



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:23 am BST

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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

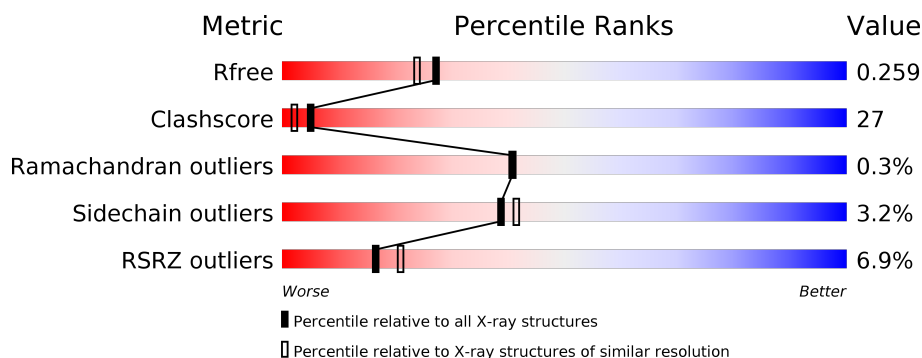
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 respectively. 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>77%</div> <div>21%</div> <div>..</div> </div>
1	B	651	<div> <div>76%</div> <div>22%</div> <div>..</div> </div>
1	C	651	<div> <div>5%</div> <div>58%</div> <div>41%</div> <div>..</div> </div>
1	D	651	<div> <div>22%</div> <div>39%</div> <div>57%</div> <div>..</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			

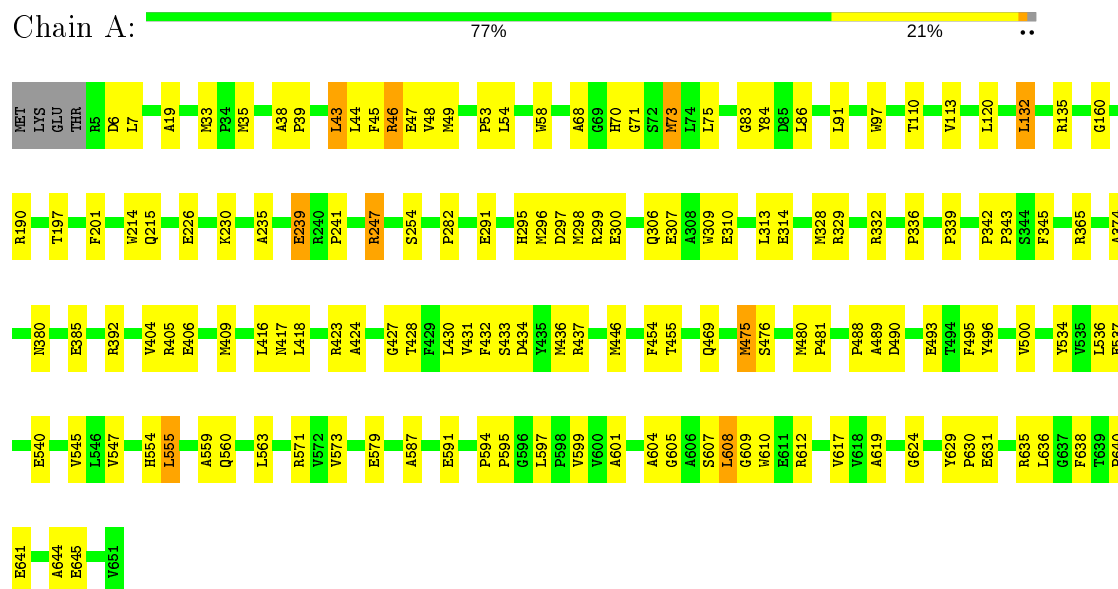
- Molecule 2 is water.

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		

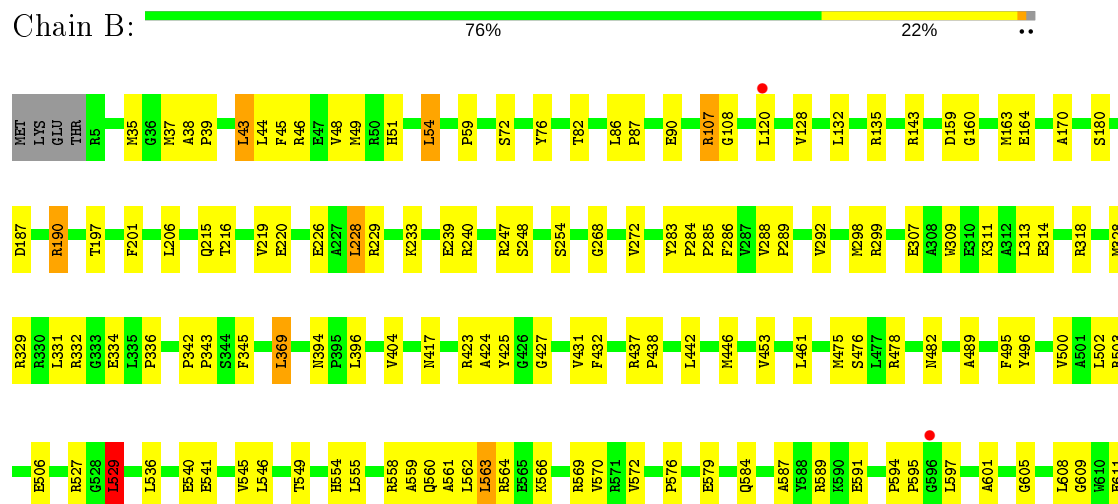
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

