



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:45 AM GMT

PDB ID : 2E6K
Title : X-ray structure of Thermus thermophilus HB8 TT0505
Authors : Yoshida, H.; Kamitori, S.; Agari, Y.; Iino, H.; Kanagawa, M.; Nakagawa, N.; Ebihara, A.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-12-27
Resolution : 2.09 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

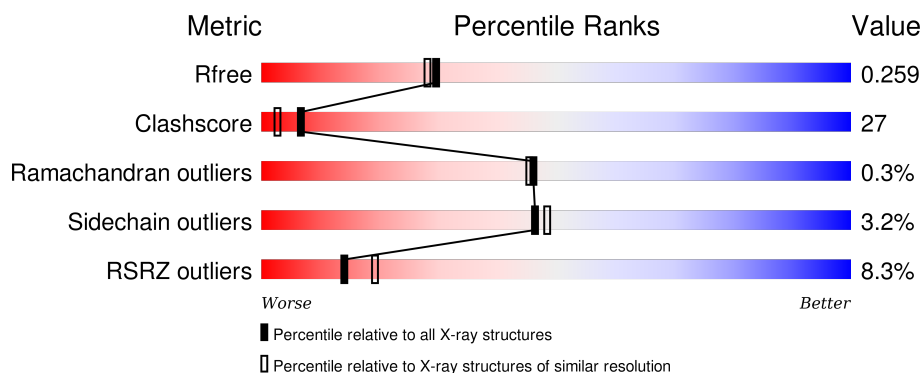
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	651	<div> <div></div> <div>77%21%..</div> </div>
1	B	651	<div> <div>%</div> <div>76%22%..</div> </div>
1	C	651	<div> <div>6%</div> <div>58%41%..</div> </div>
1	D	651	<div> <div>25%</div> <div>39%57%..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21768 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 Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			
1	B	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			
1	C	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			
1	D	647	Total	C	N	O	Se	0	0	0
			5039	3218	895	911	15			

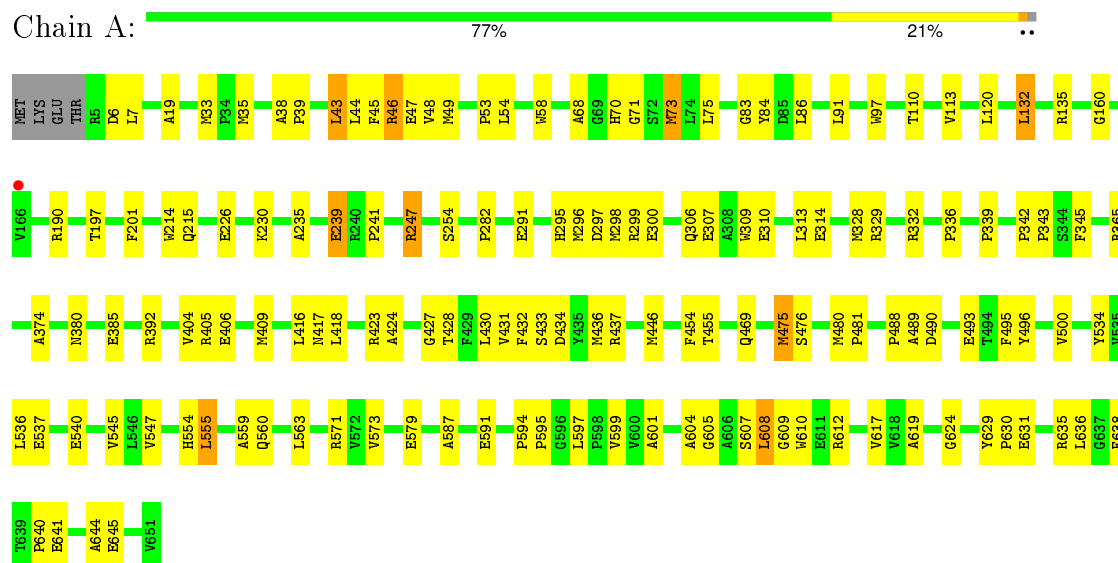
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	531	Total	O	0	0
			531	531		
2	B	496	Total	O	0	0
			496	496		
2	C	297	Total	O	0	0
			297	297		
2	D	288	Total	O	0	0
			288	288		

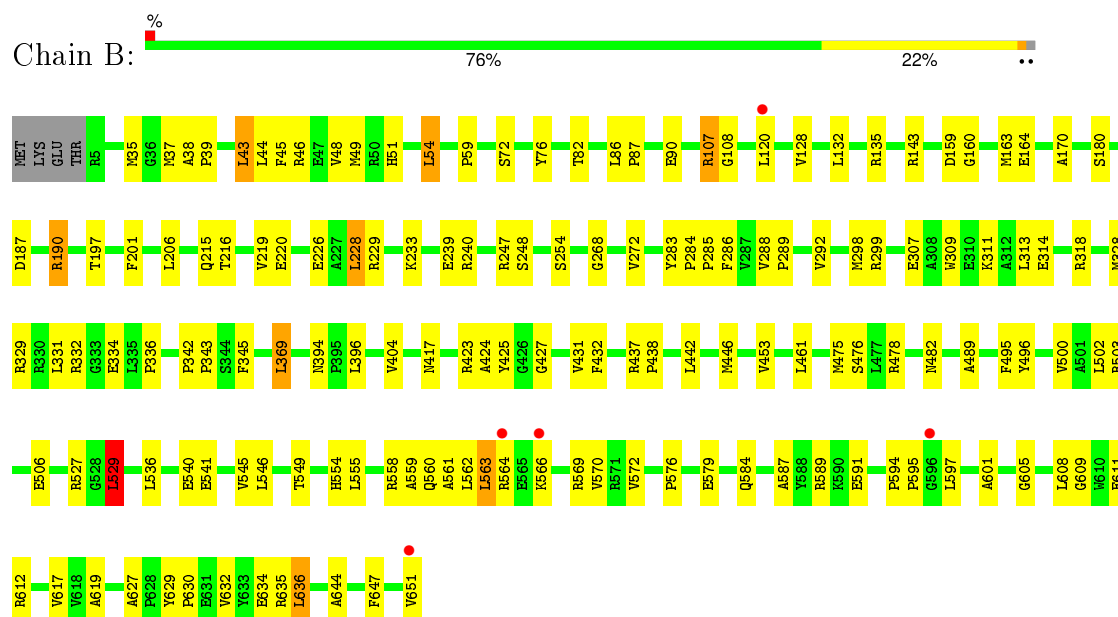
3 Residue-property plots

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: Transketolase



• Molecule 1: Transketolase



Chain C:

Sequence logo for Chain C, showing amino acid conservation across 100 positions. The y-axis lists amino acids (MET, LYS, GLU, THR, etc.) and the x-axis lists positions (A601 to V651). The color scale indicates conservation levels from 6% (red) to 41% (yellow).

Position	Amino Acid	Conservation (%)
A601	GLU	6%
V602	GLU	6%
E603	THR	6%
A604	THR	6%
G605	THR	6%
P619	THR	6%
L608	THR	6%
A619	THR	6%
A627	THR	6%
F628	THR	6%
V629	THR	6%
P630	THR	6%
E631	THR	6%
V632	THR	6%
R635	THR	6%
F638	THR	6%
E641	THR	6%
R642	THR	6%
A644	THR	6%
E645	THR	6%
A646	THR	6%
F647	THR	6%
V651	THR	6%
V512	THR	6%
L513	THR	6%
L514	THR	6%
T514	THR	6%
R515	THR	6%
P519	THR	6%
L520	THR	6%
L521	THR	6%
S522	THR	6%
P523	THR	6%
E524	THR	6%
K525	THR	6%
A526	THR	6%
R527	THR	6%
G528	THR	6%
L529	THR	6%
L530	THR	6%
R531	THR	6%
G532	THR	6%
L536	THR	6%
E537	THR	6%
D538	THR	6%
V539	THR	6%
E540	THR	6%
E541	THR	6%
P542	THR	6%
Q543	THR	6%
L546	THR	6%
V547	THR	6%
A548	THR	6%
T549	THR	6%
H554	THR	6%
L555	THR	6%
R558	THR	6%
A559	THR	6%
L562	THR	6%
L563	THR	6%
R564	THR	6%
E565	THR	6%
K566	THR	6%
R569	THR	6%
V570	THR	6%
R571	THR	6%
E579	THR	6%
L580	THR	6%
A587	THR	6%
P594	THR	6%
R595	THR	6%
G596	THR	6%
L597	THR	6%
F345	THR	6%
Y422	THR	6%
D346	THR	6%
K423	THR	6%
A424	THR	6%
Y425	THR	6%
G426	THR	6%
G427	THR	6%
T428	THR	6%
F429	THR	6%
L430	THR	6%
F431	THR	6%
F432	THR	6%
L366	THR	6%
P367	THR	6%
I440	THR	6%
I441	THR	6%
L442	THR	6%
A443	THR	6%
M446	THR	6%
G447	THR	6%
V448	THR	6%
P449	THR	6%
F452	THR	6%
V453	THR	6%
F454	THR	6%
T455	THR	6%
H456	THR	6%
D457	THR	6%
S458	THR	6%
L461	THR	6%
D464	THR	6%
Q469	THR	6%
P470	THR	6%
V471	THR	6%
E472	THR	6%
N482	THR	6%
L483	THR	6%
F494	THR	6%
G495	THR	6%
R497	THR	6%
A491	THR	6%
Y492	THR	6%
E493	THR	6%
Y496	THR	6%
E499	THR	6%
L502	THR	6%
R503	THR	6%
R504	THR	6%
K505	THR	6%
E506	THR	6%
H410	THR	6%
K411	THR	6%
I412	THR	6%
L413	THR	6%
L416	THR	6%
N417	THR	6%
L418	THR	6%
H419	THR	6%
P346	THR	6%
F347	THR	6%
V246	THR	6%
R247	THR	6%
S254	THR	6%
K261	THR	6%
G264	THR	6%
E265	THR	6%
R276	THR	6%
P289	THR	6%
E290	THR	6%
E291	THR	6%
Y292	THR	6%
Y293	THR	6%
R294	THR	6%
H295	THR	6%
D296	THR	6%
D297	THR	6%
F298	THR	6%
A299	THR	6%
M298	THR	

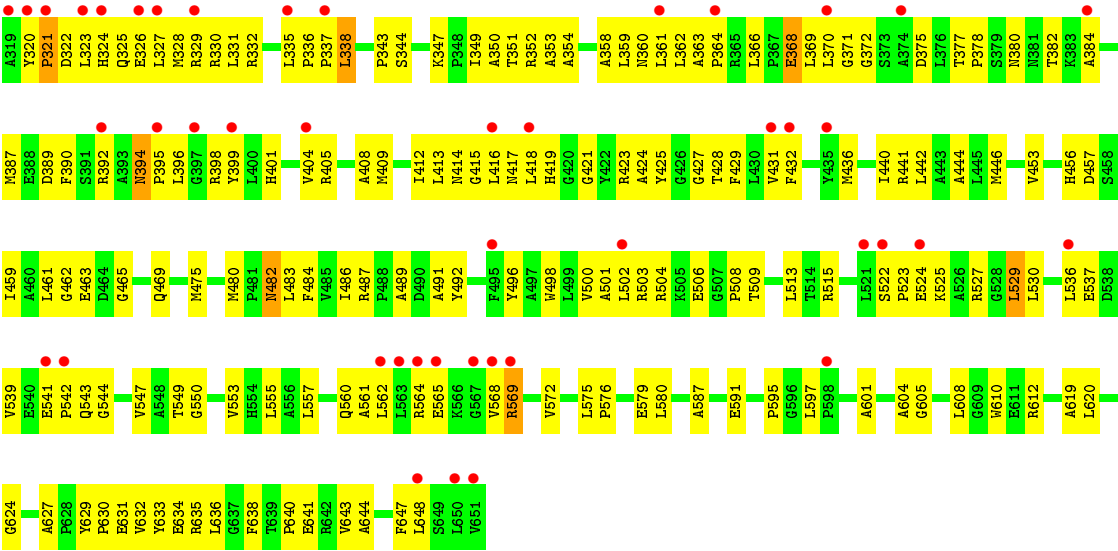
Chain D:

25%

39%

57%

AMINO ACIDS: MET, LYS, GLU, THR, PHE, D6, E8, L7, T9, L10, S11, M12, M13, A14, I15, R16, F17, L18, A19, H80, T20, D21, A22, V23, E24, K25, A26, R27, S28, G29, H30, P31, G32, N33, K34, T35, G36, G37, A38, P39, L40, A41, Y42, L43, T44, F45, R46, E47, V48, M49, N52, P53, L54, D55, P56, W58, P59, S125, D60, V328.



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.61Å 88.96Å 117.18Å 72.48° 89.13° 73.36°	Depositor
Resolution (Å)	38.59 – 2.09 38.59 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.59-2.09) 86.9 (38.59-1.94)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.94Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.259 0.217 , 0.259	Depositor DCC
R_{free} test set	15242 reflections (9.86%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 193063 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21768	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/5159	0.62	0/6995
1	B	0.34	0/5159	0.62	1/6995 (0.0%)
1	C	0.30	0/5159	0.56	0/6995
1	D	0.29	0/5159	0.55	0/6995
All	All	0.32	0/20636	0.59	1/27980 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	LEU	CA-CB-CG	6.39	130.01	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5039	0	5004	122	0
1	B	5039	0	5004	157	0
1	C	5039	0	5004	311	0
1	D	5039	0	5004	532	0
2	A	531	0	0	21	0
2	B	496	0	0	41	0
2	C	297	0	0	88	0
2	D	288	0	0	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21768	0	20016	1088	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 27.

