



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:30 AM UTC

PDB ID : 2YV3 / pdb_00002yv3
Title : Crystal Structure of Aspartate Semialdehyde Dehydrogenase from *Thermus thermophilus* HB8
Authors : Kagawa, W.; Fujikawa, N.; Kurumizaka, H.; Bessho, Y.; Ellis, M.J.; Antonyuk, S.V.; Strange, R.W.; Hasnain, S.S.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-04-07
Resolution : 2.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

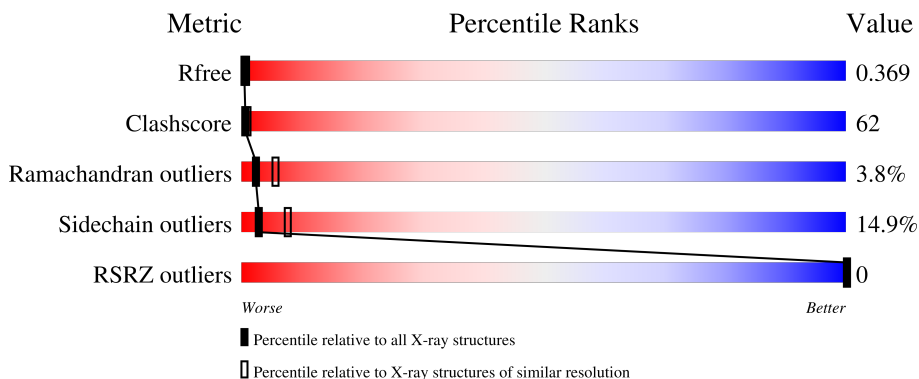
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of 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	331	
1	B	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5107 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 Aspartate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2531	1622	448	455	6			
1	B	328	Total	C	N	O	S	0	0	0
			2531	1622	448	455	6			

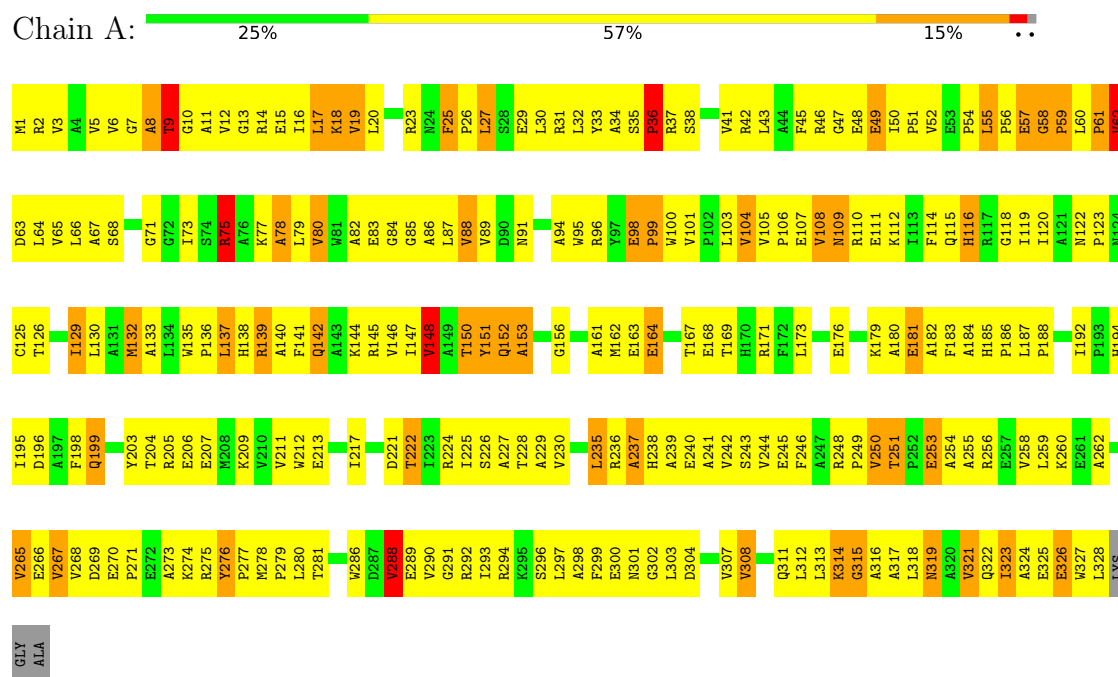
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	24	Total	O	0	0
			24	24		

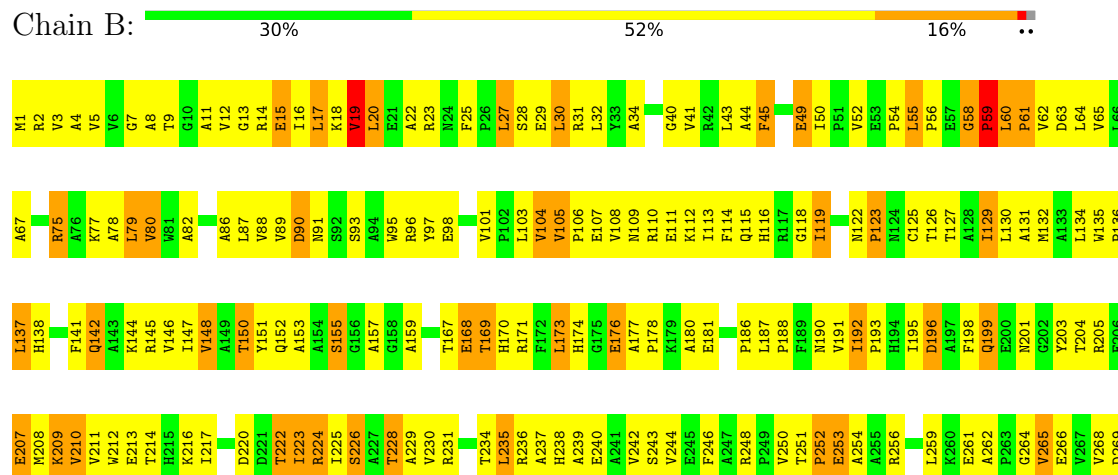
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Aspartate-semialdehyde dehydrogenase



