



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:51 PM GMT

PDB ID : 1QZX
Title : Crystal structure of the complete core of archaeal SRP and implications for inter-domain communication
Authors : Rosendal, K.R.; Wild, K.; Montoya, G.; Sinning, I.
Deposited on : 2003-09-18
Resolution : 4.00 Å(reported)

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

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

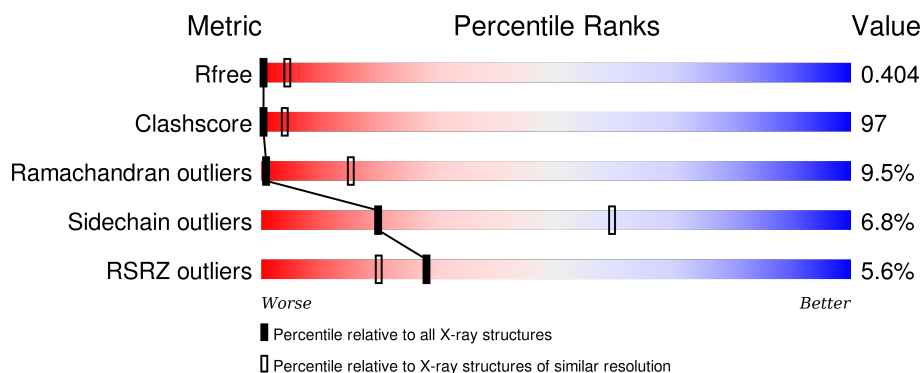
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

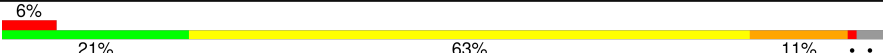
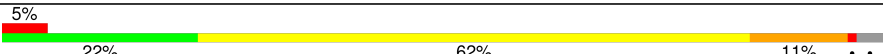
The reported resolution of this entry is 4.00 Å.

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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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 ≥ 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	440	 6% 21% 63% 11% • •
1	B	440	 5% 22% 62% 11% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6698 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 Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3349	2142	565	628	14			
1	B	425	Total	C	N	O	S	0	0	0
			3349	2142	565	628	14			

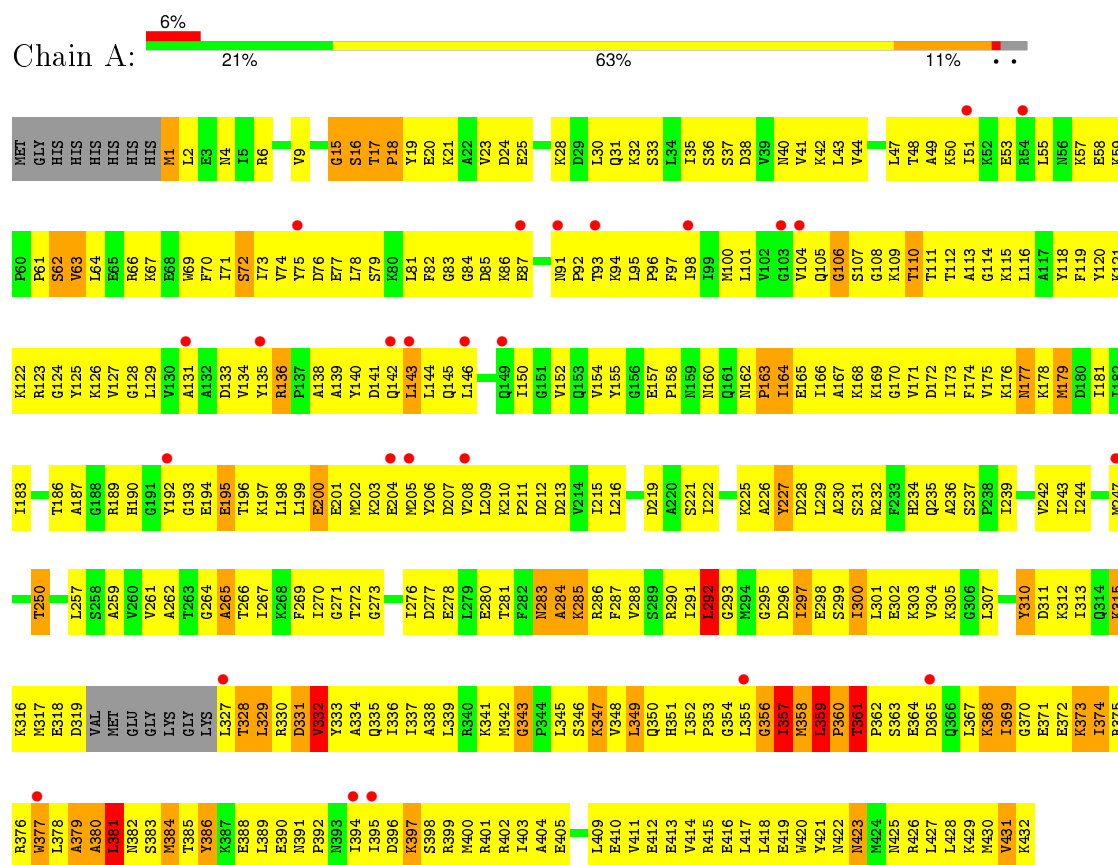
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7
A	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
A	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7
B	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
B	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
B	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7

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: Signal recognition 54 kDa protein



K121	K122	K123	K124	K125	K126	K127	K128	K129	K130	A131	A132	D133	V134	K135	A136	P137	A138	A139	D140	D141	Q142	L143		Q149	I150	G151	V152	Q153	V154	I155	I156	E157	P158	N159	M160	Q161	M162	P163	I164	E165	L166	A167	K168	K169	G170	V171	D172	I173	F174	V175	K176	M177	K178	M179	D180	I181			
K315	K316	K317	D318	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374				
K375	K376	K377	L378	A379	A380	K381	K382	S383	K384	K385	K386	K387	L388	E389	N390	P392	N393	L394	L395	D396	K397	S398	K399	N400	P401	N402	L403	E404		L409	E410	V411	E412	E413	V414	E415		E417	L418	E419	N420	V421	N422	N423	N424	N425	N426	L427	L428	K429	V430	V431	K432						
M247	I182	I183		T186	A187	G188	H189	G190	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K203	E204	M205	D206	V207	D208	L209	K210	P211	D212	D213	V214	L215	L216		D219	A220	S221	I222		K225	A226	Y227	D228	L229	A230	S231	R232	F233	G234	Q235	V304	K236	S237	L239		Y340	D342	I243	I244	I181
K316	K317	D319	VAL	MET	GLU	GLY	LYS	GLY	LNS	L327	T328	L329	A330	D331	V332	Y333	A334	A338	L339	R340	K341	M342	G343	P344	L345	S346	K347	V348	L349	Q350	H351	I352	P353	G354	L355	G356	I357	M358	L359	P360	T361	P362	S363	E364	D365	Q366	L367	K368	I369	G370	E371	E372	K373	I374					
M247	I182	I183		T186	A187	G188	H190	G191	Y192	G193	E194	T196	K197	L198	L199	E200	E201	M202	K2																																								

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	197.91Å 197.91Å 64.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 38.81 – 4.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (40.00-4.00) 97.9 (38.81-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.313 , 0.383 0.402 , 0.404	Depositor DCC
R_{free} test set	725 reflections (6.88%)	DCC
Wilson B-factor (Å ²)	171.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.6	EDS
Estimated twinning fraction	0.428 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 10545 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6698	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	0.71	5/3399 (0.1%)	0.88	4/4569 (0.1%)
1	B	0.71	5/3399 (0.1%)	0.88	4/4569 (0.1%)
All	All	0.71	10/6798 (0.1%)	0.88	8/9138 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	THR	CB-CG2	-6.78	1.29	1.52
1	B	361	THR	CB-CG2	-6.78	1.29	1.52
1	B	227	TYR	CD2-CE2	-5.99	1.30	1.39
1	A	227	TYR	CD2-CE2	-5.96	1.30	1.39
1	A	361	THR	CA-CB	5.92	1.68	1.53
1	B	361	THR	CA-CB	5.91	1.68	1.53
1	B	360	PRO	N-CD	5.33	1.55	1.47
1	A	360	PRO	N-CD	5.33	1.55	1.47
1	A	360	PRO	C-N	-5.15	1.22	1.34
1	B	360	PRO	C-N	-5.13	1.22	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	LEU	CA-CB-CG	-5.79	101.99	115.30
1	B	292	LEU	CA-CB-CG	-5.77	102.03	115.30
1	B	361	THR	N-CA-CB	5.21	120.20	110.30
1	A	361	THR	N-CA-CB	5.20	120.19	110.30
1	B	332	VAL	N-CA-C	-5.16	97.06	111.00
1	A	332	VAL	N-CA-C	-5.16	97.07	111.00
1	B	359	LEU	CB-CA-C	5.02	119.74	110.20
1	A	359	LEU	CB-CA-C	5.02	119.74	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3349	0	3486	713	43
1	B	3349	0	3486	708	43
All	All	6698	0	6972	1324	43

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 97.

