



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 AM UTC

PDB ID : 6O76 / pdb_00006o76
Title : Human cytosolic Histidyl-tRNA synthetase (HisRS) with WHEP domain
Authors : Kuhle, B.; Yang, X.L.
Deposited on : 2019-03-07
Resolution : 2.79 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
Xtrriage (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

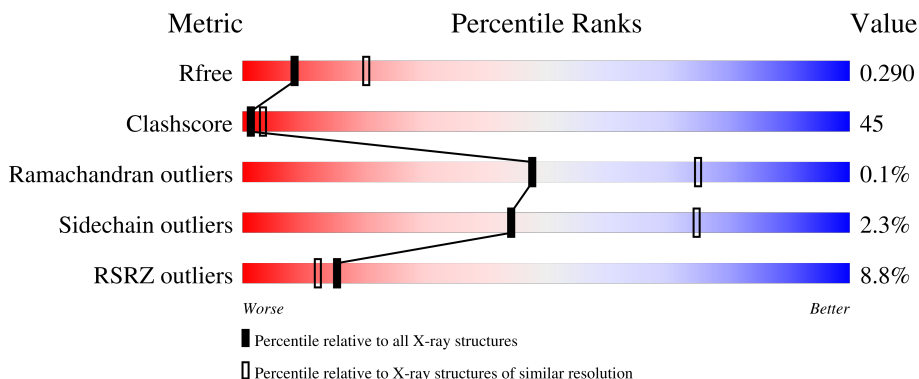
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	509	
1	B	509	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7015 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 Histidine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3469	2209	595	648	17	0	1	0
1	B	451	3482	2224	599	647	12	0	0	0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

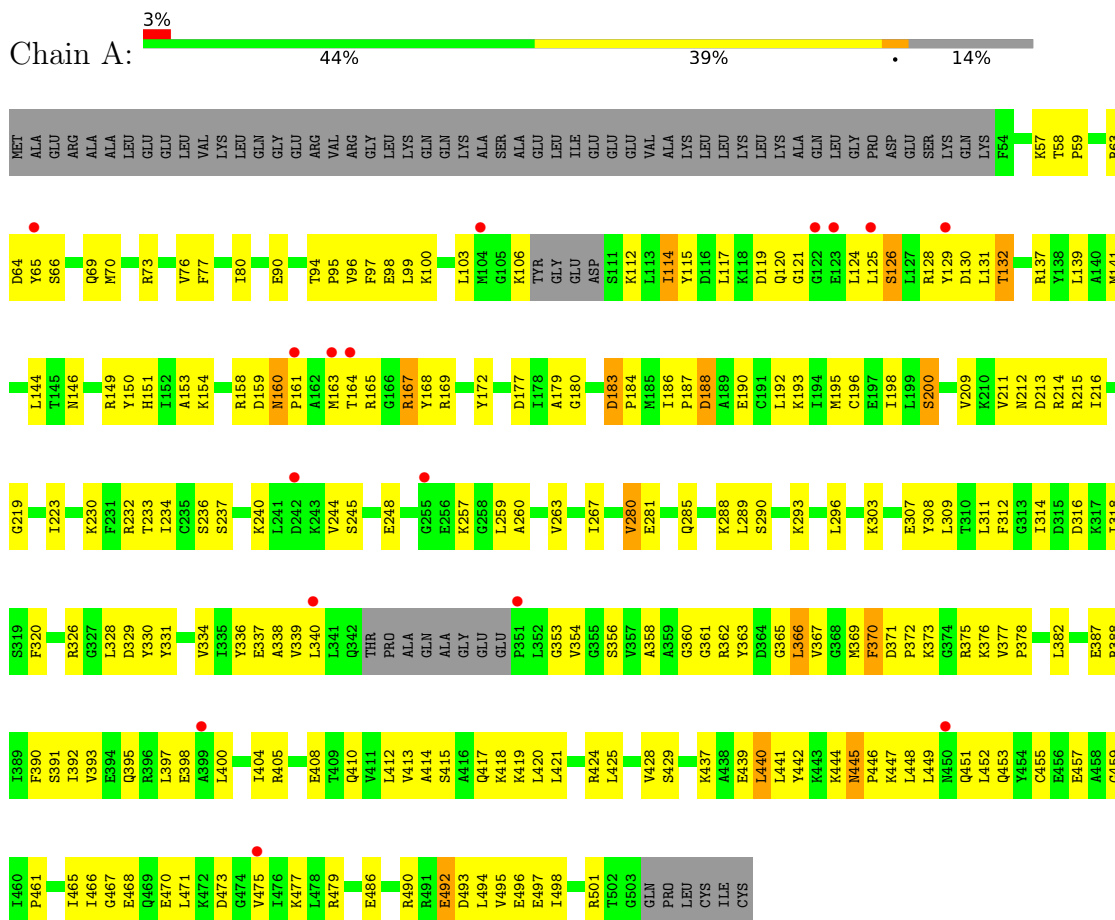
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	27	Total	O	0	0
			27	27		

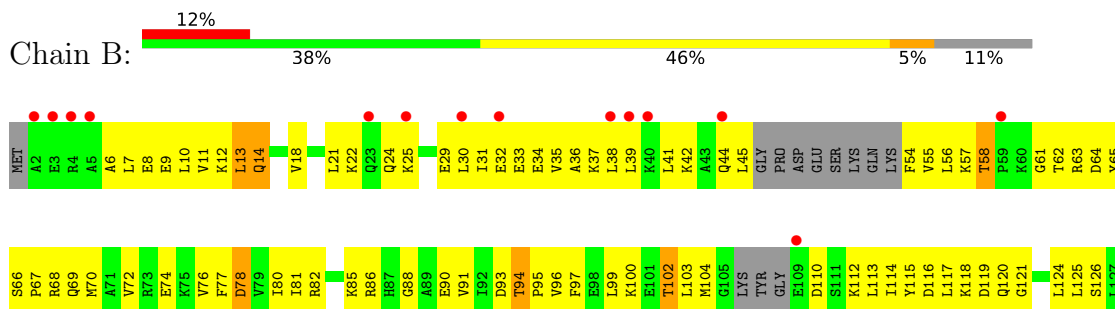
3 Residue-property plots i

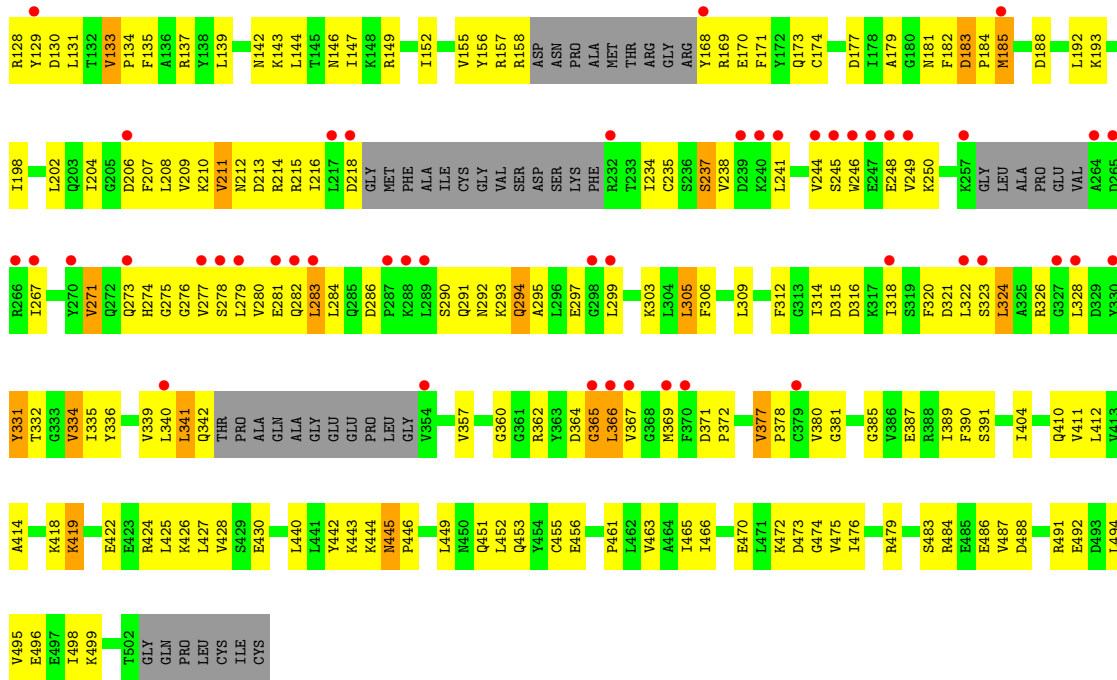
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Histidine-tRNA ligase, cytoplasmic



- Molecule 1: Histidine-tRNA ligase, cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.67Å 97.67Å 254.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.02 – 2.79 29.02 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.02-2.79) 96.8 (29.02-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.80Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.236 , 0.295 0.260 , 0.290	Depositor DCC
R_{free} test set	1555 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtrriage
Anisotropy	0.364	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7015	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

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

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	0.50	0/3519	0.89	21/4734 (0.4%)
1	B	0.55	0/3520	0.98	23/4734 (0.5%)
All	All	0.53	0/7039	0.93	44/9468 (0.5%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	GLU	O-C-N	-11.14	110.31	122.12
1	A	366	LEU	N-CA-C	8.61	120.67	111.28
1	B	366	LEU	N-CA-C	7.97	119.96	111.28
1	B	271	VAL	N-CA-C	7.37	118.16	110.72
1	A	365	GLY	N-CA-C	6.93	121.05	112.73
1	A	114	ILE	N-CA-C	6.69	117.93	108.36
1	A	132	THR	N-CA-C	6.63	118.50	111.28
1	A	293	LYS	N-CA-C	6.55	118.50	111.36
1	A	167	ARG	N-CA-C	6.31	119.50	110.10
1	A	367	VAL	N-CA-C	6.22	116.97	110.62
1	B	184	PRO	N-CA-C	6.15	120.74	111.14
1	B	419	LYS	N-CA-C	5.99	119.82	111.74
1	A	377	VAL	CA-C-N	-5.98	113.78	119.76
1	A	377	VAL	C-N-CA	-5.98	113.78	119.76
1	A	370	PHE	N-CA-C	5.96	117.78	111.28
1	B	365	GLY	N-CA-C	5.95	120.38	112.77
1	B	94	THR	CA-C-N	-5.92	114.16	120.03
1	B	94	THR	C-N-CA	-5.92	114.16	120.03
1	B	237	SER	N-CA-C	-5.74	105.03	111.28
1	B	334	VAL	N-CA-C	5.72	117.44	109.55
1	B	248	GLU	N-CA-C	-5.71	105.06	111.28
1	A	184	PRO	N-CA-C	5.71	119.82	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	VAL	CA-C-N	-5.69	114.07	119.76
1	B	377	VAL	C-N-CA	-5.69	114.07	119.76
1	A	445	ASN	CA-C-N	-5.58	114.17	119.76
1	A	445	ASN	C-N-CA	-5.58	114.17	119.76
1	B	58	THR	CA-C-N	-5.56	114.06	119.78
1	B	58	THR	C-N-CA	-5.56	114.06	119.78
1	B	445	ASN	CA-C-N	-5.48	114.33	120.14
1	B	445	ASN	C-N-CA	-5.48	114.33	120.14
1	B	133	VAL	O-C-N	5.47	123.96	120.07
1	B	211	VAL	N-CA-C	5.45	116.33	108.48
1	A	164	THR	N-CA-C	-5.42	105.37	111.28
1	B	267	ILE	N-CA-C	5.40	116.13	110.62
1	B	331	TYR	N-CA-C	5.38	118.24	110.28
1	B	185	MET	N-CA-C	5.37	121.72	113.28
1	A	165	ARG	N-CA-C	-5.29	103.70	110.53
1	A	183	ASP	CA-C-N	-5.17	114.25	119.83
1	A	183	ASP	C-N-CA	-5.17	114.25	119.83
1	B	183	ASP	CA-C-N	-5.13	114.48	119.76
1	B	183	ASP	C-N-CA	-5.13	114.48	119.76
1	A	131	LEU	N-CA-C	5.11	116.93	111.36
1	A	126	SER	CB-CA-C	-5.05	99.69	109.68
1	A	400	LEU	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

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	3469	0	3543	270	0
1	B	3482	0	3506	412	0
2	A	2	0	0	0	0
3	A	35	0	0	15	0
3	B	27	0	0	10	0
All	All	7015	0	7049	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 45.

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:246:TRP:HA	1:B:249:VAL:CG2	1.22	1.68
1:B:246:TRP:C	1:B:249:VAL:HG22	1.31	1.50
1:A:336:TYR:CE1	1:A:360:GLY:HA3	1.46	1.50
1:B:246:TRP:CA	1:B:249:VAL:CG2	1.90	1.47
