B:644:GLY:O	2.04	0.57
1:B:542:GLU:HB3	1:B:649:LYS:HG3	1.87	0.57
1:A:680:LEU:O	1:A:691:ARG:NH2	2.37	0.57
1:B:436:PHE:HB3	1:B:440:GLU:CB	2.35	0.57
1:B:404:LEU:O	1:B:408:HIS:HB2	2.03	0.57
1:D:585:MET:O	1:D:589:PHE:HD2	1.87	0.57
1:B:233:ARG:NH1	1:C:451:THR:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:605:ILE:HD11	1:F:644:GLY:HA3	1.87	0.57
1:F:507:ILE:HG21	1:F:555:LYS:NZ	2.19	0.57
1:B:306:PHE:HZ	1:B:327:PHE:HZ	1.51	0.57
1:B:307:ALA:O	1:B:311:GLU:HG2	2.03	0.57
1:E:652:LEU:CD2	1:E:657:MET:HB3	2.34	0.57
1:C:547:SER:HB2	1:C:549:LYS:HG3	1.87	0.57
1:F:546:HIS:CE1	1:F:709:LYS:H	2.23	0.57
1:D:567:ILE:HG23	1:D:601:VAL:HB	1.87	0.57
1:A:307:ALA:O	1:A:310:GLU:HG3	2.04	0.57
1:B:386:PRO:HG2	1:C:440:GLU:HG2	1.85	0.57
1:D:533:ARG:HD2	1:E:505:ASN:ND2	2.20	0.57
1:D:534:THR:OG1	1:E:715:GLU:HG2	2.05	0.57
1:F:351:VAL:HG22	1:F:380:ASP:OD2	2.05	0.57
1:D:620:ASN:O	1:D:624:GLN:HG2	2.05	0.57
1:F:257:LEU:HG	1:F:371:GLY:O	2.05	0.57
1:F:388:ARG:O	1:F:389:LEU:HD23	2.05	0.57
1:D:604:ASP:HB3	1:D:607:ARG:HB3	1.87	0.57
1:C:606:GLU:HG2	1:C:607:ARG:N	2.19	0.57
1:B:233:ARG:HH12	1:C:451:THR:HA	1.70	0.57
1:C:510:TRP:CZ3	1:C:670:ILE:HG12	2.40	0.57
1:E:236:ALA:HA	1:E:239:VAL:HG22	1.87	0.57
1:D:330:ILE:HD12	1:D:331:ASP:N	2.20	0.57
1:C:728:LYS:O	1:C:732:LEU:HG	2.05	0.57
1:F:606:GLU:OE2	1:F:647:SER:HB2	2.05	0.56
1:F:438:GLY:HA2	1:F:441:LEU:HD13	1.87	0.56
1:A:688:ASP:OD1	1:A:689:LYS:N	2.38	0.56
1:C:485:GLU:O	1:C:489:LYS:N	2.33	0.56
1:C:677:LEU:HD21	1:C:695:ALA:HB2	1.86	0.56
1:E:628:VAL:HB	1:F:574:ILE:HD12	1.86	0.56
1:E:640:LEU:HD12	1:E:641:LEU:H	1.70	0.56
1:B:407:LEU:CD1	1:B:426:ILE:HG23	2.35	0.56
1:D:651:VAL:O	1:D:654:GLU:HG2	2.05	0.56
1:B:224:ASP:O	1:B:228:SER:HB2	2.05	0.56
1:D:356:SER:HB2	1:E:288:PRO:HG3	1.87	0.56
1:A:685:ASN:HD21	1:A:714:ILE:HD13	1.70	0.56
1:D:326:ILE:HG22	1:D:370:ILE:HG13	1.86	0.56
1:F:612:VAL:HG12	1:F:617:ARG:HB2	1.87	0.56
1:F:327:PHE:HE2	1:F:330:ILE:HA	1.70	0.56
1:E:404:LEU:O	1:E:408:HIS:HB2	2.05	0.56
1:E:256:ILE:HG13	1:E:370:ILE:HG22	1.85	0.56
1:B:525:VAL:HG11	1:B:560:SER:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:542:GLU:O	1:F:666:HIS:ND1	2.37	0.56
1:B:656:GLU:OE1	1:C:648:ARG:NH2	2.38	0.56
1:F:617:ARG:HG3	1:F:617:ARG:HH11	1.70	0.56
1:F:309:ALA:HB1	1:F:367:ILE:HG21	1.88	0.56
1:D:300:ALA:O	1:D:303:ARG:HB3	2.05	0.56
1:B:508:ILE:H	2:B:801:ATP:N6	2.03	0.56
1:E:697:GLN:HG3	1:E:730:LEU:HD11	1.88	0.56
1:B:414:MET:SD	1:B:449:GLN:NE2	2.73	0.56
1:E:528:THR:HG21	1:E:641:LEU:CD2	2.36	0.56
1:F:521:GLY:O	1:F:525:VAL:HG23	2.05	0.56
1:B:649:LYS:HE3	1:B:658:LEU:HD11	1.87	0.56
1:D:326:ILE:HG22	1:D:370:ILE:CG1	2.36	0.56
1:F:711:LEU:HD11	2:F:801:ATP:C8	2.40	0.56
1:F:655:MET:O	1:F:656:GLU:CB	2.53	0.56
1:F:313:GLN:O	1:F:317:GLY:N	2.39	0.56
1:F:550:THR:OG1	2:F:801:ATP:O1A	2.24	0.56
1:A:565:ILE:HG13	1:A:599:CYS:HB3	1.87	0.55
1:D:652:LEU:HD13	1:D:657:MET:HB3	1.89	0.55
1:C:630:LEU:HD11	1:C:661:PHE:CE1	2.42	0.55
1:A:709:LYS:HA	1:A:709:LYS:HE2	1.89	0.55
1:F:235:PHE:HZ	1:F:273:ILE:HG12	1.71	0.55
1:C:624:GLN:O	1:C:628:VAL:HG23	2.05	0.55
1:F:229:ASP:OD1	1:F:230:ILE:N	2.39	0.55
1:E:563:PRO:HG2	1:E:595:SER:OG	2.06	0.55
1:A:353:GLN:HA	1:B:288:PRO:CG	2.36	0.55
1:D:239:VAL:HG13	1:D:240:PHE:CD1	2.40	0.55
1:E:556:ILE:HA	1:E:559:GLU:HG2	1.87	0.55
2:E:801:ATP:H5'2	2:E:801:ATP:N3	2.22	0.55
1:D:383:LEU:O	1:D:389:LEU:HB2	2.06	0.55
1:F:256:ILE:HG13	1:F:370:ILE:HG22	1.89	0.55
1:A:449:GLN:O	1:A:453:MET:HG2	2.07	0.55
1:E:296:GLY:H	1:E:297:GLU:CB	2.20	0.55
1:B:240:PHE:HD2	1:B:244:ILE:HG21	1.70	0.55
1:B:528:THR:O	1:B:639:LYS:HD2	2.07	0.55
1:C:611:TYR:HE1	1:C:616:PRO:HB2	1.70	0.55
1:E:652:LEU:HD22	1:E:658:LEU:HD13	1.88	0.54
1:C:490:PRO:HB2	1:C:492:PHE:N	2.22	0.54
1:C:508:ILE:HD13	1:C:683:LEU:HD21	1.90	0.54
1:D:240:PHE:CD2	1:D:244:ILE:HG21	2.40	0.54
1:A:406:ILE:HG12	2:A:802:ATP:HN61	1.71	0.54
1:C:315:ARG:HA	1:C:315:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:ARG:HG3	1:E:357:LYS:HE2	1.89	0.54
1:B:309:ALA:HA	1:B:312:GLU:OE1	2.06	0.54
1:A:612:VAL:HG11	1:F:618:PHE:HZ	1.72	0.54
1:A:724:TYR:HD1	1:A:727:ARG:HH12	1.54	0.54
1:C:428:GLU:O	1:C:432:GLU:HG2	2.07	0.54
1:A:224:ASP:OD1	1:A:225:LYS:N	2.41	0.54
1:A:457:ILE:HD11	1:F:240:PHE:CE1	2.43	0.54
1:E:538:SER:HG	1:E:662:SER:H	1.48	0.54
1:B:428:GLU:O	1:B:432:GLU:HG2	2.08	0.54
1:B:327:PHE:HB2	1:B:330:ILE:HG22	1.88	0.54
1:C:584:ALA:O	1:C:588:ILE:HG13	2.08	0.54
1:B:581:LYS:NZ	1:B:608:LEU:O	2.39	0.54
1:E:436:PHE:HB3	1:E:440:GLU:CB	2.37	0.54
1:B:710:LEU:O	1:B:714:ILE:HG13	2.07	0.54
2:D:802:ATP:O2A	2:D:802:ATP:H4'	2.08	0.54
1:A:513:PRO:O	1:A:517:VAL:HG23	2.08	0.54
1:C:404:LEU:O	1:C:408:HIS:HB2	2.07	0.54
1:A:694:ILE:O	1:A:698:VAL:HG13	2.07	0.54
1:F:538:SER:O	1:F:663:THR:HG22	2.08	0.54
1:A:300:ALA:HA	1:A:303:ARG:HG2	1.90	0.54
1:E:676:LEU:O	1:E:680:LEU:HG	2.07	0.54
1:A:236:ALA:HB1	1:B:453:MET:HB2	1.90	0.54
1:D:728:LYS:O	1:D:732:LEU:HD13	2.08	0.54
1:E:541:LEU:N	1:E:644:GLY:O	2.33	0.54
1:A:326:ILE:HG22	1:A:370:ILE:CG1	2.36	0.54
1:D:268:LEU:HD23	2:D:802:ATP:H3'	1.89	0.54
1:E:671:ALA:HB1	1:E:702:LYS:HE2	1.90	0.54
1:D:628:VAL:O	1:D:632:LYS:N	2.40	0.54
1:A:493:GLY:HA2	1:A:494:THR:CB	2.38	0.54
1:D:508:ILE:N	2:D:801:ATP:HN61	2.03	0.54
1:F:728:LYS:O	1:F:732:LEU:HG	2.08	0.54
1:E:534:THR:HG21	1:F:712:MET:HA	1.90	0.54
1:E:354:LEU:O	1:E:358:ILE:HG12	2.08	0.54
1:C:577:SER:O	1:C:579:THR:N	2.41	0.53
1:B:552:LEU:O	1:B:556:ILE:HG13	2.08	0.53
1:D:713:LEU:HD22	1:D:729:PHE:CD1	2.43	0.53
1:E:600:VAL:HG23	1:E:640:LEU:HD11	1.90	0.53
1:E:544:PRO:O	1:E:547:SER:HB3	2.07	0.53
1:E:673:GLY:HA3	1:E:698:VAL:HB	1.91	0.53
1:A:306:PHE:CD1	1:A:357:LYS:HB3	2.44	0.53
1:D:513:PRO:O	1:D:516:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:GLU:HA	1:A:691:ARG:NH1	2.22	0.53
1:F:406:ILE:O	1:F:409:ILE:HG22	2.09	0.53
1:D:402:GLY:HA2	1:D:405:GLN:OE1	2.08	0.53
