



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:24 AM UTC

PDB ID : 4DJK / pdb_00004djk
Title : Structure of glutamate-GABA antiporter GadC
Authors : Ma, D.; Lu, P.L.; Yan, C.Y.; Fan, C.; Yin, P.; Wang, J.W.; Shi, Y.G.
Deposited on : 2012-02-02
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

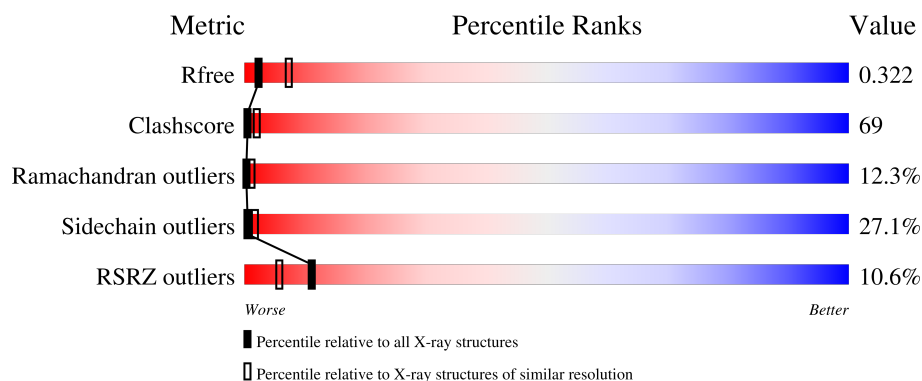
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	511	11% 19% 45% 21% • 12%
1	B	511	8% 18% 46% 22% • 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6891 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.

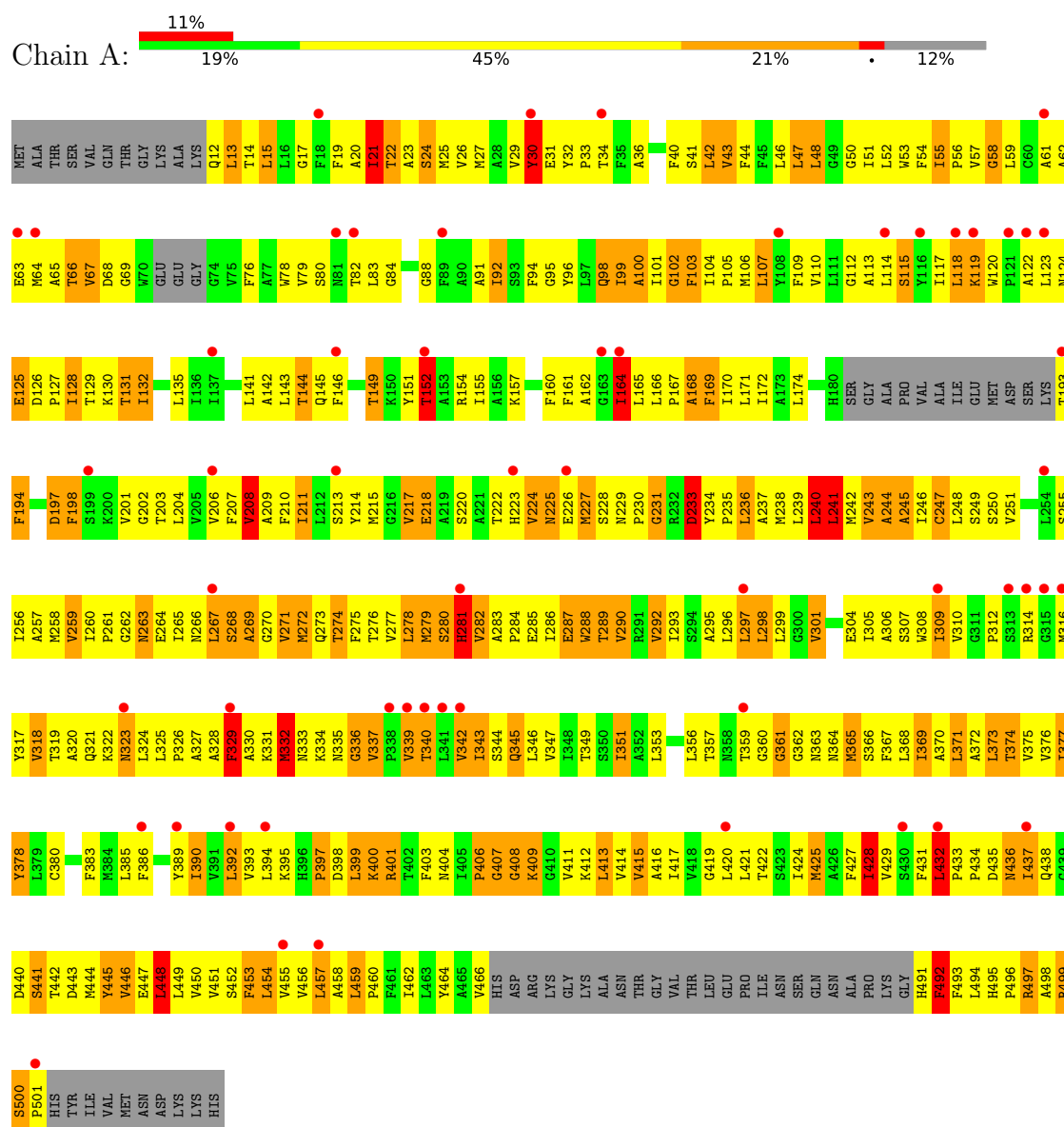
- Molecule 1 is a protein called Probable glutamate/gamma-aminobutyrate antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3436	2314	528	574	20			
1	B	453	Total	C	N	O	S	0	0	0
			3455	2324	532	579	20			

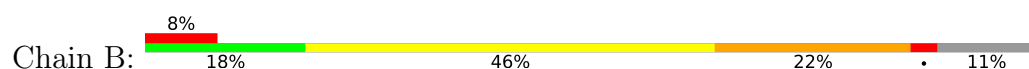
3 Residue-property plots [i](#)

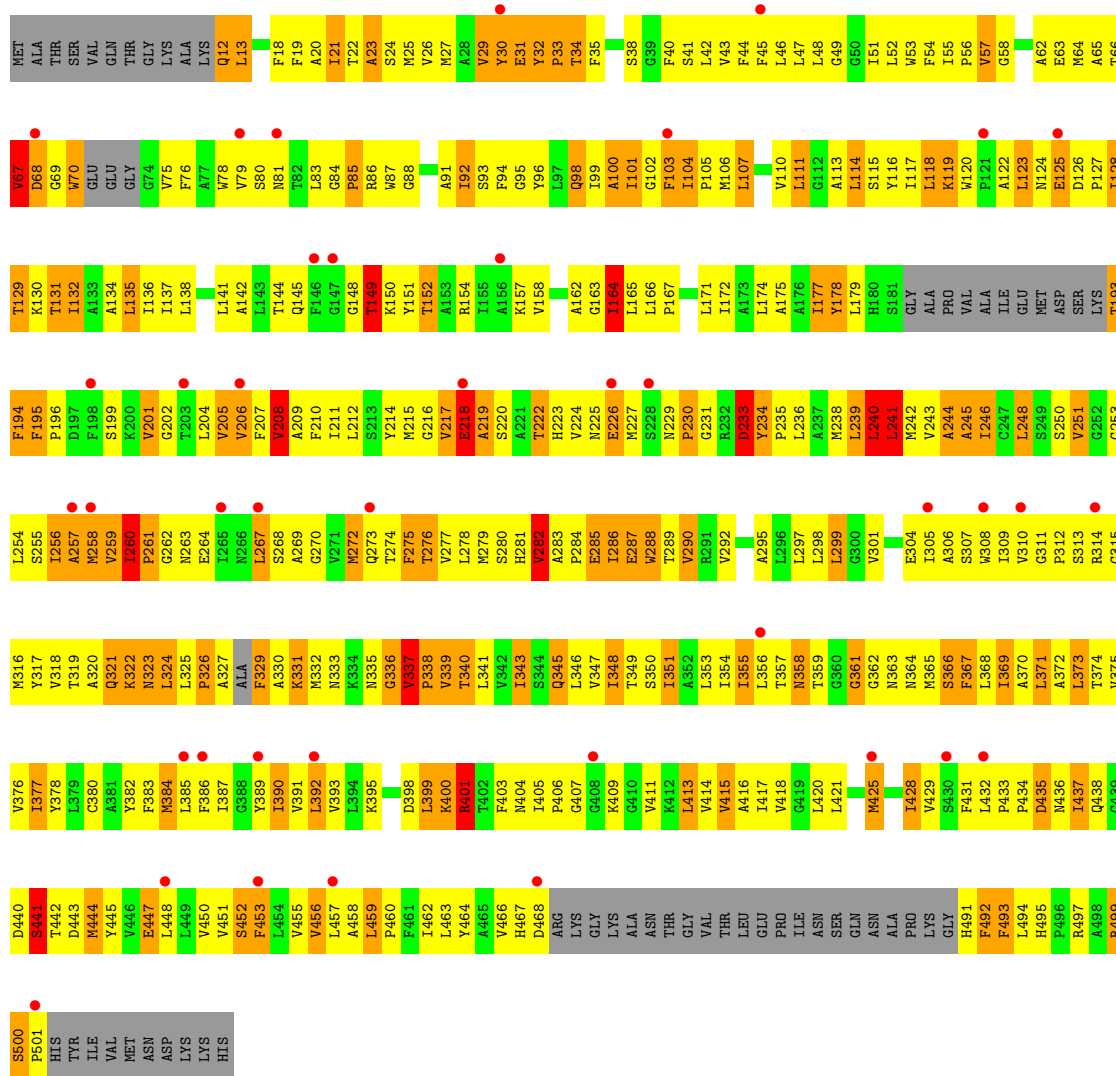
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.96Å 106.41Å 185.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.14 – 3.10 33.14 – 3.10	Depositor EDS
% Data completeness (in resolution range)	79.7 (33.14-3.10) 79.7 (33.14-3.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.282 , 0.325 0.274 , 0.322	Depositor DCC
R_{free} test set	1146 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å ²)	102.0	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 88.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6891	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.62	0/3524	1.03	11/4812 (0.2%)