1:B:331:TYR:CD2	1:B:335:ILE:HD12	1.55	1.41
1:A:414:ALA:CB	1:A:451:GLN:OE1	1.76	1.32
1:B:495:VAL:CG1	3:B:604:HOH:O	1.73	1.32
1:B:246:TRP:CA	1:B:249:VAL:HG22	1.54	1.29
1:B:12:LYS:NZ	1:B:168:TYR:CZ	1.98	1.29
1:B:130:ASP:OD2	1:B:133:VAL:HG23	1.35	1.25
1:A:414:ALA:HB1	1:A:451:GLN:OE1	1.28	1.23
1:B:331:TYR:HD2	1:B:335:ILE:CD1	1.51	1.22
1:B:234:ILE:O	1:B:238:VAL:HG23	1.35	1.22
1:B:246:TRP:CA	1:B:249:VAL:HG21	1.59	1.20
1:B:246:TRP:C	1:B:249:VAL:CG2	2.09	1.20
1:B:218:ASP:OD1	1:B:294:GLN:NE2	1.73	1.20
1:B:472:LYS:HE2	1:B:472:LYS:HA	1.24	1.19
1:B:241:LEU:CD2	1:B:271:VAL:HG11	1.74	1.16
1:B:21:LEU:HD21	1:B:342:GLN:HG2	1.20	1.15
1:A:331:TYR:CE1	1:A:361:GLY:HA3	1.81	1.14
1:B:214:ARG:NH1	1:B:332:THR:HA	1.62	1.14
1:B:246:TRP:O	1:B:249:VAL:CG2	1.97	1.13
1:B:414:ALA:HB1	1:B:451:GLN:OE1	1.49	1.12
1:B:282:GLN:HG3	1:B:283:LEU:HD23	1.23	1.11
1:B:214:ARG:NE	1:B:331:TYR:O	1.84	1.10
1:A:158:ARG:NH1	1:B:120:GLN:HB3	1.64	1.10
1:A:336:TYR:CE1	1:A:360:GLY:CA	2.33	1.09
1:B:324:LEU:HD21	1:B:335:ILE:HG21	1.32	1.08
1:A:160:ASN:O	1:A:167:ARG:NH2	1.88	1.05
1:A:369:MET:HE3	1:A:370:PHE:CE2	1.92	1.04
1:A:158:ARG:HH11	1:B:120:GLN:HB3	0.89	1.03
1:B:188:ASP:CG	1:B:362:ARG:HH21	1.67	1.03
1:B:321:ASP:CG	1:B:323:SER:HG	1.66	1.03
1:B:303:LYS:O	3:B:601:HOH:O	1.77	1.02
1:B:214:ARG:HH11	1:B:332:THR:CA	1.72	1.02
1:B:364:ASP:OD1	1:B:378:PRO:HA	1.59	1.01
1:B:277:VAL:HG12	1:B:306:PHE:CD1	1.95	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASP:HB2	1:B:113:LEU:HD13	1.41	1.00
1:B:419:LYS:H	1:B:445:ASN:ND2	1.58	1.00
1:B:112:LYS:HE2	1:B:112:LYS:HA	1.42	0.99
1:B:214:ARG:HH11	1:B:332:THR:HA	0.85	0.99
1:A:230:LYS:O	1:A:233:THR:HG22	1.63	0.98
1:A:415:SER:OG	1:A:424:ARG:NH1	1.97	0.98
1:B:244:VAL:HG13	1:B:249:VAL:HG12	1.46	0.97
1:B:246:TRP:O	1:B:249:VAL:HG22	1.57	0.97
1:B:12:LYS:NZ	1:B:168:TYR:OH	1.96	0.97
1:A:414:ALA:HB2	1:A:451:GLN:OE1	1.61	0.96
1:B:12:LYS:NZ	1:B:168:TYR:CE1	2.31	0.96
1:B:211:VAL:HG12	1:B:336:TYR:HB3	1.46	0.96
1:B:321:ASP:OD2	1:B:323:SER:OG	1.83	0.96
1:B:241:LEU:CD2	1:B:271:VAL:CG1	2.43	0.96
1:B:331:TYR:CD2	1:B:335:ILE:CD1	2.35	0.95
1:B:99:LEU:O	1:B:102:THR:OG1	1.85	0.95
1:B:321:ASP:CG	1:B:323:SER:OG	2.09	0.95
1:A:373:LYS:HD2	1:A:375:ARG:HH21	1.29	0.94
1:A:397:LEU:HD12	1:A:404:ILE:HD11	1.49	0.94
1:B:246:TRP:O	1:B:249:VAL:HG23	1.67	0.94
1:B:21:LEU:CD2	1:B:342:GLN:HG2	1.95	0.94
1:B:238:VAL:HG12	1:B:323:SER:O	1.67	0.94
1:B:96:VAL:O	1:B:128:ARG:HG3	1.68	0.93
1:A:103:LEU:HD23	1:A:129:TYR:CE1	2.04	0.92
1:B:143:LYS:NZ	1:B:371:ASP:OD2	2.02	0.92
1:A:66:SER:H	1:A:69:GLN:HE21	1.11	0.92
1:B:212:ASN:OD1	1:B:213:ASP:N	2.01	0.92
1:A:492:GLU:N	1:A:492:GLU:OE1	2.03	0.91
1:B:367:VAL:HG11	1:B:377:VAL:CG2	1.99	0.91
1:A:446:PRO:HG2	1:A:451:GLN:NE2	1.83	0.91
1:B:367:VAL:HG11	1:B:377:VAL:HG21	1.48	0.91
1:B:321:ASP:OD1	1:B:323:SER:OG	1.88	0.90
1:B:110:ASP:HB2	1:B:113:LEU:CD1	2.01	0.90
1:B:419:LYS:H	1:B:445:ASN:HD21	0.91	0.90
1:A:214:ARG:NH1	1:A:328:LEU:O	2.06	0.89
1:A:213:ASP:OD1	3:A:701:HOH:O	1.87	0.89
1:B:241:LEU:HD21	1:B:271:VAL:CG1	2.04	0.88
1:B:7:LEU:HD21	1:B:44:GLN:CB	2.03	0.87
1:B:9:GLU:O	1:B:12:LYS:HG2	1.74	0.87
1:A:63:ARG:HD3	3:A:718:HOH:O	1.73	0.87
1:B:476:ILE:HD12	1:B:494:LEU:HD22	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD21	1:B:42:LYS:HE3	1.57	0.87
1:B:100:LYS:HB3	1:B:124:LEU:CD1	2.05	0.87
1:B:495:VAL:HG12	3:B:604:HOH:O	1.53	0.86
1:A:309:LEU:HD23	1:A:314:ILE:HD11	1.55	0.86
1:A:158:ARG:HH11	1:B:120:GLN:CB	1.84	0.86
1:B:158:ARG:HA	1:B:169:ARG:HD2	1.58	0.86
1:B:218:ASP:OD1	1:B:294:GLN:CD	2.18	0.85
1:B:100:LYS:HB3	1:B:124:LEU:HD11	1.58	0.85
1:B:130:ASP:CG	1:B:133:VAL:HG23	2.00	0.85
1:A:331:TYR:CD1	1:A:361:GLY:HA3	2.13	0.84
1:A:424:ARG:HG2	1:A:466:ILE:HD12	1.59	0.83
1:B:492:GLU:OE1	1:B:492:GLU:N	2.10	0.83
1:A:66:SER:H	1:A:69:GLN:NE2	1.77	0.83
1:B:234:ILE:O	1:B:237:SER:OG	1.97	0.83
1:B:305:LEU:HD12	1:B:305:LEU:O	1.79	0.83
1:B:340:LEU:HD23	1:B:341:LEU:N	1.92	0.83
1:B:124:LEU:HD12	1:B:124:LEU:O	1.78	0.83
1:A:114:ILE:HG23	3:A:711:HOH:O	1.79	0.83
1:A:397:LEU:HD12	1:A:404:ILE:CD1	2.07	0.83
1:A:373:LYS:HD2	1:A:375:ARG:NH2	1.93	0.83
1:B:367:VAL:CG1	1:B:377:VAL:CG2	2.57	0.83
1:B:8:GLU:O	1:B:11:VAL:HG22	1.79	0.82
1:B:286:ASP:O	1:B:290:SER:OG	1.95	0.82
1:B:14:GLN:NE2	1:B:34:GLU:OE1	2.12	0.82