1:F:240:PHE:CD2	1:F:244:ILE:HG21	2.44	0.53
1:D:265:GLY:O	1:D:268:LEU:HG	2.08	0.53
1:E:686:PHE:HB2	1:E:690:GLU:OE1	2.09	0.53
1:A:671:ALA:HA	1:A:703:VAL:O	2.08	0.53
1:C:688:ASP:HA	1:C:691:ARG:HH12	1.73	0.53
1:B:548:GLY:HA3	2:B:801:ATP:C2	2.43	0.53
1:A:258:LEU:HA	1:A:393:MET:O	2.08	0.53
1:A:705:ILE:HD13	1:A:710:LEU:CD1	2.36	0.53
1:F:609:LEU:HD11	1:F:657:MET:HE1	1.91	0.53
1:C:540:LEU:HD12	1:C:644:GLY:O	2.09	0.53
1:C:326:ILE:HB	1:C:370:ILE:HD11	1.89	0.53
1:C:606:GLU:HG3	1:C:648:ARG:HH11	1.74	0.53
1:D:689:LYS:O	1:D:692:THR:OG1	2.22	0.53
1:F:311:GLU:OE1	1:F:314:ARG:NH2	2.40	0.53
1:E:281:GLU:N	1:E:282:PRO:HA	2.24	0.53
1:F:518:LEU:CD2	1:F:555:LYS:HD2	2.38	0.53
1:F:713:LEU:HD22	1:F:732:LEU:HB3	1.90	0.53
1:D:527:GLN:HE22	1:E:715:GLU:C	2.11	0.53
1:E:565:ILE:HG12	1:E:599:CYS:HB3	1.90	0.53
1:E:447:ALA:O	1:E:451:THR:HG23	2.09	0.53
1:B:307:ALA:HA	1:B:310:GLU:HG2	1.89	0.53
1:F:522:GLU:OE2	1:F:526:GLN:HG2	2.09	0.53
1:A:503:ILE:HG23	1:A:506:GLY:HA2	1.91	0.53
1:B:578:GLU:HG2	1:B:619:SER:HB2	1.90	0.53
1:F:228:SER:HA	1:F:231:PHE:CD2	2.44	0.53
1:C:711:LEU:HD23	1:C:711:LEU:N	2.24	0.53
1:B:246:GLU:HG2	1:B:247:GLN:N	2.23	0.53
1:C:441:LEU:O	1:C:444:LEU:HG	2.08	0.53
1:A:685:ASN:ND2	1:A:714:ILE:HG21	2.23	0.52
1:C:691:ARG:HB2	1:C:691:ARG:HH11	1.75	0.52
1:D:330:ILE:CD1	1:D:373:THR:HB	2.40	0.52
1:B:309:ALA:HB1	1:B:367:ILE:HG21	1.90	0.52
1:D:381:GLU:O	1:D:384:LEU:HG	2.09	0.52
1:B:571:ASP:O	1:B:574:ILE:HG13	2.09	0.52
1:B:319:ASN:HB3	1:B:320:SER:HB2	1.91	0.52
1:E:386:PRO:HA	1:E:390:GLU:HA	1.91	0.52
1:A:293:LYS:O	1:A:294:TYR:CG	2.62	0.52
1:E:608:LEU:HD23	1:E:626:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:GLU:CD	1:D:243:GLU:H	2.12	0.52
1:A:440:GLU:O	1:A:444:LEU:HG	2.09	0.52
1:B:383:LEU:O	1:B:389:LEU:HB2	2.10	0.52
1:E:526:GLN:HA	1:E:529:LYS:HG2	1.90	0.52
1:A:560:SER:HB2	1:A:562:PHE:CE1	2.45	0.52
1:F:542:GLU:N	1:F:665:ILE:O	2.39	0.52
1:E:258:LEU:HB3	1:E:395:ILE:HD11	1.91	0.52
1:D:687:LYS:O	1:D:691:ARG:HG3	2.08	0.52
1:D:527:GLN:NE2	1:E:716:MET:HA	2.24	0.52
1:C:385:ARG:NH1	1:C:388:ARG:HH22	2.08	0.52
1:D:219:GLY:N	1:D:272:GLN:HE22	2.08	0.52
1:A:542:GLU:HA	1:A:646:THR:O	2.08	0.52
1:D:223:LEU:HD11	1:D:395:ILE:HD12	1.91	0.52
1:A:598:SER:OG	1:A:640:LEU:HD12	2.10	0.52
1:E:220:ILE:HB	1:E:223:LEU:HD11	1.91	0.52
1:F:404:LEU:O	1:F:408:HIS:HB2	2.10	0.52
1:A:452:ALA:O	1:A:456:HIS:ND1	2.41	0.52
1:F:428:GLU:O	1:F:432:GLU:HG2	2.09	0.52
1:E:449:GLN:O	1:E:453:MET:HG2	2.10	0.52
1:D:406:ILE:HD11	2:D:802:ATP:N6	2.24	0.52
1:A:300:ALA:O	1:A:304:LYS:HG3	2.09	0.52
1:C:670:ILE:HG21	1:C:676:LEU:HB2	1.92	0.52
1:B:526:GLN:NE2	1:C:719:GLN:HB3	2.17	0.52
1:D:624:GLN:NE2	1:E:610:ASP:O	2.43	0.52
1:E:490:PRO:HA	1:E:491:ALA:CB	2.36	0.52
1:D:677:LEU:HD12	1:D:695:ALA:HB2	1.91	0.52
1:E:650:ASP:OD1	1:E:651:VAL:N	2.43	0.52
1:F:721:ASP:HB2	1:F:724:TYR:CD1	2.41	0.52
1:A:223:LEU:HD12	1:A:227:PHE:HB2	1.91	0.52
1:A:327:PHE:CD1	1:A:330:ILE:HG22	2.45	0.52
1:A:596:GLN:HA	1:A:638:ARG:HD3	1.92	0.52
1:A:571:ASP:OD1	1:A:572:LYS:N	2.43	0.52
1:A:299:GLU:HG3	1:B:289:GLU:CB	2.40	0.52
1:A:309:ALA:HA	1:A:323:HIS:CE1	2.45	0.52
1:F:245:VAL:O	1:F:249:GLY:N	2.40	0.52
1:F:605:ILE:O	1:F:608:LEU:HG	2.10	0.52
1:E:696:GLN:HB3	1:E:697:GLN:NE2	2.25	0.52
1:D:218:MET:C	1:D:272:GLN:HE22	2.13	0.52
1:C:240:PHE:HB3	1:C:244:ILE:HD13	1.92	0.52
1:A:526:GLN:HE21	1:A:530:ASN:HD22	1.58	0.52
1:E:664:THR:C	1:E:665:ILE:HD13	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:ARG:CZ	1:F:391:VAL:HB	2.41	0.51
1:A:564:PHE:CE1	1:A:566:LYS:HB2	2.45	0.51
1:E:628:VAL:O	1:E:632:LYS:N	2.39	0.51
1:D:543:GLY:N	1:D:549:LYS:HD3	2.24	0.51
1:F:514:VAL:O	1:F:518:LEU:HD12	2.10	0.51
1:E:708:LYS:HB2	2:E:801:ATP:O5'	2.09	0.51
1:D:688:ASP:O	1:D:692:THR:HG23	2.11	0.51
1:C:308:ASP:OD1	1:C:309:ALA:N	2.42	0.51
1:A:313:GLN:NE2	1:A:365:ASN:O	2.41	0.51
1:B:593:TYR:O	1:B:638:ARG:HD3	2.09	0.51
1:F:375:ARG:HD3	1:F:377:ASP:H	1.76	0.51
1:B:609:LEU:HD22	1:B:623:LEU:HB2	1.91	0.51
1:D:268:LEU:HD12	1:D:269:LEU:N	2.24	0.51
1:B:503:ILE:HG22	1:B:506:GLY:H	1.74	0.51
1:F:632:LYS:HD2	1:F:633:ALA:H	1.76	0.51
1:D:507:ILE:HA	2:D:801:ATP:C5	2.46	0.51
1:D:632:LYS:NZ	1:E:571:ASP:HB3	2.25	0.51
1:F:260:GLY:O	1:F:374:ASN:HA	2.10	0.51
1:B:589:PHE:CD2	1:B:629:LEU:HD13	2.45	0.51
1:F:717:SER:O	1:F:725:ARG:HG2	2.10	0.51
1:C:596:GLN:HA	1:C:638:ARG:HD3	1.92	0.51
1:A:611:TYR:CE2	1:A:651:VAL:HG11	2.45	0.51
1:A:504:MET:HB3	2:A:801:ATP:O3'	2.11	0.51
1:F:686:PHE:CE1	1:F:714:ILE:HG23	2.46	0.51
1:A:358:ILE:HD12	1:A:359:ASP:H	1.76	0.51
1:C:579:THR:O	1:C:583:GLN:HG2	2.10	0.51
1:B:306:PHE:HZ	1:B:327:PHE:CZ	2.28	0.51
1:F:261:PRO:CG	1:F:398:PRO:HD3	2.41	0.51
1:C:436:PHE:HB3	1:C:440:GLU:OE1	2.10	0.51
1:A:490:PRO:HA	1:A:491:ALA:CB	2.34	0.51
1:B:257:LEU:HB2	1:B:389:LEU:HD13	1.93	0.51
1:D:284:VAL:HG21	1:D:325:ILE:HG22	1.92	0.51
1:D:625:ALA:O	1:D:629:LEU:HG	2.11	0.51
1:E:358:ILE:HD12	1:E:388:ARG:HB3	1.93	0.51
1:E:499:TYR:O	1:E:503:ILE:HG13	2.11	0.51
1:F:686:PHE:HB3	1:F:690:GLU:CB	2.41	0.51
1:C:242:PRO:HD2	1:C:243:GLU:H	1.76	0.51
1:D:589:PHE:CD2	1:D:629:LEU:HD13	2.46	0.51
1:F:734:ARG:O	1:F:734:ARG:HD3	2.10	0.51
1:E:299:GLU:OE2	1:E:349:THR:HB	2.11	0.51
1:A:322:LEU:HD12	1:A:323:HIS:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:671:ALA:HA	1:E:703:VAL:O	2.11	0.51
1:B:570:PRO:HG3	1:B:608:LEU:HD23	1.93	0.51
1:A:625:ALA:O	1:A:629:LEU:HG	2.10	0.51
1:A:630:LEU:HD23	1:A:642:ILE:HD12	1.92	0.51
1:D:246:GLU:HG2	1:D:247:GLN:N	2.26	0.51
1:A:453:MET:SD	1:F:244:ILE:HG23	2.50	0.50
1:E:323:HIS:HB2	1:E:367:ILE:HG22	1.94	0.50
1:D:721:ASP:O	1:D:725:ARG:HG3	2.11	0.50
1:E:524:LEU:O	1:E:528:THR:HG23	2.12	0.50
1:F:710:LEU:O	1:F:714:ILE:HG13	2.10	0.50
1:C:289:GLU:O	1:C:291:LEU:N	2.34	0.50
1:C:614:ILE:O	1:C:616:PRO:HA	2.11	0.50
1:D:527:GLN:NE2	1:E:715:GLU:HG3	2.26	0.50