1	B	0.60	0/3543	1.04	14/4836 (0.3%)
All	All	0.61	0/7067	1.04	25/9648 (0.3%)

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

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

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	444	MET	N-CA-C	-9.85	101.44	112.57
1	B	444	MET	N-CA-C	-8.88	103.55	112.97
1	B	152	THR	N-CA-C	7.84	120.52	111.11
1	B	226	GLU	N-CA-C	-7.16	104.28	112.87
1	B	256	ILE	CB-CA-C	-6.97	102.78	111.70
1	B	260	ILE	CA-C-N	6.83	128.38	119.84
1	B	260	ILE	C-N-CA	6.83	128.38	119.84
1	B	358	ASN	N-CA-C	6.36	120.40	111.30
1	B	450	VAL	N-CA-C	6.21	116.36	110.53
1	B	363	ASN	N-CA-C	-6.16	105.81	113.15
1	A	82	THR	N-CA-C	6.12	120.82	113.23
1	A	448	LEU	N-CA-C	5.84	117.45	111.14
1	A	432	LEU	CA-C-N	5.80	126.35	120.38
1	A	432	LEU	C-N-CA	5.80	126.35	120.38
1	A	263	ASN	N-CA-C	-5.57	108.28	114.62
1	A	55	ILE	CB-CA-C	-5.47	108.55	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	GLY	N-CA-C	-5.41	108.40	114.40
1	A	428	ILE	N-CA-CB	5.40	116.75	110.65
1	A	397	PRO	N-CA-C	-5.34	109.12	114.68
1	B	219	ALA	CA-C-N	5.34	131.31	121.70
1	B	219	ALA	C-N-CA	5.34	131.31	121.70
1	B	128	ILE	N-CA-C	5.33	115.54	110.42
1	B	129	THR	N-CA-C	-5.33	105.16	110.97
1	A	383	PHE	N-CA-C	-5.16	105.55	111.07
1	A	201	VAL	N-CA-C	5.02	116.47	109.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	VAL	Peptide

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	3436	0	3595	468	0
1	B	3455	0	3605	509	0
All	All	6891	0	7200	970	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 69.