1:B:115:TYR:CE2	1:B:158:ARG:HB3	2.14	0.81
1:B:218:ASP:CG	1:B:294:GLN:HE22	1.88	0.81
1:A:373:LYS:CD	1:A:375:ARG:HH21	1.94	0.81
1:A:429:SER:OG	1:B:312:PHE:HD1	1.64	0.81
1:B:118:LYS:O	1:B:120:GLN:NE2	2.12	0.81
1:B:156:TYR:CE2	1:B:170:GLU:HG3	2.16	0.81
1:B:100:LYS:CB	1:B:124:LEU:HD13	2.10	0.81
1:B:100:LYS:HB2	1:B:124:LEU:HD13	1.60	0.81
1:B:340:LEU:HD23	1:B:341:LEU:H	1.44	0.80
1:B:9:GLU:CG	1:B:168:TYR:OH	2.29	0.80
1:B:282:GLN:CG	1:B:283:LEU:HD23	2.10	0.80
1:B:495:VAL:HG13	3:B:604:HOH:O	1.55	0.80
1:A:180:GLY:O	1:A:378:PRO:HG2	1.82	0.80
1:B:94:THR:HG23	1:B:95:PRO:HD2	1.64	0.80
1:B:24:GLN:O	1:B:25:LYS:HG3	1.82	0.80
1:B:238:VAL:O	1:B:241:LEU:HB3	1.82	0.80
1:B:100:LYS:CB	1:B:124:LEU:CD1	2.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:O	1:B:35:VAL:HG22	1.82	0.79
1:A:326:ARG:CZ	1:A:337:GLU:OE1	2.31	0.79
1:B:188:ASP:OD1	1:B:362:ARG:NH2	2.15	0.79
1:B:188:ASP:CG	1:B:362:ARG:NH2	2.41	0.79
1:B:246:TRP:O	1:B:250:LYS:N	2.15	0.78
1:B:7:LEU:HD21	1:B:44:GLN:HB3	1.65	0.78
1:B:282:GLN:HG3	1:B:283:LEU:CD2	2.11	0.78
1:B:367:VAL:CG1	1:B:377:VAL:HG21	2.13	0.78
1:B:9:GLU:CG	1:B:12:LYS:HE2	2.12	0.78
1:B:328:LEU:HD12	1:B:328:LEU:O	1.82	0.78
1:B:31:ILE:O	1:B:35:VAL:HG13	1.84	0.78
1:B:277:VAL:CG1	1:B:306:PHE:CD1	2.66	0.78
1:A:369:MET:HE3	1:A:370:PHE:CD2	2.18	0.78
1:A:388[A]:ARG:NH2	3:A:702:HOH:O	2.02	0.78
1:B:177:ASP:OD1	1:B:381:GLY:HA3	1.84	0.78
1:A:237:SER:OG	1:A:257:LYS:NZ	2.16	0.77
1:A:369:MET:HE3	1:A:370:PHE:HE2	1.44	0.77
1:A:159:ASP:OD1	1:A:160:ASN:N	2.17	0.77
1:A:420:LEU:N	3:A:703:HOH:O	2.05	0.77
1:B:68:ARG:NH1	1:B:404:ILE:HD12	1.99	0.77
1:B:367:VAL:HG11	1:B:377:VAL:CB	2.15	0.77
1:A:479:ARG:NH2	1:A:486:GLU:OE2	2.18	0.77
1:B:66:SER:OG	1:B:69:GLN:NE2	2.16	0.77
1:B:419:LYS:N	1:B:445:ASN:HD21	1.77	0.76
1:B:11:VAL:HG12	1:B:41:LEU:HB3	1.67	0.76
1:B:479:ARG:NH2	1:B:486:GLU:OE2	2.17	0.76
1:A:158:ARG:NH1	1:B:120:GLN:CB	2.46	0.76
1:B:38:LEU:O	1:B:38:LEU:HD23	1.86	0.76
1:B:66:SER:H	1:B:69:GLN:NE2	1.83	0.75
1:B:324:LEU:HD21	1:B:335:ILE:CG2	2.14	0.75
1:B:21:LEU:HD21	1:B:342:GLN:CG	2.11	0.75
1:A:188:ASP:OD1	1:A:362:ARG:NH2	2.19	0.75
1:A:371:ASP:OD1	1:A:372:PRO:HD2	1.86	0.75
1:A:195:MET:HE1	1:A:338:ALA:HB2	1.70	0.74
1:B:66:SER:CB	1:B:69:GLN:HE21	2.00	0.74
1:A:232:ARG:HH12	1:A:329:ASP:HB3	1.53	0.74
1:A:467:GLY:HA3	1:A:470:GLU:OE1	1.86	0.74
1:B:158:ARG:HA	1:B:169:ARG:CD	2.17	0.74
1:A:195:MET:CE	1:A:338:ALA:HB2	2.18	0.73
1:B:10:LEU:HD23	1:B:391:SER:HB2	1.71	0.73
1:A:412:LEU:HD12	1:A:413:VAL:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:HD2	1:A:149:ARG:C	2.14	0.73
1:A:448:LEU:HD23	1:A:448:LEU:C	2.14	0.73
1:A:429:SER:OG	1:B:312:PHE:CD1	2.41	0.72
1:B:449:LEU:O	1:B:453:GLN:HG3	1.88	0.72
1:B:324:LEU:C	1:B:324:LEU:HD23	2.14	0.72
1:A:285:GLN:HA	1:A:285:GLN:NE2	2.03	0.72
1:B:331:TYR:HD2	1:B:335:ILE:HD13	1.53	0.72
1:A:412:LEU:HD12	1:A:413:VAL:H	1.52	0.72
1:B:110:ASP:CB	1:B:113:LEU:HD13	2.18	0.72
1:A:223:ILE:HD11	1:A:288:LYS:HB3	1.71	0.71
1:B:39:LEU:HD12	1:B:39:LEU:H	1.54	0.71
1:B:241:LEU:HD23	1:B:271:VAL:HG11	1.69	0.71
1:A:103:LEU:HD23	1:A:129:TYR:CD1	2.25	0.71
1:A:492:GLU:CD	1:A:492:GLU:H	1.95	0.71
1:B:13:LEU:HD23	1:B:391:SER:OG	1.91	0.71
1:B:279:LEU:O	1:B:282:GLN:HG2	1.90	0.71
1:A:331:TYR:CE1	1:A:361:GLY:CA	2.69	0.70
1:A:497:GLU:O	1:A:501:ARG:HG2	1.91	0.70
1:B:61:GLY:O	1:B:168:TYR:HB3	1.91	0.70
1:B:241:LEU:HD21	1:B:271:VAL:HG11	1.62	0.70
1:A:449:LEU:O	1:A:453:GLN:HG3	1.91	0.70
1:A:373:LYS:HD2	1:A:375:ARG:HE	1.56	0.70
1:B:299:LEU:O	1:B:303:LYS:CG	2.40	0.70
1:B:410:GLN:O	1:B:461:PRO:HG2	1.91	0.70
1:B:492:GLU:CD	1:B:492:GLU:H	1.96	0.70
1:A:103:LEU:HD23	1:A:129:TYR:HE1	1.49	0.70
1:A:397:LEU:CD1	1:A:404:ILE:HD11	2.21	0.70
1:B:135:PHE:HB2	1:B:149:ARG:NH1	2.07	0.70
1:B:472:LYS:HA	1:B:472:LYS:CE	2.07	0.70
1:A:336:TYR:HE1	1:A:360:GLY:HA3	0.95	0.70
1:A:190:GLU:OE2	1:B:442:TYR:OH	2.06	0.69
1:A:425:LEU:HD23	1:A:440:LEU:HD21	1.73	0.69
1:B:112:LYS:O	1:B:112:LYS:HD3	1.91	0.69
1:B:97:PHE:CD1	1:B:125:LEU:HD22	2.28	0.69
1:B:112:LYS:HA	1:B:112:LYS:CE	2.20	0.69
1:B:283:LEU:HD23	1:B:283:LEU:N	2.07	0.69
1:B:9:GLU:CG	1:B:168:TYR:HH	2.05	0.69
1:B:277:VAL:HG12	1:B:306:PHE:CG	2.27	0.69
1:A:371:ASP:OD1	1:A:372:PRO:CD	2.41	0.69
1:B:362:ARG:NH2	3:B:602:HOH:O	2.26	0.69
1:A:440:LEU:C	1:A:440:LEU:HD12	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:723:HOH:O	1:B:102:THR:HG21	1.94	0.68