1:D:721:ASP:HB2	1:D:724:TYR:CE2	2.47	0.50
1:E:325:ILE:HG13	1:E:369:VAL:HB	1.93	0.50
1:A:721:ASP:O	1:A:725:ARG:HG3	2.12	0.50
1:E:657:MET:HG3	1:E:661:PHE:CE1	2.46	0.50
1:D:358:ILE:HD12	1:D:388:ARG:HB3	1.92	0.50
1:A:720:MET:HG3	1:A:728:LYS:HD2	1.93	0.50
1:D:377:ASP:OD1	1:D:378:LEU:N	2.45	0.50
1:C:569:SER:HB3	1:C:572:LYS:HG2	1.94	0.50
1:F:538:SER:OG	1:F:661:PHE:HD1	1.94	0.50
1:C:609:LEU:O	1:C:610:ASP:HB2	2.12	0.50
1:A:347:HIS:N	1:A:348:ASP:HA	2.27	0.50
1:C:311:GLU:HA	1:C:314:ARG:HG2	1.93	0.50
1:F:429:LEU:HD12	1:F:430:ALA:N	2.26	0.50
1:E:528:THR:HG21	1:E:641:LEU:HD23	1.94	0.50
1:F:508:ILE:HD13	1:F:510:TRP:CD1	2.47	0.50
1:B:327:PHE:HB2	1:B:330:ILE:CG2	2.41	0.50
1:A:607:ARG:HD3	1:F:624:GLN:HE22	1.77	0.50
1:B:523:LEU:HA	1:B:526:GLN:HG2	1.94	0.50
1:A:652:LEU:HA	1:A:655:MET:SD	2.52	0.50
1:F:315:ARG:HE	1:F:316:LEU:HD13	1.76	0.50
1:A:650:ASP:OD1	1:A:650:ASP:N	2.44	0.50
1:D:221:GLY:HA3	1:D:406:ILE:HD13	1.93	0.50
1:E:237:SER:HB2	1:F:453:MET:SD	2.52	0.50
1:E:629:LEU:HA	1:E:632:LYS:HB3	1.92	0.50
1:D:690:GLU:O	1:D:693:THR:OG1	2.21	0.50
1:D:510:TRP:HB3	1:D:679:ALA:HB2	1.93	0.50
1:D:407:LEU:O	1:D:411:THR:HG23	2.12	0.50
1:D:349:THR:HA	1:D:352:ASN:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:O	1:A:409:ILE:HG22	2.11	0.50
1:D:627:LEU:HD13	1:E:607:ARG:HH22	1.77	0.49
1:F:653:GLN:HA	1:F:658:LEU:HB3	1.94	0.49
1:C:677:LEU:HD21	1:C:695:ALA:CB	2.41	0.49
1:B:540:LEU:HD23	1:B:661:PHE:HD1	1.73	0.49
1:D:604:ASP:HB3	1:D:607:ARG:CB	2.42	0.49
1:A:540:LEU:HD12	1:A:644:GLY:O	2.12	0.49
1:F:311:GLU:OE1	1:F:314:ARG:NE	2.43	0.49
1:F:512:ASP:OD1	1:F:513:PRO:HD3	2.12	0.49
1:E:388:ARG:O	1:E:389:LEU:HD23	2.11	0.49
1:F:258:LEU:HA	1:F:393:MET:O	2.12	0.49
1:D:427:LYS:O	1:D:431:VAL:HG12	2.12	0.49
1:A:446:ARG:HA	1:A:449:GLN:HG3	1.94	0.49
1:F:707:ILE:HG12	2:F:801:ATP:C5	2.47	0.49
1:A:268:LEU:N	2:A:802:ATP:O2A	2.37	0.49
1:B:628:VAL:O	1:B:632:LYS:N	2.45	0.49
1:C:353:GLN:HA	1:D:288:PRO:HG3	1.93	0.49
1:C:325:ILE:HG13	1:C:369:VAL:HG23	1.93	0.49
1:B:569:SER:HA	1:B:603:ASP:HB3	1.93	0.49
1:A:309:ALA:HA	1:A:323:HIS:ND1	2.27	0.49
1:B:428:GLU:O	1:B:431:VAL:HG12	2.13	0.49
1:C:590:ASP:HA	1:C:593:TYR:CD2	2.46	0.49
1:F:566:LYS:HD2	1:F:567:ILE:H	1.76	0.49
1:E:419:LEU:HD12	1:E:420:LEU:N	2.28	0.49
1:C:676:LEU:HD12	1:C:705:ILE:HG21	1.93	0.49
1:B:236:ALA:HA	1:B:239:VAL:HG12	1.94	0.49
1:F:635:PRO:O	1:F:638:ARG:HG2	2.12	0.49
1:F:508:ILE:C	1:F:509:LYS:HD3	2.32	0.49
1:B:236:ALA:O	1:B:239:VAL:HG12	2.12	0.49
1:B:303:ARG:HB2	1:B:353:GLN:HE21	1.77	0.49
1:F:517:VAL:HG13	1:F:665:ILE:HG21	1.93	0.49
1:C:428:GLU:O	1:C:431:VAL:HG12	2.12	0.49
1:F:296:GLY:H	1:F:297:GLU:CB	2.26	0.49
1:A:708:LYS:HD3	2:A:801:ATP:H5'2	1.93	0.49
1:C:256:ILE:HA	1:C:391:VAL:HG13	1.95	0.49
1:A:257:LEU:HG	1:A:389:LEU:HD12	1.94	0.49
1:F:612:VAL:HG13	1:F:614:ILE:O	2.13	0.49
1:F:224:ASP:O	1:F:228:SER:HB2	2.12	0.49
1:D:542:GLU:OE2	1:D:649:LYS:HD2	2.12	0.49
1:F:713:LEU:HD22	1:F:732:LEU:HD13	1.94	0.49
1:F:505:ASN:HB2	2:F:801:ATP:O2'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:678:GLU:O	1:F:682:LEU:HG	2.13	0.49
1:A:242:PRO:HD2	1:A:243:GLU:CD	2.33	0.49
1:F:330:ILE:HG12	1:F:373:THR:HG22	1.95	0.49
1:E:557:ALA:HB1	1:E:565:ILE:HG21	1.94	0.49
1:B:612:VAL:HG13	1:B:614:ILE:O	2.13	0.49
1:A:270:ALA:O	1:A:273:ILE:HG22	2.12	0.49
1:A:507:ILE:HG23	2:A:801:ATP:N6	2.28	0.49
1:E:583:GLN:HA	1:E:586:LYS:HG2	1.95	0.49
1:A:222:GLY:O	1:A:224:ASP:N	2.45	0.49
1:B:354:LEU:O	1:B:358:ILE:HG12	2.12	0.49
1:B:296:GLY:H	1:B:297:GLU:CB	2.25	0.49
1:F:635:PRO:HD2	1:F:638:ARG:HH11	1.77	0.49
1:D:686:PHE:CE1	1:D:714:ILE:HG23	2.48	0.49
1:F:270:ALA:O	1:F:273:ILE:HG22	2.12	0.49
1:F:354:LEU:O	1:F:358:ILE:HG12	2.12	0.48
1:C:707:ILE:O	1:C:711:LEU:HG	2.12	0.48
1:C:618:PHE:HE1	1:C:620:ASN:OD1	1.96	0.48
1:C:578:GLU:HB3	1:C:621:LEU:HB3	1.95	0.48
1:B:272:GLN:OE1	1:B:272:GLN:HA	2.13	0.48
1:E:348:ASP:O	1:E:351:VAL:HG22	2.13	0.48
1:C:256:ILE:HG22	1:C:391:VAL:HG11	1.94	0.48
1:F:347:HIS:O	1:F:350:VAL:HG13	2.14	0.48
1:B:270:ALA:O	1:B:273:ILE:HG22	2.12	0.48
1:D:557:ALA:O	1:D:560:SER:OG	2.20	0.48
1:C:694:ILE:O	1:C:698:VAL:HG22	2.14	0.48
1:D:527:GLN:HE22	1:E:716:MET:CA	2.26	0.48
1:D:536:LEU:HD21	1:D:630:LEU:O	2.14	0.48
1:D:686:PHE:HB3	1:D:690:GLU:HG3	1.95	0.48
1:E:652:LEU:HD21	1:E:661:PHE:CE1	2.46	0.48
1:D:353:GLN:OE1	1:E:288:PRO:HG2	2.14	0.48
1:A:609:LEU:O	1:A:610:ASP:HB3	2.14	0.48
1:E:717:SER:OG	1:E:729:PHE:HB2	2.13	0.48
1:F:552:LEU:O	1:F:556:ILE:HG13	2.12	0.48
1:C:285:VAL:HG13	1:C:326:ILE:HD11	1.95	0.48
1:A:540:LEU:HD13	1:A:605:ILE:HD12	1.95	0.48
1:C:254:LYS:O	1:C:368:LEU:HA	2.13	0.48
1:A:402:GLY:O	1:A:406:ILE:HD12	2.14	0.48
1:E:257:LEU:HB2	1:E:389:LEU:HD13	1.95	0.48
1:D:261:PRO:HD2	1:D:395:ILE:O	2.14	0.48
1:E:309:ALA:HB1	1:E:367:ILE:HG21	1.94	0.48
1:A:428:GLU:O	1:A:432:GLU:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:PRO:HA	1:C:491:ALA:CB	2.39	0.48
1:F:507:ILE:HG21	1:F:555:LYS:HZ1	1.78	0.48
1:D:486:ASN:O	1:D:490:PRO:HD3	2.14	0.48
1:B:626:LEU:O	1:B:630:LEU:HG	2.14	0.48
1:E:441:LEU:HD23	1:E:444:LEU:HD21	1.96	0.48
1:C:721:ASP:O	1:C:725:ARG:HG3	2.13	0.48
1:D:510:TRP:CE3	1:D:670:ILE:HG22	2.48	0.48
1:D:256:ILE:O	1:D:370:ILE:HA	2.14	0.48
1:E:516:ARG:O	1:E:519:ASP:OD1	2.31	0.48
1:D:609:LEU:O	1:D:610:ASP:OD1	2.32	0.48
1:B:388:ARG:O	1:B:389:LEU:HD23	2.12	0.48
1:A:437:SER:O	1:A:440:GLU:HG2	2.13	0.48
1:A:610:ASP:HA	1:F:624:GLN:NE2	2.29	0.48
1:E:656:GLU:HG2	1:F:648:ARG:HH22	1.79	0.48
1:C:221:GLY:HA3	1:C:406:ILE:HG13	1.96	0.48
1:A:509:LYS:HD3	1:A:509:LYS:N	2.28	0.48
1:F:715:GLU:O	1:F:719:GLN:HG2	2.13	0.48
1:E:270:ALA:O	1:E:273:ILE:HG22	2.14	0.48
1:B:268:LEU:HD12	1:B:269:LEU:N	2.29	0.48
1:C:297:GLU:O	1:C:301:ASN:N	2.39	0.48
1:B:298:SER:O	1:B:301:ASN:HB2	2.13	0.48
1:D:540:LEU:HB2	1:D:661:PHE:CD1	2.49	0.48
1:D:245:VAL:O	1:D:249:GLY:N	2.43	0.48
1:F:686:PHE:HE1	1:F:714:ILE:HG23	1.77	0.48
