Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 07:58 PM EDT

PDB ID	:	2EGY
Title	:	Crystal structure of LysN, alpha-aminoadipate aminotransferase (substrate free form), from Thermus thermophilus HB27
Authors	:	Tomita, T.; Miyazaki, T.; Miyagawa, T.; Fushinobu, S.; Kuzuyama, T.; Nishiyama, M.
Deposited on	:	2007-03-02
Resolution	:	2.67 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 (i) 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 (i)) were used in the production of this report:

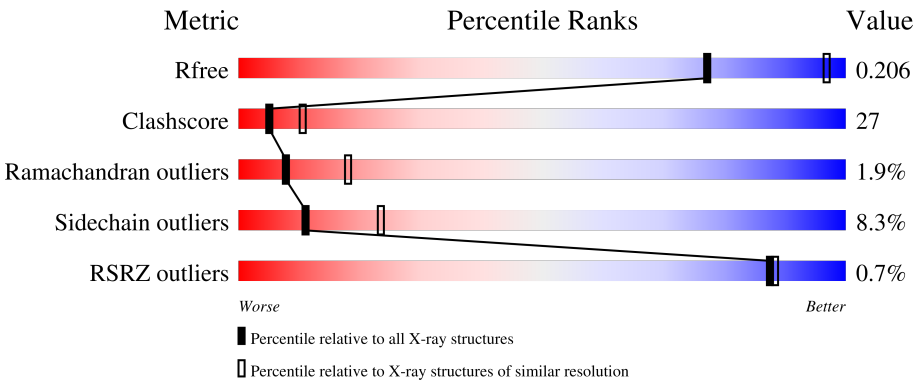
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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% 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	397	2%, 54%, 39%, 5% •
1	B	397	%, 49%, 45%, 5% •
1	C	397	54%, 40%, 6% •
1	D	397	55%, 38%, 5% •

2 Entry composition (i)

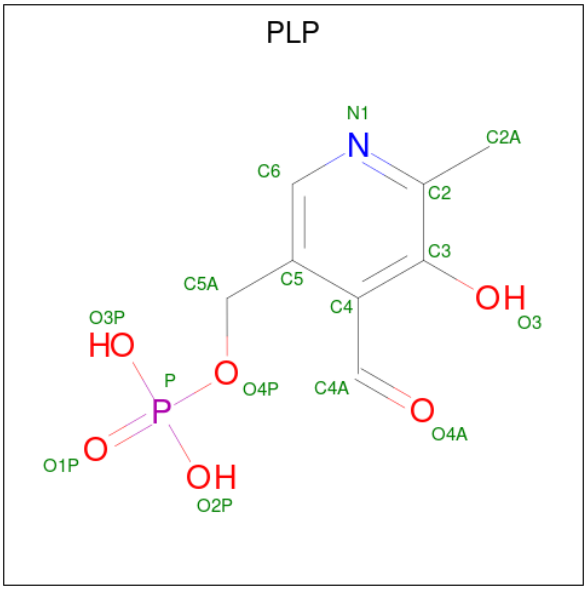
There are 3 unique types of molecules in this entry. The entry contains 12341 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-aminodipate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	3038	1949	536	545	8	0	0	0
1	B	394	3054	1960	539	547	8	0	0	0
1	C	396	3070	1971	541	550	8	0	0	0
1	D	391	3036	1946	538	544	8	0	0	0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	8	1	5	1	0	0
2	B	1	15	8	1	5	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	15	8	1	5	1	0	0
2	D	1	15	8	1	5	1	0	0

- Molecule 3 is water.

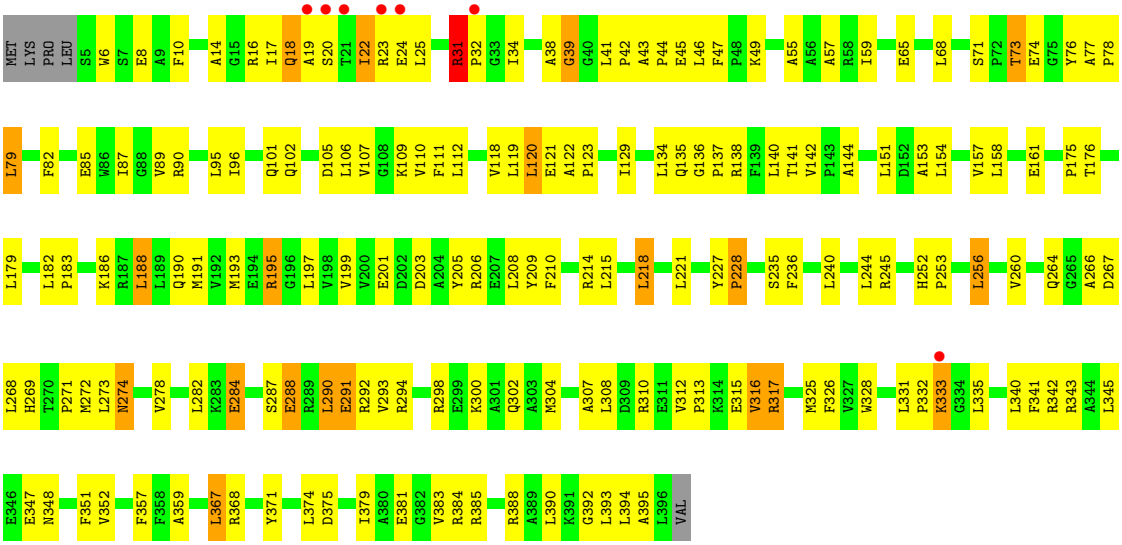
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	23	23	23	0	0
3	B	21	21	21	0	0
3	C	16	16	16	0	0
3	D	23	23	23	0	0

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 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.

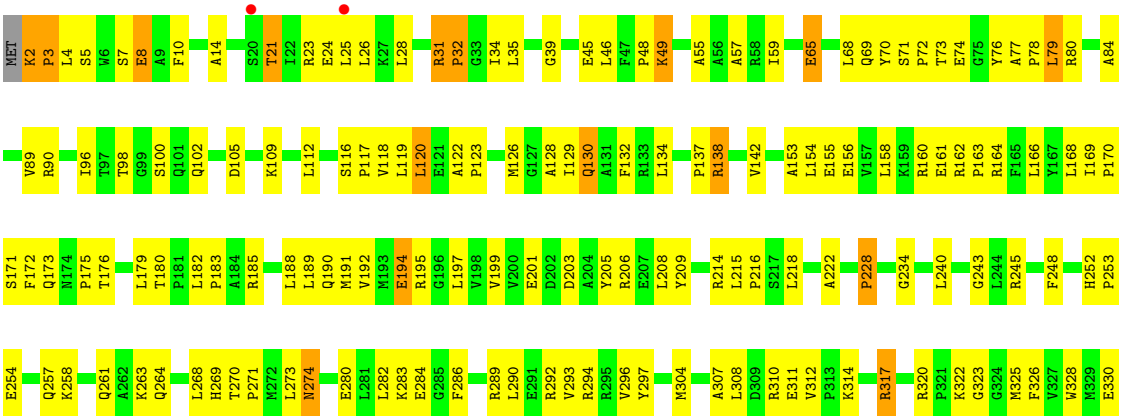
• Molecule 1: Alpha-aminodipate aminotransferase