• Molecule 1: Aspartate-semialdehyde dehydrogenase



E270	P271	K274	R275	Y276	P277	M278	P279	L280	T281	A282	S283	G284	K285	W286	D287	V288	F289	V290	G291	R292	I293	R294	K295	S296	L297	A298	F299	L303	D304	V307	V308	G309	D310	Q311	L312	L313	K314	G315	A316	A317	L318	N319	A320	V321	Q322	I323	A324	E325	E326	W327	L328	LYS	GLY	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.17Å 125.17Å 116.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 99.8 (50.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.303 , 0.368 0.303 , 0.369	Depositor DCC
R_{free} test set	2923 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5107	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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	0.60	0/2593	1.24	32/3533 (0.9%)
1	B	0.60	0/2593	1.21	27/3533 (0.8%)
All	All	0.60	0/5186	1.22	59/7066 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	GLY	CA-C-N	11.39	134.08	119.84
1	A	58	GLY	C-N-CA	11.39	134.08	119.84
1	A	104	VAL	N-CA-C	8.97	122.67	108.85
1	B	19	VAL	N-CA-C	-8.67	104.24	112.83
1	B	20	LEU	N-CA-C	-8.51	101.02	111.40
1	B	104	VAL	N-CA-C	8.39	120.56	108.48
1	A	62	VAL	N-CA-C	8.25	120.21	108.42
1	A	98	GLU	CA-C-N	8.04	129.89	119.84
1	A	98	GLU	C-N-CA	8.04	129.89	119.84
1	B	157	ALA	N-CA-C	-7.68	102.83	112.90
1	B	326	GLU	N-CA-C	-7.67	103.89	113.18
1	B	315	GLY	N-CA-C	-7.48	95.45	113.18
1	B	169	THR	N-CA-C	-7.39	102.82	111.03
1	A	315	GLY	N-CA-C	-6.90	96.83	113.18
1	A	236	ARG	N-CA-C	6.83	122.56	112.94
1	B	55	LEU	CA-C-N	6.63	126.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	LEU	C-N-CA	6.63	126.87	119.90
1	B	90	ASP	N-CA-C	6.54	119.18	108.52
1	A	84	GLY	N-CA-C	-6.43	107.33	115.31
1	A	88	VAL	N-CA-C	6.37	117.04	107.80
1	B	192	ILE	CA-C-N	6.31	127.72	119.84
1	B	192	ILE	C-N-CA	6.31	127.72	119.84
1	A	237	ALA	N-CA-C	6.21	119.06	109.07
1	A	18	LYS	N-CA-C	6.19	117.82	111.14
1	A	55	LEU	CA-C-N	6.05	127.40	119.84
1	A	55	LEU	C-N-CA	6.05	127.40	119.84
1	A	101	VAL	N-CA-C	6.02	114.45	107.89
1	A	152	GLN	N-CA-C	5.93	119.26	110.48
1	A	316	ALA	N-CA-C	5.91	119.67	112.23
1	A	109	ASN	N-CA-C	5.82	120.63	112.72
1	A	153	ALA	N-CA-C	5.79	119.04	110.46
1	B	105	VAL	N-CA-C	-5.79	96.38	108.88
1	B	101	VAL	N-CA-C	5.74	114.19	107.77
1	B	216	LYS	N-CA-C	5.73	117.61	111.36
1	A	67	ALA	N-CA-C	5.62	117.84	109.25
1	A	75	ARG	N-CA-C	-5.49	105.30	111.28
1	A	288	VAL	N-CA-C	-5.44	100.64	108.48
1	A	9	THR	N-CA-C	5.43	122.37	110.80
1	B	23	ARG	N-CA-C	-5.37	106.60	112.72
1	A	314	LYS	N-CA-C	-5.32	104.26	111.55
1	B	15	GLU	N-CA-C	-5.32	105.06	112.45
1	A	19	VAL	N-CA-C	-5.31	105.20	110.62
1	A	269	ASP	N-CA-C	5.28	116.04	107.32
1	B	252	PRO	N-CA-C	-5.27	105.93	113.47
1	B	119	ILE	N-CA-C	5.26	115.48	108.11
1	B	58	GLY	CA-C-N	5.25	126.40	119.84
1	B	58	GLY	C-N-CA	5.25	126.40	119.84
1	B	7	GLY	N-CA-C	-5.25	100.74	113.18
1	A	115	GLN	N-CA-C	-5.21	106.61	113.17
1	B	320	ALA	N-CA-C	-5.20	106.91	113.20
1	A	151	TYR	N-CA-C	-5.18	101.23	108.54
1	B	209	LYS	N-CA-C	-5.18	105.55	111.14
1	B	177	ALA	N-CA-C	5.11	118.52	109.58
1	A	25	PHE	CA-C-N	5.10	126.21	119.84
1	A	25	PHE	C-N-CA	5.10	126.21	119.84
1	A	148	VAL	N-CA-C	5.05	116.80	108.97
1	B	228	THR	N-CA-C	-5.03	99.78	108.69
1	A	246	PHE	N-CA-C	5.03	117.54	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	LEU	N-CA-C	5.01	121.48	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	TYR	Sidechain

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	2531	0	2553	348	0
1	B	2531	0	2553	316	0
2	A	21	0	0	2	0
2	B	24	0	0	4	0
All	All	5107	0	5106	635	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 62.