1:F:589:PHE:CD2	1:F:629:LEU:HD22	2.49	0.48
1:C:677:LEU:HD11	1:C:698:VAL:HG21	1.96	0.47
1:D:513:PRO:O	1:D:517:VAL:HG23	2.13	0.47
1:A:565:ILE:HA	1:A:599:CYS:O	2.13	0.47
1:A:313:GLN:OE1	1:A:317:GLY:HA2	2.14	0.47
1:B:589:PHE:HE1	1:B:600:VAL:HG11	1.79	0.47
1:B:695:ALA:HB1	1:B:699:LYS:HE3	1.95	0.47
1:F:242:PRO:HD2	1:F:243:GLU:H	1.79	0.47
1:E:648:ARG:NE	1:E:650:ASP:OD1	2.43	0.47
1:D:602:VAL:O	1:D:644:GLY:HA2	2.13	0.47
1:E:236:ALA:HB1	1:E:240:PHE:CZ	2.50	0.47
1:E:503:ILE:O	1:E:503:ILE:HD12	2.13	0.47
1:E:721:ASP:O	1:E:725:ARG:HG3	2.13	0.47
1:E:246:GLU:HG2	1:E:247:GLN:N	2.29	0.47
1:B:265:GLY:N	2:B:802:ATP:O3A	2.47	0.47
1:D:307:ALA:HA	1:D:310:GLU:OE1	2.14	0.47
1:C:653:GLN:HG3	1:C:658:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:GLU:HA	1:A:691:ARG:CZ	2.44	0.47
1:B:437:SER:O	1:B:440:GLU:HB2	2.14	0.47
1:F:528:THR:HG21	1:F:641:LEU:HB2	1.96	0.47
1:B:452:ALA:HA	1:B:455:ARG:NE	2.29	0.47
1:A:399:ASP:O	1:A:403:ARG:N	2.31	0.47
1:E:677:LEU:HA	1:E:680:LEU:HD12	1.95	0.47
1:B:452:ALA:O	1:B:455:ARG:HG3	2.15	0.47
1:A:419:LEU:O	1:A:419:LEU:HD13	2.15	0.47
1:B:281:GLU:N	1:B:282:PRO:HA	2.29	0.47
1:F:508:ILE:HG13	1:F:508:ILE:H	1.53	0.47
1:B:327:PHE:CE2	1:B:369:VAL:HG21	2.50	0.47
1:E:441:LEU:HA	1:E:444:LEU:HG	1.96	0.47
1:B:254:LYS:O	1:B:368:LEU:HA	2.14	0.47
1:C:518:LEU:HD21	1:C:552:LEU:HD22	1.97	0.47
1:C:533:ARG:C	1:D:505:ASN:HD21	2.17	0.47
1:A:531:SER:O	1:A:639:LYS:HE2	2.14	0.47
1:B:507:ILE:CG1	1:B:555:LYS:HD3	2.44	0.47
1:A:678:GLU:O	1:A:681:GLU:HG2	2.14	0.47
1:D:654:GLU:HB2	1:E:614:ILE:HD11	1.97	0.47
1:A:221:GLY:HA3	2:A:802:ATP:N6	2.29	0.47
1:F:228:SER:HA	1:F:231:PHE:CE2	2.49	0.47
1:A:720:MET:HG3	1:A:728:LYS:CD	2.45	0.47
1:F:524:LEU:O	1:F:528:THR:OG1	2.31	0.47
1:B:324:ILE:HG12	1:B:368:LEU:HD11	1.94	0.47
1:B:377:ASP:OD1	1:B:378:LEU:N	2.47	0.47
1:E:568:CYS:HB3	1:E:601:VAL:O	2.14	0.47
1:A:573:MET:HA	1:A:576:PHE:CD2	2.50	0.47
1:A:510:TRP:HE3	1:A:675:GLN:HB3	1.79	0.47
1:B:289:GLU:O	1:B:291:LEU:N	2.41	0.47
1:B:507:ILE:HG13	1:B:555:LYS:HD3	1.96	0.47
1:A:241:PRO:HA	1:A:242:PRO:HA	1.62	0.47
1:A:569:SER:HB3	1:A:571:ASP:OD1	2.14	0.47
1:B:614:ILE:O	1:B:616:PRO:HA	2.15	0.47
1:B:402:GLY:O	1:B:406:ILE:HD12	2.14	0.47
1:D:657:MET:HG2	1:D:661:PHE:HE2	1.80	0.47
1:D:548:GLY:N	2:D:801:ATP:O2B	2.47	0.47
1:A:510:TRP:CE3	1:A:670:ILE:HG12	2.49	0.47
1:D:318:ALA:O	1:D:319:ASN:ND2	2.48	0.47
1:E:546:HIS:HB3	1:E:708:LYS:HB3	1.95	0.47
1:E:438:GLY:O	1:E:441:LEU:N	2.44	0.47
1:B:440:GLU:O	1:B:444:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:GLY:HA3	1:F:586:LYS:CE	2.45	0.47
1:F:615:GLY:HA3	1:F:616:PRO:C	2.34	0.47
1:E:540:LEU:HD11	1:E:646:THR:CG2	2.44	0.46
1:E:627:LEU:HD13	1:F:607:ARG:NE	2.30	0.46
1:D:510:TRP:CB	1:D:679:ALA:HB2	2.44	0.46
1:A:550:THR:HG23	1:A:603:ASP:OD1	2.15	0.46
1:D:611:TYR:CE2	1:D:613:PRO:HA	2.51	0.46
1:A:567:ILE:HG13	1:A:601:VAL:HB	1.95	0.46
1:E:732:LEU:HD23	1:E:732:LEU:HA	1.62	0.46
1:B:707:ILE:O	1:B:711:LEU:HG	2.15	0.46
1:C:231:PHE:CE1	1:C:235:PHE:HD2	2.32	0.46
1:A:240:PHE:HA	1:A:241:PRO:HD3	1.54	0.46
1:F:428:GLU:O	1:F:431:VAL:HG12	2.15	0.46
1:B:524:LEU:HD21	1:B:663:THR:HG21	1.97	0.46
1:C:349:THR:O	1:C:352:ASN:HB3	2.15	0.46
1:B:299:GLU:HG3	1:B:349:THR:OG1	2.16	0.46
1:D:512:ASP:O	1:D:515:THR:OG1	2.26	0.46
1:E:586:LYS:HA	1:E:589:PHE:CD2	2.51	0.46
1:D:713:LEU:HD22	1:D:729:PHE:HD1	1.80	0.46
1:B:589:PHE:CE1	1:B:600:VAL:HG11	2.51	0.46
1:F:528:THR:OG1	1:F:641:LEU:HD12	2.15	0.46
1:D:694:ILE:O	1:D:698:VAL:HG22	2.15	0.46
1:B:715:GLU:O	1:B:719:GLN:HG2	2.16	0.46
1:D:240:PHE:HA	1:D:241:PRO:HD3	1.68	0.46
1:B:625:ALA:O	1:B:629:LEU:HG	2.16	0.46
1:B:576:PHE:HB3	1:B:580:ALA:HB3	1.97	0.46
1:F:281:GLU:N	1:F:282:PRO:HA	2.30	0.46
1:B:542:GLU:OE1	1:B:649:LYS:HD3	2.16	0.46
1:F:555:LYS:HG3	1:F:559:GLU:OE2	2.15	0.46
1:F:721:ASP:O	1:F:725:ARG:HG3	2.15	0.46
1:F:670:ILE:O	1:F:704:TRP:HA	2.15	0.46
1:E:569:SER:HA	1:E:570:PRO:HD3	1.82	0.46
1:E:437:SER:O	1:E:440:GLU:HB2	2.16	0.46
1:C:241:PRO:HA	1:C:242:PRO:HA	1.69	0.46
1:C:576:PHE:HB3	1:C:580:ALA:HB3	1.98	0.46
1:D:608:LEU:O	1:D:622:VAL:HG11	2.15	0.46
1:D:254:LYS:O	1:D:368:LEU:HA	2.16	0.46
1:C:380:ASP:OD1	1:C:382:ALA:N	2.40	0.46
1:F:375:ARG:HD3	1:F:376:PRO:N	2.31	0.46
1:E:669:ASN:OD1	1:E:706:GLY:HA2	2.15	0.46
1:F:315:ARG:NE	1:F:316:LEU:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:PRO:HD2	1:B:597:LEU:HB2	1.96	0.46
1:A:315:ARG:HG2	1:A:316:LEU:CD1	2.46	0.46
1:C:711:LEU:O	1:C:715:GLU:HG2	2.15	0.46
1:E:653:GLN:HB2	1:E:658:LEU:HD22	1.98	0.46
1:A:240:PHE:HD2	1:B:453:MET:SD	2.39	0.46
1:D:728:LYS:HE3	1:D:732:LEU:HD11	1.97	0.46
1:C:246:GLU:HG2	1:C:247:GLN:N	2.31	0.46
1:C:703:VAL:O	1:C:704:TRP:HD1	1.99	0.46
1:E:242:PRO:HD2	1:E:243:GLU:H	1.80	0.46
1:E:705:ILE:HD12	1:E:713:LEU:HD12	1.97	0.46
1:B:626:LEU:HA	1:B:626:LEU:HD23	1.59	0.46
1:D:690:GLU:O	1:D:694:ILE:HG13	2.17	0.45
1:D:511:GLY:HA3	1:D:675:GLN:HE21	1.80	0.45
1:D:512:ASP:N	1:D:513:PRO:CD	2.79	0.45
1:B:452:ALA:HA	1:B:455:ARG:CG	2.47	0.45
1:E:377:ASP:OD1	1:E:378:LEU:N	2.48	0.45
1:A:433:THR:HB	1:A:436:PHE:HD2	1.80	0.45
1:F:324:ILE:HG12	1:F:368:LEU:HD11	1.98	0.45
1:C:533:ARG:HB2	1:D:715:GLU:OE1	2.15	0.45
1:E:658:LEU:HD12	1:E:658:LEU:HA	1.71	0.45
1:A:713:LEU:HD23	1:A:713:LEU:HA	1.75	0.45
1:B:306:PHE:CZ	1:B:327:PHE:HZ	2.32	0.45
1:C:517:VAL:HG13	1:C:665:ILE:HG21	1.97	0.45
1:B:549:LYS:NZ	1:B:647:SER:HA	2.29	0.45
1:C:240:PHE:CD2	1:C:244:ILE:HG21	2.49	0.45
1:A:689:LYS:O	1:A:692:THR:HB	2.17	0.45
1:B:242:PRO:HD2	1:B:243:GLU:H	1.80	0.45
1:F:589:PHE:O	1:F:593:TYR:HD1	2.00	0.45
1:E:549:LYS:HG3	1:E:550:THR:N	2.32	0.45
1:D:626:LEU:O	1:D:630:LEU:HG	2.16	0.45
1:B:284:VAL:HG23	1:B:324:ILE:O	2.17	0.45
1:B:606:GLU:N	1:B:606:GLU:OE1	2.49	0.45
1:E:510:TRP:CE3	1:E:511:GLY:HA3	2.52	0.45
1:B:548:GLY:HA2	2:B:801:ATP:O1A	2.17	0.45
1:A:602:VAL:N	1:A:643:ILE:O	2.47	0.45