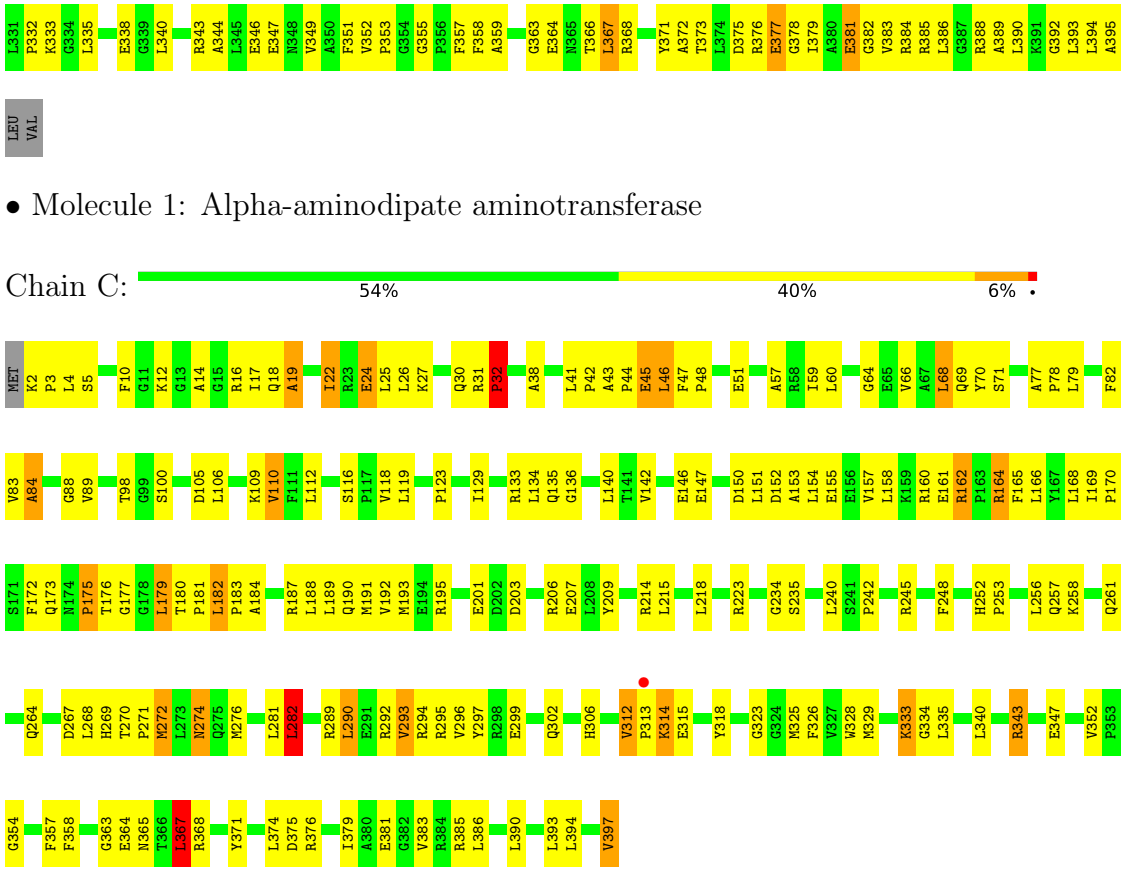
Chain A: 2% 54% 39% 5% •



• Molecule 1: Alpha-aminodipate aminotransferase

Chain B: % 49% 45% 5% •



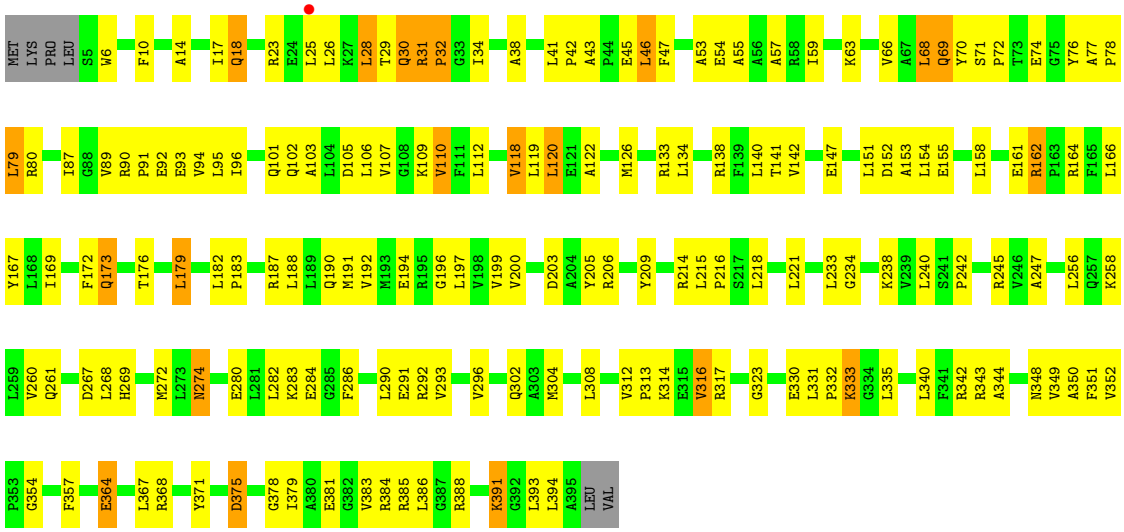


• Molecule 1: Alpha-aminodipate aminotransferase

Chain C: 54% 40% 6% •

• Molecule 1: Alpha-aminodipate aminotransferase

Chain D: 55% 38% 5% •



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.41Å 138.51Å 111.75Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	43.97 – 2.67 43.97 – 2.66	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.97-2.67) 97.8 (43.97-2.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.63 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.294 0.208 , 0.206	Depositor DCC
R_{free} test set	2391 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12341	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6286e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.36	0/3103	0.65	0/4196
1	B	0.34	0/3120	0.62	1/4219 (0.0%)
1	C	0.34	0/3136	0.63	3/4240 (0.1%)
1	D	0.35	0/3101	0.63	1/4192 (0.0%)
All	All	0.35	0/12460	0.63	5/16847 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	367	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	282	LEU	CA-CB-CG	5.74	128.49	115.30
1	C	32	PRO	N-CA-CB	5.49	109.88	103.30
1	B	32	PRO	N-CA-CB	5.26	109.61	103.30
1	D	32	PRO	N-CA-CB	5.20	109.53	103.30