All (970) 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:227:MET:HE1	1:B:234:TYR:HB2	1.28	1.11
1:A:64:MET:HE2	1:A:78:TRP:HB3	1.33	1.05
1:A:491:HIS:C	1:A:493:PHE:H	1.58	1.05
1:A:394:LEU:HD11	1:B:204:LEU:HD12	1.40	1.04
1:B:64:MET:HE2	1:B:78:TRP:HB3	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HD13	1:A:373:LEU:HD21	1.43	1.00
1:A:227:MET:HE1	1:A:234:TYR:HB2	1.41	1.00
1:B:400:LYS:H	1:B:400:LYS:HD2	1.24	1.00
1:B:279:MET:O	1:B:281:HIS:N	1.94	1.00
1:A:128:ILE:HG22	1:A:132:ILE:HG22	1.44	0.99
1:B:377:ILE:HD11	1:B:456:VAL:HG11	1.44	0.99
1:A:12:GLN:HG2	1:A:228:SER:HB3	1.45	0.98
1:A:21:ILE:HG13	1:A:492:PHE:CD1	1.99	0.97
1:B:283:ALA:HB1	1:B:284:PRO:HA	1.44	0.97
1:A:17:GLY:O	1:A:21:ILE:HG22	1.64	0.96
1:A:336:GLY:HA3	1:A:337:VAL:HB	1.46	0.96
1:B:178:TYR:HD2	1:B:178:TYR:O	1.48	0.96
1:B:219:ALA:HB3	1:B:220:SER:HB2	1.48	0.95
1:B:22:THR:O	1:B:24:SER:N	1.98	0.95
1:B:398:ASP:HA	1:B:399:LEU:HG	1.48	0.95
1:B:377:ILE:CD1	1:B:456:VAL:HG11	1.96	0.95
1:A:491:HIS:HD1	1:A:492:PHE:HD2	1.01	0.95
1:B:254:LEU:HA	1:B:257:ALA:HB3	1.49	0.94
1:A:260:ILE:HD11	1:A:277:VAL:HG21	1.51	0.93
1:A:94:PHE:CE1	1:A:460:PRO:HG2	2.03	0.93
1:B:92:ILE:HD12	1:B:316:MET:HG3	1.52	0.91
1:B:219:ALA:HB3	1:B:220:SER:CB	2.01	0.91
1:B:495:HIS:CD2	1:B:497:ARG:HG3	2.05	0.91
1:A:40:PHE:HD2	1:A:194:PHE:HB2	1.35	0.90
1:A:406:PRO:O	1:A:408:GLY:N	2.03	0.90
1:A:441:SER:O	1:A:443:ASP:N	2.05	0.89
1:B:67:VAL:CG2	1:B:400:LYS:HB2	2.02	0.89
1:A:233:ASP:H	1:A:235:PRO:HD2	1.34	0.88
1:B:284:PRO:HA	1:B:287:GLU:HB2	1.56	0.88
1:A:168:ALA:O	1:A:171:LEU:N	2.06	0.88
1:B:253:GLY:O	1:B:257:ALA:HB2	1.74	0.87
1:B:19:PHE:O	1:B:23:ALA:HB2	1.72	0.87
1:A:157:LYS:HE3	1:A:491:HIS:N	1.88	0.87
1:A:436:ASN:O	1:A:436:ASN:ND2	2.08	0.87
1:A:491:HIS:O	1:A:494:LEU:HD23	1.75	0.87
1:B:399:LEU:H	1:B:400:LYS:HD2	1.40	0.87
1:A:117:ILE:O	1:A:119:LYS:N	2.08	0.86
1:B:80:SER:HA	1:B:84:GLY:O	1.75	0.85
1:B:276:THR:HG22	1:B:290:VAL:HG11	1.56	0.85
1:A:491:HIS:C	1:A:493:PHE:N	2.32	0.84
1:B:68:ASP:CB	1:B:69:GLY:HA2	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASN:HD22	1:B:438:GLN:HB2	1.42	0.84
1:B:29:VAL:HA	1:B:32:TYR:CD1	2.12	0.84
1:A:225:ASN:C	1:A:227:MET:H	1.86	0.84
1:B:281:HIS:C	1:B:283:ALA:H	1.81	0.84
1:A:314:ARG:HH21	1:A:337:VAL:HA	1.44	0.83
1:B:222:THR:O	1:B:224:VAL:N	2.11	0.83
1:B:67:VAL:HG23	1:B:400:LYS:HB2	1.60	0.83
1:B:451:VAL:O	1:B:455:VAL:HG23	1.79	0.83
1:B:79:VAL:HG13	1:B:83:LEU:HD12	1.60	0.83
1:B:491:HIS:C	1:B:493:PHE:H	1.87	0.82
1:B:162:ALA:O	1:B:167:PRO:HD3	1.80	0.82
1:B:68:ASP:HB2	1:B:69:GLY:HA2	1.62	0.81
1:A:174:LEU:HG	1:A:278:LEU:HD23	1.60	0.81
1:B:257:ALA:O	1:B:261:PRO:HG2	1.80	0.80
1:B:110:VAL:HG11	1:B:137:ILE:HD13	1.62	0.80
1:A:364:ASN:HD22	1:A:438:GLN:HB2	1.47	0.80
1:B:240:LEU:O	1:B:243:VAL:N	2.15	0.80
1:B:279:MET:C	1:B:281:HIS:H	1.90	0.80
1:A:126:ASP:O	1:A:129:THR:OG1	1.99	0.80
1:A:451:VAL:O	1:A:455:VAL:HG23	1.81	0.80
1:B:436:ASN:HA	1:B:441:SER:CB	2.11	0.80
1:A:279:MET:O	1:A:281:HIS:N	2.15	0.79
1:A:198:PHE:O	1:B:395:LYS:HG3	1.82	0.79
1:B:258:MET:O	1:B:259:VAL:HG13	1.83	0.79
1:B:250:SER:O	1:B:254:LEU:HB2	1.82	0.79
1:A:29:VAL:O	1:A:32:TYR:N	2.15	0.78
1:B:464:TYR:HD2	1:B:464:TYR:O	1.65	0.78
1:A:283:ALA:HA	1:A:286:ILE:HB	1.64	0.78
1:B:208:VAL:HG13	1:B:375:VAL:HG21	1.66	0.78
1:B:339:VAL:O	1:B:343:ILE:HB	1.83	0.77
1:A:286:ILE:C	1:A:288:TRP:H	1.93	0.77
1:A:495:HIS:HD2	1:A:497:ARG:HB2	1.47	0.77
1:A:19:PHE:O	1:A:23:ALA:HB2	1.83	0.77
1:A:47:LEU:O	1:A:51:ILE:HG12	1.84	0.77
1:A:459:LEU:HD13	1:A:462:ILE:HD11	1.66	0.77
1:B:331:LYS:O	1:B:332:MET:HG2	1.84	0.77
1:A:19:PHE:HE1	1:A:241:LEU:HA	1.50	0.76
1:B:120:TRP:NE1	1:B:122:ALA:HB3	2.00	0.76
1:B:425:MET:O	1:B:429:VAL:HG23	1.85	0.76
1:A:322:LYS:O	1:A:325:LEU:HD13	1.85	0.76