1:F:694:ILE:O	1:F:698:VAL:HG22	2.15	0.45
1:E:383:LEU:O	1:E:389:LEU:HB2	2.16	0.45
1:A:636:GLN:HA	1:A:637:GLY:HA2	1.51	0.45
1:D:281:GLU:N	1:D:282:PRO:HA	2.31	0.45
1:D:312:GLU:OE1	1:D:323:HIS:CG	2.70	0.45
1:B:385:ARG:HH21	2:C:802:ATP:PG	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:GLN:HA	1:F:719:GLN:CD	2.37	0.45
1:A:517:VAL:HG13	1:A:665:ILE:HG21	1.98	0.45
1:D:223:LEU:HG	1:D:226:GLU:HB3	1.98	0.45
1:F:673:GLY:O	1:F:676:LEU:HB3	2.15	0.45
1:E:245:VAL:O	1:E:249:GLY:N	2.48	0.45
1:A:676:LEU:CD1	1:A:710:LEU:HD11	2.47	0.45
1:F:240:PHE:HB3	1:F:244:ILE:HD13	1.98	0.45
1:F:323:HIS:HB3	1:F:367:ILE:HG22	1.97	0.45
1:B:690:GLU:O	1:B:694:ILE:HG13	2.16	0.45
1:E:714:ILE:O	1:E:718:LEU:HG	2.16	0.45
1:C:257:LEU:O	1:C:393:MET:N	2.42	0.45
1:B:310:GLU:OE2	1:B:357:LYS:NZ	2.47	0.45
1:C:227:PHE:HA	1:C:230:ILE:HG22	1.97	0.45
1:B:436:PHE:N	1:B:436:PHE:CD1	2.84	0.45
1:D:503:ILE:HG22	1:D:506:GLY:HA2	1.97	0.45
1:D:519:ASP:O	1:D:523:LEU:HG	2.17	0.45
1:D:670:ILE:HD11	1:D:705:ILE:CG2	2.43	0.45
1:E:519:ASP:OD1	1:E:520:ASP:N	2.49	0.45
1:E:325:ILE:O	1:E:369:VAL:HA	2.16	0.45
1:B:568:CYS:SG	1:B:588:ILE:HD12	2.57	0.45
1:D:286:ASN:HB2	1:D:327:PHE:HD1	1.82	0.45
1:C:612:VAL:CG2	1:C:613:PRO:HD2	2.47	0.45
1:D:669:ASN:HD21	1:D:706:GLY:CA	2.30	0.45
1:D:669:ASN:HD21	1:D:706:GLY:N	2.15	0.45
1:A:582:CYS:SG	1:A:621:LEU:HG	2.57	0.45
1:D:596:GLN:NE2	1:D:637:GLY:O	2.49	0.45
1:E:573:MET:HB3	1:E:581:LYS:HD3	1.97	0.45
1:C:506:GLY:N	2:C:801:ATP:O2'	2.50	0.45
1:D:530:ASN:ND2	1:E:719:GLN:OE1	2.50	0.45
1:F:604:ASP:HB3	1:F:607:ARG:HB2	1.99	0.44
1:A:527:GLN:O	1:A:531:SER:N	2.51	0.44
1:C:542:GLU:HG3	1:C:649:LYS:CE	2.47	0.44
1:F:711:LEU:HD11	2:F:801:ATP:H8	1.82	0.44
1:E:562:PHE:HB3	1:E:563:PRO:HD2	1.99	0.44
1:C:402:GLY:O	1:C:405:GLN:HB2	2.17	0.44
1:B:712:MET:O	1:B:716:MET:HG3	2.16	0.44
1:C:270:ALA:O	1:C:273:ILE:HG22	2.17	0.44
1:E:596:GLN:HA	1:E:638:ARG:HA	1.98	0.44
1:E:545:PRO:HG3	1:E:647:SER:OG	2.18	0.44
1:D:510:TRP:HE3	1:D:675:GLN:HG2	1.82	0.44
1:F:546:HIS:CD2	1:F:546:HIS:H	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:LYS:HD2	1:E:645:THR:HB	1.99	0.44
2:D:802:ATP:H2'	2:D:802:ATP:N3	2.32	0.44
1:E:595:SER:OG	1:E:597:LEU:O	2.24	0.44
1:A:607:ARG:HA	1:A:607:ARG:HD3	1.78	0.44
1:C:402:GLY:O	1:C:406:ILE:HD12	2.18	0.44
1:B:268:LEU:HD11	2:B:802:ATP:H2	1.82	0.44
1:F:365:ASN:O	1:F:366:ASN:CB	2.65	0.44
1:C:691:ARG:HB2	1:C:691:ARG:NH1	2.32	0.44
1:C:686:PHE:CE1	1:C:714:ILE:HG23	2.52	0.44
1:D:546:HIS:ND1	1:D:709:LYS:HD3	2.32	0.44
1:F:709:LYS:O	1:F:713:LEU:HG	2.17	0.44
1:E:502:TYR:CZ	1:E:567:ILE:HG21	2.53	0.44
1:A:617:ARG:NH1	1:A:617:ARG:HG3	2.30	0.44
1:D:518:LEU:O	1:D:522:GLU:HG2	2.17	0.44
1:A:407:LEU:CD1	1:A:426:ILE:HG23	2.48	0.44
1:F:513:PRO:O	1:F:517:VAL:HG23	2.17	0.44
1:A:607:ARG:HG2	1:F:628:VAL:HG22	1.99	0.44
1:B:541:LEU:O	1:B:541:LEU:HD12	2.17	0.44
1:C:385:ARG:HD2	1:D:263:GLY:HA3	1.97	0.44
1:B:240:PHE:HA	1:B:241:PRO:HD3	1.65	0.44
1:A:327:PHE:CE1	1:A:330:ILE:HG22	2.53	0.44
1:B:602:VAL:N	1:B:643:ILE:O	2.31	0.44
1:C:721:ASP:HB2	1:C:724:TYR:CD1	2.52	0.44
1:D:505:ASN:C	2:D:801:ATP:H8	2.21	0.44
1:D:715:GLU:O	1:D:719:GLN:HG2	2.18	0.44
2:C:802:ATP:N3	2:C:802:ATP:H2'	2.32	0.44
1:E:654:GLU:HG2	1:F:614:ILE:HD11	1.99	0.44
1:B:240:PHE:CD2	1:B:244:ILE:HG21	2.50	0.44
1:B:516:ARG:O	1:B:519:ASP:OD1	2.36	0.44
1:B:669:ASN:OD1	1:B:706:GLY:HA2	2.17	0.44
1:F:225:LYS:HG3	1:F:226:GLU:N	2.32	0.44
1:A:631:LYS:HB2	1:A:631:LYS:NZ	2.32	0.44
1:C:299:GLU:HG2	1:C:350:VAL:HG12	2.00	0.44
1:D:507:ILE:HG23	2:D:801:ATP:N6	2.33	0.44
1:C:230:ILE:HD11	1:C:256:ILE:HB	2.00	0.44
1:E:353:GLN:O	1:E:357:LYS:HG2	2.17	0.44
1:D:223:LEU:HD23	1:D:223:LEU:O	2.18	0.44
1:A:286:ASN:HB2	1:A:327:PHE:HB3	1.99	0.44
1:C:555:LYS:HA	1:C:558:GLU:OE1	2.18	0.44
1:F:597:LEU:HA	1:F:639:LYS:O	2.18	0.44
1:D:298:SER:O	1:D:301:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:602:VAL:HG12	1:F:605:ILE:HG12	1.99	0.44
1:D:388:ARG:O	1:D:389:LEU:HD23	2.17	0.44
1:B:241:PRO:HA	1:B:242:PRO:HA	1.72	0.44
1:F:261:PRO:HG3	1:F:397:LEU:HA	1.99	0.44
1:C:445:VAL:HG12	1:C:449:GLN:HE22	1.82	0.44
1:D:453:MET:O	1:D:457:ILE:HG13	2.18	0.44
1:C:539:VAL:HG23	1:C:663:THR:HG23	1.99	0.44
1:F:536:LEU:HD11	1:F:633:ALA:HA	1.99	0.44
1:E:540:LEU:HD12	1:E:644:GLY:O	2.17	0.44
1:C:324:ILE:HD12	1:C:324:ILE:N	2.33	0.44
1:F:600:VAL:HG23	1:F:642:ILE:HA	1.99	0.44
1:B:566:LYS:HB2	1:B:566:LYS:HE2	1.71	0.44
1:B:555:LYS:O	1:B:559:GLU:HG2	2.18	0.44
1:E:232:ARG:HH22	1:F:457:ILE:HB	1.83	0.44
1:A:632:LYS:HE3	1:A:633:ALA:O	2.18	0.44
1:A:223:LEU:CD1	1:A:227:PHE:HB2	2.47	0.44
1:D:231:PHE:O	1:D:235:PHE:HB2	2.18	0.44
1:F:579:THR:O	1:F:583:GLN:HG2	2.18	0.44
1:C:436:PHE:CD1	1:C:436:PHE:N	2.83	0.43
1:E:696:GLN:HA	1:E:696:GLN:OE1	2.18	0.43
1:C:627:LEU:HD23	1:C:627:LEU:HA	1.71	0.43
1:C:618:PHE:HZ	1:D:612:VAL:HG11	1.83	0.43
1:F:240:PHE:HA	1:F:241:PRO:HD3	1.73	0.43
1:A:322:LEU:O	1:A:323:HIS:HD2	2.01	0.43
1:C:542:GLU:HG3	1:C:649:LYS:HD3	2.00	0.43
1:F:441:LEU:O	1:F:445:VAL:HG23	2.18	0.43
1:A:242:PRO:HD2	1:A:243:GLU:OE1	2.17	0.43
1:E:257:LEU:HG	1:E:371:GLY:O	2.18	0.43
1:A:270:ALA:HA	1:A:273:ILE:HG22	1.99	0.43
1:C:347:HIS:O	1:C:350:VAL:HG22	2.19	0.43
1:C:555:LYS:O	1:C:559:GLU:HG2	2.18	0.43
1:E:218:MET:HA	1:E:219:GLY:HA2	1.73	0.43
1:C:730:LEU:HD23	1:C:730:LEU:HA	1.82	0.43
1:D:331:ASP:O	1:D:332:ALA:HB3	2.18	0.43
1:B:627:LEU:HD21	1:B:657:MET:HG3	2.00	0.43
1:E:676:LEU:HD13	1:E:703:VAL:HG11	2.00	0.43
1:C:218:MET:HA	1:C:219:GLY:HA2	1.87	0.43
1:B:348:ASP:O	1:B:352:ASN:ND2	2.51	0.43
1:B:300:ALA:O	1:B:303:ARG:HB3	2.18	0.43
1:B:242:PRO:O	1:B:245:VAL:HG22	2.17	0.43
1:A:618:PHE:CZ	1:B:612:VAL:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:TYR:HA	1:A:618:PHE:HB3	2.00	0.43
1:B:611:TYR:CZ	1:B:613:PRO:HA	2.54	0.43
1:B:438:GLY:O	1:B:441:LEU:N	2.48	0.43
1:E:406:ILE:O	1:E:409:ILE:HG22	2.18	0.43