All (1324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PRO:HD3	1:B:367:LEU:CD2	1.43	1.47
1:B:190:HIS:CD2	1:B:197:LYS:HD2	1.49	1.45
1:A:190:HIS:CD2	1:A:197:LYS:HD2	1.49	1.44
1:A:362:PRO:HD3	1:A:367:LEU:CD2	1.43	1.43
1:B:359:LEU:CG	1:B:360:PRO:HD3	1.49	1.42
1:A:359:LEU:CG	1:A:360:PRO:HD3	1.49	1.39
1:A:362:PRO:CD	1:A:367:LEU:HD21	1.54	1.38
1:B:362:PRO:CD	1:B:367:LEU:HD21	1.54	1.38
1:A:361:THR:HA	1:A:367:LEU:CD1	1.54	1.36
1:A:385:THR:HG21	1:B:382:ASN:O	1.25	1.35
1:A:382:ASN:O	1:B:385:THR:HG21	1.27	1.34
1:B:361:THR:HA	1:B:367:LEU:CD1	1.54	1.34
1:A:361:THR:CA	1:A:367:LEU:HD11	1.62	1.28
1:B:361:THR:CA	1:B:367:LEU:HD11	1.62	1.27
1:A:164:ILE:CD1	1:A:208:VAL:HG21	1.66	1.24
1:B:164:ILE:CD1	1:B:208:VAL:HG21	1.66	1.24
1:B:92:PRO:HB2	1:B:97:PHE:CE2	1.75	1.21
1:B:359:LEU:CD1	1:B:360:PRO:HD3	1.70	1.20
1:A:92:PRO:HB2	1:A:97:PHE:CE2	1.75	1.20
1:A:359:LEU:CD1	1:A:360:PRO:HD3	1.70	1.20
1:A:2:LEU:HD22	1:A:291:ILE:HG21	1.23	1.17
1:B:356:GLY:O	1:B:357:ILE:HG13	1.47	1.14
1:B:164:ILE:HD11	1:B:208:VAL:HG21	1.20	1.13
1:A:190:HIS:CD2	1:A:197:LYS:CD	2.31	1.13
1:B:359:LEU:HG	1:B:360:PRO:HD3	1.15	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HG	1:A:360:PRO:HD3	1.15	1.13
1:B:190:HIS:CD2	1:B:197:LYS:CD	2.31	1.13
1:B:194:GLU:HB3	1:B:197:LYS:CE	1.80	1.11
1:A:129:LEU:HD13	1:A:143:LEU:HD21	1.29	1.11
1:A:194:GLU:HB3	1:A:197:LYS:CE	1.80	1.11
1:B:2:LEU:HD22	1:B:291:ILE:HG21	1.23	1.11
1:B:17:THR:HG22	1:B:18:PRO:CD	1.81	1.10
1:A:356:GLY:O	1:A:357:ILE:HG13	1.47	1.10
1:A:17:THR:HG22	1:A:18:PRO:CD	1.82	1.10
1:A:194:GLU:HB3	1:A:197:LYS:HE3	1.16	1.10
1:A:164:ILE:HD11	1:A:208:VAL:CG2	1.82	1.09
1:B:164:ILE:HD11	1:B:208:VAL:CG2	1.82	1.08
1:B:129:LEU:HD13	1:B:143:LEU:HD21	1.29	1.08
1:B:359:LEU:HG	1:B:360:PRO:CD	1.84	1.07
1:A:164:ILE:HD11	1:A:208:VAL:HG21	1.20	1.07
1:A:17:THR:CG2	1:A:18:PRO:HD2	1.83	1.07
1:A:359:LEU:HG	1:A:360:PRO:CD	1.84	1.07
1:B:190:HIS:CG	1:B:197:LYS:HD2	1.88	1.07
1:B:194:GLU:HB3	1:B:197:LYS:HE3	1.16	1.07
1:B:17:THR:CG2	1:B:18:PRO:HD2	1.83	1.07
1:A:126:LYS:HE3	1:B:364:GLU:OE2	1.54	1.07
1:A:122:LYS:O	1:B:359:LEU:HD13	1.55	1.06
1:A:190:HIS:CG	1:A:197:LYS:HD2	1.88	1.06
1:B:409:LEU:HD13	1:B:413:GLU:OE1	1.56	1.06
1:B:157:GLU:HB3	1:B:160:ASN:ND2	1.70	1.06
1:A:364:GLU:OE2	1:B:126:LYS:HE3	1.56	1.05
1:A:157:GLU:HB3	1:A:160:ASN:ND2	1.69	1.05
1:B:378:LEU:HA	1:B:381:LEU:HD12	1.39	1.05
1:A:409:LEU:HD13	1:A:413:GLU:OE1	1.56	1.05
1:A:348:VAL:O	1:A:352:ILE:HG13	1.56	1.05
1:A:378:LEU:HA	1:A:381:LEU:HD12	1.39	1.04
1:A:359:LEU:HD13	1:B:122:LYS:O	1.57	1.04
1:B:194:GLU:CB	1:B:197:LYS:HE3	1.87	1.04
1:B:348:VAL:O	1:B:352:ILE:HG13	1.56	1.04
1:A:385:THR:HG21	1:B:382:ASN:C	1.79	1.03
1:A:329:LEU:HD22	1:A:392:PRO:HB3	1.40	1.03
1:A:194:GLU:CB	1:A:197:LYS:HE3	1.87	1.03
1:A:359:LEU:CG	1:A:360:PRO:CD	2.36	1.03
1:B:157:GLU:HB3	1:B:160:ASN:HD22	1.18	1.03
1:A:382:ASN:C	1:B:385:THR:HG21	1.79	1.02
1:B:303:LYS:O	1:B:307:LEU:HG	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:CG	1:B:360:PRO:CD	2.36	1.02
1:B:61:PRO:HD2	1:B:64:LEU:HD12	1.40	1.02
1:A:303:LYS:O	1:A:307:LEU:HG	1.59	1.02
1:A:157:GLU:HB3	1:A:160:ASN:HD22	1.18	1.01
1:B:361:THR:HG23	1:B:362:PRO:HD2	1.40	1.01
1:B:383:SER:HB3	1:B:403:ILE:HG23	1.41	1.01
1:A:383:SER:HB3	1:A:403:ILE:HG23	1.41	1.00
1:A:402:ARG:HD3	1:B:402:ARG:HD3	1.37	1.00
1:B:378:LEU:HA	1:B:381:LEU:CD1	1.91	1.00
1:A:378:LEU:HA	1:A:381:LEU:CD1	1.91	0.99
1:A:359:LEU:HD12	1:A:360:PRO:HD3	1.42	0.99
1:A:361:THR:HG23	1:A:362:PRO:HD2	1.40	0.99
1:B:329:LEU:HD22	1:B:392:PRO:HB3	1.40	0.99
1:A:61:PRO:HD2	1:A:64:LEU:HD12	1.40	0.99
1:B:359:LEU:HD12	1:B:360:PRO:HD3	1.42	0.98
1:A:385:THR:HA	1:B:384:MET:O	1.64	0.97
1:A:384:MET:O	1:B:385:THR:HA	1.64	0.97
1:A:385:THR:CG2	1:B:382:ASN:O	2.11	0.97
1:A:382:ASN:O	1:B:385:THR:CG2	2.12	0.97
1:A:1:MET:SD	1:A:37:SER:CB	2.55	0.95
1:B:164:ILE:CG1	1:B:208:VAL:HG21	1.97	0.95
1:B:1:MET:SD	1:B:37:SER:CB	2.55	0.95
1:A:164:ILE:CG1	1:A:208:VAL:HG21	1.97	0.95
1:A:301:LEU:HG	1:A:305:LYS:HD2	1.49	0.95
1:A:397:LYS:HA	1:A:400:MET:HE3	1.49	0.94
1:A:335:GLN:O	1:A:339:LEU:HD22	1.66	0.94
1:B:94:LYS:N	1:B:97:PHE:CZ	2.36	0.94
1:B:75:TYR:CD2	1:B:297:ILE:HG23	2.02	0.94
1:A:75:TYR:CD2	1:A:297:ILE:HG23	2.02	0.94
1:A:72:SER:HB2	1:A:300:ILE:HD11	1.48	0.94
1:B:301:LEU:HG	1:B:305:LYS:HD2	1.49	0.94
1:A:94:LYS:N	1:A:97:PHE:CZ	2.36	0.93
1:B:335:GLN:O	1:B:339:LEU:HD22	1.66	0.93
1:B:72:SER:HB2	1:B:300:ILE:HD11	1.48	0.93
1:A:15:GLY:HA2	1:A:67:LYS:NZ	1.83	0.93
1:B:15:GLY:HA2	1:B:67:LYS:NZ	1.83	0.93
1:B:200:GLU:CD	1:B:201:GLU:N	2.23	0.93
1:B:397:LYS:HA	1:B:400:MET:HE3	1.49	0.92
1:B:197:LYS:O	1:B:200:GLU:OE1	1.87	0.92
1:A:200:GLU:CD	1:A:201:GLU:N	2.23	0.92
1:B:157:GLU:CB	1:B:160:ASN:HD22	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:O	1:A:200:GLU:OE1	1.87	0.92
1:B:297:ILE:O	1:B:300:ILE:HB	1.69	0.92
1:B:15:GLY:HA2	1:B:67:LYS:HZ3	1.34	0.92
1:A:327:LEU:HD12	1:A:391:ASN:OD1	1.70	0.91
1:A:297:ILE:O	1:A:300:ILE:HB	1.69	0.91
1:B:221:SER:HA	1:B:250:THR:HG21	1.53	0.91
1:A:221:SER:HA	1:A:250:THR:HG21	1.53	0.91
1:A:349:LEU:HA	1:A:352:ILE:HB	1.53	0.91
1:B:327:LEU:HD12	1:B:391:ASN:OD1	1.70	0.91
1:B:295:GLY:HA2	1:B:298:GLU:HB2	1.52	0.91
1:B:317:MET:SD	1:B:328:THR:OG1	2.29	0.91
1:B:362:PRO:CD	1:B:367:LEU:CD2	2.27	0.91
1:A:157:GLU:CB	1:A:160:ASN:HD22	1.82	0.91
1:A:331:ASP:O	1:A:332:VAL:HG23	1.71	0.90
1:A:301:LEU:HD11	1:A:305:LYS:HE3	1.51	0.90
1:A:317:MET:SD	1:A:328:THR:OG1	2.29	0.90
1:B:301:LEU:HD11	1:B:305:LYS:HE3	1.51	0.90
1:A:281:THR:HG21	1:B:315:LYS:NZ	1.86	0.90
1:B:361:THR:OG1	1:B:367:LEU:HG	1.70	0.90
1:A:295:GLY:HA2	1:A:298:GLU:HB2	1.52	0.90
1:B:331:ASP:O	1:B:332:VAL:HG23	1.71	0.90
1:B:349:LEU:HA	1:B:352:ILE:HB	1.53	0.90
1:A:85:ASP:CG	1:A:285:LYS:HD3	1.92	0.90
1:A:2:LEU:HD22	1:A:291:ILE:HD13	1.51	0.89
1:B:2:LEU:HD22	1:B:291:ILE:HD13	1.51	0.89
1:B:85:ASP:CG	1:B:285:LYS:HD3	1.92	0.89
1:A:361:THR:OG1	1:A:367:LEU:HG	1.70	0.89
1:A:362:PRO:CD	1:A:367:LEU:CD2	2.27	0.89
1:A:315:LYS:NZ	1:B:281:THR:HG21	1.87	0.89
1:B:329:LEU:CD2	1:B:392:PRO:HB3	2.03	0.89
1:A:329:LEU:CD2	1:A:392:PRO:HB3	2.03	0.89
1:B:17:THR:HG22	1:B:18:PRO:HD2	0.92	0.88
1:B:1:MET:SD	1:B:37:SER:HB3	2.15	0.87
1:B:118:TYR:HE2	1:B:277:ASP:HB3	1.40	0.87
1:A:167:ALA:HB1	1:A:209:LEU:HD11	1.57	0.87
1:A:359:LEU:CB	1:A:360:PRO:CD	2.53	0.87
1:A:118:TYR:HE2	1:A:277:ASP:HB3	1.40	0.87
1:A:150:ILE:HG13	1:A:152:VAL:HG23	1.56	0.87
1:B:167:ALA:HB1	1:B:209:LEU:HD11	1.57	0.87
1:B:359:LEU:CB	1:B:360:PRO:CD	2.53	0.86
1:A:86:LYS:HE2	1:A:266:THR:HG23	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HB3	1:B:242:VAL:HG22	1.56	0.86
1:A:383:SER:CB	1:A:403:ILE:HG23	2.06	0.86
1:A:2:LEU:CD2	1:A:291:ILE:HG21	2.06	0.86
1:B:150:ILE:HG13	1:B:152:VAL:HG23	1.56	0.86
1:A:359:LEU:HD12	1:A:360:PRO:CD	2.06	0.86
1:A:216:LEU:HB3	1:A:242:VAL:HG22	1.56	0.86
1:B:2:LEU:HD22	1:B:291:ILE:CG2	2.05	0.85
1:B:86:LYS:HE2	1:B:266:THR:HG23	1.56	0.85
1:B:383:SER:CB	1:B:403:ILE:HG23	2.06	0.85
1:B:359:LEU:HD12	1:B:360:PRO:CD	2.06	0.85
1:A:402:ARG:CZ	1:B:402:ARG:HG2	2.07	0.85
1:A:1:MET:SD	1:A:37:SER:HB3	2.15	0.85
1:B:381:LEU:N	1:B:381:LEU:HD23	1.92	0.85
1:B:422:ASN:O	1:B:426:ARG:HG3	1.77	0.84
1:A:2:LEU:HD22	1:A:291:ILE:CG2	2.05	0.84
1:A:95:LEU:HD23	1:A:97:PHE:CE1	2.12	0.84
1:A:402:ARG:HG2	1:B:402:ARG:CZ	2.07	0.84
1:B:372:GLU:O	1:B:374:ILE:N	2.10	0.84
1:A:123:ARG:CZ	1:B:318:GLU:OE1	2.26	0.84
1:B:417:LEU:HB3	1:B:421:TYR:HE1	1.41	0.84
1:A:381:LEU:N	1:A:381:LEU:HD23	1.92	0.84
1:B:95:LEU:HD23	1:B:97:PHE:CE1	2.12	0.84
1:A:422:ASN:O	1:A:426:ARG:HG3	1.77	0.84
1:A:310:TYR:OH	1:A:355:LEU:HD23	1.78	0.84
1:A:69:TRP:O	1:A:73:ILE:HG13	1.78	0.84
1:A:417:LEU:HB3	1:A:421:TYR:HE1	1.41	0.84
1:A:17:THR:HG22	1:A:18:PRO:HD2	0.92	0.83
1:A:200:GLU:OE2	1:A:201:GLU:HA	1.78	0.83
1:A:164:ILE:HG23	1:A:165:GLU:N	1.94	0.83
1:A:372:GLU:O	1:A:374:ILE:N	2.10	0.83
1:B:164:ILE:HG23	1:B:165:GLU:N	1.94	0.83
1:B:69:TRP:O	1:B:73:ILE:HG13	1.78	0.83
1:B:2:LEU:CD2	1:B:291:ILE:HG21	2.06	0.83
1:B:310:TYR:OH	1:B:355:LEU:HD23	1.78	0.83
1:A:372:GLU:C	1:A:374:ILE:H	1.78	0.83
1:A:318:GLU:OE1	1:B:123:ARG:CZ	2.26	0.82
1:B:92:PRO:HB2	1:B:97:PHE:CZ	2.14	0.82
1:A:92:PRO:HB2	1:A:97:PHE:CZ	2.14	0.82
1:B:418:LEU:HA	1:B:421:TYR:HD1	1.44	0.82
1:A:418:LEU:HA	1:A:421:TYR:HD1	1.43	0.82
1:A:313:ILE:HD11	1:A:331:ASP:OD1	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLU:OE2	1:B:201:GLU:HA	1.78	0.81
1:B:380:ALA:HA	1:B:383:SER:HB2	1.61	0.81
1:B:164:ILE:CD1	1:B:208:VAL:CG2	2.51	0.81
1:A:55:LEU:HD13	1:A:55:LEU:O	1.80	0.81
1:A:15:GLY:HA2	1:A:67:LYS:HZ3	1.40	0.81
1:A:2:LEU:CD2	1:A:291:ILE:HD13	2.11	0.81
1:B:55:LEU:HD13	1:B:55:LEU:O	1.80	0.81
1:B:100:MET:HE3	1:B:205:MET:O	1.80	0.81
1:A:380:ALA:HA	1:A:383:SER:HB2	1.61	0.81
1:B:2:LEU:CD2	1:B:291:ILE:HD13	2.11	0.81
1:B:75:TYR:HD2	1:B:297:ILE:HG23	1.45	0.81
1:A:378:LEU:O	1:A:381:LEU:HG	1.81	0.80
1:A:176:LYS:O	1:A:178:LYS:N	2.14	0.80
1:B:176:LYS:O	1:B:178:LYS:N	2.15	0.80
1:B:372:GLU:C	1:B:374:ILE:H	1.78	0.80
1:A:6:ARG:HG3	1:A:292:LEU:HD23	1.62	0.80
1:B:313:ILE:HD11	1:B:331:ASP:OD1	1.80	0.80
1:B:359:LEU:CB	1:B:360:PRO:HD3	2.11	0.80
1:B:378:LEU:O	1:B:381:LEU:HG	1.81	0.80
1:A:75:TYR:HD2	1:A:297:ILE:HG23	1.45	0.80
1:B:394:ILE:HG22	1:B:399:ARG:NH1	1.96	0.80
1:B:6:ARG:HG3	1:B:292:LEU:HD23	1.62	0.80
1:B:346:SER:O	1:B:348:VAL:N	2.15	0.80
1:A:359:LEU:CB	1:A:360:PRO:HD3	2.11	0.80
1:A:346:SER:O	1:A:348:VAL:N	2.15	0.80
1:A:129:LEU:CD1	1:A:143:LEU:HD21	2.11	0.80
1:A:163:PRO:HG2	1:A:164:ILE:H	1.47	0.79
1:B:199:LEU:HD23	1:B:202:MET:SD	2.23	0.79
1:B:94:LYS:N	1:B:97:PHE:HZ	1.81	0.79
1:A:417:LEU:HB3	1:A:421:TYR:CE1	2.18	0.79
1:B:417:LEU:HB3	1:B:421:TYR:CE1	2.18	0.78
1:B:272:THR:HG21	1:B:280:GLU:OE2	1.82	0.78
1:A:199:LEU:HD23	1:A:202:MET:SD	2.23	0.78
1:A:172:ASP:O	1:A:176:LYS:HG3	1.83	0.78
1:B:172:ASP:O	1:B:176:LYS:HG3	1.83	0.78
1:A:272:THR:HG21	1:A:280:GLU:OE2	1.82	0.78
1:A:94:LYS:N	1:A:97:PHE:HZ	1.81	0.78
1:A:100:MET:HE3	1:A:205:MET:O	1.83	0.78
1:A:394:ILE:HG22	1:A:399:ARG:NH1	1.96	0.78
1:B:129:LEU:CD1	1:B:143:LEU:HD21	2.11	0.78
1:A:124:GLY:HA3	1:B:359:LEU:CA	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:HG2	1:B:164:ILE:H	1.47	0.78
1:A:234:HIS:CE1	1:A:265:ALA:CB	2.67	0.78
1:B:82:PHE:C	1:B:261:VAL:HG21	2.04	0.78
1:A:402:ARG:HD3	1:B:402:ARG:CD	2.14	0.78
1:A:384:MET:HE2	1:A:389:LEU:HD23	1.66	0.77
1:B:234:HIS:CE1	1:B:265:ALA:CB	2.67	0.77
1:A:82:PHE:C	1:A:261:VAL:HG21	2.04	0.77
1:A:299:SER:O	1:A:303:LYS:HG2	1.85	0.77
1:B:299:SER:O	1:B:303:LYS:HG2	1.85	0.76
1:A:396:ASP:O	1:A:400:MET:HG3	1.86	0.76
1:A:222:ILE:HG21	1:A:226:ALA:HB2	1.68	0.76
1:B:222:ILE:HG21	1:B:226:ALA:HB2	1.67	0.76
1:B:194:GLU:HB3	1:B:197:LYS:CD	2.16	0.76
1:A:402:ARG:CD	1:B:402:ARG:HD3	2.14	0.76
1:A:87:GLU:HG3	1:B:315:LYS:HZ1	1.50	0.76
1:B:396:ASP:O	1:B:400:MET:HG3	1.86	0.76
1:B:383:SER:O	1:B:403:ILE:HG12	1.85	0.76
1:A:361:THR:OG1	1:A:367:LEU:CG	2.34	0.76
1:A:383:SER:O	1:A:403:ILE:HG12	1.85	0.76
1:A:124:GLY:HA3	1:B:359:LEU:HA	1.68	0.76
1:A:194:GLU:HB3	1:A:197:LYS:CD	2.16	0.76
1:A:359:LEU:CA	1:B:124:GLY:HA3	2.16	0.76
1:B:200:GLU:OE2	1:B:201:GLU:CA	2.33	0.75
1:A:200:GLU:OE2	1:A:201:GLU:CA	2.34	0.75
1:B:234:HIS:CE1	1:B:265:ALA:HB1	2.22	0.75
1:A:356:GLY:O	1:A:357:ILE:CG1	2.32	0.75
1:A:329:LEU:CD1	1:A:421:TYR:HB3	2.17	0.75
1:A:402:ARG:HG2	1:B:402:ARG:NH2	2.02	0.75
1:A:234:HIS:CE1	1:A:265:ALA:HB1	2.22	0.75
1:B:361:THR:OG1	1:B:367:LEU:CG	2.34	0.75
1:B:335:GLN:HB3	1:B:355:LEU:HD22	1.70	0.74
1:A:122:LYS:O	1:B:359:LEU:CD1	2.33	0.74
1:B:92:PRO:HB2	1:B:97:PHE:CD2	2.22	0.74
1:B:222:ILE:CG2	1:B:226:ALA:HB2	2.17	0.74
1:A:335:GLN:HB3	1:A:355:LEU:HD22	1.70	0.74
1:A:382:ASN:CA	1:B:385:THR:HG21	2.18	0.74
1:A:359:LEU:HA	1:B:124:GLY:HA3	1.68	0.74
1:B:118:TYR:CE2	1:B:277:ASP:HB3	2.22	0.74
1:B:329:LEU:CD1	1:B:421:TYR:HB3	2.17	0.74
1:B:329:LEU:HD22	1:B:392:PRO:CB	2.17	0.74
1:A:349:LEU:HD22	1:A:371:GLU:HG2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:NH2	1:B:402:ARG:HG2	2.03	0.74
1:B:378:LEU:O	1:B:380:ALA:O	2.06	0.74
1:A:164:ILE:HG23	1:A:165:GLU:H	1.50	0.74
1:A:118:TYR:CE2	1:A:277:ASP:HB3	2.22	0.74
1:A:222:ILE:CG2	1:A:226:ALA:HB2	2.17	0.74
1:A:92:PRO:HB2	1:A:97:PHE:CD2	2.22	0.74
1:A:384:MET:CE	1:A:389:LEU:HD23	2.18	0.73
1:B:200:GLU:OE2	1:B:201:GLU:N	2.22	0.73
1:A:362:PRO:HD3	1:A:367:LEU:HD23	1.66	0.73
1:A:378:LEU:O	1:A:380:ALA:O	2.06	0.73
1:A:206:TYR:OH	1:A:239:ILE:HD11	1.88	0.73
1:A:382:ASN:HA	1:B:385:THR:CG2	2.18	0.73
1:B:164:ILE:HG23	1:B:165:GLU:H	1.50	0.73
1:A:385:THR:CG2	1:B:382:ASN:HA	2.19	0.73
1:B:346:SER:C	1:B:348:VAL:H	1.92	0.73
1:B:356:GLY:O	1:B:357:ILE:CG1	2.31	0.73
1:A:346:SER:C	1:A:348:VAL:H	1.92	0.73
1:A:402:ARG:HB3	1:B:402:ARG:NH1	2.04	0.73
1:B:206:TYR:OH	1:B:239:ILE:HD11	1.88	0.73
1:A:385:THR:HG21	1:B:382:ASN:CA	2.19	0.73
1:A:373:LYS:HE3	1:A:377:TRP:CH2	2.24	0.73
1:B:349:LEU:HD22	1:B:371:GLU:HG2	1.70	0.72
1:A:123:ARG:NH1	1:B:318:GLU:CD	2.42	0.72
1:A:318:GLU:CD	1:B:123:ARG:NH1	2.43	0.72
1:A:95:LEU:HD23	1:A:97:PHE:CD1	2.24	0.72
1:B:174:PHE:O	1:B:179:MET:HB2	1.90	0.72
1:B:373:LYS:HE3	1:B:377:TRP:CH2	2.24	0.72
1:B:384:MET:HE2	1:B:389:LEU:HD23	1.69	0.72
1:B:155:TYR:CD2	1:B:170:GLY:HA2	2.24	0.72
1:A:155:TYR:CD2	1:A:170:GLY:HA2	2.24	0.72
1:A:342:MET:O	1:A:348:VAL:HG21	1.90	0.72
1:B:383:SER:HB3	1:B:403:ILE:CG2	2.19	0.72
1:A:372:GLU:O	1:A:374:ILE:HG22	1.88	0.72
1:B:95:LEU:HD23	1:B:97:PHE:CD1	2.24	0.72
1:A:357:ILE:O	1:A:358:MET:HB2	1.88	0.72
1:B:164:ILE:HG13	1:B:208:VAL:HG21	1.70	0.72
1:A:281:THR:HG21	1:B:315:LYS:CE	2.19	0.72
1:B:342:MET:O	1:B:348:VAL:HG21	1.90	0.72
1:B:372:GLU:O	1:B:374:ILE:HG22	1.88	0.72
1:B:234:HIS:NE2	1:B:265:ALA:HB2	2.04	0.72
1:A:83:GLY:N	1:A:261:VAL:HG11	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:NH1	1:B:318:GLU:OE2	2.23	0.72
1:B:334:ALA:O	1:B:337:ILE:HG22	1.90	0.72
1:B:384:MET:CE	1:B:389:LEU:HD23	2.18	0.72
1:B:329:LEU:HD11	1:B:421:TYR:HB3	1.72	0.72
1:A:200:GLU:OE2	1:A:201:GLU:N	2.22	0.72
1:A:234:HIS:NE2	1:A:265:ALA:HB2	2.04	0.72
1:B:362:PRO:HD3	1:B:367:LEU:HD23	1.66	0.71
1:A:329:LEU:HD11	1:A:421:TYR:HB3	1.72	0.71
1:A:334:ALA:O	1:A:337:ILE:HG22	1.90	0.71
1:A:42:LYS:O	1:A:42:LYS:HD3	1.91	0.71
1:B:357:ILE:O	1:B:358:MET:HB2	1.88	0.71
1:A:164:ILE:HG13	1:A:208:VAL:HG21	1.70	0.71
1:A:301:LEU:HD21	1:A:305:LYS:NZ	2.06	0.71
1:A:329:LEU:HD22	1:A:392:PRO:CB	2.17	0.71