1:A:222:THR:O	1:A:224:VAL:N	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:THR:HG22	1:A:290:VAL:HG11	1.67	0.76
1:B:442:THR:HG21	1:B:444:MET:HE2	1.67	0.75
1:A:117:ILE:C	1:A:119:LYS:H	1.93	0.75
1:A:411:VAL:HA	1:A:414:VAL:HG12	1.68	0.75
1:B:83:LEU:HB3	1:B:87:TRP:HE3	1.52	0.75
1:B:398:ASP:HA	1:B:399:LEU:CG	2.16	0.75
1:A:491:HIS:O	1:A:493:PHE:N	2.18	0.75
1:B:94:PHE:CE1	1:B:460:PRO:HG2	2.21	0.75
1:A:52:LEU:HB3	1:A:422:THR:HG21	1.67	0.74
1:A:222:THR:C	1:A:224:VAL:H	1.95	0.74
1:B:491:HIS:O	1:B:494:LEU:HD23	1.86	0.74
1:B:500:SER:H	1:B:501:PRO:HD3	1.53	0.74
1:A:106:MET:HB3	1:A:305:ILE:HD11	1.69	0.74
1:A:284:PRO:C	1:A:286:ILE:H	1.94	0.74
1:B:306:ALA:HA	1:B:309:ILE:HG12	1.70	0.74
1:B:414:VAL:O	1:B:418:VAL:HG23	1.88	0.73
1:A:325:LEU:HB2	1:A:326:PRO:HD3	1.71	0.73
1:A:491:HIS:ND1	1:A:492:PHE:CD2	2.55	0.73
1:B:361:GLY:N	1:B:442:THR:OG1	2.19	0.73
1:B:68:ASP:OD1	1:B:81:ASN:ND2	2.20	0.73
1:B:41:SER:CB	1:B:196:PRO:HB3	2.19	0.73
1:B:229:ASN:ND2	1:B:229:ASN:O	2.22	0.73
1:A:44:PHE:HB2	1:A:193:THR:HG22	1.71	0.72
1:B:157:LYS:HE3	1:B:491:HIS:N	2.03	0.72
1:B:392:LEU:HD12	1:B:392:LEU:O	1.88	0.72
1:B:491:HIS:O	1:B:493:PHE:N	2.22	0.72
1:B:202:GLY:HA3	1:B:434:PRO:CA	2.19	0.72
1:A:327:ALA:O	1:A:329:PHE:N	2.23	0.72
1:B:436:ASN:HA	1:B:441:SER:OG	1.88	0.72
1:B:202:GLY:HA3	1:B:434:PRO:N	2.05	0.72
1:A:293:ILE:HA	1:A:296:LEU:HD13	1.71	0.72
1:B:464:TYR:HE2	1:B:468:ASP:O	1.72	0.71
1:A:292:VAL:O	1:A:296:LEU:HD12	1.89	0.71
1:A:395:LYS:HG3	1:B:201:VAL:HG21	1.70	0.71
1:A:316:MET:HG2	1:A:316:MET:O	1.91	0.71
1:B:284:PRO:C	1:B:286:ILE:H	1.98	0.71
1:A:66:THR:HG21	1:A:403:PHE:HB3	1.73	0.71
1:A:66:THR:O	1:A:67:VAL:HB	1.91	0.71
1:B:66:THR:HG22	1:B:224:VAL:HG11	1.73	0.71
1:A:339:VAL:HG13	1:A:340:THR:N	2.05	0.70
1:B:29:VAL:O	1:B:31:GLU:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ALA:O	1:B:66:THR:HG23	1.90	0.70
1:B:222:THR:C	1:B:224:VAL:H	1.99	0.70
1:B:262:GLY:O	1:B:264:GLU:N	2.23	0.70
1:A:101:ILE:HG22	1:A:374:THR:OG1	1.91	0.70
1:B:67:VAL:HG21	1:B:400:LYS:HB2	1.72	0.70
1:B:103:PHE:HZ	1:B:309:ILE:HD13	1.57	0.70
1:B:398:ASP:HA	1:B:399:LEU:CB	2.21	0.70
1:B:283:ALA:HB1	1:B:284:PRO:CA	2.21	0.70
1:A:149:THR:O	1:A:149:THR:OG1	2.10	0.69
1:A:30:TYR:N	1:A:30:TYR:CD2	2.59	0.69
1:A:53:TRP:C	1:A:56:PRO:HD2	2.17	0.69
1:A:431:PHE:C	1:A:432:LEU:HD23	2.18	0.69
1:B:178:TYR:O	1:B:178:TYR:CD2	2.38	0.69
1:A:46:LEU:HD23	1:A:246:ILE:HA	1.72	0.69
1:B:68:ASP:HB2	1:B:69:GLY:CA	2.22	0.69
1:A:118:LEU:HD23	1:A:118:LEU:O	1.93	0.69
1:B:304:GLU:O	1:B:307:SER:OG	2.09	0.69
1:B:495:HIS:NE2	1:B:497:ARG:HG3	2.08	0.69
1:B:174:LEU:HG	1:B:278:LEU:HD22	1.74	0.69
1:B:314:ARG:HB2	1:B:337:VAL:HG21	1.75	0.69
1:B:350:SER:O	1:B:354:ILE:HG13	1.92	0.69
1:B:491:HIS:C	1:B:493:PHE:N	2.46	0.69
1:B:276:THR:CG2	1:B:290:VAL:HG11	2.22	0.69
1:A:46:LEU:HD12	1:A:210:PHE:CD1	2.27	0.69
1:A:279:MET:HE2	1:A:289:THR:HG21	1.75	0.69
1:A:101:ILE:HD13	1:A:373:LEU:CD2	2.21	0.68
1:B:43:VAL:O	1:B:47:LEU:HG	1.94	0.68
1:B:21:ILE:HB	1:B:492:PHE:CD1	2.29	0.68
1:B:68:ASP:CB	1:B:69:GLY:CA	2.71	0.68
1:A:67:VAL:HG11	1:A:400:LYS:HB2	1.76	0.68
1:A:101:ILE:C	1:A:103:PHE:H	1.99	0.68
1:A:307:SER:HB2	1:A:494:LEU:HD12	1.74	0.68
1:A:365:MET:HA	1:A:437:ILE:HD11	1.74	0.68
1:B:38:SER:O	1:B:41:SER:OG	2.10	0.68
1:B:99:ILE:O	1:B:101:ILE:N	2.27	0.68
1:A:98:GLN:HG3	1:A:378:TYR:CD2	2.28	0.68
1:A:274:THR:O	1:A:278:LEU:HB2	1.94	0.68
1:B:329:PHE:O	1:B:340:THR:HG21	1.93	0.68
1:A:46:LEU:HD12	1:A:210:PHE:HD1	1.59	0.68
1:A:128:ILE:N	1:A:128:ILE:HD12	2.08	0.67
1:A:333:ASN:CG	1:A:334:LYS:H	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HG3	1:A:445:TYR:CD2	2.30	0.67
1:A:237:ALA:O	1:A:241:LEU:HB2	1.95	0.67
1:B:314:ARG:HG2	1:B:500:SER:OG	1.95	0.67
1:A:166:LEU:HB3	1:A:167:PRO:HD3	1.76	0.67
1:B:86:ARG:HA	1:B:464:TYR:CE1	2.30	0.67