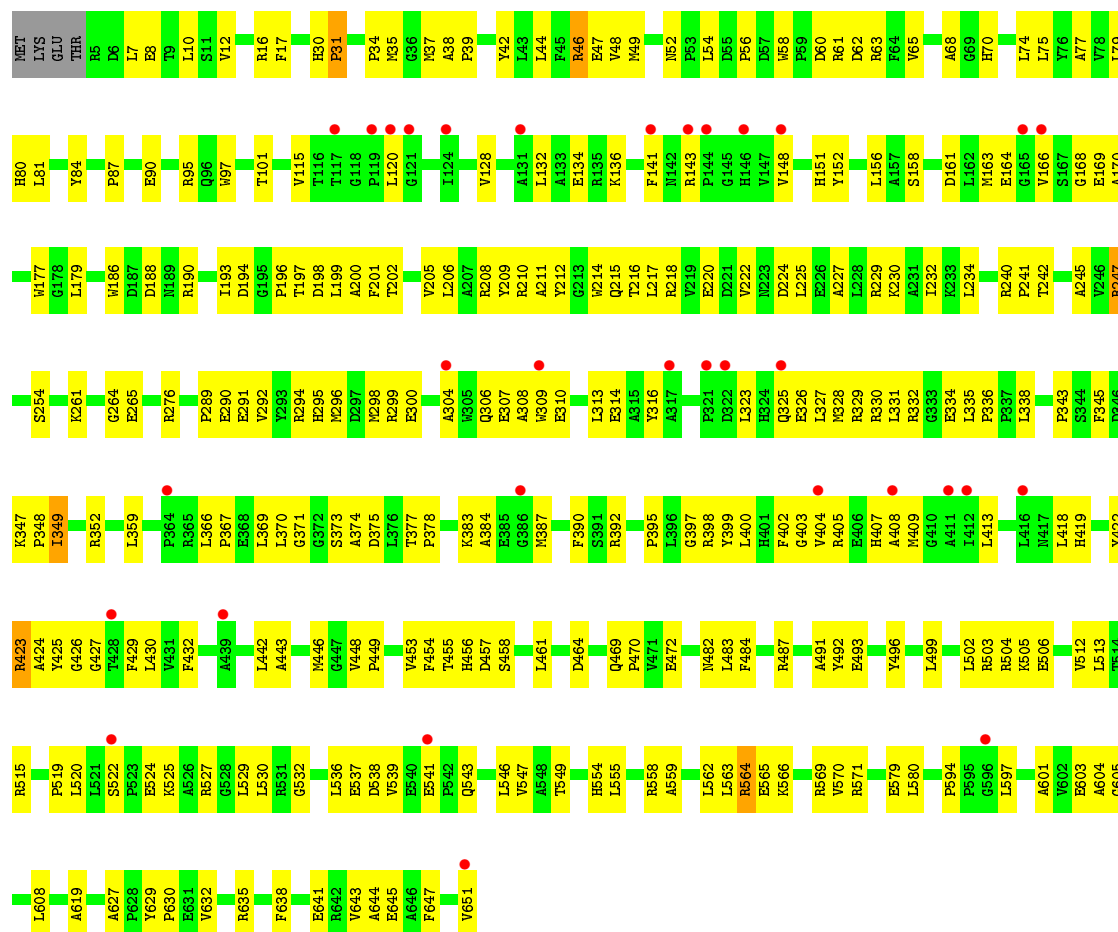


• Molecule 1: Transketolase

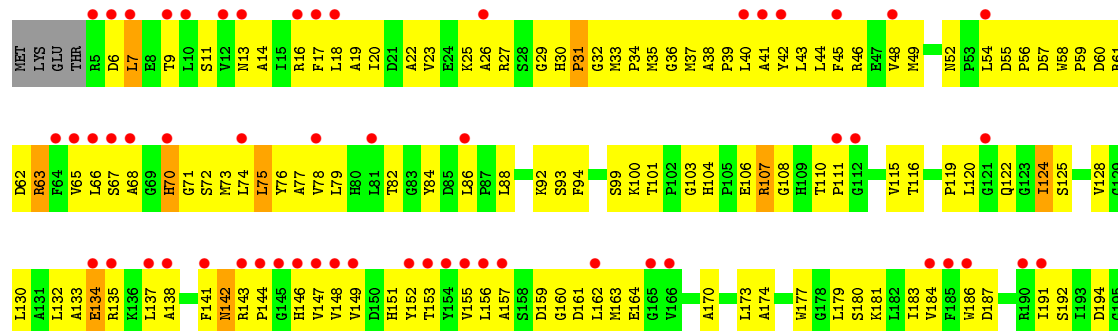


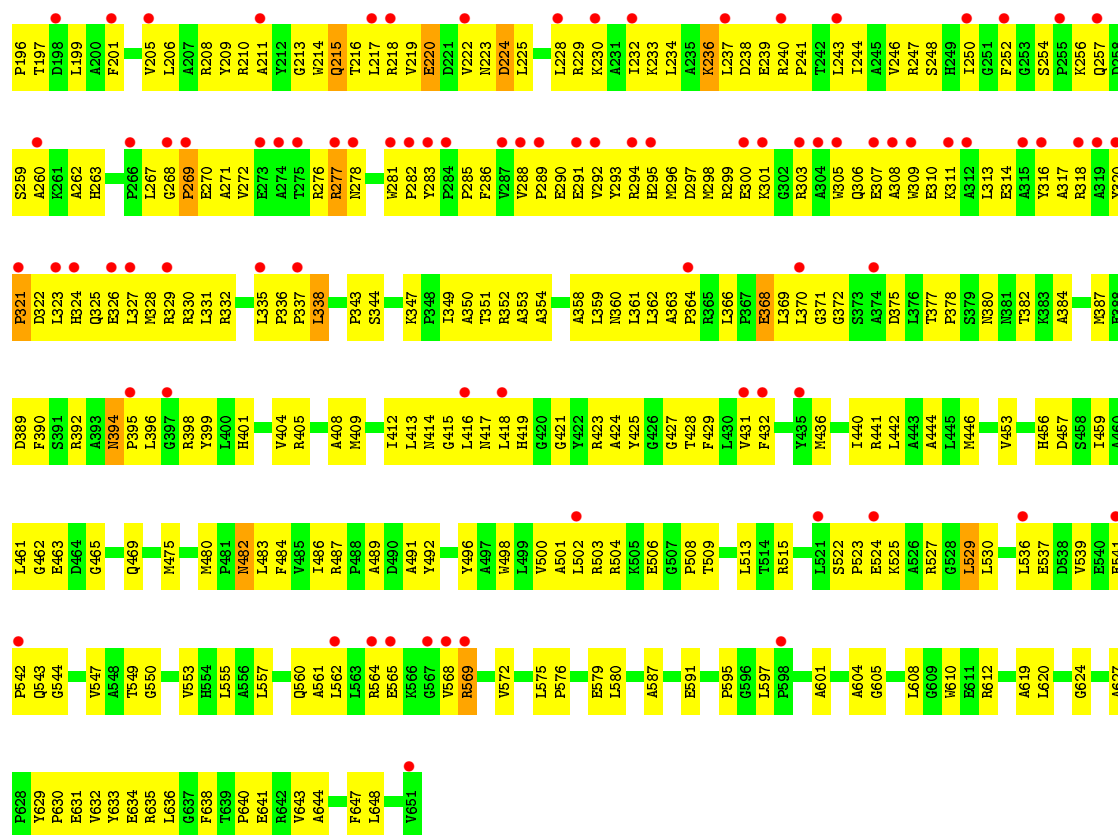


• Molecule 1: Transketolase



• Molecule 1: Transketolase





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) 97.6 (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 (7.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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:C:31:PRO:HD2	2:C:935:HOH:O	1.81	0.81
1:C:387:MSE:HE2	1:C:399:TYR:HB2	1.63	0.81
1:D:73:MSE:HG3	2:D:867: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:244:ILE:HG13	2:D:889:HOH:O	1.83	0.79
1:D:240:ARG:NE	1:D:392:ARG:HH22	1.79	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:C:374:ALA:HA	2:C:928:HOH:O	1.82	0.78
1:D:210:ARG:HD2	2:D:790:HOH:O	1.83	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:B:417:ASN:HD21	1:B:424:ALA:N	1.81	0.77
1:C:543:GLN:NE2	1:C:569:ARG:H	1.82	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:C:594:PRO:HG2	1:C:597:LEU:HD12	1.66	0.76
1:D:134:GLU:HA	2:D:883:HOH:O	1.85	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:115:VAL:HG22	2:D:872:HOH:O	1.86	0.76
1:D:267:LEU:N	2:D:858:HOH:O	2.18	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:C:367:PRO:HG2	2:C:909:HOH:O	1.86	0.75
1:D:191:ILE:HD12	2:D:887:HOH:O	1.87	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: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:44:LEU:HA	1:D:48:VAL:CG1	2.16	0.74
1:A:476:SER:HB2	1:B:476:SER:HB2	1.70	0.74
1:D:192:SER:OG	1:D:197:THR:HG22	1.88	0.74
1:C:409:MSE:O	1:C:413:LEU:HG	1.88	0.74
1:C:569:ARG:NH2	1:C:569:ARG:HB2	2.02	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:C:564:ARG:HH11	1:C:564:ARG:HB2	1.54	0.72
1:D:128:VAL:HG21	1:D:170:ALA:HB1	1.71	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:C:443:ALA:HB1	2:C:940:HOH:O	1.90	0.72
1:D:56:PRO:HD3	2:D:902:HOH:O	1.88	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:C:569:ARG:HH21	1:C:569:ARG:HB2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:LEU:HD23	2:D:888:HOH:O	1.90	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:C:151:HIS:HB3	2:C:924:HOH:O	1.90	0.71
1:D:215:GLN:HG3	2:D:756:HOH:O	1.90	0.71
1:C:152:TYR:HB2	2:C:906:HOH:O	1.89	0.71
1:D:307:GLU:HG3	1:D:308:ALA:N	2.06	0.71
1:D:390:PHE:HE1	1:D:395:PRO:HA	1.56	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:C:513:LEU:HD12	2:C:907:HOH:O	1.91	0.70
1:D:306:GLN:O	1:D:310:GLU:HG2	1.90	0.70
1:D:162:LEU:HG	2:D:878:HOH:O	1.91	0.70
1:D:20:ILE:HD11	1:D:35:MSE:HG2	1.73	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:B:564:ARG:HH22	1:B:569:ARG:HG2	1.58	0.69
1:C:522:SER:OG	1:C:524:GLU:HG2	1.93	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:B:560:GLN:HG2	2:B:1144:HOH:O	1.93	0.68
1:C:194:ASP:OD2	1:D:375:ASP:HA	1.94	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:B:197:THR:HG22	1:B:201:PHE:HB3	1.76	0.67
1:D:23:VAL:HG23	2:D:867:HOH:O	1.94	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:C:383:LYS:HD2	2:C:927:HOH:O	1.94	0.67
1:D:79:LEU:HA	2:D:888:HOH:O	1.93	0.67
1:B:159:ASP:HB2	2:B:1062:HOH:O	1.94	0.67
1:C:215:GLN:HG3	1:C:240:ARG:NH1	2.10	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:C:316:TYR:OH	1:C:323:LEU:HB3	1.94	0.67
1:D:130:LEU:O	1:D:133:ALA:HB3	1.95	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:B:289:PRO:HD3	2:B:1076:HOH:O	1.95	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:A:239:GLU:HG3	2:A:949:HOH:O	1.96	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: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:B:298:MSE:HG3	2:B:1087:HOH:O	1.95	0.66
1:D:587:ALA:O	1:D:591:GLU:HG3	1.96	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:416:LEU:HD22	1:D:416:LEU:H	1.61	0.65
1:D:63:ARG:HH21	1:D:63:ARG:HG3	1.62	0.65
1:A:640:PRO:HA	2:A:1113:HOH:O	1.97	0.65
1:D:543:GLN:HE21	1:D:569:ARG:H	1.44	0.65
1:D:327:LEU:O	1:D:331:LEU:HB2	1.96	0.65
1:A:555:LEU:HD22	2:A:1113:HOH:O	1.95	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:D:18:LEU:HB2	2:D:907:HOH:O	1.96	0.65
1:D:289:PRO:HG2	1:D:292:VAL:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ASN:OD1	1:D:54:LEU:HB3	1.97	0.65
1:D:487:ARG:HG2	1:D:550:GLY:HA3	1.78	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:C:217:LEU:HD11	2:C:916:HOH:O	1.95	0.64
1:D:219:VAL:O	1:D:247:ARG:HG2	1.96	0.64
1:D:94:PHE:HB3	2:D:891:HOH:O	1.97	0.64
1:D:324:HIS:C	1:D:326:GLU:H	2.01	0.64
1:D:405:ARG:HD2	2:D:855:HOH:O	1.96	0.64
1:C:242:THR:HG22	2:C:939:HOH:O	1.97	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:563:LEU:HD11	1:C:644:ALA:HA	1.79	0.64
1:C:423:ARG:HH21	1:C:449:PRO:HB2	1.63	0.64
1:D:289:PRO:HG2	1:D:292:VAL:HG23	1.79	0.64
1:B:288:VAL:HA	2:B:1076:HOH:O	1.97	0.64
1:A:608:LEU:HD12	1:B:475:MSE:HE1	1.78	0.64
1:B:605:GLY:O	1:B:619:ALA:HB1	1.98	0.64
1:D:22:ALA:HA	2:D:926:HOH:O	1.97	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:B:478:ARG:HB3	2:B:1088:HOH:O	1.97	0.64
1:D:384:ALA:HA	2:D:840:HOH:O	1.98	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:A:46:ARG:HE	1:A:295:HIS:CE1	2.17	0.63
1:D:267:LEU:HG	2:D:858:HOH:O	1.97	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:A:19:ALA:HA	1:A:73:MSE:HG3	1.81	0.63
1:B:564:ARG:NH2	1:B:569:ARG:HG2	2.13	0.63
1:C:327:LEU:HB2	2:C:870:HOH:O	1.98	0.63
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:88:LEU:HD11	2:D:905:HOH:O	1.98	0.62
1:D:323:LEU:HB3	2:D:801:HOH:O	1.99	0.62
1:D:371:GLY:C	2:D:861:HOH:O	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LEU:HD11	2:D:892:HOH:O	1.98	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:B:309:TRP:CZ2	1:B:313:LEU:HD11	2.34	0.62
1:B:44:LEU:HB3	1:B:49:MSE:HE2	1.80	0.62
1:D:416:LEU:HA	2:D:849:HOH:O	1.99	0.62
1:D:88:LEU:O	1:D:92:LYS:HG3	2.00	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:327:LEU:HG	1:C:331:LEU:HD22	1.81	0.62