1:A:359:LEU:CD1	1:B:122:LYS:O	2.35	0.71
1:B:403:ILE:HG22	1:B:414:VAL:HG21	1.73	0.71
1:B:385:THR:HG22	1:B:386:TYR:N	2.05	0.71
1:A:169:LYS:O	1:A:173:ILE:HG13	1.91	0.71
1:A:174:PHE:O	1:A:179:MET:HB2	1.90	0.71
1:A:432:LYS:HE2	1:B:277:ASP:HB2	1.72	0.71
1:A:134:VAL:HA	1:A:140:TYR:HE1	1.55	0.71
1:B:134:VAL:HA	1:B:140:TYR:HE1	1.55	0.71
1:B:83:GLY:N	1:B:261:VAL:HG11	2.05	0.71
1:B:355:LEU:O	1:B:356:GLY:C	2.29	0.70
1:A:318:GLU:OE2	1:B:123:ARG:NH1	2.24	0.70
1:A:403:ILE:HG22	1:A:414:VAL:HG21	1.73	0.70
1:A:355:LEU:O	1:A:356:GLY:C	2.30	0.70
1:A:402:ARG:NH1	1:B:402:ARG:HB3	2.05	0.70
1:A:402:ARG:CG	1:B:402:ARG:CZ	2.70	0.70
1:A:402:ARG:CZ	1:B:402:ARG:CG	2.70	0.70
1:B:301:LEU:O	1:B:305:LYS:HD2	1.92	0.70
1:B:169:LYS:O	1:B:173:ILE:HG13	1.91	0.70
1:A:179:MET:HA	1:A:179:MET:CE	2.21	0.70
1:A:63:VAL:HG12	1:A:63:VAL:O	1.92	0.70
1:A:176:LYS:C	1:A:178:LYS:H	1.96	0.70
1:B:42:LYS:HD3	1:B:42:LYS:O	1.91	0.70
1:A:200:GLU:CD	1:A:200:GLU:C	2.51	0.69
1:A:277:ASP:HB2	1:B:432:LYS:HE2	1.73	0.69
1:A:303:LYS:HG3	1:A:304:VAL:H	1.57	0.69
1:A:315:LYS:HZ3	1:B:281:THR:HG21	1.55	0.69
1:B:303:LYS:HG3	1:B:304:VAL:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:THR:HG22	1:A:386:TYR:N	2.05	0.69
1:B:200:GLU:CD	1:B:200:GLU:C	2.51	0.69
1:B:136:ARG:HD3	1:B:139:ALA:HB2	1.74	0.69
1:A:301:LEU:O	1:A:305:LYS:HD2	1.92	0.69
1:B:301:LEU:HD21	1:B:305:LYS:NZ	2.06	0.69
1:B:397:LYS:CA	1:B:400:MET:HE3	2.23	0.69
1:A:247:MET:CE	1:A:270:ILE:HD11	2.23	0.69
1:B:176:LYS:C	1:B:178:LYS:H	1.96	0.69
1:B:401:ARG:O	1:B:405:GLU:HG2	1.92	0.69
1:B:310:TYR:HA	1:B:335:GLN:HE22	1.57	0.69
1:B:78:LEU:O	1:B:81:LEU:HB3	1.93	0.69
1:A:315:LYS:CE	1:B:281:THR:HG21	2.21	0.69
1:B:179:MET:CE	1:B:179:MET:HA	2.21	0.69
1:B:384:MET:HA	1:B:388:GLU:OE1	1.92	0.69
1:B:361:THR:HG23	1:B:362:PRO:CD	2.20	0.69
1:B:369:ILE:HG22	1:B:370:GLY:H	1.58	0.69
1:A:401:ARG:O	1:A:405:GLU:HG2	1.92	0.69
1:A:369:ILE:HG22	1:A:370:GLY:H	1.58	0.68
1:A:78:LEU:O	1:A:81:LEU:HB3	1.93	0.68
1:A:384:MET:HA	1:A:388:GLU:OE1	1.92	0.68
1:A:300:ILE:O	1:A:303:LYS:HG2	1.93	0.68
1:A:315:LYS:HZ1	1:B:87:GLU:HG3	1.57	0.68
1:A:310:TYR:HA	1:A:335:GLN:HE22	1.58	0.68
1:B:100:MET:CE	1:B:205:MET:O	2.42	0.68
1:B:300:ILE:O	1:B:303:LYS:HG2	1.93	0.68
1:B:235:GLN:O	1:B:237:SER:N	2.27	0.68
1:B:247:MET:CE	1:B:270:ILE:HD11	2.23	0.68
1:B:302:GLU:OE1	1:B:341:LYS:HE3	1.94	0.68
1:A:412:GLU:OE1	1:A:415:ARG:HD2	1.93	0.68
1:A:190:HIS:CD2	1:A:194:GLU:OE1	2.47	0.68
1:A:383:SER:HB3	1:A:403:ILE:CG2	2.19	0.68
1:A:394:ILE:O	1:A:399:ARG:NH1	2.27	0.68
1:A:136:ARG:HD3	1:A:139:ALA:HB2	1.74	0.68
1:B:63:VAL:HG12	1:B:63:VAL:O	1.92	0.68
1:A:409:LEU:HB3	1:A:413:GLU:CD	2.14	0.67
1:A:234:HIS:CE1	1:A:265:ALA:HB2	2.30	0.67
1:B:361:THR:OG1	1:B:367:LEU:CD1	2.42	0.67
1:A:378:LEU:HA	1:A:381:LEU:HD11	1.76	0.67
1:A:397:LYS:HA	1:A:400:MET:CE	2.24	0.67
1:B:394:ILE:O	1:B:399:ARG:NH1	2.27	0.67
1:B:412:GLU:OE1	1:B:415:ARG:HD2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HA	1:B:381:LEU:HD11	1.76	0.67
1:B:397:LYS:HA	1:B:400:MET:CE	2.24	0.67
1:A:100:MET:CE	1:A:205:MET:O	2.42	0.67
1:B:374:ILE:C	1:B:376:ARG:H	1.96	0.67
1:A:302:GLU:OE1	1:A:341:LYS:HE3	1.94	0.67
1:A:235:GLN:O	1:A:237:SER:N	2.27	0.67
1:B:374:ILE:HG23	1:B:375:ARG:H	1.60	0.67
1:B:373:LYS:HE3	1:B:377:TRP:CZ3	2.30	0.67
1:B:190:HIS:CD2	1:B:194:GLU:OE1	2.47	0.67
1:B:369:ILE:HG22	1:B:370:GLY:N	2.10	0.67
1:B:409:LEU:HB3	1:B:413:GLU:CD	2.14	0.67
1:A:373:LYS:HE3	1:A:377:TRP:CZ3	2.30	0.67
1:A:397:LYS:CA	1:A:400:MET:HE3	2.23	0.67
1:A:361:THR:OG1	1:A:367:LEU:CD1	2.42	0.67
1:B:234:HIS:CE1	1:B:265:ALA:HB2	2.30	0.67
1:B:247:MET:HE2	1:B:257:LEU:HD21	1.77	0.67
1:A:95:LEU:CD2	1:A:97:PHE:HE1	2.08	0.66
1:B:301:LEU:HG	1:B:305:LYS:CD	2.24	0.66
1:B:75:TYR:OH	1:B:292:LEU:HD12	1.95	0.66
1:A:369:ILE:HG22	1:A:370:GLY:N	2.10	0.66
1:A:94:LYS:C	1:A:97:PHE:CZ	2.69	0.66
1:B:378:LEU:O	1:B:379:ALA:C	2.34	0.66
1:A:374:ILE:C	1:A:376:ARG:H	1.96	0.66
1:A:374:ILE:HG23	1:A:375:ARG:H	1.60	0.66
1:A:1:MET:O	1:A:4:ASN:N	2.28	0.66
1:A:280:GLU:OE1	1:A:290:ARG:NH2	2.28	0.66
1:B:190:HIS:HD2	1:B:194:GLU:OE1	1.79	0.66
1:B:118:TYR:HE2	1:B:277:ASP:CB	2.09	0.66
1:B:95:LEU:CD2	1:B:97:PHE:HE1	2.08	0.66
1:A:348:VAL:HG12	1:A:352:ILE:HD11	1.77	0.66
1:A:31:GLN:HG3	1:A:48:THR:HG21	1.78	0.66
1:B:119:PHE:CZ	1:B:123:ARG:NH2	2.64	0.66
1:B:276:ILE:HG23	1:B:277:ASP:N	2.10	0.66
1:B:361:THR:CA	1:B:367:LEU:CD1	2.44	0.66
1:B:379:ALA:O	1:B:380:ALA:O	2.14	0.66
1:A:348:VAL:O	1:A:352:ILE:CG1	2.39	0.66
1:B:1:MET:O	1:B:4:ASN:N	2.28	0.66
1:B:31:GLN:HG3	1:B:48:THR:HG21	1.78	0.66
1:A:164:ILE:CG2	1:A:165:GLU:H	2.09	0.65
1:B:280:GLU:OE1	1:B:290:ARG:NH2	2.28	0.65
1:A:119:PHE:CZ	1:A:123:ARG:NH2	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:HA	1:B:376:ARG:HG3	1.78	0.65
1:A:361:THR:HG23	1:A:362:PRO:CD	2.20	0.65
1:A:373:LYS:HA	1:A:376:ARG:HG3	1.78	0.65
1:A:276:ILE:HG23	1:A:277:ASP:N	2.10	0.65
1:B:409:LEU:CD1	1:B:413:GLU:OE1	2.41	0.65
1:A:301:LEU:HG	1:A:305:LYS:CD	2.24	0.65
1:B:301:LEU:HD21	1:B:305:LYS:HZ1	1.62	0.65
1:B:94:LYS:C	1:B:97:PHE:CZ	2.69	0.65
1:B:348:VAL:HG12	1:B:352:ILE:HD11	1.77	0.65
1:A:190:HIS:HD2	1:A:194:GLU:OE1	1.79	0.65
1:A:339:LEU:HD22	1:A:339:LEU:H	1.62	0.65
1:B:423:ASN:O	1:B:427:LEU:HG	1.97	0.65
1:A:310:TYR:O	1:A:313:ILE:HG22	1.97	0.64
1:A:75:TYR:OH	1:A:292:LEU:HD12	1.95	0.64
1:A:53:GLU:HG3	1:A:57:LYS:HE3	1.79	0.64
1:B:53:GLU:HG3	1:B:57:LYS:HE3	1.79	0.64
1:A:297:ILE:O	1:A:300:ILE:CB	2.45	0.64
1:A:423:ASN:O	1:A:427:LEU:HG	1.97	0.64
1:B:164:ILE:CG2	1:B:165:GLU:N	2.59	0.64
1:A:378:LEU:O	1:A:379:ALA:C	2.34	0.64
1:A:379:ALA:O	1:A:380:ALA:O	2.15	0.64
1:A:359:LEU:HA	1:B:124:GLY:CA	2.28	0.64
1:A:2:LEU:HD13	1:A:291:ILE:HG23	1.79	0.64
1:B:167:ALA:HB1	1:B:209:LEU:HD21	1.79	0.64
1:A:21:LYS:HD3	1:A:25:GLU:OE2	1.97	0.64
1:A:361:THR:CA	1:A:367:LEU:CD1	2.44	0.64
1:A:124:GLY:CA	1:B:359:LEU:HA	2.27	0.64
1:A:86:LYS:CE	1:A:266:THR:HG23	2.28	0.64
1:B:21:LYS:HD3	1:B:25:GLU:OE2	1.97	0.64
1:B:310:TYR:O	1:B:313:ILE:HG22	1.98	0.64
1:B:335:GLN:O	1:B:339:LEU:CD2	2.45	0.64
1:A:385:THR:CA	1:B:384:MET:O	2.44	0.64
1:B:288:VAL:O	1:B:291:ILE:HG12	1.97	0.64
1:A:87:GLU:OE2	1:B:315:LYS:HD2	1.98	0.64
1:B:164:ILE:CG2	1:B:165:GLU:H	2.09	0.64
1:B:176:LYS:C	1:B:178:LYS:N	2.51	0.64
1:A:167:ALA:HB1	1:A:209:LEU:HD21	1.79	0.64
1:A:119:PHE:CZ	1:A:123:ARG:NE	2.66	0.63
1:A:95:LEU:CD2	1:A:97:PHE:CE1	2.82	0.63
1:A:385:THR:CG2	1:B:382:ASN:C	2.63	0.63
1:A:384:MET:O	1:B:385:THR:CA	2.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:O	1:A:291:ILE:HG12	1.97	0.63
1:A:129:LEU:HD13	1:A:143:LEU:CD2	2.18	0.63
1:A:281:THR:HG21	1:B:315:LYS:HZ3	1.63	0.63
1:B:339:LEU:HD22	1:B:339:LEU:H	1.62	0.63
1:A:335:GLN:O	1:A:339:LEU:CD2	2.45	0.63
1:A:87:GLU:HG3	1:B:315:LYS:NZ	2.14	0.63
1:B:244:ILE:O	1:B:271:GLY:N	2.24	0.63
1:B:196:THR:OG1	1:B:232:ARG:NH1	2.32	0.63
1:B:372:GLU:C	1:B:374:ILE:N	2.52	0.63
1:A:247:MET:HE1	1:A:257:LEU:HD21	1.81	0.63
1:B:362:PRO:HD3	1:B:367:LEU:HD21	0.68	0.63
1:A:118:TYR:HE2	1:A:277:ASP:CB	2.09	0.63
1:B:119:PHE:HZ	1:B:123:ARG:NH2	1.95	0.63
1:A:69:TRP:NE1	1:A:73:ILE:HD11	2.14	0.63
1:B:2:LEU:HD13	1:B:291:ILE:HG23	1.79	0.63
1:B:362:PRO:O	1:B:363:SER:C	2.36	0.63
1:B:9:VAL:HG13	1:B:71:ILE:CD1	2.28	0.63
1:B:348:VAL:O	1:B:352:ILE:CG1	2.39	0.63
1:B:85:ASP:OD1	1:B:285:LYS:HD3	1.99	0.63
1:A:33:SER:O	1:A:36:SER:HB2	1.99	0.63
1:B:357:ILE:HD12	1:B:358:MET:H	1.64	0.62
1:A:9:VAL:HG13	1:A:71:ILE:CD1	2.28	0.62
1:A:167:ALA:CB	1:A:209:LEU:HD21	2.29	0.62
1:B:379:ALA:HB2	1:B:409:LEU:HD11	1.80	0.62
1:A:379:ALA:HB2	1:A:409:LEU:HD11	1.80	0.62
1:B:359:LEU:HB3	1:B:360:PRO:HD2	1.81	0.62
1:A:164:ILE:CD1	1:A:208:VAL:CG2	2.51	0.62
1:B:69:TRP:NE1	1:B:73:ILE:HD11	2.14	0.62
1:B:33:SER:O	1:B:36:SER:HB2	1.99	0.62
1:A:196:THR:OG1	1:A:232:ARG:NH1	2.32	0.62
1:A:119:PHE:HZ	1:A:123:ARG:NH2	1.95	0.62
1:B:379:ALA:CB	1:B:409:LEU:HD11	2.30	0.62
1:A:376:ARG:O	1:A:377:TRP:C	2.38	0.62
1:B:283:ASN:C	1:B:283:ASN:HD22	2.03	0.62
1:A:362:PRO:HD3	1:A:367:LEU:HD21	0.68	0.62
1:A:357:ILE:HD12	1:A:358:MET:H	1.64	0.62
1:B:1:MET:SD	1:B:37:SER:HB2	2.40	0.62
1:A:283:ASN:HD22	1:A:283:ASN:C	2.03	0.62
1:A:291:ILE:O	1:A:292:LEU:HB2	2.00	0.62
1:A:75:TYR:O	1:A:76:ASP:C	2.38	0.62
1:A:315:LYS:NZ	1:B:87:GLU:HG3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:HIS:O	1:B:353:PRO:HD3	2.00	0.62
1:A:315:LYS:HD2	1:B:87:GLU:OE2	2.00	0.62
1:A:82:PHE:O	1:A:261:VAL:HG21	1.99	0.62
1:A:244:ILE:O	1:A:271:GLY:N	2.24	0.62
1:A:379:ALA:CB	1:A:409:LEU:HD11	2.30	0.61
1:B:167:ALA:CB	1:B:209:LEU:HD21	2.29	0.61
1:A:359:LEU:HB3	1:A:360:PRO:HD2	1.81	0.61
1:B:119:PHE:CZ	1:B:123:ARG:NE	2.66	0.61
1:B:75:TYR:O	1:B:76:ASP:C	2.38	0.61
1:B:129:LEU:HD13	1:B:143:LEU:CD2	2.18	0.61
1:A:351:HIS:O	1:A:353:PRO:HD3	2.00	0.61
1:A:382:ASN:C	1:B:385:THR:CG2	2.64	0.61
1:B:297:ILE:O	1:B:300:ILE:CB	2.45	0.61
1:A:85:ASP:OD1	1:A:285:LYS:HD3	1.99	0.61
1:B:394:ILE:CG2	1:B:399:ARG:NH1	2.63	0.61
1:A:194:GLU:CA	1:A:197:LYS:HE3	2.30	0.61
1:A:329:LEU:HD11	1:A:421:TYR:CB	2.31	0.61
1:B:242:VAL:CG1	1:B:243:ILE:N	2.64	0.61
1:A:394:ILE:CG2	1:A:399:ARG:NH1	2.64	0.61
1:A:394:ILE:CG2	1:A:399:ARG:HH12	2.14	0.61
1:B:380:ALA:C	1:B:381:LEU:HG	2.21	0.61
1:B:116:LEU:HD11	1:B:120:TYR:CE2	2.36	0.61
1:A:394:ILE:HG22	1:A:394:ILE:O	2.00	0.61
1:A:380:ALA:C	1:A:381:LEU:HG	2.21	0.61
1:B:291:ILE:O	1:B:292:LEU:HB2	2.00	0.61
1:B:82:PHE:O	1:B:261:VAL:HG21	2.00	0.61
1:B:273:GLY:HA3	1:B:278:GLU:OE1	2.00	0.61
1:A:87:GLU:HB3	1:B:312:LYS:HE2	1.82	0.61
1:B:300:ILE:HD13	1:B:303:LYS:CE	2.31	0.61
1:B:394:ILE:HG22	1:B:394:ILE:O	2.00	0.61
1:B:377:TRP:CE3	1:B:377:TRP:HA	2.35	0.60
1:B:6:ARG:HA	1:B:292:LEU:HD21	1.83	0.60
1:A:247:MET:HE1	1:A:270:ILE:HD11	1.82	0.60
1:A:273:GLY:HA3	1:A:278:GLU:OE1	2.00	0.60
1:A:91:ASN:ND2	1:B:357:ILE:HG21	2.16	0.60
1:A:328:THR:HG23	1:A:331:ASP:OD2	2.01	0.60
1:A:377:TRP:HA	1:A:377:TRP:CE3	2.35	0.60
1:A:176:LYS:C	1:A:178:LYS:N	2.51	0.60
1:A:6:ARG:HA	1:A:292:LEU:HD21	1.83	0.60
1:B:378:LEU:HD23	1:B:378:LEU:C	2.22	0.60
1:B:378:LEU:CA	1:B:381:LEU:CD1	2.76	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:CD	1:B:402:ARG:CD	2.78	0.60
1:A:234:HIS:CD2	1:A:265:ALA:HB2	2.36	0.60
1:B:247:MET:HE2	1:B:257:LEU:CD2	2.31	0.60
1:B:376:ARG:O	1:B:377:TRP:C	2.38	0.60
1:B:301:LEU:CD1	1:B:305:LYS:HE3	2.28	0.60
1:B:329:LEU:HD11	1:B:421:TYR:CB	2.31	0.60
1:A:327:LEU:HB2	1:A:390:GLU:O	2.01	0.60
1:A:378:LEU:HD23	1:A:378:LEU:C	2.22	0.60
1:B:122:LYS:C	1:B:124:GLY:H	2.05	0.60
1:A:300:ILE:HD13	1:A:303:LYS:CE	2.31	0.60
1:A:116:LEU:HD11	1:A:120:TYR:CE2	2.36	0.60
1:B:234:HIS:CD2	1:B:265:ALA:HB2	2.36	0.60
1:A:30:LEU:HD23	1:A:48:THR:HG22	1.84	0.60
1:A:119:PHE:HZ	1:A:123:ARG:HH21	1.48	0.60
1:B:327:LEU:HB2	1:B:390:GLU:O	2.01	0.60
1:B:328:THR:HG23	1:B:331:ASP:OD2	2.01	0.60
1:A:378:LEU:CA	1:A:381:LEU:CD1	2.76	0.60
1:B:394:ILE:CG2	1:B:399:ARG:HH12	2.14	0.60
1:B:194:GLU:CA	1:B:197:LYS:HE3	2.30	0.60
1:A:123:ARG:NH2	1:B:318:GLU:OE1	2.35	0.59
1:A:276:ILE:CG2	1:A:277:ASP:N	2.65	0.59
1:B:85:ASP:OD1	1:B:285:LYS:CD	2.50	0.59
1:A:382:ASN:CA	1:B:385:THR:CG2	2.79	0.59
1:A:302:GLU:OE1	1:A:341:LYS:HG3	2.02	0.59
1:A:122:LYS:C	1:A:124:GLY:H	2.05	0.59
1:A:85:ASP:OD1	1:A:285:LYS:CD	2.50	0.59
1:A:312:LYS:HE2	1:B:87:GLU:HB3	1.83	0.59
1:A:41:VAL:O	1:A:41:VAL:HG12	2.02	0.59
1:A:372:GLU:C	1:A:374:ILE:N	2.52	0.59
1:A:242:VAL:CG1	1:A:243:ILE:N	2.64	0.59
1:A:385:THR:CG2	1:B:382:ASN:CA	2.79	0.59
1:B:276:ILE:CG2	1:B:277:ASP:N	2.65	0.59
1:A:377:TRP:CA	1:A:377:TRP:CE3	2.85	0.59
1:B:302:GLU:OE1	1:B:341:LYS:HG3	2.02	0.59
1:B:30:LEU:HD23	1:B:48:THR:HG22	1.84	0.59
1:A:331:ASP:O	1:A:332:VAL:CG2	2.49	0.59
1:A:357:ILE:HG21	1:B:91:ASN:ND2	2.18	0.59
1:B:346:SER:C	1:B:348:VAL:N	2.55	0.59
1:B:348:VAL:CG1	1:B:352:ILE:HD11	2.33	0.59
1:B:86:LYS:CE	1:B:266:THR:HG23	2.28	0.59
1:B:331:ASP:O	1:B:332:VAL:CG2	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:PRO:O	1:A:363:SER:C	2.36	0.59
1:B:377:TRP:CA	1:B:377:TRP:CE3	2.85	0.58
1:A:318:GLU:OE1	1:B:123:ARG:NH2	2.36	0.58
1:B:109:LYS:O	1:B:110:THR:CB	2.51	0.58
1:B:318:GLU:O	1:B:319:ASP:OD1	2.22	0.58
1:B:418:LEU:HA	1:B:421:TYR:CD1	2.34	0.58
1:B:41:VAL:HG12	1:B:41:VAL:O	2.02	0.58
1:A:109:LYS:O	1:A:110:THR:CB	2.51	0.58
1:B:377:TRP:HE3	1:B:377:TRP:N	2.02	0.58
1:B:100:MET:CE	1:B:209:LEU:HD12	2.34	0.58
1:A:335:GLN:HB3	1:A:355:LEU:CD2	2.33	0.58
1:A:409:LEU:CD1	1:A:413:GLU:OE1	2.41	0.58
1:A:2:LEU:HB3	1:A:291:ILE:CG2	2.34	0.58
1:B:335:GLN:HB3	1:B:355:LEU:CD2	2.33	0.57
1:A:346:SER:C	1:A:348:VAL:N	2.55	0.57
1:A:123:ARG:O	1:B:358:MET:O	2.22	0.57
1:B:359:LEU:HB3	1:B:360:PRO:CD	2.33	0.57
1:A:301:LEU:O	1:A:305:LYS:HB2	2.04	0.57
1:B:131:ALA:O	1:B:140:TYR:HE2	1.87	0.57
1:A:1:MET:SD	1:A:37:SER:HB2	2.40	0.57
1:B:199:LEU:CD2	1:B:202:MET:SD	2.92	0.57
1:A:402:ARG:CD	1:B:402:ARG:NE	2.68	0.57
1:A:402:ARG:NE	1:B:402:ARG:NE	2.51	0.57
1:A:359:LEU:HB3	1:A:360:PRO:CD	2.33	0.57
1:A:367:LEU:O	1:A:368:LYS:HB2	2.04	0.57
1:B:359:LEU:CD1	1:B:360:PRO:CD	2.60	0.57
1:B:118:TYR:OH	1:B:122:LYS:HE3	2.04	0.57
1:B:2:LEU:HB3	1:B:291:ILE:CG2	2.34	0.57
1:A:87:GLU:HG2	1:B:312:LYS:HG2	1.86	0.57
1:B:367:LEU:O	1:B:368:LYS:HB2	2.04	0.57
1:A:299:SER:O	1:A:303:LYS:N	2.37	0.57
1:A:300:ILE:HG22	1:A:301:LEU:N	2.20	0.57
1:A:348:VAL:CG1	1:A:352:ILE:HD11	2.33	0.57
1:A:377:TRP:N	1:A:377:TRP:HE3	2.02	0.57
1:B:301:LEU:O	1:B:305:LYS:HB2	2.04	0.57
1:A:199:LEU:CD2	1:A:202:MET:SD	2.92	0.57
1:B:283:ASN:O	1:B:284:ALA:C	2.42	0.57
1:B:369:ILE:CG2	1:B:370:GLY:H	2.18	0.56
1:A:361:THR:OG1	1:A:367:LEU:HD12	2.04	0.56
1:A:402:ARG:NE	1:B:402:ARG:CD	2.69	0.56
1:A:100:MET:CE	1:A:209:LEU:HD12	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:THR:OG1	1:B:367:LEU:HD12	2.04	0.56
1:A:318:GLU:O	1:A:319:ASP:OD1	2.21	0.56
1:A:318:GLU:OE1	1:B:123:ARG:NH1	2.39	0.56
1:B:299:SER:O	1:B:303:LYS:N	2.37	0.56
1:B:300:ILE:HG22	1:B:301:LEU:N	2.20	0.56
1:B:77:GLU:O	1:B:78:LEU:C	2.41	0.56
1:A:283:ASN:O	1:A:284:ALA:C	2.42	0.56
1:A:118:TYR:OH	1:A:122:LYS:HE3	2.04	0.56
1:A:300:ILE:HD13	1:A:303:LYS:HE3	1.88	0.56
1:A:116:LEU:HD11	1:A:120:TYR:HE2	1.69	0.56
1:A:342:MET:O	1:A:343:GLY:O	2.23	0.56
1:A:358:MET:O	1:B:123:ARG:O	2.23	0.56
1:A:131:ALA:O	1:A:140:TYR:HE2	1.87	0.56
1:B:116:LEU:HD11	1:B:120:TYR:HE2	1.69	0.56
1:B:427:LEU:O	1:B:431:VAL:HG23	2.06	0.56
1:B:95:LEU:CD2	1:B:97:PHE:CE1	2.82	0.56
1:A:301:LEU:CD1	1:A:305:LYS:HE3	2.28	0.56