1:B:281:HIS:C	1:B:283:ALA:N	2.50	0.67
1:A:240:LEU:O	1:A:243:VAL:N	2.28	0.67
1:B:22:THR:C	1:B:24:SER:H	2.01	0.67
1:A:101:ILE:O	1:A:103:PHE:N	2.28	0.67
1:A:124:ASN:HD21	1:A:268:SER:HB2	1.59	0.67
1:A:333:ASN:O	1:A:334:LYS:HG3	1.95	0.67
1:A:361:GLY:O	1:A:440:ASP:HB3	1.95	0.66
1:B:282:VAL:HG13	1:B:286:ILE:HG21	1.76	0.66
1:A:369:ILE:HG13	1:A:445:TYR:CE1	2.30	0.66
1:B:76:PHE:O	1:B:80:SER:OG	2.10	0.66
1:B:243:VAL:HA	1:B:246:ILE:HD12	1.77	0.66
1:B:364:ASN:HD22	1:B:438:GLN:CB	2.08	0.66
1:A:408:GLY:O	1:A:412:LYS:HE3	1.95	0.66
1:B:42:LEU:HD12	1:B:43:VAL:N	2.10	0.66
1:A:25:MET:HB2	1:A:495:HIS:HE1	1.61	0.66
1:A:67:VAL:HG11	1:A:401:ARG:H	1.60	0.66
1:A:229:ASN:O	1:A:230:PRO:C	2.37	0.66
1:B:157:LYS:HZ1	1:B:491:HIS:N	1.94	0.66
1:A:269:ALA:O	1:A:271:VAL:N	2.29	0.66
1:B:453:PHE:C	1:B:453:PHE:CD2	2.73	0.66
1:A:29:VAL:O	1:A:31:GLU:N	2.28	0.65
1:A:336:GLY:CA	1:A:337:VAL:HB	2.22	0.65
1:B:83:LEU:HB3	1:B:87:TRP:CE3	2.31	0.65
1:B:233:ASP:H	1:B:235:PRO:HD2	1.60	0.65
1:B:234:TYR:C	1:B:234:TYR:CD2	2.74	0.65
1:B:365:MET:HA	1:B:437:ILE:CD1	2.25	0.65
1:A:66:THR:O	1:A:66:THR:OG1	2.10	0.65
1:A:171:LEU:HB2	1:A:275:PHE:CZ	2.31	0.65
1:A:377:ILE:HG12	1:A:456:VAL:HG11	1.78	0.65
1:B:274:THR:O	1:B:278:LEU:HB2	1.97	0.65
1:B:283:ALA:HB1	1:B:287:GLU:HB2	1.77	0.65
1:B:46:LEU:HD23	1:B:246:ILE:HA	1.79	0.65
1:B:53:TRP:C	1:B:56:PRO:HD2	2.21	0.65
1:B:94:PHE:HE1	1:B:460:PRO:HG2	1.62	0.65
1:B:175:ALA:HB2	1:B:278:LEU:HD11	1.77	0.65
1:B:120:TRP:CD1	1:B:122:ALA:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:O	1:B:289:THR:HG22	1.97	0.65
1:B:233:ASP:OD2	1:B:234:TYR:N	2.29	0.65
1:B:356:LEU:HD11	1:B:369:ILE:HD13	1.79	0.65
1:B:365:MET:HA	1:B:437:ILE:HD11	1.78	0.65
1:A:496:PRO:C	1:A:498:ALA:H	2.05	0.65
1:B:209:ALA:HB2	1:B:371:LEU:HD12	1.79	0.65
1:B:448:LEU:O	1:B:452:SER:HB2	1.96	0.65
1:B:433:PRO:HG3	1:B:445:TYR:HD2	1.62	0.64
1:A:323:ASN:HB3	1:A:325:LEU:CD1	2.26	0.64
1:B:34:THR:HG22	1:B:267:LEU:HD12	1.79	0.64
1:A:99:ILE:O	1:A:101:ILE:N	2.30	0.64
1:A:225:ASN:C	1:A:227:MET:N	2.54	0.64
1:B:411:VAL:HA	1:B:414:VAL:HG12	1.80	0.64
1:A:197:ASP:O	1:A:203:THR:HG21	1.96	0.64
1:A:295:ALA:O	1:A:298:LEU:HD23	1.97	0.64
1:B:98:GLN:HB2	1:B:378:TYR:HB2	1.80	0.64
1:B:103:PHE:CZ	1:B:309:ILE:HD13	2.32	0.64
1:B:117:ILE:HD11	1:B:295:ALA:HA	1.78	0.64
1:B:317:TYR:CE1	1:B:330:ALA:HB1	2.32	0.64
1:B:365:MET:O	1:B:366:SER:C	2.41	0.64
1:A:356:LEU:HD11	1:A:369:ILE:HD13	1.80	0.64
1:B:127:PRO:O	1:B:131:THR:HG22	1.97	0.64
1:A:409:LYS:HA	1:A:412:LYS:HB2	1.79	0.64
1:A:440:ASP:N	1:A:441:SER:OG	2.26	0.64
1:B:219:ALA:HB3	1:B:220:SER:HB3	1.80	0.64
1:A:347:VAL:O	1:A:351:ILE:CG1	2.46	0.64
1:B:12:GLN:N	1:B:12:GLN:OE1	2.31	0.64
1:A:399:LEU:C	1:A:400:LYS:HD2	2.22	0.63
1:B:22:THR:OG1	1:B:241:LEU:HD11	1.98	0.63
1:A:356:LEU:HD11	1:A:369:ILE:HG21	1.79	0.63
1:A:64:MET:CE	1:A:78:TRP:HB3	2.19	0.63
1:A:373:LEU:HB2	1:A:449:LEU:HD12	1.81	0.63
1:A:104:ILE:N	1:A:105:PRO:HD2	2.14	0.63
1:A:279:MET:HE2	1:A:289:THR:CG2	2.29	0.63
1:B:30:TYR:N	1:B:30:TYR:CD2	2.65	0.63
1:B:124:ASN:ND2	1:B:269:ALA:HB2	2.14	0.63
1:B:400:LYS:H	1:B:400:LYS:CD	1.97	0.63
1:A:80:SER:HA	1:A:84:GLY:O	1.99	0.63
1:B:31:GLU:O	1:B:32:TYR:C	2.42	0.63
1:B:92:ILE:HD12	1:B:316:MET:CG	2.27	0.63
1:B:94:PHE:C	1:B:96:TYR:H	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HG22	1:B:118:LEU:HD12	1.79	0.63
1:A:339:VAL:CG1	1:A:340:THR:N	2.62	0.62
1:B:317:TYR:O	1:B:320:ALA:N	2.32	0.62
1:A:492:PHE:CD2	1:A:492:PHE:N	2.68	0.62
1:B:194:PHE:O	1:B:196:PRO:N	2.32	0.62
1:B:208:VAL:CG1	1:B:371:LEU:HB3	2.29	0.62
1:B:215:MET:HE2	1:B:378:TYR:HD2	1.64	0.62
1:B:225:ASN:C	1:B:227:MET:N	2.57	0.62
1:B:240:LEU:O	1:B:242:MET:N	2.32	0.62
1:A:19:PHE:CE1	1:A:241:LEU:HA	2.33	0.62
1:A:101:ILE:C	1:A:103:PHE:N	2.56	0.62
