



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:21 AM GMT

PDB ID : 3LRB  
Title : Structure of E. coli AdiC  
Authors : Gao, X.; Lu, F.; Zhou, L.; Shi, Y.  
Deposited on : 2010-02-10  
Resolution : 3.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

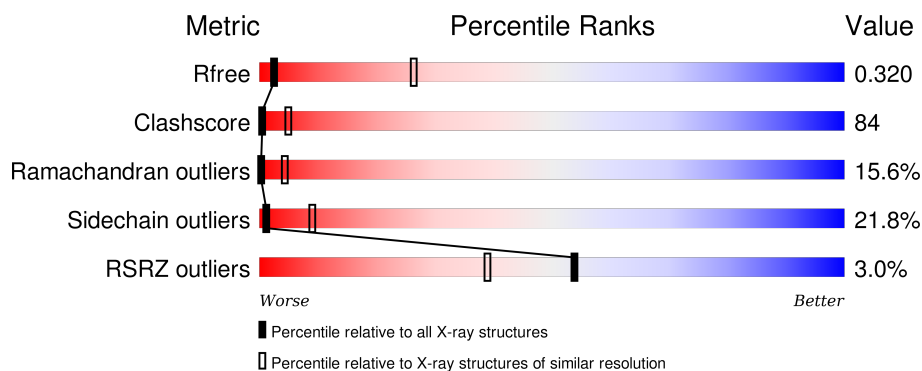
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

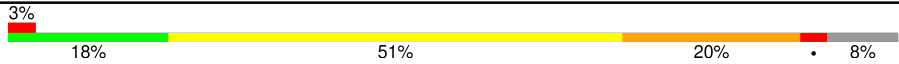
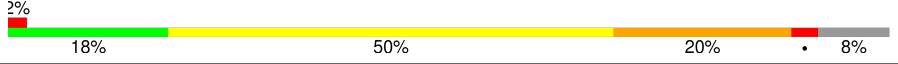
The reported resolution of this entry is 3.61 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	
1	B	445	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

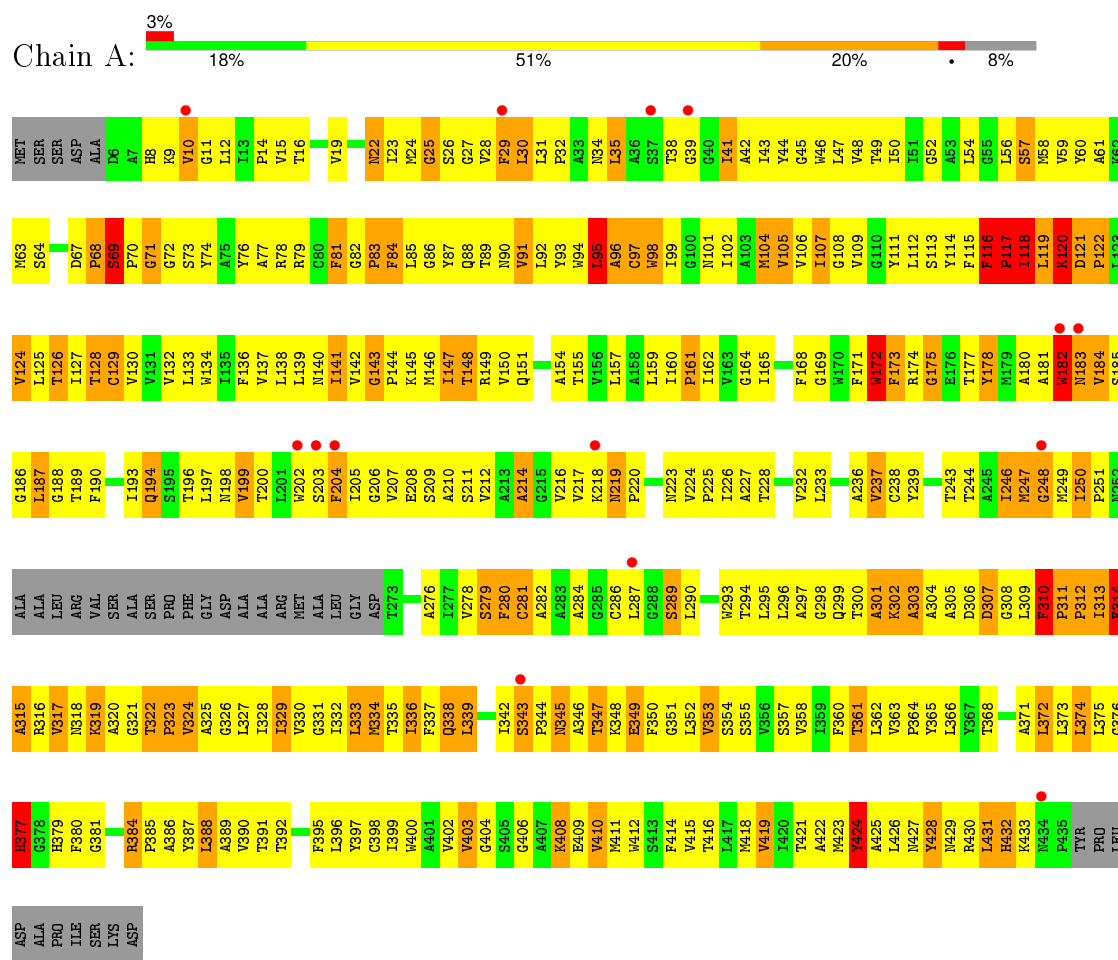
- Molecule 1 is a protein called Arginine/agmatine antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			
1	B	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Arginine/agmatine antiporter



PRO	L375	G376	F377	G378	H379	F380	G381											R384	F385	A386	Y387	I388	A389	V390	T391	T392											F395	L396	Y397	C398	I399	W400	A401	V402	W403	G404											S405	P343	A407	K408	E409	W410	M411	W412	S413	F414	W415	T416	L417	M418	W419	I420	T421	A422	M423	A424	L425	L426	M427	Y428	M429	R430	L431	H432	K433	M434	P435	TYR
LEU	I313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	T329	V330	G331	L332	M333	M334	T335	I336	F337	Q338	L339											T342	S343	P344	N345	A346	T347	K348	E349	F350	G351	L352	V353	S354	S355	V356	S357	V358	I359	F360	T361	L362	V363	P364	Y365	L366	Y367	T368											A371	L372	L373	L374										
ASP	G185	L186	L187	G188	T189	F190											I193	Q194	S195	T196	L197	N198	V199	T200	L201	W202	S203	F204	L205	G206	E208	S209	A210	S211	V212	A213	Q214	G215	V216	V217	K218	N219	P220	N223	Y224	P225	I226	A227	T228	V232	L233	A236	V237	C238	R174	Y239											T243	T244	A245	I246	W247	G248	M249	P251														
ALA	N252	ALA	ALA	LEU	ARG	VAL	SER	ALA	SER	PRO	PHE	GLY	ASP	ALA	ARG	MET	ALA	LEU	GLY	ASP	T273	A276	I277	V278	S279	F280	C281	A282	A283	A284	G285	C286	L287	G288	S289	L290	G291	G292	W293	T294	L295	L296	A297	Q298	Q299	T300	A301	C302	A303	A304	A305	D306	D307	G308	L309	F310	P311	T250	P312																													
PRO	L375	G376	F377	G378	H379	F380	G381											R384	F385	A386	Y387	I388	A389	V390	T391	T392											F395	L396	Y397	C398	I399	W400	A401	V402	W403	G404											S405	P343	A407	K408	E409	W410	M411	W412	S413	F414	W415	T416	L417	M418	W419	I420	T421	A422	M423	A424	L425	L426	M427	Y428	M429	R430	L431	H432	K433	M434	P435	TYR
LEU	I313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	T329	V330	G331	L332	M333	M334	T335	I336	F337	Q338	L339											T342	S343	P344	N345	A346	T347	K348	E349	F350	G351	L352	V353	S354	S355	V356	S357	V358	I359	F360	T361	L362	V363	P364	Y365	L366	Y367	T368											A371	L372	L373	L374										
ASP	G185	L186	L187	G188	T189	F190											I193	Q194	S195	T196	L197	N198	V199	T200	L201	W202	S203	F204	L205	G206	E208	S209	A210	S211	V212	A213	Q214	G215	V216	V217	K218	N219	P220	N223	Y224	P225	I226	A227	T228	V232	L233	A236	V237	C238	R174	Y239											T243	T244	A245	I246	W247	G248	M249	P251														
ALA	N252	ALA	ALA	LEU	ARG	VAL	SER	ALA	SER	PRO	PHE	GLY	ASP	ALA	ARG	MET	ALA	LEU	GLY	ASP	T273	A276	I277	V278	S279	F280	C281	A282	A283	A284	G285	C286	L287	G288	S289	L290	G291	G292	W293	T294	L295	L296	A297	Q298	Q299	T300	A301	C302	A303	A304	A305	D306	D307	G308	L309	F310	P311	T250	P312																													
PRO	L375	G376	F377	G378	H379	F380	G381											R384	F385	A386	Y387	I388	A389	V390	T391	T392											F395	L396	Y397	C398	I399	W400	A401	V402	W403	G404											S405	P343	A407	K408	E409	W410	M411	W412	S413	F414	W415	T416	L417	M418	W419	I420	T421	A422	M423	A424	L425	L426	M427	Y428	M429	R430	L431	H432	K433	M434	P435	TYR
LEU	I313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	T329	V330	G331	L332	M333	M334	T335	I336	F337	Q338	L339											T342	S343	P344	N345	A346	T347	K348	E349	F350	G351	L352	V353	S354	S355	V356	S357	V358	I359	F360	T361	L362	V363	P364	Y365	L366	Y367	T368											A371	L372	L373	L374										
ASP	G185	L186	L187	G188	T189	F190											I193	Q194	S195	T196	L197	N198	V199	T200	L201	W202	S203	F204	L205	G206	E208	S209	A210	S211	V212	A213	Q214	G215	V216	V217	K218	N219	P220	N223	Y224	P225	I226	A227	T228	V232	L233	A236	V237	C238	R174	Y239											T243	T244	A245	I246	W247	G248	M249	P251														
ALA	N252	ALA	ALA	LEU	ARG	VAL	SER	ALA	SER	PRO	PHE	GLY	ASP	ALA	ARG	MET	ALA	LEU	GLY	ASP	T273	A276	I277	V278	S279	F280	C281	A282	A283	A284	G285	C286	L287	G288	S289	L290	G291	G292	W293	T294	L295	L296	A297	Q298	Q299	T300	A301	C302	A303	A304	A305	D306	D307	G308	L309	F310	P311	T250	P312																													
PRO	L375	G376	F377	G378	H379	F380	G381											R384	F385	A386	Y387	I388	A389	V390	T391	T392											F395	L396	Y397	C398	I399	W400	A401	V402	W403	G404											S405	P343	A407	K408	E409	W410	M411	W412	S413	F414	W415	T416	L417	M418	W419	I420	T421	A422	M423	A424	L425	L426	M427	Y428	M429	R430	L431	H432	K433	M434	P435	TYR
LEU	I313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	T329	V330	G331	L332	M333	M334	T335	I336	F337	Q338	L339											T342	S343	P344	N345	A346	T347	K348	E349	F350	G351	L352	V353	S354	S355	V356	S357	V358	I359	F360	T361	L362	V363	P364	Y365	L366	Y367	T368											A371	L372	L373	L374										
ASP	G185	L186	L187	G188	T189	F190											I193	Q194	S195	T196	L197	N198	V199	T200	L201	W202	S203	F204	L205	G206	E208	S209	A210	S211	V212	A213	Q214	G215	V216	V217	K218	N219	P220	N223	Y224	P225	I226	A227	T228	V232	L233	A236	V237	C238	R174	Y239											T243	T244	A245	I246	W247	G248	M249	P251														
ALA	N252	ALA	ALA	LEU	ARG	VAL	SER	ALA	SER	PRO	PHE	GLY	ASP	ALA	ARG	MET	ALA	LEU	GLY	ASP	T273	A276	I277	V278	S279	F280	C281	A282	A283	A284	G285	C286	L287	G288	S289	L290	G291	G292	W293	T294	L295	L296	A297	Q298	Q299	T300	A301	C302	A303	A304	A305	D306	D307	G308	L309	F310	P311	T250	P312																													
PRO	L375	G376	F377	G378	H379	F380	G381											R384	F385	A386	Y387	I388	A389	V390	T391	T392											F395	L396	Y397	C398	I399	W400	A401	V402	W403	G404											S405	P343	A407	K408	E409	W410	M411	W412	S413	F414	W415	T416	L417	M418	W419	I420	T421	A422	M423	A424	L425	L426	M427	Y428	M429	R430	L431	H432	K433	M434	P435	TYR
LEU	I313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	T329	V330	G331	L332	M333	M334	T335	I336	F337	Q338	L339											T342	S343	P344	N345	A346	T347	K348	E349	F350	G351	L352	V353	S354	S355	V356	S357	V358	I359	F360	T361	L362	V363	P364	Y365	L366	Y367	T368											A371	L372	L373	L374										
ASP	G185	L186	L187	G188	T189	F190											I193	Q194	S195	T196	L197	N198	V199	T200	L201	W202	S203	F204	L205	G206	E208	S209	A210	S211	V212	A213	Q214	G215	V216	V217	K218	N219	P220	N223	Y224	P225	I226	A227	T228	V232	L233	A236	V237	C238	R174	Y239											T243	T244	A245	I246	W247	G248	M249	P251														
ALA	N252	ALA	ALA	LEU	ARG	VAL	SER	ALA	SER	PRO	PHE	GLY	ASP	ALA	ARG	MET	ALA	LEU	GLY	ASP	T273	A276	I277	V278	S279	F280	C281	A282	A283	A284	G285	C286	L287	G288	S289	L290	G291	G292	W293	T294	L295	L296	A297	Q298	Q299	T300	A301	C302	A303	A304	A305	D306	D307	G308	L309	F310	P311	T250	P312																													
PRO	L375	G376	F377	G378	H379	F380	G381											R384	F385	A386	Y387	I388	A389	V390	T391	T392											F395	L396	Y397	C398	I399	W400	A401	V402	W403	G404											S405	P343	A407	K408	E409	W410	M411	W412	S413	F414	W415	T416	L417	M418	W419	I420	T421	A422	M423	A424	L425	L426	M427	Y428	M429	R430	L431	H432	K433	M434	P435	TYR
LEU	I313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	T329	V330	G331	L332	M333	M334	T335	I336	F337	Q338	L339											T342	S343	P344	N345	A346	T347	K348	E349	F350	G351	L352	V353	S354	S355	V356	S357	V358	I359	F360	T361	L362	V363	P364	Y365	L366	Y367	T368											A371	L372	L373	L374										
ASP	G185	L186	L187	G188	T189	F190											I193	Q194	S195	T196	L197	N198	V199	T200	L201	W202	S203	F204	L205	G206	E208	S209	A210	S211	V212	A213	Q214	G215	V216	V217	K218	N219	P220	N223	Y224	P225	I226	A227	T228	V232	L233	A236	V237	C238	R174	Y239											T243	T244	A245	I246	W247	G248	M249	P251														
ALA	N252	ALA	ALA	LEU	ARG	VAL	SER	ALA	SER	PRO	PHE	GLY	ASP	ALA	ARG	MET	ALA	LEU	GLY	ASP	T273	A276	I277	V278	S279	F280	C281	A282	A283	A284	G285	C286	L287	G288	S289	L290	G291	G292	W293	T294	L295	L296	A297	Q298	Q299	T300	A301	C302	A303	A304	A305	D306	D307	G308	L309	F310	P311	T250	P312																													
PRO	L375	G376	F377	G378	H379	F380	G381											R384	F385	A386	Y387	I388	A389	V390	T391	T392											F395	L396	Y397	C398	I399	W400	A401	V402	W403	G404											S405	P343	A407	K408	E409	W410	M411	W412	S413	F414	W415	T416	L417	M418	W419	I420	T421	A422	M423	A424	L425	L426	M427	Y428	M429	R430	L431	H432	K433	M434	P435	TYR
LEU	I313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	T329	V330	G331	L332	M333	M334	T335	I336	F337	Q338	L339											T342	S343	P344	N345	A346	T347	K348	E34																																											