All (1088) 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:428:THR:HB	2:A:1149:HOH:O	1.51	1.08
1:C:405:ARG:NH1	1:D:163:MSE:HE2	1.74	1.03
1:D:76:TYR:HA	2:D:854:HOH:O	1.60	1.00
1:B:475:MSE:HE2	1:B:609:GLY:HA3	1.43	0.99
1:A:493:GLU:HB2	2:A:1175:HOH:O	1.62	0.97
1:A:405:ARG:NH2	1:B:163:MSE:HE2	1.78	0.96
1:C:543:GLN:HE21	1:C:569:ARG:H	1.04	0.95
1:C:487:ARG:HH21	1:C:549:THR:HG23	1.32	0.95
1:C:39:PRO:HG2	1:C:222:VAL:HG22	1.49	0.94
1:B:546:LEU:HD13	1:B:570:VAL:HG11	1.50	0.94
1:C:241:PRO:HD3	2:C:915:HOH:O	1.68	0.94
1:D:31:PRO:HG3	2:D:858:HOH:O	1.69	0.93
1:B:417:ASN:HD21	1:B:424:ALA:H	1.02	0.92
1:C:405:ARG:HH12	1:D:163:MSE:HE2	1.27	0.90
1:C:163:MSE:HE2	1:D:405:ARG:NH2	1.86	0.89
1:D:215:GLN:NE2	1:D:240:ARG:HB2	1.86	0.88
1:D:240:ARG:HA	2:D:846:HOH:O	1.74	0.88
1:B:546:LEU:HB2	2:B:1114:HOH:O	1.73	0.88
1:B:647:PHE:HB3	2:B:1146:HOH:O	1.74	0.87
1:C:205:VAL:HG23	1:C:206:LEU:HD12	1.56	0.87
1:A:417:ASN:HD21	1:A:424:ALA:H	1.15	0.87
1:D:399:TYR:HA	2:D:861:HOH:O	1.74	0.87
1:C:369:LEU:HD11	1:C:425:TYR:HE2	1.39	0.87
1:A:405:ARG:CZ	1:B:163:MSE:HE2	2.06	0.86
1:C:330:ARG:HD2	2:C:909:HOH:O	1.75	0.86
1:B:163:MSE:HE3	1:B:201:PHE:HB2	1.58	0.86
1:D:137:LEU:HB3	2:D:883:HOH:O	1.76	0.86
1:D:263:HIS:HA	2:D:860:HOH:O	1.77	0.85
1:A:332:ARG:HD3	2:A:1176:HOH:O	1.77	0.85
1:D:16:ARG:O	1:D:20:ILE:HG12	1.77	0.85
1:D:41:ALA:HB2	1:D:74:LEU:HD11	1.59	0.85
1:C:306:GLN:HB2	2:C:929:HOH:O	1.76	0.85
1:D:37:MSE:HB2	2:D:842:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:LEU:HD12	2:D:854:HOH:O	1.74	0.84
1:C:44:LEU:HB3	1:C:49:MSE:HE2	1.59	0.84
1:C:148:VAL:HG21	2:C:914:HOH:O	1.76	0.84
1:C:220:GLU:HA	2:C:903:HOH:O	1.79	0.83
1:A:428:THR:OG1	1:A:436:MSE:HE1	1.79	0.83
1:D:148:VAL:HG13	1:D:149:VAL:HG23	1.60	0.83
1:D:161:ASP:HB2	2:D:878:HOH:O	1.80	0.82
1:A:475:MSE:HG2	1:A:608:LEU:O	1.80	0.81
1:C:549:THR:HG21	1:C:603:GLU:OE2	1.80	0.81
1:D:153:THR:HG23	2:D:863:HOH:O	1.80	0.81
1:D:73:MSE:HG3	2:D:867:HOH:O	1.81	0.81
1:C:387:MSE:HE2	1:C:399:TYR:HB2	1.63	0.81
1:C:31:PRO:HD2	2:C:935:HOH:O	1.81	0.81
1:D:44:LEU:HB3	1:D:49:MSE:HE2	1.63	0.80
1:D:73:MSE:HB3	2:D:932:HOH:O	1.80	0.80
1:A:488:PRO:HB2	2:A:1175:HOH:O	1.80	0.80
1:D:326:GLU:HB2	2:D:805:HOH:O	1.81	0.80
1:A:405:ARG:HH22	1:B:163:MSE:HE2	1.47	0.79
1:C:30:HIS:HA	2:C:935:HOH:O	1.81	0.79
1:D:335:LEU:H	1:D:335:LEU:HD23	1.47	0.79
1:D:240:ARG:NE	1:D:392:ARG:HH22	1.79	0.79
1:D:244:ILE:HG13	2:D:889:HOH:O	1.83	0.79
1:B:59:PRO:HG2	1:B:309:TRP:CH2	2.18	0.79
1:D:236:LYS:HA	1:D:236:LYS:HZ3	1.48	0.78
1:C:46:ARG:HA	1:C:298:MSE:HE3	1.65	0.78
1:D:232:ILE:O	1:D:236:LYS:HG2	1.83	0.78
1:D:210:ARG:HD2	2:D:790:HOH:O	1.83	0.78
1:C:374:ALA:HA	2:C:928:HOH:O	1.82	0.78
1:D:22:ALA:HB3	2:D:867:HOH:O	1.83	0.78
1:D:29:GLY:HA3	2:D:853:HOH:O	1.83	0.78
1:D:74:LEU:HD13	2:D:829:HOH:O	1.81	0.78
1:C:543:GLN:NE2	1:C:569:ARG:H	1.82	0.77
1:B:417:ASN:HD21	1:B:424:ALA:N	1.81	0.77
1:D:457:ASP:HB3	2:D:929:HOH:O	1.84	0.77
1:B:309:TRP:CH2	1:B:313:LEU:HD11	2.18	0.77
1:B:576:PRO:HA	2:B:1117:HOH:O	1.83	0.77
1:C:424:ALA:HB1	2:C:894:HOH:O	1.83	0.77
1:B:37:MSE:HE1	1:B:248:SER:HB3	1.66	0.77
1:D:530:LEU:HG	2:D:896:HOH:O	1.85	0.76
1:D:134:GLU:HA	2:D:883:HOH:O	1.85	0.76
1:C:594:PRO:HG2	1:C:597:LEU:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLN:HE21	1:D:215:GLN:N	1.83	0.76
1:D:390:PHE:CE1	1:D:395:PRO:HA	2.20	0.76
1:D:267:LEU:N	2:D:858:HOH:O	2.18	0.76
1:D:115:VAL:HG22	2:D:872:HOH:O	1.86	0.76
1:B:442:LEU:HG	1:B:446:MSE:HE2	1.68	0.75
1:D:442:LEU:HG	1:D:446:MSE:HE3	1.67	0.75
1:B:163:MSE:HE3	1:B:201:PHE:CB	2.17	0.75
1:D:191:ILE:HD12	2:D:887:HOH:O	1.87	0.75
1:C:367:PRO:HG2	2:C:909:HOH:O	1.86	0.75
1:D:116:THR:H	1:D:446:MSE:HE2	1.51	0.75
1:D:250:ILE:HG21	2:D:937:HOH:O	1.85	0.74
1:D:44:LEU:HA	1:D:48:VAL:CG1	2.16	0.74
1:C:81:LEU:HG	2:C:932:HOH:O	1.87	0.74
1:D:361:LEU:HD23	2:D:870:HOH:O	1.88	0.74
1:D:192:SER:OG	1:D:197:THR:HG22	1.88	0.74
1:A:476:SER:HB2	1:B:476:SER:HB2	1.70	0.74
1:C:569:ARG:NH2	1:C:569:ARG:HB2	2.02	0.74
1:C:409:MSE:O	1:C:413:LEU:HG	1.88	0.74
2:C:910:HOH:O	1:D:199:LEU:HD22	1.88	0.74
1:C:327:LEU:HD13	2:C:897:HOH:O	1.87	0.73
1:C:216:THR:HG23	2:C:902:HOH:O	1.89	0.73
1:D:25:LYS:HB3	2:D:926:HOH:O	1.89	0.73
1:D:73:MSE:HE3	2:D:932:HOH:O	1.89	0.73
1:B:54:LEU:HD13	1:B:299:ARG:HG2	1.71	0.73
1:D:128:VAL:HG21	1:D:170:ALA:HB1	1.71	0.72
1:C:564:ARG:HH11	1:C:564:ARG:HB2	1.54	0.72
1:D:68:ALA:HB1	1:D:70:HIS:NE2	2.04	0.72
1:B:417:ASN:ND2	1:B:424:ALA:H	1.82	0.72
1:B:563:LEU:HD11	2:B:1146:HOH:O	1.89	0.72
1:A:409:MSE:HE1	1:A:428:THR:HG23	1.72	0.72
1:D:191:ILE:HG21	2:D:937:HOH:O	1.86	0.72
1:D:484:PHE:HA	1:D:579:GLU:HG3	1.72	0.72
1:D:56:PRO:HD3	2:D:902:HOH:O	1.88	0.72
1:C:443:ALA:HB1	2:C:940:HOH:O	1.90	0.72
1:D:94:PHE:HA	1:D:101:THR:OG1	1.90	0.72
1:B:313:LEU:HD13	2:B:1132:HOH:O	1.90	0.72
1:D:369:LEU:HD23	1:D:423:ARG:O	1.89	0.72
1:D:27:ARG:HD2	2:D:928:HOH:O	1.89	0.71
1:C:409:MSE:HE2	1:C:426:GLY:HA3	1.70	0.71
1:C:402:PHE:CD2	1:C:409:MSE:HE3	2.26	0.71
1:D:79:LEU:HD23	2:D:888:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ARG:HH21	1:C:569:ARG:HB2	1.54	0.71
1:A:43:LEU:HD22	1:A:48:VAL:HG23	1.72	0.71
1:B:549:THR:HB	2:B:1117:HOH:O	1.90	0.71
1:D:215:GLN:HG3	2:D:756:HOH:O	1.90	0.71
1:C:151:HIS:HB3	2:C:924:HOH:O	1.90	0.71
1:D:390:PHE:HE1	1:D:395:PRO:HA	1.56	0.71
1:D:307:GLU:HG3	1:D:308:ALA:N	2.06	0.71
1:C:152:TYR:HB2	2:C:906:HOH:O	1.89	0.71
1:D:220:GLU:HG3	2:D:662:HOH:O	1.88	0.71
1:D:34:PRO:HA	2:D:842:HOH:O	1.89	0.70
1:D:20:ILE:HG23	1:D:267:LEU:HD12	1.73	0.70
1:A:374:ALA:HB3	1:A:428:THR:HG22	1.72	0.70
1:D:306:GLN:O	1:D:310:GLU:HG2	1.90	0.70
1:C:513:LEU:HD12	2:C:907:HOH:O	1.91	0.70
1:D:20:ILE:HD11	1:D:35:MSE:HG2	1.73	0.70
1:D:162:LEU:HG	2:D:878:HOH:O	1.91	0.70
1:D:363:ALA:HB3	1:D:364:PRO:HD3	1.74	0.70
1:D:39:PRO:HG2	1:D:222:VAL:HG22	1.73	0.70
1:A:610:TRP:HB3	1:A:617:VAL:HG11	1.74	0.70
1:D:328:MSE:O	1:D:332:ARG:HG3	1.92	0.69
1:A:559:ALA:O	1:A:563:LEU:HD13	1.92	0.69
1:D:444:ALA:HA	2:D:874:HOH:O	1.92	0.69
1:D:184:VAL:HG13	2:D:824:HOH:O	1.91	0.69
1:D:366:LEU:HD11	1:D:502:LEU:HD21	1.73	0.69
1:D:215:GLN:NE2	1:D:215:GLN:N	2.40	0.69
1:C:329:ARG:HH22	1:C:336:PRO:HD3	1.57	0.69
1:C:329:ARG:NH2	1:C:336:PRO:HD3	2.07	0.69
1:D:217:LEU:HG	2:D:838:HOH:O	1.92	0.69
1:C:522:SER:OG	1:C:524:GLU:HG2	1.93	0.69
1:B:564:ARG:HH22	1:B:569:ARG:HG2	1.58	0.69
1:A:405:ARG:NH1	1:B:163:MSE:HE2	2.08	0.69
1:A:417:ASN:HD21	1:A:424:ALA:N	1.89	0.68
1:C:194:ASP:OD2	1:D:375:ASP:HA	1.94	0.68
1:B:560:GLN:HG2	2:B:1144:HOH:O	1.93	0.68
1:C:532:GLY:N	1:C:580:LEU:HD22	2.08	0.68
1:B:163:MSE:CE	1:B:201:PHE:HB2	2.23	0.68
1:D:482:ASN:ND2	1:D:504:ARG:HH12	1.92	0.68
1:D:543:GLN:NE2	1:D:569:ARG:H	1.90	0.68
1:C:310:GLU:O	1:C:314:GLU:HG2	1.93	0.68
1:D:298:MSE:HB2	2:D:903:HOH:O	1.94	0.68
1:D:133:ALA:HA	2:D:873:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:HD3	1:C:298:MSE:HE1	1.76	0.68
1:C:54:LEU:HD21	1:C:299:ARG:HG2	1.75	0.67
1:D:23:VAL:HG23	2:D:867:HOH:O	1.94	0.67
1:B:197:THR:HG22	1:B:201:PHE:HB3	1.76	0.67
1:D:240:ARG:HE	1:D:392:ARG:HH22	1.39	0.67
1:D:569:ARG:HD2	2:D:815:HOH:O	1.94	0.67
1:D:79:LEU:HA	2:D:888:HOH:O	1.93	0.67
1:C:383:LYS:HD2	2:C:927:HOH:O	1.94	0.67
1:C:215:GLN:HG3	1:C:240:ARG:NH1	2.10	0.67
1:B:159:ASP:HB2	2:B:1062:HOH:O	1.94	0.67
1:C:241:PRO:HA	2:C:946:HOH:O	1.95	0.67
1:C:295:HIS:CD2	1:C:296:MSE:HE3	2.30	0.67
1:C:336:PRO:O	1:C:338:LEU:HD22	1.95	0.67
1:D:130:LEU:O	1:D:133:ALA:HB3	1.95	0.67
1:C:316:TYR:OH	1:C:323:LEU:HB3	1.94	0.67
1:C:370:LEU:HA	2:C:917:HOH:O	1.95	0.66
1:D:311:LYS:HA	1:D:314:GLU:HG2	1.76	0.66
1:D:268:GLY:O	1:D:272:VAL:HG23	1.96	0.66
1:C:409:MSE:HE2	1:C:426:GLY:CA	2.26	0.66
1:D:30:HIS:HB2	1:D:70:HIS:O	1.95	0.66
1:B:289:PRO:HD3	2:B:1076:HOH:O	1.95	0.66
1:D:309:TRP:O	1:D:313:LEU:HG	1.95	0.66
1:D:605:GLY:O	1:D:619:ALA:HB1	1.96	0.66
1:A:239:GLU:HG3	2:A:949:HOH:O	1.96	0.66
1:D:157:ALA:HB1	2:D:878:HOH:O	1.95	0.66
1:C:247:ARG:HB2	2:C:903:HOH:O	1.95	0.66
1:B:37:MSE:CE	1:B:248:SER:HB3	2.26	0.66
1:D:587:ALA:O	1:D:591:GLU:HG3	1.96	0.66
1:B:298:MSE:HG3	2:B:1087:HOH:O	1.95	0.66
1:A:73:MSE:HE1	1:A:91:LEU:HD22	1.78	0.65
1:B:229:ARG:O	1:B:233:LYS:HG3	1.96	0.65
1:D:63:ARG:HH21	1:D:63:ARG:HG3	1.62	0.65
1:D:416:LEU:HD22	1:D:416:LEU:H	1.61	0.65
1:D:543:GLN:HE21	1:D:569:ARG:H	1.44	0.65
1:A:640:PRO:HA	2:A:1113:HOH:O	1.97	0.65
1:D:327:LEU:O	1:D:331:LEU:HB2	1.96	0.65
1:C:166:VAL:HG23	2:C:904:HOH:O	1.95	0.65
1:C:403:GLY:N	2:C:928:HOH:O	2.28	0.65
1:A:555:LEU:HD22	2:A:1113:HOH:O	1.95	0.65
1:D:52:ASN:OD1	1:D:54:LEU:HB3	1.97	0.65
1:D:18:LEU:HB2	2:D:907:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:ARG:HG2	1:D:550:GLY:HA3	1.78	0.65
1:D:289:PRO:HG2	1:D:292:VAL:CG2	2.27	0.65
1:C:329:ARG:O	1:C:334:GLU:HB2	1.97	0.65
1:C:163:MSE:HE2	1:D:405:ARG:HH22	1.58	0.65
1:D:94:PHE:HB3	2:D:891:HOH:O	1.97	0.64
1:D:219:VAL:O	1:D:247:ARG:HG2	1.96	0.64
1:C:217:LEU:HD11	2:C:916:HOH:O	1.95	0.64
1:D:405:ARG:HD2	2:D:855:HOH:O	1.96	0.64
1:D:324:HIS:C	1:D:326:GLU:H	2.01	0.64
1:D:20:ILE:HD12	1:D:267:LEU:HD11	1.79	0.64
1:D:370:LEU:HB2	1:D:424:ALA:HB2	1.79	0.64
1:C:242:THR:HG22	2:C:939:HOH:O	1.97	0.64
1:C:563:LEU:HD11	1:C:644:ALA:HA	1.79	0.64
1:D:289:PRO:HG2	1:D:292:VAL:HG23	1.79	0.64
1:C:423:ARG:HH21	1:C:449:PRO:HB2	1.63	0.64
1:D:22:ALA:HA	2:D:926:HOH:O	1.97	0.64
1:A:608:LEU:HD12	1:B:475:MSE:HE1	1.78	0.64
1:B:288:VAL:HA	2:B:1076:HOH:O	1.97	0.64
1:B:605:GLY:O	1:B:619:ALA:HB1	1.98	0.64
1:D:384:ALA:HB3	1:D:387:MSE:SE	2.48	0.64
1:D:37:MSE:HE2	1:D:156:LEU:HD11	1.79	0.64
1:B:475:MSE:CE	1:B:609:GLY:HA3	2.22	0.64
1:D:384:ALA:HA	2:D:840:HOH:O	1.98	0.64
1:B:478:ARG:HB3	2:B:1088:HOH:O	1.97	0.64