1:B:7:LEU:O	1:B:11:VAL:HG13	1.92	0.68
1:B:367:VAL:CB	1:B:377:VAL:HB	2.24	0.68
1:B:54:PHE:O	1:B:55:VAL:HG12	1.93	0.68
1:B:414:ALA:O	1:B:465:ILE:HA	1.93	0.68
1:B:206:ASP:O	1:B:340:LEU:HD23	1.94	0.68
1:B:241:LEU:HD21	1:B:271:VAL:HG12	1.74	0.68
1:B:215:ARG:HA	1:B:218:ASP:OD2	1.95	0.67
1:B:24:GLN:OE1	1:B:342:GLN:NE2	2.27	0.67
1:B:241:LEU:HD23	1:B:271:VAL:CG1	2.23	0.67
1:B:472:LYS:HE2	1:B:472:LYS:CA	2.14	0.67
1:A:212:ASN:OD1	1:A:213:ASP:N	2.27	0.67
1:B:142:ASN:HB2	1:B:144:LEU:CD1	2.24	0.67
1:A:196:CYS:O	1:A:200:SER:OG	2.06	0.67
1:A:146:ASN:HA	1:A:179:ALA:O	1.94	0.67
1:B:419:LYS:N	1:B:445:ASN:ND2	2.39	0.67
1:A:497:GLU:OE2	1:A:501:ARG:NH1	2.24	0.67
1:B:68:ARG:CZ	1:B:404:ILE:HD12	2.25	0.67
1:B:77:PHE:O	1:B:81:ILE:HG12	1.94	0.67
1:B:275:GLY:O	1:B:320:PHE:N	2.27	0.66
1:A:307:GLU:OE2	1:B:422:GLU:OE2	2.13	0.66
1:A:336:TYR:CD1	1:A:360:GLY:HA3	2.26	0.66
1:B:470:GLU:OE1	1:B:470:GLU:N	2.26	0.66
1:A:439:GLU:HG3	3:A:719:HOH:O	1.93	0.66
1:B:113:LEU:O	1:B:158:ARG:HG2	1.95	0.66
1:B:367:VAL:HG11	1:B:377:VAL:HB	1.78	0.66
1:A:66:SER:N	1:A:69:GLN:HE21	1.89	0.65
1:A:448:LEU:HD23	1:A:448:LEU:O	1.97	0.65
1:A:80:ILE:HG23	1:A:198:ILE:HD13	1.78	0.65
1:B:214:ARG:HE	1:B:331:TYR:C	2.03	0.65
1:B:103:LEU:HD22	1:B:129:TYR:CE2	2.31	0.65
1:B:188:ASP:OD1	1:B:380:VAL:HG21	1.96	0.65
1:B:276:GLY:O	1:B:280:VAL:HG23	1.96	0.65
1:B:142:ASN:HB2	1:B:144:LEU:HD11	1.78	0.65
1:B:142:ASN:CB	1:B:144:LEU:HD11	2.26	0.65
1:B:155:VAL:HG11	1:B:173:GLN:OE1	1.96	0.65
1:A:281:GLU:HG3	1:A:303:LYS:NZ	2.11	0.65
1:A:160:ASN:N	1:A:160:ASN:HD22	1.95	0.65
1:A:340:LEU:O	1:A:353:GLY:HA2	1.96	0.65
1:B:146:ASN:HA	1:B:179:ALA:O	1.97	0.64
1:A:115:TYR:OH	1:A:169:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ARG:HG2	1:A:492:GLU:CD	2.22	0.64
1:B:88:GLY:HA2	3:B:614:HOH:O	1.96	0.64
1:B:124:LEU:HD12	1:B:124:LEU:C	2.22	0.64
1:A:244:VAL:HG22	1:A:245:SER:H	1.60	0.64
1:A:338:ALA:HB3	1:A:358:ALA:HB3	1.80	0.64
1:B:24:GLN:C	1:B:25:LYS:HG3	2.22	0.64
1:A:370:PHE:CE1	1:B:56:LEU:HD21	2.33	0.63
1:A:370:PHE:CD1	1:B:56:LEU:HD21	2.33	0.63
1:B:39:LEU:HD12	1:B:39:LEU:N	2.13	0.63
1:B:241:LEU:HD22	1:B:271:VAL:HG11	1.75	0.63
1:B:476:ILE:HD12	1:B:494:LEU:CD2	2.28	0.63
1:B:192:LEU:HD21	1:B:336:TYR:CD1	2.34	0.63
1:A:370:PHE:HD1	1:B:56:LEU:HD11	1.63	0.63
1:B:425:LEU:HD23	1:B:440:LEU:HD11	1.80	0.63
1:B:13:LEU:HD12	1:B:13:LEU:O	1.99	0.63
1:B:367:VAL:CG1	1:B:377:VAL:HB	2.28	0.63
1:B:367:VAL:HB	1:B:377:VAL:HB	1.79	0.63
1:A:376:LYS:HG3	1:A:376:LYS:O	1.98	0.62
1:A:366:LEU:O	1:A:366:LEU:HD23	1.98	0.62
1:A:373:LYS:HD2	1:A:375:ARG:NE	2.13	0.62
1:A:120:GLN:HB3	1:B:158:ARG:NH1	2.14	0.62
1:A:429:SER:HG	1:B:312:PHE:HD1	1.48	0.62
1:B:38:LEU:HD23	1:B:38:LEU:C	2.24	0.62
1:B:246:TRP:HA	1:B:249:VAL:HG21	0.63	0.62
1:A:117:LEU:CD2	1:B:115:TYR:HD1	2.13	0.62
1:B:7:LEU:HD21	1:B:44:GLN:HB2	1.81	0.62
1:B:135:PHE:HB2	1:B:149:ARG:HH11	1.65	0.62
1:A:405:ARG:HD3	1:A:459:GLY:HA3	1.82	0.62
1:B:495:VAL:O	1:B:499:LYS:HG3	2.00	0.61
1:A:370:PHE:CD1	1:B:56:LEU:HD11	2.35	0.61
1:B:284:LEU:O	1:B:290:SER:OG	2.18	0.61
1:B:494:LEU:O	1:B:498:ILE:HG13	2.00	0.61
1:B:38:LEU:CD2	1:B:42:LYS:HE3	2.28	0.61
1:A:259:LEU:HD12	1:A:260:ALA:H	1.66	0.61
1:A:223:ILE:CD1	1:A:288:LYS:HB3	2.29	0.61
1:B:157:ARG:NH1	1:B:171:PHE:HZ	1.99	0.61
1:B:274:HIS:HB2	1:B:320:PHE:O	2.00	0.61
1:B:81:ILE:HD11	1:B:152:ILE:HD12	1.82	0.61
1:B:322:LEU:N	1:B:322:LEU:HD12	2.16	0.61
1:B:414:ALA:CB	1:B:451:GLN:OE1	2.38	0.61
1:A:421:LEU:HD12	1:A:421:LEU:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:VAL:HG13	1:B:55:VAL:O	2.01	0.60
1:A:441:LEU:O	3:A:704:HOH:O	2.15	0.60
1:A:414:ALA:O	1:A:465:ILE:HA	2.00	0.60
1:B:483:SER:O	1:B:484:ARG:HB2	2.00	0.60
1:B:30:LEU:HD12	1:B:30:LEU:N	2.16	0.60
1:B:244:VAL:HG22	1:B:245:SER:N	2.17	0.60
1:A:65:TYR:HB2	1:B:93:ASP:HB3	1.83	0.60
1:A:309:LEU:HD23	1:A:314:ILE:CD1	2.32	0.59
1:B:57:LYS:HE2	1:B:58:THR:O	2.02	0.59
1:A:425:LEU:O	1:A:428:VAL:HG12	2.02	0.59
1:A:336:TYR:CD1	1:A:360:GLY:CA	2.85	0.59
1:B:473:ASP:HB2	1:B:475:VAL:HG22	1.85	0.59
1:A:120:GLN:CB	1:B:158:ARG:NH1	2.65	0.59
1:A:215:ARG:NH2	3:A:701:HOH:O	2.35	0.59
1:B:238:VAL:CG1	1:B:323:SER:O	2.47	0.59
1:B:291:GLN:HG3	1:B:291:GLN:O	2.02	0.59
1:B:452:LEU:O	1:B:456:GLU:HG3	2.02	0.59
1:B:476:ILE:CD1	1:B:494:LEU:HD22	2.32	0.59