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.81Å 108.30Å 138.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.61 49.32 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.32-3.61) 99.8 (49.32-3.61)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.295 , 0.318 0.294 , 0.320	Depositor DCC
$R_{free}$ test set	876 reflections (5.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	152.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 132.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 16551 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.48	0/3115	0.74	2/4264 (0.0%)
1	B	0.48	0/3115	0.74	2/4264 (0.0%)
All	All	0.48	0/6230	0.74	4/8528 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	311	PRO	C-N-CD	-6.25	106.85	120.60
1	B	311	PRO	C-N-CD	-5.78	107.89	120.60
1	A	432	HIS	N-CA-C	5.72	126.45	111.00
1	B	432	HIS	N-CA-C	5.38	125.52	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	PHE	Peptide
1	A	377	HIS	Peptide
1	A	424	TYR	Peptide
1	B	116	PHE	Peptide
1	B	377	HIS	Peptide

*Continued on next page...*

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Mol	Chain	Res	Type	Group
1	B	424	TYR	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	3036	0	3141	537	0
1	B	3036	0	3141	538	0
All	All	6072	0	6282	1040	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 84.

All (1040) 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:315:ALA:HB1	1:A:316:ARG:HA	1.19	1.16
1:A:430:ARG:HG2	1:B:374:LEU:HD23	1.28	1.15
1:B:38:THR:HB	1:B:39:GLY:HA3	1.18	1.14
1:B:315:ALA:HB1	1:B:316:ARG:HA	1.15	1.14
1:A:38:THR:HB	1:A:39:GLY:HA3	1.19	1.12
1:B:342:ILE:HB	1:B:343:SER:HB2	1.37	1.06
1:B:425:ALA:HA	1:B:428:TYR:CZ	1.90	1.05
1:A:425:ALA:HA	1:A:428:TYR:CZ	1.91	1.03
1:A:105:VAL:HB	1:A:129:CYS:SG	1.97	1.03
1:A:374:LEU:HD23	1:B:430:ARG:HG2	1.36	1.02
1:A:342:ILE:HB	1:A:343:SER:HB2	1.38	1.02
1:B:105:VAL:HB	1:B:129:CYS:SG	2.00	1.00
1:B:327:LEU:H	1:B:327:LEU:HD12	1.27	0.99
1:A:327:LEU:HD12	1:A:327:LEU:H	1.27	0.99
1:A:173:PHE:HA	1:A:174:ARG:HB2	1.44	0.98
1:B:173:PHE:HA	1:B:174:ARG:HB2	1.44	0.98
1:A:164:GLY:O	1:A:168:PHE:HB2	1.62	0.98
1:B:38:THR:CB	1:B:39:GLY:HA3	1.93	0.97
1:B:164:GLY:O	1:B:168:PHE:HB2	1.64	0.96
1:A:116:PHE:O	1:A:118:ILE:HG22	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:CB	1:A:39:GLY:HA3	1.94	0.94
1:B:91:VAL:O	1:B:95:LEU:HB2	1.67	0.93
1:A:424:TYR:HD1	1:A:430:ARG:NH2	1.66	0.93
1:B:210:ALA:HB3	1:B:228:THR:HG22	1.49	0.92
1:A:107:ILE:HG23	1:A:111:TYR:HE1	1.34	0.92
1:A:422:ALA:HA	1:B:395:PHE:CE1	2.04	0.92
1:B:79:ARG:HB2	1:B:375:LEU:HD11	1.51	0.92
1:A:91:VAL:O	1:A:95:LEU:HB2	1.69	0.91
1:A:24:MET:HB3	1:A:25:GLY:HA2	1.52	0.91
1:A:210:ALA:HB3	1:A:228:THR:HG22	1.49	0.91
1:B:424:TYR:HD1	1:B:430:ARG:NH2	1.67	0.91
1:B:116:PHE:O	1:B:118:ILE:HG22	1.70	0.91
1:A:93:TYR:HD2	1:A:300:THR:HG21	1.33	0.91
1:B:302:LYS:HG3	1:B:314:PHE:HB2	1.50	0.90
1:B:346:ALA:HB3	1:B:351:GLY:HA2	1.51	0.90
1:A:428:TYR:OH	1:B:373:LEU:HD13	1.71	0.90
1:B:102:ILE:HD13	1:B:337:PHE:HD2	1.37	0.90
1:B:24:MET:HB3	1:B:25:GLY:HA2	1.54	0.90
1:B:107:ILE:HG23	1:B:111:TYR:HE1	1.36	0.89
1:B:10:VAL:HG12	1:B:11:GLY:H	1.36	0.89
1:A:10:VAL:HG12	1:A:11:GLY:H	1.37	0.88
1:A:302:LYS:HG3	1:A:314:PHE:HB2	1.54	0.88
1:B:342:ILE:CB	1:B:343:SER:HB2	2.03	0.88
1:A:16:THR:HG22	1:A:227:ALA:HA	1.53	0.88
1:A:342:ILE:CB	1:A:343:SER:HB2	2.04	0.87
1:B:93:TYR:HD2	1:B:300:THR:HG21	1.37	0.87
1:A:384:ARG:HE	1:A:388:LEU:HD12	1.39	0.87
1:B:16:THR:HG22	1:B:227:ALA:HA	1.55	0.87
1:A:374:LEU:O	1:A:375:LEU:HD23	1.74	0.87
1:A:346:ALA:HB3	1:A:351:GLY:HA2	1.53	0.86
1:A:315:ALA:CB	1:A:316:ARG:HA	2.05	0.86
1:A:102:ILE:HD13	1:A:337:PHE:HD2	1.38	0.86
1:A:57:SER:HB2	1:A:232:VAL:HG21	1.58	0.85
1:B:374:LEU:O	1:B:375:LEU:HD23	1.76	0.85
1:B:315:ALA:CB	1:B:316:ARG:HA	2.01	0.85
1:A:425:ALA:HA	1:A:428:TYR:CE1	2.11	0.85
1:A:424:TYR:CD1	1:A:430:ARG:NH2	2.45	0.85
1:B:384:ARG:HE	1:B:388:LEU:HD12	1.41	0.85
1:B:315:ALA:HB1	1:B:316:ARG:CA	2.03	0.85
1:A:28:VAL:HG11	1:A:162:ILE:HD11	1.56	0.85
1:B:425:ALA:HA	1:B:428:TYR:CE1	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:TYR:O	1:A:429:ASN:ND2	2.10	0.85
1:A:313:ILE:HG22	1:A:314:PHE:H	1.40	0.84
1:A:79:ARG:HB2	1:A:375:LEU:HD11	1.57	0.84
1:B:330:VAL:O	1:B:334:MET:HB2	1.77	0.84
1:A:118:ILE:HA	1:A:119:LEU:O	1.78	0.84
1:A:228:THR:O	1:A:232:VAL:HG23	1.78	0.84
1:B:22:ASN:HB3	1:B:293:TRP:NE1	1.93	0.83
1:A:139:LEU:HD13	1:A:150:VAL:HG21	1.59	0.83
1:B:139:LEU:HD13	1:B:150:VAL:HG21	1.59	0.83
1:B:290:LEU:O	1:B:294:THR:HG23	1.79	0.83
1:A:315:ALA:HB1	1:A:316:ARG:CA	2.07	0.83
1:B:228:THR:O	1:B:232:VAL:HG23	1.79	0.83
1:B:342:ILE:HB	1:B:343:SER:CB	2.09	0.82
1:A:160:ILE:HB	1:A:161:PRO:HD3	1.61	0.82
1:A:330:VAL:O	1:A:334:MET:HB2	1.79	0.82
1:A:138:LEU:HA	1:A:141:ILE:HG13	1.59	0.82
1:B:160:ILE:HB	1:B:161:PRO:HD3	1.62	0.82
1:A:342:ILE:HB	1:A:343:SER:CB	2.09	0.82
1:B:424:TYR:CD1	1:B:430:ARG:NH2	2.48	0.82
1:A:290:LEU:O	1:A:294:THR:HG23	1.79	0.82
1:B:138:LEU:HA	1:B:141:ILE:HG13	1.60	0.82
1:B:28:VAL:HG11	1:B:162:ILE:HD11	1.62	0.81
1:B:104:MET:HE3	1:B:286:CYS:SG	2.21	0.81
1:A:19:VAL:O	1:A:23:ILE:HD13	1.81	0.81
1:A:118:ILE:HA	1:A:119:LEU:C	2.01	0.81
1:A:102:ILE:HD13	1:A:337:PHE:CD2	2.16	0.81
1:A:130:VAL:HG21	1:A:339:LEU:HD23	1.61	0.81
1:B:57:SER:HB2	1:B:232:VAL:HG21	1.62	0.81
1:B:44:TYR:HD2	1:B:193:ILE:HD11	1.46	0.81
1:B:130:VAL:HG21	1:B:339:LEU:HD23	1.62	0.80
1:A:41:ILE:HG13	1:A:43:ILE:HG13	1.64	0.80
1:B:102:ILE:HD13	1:B:337:PHE:CD2	2.17	0.79
1:B:311:PRO:HD3	1:B:426:LEU:HD21	1.64	0.79
1:B:41:ILE:HG13	1:B:43:ILE:HG13	1.65	0.79
1:B:67:ASP:CG	1:B:79:ARG:HH12	1.86	0.79
1:A:104:MET:HE3	1:A:286:CYS:SG	2.22	0.79
1:B:313:ILE:HG22	1:B:314:PHE:H	1.46	0.79
1:A:22:ASN:HB3	1:A:293:TRP:NE1	1.98	0.79
1:A:219:ASN:H	1:A:223:ASN:HD22	1.31	0.79
1:A:327:LEU:HD12	1:A:327:LEU:N	1.98	0.79
1:B:118:ILE:HA	1:B:119:LEU:C	2.03	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HA	1:B:119:LEU:O	1.81	0.79
1:B:10:VAL:HG12	1:B:11:GLY:N	1.97	0.78
1:B:428:TYR:O	1:B:429:ASN:ND2	2.16	0.78
1:B:327:LEU:N	1:B:327:LEU:HD12	1.98	0.78
1:B:219:ASN:H	1:B:223:ASN:HD22	1.30	0.78
1:B:323:PRO:HD2	1:B:327:LEU:HD11	1.64	0.78
1:B:372:LEU:O	1:B:372:LEU:HG	1.83	0.78
1:A:207:VAL:HG12	1:A:232:VAL:HG22	1.65	0.77
1:B:312:PRO:HA	1:B:313:ILE:HB	1.64	0.77
1:A:312:PRO:HA	1:A:313:ILE:HB	1.66	0.77
1:B:121:ASP:HB2	1:B:122:PRO:HD3	1.67	0.77
1:A:86:GLY:O	1:A:89:THR:HG22	1.84	0.77
1:A:313:ILE:O	1:A:315:ALA:HB3	1.85	0.76
1:A:107:ILE:HG23	1:A:111:TYR:CE1	2.20	0.76
1:A:126:THR:HG21	1:A:342:ILE:HG23	1.66	0.76
1:A:323:PRO:HD2	1:A:327:LEU:HD11	1.66	0.76
1:A:311:PRO:HD3	1:A:426:LEU:HD21	1.65	0.76
1:A:374:LEU:HD12	1:A:374:LEU:H	1.51	0.76
1:B:126:THR:HG21	1:B:342:ILE:HG23	1.65	0.76
1:A:430:ARG:HG2	1:B:374:LEU:CD2	2.14	0.76
1:B:72:GLY:H	1:B:212:VAL:HA	1.50	0.76
1:A:32:PRO:HG3	1:A:243:THR:HG22	1.68	0.76
1:A:140:ASN:HB3	1:A:327:LEU:CD2	2.16	0.75
1:A:10:VAL:HG12	1:A:11:GLY:N	2.00	0.75
1:A:44:TYR:HD2	1:A:193:ILE:HD11	1.50	0.75
1:A:67:ASP:CG	1:A:79:ARG:HH12	1.89	0.75
1:B:19:VAL:O	1:B:23:ILE:HD13	1.87	0.75
1:A:395:PHE:CE1	1:B:422:ALA:HA	2.21	0.75
1:A:314:PHE:HA	1:A:315:ALA:C	2.07	0.75
1:A:302:LYS:N	1:A:302:LYS:HD3	2.01	0.75
1:B:140:ASN:HB3	1:B:327:LEU:CD2	2.17	0.74
1:B:376:GLY:HA3	1:B:379:HIS:CD2	2.22	0.74
1:B:44:TYR:CD2	1:B:193:ILE:HD11	2.22	0.74
1:A:219:ASN:HD22	1:A:223:ASN:ND2	1.85	0.74
1:B:64:SER:O	1:B:68:PRO:HG3	1.88	0.74
1:B:374:LEU:HD12	1:B:374:LEU:H	1.52	0.74
1:B:313:ILE:O	1:B:315:ALA:HB3	1.87	0.74
1:B:207:VAL:HG12	1:B:232:VAL:HG22	1.68	0.74
1:B:219:ASN:HD22	1:B:223:ASN:ND2	1.85	0.73
1:B:379:HIS:C	1:B:381:GLY:H	1.91	0.73
1:A:376:GLY:HA3	1:A:379:HIS:CD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:CA	1:B:343:SER:HB2	2.18	0.73
1:B:22:ASN:HB3	1:B:293:TRP:HE1	1.53	0.73
1:B:32:PRO:HG3	1:B:243:THR:HG22	1.70	0.73
1:A:372:LEU:HG	1:A:372:LEU:O	1.88	0.73
1:A:72:GLY:H	1:A:212:VAL:HA	1.53	0.73
1:B:107:ILE:HG23	1:B:111:TYR:CE1	2.22	0.72
1:A:302:LYS:HD3	1:A:302:LYS:H	1.54	0.72
1:A:50:ILE:HD13	1:A:236:ALA:HB1	1.71	0.72
1:A:209:SER:HB3	1:A:296:LEU:HD11	1.71	0.72
1:A:342:ILE:CA	1:A:343:SER:HB2	2.18	0.72
1:A:102:ILE:HD13	1:A:337:PHE:HB3	1.72	0.72
1:A:121:ASP:HB2	1:A:122:PRO:HD3	1.71	0.72
1:A:184:VAL:HG12	1:A:185:SER:H	1.54	0.72
1:A:379:HIS:C	1:A:381:GLY:H	1.93	0.72
1:B:302:LYS:N	1:B:302:LYS:HD3	2.03	0.72
1:A:44:TYR:CD2	1:A:193:ILE:HD11	2.24	0.72
1:B:72:GLY:N	1:B:212:VAL:HA	2.05	0.71
1:B:184:VAL:HG12	1:B:185:SER:H	1.56	0.71
1:B:302:LYS:H	1:B:302:LYS:HD3	1.56	0.71
1:A:105:VAL:HG13	1:A:290:LEU:HD11	1.72	0.71
1:A:64:SER:O	1:A:68:PRO:HG3	1.90	0.70
1:B:23:ILE:HD11	1:B:206:GLY:C	2.12	0.70
1:A:424:TYR:HD1	1:A:430:ARG:HH21	1.39	0.70
1:B:90:ASN:OD1	1:B:300:THR:O	2.08	0.70
1:B:38:THR:HB	1:B:39:GLY:CA	2.11	0.70
1:A:428:TYR:HE2	1:B:388:LEU:HD21	1.56	0.70
1:B:209:SER:HB3	1:B:296:LEU:HD11	1.74	0.70
1:A:310:PHE:HB3	1:A:311:PRO:O	1.92	0.70
1:B:335:THR:O	1:B:338:GLN:N	2.25	0.70
1:B:424:TYR:HD1	1:B:430:ARG:HH21	1.38	0.69
1:B:104:MET:O	1:B:104:MET:HE2	1.93	0.69
1:B:86:GLY:O	1:B:89:THR:HG22	1.92	0.69
1:B:305:ALA:HB1	1:B:312:PRO:HB3	1.74	0.69
1:B:327:LEU:H	1:B:327:LEU:CD1	2.04	0.69
1:B:38:THR:CB	1:B:39:GLY:CA	2.70	0.69
1:A:388:LEU:HD21	1:B:428:TYR:HE2	1.58	0.69
1:A:101:ASN:O	1:A:104:MET:N	2.26	0.69
1:A:22:ASN:HB3	1:A:293:TRP:HE1	1.57	0.69
1:B:34:ASN:HB3	1:B:199:VAL:HG11	1.75	0.69
1:A:72:GLY:N	1:A:212:VAL:HA	2.08	0.69
1:A:250:ILE:H	1:A:251:PRO:HD2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:CD1	1:A:327:LEU:H	2.04	0.68
1:B:314:PHE:HA	1:B:315:ALA:C	2.11	0.68
1:B:347:THR:O	1:B:348:LYS:HG3	1.94	0.68
1:A:344:PRO:HA	1:A:347:THR:HG22	1.75	0.68
1:B:138:LEU:O	1:B:142:VAL:HG23	1.94	0.68
1:A:428:TYR:CZ	1:B:373:LEU:HD13	2.28	0.68
1:B:323:PRO:HD2	1:B:327:LEU:CD1	2.23	0.68
1:B:102:ILE:HD13	1:B:337:PHE:HB3	1.76	0.68
1:B:139:LEU:HD22	1:B:146:MET:HE1	1.75	0.68
1:B:379:HIS:HD1	1:B:387:TYR:HD2	1.41	0.68
1:A:374:LEU:CD2	1:B:430:ARG:HG2	2.19	0.68
1:A:250:ILE:H	1:A:251:PRO:CD	2.07	0.68
1:A:34:ASN:HB3	1:A:199:VAL:HG11	1.74	0.68
1:A:143:GLY:HA2	1:A:146:MET:H	1.57	0.68
1:B:93:TYR:CD2	1:B:300:THR:HG21	2.26	0.68
1:B:81:PHE:HB3	1:B:82:GLY:HA2	1.74	0.68
1:B:72:GLY:C	1:B:74:TYR:H	1.97	0.68
1:B:205:ILE:HD11	1:B:358:VAL:HG13	1.75	0.68
1:A:300:THR:HG22	1:A:300:THR:O	1.93	0.67
1:B:250:ILE:H	1:B:251:PRO:HD2	1.59	0.67
1:B:250:ILE:H	1:B:251:PRO:CD	2.08	0.67
1:A:44:TYR:HB2	1:A:193:ILE:HD11	1.77	0.67
1:B:379:HIS:ND1	1:B:387:TYR:HD2	1.93	0.67
1:B:144:PRO:HB2	1:B:216:VAL:HG11	1.77	0.67
1:B:120:LYS:HE3	1:B:120:LYS:HA	1.76	0.67
1:A:178:TYR:HD2	1:A:247:MET:HA	1.59	0.67
1:A:95:LEU:HD23	1:A:95:LEU:O	1.95	0.67
1:B:424:TYR:N	1:B:424:TYR:HD2	1.93	0.67
1:B:50:ILE:HD13	1:B:236:ALA:HB1	1.76	0.67
1:A:90:ASN:OD1	1:A:300:THR:O	2.12	0.66
1:A:424:TYR:CD2	1:A:424:TYR:N	2.63	0.66
1:B:105:VAL:HG13	1:B:290:LEU:HD11	1.76	0.66
1:A:93:TYR:CD2	1:A:300:THR:HG21	2.23	0.66
1:B:424:TYR:N	1:B:424:TYR:CD2	2.64	0.66
1:A:104:MET:HE2	1:A:104:MET:O	1.95	0.66
1:B:41:ILE:O	1:B:183:ASN:HA	1.96	0.66
1:A:347:THR:O	1:A:348:LYS:HG3	1.94	0.66
1:A:78:ARG:HA	1:A:82:GLY:HA3	1.77	0.66
1:B:69:SER:OG	1:B:70:PRO:HA	1.95	0.66
1:A:84:PHE:HZ	1:A:421:THR:HG1	1.41	0.66
1:B:83:PRO:HB3	1:B:430:ARG:NH1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:N	1:A:343:SER:HB2	2.10	0.66
1:A:72:GLY:C	1:A:74:TYR:H	1.98	0.66
1:B:126:THR:CG2	1:B:342:ILE:HG23	2.25	0.66
1:B:300:THR:O	1:B:300:THR:HG22	1.95	0.66
1:B:81:PHE:HB3	1:B:82:GLY:CA	2.26	0.66
1:A:23:ILE:HD11	1:A:206:GLY:C	2.16	0.66
1:B:325:ALA:O	1:B:329:ILE:HG13	1.95	0.66
1:A:379:HIS:ND1	1:A:387:TYR:HD2	1.94	0.66