1:D:138:ALA:O	1:D:142:ASN:HB2	1.99	0.63
1:D:416:LEU:HD22	2:D:923:HOH:O	1.98	0.63
1:D:148:VAL:HG23	1:D:313:LEU:CD2	2.27	0.63
1:D:115:VAL:HG13	1:D:446:MSE:HE1	1.79	0.63
1:D:267:LEU:HG	2:D:858:HOH:O	1.97	0.63
1:A:46:ARG:HE	1:A:295:HIS:CE1	2.17	0.63
1:D:604:ALA:HA	1:D:638:PHE:CZ	2.33	0.63
1:D:9:THR:HG22	2:D:798:HOH:O	1.98	0.63
1:D:612:ARG:HG2	2:D:885:HOH:O	1.98	0.63
1:C:327:LEU:HB2	2:C:870:HOH:O	1.98	0.63
1:B:564:ARG:NH2	1:B:569:ARG:HG2	2.13	0.63
1:A:19:ALA:HA	1:A:73:MSE:HG3	1.81	0.63
1:D:88:LEU:HD11	2:D:905:HOH:O	1.98	0.62
1:D:124:ILE:HG21	2:D:844:HOH:O	1.99	0.62
1:D:187:ASP:OD1	1:D:248:SER:HB3	1.99	0.62
1:D:371:GLY:C	2:D:861:HOH:O	2.37	0.62
1:D:66:LEU:HD11	2:D:892:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:LEU:HB3	2:D:801:HOH:O	1.99	0.62
1:C:101:THR:HG22	2:C:913:HOH:O	1.98	0.62
1:C:169:GLU:CA	1:C:405:ARG:HD3	2.30	0.62
1:D:163:MSE:HE3	1:D:201:PHE:HB2	1.80	0.62
1:D:222:VAL:HG23	2:D:894:HOH:O	1.99	0.62
1:D:7:LEU:HG	2:D:879:HOH:O	2.00	0.62
1:A:433:SER:HA	1:A:436:MSE:HE3	1.81	0.62
1:D:88:LEU:O	1:D:92:LYS:HG3	2.00	0.62
1:B:309:TRP:CZ2	1:B:313:LEU:HD11	2.34	0.62
1:D:416:LEU:HA	2:D:849:HOH:O	1.99	0.62
1:B:44:LEU:HB3	1:B:49:MSE:HE2	1.80	0.62
1:D:63:ARG:HE	1:D:151:HIS:CD2	2.17	0.62
1:C:327:LEU:HG	1:C:331:LEU:HD22	1.81	0.62
1:A:83:GLY:HA3	1:A:299:ARG:HD2	1.81	0.62
1:C:261:LYS:HB3	1:C:261:LYS:NZ	2.15	0.62
1:C:369:LEU:HD11	1:C:425:TYR:CE2	2.30	0.62
1:D:94:PHE:HD1	1:D:101:THR:HB	1.65	0.62
1:D:71:GLY:O	1:D:74:LEU:HB3	1.98	0.62
1:D:384:ALA:O	1:D:387:MSE:HB2	2.00	0.61
1:C:143:ARG:HH11	1:C:143:ARG:HG3	1.65	0.61
1:C:647:PHE:O	1:C:651:VAL:HG23	1.99	0.61
1:D:409:MSE:SE	2:D:809:HOH:O	2.68	0.61
1:C:169:GLU:HA	1:C:405:ARG:HD3	1.83	0.61
1:D:252:PHE:HA	1:D:257:GLN:NE2	2.16	0.61
1:D:366:LEU:HB3	1:D:368:GLU:OE2	2.01	0.61
1:D:26:ALA:HB2	2:D:891:HOH:O	2.01	0.61
1:D:225:LEU:HB3	1:D:229:ARG:NH1	2.15	0.61
1:D:45:PHE:CD1	1:D:78:VAL:HG21	2.35	0.61
1:C:163:MSE:HE2	1:D:405:ARG:CZ	2.29	0.61
1:A:197:THR:HG22	1:A:201:PHE:HB3	1.81	0.61
1:A:608:LEU:HD22	1:B:612:ARG:CZ	2.30	0.61
1:C:143:ARG:HB3	2:C:918:HOH:O	2.00	0.61
1:D:394:ASN:HD21	1:D:396:LEU:HB2	1.63	0.61
1:C:605:GLY:O	1:C:619:ALA:HB1	2.01	0.61
1:D:483:LEU:HD23	1:D:508:PRO:HG2	1.83	0.61
1:D:116:THR:N	1:D:446:MSE:HE2	2.14	0.61
1:B:54:LEU:CD1	1:B:299:ARG:HG2	2.31	0.61
1:A:297:ASP:O	1:A:298:MSE:HE2	2.00	0.61
1:D:82:THR:HB	2:D:903:HOH:O	2.00	0.61
1:C:449:PRO:HB3	1:C:505:LYS:HA	1.83	0.61
1:B:190:ARG:HH11	1:B:190:ARG:HG3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:VAL:HA	2:D:868:HOH:O	2.00	0.60
1:D:133:ALA:HB1	1:D:419:HIS:CG	2.36	0.60
1:D:66:LEU:HD21	2:D:892:HOH:O	2.00	0.60
1:D:636:LEU:HD13	2:D:847:HOH:O	1.99	0.60
1:B:37:MSE:HE3	1:B:187:ASP:OD1	2.00	0.60
1:C:555:LEU:HD22	1:C:643:VAL:HG21	1.84	0.60
1:C:522:SER:HB3	1:C:525:LYS:CG	2.31	0.60
1:D:277:ARG:HD3	1:D:277:ARG:O	2.01	0.60
1:D:215:GLN:HE22	1:D:240:ARG:HB2	1.64	0.60
1:D:225:LEU:HA	2:D:884:HOH:O	2.01	0.60
1:B:437:ARG:HB3	1:B:438:PRO:HD3	1.83	0.60
1:C:487:ARG:HD3	1:C:549:THR:HG23	1.83	0.60
1:B:394:ASN:ND2	2:B:1057:HOH:O	2.34	0.60
1:D:197:THR:HB	2:D:839:HOH:O	2.02	0.60
1:D:236:LYS:NZ	1:D:236:LYS:HA	2.15	0.60
1:C:46:ARG:HG3	1:C:296:MSE:HE1	1.84	0.59
1:D:13:ASN:O	1:D:17:PHE:HD1	1.85	0.59
1:D:543:GLN:HE22	1:D:568:VAL:HA	1.66	0.59
1:A:44:LEU:HB3	1:A:49:MSE:HE2	1.84	0.59
1:C:56:PRO:HA	2:C:930:HOH:O	2.02	0.59
1:C:37:MSE:HG2	2:C:922:HOH:O	2.01	0.59
1:A:385:GLU:HB3	2:A:790:HOH:O	2.02	0.59
1:D:228:LEU:HD22	2:D:884:HOH:O	2.02	0.59
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.67	0.59
1:B:190:ARG:HD2	1:B:190:ARG:N	2.17	0.59
1:D:629:TYR:CD1	1:D:630:PRO:HA	2.37	0.59
1:D:252:PHE:HA	1:D:257:GLN:HE21	1.67	0.59
1:A:608:LEU:HD22	1:B:612:ARG:NH2	2.18	0.59
1:D:7:LEU:CD2	1:D:7:LEU:H	2.15	0.59
1:D:67:SER:HB2	2:D:837:HOH:O	2.03	0.59
1:A:417:ASN:ND2	1:A:424:ALA:H	1.94	0.59
1:C:387:MSE:HE2	1:C:399:TYR:CB	2.31	0.59
1:C:538:ASP:HA	2:C:853:HOH:O	2.02	0.59
1:D:368:GLU:CD	1:D:368:GLU:H	2.06	0.59
1:D:132:LEU:HD23	1:D:132:LEU:O	2.02	0.59
1:D:303:ARG:HB3	2:D:788:HOH:O	2.03	0.59
1:C:349:ILE:N	1:C:349:ILE:HD13	2.16	0.59
1:C:289:PRO:HB2	1:C:291:GLU:OE2	2.02	0.59
1:C:306:GLN:O	1:C:310:GLU:HG3	2.03	0.59
1:A:427:GLY:O	1:A:428:THR:HG23	2.02	0.59
1:D:76:TYR:HD1	2:D:854:HOH:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LEU:HD22	2:C:897:HOH:O	2.02	0.59
1:B:247:ARG:HG2	2:B:1103:HOH:O	2.02	0.59
1:C:569:ARG:HH21	1:C:569:ARG:CB	2.16	0.59
1:D:272:VAL:O	1:D:276:ARG:HG3	2.03	0.59
1:D:120:LEU:H	1:D:120:LEU:HD22	1.68	0.58
1:D:297:ASP:HB2	2:D:901:HOH:O	2.01	0.58
1:C:136:LYS:HG3	1:C:422:TYR:OH	2.03	0.58
1:C:348:PRO:HA	1:C:520:LEU:CD2	2.33	0.58
1:D:31:PRO:O	1:D:34:PRO:HG2	2.02	0.58
1:A:328:MSE:O	1:A:332:ARG:HD2	2.03	0.58
1:C:347:LYS:O	1:C:349:ILE:HG23	2.02	0.58
1:C:169:GLU:CB	1:C:405:ARG:HD3	2.33	0.58
1:D:94:PHE:HE2	2:D:853:HOH:O	1.86	0.58
1:D:417:ASN:HB2	2:D:808:HOH:O	2.03	0.58
1:C:538:ASP:OD1	1:C:539:VAL:N	2.37	0.58
1:D:415:GLY:HA2	2:D:856:HOH:O	2.03	0.58
1:D:529:LEU:HG	2:D:933:HOH:O	2.02	0.58
1:D:330:ARG:HB3	1:D:421:GLY:HA2	1.85	0.58
1:C:193:ILE:HD13	1:D:375:ASP:OD2	2.03	0.58
1:B:43:LEU:HD13	1:B:48:VAL:HG23	1.85	0.58
1:A:579:GLU:CD	1:A:579:GLU:H	2.06	0.58
1:D:163:MSE:HE3	1:D:201:PHE:CB	2.33	0.58
1:D:250:ILE:HD11	2:D:860:HOH:O	2.03	0.58
1:D:46:ARG:HG2	1:D:46:ARG:HH11	1.68	0.58
1:D:180:SER:HB3	1:D:239:GLU:C	2.24	0.58
1:C:562:LEU:O	1:C:565:GLU:HB3	2.03	0.58
1:B:594:PRO:HG2	1:B:597:LEU:HD11	1.86	0.58
1:C:487:ARG:HH21	1:C:549:THR:CG2	2.12	0.58
1:D:224:ASP:O	1:D:228:LEU:HD13	2.04	0.58
1:A:7:LEU:HD11	1:A:291:GLU:HG2	1.84	0.58
1:B:240:ARG:HB2	2:B:1134:HOH:O	2.04	0.57
2:C:849:HOH:O	1:D:104:HIS:HE1	1.86	0.57
2:C:901:HOH:O	1:D:480:MSE:HG3	2.03	0.57
1:D:135:ARG:NH2	1:D:181:LYS:HG3	2.19	0.57
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.86	0.57
1:C:546:LEU:HG	1:C:570:VAL:HG21	1.86	0.57
1:D:119:PRO:HB2	1:D:122:GLN:CG	2.34	0.57
1:B:627:ALA:HB3	1:B:632:VAL:HB	1.87	0.57
1:D:151:HIS:HB2	2:D:852:HOH:O	2.05	0.57
1:D:527:ARG:HA	2:D:896:HOH:O	2.04	0.57
1:A:631:GLU:O	1:A:635:ARG:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:PRO:HD3	2:D:916:HOH:O	2.03	0.57
2:C:901:HOH:O	1:D:441:ARG:HG3	2.04	0.57
1:D:290:GLU:O	1:D:294:ARG:HG3	2.05	0.57
1:D:32:GLY:HA3	2:D:860:HOH:O	2.05	0.57
1:D:366:LEU:CD1	1:D:502:LEU:HD21	2.34	0.57
1:D:130:LEU:HD12	2:D:856:HOH:O	2.04	0.57
1:C:559:ALA:O	1:C:563:LEU:HD13	2.04	0.57
1:A:537:GLU:HB3	2:A:1170:HOH:O	2.05	0.57
1:D:179:LEU:N	1:D:179:LEU:HD22	2.20	0.57
1:C:461:LEU:CD1	1:C:464:ASP:HB2	2.35	0.57
1:A:343:PRO:HG2	1:A:345:PHE:CE2	2.39	0.57
1:D:292:VAL:HG21	2:D:871:HOH:O	2.04	0.57
1:A:300:GLU:HG3	2:A:1128:HOH:O	2.03	0.57
1:D:522:SER:HB2	1:D:525:LYS:CG	2.35	0.56
1:C:484:PHE:HA	1:C:579:GLU:HG3	1.86	0.56
1:D:522:SER:HB3	2:D:890:HOH:O	2.05	0.56
1:B:107:ARG:HD2	1:B:108:GLY:N	2.20	0.56
1:D:86:LEU:HD21	1:D:110:THR:HG23	1.87	0.56
1:C:46:ARG:O	1:C:46:ARG:HD3	2.04	0.56
1:D:177:TRP:O	1:D:392:ARG:HB3	2.04	0.56
1:C:205:VAL:HG23	1:C:206:LEU:N	2.20	0.56
1:C:289:PRO:HG2	1:C:292:VAL:HG23	1.87	0.56
1:C:579:GLU:H	1:C:579:GLU:CD	2.09	0.56
1:B:219:VAL:HG11	1:B:228:LEU:HD13	1.86	0.56
1:A:489:ALA:O	1:A:554:HIS:HE1	1.88	0.56
1:D:416:LEU:HD13	2:D:849:HOH:O	2.04	0.56
1:C:349:ILE:HD11	1:C:520:LEU:HD11	1.86	0.56
1:C:132:LEU:CD2	1:C:136:LYS:HD2	2.35	0.56
1:C:7:LEU:HG	1:C:295:HIS:CD2	2.40	0.56
1:C:37:MSE:HE2	1:C:156:LEU:HD11	1.88	0.56
1:C:164:GLU:HB3	1:C:166:VAL:HG12	1.87	0.56
1:A:563:LEU:HD11	1:A:644:ALA:HA	1.87	0.56
1:D:278:ASN:HB3	2:D:687:HOH:O	2.06	0.56
1:C:338:LEU:HD11	1:C:366:LEU:HD21	1.87	0.55
1:D:116:THR:HB	1:D:446:MSE:HE2	1.87	0.55
1:D:343:PRO:HD3	2:D:870:HOH:O	2.06	0.55
1:B:594:PRO:HG2	1:B:597:LEU:HD21	1.88	0.55
1:D:359:LEU:HD12	2:D:877:HOH:O	2.07	0.55
1:C:198:ASP:HA	2:C:908:HOH:O	2.06	0.55
1:C:201:PHE:N	2:C:908:HOH:O	2.35	0.55
1:D:124:ILE:HD13	1:D:124:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:VAL:HG12	2:D:824:HOH:O	2.06	0.55
1:D:141:PHE:HE1	2:D:805:HOH:O	1.90	0.55
1:D:557:LEU:O	1:D:560:GLN:HG2	2.06	0.55
1:C:506:GLU:N	1:C:506:GLU:OE1	2.39	0.55
1:B:307:GLU:HB2	2:B:1039:HOH:O	2.06	0.55
1:B:37:MSE:CE	1:B:248:SER:CB	2.83	0.55
1:C:218:ARG:NH1	1:C:245:ALA:HB1	2.21	0.55
1:D:465:GLY:O	1:D:469:GLN:HG3	2.07	0.55
1:D:201:PHE:HB3	2:D:839:HOH:O	2.06	0.55
1:D:6:ASP:HA	2:D:798:HOH:O	2.05	0.55
1:C:304:ALA:HA	1:C:307:GLU:HG2	1.88	0.55
1:A:215:GLN:HE22	1:A:235:ALA:HA	1.71	0.55
1:C:571:ARG:HG3	2:C:853:HOH:O	2.07	0.55
1:D:475:MSE:HE3	1:D:608:LEU:O	2.07	0.55
1:D:215:GLN:HE22	1:D:240:ARG:CB	2.20	0.55
1:B:314:GLU:O	1:B:318:ARG:HG3	2.06	0.55
1:C:209:TYR:HA	1:C:212:TYR:HD2	1.72	0.55
1:C:408:ALA:N	2:C:904:HOH:O	2.40	0.55
1:A:197:THR:CG2	1:A:201:PHE:HB3	2.37	0.55
1:C:65:VAL:HG13	1:C:115:VAL:CG1	2.36	0.55
1:C:404:VAL:H	1:D:163:MSE:SE	2.40	0.55
1:B:82:THR:HG21	2:B:1087:HOH:O	2.06	0.55
1:D:461:LEU:HA	1:D:515:ARG:HD3	1.87	0.55
1:C:54:LEU:HD11	1:C:299:ARG:HG2	1.89	0.55
1:C:77:ALA:HB1	2:C:905:HOH:O	2.07	0.55
1:D:547:VAL:O	1:D:601:ALA:HA	2.06	0.55
1:D:75:LEU:HD22	1:D:75:LEU:O	2.07	0.54
1:A:610:TRP:CB	1:A:617:VAL:HG11	2.37	0.54
1:C:218:ARG:HH11	1:C:245:ALA:CB	2.19	0.54
1:C:17:PHE:CE2	1:C:276:ARG:HG2	2.42	0.54
1:A:608:LEU:CD1	1:B:475:MSE:HE1	2.36	0.54
1:D:236:LYS:CA	1:D:236:LYS:HZ3	2.20	0.54
1:C:120:LEU:HD22	1:C:120:LEU:H	1.73	0.54
1:D:174:ALA:HA	1:D:179:LEU:HD23	1.90	0.54
1:D:300:GLU:HA	2:D:788:HOH:O	2.08	0.54
1:B:506:GLU:H	1:B:506:GLU:CD	2.10	0.54
1:C:54:LEU:HD21	1:C:299:ARG:CG	2.37	0.54
1:D:291:GLU:N	1:D:291:GLU:OE1	2.40	0.54
1:D:459:ILE:HD13	1:D:636:LEU:HD23	1.88	0.54