1:A:232:ARG:NH1	1:A:329:ASP:HB3	2.16	0.59
1:A:76:VAL:CG2	1:A:390:PHE:HE1	2.16	0.59
1:B:234:ILE:C	1:B:238:VAL:HG23	2.23	0.59
1:B:316:ASP:OD1	1:B:316:ASP:N	2.35	0.59
1:A:373:LYS:CE	1:A:375:ARG:HH21	2.14	0.59
1:A:373:LYS:HD2	1:A:375:ARG:CZ	2.32	0.58
1:A:180:GLY:C	1:A:378:PRO:HG2	2.28	0.58
1:A:124:LEU:N	1:A:124:LEU:HD12	2.18	0.58
1:B:54:PHE:CG	1:B:55:VAL:N	2.72	0.58
1:B:479:ARG:HB2	1:B:486:GLU:HG2	1.84	0.58
1:B:72:VAL:O	1:B:76:VAL:HG23	2.04	0.58
1:A:440:LEU:HD12	1:A:440:LEU:O	2.04	0.58
1:A:446:PRO:HG2	1:A:451:GLN:HE21	1.65	0.58
1:B:100:LYS:HE3	1:B:124:LEU:HD13	1.86	0.58
1:B:214:ARG:CD	1:B:328:LEU:CD1	2.81	0.58
1:A:177:ASP:OD2	1:A:363:TYR:OH	2.22	0.57
1:A:211:VAL:HG12	1:A:336:TYR:HB3	1.85	0.57
1:A:388[B]:ARG:O	1:A:392:ILE:HG13	2.04	0.57
1:A:437:LYS:HG2	1:B:86:ARG:HA	1.85	0.57
1:A:158:ARG:HH12	1:B:120:GLN:C	2.12	0.57
1:B:157:ARG:O	1:B:169:ARG:HB3	2.05	0.57
1:A:397:LEU:CD1	1:A:404:ILE:CD1	2.78	0.57
1:A:417:GLN:OE1	1:A:468:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:NH2	1:B:65:TYR:CZ	2.73	0.57
1:B:103:LEU:HB3	1:B:129:TYR:HE2	1.68	0.57
1:B:241:LEU:HD12	1:B:249:VAL:HG11	1.87	0.57
1:A:128:ARG:HH12	1:A:153:ALA:CB	2.16	0.57
1:A:388[A]:ARG:O	1:A:392:ILE:HG13	2.04	0.57
1:B:68:ARG:NH2	1:B:404:ILE:HB	2.19	0.57
1:A:336:TYR:CE1	1:A:360:GLY:C	2.83	0.57
1:B:214:ARG:CZ	1:B:332:THR:HA	2.33	0.56
1:A:442:TYR:HB2	1:B:182:PHE:HB3	1.87	0.56
1:B:97:PHE:HD1	1:B:125:LEU:HD22	1.69	0.56
1:B:29:GLU:O	1:B:33:GLU:HG3	2.05	0.56
1:B:94:THR:CG2	1:B:95:PRO:HD2	2.35	0.56
1:A:285:GLN:HA	1:A:285:GLN:HE21	1.69	0.56
1:A:192:LEU:HD11	1:A:336:TYR:CD2	2.40	0.56
1:B:234:ILE:O	1:B:238:VAL:CG2	2.30	0.56
1:B:367:VAL:CG1	1:B:377:VAL:CB	2.84	0.56
1:B:411:VAL:HG22	1:B:412:LEU:N	2.21	0.56
1:B:424:ARG:NE	3:B:605:HOH:O	2.35	0.56
1:A:209:VAL:HB	1:A:318:ILE:HD13	1.87	0.56
1:B:334:VAL:HG12	1:B:335:ILE:N	2.19	0.55
1:A:132:THR:HG21	1:A:330:TYR:OH	2.06	0.55
1:A:183:ASP:OD2	1:B:444:LYS:N	2.39	0.55
1:A:421:LEU:HD22	1:A:444:LYS:HA	1.88	0.55
1:A:490:ARG:HG2	1:A:492:GLU:OE2	2.06	0.55
1:B:305:LEU:HD12	1:B:305:LEU:C	2.31	0.55
1:A:395:GLN:HA	1:A:398:GLU:HB3	1.88	0.55
1:B:18:VAL:HG22	1:B:34:GLU:HB3	1.89	0.55
1:A:444:LYS:N	1:B:183:ASP:OD2	2.39	0.55
1:B:158:ARG:CA	1:B:169:ARG:HD2	2.35	0.55
1:B:214:ARG:CD	1:B:328:LEU:HD12	2.37	0.54
1:B:425:LEU:O	1:B:428:VAL:HG12	2.08	0.54
1:B:115:TYR:OH	1:B:169:ARG:NE	2.41	0.54
1:B:116:ASP:OD1	1:B:126:SER:HB3	2.07	0.54
1:A:453:GLN:O	1:A:457:GLU:HG3	2.07	0.54
1:B:249:VAL:HG23	1:B:250:LYS:N	2.21	0.54
1:B:39:LEU:H	1:B:39:LEU:CD1	2.21	0.54
1:A:330:TYR:CE2	1:A:366:LEU:HD13	2.42	0.54
1:B:271:VAL:HG13	1:B:323:SER:HA	1.89	0.54
1:B:326:ARG:HD2	1:B:326:ARG:N	2.22	0.54
1:A:418:LYS:O	1:A:419:LYS:HB3	2.07	0.54
1:B:275:GLY:N	1:B:320:PHE:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:HG3	1:A:303:LYS:HZ1	1.73	0.53
1:A:366:LEU:HD23	1:A:366:LEU:C	2.33	0.53
1:A:493:ASP:O	1:A:496:GLU:HG3	2.08	0.53
1:A:106:LYS:CB	1:A:129:TYR:OH	2.55	0.53
1:A:421:LEU:HB3	3:A:727:HOH:O	2.09	0.53
1:A:309:LEU:CD2	1:A:314:ILE:HD11	2.31	0.53
1:A:370:PHE:CE1	1:B:56:LEU:CD2	2.91	0.53
1:B:8:GLU:N	1:B:45:LEU:HD21	2.23	0.53
1:A:308:TYR:HA	1:A:311:LEU:HD12	1.89	0.53
1:A:354:VAL:O	1:A:354:VAL:HG12	2.09	0.53
1:B:367:VAL:HG12	1:B:377:VAL:CG2	2.37	0.53
1:A:119:ASP:OD1	1:A:121:GLY:N	2.42	0.53
1:A:281:GLU:CG	1:A:303:LYS:NZ	2.72	0.53
1:B:364:ASP:OD1	1:B:378:PRO:CA	2.44	0.53
1:B:130:ASP:CG	1:B:133:VAL:CG2	2.80	0.53
1:B:214:ARG:HD2	1:B:328:LEU:CD1	2.40	0.52
1:A:439:GLU:CG	3:A:719:HOH:O	2.54	0.52
1:A:479:ARG:HB2	1:A:486:GLU:HG2	1.91	0.52
1:B:131:LEU:C	1:B:134:PRO:HD2	2.33	0.52
1:A:130:ASP:OD2	1:A:132:THR:OG1	2.27	0.52
1:A:95:PRO:HD3	1:B:64:ASP:OD1	2.09	0.52
1:B:30:LEU:N	1:B:30:LEU:CD1	2.73	0.52
1:B:7:LEU:HD21	1:B:44:GLN:C	2.35	0.52
1:B:112:LYS:HE2	1:B:112:LYS:CA	2.17	0.52
1:B:339:VAL:HG23	1:B:339:VAL:O	2.08	0.52
1:B:446:PRO:HG2	1:B:451:GLN:NE2	2.24	0.52
1:A:188:ASP:OD1	1:A:188:ASP:N	2.41	0.52
1:B:142:ASN:CB	1:B:144:LEU:CD1	2.85	0.52
1:B:245:SER:O	1:B:249:VAL:N	2.43	0.52
1:B:214:ARG:HD3	1:B:328:LEU:HD12	1.91	0.52
1:A:334:VAL:HG22	3:A:712:HOH:O	2.10	0.51
1:B:446:PRO:CG	1:B:451:GLN:NE2	2.73	0.51
1:A:97:PHE:HE1	1:B:62:THR:HG21	1.74	0.51
1:A:59:PRO:HB3	1:B:125:LEU:HD21	1.92	0.51
1:A:213:ASP:HB3	1:A:216:ILE:HG13	1.92	0.51