All (635) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:THR:HG21	1:B:152:GLN:HE21	1.13	1.13
1:A:60:LEU:HG	1:A:61:PRO:HB3	1.34	1.05
1:B:65:VAL:HG11	1:B:88:VAL:HG22	1.41	1.03
1:B:146:VAL:HG22	1:B:244:VAL:HG22	1.42	1.02
1:A:151:TYR:HB2	1:A:239:ALA:HB3	1.37	1.02
1:B:75:ARG:HB2	1:B:75:ARG:HH11	1.23	1.00
1:B:269:ASP:OD2	1:B:293:ILE:HG13	1.62	0.99
1:B:278:MET:HB2	1:B:281:THR:HG22	1.42	0.97
1:A:171:ARG:HH22	1:A:179:LYS:HG3	1.29	0.96
1:A:139:ARG:HH11	1:A:139:ARG:HB3	1.34	0.93
1:B:106:PRO:HG2	1:B:321:VAL:HG13	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:GLU:HG2	1:B:275:ARG:HD2	1.51	0.93
1:A:75:ARG:HD3	1:A:94:ALA:HB1	1.53	0.89
1:A:65:VAL:HG11	1:A:88:VAL:HG22	1.54	0.89
1:B:60:LEU:HG	1:B:61:PRO:HB3	1.54	0.89
1:B:65:VAL:HG13	1:B:88:VAL:HA	1.55	0.88
1:B:134:LEU:HD21	1:B:146:VAL:HG21	1.56	0.88
1:A:27:LEU:HD21	1:A:46:ARG:HH12	1.36	0.87
1:A:136:PRO:HA	1:A:139:ARG:HD3	1.56	0.87
1:B:89:VAL:HG21	1:B:323:ILE:HD11	1.55	0.86
1:B:251:THR:HB	1:B:254:ALA:HB3	1.58	0.86
1:B:293:ILE:HD12	1:B:293:ILE:O	1.75	0.86
1:A:171:ARG:HB3	1:A:176:GLU:HG3	1.57	0.85
1:A:150:THR:HG22	1:A:230:VAL:H	1.41	0.85
1:B:319:ASN:O	1:B:323:ILE:HD13	1.75	0.85
1:B:1:MET:HE2	1:B:1:MET:HA	1.57	0.84
1:B:205:ARG:O	1:B:209:LYS:HG3	1.77	0.84
1:B:129:ILE:HG22	1:B:314:LYS:HG3	1.59	0.84
1:B:315:GLY:O	1:B:319:ASN:ND2	2.11	0.83
1:A:77:LYS:O	1:A:80:VAL:HG23	1.78	0.83
1:B:253:GLU:HA	1:B:256:ARG:NH1	1.93	0.83
1:A:59:PRO:HG2	1:A:80:VAL:HG12	1.59	0.82
1:A:132:MET:HA	1:A:132:MET:HE2	1.62	0.81
1:A:270:GLU:HB3	1:A:275:ARG:HB3	1.60	0.81
1:A:2:ARG:H	1:A:2:ARG:HD3	1.44	0.81
1:B:211:VAL:HG22	1:B:225:ILE:HG22	1.63	0.81
1:A:105:VAL:HG13	1:A:318:LEU:HD11	1.62	0.80
1:B:91:ASN:HA	1:B:122:ASN:HD22	1.44	0.80
1:B:310:ASP:OD2	1:B:313:LEU:HG	1.82	0.80
1:B:30:LEU:H	1:B:30:LEU:HD23	1.46	0.80
1:A:109:ASN:HB2	1:A:112:LYS:HG2	1.62	0.80
1:B:251:THR:HB	1:B:254:ALA:CB	2.11	0.80
1:A:279:PRO:HG2	1:B:190:ASN:OD1	1.80	0.80
1:B:150:THR:HG21	1:B:152:GLN:NE2	1.95	0.80
1:B:88:VAL:HB	1:B:119:ILE:HD12	1.64	0.79
1:A:317:ALA:O	1:A:321:VAL:HB	1.82	0.79
1:B:14:ARG:HA	1:B:17:LEU:HD11	1.64	0.79
1:B:65:VAL:CG1	1:B:88:VAL:HG22	2.13	0.79
1:B:155:SER:HB3	1:B:236:ARG:HA	1.64	0.78
1:A:262:ALA:HB3	1:A:265:VAL:HG11	1.64	0.78
1:B:32:LEU:HD13	1:B:43:LEU:HD22	1.66	0.78
1:A:65:VAL:CG1	1:A:88:VAL:HG22	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:HG21	1:A:152:GLN:NE2	1.99	0.78
1:A:2:ARG:HA	1:A:29:GLU:HB3	1.67	0.77
1:A:64:LEU:HD21	1:A:323:ILE:HG12	1.65	0.76
1:B:107:GLU:CD	1:B:107:GLU:H	1.91	0.76
1:A:27:LEU:HD21	1:A:46:ARG:NH1	2.00	0.76
1:B:150:THR:HG22	1:B:229:ALA:HA	1.66	0.76
1:A:75:ARG:HH11	1:A:75:ARG:HB2	1.50	0.76
1:A:136:PRO:HA	1:A:139:ARG:CD	2.16	0.76
1:B:106:PRO:HB2	1:B:107:GLU:OE2	1.86	0.76
1:A:91:ASN:HA	1:A:122:ASN:HB3	1.67	0.76
1:A:32:LEU:HD13	1:A:43:LEU:HD22	1.68	0.76
1:A:105:VAL:HG13	1:A:318:LEU:CD1	2.16	0.75
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.53	0.74
1:A:129:ILE:HG13	1:A:130:LEU:N	2.01	0.74
1:B:65:VAL:CG1	1:B:88:VAL:HA	2.18	0.74
1:A:11:ALA:HB1	1:A:312:LEU:HD11	1.69	0.74
1:A:89:VAL:HG21	1:A:323:ILE:HD11	1.67	0.73
1:B:34:ALA:O	1:B:54:PRO:HA	1.88	0.73
1:A:17:LEU:HD23	1:A:45:PHE:HD1	1.52	0.73
1:A:60:LEU:HG	1:A:61:PRO:CB	2.13	0.73
1:A:12:VAL:O	1:A:16:ILE:HG13	1.88	0.72
1:B:141:PHE:O	1:B:248:ARG:HG3	1.89	0.72
1:A:1:MET:SD	1:A:63:ASP:HB3	2.29	0.72
1:A:141:PHE:HA	1:A:248:ARG:HD2	1.71	0.72
1:B:88:VAL:HB	1:B:119:ILE:CD1	2.19	0.72
1:B:171:ARG:HH21	1:B:176:GLU:HB2	1.55	0.72
1:A:139:ARG:HH11	1:A:139:ARG:CB	2.02	0.72
1:A:150:THR:HG23	1:A:152:GLN:HG3	1.72	0.72
1:A:323:ILE:N	1:A:323:ILE:HD12	2.05	0.72
1:A:79:LEU:HD22	1:A:79:LEU:H	1.55	0.71
1:A:319:ASN:O	1:A:323:ILE:HD13	1.90	0.71
1:B:104:VAL:HG12	1:B:322:GLN:HE21	1.56	0.71
1:B:270:GLU:CG	1:B:275:ARG:HD2	2.21	0.71
1:B:96:ARG:HH12	1:B:209:LYS:NZ	1.89	0.70
1:A:14:ARG:O	1:A:17:LEU:HD12	1.91	0.70
1:B:187:LEU:HD13	1:B:192:ILE:HD12	1.72	0.70
1:A:110:ARG:HH21	1:A:328:LEU:HB3	1.56	0.70
1:B:318:LEU:O	1:B:322:GLN:HG3	1.90	0.70
1:B:151:TYR:HB2	1:B:239:ALA:HB3	1.71	0.70
1:B:60:LEU:HG	1:B:61:PRO:CB	2.22	0.70
1:A:145:ARG:NH2	1:B:145:ARG:HH22	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASN:HD21	1:B:217:ILE:HG23	1.57	0.70
1:B:3:VAL:HG12	1:B:64:LEU:HB3	1.72	0.69
1:A:105:VAL:HA	1:A:318:LEU:HD11	1.74	0.69
1:A:12:VAL:HG12	1:A:16:ILE:HD11	1.74	0.69
1:A:106:PRO:HG2	1:A:321:VAL:HG13	1.72	0.69
1:B:13:GLY:O	1:B:17:LEU:HD12	1.92	0.69
1:B:248:ARG:HG2	1:B:248:ARG:HH11	1.58	0.69
1:A:56:PRO:O	1:A:58:GLY:N	2.27	0.68
1:B:104:VAL:CG1	1:B:322:GLN:HE21	2.05	0.68
1:B:150:THR:HG22	1:B:230:VAL:H	1.59	0.68
1:A:59:PRO:CG	1:A:80:VAL:HG12	2.23	0.68
1:B:292:ARG:HH12	1:B:294:ARG:NH1	1.90	0.68
1:A:169:THR:O	1:A:173:LEU:HD23	1.92	0.68
1:B:75:ARG:HH11	1:B:75:ARG:CB	2.03	0.68
1:A:298:ALA:HB2	1:B:226:SER:HB2	1.75	0.67
1:A:171:ARG:NH2	1:A:179:LYS:HG3	2.06	0.67
1:B:109:ASN:HB2	1:B:112:LYS:HG2	1.77	0.67
1:B:62:VAL:HG22	1:B:63:ASP:H	1.61	0.67
1:B:31:ARG:HG2	1:B:31:ARG:HH11	1.60	0.66
1:B:59:PRO:O	1:B:60:LEU:HB2	1.93	0.66
1:B:292:ARG:HH11	1:B:292:ARG:HB3	1.60	0.66
1:A:145:ARG:HH21	1:B:145:ARG:HH22	1.43	0.66
1:B:211:VAL:HG22	1:B:225:ILE:CG2	2.25	0.66
1:A:2:ARG:O	1:A:63:ASP:HB2	1.94	0.66
1:A:16:ILE:O	1:A:20:LEU:HB2	1.96	0.66
1:A:110:ARG:HH12	1:A:114:PHE:HE2	1.44	0.66
1:A:139:ARG:CB	1:A:139:ARG:NH1	2.59	0.65
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.61	0.65
1:A:15:GLU:OE2	1:A:15:GLU:HA	1.95	0.65
1:B:8:ALA:O	1:B:43:LEU:HD21	1.97	0.65
1:A:139:ARG:HB3	1:A:139:ARG:NH1	2.11	0.65
1:B:168:GLU:HB3	1:B:188:PRO:HG2	1.78	0.65
1:A:64:LEU:HD12	1:A:87:LEU:HB3	1.79	0.65
1:B:14:ARG:HA	1:B:17:LEU:CD1	2.27	0.65
1:A:49:GLU:O	1:A:50:ILE:HD13	1.96	0.65
1:A:137:LEU:HD11	1:A:259:LEU:HD21	1.78	0.65
1:A:296:SER:HB3	1:A:302:GLY:C	2.22	0.64
1:B:168:GLU:OE1	1:B:168:GLU:HA	1.97	0.64
1:A:95:TRP:C	1:A:98:GLU:HG2	2.22	0.64
1:A:171:ARG:HG2	1:A:176:GLU:OE1	1.97	0.64
1:A:226:SER:CB	1:B:298:ALA:HB2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG13	1:A:55:LEU:HD11	1.80	0.64
1:B:96:ARG:NH1	1:B:209:LYS:HZ1	1.95	0.64
1:A:150:THR:HG21	1:A:152:GLN:HE21	1.63	0.64
1:A:226:SER:HB2	1:B:298:ALA:HB2	1.79	0.64
1:B:30:LEU:HD23	1:B:30:LEU:N	2.12	0.64
1:A:82:ALA:HA	1:A:86:ALA:O	1.98	0.63
1:A:171:ARG:NH1	1:A:179:LYS:HD3	2.13	0.63
1:A:179:LYS:O	1:A:181:GLU:HG2	1.98	0.63
1:B:8:ALA:HB1	1:B:32:LEU:HD22	1.80	0.63
1:B:40:GLY:O	1:B:41:VAL:HG23	1.98	0.63
1:B:237:ALA:HB3	1:B:279:PRO:HB3	1.79	0.63
1:B:1:MET:HG3	1:B:27:LEU:HA	1.81	0.63
1:B:256:ARG:HD3	1:B:293:ILE:CD1	2.29	0.63
1:A:95:TRP:O	1:A:98:GLU:HG2	1.98	0.63
1:A:248:ARG:HB3	1:A:249:PRO:HD2	1.81	0.63
1:A:9:THR:HA	1:A:14:ARG:NH1	2.13	0.63
1:A:14:ARG:O	1:A:17:LEU:CD1	2.47	0.63
1:A:141:PHE:HA	1:A:248:ARG:CD	2.28	0.63
1:B:144:LYS:O	1:B:145:ARG:HG2	1.98	0.62
1:A:73:ILE:HG23	1:A:77:LYS:HZ3	1.64	0.62
1:A:281:THR:HG23	1:A:289:GLU:OE2	1.98	0.62
1:A:29:GLU:HG3	1:A:30:LEU:N	2.14	0.62
1:A:248:ARG:HG3	1:A:248:ARG:HH11	1.64	0.62
1:A:290:VAL:HG22	1:A:307:VAL:HG13	1.82	0.62