1:D:63:ARG:HE	1:D:151:HIS:CD2	2.17	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: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:384:ALA:O	1:D:387:MSE:HB2	2.00	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:A:197:THR:HG22	1:A:201:PHE:HB3	1.81	0.61
1:D:225:LEU:HB3	1:D:229:ARG:NH1	2.15	0.61
1:D:26:ALA:HB2	2:D:891:HOH:O	2.01	0.61
1:C:163:MSE:HE2	1:D:405:ARG:CZ	2.29	0.61
1:D:45:PHE:CD1	1:D:78:VAL:HG21	2.35	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:C:605:GLY:O	1:C:619:ALA:HB1	2.01	0.61
1:D:394:ASN:HD21	1:D:396:LEU:HB2	1.63	0.61
1:D:483:LEU:HD23	1:D:508:PRO:HG2	1.83	0.61
1:A:297:ASP:O	1:A:298:MSE:HE2	2.00	0.61
1:B:54:LEU:CD1	1:B:299:ARG:HG2	2.31	0.61
1:D:116:THR:N	1:D:446:MSE:HE2	2.14	0.61
1:D:82:THR:HB	2:D:903:HOH:O	2.00	0.61
1:B:190:ARG:HH11	1:B:190:ARG:HG3	1.64	0.61
1:C:449:PRO:HB3	1:C:505:LYS:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ALA:HB1	1:D:419:HIS:CG	2.36	0.60
1:D:149:VAL:HA	2:D:868:HOH:O	2.00	0.60
1:D:636:LEU:HD13	2:D:847:HOH:O	1.99	0.60
1:D:66:LEU:HD21	2:D:892:HOH:O	2.00	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:B:437:ARG:HB3	1:B:438:PRO:HD3	1.83	0.60
1:D:225:LEU:HA	2:D:884:HOH:O	2.01	0.60
1:B:394:ASN:ND2	2:B:1057:HOH:O	2.34	0.60
1:C:487:ARG:HD3	1:C:549:THR:HG23	1.83	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:A:44:LEU:HB3	1:A:49:MSE:HE2	1.84	0.59
1:C:46:ARG:HG3	1:C:296:MSE:HE1	1.84	0.59
1:C:56:PRO:HA	2:C:930:HOH:O	2.02	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: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:B:190:ARG:HD2	1:B:190:ARG:N	2.17	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:D:629:TYR:CD1	1:D:630:PRO:HA	2.37	0.59
1:A:608:LEU:HD22	1:B:612:ARG:NH2	2.18	0.59
1:D:252:PHE:HA	1:D:257:GLN:HE21	1.67	0.59
1:D:67:SER:HB2	2:D:837:HOH:O	2.03	0.59
1:D:7:LEU:CD2	1:D:7:LEU:H	2.15	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:C:289:PRO:HB2	1:C:291:GLU:OE2	2.02	0.59
1:C:349:ILE:N	1:C:349:ILE:HD13	2.16	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:D:368:GLU:CD	1:D:368:GLU:H	2.06	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:B:247:ARG:HG2	2:B:1103:HOH:O	2.02	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:D:76:TYR:HD1	2:D:854:HOH:O	1.85	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:C:136:LYS:HG3	1:C:422:TYR:OH	2.03	0.58
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:348:PRO:HA	1:C:520:LEU:CD2	2.33	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:D:31:PRO:O	1:D:34:PRO:HG2	2.02	0.58
1:C:169:GLU:CB	1:C:405:ARG:HD3	2.33	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:417:ASN:HB2	2:D:808:HOH:O	2.03	0.58
1:D:330:ARG:HB3	1:D:421:GLY:HA2	1.85	0.58
1:D:529:LEU:HG	2:D:933:HOH:O	2.02	0.58
1:D:94:PHE:HE2	2:D:853:HOH:O	1.86	0.58
1:C:193:ILE:HD13	1:D:375:ASP:OD2	2.03	0.58
1:A:579:GLU:CD	1:A:579:GLU:H	2.06	0.58
1:B:43:LEU:HD13	1:B:48:VAL:HG23	1.85	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:B:594:PRO:HG2	1:B:597:LEU:HD11	1.86	0.58
1:C:562:LEU:O	1:C:565:GLU:HB3	2.03	0.58
1:D:180:SER:HB3	1:D:239:GLU:C	2.24	0.58
1:A:7:LEU:HD11	1:A:291:GLU:HG2	1.84	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: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
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:135:ARG:NH2	1:D:181:LYS:HG3	2.19	0.57
2:C:901:HOH:O	1:D:480:MSE:HG3	2.03	0.57
1:B:627:ALA:HB3	1:B:632:VAL:HB	1.87	0.57
1:D:119:PRO:HB2	1:D:122:GLN:CG	2.34	0.57
1:A:631:GLU:O	1:A:635:ARG:HG3	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:GLU:O	1:D:294:ARG:HG3	2.05	0.57
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:A:537:GLU:HB3	2:A:1170:HOH:O	2.05	0.57
1:C:559:ALA:O	1:C:563:LEU:HD13	2.04	0.57
1:D:130:LEU:HD12	2:D:856:HOH:O	2.04	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:A:343:PRO:HG2	1:A:345:PHE:CE2	2.39	0.57
1:C:461:LEU:CD1	1:C:464:ASP:HB2	2.35	0.57
1:D:179:LEU:N	1:D:179:LEU:HD22	2.20	0.57
1:A:300:GLU:HG3	2:A:1128:HOH:O	2.03	0.57
1:D:292:VAL:HG21	2:D:871:HOH:O	2.04	0.57
1:C:484:PHE:HA	1:C:579:GLU:HG3	1.86	0.56
1:D:522:SER:HB2	1:D:525:LYS:CG	2.35	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:D:522:SER:HB3	2:D:890:HOH:O	2.05	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:B:219:VAL:HG11	1:B:228:LEU:HD13	1.86	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: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:132:LEU:CD2	1:C:136:LYS:HD2	2.35	0.56
1:C:349:ILE:HD11	1:C:520:LEU:HD11	1.86	0.56
1:C:37:MSE:HE2	1:C:156:LEU:HD11	1.88	0.56
1:C:7:LEU:HG	1:C:295:HIS:CD2	2.40	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:343:PRO:HD3	2:D:870:HOH:O	2.06	0.55
1:D:116:THR:HB	1:D:446:MSE:HE2	1.87	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:B:307:GLU:HB2	2:B:1039:HOH:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:GLU:N	1:C:506:GLU:OE1	2.39	0.55
1:D:124:ILE:HD13	1:D:124:ILE:O	2.06	0.55
1:D:141:PHE:HE1	2:D:805:HOH:O	1.90	0.55
1:D:155:VAL:HG12	2:D:824:HOH:O	2.06	0.55
1:D:557:LEU:O	1:D:560:GLN:HG2	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:A:215:GLN:HE22	1:A:235:ALA:HA	1.71	0.55
1:C:304:ALA:HA	1:C:307:GLU:HG2	1.88	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: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: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:D:215:GLN:HE22	1:D:240:ARG:CB	2.20	0.55
1:A:197:THR:CG2	1:A:201:PHE:HB3	2.37	0.55
1:C:408:ALA:N	2:C:904:HOH:O	2.40	0.55
1:C:65:VAL:HG13	1:C:115:VAL:CG1	2.36	0.55
1:B:82:THR:HG21	2:B:1087:HOH:O	2.06	0.55
1:C:404:VAL:H	1:D:163:MSE:SE	2.40	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: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:D:75:LEU:HD22	1:D:75:LEU:O	2.07	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:B:506:GLU:CD	1:B:506:GLU:H	2.10	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:601:ALA:HB3	1:B:617:VAL:HG13	1.90	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:A:641:GLU:O	1:A:645:GLU:HG3	2.08	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:C:63:ARG:NH1	1:C:419:HIS:HA	2.22	0.54