1:B:331:TYR:OH	1:B:360:GLY:HA2	2.09	0.51
1:B:212:ASN:O	1:B:335:ILE:N	2.30	0.51
1:A:76:VAL:CG2	1:A:390:PHE:CE1	2.93	0.51
1:A:444:LYS:HG2	1:B:183:ASP:OD2	2.11	0.51
1:B:119:ASP:O	1:B:121:GLY:N	2.35	0.51
1:B:114:ILE:HG23	3:B:616:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LYS:HA	1:B:314:ILE:HD13	1.92	0.50
1:A:96:VAL:O	1:A:128:ARG:HG2	2.11	0.50
1:B:18:VAL:O	1:B:22:LYS:HG3	2.11	0.50
1:A:446:PRO:CG	1:A:451:GLN:NE2	2.67	0.50
1:B:110:ASP:HB2	1:B:113:LEU:HD11	1.93	0.50
1:A:425:LEU:HD23	1:A:440:LEU:CD2	2.42	0.50
1:B:244:VAL:CG2	1:B:245:SER:N	2.74	0.50
1:A:447:LYS:O	1:A:451:GLN:HG3	2.11	0.50
1:A:473:ASP:HB3	1:A:475:VAL:HG22	1.94	0.50
1:B:142:ASN:HB3	1:B:144:LEU:HD11	1.93	0.50
1:B:24:GLN:C	1:B:25:LYS:CG	2.85	0.49
1:B:185:MET:HE3	1:B:305:LEU:HB2	1.94	0.49
1:B:244:VAL:O	1:B:249:VAL:HG11	2.12	0.49
1:A:214:ARG:NH1	1:A:328:LEU:C	2.70	0.49
1:A:408:GLU:OE1	1:B:85:LYS:HD3	2.12	0.49
1:B:9:GLU:CB	1:B:168:TYR:OH	2.59	0.49
1:A:240:LYS:O	1:A:244:VAL:HG12	2.12	0.49
1:A:309:LEU:HD22	1:A:314:ILE:HG13	1.94	0.49
1:A:59:PRO:HB3	1:B:125:LEU:CD2	2.43	0.49
1:A:103:LEU:CD2	1:A:129:TYR:CD1	2.94	0.49
1:A:316:ASP:OD1	1:A:316:ASP:N	2.45	0.49
1:B:113:LEU:CD1	1:B:113:LEU:N	2.75	0.49
1:B:292:ASN:OD1	1:B:295:ALA:N	2.33	0.49
1:A:371:ASP:OD1	1:A:372:PRO:N	2.46	0.49
1:B:7:LEU:CD2	1:B:44:GLN:HB3	2.39	0.49
1:A:245:SER:HB3	1:A:248:GLU:OE1	2.13	0.49
1:B:38:LEU:C	1:B:38:LEU:CD2	2.86	0.49
1:B:331:TYR:OH	1:B:360:GLY:CA	2.61	0.49
1:A:219:GLY:O	1:A:223:ILE:HG22	2.13	0.49
1:B:321:ASP:OD2	1:B:323:SER:N	2.37	0.49
1:B:8:GLU:CG	1:B:45:LEU:HD22	2.43	0.48
1:B:10:LEU:CD2	1:B:391:SER:HB2	2.42	0.48
1:B:66:SER:CB	1:B:69:GLN:NE2	2.73	0.48
1:B:445:ASN:ND2	3:B:609:HOH:O	2.43	0.48
1:B:9:GLU:HB2	1:B:168:TYR:OH	2.12	0.48
1:B:293:LYS:O	1:B:297:GLU:CG	2.61	0.48
1:B:336:TYR:CE2	1:B:360:GLY:C	2.91	0.48
1:A:120:GLN:HB2	1:B:158:ARG:HH12	1.77	0.48
1:A:193:LYS:HA	1:A:314:ILE:HD13	1.95	0.48
1:B:324:LEU:C	1:B:324:LEU:CD2	2.85	0.48
1:A:120:GLN:CB	1:B:158:ARG:HH12	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:OD2	1:B:444:LYS:HG2	2.12	0.48
1:A:326:ARG:NH1	1:A:337:GLU:OE1	2.47	0.48
1:B:282:GLN:HG3	1:B:283:LEU:N	2.28	0.48
1:A:259:LEU:HD12	1:A:260:ALA:N	2.27	0.48
1:B:237:SER:O	1:B:241:LEU:N	2.46	0.48
1:A:57:LYS:HE2	1:A:58:THR:O	2.14	0.48
1:A:96:VAL:HA	1:A:128:ARG:HE	1.79	0.48
1:A:440:LEU:C	1:A:440:LEU:CD1	2.85	0.48
1:A:76:VAL:HG21	1:A:390:PHE:CE1	2.48	0.48
1:A:97:PHE:HA	1:A:126:SER:O	2.13	0.48
1:A:149:ARG:HD2	1:A:150:TYR:N	2.29	0.48
1:B:202:LEU:HD13	1:B:389:ILE:HG21	1.96	0.48
1:B:331:TYR:N	1:B:331:TYR:CD1	2.81	0.48
1:B:177:ASP:OD1	1:B:381:GLY:CA	2.59	0.47
1:A:195:MET:HE3	1:A:338:ALA:HB2	1.93	0.47
1:B:280:VAL:HG22	1:B:320:PHE:CD2	2.49	0.47
1:A:117:LEU:HD23	1:B:115:TYR:HD1	1.79	0.47
1:A:494:LEU:HD12	1:A:494:LEU:O	2.14	0.47
1:B:14:GLN:CA	1:B:14:GLN:HE21	2.27	0.47
1:A:214:ARG:HH12	1:A:328:LEU:C	2.22	0.47
1:A:493:ASP:O	1:A:496:GLU:CG	2.62	0.47
1:A:281:GLU:HG3	1:A:303:LYS:HZ3	1.78	0.47
1:A:408:GLU:CD	1:B:85:LYS:HD3	2.39	0.47
1:A:281:GLU:CG	1:A:303:LYS:HZ1	2.28	0.47
1:A:419:LYS:HG2	1:A:419:LYS:O	2.15	0.47
1:A:441:LEU:HD12	1:A:451:GLN:HG2	1.97	0.47
1:A:137:ARG:O	1:A:141:MET:HB2	2.14	0.47
1:A:160:ASN:HD22	1:A:160:ASN:H	1.62	0.47
1:A:329:ASP:OD2	1:A:329:ASP:N	2.45	0.47
1:B:8:GLU:CG	1:B:45:LEU:CD2	2.93	0.47
1:B:94:THR:HG21	1:B:134:PRO:HB3	1.96	0.47
1:B:113:LEU:N	1:B:113:LEU:HD12	2.30	0.47
1:B:213:ASP:HA	1:B:334:VAL:HA	1.96	0.47
1:B:340:LEU:CD2	1:B:341:LEU:N	2.73	0.47
1:B:426:LYS:O	1:B:430:GLU:HG3	2.14	0.47
1:A:233:THR:O	1:A:236:SER:OG	2.25	0.47
1:B:322:LEU:HD12	1:B:322:LEU:H	1.80	0.47
1:A:192:LEU:HD13	3:A:731:HOH:O	2.13	0.47
1:B:207:PHE:O	1:B:208:LEU:HD23	2.15	0.47
1:A:193:LYS:HD3	1:A:312:PHE:HB3	1.96	0.47
1:B:63:ARG:NH2	1:B:65:TYR:OH	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:O	1:B:78:ASP:HB2	2.14	0.47
1:B:103:LEU:HD12	1:B:126:SER:OG	2.15	0.47
1:B:331:TYR:N	1:B:331:TYR:HD1	2.13	0.47
1:A:96:VAL:HB	1:B:156:TYR:OH	2.15	0.46
1:A:195:MET:HG3	1:A:382:LEU:HD22	1.97	0.46
1:B:130:ASP:OD2	1:B:133:VAL:CG2	2.30	0.46
1:B:244:VAL:O	1:B:249:VAL:CG1	2.63	0.46
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.77	0.46
1:A:233:THR:HG23	1:A:234:ILE:N	2.30	0.46
1:A:160:ASN:HB2	1:A:167:ARG:HH22	1.81	0.46
1:A:309:LEU:CD2	1:A:314:ILE:CD1	2.93	0.46