1:B:103:LEU:HD23	1:B:217:ILE:HG13	1.79	0.62
1:B:12:VAL:O	1:B:16:ILE:HG13	1.99	0.62
1:B:220:ASP:OD1	1:B:223:ILE:HG13	2.00	0.62
1:B:4:ALA:HA	1:B:31:ARG:O	1.99	0.61
1:A:237:ALA:HB3	1:A:279:PRO:HB3	1.81	0.61
1:B:256:ARG:HD3	1:B:293:ILE:HD11	1.81	0.61
1:A:132:MET:HA	1:A:132:MET:CE	2.29	0.61
1:B:126:THR:O	1:B:126:THR:HG22	1.99	0.61
1:B:153:ALA:H	1:B:238:HIS:CD2	2.17	0.61
1:B:1:MET:HG2	1:B:327:TRP:HZ2	1.64	0.61
1:B:15:GLU:HG3	1:B:312:LEU:HB3	1.82	0.61
1:A:129:ILE:HG22	1:A:314:LYS:HG3	1.80	0.61
1:A:270:GLU:HB2	1:A:275:ARG:HD2	1.83	0.61
1:B:15:GLU:O	1:B:19:VAL:HG13	2.00	0.61
1:A:129:ILE:HD12	1:A:307:VAL:HG12	1.83	0.60
1:A:34:ALA:O	1:A:54:PRO:HA	2.01	0.60
1:B:296:SER:HB3	1:B:304:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HA	1:B:318:LEU:HD11	1.82	0.60
1:A:110:ARG:NH1	1:A:114:PHE:HE2	1.97	0.60
1:B:17:LEU:HA	1:B:20:LEU:HB2	1.83	0.60
1:A:107:GLU:HG2	1:A:132:MET:SD	2.42	0.60
1:A:296:SER:HA	1:B:203:TYR:OH	2.01	0.60
1:B:110:ARG:O	1:B:113:ILE:HG13	2.02	0.60
1:A:87:LEU:HD11	1:A:116:HIS:NE2	2.16	0.60
1:A:147:ILE:HD12	1:B:147:ILE:CD1	2.31	0.59
1:B:130:LEU:HB2	1:B:240:GLU:OE1	2.02	0.59
1:B:134:LEU:HD21	1:B:146:VAL:CG2	2.32	0.59
1:B:292:ARG:NH1	1:B:294:ARG:NH1	2.49	0.59
1:B:167:THR:O	1:B:171:ARG:HG3	2.02	0.59
1:A:45:PHE:O	1:A:48:GLU:N	2.35	0.59
1:B:150:THR:CG2	1:B:229:ALA:HA	2.32	0.59
1:B:95:TRP:O	1:B:98:GLU:HG2	2.01	0.59
1:A:27:LEU:HD22	1:A:27:LEU:H	1.68	0.59
1:A:293:ILE:HD12	1:A:293:ILE:O	2.03	0.59
1:B:153:ALA:HB1	1:B:234:THR:O	2.03	0.59
1:B:242:VAL:HG12	1:B:243:SER:N	2.18	0.59
1:A:29:GLU:CD	1:A:30:LEU:H	2.10	0.59
1:A:142:GLN:HE21	1:A:248:ARG:HH22	1.50	0.58
1:A:168:GLU:OE2	1:A:179:LYS:N	2.32	0.58
1:B:91:ASN:CA	1:B:122:ASN:HD22	2.12	0.58
1:A:171:ARG:HH12	1:A:179:LYS:HB2	1.68	0.58
1:A:29:GLU:CG	1:A:30:LEU:N	2.67	0.58
1:A:64:LEU:HD22	1:A:323:ILE:HG21	1.85	0.58
1:A:278:MET:HE3	1:A:280:LEU:HB3	1.85	0.58
1:B:25:PHE:HZ	1:B:323:ILE:HG21	1.68	0.58
1:A:77:LYS:C	1:A:80:VAL:HG23	2.28	0.58
1:B:253:GLU:HA	1:B:256:ARG:HH12	1.66	0.58
1:A:237:ALA:HB3	1:A:279:PRO:CB	2.33	0.58
1:A:277:PRO:HD3	1:A:291:GLY:HA3	1.86	0.58
1:A:110:ARG:HH21	1:A:328:LEU:CB	2.17	0.58
1:B:62:VAL:HG22	1:B:63:ASP:N	2.19	0.57
1:A:251:THR:HG22	1:A:253:GLU:OE2	2.04	0.57
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.17	0.57
1:B:104:VAL:HB	1:B:322:GLN:NE2	2.19	0.57
1:B:109:ASN:HB2	1:B:112:LYS:CG	2.34	0.57
1:B:91:ASN:OD1	1:B:122:ASN:ND2	2.37	0.57
1:B:96:ARG:NH1	1:B:209:LYS:NZ	2.50	0.57
1:A:325:GLU:O	1:A:326:GLU:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLY:N	1:A:33:TYR:O	2.30	0.57
1:B:268:VAL:O	1:B:291:GLY:HA3	2.04	0.57
1:B:49:GLU:CD	1:B:49:GLU:H	2.13	0.57
1:A:105:VAL:HG22	1:A:123:PRO:HG3	1.86	0.57
1:B:132:MET:HB3	1:B:288:VAL:HG11	1.85	0.57
1:B:323:ILE:HA	1:B:326:GLU:HB3	1.87	0.57
1:A:325:GLU:OE1	1:A:328:LEU:HD12	2.04	0.56
1:A:30:LEU:HG	1:A:30:LEU:O	2.04	0.56
1:A:288:VAL:HG23	1:A:308:VAL:O	2.05	0.56
1:B:64:LEU:HD21	1:B:323:ILE:HG12	1.87	0.56
1:B:77:LYS:HD2	2:B:347:HOH:O	2.04	0.56
1:A:278:MET:CE	1:A:280:LEU:HD23	2.35	0.56
1:B:3:VAL:CG1	1:B:64:LEU:HD23	2.35	0.56
1:B:292:ARG:HB3	1:B:292:ARG:NH1	2.20	0.56
1:B:318:LEU:C	1:B:321:VAL:HG12	2.30	0.56
1:A:325:GLU:O	1:A:328:LEU:N	2.39	0.56
1:A:110:ARG:NH2	1:A:328:LEU:HB3	2.21	0.56
1:A:270:GLU:CB	1:A:275:ARG:HB3	2.33	0.56
1:A:185:HIS:CG	1:B:278:MET:HE1	2.40	0.56
1:A:168:GLU:HB3	1:A:188:PRO:HG2	1.88	0.56
1:A:323:ILE:HD12	1:A:323:ILE:H	1.70	0.56
1:B:1:MET:O	1:B:28:SER:HB3	2.06	0.56
1:B:1:MET:HG2	1:B:327:TRP:CZ2	2.39	0.56
1:A:206:GLU:HA	1:A:209:LYS:HD3	1.87	0.56
1:B:64:LEU:HD22	1:B:323:ILE:HG21	1.88	0.56
1:A:116:HIS:ND1	1:A:116:HIS:C	2.64	0.55
1:B:96:ARG:HH12	1:B:209:LYS:HZ1	1.53	0.55
1:A:65:VAL:HG13	1:A:88:VAL:HA	1.88	0.55
1:A:125:CYS:SG	1:A:238:HIS:HE1	2.29	0.55
1:A:153:ALA:H	1:A:238:HIS:CD2	2.25	0.55
1:A:15:GLU:HG2	1:A:312:LEU:HD13	1.87	0.55
1:A:136:PRO:HA	1:A:139:ARG:CG	2.37	0.55
1:A:323:ILE:N	1:A:323:ILE:CD1	2.70	0.55
1:B:250:VAL:HG11	1:B:303:LEU:CD1	2.37	0.55
1:B:251:THR:CG2	1:B:253:GLU:HG2	2.37	0.55
1:B:323:ILE:HD12	1:B:323:ILE:N	2.22	0.55
1:A:17:LEU:C	1:A:17:LEU:HD22	2.32	0.55
1:B:30:LEU:N	1:B:30:LEU:CD2	2.70	0.55
1:B:292:ARG:HH12	1:B:294:ARG:CZ	2.19	0.55
1:A:12:VAL:HB	1:A:68:SER:OG	2.07	0.54
1:A:79:LEU:H	1:A:79:LEU:CD2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:CD1	1:B:147:ILE:HD12	2.38	0.54
1:A:278:MET:HE1	1:A:280:LEU:HD23	1.89	0.54
1:A:318:LEU:HD23	1:A:322:GLN:OE1	2.08	0.54
1:A:319:ASN:O	1:A:323:ILE:CD1	2.56	0.54
1:B:323:ILE:O	1:B:327:TRP:HD1	1.91	0.54
1:A:163:GLU:O	1:A:167:THR:HG22	2.08	0.54
1:B:115:GLN:O	1:B:115:GLN:HG2	2.07	0.54
1:A:238:HIS:NE2	1:A:311:GLN:HG3	2.23	0.54
1:B:89:VAL:HG21	1:B:323:ILE:CD1	2.32	0.54
1:B:125:CYS:O	1:B:129:ILE:HG23	2.08	0.54
1:B:299:PHE:N	1:B:299:PHE:CD1	2.76	0.54
1:B:3:VAL:HG12	1:B:64:LEU:HD23	1.90	0.54
1:B:246:PHE:HB2	1:B:250:VAL:HG21	1.88	0.54
1:A:78:ALA:HB2	1:A:95:TRP:NE1	2.23	0.54
1:A:88:VAL:HB	1:A:119:ILE:CD1	2.38	0.54
1:A:125:CYS:SG	1:A:126:THR:N	2.79	0.54
1:A:130:LEU:HD13	1:A:240:GLU:OE1	2.08	0.53
1:A:150:THR:CG2	1:A:152:GLN:HG3	2.37	0.53
1:A:75:ARG:HB2	1:A:75:ARG:NH1	2.21	0.53
1:A:78:ALA:HB3	1:A:95:TRP:CZ2	2.43	0.53
1:B:169:THR:HG22	1:B:173:LEU:CD2	2.38	0.53
1:B:313:LEU:O	1:B:317:ALA:HB3	2.09	0.53
1:B:251:THR:HG22	1:B:253:GLU:HG2	1.89	0.53
1:A:65:VAL:HG13	1:A:65:VAL:O	2.07	0.53
1:A:184:ALA:HB1	1:B:274:LYS:HD3	1.89	0.53
1:A:323:ILE:H	1:A:323:ILE:CD1	2.22	0.53
1:A:79:LEU:HD22	1:A:79:LEU:N	2.20	0.53
1:B:109:ASN:ND2	1:B:217:ILE:HG23	2.21	0.53
1:A:29:GLU:CG	1:A:30:LEU:H	2.21	0.53
1:B:43:LEU:HD13	1:B:52:VAL:CG2	2.39	0.53
1:A:276:TYR:CD1	1:B:193:PRO:HG2	2.43	0.53
1:B:145:ARG:O	1:B:244:VAL:HA	2.08	0.53
1:A:30:LEU:N	1:A:30:LEU:HD23	2.23	0.53
1:B:60:LEU:HG	1:B:61:PRO:CA	2.39	0.53
1:B:195:ILE:HG13	1:B:229:ALA:HB1	1.90	0.53
1:A:71:GLY:O	1:A:75:ARG:HB2	2.09	0.53
1:A:318:LEU:C	1:A:321:VAL:HG12	2.34	0.53
1:A:180:ALA:HB2	1:A:186:PRO:HG3	1.91	0.52
1:A:298:ALA:HB2	1:B:226:SER:CB	2.38	0.52
1:B:106:PRO:HG2	1:B:321:VAL:CG1	2.34	0.52
1:B:222:THR:O	1:B:223:ILE:HG13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:GLU:HG3	1:B:275:ARG:NH1	2.24	0.52
1:A:195:ILE:HG21	1:A:206:GLU:HG2	1.92	0.52
1:B:30:LEU:HB2	2:B:346:HOH:O	2.08	0.52
1:A:133:ALA:O	1:A:137:LEU:HD13	2.10	0.52
1:A:12:VAL:HG12	1:A:16:ILE:CD1	2.40	0.52
1:A:17:LEU:HD13	1:A:18:LYS:H	1.74	0.52
1:A:136:PRO:HA	1:A:139:ARG:HG2	1.92	0.52
1:B:220:ASP:CG	1:B:223:ILE:HG13	2.34	0.52
1:A:141:PHE:C	1:A:248:ARG:HD2	2.35	0.51
1:A:43:LEU:N	1:A:43:LEU:HD12	2.26	0.51
1:B:129:ILE:HG13	1:B:130:LEU:N	2.23	0.51
1:B:262:ALA:HB3	1:B:265:VAL:HG11	1.91	0.51
1:B:291:GLY:O	1:B:292:ARG:HB2	2.09	0.51
1:A:15:GLU:CG	1:A:312:LEU:HD13	2.40	0.51
1:B:78:ALA:HB3	1:B:95:TRP:CZ2	2.46	0.51
1:B:107:GLU:CD	1:B:107:GLU:N	2.61	0.51
1:B:250:VAL:CG1	1:B:303:LEU:HD11	2.40	0.51
1:A:65:VAL:HG13	1:A:88:VAL:HG13	1.93	0.51
1:A:107:GLU:OE1	1:A:132:MET:HE1	2.10	0.51
1:A:297:LEU:HD23	1:B:203:TYR:CE2	2.45	0.51