1:B:601:ALA:HB3	1:B:617:VAL:HG13	1.90	0.54
1:C:63:ARG:NH1	1:C:419:HIS:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:NH2	1:B:336:PRO:HD3	2.22	0.54
1:A:641:GLU:O	1:A:645:GLU:HG3	2.08	0.54
1:D:7:LEU:HD23	1:D:7:LEU:H	1.71	0.54
1:D:338:LEU:CD2	1:D:338:LEU:H	2.21	0.54
1:A:247:ARG:NE	2:A:759:HOH:O	2.40	0.54
1:D:142:ASN:ND2	1:D:147:VAL:HG13	2.22	0.54
1:A:431:VAL:HG13	1:A:432:PHE:CD1	2.43	0.54
1:C:349:ILE:H	1:C:349:ILE:HD13	1.73	0.54
1:D:119:PRO:HB2	1:D:122:GLN:HG2	1.89	0.54
1:C:493:GLU:HG2	1:C:529:LEU:HB2	1.90	0.54
1:D:134:GLU:HG3	2:D:685:HOH:O	2.07	0.54
1:D:213:GLY:HA3	2:D:876:HOH:O	2.07	0.54
1:A:342:PRO:HB3	1:A:495:PHE:CD2	2.43	0.54
1:C:294:ARG:HA	1:C:294:ARG:NE	2.23	0.54
1:D:45:PHE:HA	1:D:49:MSE:HE3	1.89	0.53
1:D:148:VAL:HG21	1:D:327:LEU:HD21	1.90	0.53
1:D:413:LEU:C	1:D:415:GLY:H	2.11	0.53
1:D:52:ASN:C	1:D:54:LEU:H	2.12	0.53
1:C:461:LEU:HD13	1:C:464:ASP:HB2	1.90	0.53
1:D:239:GLU:O	1:D:240:ARG:HD3	2.08	0.53
1:D:442:LEU:CG	1:D:446:MSE:HE3	2.36	0.53
1:D:138:ALA:HA	1:D:149:VAL:HB	1.91	0.53
1:C:193:ILE:H	1:C:193:ILE:HD12	1.74	0.53
1:C:225:LEU:O	1:C:229:ARG:HG3	2.08	0.53
1:C:594:PRO:CG	1:C:597:LEU:HD12	2.36	0.53
1:C:566:LYS:NZ	2:C:695:HOH:O	2.42	0.53
1:C:402:PHE:CE2	1:C:409:MSE:HE3	2.44	0.53
1:D:323:LEU:N	1:D:323:LEU:HD12	2.23	0.53
1:D:301:LYS:HE2	2:D:759:HOH:O	2.09	0.53
1:D:20:ILE:HD12	1:D:267:LEU:CD1	2.39	0.53
1:C:398:ARG:HB3	2:C:917:HOH:O	2.09	0.53
1:C:202:THR:HG23	2:C:908:HOH:O	2.08	0.52
1:C:423:ARG:CZ	2:C:850:HOH:O	2.55	0.52
1:D:529:LEU:HD23	1:D:576:PRO:CG	2.38	0.52
1:A:605:GLY:O	1:A:619:ALA:HB1	2.09	0.52
1:B:587:ALA:O	1:B:591:GLU:HG3	2.09	0.52
1:C:179:LEU:N	2:C:915:HOH:O	2.41	0.52
1:D:215:GLN:NE2	1:D:240:ARG:CB	2.66	0.52
1:B:332:ARG:NH2	1:B:334:GLU:OE1	2.42	0.52
1:A:132:LEU:HD13	1:A:416:LEU:HD21	1.91	0.52
1:B:309:TRP:CZ3	1:B:313:LEU:HD11	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:LEU:HD23	1:D:576:PRO:HB2	1.92	0.52
1:D:338:LEU:H	1:D:338:LEU:HD23	1.73	0.52
1:B:328:MSE:HB3	1:B:332:ARG:NH1	2.25	0.52
1:D:635:ARG:HD2	2:D:831:HOH:O	2.09	0.52
1:D:74:LEU:O	1:D:78:VAL:HG12	2.09	0.52
1:D:116:THR:CB	1:D:446:MSE:HE2	2.40	0.52
1:D:483:LEU:C	1:D:483:LEU:HD13	2.30	0.52
1:B:43:LEU:HD13	1:B:48:VAL:CG2	2.39	0.52
1:D:562:LEU:O	1:D:565:GLU:HG2	2.09	0.52
1:C:329:ARG:NH1	2:C:909:HOH:O	2.41	0.52
1:D:360:ASN:C	2:D:886:HOH:O	2.48	0.52
1:D:459:ILE:CD1	1:D:636:LEU:HD23	2.39	0.52
1:D:529:LEU:HD22	1:D:529:LEU:O	2.09	0.52
1:A:35:MSE:HE1	1:A:254:SER:HB3	1.90	0.52
1:A:83:GLY:HA3	1:A:299:ARG:CD	2.40	0.52
1:B:343:PRO:HG2	1:B:345:PHE:CE1	2.45	0.52
1:A:406:GLU:HB3	1:A:436:MSE:HE2	1.90	0.52
1:C:214:TRP:CG	1:C:241:PRO:HG2	2.45	0.52
1:C:373:SER:N	1:C:409:MSE:HE1	2.24	0.52
1:D:252:PHE:HB2	2:D:848:HOH:O	2.10	0.52
1:D:19:ALA:HB2	2:D:932:HOH:O	2.10	0.52
1:D:179:LEU:N	2:D:846:HOH:O	2.43	0.52
1:D:529:LEU:HD23	1:D:576:PRO:CB	2.40	0.52
1:D:55:ASP:HB2	2:D:825:HOH:O	2.10	0.52
1:C:377:THR:N	1:C:378:PRO:HD2	2.25	0.52
1:D:173:LEU:HD13	1:D:177:TRP:CH2	2.45	0.52
1:B:529:LEU:HD22	1:B:576:PRO:CG	2.40	0.52
1:D:414:ASN:C	2:D:808:HOH:O	2.49	0.52
1:B:431:VAL:HG13	1:B:432:PHE:CD1	2.45	0.52
1:C:58:TRP:HB2	1:C:306:GLN:OE1	2.10	0.51
1:D:11:SER:HB3	2:D:909:HOH:O	2.09	0.51
1:D:156:LEU:HB2	2:D:881:HOH:O	2.10	0.51
1:D:183:ILE:HD11	1:D:236:LYS:NZ	2.26	0.51
1:D:527:ARG:HE	1:D:530:LEU:CD1	2.23	0.51
1:C:115:VAL:HG23	1:C:446:MSE:SE	2.61	0.51
1:D:41:ALA:CB	1:D:74:LEU:HD11	2.35	0.51
1:D:579:GLU:H	1:D:579:GLU:CD	2.12	0.51
1:C:151:HIS:NE2	1:C:419:HIS:NE2	2.57	0.51
1:C:387:MSE:HE3	2:C:917:HOH:O	2.10	0.51
1:D:323:LEU:H	1:D:323:LEU:HD12	1.76	0.51
1:C:442:LEU:HG	1:C:446:MSE:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:TYR:HB2	2:C:925:HOH:O	2.10	0.51
1:C:604:ALA:HA	1:C:638:PHE:CZ	2.46	0.51
1:A:405:ARG:HH22	1:B:163:MSE:CE	2.21	0.51
1:D:31:PRO:O	1:D:35:MSE:HG3	2.11	0.51
1:C:48:VAL:HG21	1:C:232:ILE:HD13	1.92	0.51
1:B:215:GLN:CB	2:B:1134:HOH:O	2.57	0.51
1:D:354:ALA:HB1	1:D:491:ALA:HA	1.93	0.51
1:C:44:LEU:HA	1:C:48:VAL:HB	1.93	0.51
1:D:11:SER:O	1:D:14:ALA:HB3	2.11	0.51
1:D:501:ALA:HB2	1:D:509:THR:HG21	1.92	0.51
1:D:358:ALA:O	1:D:362:LEU:HG	2.11	0.51
1:C:163:MSE:HE3	1:C:201:PHE:HB2	1.93	0.51
1:D:157:ALA:N	2:D:824:HOH:O	2.44	0.51
1:C:63:ARG:HG2	2:C:941:HOH:O	2.11	0.51
1:D:344:SER:HA	2:D:845:HOH:O	2.11	0.51
1:D:321:PRO:HG2	1:D:322:ASP:H	1.76	0.51
1:D:7:LEU:HG	1:D:295:HIS:CE1	2.46	0.51
1:D:215:GLN:CD	1:D:240:ARG:HB2	2.30	0.50
1:C:35:MSE:HE1	1:C:254:SER:HB3	1.93	0.50
1:D:536:LEU:HD23	1:D:536:LEU:C	2.30	0.50
1:D:636:LEU:HB2	2:D:847:HOH:O	2.10	0.50
1:D:107:ARG:HD3	1:D:108:GLY:N	2.25	0.50
1:C:325:GLN:HG3	1:C:326:GLU:N	2.26	0.50
1:C:343:PRO:HG2	1:C:345:PHE:CE1	2.46	0.50
1:A:247:ARG:HG3	1:A:247:ARG:HH21	1.76	0.50
1:C:325:GLN:HG3	1:C:326:GLU:H	1.76	0.50
1:B:570:VAL:HG12	2:B:1114:HOH:O	2.11	0.50
1:C:369:LEU:HD13	1:C:369:LEU:C	2.32	0.50
1:B:313:LEU:HB3	2:B:1132:HOH:O	2.12	0.50
1:C:60:ASP:CG	2:C:924:HOH:O	2.49	0.50
1:B:220:GLU:CD	1:B:247:ARG:HH11	2.14	0.50
1:D:246:VAL:HG13	2:D:898:HOH:O	2.10	0.50
1:D:267:LEU:HD13	2:D:789:HOH:O	2.11	0.50
1:C:332:ARG:HD2	1:C:334:GLU:OE2	2.12	0.50
1:D:414:ASN:O	1:D:418:LEU:HD12	2.10	0.50
1:D:423:ARG:HG2	1:D:423:ARG:HH11	1.76	0.50
1:C:61:ARG:NE	2:C:941:HOH:O	2.43	0.50
1:B:190:ARG:NH1	1:B:190:ARG:HG3	2.27	0.50
1:D:456:HIS:CD2	1:D:515:ARG:HD2	2.47	0.50
1:D:484:PHE:CD2	1:D:579:GLU:HG3	2.46	0.50
1:C:218:ARG:HH11	1:C:245:ALA:HB1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:NH2	2:B:1129:HOH:O	2.45	0.50
1:C:522:SER:HB3	1:C:525:LYS:HG2	1.92	0.50
1:C:265:GLU:N	2:C:935:HOH:O	2.44	0.50
1:A:392:ARG:HG3	2:A:716:HOH:O	2.11	0.50
1:B:651:VAL:OXT	1:B:651:VAL:HG22	2.12	0.50
1:D:163:MSE:HE3	1:D:201:PHE:CD1	2.46	0.50
1:C:413:LEU:CD2	2:C:894:HOH:O	2.59	0.50
1:D:46:ARG:HG3	1:D:298:MSE:CE	2.41	0.50
1:C:218:ARG:HH11	1:C:245:ALA:C	2.14	0.50
1:B:284:PRO:HG3	2:B:1145:HOH:O	2.10	0.50
1:A:120:LEU:HD12	1:B:404:VAL:HG11	1.94	0.49
1:B:226:GLU:OE2	1:B:229:ARG:NH2	2.45	0.49
1:A:554:HIS:HD2	2:A:945:HOH:O	1.94	0.49
1:D:18:LEU:HD12	1:D:77:ALA:HB1	1.94	0.49
1:D:42:TYR:HD1	1:D:296:MSE:HE1	1.77	0.49
1:A:120:LEU:HD13	1:A:160:GLY:HA3	1.93	0.49
1:C:496:TYR:CZ	1:C:527:ARG:HG2	2.48	0.49
1:D:543:GLN:NE2	1:D:568:VAL:HA	2.26	0.49
1:D:311:LYS:CA	1:D:314:GLU:HG2	2.43	0.49
1:D:631:GLU:HG3	1:D:635:ARG:HD2	1.94	0.49
1:D:208:ARG:O	1:D:211:ALA:HB3	2.12	0.49
1:D:36:GLY:HA2	2:D:848:HOH:O	2.10	0.49
1:D:23:VAL:HG22	2:D:853:HOH:O	2.12	0.49
1:D:33:MSE:N	1:D:34:PRO:HD2	2.28	0.49
1:C:166:VAL:HA	2:C:904:HOH:O	2.12	0.49
1:D:163:MSE:CE	1:D:201:PHE:HB2	2.42	0.49
1:C:205:VAL:HG23	1:C:206:LEU:H	1.78	0.49
1:A:601:ALA:HB3	1:A:617:VAL:HG12	1.94	0.49
1:D:496:TYR:HB3	1:D:529:LEU:HD12	1.94	0.49
1:D:119:PRO:O	1:D:122:GLN:HG2	2.13	0.49
1:D:318:ARG:HH21	1:D:318:ARG:HG2	1.78	0.49
1:D:23:VAL:N	2:D:867:HOH:O	2.45	0.49
1:D:214:TRP:C	1:D:215:GLN:NE2	2.65	0.49
1:B:128:VAL:HG21	1:B:170:ALA:HB1	1.95	0.49
1:D:219:VAL:HG11	1:D:228:LEU:HD12	1.93	0.49
1:C:455:THR:HB	2:C:907:HOH:O	2.13	0.49
1:D:415:GLY:HA2	2:D:841:HOH:O	2.13	0.49
1:D:549:THR:HG22	1:D:575:LEU:O	2.13	0.49
1:D:285:PRO:O	1:D:286:PHE:HB2	2.12	0.49
1:C:541:GLU:O	1:C:569:ARG:NH2	2.45	0.49
1:C:327:LEU:CD1	1:C:331:LEU:HD13	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HG3	2:C:941:HOH:O	2.13	0.49
1:C:499:LEU:HB3	1:C:503:ARG:HH21	1.77	0.49
1:D:267:LEU:O	1:D:271:ALA:HB3	2.12	0.49
1:C:456:HIS:CE1	1:C:515:ARG:HG3	2.48	0.49
1:D:364:PRO:CD	2:D:886:HOH:O	2.60	0.49
1:C:143:ARG:HG3	1:C:143:ARG:NH1	2.27	0.49
1:C:482:ASN:ND2	1:C:504:ARG:HH22	2.10	0.49
1:B:554:HIS:HD2	2:B:1072:HOH:O	1.95	0.49
1:D:39:PRO:O	1:D:43:LEU:HB2	2.13	0.48
1:C:186:TRP:CZ3	1:C:205:VAL:HG21	2.48	0.48
1:B:644:ALA:HA	2:B:1146:HOH:O	2.12	0.48
1:D:394:ASN:ND2	1:D:396:LEU:H	2.10	0.48
1:D:107:ARG:CD	1:D:108:GLY:N	2.75	0.48
1:A:97:TRP:HH2	1:B:636:LEU:HD13	1.78	0.48
1:D:597:LEU:N	1:D:597:LEU:HD12	2.28	0.48
1:A:490:ASP:N	2:A:1175:HOH:O	2.20	0.48
1:D:37:MSE:HE2	1:D:156:LEU:CD1	2.43	0.48
1:D:206:LEU:HG	1:D:216:THR:HB	1.95	0.48
1:D:289:PRO:HB2	1:D:291:GLU:OE1	2.14	0.48
1:A:629:TYR:CD2	1:A:630:PRO:HA	2.47	0.48
1:B:206:LEU:HG	1:B:216:THR:HB	1.95	0.48
1:C:169:GLU:HB3	1:C:408:ALA:HB2	1.96	0.48
1:D:322:ASP:C	1:D:324:HIS:H	2.15	0.48
1:D:569:ARG:NE	2:D:724:HOH:O	2.46	0.48
1:C:423:ARG:HG3	1:C:423:ARG:HH11	1.78	0.48
1:C:348:PRO:HA	1:C:520:LEU:HD21	1.95	0.48
1:C:38:ALA:N	1:C:39:PRO:HD2	2.28	0.48
1:D:35:MSE:HE1	1:D:254:SER:HB3	1.95	0.48
1:B:496:TYR:O	1:B:500:VAL:HG23	2.14	0.48
1:B:120:LEU:HD13	1:B:160:GLY:HA3	1.94	0.48
1:B:87:PRO:HG2	1:B:90:GLU:HG2	1.96	0.48
1:D:363:ALA:N	2:D:886:HOH:O	2.46	0.48
1:D:135:ARG:NH2	1:D:181:LYS:HE3	2.28	0.48
1:B:545:VAL:HG23	1:B:597:LEU:HD13	1.96	0.48
1:B:579:GLU:CD	1:B:579:GLU:H	2.17	0.48
1:D:186:TRP:CZ3	1:D:205:VAL:HG21	2.48	0.48
1:C:218:ARG:HD2	1:C:245:ALA:O	2.13	0.48
1:B:332:ARG:NH1	2:B:860:HOH:O	2.45	0.48
1:A:33:MSE:HE2	2:A:1173:HOH:O	2.12	0.48
1:B:570:VAL:HA	2:B:1138:HOH:O	2.13	0.48
1:D:173:LEU:HD11	2:D:855:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:PRO:CD	2:C:935:HOH:O	2.49	0.48
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.96	0.48
1:A:310:GLU:O	1:A:314:GLU:HG2	2.14	0.48
1:D:191:ILE:O	2:D:827:HOH:O	2.20	0.48
1:D:38:ALA:N	1:D:39:PRO:HD2	2.29	0.48
1:C:52:ASN:OD1	1:C:54:LEU:HD23	2.14	0.48
1:C:97:TRP:HZ3	2:D:847:HOH:O	1.97	0.48
1:C:37:MSE:HE2	1:C:156:LEU:CD1	2.44	0.48
1:C:461:LEU:C	1:C:461:LEU:HD12	2.33	0.48
1:C:309:TRP:O	1:C:313:LEU:HD23	2.14	0.48
1:B:635:ARG:HD3	2:B:1116:HOH:O	2.14	0.48
1:B:369:LEU:HD11	1:B:425:TYR:HE2	1.78	0.48
1:C:8:GLU:O	1:C:12:VAL:HG23	2.14	0.48
1:D:555:LEU:HD22	1:D:643:VAL:HG21	1.95	0.48