1:A:143:LEU:HD13	1:A:154:VAL:HG13	1.88	0.56
1:B:347:LYS:O	1:B:347:LYS:HG3	2.06	0.56
1:A:293:GLY:HA3	1:A:296:ASP:OD2	2.06	0.56
1:B:293:GLY:HA3	1:B:296:ASP:OD2	2.06	0.56
1:A:135:TYR:CD1	1:A:189:ARG:CZ	2.88	0.56
1:A:427:LEU:O	1:A:431:VAL:HG23	2.05	0.56
1:B:1:MET:CG	1:B:37:SER:HB3	2.36	0.56
1:A:312:LYS:HG2	1:B:87:GLU:HG2	1.87	0.56
1:B:135:TYR:CD1	1:B:189:ARG:CZ	2.88	0.56
1:B:380:ALA:C	1:B:381:LEU:CG	2.74	0.56
1:B:300:ILE:HD13	1:B:303:LYS:HE3	1.88	0.56
1:A:385:THR:CG2	1:A:386:TYR:N	2.69	0.56
1:A:347:LYS:HG3	1:A:347:LYS:O	2.06	0.56
1:A:369:ILE:CG2	1:A:370:GLY:H	2.18	0.55
1:B:95:LEU:HD23	1:B:97:PHE:HE1	1.63	0.55
1:B:219:ASP:OD1	1:B:221:SER:OG	2.23	0.55
1:A:293:GLY:O	1:A:296:ASP:N	2.32	0.55
1:B:247:MET:HE2	1:B:270:ILE:HD11	1.89	0.55
1:A:123:ARG:NH1	1:B:318:GLU:OE1	2.39	0.55
1:B:376:ARG:O	1:B:379:ALA:N	2.40	0.55
1:B:342:MET:O	1:B:343:GLY:O	2.24	0.55
1:A:219:ASP:OD1	1:A:221:SER:OG	2.23	0.55
1:B:425:ASN:O	1:B:429:LYS:HG3	2.06	0.55
1:B:427:LEU:O	1:B:428:LEU:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:CD2	1:B:297:ILE:CG2	2.85	0.55
1:A:379:ALA:HB3	1:A:417:LEU:HD11	1.88	0.55
1:A:376:ARG:O	1:A:379:ALA:N	2.40	0.55
1:B:293:GLY:O	1:B:296:ASP:N	2.32	0.55
1:A:51:ILE:HD13	1:A:74:VAL:HG22	1.88	0.55
1:B:85:ASP:OD1	1:B:285:LYS:CE	2.54	0.55
1:A:416:GLU:O	1:A:417:LEU:C	2.45	0.55
1:B:267:ILE:HG22	1:B:267:ILE:O	2.07	0.55
1:A:409:LEU:HB3	1:A:413:GLU:OE1	2.07	0.55
1:A:85:ASP:OD1	1:A:285:LYS:CE	2.54	0.55
1:B:379:ALA:HB3	1:B:417:LEU:HD11	1.88	0.54
1:B:329:LEU:O	1:B:329:LEU:HG	2.07	0.54
1:B:385:THR:CG2	1:B:386:TYR:N	2.69	0.54
1:B:143:LEU:HD13	1:B:154:VAL:HG13	1.88	0.54
1:B:416:GLU:O	1:B:417:LEU:C	2.45	0.54
1:A:300:ILE:HD13	1:A:303:LYS:HZ2	1.72	0.54
1:B:129:LEU:HD23	1:B:183:ILE:HB	1.89	0.54
1:A:40:ASN:HD22	1:A:42:LYS:CB	2.20	0.54
1:A:77:GLU:O	1:A:78:LEU:C	2.41	0.54
1:B:75:TYR:CE2	1:B:297:ILE:HG23	2.42	0.54
1:A:1:MET:CG	1:A:37:SER:HB3	2.36	0.54
1:A:247:MET:HE1	1:A:257:LEU:CD2	2.37	0.54
1:A:270:ILE:HG23	1:A:270:ILE:O	2.08	0.54
1:B:361:THR:CB	1:B:367:LEU:HG	2.38	0.54
1:A:163:PRO:O	1:A:164:ILE:C	2.46	0.54
1:A:129:LEU:HD23	1:A:183:ILE:HB	1.89	0.54
1:A:221:SER:CA	1:A:250:THR:HG21	2.33	0.54
1:B:361:THR:HA	1:B:367:LEU:HD11	0.66	0.54
1:B:369:ILE:HA	1:B:373:LYS:HG2	1.89	0.54
1:A:329:LEU:HG	1:A:329:LEU:O	2.07	0.54
1:B:28:LYS:O	1:B:32:LYS:HD3	2.07	0.54
1:B:409:LEU:HB3	1:B:413:GLU:OE1	2.07	0.54
1:A:336:ILE:HD11	1:A:377:TRP:HD1	1.73	0.54
1:A:101:LEU:HD12	1:A:113:ALA:HB2	1.90	0.54
1:A:267:ILE:O	1:A:267:ILE:HG22	2.07	0.54
1:A:425:ASN:O	1:A:429:LYS:HG3	2.06	0.54
1:B:190:HIS:HB3	1:B:194:GLU:HB2	1.89	0.54
1:A:369:ILE:HA	1:A:373:LYS:HG2	1.89	0.54
1:B:101:LEU:HD12	1:B:113:ALA:HB2	1.90	0.54
1:A:385:THR:HG23	1:B:384:MET:O	2.08	0.54
1:B:94:LYS:N	1:B:97:PHE:CE2	2.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TYR:CE2	1:A:297:ILE:HG23	2.42	0.54
1:B:155:TYR:CE1	1:B:173:ILE:HD12	2.43	0.54
1:A:247:MET:HG3	1:A:270:ILE:HD11	1.90	0.54
1:A:293:GLY:CA	1:A:296:ASP:OD2	2.56	0.54
1:A:28:LYS:O	1:A:32:LYS:HD3	2.07	0.54
1:B:381:LEU:N	1:B:381:LEU:CD2	2.62	0.53
1:B:403:ILE:CG2	1:B:414:VAL:HG21	2.37	0.53
1:A:359:LEU:CD1	1:A:360:PRO:CD	2.60	0.53
1:A:403:ILE:CG2	1:A:414:VAL:HG21	2.38	0.53
1:B:162:ASN:O	1:B:166:ILE:HG13	2.08	0.53
1:B:51:ILE:HD13	1:B:74:VAL:HG22	1.88	0.53
1:B:209:LEU:O	1:B:210:LYS:C	2.46	0.53
1:B:105:GLN:O	1:B:106:GLY:O	2.26	0.53
1:B:380:ALA:O	1:B:381:LEU:CB	2.56	0.53
1:B:380:ALA:O	1:B:381:LEU:HG	2.08	0.53
1:A:361:THR:CB	1:A:367:LEU:HG	2.38	0.53
1:B:40:ASN:HD22	1:B:42:LYS:CB	2.20	0.53
1:A:105:GLN:O	1:A:106:GLY:O	2.26	0.53
1:A:19:TYR:CD2	1:A:66:ARG:NH2	2.76	0.53
1:B:336:ILE:HD11	1:B:377:TRP:HD1	1.73	0.53
1:A:380:ALA:C	1:A:381:LEU:CG	2.74	0.53
1:A:380:ALA:O	1:A:382:ASN:OD1	2.26	0.53
1:A:427:LEU:O	1:A:428:LEU:C	2.45	0.53
1:B:270:ILE:HG23	1:B:270:ILE:O	2.08	0.53
1:B:118:TYR:CZ	1:B:122:LYS:HE3	2.44	0.53
1:A:162:ASN:O	1:A:166:ILE:HG13	2.08	0.53
1:B:343:GLY:O	1:B:348:VAL:HG21	2.09	0.53
1:B:247:MET:HG3	1:B:270:ILE:HD11	1.91	0.53
1:B:19:TYR:CD2	1:B:66:ARG:NH2	2.76	0.53
1:B:310:TYR:CZ	1:B:355:LEU:HD23	2.44	0.53
1:A:9:VAL:HG13	1:A:71:ILE:HD12	1.90	0.53
1:B:75:TYR:OH	1:B:292:LEU:CD1	2.55	0.53
1:B:1:MET:HG2	1:B:37:SER:HB3	1.91	0.53
1:B:380:ALA:O	1:B:382:ASN:OD1	2.26	0.53
1:A:380:ALA:O	1:A:381:LEU:HG	2.08	0.53
1:B:9:VAL:HG13	1:B:71:ILE:HD12	1.90	0.53
1:A:23:VAL:O	1:A:24:ASP:C	2.46	0.53
1:B:155:TYR:CD2	1:B:170:GLY:CA	2.91	0.53
1:A:190:HIS:HB3	1:A:194:GLU:HB2	1.89	0.53
1:A:394:ILE:HG22	1:A:399:ARG:CZ	2.39	0.53
1:B:163:PRO:O	1:B:164:ILE:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ILE:O	1:A:303:LYS:CG	2.57	0.53
1:A:75:TYR:OH	1:A:292:LEU:CD1	2.55	0.53
1:A:155:TYR:CE1	1:A:173:ILE:HD12	2.43	0.53
1:A:167:ALA:HB1	1:A:209:LEU:CD1	2.36	0.53
1:B:167:ALA:HB1	1:B:209:LEU:CD1	2.36	0.53
1:B:293:GLY:CA	1:B:296:ASP:OD2	2.56	0.53
1:A:380:ALA:O	1:A:381:LEU:CB	2.56	0.53
1:A:70:PHE:O	1:A:71:ILE:C	2.46	0.53
1:B:300:ILE:O	1:B:303:LYS:CG	2.57	0.53
1:B:70:PHE:O	1:B:71:ILE:C	2.46	0.52
1:A:15:GLY:HA2	1:A:67:LYS:HZ2	1.71	0.52
1:B:431:VAL:O	1:B:432:LYS:HB2	2.09	0.52
1:A:299:SER:O	1:A:303:LYS:CG	2.56	0.52
1:B:23:VAL:O	1:B:24:ASP:C	2.45	0.52
1:A:155:TYR:CD2	1:A:170:GLY:CA	2.91	0.52
1:A:313:ILE:CD1	1:A:331:ASP:OD1	2.56	0.52
1:B:143:LEU:O	1:B:143:LEU:HD22	2.10	0.52
1:B:394:ILE:HG22	1:B:399:ARG:CZ	2.39	0.52
1:B:362:PRO:CD	1:B:367:LEU:HD23	2.33	0.52
1:A:372:GLU:C	1:A:374:ILE:HG22	2.30	0.52
1:B:64:LEU:HD11	1:B:303:LYS:HZ3	1.73	0.52
1:B:345:LEU:HG	1:B:346:SER:H	1.74	0.52
1:A:357:ILE:O	1:A:358:MET:CB	2.57	0.52
1:A:377:TRP:CZ3	1:A:417:LEU:CD2	2.93	0.52
1:B:428:LEU:O	1:B:431:VAL:HG23	2.10	0.52
1:A:75:TYR:CE1	1:A:292:LEU:HD12	2.44	0.52
1:A:343:GLY:O	1:A:348:VAL:HG21	2.09	0.52
1:A:1:MET:HG2	1:A:37:SER:HB3	1.91	0.52
1:A:310:TYR:CZ	1:A:355:LEU:HD23	2.44	0.52
1:B:75:TYR:HD2	1:B:297:ILE:CG2	2.19	0.52
1:B:225:LYS:C	1:B:227:TYR:H	2.12	0.52
1:A:384:MET:O	1:B:385:THR:HG23	2.09	0.52
1:A:100:MET:HE3	1:A:209:LEU:HD12	1.90	0.52
1:B:372:GLU:C	1:B:374:ILE:HG22	2.30	0.52
1:A:428:LEU:O	1:A:431:VAL:HG23	2.10	0.52
1:B:361:THR:CG2	1:B:365:ASP:O	2.58	0.52
1:B:374:ILE:HG23	1:B:375:ARG:N	2.24	0.52
1:A:118:TYR:CZ	1:A:122:LYS:HE3	2.44	0.52
1:B:295:GLY:HA2	1:B:298:GLU:CB	2.33	0.52
1:A:209:LEU:O	1:A:210:LYS:C	2.46	0.52
1:B:377:TRP:CZ3	1:B:417:LEU:CD2	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HB3	1:A:389:LEU:O	2.10	0.51
1:A:58:GLU:O	1:A:69:TRP:NE1	2.43	0.51
1:A:225:LYS:C	1:A:227:TYR:H	2.13	0.51
1:A:190:HIS:CG	1:A:197:LYS:CD	2.79	0.51
1:A:164:ILE:CG2	1:A:165:GLU:N	2.59	0.51
1:A:283:ASN:ND2	1:A:283:ASN:C	2.62	0.51
1:B:133:ASP:OD1	1:B:187:ALA:HB2	2.09	0.51
1:A:133:ASP:OD1	1:A:187:ALA:HB2	2.09	0.51
1:B:329:LEU:HD11	1:B:421:TYR:CG	2.45	0.51
1:A:329:LEU:HD11	1:A:421:TYR:CG	2.45	0.51
1:A:75:TYR:HD2	1:A:297:ILE:CG2	2.19	0.51
1:B:83:GLY:HA2	1:B:261:VAL:HG13	1.92	0.51
1:A:361:THR:CG2	1:A:365:ASP:O	2.58	0.51
1:A:417:LEU:O	1:A:421:TYR:CD1	2.64	0.51
1:A:431:VAL:O	1:A:432:LYS:HB2	2.09	0.51
1:B:75:TYR:CE1	1:B:292:LEU:HD12	2.44	0.51
1:B:417:LEU:O	1:B:421:TYR:CD1	2.64	0.51
1:A:380:ALA:HB1	1:A:384:MET:SD	2.51	0.51
1:A:40:ASN:ND2	1:A:42:LYS:CB	2.73	0.51
1:A:225:LYS:C	1:A:227:TYR:N	2.64	0.51
1:A:143:LEU:HD22	1:A:143:LEU:O	2.10	0.51
1:B:144:LEU:HD23	1:B:154:VAL:HB	1.91	0.51
1:B:168:LYS:HE3	1:B:208:VAL:HG13	1.93	0.51
1:B:310:TYR:OH	1:B:355:LEU:HA	2.11	0.51
1:B:374:ILE:C	1:B:376:ARG:N	2.64	0.51
1:A:310:TYR:OH	1:A:355:LEU:HA	2.11	0.51
1:A:361:THR:HA	1:A:367:LEU:HD11	0.66	0.51
1:A:374:ILE:HG23	1:A:375:ARG:N	2.24	0.51
1:A:346:SER:O	1:A:349:LEU:N	2.43	0.51
1:B:283:ASN:C	1:B:283:ASN:ND2	2.62	0.51
1:A:40:ASN:HB3	1:A:43:LEU:HG	1.92	0.51
1:A:53:GLU:CG	1:A:57:LYS:HE3	2.40	0.51
1:B:53:GLU:CG	1:B:57:LYS:HE3	2.40	0.51
1:B:225:LYS:C	1:B:227:TYR:N	2.64	0.51
1:A:259:ALA:O	1:A:262:ALA:HB3	2.11	0.51
1:B:330:ARG:HB3	1:B:389:LEU:O	2.10	0.51
1:B:380:ALA:HB1	1:B:384:MET:SD	2.51	0.51
1:A:163:PRO:HG2	1:A:164:ILE:N	2.22	0.51
1:A:295:GLY:HA2	1:A:298:GLU:CB	2.33	0.51
1:B:40:ASN:HB3	1:B:43:LEU:HG	1.92	0.51
1:A:168:LYS:HE3	1:A:208:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:O	1:B:303:LYS:CG	2.56	0.51
1:A:384:MET:O	1:B:385:THR:CB	2.59	0.50
1:A:75:TYR:CD2	1:A:297:ILE:CG2	2.85	0.50
1:B:301:LEU:O	1:B:301:LEU:HG	2.11	0.50
1:B:61:PRO:O	1:B:62:SER:C	2.48	0.50
1:A:63:VAL:CG1	1:A:63:VAL:O	2.59	0.50
1:B:40:ASN:ND2	1:B:42:LYS:CB	2.73	0.50
1:A:114:GLY:O	1:A:115:LYS:C	2.49	0.50
1:A:301:LEU:HG	1:A:301:LEU:O	2.11	0.50
1:A:61:PRO:O	1:A:62:SER:C	2.48	0.50
1:B:131:ALA:HB2	1:B:143:LEU:HD12	1.92	0.50
1:B:369:ILE:CG2	1:B:370:GLY:N	2.75	0.50
1:A:6:ARG:HG3	1:A:292:LEU:CD2	2.37	0.50
1:A:345:LEU:HG	1:A:346:SER:H	1.74	0.50
1:A:83:GLY:HA2	1:A:261:VAL:HG13	1.92	0.50
1:A:195:GLU:O	1:A:196:THR:C	2.49	0.50
1:A:420:TRP:O	1:A:423:ASN:N	2.45	0.50
1:B:6:ARG:HG3	1:B:292:LEU:CD2	2.37	0.50
1:A:119:PHE:CE1	1:A:123:ARG:NE	2.73	0.50
1:B:374:ILE:HD13	1:B:374:ILE:C	2.31	0.50
1:B:101:LEU:HD23	1:B:215:ILE:HB	1.94	0.50
1:A:359:LEU:CB	1:A:360:PRO:HD2	2.36	0.50
1:A:369:ILE:CG2	1:A:370:GLY:N	2.75	0.50
1:B:420:TRP:O	1:B:423:ASN:N	2.45	0.50
1:A:144:LEU:HD23	1:A:154:VAL:HB	1.91	0.50
1:A:101:LEU:HD23	1:A:215:ILE:HB	1.94	0.50
1:B:346:SER:O	1:B:349:LEU:N	2.43	0.50
1:B:374:ILE:HD13	1:B:375:ARG:N	2.27	0.50
1:A:374:ILE:C	1:A:374:ILE:HD13	2.31	0.50
1:A:243:ILE:HG12	1:A:269:PHE:HB2	1.94	0.50
1:A:123:ARG:C	1:B:358:MET:O	2.50	0.50
1:B:115:LYS:O	1:B:118:TYR:HB3	2.12	0.50
1:B:349:LEU:HA	1:B:352:ILE:CB	2.36	0.50
1:A:374:ILE:HD13	1:A:375:ARG:N	2.27	0.50
1:B:87:GLU:OE1	1:B:283:ASN:OD1	2.30	0.49
1:B:259:ALA:O	1:B:262:ALA:HB3	2.11	0.49
1:A:385:THR:CB	1:B:384:MET:O	2.60	0.49
1:A:418:LEU:HA	1:A:421:TYR:CD1	2.34	0.49
1:A:244:ILE:HB	1:A:270:ILE:HG13	1.94	0.49
1:A:374:ILE:C	1:A:376:ARG:N	2.64	0.49
1:B:114:GLY:O	1:B:115:LYS:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ALA:HB2	1:A:143:LEU:HD12	1.92	0.49
1:B:58:GLU:O	1:B:69:TRP:NE1	2.44	0.49
1:B:195:GLU:O	1:B:196:THR:C	2.49	0.49
1:B:243:ILE:HG12	1:B:269:PHE:HB2	1.94	0.49
1:B:200:GLU:OE2	1:B:200:GLU:C	2.49	0.49
1:A:300:ILE:HA	1:A:303:LYS:HE3	1.94	0.49
1:B:300:ILE:HD13	1:B:303:LYS:HZ2	1.77	0.49
1:A:281:THR:CB	1:B:315:LYS:HD3	2.42	0.49
1:A:115:LYS:O	1:A:118:TYR:HB3	2.12	0.49
1:A:200:GLU:OE1	1:A:201:GLU:N	2.46	0.49
1:A:40:ASN:HD22	1:A:42:LYS:H	1.61	0.49
1:B:63:VAL:O	1:B:63:VAL:CG1	2.59	0.49
1:B:357:ILE:O	1:B:358:MET:CB	2.57	0.49
1:B:377:TRP:N	1:B:377:TRP:CE3	2.81	0.49
1:A:242:VAL:HG12	1:A:243:ILE:N	2.27	0.49
1:B:163:PRO:CG	1:B:164:ILE:H	2.23	0.48
1:A:349:LEU:O	1:A:352:ILE:N	2.43	0.48
1:B:100:MET:HE2	1:B:209:LEU:HD12	1.95	0.48
1:B:244:ILE:HB	1:B:270:ILE:HG13	1.94	0.48
1:A:127:VAL:HA	1:A:181:ILE:O	2.14	0.48
1:B:242:VAL:HG12	1:B:243:ILE:N	2.27	0.48
1:A:207:ASP:OD1	1:A:207:ASP:C	2.52	0.48
1:B:207:ASP:OD1	1:B:207:ASP:C	2.52	0.48
1:B:100:MET:HE3	1:B:209:LEU:HD12	1.95	0.48
1:B:330:ARG:HB3	1:B:389:LEU:HB3	1.95	0.48
1:A:358:MET:O	1:B:123:ARG:C	2.52	0.48
1:A:215:ILE:HG21	1:A:243:ILE:CD1	2.43	0.48
1:B:300:ILE:HA	1:B:303:LYS:HE3	1.94	0.48
1:A:200:GLU:C	1:A:200:GLU:OE2	2.49	0.48
1:A:432:LYS:HE2	1:B:277:ASP:CB	2.40	0.48
1:B:168:LYS:CE	1:B:208:VAL:HG13	2.44	0.48
1:A:87:GLU:OE1	1:A:283:ASN:OD1	2.30	0.48
1:B:107:SER:OG	1:B:109:LYS:HB2	2.13	0.48
1:A:362:PRO:HD2	1:A:367:LEU:CD2	2.38	0.48
1:A:432:LYS:HE2	1:B:277:ASP:OD2	2.14	0.48
1:B:396:ASP:C	1:B:396:ASP:OD1	2.52	0.48
1:A:234:HIS:NE2	1:A:265:ALA:CB	2.75	0.48
1:A:108:GLY:O	1:A:112:THR:OG1	2.25	0.48
1:B:164:ILE:HD11	1:B:208:VAL:HG22	1.88	0.48
1:A:20:GLU:O	1:A:24:ASP:OD2	2.32	0.48
1:A:277:ASP:OD2	1:B:432:LYS:HE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASN:HD22	1:B:42:LYS:H	1.61	0.48
1:A:107:SER:OG	1:A:109:LYS:HB2	2.13	0.48
1:B:430:MET:HA	1:B:430:MET:HE3	1.95	0.48
1:B:370:GLY:O	1:B:373:LYS:HB3	2.14	0.48
1:B:194:GLU:O	1:B:197:LYS:HG2	2.14	0.48
1:A:373:LYS:HE3	1:A:377:TRP:HH2	1.78	0.48
1:A:168:LYS:CE	1:A:208:VAL:HG13	2.44	0.48
1:B:303:LYS:C	1:B:307:LEU:HG	2.31	0.48
1:B:215:ILE:HG21	1:B:243:ILE:CD1	2.43	0.48
1:A:377:TRP:N	1:A:377:TRP:CE3	2.81	0.47
1:A:315:LYS:HD3	1:B:281:THR:CB	2.44	0.47
1:B:127:VAL:HA	1:B:181:ILE:O	2.14	0.47
1:A:194:GLU:HA	1:A:197:LYS:HE3	1.96	0.47
1:A:194:GLU:O	1:A:197:LYS:HG2	2.14	0.47
1:A:376:ARG:O	1:A:379:ALA:CB	2.62	0.47
1:A:417:LEU:C	1:A:421:TYR:CD1	2.88	0.47
1:A:430:MET:HA	1:A:430:MET:HE3	1.96	0.47
1:B:177:ASN:O	1:B:178:LYS:HB2	2.14	0.47
1:A:291:ILE:O	1:A:292:LEU:CB	2.62	0.47
1:A:74:VAL:O	1:A:75:TYR:C	2.53	0.47
1:A:383:SER:HB3	1:A:403:ILE:CA	2.44	0.47
1:A:277:ASP:CB	1:B:432:LYS:HE2	2.41	0.47
1:B:163:PRO:HG2	1:B:164:ILE:N	2.22	0.47
1:A:70:PHE:O	1:A:73:ILE:N	2.47	0.47
1:B:247:MET:SD	1:B:270:ILE:HD11	2.55	0.47
1:B:417:LEU:C	1:B:421:TYR:CD1	2.88	0.47
1:B:300:ILE:HD13	1:B:303:LYS:NZ	2.29	0.47
1:B:302:GLU:CD	1:B:341:LYS:HE3	2.35	0.47
1:B:221:SER:CA	1:B:250:THR:HG21	2.33	0.47
1:B:376:ARG:O	1:B:379:ALA:CB	2.62	0.47
1:B:383:SER:HB3	1:B:403:ILE:CA	2.44	0.47
1:A:141:ASP:O	1:A:145:GLN:HG3	2.15	0.47
1:B:194:GLU:HA	1:B:197:LYS:HE3	1.96	0.47
1:B:200:GLU:OE1	1:B:201:GLU:N	2.46	0.47
1:A:370:GLY:O	1:A:373:LYS:HB3	2.14	0.47
1:A:418:LEU:CA	1:A:421:TYR:HD1	2.21	0.47
1:A:177:ASN:O	1:A:178:LYS:HB2	2.14	0.47
1:A:302:GLU:HB3	1:A:341:LYS:HB3	1.97	0.47
1:B:20:GLU:O	1:B:24:ASP:OD2	2.32	0.47
1:B:61:PRO:O	1:B:62:SER:O	2.33	0.47
1:A:334:ALA:HA	1:A:337:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:MET:SD	1:A:270:ILE:HD11	2.55	0.47
1:A:98:ILE:HD13	1:A:171:VAL:HG11	1.97	0.47
1:A:317:MET:CE	1:A:328:THR:HB	2.45	0.47
1:A:61:PRO:O	1:A:62:SER:O	2.33	0.47
1:B:98:ILE:HD13	1:B:171:VAL:HG11	1.97	0.47
1:A:362:PRO:CD	1:A:367:LEU:HD23	2.33	0.47
1:B:302:GLU:HB3	1:B:341:LYS:HB3	1.97	0.47
1:B:367:LEU:O	1:B:368:LYS:CB	2.63	0.47
1:A:300:ILE:HD13	1:A:303:LYS:NZ	2.29	0.47
1:A:302:GLU:CD	1:A:341:LYS:HE3	2.34	0.47
1:A:85:ASP:OD1	1:A:285:LYS:HE2	2.15	0.47
1:B:235:GLN:C	1:B:237:SER:H	2.18	0.47
1:B:378:LEU:O	1:B:381:LEU:CG	2.60	0.46
1:B:190:HIS:CG	1:B:197:LYS:CD	2.79	0.46
1:A:330:ARG:HB3	1:A:389:LEU:HB3	1.95	0.46
1:B:115:LYS:HG2	1:B:276:ILE:O	2.14	0.46
1:A:115:LYS:HG2	1:A:276:ILE:O	2.14	0.46
1:B:40:ASN:ND2	1:B:42:LYS:H	2.13	0.46
1:A:235:GLN:C	1:A:237:SER:H	2.18	0.46
1:A:119:PHE:CZ	1:A:123:ARG:CZ	2.98	0.46
1:B:317:MET:CE	1:B:328:THR:HB	2.45	0.46
1:A:367:LEU:O	1:A:368:LYS:CB	2.63	0.46
1:A:417:LEU:C	1:A:421:TYR:CE1	2.89	0.46