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	3038	0	3072	161	0
1	B	3054	0	3092	185	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3070	0	3112	195	0
1	D	3036	0	3073	173	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
3	A	23	0	0	1	0
3	B	21	0	0	1	0
3	C	16	0	0	0	0
3	D	23	0	0	0	0
All	All	12341	0	12377	668	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 (668) 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:48:PRO:HB3	1:B:289:ARG:HH22	1.25	1.02
1:D:140:LEU:HD11	1:D:161:GLU:HG2	1.45	0.98
1:C:119:LEU:HD22	1:C:166:LEU:HG	1.44	0.96
1:B:274:ASN:HD22	1:B:274:ASN:H	1.12	0.95
1:D:274:ASN:HD22	1:D:274:ASN:H	0.98	0.94
1:D:343:ARG:HH12	1:D:393:LEU:HA	1.32	0.94
1:C:274:ASN:H	1:C:274:ASN:HD22	1.14	0.93
1:C:116:SER:HB2	1:C:164:ARG:HH11	1.33	0.93
1:C:27:LYS:HA	1:C:30:GLN:HE21	1.32	0.92
1:C:134:LEU:HD11	1:D:109:LYS:HD3	1.52	0.91
1:A:140:LEU:HD11	1:A:161:GLU:HG2	1.51	0.91
1:D:274:ASN:HD22	1:D:274:ASN:N	1.65	0.91
1:D:31:ARG:H	1:D:31:ARG:HD3	1.37	0.89
1:A:384:ARG:CZ	1:A:388:ARG:HH22	1.84	0.89
1:C:274:ASN:HD22	1:C:274:ASN:N	1.69	0.89
1:D:46:LEU:HD11	1:D:296:VAL:HG21	1.55	0.89
1:A:74:GLU:H	1:A:74:GLU:CD	1.76	0.88
1:B:2:LYS:NZ	1:B:2:LYS:HA	1.88	0.88
1:D:59:ILE:HD11	1:D:280:GLU:HG3	1.54	0.88
1:C:176:THR:HA	1:C:328:TRP:HB2	1.57	0.86
1:C:140:LEU:HD11	1:C:161:GLU:HG2	1.58	0.85
1:B:290:LEU:O	1:B:293:VAL:HG12	1.77	0.84
1:C:41:LEU:HB3	1:D:69:GLN:HE22	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ILE:HD11	1:D:258:LYS:HE3	1.60	0.83
1:C:390:LEU:O	1:C:394:LEU:HD23	1.79	0.82
1:B:332:PRO:HG2	1:B:335:LEU:HD12	1.61	0.82
1:B:77:ALA:HB3	1:B:78:PRO:HD3	1.60	0.82
1:D:17:ILE:HG23	1:D:134:LEU:HD23	1.60	0.82
1:D:79:LEU:HD13	1:D:96:ILE:HD13	1.62	0.81
1:B:48:PRO:HB3	1:B:289:ARG:NH2	1.94	0.81
1:C:116:SER:HB2	1:C:164:ARG:NH1	1.94	0.81
1:A:186:LYS:O	1:A:190:GLN:HG2	1.81	0.80
1:A:122:ALA:HB2	1:A:141:THR:HB	1.62	0.79
1:B:376:ARG:HH11	1:B:376:ARG:HB3	1.49	0.78
1:C:333:LYS:HE2	1:C:365:ASN:HD21	1.49	0.78
1:A:43:ALA:HB3	1:A:46:LEU:HD23	1.65	0.78
1:B:119:LEU:HD21	1:B:154:LEU:HD11	1.67	0.77
1:D:55:ALA:O	1:D:59:ILE:HG12	1.85	0.77
1:D:182:LEU:HD13	1:D:216:PRO:HD2	1.65	0.77
1:D:274:ASN:H	1:D:274:ASN:ND2	1.75	0.77
1:A:274:ASN:N	1:A:274:ASN:HD22	1.83	0.76
1:B:2:LYS:HA	1:B:2:LYS:HZ2	1.50	0.76
1:B:2:LYS:HD3	1:B:3:PRO:HD2	1.66	0.76
1:C:43:ALA:HB3	1:C:46:LEU:HD22	1.67	0.75
1:B:253:PRO:O	1:B:257:GLN:HG3	1.86	0.75
1:B:45:GLU:HG2	1:B:46:LEU:HD12	1.68	0.75
1:C:31:ARG:HG3	1:C:32:PRO:N	2.03	0.74
1:D:18:GLN:NE2	1:D:133:ARG:HD3	2.03	0.73
1:A:95:LEU:HB2	1:A:256:LEU:HD21	1.69	0.73
1:D:74:GLU:HB3	1:D:80:ARG:NH2	2.03	0.73
1:A:6:TRP:CB	1:B:254:GLU:HG2	2.19	0.73
1:A:274:ASN:HD22	1:A:274:ASN:H	1.37	0.73
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.71	0.73
1:A:79:LEU:HD13	1:A:96:ILE:HD13	1.71	0.73
1:D:343:ARG:NH1	1:D:393:LEU:HA	2.04	0.73
1:C:162:ARG:HG2	1:C:162:ARG:HH21	1.53	0.73
1:C:203:ASP:OD2	1:C:206:ARG:HB2	1.89	0.72
1:C:293:VAL:HG23	1:C:297:TYR:CE1	2.23	0.72
1:D:381:GLU:OE1	1:D:384:ARG:HD3	1.89	0.72
1:B:71:SER:HB2	1:B:72:PRO:HD2	1.71	0.72
1:C:234:GLY:HA3	1:C:248:PHE:CZ	2.25	0.72
1:B:117:PRO:HB2	1:B:163:PRO:HA	1.70	0.71
1:D:18:GLN:HE22	1:D:133:ARG:HD3	1.56	0.71
1:B:176:THR:HA	1:B:328:TRP:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLN:O	1:B:194:GLU:HB2	1.91	0.71
1:B:274:ASN:HD22	1:B:274:ASN:N	1.88	0.71
1:B:119:LEU:HD21	1:B:154:LEU:CD1	2.21	0.70
1:C:223:ARG:HE	1:C:223:ARG:HA	1.56	0.70
1:A:112:LEU:HD11	1:A:118:VAL:HG11	1.74	0.70
1:B:344:ALA:HB1	1:B:349:VAL:HG13	1.74	0.70
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.55	0.70
1:B:179:LEU:HD11	1:B:215:LEU:HD12	1.71	0.69
1:B:21:THR:O	1:B:25:LEU:HD13	1.92	0.69
1:B:84:ALA:HB1	1:B:89:VAL:O	1.93	0.69
1:C:151:LEU:HD11	1:C:184:ALA:HB1	1.75	0.69
1:A:49:LYS:HB2	1:A:49:LYS:NZ	2.08	0.69
1:B:203:ASP:OD2	1:B:206:ARG:HB2	1.93	0.69
1:D:274:ASN:N	1:D:274:ASN:ND2	2.37	0.69
1:A:300:LYS:HE2	1:A:374:LEU:O	1.93	0.68
1:B:317:ARG:HD3	1:B:317:ARG:N	2.08	0.68
1:D:102:GLN:O	1:D:106:LEU:HG	1.93	0.68
1:B:199:VAL:HG11	1:B:218:LEU:HD23	1.76	0.68
1:B:74:GLU:HB3	1:B:80:ARG:NH2	2.09	0.68
1:A:22:ILE:HG12	1:B:264:GLN:HE22	1.59	0.68
1:C:168:LEU:CD1	1:C:188:LEU:HD21	2.24	0.68
1:C:293:VAL:HG23	1:C:297:TYR:HE1	1.59	0.68
1:C:274:ASN:N	1:C:274:ASN:ND2	2.41	0.67
1:A:151:LEU:HD21	1:A:188:LEU:HD12	1.75	0.67
1:B:100:SER:HA	3:B:413:HOH:O	1.94	0.67
1:D:87:ILE:HG22	1:D:89:VAL:HG13	1.77	0.67
1:C:245:ARG:HD3	1:D:269:HIS:CE1	2.30	0.67
1:A:343:ARG:HH21	1:A:393:LEU:HD12	1.60	0.67
1:B:376:ARG:HB3	1:B:376:ARG:NH1	2.09	0.67
1:C:274:ASN:H	1:C:274:ASN:ND2	1.90	0.67
1:A:269:HIS:CE1	1:B:245:ARG:HD3	2.31	0.66
1:B:340:LEU:HD21	1:B:390:LEU:HA	1.77	0.66
1:B:162:ARG:NH2	1:B:162:ARG:HB3	2.10	0.66
1:C:335:LEU:HD11	1:C:393:LEU:HD23	1.76	0.66
1:B:79:LEU:HD13	1:B:96:ILE:HD12	1.77	0.66
1:C:16:ARG:HE	1:C:136:GLY:HA3	1.61	0.65
1:D:134:LEU:HD13	1:D:134:LEU:O	1.96	0.65
1:C:295:ARG:O	1:C:299:GLU:HG2	1.95	0.65
1:B:59:ILE:HD11	1:B:280:GLU:HG3	1.77	0.65
1:B:24:GLU:O	1:B:28:LEU:HG	1.97	0.65
1:B:156:GLU:O	1:B:160:ARG:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ILE:HD11	1:D:280:GLU:CG	2.27	0.65
1:A:6:TRP:HB3	1:B:254:GLU:HG2	1.79	0.65
1:D:106:LEU:O	1:D:110:VAL:HG12	1.97	0.65
1:B:23:ARG:HA	1:B:26:LEU:HG	1.80	0.64
1:D:17:ILE:HD12	1:D:18:GLN:N	2.13	0.64
1:B:332:PRO:HG2	1:B:335:LEU:CD1	2.27	0.64
1:C:47:PHE:CE2	1:D:69:GLN:HG2	2.32	0.64
1:D:76:TYR:CE2	1:D:78:PRO:HB2	2.33	0.64
1:A:22:ILE:HG12	1:B:264:GLN:NE2	2.12	0.63
1:D:169:ILE:HG21	1:D:173:GLN:HA	1.80	0.63
1:D:364:GLU:H	1:D:364:GLU:CD	2.01	0.63
1:C:152:ASP:O	1:C:155:GLU:HG2	1.99	0.63
1:D:29:THR:O	1:D:30:GLN:HB2	1.98	0.63
1:C:258:LYS:HD2	1:D:17:ILE:HD11	1.80	0.63
1:C:27:LYS:HA	1:C:30:GLN:NE2	2.11	0.63
1:A:298:ARG:O	1:A:302:GLN:HG3	1.99	0.63
1:C:182:LEU:HB3	1:C:183:PRO:HD3	1.79	0.63
1:D:10:PHE:HB3	1:D:14:ALA:CB	2.29	0.63
1:D:381:GLU:O	1:D:384:ARG:HB3	1.99	0.63
1:A:31:ARG:HH21	1:A:31:ARG:HG2	1.63	0.62
1:B:112:LEU:CD2	1:B:118:VAL:HG22	2.29	0.62
1:A:90:ARG:NH1	1:D:90:ARG:HG2	2.13	0.62
1:C:38:ALA:HA	1:C:352:VAL:HG23	1.82	0.62
1:C:48:PRO:HB2	1:C:51:GLU:HB3	1.81	0.62
1:C:218:LEU:HD12	1:C:218:LEU:H	1.64	0.62
1:D:256:LEU:O	1:D:260:VAL:HG23	1.98	0.62
1:D:375:ASP:HB3	1:D:378:GLY:H	1.64	0.62
1:A:140:LEU:CD1	1:A:161:GLU:HG2	2.26	0.62
1:A:304:MET:CE	1:A:371:TYR:HB3	2.30	0.62
1:D:31:ARG:HD3	1:D:31:ARG:N	2.07	0.62
1:C:14:ALA:O	1:C:17:ILE:HG12	2.00	0.61
1:A:290:LEU:O	1:A:293:VAL:HG22	1.99	0.61
1:C:22:ILE:N	1:C:25:LEU:HD13	2.16	0.61
1:C:261:GLN:HE21	1:D:17:ILE:HD13	1.65	0.61
1:C:170:PRO:HG2	1:C:218:LEU:HD13	1.82	0.61
1:A:153:ALA:O	1:A:157:VAL:HG23	2.00	0.61
1:A:287:SER:HB2	1:A:288:GLU:OE1	2.00	0.61
1:D:169:ILE:HB	1:D:173:GLN:HB2	1.83	0.61
1:B:2:LYS:HB3	1:B:3:PRO:HD2	1.82	0.61
1:D:119:LEU:HD23	1:D:119:LEU:C	2.21	0.61
1:C:71:SER:OG	1:C:272:MET:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLU:O	1:C:181:PRO:HD3	2.00	0.61
1:D:179:LEU:HD21	1:D:215:LEU:HD12	1.83	0.61
1:B:142:VAL:HG23	1:B:153:ALA:HB3	1.82	0.60
1:C:116:SER:CB	1:C:164:ARG:NH1	2.64	0.60
1:C:147:GLU:HG2	1:C:181:PRO:HG2	1.82	0.60
1:A:256:LEU:O	1:A:260:VAL:HG23	2.00	0.60
1:A:304:MET:HE3	1:A:371:TYR:HB3	1.83	0.60
1:C:10:PHE:HB3	1:C:14:ALA:HB2	1.84	0.60
1:D:162:ARG:HH21	1:D:162:ARG:HG2	1.66	0.60
1:D:169:ILE:HD12	1:D:169:ILE:N	2.15	0.60
1:A:95:LEU:CB	1:A:256:LEU:HD21	2.32	0.60
1:B:2:LYS:HA	1:B:2:LYS:HZ3	1.65	0.60
1:B:375:ASP:O	1:B:379:ILE:HG12	2.01	0.60
1:D:17:ILE:CG2	1:D:134:LEU:HD23	2.31	0.60