1:A:247:ARG:NE	2:A:759:HOH:O	2.40	0.54
1:D:338:LEU:CD2	1:D:338:LEU:H	2.21	0.54
1:D:7:LEU:HD23	1:D:7:LEU:H	1.71	0.54
1:A:431:VAL:HG13	1:A:432:PHE:CD1	2.43	0.54
1:D:142:ASN:ND2	1:D:147:VAL:HG13	2.22	0.54
1:C:349:ILE:H	1:C:349:ILE:HD13	1.73	0.54
1:C:493:GLU:HG2	1:C:529:LEU:HB2	1.90	0.54
1:D:119:PRO:HB2	1:D:122:GLN:HG2	1.89	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: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:C:461:LEU:HD13	1:C:464:ASP:HB2	1.90	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:45:PHE:HA	1:D:49:MSE:HE3	1.89	0.53
1:D:52:ASN:C	1:D:54:LEU:H	2.12	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: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:D:138:ALA:HA	1:D:149:VAL:HB	1.91	0.53
1:C:566:LYS:NZ	2:C:695:HOH:O	2.42	0.53
1:C:594:PRO:CG	1:C:597:LEU:HD12	2.36	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:C:398:ARG:HB3	2:C:917:HOH:O	2.09	0.53
1:D:20:ILE:HD12	1:D:267:LEU:CD1	2.39	0.53
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: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:132:LEU:HD13	1:A:416:LEU:HD21	1.91	0.52
1:B:332:ARG:NH2	1:B:334:GLU:OE1	2.42	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: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:B:328:MSE:HB3	1:B:332:ARG:NH1	2.25	0.52
1:D:338:LEU:H	1:D:338:LEU:HD23	1.73	0.52
1:D:529:LEU:HD23	1:D:576:PRO:HB2	1.92	0.52
1:D:635:ARG:HD2	2:D:831:HOH:O	2.09	0.52
1:B:43:LEU:HD13	1:B:48:VAL:CG2	2.39	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:D:562:LEU:O	1:D:565:GLU:HG2	2.09	0.52
1:D:74:LEU:O	1:D:78:VAL:HG12	2.09	0.52
1:A:35:MSE:HE1	1:A:254:SER:HB3	1.90	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: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:179:LEU:N	2:D:846:HOH:O	2.43	0.52
1:D:19:ALA:HB2	2:D:932:HOH:O	2.10	0.52
1:D:252:PHE:HB2	2:D:848:HOH:O	2.10	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:B:431:VAL:HG13	1:B:432:PHE:CD1	2.45	0.52
1:B:529:LEU:HD22	1:B:576:PRO:CG	2.40	0.52
1:D:173:LEU:HD13	1:D:177:TRP:CH2	2.45	0.52
1:D:414:ASN:C	2:D:808:HOH:O	2.49	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:C:115:VAL:HG23	1:C:446:MSE:SE	2.61	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:151:HIS:NE2	1:C:419:HIS:NE2	2.57	0.51
1:D:579:GLU:H	1:D:579:GLU:CD	2.12	0.51
1:D:41:ALA:CB	1:D:74:LEU:HD11	2.35	0.51
1:C:387:MSE:HE3	2:C:917:HOH:O	2.10	0.51
1:C:442:LEU:HG	1:C:446:MSE:HE2	1.91	0.51
1:C:492:TYR:HB2	2:C:925:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:ALA:HA	1:C:638:PHE:CZ	2.46	0.51
1:D:323:LEU:H	1:D:323:LEU:HD12	1.76	0.51
1:A:405:ARG:HH22	1:B:163:MSE:CE	2.21	0.51
1:B:215:GLN:CB	2:B:1134:HOH:O	2.57	0.51
1:C:48:VAL:HG21	1:C:232:ILE:HD13	1.92	0.51
1:D:354:ALA:HB1	1:D:491:ALA:HA	1.93	0.51
1:D:31:PRO:O	1:D:35:MSE:HG3	2.11	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:C:63:ARG:HG2	2:C:941:HOH:O	2.11	0.51
1:D:157:ALA:N	2:D:824:HOH:O	2.44	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:C:35:MSE:HE1	1:C:254:SER:HB3	1.93	0.50
1:D:215:GLN:CD	1:D:240:ARG:HB2	2.30	0.50
1:D:536:LEU:HD23	1:D:536:LEU:C	2.30	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:D:107:ARG:HD3	1:D:108:GLY:N	2.25	0.50
1:D:636:LEU:HB2	2:D:847:HOH:O	2.10	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:220:GLU:CD	1:B:247:ARG:HH11	2.14	0.50
1:B:313:LEU:HB3	2:B:1132:HOH:O	2.12	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:C:60:ASP:CG	2:C:924:HOH:O	2.49	0.50
1:D:246:VAL:HG13	2:D:898:HOH:O	2.10	0.50
1:B:190:ARG:NH1	1:B:190:ARG:HG3	2.27	0.50
1:C:332:ARG:HD2	1:C:334:GLU:OE2	2.12	0.50
1:C:61:ARG:NE	2:C:941:HOH:O	2.43	0.50
1:D:267:LEU:HD13	2:D:789:HOH:O	2.11	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:D:456:HIS:CD2	1:D:515:ARG:HD2	2.47	0.50
1:B:143:ARG:NH2	2:B:1129:HOH:O	2.45	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:D:484:PHE:CD2	1:D:579:GLU:HG3	2.46	0.50
1:C:522:SER:HB3	1:C:525:LYS:HG2	1.92	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:C:265:GLU:N	2:C:935:HOH:O	2.44	0.50
1:B:284:PRO:HG3	2:B:1145:HOH:O	2.10	0.50
1:C:218:ARG:HH11	1:C:245:ALA:C	2.14	0.50
1:C:413:LEU:CD2	2:C:894:HOH:O	2.59	0.50
1:D:163:MSE:HE3	1:D:201:PHE:CD1	2.46	0.50
1:D:46:ARG:HG3	1:D:298:MSE:CE	2.41	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:120:LEU:HD13	1:A:160:GLY:HA3	1.93	0.49
1:A:554:HIS:HD2	2:A:945:HOH:O	1.94	0.49
1:C:496:TYR:CZ	1:C:527:ARG:HG2	2.48	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:D:208:ARG:O	1:D:211:ALA:HB3	2.12	0.49
1:D:311:LYS:CA	1:D:314:GLU:HG2	2.43	0.49
1:D:543:GLN:NE2	1:D:568:VAL:HA	2.26	0.49
1:D:631:GLU:HG3	1:D:635:ARG:HD2	1.94	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:D:36:GLY:HA2	2:D:848:HOH:O	2.10	0.49
1:A:601:ALA:HB3	1:A:617:VAL:HG12	1.94	0.49
1:C:166:VAL:HA	2:C:904:HOH:O	2.12	0.49
1:C:205:VAL:HG23	1:C:206:LEU:H	1.78	0.49
1:D:119:PRO:O	1:D:122:GLN:HG2	2.13	0.49
1:D:163:MSE:CE	1:D:201:PHE:HB2	2.42	0.49
1:D:318:ARG:HH21	1:D:318:ARG:HG2	1.78	0.49
1:D:496:TYR:HB3	1:D:529:LEU:HD12	1.94	0.49
1:B:128:VAL:HG21	1:B:170:ALA:HB1	1.95	0.49
1:D:214:TRP:C	1:D:215:GLN:NE2	2.65	0.49
1:D:23:VAL:N	2:D:867:HOH:O	2.45	0.49
1:C:455:THR:HB	2:C:907:HOH:O	2.13	0.49
1:D:219:VAL:HG11	1:D:228:LEU:HD12	1.93	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:C:327:LEU:CD1	1:C:331:LEU:HD13	2.43	0.49
1:C:499:LEU:HB3	1:C:503:ARG:HH21	1.77	0.49
1:C:541:GLU:O	1:C:569:ARG:NH2	2.45	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:D:285:PRO:O	1:D:286:PHE:HB2	2.12	0.49
1:B:554:HIS:HD2	2:B:1072:HOH:O	1.95	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:C:456:HIS:CE1	1:C:515:ARG:HG3	2.48	0.49
1:D:267:LEU:O	1:D:271:ALA:HB3	2.12	0.49
1:D:364:PRO:CD	2:D:886:HOH:O	2.60	0.49
1:C:186:TRP:CZ3	1:C:205:VAL:HG21	2.48	0.48
1:D:39:PRO:O	1:D:43:LEU:HB2	2.13	0.48