1:A:81:PHE:HB3	1:A:82:GLY:HA2	1.77	0.65
1:B:105:VAL:HG21	1:B:133:LEU:HD21	1.78	0.65
1:A:311:PRO:CD	1:A:426:LEU:HD21	2.26	0.65
1:A:98:TRP:CD1	1:A:98:TRP:C	2.69	0.65
1:A:128:THR:O	1:A:132:VAL:HG23	1.96	0.65
1:A:126:THR:CG2	1:A:342:ILE:HG23	2.25	0.65
1:B:178:TYR:HD2	1:B:247:MET:HA	1.58	0.65
1:A:305:ALA:HB1	1:A:312:PRO:HB3	1.77	0.65
1:A:8:HIS:HA	1:A:145:LYS:HD2	1.78	0.65
1:A:373:LEU:HD13	1:B:428:TYR:OH	1.95	0.65
1:A:120:LYS:HE3	1:A:120:LYS:HA	1.78	0.65
1:B:312:PRO:HA	1:B:313:ILE:CB	2.27	0.65
1:B:342:ILE:N	1:B:343:SER:HB2	2.10	0.65
1:B:128:THR:O	1:B:132:VAL:HG23	1.96	0.65
1:B:143:GLY:HA2	1:B:146:MET:H	1.61	0.65
1:A:144:PRO:HB2	1:A:216:VAL:HG11	1.78	0.65
1:B:344:PRO:HA	1:B:347:THR:HG22	1.78	0.65
1:A:38:THR:CB	1:A:39:GLY:CA	2.71	0.65
1:B:72:GLY:O	1:B:74:TYR:N	2.30	0.65
1:A:41:ILE:O	1:A:183:ASN:HA	1.97	0.65
1:B:95:LEU:O	1:B:95:LEU:HD23	1.97	0.65
1:A:19:VAL:HG11	1:A:228:THR:HA	1.77	0.65
1:A:105:VAL:HG21	1:A:133:LEU:HD21	1.78	0.65
1:A:69:SER:OG	1:A:70:PRO:HA	1.97	0.64
1:A:249:MET:SD	1:A:251:PRO:HD2	2.37	0.64
1:A:97:CYS:HB2	1:A:297:ALA:HB2	1.79	0.64
1:A:323:PRO:HD2	1:A:327:LEU:CD1	2.27	0.64
1:A:424:TYR:HD2	1:A:424:TYR:N	1.95	0.64
1:A:59:VAL:HG22	1:A:391:THR:HG22	1.79	0.64
1:A:325:ALA:O	1:A:329:ILE:HG13	1.98	0.64
1:A:312:PRO:HA	1:A:313:ILE:CB	2.27	0.63
1:B:140:ASN:ND2	1:B:147:ILE:HG12	2.12	0.63
1:B:19:VAL:HG11	1:B:228:THR:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:VAL:HG12	1:A:232:VAL:CG2	2.27	0.63
1:A:430:ARG:HG3	1:A:431:LEU:H	1.63	0.63
1:B:311:PRO:CD	1:B:426:LEU:HD21	2.26	0.63
1:A:298:GLY:HA2	1:A:302:LYS:HE2	1.79	0.63
1:B:78:ARG:HA	1:B:82:GLY:HA3	1.78	0.63
1:B:207:VAL:HG12	1:B:232:VAL:CG2	2.29	0.63
1:B:302:LYS:CG	1:B:314:PHE:HB2	2.27	0.63
1:B:97:CYS:HB2	1:B:297:ALA:HB2	1.81	0.63
1:A:371:ALA:C	1:A:373:LEU:H	2.02	0.63
1:B:101:ASN:O	1:B:104:MET:N	2.30	0.63
1:A:84:PHE:CD1	1:B:85:LEU:HD11	2.34	0.63
1:B:133:LEU:HD11	1:B:338:GLN:HG3	1.81	0.63
1:B:376:GLY:HA3	1:B:379:HIS:HD2	1.62	0.63
1:A:81:PHE:HB3	1:A:82:GLY:CA	2.29	0.62
1:B:372:LEU:CG	1:B:372:LEU:O	2.47	0.62
1:B:59:VAL:HG22	1:B:391:THR:HG22	1.82	0.62
1:B:120:LYS:CA	1:B:120:LYS:HE3	2.29	0.62
1:A:310:PHE:HB3	1:A:311:PRO:C	2.20	0.62
1:A:376:GLY:HA3	1:A:379:HIS:HD2	1.62	0.62
1:B:173:PHE:CA	1:B:174:ARG:HB2	2.25	0.62
1:B:301:ALA:HB1	1:B:310:PHE:HE1	1.65	0.62
1:A:306:ASP:O	1:A:308:GLY:N	2.33	0.62
1:B:98:TRP:CD1	1:B:98:TRP:C	2.72	0.62
1:B:249:MET:SD	1:B:251:PRO:HD2	2.38	0.62
1:B:306:ASP:O	1:B:308:GLY:N	2.33	0.62
1:A:173:PHE:CA	1:A:174:ARG:HB2	2.25	0.62
1:B:44:TYR:HB2	1:B:193:ILE:HD11	1.81	0.62
1:B:379:HIS:CE1	1:B:387:TYR:CD2	2.88	0.61
1:B:50:ILE:O	1:B:54:LEU:HB2	2.00	0.61
1:B:8:HIS:HA	1:B:145:LYS:HD2	1.81	0.61
1:A:379:HIS:CE1	1:A:387:TYR:CD2	2.88	0.61
1:A:24:MET:HB3	1:A:25:GLY:CA	2.29	0.61
1:B:430:ARG:HG3	1:B:431:LEU:H	1.64	0.61
1:A:114:TYR:CD1	1:A:118:ILE:HG12	2.35	0.61
1:A:173:PHE:HA	1:A:174:ARG:CB	2.18	0.61
1:A:50:ILE:O	1:A:54:LEU:HB2	2.01	0.61
1:A:205:ILE:HD11	1:A:358:VAL:HG13	1.83	0.61
1:A:72:GLY:O	1:A:74:TYR:N	2.34	0.61
1:A:139:LEU:HD22	1:A:146:MET:HE1	1.83	0.60
1:B:298:GLY:HA2	1:B:302:LYS:HE2	1.81	0.60
1:B:371:ALA:C	1:B:373:LEU:H	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:HB3	1:B:25:GLY:CA	2.30	0.60
1:A:140:ASN:ND2	1:A:147:ILE:HG12	2.16	0.60
1:B:71:GLY:O	1:B:212:VAL:HG13	2.01	0.60
1:B:142:VAL:CG1	1:B:146:MET:HG3	2.31	0.60
1:B:280:PHE:C	1:B:282:ALA:H	2.04	0.60
1:A:301:ALA:HB1	1:A:310:PHE:HE1	1.66	0.60
1:A:422:ALA:HA	1:B:395:PHE:CD1	2.37	0.60
1:B:310:PHE:HB3	1:B:311:PRO:O	2.01	0.60
1:B:19:VAL:HG21	1:B:210:ALA:HB2	1.84	0.60
1:B:427:ASN:O	1:B:429:ASN:N	2.30	0.60
1:A:406:GLY:HA3	1:A:409:GLU:OE1	2.02	0.60
1:B:314:PHE:N	1:B:314:PHE:CD2	2.67	0.60
1:B:406:GLY:HA3	1:B:409:GLU:OE1	2.00	0.60
1:B:173:PHE:HA	1:B:174:ARG:CB	2.18	0.60
1:B:99:ILE:HG21	1:B:357:SER:HB3	1.82	0.59
1:B:376:GLY:O	1:B:377:HIS:C	2.40	0.59
1:B:94:TRP:CZ3	1:B:98:TRP:HZ3	2.18	0.59
1:A:142:VAL:CG1	1:A:146:MET:HG3	2.31	0.59
1:A:376:GLY:O	1:A:377:HIS:C	2.39	0.59
1:A:138:LEU:O	1:A:142:VAL:HG23	2.02	0.59
1:A:78:ARG:HA	1:A:82:GLY:CA	2.32	0.59
1:B:310:PHE:HB3	1:B:311:PRO:C	2.22	0.59
1:A:120:LYS:HE3	1:A:120:LYS:CA	2.32	0.59
1:B:139:LEU:HD22	1:B:146:MET:CE	2.32	0.59
1:A:19:VAL:HG21	1:A:210:ALA:HB2	1.85	0.59
1:B:204:PHE:HE1	1:B:232:VAL:HG13	1.67	0.59
1:B:114:TYR:CD1	1:B:118:ILE:HG12	2.37	0.59
1:A:94:TRP:CZ3	1:A:98:TRP:HZ3	2.21	0.59
1:B:15:VAL:HG21	1:B:217:VAL:HG13	1.85	0.59
1:A:105:VAL:HG13	1:A:290:LEU:CD1	2.33	0.59
1:A:335:THR:O	1:A:338:GLN:N	2.35	0.59
1:B:118:ILE:O	1:B:118:ILE:HG13	2.03	0.59
1:A:280:PHE:C	1:A:282:ALA:H	2.06	0.59
1:A:72:GLY:C	1:A:74:TYR:N	2.57	0.58
1:A:83:PRO:HB3	1:A:430:ARG:NH1	2.17	0.58
1:B:286:CYS:HA	1:B:289:SER:HB3	1.85	0.58
1:A:355:SER:O	1:A:358:VAL:HB	2.03	0.58
1:A:139:LEU:CD1	1:A:150:VAL:HG21	2.31	0.58
1:B:79:ARG:CB	1:B:375:LEU:HD11	2.29	0.58
1:A:133:LEU:HD11	1:A:338:GLN:HG3	1.85	0.58
1:B:113:SER:O	1:B:118:ILE:HB	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG21	1:A:217:VAL:HG13	1.85	0.58
1:B:96:ALA:HB1	1:B:357:SER:O	2.04	0.58
1:B:78:ARG:HA	1:B:82:GLY:CA	2.32	0.58
1:A:314:PHE:HA	1:A:315:ALA:O	2.03	0.58
1:B:379:HIS:CE1	1:B:387:TYR:HD2	2.21	0.58
1:B:360:PHE:CE1	1:B:416:THR:HG21	2.39	0.58
1:B:81:PHE:HB2	1:B:85:LEU:HB2	1.85	0.58
1:B:411:MET:HG3	1:B:412:TRP:N	2.19	0.58
1:A:125:LEU:O	1:A:125:LEU:HD23	2.03	0.58
1:A:85:LEU:HD11	1:B:84:PHE:CD1	2.39	0.58
1:A:96:ALA:HB1	1:A:357:SER:O	2.04	0.58
1:A:302:LYS:CG	1:A:314:PHE:HB2	2.33	0.57
1:A:38:THR:HB	1:A:39:GLY:CA	2.12	0.57
1:B:139:LEU:CD1	1:B:150:VAL:HG21	2.32	0.57
1:A:286:CYS:HA	1:A:289:SER:HB3	1.87	0.57
1:B:105:VAL:HG13	1:B:290:LEU:CD1	2.35	0.57
1:B:116:PHE:O	1:B:117:PRO:C	2.42	0.57
1:B:137:VAL:O	1:B:141:ILE:HG12	2.03	0.57
1:B:379:HIS:C	1:B:381:GLY:N	2.58	0.57
1:A:411:MET:HA	1:B:410:VAL:HG12	1.87	0.57
1:B:72:GLY:C	1:B:74:TYR:N	2.57	0.57
1:B:120:LYS:CE	1:B:120:LYS:HA	2.34	0.57
1:B:384:ARG:O	1:B:386:ALA:N	2.38	0.57
1:A:133:LEU:HD13	1:A:334:MET:HG2	1.87	0.57
1:A:379:HIS:CE1	1:A:387:TYR:HD2	2.22	0.57
1:A:212:VAL:HG11	1:A:296:LEU:HB3	1.87	0.56
1:A:165:ILE:HA	1:A:169:GLY:H	1.70	0.56
1:A:384:ARG:O	1:A:386:ALA:N	2.38	0.56
1:A:113:SER:O	1:A:118:ILE:HB	2.05	0.56
1:A:102:ILE:CD1	1:A:337:PHE:HD2	2.13	0.56
1:B:48:VAL:HG11	1:B:197:LEU:HD11	1.86	0.56
1:A:48:VAL:HG11	1:A:197:LEU:HD11	1.87	0.56
1:A:414:PHE:HD1	1:B:414:PHE:HD1	1.53	0.56
1:A:386:ALA:O	1:A:389:ALA:HB3	2.06	0.56
1:B:342:ILE:CB	1:B:343:SER:CB	2.78	0.56
1:B:22:ASN:HB3	1:B:293:TRP:CD1	2.39	0.56
1:A:372:LEU:O	1:A:372:LEU:CG	2.53	0.56
1:A:114:TYR:O	1:A:115:PHE:HB2	2.06	0.56
1:A:118:ILE:HD12	1:A:119:LEU:N	2.20	0.56
1:A:99:ILE:HG21	1:A:357:SER:HB3	1.87	0.56
1:B:373:LEU:HD11	1:B:391:THR:OG1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TRP:CZ3	1:B:98:TRP:CZ3	2.92	0.56
1:A:118:ILE:HG13	1:A:118:ILE:O	2.06	0.56
1:B:12:LEU:O	1:B:16:THR:HG23	2.06	0.56
1:A:44:TYR:O	1:A:47:LEU:N	2.39	0.56
1:A:78:ARG:CA	1:A:82:GLY:HA3	2.36	0.56
1:B:165:ILE:HA	1:B:169:GLY:H	1.71	0.56
1:A:120:LYS:HA	1:A:120:LYS:CE	2.35	0.55
1:B:216:VAL:HG23	1:B:299:GLN:NE2	2.22	0.55
1:A:216:VAL:O	1:A:216:VAL:HG12	2.06	0.55
1:B:102:ILE:CD1	1:B:337:PHE:HD2	2.14	0.55
1:A:105:VAL:CG2	1:A:133:LEU:HD21	2.37	0.55
1:A:351:GLY:C	1:A:353:VAL:H	2.10	0.55
1:B:44:TYR:O	1:B:47:LEU:N	2.39	0.55
1:A:54:LEU:HD11	1:A:233:LEU:HD23	1.88	0.55
1:A:216:VAL:HG23	1:A:299:GLN:NE2	2.22	0.55
1:A:302:LYS:HA	1:A:314:PHE:O	2.06	0.55
1:A:306:ASP:O	1:A:307:ASP:C	2.45	0.55
1:A:316:ARG:C	1:A:317:VAL:HG23	2.27	0.55
1:A:379:HIS:C	1:A:381:GLY:N	2.59	0.55
1:B:83:PRO:HB3	1:B:430:ARG:HH11	1.71	0.55
1:A:116:PHE:O	1:A:117:PRO:C	2.42	0.55
1:A:81:PHE:CZ	1:B:81:PHE:HA	2.42	0.55
1:B:317:VAL:HG13	1:B:322:THR:O	2.07	0.55
1:B:82:GLY:N	1:B:83:PRO:HD2	2.22	0.55
1:B:181:ALA:O	1:B:182:TRP:O	2.25	0.55
1:A:137:VAL:O	1:A:141:ILE:HG12	2.06	0.55
1:B:386:ALA:O	1:B:389:ALA:HB3	2.06	0.55
1:A:181:ALA:O	1:A:182:TRP:O	2.24	0.55
1:B:97:CYS:HB3	1:B:293:TRP:HE3	1.71	0.55
1:B:45:GLY:HA3	1:B:196:THR:OG1	2.06	0.55
1:B:355:SER:O	1:B:358:VAL:HB	2.06	0.55
1:B:205:ILE:CD1	1:B:358:VAL:HG13	2.36	0.55
1:A:280:PHE:CD2	1:A:281:CYS:N	2.75	0.55
1:A:78:ARG:O	1:A:82:GLY:HA3	2.07	0.55
1:B:302:LYS:HA	1:B:314:PHE:O	2.07	0.55
1:A:119:LEU:HD13	1:A:124:VAL:HG21	1.88	0.55
1:B:408:LYS:HD2	1:B:408:LYS:H	1.72	0.55
1:B:140:ASN:OD1	1:B:147:ILE:HG21	2.07	0.55
1:B:81:PHE:CD2	1:B:81:PHE:C	2.80	0.55
1:B:78:ARG:CA	1:B:82:GLY:HA3	2.36	0.55
1:B:236:ALA:O	1:B:239:TYR:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:CD2	1:A:314:PHE:N	2.74	0.55
1:A:81:PHE:HB2	1:A:85:LEU:HB2	1.87	0.55
1:A:129:CYS:SG	1:A:338:GLN:NE2	2.80	0.55
1:A:410:VAL:HG12	1:B:411:MET:HA	1.89	0.55
1:B:306:ASP:O	1:B:307:ASP:C	2.44	0.54
1:B:54:LEU:HD11	1:B:233:LEU:HD23	1.89	0.54
1:A:11:GLY:O	1:A:15:VAL:HG23	2.07	0.54
1:A:360:PHE:CE1	1:A:416:THR:HG21	2.42	0.54
1:A:76:TYR:HH	1:A:211:SER:HG	1.53	0.54
1:B:177:THR:O	1:B:180:ALA:HB3	2.08	0.54
1:A:204:PHE:HE1	1:A:232:VAL:HG13	1.71	0.54
1:A:82:GLY:N	1:A:83:PRO:HD2	2.23	0.54
1:A:114:TYR:C	1:A:115:PHE:HD2	2.11	0.54
1:B:280:PHE:CD2	1:B:281:CYS:N	2.75	0.54
1:A:318:ASN:O	1:A:319:LYS:O	2.26	0.54
1:B:314:PHE:HA	1:B:315:ALA:O	2.06	0.54
1:A:408:LYS:HD2	1:A:408:LYS:H	1.73	0.54
1:A:9:LYS:C	1:A:10:VAL:HG23	2.28	0.54
1:B:102:ILE:HG21	1:B:337:PHE:CD2	2.43	0.54
1:A:97:CYS:HB3	1:A:293:TRP:HE3	1.73	0.54
1:B:114:TYR:C	1:B:115:PHE:HD2	2.11	0.54
1:A:15:VAL:O	1:A:19:VAL:HG23	2.08	0.54
1:B:114:TYR:O	1:B:115:PHE:HB2	2.08	0.54
1:B:338:GLN:OE1	1:B:338:GLN:O	2.26	0.54
1:B:79:ARG:HB3	1:B:375:LEU:HD21	1.88	0.54
1:A:31:LEU:HD21	1:A:203:SER:OG	2.08	0.54
1:B:144:PRO:HD3	1:B:322:THR:HG23	1.90	0.53
1:B:77:ALA:HB3	1:B:89:THR:HG21	1.90	0.53
1:A:337:PHE:HZ	1:A:345:ASN:ND2	2.05	0.53
1:A:177:THR:O	1:A:180:ALA:HB3	2.08	0.53
1:B:118:ILE:HD12	1:B:119:LEU:N	2.22	0.53
1:A:139:LEU:HD22	1:A:146:MET:CE	2.38	0.53
1:A:94:TRP:CZ3	1:A:98:TRP:CZ3	2.95	0.53
1:A:338:GLN:OE1	1:A:338:GLN:O	2.26	0.53
1:A:79:ARG:HB3	1:A:375:LEU:HD21	1.90	0.53
1:B:329:ILE:O	1:B:333:LEU:HB2	2.08	0.53
1:B:376:GLY:O	1:B:379:HIS:N	2.42	0.53
1:B:86:GLY:HA2	1:B:89:THR:HG22	1.91	0.53
1:A:41:ILE:HA	1:A:42:ALA:C	2.28	0.53
1:A:41:ILE:HG13	1:A:43:ILE:CG1	2.36	0.53
1:A:45:GLY:HA3	1:A:196:THR:OG1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLY:O	1:B:15:VAL:HG23	2.07	0.53
1:A:102:ILE:HG21	1:A:337:PHE:CD2	2.44	0.53
1:A:8:HIS:O	1:A:9:LYS:HD3	2.09	0.53
1:B:316:ARG:C	1:B:317:VAL:HG23	2.28	0.53
1:A:225:PRO:O	1:A:226:ILE:C	2.46	0.53
1:A:428:TYR:CE1	1:B:373:LEU:HB3	2.44	0.53
1:B:82:GLY:H	1:B:83:PRO:HD2	1.74	0.53
1:B:9:LYS:C	1:B:10:VAL:HG23	2.29	0.53
1:B:161:PRO:HB3	1:B:278:VAL:HG22	1.90	0.53
1:A:408:LYS:H	1:A:408:LYS:CD	2.22	0.53
1:A:411:MET:HG3	1:A:412:TRP:N	2.24	0.53
1:B:52:GLY:HA3	1:B:397:TYR:HD2	1.74	0.53
1:A:427:ASN:O	1:A:429:ASN:N	2.34	0.53
1:A:101:ASN:CG	1:A:290:LEU:HD22	2.29	0.53
1:B:172:TRP:HE3	1:B:173:PHE:N	2.06	0.53
1:A:12:LEU:O	1:A:16:THR:HG23	2.09	0.53
1:A:143:GLY:HA2	1:A:146:MET:HB2	1.90	0.53
1:A:154:ALA:HB1	1:A:284:ALA:O	2.09	0.53
1:A:323:PRO:O	1:A:324:VAL:C	2.47	0.52
1:B:11:GLY:O	1:B:14:PRO:HD2	2.09	0.52
1:B:154:ALA:HB1	1:B:284:ALA:O	2.09	0.52
1:B:105:VAL:O	1:B:107:ILE:N	2.42	0.52
1:A:107:ILE:O	1:A:111:TYR:HD1	1.92	0.52
1:B:31:LEU:HD21	1:B:203:SER:OG	2.09	0.52
1:A:373:LEU:HD11	1:A:391:THR:OG1	2.09	0.52
1:A:118:ILE:HD12	1:A:118:ILE:C	2.29	0.52
1:A:124:VAL:O	1:A:128:THR:HB	2.09	0.52
1:B:351:GLY:C	1:B:353:VAL:H	2.13	0.52
1:B:143:GLY:HA2	1:B:146:MET:HB2	1.91	0.52
1:A:22:ASN:HB3	1:A:293:TRP:CD1	2.43	0.52
1:A:302:LYS:N	1:A:302:LYS:CD	2.72	0.52
1:A:303:ALA:O	1:A:306:ASP:N	2.26	0.52