1:B:41:SER:HB2	1:B:196:PRO:HB3	1.82	0.62
1:A:119:LYS:HE3	1:A:119:LYS:HA	1.81	0.62
1:A:347:VAL:O	1:A:351:ILE:HG13	1.99	0.62
1:A:368:LEU:HD23	1:A:437:ILE:HG21	1.80	0.62
1:A:67:VAL:HG21	1:A:400:LYS:HB3	1.80	0.62
1:A:492:PHE:HD2	1:A:492:PHE:N	1.96	0.62
1:B:225:ASN:C	1:B:227:MET:H	2.07	0.62
1:B:18:PHE:CD1	1:B:21:ILE:HD11	2.34	0.62
1:B:376:VAL:HG23	1:B:453:PHE:HD1	1.65	0.62
1:A:356:LEU:HD11	1:A:369:ILE:CG2	2.30	0.62
1:B:244:ALA:O	1:B:246:ILE:N	2.33	0.62
1:B:365:MET:HG3	1:B:437:ILE:HD11	1.82	0.62
1:B:377:ILE:HG22	1:B:378:TYR:N	2.15	0.62
1:A:40:PHE:HD2	1:A:194:PHE:CB	2.11	0.61
1:A:317:TYR:OH	1:A:330:ALA:HB1	2.00	0.61
1:A:327:ALA:C	1:A:329:PHE:H	2.07	0.61
1:A:377:ILE:HD11	1:A:456:VAL:HG21	1.81	0.61
1:B:240:LEU:O	1:B:241:LEU:C	2.43	0.61
1:B:260:ILE:H	1:B:261:PRO:HD2	1.65	0.61
1:B:431:PHE:O	1:B:432:LEU:HD23	1.99	0.61
1:A:215:MET:CE	1:A:375:VAL:HG13	2.31	0.61
1:B:362:GLY:HA3	1:B:440:ASP:HB3	1.82	0.61
1:B:431:PHE:C	1:B:432:LEU:HD23	2.25	0.61
1:B:255:SER:O	1:B:259:VAL:HG22	2.00	0.61
1:B:417:ILE:O	1:B:421:LEU:HD13	2.00	0.61
1:A:259:VAL:HG21	1:A:278:LEU:HD12	1.83	0.61
1:A:40:PHE:O	1:A:43:VAL:HG23	1.99	0.61
1:A:117:ILE:HD11	1:A:295:ALA:N	2.15	0.61
1:B:234:TYR:C	1:B:234:TYR:HD2	2.06	0.61
1:B:104:ILE:HG12	1:B:353:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PHE:O	1:A:390:ILE:HG12	2.00	0.61
1:B:104:ILE:HG22	1:B:105:PRO:N	2.16	0.61
1:B:128:ILE:O	1:B:132:ILE:HG23	2.01	0.61
1:A:32:TYR:N	1:A:33:PRO:HD2	2.16	0.61
1:B:207:PHE:O	1:B:208:VAL:C	2.44	0.61
1:B:456:VAL:HG12	1:B:457:LEU:N	2.15	0.61
1:A:142:ALA:O	1:A:146:PHE:HD2	1.84	0.61
1:A:152:THR:HG21	1:A:307:SER:HA	1.83	0.61
1:B:307:SER:HB2	1:B:494:LEU:HD12	1.83	0.60
1:B:433:PRO:HG3	1:B:445:TYR:CD2	2.36	0.60
1:A:112:GLY:O	1:A:115:SER:HB3	2.01	0.60
1:B:256:ILE:HG23	1:B:274:THR:OG1	2.01	0.60
1:B:113:ALA:HA	1:B:272:MET:SD	2.42	0.60
1:B:371:LEU:O	1:B:375:VAL:HG23	2.01	0.60
1:A:120:TRP:CD1	1:A:122:ALA:HB3	2.36	0.60
1:A:368:LEU:O	1:A:371:LEU:HB2	2.01	0.60
1:B:215:MET:HE2	1:B:378:TYR:CD2	2.36	0.60
1:A:12:GLN:HG2	1:A:228:SER:CB	2.28	0.60
1:B:253:GLY:O	1:B:257:ALA:CB	2.48	0.60
1:B:47:LEU:O	1:B:51:ILE:HG12	2.02	0.60
1:B:174:LEU:HG	1:B:278:LEU:CD2	2.31	0.60
1:A:21:ILE:HG13	1:A:492:PHE:CE1	2.37	0.59
1:A:244:ALA:O	1:A:246:ILE:N	2.35	0.59
1:A:306:ALA:O	1:A:309:ILE:HG12	2.02	0.59
1:A:124:ASN:O	1:A:363:ASN:ND2	2.35	0.59
1:B:55:ILE:HA	1:B:238:MET:CE	2.33	0.59
1:A:361:GLY:HA3	1:A:441:SER:HA	1.84	0.59
1:A:30:TYR:CE2	1:A:301:VAL:HG23	2.37	0.59
1:B:98:GLN:HG3	1:B:378:TYR:CD2	2.38	0.59
1:B:367:PHE:O	1:B:370:ALA:N	2.35	0.59
1:A:128:ILE:O	1:A:131:THR:HG23	2.01	0.59
1:A:256:ILE:HA	1:A:274:THR:OG1	2.03	0.59
1:A:284:PRO:C	1:A:286:ILE:N	2.61	0.59
1:B:499:ARG:O	1:B:500:SER:HB2	2.02	0.59
1:A:54:PHE:CD1	1:A:214:TYR:HD1	2.21	0.59
1:B:29:VAL:HA	1:B:32:TYR:CE1	2.37	0.59
1:B:361:GLY:H	1:B:442:THR:HG1	1.46	0.59
1:B:233:ASP:O	1:B:236:LEU:HB2	2.03	0.59
1:A:286:ILE:C	1:A:288:TRP:N	2.57	0.59
1:B:279:MET:C	1:B:281:HIS:N	2.51	0.59
1:A:79:VAL:CG1	1:A:88:GLY:HA2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:HIS:HA	1:A:494:LEU:HD22	1.85	0.58
1:A:498:ALA:O	1:A:499:ARG:O	2.21	0.58
1:B:44:PHE:HA	1:B:193:THR:HG22	1.85	0.58
1:A:61:ALA:HB2	1:A:385:LEU:HD11	1.84	0.58
1:A:314:ARG:NH2	1:A:336:GLY:HA3	2.18	0.58
1:B:64:MET:CE	1:B:78:TRP:HB3	2.25	0.58
1:B:236:LEU:HA	1:B:239:LEU:HB2	1.85	0.58
1:A:98:GLN:HG3	1:A:378:TYR:CG	2.38	0.58
1:B:314:ARG:NH2	1:B:335:ASN:HB3	2.19	0.58
1:B:215:MET:HE1	1:B:375:VAL:HA	1.86	0.58
1:A:168:ALA:O	1:A:169:PHE:C	2.47	0.58
1:B:163:GLY:O	1:B:164:ILE:HG13	2.03	0.58
1:B:208:VAL:HG12	1:B:209:ALA:N	2.18	0.58
1:B:101:ILE:HG22	1:B:374:THR:OG1	2.04	0.58
1:B:145:GLN:NE2	1:B:152:THR:HG21	2.19	0.58
1:B:283:ALA:HA	1:B:285:GLU:N	2.18	0.58
1:A:52:LEU:CB	1:A:422:THR:HG21	2.34	0.58