1:B:530:ASN:HD22	1:B:530:ASN:HA	1.64	0.43
1:C:375:ARG:HA	1:C:376:PRO:HD2	1.86	0.43
1:F:605:ILE:N	1:F:606:GLU:OE1	2.51	0.43
1:C:627:LEU:HD12	1:D:607:ARG:NH1	2.27	0.43
1:E:235:PHE:CZ	1:E:273:ILE:HG12	2.51	0.43
1:D:241:PRO:HA	1:D:242:PRO:HA	1.77	0.43
1:A:508:ILE:HB	1:A:682:LEU:HD22	2.01	0.43
1:A:355:LEU:HA	1:A:358:ILE:HD11	1.99	0.43
1:E:358:ILE:HG13	1:E:388:ARG:HD3	2.00	0.43
1:C:325:ILE:HD12	1:C:327:PHE:HE2	1.83	0.43
1:B:517:VAL:HG21	1:B:667:VAL:HG22	2.00	0.43
1:C:423:ASP:OD1	1:C:423:ASP:N	2.51	0.43
1:E:232:ARG:NH2	1:F:454:ASN:O	2.52	0.43
1:C:638:ARG:NH1	1:C:638:ARG:HG3	2.31	0.43
1:C:518:LEU:HD23	1:C:518:LEU:HA	1.83	0.43
1:E:270:ALA:HA	1:E:273:ILE:HG22	2.01	0.43
1:A:687:LYS:HB2	1:A:690:GLU:HG3	1.99	0.43
1:F:525:VAL:HG11	1:F:560:SER:CB	2.48	0.43
1:D:677:LEU:O	1:D:691:ARG:NH2	2.51	0.43
1:F:570:PRO:HG2	1:F:604:ASP:CB	2.44	0.43
1:A:285:VAL:HG13	1:A:326:ILE:CD1	2.46	0.43
1:B:627:LEU:HB3	1:C:607:ARG:NH2	2.34	0.43
1:D:441:LEU:HD12	1:D:441:LEU:HA	1.90	0.43
1:F:499:TYR:CD1	1:F:558:GLU:HG2	2.53	0.43
1:E:428:GLU:O	1:E:431:VAL:HG12	2.18	0.43
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.80	0.43
1:F:541:LEU:HD23	1:F:549:LYS:HB2	2.01	0.43
1:A:627:LEU:HD13	1:B:607:ARG:NH1	2.32	0.43
1:A:380:ASP:OD1	1:A:381:GLU:N	2.50	0.43
1:E:522:GLU:HA	1:E:525:VAL:HG22	2.01	0.43
1:E:592:ALA:HB1	1:E:640:LEU:HD22	2.00	0.43
1:A:678:GLU:HA	1:A:681:GLU:HG2	2.00	0.43
1:E:711:LEU:HD11	2:E:801:ATP:C1'	2.48	0.43
1:A:236:ALA:HB1	1:B:453:MET:CB	2.49	0.43
1:A:544:PRO:HB2	1:A:669:ASN:HD21	1.84	0.43
1:C:683:LEU:HD11	1:C:711:LEU:HD22	2.01	0.43
1:C:686:PHE:HE1	1:C:714:ILE:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LEU:HG	1:B:371:GLY:O	2.19	0.43
1:C:673:GLY:O	1:C:676:LEU:HB3	2.19	0.43
1:A:221:GLY:O	1:A:223:LEU:HG	2.18	0.43
1:F:589:PHE:HD2	1:F:629:LEU:HD13	1.83	0.43
1:B:694:ILE:O	1:B:698:VAL:HG22	2.19	0.43
1:A:357:LYS:HE3	1:A:357:LYS:HA	2.00	0.43
1:C:284:VAL:O	1:C:326:ILE:HG13	2.19	0.43
1:C:385:ARG:NH1	1:C:388:ARG:HH12	2.17	0.43
1:E:635:PRO:HG2	1:E:638:ARG:HH22	1.84	0.42
1:D:609:LEU:CD1	1:D:611:TYR:HB2	2.49	0.42
1:A:449:GLN:HG2	1:A:449:GLN:H	1.66	0.42
1:B:612:VAL:HG12	1:B:617:ARG:O	2.19	0.42
1:B:439:ALA:HA	2:B:802:ATP:H1'	2.01	0.42
1:E:722:PRO:HA	1:E:725:ARG:HD2	2.00	0.42
1:B:259:TYR:CD2	1:B:376:PRO:HD3	2.54	0.42
1:D:413:ARG:HH12	1:D:417:HIS:CE1	2.36	0.42
1:C:626:LEU:HA	1:C:626:LEU:HD23	1.80	0.42
1:A:670:ILE:HG23	1:A:675:GLN:HB2	2.01	0.42
1:B:720:MET:HG3	1:B:728:LYS:CG	2.45	0.42
1:C:611:TYR:CZ	1:C:651:VAL:HG11	2.54	0.42
1:D:263:GLY:O	1:D:437:SER:HB3	2.18	0.42
1:F:499:TYR:HB3	1:F:558:GLU:OE1	2.19	0.42
1:D:632:LYS:HZ3	1:E:571:ASP:HB3	1.84	0.42
1:C:671:ALA:HA	1:C:703:VAL:O	2.19	0.42
1:C:233:ARG:HB2	1:C:233:ARG:CZ	2.49	0.42
1:E:540:LEU:HD12	1:E:541:LEU:H	1.84	0.42
1:A:388:ARG:O	1:A:389:LEU:HD22	2.19	0.42
1:E:232:ARG:HH22	1:F:457:ILE:H	1.66	0.42
1:D:406:ILE:HB	1:D:441:LEU:HD23	2.01	0.42
1:C:236:ALA:HB1	1:D:453:MET:HB3	2.01	0.42
1:F:658:LEU:HA	1:F:661:PHE:CD2	2.50	0.42
1:E:620:ASN:O	1:E:624:GLN:HG2	2.18	0.42
1:B:303:ARG:CG	1:B:357:LYS:HE2	2.40	0.42
1:D:236:ALA:HB1	1:E:453:MET:HB2	2.02	0.42
1:E:507:ILE:CG1	1:E:555:LYS:HD3	2.49	0.42
1:E:643:ILE:N	1:E:643:ILE:HD12	2.34	0.42
1:D:258:LEU:O	1:D:258:LEU:HD12	2.19	0.42
1:B:728:LYS:HA	1:B:728:LYS:HD3	1.82	0.42
1:E:677:LEU:HD11	1:E:695:ALA:HA	2.01	0.42
1:A:258:LEU:HD12	1:A:258:LEU:O	2.19	0.42
1:E:351:VAL:HG23	1:E:352:ASN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:THR:OG1	1:C:537:VAL:HG21	2.19	0.42
1:D:300:ALA:O	1:D:304:LYS:HG3	2.20	0.42
1:A:267:THR:HG23	1:A:326:ILE:HD13	2.01	0.42
1:E:300:ALA:O	1:E:303:ARG:HB3	2.20	0.42
1:B:718:LEU:HD12	1:B:718:LEU:HA	1.84	0.42
1:E:445:VAL:O	1:E:449:GLN:HG2	2.19	0.42
1:B:249:GLY:HA3	1:C:413:ARG:NH1	2.35	0.42
1:C:536:LEU:HD12	1:C:640:LEU:HB3	2.02	0.42
1:C:525:VAL:HG11	1:C:560:SER:HA	2.01	0.42
1:E:436:PHE:CD1	1:E:436:PHE:N	2.86	0.42
1:F:542:GLU:HB2	1:F:666:HIS:HA	2.02	0.42
1:F:525:VAL:HG11	1:F:560:SER:HB2	2.00	0.42
1:F:227:PHE:HA	1:F:230:ILE:HG22	2.02	0.42
1:D:307:ALA:HA	1:D:310:GLU:CD	2.39	0.42
1:E:241:PRO:HA	1:E:242:PRO:HA	1.65	0.42
1:B:601:VAL:HG22	1:B:643:ILE:HB	2.02	0.42
1:B:322:LEU:HA	1:B:366:ASN:O	2.19	0.42
1:A:322:LEU:HD13	1:A:366:ASN:O	2.20	0.42
1:C:705:ILE:HD13	1:C:710:LEU:HD13	2.02	0.42
1:E:664:THR:O	1:E:665:ILE:HD13	2.20	0.42
1:B:266:LYS:O	1:B:269:LEU:HB3	2.19	0.42
1:A:262:PRO:HA	1:A:263:GLY:HA2	1.70	0.42
1:A:219:GLY:O	1:A:272:GLN:HG2	2.19	0.42
1:D:730:LEU:HB3	1:D:734:ARG:NH1	2.35	0.42
1:B:590:ASP:HA	1:B:593:TYR:CD2	2.55	0.42
1:F:375:ARG:HD3	1:F:376:PRO:CD	2.50	0.42
1:E:232:ARG:HH22	1:F:457:ILE:CA	2.33	0.42
1:E:654:GLU:CG	1:F:614:ILE:HD11	2.50	0.42
1:D:384:LEU:HD12	1:D:385:ARG:N	2.35	0.42
1:D:518:LEU:HD21	1:D:552:LEU:HD13	2.02	0.42
1:A:377:ASP:OD2	1:A:378:LEU:HD23	2.19	0.42
1:F:319:ASN:HB2	1:F:320:SER:HB2	2.00	0.42
1:A:550:THR:OG1	2:A:801:ATP:O1G	2.33	0.42
1:E:263:GLY:H	2:E:802:ATP:PG	2.43	0.42
1:D:540:LEU:HD12	1:D:661:PHE:CE1	2.55	0.42
1:C:686:PHE:HB3	1:C:690:GLU:OE2	2.18	0.42
1:C:730:LEU:O	1:C:734:ARG:HG3	2.19	0.42
1:B:385:ARG:CZ	1:C:263:GLY:HA2	2.50	0.42
1:C:320:SER:O	1:C:320:SER:OG	2.34	0.42
1:A:624:GLN:HG3	1:B:610:ASP:CG	2.40	0.42
1:D:307:ALA:HA	1:D:310:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:ASN:HA	1:F:320:SER:HA	1.90	0.42
1:A:283:LYS:HA	1:A:324:ILE:O	2.20	0.42
1:E:624:GLN:HG3	1:F:610:ASP:OD2	2.20	0.41
1:E:641:LEU:HD12	1:E:641:LEU:O	2.20	0.41
1:D:609:LEU:HD12	1:D:611:TYR:H	1.85	0.41
1:A:560:SER:O	1:A:561:ASN:OD1	2.38	0.41
1:F:326:ILE:HG22	1:F:370:ILE:HG13	2.01	0.41
1:D:527:GLN:NE2	1:E:715:GLU:O	2.51	0.41
1:E:674:GLU:HA	1:E:677:LEU:HD12	2.02	0.41
1:A:513:PRO:O	1:A:516:ARG:HB3	2.19	0.41
1:A:492:PHE:HA	1:A:493:GLY:HA2	1.82	0.41
1:A:526:GLN:NE2	1:A:530:ASN:HD22	2.18	0.41
1:B:611:TYR:OH	1:B:613:PRO:HA	2.19	0.41