1:A:97:TRP:HH2	1:B:636:LEU:HD13	1.78	0.48
1:B:644:ALA:HA	2:B:1146:HOH:O	2.12	0.48
1:D:107:ARG:CD	1:D:108:GLY:N	2.75	0.48
1:D:394:ASN:ND2	1:D:396:LEU:H	2.10	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: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: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:D:37:MSE:HE2	1:D:156:LEU:CD1	2.43	0.48
1:C:169:GLU:HB3	1:C:408:ALA:HB2	1.96	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: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:B:120:LEU:HD13	1:B:160:GLY:HA3	1.94	0.48
1:B:496:TYR:O	1:B:500:VAL:HG23	2.14	0.48
1:B:87:PRO:HG2	1:B:90:GLU:HG2	1.96	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:D:135:ARG:NH2	1:D:181:LYS:HE3	2.28	0.48
1:D:363:ALA:N	2:D:886:HOH:O	2.46	0.48
1:B:579:GLU:CD	1:B:579:GLU:H	2.17	0.48
1:B:545:VAL:HG23	1:B:597:LEU:HD13	1.96	0.48
1:A:33:MSE:HE2	2:A:1173:HOH:O	2.12	0.48
1:B:332:ARG:NH1	2:B:860:HOH:O	2.45	0.48
1:C:218:ARG:HD2	1:C:245:ALA:O	2.13	0.48
1:D:186:TRP:CZ3	1:D:205:VAL:HG21	2.48	0.48
1:A:310:GLU:O	1:A:314:GLU:HG2	2.14	0.48
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:VAL:HA	2:B:1138:HOH:O	2.13	0.48
1:C:31:PRO:CD	2:C:935:HOH:O	2.49	0.48
1:D:173:LEU:HD11	2:D:855:HOH:O	2.14	0.48
1:B:369:LEU:HD11	1:B:425:TYR:HE2	1.78	0.48
1:B:635:ARG:HD3	2:B:1116:HOH:O	2.14	0.48
1:C:8:GLU:O	1:C:12:VAL:HG23	2.14	0.48
1:C:37:MSE:HE2	1:C:156:LEU:CD1	2.44	0.48
1:C:309:TRP:O	1:C:313:LEU:HD23	2.14	0.48
1:C:461:LEU:C	1:C:461:LEU:HD12	2.33	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: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: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:C:196:PRO:O	1:C:199:LEU:HD13	2.13	0.47
1:C:209:TYR:HA	1:C:212:TYR:CD2	2.47	0.47
1:C:327:LEU:HD12	1:C:331:LEU:HD13	1.96	0.47
1:D:252:PHE:HD2	1:D:257:GLN:HE22	1.62	0.47
1:D:459:ILE:HD13	1:D:620:LEU:HD22	1.96	0.47
1:D:79:LEU:O	1:D:84:TYR:HB2	2.14	0.47
1:C:310:GLU:HG2	2:C:723:HOH:O	2.13	0.47
1:D:404:VAL:HG12	1:D:404:VAL:O	2.15	0.47
1:D:370:LEU:O	1:D:424:ALA:HA	2.14	0.47
1:D:427:GLY:HA2	1:D:453:VAL:O	2.14	0.47
1:D:536:LEU:O	1:D:536:LEU:HD23	2.15	0.47
1:B:328:MSE:O	1:B:332:ARG:HG3	2.14	0.47
1:B:417:ASN:ND2	1:B:423:ARG:HA	2.29	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:A:545:VAL:HG22	1:A:571:ARG:CG	2.43	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: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:C:519:PRO:HB2	1:C:554:HIS:CD2	2.49	0.47
1:D:44:LEU:HD23	1:D:48:VAL:HG11	1.97	0.47
1:A:475:MSE:HE3	1:A:608:LEU:O	2.14	0.47
1:C:555:LEU:O	1:C:555:LEU:HD23	2.15	0.47
1:D:329:ARG:NH1	2:D:916:HOH:O	2.47	0.47
1:C:210:ARG:HA	2:C:902:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:CG	1:C:296:MSE:HE1	2.45	0.47
1:D:223:ASN:O	1:D:225:LEU:HD12	2.15	0.47
1:D:311:LYS:HA	1:D:314:GLU:CG	2.44	0.47
1:D:44:LEU:HA	1:D:48:VAL:HG12	1.95	0.47
1:A:547:VAL:O	1:A:601:ALA:HA	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:B:328:MSE:HB3	1:B:332:ARG:HH12	1.79	0.47
1:B:396:LEU:HD23	2:B:1057:HOH:O	2.14	0.47
1:B:475:MSE:HE2	1:B:608:LEU:O	2.15	0.47
1:C:352:ARG:NH2	1:C:456:HIS:HE1	2.12	0.47
1:D:418:LEU:HD13	2:D:872:HOH:O	2.14	0.47
1:C:136:LYS:HB2	2:C:729:HOH:O	2.14	0.47
1:C:375:ASP:OD1	1:D:192:SER:HB3	2.15	0.47
1:C:390:PHE:HA	1:C:397:GLY:HA3	1.97	0.47
1:D:119:PRO:HB2	1:D:122:GLN:HG3	1.96	0.47
1:D:230:LYS:HB3	1:D:230:LYS:NZ	2.30	0.47
1:D:46:ARG:NH2	1:D:295:HIS:CD2	2.83	0.47
1:D:414:ASN:O	1:D:418:LEU:HB2	2.14	0.47
1:A:45:PHE:CE1	1:A:49:MSE:HE1	2.50	0.47
1:A:607:SER:HB2	1:A:617:VAL:HG21	1.96	0.47
1:C:427:GLY:HA2	1:C:453:VAL:O	2.15	0.47
1:D:230:LYS:O	1:D:234:LEU:HG	2.15	0.47
1:D:336:PRO:HD3	2:D:766:HOH:O	2.14	0.47
1:A:314:GLU:HB2	2:A:1120:HOH:O	2.15	0.46
1:D:217:LEU:HB2	1:D:244:ILE:HG12	1.98	0.46
1:C:46:ARG:HD3	1:C:298:MSE:CE	2.44	0.46
1:D:120:LEU:O	1:D:164:GLU:HG3	2.14	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:C:564:ARG:NH1	1:C:564:ARG:HB2	2.27	0.46
1:D:159:ASP:OD2	1:D:197:THR:HG21	2.15	0.46
1:D:289:PRO:HG2	1:D:292:VAL:HG21	1.97	0.46
1:D:37:MSE:HE3	1:D:40:LEU:HD23	1.97	0.46
1:B:215:GLN:HB3	2:B:1134:HOH:O	2.14	0.46
1:D:149:VAL:HG11	2:D:883:HOH:O	2.15	0.46
1:B:299:ARG:NH2	2:B:731:HOH:O	2.49	0.46
1:D:240:ARG:NH2	1:D:392:ARG:HH12	2.13	0.46
1:D:295:HIS:HE1	2:D:879:HOH:O	1.98	0.46
1:D:372:GLY:C	2:D:809:HOH:O	2.53	0.46
1:D:389:ASP:OD1	1:D:401:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:HIS:ND1	2:D:866:HOH:O	2.36	0.46
1:D:560:GLN:HG3	1:D:561:ALA:N	2.30	0.46
1:D:627:ALA:HB3	1:D:632:VAL:HB	1.96	0.46
1:C:193:ILE:N	1:C:193:ILE:HD12	2.31	0.46
1:C:387:MSE:HE3	1:C:398:ARG:O	2.16	0.46
1:C:580:LEU:O	1:C:580:LEU:HD23	2.16	0.46
1:D:527:ARG:HE	1:D:530:LEU:HD12	1.80	0.46
1:C:234:LEU:HB3	2:C:916:HOH:O	2.15	0.46
1:D:541:GLU:HB2	2:D:724:HOH:O	2.14	0.46
1:D:30:HIS:CD2	1:D:70:HIS:HB2	2.51	0.46
1:D:76:TYR:HE2	1:D:94:PHE:HE1	1.64	0.46
1:B:107:ARG:HD2	1:B:107:ARG:C	2.36	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:C:31:PRO:C	1:C:34:PRO:HD2	2.36	0.46
1:C:487:ARG:HG3	1:C:512:VAL:HB	1.97	0.46
1:D:134:GLU:HB2	1:D:151:HIS:CE1	2.51	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:106:GLU:HA	1:D:116:THR:HG23	1.97	0.46
1:A:612:ARG:HA	1:B:611:GLU:HG2	1.97	0.45
1:D:297:ASP:OD1	1:D:299:ARG:HB2	2.16	0.45
1:D:364:PRO:HD3	2:D:886:HOH:O	2.16	0.45
1:D:557:LEU:HD23	1:D:572:VAL:HG11	1.99	0.45
1:D:7:LEU:HD23	1:D:7:LEU:N	2.31	0.45
1:B:369:LEU:CD1	1:B:425:TYR:HE2	2.30	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:C:158:SER:HB2	2:C:912:HOH:O	2.16	0.45
1:D:362:LEU:O	1:D:366:LEU:HG	2.16	0.45
1:B:215:GLN:HB2	2:B:1134:HOH:O	2.17	0.45
1:D:209:TYR:O	1:D:214:TRP:HB2	2.16	0.45
1:D:431:VAL:HG13	1:D:432:PHE:CD1	2.52	0.45
1:D:496:TYR:O	1:D:500:VAL:HG12	2.16	0.45
1:D:496:TYR:CB	1:D:529:LEU:HD12	2.47	0.45
1:D:539:VAL:O	1:D:542:PRO:HD3	2.16	0.45
1:D:76:TYR:CE2	1:D:94:PHE:HE1	2.34	0.45
1:A:214:TRP:CG	1:A:241:PRO:HG2	2.51	0.45
1:B:541:GLU:HB2	1:B:569:ARG:NH2	2.32	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