1:C:314:LYS:N	1:C:314:LYS:HD2	2.17	0.60
1:A:151:LEU:CD2	1:A:188:LEU:HD12	2.32	0.60
1:A:326:PHE:CD1	1:A:368:ARG:HD2	2.37	0.59
1:C:169:ILE:HD12	1:C:173:GLN:HG2	1.85	0.59
1:D:209:TYR:CE2	1:D:214:ARG:HB3	2.37	0.59
1:B:347:GLU:OE2	1:B:388:ARG:HD2	2.02	0.59
1:D:95:LEU:HB3	1:D:256:LEU:HD11	1.84	0.59
1:A:154:LEU:HD23	1:A:191:MET:CE	2.33	0.59
1:C:135:GLN:HE21	1:C:135:GLN:HA	1.66	0.59
1:A:206:ARG:HG3	1:A:214:ARG:HD2	1.83	0.59
1:B:297:TYR:HE2	1:B:372:ALA:HB1	1.67	0.59
1:A:176:THR:HA	1:A:328:TRP:HB2	1.85	0.59
1:B:364:GLU:CB	1:C:364:GLU:HG3	2.32	0.59
1:C:140:LEU:CD1	1:C:161:GLU:HG2	2.30	0.59
1:C:313:PRO:HB2	1:C:315:GLU:OE1	2.02	0.59
1:D:28:LEU:HD13	1:D:28:LEU:H	1.65	0.59
1:D:343:ARG:NH1	1:D:393:LEU:HD12	2.17	0.59
1:B:119:LEU:HD23	1:B:166:LEU:HG	1.86	0.58
1:C:187:ARG:HH11	1:C:187:ARG:HG3	1.67	0.58
1:C:302:GLN:HE21	1:C:306:HIS:CE1	2.21	0.58
1:D:192:VAL:HG11	1:D:199:VAL:HG23	1.85	0.58
1:B:138:ARG:HH22	1:B:161:GLU:CD	2.06	0.58
1:C:292:ARG:HH21	1:C:292:ARG:HG3	1.68	0.58
1:A:195:ARG:HB3	1:A:197:LEU:HG	1.84	0.58
1:B:282:LEU:HG	1:B:286:PHE:CD1	2.38	0.58
1:C:135:GLN:HA	1:C:135:GLN:NE2	2.19	0.58
1:C:161:GLU:HG3	1:C:162:ARG:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:O	1:D:293:VAL:HG12	2.04	0.58
1:A:77:ALA:HB3	1:A:78:PRO:HD3	1.86	0.57
1:C:71:SER:HB2	1:C:269:HIS:CD2	2.39	0.57
1:C:98:THR:O	1:C:98:THR:HG22	2.05	0.57
1:D:290:LEU:HA	1:D:293:VAL:HG12	1.85	0.57
1:D:391:LYS:HE3	1:D:391:LYS:HA	1.86	0.57
1:A:154:LEU:HD23	1:A:191:MET:HE1	1.87	0.57
1:B:310:ARG:HB2	1:B:310:ARG:NH2	2.19	0.57
1:C:272:MET:O	1:C:276:MET:HG3	2.04	0.57
1:D:28:LEU:HD13	1:D:28:LEU:N	2.19	0.57
1:D:209:TYR:CD2	1:D:214:ARG:HB3	2.40	0.57
1:D:169:ILE:CG2	1:D:173:GLN:HA	2.35	0.57
1:C:379:ILE:O	1:C:383:VAL:HG23	2.03	0.57
1:A:101:GLN:HA	1:A:101:GLN:NE2	2.19	0.57
1:B:364:GLU:HB3	1:C:364:GLU:HG3	1.86	0.57
1:D:283:LYS:HG3	1:D:284:GLU:HG2	1.87	0.57
1:B:330:GLU:HG2	1:B:366:THR:HG22	1.86	0.56
1:D:103:ALA:HB1	1:D:233:LEU:HD22	1.87	0.56
1:A:307:ALA:C	1:A:383:VAL:HG11	2.26	0.56
1:A:342:ARG:HG3	1:A:342:ARG:NH1	2.20	0.56
1:B:317:ARG:HD3	1:B:317:ARG:H	1.69	0.56
1:C:71:SER:H	1:C:269:HIS:CE1	2.23	0.56
1:C:158:LEU:HB3	1:C:195:ARG:NE	2.19	0.56
1:C:170:PRO:HG2	1:C:218:LEU:CD1	2.35	0.56
1:D:167:TYR:CE2	1:D:169:ILE:HD11	2.40	0.56
1:D:192:VAL:HG13	1:D:197:LEU:HB2	1.87	0.56
1:B:206:ARG:HG3	1:B:214:ARG:HD2	1.87	0.56
1:D:77:ALA:HB3	1:D:78:PRO:HD3	1.87	0.56
1:B:189:LEU:HD11	1:B:222:ALA:HB2	1.86	0.56
1:A:375:ASP:O	1:A:379:ILE:HG12	2.06	0.56
1:C:257:GLN:NE2	1:C:257:GLN:HA	2.21	0.56
1:A:381:GLU:O	1:A:385:ARG:HG3	2.05	0.56
1:B:120:LEU:HD11	1:B:129:ILE:CD1	2.36	0.56
1:A:201:GLU:OE2	1:A:218:LEU:HB2	2.06	0.56
1:B:45:GLU:HG2	1:B:46:LEU:CD1	2.35	0.56
1:C:47:PHE:HE2	1:D:69:GLN:HG2	1.69	0.56
1:B:169:ILE:CG2	1:B:173:GLN:HA	2.36	0.55
1:A:158:LEU:HD22	1:A:191:MET:HE3	1.88	0.55
1:A:343:ARG:HH21	1:A:393:LEU:CD1	2.19	0.55
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.69	0.55
1:D:343:ARG:HH11	1:D:343:ARG:HG3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ALA:HA	1:A:352:VAL:HG23	1.88	0.55
1:A:31:ARG:HD2	1:A:31:ARG:C	2.27	0.55
1:A:122:ALA:HB2	1:A:141:THR:CB	2.36	0.55
1:B:340:LEU:HD12	1:B:351:PHE:CZ	2.42	0.55
1:D:391:LYS:HE3	1:D:391:LYS:O	2.07	0.55
1:A:95:LEU:HB2	1:A:256:LEU:CD2	2.37	0.55
1:C:16:ARG:HD2	1:C:134:LEU:O	2.06	0.55
1:C:154:LEU:HG	1:C:191:MET:CE	2.36	0.55
1:C:312:VAL:HG21	1:C:318:TYR:CE1	2.42	0.55
1:D:384:ARG:HH22	1:D:388:ARG:NH1	2.05	0.55
1:A:79:LEU:HD13	1:A:96:ILE:CD1	2.36	0.55
1:B:158:LEU:HD21	1:B:197:LEU:HD12	1.89	0.55
1:C:18:GLN:NE2	1:C:133:ARG:HD3	2.22	0.55
1:C:252:HIS:CG	1:D:6:TRP:HE1	2.25	0.55
1:A:55:ALA:O	1:A:59:ILE:HG13	2.06	0.55
1:A:136:GLY:N	1:A:137:PRO:CD	2.70	0.55
1:A:312:VAL:HG12	1:A:316:VAL:HG13	1.88	0.55
1:B:364:GLU:HG3	1:C:333:LYS:HE2	1.88	0.55
1:C:261:GLN:HE21	1:D:17:ILE:CD1	2.20	0.54
1:B:180:THR:O	1:B:185:ARG:NE	2.38	0.54
1:B:292:ARG:O	1:B:296:VAL:HG23	2.07	0.54
1:C:168:LEU:HD11	1:C:188:LEU:HD21	1.89	0.54
1:C:333:LYS:HE2	1:C:365:ASN:ND2	2.19	0.54
1:D:314:LYS:O	1:D:314:LYS:HG2	2.07	0.54
1:C:258:LYS:CD	1:D:17:ILE:HD11	2.37	0.54
1:C:358:PHE:CE2	1:C:363:GLY:HA3	2.42	0.54
1:A:120:LEU:HD11	1:A:129:ILE:HD13	1.89	0.54
1:A:274:ASN:N	1:A:274:ASN:ND2	2.53	0.54
1:B:343:ARG:HE	1:B:392:GLY:HA3	1.72	0.54
1:C:154:LEU:HG	1:C:191:MET:HE1	1.90	0.54
1:D:155:GLU:HA	1:D:191:MET:HE1	1.89	0.54
1:A:271:PRO:HG3	1:B:271:PRO:HG2	1.90	0.54
1:A:293:VAL:HG23	1:A:294:ARG:N	2.22	0.54
1:B:134:LEU:HD13	1:B:134:LEU:O	2.08	0.54
1:B:243:GLY:O	1:B:245:ARG:HG2	2.08	0.54
1:D:304:MET:HG3	1:D:371:TYR:CD2	2.43	0.53
1:B:340:LEU:HD23	1:B:393:LEU:HD22	1.90	0.53
1:C:253:PRO:O	1:C:257:GLN:HG2	2.07	0.53
1:D:173:GLN:HG2	1:D:176:THR:OG1	2.08	0.53
1:A:31:ARG:NH1	1:A:348:ASN:HD22	2.07	0.53
1:D:29:THR:HA	1:D:34:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ARG:HG2	1:C:162:ARG:NH2	2.23	0.53
1:D:105:ASP:O	1:D:109:LYS:HG3	2.08	0.53
1:B:205:TYR:HD1	1:B:208:LEU:HD22	1.74	0.53
1:B:234:GLY:HA3	1:B:248:PHE:CZ	2.43	0.53
1:D:352:VAL:CG1	1:D:368:ARG:HB3	2.38	0.53
1:A:79:LEU:CD1	1:A:96:ILE:HD13	2.37	0.52
1:A:129:ILE:HD12	1:A:359:ALA:HB2	1.91	0.52
1:B:112:LEU:HD21	1:B:118:VAL:HG22	1.92	0.52
1:C:142:VAL:HG22	1:C:150:ASP:HB3	1.92	0.52
1:C:289:ARG:O	1:C:293:VAL:HG12	2.08	0.52
1:B:155:GLU:HG3	1:B:191:MET:HE3	1.90	0.52
1:A:49:LYS:HB2	1:A:49:LYS:HZ3	1.74	0.52
1:C:31:ARG:CG	1:C:32:PRO:N	2.71	0.52
1:D:216:PRO:HB2	1:D:221:LEU:HD21	1.91	0.52
1:B:326:PHE:CD1	1:B:368:ARG:HD2	2.44	0.52
1:D:352:VAL:HG13	1:D:352:VAL:O	2.10	0.52
1:A:315:GLU:CD	1:A:315:GLU:N	2.62	0.52
1:C:325:MET:HA	1:C:371:TYR:CZ	2.45	0.52
1:A:119:LEU:HD11	1:A:154:LEU:CD1	2.39	0.52
1:A:267:ASP:O	1:A:268:LEU:HB2	2.09	0.52
1:D:90:ARG:HD3	1:D:91:PRO:HD2	1.92	0.52
1:B:274:ASN:H	1:B:274:ASN:ND2	1.89	0.52
1:D:234:GLY:O	1:D:247:ALA:HB1	2.10	0.52
1:D:313:PRO:O	1:D:316:VAL:HG13	2.10	0.52
1:B:112:LEU:HD22	1:B:118:VAL:HG22	1.92	0.52
1:B:166:LEU:HD12	1:B:166:LEU:N	2.24	0.52
1:C:18:GLN:O	1:C:19:ALA:C	2.48	0.52
1:A:199:VAL:HG11	1:A:218:LEU:HD23	1.92	0.51
1:A:347:GLU:OE1	1:A:388:ARG:HD2	2.10	0.51
1:C:27:LYS:CA	1:C:30:GLN:HE21	2.16	0.51
1:B:46:LEU:CD2	1:B:293:VAL:HG23	2.41	0.51
1:A:44:PRO:HA	1:A:47:PHE:CE2	2.45	0.51
1:B:71:SER:H	1:B:269:HIS:CE1	2.29	0.51
1:B:286:PHE:O	1:B:290:LEU:HD13	2.11	0.51
1:C:45:GLU:HG2	1:C:46:LEU:HD13	1.92	0.51
1:C:207:GLU:O	1:C:294:ARG:HD3	2.10	0.51
1:A:392:GLY:O	1:A:395:ALA:HB3	2.11	0.51
1:B:31:ARG:H	1:B:34:ILE:HG21	1.75	0.51
1:D:95:LEU:CB	1:D:256:LEU:HD11	2.40	0.51
1:D:317:ARG:NH2	1:D:330:GLU:HB3	2.25	0.51
1:B:325:MET:HA	1:B:371:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:MET:HG3	1:D:371:TYR:HD2	1.76	0.51
1:D:375:ASP:O	1:D:379:ILE:HG13	2.10	0.51
1:A:315:GLU:CD	1:A:315:GLU:H	2.14	0.51
1:B:112:LEU:CD1	1:B:118:VAL:HG21	2.41	0.51
1:B:138:ARG:NH2	1:B:161:GLU:OE1	2.43	0.51
1:D:162:ARG:HG3	1:D:197:LEU:HD21	1.92	0.51
1:D:343:ARG:NH1	1:D:343:ARG:HG3	2.26	0.51
1:B:119:LEU:CD2	1:B:154:LEU:HD11	2.40	0.51
1:A:274:ASN:HD21	1:B:274:ASN:HD21	1.59	0.51
1:D:23:ARG:HH21	1:D:23:ARG:HG3	1.75	0.51
1:D:79:LEU:HD13	1:D:96:ILE:CD1	2.39	0.51
1:C:293:VAL:O	1:C:297:TYR:HD1	1.94	0.50
1:D:122:ALA:HB2	1:D:141:THR:HB	1.93	0.50
1:D:203:ASP:OD2	1:D:206:ARG:HB2	2.11	0.50
1:A:8:GLU:O	1:A:8:GLU:HG3	2.11	0.50
1:A:76:TYR:CE2	1:A:78:PRO:HB2	2.46	0.50
1:A:119:LEU:HD11	1:A:154:LEU:HD11	1.94	0.50
1:C:335:LEU:HD22	1:C:394:LEU:HD21	1.93	0.50
1:B:98:THR:HG22	1:B:98:THR:O	2.12	0.50
1:D:63:LYS:HB3	1:D:66:VAL:CG1	2.41	0.50