1:E:284:VAL:HG23	1:E:324:ILE:O	2.20	0.41
1:F:577:SER:O	1:F:581:LYS:HG3	2.20	0.41
1:D:544:PRO:O	1:D:547:SER:HB3	2.19	0.41
1:F:516:ARG:HB3	1:F:516:ARG:NH1	2.35	0.41
1:D:566:LYS:HD3	1:D:566:LYS:HA	1.83	0.41
1:B:526:GLN:HG3	1:C:719:GLN:OE1	2.20	0.41
1:D:624:GLN:OE1	1:D:624:GLN:HA	2.19	0.41
1:E:528:THR:HG21	1:E:641:LEU:HD22	2.01	0.41
1:F:690:GLU:O	1:F:694:ILE:HG13	2.20	0.41
1:E:708:LYS:HA	2:E:801:ATP:H4'	2.02	0.41
1:E:706:GLY:O	1:E:710:LEU:N	2.51	0.41
1:E:713:LEU:HD23	1:E:713:LEU:HA	1.77	0.41
1:D:720:MET:HB3	1:D:724:TYR:CE1	2.55	0.41
1:D:562:PHE:CD2	1:D:597:LEU:HG	2.55	0.41
1:B:402:GLY:O	1:B:405:GLN:HB2	2.19	0.41
1:B:693:THR:O	1:B:697:GLN:HG2	2.19	0.41
1:F:304:LYS:HA	1:F:304:LYS:HD2	1.90	0.41
1:E:230:ILE:HD12	1:E:230:ILE:HA	1.85	0.41
1:C:627:LEU:HD21	1:C:657:MET:SD	2.60	0.41
1:F:557:ALA:HB1	1:F:565:ILE:HG21	2.02	0.41
1:C:319:ASN:HA	1:C:320:SER:HA	1.85	0.41
1:C:385:ARG:HH11	1:C:388:ARG:HH22	1.68	0.41
1:D:257:LEU:HG	1:D:371:GLY:O	2.20	0.41
1:E:630:LEU:HD22	1:E:660:ALA:CB	2.50	0.41
1:F:502:TYR:HD2	1:F:503:ILE:HG13	1.85	0.41
1:B:386:PRO:HB2	1:C:440:GLU:HA	2.02	0.41
1:E:697:GLN:HG3	1:E:730:LEU:CD1	2.51	0.41
1:E:512:ASP:N	1:E:513:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:LEU:O	1:D:556:ILE:HG13	2.20	0.41
1:B:437:SER:OG	1:B:440:GLU:HG2	2.20	0.41
1:D:231:PHE:CD1	1:D:235:PHE:HD2	2.39	0.41
1:C:272:GLN:HA	1:C:272:GLN:OE1	2.20	0.41
1:B:218:MET:HA	1:B:219:GLY:HA2	1.78	0.41
1:A:551:ALA:HB1	2:A:801:ATP:H3'	2.02	0.41
1:E:607:ARG:HD3	1:E:607:ARG:HA	1.75	0.41
1:A:256:ILE:CG1	1:A:370:ILE:HG22	2.48	0.41
1:A:299:GLU:CD	1:A:303:ARG:HE	2.23	0.41
1:A:502:TYR:N	1:A:502:TYR:CD1	2.88	0.41
1:F:379:ILE:HD12	1:F:379:ILE:H	1.85	0.41
1:F:406:ILE:CB	1:F:441:LEU:HD22	2.49	0.41
1:D:268:LEU:O	1:D:271:ARG:HG2	2.21	0.41
1:E:713:LEU:CD2	1:E:732:LEU:HD13	2.51	0.41
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.76	0.41
1:D:626:LEU:HD23	1:D:626:LEU:HA	1.76	0.41
1:B:607:ARG:HA	1:B:607:ARG:HD3	1.77	0.41
1:F:503:ILE:HD11	1:F:551:ALA:O	2.20	0.41
1:C:334:CYS:HA	1:C:351:VAL:HG22	2.01	0.41
1:B:562:PHE:HD2	1:B:599:CYS:HB2	1.86	0.41
1:A:614:ILE:HG23	1:A:614:ILE:O	2.21	0.41
1:F:635:PRO:HB2	1:F:638:ARG:NH1	2.36	0.41
1:D:312:GLU:CG	1:D:313:GLN:H	2.34	0.41
1:F:553:ALA:HB1	1:F:643:ILE:HG21	2.01	0.41
1:D:236:ALA:HA	1:D:239:VAL:HG12	2.02	0.41
1:A:566:LYS:HA	1:A:566:LYS:HD3	1.77	0.41
1:A:428:GLU:O	1:A:431:VAL:HG12	2.21	0.41
1:B:268:LEU:CD1	2:B:802:ATP:H2	2.34	0.41
1:D:231:PHE:HA	1:D:235:PHE:CD2	2.56	0.41
1:C:560:SER:HB2	1:C:562:PHE:CE1	2.54	0.41
1:E:612:VAL:CG2	1:E:613:PRO:HD2	2.51	0.41
1:C:709:LYS:HE2	1:C:713:LEU:HD21	2.02	0.41
1:F:677:LEU:O	1:F:681:GLU:HG3	2.21	0.41
1:D:386:PRO:O	1:E:439:ALA:HB1	2.21	0.41
1:B:717:SER:O	1:B:725:ARG:HG2	2.20	0.41
1:D:242:PRO:O	1:D:245:VAL:HG12	2.20	0.41
1:D:531:SER:OG	1:D:534:THR:OG1	2.26	0.41
1:B:623:LEU:O	1:B:627:LEU:HG	2.20	0.41
1:C:407:LEU:HD13	1:C:426:ILE:HG22	2.03	0.41
1:A:240:PHE:CD2	1:B:453:MET:SD	3.14	0.41
1:B:265:GLY:O	1:B:268:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:HIS:HB3	1:A:708:LYS:HB3	2.02	0.41
1:E:726:VAL:O	1:E:730:LEU:HG	2.21	0.41
1:E:670:ILE:HG22	1:E:672:THR:N	2.33	0.41
1:D:242:PRO:HD2	1:D:243:GLU:H	1.85	0.41
1:E:680:LEU:HB3	1:E:686:PHE:HZ	1.84	0.41
1:A:235:PHE:HE1	1:A:277:LEU:CB	2.34	0.41
1:D:325:ILE:O	1:D:369:VAL:HA	2.21	0.41
1:E:666:HIS:ND1	1:E:668:PRO:HD3	2.35	0.41
1:E:497:GLU:N	1:E:497:GLU:OE1	2.54	0.41
1:C:295:VAL:O	1:D:294:TYR:HB2	2.20	0.41
1:A:551:ALA:CB	2:A:801:ATP:H3'	2.51	0.41
1:D:386:PRO:HB2	1:E:439:ALA:O	2.20	0.41
1:E:605:ILE:HA	1:E:608:LEU:HB3	2.01	0.41
1:D:687:LYS:O	1:D:690:GLU:HG2	2.21	0.41
1:D:711:LEU:O	1:D:715:GLU:HG2	2.21	0.41
1:C:616:PRO:CG	1:D:614:ILE:HD13	2.44	0.41
1:D:319:ASN:HA	1:D:320:SER:HA	1.88	0.41
1:A:358:ILE:HD12	1:A:359:ASP:N	2.35	0.41
1:D:271:ARG:HG2	1:D:272:GLN:N	2.36	0.41
1:B:256:ILE:O	1:B:370:ILE:HA	2.21	0.41
1:B:302:ILE:O	1:B:306:PHE:HD2	2.04	0.41
1:F:228:SER:HB3	1:F:232:ARG:HH21	1.85	0.41
1:D:570:PRO:HG3	1:D:608:LEU:HD21	2.02	0.41
1:C:236:ALA:HB1	1:D:453:MET:CB	2.51	0.41
1:A:261:PRO:HD2	1:A:395:ILE:O	2.21	0.41
1:F:218:MET:HA	1:F:219:GLY:HA2	1.75	0.41
1:C:534:THR:HA	1:C:535:PRO:HD2	1.86	0.41
1:C:690:GLU:HB2	1:C:726:VAL:CG2	2.48	0.41
1:E:540:LEU:HD22	1:E:661:PHE:CE1	2.56	0.41
1:A:299:GLU:HG2	1:A:353:GLN:HG2	2.03	0.41
1:F:236:ALA:HA	1:F:239:VAL:CG1	2.47	0.41
1:C:240:PHE:HA	1:C:241:PRO:HD3	1.76	0.41
1:A:706:GLY:O	1:A:709:LYS:HB3	2.21	0.41
1:E:612:VAL:HG22	1:E:613:PRO:HD2	2.02	0.41
1:C:409:ILE:HG23	1:C:410:HIS:ND1	2.36	0.41
1:B:534:THR:HA	1:B:535:PRO:HD3	1.81	0.41
1:C:267:THR:OG1	2:C:802:ATP:H5'1	2.22	0.40
1:F:728:LYS:HE3	1:F:732:LEU:HD21	2.03	0.40
1:E:705:ILE:CD1	1:E:713:LEU:HD12	2.51	0.40
1:E:685:ASN:HB3	1:E:718:LEU:HD11	2.02	0.40
1:A:685:ASN:N	1:A:685:ASN:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:ALA:HA	2:E:802:ATP:H1'	2.03	0.40
1:D:312:GLU:HG2	1:D:313:GLN:H	1.86	0.40
1:C:683:LEU:CD1	1:C:711:LEU:HD22	2.51	0.40
1:A:322:LEU:HD12	1:A:323:HIS:N	2.36	0.40
1:E:708:LYS:HA	1:E:711:LEU:HD12	2.02	0.40
1:D:514:VAL:O	1:D:518:LEU:HG	2.22	0.40
1:B:576:PHE:N	1:B:576:PHE:CD1	2.90	0.40
1:C:359:ASP:O	1:D:267:THR:HG21	2.21	0.40
1:A:507:ILE:HG23	2:A:801:ATP:C6	2.56	0.40
1:A:546:HIS:HA	1:A:708:LYS:HB3	2.02	0.40
1:B:527:GLN:HB2	1:C:719:GLN:HG3	2.03	0.40
1:E:540:LEU:HD12	1:E:541:LEU:N	2.35	0.40
1:E:627:LEU:HG	1:E:657:MET:HE1	2.02	0.40
1:B:445:VAL:O	1:B:449:GLN:HG2	2.21	0.40
1:B:615:GLY:HA3	1:B:616:PRO:HA	1.86	0.40
1:A:417:HIS:HB3	1:A:419:LEU:HD12	2.02	0.40
1:A:262:PRO:HG2	1:A:374:ASN:OD1	2.21	0.40
1:E:606:GLU:OE2	1:E:647:SER:N	2.55	0.40
1:C:615:GLY:N	1:C:616:PRO:HA	2.35	0.40
1:D:348:ASP:O	1:D:351:VAL:HG22	2.21	0.40
1:F:618:PHE:HE1	1:F:620:ASN:HA	1.86	0.40
1:D:560:SER:HB2	1:D:562:PHE:CD1	2.56	0.40
1:B:539:VAL:HA	1:B:663:THR:O	2.22	0.40