1:C:352:ARG:HH21	1:C:456:HIS:HE1	1.60	0.47
1:D:252:PHE:HD2	1:D:257:GLN:HE22	1.62	0.47
1:D:79:LEU:O	1:D:84:TYR:HB2	2.14	0.47
1:C:327:LEU:HD12	1:C:331:LEU:HD13	1.96	0.47
1:D:459:ILE:HD13	1:D:620:LEU:HD22	1.96	0.47
1:C:209:TYR:HA	1:C:212:TYR:CD2	2.47	0.47
1:C:196:PRO:O	1:C:199:LEU:HD13	2.13	0.47
1:C:310:GLU:HG2	2:C:723:HOH:O	2.13	0.47
1:D:370:LEU:O	1:D:424:ALA:HA	2.14	0.47
1:D:536:LEU:O	1:D:536:LEU:HD23	2.15	0.47
1:D:427:GLY:HA2	1:D:453:VAL:O	2.14	0.47
1:D:404:VAL:HG12	1:D:404:VAL:O	2.15	0.47
1:B:417:ASN:ND2	1:B:423:ARG:HA	2.29	0.47
1:B:328:MSE:O	1:B:332:ARG:HG3	2.14	0.47
1:B:558:ARG:NH2	2:B:666:HOH:O	2.46	0.47
1:C:390:PHE:CE1	1:C:395:PRO:HA	2.49	0.47
1:D:44:LEU:HD23	1:D:48:VAL:HG11	1.97	0.47
1:B:563:LEU:HD21	2:B:1146:HOH:O	2.15	0.47
1:C:264:GLY:CA	2:C:935:HOH:O	2.63	0.47
1:A:545:VAL:HG22	1:A:571:ARG:CG	2.43	0.47
1:C:519:PRO:HB2	1:C:554:HIS:CD2	2.49	0.47
1:B:180:SER:HB3	1:B:239:GLU:O	2.15	0.47
1:B:562:LEU:HD23	1:B:562:LEU:O	2.15	0.47
1:A:475:MSE:HE3	1:A:608:LEU:O	2.14	0.47
1:D:329:ARG:NH1	2:D:916:HOH:O	2.47	0.47
1:C:555:LEU:O	1:C:555:LEU:HD23	2.15	0.47
1:C:46:ARG:CG	1:C:296:MSE:HE1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASN:O	1:D:225:LEU:HD12	2.15	0.47
1:D:44:LEU:HA	1:D:48:VAL:HG12	1.95	0.47
1:C:210:ARG:HA	2:C:902:HOH:O	2.15	0.47
1:C:210:ARG:HG3	2:C:902:HOH:O	2.14	0.47
1:C:448:VAL:HB	2:C:940:HOH:O	2.14	0.47
1:A:547:VAL:O	1:A:601:ALA:HA	2.15	0.47
1:D:311:LYS:HA	1:D:314:GLU:CG	2.44	0.47
1:B:475:MSE:HE2	1:B:608:LEU:O	2.15	0.47
1:D:418:LEU:HD13	2:D:872:HOH:O	2.14	0.47
1:C:352:ARG:NH2	1:C:456:HIS:HE1	2.12	0.47
1:B:396:LEU:HD23	2:B:1057:HOH:O	2.14	0.47
1:B:328:MSE:HB3	1:B:332:ARG:HH12	1.79	0.47
1:C:375:ASP:OD1	1:D:192:SER:HB3	2.15	0.47
1:D:414:ASN:O	1:D:418:LEU:HB2	2.14	0.47
1:D:46:ARG:NH2	1:D:295:HIS:CD2	2.83	0.47
1:C:136:LYS:HB2	2:C:729:HOH:O	2.14	0.47
1:D:119:PRO:HB2	1:D:122:GLN:HG3	1.96	0.47
1:C:390:PHE:HA	1:C:397:GLY:HA3	1.97	0.47
1:D:230:LYS:HB3	1:D:230:LYS:NZ	2.30	0.47
1:D:336:PRO:HD3	2:D:766:HOH:O	2.14	0.47
1:A:607:SER:HB2	1:A:617:VAL:HG21	1.96	0.47
1:A:45:PHE:CE1	1:A:49:MSE:HE1	2.50	0.47
1:D:230:LYS:O	1:D:234:LEU:HG	2.15	0.47
1:C:427:GLY:HA2	1:C:453:VAL:O	2.15	0.47
1:D:217:LEU:HB2	1:D:244:ILE:HG12	1.98	0.46
1:A:314:GLU:HB2	2:A:1120:HOH:O	2.15	0.46
1:D:120:LEU:O	1:D:164:GLU:HG3	2.14	0.46
1:C:46:ARG:HD3	1:C:298:MSE:CE	2.44	0.46
1:D:206:LEU:HD21	1:D:218:ARG:HG2	1.97	0.46
2:C:901:HOH:O	1:D:480:MSE:SE	2.83	0.46
1:D:159:ASP:OD2	1:D:197:THR:HG21	2.15	0.46
1:D:37:MSE:HE3	1:D:40:LEU:HD23	1.97	0.46
1:C:564:ARG:NH1	1:C:564:ARG:HB2	2.27	0.46
1:D:289:PRO:HG2	1:D:292:VAL:HG21	1.97	0.46
1:D:149:VAL:HG11	2:D:883:HOH:O	2.15	0.46
1:B:215:GLN:HB3	2:B:1134:HOH:O	2.14	0.46
1:D:240:ARG:NH2	1:D:392:ARG:HH12	2.13	0.46
1:D:372:GLY:C	2:D:809:HOH:O	2.53	0.46
1:B:299:ARG:NH2	2:B:731:HOH:O	2.49	0.46
1:D:295:HIS:HE1	2:D:879:HOH:O	1.98	0.46
1:D:419:HIS:ND1	2:D:866:HOH:O	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:ALA:HB3	1:D:632:VAL:HB	1.96	0.46
1:D:560:GLN:HG3	1:D:561:ALA:N	2.30	0.46
1:D:389:ASP:OD1	1:D:401:HIS:HE1	1.99	0.46
1:C:387:MSE:HE3	1:C:398:ARG:O	2.16	0.46
1:D:527:ARG:HE	1:D:530:LEU:HD12	1.80	0.46
1:C:193:ILE:N	1:C:193:ILE:HD12	2.31	0.46
1:C:580:LEU:O	1:C:580:LEU:HD23	2.16	0.46
1:D:76:TYR:HE2	1:D:94:PHE:HE1	1.64	0.46
1:D:30:HIS:CD2	1:D:70:HIS:HB2	2.51	0.46
1:D:541:GLU:HB2	2:D:724:HOH:O	2.14	0.46
1:C:234:LEU:HB3	2:C:916:HOH:O	2.15	0.46
1:C:530:LEU:O	1:C:580:LEU:HD21	2.15	0.46
1:D:413:LEU:HA	1:D:416:LEU:HD23	1.98	0.46
1:B:107:ARG:HD2	1:B:107:ARG:C	2.36	0.46
1:C:487:ARG:HG3	1:C:512:VAL:HB	1.97	0.46
1:D:16:ARG:HH12	1:D:223:ASN:ND2	2.14	0.46
1:D:180:SER:HB2	1:D:238:ASP:O	2.16	0.46
1:D:134:GLU:HB2	1:D:151:HIS:CE1	2.51	0.46
1:C:31:PRO:C	1:C:34:PRO:HD2	2.36	0.46
1:D:106:GLU:HA	1:D:116:THR:HG23	1.97	0.46
1:D:364:PRO:HD3	2:D:886:HOH:O	2.16	0.45
1:D:7:LEU:HD23	1:D:7:LEU:N	2.31	0.45
1:D:297:ASP:OD1	1:D:299:ARG:HB2	2.16	0.45
1:D:557:LEU:HD23	1:D:572:VAL:HG11	1.99	0.45
1:A:612:ARG:HA	1:B:611:GLU:HG2	1.97	0.45
1:D:335:LEU:H	1:D:335:LEU:CD2	2.22	0.45
1:D:543:GLN:HE21	1:D:569:ARG:HD3	1.81	0.45
1:B:369:LEU:CD1	1:B:425:TYR:HE2	2.30	0.45
1:D:362:LEU:O	1:D:366:LEU:HG	2.16	0.45
1:C:158:SER:HB2	2:C:912:HOH:O	2.16	0.45
1:D:76:TYR:CE2	1:D:94:PHE:HE1	2.34	0.45
1:D:209:TYR:O	1:D:214:TRP:HB2	2.16	0.45
1:D:496:TYR:CB	1:D:529:LEU:HD12	2.47	0.45
1:D:496:TYR:O	1:D:500:VAL:HG12	2.16	0.45
1:B:215:GLN:HB2	2:B:1134:HOH:O	2.17	0.45
1:D:431:VAL:HG13	1:D:432:PHE:CD1	2.52	0.45
1:D:539:VAL:O	1:D:542:PRO:HD3	2.16	0.45
1:C:120:LEU:O	1:C:164:GLU:HG3	2.16	0.45
1:C:42:TYR:HE1	1:C:296:MSE:HE1	1.81	0.45
1:B:541:GLU:HB2	1:B:569:ARG:NH2	2.32	0.45
1:A:214:TRP:CG	1:A:241:PRO:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ARG:HG3	1:D:353:ALA:N	2.31	0.45
1:A:406:GLU:HG3	1:A:428:THR:HG21	1.98	0.45
1:D:46:ARG:HH21	1:D:295:HIS:CD2	2.34	0.45
1:D:132:LEU:HD22	1:D:416:LEU:HD11	1.98	0.45
1:C:430:LEU:HA	1:C:454:PHE:HB3	1.99	0.45
1:D:281:TRP:NE1	1:D:283:TYR:HB2	2.32	0.45
1:C:413:LEU:HD22	2:C:894:HOH:O	2.17	0.45
1:C:80:HIS:HB3	2:C:932:HOH:O	2.17	0.45
1:D:632:VAL:O	1:D:636:LEU:HB2	2.16	0.45
1:C:390:PHE:HB2	1:C:397:GLY:O	2.17	0.45
1:B:503:ARG:HD2	2:B:1095:HOH:O	2.16	0.45
1:A:594:PRO:HG2	1:A:597:LEU:HD22	1.98	0.45
1:B:566:LYS:HB3	1:B:566:LYS:NZ	2.31	0.45
1:C:457:ASP:CB	1:C:512:VAL:HG12	2.47	0.45
1:C:292:VAL:N	2:C:895:HOH:O	2.50	0.45
1:A:190:ARG:NH2	1:A:247:ARG:NH1	2.64	0.45
1:C:177:TRP:O	1:C:392:ARG:HG2	2.17	0.45
1:D:191:ILE:HG23	2:D:887:HOH:O	2.16	0.45
1:D:252:PHE:CD2	1:D:257:GLN:NE2	2.85	0.45
1:D:241:PRO:HD3	2:D:846:HOH:O	2.16	0.45
1:B:107:ARG:HD3	2:B:1069:HOH:O	2.17	0.45
1:A:418:LEU:HD11	1:A:446:MSE:SE	2.67	0.45
1:D:436:MSE:O	1:D:440:ILE:HG13	2.17	0.45
1:B:475:MSE:HG3	1:B:608:LEU:O	2.17	0.45
1:D:228:LEU:HD21	2:D:894:HOH:O	2.15	0.45
1:C:141:PHE:HB3	2:C:914:HOH:O	2.16	0.45
1:D:18:LEU:CD1	1:D:77:ALA:HB1	2.47	0.45
1:C:261:LYS:HB3	1:C:261:LYS:HZ2	1.80	0.45
1:C:349:ILE:CD1	1:C:520:LEU:HD11	2.47	0.45
1:C:469:GLN:HA	1:C:470:PRO:HD3	1.82	0.45
1:D:489:ALA:HB2	1:D:553:VAL:HG21	1.98	0.45
1:C:79:LEU:O	1:C:84:TYR:HB2	2.16	0.45
1:D:398:ARG:HG3	1:D:398:ARG:HH11	1.82	0.45
1:B:595:PRO:HG2	2:B:1040:HOH:O	2.15	0.45
1:C:375:ASP:HA	1:D:194:ASP:OD1	2.17	0.44
1:D:250:ILE:O	1:D:257:GLN:HA	2.16	0.44
1:D:88:LEU:HD11	1:D:286:PHE:HD1	1.82	0.44
1:A:609:GLY:HA2	1:B:609:GLY:HA2	1.99	0.44
1:C:429:PHE:HD2	1:C:432:PHE:CE2	2.35	0.44
1:C:352:ARG:HA	1:C:513:LEU:HD13	1.99	0.44
1:B:45:PHE:CE1	1:B:49:MSE:HE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:GLU:HB3	2:D:890:HOH:O	2.16	0.44
1:A:594:PRO:HA	1:A:595:PRO:HD2	1.88	0.44
1:C:95:ARG:HH11	1:D:463:GLU:HB3	1.81	0.44
1:D:259:SER:C	2:D:937:HOH:O	2.55	0.44
1:D:22:ALA:HB3	1:D:73:MSE:HE2	1.99	0.44
1:D:39:PRO:CG	1:D:222:VAL:HG22	2.45	0.44
1:C:571:ARG:NE	2:C:853:HOH:O	2.41	0.44
1:D:77:ALA:HB2	2:D:907:HOH:O	2.17	0.44
1:D:65:VAL:HG12	2:D:837:HOH:O	2.17	0.44
1:B:584:GLN:HA	2:B:1120:HOH:O	2.17	0.44
1:C:42:TYR:O	1:C:46:ARG:HB2	2.18	0.44
1:D:61:ARG:CZ	1:D:63:ARG:NH2	2.80	0.44
1:D:205:VAL:CG2	1:D:206:LEU:N	2.80	0.44
1:A:68:ALA:HB1	1:A:70:HIS:CE1	2.53	0.44
1:D:644:ALA:O	1:D:648:LEU:HG	2.18	0.44
1:D:282:PRO:HG2	2:D:880:HOH:O	2.17	0.44
1:A:374:ALA:HB3	1:A:428:THR:CG2	2.43	0.44
1:A:58:TRP:CD1	1:A:306:GLN:HG3	2.52	0.44
1:C:404:VAL:HG12	1:D:164:GLU:OE2	2.17	0.44
1:C:39:PRO:O	1:C:42:TYR:HB3	2.18	0.44
1:C:423:ARG:NH2	2:C:850:HOH:O	2.50	0.44
1:B:594:PRO:CG	1:B:597:LEU:HD21	2.46	0.44
1:D:349:ILE:HG13	1:D:353:ALA:HB3	2.00	0.44
1:D:595:PRO:HB3	2:D:922:HOH:O	2.17	0.44
1:B:527:ARG:HB2	1:B:527:ARG:NH1	2.33	0.44
1:D:36:GLY:CA	2:D:848:HOH:O	2.65	0.44
1:D:229:ARG:O	1:D:233:LYS:HG2	2.17	0.44
1:D:59:PRO:HB2	1:D:309:TRP:CH2	2.52	0.44
1:D:63:ARG:CG	1:D:63:ARG:HH21	2.26	0.44
1:C:405:ARG:HH12	1:D:163:MSE:CE	2.13	0.44
1:D:324:HIS:C	1:D:326:GLU:N	2.69	0.44
1:D:336:PRO:HB2	1:D:337:PRO:HD2	1.99	0.44
1:D:492:TYR:CE1	1:D:523:PRO:HG3	2.53	0.44
1:A:496:TYR:O	1:A:500:VAL:HG23	2.18	0.44
1:D:269:PRO:HG2	1:D:270:GLU:H	1.81	0.44
1:D:148:VAL:HG12	2:D:899:HOH:O	2.17	0.44
1:C:80:HIS:CD2	2:C:932:HOH:O	2.71	0.44
1:D:52:ASN:C	1:D:54:LEU:N	2.71	0.44
1:A:247:ARG:HG3	2:A:1178:HOH:O	2.17	0.44
1:B:283:TYR:HA	1:B:284:PRO:HD3	1.79	0.44
1:B:342:PRO:HB3	1:B:495:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:610:TRP:C	1:D:612:ARG:H	2.20	0.44
1:A:545:VAL:HB	1:A:599:VAL:HG22	2.00	0.44
1:B:35:MSE:HE1	1:B:254:SER:HB3	1.99	0.44
1:B:540:GLU:HG2	2:B:1110:HOH:O	2.18	0.44
1:C:359:LEU:HB3	1:C:384:ALA:HB2	1.98	0.44
1:D:19:ALA:HA	1:D:73:MSE:HE2	2.00	0.43
1:D:124:ILE:CG2	1:D:125:SER:N	2.81	0.43
1:D:196:PRO:HD2	1:D:199:LEU:HD11	2.00	0.43
1:D:295:HIS:CE1	2:D:879:HOH:O	2.71	0.43
1:B:289:PRO:HG2	1:B:292:VAL:HG23	2.00	0.43
1:C:608:LEU:HD13	1:D:612:ARG:HH11	1.83	0.43
1:D:352:ARG:HA	1:D:513:LEU:HD13	1.99	0.43
1:D:133:ALA:HB2	2:D:849:HOH:O	2.17	0.43
1:B:220:GLU:OE1	1:B:247:ARG:NH1	2.51	0.43
1:A:6:ASP:OD1	1:A:7:LEU:HD22	2.18	0.43
1:D:256:LYS:O	1:D:262:ALA:HB2	2.18	0.43
1:D:288:VAL:O	1:D:293:TYR:HE2	2.01	0.43
1:D:416:LEU:HB2	1:D:424:ALA:HB3	2.00	0.43
1:C:188:ASP:OD1	1:C:190:ARG:CZ	2.67	0.43
1:D:93:SER:HA	2:D:906:HOH:O	2.17	0.43
1:D:44:LEU:HA	1:D:48:VAL:HG13	1.96	0.43
1:D:116:THR:OG1	1:D:446:MSE:HG2	2.19	0.43
1:D:416:LEU:HD13	2:D:923:HOH:O	2.18	0.43
1:D:630:PRO:O	1:D:634:GLU:HG3	2.18	0.43
2:C:901:HOH:O	1:D:480:MSE:HE2	2.17	0.43
1:B:527:ARG:HH11	1:B:527:ARG:HB2	1.83	0.43
1:B:629:TYR:CD1	1:B:630:PRO:HA	2.53	0.43
1:C:335:LEU:HD12	1:C:336:PRO:HD2	2.00	0.43
1:D:62:ASP:HA	2:D:852:HOH:O	2.18	0.43
1:B:506:GLU:CD	1:B:506:GLU:N	2.72	0.43