1:B:120:LEU:HD11	1:B:129:ILE:HD13	1.94	0.50
1:C:134:LEU:O	1:C:134:LEU:HD23	2.11	0.50
1:C:173:GLN:O	1:C:177:GLY:N	2.40	0.50
1:A:193:MET:HG2	1:A:227:TYR:CG	2.45	0.50
1:B:377:GLU:O	1:B:381:GLU:HB2	2.11	0.50
1:C:158:LEU:HB3	1:C:195:ARG:CD	2.42	0.50
1:C:292:ARG:O	1:C:296:VAL:HG23	2.12	0.50
1:C:312:VAL:HG21	1:C:318:TYR:HE1	1.76	0.50
1:C:17:ILE:HD11	1:D:258:LYS:CE	2.36	0.50
1:D:340:LEU:HD12	1:D:351:PHE:CZ	2.46	0.50
1:D:342:ARG:HG2	1:D:342:ARG:HH11	1.75	0.50
1:C:41:LEU:HD23	1:D:69:GLN:NE2	2.26	0.50
1:D:340:LEU:HD23	1:D:393:LEU:HD22	1.93	0.50
1:B:118:VAL:HG23	1:B:137:PRO:HB2	1.93	0.49
1:C:12:LYS:HB2	1:C:16:ARG:HH12	1.77	0.49
1:A:138:ARG:NH2	1:A:161:GLU:CD	2.65	0.49
1:C:206:ARG:NH2	1:C:214:ARG:NH2	2.59	0.49
1:C:38:ALA:HB1	1:C:352:VAL:HG22	1.93	0.49
1:C:290:LEU:O	1:C:293:VAL:HG13	2.13	0.49
1:A:112:LEU:HD21	1:A:118:VAL:CG1	2.43	0.49
1:A:123:PRO:HB2	1:A:357:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:CD	1:A:294:ARG:HH21	2.16	0.49
1:B:5:SER:HB3	1:B:8:GLU:HG2	1.95	0.49
1:B:55:ALA:O	1:B:59:ILE:HG13	2.12	0.49
1:C:147:GLU:HG2	1:C:181:PRO:CG	2.41	0.49
1:B:2:LYS:CB	1:B:3:PRO:HD2	2.42	0.49
1:B:69:GLN:HG3	1:B:70:TYR:N	2.28	0.49
1:B:347:GLU:O	1:B:385:ARG:HD3	2.13	0.49
1:A:209:TYR:CE2	1:A:214:ARG:HB2	2.48	0.49
1:C:82:PHE:CZ	1:C:282:LEU:HD23	2.48	0.49
1:A:119:LEU:HD23	1:A:120:LEU:N	2.28	0.49
1:C:69:GLN:HB2	1:D:47:PHE:HE2	1.78	0.49
1:C:69:GLN:NE2	1:D:41:LEU:HB3	2.28	0.49
1:C:375:ASP:O	1:C:379:ILE:HG13	2.13	0.49
1:D:291:GLU:OE1	1:D:291:GLU:HA	2.13	0.49
1:A:313:PRO:HG2	1:A:394:LEU:HD12	1.95	0.49
1:A:210:PHE:HB3	1:A:298:ARG:HG3	1.95	0.48
1:D:30:GLN:O	1:D:30:GLN:HG2	2.13	0.48
1:A:57:ALA:HB2	1:B:57:ALA:HB2	1.93	0.48
1:A:119:LEU:HD23	1:A:119:LEU:C	2.33	0.48
1:B:172:PHE:CD1	1:B:179:LEU:HD23	2.48	0.48
1:B:304:MET:O	1:B:308:LEU:HG	2.12	0.48
1:A:135:GLN:HA	1:A:135:GLN:NE2	2.28	0.48
1:B:269:HIS:HD2	1:B:270:THR:O	1.96	0.48
1:B:340:LEU:HD21	1:B:390:LEU:HD12	1.96	0.48
1:C:326:PHE:CD1	1:C:368:ARG:HD2	2.48	0.48
1:D:107:VAL:HG11	1:D:200:VAL:HG21	1.96	0.48
1:D:119:LEU:HD22	1:D:166:LEU:HG	1.94	0.48
1:A:307:ALA:HA	1:A:310:ARG:NH2	2.29	0.48
1:B:172:PHE:CE1	1:B:323:GLY:HA3	2.49	0.48
1:B:343:ARG:HH21	1:B:392:GLY:HA3	1.79	0.48
1:B:310:ARG:CB	1:B:310:ARG:HH21	2.26	0.48
1:C:57:ALA:HB2	1:D:57:ALA:HB2	1.95	0.48
1:C:256:LEU:O	1:C:256:LEU:HD13	2.14	0.48
1:A:105:ASP:O	1:A:109:LYS:HG3	2.12	0.48
1:C:172:PHE:CE1	1:C:323:GLY:HA3	2.48	0.48
1:A:38:ALA:O	1:A:39:GLY:O	2.31	0.48
1:B:154:LEU:HD23	1:B:191:MET:CE	2.43	0.48
1:B:154:LEU:HD23	1:B:191:MET:HE2	1.96	0.48
1:A:304:MET:HE1	1:A:379:ILE:HG23	1.96	0.48
1:D:267:ASP:O	1:D:268:LEU:HB2	2.14	0.48
1:A:44:PRO:HA	1:A:47:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG23	1:A:153:ALA:HB3	1.96	0.48
1:B:35:LEU:O	1:B:349:VAL:HA	2.14	0.48
1:D:292:ARG:O	1:D:296:VAL:HG23	2.14	0.48
1:A:19:ALA:H	1:B:261:GLN:NE2	2.11	0.47
1:A:312:VAL:HG13	1:A:390:LEU:HD13	1.95	0.47
1:B:347:GLU:HG3	1:B:389:ALA:HB2	1.94	0.47
1:C:218:LEU:HD12	1:C:218:LEU:N	2.26	0.47
1:A:107:VAL:HG13	1:A:111:PHE:CD2	2.49	0.47
1:A:138:ARG:HH21	1:A:161:GLU:CD	2.17	0.47
1:C:270:THR:O	1:C:271:PRO:C	2.52	0.47
1:A:332:PRO:HG2	1:A:335:LEU:HD12	1.94	0.47
1:B:340:LEU:HD23	1:B:393:LEU:CD2	2.44	0.47
1:C:168:LEU:C	1:C:170:PRO:HD3	2.35	0.47
1:A:121:GLU:HB3	1:A:144:ALA:HB2	1.97	0.47
1:C:16:ARG:NE	1:C:136:GLY:HA3	2.26	0.47
1:C:105:ASP:O	1:C:109:LYS:HG3	2.12	0.47
1:C:105:ASP:OD2	1:C:109:LYS:HE3	2.15	0.47
1:A:65:GLU:CD	1:A:65:GLU:H	2.17	0.47
1:B:77:ALA:CB	1:B:78:PRO:HD3	2.40	0.47
1:C:26:LEU:O	1:C:30:GLN:HG2	2.14	0.47
1:C:44:PRO:O	1:C:46:LEU:N	2.47	0.47
1:D:38:ALA:HB2	1:D:351:PHE:C	2.34	0.47
1:D:190:GLN:O	1:D:194:GLU:HB2	2.15	0.47
1:A:73:THR:OG1	1:A:264:GLN:HG2	2.13	0.47
1:B:343:ARG:HG3	1:B:343:ARG:HH11	1.80	0.47
1:C:79:LEU:O	1:C:83:VAL:HG23	2.14	0.47
1:C:168:LEU:HD13	1:C:188:LEU:HD21	1.94	0.47
1:D:349:VAL:HG22	1:D:350:ALA:N	2.29	0.47
1:B:116:SER:OG	1:B:164:ARG:NH1	2.47	0.47
1:B:175:PRO:HB3	1:B:368:ARG:HD3	1.96	0.47
1:C:269:HIS:CE1	1:D:245:ARG:HD3	2.49	0.47
1:C:302:GLN:NE2	1:C:306:HIS:NE2	2.62	0.47
1:A:22:ILE:HG23	1:A:23:ARG:N	2.30	0.47
1:B:286:PHE:CZ	1:B:290:LEU:HD11	2.50	0.46
1:C:25:LEU:HD21	1:C:352:VAL:HG13	1.97	0.46
1:C:119:LEU:HD22	1:C:166:LEU:CG	2.31	0.46
1:A:253:PRO:HG2	1:D:92:GLU:HG2	1.95	0.46
1:C:188:LEU:O	1:C:192:VAL:HG23	2.15	0.46
1:A:43:ALA:HB3	1:A:46:LEU:CD2	2.41	0.46
1:A:134:LEU:O	1:A:134:LEU:HD13	2.15	0.46
1:B:46:LEU:HD11	1:B:296:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:HIS:CE1	1:B:254:GLU:H	2.34	0.46
1:C:189:LEU:O	1:C:193:MET:HG2	2.15	0.46
1:C:218:LEU:H	1:C:218:LEU:CD1	2.28	0.46
1:A:293:VAL:CG2	1:A:294:ARG:N	2.78	0.46
1:B:34:ILE:HG23	1:B:34:ILE:O	2.16	0.46
1:B:73:THR:CG2	1:B:263:LYS:HD2	2.45	0.46
1:C:223:ARG:HA	1:C:223:ARG:NE	2.28	0.46
1:B:74:GLU:HB3	1:B:80:ARG:CZ	2.45	0.46
1:C:206:ARG:HG2	1:C:207:GLU:OE2	2.15	0.46
1:D:71:SER:HB3	1:D:272:MET:HE1	1.97	0.46
1:D:187:ARG:O	1:D:191:MET:HG3	2.15	0.46
1:D:391:LYS:HE3	1:D:391:LYS:CA	2.46	0.46
1:C:129:ILE:O	1:C:133:ARG:HB2	2.15	0.46
1:C:257:GLN:HA	1:C:257:GLN:HE21	1.80	0.46
1:D:340:LEU:HD13	1:D:340:LEU:O	2.16	0.46
1:B:364:GLU:H	1:B:364:GLU:CD	2.16	0.46
1:A:179:LEU:HD11	1:A:215:LEU:CD1	2.46	0.46
1:B:172:PHE:CE1	1:B:179:LEU:HD23	2.51	0.46
1:D:290:LEU:C	1:D:293:VAL:HG12	2.36	0.46
1:D:354:GLY:HA2	1:D:357:PHE:HD2	1.80	0.46
1:B:367:LEU:HD13	1:B:367:LEU:N	2.32	0.46
1:D:74:GLU:HB3	1:D:80:ARG:HH21	1.80	0.46
1:D:120:LEU:O	1:D:120:LEU:HD23	2.16	0.46
1:B:73:THR:HG23	1:B:263:LYS:HD2	1.98	0.45
1:C:106:LEU:O	1:C:110:VAL:HG13	2.16	0.45
1:D:152:ASP:O	1:D:155:GLU:HB3	2.16	0.45
1:A:14:ALA:HA	1:A:17:ILE:HD11	1.97	0.45
1:A:71:SER:HB2	1:A:272:MET:HE2	1.98	0.45
1:C:4:LEU:HD22	1:C:5:SER:N	2.31	0.45
1:C:68:LEU:HD23	1:D:47:PHE:HB3	1.97	0.45
1:C:119:LEU:HD12	1:C:157:VAL:HG11	1.97	0.45
1:C:209:TYR:CD2	1:C:214:ARG:HB3	2.51	0.45
1:A:307:ALA:HB1	1:A:383:VAL:HB	1.97	0.45
1:B:112:LEU:HD13	1:B:118:VAL:HG21	1.99	0.45
1:B:358:PHE:CE2	1:B:363:GLY:HA3	2.51	0.45
1:C:164:ARG:HD2	1:C:164:ARG:HA	1.68	0.45
1:D:172:PHE:CE1	1:D:323:GLY:HA3	2.52	0.45
1:D:290:LEU:CA	1:D:293:VAL:HG12	2.46	0.45
1:A:340:LEU:HD22	1:A:351:PHE:CE1	2.51	0.45
1:B:128:ALA:HB1	1:B:132:PHE:CE2	2.51	0.45
1:B:201:GLU:OE2	1:B:218:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD11	1:C:154:LEU:CD1	2.46	0.45
1:C:245:ARG:NH2	1:D:268:LEU:HB2	2.31	0.45
1:C:381:GLU:O	1:C:385:ARG:HG3	2.16	0.45
1:A:49:LYS:HB2	1:A:49:LYS:HZ2	1.81	0.45
1:A:292:ARG:HB3	3:A:417:HOH:O	2.17	0.45
1:B:123:PRO:HB2	1:B:357:PHE:HB3	1.98	0.45
1:A:102:GLN:O	1:A:105:ASP:N	2.48	0.45
1:B:376:ARG:HH11	1:B:376:ARG:CB	2.24	0.45
1:C:4:LEU:HD22	1:C:5:SER:H	1.82	0.45
1:D:140:LEU:CD1	1:D:161:GLU:HG2	2.33	0.45
1:A:332:PRO:HG2	1:A:335:LEU:CD1	2.46	0.45
1:C:302:GLN:HG3	1:C:306:HIS:CE1	2.51	0.45
1:A:107:VAL:HG13	1:A:111:PHE:HD2	1.81	0.45
1:B:76:TYR:CE1	1:B:78:PRO:HD2	2.51	0.45
1:C:201:GLU:OE2	1:C:218:LEU:HD13	2.16	0.45
1:A:45:GLU:H	1:A:45:GLU:HG2	1.48	0.45
1:C:84:ALA:O	1:C:88:GLY:N	2.37	0.45
1:D:364:GLU:CD	1:D:364:GLU:N	2.69	0.45
1:D:138:ARG:HH22	1:D:161:GLU:CD	2.20	0.45
1:D:308:LEU:O	1:D:312:VAL:HB	2.17	0.45
1:B:394:LEU:O	1:B:395:ALA:HB2	2.17	0.44
1:C:2:LYS:HB3	1:C:3:PRO:CD	2.47	0.44
1:D:147:GLU:OE1	1:D:147:GLU:HA	2.17	0.44
1:A:384:ARG:NH1	1:A:388:ARG:HH22	2.14	0.44
1:C:82:PHE:CE2	1:C:282:LEU:HD23	2.52	0.44
1:D:188:LEU:O	1:D:188:LEU:HD13	2.16	0.44
1:B:175:PRO:CB	1:B:368:ARG:HD3	2.47	0.44
1:B:10:PHE:HB3	1:B:14:ALA:CB	2.47	0.44
1:B:252:HIS:CE1	1:B:253:PRO:HG2	2.51	0.44