1:A:301:LEU:HD21	1:A:305:LYS:HZ1	1.77	0.46
1:B:300:ILE:HA	1:B:303:LYS:HG2	1.97	0.46
1:B:334:ALA:CA	1:B:337:ILE:HG22	2.46	0.46
1:A:40:ASN:ND2	1:A:42:LYS:HB2	2.31	0.46
1:A:135:TYR:CE1	1:A:189:ARG:NE	2.83	0.46
1:B:119:PHE:CE1	1:B:123:ARG:NE	2.74	0.46
1:A:94:LYS:N	1:A:97:PHE:CE2	2.68	0.46
1:B:74:VAL:O	1:B:75:TYR:C	2.53	0.46
1:B:85:ASP:OD1	1:B:285:LYS:HE2	2.15	0.46
1:B:230:ALA:O	1:B:231:SER:C	2.54	0.46
1:B:313:ILE:CD1	1:B:331:ASP:OD1	2.56	0.46
1:B:336:ILE:HG13	1:B:377:TRP:HB3	1.98	0.46
1:B:379:ALA:C	1:B:380:ALA:O	2.52	0.46
1:A:317:MET:SD	1:A:328:THR:CB	3.04	0.46
1:B:207:ASP:O	1:B:210:LYS:HG3	2.16	0.46
1:A:40:ASN:ND2	1:A:42:LYS:H	2.13	0.46
1:A:163:PRO:CG	1:A:164:ILE:H	2.23	0.46
1:A:300:ILE:HA	1:A:303:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:CG2	1:A:243:ILE:HG13	2.46	0.46
1:B:298:GLU:O	1:B:302:GLU:HG2	2.16	0.46
1:B:270:ILE:O	1:B:270:ILE:CG2	2.64	0.46
1:A:109:LYS:O	1:A:110:THR:HB	2.16	0.46
1:A:230:ALA:O	1:A:231:SER:C	2.54	0.46
1:B:362:PRO:HD2	1:B:367:LEU:CD2	2.38	0.46
1:B:417:LEU:C	1:B:421:TYR:CE1	2.89	0.46
1:A:361:THR:CB	1:A:367:LEU:CD1	2.93	0.46
1:A:361:THR:HG23	1:A:367:LEU:HG	1.98	0.46
1:A:334:ALA:CA	1:A:337:ILE:HG22	2.46	0.46
1:A:193:GLY:N	1:A:195:GLU:OE2	2.42	0.46
1:B:141:ASP:O	1:B:145:GLN:HG3	2.15	0.46
1:A:301:LEU:O	1:A:305:LYS:CD	2.61	0.46
1:A:300:ILE:C	1:A:302:GLU:N	2.69	0.46
1:A:303:LYS:C	1:A:307:LEU:HG	2.31	0.46
1:B:9:VAL:HG11	1:B:292:LEU:HD13	1.98	0.46
1:B:397:LYS:O	1:B:398:SER:C	2.53	0.46
1:A:270:ILE:CG2	1:A:270:ILE:O	2.63	0.46
1:B:135:TYR:CE1	1:B:189:ARG:NE	2.83	0.46
1:A:125:TYR:CD2	1:B:358:MET:SD	3.09	0.46
1:A:336:ILE:HG13	1:A:377:TRP:HB3	1.98	0.46
1:B:303:LYS:O	1:B:307:LEU:CG	2.49	0.46
1:A:330:ARG:CB	1:A:389:LEU:HB3	2.46	0.46
1:B:310:TYR:HA	1:B:335:GLN:NE2	2.29	0.46
1:B:361:THR:CB	1:B:367:LEU:CD1	2.93	0.46
1:B:378:LEU:CA	1:B:381:LEU:HD11	2.45	0.46
1:A:300:ILE:CD1	1:A:303:LYS:HZ2	2.28	0.46
1:B:298:GLU:C	1:B:300:ILE:N	2.67	0.46
1:B:334:ALA:HA	1:B:337:ILE:HG22	1.97	0.46
1:A:122:LYS:C	1:A:124:GLY:N	2.70	0.45
1:A:75:TYR:CZ	1:A:292:LEU:HD12	2.50	0.45
1:B:307:LEU:N	1:B:307:LEU:HD23	2.31	0.45
1:B:392:PRO:O	1:B:395:ILE:HG13	2.16	0.45
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.61	0.45
1:A:396:ASP:C	1:A:396:ASP:OD1	2.52	0.45
1:A:378:LEU:O	1:A:381:LEU:CG	2.60	0.45
1:B:94:LYS:O	1:B:96:PRO:O	2.34	0.45
1:B:2:LEU:HD13	1:B:291:ILE:CG2	2.46	0.45
1:B:119:PHE:CZ	1:B:123:ARG:CZ	2.98	0.45
1:B:301:LEU:O	1:B:305:LYS:CD	2.61	0.45
1:B:70:PHE:O	1:B:73:ILE:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ILE:CG2	1:B:243:ILE:HG13	2.46	0.45
1:B:40:ASN:ND2	1:B:42:LYS:HB2	2.31	0.45
1:A:335:GLN:O	1:A:338:ALA:HB3	2.17	0.45
1:A:307:LEU:HD23	1:A:307:LEU:N	2.31	0.45
1:B:75:TYR:CZ	1:B:292:LEU:HD12	2.50	0.45
1:B:2:LEU:HD11	1:B:288:VAL:HA	1.98	0.45
1:A:235:GLN:C	1:A:237:SER:N	2.70	0.45
1:B:335:GLN:O	1:B:338:ALA:HB3	2.17	0.45
1:A:392:PRO:O	1:A:395:ILE:HG13	2.17	0.45
1:B:111:THR:HG22	1:B:115:LYS:HE3	1.98	0.45
1:A:298:GLU:O	1:A:302:GLU:HG2	2.16	0.45
1:A:9:VAL:HG11	1:A:292:LEU:HD13	1.98	0.45
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.70	0.45
1:A:349:LEU:HA	1:A:352:ILE:CB	2.36	0.45
1:A:207:ASP:O	1:A:210:LYS:HG3	2.16	0.45
1:B:109:LYS:O	1:B:110:THR:HB	2.16	0.45
1:A:93:THR:O	1:A:93:THR:HG22	2.16	0.45
1:B:93:THR:O	1:B:93:THR:HG22	2.16	0.45
1:B:212:ASP:O	1:B:213:ASP:OD1	2.35	0.45
1:B:317:MET:SD	1:B:328:THR:CB	3.04	0.45
1:A:125:TYR:CG	1:B:358:MET:SD	3.10	0.45
1:B:391:ASN:O	1:B:392:PRO:C	2.55	0.45
1:A:417:LEU:CB	1:A:421:TYR:HE1	2.21	0.45
1:A:2:LEU:HD11	1:A:288:VAL:HA	1.98	0.45
1:B:300:ILE:CA	1:B:303:LYS:HG2	2.47	0.45
1:A:164:ILE:HD11	1:A:208:VAL:HG22	1.88	0.45
1:A:168:LYS:HG3	1:A:172:ASP:OD2	2.17	0.45
1:A:94:LYS:O	1:A:96:PRO:O	2.34	0.45
1:B:300:ILE:C	1:B:302:GLU:H	2.19	0.45
1:B:300:ILE:HA	1:B:303:LYS:CD	2.47	0.45
1:B:40:ASN:HD22	1:B:42:LYS:HB3	1.82	0.45
1:B:372:GLU:O	1:B:374:ILE:CG2	2.62	0.45
1:B:330:ARG:CB	1:B:389:LEU:HB3	2.46	0.45
1:A:336:ILE:HD11	1:A:377:TRP:CD1	2.52	0.45
1:A:94:LYS:CA	1:A:97:PHE:CZ	3.00	0.45
1:A:50:LYS:HD3	1:A:77:GLU:OE1	2.17	0.45
1:B:301:LEU:O	1:B:305:LYS:CG	2.65	0.45
1:A:397:LYS:O	1:A:398:SER:C	2.53	0.45
1:B:373:LYS:O	1:B:373:LYS:HG3	2.17	0.44
1:A:373:LYS:HG3	1:A:373:LYS:O	2.17	0.44
1:A:300:ILE:C	1:A:302:GLU:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ILE:CA	1:A:303:LYS:HG2	2.47	0.44
1:A:100:MET:HE2	1:A:209:LEU:HD12	2.00	0.44
1:B:418:LEU:CA	1:B:421:TYR:HD1	2.22	0.44
1:A:335:GLN:OE1	1:A:335:GLN:HA	2.17	0.44
1:A:300:ILE:HA	1:A:303:LYS:CD	2.47	0.44
1:A:301:LEU:O	1:A:305:LYS:CG	2.65	0.44
1:B:207:ASP:OD1	1:B:210:LYS:NZ	2.50	0.44
1:B:234:HIS:NE2	1:B:265:ALA:CB	2.75	0.44
1:A:212:ASP:O	1:A:213:ASP:OD1	2.35	0.44
1:B:361:THR:HG23	1:B:367:LEU:HG	1.98	0.44
1:A:336:ILE:HA	1:A:339:LEU:HD23	1.99	0.44
1:B:168:LYS:HG3	1:B:172:ASP:OD2	2.17	0.44
1:B:47:LEU:CD1	1:B:77:GLU:HB3	2.48	0.44
1:A:157:GLU:OE2	1:A:169:LYS:HD2	2.17	0.44
1:B:349:LEU:O	1:B:352:ILE:N	2.43	0.44
1:B:150:ILE:HG13	1:B:152:VAL:CG2	2.39	0.44
1:B:30:LEU:HD23	1:B:48:THR:CG2	2.47	0.44
1:B:336:ILE:HA	1:B:339:LEU:HD23	1.99	0.44
1:A:298:GLU:C	1:A:300:ILE:N	2.67	0.44
1:B:23:VAL:HG13	1:B:70:PHE:CZ	2.53	0.44
1:B:192:TYR:HE1	1:B:229:LEU:HD23	1.83	0.44
1:A:198:LEU:O	1:A:201:GLU:HB3	2.18	0.44
1:A:111:THR:HG22	1:A:115:LYS:HE3	1.98	0.44
1:A:47:LEU:CD1	1:A:77:GLU:HB3	2.48	0.44
1:B:157:GLU:OE2	1:B:169:LYS:HD2	2.17	0.44
1:B:333:TYR:O	1:B:334:ALA:C	2.55	0.44
1:A:53:GLU:O	1:A:57:LYS:HG3	2.18	0.44
1:B:53:GLU:O	1:B:57:LYS:HG3	2.18	0.44
1:A:378:LEU:CA	1:A:381:LEU:HD11	2.45	0.44
1:B:94:LYS:CA	1:B:97:PHE:CZ	3.00	0.44
1:A:71:ILE:O	1:A:74:VAL:HB	2.18	0.44
1:A:302:GLU:CD	1:A:341:LYS:CD	2.86	0.44
1:A:402:ARG:CB	1:B:402:ARG:NH1	2.79	0.44
1:A:40:ASN:HD22	1:A:42:LYS:HB3	1.82	0.44
1:B:410:GLU:HG2	1:B:411:VAL:N	2.33	0.44
1:B:335:GLN:OE1	1:B:335:GLN:HA	2.17	0.44
1:B:361:THR:HA	1:B:367:LEU:CG	2.40	0.44
1:B:164:ILE:O	1:B:165:GLU:C	2.56	0.44
1:A:23:VAL:HG13	1:A:70:PHE:CZ	2.53	0.44
1:B:291:ILE:O	1:B:292:LEU:CB	2.62	0.44
1:B:300:ILE:C	1:B:302:GLU:N	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:HD3	1:B:77:GLU:OE1	2.17	0.44
1:A:164:ILE:O	1:A:165:GLU:C	2.56	0.44
1:A:303:LYS:HG3	1:A:304:VAL:N	2.30	0.44
1:B:298:GLU:O	1:B:299:SER:C	2.56	0.44
1:B:69:TRP:CD1	1:B:73:ILE:HD11	2.53	0.44
1:A:348:VAL:HG12	1:A:352:ILE:CD1	2.45	0.44
1:B:198:LEU:O	1:B:201:GLU:HB3	2.18	0.43
1:B:122:LYS:C	1:B:124:GLY:N	2.70	0.43
1:A:207:ASP:OD1	1:A:210:LYS:NZ	2.50	0.43
1:A:244:ILE:HG13	1:A:267:ILE:HD13	1.99	0.43
1:A:64:LEU:HD11	1:A:303:LYS:HZ3	1.83	0.43
1:A:69:TRP:CD1	1:A:73:ILE:HD11	2.53	0.43
1:B:302:GLU:CD	1:B:341:LYS:CD	2.86	0.43
1:B:71:ILE:O	1:B:74:VAL:HB	2.18	0.43
1:B:78:LEU:O	1:B:79:SER:C	2.56	0.43
1:A:41:VAL:CG1	1:A:41:VAL:O	2.65	0.43
1:A:372:GLU:O	1:A:374:ILE:CG2	2.62	0.43
1:A:176:LYS:O	1:A:177:ASN:C	2.56	0.43
1:A:176:LYS:O	1:A:178:LYS:HG2	2.18	0.43
1:A:298:GLU:O	1:A:299:SER:C	2.56	0.43
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.79	0.43
1:A:349:LEU:HA	1:A:352:ILE:HD12	2.00	0.43
1:B:41:VAL:CG1	1:B:41:VAL:O	2.65	0.43
1:A:109:LYS:HE2	1:A:186:THR:O	2.18	0.43
1:A:104:VAL:HG21	1:A:192:TYR:CE2	2.53	0.43
1:A:2:LEU:HD13	1:A:291:ILE:CG2	2.46	0.43
1:B:349:LEU:HA	1:B:352:ILE:HD12	2.00	0.43
1:B:235:GLN:C	1:B:237:SER:N	2.70	0.43
1:A:163:PRO:O	1:A:166:ILE:N	2.52	0.43
1:B:131:ALA:O	1:B:140:TYR:CE2	2.69	0.43
1:A:199:LEU:HA	1:A:202:MET:SD	2.59	0.43
1:A:83:GLY:HA2	1:A:261:VAL:CG1	2.48	0.43
1:A:410:GLU:HG2	1:A:411:VAL:N	2.33	0.43
1:B:403:ILE:HG22	1:B:414:VAL:CG2	2.45	0.43
1:B:417:LEU:CB	1:B:421:TYR:HE1	2.21	0.43
1:B:119:PHE:HZ	1:B:123:ARG:HH21	1.48	0.43
1:B:2:LEU:HA	1:B:2:LEU:HD23	1.79	0.43
1:B:244:ILE:HG13	1:B:267:ILE:HD13	1.99	0.43
1:B:293:GLY:O	1:B:296:ASP:HB2	2.18	0.43
1:A:192:TYR:HE1	1:A:229:LEU:HD23	1.83	0.43
1:B:163:PRO:O	1:B:166:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLU:CD	1:B:341:LYS:HD2	2.39	0.43
1:A:293:GLY:O	1:A:296:ASP:HB2	2.18	0.43
1:B:105:GLN:O	1:B:106:GLY:C	2.56	0.43
1:B:336:ILE:HD11	1:B:377:TRP:CD1	2.52	0.43
1:A:358:MET:SD	1:B:125:TYR:CD2	3.12	0.43
1:A:291:ILE:HG13	1:A:291:ILE:O	2.19	0.43
1:A:301:LEU:HD21	1:A:305:LYS:HZ2	1.83	0.43
1:B:2:LEU:HB3	1:B:291:ILE:HG22	2.01	0.43
1:B:348:VAL:HG12	1:B:352:ILE:CD1	2.45	0.43
1:B:199:LEU:HA	1:B:202:MET:SD	2.59	0.43
1:A:247:MET:HG3	1:A:270:ILE:CD1	2.48	0.43
1:B:291:ILE:O	1:B:291:ILE:HG13	2.19	0.43
1:B:303:LYS:HG3	1:B:304:VAL:N	2.30	0.43
1:B:247:MET:HG3	1:B:270:ILE:CD1	2.48	0.43
1:B:109:LYS:HE2	1:B:186:THR:O	2.18	0.43
1:B:146:LEU:HD22	1:B:276:ILE:HD13	2.00	0.43
1:A:131:ALA:O	1:A:140:TYR:CE2	2.69	0.43
1:B:210:LYS:N	1:B:211:PRO:CD	2.82	0.43
1:B:127:VAL:HG12	1:B:128:GLY:N	2.34	0.43
1:A:175:VAL:HG12	1:A:175:VAL:O	2.19	0.43
1:A:391:ASN:O	1:A:392:PRO:C	2.55	0.42
1:A:124:GLY:HA3	1:B:359:LEU:N	2.34	0.42
1:B:163:PRO:CG	1:B:164:ILE:N	2.82	0.42
1:A:219:ASP:CG	1:A:221:SER:HG	2.19	0.42
1:A:333:TYR:O	1:A:334:ALA:C	2.55	0.42
1:B:104:VAL:HG21	1:B:192:TYR:CE2	2.53	0.42
1:A:403:ILE:HG22	1:A:414:VAL:CG2	2.45	0.42
1:B:176:LYS:O	1:B:178:LYS:HG2	2.18	0.42
1:B:40:ASN:O	1:B:44:VAL:HG23	2.19	0.42
1:B:335:GLN:CB	1:B:355:LEU:HD22	2.46	0.42
1:A:302:GLU:CD	1:A:341:LYS:HD2	2.39	0.42
1:B:107:SER:C	1:B:109:LYS:N	2.71	0.42
1:B:157:GLU:HB2	1:B:160:ASN:HD22	1.77	0.42
1:A:37:SER:O	1:A:38:ASP:HB3	2.19	0.42
1:B:83:GLY:HA2	1:B:261:VAL:CG1	2.48	0.42
1:B:383:SER:O	1:B:384:MET:HG3	2.20	0.42
1:A:210:LYS:N	1:A:211:PRO:CD	2.82	0.42
1:B:368:LYS:O	1:B:369:ILE:HB	2.20	0.42
1:A:383:SER:O	1:A:384:MET:HG3	2.20	0.42
1:A:2:LEU:HB3	1:A:291:ILE:HG22	2.01	0.42
1:A:299:SER:C	1:A:303:LYS:HE3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:OG	1:A:73:ILE:N	2.53	0.42
1:A:76:ASP:O	1:A:79:SER:HB3	2.19	0.42
1:B:302:GLU:CD	1:B:341:LYS:CE	2.88	0.42
1:A:222:ILE:HA	1:A:222:ILE:HD12	1.93	0.42
1:A:30:LEU:HD23	1:A:48:THR:CG2	2.47	0.42
1:A:310:TYR:OH	1:A:354:GLY:O	2.37	0.42
1:A:376:ARG:O	1:A:379:ALA:HB3	2.19	0.42
1:A:358:MET:SD	1:B:125:TYR:CG	3.13	0.42
1:B:283:ASN:HD21	1:B:285:LYS:HG2	1.85	0.42
1:A:383:SER:HB2	1:A:403:ILE:HG23	1.97	0.42
1:A:146:LEU:HD22	1:A:276:ILE:HD13	2.00	0.42
1:B:37:SER:O	1:B:38:ASP:HB3	2.20	0.42
1:A:334:ALA:C	1:A:337:ILE:HG22	2.40	0.42
1:A:40:ASN:O	1:A:44:VAL:HG23	2.19	0.42
1:B:35:ILE:O	1:B:36:SER:C	2.57	0.42
1:A:303:LYS:O	1:A:307:LEU:CG	2.49	0.42
1:A:167:ALA:C	1:A:209:LEU:HD21	2.40	0.42
1:A:227:TYR:O	1:A:228:ASP:C	2.57	0.42
1:B:13:LEU:HD23	1:B:13:LEU:HA	1.84	0.42
1:B:76:ASP:O	1:B:79:SER:HB3	2.19	0.42
1:A:283:ASN:HD21	1:A:285:LYS:HG2	1.85	0.42
1:B:227:TYR:O	1:B:228:ASP:C	2.57	0.42
1:B:121:LYS:O	1:B:124:GLY:N	2.52	0.41
1:A:302:GLU:CD	1:A:341:LYS:CE	2.88	0.41
1:B:202:MET:O	1:B:203:LYS:C	2.59	0.41
1:B:347:LYS:HD2	1:B:350:GLN:HE21	1.84	0.41
1:A:105:GLN:O	1:A:106:GLY:C	2.56	0.41
1:B:377:TRP:CA	1:B:377:TRP:HE3	2.33	0.41
1:B:20:GLU:OE1	1:B:20:GLU:HA	2.20	0.41
1:B:298:GLU:O	1:B:300:ILE:N	2.54	0.41
1:A:127:VAL:HG12	1:A:128:GLY:N	2.34	0.41
1:B:64:LEU:CD1	1:B:303:LYS:HZ3	2.33	0.41
1:B:113:ALA:O	1:B:129:LEU:HD21	2.21	0.41
1:B:116:LEU:HD23	1:B:183:ILE:HD13	2.03	0.41
1:A:284:ALA:O	1:A:286:ARG:N	2.52	0.41
1:B:373:LYS:HE3	1:B:377:TRP:HH2	1.78	0.41
1:B:383:SER:HB3	1:B:403:ILE:HA	2.03	0.41
1:A:379:ALA:C	1:A:380:ALA:O	2.52	0.41
1:A:381:LEU:HB2	1:A:382:ASN:H	1.54	0.41
1:A:116:LEU:HD23	1:A:183:ILE:HD13	2.03	0.41
1:B:299:SER:C	1:B:303:LYS:HE3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:37:SER:OG	2.79	0.41
1:B:334:ALA:C	1:B:337:ILE:HG22	2.39	0.41
1:A:138:ALA:O	1:A:142:GLN:HB2	2.20	0.41
1:B:376:ARG:O	1:B:379:ALA:HB3	2.19	0.41
1:B:15:GLY:HA2	1:B:67:LYS:HZ2	1.78	0.41
1:B:284:ALA:O	1:B:286:ARG:N	2.52	0.41
1:B:350:GLN:HG3	1:B:351:HIS:CD2	2.56	0.41
1:A:350:GLN:HG3	1:A:351:HIS:CD2	2.56	0.41
1:B:138:ALA:O	1:B:142:GLN:HB2	2.20	0.41
1:A:368:LYS:O	1:A:369:ILE:HB	2.20	0.41
1:A:381:LEU:N	1:A:381:LEU:CD2	2.62	0.41
1:B:219:ASP:CG	1:B:221:SER:HG	2.21	0.41
1:B:244:ILE:HG21	1:B:257:LEU:CD1	2.51	0.41
1:B:383:SER:HB2	1:B:403:ILE:HG23	1.97	0.41
1:A:402:ARG:NH1	1:B:402:ARG:CB	2.79	0.41
1:A:202:MET:O	1:A:203:LYS:C	2.58	0.41
1:A:333:TYR:O	1:A:337:ILE:HG22	2.21	0.41
1:A:107:SER:C	1:A:109:LYS:N	2.71	0.41
1:A:335:GLN:CB	1:A:355:LEU:HD22	2.46	0.41
1:A:379:ALA:HB1	1:A:409:LEU:HD11	2.03	0.41
1:A:430:MET:CE	1:A:430:MET:HA	2.50	0.41
1:B:168:LYS:HE3	1:B:208:VAL:CG1	2.51	0.41
1:A:143:LEU:HA	1:A:143:LEU:HD23	1.81	0.41
1:A:78:LEU:O	1:A:79:SER:C	2.56	0.41
1:A:20:GLU:HA	1:A:20:GLU:OE1	2.20	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.70	0.41
1:A:113:ALA:O	1:A:129:LEU:HD21	2.20	0.41
1:A:131:ALA:HB1	1:A:140:TYR:CD2	2.56	0.41
1:B:300:ILE:CD1	1:B:303:LYS:HZ2	2.33	0.41
1:A:157:GLU:HB2	1:A:160:ASN:HD22	1.77	0.41
1:A:284:ALA:O	1:A:287:PHE:N	2.54	0.41
1:B:167:ALA:C	1:B:209:LEU:HD21	2.40	0.41
1:A:347:LYS:HD2	1:A:350:GLN:HE21	1.84	0.41
1:B:175:VAL:HG12	1:B:175:VAL:O	2.19	0.41
1:B:381:LEU:HB2	1:B:382:ASN:H	1.53	0.41
1:A:310:TYR:HA	1:A:335:GLN:NE2	2.29	0.41
1:A:168:LYS:HE3	1:A:208:VAL:CG1	2.51	0.41
1:A:47:LEU:C	1:A:49:ALA:H	2.24	0.41
1:B:264:GLY:O	1:B:265:ALA:O	2.39	0.41
1:A:179:MET:HA	1:A:179:MET:HE1	1.99	0.41
1:B:377:TRP:O	1:B:381:LEU:HD11	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:MET:O	1:A:432:LYS:N	2.55	0.40
1:B:423:ASN:ND2	1:B:423:ASN:O	2.55	0.40
1:B:6:ARG:CA	1:B:292:LEU:HD21	2.51	0.40
1:B:131:ALA:HB1	1:B:140:TYR:CD2	2.56	0.40
1:A:347:LYS:CG	1:A:347:LYS:O	2.69	0.40
1:A:119:PHE:CE1	1:A:123:ARG:NH2	2.88	0.40
1:B:331:ASP:O	1:B:332:VAL:CB	2.70	0.40
1:A:383:SER:HB3	1:A:403:ILE:HA	2.03	0.40
1:A:420:TRP:O	1:A:421:TYR:C	2.60	0.40
1:A:121:LYS:O	1:A:124:GLY:N	2.52	0.40
1:A:281:THR:HG21	1:B:315:LYS:HZ2	1.77	0.40
1:B:312:LYS:O	1:B:315:LYS:N	2.54	0.40
1:A:264:GLY:O	1:A:265:ALA:O	2.39	0.40
1:A:35:ILE:O	1:A:36:SER:C	2.57	0.40
1:B:127:VAL:HG13	1:B:181:ILE:O	2.22	0.40
1:B:329:LEU:HD22	1:B:392:PRO:CG	2.51	0.40
1:B:380:ALA:O	1:B:381:LEU:CG	2.70	0.40
1:A:377:TRP:O	1:A:381:LEU:HD11	2.21	0.40
1:A:298:GLU:O	1:A:300:ILE:N	2.54	0.40
1:B:47:LEU:C	1:B:49:ALA:H	2.24	0.40
1:B:349:LEU:N	1:B:352:ILE:HD12	2.37	0.40
1:A:397:LYS:N	1:A:400:MET:CE	2.85	0.40
1:A:419:GLU:HG3	1:A:419:GLU:O	2.21	0.40
1:A:313:ILE:HG21	1:A:335:GLN:NE2	2.37	0.40
1:B:333:TYR:O	1:B:337:ILE:HG22	2.21	0.40
1:A:127:VAL:HG13	1:A:181:ILE:O	2.22	0.40
1:B:83:GLY:CA	1:B:261:VAL:CG1	3.00	0.40
1:B:430:MET:HA	1:B:430:MET:CE	2.51	0.40