1:D:349:ILE:HG13	1:D:350:ALA:N	2.34	0.43
1:D:506:GLU:H	1:D:506:GLU:CD	2.21	0.43
1:C:407:HIS:HB3	2:C:904:HOH:O	2.18	0.43
1:D:191:ILE:HG13	2:D:937:HOH:O	2.18	0.43
1:D:368:GLU:CD	1:D:368:GLU:N	2.72	0.43
1:D:413:LEU:C	1:D:415:GLY:N	2.71	0.43
1:C:230:LYS:HB3	1:C:230:LYS:HE2	1.89	0.43
1:C:418:LEU:HD11	1:C:446:MSE:SE	2.68	0.43
1:C:627:ALA:HB3	1:C:632:VAL:HB	2.00	0.43
1:C:429:PHE:HD1	1:C:455:THR:HG23	1.84	0.43
1:D:46:ARG:HA	1:D:298:MSE:SE	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ALA:N	2:D:887:HOH:O	2.52	0.43
1:A:405:ARG:HH12	1:B:163:MSE:HE2	1.82	0.43
1:C:34:PRO:HA	1:C:74:LEU:HD13	2.00	0.43
1:D:133:ALA:HA	2:D:812:HOH:O	2.19	0.43
1:D:277:ARG:HD3	1:D:277:ARG:C	2.39	0.43
1:C:10:LEU:HD23	2:C:895:HOH:O	2.18	0.43
1:C:136:LYS:HG3	1:C:422:TYR:CZ	2.54	0.43
1:A:404:VAL:HG12	1:B:164:GLU:OE2	2.19	0.43
1:A:282:PRO:HA	2:A:990:HOH:O	2.19	0.43
1:D:252:PHE:CB	2:D:848:HOH:O	2.67	0.43
1:D:141:PHE:HA	2:D:908:HOH:O	2.19	0.43
1:D:364:PRO:HD2	2:D:886:HOH:O	2.18	0.43
1:C:349:ILE:HD11	1:C:491:ALA:HB2	2.01	0.43
1:D:191:ILE:N	1:D:197:THR:HG23	2.33	0.43
1:C:247:ARG:HG2	1:C:247:ARG:HH11	1.82	0.43
1:A:46:ARG:NH2	1:A:298:MSE:HE1	2.34	0.43
1:D:461:LEU:HD12	1:D:462:GLY:N	2.33	0.43
1:C:224:ASP:OD2	1:C:227:ALA:HB2	2.19	0.43
1:D:380:ASN:HB3	1:D:382:THR:HG23	2.01	0.43
1:D:111:PRO:HG3	2:D:792:HOH:O	2.18	0.42
1:D:25:LYS:NZ	1:D:92:LYS:HB3	2.34	0.42
1:D:34:PRO:HA	2:D:829:HOH:O	2.19	0.42
1:C:242:THR:CG2	2:C:939:HOH:O	2.64	0.42
1:A:33:MSE:CE	1:A:71:GLY:HA3	2.49	0.42
1:C:87:PRO:HG2	1:C:90:GLU:HG2	2.02	0.42
1:C:629:TYR:CD1	1:C:630:PRO:HA	2.55	0.42
1:C:400:LEU:HD12	1:C:400:LEU:N	2.34	0.42
1:A:540:GLU:HA	1:A:540:GLU:OE1	2.19	0.42
1:B:311:LYS:HD2	2:B:885:HOH:O	2.19	0.42
1:D:120:LEU:H	1:D:120:LEU:CD2	2.32	0.42
1:D:240:ARG:HB3	1:D:241:PRO:HD2	2.00	0.42
1:D:148:VAL:HG23	1:D:313:LEU:HD22	2.01	0.42
1:C:392:ARG:NH1	2:C:884:HOH:O	2.50	0.42
1:C:635:ARG:HG2	1:C:635:ARG:HH11	1.84	0.42
1:C:404:VAL:HG21	1:D:160:GLY:CA	2.50	0.42
1:D:79:LEU:HD13	1:D:111:PRO:O	2.19	0.42
1:C:295:HIS:CD2	1:C:296:MSE:CE	3.02	0.42
1:C:329:ARG:NH2	1:C:334:GLU:O	2.52	0.42
1:D:61:ARG:NH1	1:D:63:ARG:NH2	2.68	0.42
1:D:68:ALA:HB1	1:D:70:HIS:CD2	2.53	0.42
1:D:508:PRO:HD2	2:D:874:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:MSE:O	1:A:298:MSE:HG2	2.18	0.42
1:D:557:LEU:CD2	1:D:572:VAL:HG11	2.49	0.42
1:A:437:ARG:HG2	2:A:1162:HOH:O	2.19	0.42
1:D:186:TRP:N	2:D:834:HOH:O	2.52	0.42
1:D:107:ARG:HD3	1:D:108:GLY:H	1.85	0.42
1:D:58:TRP:CH2	1:D:305:TRP:HB3	2.54	0.42
1:A:534:TYR:O	1:A:573:VAL:HG13	2.20	0.42
1:A:489:ALA:N	2:A:1175:HOH:O	2.52	0.42
1:D:498:TRP:O	1:D:502:LEU:HB2	2.19	0.42
1:C:647:PHE:CE2	1:C:651:VAL:HG22	2.55	0.42
1:D:636:LEU:HD12	1:D:636:LEU:HA	1.80	0.42
1:B:630:PRO:O	1:B:634:GLU:HG3	2.19	0.42
1:C:169:GLU:HB3	1:C:405:ARG:HD3	2.01	0.42
1:A:608:LEU:HD22	1:B:612:ARG:NH1	2.35	0.42
1:D:20:ILE:HD11	1:D:35:MSE:CG	2.44	0.42
1:D:327:LEU:O	1:D:331:LEU:CB	2.67	0.42
1:D:314:GLU:O	1:D:317:ALA:HB3	2.19	0.42
1:D:631:GLU:O	1:D:635:ARG:HG3	2.20	0.42
1:B:427:GLY:HA2	1:B:453:VAL:O	2.19	0.42
1:C:128:VAL:HG21	1:C:170:ALA:HB1	2.01	0.42
1:A:110:THR:HB	1:A:113:VAL:CG2	2.48	0.42
1:D:72:SER:HB2	1:D:76:TYR:CE2	2.54	0.42
1:A:417:ASN:ND2	1:A:423:ARG:HA	2.34	0.42
1:D:216:THR:HG22	1:D:243:LEU:HB3	2.01	0.42
1:C:218:ARG:HD3	1:C:245:ALA:HB3	2.01	0.42
1:D:301:LYS:HB2	2:D:807:HOH:O	2.19	0.42
1:D:354:ALA:CB	1:D:491:ALA:HA	2.50	0.42
1:A:339:PRO:HB3	1:A:365:ARG:NH1	2.34	0.42
1:A:226:GLU:HG3	1:A:230:LYS:HE3	2.02	0.42
1:C:31:PRO:O	1:C:34:PRO:HD2	2.20	0.42
1:D:484:PHE:HA	1:D:579:GLU:CG	2.47	0.42
1:C:230:LYS:O	1:C:234:LEU:HG	2.20	0.42
1:A:329:ARG:NH1	1:A:336:PRO:HD3	2.34	0.42
1:D:46:ARG:HG2	1:D:46:ARG:NH1	2.34	0.42
1:C:323:LEU:HD12	1:C:323:LEU:N	2.34	0.42
1:C:132:LEU:O	1:C:132:LEU:HD23	2.20	0.42
1:D:537:GLU:HG2	1:D:560:GLN:HE22	1.85	0.42
1:C:208:ARG:O	1:C:211:ALA:HB3	2.19	0.42
1:A:636:LEU:HA	1:A:636:LEU:HD23	1.91	0.42
1:D:640:PRO:HG2	1:D:641:GLU:OE1	2.19	0.42
1:D:252:PHE:CA	1:D:257:GLN:HE21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:PHE:HA	2:D:905:HOH:O	2.20	0.42
1:D:222:VAL:HG13	1:D:223:ASN:N	2.35	0.42
1:D:329:ARG:NH1	1:D:329:ARG:HG2	2.32	0.42
1:C:493:GLU:HG2	1:C:529:LEU:CD1	2.50	0.42
1:C:68:ALA:HB1	1:C:70:HIS:CE1	2.55	0.42
1:B:72:SER:HB2	1:B:76:TYR:CE2	2.55	0.42
1:D:63:ARG:CG	1:D:63:ARG:NH2	2.83	0.41
1:C:373:SER:CA	1:C:409:MSE:HE1	2.50	0.41
1:C:429:PHE:HD2	1:C:432:PHE:HE2	1.68	0.41
1:D:561:ALA:O	1:D:564:ARG:HB3	2.20	0.41
1:C:307:GLU:HG3	1:C:308:ALA:N	2.34	0.41
1:A:545:VAL:HG22	1:A:571:ARG:HG2	2.02	0.41
1:C:457:ASP:HB3	1:C:512:VAL:HG12	2.03	0.41
1:D:461:LEU:CA	1:D:515:ARG:HD3	2.51	0.41
1:B:285:PRO:O	1:B:286:PHE:HB2	2.19	0.41
1:D:544:GLY:HA3	1:D:647:PHE:CE1	2.55	0.41
1:A:587:ALA:O	1:A:591:GLU:HG3	2.20	0.41
1:D:326:GLU:OE2	1:D:329:ARG:NH2	2.54	0.41
1:C:80:HIS:HD2	2:C:932:HOH:O	2.04	0.41
1:D:610:TRP:C	1:D:612:ARG:N	2.73	0.41
1:D:338:LEU:HD21	1:D:503:ARG:NH1	2.35	0.41
1:C:95:ARG:HH11	1:D:463:GLU:CB	2.34	0.41
1:D:100:LYS:HD2	2:D:882:HOH:O	2.20	0.41
1:D:347:LYS:HA	2:D:925:HOH:O	2.21	0.41
1:B:461:LEU:C	1:B:461:LEU:HD12	2.40	0.41
1:D:377:THR:N	1:D:378:PRO:HD2	2.35	0.41
1:C:163:MSE:HE3	1:C:200:ALA:O	2.20	0.41
1:C:197:THR:HG22	1:C:201:PHE:HB3	2.01	0.41
1:B:59:PRO:CG	1:B:309:TRP:CH2	2.99	0.41
1:D:143:ARG:HB3	1:D:144:PRO:HD2	2.03	0.41
1:D:206:LEU:HB3	1:D:210:ARG:HH22	1.86	0.41
1:A:43:LEU:HD23	1:A:47:GLU:HB2	2.02	0.41
1:B:190:ARG:CD	1:B:190:ARG:N	2.82	0.41
1:A:434:ASP:OD1	1:B:437:ARG:HG2	2.20	0.41
1:B:228:LEU:HA	1:B:228:LEU:HD12	1.90	0.41
1:C:16:ARG:HG2	1:C:35:MSE:HA	2.03	0.41
1:D:25:LYS:HD2	2:D:919:HOH:O	2.20	0.41
1:D:61:ARG:HH21	1:D:61:ARG:HG2	1.85	0.41
1:D:527:ARG:NE	1:D:530:LEU:HD12	2.36	0.41
1:B:541:GLU:CB	1:B:569:ARG:NH2	2.83	0.41
1:D:292:VAL:O	1:D:296:MSE:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ALA:O	1:B:554:HIS:HE1	2.02	0.41
1:D:120:LEU:N	1:D:120:LEU:HD22	2.34	0.41
1:D:94:PHE:HD2	2:D:891:HOH:O	2.03	0.41
1:B:163:MSE:HE3	1:B:201:PHE:CG	2.55	0.41
1:B:559:ALA:O	1:B:563:LEU:HD22	2.21	0.41
1:D:62:ASP:OD1	1:D:152:TYR:HB2	2.21	0.41
1:C:571:ARG:CG	2:C:853:HOH:O	2.67	0.41
1:C:458:SER:HA	1:C:470:PRO:HD2	2.03	0.41
1:D:522:SER:HB2	1:D:525:LYS:HB2	2.03	0.41
1:A:380:ASN:HA	1:A:455:THR:HG21	2.03	0.41
1:A:480:MSE:HA	1:A:481:PRO:HD3	1.93	0.41
1:C:42:TYR:CE1	1:C:296:MSE:HE1	2.56	0.41
1:D:60:ASP:O	1:D:151:HIS:HB3	2.21	0.41
1:D:61:ARG:NH1	1:D:63:ARG:HH22	2.18	0.41
1:D:318:ARG:NH2	1:D:318:ARG:HG2	2.36	0.41
1:A:53:PRO:HB3	1:A:84:TYR:CD1	2.56	0.41
1:C:169:GLU:CB	1:C:408:ALA:HB2	2.51	0.41
1:D:35:MSE:SE	1:D:267:LEU:HD11	2.70	0.41
1:D:372:GLY:N	2:D:861:HOH:O	2.52	0.41
1:C:52:ASN:HB2	2:C:929:HOH:O	2.21	0.41
1:D:124:ILE:HG23	1:D:125:SER:N	2.35	0.41
1:C:327:LEU:CA	2:C:870:HOH:O	2.69	0.41
1:D:317:ALA:O	1:D:320:TYR:O	2.39	0.41
1:B:51:HIS:CE1	2:B:1087:HOH:O	2.74	0.41
1:D:205:VAL:HG23	1:D:206:LEU:N	2.34	0.41
1:D:359:LEU:HD13	1:D:425:TYR:OH	2.21	0.41
1:C:65:VAL:HG13	1:C:115:VAL:HG12	2.02	0.41
1:D:408:ALA:O	1:D:412:ILE:HG13	2.21	0.41
1:C:547:VAL:O	1:C:601:ALA:HA	2.21	0.41
1:D:17:PHE:HA	1:D:20:ILE:CG1	2.50	0.40
1:C:409:MSE:HE2	1:C:426:GLY:HA2	2.03	0.40
1:A:54:LEU:HD21	1:A:299:ARG:CB	2.51	0.40
1:D:632:VAL:HG13	1:D:633:TYR:N	2.37	0.40
1:C:472:GLU:OE2	2:C:901:HOH:O	2.22	0.40
1:D:351:THR:HA	1:D:354:ALA:HB3	2.03	0.40
1:A:309:TRP:CH2	1:A:313:LEU:HD11	2.56	0.40
1:D:75:LEU:HD22	1:D:79:LEU:HG	2.02	0.40
1:C:214:TRP:CD2	1:C:241:PRO:HG2	2.56	0.40
1:D:20:ILE:CD1	1:D:35:MSE:SE	3.19	0.40
1:B:561:ALA:O	1:B:564:ARG:HB3	2.21	0.40
1:C:558:ARG:NH1	2:C:814:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HA	1:A:454:PHE:HB3	2.02	0.40
1:B:268:GLY:O	1:B:272:VAL:HG23	2.21	0.40
1:B:572:VAL:HG22	2:B:1114:HOH:O	2.20	0.40
1:D:233:LYS:O	1:D:237:LEU:HD13	2.21	0.40
1:D:161:ASP:HB3	2:D:844:HOH:O	2.21	0.40
1:C:371:GLY:HA3	1:C:387:MSE:HE1	2.04	0.40
1:C:62:ASP:CG	2:C:906:HOH:O	2.60	0.40
1:C:461:LEU:HG	1:C:469:GLN:HG2	2.02	0.40
1:C:377:THR:HB	1:C:378:PRO:CD	2.51	0.40
1:D:555:LEU:HD23	1:D:555:LEU:O	2.21	0.40
1:A:594:PRO:HG2	1:A:597:LEU:CD2	2.51	0.40
1:D:146:HIS:HB3	1:D:316:TYR:CD1	2.56	0.40
1:C:168:GLY:N	2:C:787:HOH:O	2.54	0.40
1:C:641:GLU:O	1:C:645:GLU:HG3	2.21	0.40
1:C:120:LEU:HD12	1:C:161:ASP:OD1	2.22	0.40
1:C:539:VAL:HG12	1:C:564:ARG:HH22	1.86	0.40
1:C:563:LEU:HD11	1:C:644:ALA:CA	2.50	0.40
1:D:486:ILE:HA	1:D:576:PRO:O	2.22	0.40
1:D:469:GLN:OE1	1:D:624:GLY:HA3	2.21	0.40
1:C:343:PRO:HG2	1:C:345:PHE:CZ	2.56	0.40
1:A:604:ALA:HA	1:A:638:PHE:CZ	2.56	0.40
1:A:469:GLN:OE1	1:A:624:GLY:HA3	2.21	0.40
1:B:442:LEU:CG	1:B:446:MSE:HE2	2.46	0.40
1:B:220:GLU:OE2	1:B:247:ARG:NH1	2.55	0.40
2:C:901:HOH:O	1:D:441:ARG:CG	2.66	0.40
1:A:560:GLN:NE2	2:A:1170:HOH:O	2.54	0.40
1:B:584:GLN:O	1:B:589:ARG:NH2	2.54	0.40
1:D:506:GLU:N	1:D:506:GLU:CD	2.75	0.40
1:D:144:PRO:C	1:D:146:HIS:H	2.24	0.40
1:D:428:THR:OG1	1:D:429:PHE:N	2.54	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	645/651 (99%)	632 (98%)	13 (2%)	0	100	100
1	B	645/651 (99%)	628 (97%)	17 (3%)	0	100	100
1	C	645/651 (99%)	619 (96%)	25 (4%)	1 (0%)	52	53
1	D	645/651 (99%)	584 (90%)	54 (8%)	7 (1%)	17	11
All	All	2580/2604 (99%)	2463 (96%)	109 (4%)	8 (0%)	46	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	321	PRO
1	D	142	ASN
1	D	31	PRO
1	D	224	ASP
1	D	325	GLN
1	C	31	PRO
1	D	103	GLY
1	D	269	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	517/507 (102%)	503 (97%)	14 (3%)	52	56
1	B	517/507 (102%)	499 (96%)	18 (4%)	43	44
1	C	517/507 (102%)	502 (97%)	15 (3%)	50	53
1	D	517/507 (102%)	497 (96%)	20 (4%)	39	39
All	All	2068/2028 (102%)	2001 (97%)	67 (3%)	46	48