1:B:135:TRP:HB3	1:B:136:PRO:CD	2.40	0.51
1:A:318:LEU:HD23	1:A:318:LEU:O	2.10	0.51
1:A:108:VAL:HG22	1:A:135:TRP:CG	2.46	0.51
1:B:150:THR:HG23	1:B:152:GLN:HG3	1.92	0.51
1:B:171:ARG:O	1:B:176:GLU:HG3	2.10	0.51
1:A:83:GLU:C	1:A:85:GLY:H	2.19	0.51
1:B:1:MET:CG	1:B:327:TRP:HZ2	2.24	0.51
1:B:93:SER:HB3	1:B:209:LYS:HZ1	1.75	0.51
1:A:135:TRP:CZ3	1:A:138:HIS:HD2	2.28	0.51
1:A:277:PRO:HG2	1:A:291:GLY:N	2.26	0.51
1:A:145:ARG:HH21	1:B:145:ARG:NH2	2.09	0.51
1:A:135:TRP:HA	1:A:135:TRP:CE3	2.46	0.50
1:B:63:ASP:O	1:B:86:ALA:HA	2.11	0.50
1:B:150:THR:CG2	1:B:152:GLN:HG3	2.41	0.50
1:B:222:THR:O	1:B:223:ILE:CG1	2.59	0.50
1:A:203:TYR:CE2	1:B:297:LEU:HD22	2.46	0.50
1:A:260:LYS:HZ2	1:A:267:VAL:CG1	2.23	0.50
1:A:151:TYR:CB	1:A:239:ALA:HB3	2.25	0.50
1:A:318:LEU:HA	1:A:321:VAL:CG1	2.41	0.50
1:B:180:ALA:C	1:B:181:GLU:HG2	2.36	0.50
1:A:65:VAL:CG1	1:A:88:VAL:HA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:O	1:B:321:VAL:HG12	2.11	0.50
1:B:323:ILE:N	1:B:323:ILE:CD1	2.74	0.50
1:A:50:ILE:HG23	1:A:51:PRO:HD2	1.93	0.50
1:A:77:LYS:HA	1:A:80:VAL:CG2	2.41	0.50
1:A:171:ARG:HH12	1:A:179:LYS:CG	2.24	0.50
1:A:29:GLU:OE2	1:A:30:LEU:HD23	2.11	0.50
1:A:104:VAL:HB	1:A:322:GLN:HE21	1.76	0.50
1:A:135:TRP:HB3	1:A:136:PRO:CD	2.42	0.50
1:A:294:ARG:HD2	1:B:203:TYR:CD2	2.47	0.50
1:B:108:VAL:HG13	1:B:135:TRP:CE2	2.47	0.50
1:A:145:ARG:HG3	1:A:224:ARG:HB2	1.93	0.50
1:A:256:ARG:O	1:A:260:LYS:N	2.39	0.49
2:A:351:HOH:O	1:B:280:LEU:HB2	2.12	0.49
1:B:43:LEU:HD13	1:B:52:VAL:HG23	1.94	0.49
1:B:122:ASN:ND2	1:B:319:ASN:HD21	2.10	0.49
1:A:106:PRO:HD2	1:A:318:LEU:HG	1.94	0.49
1:A:318:LEU:O	1:A:321:VAL:HG12	2.13	0.49
1:B:209:LYS:HE2	1:B:213:GLU:OE1	2.13	0.49
1:A:35:SER:O	1:A:36:PRO:C	2.56	0.49
1:A:150:THR:HB	1:A:229:ALA:HA	1.95	0.49
1:B:65:VAL:HG13	1:B:65:VAL:O	2.11	0.49
1:A:32:LEU:CD1	1:A:43:LEU:HD22	2.42	0.49
1:A:15:GLU:HG3	1:A:312:LEU:HB3	1.95	0.48
1:A:192:ILE:C	1:A:194:HIS:H	2.21	0.48
1:A:268:VAL:HG21	1:A:289:GLU:HG2	1.95	0.48
1:B:16:ILE:HA	1:B:316:ALA:HB1	1.94	0.48
1:B:65:VAL:HG12	1:B:87:LEU:O	2.13	0.48
1:B:270:GLU:HB2	1:B:275:ARG:HB3	1.95	0.48
1:A:17:LEU:HD13	1:A:18:LYS:N	2.29	0.48
1:A:300:GLU:HG2	1:B:224:ARG:NH1	2.28	0.48
1:B:250:VAL:HG12	1:B:251:THR:H	1.78	0.48
1:B:251:THR:HB	1:B:254:ALA:H	1.78	0.48
1:A:77:LYS:O	1:A:78:ALA:C	2.56	0.48
1:A:226:SER:HB3	1:B:298:ALA:HB2	1.96	0.48
1:A:265:VAL:O	1:A:265:VAL:HG22	2.12	0.48
1:A:251:THR:HG22	1:A:253:GLU:HG2	1.96	0.48
1:B:253:GLU:CA	1:B:256:ARG:HH12	2.26	0.48
1:A:132:MET:CE	1:A:132:MET:CA	2.92	0.48
1:A:192:ILE:HG22	1:A:194:HIS:HB3	1.95	0.48
1:B:250:VAL:HG11	1:B:303:LEU:HD12	1.96	0.48
1:B:290:VAL:HG22	1:B:307:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HG2	1:B:31:ARG:NH1	2.27	0.48
1:B:153:ALA:H	1:B:238:HIS:HD2	1.59	0.48
1:A:96:ARG:HH12	1:A:209:LYS:HE3	1.78	0.47
1:B:145:ARG:HD2	1:B:224:ARG:HB2	1.95	0.47
1:A:10:GLY:O	1:A:14:ARG:HB2	2.14	0.47
1:B:1:MET:SD	1:B:327:TRP:HZ2	2.37	0.47
1:A:30:LEU:HD12	1:A:50:ILE:HG13	1.95	0.47
1:A:96:ARG:NH1	1:A:209:LYS:HE3	2.29	0.47
1:A:141:PHE:CA	1:A:248:ARG:HD2	2.41	0.47
1:B:209:LYS:C	1:B:211:VAL:N	2.70	0.47
1:B:220:ASP:OD1	1:B:222:THR:O	2.31	0.47
1:A:8:ALA:HB1	1:A:43:LEU:HD21	1.96	0.47
1:A:36:PRO:O	1:A:37:ARG:C	2.57	0.47
1:A:64:LEU:CD2	1:A:323:ILE:HG21	2.43	0.47
1:A:161:ALA:HB1	1:A:183:PHE:CZ	2.50	0.47
1:A:171:ARG:HH12	1:A:179:LYS:CB	2.27	0.47
1:A:43:LEU:HD13	1:A:52:VAL:CG2	2.44	0.47
1:A:116:HIS:ND1	1:A:118:GLY:N	2.62	0.47
1:A:145:ARG:O	1:A:244:VAL:HA	2.14	0.47
1:B:123:PRO:HB3	1:B:217:ILE:HD11	1.97	0.47
1:A:248:ARG:C	1:A:301:ASN:HD21	2.22	0.47
1:A:300:GLU:OE1	1:A:300:GLU:O	2.31	0.47
1:B:187:LEU:N	1:B:188:PRO:CD	2.78	0.47
1:A:150:THR:HG22	1:A:230:VAL:N	2.21	0.47
1:A:207:GLU:OE2	1:A:228:THR:HA	2.15	0.47
1:A:318:LEU:HA	1:A:321:VAL:HG12	1.96	0.47
1:B:209:LYS:C	1:B:211:VAL:H	2.22	0.47
1:B:225:ILE:CG2	1:B:226:SER:N	2.78	0.47
1:A:88:VAL:HB	1:A:119:ILE:HD13	1.96	0.47
1:A:141:PHE:O	1:A:142:GLN:O	2.31	0.47
1:B:253:GLU:HA	1:B:256:ARG:CZ	2.43	0.47
1:A:277:PRO:CB	1:A:308:VAL:HG23	2.44	0.47
1:A:281:THR:HG23	1:A:289:GLU:CD	2.40	0.47
1:A:2:ARG:O	1:A:62:VAL:HG22	2.15	0.47
1:A:194:HIS:CE1	1:A:198:PHE:HE2	2.33	0.47
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.29	0.47
1:A:294:ARG:NE	1:B:203:TYR:CE1	2.83	0.47
1:A:108:VAL:HG12	1:A:109:ASN:N	2.30	0.46
1:A:164:GLU:OE1	1:A:182:ALA:HB3	2.15	0.46
1:B:110:ARG:NH2	1:B:328:LEU:HB3	2.29	0.46
1:B:113:ILE:O	1:B:116:HIS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HG2	1:A:110:ARG:NH1	2.30	0.46
1:A:205:ARG:O	1:A:209:LYS:HG3	2.15	0.46
1:A:300:GLU:HG2	1:B:224:ARG:HH11	1.80	0.46
1:B:134:LEU:HD11	1:B:244:VAL:HG21	1.97	0.46
1:A:238:HIS:CE1	1:A:311:GLN:HG3	2.50	0.46
1:A:130:LEU:HB2	1:A:240:GLU:OE1	2.15	0.46
1:B:129:ILE:HD12	1:B:307:VAL:HG12	1.98	0.46
1:A:41:VAL:CG1	1:A:42:ARG:N	2.78	0.46
1:A:213:GLU:O	1:A:217:ILE:HG13	2.16	0.46
1:A:265:VAL:O	1:A:265:VAL:HG13	2.16	0.46
1:B:237:ALA:CB	1:B:279:PRO:HA	2.45	0.46
1:A:135:TRP:HB3	1:A:136:PRO:HD3	1.97	0.46
1:A:273:ALA:O	1:A:274:LYS:C	2.58	0.46
1:B:170:HIS:HD2	1:B:174:HIS:CD2	2.34	0.46
1:A:2:ARG:C	1:A:62:VAL:HG22	2.40	0.46
1:A:118:GLY:O	1:A:119:ILE:HD13	2.16	0.46
1:A:171:ARG:HH12	1:A:179:LYS:HD3	1.81	0.46
1:B:134:LEU:CD1	1:B:244:VAL:HG21	2.46	0.46
1:B:146:VAL:HG22	1:B:244:VAL:CG2	2.28	0.46
1:A:25:PHE:HZ	1:A:323:ILE:HG22	1.81	0.46
1:A:142:GLN:HG3	1:A:248:ARG:NH2	2.30	0.46
1:B:262:ALA:HB3	1:B:265:VAL:CG1	2.45	0.46
1:A:95:TRP:HA	1:A:98:GLU:CG	2.45	0.46
1:A:313:LEU:O	1:A:317:ALA:HB3	2.15	0.46
1:B:75:ARG:HA	1:B:95:TRP:CZ2	2.51	0.46
1:B:97:TYR:OH	1:B:209:LYS:HE3	2.16	0.46
1:A:5:VAL:N	1:A:31:ARG:O	2.45	0.46
1:A:7:GLY:O	1:A:8:ALA:C	2.58	0.46
1:A:187:LEU:O	1:A:187:LEU:HG	2.15	0.46
1:A:262:ALA:HB3	1:A:265:VAL:CG1	2.40	0.46
1:B:313:LEU:C	1:B:315:GLY:H	2.22	0.46
1:A:13:GLY:HA2	1:A:16:ILE:HD12	1.97	0.45
1:A:203:TYR:OH	1:B:296:SER:HA	2.15	0.45
1:A:260:LYS:HZ2	1:A:267:VAL:HG12	1.82	0.45
1:B:199:GLN:HE22	1:B:205:ARG:HH11	1.65	0.45
1:A:25:PHE:HZ	1:A:323:ILE:CG2	2.29	0.45
1:B:250:VAL:HG12	1:B:251:THR:N	2.31	0.45
1:A:105:VAL:CG1	1:A:318:LEU:HD11	2.41	0.45
1:B:17:LEU:HA	1:B:20:LEU:HD22	1.97	0.45
1:B:122:ASN:OD1	1:B:318:LEU:HD23	2.16	0.45
1:B:269:ASP:O	1:B:271:PRO:HD3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:CG	1:A:91:ASN:O	2.59	0.45
1:A:185:HIS:HB3	1:A:186:PRO:CD	2.46	0.45
1:B:211:VAL:O	1:B:212:TRP:C	2.58	0.45
1:A:25:PHE:O	1:A:27:LEU:HD13	2.17	0.45
1:B:2:ARG:HA	1:B:29:GLU:HB3	1.98	0.45
1:B:64:LEU:HD12	1:B:65:VAL:H	1.81	0.45
1:B:104:VAL:CB	1:B:322:GLN:HE21	2.29	0.45
1:B:25:PHE:HD1	1:B:27:LEU:HB3	1.82	0.45
1:B:105:VAL:HG13	1:B:318:LEU:HD11	1.99	0.45
1:B:250:VAL:HG11	1:B:303:LEU:HD11	1.99	0.45
1:A:296:SER:HB2	1:A:304:ASP:OD1	2.16	0.45
1:B:2:ARG:O	1:B:62:VAL:HG22	2.16	0.45
1:B:321:VAL:O	1:B:325:GLU:HG2	2.17	0.45
1:A:137:LEU:N	1:A:137:LEU:CD1	2.80	0.45
1:A:198:PHE:CG	1:B:271:PRO:HB3	2.51	0.45
1:A:1:MET:O	1:A:3:VAL:HG13	2.16	0.45
1:B:56:PRO:C	1:B:58:GLY:H	2.25	0.45
1:B:242:VAL:CG1	1:B:243:SER:N	2.80	0.45