1:A:209:SER:CB	1:A:296:LEU:HD11	2.40	0.52
1:B:337:PHE:HZ	1:B:345:ASN:ND2	2.07	0.52
1:A:105:VAL:O	1:A:107:ILE:N	2.42	0.52
1:A:337:PHE:HZ	1:A:345:ASN:HD21	1.58	0.52
1:A:172:TRP:HE3	1:A:173:PHE:N	2.08	0.52
1:B:125:LEU:HD23	1:B:125:LEU:O	2.08	0.52
1:A:71:GLY:O	1:A:212:VAL:HG13	2.10	0.52
1:A:78:ARG:C	1:A:82:GLY:HA3	2.30	0.52
1:B:216:VAL:HG12	1:B:216:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PHE:HB3	1:B:117:PRO:HD2	1.90	0.52
1:B:408:LYS:CD	1:B:408:LYS:H	2.21	0.52
1:B:92:LEU:HD21	1:B:363:VAL:HB	1.91	0.52
1:A:144:PRO:HD3	1:A:322:THR:HG23	1.92	0.52
1:B:318:ASN:O	1:B:319:LYS:O	2.28	0.52
1:B:173:PHE:CE1	1:B:247:MET:HB3	2.44	0.52
1:A:205:ILE:CD1	1:A:358:VAL:HG13	2.39	0.52
1:A:373:LEU:O	1:A:375:LEU:N	2.43	0.52
1:B:78:ARG:O	1:B:82:GLY:HA3	2.10	0.52
1:B:69:SER:OG	1:B:214:ALA:HB2	2.10	0.52
1:A:411:MET:HA	1:B:410:VAL:CG1	2.40	0.52
1:B:41:ILE:HA	1:B:42:ALA:C	2.30	0.52
1:A:317:VAL:HG13	1:A:322:THR:O	2.10	0.51
1:A:8:HIS:HB3	1:A:9:LYS:HE2	1.92	0.51
1:B:225:PRO:O	1:B:226:ILE:C	2.48	0.51
1:B:301:ALA:HB1	1:B:310:PHE:CE1	2.44	0.51
1:A:79:ARG:CB	1:A:375:LEU:HD11	2.37	0.51
1:A:81:PHE:CD2	1:A:81:PHE:C	2.82	0.51
1:B:371:ALA:O	1:B:373:LEU:N	2.43	0.51
1:B:384:ARG:NE	1:B:388:LEU:HD12	2.20	0.51
1:B:28:VAL:O	1:B:30:LEU:N	2.40	0.51
1:A:430:ARG:CG	1:B:374:LEU:HD23	2.20	0.51
1:B:237:VAL:HG12	1:B:238:CYS:N	2.25	0.51
1:A:236:ALA:O	1:A:239:TYR:HB2	2.09	0.51
1:A:136:PHE:CZ	1:A:287:LEU:O	2.63	0.51
1:A:391:THR:O	1:A:395:PHE:HD2	1.93	0.51
1:B:305:ALA:HB1	1:B:312:PRO:CB	2.40	0.51
1:A:344:PRO:O	1:A:345:ASN:HB2	2.11	0.51
1:B:22:ASN:N	1:B:22:ASN:HD22	2.06	0.51
1:B:136:PHE:CZ	1:B:287:LEU:O	2.64	0.51
1:A:46:TRP:HA	1:A:49:THR:HG22	1.93	0.51
1:A:416:THR:O	1:A:419:VAL:HG12	2.10	0.51
1:A:173:PHE:CE1	1:A:247:MET:HB3	2.45	0.51
1:B:173:PHE:CG	1:B:174:ARG:O	2.64	0.51
1:A:418:MET:SD	1:B:402:VAL:HG21	2.50	0.51
1:A:376:GLY:O	1:A:379:HIS:N	2.44	0.51
1:A:173:PHE:CG	1:A:174:ARG:O	2.63	0.51
1:A:371:ALA:O	1:A:373:LEU:N	2.43	0.51
1:A:342:ILE:CB	1:A:343:SER:CB	2.78	0.51
1:B:118:ILE:HD12	1:B:118:ILE:C	2.32	0.51
1:B:107:ILE:O	1:B:111:TYR:HD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:OD2	1:B:79:ARG:NH1	2.36	0.51
1:B:178:TYR:CD2	1:B:247:MET:HA	2.44	0.51
1:B:280:PHE:C	1:B:282:ALA:N	2.64	0.51
1:A:165:ILE:HG23	1:A:169:GLY:HA3	1.92	0.51
1:A:92:LEU:HD21	1:A:363:VAL:HB	1.93	0.51
1:B:344:PRO:O	1:B:345:ASN:HB2	2.11	0.51
1:B:371:ALA:C	1:B:373:LEU:N	2.65	0.51
1:B:247:MET:HG2	1:B:248:GLY:N	2.26	0.51
1:A:52:GLY:HA3	1:A:397:TYR:HD2	1.75	0.51
1:A:94:TRP:C	1:A:96:ALA:H	2.15	0.50
1:B:78:ARG:C	1:B:82:GLY:HA3	2.31	0.50
1:B:112:LEU:O	1:B:113:SER:C	2.50	0.50
1:B:24:MET:HE3	1:B:238:CYS:HB3	1.93	0.50
1:B:8:HIS:O	1:B:9:LYS:HD3	2.10	0.50
1:B:119:LEU:HD13	1:B:124:VAL:HG21	1.92	0.50
1:A:280:PHE:C	1:A:282:ALA:N	2.65	0.50
1:B:363:VAL:HB	1:B:364:PRO:HD3	1.93	0.50
1:B:365:TYR:HB3	1:B:398:CYS:SG	2.51	0.50
1:B:313:ILE:HG22	1:B:314:PHE:N	2.23	0.50
1:B:416:THR:O	1:B:419:VAL:HG12	2.12	0.50
1:B:96:ALA:HA	1:B:357:SER:HB2	1.92	0.50
1:A:216:VAL:CG2	1:A:299:GLN:NE2	2.74	0.50
1:A:94:TRP:O	1:A:96:ALA:N	2.40	0.50
1:A:116:PHE:HB3	1:A:117:PRO:HD2	1.91	0.50
1:A:161:PRO:HB3	1:A:278:VAL:HG22	1.92	0.50
1:B:57:SER:CB	1:B:232:VAL:HG21	2.39	0.50
1:B:101:ASN:CG	1:B:290:LEU:HD22	2.31	0.50
1:A:22:ASN:N	1:A:22:ASN:HD22	2.08	0.50
1:B:165:ILE:HG23	1:B:169:GLY:HA3	1.92	0.50
1:B:8:HIS:HB3	1:B:9:LYS:HE2	1.93	0.50
1:B:219:ASN:H	1:B:223:ASN:ND2	2.04	0.50
1:B:187:LEU:N	1:B:187:LEU:HD23	2.27	0.50
1:A:371:ALA:C	1:A:373:LEU:N	2.65	0.50
1:B:133:LEU:HD13	1:B:334:MET:HG2	1.94	0.50
1:A:102:ILE:CD1	1:A:337:PHE:HB3	2.42	0.50
1:B:27:GLY:O	1:B:30:LEU:HB2	2.12	0.50
1:B:105:VAL:CG2	1:B:133:LEU:HD21	2.40	0.49
1:B:71:GLY:C	1:B:212:VAL:HA	2.33	0.49
1:A:178:TYR:CD2	1:A:247:MET:HA	2.46	0.49
1:A:81:PHE:CE2	1:A:83:PRO:HB2	2.46	0.49
1:A:83:PRO:O	1:A:84:PHE:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:O	1:B:128:THR:HG22	2.11	0.49
1:B:22:ASN:N	1:B:22:ASN:ND2	2.60	0.49
1:A:44:TYR:CB	1:A:193:ILE:HD11	2.42	0.49
1:A:71:GLY:O	1:A:212:VAL:HA	2.12	0.49
1:B:403:VAL:CG1	1:B:404:GLY:N	2.75	0.49
1:B:302:LYS:N	1:B:302:LYS:CD	2.73	0.49
1:A:403:VAL:CG1	1:A:404:GLY:N	2.75	0.49
1:A:101:ASN:ND2	1:A:290:LEU:HD22	2.27	0.49
1:A:27:GLY:O	1:A:30:LEU:HB2	2.12	0.49
1:B:212:VAL:HG13	1:B:300:THR:OG1	2.13	0.49
1:B:81:PHE:C	1:B:81:PHE:HD2	2.16	0.49
1:B:122:PRO:C	1:B:124:VAL:H	2.15	0.49
1:A:82:GLY:H	1:A:83:PRO:HD2	1.78	0.49
1:B:151:GLN:HE21	1:B:155:THR:CG2	2.26	0.49
1:B:384:ARG:C	1:B:386:ALA:N	2.66	0.49
1:B:67:ASP:CG	1:B:79:ARG:NH1	2.61	0.49
1:A:54:LEU:O	1:A:58:MET:HE2	2.13	0.49
1:B:140:ASN:HB3	1:B:327:LEU:HD22	1.94	0.49
1:B:302:LYS:HE3	1:B:326:GLY:HA3	1.94	0.49
1:B:74:TYR:OH	1:B:87:TYR:CE1	2.66	0.49
1:A:104:MET:CE	1:A:286:CYS:HB3	2.42	0.49
1:A:58:MET:HA	1:A:61:ALA:HB3	1.94	0.49
1:B:323:PRO:O	1:B:324:VAL:C	2.51	0.48
1:A:247:MET:HG2	1:A:248:GLY:N	2.28	0.48
1:A:302:LYS:HE3	1:A:326:GLY:HA3	1.95	0.48
1:B:104:MET:CE	1:B:286:CYS:HB3	2.43	0.48
1:B:10:VAL:CG1	1:B:11:GLY:H	2.06	0.48
1:A:305:ALA:HB1	1:A:312:PRO:CB	2.42	0.48
1:B:101:ASN:ND2	1:B:294:THR:HG22	2.28	0.48
1:A:373:LEU:C	1:A:375:LEU:H	2.16	0.48
1:B:209:SER:CB	1:B:296:LEU:HD11	2.44	0.48
1:B:323:PRO:CD	1:B:327:LEU:HD11	2.40	0.48
1:B:384:ARG:HH21	1:B:388:LEU:HD11	1.78	0.48
1:A:373:LEU:HD13	1:B:428:TYR:CZ	2.48	0.48
1:A:140:ASN:OD1	1:A:147:ILE:HG21	2.14	0.48
1:A:83:PRO:HB3	1:A:430:ARG:HH11	1.79	0.48
1:A:112:LEU:O	1:A:113:SER:C	2.51	0.48
1:A:196:THR:O	1:A:200:THR:HG23	2.13	0.48
1:A:301:ALA:HB1	1:A:310:PHE:CE1	2.46	0.48
1:B:142:VAL:HG11	1:B:146:MET:HG3	1.96	0.48
1:A:11:GLY:O	1:A:14:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ILE:HG13	1:B:43:ILE:CG1	2.37	0.48
1:A:42:ALA:O	1:A:196:THR:HG21	2.14	0.48
1:A:410:VAL:CG1	1:B:411:MET:HA	2.43	0.48
1:A:154:ALA:HA	1:A:157:LEU:HD12	1.94	0.48
1:A:71:GLY:C	1:A:212:VAL:HA	2.34	0.48
1:B:19:VAL:CG2	1:B:210:ALA:HB2	2.44	0.48
1:B:216:VAL:CG2	1:B:299:GLN:NE2	2.76	0.48
1:A:151:GLN:HE21	1:A:155:THR:CG2	2.26	0.48
1:B:46:TRP:HA	1:B:49:THR:HG22	1.96	0.48
1:A:98:TRP:CD1	1:A:99:ILE:N	2.82	0.48
1:B:324:VAL:HG12	1:B:325:ALA:N	2.28	0.48
1:B:129:CYS:SG	1:B:338:GLN:NE2	2.87	0.48
1:B:93:TYR:HD2	1:B:300:THR:CG2	2.18	0.48
1:A:28:VAL:HG11	1:A:162:ILE:CD1	2.36	0.48
1:B:124:VAL:O	1:B:128:THR:HB	2.13	0.48
1:B:280:PHE:O	1:B:282:ALA:N	2.47	0.48
1:A:365:TYR:HB3	1:A:398:CYS:SG	2.53	0.48
1:A:187:LEU:N	1:A:187:LEU:HD23	2.29	0.48
1:A:83:PRO:O	1:A:86:GLY:N	2.44	0.48
1:B:333:LEU:HA	1:B:336:ILE:HD12	1.96	0.48
1:B:126:THR:HG21	1:B:342:ILE:CG2	2.40	0.48
1:A:44:TYR:O	1:A:45:GLY:C	2.50	0.48
1:B:408:LYS:O	1:B:411:MET:HG2	2.14	0.48
1:B:92:LEU:CD2	1:B:364:PRO:HD3	2.44	0.48
1:A:375:LEU:C	1:A:377:HIS:H	2.17	0.47
1:A:93:TYR:HD2	1:A:300:THR:CG2	2.17	0.47
1:A:402:VAL:HG21	1:B:418:MET:SD	2.54	0.47
1:A:57:SER:CB	1:A:232:VAL:HG21	2.36	0.47
1:A:96:ALA:HA	1:A:357:SER:HB2	1.96	0.47
1:B:71:GLY:O	1:B:212:VAL:HA	2.14	0.47
1:B:337:PHE:HZ	1:B:345:ASN:HD21	1.61	0.47
1:B:120:LYS:O	1:B:121:ASP:OD1	2.32	0.47
1:A:219:ASN:H	1:A:223:ASN:ND2	2.06	0.47
1:A:384:ARG:C	1:A:386:ALA:N	2.67	0.47
1:A:81:PHE:HD2	1:A:81:PHE:C	2.18	0.47
1:A:74:TYR:OH	1:A:87:TYR:CE1	2.67	0.47
1:A:92:LEU:CD2	1:A:364:PRO:HD3	2.44	0.47
1:B:15:VAL:O	1:B:19:VAL:HG23	2.14	0.47
1:B:328:ILE:O	1:B:332:ILE:HG13	2.15	0.47
1:B:99:ILE:CG2	1:B:357:SER:HB3	2.45	0.47
1:A:206:GLY:C	1:A:208:GLU:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASN:ND2	1:B:290:LEU:HD22	2.29	0.47
1:B:83:PRO:O	1:B:84:PHE:C	2.52	0.47
1:A:24:MET:HE3	1:A:238:CYS:HB3	1.96	0.47
1:A:41:ILE:N	1:A:42:ALA:HB3	2.29	0.47
1:A:120:LYS:O	1:A:121:ASP:OD1	2.33	0.47
1:A:126:THR:HG21	1:A:342:ILE:CG2	2.40	0.47
1:B:41:ILE:N	1:B:42:ALA:HB3	2.29	0.47
1:A:86:GLY:HA2	1:A:89:THR:HG22	1.97	0.47
1:B:391:THR:O	1:B:395:PHE:HD2	1.97	0.47
1:A:212:VAL:HG13	1:A:300:THR:OG1	2.15	0.47
1:A:384:ARG:HH21	1:A:388:LEU:HD11	1.79	0.47
1:A:71:GLY:O	1:A:212:VAL:O	2.33	0.47
1:A:105:VAL:CB	1:A:129:CYS:SG	2.86	0.47
1:B:16:THR:HG22	1:B:227:ALA:CA	2.37	0.47
1:A:54:LEU:HD11	1:A:233:LEU:CD2	2.45	0.47
1:B:412:TRP:HA	1:B:412:TRP:CE3	2.49	0.47
1:A:142:VAL:HG11	1:A:146:MET:HG3	1.96	0.47
1:B:208:GLU:O	1:B:212:VAL:HG23	2.15	0.47
1:A:114:TYR:CE1	1:A:118:ILE:HG12	2.49	0.47
1:A:351:GLY:C	1:A:353:VAL:N	2.68	0.47
1:B:115:PHE:O	1:B:116:PHE:O	2.33	0.47
1:A:19:VAL:CG2	1:A:210:ALA:HB2	2.44	0.47
1:A:74:TYR:HE1	1:A:86:GLY:C	2.18	0.47
1:B:421:THR:O	1:B:422:ALA:C	2.53	0.47
1:A:361:THR:C	1:A:364:PRO:HD2	2.35	0.47
1:A:421:THR:O	1:A:422:ALA:C	2.54	0.47
1:A:63:MET:CE	1:A:375:LEU:HD12	2.45	0.47
1:B:94:TRP:C	1:B:96:ALA:H	2.18	0.47
1:B:116:PHE:HB3	1:B:117:PRO:CD	2.45	0.47
1:A:428:TYR:CD1	1:B:373:LEU:HB3	2.50	0.46
1:B:42:ALA:O	1:B:196:THR:HG21	2.15	0.46
1:B:58:MET:HA	1:B:61:ALA:HB3	1.97	0.46
1:A:329:ILE:O	1:A:333:LEU:HB2	2.15	0.46
1:B:93:TYR:OH	1:B:208:GLU:CD	2.53	0.46
1:B:323:PRO:O	1:B:326:GLY:N	2.48	0.46
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.70	0.46
1:A:342:ILE:H	1:A:343:SER:HB2	1.78	0.46
1:A:173:PHE:HB3	1:A:178:TYR:OH	2.16	0.46
1:B:116:PHE:O	1:B:118:ILE:CG2	2.55	0.46
1:A:160:ILE:CB	1:A:161:PRO:HD3	2.41	0.46
1:A:69:SER:OG	1:A:214:ALA:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:HD12	1:A:147:ILE:O	2.15	0.46
1:A:119:LEU:HB3	1:A:120:LYS:H	1.51	0.46
1:B:31:LEU:HB2	1:B:32:PRO:HD3	1.98	0.46
1:A:317:VAL:O	1:A:318:ASN:C	2.52	0.46
1:B:72:GLY:N	1:B:211:SER:O	2.49	0.46
1:A:92:LEU:CD2	1:A:363:VAL:HB	2.46	0.46
1:B:305:ALA:HA	1:B:312:PRO:HG3	1.97	0.46
1:B:310:PHE:H	1:B:312:PRO:HD3	1.80	0.46
1:B:196:THR:O	1:B:200:THR:HG23	2.16	0.46
1:A:22:ASN:N	1:A:22:ASN:ND2	2.62	0.46
1:A:412:TRP:CE3	1:A:412:TRP:HA	2.51	0.46
1:A:77:ALA:HB3	1:A:89:THR:HG21	1.96	0.46
1:A:116:PHE:HB3	1:A:117:PRO:CD	2.46	0.46
1:A:332:ILE:HG22	1:A:336:ILE:HD11	1.97	0.46
1:B:302:LYS:HE3	1:B:326:GLY:CA	2.46	0.46
1:B:102:ILE:CD1	1:B:337:PHE:HB3	2.46	0.46
1:B:357:SER:HA	1:B:360:PHE:HD2	1.80	0.46
1:A:428:TYR:CE1	1:B:373:LEU:CB	2.99	0.46
1:B:425:ALA:CA	1:B:428:TYR:CZ	2.82	0.46
1:B:173:PHE:HB3	1:B:178:TYR:OH	2.16	0.46
1:A:237:VAL:HG12	1:A:238:CYS:N	2.31	0.46
1:A:408:LYS:O	1:A:411:MET:HG2	2.16	0.46
1:A:177:THR:CG2	1:A:247:MET:HB2	2.46	0.46
1:B:177:THR:CG2	1:B:247:MET:HB2	2.44	0.46
1:A:92:LEU:HD21	1:A:360:PHE:O	2.15	0.46
1:B:389:ALA:O	1:B:392:THR:N	2.49	0.46
1:B:342:ILE:H	1:B:343:SER:HB2	1.79	0.46
1:B:54:LEU:HD11	1:B:233:LEU:CD2	2.46	0.46
1:A:206:GLY:O	1:A:208:GLU:N	2.50	0.45
1:A:305:ALA:HA	1:A:312:PRO:HG3	1.97	0.45
1:B:376:GLY:CA	1:B:379:HIS:HA	2.46	0.45
1:B:81:PHE:HD2	1:B:82:GLY:N	2.14	0.45
1:A:102:ILE:O	1:A:106:VAL:HG23	2.16	0.45
1:B:140:ASN:HD21	1:B:147:ILE:HG12	1.78	0.45
1:B:126:THR:O	1:B:130:VAL:HG23	2.16	0.45
1:B:305:ALA:HA	1:B:312:PRO:CG	2.46	0.45
1:B:345:ASN:O	1:B:346:ALA:HB3	2.17	0.45
1:A:28:VAL:O	1:A:30:LEU:N	2.42	0.45
1:A:31:LEU:HB2	1:A:32:PRO:HD3	1.98	0.45
1:A:324:VAL:HG12	1:A:325:ALA:N	2.31	0.45
1:A:376:GLY:CA	1:A:379:HIS:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:CZ	1:A:421:THR:OG1	2.65	0.45
1:B:101:ASN:HD21	1:B:294:THR:HG22	1.81	0.45
1:B:209:SER:HB3	1:B:296:LEU:CD1	2.46	0.45
1:B:142:VAL:O	1:B:143:GLY:O	2.35	0.45
1:A:349:GLU:O	1:A:350:PHE:HB2	2.17	0.45
1:A:305:ALA:HA	1:A:312:PRO:CG	2.47	0.45
1:B:296:LEU:HD23	1:B:296:LEU:N	2.31	0.45
1:A:68:PRO:HA	1:A:69:SER:CB	2.46	0.45
1:A:314:PHE:CA	1:A:315:ALA:O	2.65	0.45
1:A:10:VAL:CG1	1:A:11:GLY:H	2.07	0.45
1:B:8:HIS:HA	1:B:145:LYS:CD	2.46	0.45
1:B:84:PHE:CZ	1:B:421:THR:OG1	2.68	0.45
1:A:339:LEU:HA	1:A:342:ILE:HG13	1.98	0.45
1:B:247:MET:CE	1:B:249:MET:HB2	2.47	0.45
1:B:81:PHE:CE1	1:B:84:PHE:HB3	2.52	0.45
1:A:81:PHE:HA	1:B:81:PHE:CZ	2.52	0.45
1:A:122:PRO:C	1:A:124:VAL:H	2.19	0.45