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	46	ARG
1	A	73	MSE
1	A	75	LEU
1	A	86	LEU
1	A	132	LEU
1	A	135	ARG
1	A	239	GLU
1	A	247	ARG
1	A	307	GLU
1	A	475	MSE
1	A	536	LEU
1	A	555	LEU
1	A	608	LEU
1	B	43	LEU
1	B	46	ARG
1	B	54	LEU
1	B	86	LEU
1	B	107	ARG
1	B	132	LEU
1	B	135	ARG
1	B	190	ARG
1	B	228	LEU
1	B	331	LEU
1	B	369	LEU
1	B	482	ASN
1	B	502	LEU
1	B	529	LEU
1	B	536	LEU
1	B	555	LEU
1	B	563	LEU
1	B	636	LEU
1	C	46	ARG
1	C	47	GLU
1	C	75	LEU
1	C	134	GLU
1	C	247	ARG
1	C	290	GLU
1	C	300	GLU
1	C	328	MSE
1	C	349	ILE
1	C	423	ARG
1	C	483	LEU

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Mol	Chain	Res	Type
1	C	502	LEU
1	C	536	LEU
1	C	537	GLU
1	C	564	ARG
1	D	7	LEU
1	D	57	ASP
1	D	63	ARG
1	D	70	HIS
1	D	75	LEU
1	D	99	SER
1	D	107	ARG
1	D	124	ILE
1	D	134	GLU
1	D	215	GLN
1	D	220	GLU
1	D	236	LYS
1	D	277	ARG
1	D	338	LEU
1	D	368	GLU
1	D	394	ASN
1	D	482	ASN
1	D	529	LEU
1	D	569	ARG
1	D	580	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	215	GLN
1	A	380	ASN
1	A	394	ASN
1	A	417	ASN
1	A	554	HIS
1	A	560	GLN
1	B	109	HIS
1	B	122	GLN
1	B	215	GLN
1	B	278	ASN
1	B	324	HIS
1	B	380	ASN
1	B	394	ASN