1:A:55:LEU:HA	1:A:55:LEU:HD23	1.69	0.45
1:B:283:SER:O	1:B:283:SER:OG	2.30	0.45
1:A:196:ASP:OD2	1:A:205:ARG:HB3	2.17	0.44
1:B:30:LEU:HD12	1:B:50:ILE:HD11	1.99	0.44
1:B:251:THR:CB	1:B:254:ALA:HB3	2.39	0.44
1:B:324:ALA:O	1:B:327:TRP:HB2	2.17	0.44
1:A:43:LEU:N	1:A:43:LEU:CD1	2.80	0.44
1:B:5:VAL:HB	1:B:32:LEU:HD23	1.99	0.44
1:B:223:ILE:O	1:B:225:ILE:N	2.50	0.44
1:A:129:ILE:CG1	1:A:130:LEU:N	2.78	0.44
1:B:11:ALA:HB2	1:B:159:ALA:HB2	1.99	0.44
1:B:19:VAL:HA	1:B:22:ALA:HB3	1.99	0.44
1:B:223:ILE:O	1:B:223:ILE:HG22	2.18	0.44
1:B:248:ARG:NH1	1:B:248:ARG:CG	2.80	0.44
1:A:319:ASN:C	1:A:321:VAL:N	2.73	0.44
1:A:319:ASN:C	1:A:321:VAL:H	2.25	0.44
1:B:64:LEU:CD2	1:B:323:ILE:HG21	2.48	0.44
1:A:130:LEU:CD1	1:A:242:VAL:HG21	2.48	0.44
1:A:240:GLU:O	1:A:242:VAL:HG23	2.16	0.44
1:B:29:GLU:HG3	1:B:31:ARG:HG3	2.00	0.44
1:B:58:GLY:N	1:B:59:PRO:HD3	2.32	0.44
1:B:251:THR:HG22	1:B:253:GLU:OE2	2.17	0.44
1:A:83:GLU:C	1:A:85:GLY:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ALA:O	1:A:248:ARG:HD3	2.17	0.44
1:B:220:ASP:OD1	1:B:222:THR:HG23	2.17	0.44
1:B:246:PHE:HB2	1:B:250:VAL:CG2	2.47	0.44
1:A:26:PRO:HG2	1:A:327:TRP:CZ2	2.53	0.44
1:B:59:PRO:HG3	2:B:347:HOH:O	2.18	0.44
1:A:45:PHE:O	1:A:46:ARG:C	2.61	0.43
1:A:187:LEU:N	1:A:188:PRO:CD	2.81	0.43
1:A:260:LYS:NZ	1:A:267:VAL:CG1	2.81	0.43
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.86	0.43
1:B:2:ARG:CB	1:B:62:VAL:HG23	2.47	0.43
1:A:278:MET:C	1:A:280:LEU:N	2.76	0.43
1:B:292:ARG:HH11	1:B:292:ARG:CB	2.28	0.43
1:A:45:PHE:HE2	1:A:46:ARG:NH1	2.16	0.43
1:B:9:THR:O	1:B:14:ARG:NH1	2.51	0.43
1:B:259:LEU:HD13	1:B:290:VAL:HG11	2.00	0.43
1:A:45:PHE:CE2	1:A:46:ARG:NH1	2.87	0.43
1:B:266:GLU:OE2	1:B:285:LYS:NZ	2.46	0.43
1:B:252:PRO:HG2	1:B:253:GLU:OE2	2.19	0.43
1:A:107:GLU:N	1:A:107:GLU:CD	2.76	0.43
1:B:223:ILE:HG22	1:B:225:ILE:HG13	2.00	0.43
1:A:104:VAL:O	1:A:318:LEU:HD21	2.19	0.43
1:B:118:GLY:O	1:B:119:ILE:HD13	2.19	0.43
1:A:14:ARG:HG3	1:A:14:ARG:HH11	1.84	0.43
1:B:138:HIS:O	1:B:142:GLN:HA	2.19	0.43
1:B:150:THR:CG2	1:B:152:GLN:HE21	2.05	0.43
1:A:77:LYS:HA	1:A:80:VAL:HG23	2.01	0.43
1:B:126:THR:O	1:B:126:THR:CG2	2.67	0.43
1:B:201:ASN:HD21	1:B:203:TYR:HB2	1.84	0.43
1:B:211:VAL:O	1:B:214:THR:N	2.52	0.43
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.82	0.43
1:A:250:VAL:HG11	1:A:303:LEU:CD1	2.49	0.43
1:B:248:ARG:HH11	1:B:248:ARG:CG	2.24	0.43
1:B:278:MET:O	1:B:279:PRO:C	2.62	0.43
1:A:45:PHE:C	1:A:47:GLY:N	2.75	0.42
1:B:108:VAL:HG13	1:B:135:TRP:CD2	2.53	0.42
1:B:210:VAL:O	1:B:214:THR:OG1	2.35	0.42
1:A:103:LEU:HD21	1:A:213:GLU:HG2	2.01	0.42
1:A:277:PRO:HB3	1:A:308:VAL:HG23	2.01	0.42
1:A:323:ILE:HA	1:A:326:GLU:HB3	2.01	0.42
1:B:204:THR:OG1	1:B:207:GLU:HG2	2.19	0.42
1:A:73:ILE:CG2	1:A:77:LYS:HZ3	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLN:HE22	1:A:212:TRP:HH2	1.67	0.42
1:B:195:ILE:HG23	1:B:231:ARG:NH2	2.35	0.42
1:A:148:VAL:O	1:A:227:ALA:HA	2.19	0.42
1:B:224:ARG:H	1:B:224:ARG:HG2	1.63	0.42
1:B:256:ARG:HH11	1:B:293:ILE:HD13	1.83	0.42
1:A:30:LEU:H	1:A:30:LEU:HD23	1.83	0.42
1:A:87:LEU:CD1	1:A:116:HIS:NE2	2.82	0.42
1:A:147:ILE:HD13	1:B:147:ILE:HD12	2.01	0.42
1:A:254:ALA:O	1:A:258:VAL:HG23	2.19	0.42
1:A:262:ALA:CB	1:A:265:VAL:HG11	2.41	0.42
1:B:264:GLY:O	1:B:287:ASP:HA	2.19	0.42
1:A:100:TRP:CD1	1:A:100:TRP:C	2.97	0.42
1:B:88:VAL:HB	1:B:119:ILE:HD13	2.00	0.42
1:A:58:GLY:HA2	1:A:59:PRO:HD3	1.70	0.42
1:A:139:ARG:NH1	1:A:139:ARG:HB2	2.33	0.42
1:A:185:HIS:ND1	1:B:278:MET:HE1	2.35	0.42
1:A:255:ALA:O	1:A:259:LEU:HG	2.19	0.42
1:B:171:ARG:NH2	1:B:176:GLU:HB2	2.28	0.42
1:B:207:GLU:HG2	1:B:207:GLU:H	1.19	0.42
1:A:42:ARG:C	1:A:43:LEU:HD12	2.45	0.42
1:B:17:LEU:HD22	1:B:17:LEU:C	2.44	0.42
1:B:61:PRO:O	1:B:61:PRO:HG2	2.19	0.42
1:A:271:PRO:HB3	1:B:198:PHE:CG	2.55	0.42
1:B:91:ASN:HA	1:B:122:ASN:ND2	2.24	0.42
1:B:144:LYS:C	1:B:145:ARG:HG2	2.45	0.42
1:B:145:ARG:CD	1:B:224:ARG:HB2	2.50	0.42
1:A:207:GLU:OE1	1:B:292:ARG:NH2	2.53	0.41
1:B:104:VAL:CB	1:B:322:GLN:NE2	2.83	0.41
1:B:269:ASP:OD2	1:B:293:ILE:CG1	2.51	0.41
1:A:87:LEU:HD11	1:A:116:HIS:CD2	2.55	0.41
1:A:104:VAL:HG12	1:A:105:VAL:N	2.36	0.41
1:A:156:GLY:HA3	2:A:346:HOH:O	2.18	0.41
1:A:199:GLN:NE2	1:A:212:TRP:HH2	2.18	0.41
1:A:242:VAL:HG12	1:A:243:SER:N	2.35	0.41
1:A:266:GLU:HG2	1:A:268:VAL:HG23	2.02	0.41
1:B:5:VAL:CG2	1:B:32:LEU:HD23	2.51	0.41
1:B:80:VAL:C	1:B:82:ALA:N	2.76	0.41
1:B:259:LEU:C	1:B:261:GLU:N	2.77	0.41
1:A:209:LYS:C	1:A:211:VAL:N	2.77	0.41
1:B:127:THR:O	1:B:131:ALA:N	2.50	0.41
1:B:67:ALA:HB3	1:B:90:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:VAL:HG12	1:A:42:ARG:N	2.35	0.41
1:A:244:VAL:HG12	1:A:245:GLU:N	2.36	0.41
1:B:277:PRO:HB2	1:B:308:VAL:HG23	2.03	0.41
1:A:119:ILE:HG22	1:A:120:ILE:N	2.36	0.41
1:A:299:PHE:CD2	1:B:145:ARG:NH2	2.88	0.41
1:B:30:LEU:HD12	1:B:50:ILE:CD1	2.51	0.41
1:A:142:GLN:HB2	1:A:248:ARG:NH1	2.35	0.41
1:B:25:PHE:CZ	1:B:323:ILE:HG21	2.51	0.41
1:B:292:ARG:HD2	1:B:292:ARG:HA	1.79	0.41
1:A:109:ASN:ND2	1:A:217:ILE:O	2.53	0.41
1:B:253:GLU:HB3	1:B:256:ARG:HH22	1.85	0.41
1:A:57:GLU:HA	1:A:57:GLU:OE1	2.21	0.41
1:A:142:GLN:HG3	1:A:248:ARG:CZ	2.50	0.41
1:A:192:ILE:C	1:A:194:HIS:N	2.79	0.41
1:B:3:VAL:HG11	1:B:64:LEU:HD23	2.03	0.41
1:B:15:GLU:OE2	1:B:313:LEU:HD21	2.21	0.41
1:B:79:LEU:O	1:B:82:ALA:HB3	2.21	0.41
1:B:93:SER:HA	1:B:96:ARG:HD2	2.03	0.41
1:B:148:VAL:HB	1:B:242:VAL:HG22	2.02	0.41
1:B:178:PRO:CG	1:B:186:PRO:HB3	2.51	0.41
1:B:186:PRO:HA	2:B:332:HOH:O	2.20	0.41
1:B:253:GLU:CD	1:B:253:GLU:H	2.29	0.41
1:A:12:VAL:HA	1:A:312:LEU:HD22	2.03	0.41
1:A:62:VAL:O	1:A:86:ALA:HB2	2.21	0.41
1:A:110:ARG:NH2	1:A:328:LEU:CB	2.82	0.41
1:A:132:MET:HG2	1:A:288:VAL:CG1	2.51	0.41
1:A:222:THR:O	1:A:222:THR:HG23	2.20	0.41
1:A:314:LYS:HD2	1:A:314:LYS:HA	1.82	0.41
1:B:137:LEU:HB3	1:B:246:PHE:CZ	2.55	0.41
1:B:152:GLN:O	1:B:231:ARG:HA	2.20	0.41
1:A:15:GLU:OE2	1:A:15:GLU:CA	2.67	0.40
1:A:105:VAL:HG13	1:A:318:LEU:HD12	2.01	0.40
1:A:241:ALA:HB1	1:B:228:THR:HG21	2.03	0.40
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.83	0.40
1:A:204:THR:HG23	1:A:207:GLU:OE1	2.22	0.40
1:A:324:ALA:O	1:A:327:TRP:HB2	2.21	0.40
1:B:44:ALA:O	1:B:45:PHE:HB2	2.20	0.40
1:B:91:ASN:CB	1:B:122:ASN:HD22	2.34	0.40
1:B:196:ASP:HB3	1:B:205:ARG:HB3	2.04	0.40
1:A:195:ILE:HG21	1:A:206:GLU:CG	2.51	0.40
1:B:313:LEU:HA	1:B:313:LEU:HD23	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD22	1:A:27:LEU:N	2.35	0.40
1:A:45:PHE:O	1:A:47:GLY:N	2.54	0.40
1:A:65:VAL:HG12	1:A:87:LEU:O	2.21	0.40
1:A:146:VAL:HB	1:A:225:ILE:HG23	2.04	0.40
1:B:150:THR:HG22	1:B:230:VAL:N	2.33	0.40
1:A:23:ARG:NH2	1:A:286:TRP:CE3	2.83	0.40
1:A:30:LEU:N	1:A:30:LEU:CD2	2.85	0.40
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.93	0.40
1:B:58:GLY:N	1:B:59:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	326/331 (98%)	261 (80%)	52 (16%)	13 (4%)	2	5
1	B	326/331 (98%)	266 (82%)	48 (15%)	12 (4%)	2	6
All	All	652/662 (98%)	527 (81%)	100 (15%)	25 (4%)	2	5