1:B:147:ILE:O	1:B:147:ILE:HD12	2.17	0.45
1:B:29:PHE:CD2	1:B:111:TYR:HE2	2.35	0.45
1:B:310:PHE:HB2	1:B:312:PRO:HG3	1.98	0.45
1:B:311:PRO:HG2	1:B:426:LEU:HD11	1.97	0.45
1:B:114:TYR:CE1	1:B:118:ILE:HG12	2.52	0.45
1:A:60:TYR:CE2	1:A:368:THR:HG21	2.52	0.45
1:B:104:MET:C	1:B:104:MET:HE2	2.36	0.45
1:A:337:PHE:CZ	1:A:345:ASN:ND2	2.85	0.45
1:B:120:LYS:CA	1:B:120:LYS:CE	2.95	0.45
1:A:184:VAL:C	1:A:186:GLY:H	2.20	0.45
1:B:194:GLN:O	1:B:198:ASN:HB2	2.17	0.45
1:B:105:VAL:C	1:B:107:ILE:N	2.69	0.44
1:B:311:PRO:HA	1:B:312:PRO:HD3	1.36	0.44
1:B:44:TYR:CB	1:B:193:ILE:HD11	2.45	0.44
1:B:44:TYR:O	1:B:45:GLY:C	2.54	0.44
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.71	0.44
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.71	0.44
1:A:323:PRO:CD	1:A:327:LEU:HD11	2.43	0.44
1:A:333:LEU:HA	1:A:336:ILE:HD12	1.99	0.44
1:A:93:TYR:O	1:A:94:TRP:C	2.56	0.44
1:B:60:TYR:HD1	1:B:211:SER:CB	2.30	0.44
1:A:247:MET:CE	1:A:249:MET:HB2	2.47	0.44
1:A:173:PHE:HE1	1:A:247:MET:HB3	1.82	0.44
1:B:114:TYR:C	1:B:115:PHE:CD2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:HA	1:B:157:LEU:HD12	1.98	0.44
1:B:361:THR:C	1:B:364:PRO:HD2	2.37	0.44
1:A:384:ARG:N	1:A:385:PRO:CD	2.81	0.44
1:B:374:LEU:N	1:B:374:LEU:HD12	2.26	0.44
1:A:422:ALA:CB	1:B:395:PHE:CD1	3.00	0.44
1:B:219:ASN:O	1:B:223:ASN:HB2	2.18	0.44
1:A:310:PHE:HB2	1:A:312:PRO:HG3	1.99	0.44
1:A:72:GLY:N	1:A:211:SER:O	2.50	0.44
1:B:102:ILE:O	1:B:106:VAL:HG23	2.17	0.44
1:B:133:LEU:HD11	1:B:338:GLN:CG	2.47	0.44
1:B:212:VAL:HG11	1:B:296:LEU:HB3	1.98	0.44
1:B:317:VAL:O	1:B:318:ASN:C	2.55	0.44
1:A:125:LEU:O	1:A:128:THR:HG22	2.17	0.44
1:A:346:ALA:O	1:A:348:LYS:N	2.45	0.44
1:A:428:TYR:HH	1:B:373:LEU:HD13	1.76	0.44
1:A:114:TYR:C	1:A:115:PHE:CD2	2.91	0.44
1:A:345:ASN:O	1:A:346:ALA:HB3	2.16	0.44
1:A:84:PHE:HZ	1:A:421:THR:OG1	1.98	0.44
1:B:322:THR:HA	1:B:323:PRO:HD3	1.83	0.44
1:B:360:PHE:CZ	1:B:416:THR:HG21	2.52	0.44
1:B:74:TYR:HE1	1:B:86:GLY:C	2.21	0.44
1:B:98:TRP:CD1	1:B:99:ILE:N	2.85	0.44
1:A:119:LEU:HD22	1:A:124:VAL:HG11	1.99	0.44
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.77	0.44
1:A:374:LEU:HD23	1:B:430:ARG:CG	2.27	0.44
1:A:81:PHE:CB	1:A:85:LEU:HB2	2.48	0.44
1:B:107:ILE:HG22	1:B:108:GLY:N	2.33	0.44
1:B:133:LEU:CD1	1:B:338:GLN:HG3	2.46	0.44
1:A:114:TYR:O	1:A:115:PHE:CB	2.65	0.44
1:B:54:LEU:O	1:B:58:MET:HE2	2.17	0.44
1:A:399:ILE:HG12	1:B:418:MET:HE2	1.99	0.44
1:B:350:PHE:C	1:B:352:LEU:H	2.22	0.44
1:A:299:GLN:C	1:A:301:ALA:H	2.21	0.44
1:A:363:VAL:HB	1:A:364:PRO:HD3	2.00	0.44
1:A:384:ARG:NE	1:A:388:LEU:HD12	2.20	0.44
1:B:60:TYR:CE2	1:B:368:THR:HG21	2.53	0.44
1:B:97:CYS:HB3	1:B:293:TRP:CE3	2.52	0.44
1:B:142:VAL:HG12	1:B:146:MET:HG3	1.98	0.44
1:A:193:ILE:HG23	1:A:197:LEU:HG	1.99	0.44
1:B:69:SER:CB	1:B:70:PRO:HA	2.48	0.44
1:A:280:PHE:CD2	1:A:280:PHE:C	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLY:O	1:B:212:VAL:O	2.36	0.43
1:A:188:GLY:O	1:A:189:THR:C	2.56	0.43
1:A:194:GLN:O	1:A:198:ASN:HB2	2.18	0.43
1:A:303:ALA:O	1:A:305:ALA:N	2.51	0.43
1:B:59:VAL:HG13	1:B:372:LEU:CD2	2.47	0.43
1:B:68:PRO:HG2	1:B:220:PRO:HB2	2.01	0.43
1:B:92:LEU:CD2	1:B:363:VAL:HB	2.47	0.43
1:A:319:LYS:H	1:A:319:LYS:HG3	1.65	0.43
1:A:76:TYR:CD2	1:A:76:TYR:N	2.86	0.43
1:B:98:TRP:HB2	1:B:330:VAL:HG13	2.00	0.43
1:B:375:LEU:C	1:B:377:HIS:H	2.21	0.43
1:A:395:PHE:CD1	1:B:422:ALA:HA	2.53	0.43
1:A:101:ASN:ND2	1:A:294:THR:HG22	2.33	0.43
1:A:16:THR:HG22	1:A:227:ALA:CA	2.35	0.43
1:A:276:ALA:HA	1:A:279:SER:OG	2.18	0.43
1:B:17:LEU:HD23	1:B:17:LEU:HA	1.76	0.43
1:A:59:VAL:HG13	1:A:372:LEU:CD2	2.49	0.43
1:A:389:ALA:O	1:A:392:THR:N	2.51	0.43
1:A:360:PHE:CZ	1:A:416:THR:HG21	2.54	0.43
1:A:421:THR:C	1:A:423:MET:N	2.71	0.43
1:B:63:MET:CE	1:B:375:LEU:HD12	2.48	0.43
1:B:250:ILE:N	1:B:251:PRO:CD	2.75	0.43
1:A:350:PHE:C	1:A:352:LEU:H	2.22	0.43
1:B:349:GLU:O	1:B:350:PHE:HB2	2.18	0.43
1:A:143:GLY:HA2	1:A:146:MET:CB	2.49	0.43
1:A:302:LYS:HE3	1:A:326:GLY:CA	2.49	0.43
1:B:74:TYR:OH	1:B:87:TYR:HE1	2.02	0.43
1:B:83:PRO:O	1:B:86:GLY:N	2.52	0.43
1:B:114:TYR:O	1:B:115:PHE:CB	2.67	0.43
1:A:142:VAL:O	1:A:143:GLY:O	2.36	0.43
1:A:74:TYR:OH	1:A:87:TYR:HE1	2.02	0.43
1:A:8:HIS:HA	1:A:145:LYS:CD	2.45	0.43
1:B:105:VAL:CB	1:B:129:CYS:SG	2.91	0.43
1:B:430:ARG:HG3	1:B:431:LEU:N	2.32	0.43
1:A:115:PHE:O	1:A:116:PHE:O	2.37	0.43
1:A:280:PHE:O	1:A:282:ALA:N	2.51	0.43
1:A:357:SER:HA	1:A:360:PHE:HD2	1.82	0.43
1:B:319:LYS:O	1:B:320:ALA:HB3	2.18	0.43
1:B:357:SER:HA	1:B:360:PHE:CD2	2.53	0.43
1:B:339:LEU:HA	1:B:342:ILE:HG13	2.01	0.43
1:A:102:ILE:HG23	1:A:338:GLN:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ARG:HA	1:B:175:GLY:HA3	1.83	0.43
1:B:193:ILE:HG23	1:B:197:LEU:HG	2.00	0.43
1:B:219:ASN:HD22	1:B:223:ASN:HD21	1.65	0.43
1:B:219:ASN:ND2	1:B:219:ASN:N	2.66	0.43
1:B:276:ALA:HA	1:B:279:SER:OG	2.18	0.43
1:A:357:SER:HA	1:A:360:PHE:CD2	2.53	0.43
1:B:173:PHE:HE1	1:B:247:MET:HB3	1.82	0.43
1:A:219:ASN:HD22	1:A:223:ASN:HD21	1.64	0.43
1:A:322:THR:HA	1:A:323:PRO:HD3	1.82	0.43
1:A:323:PRO:O	1:A:326:GLY:N	2.51	0.43
1:B:303:ALA:O	1:B:305:ALA:N	2.52	0.43
1:B:303:ALA:O	1:B:306:ASP:N	2.28	0.43
1:B:76:TYR:CD2	1:B:76:TYR:N	2.86	0.43
1:A:140:ASN:CB	1:A:327:LEU:CD2	2.94	0.43
1:B:332:ILE:HG22	1:B:336:ILE:HD11	2.01	0.43
1:B:373:LEU:C	1:B:375:LEU:H	2.22	0.43
1:B:102:ILE:HG23	1:B:338:GLN:HA	2.00	0.42
1:B:81:PHE:CE2	1:B:83:PRO:HB2	2.53	0.42
1:B:87:TYR:HE2	1:B:430:ARG:HH12	1.66	0.42
1:A:29:PHE:CD2	1:A:111:TYR:HE2	2.37	0.42
1:A:250:ILE:N	1:A:251:PRO:CD	2.74	0.42
1:A:219:ASN:O	1:A:223:ASN:HB2	2.19	0.42
1:A:311:PRO:HA	1:A:312:PRO:HD3	1.35	0.42
1:A:311:PRO:HG2	1:A:426:LEU:HD11	2.00	0.42
1:A:35:LEU:HA	1:A:38:THR:OG1	2.19	0.42
1:A:142:VAL:HG12	1:A:146:MET:HG3	2.00	0.42
1:A:147:ILE:HG23	1:A:148:THR:N	2.34	0.42
1:A:319:LYS:O	1:A:320:ALA:HB3	2.18	0.42
1:B:10:VAL:O	1:B:218:LYS:HG3	2.18	0.42
1:B:314:PHE:CA	1:B:315:ALA:O	2.67	0.42
1:B:346:ALA:O	1:B:348:LYS:N	2.45	0.42
1:A:105:VAL:C	1:A:107:ILE:N	2.70	0.42
1:A:250:ILE:HB	1:A:251:PRO:HD3	2.01	0.42
1:B:180:ALA:C	1:B:182:TRP:H	2.21	0.42
1:B:119:LEU:HD22	1:B:124:VAL:HG11	1.99	0.42
1:B:295:LEU:O	1:B:295:LEU:HD22	2.18	0.42
1:A:313:ILE:HG22	1:A:314:PHE:N	2.19	0.42
1:A:99:ILE:CG2	1:A:357:SER:HB3	2.49	0.42
1:A:89:THR:HG23	1:A:90:ASN:N	2.34	0.42
1:B:104:MET:HE1	1:B:286:CYS:HB3	2.00	0.42
1:B:147:ILE:HD11	1:B:291:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLY:C	1:B:353:VAL:N	2.70	0.42
1:A:67:ASP:OD2	1:A:79:ARG:NH1	2.44	0.42
1:A:81:PHE:CE1	1:A:84:PHE:HB3	2.54	0.42
1:B:144:PRO:CB	1:B:216:VAL:HG11	2.49	0.42
1:B:332:ILE:H	1:B:332:ILE:HG13	1.61	0.42
1:B:87:TYR:CB	1:B:424:TYR:OH	2.68	0.42
1:A:310:PHE:H	1:A:312:PRO:HD3	1.83	0.42
1:A:379:HIS:ND1	1:A:387:TYR:CD2	2.82	0.42
1:B:84:PHE:HZ	1:B:421:THR:OG1	2.01	0.42
1:B:93:TYR:O	1:B:96:ALA:HB3	2.20	0.42
1:A:174:ARG:HA	1:A:175:GLY:HA3	1.85	0.42
1:A:140:ASN:HB3	1:A:327:LEU:HD22	1.96	0.42
1:A:60:TYR:HD1	1:A:211:SER:CB	2.33	0.42
1:B:299:GLN:C	1:B:301:ALA:H	2.21	0.42
1:A:126:THR:O	1:A:130:VAL:HG23	2.19	0.42
1:B:177:THR:HB	1:B:247:MET:HB2	2.00	0.42
1:B:119:LEU:HB3	1:B:120:LYS:H	1.50	0.42
1:A:208:GLU:O	1:A:212:VAL:HG23	2.20	0.42
1:A:87:TYR:CB	1:A:424:TYR:OH	2.68	0.42
1:A:98:TRP:CG	1:A:99:ILE:N	2.87	0.42
1:B:101:ASN:O	1:B:102:ILE:C	2.58	0.42
1:A:84:PHE:HD1	1:B:85:LEU:HD11	1.82	0.42
1:A:180:ALA:C	1:A:182:TRP:H	2.22	0.42
1:B:34:ASN:CB	1:B:199:VAL:HG11	2.48	0.42
1:B:188:GLY:O	1:B:189:THR:C	2.57	0.42
1:A:296:LEU:HD23	1:A:296:LEU:N	2.34	0.42
1:A:63:MET:HE1	1:A:375:LEU:HD12	2.02	0.42
1:A:105:VAL:O	1:A:106:VAL:C	2.57	0.42
1:B:183:ASN:O	1:B:184:VAL:O	2.37	0.42
1:B:184:VAL:C	1:B:186:GLY:H	2.22	0.42
1:A:400:TRP:O	1:A:403:VAL:HG12	2.20	0.42
1:A:134:TRP:CH2	1:A:331:GLY:HA3	2.55	0.42
1:A:81:PHE:HD2	1:A:82:GLY:N	2.17	0.42
1:A:93:TYR:O	1:A:96:ALA:HB3	2.19	0.42
1:A:104:MET:C	1:A:104:MET:HE2	2.39	0.42
1:B:280:PHE:C	1:B:280:PHE:CD2	2.94	0.42
1:A:411:MET:O	1:A:415:VAL:HG23	2.20	0.42
1:B:98:TRP:CG	1:B:99:ILE:N	2.88	0.41
1:B:173:PHE:HE1	1:B:247:MET:CG	2.33	0.41
1:A:31:LEU:CB	1:A:32:PRO:HD3	2.50	0.41
1:A:428:TYR:CE2	1:B:373:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PRO:O	1:B:228:THR:N	2.54	0.41
1:B:35:LEU:HA	1:B:38:THR:OG1	2.20	0.41
1:A:97:CYS:HB3	1:A:293:TRP:CE3	2.53	0.41
1:A:209:SER:HB3	1:A:296:LEU:CD1	2.43	0.41
1:A:430:ARG:HG3	1:A:431:LEU:N	2.32	0.41
1:B:105:VAL:O	1:B:106:VAL:C	2.58	0.41
1:B:206:GLY:O	1:B:208:GLU:N	2.54	0.41
1:A:172:TRP:HB3	1:A:173:PHE:H	1.64	0.41
1:B:244:THR:C	1:B:246:ILE:HG22	2.40	0.41
1:B:104:MET:O	1:B:104:MET:CE	2.65	0.41
1:B:81:PHE:CB	1:B:85:LEU:HB2	2.48	0.41
1:B:24:MET:HE3	1:B:238:CYS:CB	2.49	0.41
1:B:384:ARG:N	1:B:385:PRO:CD	2.83	0.41
1:B:93:TYR:O	1:B:94:TRP:C	2.57	0.41
1:A:133:LEU:CD1	1:A:338:GLN:HG3	2.48	0.41
1:B:143:GLY:HA2	1:B:146:MET:CB	2.50	0.41
1:A:183:ASN:O	1:A:184:VAL:O	2.38	0.41
1:A:374:LEU:N	1:A:374:LEU:HD12	2.26	0.41
1:A:105:VAL:O	1:A:108:GLY:N	2.54	0.41
1:A:44:TYR:HB2	1:A:193:ILE:CD1	2.49	0.41
1:B:411:MET:O	1:B:415:VAL:HG23	2.20	0.41
1:A:10:VAL:CG1	1:A:11:GLY:N	2.69	0.41
1:A:129:CYS:HB3	1:A:338:GLN:NE2	2.36	0.41
1:B:172:TRP:CE3	1:B:173:PHE:N	2.88	0.41
1:B:206:GLY:C	1:B:208:GLU:N	2.73	0.41
1:B:335:THR:O	1:B:336:ILE:C	2.59	0.41
1:A:328:ILE:O	1:A:332:ILE:HG13	2.20	0.41
1:B:301:ALA:C	1:B:303:ALA:N	2.74	0.41
1:B:423:MET:C	1:B:424:TYR:HD2	2.24	0.41
1:B:90:ASN:O	1:B:93:TYR:N	2.53	0.41
1:B:310:PHE:CB	1:B:312:PRO:HG3	2.51	0.41
1:B:60:TYR:CD2	1:B:368:THR:HG21	2.56	0.41
1:A:120:LYS:CE	1:A:120:LYS:CA	2.97	0.41
1:A:132:VAL:O	1:A:133:LEU:C	2.59	0.41
1:A:107:ILE:O	1:A:111:TYR:CD1	2.74	0.41
1:A:119:LEU:HB3	1:A:124:VAL:HG11	2.02	0.41
1:B:172:TRP:HB3	1:B:173:PHE:H	1.65	0.41
1:B:250:ILE:HB	1:B:251:PRO:HD3	2.02	0.41
1:B:122:PRO:C	1:B:124:VAL:N	2.74	0.41
1:B:109:VAL:HB	1:B:125:LEU:HD21	2.02	0.41
1:B:28:VAL:HG11	1:B:162:ILE:CD1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:N	1:A:219:ASN:ND2	2.68	0.41
1:A:68:PRO:HA	1:A:69:SER:HB3	2.03	0.41
1:A:68:PRO:HG2	1:A:220:PRO:HB2	2.03	0.41
1:B:362:LEU:O	1:B:365:TYR:N	2.54	0.41
1:B:134:TRP:CH2	1:B:331:GLY:HA3	2.55	0.41
1:A:301:ALA:C	1:A:303:ALA:N	2.73	0.41
1:A:87:TYR:HE2	1:A:430:ARG:HH12	1.69	0.41
1:B:321:GLY:O	1:B:322:THR:O	2.39	0.41
1:A:109:VAL:HB	1:A:125:LEU:HD21	2.03	0.41
1:A:173:PHE:HE1	1:A:247:MET:CG	2.34	0.41
1:B:160:ILE:CB	1:B:161:PRO:HD3	2.42	0.41
1:A:244:THR:C	1:A:246:ILE:HG22	2.42	0.41
1:A:299:GLN:HA	1:A:299:GLN:OE1	2.21	0.40
1:A:374:LEU:CD1	1:A:374:LEU:H	2.27	0.40
1:A:29:PHE:O	1:A:30:LEU:HG	2.21	0.40
1:B:400:TRP:O	1:B:403:VAL:HG12	2.21	0.40
1:B:423:MET:C	1:B:424:TYR:CD2	2.95	0.40
1:A:177:THR:HB	1:A:247:MET:HB2	2.03	0.40
1:A:224:VAL:HB	1:A:225:PRO:HD3	2.02	0.40
1:A:224:VAL:O	1:A:227:ALA:HB3	2.21	0.40
1:A:47:LEU:HA	1:A:47:LEU:HD22	1.90	0.40
1:A:144:PRO:C	1:A:146:MET:N	2.75	0.40
1:A:391:THR:O	1:A:395:PHE:CD2	2.74	0.40
1:B:10:VAL:CG1	1:B:11:GLY:N	2.66	0.40
1:B:384:ARG:O	1:B:385:PRO:C	2.59	0.40
1:A:289:SER:O	1:A:290:LEU:C	2.59	0.40
1:B:154:ALA:O	1:B:157:LEU:HB2	2.22	0.40
1:A:321:GLY:O	1:A:322:THR:O	2.39	0.40
1:A:81:PHE:CB	1:A:82:GLY:CA	2.95	0.40
1:B:337:PHE:CZ	1:B:345:ASN:ND2	2.88	0.40
1:B:374:LEU:CD1	1:B:374:LEU:H	2.30	0.40
1:A:141:ILE:CG2	1:A:324:VAL:HG22	2.50	0.40
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.70	0.40
1:B:379:HIS:ND1	1:B:387:TYR:CD2	2.81	0.40
1:A:104:MET:HE1	1:A:286:CYS:HB3	2.02	0.40
1:A:101:ASN:HD21	1:A:294:THR:HG22	1.87	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/445 (91%)	261 (64%)	82 (20%)	63 (16%)	0	4
1	B	406/445 (91%)	262 (64%)	80 (20%)	64 (16%)	0	4
All	All	812/890 (91%)	523 (64%)	162 (20%)	127 (16%)	0	4