1:B:407:GLY:HA3	1:B:411:VAL:HB	1.85	0.58
1:A:332:MET:HA	1:A:337:VAL:O	2.04	0.58
1:B:45:PHE:HD2	1:B:210:PHE:CE2	2.22	0.58
1:B:329:PHE:C	1:B:329:PHE:CD2	2.82	0.58
1:A:245:ALA:O	1:A:249:SER:OG	2.16	0.57
1:B:99:ILE:HG21	1:B:312:PRO:HG2	1.85	0.57
1:A:21:ILE:O	1:A:499:ARG:NH2	2.36	0.57
1:A:40:PHE:CD2	1:A:194:PHE:HB2	2.27	0.57
1:A:79:VAL:HG12	1:A:88:GLY:HA2	1.86	0.57
1:B:307:SER:HB2	1:B:494:LEU:CD1	2.35	0.57
1:B:365:MET:CG	1:B:437:ILE:HD11	2.34	0.57
1:A:215:MET:HE1	1:A:375:VAL:HG13	1.86	0.57
1:B:145:GLN:HG3	1:B:309:ILE:HB	1.85	0.57
1:B:204:LEU:O	1:B:206:VAL:N	2.37	0.57
1:B:215:MET:CE	1:B:378:TYR:HB3	2.35	0.57
1:B:377:ILE:HD11	1:B:456:VAL:CG1	2.27	0.57
1:A:92:ILE:HG23	1:A:316:MET:SD	2.45	0.57
1:B:63:GLU:OE2	1:B:404:ASN:HA	2.03	0.57
1:B:405:ILE:HG23	1:B:406:PRO:HD2	1.87	0.57
1:B:431:PHE:O	1:B:433:PRO:HD3	2.04	0.57
1:A:20:ALA:O	1:A:23:ALA:N	2.33	0.57
1:A:428:ILE:O	1:A:431:PHE:N	2.36	0.57
1:B:463:LEU:O	1:B:466:VAL:HG22	2.04	0.57
1:A:247:CYS:O	1:A:251:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:O	1:A:227:MET:N	2.38	0.57
1:B:21:ILE:HB	1:B:492:PHE:HD1	1.69	0.57
1:A:42:LEU:C	1:A:42:LEU:HD12	2.30	0.56
1:B:349:THR:O	1:B:353:LEU:HB2	2.05	0.56
1:A:209:ALA:HB2	1:A:371:LEU:CD1	2.35	0.56
1:A:361:GLY:H	1:A:365:MET:HE3	1.70	0.56
1:B:40:PHE:O	1:B:40:PHE:HD1	1.88	0.56
1:B:284:PRO:C	1:B:286:ILE:N	2.62	0.56
1:A:68:ASP:HB2	1:A:69:GLY:HA2	1.88	0.56
1:A:145:GLN:HA	1:A:145:GLN:NE2	2.20	0.56
1:A:161:PHE:CE2	1:A:493:PHE:HE1	2.24	0.56
1:A:411:VAL:HA	1:A:414:VAL:CG1	2.35	0.56
1:B:46:LEU:HD12	1:B:210:PHE:CD1	2.41	0.56
1:A:228:SER:HA	1:A:230:PRO:HD3	1.87	0.56
1:A:392:LEU:HD12	1:A:401:ARG:HH21	1.70	0.56
1:B:92:ILE:HG23	1:B:316:MET:HG3	1.86	0.56
1:B:458:ALA:O	1:B:462:ILE:HG23	2.05	0.56
1:B:284:PRO:HA	1:B:287:GLU:CB	2.34	0.56
1:A:222:THR:C	1:A:224:VAL:N	2.63	0.56
1:A:456:VAL:HG12	1:A:457:LEU:N	2.19	0.56
1:B:27:MET:HG2	1:B:164:ILE:CG2	2.35	0.56
1:B:369:ILE:HG13	1:B:445:TYR:CE1	2.41	0.56
1:A:99:ILE:C	1:A:101:ILE:N	2.64	0.56
1:B:94:PHE:CD2	1:B:380:CYS:HB2	2.40	0.56
1:B:229:ASN:O	1:B:230:PRO:O	2.24	0.56
1:B:272:MET:O	1:B:273:GLN:C	2.47	0.56
1:B:338:PRO:O	1:B:339:VAL:C	2.48	0.56
1:B:464:TYR:C	1:B:464:TYR:CD2	2.84	0.56
1:B:365:MET:CB	1:B:437:ILE:HD11	2.36	0.55
1:B:411:VAL:HA	1:B:414:VAL:CG1	2.35	0.55
1:A:25:MET:HB2	1:A:495:HIS:CE1	2.40	0.55
1:A:229:ASN:O	1:A:229:ASN:CG	2.49	0.55
1:B:149:THR:HG21	1:B:314:ARG:HH22	1.71	0.55
1:B:400:LYS:HD2	1:B:400:LYS:N	2.08	0.55
1:A:339:VAL:CG1	1:A:340:THR:H	2.19	0.55
1:B:157:LYS:CE	1:B:491:HIS:N	2.70	0.55
1:B:337:VAL:N	1:B:338:PRO:HD3	2.22	0.55
1:B:351:ILE:O	1:B:355:ILE:HD12	2.07	0.55
1:B:436:ASN:HA	1:B:441:SER:HB2	1.88	0.55
1:A:209:ALA:HB2	1:A:371:LEU:HD12	1.89	0.55
1:A:500:SER:H	1:A:501:PRO:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:TYR:CD1	1:B:272:MET:HB2	2.42	0.55
1:A:453:PHE:C	1:A:453:PHE:CD2	2.84	0.55
1:B:31:GLU:O	1:B:33:PRO:N	2.40	0.55
1:A:365:MET:HA	1:A:437:ILE:CD1	2.37	0.55
1:A:398:ASP:HA	1:A:399:LEU:HB2	1.89	0.55
1:A:22:THR:HA	1:A:499:ARG:HH22	1.72	0.55
1:B:99:ILE:C	1:B:101:ILE:N	2.65	0.55
1:A:168:ALA:O	1:A:170:ILE:N	2.40	0.54
1:A:261:PRO:O	1:A:263:ASN:N	2.39	0.54
1:A:41:SER:HB3	1:A:194:PHE:O	2.07	0.54
1:B:31:GLU:HB2	1:B:35:PHE:CE2	2.41	0.54
1:B:145:GLN:OE1	1:B:145:GLN:HA	2.05	0.54
1:B:362:GLY:CA	1:B:440:ASP:HB3	2.37	0.54
1:B:131:THR:O	1:B:135:LEU:HB2	2.07	0.54
1:B:330:ALA:O	1:B:331:LYS:HD3	2.07	0.54
1:A:124:ASN:HD21	1:A:269:ALA:H	1.55	0.54
1:B:218:GLU:OE2	1:B:378:TYR:OH	2.12	0.54
1:B:301:VAL:O	1:B:305:ILE:HG13	2.07	0.54
1:B:464:TYR:HD2	1:B:464:TYR:C	2.16	0.54
1:A:124:ASN:ND2	1:A:268:SER:HB2	2.22	0.54
1:A:246:ILE:O	1:A:250:SER:OG	2.24	0.54
1:A:44:PHE:HB2	1:A:193:THR:CG2	2.38	0.54
1:B:20:ALA:O	1:B:21:ILE:C	2.51	0.54