1:B:273:GLN:O	1:B:322:LEU:HD13	2.16	0.46
1:B:8:GLU:CA	1:B:45:LEU:HD21	2.46	0.46
1:A:64:ASP:CG	1:B:137:ARG:HH22	2.24	0.46
1:B:328:LEU:HD12	1:B:328:LEU:C	2.37	0.46
1:A:479:ARG:NE	1:A:486:GLU:OE2	2.49	0.46
1:A:154:LYS:HE2	1:A:172:TYR:CE2	2.51	0.45
1:A:290:SER:O	1:A:296:LEU:HD21	2.16	0.45
1:B:66:SER:N	1:B:69:GLN:NE2	2.60	0.45
1:B:97:PHE:CE1	1:B:125:LEU:HD22	2.51	0.45
1:B:209:VAL:HB	1:B:318:ILE:HD13	1.98	0.45
1:B:414:ALA:HB1	1:B:451:GLN:CD	2.33	0.45
1:A:90:GLU:HB3	1:B:67:PRO:HB3	1.99	0.45
1:B:282:GLN:CG	1:B:283:LEU:CD2	2.86	0.45
1:A:369:MET:HG3	1:A:370:PHE:N	2.31	0.45
1:B:455:CYS:SG	1:B:463:VAL:HG22	2.56	0.45
1:B:185:MET:CE	1:B:305:LEU:HB2	2.47	0.45
1:A:470:GLU:OE2	1:A:477:LYS:HE3	2.17	0.45
1:A:495:VAL:HG13	1:A:496:GLU:N	2.31	0.45
1:B:80:ILE:HG12	1:B:198:ILE:HG21	1.97	0.45
1:A:124:LEU:N	1:A:124:LEU:CD1	2.80	0.45
1:A:336:TYR:HE2	3:A:731:HOH:O	2.00	0.45
1:A:369:MET:CE	1:A:370:PHE:HE2	2.24	0.45
1:A:370:PHE:CD1	1:B:56:LEU:CD2	3.00	0.45
1:A:373:LYS:CD	1:A:375:ARG:HE	2.27	0.45
1:A:448:LEU:C	1:A:448:LEU:CD2	2.85	0.45
1:A:448:LEU:CD2	1:A:452:LEU:HD12	2.46	0.45
1:B:411:VAL:CG2	1:B:412:LEU:N	2.80	0.45
1:A:397:LEU:HD12	1:A:404:ILE:HD13	1.96	0.45
1:B:115:TYR:HE2	1:B:157:ARG:C	2.25	0.45
1:B:418:LYS:HA	1:B:445:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG12	1:A:320:PHE:CD2	2.52	0.44
1:A:393:VAL:O	1:A:397:LEU:HG	2.17	0.44
1:B:12:LYS:CE	1:B:168:TYR:OH	2.64	0.44
1:B:366:LEU:HA	1:B:369:MET:CG	2.46	0.44
1:B:387:GLU:O	1:B:390:PHE:HB2	2.17	0.44
1:A:467:GLY:CA	1:A:470:GLU:OE1	2.59	0.44
1:B:249:VAL:CG2	1:B:250:LYS:N	2.81	0.44
1:B:335:ILE:HG23	3:B:612:HOH:O	2.18	0.44
1:A:494:LEU:O	1:A:498:ILE:HG13	2.17	0.44
1:A:73:ARG:HA	1:A:390:PHE:CE1	2.53	0.44
1:B:11:VAL:HG12	1:B:41:LEU:CB	2.44	0.44
1:B:214:ARG:HH11	1:B:332:THR:CB	2.30	0.44
1:A:370:PHE:CD1	1:B:56:LEU:CD1	3.01	0.44
1:A:124:LEU:CD1	1:A:124:LEU:H	2.31	0.44
1:B:7:LEU:HD23	1:B:45:LEU:HA	2.00	0.44
1:B:103:LEU:HD22	1:B:129:TYR:HE2	1.82	0.44
1:B:331:TYR:OH	1:B:360:GLY:C	2.60	0.44
1:B:366:LEU:HD12	1:B:366:LEU:O	2.18	0.44
1:B:68:ARG:NH1	1:B:404:ILE:CD1	2.78	0.44
1:B:70:MET:O	1:B:74:GLU:HG3	2.17	0.44
1:A:448:LEU:HD21	1:A:452:LEU:HD12	2.00	0.43
1:B:14:GLN:NE2	1:B:14:GLN:HA	2.33	0.43
1:A:98:GLU:HB2	1:A:103:LEU:HD11	2.00	0.43
1:A:370:PHE:HD1	1:B:56:LEU:HD21	1.83	0.43
1:B:277:VAL:CG1	1:B:306:PHE:HD1	2.27	0.43
1:A:99:LEU:HD11	1:B:57:LYS:HG3	2.01	0.43
1:B:427:LEU:HD22	1:B:466:ILE:HD11	2.00	0.43
1:B:334:VAL:CG1	1:B:335:ILE:N	2.81	0.43
1:B:90:GLU:O	1:B:149:ARG:HA	2.18	0.43
1:B:371:ASP:OD1	1:B:372:PRO:HD2	2.19	0.43
1:B:479:ARG:NE	1:B:486:GLU:OE2	2.51	0.43
1:A:149:ARG:C	1:A:149:ARG:CD	2.85	0.43
1:B:124:LEU:CD1	1:B:124:LEU:C	2.90	0.43
1:B:130:ASP:OD1	1:B:133:VAL:CG2	2.67	0.43
1:B:315:ASP:OD2	1:B:315:ASP:N	2.49	0.43
1:A:420:LEU:CA	3:A:703:HOH:O	2.57	0.43
1:A:97:PHE:CE1	1:B:62:THR:HG21	2.54	0.43
1:A:421:LEU:HD12	1:A:421:LEU:C	2.43	0.43
1:B:213:ASP:OD2	1:B:215:ARG:N	2.48	0.43
1:B:357:VAL:O	1:B:385:GLY:N	2.39	0.42
1:A:163:MET:HE2	1:A:163:MET:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLY:O	1:A:471:LEU:HB2	2.19	0.42
1:B:282:GLN:HE21	1:B:283:LEU:CD2	2.31	0.42
1:B:235:CYS:O	1:B:238:VAL:HB	2.20	0.42
1:A:339:VAL:HG12	1:A:356:SER:HA	2.01	0.42
1:B:66:SER:H	1:B:69:GLN:HE21	1.59	0.42
1:A:98:GLU:HB2	1:A:103:LEU:CD1	2.50	0.42
1:A:195:MET:HE2	1:A:195:MET:HB3	1.73	0.42
1:B:192:LEU:HD12	1:B:309:LEU:HD21	2.00	0.42
1:A:137:ARG:HH22	1:B:64:ASP:CG	2.28	0.42
1:A:139:LEU:HD22	1:A:144:LEU:HB2	2.01	0.42
1:A:412:LEU:HD23	1:A:455:CYS:SG	2.59	0.42
1:B:78:ASP:O	1:B:82:ARG:HG3	2.20	0.42
1:A:99:LEU:HD23	1:A:125:LEU:CD2	2.49	0.42
1:A:370:PHE:HE1	1:B:56:LEU:HD21	1.83	0.42
1:B:36:ALA:HA	1:B:39:LEU:HD13	2.00	0.42
1:B:37:LYS:O	1:B:41:LEU:HG	2.19	0.42
1:B:367:VAL:HG12	1:B:377:VAL:HG23	2.01	0.42
1:A:263:VAL:O	1:A:267:ILE:HG13	2.20	0.41
1:B:36:ALA:CA	1:B:39:LEU:HD13	2.50	0.41
1:B:143:LYS:HD2	1:B:143:LYS:HA	1.90	0.41
1:B:214:ARG:HD2	1:B:328:LEU:HD11	2.01	0.41
1:B:369:MET:HE3	1:B:369:MET:HB3	1.85	0.41
1:A:76:VAL:HG22	1:A:390:PHE:HE1	1.83	0.41
1:B:204:ILE:O	1:B:340:LEU:HD11	2.20	0.41
1:B:210:LYS:HE2	1:B:321:ASP:HB2	2.02	0.41
1:B:495:VAL:HG13	1:B:496:GLU:N	2.35	0.41
1:B:487:VAL:HG12	1:B:488:ASP:N	2.36	0.41
1:A:296:LEU:N	1:A:296:LEU:HD22	2.36	0.41
1:B:103:LEU:O	1:B:104:MET:HG2	2.20	0.41