All (43) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PRO:CB	1:B:362:PRO:CA[8_454]	1.18	1.02
1:A:362:PRO:CA	1:B:360:PRO:CB[8_454]	1.24	0.96
1:A:200:GLU:CB	1:B:203:LYS:CB[6_555]	1.41	0.79
1:A:203:LYS:CB	1:B:200:GLU:CB[6_555]	1.45	0.75
1:A:360:PRO:CB	1:B:362:PRO:CB[8_454]	1.57	0.63
1:A:362:PRO:CB	1:B:360:PRO:CB[8_454]	1.69	0.51
1:A:362:PRO:C	1:B:360:PRO:CB[8_454]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PRO:CB	1:B:362:PRO:C[8_454]	1.79	0.41
1:A:367:LEU:CD1	1:B:367:LEU:CD2[8_454]	1.83	0.37
1:A:207:ASP:CB	1:B:196:THR:CB[6_555]	1.85	0.35
1:A:196:THR:CB	1:B:207:ASP:CB[6_555]	1.85	0.35
1:A:200:GLU:O	1:B:200:GLU:O[6_555]	1.89	0.31
1:A:204:GLU:CB	1:B:197:LYS:CA[6_555]	1.90	0.30
1:A:367:LEU:CD2	1:B:367:LEU:CD1[8_454]	1.90	0.30
1:A:207:ASP:CB	1:B:196:THR:CG2[6_555]	1.92	0.28
1:A:197:LYS:CA	1:B:204:GLU:CB[6_555]	1.92	0.28
1:A:196:THR:CG2	1:B:207:ASP:CB[6_555]	1.93	0.27
1:A:204:GLU:N	1:B:200:GLU:CG[6_555]	2.03	0.17
1:A:200:GLU:CG	1:B:204:GLU:N[6_555]	2.03	0.17
1:A:41:VAL:CG1	1:B:41:VAL:CG1[6_554]	2.04	0.16
1:A:207:ASP:OD2	1:B:196:THR:OG1[6_555]	2.04	0.16
1:A:360:PRO:CA	1:B:362:PRO:CA[8_454]	2.04	0.16
1:A:196:THR:OG1	1:B:207:ASP:OD2[6_555]	2.07	0.13
1:A:207:ASP:CG	1:B:196:THR:OG1[6_555]	2.10	0.10
1:A:362:PRO:CA	1:B:360:PRO:CA[8_454]	2.10	0.10
1:A:207:ASP:OD2	1:B:196:THR:CB[6_555]	2.12	0.08
1:A:363:SER:N	1:B:360:PRO:CB[8_454]	2.12	0.08
1:A:196:THR:OG1	1:B:207:ASP:CG[6_555]	2.13	0.07
1:A:196:THR:CB	1:B:207:ASP:OD2[6_555]	2.13	0.07
1:A:204:GLU:CA	1:B:197:LYS:CA[6_555]	2.14	0.06
1:A:197:LYS:CA	1:B:204:GLU:CA[6_555]	2.14	0.06
1:A:200:GLU:C	1:B:200:GLU:O[6_555]	2.15	0.05
1:A:200:GLU:O	1:B:200:GLU:C[6_555]	2.15	0.05
1:A:200:GLU:CG	1:B:200:GLU:O[6_555]	2.16	0.04
1:A:204:GLU:CB	1:B:197:LYS:CB[6_555]	2.16	0.04
1:A:197:LYS:CB	1:B:204:GLU:CB[6_555]	2.16	0.04
1:A:200:GLU:O	1:B:200:GLU:CG[6_555]	2.17	0.03
1:A:200:GLU:CA	1:B:203:LYS:CB[6_555]	2.17	0.03
1:A:204:GLU:CB	1:B:200:GLU:OE1[6_555]	2.19	0.01
1:A:200:GLU:OE2	1:B:200:GLU:OE2[6_555]	2.19	0.01
1:A:200:GLU:OE1	1:B:204:GLU:CB[6_555]	2.19	0.01
1:A:200:GLU:CB	1:B:203:LYS:CA[6_555]	2.19	0.01
1:A:203:LYS:CB	1:B:200:GLU:CA[6_555]	2.19	0.01