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	68	PRO
1	A	83	PRO
1	A	116	PHE
1	A	117	PRO
1	A	118	ILE
1	A	182	TRP
1	A	183	ASN
1	A	184	VAL
1	A	218	LYS
1	A	312	PRO
1	A	313	ILE
1	A	319	LYS
1	A	323	PRO
1	A	345	ASN
1	A	377	HIS
1	A	428	TYR
1	A	431	LEU
1	A	432	HIS
1	B	10	VAL
1	B	68	PRO
1	B	83	PRO
1	B	116	PHE
1	B	117	PRO
1	B	118	ILE

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Mol	Chain	Res	Type
1	B	182	TRP
1	B	184	VAL
1	B	218	LYS
1	B	312	PRO
1	B	313	ILE
1	B	319	LYS
1	B	345	ASN
1	B	377	HIS
1	B	428	TYR
1	B	431	LEU
1	B	432	HIS
1	A	30	LEU
1	A	95	LEU
1	A	119	LEU
1	A	122	PRO
1	A	143	GLY
1	A	172	TRP
1	A	250	ILE
1	A	304	ALA
1	A	307	ASP
1	A	315	ALA
1	A	374	LEU
1	B	30	LEU
1	B	95	LEU
1	B	119	LEU
1	B	122	PRO
1	B	143	GLY
1	B	172	TRP
1	B	183	ASN
1	B	250	ILE
1	B	304	ALA
1	B	307	ASP
1	B	315	ALA
1	B	323	PRO
1	B	336	ILE
1	B	374	LEU
1	A	41	ILE
1	A	69	SER
1	A	121	ASP
1	A	303	ALA
1	A	310	PHE
1	A	314	PHE

