Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 08:05 PM EDT

PDB ID	:	2YV3
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:

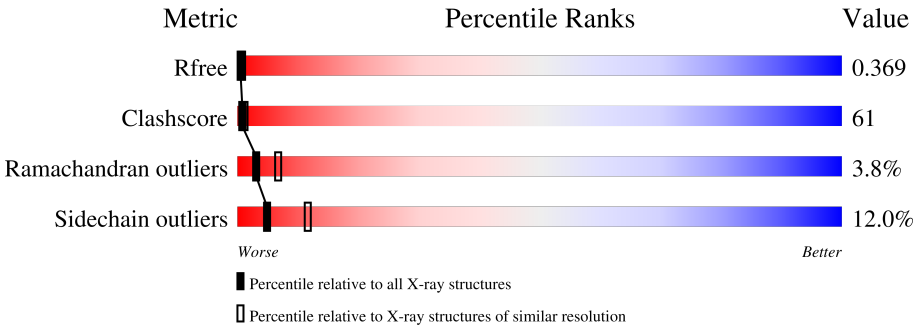
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	331	29% 60% 9% ··
1	B	331	34% 54% 11% ··

2 Entry composition (i)

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.

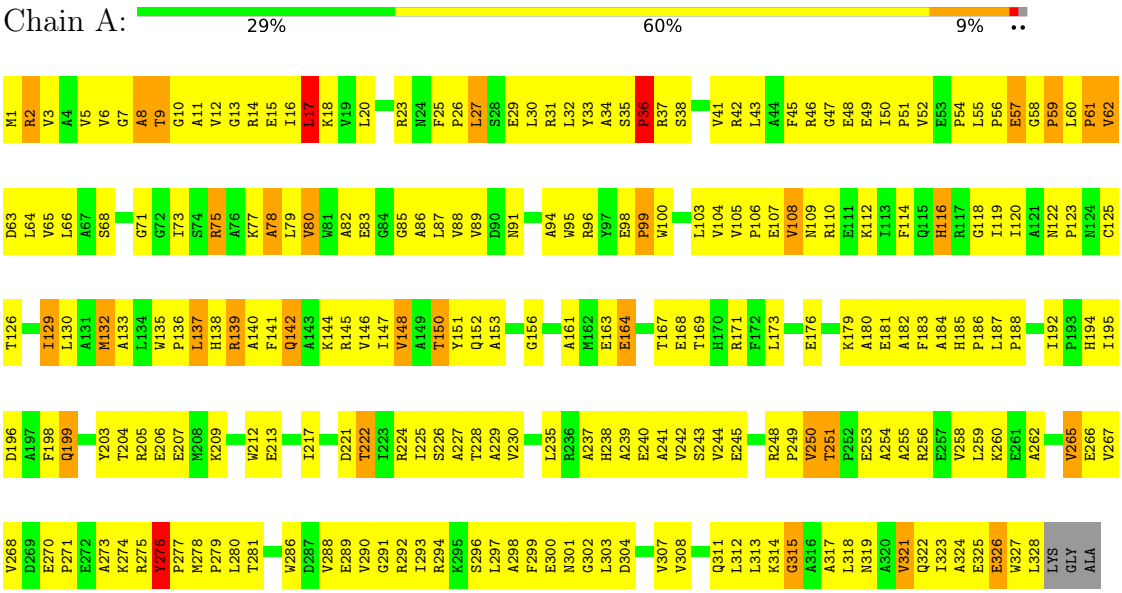
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	24	Total	O	0	0
			24	24		

3 Residue-property plots (i)

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. 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. 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.