1:C:187:ARG:HH11	1:C:187:ARG:CG	2.28	0.44
1:A:351:PHE:CE2	1:A:367:LEU:HG	2.53	0.44
1:B:105:ASP:OD2	1:B:109:LYS:HE3	2.18	0.44
1:B:169:ILE:HB	1:B:173:GLN:HG3	1.99	0.44
1:B:274:ASN:N	1:B:274:ASN:ND2	2.55	0.44
1:C:176:THR:HA	1:C:328:TRP:CB	2.37	0.44
1:C:354:GLY:HA2	1:C:357:PHE:HD2	1.83	0.44
1:A:18:GLN:HA	1:B:261:GLN:HE22	1.83	0.44
1:C:147:GLU:O	1:C:180:THR:HA	2.17	0.44
1:C:289:ARG:HG3	1:C:289:ARG:HH11	1.81	0.44
1:D:25:LEU:C	1:D:25:LEU:HD12	2.38	0.44
1:D:80:ARG:NH2	1:D:94:VAL:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HD13	1:B:188:LEU:HD21	1.99	0.44
1:C:123:PRO:HB2	1:C:357:PHE:HB3	1.99	0.44
1:C:293:VAL:HG23	1:C:297:TYR:CD1	2.51	0.44
1:D:282:LEU:HG	1:D:286:PHE:CD1	2.53	0.44
1:A:245:ARG:HD3	1:B:269:HIS:NE2	2.33	0.43
1:C:4:LEU:HD23	1:D:196:GLY:O	2.18	0.43
1:C:17:ILE:HD12	1:D:261:GLN:HB2	2.00	0.43
1:D:188:LEU:HD12	1:D:218:LEU:HD11	2.00	0.43
1:A:205:TYR:HE1	1:A:325:MET:HE3	1.83	0.43
1:B:192:VAL:HG21	1:B:199:VAL:HG21	2.00	0.43
1:C:24:GLU:CD	1:C:25:LEU:HD12	2.38	0.43
1:C:112:LEU:HD21	1:C:165:PHE:CE2	2.52	0.43
1:C:295:ARG:HG2	1:C:299:GLU:OE2	2.18	0.43
1:A:74:GLU:CD	1:A:74:GLU:N	2.54	0.43
1:A:101:GLN:HG2	1:B:268:LEU:HG	2.01	0.43
1:B:282:LEU:HG	1:B:286:PHE:CE1	2.52	0.43
1:C:77:ALA:HB3	1:C:78:PRO:CD	2.48	0.43
1:C:343:ARG:HH11	1:C:347:GLU:CG	2.31	0.43
1:A:300:LYS:CE	1:A:374:LEU:O	2.64	0.43
1:B:206:ARG:HG3	1:B:214:ARG:CD	2.48	0.43
1:A:20:SER:HA	1:A:24:GLU:OE1	2.18	0.43
1:A:31:ARG:HG2	1:A:31:ARG:NH2	2.31	0.43
1:A:235:SER:OG	1:A:236:PHE:N	2.51	0.43
1:A:284:GLU:OE1	1:A:284:GLU:HA	2.19	0.43
1:C:10:PHE:HB3	1:C:14:ALA:CB	2.46	0.43
1:A:87:ILE:HG22	1:A:89:VAL:HG13	2.00	0.43
1:A:317:ARG:HD3	1:A:317:ARG:H	1.84	0.43
1:B:169:ILE:N	1:B:170:PRO:HD3	2.33	0.43
1:B:263:LYS:HE3	1:B:269:HIS:HA	2.01	0.43
1:B:307:ALA:HA	1:B:310:ARG:NH1	2.34	0.43
1:C:376:ARG:HH11	1:C:376:ARG:HB2	1.84	0.43
1:D:25:LEU:HD12	1:D:26:LEU:N	2.34	0.43
1:B:171:SER:HA	1:B:179:LEU:HD22	2.00	0.43
1:B:286:PHE:CE1	1:B:290:LEU:HD11	2.54	0.43
1:C:84:ALA:HB1	1:C:89:VAL:O	2.19	0.43
1:C:268:LEU:HG	1:D:101:GLN:HG2	2.01	0.43
1:A:45:GLU:HG3	1:A:46:LEU:HD22	2.01	0.43
1:A:288:GLU:OE1	1:A:288:GLU:N	2.52	0.43
1:D:43:ALA:HB1	1:D:45:GLU:OE1	2.19	0.43
1:D:126:MET:HG3	1:D:357:PHE:CD1	2.54	0.43
1:D:142:VAL:HG23	1:D:153:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:GLY:HA2	1:D:357:PHE:CD2	2.54	0.43
1:A:331:LEU:HD11	1:A:340:LEU:HD12	2.01	0.43
1:D:42:PRO:HD2	1:D:242:PRO:HG3	2.00	0.43
1:B:122:ALA:HA	1:B:123:PRO:HA	1.87	0.42
1:B:352:VAL:HG12	1:B:353:PRO:O	2.19	0.42
1:C:47:PHE:HB3	1:D:68:LEU:HD23	2.01	0.42
1:C:71:SER:HB3	1:C:272:MET:CE	2.49	0.42
1:D:331:LEU:HB3	1:D:332:PRO:HD2	2.00	0.42
1:B:65:GLU:H	1:B:65:GLU:CD	2.23	0.42
1:B:162:ARG:HB3	1:B:162:ARG:CZ	2.49	0.42
1:B:192:VAL:HG13	1:B:197:LEU:O	2.19	0.42
1:A:208:LEU:N	1:A:208:LEU:HD12	2.34	0.42
1:A:381:GLU:O	1:A:384:ARG:HB3	2.19	0.42
1:B:169:ILE:HG22	1:B:173:GLN:HA	1.99	0.42
1:C:44:PRO:HA	1:C:47:PHE:CE2	2.54	0.42
1:C:161:GLU:HG3	1:C:162:ARG:H	1.83	0.42
1:C:334:GLY:O	1:C:397:VAL:HG21	2.19	0.42
1:D:71:SER:HB3	1:D:72:PRO:HD2	2.01	0.42
1:D:332:PRO:O	1:D:333:LYS:C	2.57	0.42
1:B:129:ILE:HD12	1:B:359:ALA:HB2	2.01	0.42
1:C:192:VAL:HG12	1:C:193:MET:N	2.34	0.42
1:D:112:LEU:HD21	1:D:118:VAL:CG1	2.49	0.42
1:D:205:TYR:CZ	1:D:238:LYS:HE2	2.54	0.42
1:A:158:LEU:HB3	1:A:195:ARG:CZ	2.49	0.42
1:A:304:MET:HB2	1:A:304:MET:HE2	1.93	0.42
1:A:308:LEU:HD22	1:A:312:VAL:HG21	2.02	0.42
1:A:341:PHE:O	1:A:345:LEU:HG	2.20	0.42
1:B:311:GLU:HG3	1:B:384:ARG:HA	2.00	0.42
1:B:343:ARG:HG3	1:B:343:ARG:NH1	2.34	0.42
1:C:376:ARG:HB2	1:C:376:ARG:NH1	2.34	0.42
1:D:105:ASP:OD2	1:D:109:LYS:HE3	2.20	0.42
1:C:290:LEU:HD12	1:C:290:LEU:HA	1.88	0.42
1:C:333:LYS:CE	1:C:365:ASN:ND2	2.82	0.42
1:D:54:GLU:OE2	1:D:55:ALA:N	2.53	0.42
1:C:175:PRO:CB	1:C:368:ARG:HD3	2.50	0.42
1:C:252:HIS:CD2	1:D:6:TRP:HE1	2.37	0.42
1:D:29:THR:O	1:D:30:GLN:CB	2.65	0.42
1:D:182:LEU:HB3	1:D:183:PRO:HD3	2.01	0.42
1:A:25:LEU:HD23	1:A:25:LEU:O	2.20	0.42
1:C:381:GLU:HA	1:C:381:GLU:OE1	2.20	0.42
1:D:349:VAL:HB	1:D:385:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD23	1:A:191:MET:HE2	2.01	0.41
1:B:258:LYS:HD3	1:B:258:LYS:HA	1.86	0.41
1:C:160:ARG:HG3	1:C:160:ARG:HH11	1.85	0.41
1:C:267:ASP:OD2	1:C:267:ASP:C	2.58	0.41
1:D:155:GLU:CA	1:D:191:MET:HE1	2.50	0.41
1:D:352:VAL:HG12	1:D:368:ARG:O	2.19	0.41
1:B:182:LEU:N	1:B:183:PRO:CD	2.83	0.41
1:C:267:ASP:O	1:C:269:HIS:N	2.51	0.41
1:D:71:SER:H	1:D:269:HIS:CE1	2.38	0.41
1:D:256:LEU:HD12	1:D:256:LEU:HA	1.92	0.41
1:A:266:ALA:O	1:B:102:GLN:HA	2.21	0.41
1:B:158:LEU:HD23	1:B:195:ARG:HD2	2.01	0.41
1:C:100:SER:OG	1:C:235:SER:HB2	2.20	0.41
1:C:142:VAL:HG13	1:C:142:VAL:O	2.21	0.41
1:D:31:ARG:N	1:D:31:ARG:CD	2.75	0.41
1:B:192:VAL:HG21	1:B:199:VAL:CG2	2.51	0.41
1:C:42:PRO:CG	1:C:242:PRO:HG3	2.49	0.41
1:A:82:PHE:CZ	1:A:282:LEU:HB3	2.55	0.41
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.93	0.41
1:B:168:LEU:CD1	1:B:188:LEU:HD21	2.50	0.41
1:B:307:ALA:C	1:B:383:VAL:HG11	2.41	0.41
1:B:312:VAL:HG13	1:B:390:LEU:CD2	2.51	0.41
1:B:333:LYS:NZ	1:C:333:LYS:HG2	2.35	0.41
1:C:69:GLN:HG3	1:C:70:TYR:N	2.35	0.41
1:A:41:LEU:HA	1:A:42:PRO:HD3	1.93	0.41
1:A:106:LEU:O	1:A:110:VAL:HG23	2.20	0.41
1:C:312:VAL:CG2	1:C:318:TYR:HE1	2.33	0.41
1:D:290:LEU:O	1:D:293:VAL:CG1	2.69	0.41
1:D:344:ALA:HB1	1:D:349:VAL:HG13	2.01	0.41
1:D:381:GLU:O	1:D:385:ARG:HG3	2.20	0.41
1:A:179:LEU:HD11	1:A:215:LEU:HD11	2.01	0.41
1:C:182:LEU:N	1:C:183:PRO:CD	2.83	0.41
1:A:34:ILE:HG23	1:A:34:ILE:O	2.20	0.41
1:A:317:ARG:HD3	1:A:317:ARG:N	2.35	0.41
1:B:182:LEU:HD13	1:B:216:PRO:HG2	2.02	0.41
1:C:315:GLU:CD	1:C:315:GLU:H	2.24	0.41
1:D:80:ARG:NH1	1:D:92:GLU:HA	2.35	0.41
1:A:119:LEU:HA	1:A:140:LEU:O	2.21	0.41
1:A:140:LEU:HD11	1:A:161:GLU:CG	2.35	0.41
1:A:313:PRO:O	1:A:316:VAL:HG13	2.21	0.41
1:C:179:LEU:HD21	1:C:215:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HD11	1:D:394:LEU:HD23	2.03	0.41
1:A:22:ILE:CG2	1:A:23:ARG:N	2.84	0.41
1:A:343:ARG:O	1:A:347:GLU:HG2	2.21	0.41
1:B:49:LYS:HB2	1:B:49:LYS:NZ	2.36	0.41
1:B:126:MET:O	1:B:130:GLN:HB2	2.21	0.41
1:B:205:TYR:HE1	1:B:325:MET:HE3	1.86	0.41
1:B:320:ARG:O	1:B:322:LYS:HD2	2.21	0.41
1:A:244:LEU:HD13	1:A:278:VAL:HG23	2.02	0.40
1:A:260:VAL:O	1:A:264:GLN:HG3	2.20	0.40
1:B:162:ARG:HB3	1:B:162:ARG:HH21	1.85	0.40
1:B:257:GLN:O	1:B:261:GLN:HG3	2.21	0.40
1:C:48:PRO:HG3	1:C:281:LEU:HD13	2.03	0.40
1:C:60:LEU:HD12	1:D:53:ALA:HA	2.03	0.40
1:D:90:ARG:O	1:D:93:GLU:HB2	2.21	0.40
1:D:151:LEU:HA	1:D:154:LEU:HB3	2.02	0.40
1:D:383:VAL:HG12	1:D:383:VAL:O	2.21	0.40
1:A:46:LEU:HG	1:A:293:VAL:HG12	2.02	0.40
1:A:274:ASN:ND2	1:B:274:ASN:HD21	2.19	0.40
1:D:333:LYS:C	1:D:333:LYS:HD3	2.41	0.40
1:B:310:ARG:NH2	1:B:310:ARG:CB	2.82	0.40
1:B:378:GLY:O	1:B:382:GLY:N	2.45	0.40
1:C:245:ARG:NH2	1:D:267:ASP:O	2.43	0.40
1:C:329:MET:SD	1:C:367:LEU:HD11	2.62	0.40
1:D:34:ILE:HG13	1:D:348:ASN:O	2.22	0.40
1:B:283:LYS:HG3	1:B:284:GLU:HG2	2.04	0.40
1:C:12:LYS:CB	1:C:16:ARG:HH12	2.33	0.40
1:C:142:VAL:HG23	1:C:153:ALA:HB3	2.04	0.40
1:A:252:HIS:CD2	1:A:253:PRO:HD2	2.57	0.40
1:B:209:TYR:CE2	1:B:214:ARG:HB2	2.57	0.40
1:B:280:GLU:HA	1:B:283:LYS:HE2	2.04	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	390/397 (98%)	347 (89%)	34 (9%)	9 (2%)	6	14
1	B	392/397 (99%)	351 (90%)	32 (8%)	9 (2%)	6	14
1	C	394/397 (99%)	353 (90%)	34 (9%)	7 (2%)	8	19
1	D	389/397 (98%)	355 (91%)	30 (8%)	4 (1%)	15	34
All	All	1565/1588 (99%)	1406 (90%)	130 (8%)	29 (2%)	8	18