1:E:611:TYR:CE1	1:E:616:PRO:HB2	2.57	0.40
1:B:307:ALA:O	1:B:310:GLU:HG2	2.22	0.40
1:F:359:ASP:CB	1:F:388:ARG:HD2	2.52	0.40
1:D:511:GLY:HA3	1:D:675:GLN:NE2	2.37	0.40
1:B:724:TYR:O	1:B:728:LYS:HB2	2.20	0.40
1:A:299:GLU:CD	1:A:303:ARG:HH21	2.25	0.40
1:A:442:GLU:HA	1:A:445:VAL:HG23	2.03	0.40
1:B:721:ASP:O	1:B:725:ARG:HG3	2.21	0.40
1:B:221:GLY:HA3	1:B:406:ILE:HG13	2.03	0.40
1:E:573:MET:O	1:E:576:PHE:HB2	2.22	0.40
1:D:499:TYR:N	1:D:499:TYR:CD1	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/747 (65%)	452 (93%)	20 (4%)	12 (2%)	7	48
1	B	478/747 (64%)	436 (91%)	31 (6%)	11 (2%)	8	50
1	C	482/747 (64%)	454 (94%)	19 (4%)	9 (2%)	10	54
1	D	479/747 (64%)	448 (94%)	25 (5%)	6 (1%)	15	60
1	E	474/747 (64%)	443 (94%)	21 (4%)	10 (2%)	9	52
1	F	460/747 (62%)	425 (92%)	26 (6%)	9 (2%)	9	53
All	All	2857/4482 (64%)	2658 (93%)	142 (5%)	57 (2%)	14	53

All (57) 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	A	498	ASP
1	A	504	MET
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	497	GLU
1	C	498	ASP
1	C	578	GLU
1	D	283	LYS
1	D	318	ALA

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Mol	Chain	Res	Type
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	439	ALA
1	C	293	LYS
1	E	507	ILE
1	A	242	PRO
1	A	264	CYS
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	241	PRO
1	D	500	ALA
1	A	668	PRO
1	B	438	GLY
1	B	490	PRO
1	D	241	PRO
1	B	546	HIS
1	E	490	PRO
1	C	490	PRO
1	E	438	GLY
1	F	438	GLY
1	F	668	PRO
1	F	684	GLY

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	348/638 (54%)	344 (99%)	4 (1%)	80	91
1	B	356/638 (56%)	353 (99%)	3 (1%)	86	93
1	C	353/638 (55%)	351 (99%)	2 (1%)	90	95
1	D	348/638 (54%)	347 (100%)	1 (0%)	94	97
1	E	350/638 (55%)	349 (100%)	1 (0%)	94	97
1	F	339/638 (53%)	334 (98%)	5 (2%)	72	89
All	All	2094/3828 (55%)	2078 (99%)	16 (1%)	87	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	LEU
1	A	322	LEU
1	A	367	ILE
1	A	419	LEU
1	B	305	LEU
1	B	322	LEU
1	B	456	HIS
1	C	305	LEU
1	C	676	LEU
1	D	305	LEU
1	E	305	LEU
1	F	305	LEU
1	F	322	LEU
1	F	365	ASN
1	F	528	THR
1	F	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	A	353	GLN
1	A	530	ASN
1	B	352	ASN
1	B	526	GLN

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Mol	Chain	Res	Type
1	B	561	ASN
1	C	319	ASN
1	D	272	GLN
1	D	319	ASN
1	D	352	ASN
1	D	527	GLN
1	D	596	GLN
1	D	675	GLN
1	E	505	ASN
1	E	527	GLN
1	F	526	GLN
1	F	546	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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	ATP	A	801	-	26,33,33	1.12	2 (7%)	26,52,52	1.80	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	802	-	26,33,33	0.94	1 (3%)	26,52,52	1.67	1 (3%)
2	ATP	B	801	-	26,33,33	1.00	1 (3%)	26,52,52	1.91	2 (7%)
2	ATP	B	802	-	26,33,33	0.99	1 (3%)	26,52,52	1.40	2 (7%)
2	ATP	C	801	-	26,33,33	0.93	1 (3%)	26,52,52	1.85	4 (15%)
2	ATP	C	802	-	26,33,33	1.06	1 (3%)	26,52,52	1.71	2 (7%)
2	ATP	D	801	-	26,33,33	0.94	1 (3%)	26,52,52	1.41	2 (7%)
2	ATP	D	802	-	26,33,33	1.02	1 (3%)	26,52,52	2.34	5 (19%)
2	ATP	E	801	-	26,33,33	1.02	2 (7%)	26,52,52	2.67	4 (15%)
2	ATP	E	802	-	26,33,33	1.00	1 (3%)	26,52,52	1.69	1 (3%)
2	ATP	F	801	-	26,33,33	1.01	1 (3%)	26,52,52	1.71	4 (15%)

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	ATP	A	801	-	-	0/18/38/38	0/3/3/3
2	ATP	A	802	-	-	0/18/38/38	0/3/3/3
2	ATP	B	801	-	-	0/18/38/38	0/3/3/3
2	ATP	B	802	-	-	0/18/38/38	0/3/3/3
2	ATP	C	801	-	-	0/18/38/38	0/3/3/3
2	ATP	C	802	-	-	0/18/38/38	0/3/3/3
2	ATP	D	801	-	-	0/18/38/38	0/3/3/3
2	ATP	D	802	-	-	0/18/38/38	0/3/3/3
2	ATP	E	801	-	-	0/18/38/38	0/3/3/3
2	ATP	E	802	-	-	0/18/38/38	0/3/3/3
2	ATP	F	801	-	-	0/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ATP	O2'-C2'	2.31	1.48	1.43
2	E	801	ATP	O4'-C1'	2.33	1.44	1.41
2	C	801	ATP	C5-C4	2.79	1.46	1.40
2	D	801	ATP	C5-C4	2.97	1.47	1.40
2	A	802	ATP	C5-C4	2.99	1.47	1.40
2	F	801	ATP	C5-C4	3.06	1.47	1.40
2	D	802	ATP	C5-C4	3.13	1.47	1.40
2	E	801	ATP	C5-C4	3.23	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ATP	C5-C4	3.27	1.47	1.40
2	E	802	ATP	C5-C4	3.28	1.47	1.40
2	A	801	ATP	C5-C4	3.30	1.48	1.40
2	C	802	ATP	C5-C4	3.60	1.48	1.40
2	B	802	ATP	C5-C4	3.62	1.48	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	801	ATP	N3-C2-N1	-10.51	120.62	128.87
2	D	802	ATP	N3-C2-N1	-9.44	121.46	128.87
2	B	801	ATP	N3-C2-N1	-7.30	123.14	128.87
2	C	801	ATP	N3-C2-N1	-6.95	123.41	128.87
2	A	802	ATP	N3-C2-N1	-6.71	123.60	128.87
2	E	802	ATP	N3-C2-N1	-6.70	123.61	128.87
2	A	801	ATP	N3-C2-N1	-6.60	123.69	128.87
2	C	802	ATP	N3-C2-N1	-6.14	124.05	128.87
2	F	801	ATP	N3-C2-N1	-6.06	124.11	128.87
2	D	801	ATP	N3-C2-N1	-5.06	124.89	128.87
2	E	801	ATP	C1'-N9-C4	-4.55	121.73	126.81
2	B	802	ATP	N3-C2-N1	-4.41	125.40	128.87
2	D	802	ATP	C1'-N9-C4	-3.70	122.67	126.81
2	B	801	ATP	C1'-N9-C4	-3.65	122.73	126.81
2	E	801	ATP	N6-C6-N1	-3.40	112.82	118.52
2	C	801	ATP	C2'-C1'-N9	-3.19	104.92	113.47
2	F	801	ATP	C4'-O4'-C1'	-2.36	107.14	109.64
2	C	801	ATP	C1'-N9-C4	-2.26	124.28	126.81
2	D	801	ATP	C1'-N9-C4	-2.10	124.46	126.81
2	D	802	ATP	O4'-C1'-N9	-2.09	104.15	108.11
2	D	802	ATP	O3G-PG-O2G	2.01	114.83	107.44
2	C	801	ATP	O3G-PG-O2G	2.07	115.04	107.44
2	A	801	ATP	O3G-PG-O2G	2.08	115.07	107.44
2	A	801	ATP	C1'-N9-C4	2.10	129.15	126.81
2	B	802	ATP	C4'-O4'-C1'	2.19	111.96	109.64
2	F	801	ATP	N6-C6-N1	2.28	122.33	118.52
2	F	801	ATP	C1'-N9-C4	2.44	129.53	126.81
2	D	802	ATP	C2-N1-C6	2.45	123.14	118.77
2	A	801	ATP	C2'-C3'-C4'	2.64	108.04	102.64
2	E	801	ATP	C2-N1-C6	2.83	123.83	118.77
2	C	802	ATP	C4'-O4'-C1'	3.26	113.10	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ATP	8	0
2	A	802	ATP	3	0
2	B	801	ATP	7	0
2	B	802	ATP	4	0
2	C	801	ATP	1	0
2	C	802	ATP	8	0
2	D	801	ATP	13	0
2	D	802	ATP	5	0
2	E	801	ATP	5	0
2	E	802	ATP	4	0
2	F	801	ATP	5	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.