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Mol	Chain	Res	Type
1	A	349	GLU
1	A	380	PHE
1	A	433	LYS
1	B	69	SER
1	B	121	ASP
1	B	310	PHE
1	B	347	THR
1	B	349	GLU
1	B	372	LEU
1	B	380	PHE
1	A	84	PHE
1	A	96	ALA
1	A	120	LYS
1	A	190	PHE
1	A	214	ALA
1	A	248	GLY
1	A	289	SER
1	A	343	SER
1	A	347	THR
1	A	372	LEU
1	B	41	ILE
1	B	73	SER
1	B	96	ALA
1	B	120	LYS
1	B	214	ALA
1	B	248	GLY
1	B	281	CYS
1	B	289	SER
1	B	303	ALA
1	B	314	PHE
1	B	335	THR
1	B	343	SER
1	B	433	LYS
1	A	322	THR
1	B	84	PHE
1	B	190	PHE
1	B	301	ALA
1	B	322	THR
1	A	73	SER
1	A	281	CYS
1	A	301	ALA
1	B	91	VAL

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Mol	Chain	Res	Type
1	B	246	ILE
1	A	25	GLY
1	A	246	ILE
1	A	336	ILE
1	A	317	VAL
1	B	25	GLY
1	B	161	PRO
1	B	317	VAL
1	A	161	PRO
1	A	324	VAL
1	A	353	VAL
1	B	353	VAL
1	A	71	GLY
1	A	91	VAL
1	A	175	GLY
1	B	175	GLY
1	B	71	GLY
1	B	106	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/343 (92%)	246 (78%)	68 (22%)	1	9
1	B	314/343 (92%)	245 (78%)	69 (22%)	1	8
All	All	628/686 (92%)	491 (78%)	137 (22%)	1	9