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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:C:430:LEU:HA	1:C:454:PHE:HB3	1.99	0.45
1:D:132:LEU:HD22	1:D:416:LEU:HD11	1.98	0.45
1:D:281:TRP:NE1	1:D:283:TYR:HB2	2.32	0.45
1:D:46:ARG:HH21	1:D:295:HIS:CD2	2.34	0.45
1:A:594:PRO:HG2	1:A:597:LEU:HD22	1.98	0.45
1:B:503:ARG:HD2	2:B:1095:HOH:O	2.16	0.45
1:B:566:LYS:HB3	1:B:566:LYS:NZ	2.31	0.45
1:C:390:PHE:HB2	1:C:397:GLY:O	2.17	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: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:C:292:VAL:N	2:C:895:HOH:O	2.50	0.45
1:C:457:ASP:CB	1:C:512:VAL:HG12	2.47	0.45
1:A:418:LEU:HD11	1:A:446:MSE:SE	2.67	0.45
1:B:107:ARG:HD3	2:B:1069:HOH:O	2.17	0.45
1:D:191:ILE:HG23	2:D:887:HOH:O	2.16	0.45
1:D:241:PRO:HD3	2:D:846:HOH:O	2.16	0.45
1:D:252:PHE:CD2	1:D:257:GLN:NE2	2.85	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:B:595:PRO:HG2	2:B:1040:HOH:O	2.15	0.45
1:C:141:PHE:HB3	2:C:914:HOH:O	2.16	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:C:79:LEU:O	1:C:84:TYR:HB2	2.16	0.45
1:D:18:LEU:CD1	1:D:77:ALA:HB1	2.47	0.45
1:D:228:LEU:HD21	2:D:894:HOH:O	2.15	0.45
1:D:398:ARG:HH11	1:D:398:ARG:HG3	1.82	0.45
1:D:489:ALA:HB2	1:D:553:VAL:HG21	1.98	0.45
1:A:594:PRO:HA	1:A:595:PRO:HD2	1.88	0.44
1:A:609:GLY:HA2	1:B:609:GLY:HA2	1.99	0.44
1:B:45:PHE:CE1	1:B:49:MSE:HE1	2.53	0.44
1:C:375:ASP:HA	1:D:194:ASP:OD1	2.17	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:D:250:ILE:O	1:D:257:GLN:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:HH11	1:D:463:GLU:HB3	1.81	0.44
1:D:524:GLU:HB3	2:D:890:HOH:O	2.16	0.44
1:D:88:LEU:HD11	1:D:286:PHE:HD1	1.82	0.44
1:B:584:GLN:HA	2:B:1120:HOH:O	2.17	0.44
1:C:571:ARG:NE	2:C:853:HOH:O	2.41	0.44
1:D:39:PRO:CG	1:D:222:VAL:HG22	2.45	0.44
1:D:22:ALA:HB3	1:D:73:MSE:HE2	1.99	0.44
1:D:259:SER:C	2:D:937:HOH:O	2.55	0.44
1:D:65:VAL:HG12	2:D:837:HOH:O	2.17	0.44
1:D:77:ALA:HB2	2:D:907:HOH:O	2.17	0.44
1:A:68:ALA:HB1	1:A:70:HIS:CE1	2.53	0.44
1:C:42:TYR:O	1:C:46:ARG:HB2	2.18	0.44
1:D:205:VAL:CG2	1:D:206:LEU:N	2.80	0.44
1:D:282:PRO:HG2	2:D:880:HOH:O	2.17	0.44
1:D:61:ARG:CZ	1:D:63:ARG:NH2	2.80	0.44
1:D:644:ALA:O	1:D:648:LEU:HG	2.18	0.44
1:A:58:TRP:CD1	1:A:306:GLN:HG3	2.52	0.44
1:A:374:ALA:HB3	1:A:428:THR:CG2	2.43	0.44
1:B:527:ARG:HB2	1:B:527:ARG:NH1	2.33	0.44
1:B:594:PRO:CG	1:B:597:LEU:HD21	2.46	0.44
1:C:39:PRO:O	1:C:42:TYR:HB3	2.18	0.44
1:C:404:VAL:HG12	1:D:164:GLU:OE2	2.17	0.44
1:C:423:ARG:NH2	2:C:850:HOH:O	2.50	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:D:229:ARG:O	1:D:233:LYS:HG2	2.17	0.44
1:D:36:GLY:CA	2:D:848:HOH:O	2.65	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:A:496:TYR:O	1:A:500:VAL:HG23	2.18	0.44
1:C:405:ARG:HH12	1:D:163:MSE:CE	2.13	0.44
1:D:269:PRO:HG2	1:D:270:GLU:H	1.81	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: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
1:C:80:HIS:CD2	2:C:932:HOH:O	2.71	0.44
1:D:148:VAL:HG12	2:D:899:HOH:O	2.17	0.44
1:D:52:ASN:C	1:D:54:LEU:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:610:TRP:C	1:D:612:ARG:H	2.20	0.44
1:B:289:PRO:HG2	1:B:292:VAL:HG23	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:19:ALA:HA	1:D:73:MSE:HE2	2.00	0.43
1:D:295:HIS:CE1	2:D:879:HOH:O	2.71	0.43
1:D:352:ARG:HA	1:D:513:LEU:HD13	1.99	0.43
1:C:608:LEU:HD13	1:D:612:ARG:HH11	1.83	0.43
1:A:6:ASP:OD1	1:A:7:LEU:HD22	2.18	0.43
1:B:220:GLU:OE1	1:B:247:ARG:NH1	2.51	0.43
1:D:133:ALA:HB2	2:D:849:HOH:O	2.17	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:C:188:ASP:OD1	1:C:190:ARG:CZ	2.67	0.43
1:D:416:LEU:HB2	1:D:424:ALA:HB3	2.00	0.43
1:D:93:SER:HA	2:D:906:HOH:O	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: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:44:LEU:HA	1:D:48:VAL:HG13	1.96	0.43
2:C:901:HOH:O	1:D:480:MSE:HE2	2.17	0.43
1:D:630:PRO:O	1:D:634:GLU:HG3	2.18	0.43
1:B:506:GLU:N	1:B:506:GLU:CD	2.72	0.43
1:C:335:LEU:HD12	1:C:336:PRO:HD2	2.00	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:D:62:ASP:HA	2:D:852:HOH:O	2.18	0.43
1:C:230:LYS:HB3	1:C:230:LYS:HE2	1.89	0.43
1:C:407:HIS:HB3	2:C:904:HOH:O	2.18	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: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: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:A:282:PRO:HA	2:A:990:HOH:O	2.19	0.43
1:A:404:VAL:HG12	1:B:164:GLU:OE2	2.19	0.43
1:A:405:ARG:HH12	1:B:163:MSE:HE2	1.82	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: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:260:ALA:N	2:D:887:HOH:O	2.52	0.43
1:D:277:ARG:HD3	1:D:277:ARG:C	2.39	0.43
1:C:349:ILE:HD11	1:C:491:ALA:HB2	2.01	0.43
1:D:141:PHE:HA	2:D:908:HOH:O	2.19	0.43
1:D:252:PHE:CB	2:D:848:HOH:O	2.67	0.43
1:D:364:PRO:HD2	2:D:886:HOH:O	2.18	0.43
1:A:46:ARG:NH2	1:A:298:MSE:HE1	2.34	0.43
1:C:224:ASP:OD2	1:C:227:ALA:HB2	2.19	0.43
1:C:247:ARG:HG2	1:C:247:ARG:HH11	1.82	0.43
1:D:191:ILE:N	1:D:197:THR:HG23	2.33	0.43
1:D:380:ASN:HB3	1:D:382:THR:HG23	2.01	0.43
1:D:461:LEU:HD12	1:D:462:GLY:N	2.33	0.43
1:A:540:GLU:HA	1:A:540:GLU:OE1	2.19	0.42
1:A:33:MSE:CE	1:A:71:GLY:HA3	2.49	0.42
1:B:311:LYS:HD2	2:B:885:HOH:O	2.19	0.42
1:C:242:THR:CG2	2:C:939:HOH:O	2.64	0.42
1:C:400:LEU:HD12	1:C:400:LEU:N	2.34	0.42
1:C:629:TYR:CD1	1:C:630:PRO:HA	2.55	0.42
1:C:87:PRO:HG2	1:C:90:GLU:HG2	2.02	0.42
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: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:D:120:LEU:H	1:D:120:LEU:CD2	2.32	0.42
1:D:148:VAL:HG23	1:D:313:LEU:HD22	2.01	0.42
1:D:240:ARG:HB3	1:D:241:PRO:HD2	2.00	0.42
1:A:296:MSE:O	1:A:298:MSE:HG2	2.18	0.42
1:A:437:ARG:HG2	2:A:1162:HOH: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:C:404:VAL:HG21	1:D:160:GLY:CA	2.50	0.42
1:D:508:PRO:HD2	2:D:874:HOH:O	2.18	0.42
1:D:557:LEU:CD2	1:D:572:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:LEU:HD13	1:D:111:PRO:O	2.19	0.42