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Mol	Chain	Res	Type
1	B	417	ASN
1	B	482	ASN
1	B	554	HIS
1	C	122	GLN
1	C	146	HIS
1	C	215	GLN
1	C	394	ASN
1	C	482	ASN
1	C	543	GLN
1	D	122	GLN
1	D	215	GLN
1	D	257	GLN
1	D	295	HIS
1	D	394	ASN
1	D	401	HIS
1	D	482	ASN
1	D	543	GLN
1	D	560	GLN

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 [i](#)

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	632/651 (97%)	-0.11	1 (0%) 95 96	14, 24, 38, 46	0
1	B	632/651 (97%)	-0.15	5 (0%) 87 90	14, 25, 38, 54	0
1	C	632/651 (97%)	0.50	40 (6%) 23 31	27, 39, 52, 59	0
1	D	632/651 (97%)	1.20	163 (25%) 1 1	28, 47, 59, 64	0
All	All	2528/2604 (97%)	0.36	209 (8%) 14 19	14, 34, 55, 64	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	PHE	6.7
1	D	284	PRO	6.1
1	D	315	ALA	5.7
1	D	282	PRO	5.6
1	D	148	VAL	5.2
1	B	651	VAL	5.1
1	D	316	TYR	5.0
1	D	320	TYR	5.0
1	D	269	PRO	4.9
1	C	166	VAL	4.8
1	D	149	VAL	4.7
1	D	42	TYR	4.7
1	D	10	LEU	4.7
1	C	386	GLY	4.5
1	D	45	PHE	4.4
1	D	147	VAL	4.4
1	D	289	PRO	4.2
1	D	237	LEU	4.1
1	D	651	VAL	4.1
1	D	218	ARG	4.1
1	C	120	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	287	VAL	4.0
1	D	288	VAL	4.0
1	D	395	PRO	4.0
1	D	301	LYS	4.0
1	D	309	TRP	3.9
1	D	312	ALA	3.9
1	D	337	PRO	3.9
1	D	6	ASP	3.9
1	D	240	ARG	3.9
1	D	283	TYR	3.9
1	D	185	PHE	3.9
1	D	295	HIS	3.8
1	D	303	ARG	3.8
1	D	291	GLU	3.8
1	D	155	VAL	3.8
1	D	292	VAL	3.8
1	D	17	PHE	3.7
1	D	335	LEU	3.7
1	C	322	ASP	3.6
1	D	260	ALA	3.6
1	D	327	LEU	3.5
1	D	323	LEU	3.5
1	D	7	LEU	3.4
1	C	148	VAL	3.4
1	D	277	ARG	3.4
1	D	397	GLY	3.4
1	C	364	PRO	3.3
1	D	294	ARG	3.3
1	D	144	PRO	3.3
1	D	324	HIS	3.2
1	D	54	LEU	3.2
1	D	162	LEU	3.2
1	C	143	ARG	3.1
1	C	439	ALA	3.1
1	D	250	ILE	3.1
1	D	112	GLY	3.1
1	D	321	PRO	3.1
1	D	562	LEU	3.1
1	C	141	PHE	3.1
1	D	191	ILE	3.1
1	D	329	ARG	3.1
1	D	222	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	522	SER	3.0
1	C	121	GLY	3.0
1	D	12	VAL	3.0
1	D	48	VAL	3.0
1	D	266	PRO	3.0
1	D	568	VAL	2.9
1	D	74	LEU	2.9
1	D	273	GLU	2.9
1	D	186	TRP	2.9
1	C	131	ALA	2.9
1	D	217	LEU	2.8
1	D	228	LEU	2.8
1	D	416	LEU	2.8
1	D	153	THR	2.8
1	C	321	PRO	2.8
1	C	651	VAL	2.8
1	D	152	TYR	2.8
1	D	157	ALA	2.8
1	D	156	LEU	2.8
1	D	13	ASN	2.8
1	D	86	LEU	2.8
1	D	138	ALA	2.7
1	D	65	VAL	2.7
1	D	255	PRO	2.7
1	C	124	ILE	2.7
1	C	404	VAL	2.7
1	D	243	LEU	2.7
1	C	309	TRP	2.7
1	C	304	ALA	2.7
1	D	232	ILE	2.7
1	C	408	ALA	2.7
1	D	154	TYR	2.7
1	C	411	ALA	2.6
1	D	26	ALA	2.6
1	C	119	PRO	2.6
1	D	326	GLU	2.6
1	D	318	ARG	2.6
1	C	428	THR	2.6
1	D	145	GLY	2.6
1	D	432	PHE	2.6
1	D	66	LEU	2.6
1	D	198	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	268	GLY	2.6
1	D	64	PHE	2.6
1	B	596	GLY	2.6
1	D	9	THR	2.6
1	D	121	GLY	2.6
1	D	370	LEU	2.6
1	D	257	GLN	2.5
1	D	16	ARG	2.5
1	D	564	ARG	2.5
1	D	18	LEU	2.5
1	D	190	ARG	2.5
1	D	541	GLU	2.5
1	C	412	ILE	2.5
1	D	565	GLU	2.4
1	C	144	PRO	2.4
1	D	143	ARG	2.4
1	D	274	ALA	2.4
1	D	166	VAL	2.4
1	D	205	VAL	2.4
1	D	431	VAL	2.4
1	D	111	PRO	2.4
1	C	317	ALA	2.4
1	D	281	TRP	2.4
1	D	300	GLU	2.4
1	D	81	LEU	2.4
1	D	275	THR	2.4
1	D	308	ALA	2.3
1	C	165	GLY	2.3
1	D	311	LYS	2.3
1	C	117	THR	2.3
1	B	120	LEU	2.3
1	D	252	PHE	2.3
1	D	364	PRO	2.3
1	D	68	ALA	2.3
1	D	319	ALA	2.3
1	D	307	GLU	2.3
1	D	165	GLY	2.3
1	D	146	HIS	2.3
1	D	278	ASN	2.3
1	D	40	LEU	2.3
1	D	502	LEU	2.3
1	D	542	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	78	VAL	2.3
1	D	5	ARG	2.3
1	D	435	TYR	2.3
1	D	211	ALA	2.3
1	D	521	LEU	2.3
1	D	524	GLU	2.3
1	D	134	GLU	2.3
1	D	230	LYS	2.3
1	D	41	ALA	2.3
1	D	598	PRO	2.2
1	D	305	TRP	2.2
1	C	416	LEU	2.2
1	D	536	LEU	2.2
1	D	184	VAL	2.2
1	D	137	LEU	2.2
1	D	567	GLY	2.2
1	D	201	PHE	2.2
1	C	325	GLN	2.2
1	D	569	ARG	2.2
1	D	183	ILE	2.2
1	D	227	ALA	2.2
1	D	374	ALA	2.2
1	C	541	GLU	2.2
1	D	75	LEU	2.2
1	D	179	LEU	2.2
1	C	596	GLY	2.2
1	D	67	SER	2.2
1	D	304	ALA	2.2
1	D	135	ARG	2.1
1	C	413	LEU	2.1
1	D	650	LEU	2.1
1	D	21	ASP	2.1
1	C	587	ALA	2.1
1	C	146	HIS	2.1
1	C	108	GLY	2.1
1	D	117	THR	2.1
1	C	374	ALA	2.1
1	D	209	TYR	2.1
1	D	384	ALA	2.1
1	B	566	LYS	2.1
1	D	70	HIS	2.1
1	D	187	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	418	LEU	2.1
1	C	177	TRP	2.1
1	B	564	ARG	2.1
1	C	440	ILE	2.1
1	C	214	TRP	2.1
1	D	272	VAL	2.1
1	D	238	ASP	2.1
1	D	563	LEU	2.1
1	D	241	PRO	2.1
1	D	180	SER	2.1
1	D	399	TYR	2.1
1	A	166	VAL	2.1
1	D	270	GLU	2.0
1	D	648	LEU	2.0
1	D	495	PHE	2.0
1	D	392	ARG	2.0
1	D	361	LEU	2.0
1	D	522	SER	2.0
1	C	452	PHE	2.0
1	D	404	VAL	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.