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	57	GLU
1	A	61	PRO
1	A	142	GLN
1	B	60	LEU
1	B	224	ARG
1	A	9	THR
1	A	235	LEU
1	A	315	GLY

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Mol	Chain	Res	Type
1	B	59	PRO
1	B	223	ILE
1	A	59	PRO
1	A	78	ALA
1	B	45	PHE
1	B	114	PHE
1	B	208	MET
1	B	282	ALA
1	B	61	PRO
1	B	142	GLN
1	B	315	GLY
1	B	123	PRO
1	A	36	PRO
1	A	99	PRO
1	A	108	VAL
1	A	265	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/259 (100%)	221 (86%)	37 (14%)	3	8
1	B	258/259 (100%)	218 (84%)	40 (16%)	2	7
All	All	516/518 (100%)	439 (85%)	77 (15%)	3	8

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	19	VAL
1	A	27	LEU
1	A	36	PRO
1	A	38	SER
1	A	49	GLU
1	A	62	VAL

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Mol	Chain	Res	Type
1	A	66	LEU
1	A	75	ARG
1	A	80	VAL
1	A	111	GLU
1	A	116	HIS
1	A	129	ILE
1	A	132	MET
1	A	137	LEU
1	A	139	ARG
1	A	144	LYS
1	A	148	VAL
1	A	150	THR
1	A	162	MET
1	A	164	GLU
1	A	181	GLU
1	A	199	GLN
1	A	221	ASP
1	A	222	THR
1	A	235	LEU
1	A	250	VAL
1	A	251	THR
1	A	253	GLU
1	A	267	VAL
1	A	288	VAL
1	A	292	ARG
1	A	308	VAL
1	A	319	ASN
1	A	321	VAL
1	A	323	ILE
1	A	326	GLU
1	B	17	LEU
1	B	18	LYS
1	B	19	VAL
1	B	27	LEU
1	B	30	LEU
1	B	49	GLU
1	B	55	LEU
1	B	59	PRO
1	B	75	ARG
1	B	79	LEU
1	B	80	VAL
1	B	111	GLU