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	421/440 (96%)	294 (70%)	87 (21%)	40 (10%)	1	15
1	B	421/440 (96%)	293 (70%)	88 (21%)	40 (10%)	1	15
All	All	842/880 (96%)	587 (70%)	175 (21%)	80 (10%)	1	15

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	236	ALA
1	A	265	ALA
1	A	332	VAL
1	A	343	GLY
1	A	347	LYS
1	A	357	ILE
1	A	358	MET
1	A	359	LEU
1	A	369	ILE
1	A	373	LYS
1	A	379	ALA
1	A	380	ALA
1	B	63	VAL
1	B	236	ALA
1	B	265	ALA
1	B	332	VAL
1	B	343	GLY
1	B	347	LYS
1	B	357	ILE
1	B	358	MET
1	B	359	LEU
1	B	369	ILE
1	B	373	LYS
1	B	379	ALA

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Mol	Chain	Res	Type
1	B	380	ALA
1	A	15	GLY
1	A	16	SER
1	A	62	SER
1	A	106	GLY
1	A	110	THR
1	A	177	ASN
1	A	179	MET
1	A	284	ALA
1	A	292	LEU
1	A	300	ILE
1	A	329	LEU
1	A	356	GLY
1	A	368	LYS
1	A	404	ALA
1	B	15	GLY
1	B	16	SER
1	B	62	SER
1	B	106	GLY
1	B	110	THR
1	B	177	ASN
1	B	179	MET
1	B	284	ALA
1	B	292	LEU
1	B	300	ILE
1	B	329	LEU
1	B	356	GLY
1	B	368	LYS
1	B	404	ALA
1	A	195	GLU
1	A	316	LYS
1	B	195	GLU
1	B	316	LYS
1	A	84	GLY
1	A	285	LYS
1	A	315	LYS
1	A	397	LYS
1	B	84	GLY
1	B	285	LYS
1	B	315	LYS
1	B	397	LYS
1	A	18	PRO