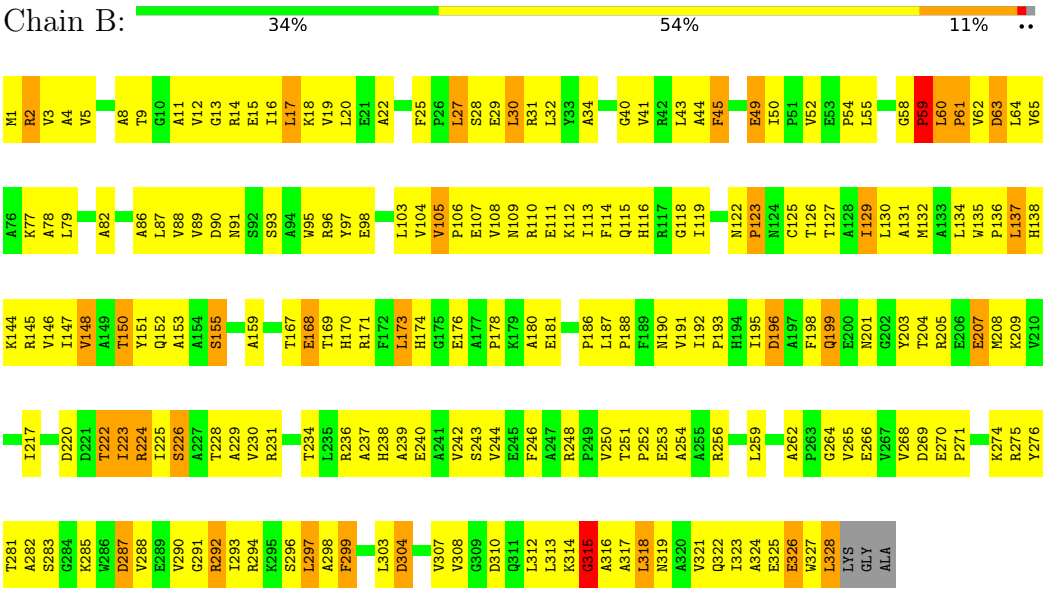
- Molecule 1: Aspartate-semialdehyde dehydrogenase

Chain A:



- Molecule 1: Aspartate-semialdehyde dehydrogenase

Chain B:



4 Data and refinement statistics (i)

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 49.14 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 99.3 (49.14-2.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.34 , 18.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.47	0/2593	0.78	2/3533 (0.1%)
1	B	0.49	0/2593	0.77	2/3533 (0.1%)
All	All	0.48	0/5186	0.78	4/7066 (0.1%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	315	GLY	N-CA-C	-7.06	95.45	113.10
1	A	315	GLY	N-CA-C	-6.51	96.83	113.10
1	A	17	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	105	VAL	N-CA-C	-5.42	96.38	111.00

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

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	338	0
1	B	2531	0	2553	307	0
2	A	21	0	0	2	0
2	B	24	0	0	4	0
All	All	5107	0	5106	618	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 61.