1:A:534:TYR:O	1:A:573:VAL:HG13	2.20	0.42
1:D:107:ARG:HD3	1:D:108:GLY:H	1.85	0.42
1:D:186:TRP:N	2:D:834:HOH:O	2.52	0.42
1:D:58:TRP:CH2	1:D:305:TRP:HB3	2.54	0.42
1:A:489:ALA:N	2:A:1175:HOH:O	2.52	0.42
1:B:630:PRO:O	1:B:634:GLU:HG3	2.19	0.42
1:C:647:PHE:CE2	1:C:651:VAL:HG22	2.55	0.42
1:D:498:TRP:O	1:D:502:LEU:HB2	2.19	0.42
1:D:636:LEU:HD12	1:D:636:LEU:HA	1.80	0.42
1:A:110:THR:HB	1:A:113:VAL:CG2	2.48	0.42
1:A:608:LEU:HD22	1:B:612:ARG:NH1	2.35	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:C:169:GLU:HB3	1:C:405:ARG:HD3	2.01	0.42
1:D:20:ILE:HD11	1:D:35:MSE:CG	2.44	0.42
1:D:314:GLU:O	1:D:317:ALA:HB3	2.19	0.42
1:D:327:LEU:O	1:D:331:LEU:CB	2.67	0.42
1:D:631:GLU:O	1:D:635:ARG:HG3	2.20	0.42
1:A:226:GLU:HG3	1:A:230:LYS:HE3	2.02	0.42
1:A:339:PRO:HB3	1:A:365:ARG:NH1	2.34	0.42
1:A:417:ASN:ND2	1:A:423:ARG:HA	2.34	0.42
1:C:218:ARG:HD3	1:C:245:ALA:HB3	2.01	0.42
1:D:216:THR:HG22	1:D:243:LEU: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:D:72:SER:HB2	1:D:76:TYR:CE2	2.54	0.42
1:A:329:ARG:NH1	1:A:336:PRO:HD3	2.34	0.42
1:C:230:LYS:O	1:C:234:LEU:HG	2.20	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:A:636:LEU:HA	1:A:636:LEU:HD23	1.91	0.42
1:C:132:LEU:O	1:C:132:LEU:HD23	2.20	0.42
1:C:208:ARG:O	1:C:211:ALA:HB3	2.19	0.42
1:C:323:LEU:HD12	1:C:323:LEU:N	2.34	0.42
1:D:46:ARG:HG2	1:D:46:ARG:NH1	2.34	0.42
1:D:537:GLU:HG2	1:D:560:GLN:HE22	1.85	0.42
1:D:640:PRO:HG2	1:D:641:GLU:OE1	2.19	0.42
1:B:72:SER:HB2	1:B:76:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:222:VAL:HG13	1:D:223:ASN:N	2.35	0.42
1:D:252:PHE:CA	1:D:257:GLN:HE21	2.33	0.42
1:D:286:PHE:HA	2:D:905:HOH:O	2.20	0.42
1:D:329:ARG:NH1	1:D:329:ARG:HG2	2.32	0.42
1:A:545:VAL:HG22	1:A:571:ARG:HG2	2.02	0.41
1:C:307:GLU:HG3	1:C:308:ALA:N	2.34	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:D:63:ARG:CG	1:D:63:ARG:NH2	2.83	0.41
1:A:587:ALA:O	1:A:591:GLU:HG3	2.20	0.41
1:B:285:PRO:O	1:B:286:PHE:HB2	2.19	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:D:544:GLY:HA3	1:D:647:PHE:CE1	2.55	0.41
1:B:461:LEU:C	1:B:461:LEU:HD12	2.40	0.41
1:C:80:HIS:HD2	2:C:932:HOH:O	2.04	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:326:GLU:OE2	1:D:329:ARG:NH2	2.54	0.41
1:D:347:LYS:HA	2:D:925:HOH:O	2.21	0.41
1:D:377:THR:N	1:D:378:PRO:HD2	2.35	0.41
1:D:338:LEU:HD21	1:D:503:ARG:NH1	2.35	0.41
1:D:610:TRP:C	1:D:612:ARG:N	2.73	0.41
1:B:59:PRO:CG	1:B:309:TRP:CH2	2.99	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:D:143:ARG:HB3	1:D:144:PRO:HD2	2.03	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:B:228:LEU:HA	1:B:228:LEU:HD12	1.90	0.41
1:A:434:ASP:OD1	1:B:437:ARG:HG2	2.20	0.41
1:C:16:ARG:HG2	1:C:35:MSE:HA	2.03	0.41
1:D:206:LEU:HB3	1:D:210:ARG:HH22	1.86	0.41
1:B:541:GLU:CB	1:B:569:ARG:NH2	2.83	0.41
1:B:489:ALA:O	1:B:554:HIS:HE1	2.02	0.41
1:D:25:LYS:HD2	2:D:919:HOH:O	2.20	0.41
1:D:292:VAL:O	1:D:296:MSE:HG2	2.20	0.41
1:D:527:ARG:NE	1:D:530:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ARG:HH21	1:D:61:ARG:HG2	1.85	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: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:C:458:SER:HA	1:C:470:PRO:HD2	2.03	0.41
1:C:571:ARG:CG	2:C:853:HOH:O	2.67	0.41
1:D:120:LEU:N	1:D:120:LEU:HD22	2.34	0.41
1:D:62:ASP:OD1	1:D:152:TYR:HB2	2.21	0.41
1:D:522:SER:HB2	1:D:525:LYS:HB2	2.03	0.41
1:D:94:PHE:HD2	2:D:891:HOH:O	2.03	0.41
1:A:53:PRO:HB3	1:A:84:TYR:CD1	2.56	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:318:ARG:NH2	1:D:318:ARG:HG2	2.36	0.41
1:D:61:ARG:NH1	1:D:63:ARG:HH22	2.18	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: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:B:51:HIS:CE1	2:B:1087:HOH:O	2.74	0.41
1:C:169:GLU:CB	1:C:408:ALA:HB2	2.51	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:547:VAL:O	1:C:601:ALA:HA	2.21	0.41
1:C:65:VAL:HG13	1:C:115:VAL:HG12	2.02	0.41
1:D:205:VAL:HG23	1:D:206:LEU:N	2.34	0.41
1:D:408:ALA:O	1:D:412:ILE:HG13	2.21	0.41
1:D:359:LEU:HD13	1:D:425:TYR:OH	2.21	0.41
1:A:309:TRP:CH2	1:A:313:LEU:HD11	2.56	0.40
1:A:54:LEU:HD21	1:A:299:ARG:CB	2.51	0.40
1:C:409:MSE:HE2	1:C:426:GLY:HA2	2.03	0.40
1:C:472:GLU:OE2	2:C:901:HOH:O	2.22	0.40
1:D:17:PHE:HA	1:D:20:ILE:CG1	2.50	0.40
1:D:351:THR:HA	1:D:354:ALA:HB3	2.03	0.40
1:D:632:VAL:HG13	1:D:633:TYR:N	2.37	0.40
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:561:ALA:O	1:B:564:ARG:HB3	2.21	0.40
1:C:214:TRP:CD2	1:C:241:PRO:HG2	2.56	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:D:20:ILE:CD1	1:D:35:MSE:SE	3.19	0.40
1:D:75:LEU:HD22	1:D:79:LEU:HG	2.02	0.40
1:A:594:PRO:HG2	1:A:597:LEU:CD2	2.51	0.40
1:B:572:VAL:HG22	2:B:1114:HOH:O	2.20	0.40
1:C:168:GLY:N	2:C:787:HOH:O	2.54	0.40
1:C:377:THR:HB	1:C:378:PRO:CD	2.51	0.40
1:C:371:GLY:HA3	1:C:387:MSE:HE1	2.04	0.40
1:C:461:LEU:HG	1:C:469:GLN:HG2	2.02	0.40
1:C:62:ASP:CG	2:C:906:HOH:O	2.60	0.40
1:C:641:GLU:O	1:C:645:GLU:HG3	2.21	0.40
1:D:146:HIS:HB3	1:D:316:TYR:CD1	2.56	0.40
1:D:161:ASP:HB3	2:D:844:HOH:O	2.21	0.40
1:D:233:LYS:O	1:D:237:LEU:HD13	2.21	0.40
1:D:555:LEU:HD23	1:D:555:LEU:O	2.21	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:C:120:LEU:HD12	1:C:161:ASP:OD1	2.22	0.40
1:C:343:PRO:HG2	1:C:345:PHE:CZ	2.56	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:469:GLN:OE1	1:D:624:GLY:HA3	2.21	0.40
1:D:486:ILE:HA	1:D:576:PRO:O	2.22	0.40
1:A:560:GLN:NE2	2:A:1170:HOH:O	2.54	0.40
1:B:220:GLU:OE2	1:B:247:ARG:NH1	2.55	0.40
1:B:442:LEU:CG	1:B:446:MSE:HE2	2.46	0.40
1:B:584:GLN:O	1:B:589:ARG:NH2	2.54	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
2:C:901:HOH:O	1:D:441:ARG:CG	2.66	0.40
1:D:506:GLU:N	1:D:506:GLU:CD	2.75	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%)	47	49
1	D	645/651 (99%)	584 (90%)	54 (8%)	7 (1%)	14	9
All	All	2580/2604 (99%)	2463 (96%)	109 (4%)	8 (0%)	41	41