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Mol	Chain	Res	Type
1	A	361	THR
1	A	381	LEU
1	A	431	VAL
1	B	18	PRO
1	B	361	THR
1	B	381	LEU
1	B	431	VAL
1	A	158	PRO
1	A	164	ILE
1	B	158	PRO
1	B	164	ILE
1	A	163	PRO
1	B	163	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	365/377 (97%)	340 (93%)	25 (7%)	20	59
1	B	365/377 (97%)	340 (93%)	25 (7%)	20	59
All	All	730/754 (97%)	680 (93%)	50 (7%)	20	59

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	SER
1	A	17	THR
1	A	59	LYS
1	A	72	SER
1	A	136	ARG
1	A	143	LEU
1	A	200	GLU
1	A	250	THR
1	A	283	ASN

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Mol	Chain	Res	Type
1	A	297	ILE
1	A	310	TYR
1	A	311	ASP
1	A	328	THR
1	A	331	ASP
1	A	349	LEU
1	A	357	ILE
1	A	359	LEU
1	A	361	THR
1	A	374	ILE
1	A	377	TRP
1	A	381	LEU
1	A	384	MET
1	A	386	TYR
1	A	423	ASN
1	B	1	MET
1	B	16	SER
1	B	17	THR
1	B	59	LYS
1	B	72	SER
1	B	136	ARG
1	B	143	LEU
1	B	200	GLU
1	B	250	THR
1	B	283	ASN
1	B	297	ILE
1	B	310	TYR
1	B	311	ASP
1	B	328	THR
1	B	331	ASP
1	B	349	LEU
1	B	357	ILE
1	B	359	LEU
1	B	361	THR
1	B	374	ILE
1	B	377	TRP
1	B	381	LEU
1	B	384	MET
1	B	386	TYR
1	B	423	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	31	GLN
1	A	40	ASN
1	A	91	ASN
1	A	148	ASN
1	A	160	ASN
1	A	190	HIS
1	A	224	GLN
1	A	234	HIS
1	A	235	GLN
1	A	283	ASN
1	A	350	GLN
1	A	351	HIS
1	B	4	ASN
1	B	31	GLN
1	B	40	ASN
1	B	91	ASN
1	B	148	ASN
1	B	160	ASN
1	B	190	HIS
1	B	224	GLN
1	B	234	HIS
1	B	235	GLN
1	B	283	ASN
1	B	350	GLN
1	B	351	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/440 (96%)	0.37	26 (6%) 25 16	80, 85, 85, 85	0
1	B	425/440 (96%)	0.32	22 (5%) 31 23	80, 85, 85, 85	0
All	All	850/880 (96%)	0.35	48 (5%) 28 20	80, 85, 85, 85	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	TYR	5.9
1	A	142	GLN	5.4
1	B	192	TYR	5.1
1	A	205	MET	4.9
1	B	142	GLN	4.9
1	A	143	LEU	4.9
1	B	143	LEU	4.8
1	A	104	VAL	4.6
1	B	205	MET	3.8
1	A	208	VAL	3.7
1	B	104	VAL	3.6
1	A	204	GLU	3.3
1	B	135	TYR	3.3
1	A	146	LEU	3.3
1	B	146	LEU	3.3
1	B	131	ALA	3.2
1	A	91	ASN	3.2
1	A	247	MET	3.1
1	A	135	TYR	3.0
1	B	355	LEU	2.9
1	B	204	GLU	2.8
1	B	247	MET	2.8
1	A	98	ILE	2.8
1	A	131	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	75	TYR	2.6
1	B	98	ILE	2.6
1	A	395	ILE	2.6
1	A	327	LEU	2.6
1	A	75	TYR	2.5
1	B	327	LEU	2.5
1	A	51	ILE	2.5
1	B	134	VAL	2.5
1	A	377	TRP	2.4
1	B	51	ILE	2.4
1	A	394	ILE	2.4
1	A	54	ARG	2.3
1	B	395	ILE	2.3
1	B	60	PRO	2.3
1	B	208	VAL	2.2
1	A	149	GLN	2.1
1	B	149	GLN	2.1
1	A	355	LEU	2.1
1	B	54	ARG	2.1
1	A	103	GLY	2.0
1	A	87	GLU	2.0
1	A	365	ASP	2.0
1	A	93	THR	2.0
1	B	344	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.