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	B	21	THR
1	B	31	ARG
1	B	32	PRO
1	C	22	ILE
1	C	32	PRO
1	D	30	GLN
1	D	32	PRO
1	A	10	PHE
1	A	18	GLN
1	A	22	ILE
1	A	39	GLY
1	A	333	LYS
1	B	39	GLY
1	B	49	LYS
1	C	19	ALA
1	C	45	GLU
1	D	18	GLN
1	C	84	ALA
1	C	374	LEU
1	D	333	LYS
1	A	31	ARG
1	A	73	THR
1	B	7	SER
1	B	3	PRO
1	B	228	PRO
1	A	228	PRO
1	C	64	GLY
1	B	355	GLY

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	305/316 (96%)	280 (92%)	25 (8%)	11 24
1	B	307/316 (97%)	283 (92%)	24 (8%)	12 27
1	C	309/316 (98%)	280 (91%)	29 (9%)	8 18
1	D	305/316 (96%)	281 (92%)	24 (8%)	12 26
All	All	1226/1264 (97%)	1124 (92%)	102 (8%)	11 23

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	31	ARG
1	A	68	LEU
1	A	79	LEU
1	A	85	GLU
1	A	120	LEU
1	A	175	PRO
1	A	188	LEU
1	A	195	ARG
1	A	203	ASP
1	A	218	LEU
1	A	221	LEU
1	A	228	PRO
1	A	240	LEU
1	A	256	LEU
1	A	273	LEU
1	A	274	ASN
1	A	284	GLU
1	A	288	GLU
1	A	290	LEU
1	A	291	GLU
1	A	316	VAL
1	A	317	ARG
1	A	333	LYS