1:B:208:LEU:CD1	1:B:341:LEU:HD21	2.51	0.41
1:B:365:GLY:O	1:B:369:MET:SD	2.79	0.41
1:A:94:THR:HG23	1:A:151:HIS:CE1	2.56	0.41
1:A:117:LEU:HA	1:B:117:LEU:HA	2.02	0.41
1:A:186:ILE:CG2	1:B:442:TYR:HD1	2.34	0.41
1:A:391:SER:O	1:A:395:GLN:HG3	2.21	0.41
1:B:39:LEU:N	1:B:39:LEU:CD1	2.82	0.41
1:B:281:GLU:OE1	1:B:281:GLU:HA	2.21	0.41
1:A:65:TYR:HA	1:A:69:GLN:NE2	2.35	0.41
1:A:373:LYS:NZ	1:A:375:ARG:HH21	2.19	0.41
1:A:448:LEU:HD21	1:A:452:LEU:CD1	2.50	0.41
1:B:6:ALA:HB2	1:B:69:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:CG2	1:B:95:PRO:CD	2.98	0.41
1:A:100:LYS:HE3	1:A:112:LYS:NZ	2.35	0.41
1:A:187:PRO:HG2	1:A:188:ASP:OD1	2.21	0.41
1:A:330:TYR:CE2	1:A:366:LEU:CD1	3.03	0.41
1:A:410:GLN:O	1:A:461:PRO:HG2	2.21	0.41
1:B:442:TYR:O	1:B:443:LYS:HD3	2.20	0.41
1:A:63:ARG:HD2	1:A:168:TYR:CE1	2.56	0.41
1:B:99:LEU:HD23	1:B:125:LEU:HD23	2.02	0.41
1:B:103:LEU:O	1:B:104:MET:SD	2.79	0.41
1:B:139:LEU:HD21	1:B:147:ILE:HG21	2.03	0.41
1:B:306:PHE:HA	1:B:309:LEU:HD12	2.02	0.41
1:B:80:ILE:HG21	1:B:174:CYS:SG	2.61	0.40
1:B:94:THR:HG22	1:B:95:PRO:N	2.35	0.40
1:B:292:ASN:OD1	1:B:295:ALA:CB	2.69	0.40
1:A:77:PHE:HD1	1:A:77:PHE:HA	1.76	0.40
1:A:418:LYS:HG2	1:A:445:ASN:HB3	2.02	0.40
1:B:13:LEU:HD12	1:B:13:LEU:C	2.44	0.40
1:B:474:GLY:O	1:B:491:ARG:HG2	2.21	0.40
1:A:223:ILE:HD11	1:A:288:LYS:CB	2.45	0.40
1:A:330:TYR:CD2	1:A:366:LEU:CD1	3.05	0.40
1:B:181:ASN:OD1	1:B:378:PRO:HG2	2.22	0.40
1:B:334:VAL:C	1:B:335:ILE:HD13	2.45	0.40
1:A:70:MET:CB	1:B:91:VAL:HG13	2.52	0.40
1:A:363:TYR:CD1	1:A:363:TYR:N	2.90	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	433/509 (85%)	417 (96%)	15 (4%)	1 (0%)	43 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	437/509 (86%)	428 (98%)	9 (2%)	0	100	100
All	All	870/1018 (86%)	845 (97%)	24 (3%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO

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	376/438 (86%)	370 (98%)	6 (2%)	55	81
1	B	356/438 (81%)	345 (97%)	11 (3%)	35	68
All	All	732/876 (84%)	715 (98%)	17 (2%)	44	75

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	188	ASP
1	A	200	SER
1	A	280	VAL
1	A	440	LEU
1	A	492	GLU
1	B	13	LEU
1	B	14	GLN
1	B	78	ASP
1	B	102	THR
1	B	216	ILE
1	B	278	SER
1	B	283	LEU
1	B	294	GLN
1	B	305	LEU

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Mol	Chain	Res	Type
1	B	324	LEU
1	B	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	160	ASN
1	A	273	GLN
1	A	285	GLN
1	B	23	GLN
1	B	69	GLN
1	B	282	GLN
1	B	294	GLN
1	B	445	ASN
1	B	451	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/509 (86%)	0.16	16 (3%) 45 38	26, 71, 126, 174	1 (0%)
1	B	451/509 (88%)	0.75	62 (13%) 6 5	25, 93, 211, 282	0
All	All	889/1018 (87%)	0.46	78 (8%) 15 12	25, 79, 187, 282	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	GLN	4.9
1	B	246	TRP	4.8
1	B	249	VAL	4.7
1	B	217	LEU	4.6
1	B	322	LEU	4.5
1	B	241	LEU	4.2
1	B	265	ASP	4.1
1	B	289	LEU	4.0
1	B	366	LEU	3.9
1	B	239	ASP	3.9
1	B	2	ALA	3.8
1	B	369	MET	3.8
1	B	245	SER	3.7
1	B	38	LEU	3.7
1	B	330	TYR	3.7
1	B	318	ILE	3.6
1	B	30	LEU	3.6
1	A	161	PRO	3.6
1	B	283	LEU	3.6
1	B	288	LYS	3.6
1	B	4	ARG	3.6
1	B	109	GLU	3.6
1	A	163	MET	3.5
1	B	129	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	370	PHE	3.5
1	B	39	LEU	3.4
1	A	351	PRO	3.3
1	B	248	GLU	3.3
1	B	247	GLU	3.2
1	B	25	LYS	3.2
1	A	255	GLY	3.1
1	B	298	GLY	3.1
1	B	218	ASP	3.1
1	B	44	GLN	3.1
1	B	266	ARG	3.0
1	B	354	VAL	3.0
1	B	282	GLN	2.9
1	B	270	TYR	2.9
1	B	257	LYS	2.9
1	B	23	GLN	2.8
1	B	232	ARG	2.8
1	B	32	GLU	2.8
1	B	240	LYS	2.8
1	B	287	PRO	2.8
1	B	264	ALA	2.8
1	B	277	VAL	2.7
1	B	281	GLU	2.7
1	B	244	VAL	2.7
1	B	367	VAL	2.6
1	B	327	GLY	2.6
1	B	279	LEU	2.5
1	A	475	VAL	2.5
1	B	365	GLY	2.5
1	B	340	LEU	2.5
1	A	122	GLY	2.5
1	B	168	TYR	2.4
1	A	399	ALA	2.4
1	B	328	LEU	2.4
1	B	40	LYS	2.3
1	A	125	LEU	2.3
1	B	267	ILE	2.2
1	B	5	ALA	2.2
1	B	206	ASP	2.2
1	B	299	LEU	2.2
1	B	278	SER	2.2
1	B	323	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	123	GLU	2.1
1	B	3	GLU	2.1
1	A	104	MET	2.1
1	A	65	TYR	2.1
1	A	164	THR	2.1
1	B	379	CYS	2.1
1	A	242	ASP	2.1
1	B	185	MET	2.1
1	A	450	ASN	2.1
1	B	59	PRO	2.0
1	A	129	TYR	2.0
1	A	340	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	CL	A	601	1/1	0.96	0.19	67,67,67,67	0
2	CL	A	602	1/1	0.96	0.19	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.