All (618) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:150:THR:HG21	1:A:152:GLN:NE2	1.99	0.78
1:A:132:MET:HA	1:A:132:MET:HE2	1.66	0.77
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:107:GLU:CD	1:B:107:GLU:H	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:168:GLU:OE1	1:B:168:GLU:HA	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MET:HE2	1:B:1:MET:HA	1.81	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
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:296:SER:HB3	1:A:302:GLY:C	2.22	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:A:95:TRP:C	1:A:98:GLU:HG2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:ILE:HG23	1:A:77:LYS:HZ3	1.68	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:B:25:PHE:HZ	1:B:323:ILE:HG21	1.68	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:278:MET:HE3	1:A:280:LEU:HB3	1.88	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: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
1:A:147:ILE:CD1	1:B:147:ILE:HD12	2.38	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:29:GLU:CD	1:A:30:LEU:H	2.10	0.53
1:A:75:ARG:HB2	1:A:75:ARG:NH1	2.21	0.53
1:A:77:LYS:C	1:A:80:VAL:HG23	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:278:MET:HE3	1:A:280:LEU:HD23	1.91	0.53
1:B:43:LEU:HD13	1:B:52:VAL:CG2	2.39	0.53
1:B:129:ILE:HG13	1:B:130:LEU:N	2.23	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: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:A:325:GLU:O	1:A:326:GLU:C	2.47	0.52
1:B:291:GLY:O	1:B:292:ARG:HB2	2.09	0.52
1:B:222:THR:O	1:B:223:ILE:HG13	2.08	0.52
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:B:107:GLU:CD	1:B:107:GLU:N	2.61	0.52
1:B:318:LEU:C	1:B:321:VAL:HG12	2.30	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:49:GLU:CD	1:B:49:GLU:H	2.13	0.52
1:A:43:LEU:N	1:A:43:LEU:HD12	2.26	0.51
1:B:262:ALA:HB3	1:B:265:VAL:HG11	1.91	0.51
1:A:15:GLU:CG	1:A:312:LEU:HD13	2.40	0.51
1:B:1:MET:HA	1:B:1:MET:CE	2.40	0.51
1:B:78:ALA:HB3	1:B:95:TRP:CZ2	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:HIS:ND1	1:A:116:HIS:C	2.64	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:B:283:SER:O	1:B:283:SER:OG	2.30	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:A:65:VAL:CG1	1:A:88:VAL:HA	2.42	0.50
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:17:LEU:C	1:A:17:LEU:HD22	2.32	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:107:GLU:OE1	1:A:132:MET:HE1	2.11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:318:LEU:C	1:A:321:VAL:HG12	2.34	0.48
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HA	1:A:321:VAL:HG12	1.96	0.47
1:B:220:ASP:CG	1:B:223:ILE:HG13	2.34	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:C	1:A:248:ARG:HD2	2.35	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: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
1:A:73:ILE:CG2	1:A:77:LYS:HZ3	2.29	0.46
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:83:GLU:C	1:A:85:GLY:H	2.19	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:B:170:HIS:HD2	1:B:174:HIS:CD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:185:HIS:HB3	1:A:186:PRO:CD	2.46	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:180:ALA:C	1:B:181:GLU:HG2	2.36	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:B:209:LYS:C	1:B:211:VAL:N	2.70	0.45
1:A:1:MET:O	1:A:3:VAL:HG13	2.16	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: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:A:35:SER:O	1:A:36:PRO:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:192:ILE:C	1:A:194:HIS:H	2.21	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: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: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: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:A:77:LYS:O	1:A:78:ALA:C	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PRO:O	1:A:37:ARG:C	2.57	0.42
1:B:108:VAL:HG13	1:B:135:TRP:CD2	2.53	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:199:GLN:HE22	1:A:212:TRP:HH2	1.67	0.42
1:A:248:ARG:C	1:A:301:ASN:HD21	2.22	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:83:GLU:C	1:A:85:GLY:N	2.73	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:281:THR:HG23	1:A:289:GLU:CD	2.40	0.42
1:A:319:ASN:C	1:A:321:VAL:N	2.73	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ALA:O	1:B:45:PHE:HB2	2.20	0.41
1:B:127:THR:O	1:B:131:ALA:N	2.50	0.41
1:A:2:ARG:C	1:A:62:VAL:HG22	2.40	0.41
1:A:273:ALA:O	1:A:274:LYS:C	2.58	0.41
1:B:67:ALA:HB3	1:B:90:ASP:OD1	2.20	0.41
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:209:LYS:C	1:B:211:VAL:H	2.22	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:7:GLY:O	1:A:8:ALA:C	2.58	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:B:313:LEU:C	1:B:315:GLY:H	2.22	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: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:A:12:VAL:HA	1:A:312:LEU:HD22	2.03	0.41
1:A:45:PHE:C	1:A:47:GLY:N	2.75	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:91:ASN:O	1:A:91:ASN:CG	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:O	1:B:212:TRP:C	2.58	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: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
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 (i)

5.3.1 Protein backbone (i)

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%)	3 6
1	B	326/331 (98%)	266 (82%)	48 (15%)	12 (4%)	3 7
All	All	652/662 (98%)	527 (81%)	100 (15%)	25 (4%)	3 7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA

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Mol	Chain	Res	Type
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
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 (i)

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%)	230 (89%)	28 (11%)	6 14
1	B	258/259 (100%)	224 (87%)	34 (13%)	4 9
All	All	516/518 (100%)	454 (88%)	62 (12%)	5 11

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	17	LEU
1	A	27	LEU
1	A	36	PRO
1	A	38	SER
1	A	62	VAL
1	A	66	LEU
1	A	75	ARG
1	A	80	VAL
1	A	100	TRP
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	164	GLU
1	A	199	GLN
1	A	221	ASP
1	A	222	THR
1	A	250	VAL
1	A	251	THR
1	A	276	TYR
1	A	292	ARG
1	A	321	VAL
1	A	326	GLU
1	B	2	ARG
1	B	17	LEU
1	B	18	LYS
1	B	27	LEU
1	B	30	LEU
1	B	49	GLU
1	B	55	LEU
1	B	59	PRO
1	B	63	ASP
1	B	75	ARG
1	B	111	GLU
1	B	129	ILE
1	B	137	LEU
1	B	148	VAL
1	B	150	THR

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Mol	Chain	Res	Type
1	B	155	SER
1	B	168	GLU
1	B	173	LEU
1	B	191	VAL
1	B	196	ASP
1	B	199	GLN
1	B	207	GLU
1	B	222	THR
1	B	226	SER
1	B	276	TYR
1	B	279	PRO
1	B	287	ASP
1	B	292	ARG
1	B	297	LEU
1	B	299	PHE
1	B	304	ASP
1	B	318	LEU
1	B	326	GLU
1	B	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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	122	ASN
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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.