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Mol	Chain	Res	Type
1	A	367	LEU
1	B	2	LYS
1	B	4	LEU
1	B	8	GLU
1	B	65	GLU
1	B	68	LEU
1	B	79	LEU
1	B	120	LEU
1	B	130	GLN
1	B	138	ARG
1	B	194	GLU
1	B	228	PRO
1	B	240	LEU
1	B	273	LEU
1	B	274	ASN
1	B	294	ARG
1	B	314	LYS
1	B	317	ARG
1	B	338	GLU
1	B	346	GLU
1	B	367	LEU
1	B	373	THR
1	B	377	GLU
1	B	381	GLU
1	B	386	LEU
1	C	24	GLU
1	C	46	LEU
1	C	59	ILE
1	C	66	VAL
1	C	68	LEU
1	C	110	VAL
1	C	118	VAL
1	C	146	GLU
1	C	162	ARG
1	C	164	ARG
1	C	175	PRO
1	C	179	LEU
1	C	182	LEU
1	C	190	GLN
1	C	240	LEU
1	C	264	GLN
1	C	272	MET

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Mol	Chain	Res	Type
1	C	274	ASN
1	C	282	LEU
1	C	290	LEU
1	C	293	VAL
1	C	312	VAL
1	C	314	LYS
1	C	333	LYS
1	C	340	LEU
1	C	343	ARG
1	C	367	LEU
1	C	386	LEU
1	C	397	VAL
1	D	28	LEU
1	D	31	ARG
1	D	46	LEU
1	D	68	LEU
1	D	69	GLN
1	D	70	TYR
1	D	79	LEU
1	D	110	VAL
1	D	118	VAL
1	D	120	LEU
1	D	158	LEU
1	D	162	ARG
1	D	164	ARG
1	D	173	GLN
1	D	179	LEU
1	D	240	LEU
1	D	274	ASN
1	D	302	GLN
1	D	316	VAL
1	D	364	GLU
1	D	367	LEU
1	D	375	ASP
1	D	386	LEU
1	D	391	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	130	GLN

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Mol	Chain	Res	Type
1	A	135	GLN
1	A	261	GLN
1	A	264	GLN
1	A	269	HIS
1	A	274	ASN
1	A	348	ASN
1	A	360	ASN
1	B	101	GLN
1	B	190	GLN
1	B	257	GLN
1	B	261	GLN
1	B	264	GLN
1	B	269	HIS
1	B	274	ASN
1	B	279	HIS
1	B	348	ASN
1	B	360	ASN
1	C	18	GLN
1	C	30	GLN
1	C	101	GLN
1	C	135	GLN
1	C	257	GLN
1	C	261	GLN
1	C	269	HIS
1	C	274	ASN
1	C	279	HIS
1	C	302	GLN
1	C	360	ASN
1	C	365	ASN
1	D	18	GLN
1	D	101	GLN
1	D	135	GLN
1	D	173	GLN
1	D	269	HIS
1	D	274	ASN
1	D	360	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	C	400	1	15,15,16	2.38	7 (46%)	20,22,23	0.99	1 (5%)
2	PLP	D	400	1	15,15,16	2.51	7 (46%)	20,22,23	1.01	1 (5%)
2	PLP	B	400	1	15,15,16	2.22	6 (40%)	20,22,23	1.01	1 (5%)
2	PLP	A	400	1	15,15,16	2.48	7 (46%)	20,22,23	0.98	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	400	1	-	0/6/6/8	0/1/1/1
2	PLP	D	400	1	-	0/6/6/8	0/1/1/1
2	PLP	B	400	1	-	0/6/6/8	0/1/1/1
2	PLP	A	400	1	-	2/6/6/8	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	PLP	C3-C2	4.86	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	PLP	C3-C2	4.48	1.45	1.40
2	C	400	PLP	P-O4P	-4.15	1.46	1.60
2	A	400	PLP	P-O4P	-4.09	1.47	1.60
2	D	400	PLP	P-O4P	-4.04	1.47	1.60
2	B	400	PLP	P-O4P	-3.86	1.47	1.60
2	C	400	PLP	C3-C2	3.62	1.44	1.40
2	B	400	PLP	C2-N1	3.61	1.40	1.33
2	C	400	PLP	C2A-C2	-3.57	1.44	1.50
2	A	400	PLP	P-O1P	3.54	1.62	1.50
2	D	400	PLP	P-O1P	3.52	1.61	1.50
2	B	400	PLP	C6-C5	3.47	1.45	1.37
2	D	400	PLP	C6-C5	3.38	1.44	1.37
2	C	400	PLP	C6-C5	3.20	1.44	1.37
2	D	400	PLP	C2-N1	3.10	1.39	1.33
2	A	400	PLP	C6-C5	3.09	1.44	1.37
2	C	400	PLP	C2-N1	3.06	1.39	1.33
2	B	400	PLP	C3-C2	3.01	1.43	1.40
2	A	400	PLP	C6-N1	2.99	1.40	1.34
2	B	400	PLP	C6-N1	2.80	1.40	1.34
2	A	400	PLP	C5A-C5	2.75	1.58	1.50
2	D	400	PLP	C6-N1	2.63	1.40	1.34
2	C	400	PLP	C6-N1	2.62	1.39	1.34
2	D	400	PLP	C5-C4	2.57	1.43	1.40
2	B	400	PLP	P-O1P	2.45	1.58	1.50
2	A	400	PLP	C2-N1	2.33	1.38	1.33
2	C	400	PLP	P-O1P	2.04	1.57	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	PLP	C5-C6-N1	-2.43	119.77	123.82
2	C	400	PLP	C5-C6-N1	-2.36	119.88	123.82
2	D	400	PLP	C5-C6-N1	-2.30	119.99	123.82
2	A	400	PLP	C5-C6-N1	-2.30	120.00	123.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	PLP	C5A-O4P-P-O1P
2	A	400	PLP	C5A-O4P-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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	392/397 (98%)	-0.35	7 (1%)	68	69	26, 46, 86, 126	0
1	B	394/397 (99%)	-0.37	2 (0%)	91	92	30, 53, 82, 111	0
1	C	396/397 (99%)	-0.41	1 (0%)	94	95	32, 52, 77, 110	0
1	D	391/397 (98%)	-0.39	1 (0%)	94	95	26, 47, 79, 125	0
All	All	1573/1588 (99%)	-0.38	11 (0%)	87	88	26, 49, 81, 126	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ARG	3.9
1	A	20	SER	3.7
1	A	21	THR	3.6
1	B	20	SER	3.3
1	D	25	LEU	3.1
1	A	19	ALA	2.8
1	A	333	LYS	2.6
1	B	25	LEU	2.3
1	A	32	PRO	2.2
1	A	24	GLU	2.1
1	C	313	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	C	400	15/16	0.96	0.14	34,42,50,50	0
2	PLP	A	400	15/16	0.97	0.19	31,41,47,48	0
2	PLP	D	400	15/16	0.97	0.16	33,42,51,51	0
2	PLP	B	400	15/16	0.98	0.14	39,50,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.