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	26	SER
1	A	29	PHE
1	A	35	LEU
1	A	56	LEU

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Mol	Chain	Res	Type
1	A	57	SER
1	A	69	SER
1	A	81	PHE
1	A	88	GLN
1	A	95	LEU
1	A	97	CYS
1	A	98	TRP
1	A	104	MET
1	A	105	VAL
1	A	107	ILE
1	A	116	PHE
1	A	117	PRO
1	A	118	ILE
1	A	120	LYS
1	A	124	VAL
1	A	126	THR
1	A	127	ILE
1	A	128	THR
1	A	129	CYS
1	A	141	ILE
1	A	147	ILE
1	A	148	THR
1	A	149	ARG
1	A	159	LEU
1	A	171	PHE
1	A	172	TRP
1	A	173	PHE
1	A	178	TYR
1	A	182	TRP
1	A	187	LEU
1	A	194	GLN
1	A	199	VAL
1	A	202	TRP
1	A	204	PHE
1	A	219	ASN
1	A	237	VAL
1	A	247	MET
1	A	279	SER
1	A	280	PHE
1	A	295	LEU
1	A	302	LYS
1	A	309	LEU

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Mol	Chain	Res	Type
1	A	310	PHE
1	A	314	PHE
1	A	329	ILE
1	A	333	LEU
1	A	334	MET
1	A	338	GLN
1	A	339	LEU
1	A	354	SER
1	A	361	THR
1	A	362	LEU
1	A	366	LEU
1	A	377	HIS
1	A	384	ARG
1	A	388	LEU
1	A	390	VAL
1	A	396	LEU
1	A	403	VAL
1	A	408	LYS
1	A	410	VAL
1	A	419	VAL
1	A	424	TYR
1	B	22	ASN
1	B	26	SER
1	B	29	PHE
1	B	35	LEU
1	B	47	LEU
1	B	56	LEU
1	B	57	SER
1	B	69	SER
1	B	81	PHE
1	B	88	GLN
1	B	95	LEU
1	B	97	CYS
1	B	98	TRP
1	B	104	MET
1	B	105	VAL
1	B	107	ILE
1	B	116	PHE
1	B	117	PRO
1	B	118	ILE
1	B	120	LYS
1	B	124	VAL

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Mol	Chain	Res	Type
1	B	126	THR
1	B	127	ILE
1	B	128	THR
1	B	129	CYS
1	B	141	ILE
1	B	147	ILE
1	B	148	THR
1	B	149	ARG
1	B	159	LEU
1	B	171	PHE
1	B	172	TRP
1	B	173	PHE
1	B	178	TYR
1	B	182	TRP
1	B	185	SER
1	B	187	LEU
1	B	194	GLN
1	B	199	VAL
1	B	202	TRP
1	B	204	PHE
1	B	219	ASN
1	B	237	VAL
1	B	247	MET
1	B	279	SER
1	B	280	PHE
1	B	295	LEU
1	B	302	LYS
1	B	309	LEU
1	B	310	PHE
1	B	314	PHE
1	B	329	ILE
1	B	333	LEU
1	B	334	MET
1	B	338	GLN
1	B	339	LEU
1	B	347	THR
1	B	354	SER
1	B	362	LEU
1	B	366	LEU
1	B	377	HIS
1	B	384	ARG
1	B	388	LEU

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Mol	Chain	Res	Type
1	B	390	VAL
1	B	396	LEU
1	B	403	VAL
1	B	408	LYS
1	B	419	VAL
1	B	424	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	151	GLN
1	A	223	ASN
1	A	338	GLN
1	A	379	HIS
1	B	22	ASN
1	B	151	GLN
1	B	223	ASN
1	B	379	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](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	410/445 (92%)	-0.05	14 (3%) 49 35	109, 173, 311, 406	0
1	B	410/445 (92%)	-0.17	11 (2%) 58 43	108, 172, 311, 406	0
All	All	820/890 (92%)	-0.11	25 (3%) 54 39	108, 172, 313, 406	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ALA	7.3
1	A	37	SER	4.1
1	A	248	GLY	4.1
1	B	170	TRP	3.9
1	A	287	LEU	3.4
1	B	167	VAL	3.4
1	A	343	SER	3.4
1	B	287	LEU	3.1
1	A	204	PHE	3.1
1	B	168	PHE	3.0
1	A	182	TRP	2.9
1	B	288	GLY	2.8
1	B	171	PHE	2.6
1	B	190	PHE	2.5
1	B	202	TRP	2.5
1	A	183	ASN	2.5
1	A	218	LYS	2.4
1	B	349	GLU	2.4
1	A	39	GLY	2.3
1	A	10	VAL	2.3
1	A	434	ASN	2.2
1	B	204	PHE	2.1
1	A	203	SER	2.1
1	A	29	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	TRP	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.