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Mol	Chain	Res	Type
1	B	129	ILE
1	B	137	LEU
1	B	148	VAL
1	B	150	THR
1	B	155	SER
1	B	168	GLU
1	B	173	LEU
1	B	176	GLU
1	B	191	VAL
1	B	196	ASP
1	B	199	GLN
1	B	207	GLU
1	B	210	VAL
1	B	222	THR
1	B	226	SER
1	B	235	LEU
1	B	253	GLU
1	B	265	VAL
1	B	279	PRO
1	B	280	LEU
1	B	287	ASP
1	B	292	ARG
1	B	297	LEU
1	B	299	PHE
1	B	304	ASP
1	B	323	ILE
1	B	326	GLU
1	B	328	LEU

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

Mol	Chain	Res	Type
1	A	124	ASN
1	A	138	HIS
1	A	142	GLN
1	A	152	GLN
1	A	199	GLN
1	A	238	HIS
1	A	322	GLN
1	B	91	ASN
1	B	109	ASN
1	B	122	ASN

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Mol	Chain	Res	Type
1	B	124	ASN
1	B	152	GLN
1	B	170	HIS
1	B	199	GLN
1	B	238	HIS
1	B	311	GLN
1	B	322	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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	328/331 (99%)	-1.41	0 100 100	11, 30, 47, 67	0
1	B	328/331 (99%)	-1.40	0 100 100	9, 31, 52, 65	0
All	All	656/662 (99%)	-1.41	0 100 100	9, 31, 49, 67	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.