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%)	44	48
1	B	517/507 (102%)	499 (96%)	18 (4%)	36	38
1	C	517/507 (102%)	502 (97%)	15 (3%)	42	46
1	D	517/507 (102%)	497 (96%)	20 (4%)	32	33
All	All	2068/2028 (102%)	2001 (97%)	67 (3%)	39	41

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%)	-0.17	0 100 100	14, 24, 38, 46	0
1	B	632/651 (97%)	-0.21	3 (0%) 91 92	14, 25, 38, 54	0
1	C	632/651 (97%)	0.43	32 (5%) 28 33	27, 39, 52, 59	0
1	D	632/651 (97%)	1.11	140 (22%) 0 0	28, 47, 59, 64	0
All	All	2528/2604 (97%)	0.29	175 (6%) 16 21	14, 34, 55, 64	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	PHE	6.3
1	D	284	PRO	5.8
1	D	315	ALA	5.4
1	D	282	PRO	5.4
1	D	316	TYR	4.8
1	D	148	VAL	4.8
1	D	320	TYR	4.8
1	B	651	VAL	4.7
1	D	269	PRO	4.6
1	D	149	VAL	4.5
1	D	42	TYR	4.5
1	D	10	LEU	4.4
1	C	386	GLY	4.3
1	C	166	VAL	4.3
1	D	45	PHE	4.1
1	D	147	VAL	4.0
1	D	218	ARG	4.0
1	D	289	PRO	3.9
1	D	237	LEU	3.9
1	D	651	VAL	3.8
1	D	301	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	395	PRO	3.8
1	D	287	VAL	3.8
1	D	312	ALA	3.8
1	D	6	ASP	3.8
1	D	337	PRO	3.7
1	C	120	LEU	3.7
1	D	309	TRP	3.7
1	D	303	ARG	3.7
1	D	240	ARG	3.7
1	D	295	HIS	3.7
1	D	283	TYR	3.7
1	D	291	GLU	3.7
1	D	288	VAL	3.6
1	D	185	PHE	3.6
1	D	155	VAL	3.6
1	D	292	VAL	3.6
1	D	17	PHE	3.5
1	D	335	LEU	3.4
1	D	323	LEU	3.4
1	C	322	ASP	3.4
1	D	327	LEU	3.3
1	D	277	ARG	3.3
1	D	260	ALA	3.3
1	D	294	ARG	3.2
1	D	144	PRO	3.2
1	D	7	LEU	3.1
1	D	397	GLY	3.1
1	D	324	HIS	3.1
1	C	364	PRO	3.1
1	C	148	VAL	3.0
1	C	143	ARG	3.0
1	D	162	LEU	3.0
1	D	329	ARG	3.0
1	D	321	PRO	3.0
1	D	250	ILE	2.9
1	D	54	LEU	2.9
1	D	562	LEU	2.9
1	C	141	PHE	2.9
1	C	439	ALA	2.9
1	D	112	GLY	2.9
1	D	222	VAL	2.9
1	D	12	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	121	GLY	2.8
1	D	48	VAL	2.8
1	D	273	GLU	2.8
1	D	74	LEU	2.8
1	D	228	LEU	2.8
1	D	568	VAL	2.8
1	D	266	PRO	2.8
1	C	522	SER	2.8
1	D	191	ILE	2.8
1	D	153	THR	2.7
1	D	186	TRP	2.7
1	D	217	LEU	2.7
1	D	416	LEU	2.7
1	C	321	PRO	2.7
1	D	152	TYR	2.6
1	D	13	ASN	2.6
1	D	138	ALA	2.6
1	D	86	LEU	2.6
1	D	255	PRO	2.6
1	C	309	TRP	2.6
1	D	156	LEU	2.6
1	D	318	ARG	2.6
1	C	131	ALA	2.5
1	C	651	VAL	2.5
1	D	65	VAL	2.5
1	D	157	ALA	2.5
1	D	16	ARG	2.5
1	C	119	PRO	2.5
1	D	243	LEU	2.5
1	C	304	ALA	2.5
1	D	326	GLU	2.5
1	D	154	TYR	2.5
1	D	145	GLY	2.5
1	C	408	ALA	2.5
1	D	257	GLN	2.5
1	B	596	GLY	2.5
1	C	124	ILE	2.5
1	D	26	ALA	2.5
1	D	121	GLY	2.4
1	D	232	ILE	2.4
1	D	9	THR	2.4
1	D	541	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	404	VAL	2.4
1	D	564	ARG	2.4
1	D	18	LEU	2.4
1	D	66	LEU	2.4
1	D	370	LEU	2.4
1	D	268	GLY	2.4
1	D	190	ARG	2.4
1	C	411	ALA	2.4
1	D	64	PHE	2.4
1	D	565	GLU	2.4
1	D	198	ASP	2.4
1	D	432	PHE	2.3
1	D	143	ARG	2.3
1	C	428	THR	2.3
1	D	281	TRP	2.3
1	D	274	ALA	2.3
1	D	205	VAL	2.3
1	C	144	PRO	2.3
1	C	317	ALA	2.3
1	D	68	ALA	2.3
1	D	364	PRO	2.3
1	D	5	ARG	2.3
1	D	300	GLU	2.2
1	D	311	LYS	2.2
1	C	412	ILE	2.2
1	D	435	TYR	2.2
1	D	146	HIS	2.2
1	D	319	ALA	2.2
1	C	165	GLY	2.2
1	D	111	PRO	2.2
1	D	431	VAL	2.2
1	D	307	GLU	2.2
1	D	81	LEU	2.2
1	D	524	GLU	2.2
1	D	502	LEU	2.2
1	D	542	PRO	2.2
1	D	598	PRO	2.2
1	D	166	VAL	2.2
1	D	184	VAL	2.2
1	D	252	PHE	2.2
1	C	117	THR	2.2
1	D	308	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	40	LEU	2.1
1	D	521	LEU	2.1
1	D	165	GLY	2.1
1	D	278	ASN	2.1
1	D	67	SER	2.1
1	D	211	ALA	2.1
1	D	275	THR	2.1
1	B	120	LEU	2.1
1	D	536	LEU	2.1
1	D	569	ARG	2.1
1	D	305	TRP	2.1
1	D	230	LYS	2.1
1	C	325	GLN	2.1
1	D	78	VAL	2.1
1	D	134	GLU	2.1
1	C	416	LEU	2.1
1	D	41	ALA	2.1
1	D	135	ARG	2.1
1	D	70	HIS	2.1
1	D	567	GLY	2.1
1	C	541	GLU	2.0
1	D	374	ALA	2.0
1	D	201	PHE	2.0
1	C	596	GLY	2.0
1	D	137	LEU	2.0
1	C	146	HIS	2.0
1	D	304	ALA	2.0
1	D	418	LEU	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.