1:A:29:VAL:O	1:A:30:TYR:C	2.51	0.54
1:A:377:ILE:CD1	1:A:456:VAL:HG11	2.37	0.54
1:B:70:TRP:CD1	1:B:222:THR:HB	2.43	0.54
1:B:99:ILE:C	1:B:101:ILE:H	2.16	0.54
1:A:36:ALA:HB1	1:A:257:ALA:HA	1.90	0.54
1:B:358:ASN:O	1:B:359:THR:HG23	2.07	0.54
1:A:46:LEU:HD22	1:A:250:SER:HB3	1.90	0.54
1:A:79:VAL:HG12	1:A:88:GLY:CA	2.37	0.54
1:A:120:TRP:NE1	1:A:122:ALA:HB3	2.23	0.53
1:A:206:VAL:HG13	1:A:210:PHE:HE2	1.73	0.53
1:A:411:VAL:O	1:A:412:LYS:C	2.51	0.53
1:B:142:ALA:HB2	1:B:346:LEU:HD11	1.89	0.53
1:B:244:ALA:O	1:B:245:ALA:C	2.51	0.53
1:A:12:GLN:CG	1:A:228:SER:HB3	2.30	0.53
1:A:296:LEU:HD12	1:A:296:LEU:H	1.73	0.53
1:A:312:PRO:HG3	1:A:498:ALA:HA	1.90	0.53
1:A:323:ASN:HB3	1:A:325:LEU:HD12	1.89	0.53
1:A:389:TYR:O	1:A:393:VAL:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:HB3	1:B:167:PRO:HD3	1.88	0.53
1:B:44:PHE:HB2	1:B:193:THR:HG22	1.91	0.53
1:B:86:ARG:HA	1:B:464:TYR:CD1	2.43	0.53
1:B:304:GLU:O	1:B:307:SER:N	2.42	0.53
1:A:204:LEU:HB3	1:A:429:VAL:CG1	2.39	0.53
1:A:376:VAL:HG23	1:A:453:PHE:HD1	1.74	0.53
1:A:441:SER:O	1:A:443:ASP:OD1	2.26	0.53
1:B:31:GLU:HB2	1:B:35:PHE:CD2	2.43	0.53
1:A:41:SER:O	1:A:44:PHE:HB3	2.08	0.53
1:A:119:LYS:HA	1:A:119:LYS:CE	2.38	0.53
1:A:131:THR:HG22	1:A:357:THR:HG21	1.89	0.53
1:A:267:LEU:HB3	1:A:367:PHE:CD2	2.44	0.53
1:B:275:PHE:O	1:B:276:THR:C	2.51	0.53
1:A:106:MET:O	1:A:110:VAL:HG23	2.08	0.53
1:A:500:SER:O	1:A:501:PRO:C	2.51	0.53
1:B:317:TYR:OH	1:B:330:ALA:HB1	2.08	0.53
1:B:373:LEU:O	1:B:373:LEU:HD23	2.09	0.53
1:A:385:LEU:HD23	1:A:385:LEU:C	2.33	0.53
1:B:351:ILE:HG22	1:B:355:ILE:HD12	1.91	0.53
1:B:66:THR:HG22	1:B:224:VAL:CG1	2.39	0.52
1:B:219:ALA:CB	1:B:220:SER:CB	2.82	0.52
1:A:99:ILE:C	1:A:101:ILE:H	2.17	0.52
1:B:366:SER:O	1:B:369:ILE:HG22	2.08	0.52
1:A:271:VAL:O	1:A:274:THR:HB	2.09	0.52
1:B:262:GLY:C	1:B:264:GLU:H	2.16	0.52
1:B:286:ILE:C	1:B:288:TRP:H	2.17	0.52
1:A:130:LYS:NZ	1:A:363:ASN:HB2	2.25	0.52
1:B:70:TRP:CE3	1:B:70:TRP:N	2.78	0.52
1:B:175:ALA:CB	1:B:278:LEU:HD11	2.40	0.52
1:B:389:TYR:C	1:B:389:TYR:CD2	2.88	0.52
1:A:29:VAL:C	1:A:31:GLU:N	2.63	0.52
1:A:110:VAL:HG22	1:A:301:VAL:HG11	1.90	0.52
1:A:377:ILE:CG1	1:A:456:VAL:HG11	2.39	0.52
1:A:491:HIS:ND1	1:A:492:PHE:CE2	2.78	0.52
1:B:204:LEU:O	1:B:205:VAL:C	2.52	0.52
1:B:18:PHE:HD1	1:B:21:ILE:HD11	1.74	0.52
1:B:29:VAL:C	1:B:31:GLU:N	2.67	0.52
1:B:120:TRP:HE1	1:B:122:ALA:HB3	1.71	0.52
1:B:260:ILE:HD11	1:B:274:THR:HA	1.91	0.52
1:B:68:ASP:HB3	1:B:69:GLY:HA2	1.89	0.52
1:A:500:SER:H	1:A:501:PRO:CD	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:HD22	1:B:269:ALA:HB2	1.75	0.52
1:B:132:ILE:HD12	1:B:132:ILE:O	2.09	0.52
1:B:308:TRP:N	1:B:308:TRP:CD1	2.78	0.52
1:B:393:VAL:HG11	1:B:413:LEU:HD13	1.91	0.52
1:A:141:LEU:HA	1:A:144:THR:CG2	2.39	0.52
1:A:401:ARG:HH12	1:A:412:LYS:NZ	2.07	0.52
1:B:104:ILE:O	1:B:107:LEU:N	2.42	0.52
1:B:289:THR:O	1:B:292:VAL:HB	2.10	0.52
1:A:307:SER:HB2	1:A:494:LEU:CD1	2.40	0.52
1:A:417:ILE:HG21	1:B:425:MET:HE3	1.92	0.52
1:A:152:THR:CG2	1:A:307:SER:HA	2.40	0.51
1:A:360:GLY:O	1:A:362:GLY:N	2.37	0.51
1:B:256:ILE:O	1:B:258:MET:N	2.43	0.51
1:A:395:LYS:HG3	1:B:201:VAL:CG2	2.39	0.51
1:B:279:MET:HE2	1:B:289:THR:HG21	1.91	0.51
1:A:495:HIS:ND1	1:A:496:PRO:HD2	2.25	0.51
1:B:149:THR:O	1:B:149:THR:OG1	2.28	0.51
1:B:336:GLY:HA3	1:B:338:PRO:HG3	1.92	0.51
1:A:160:PHE:CE1	1:A:165:LEU:HD21	2.46	0.51
1:B:20:ALA:O	1:B:22:THR:N	2.44	0.51
1:B:46:LEU:CD1	1:B:210:PHE:CD1	2.94	0.51
1:B:435:ASP:OD2	1:B:435:ASP:N	2.43	0.51
1:A:65:ALA:HB2	1:A:78:TRP:CZ2	2.46	0.51
1:A:127:PRO:HA	1:A:128:ILE:C	2.36	0.51
1:A:436:ASN:HD22	1:A:436:ASN:C	2.17	0.51
1:B:22:THR:HA	1:B:499:ARG:HH22	1.76	0.51
1:B:317:TYR:HE1	1:B:330:ALA:HB1	1.76	0.51
1:A:398:ASP:OD2	1:A:398:ASP:N	2.42	0.51
1:A:243:VAL:HG12	1:A:244:ALA:N	2.23	0.51
1:B:209:ALA:HB2	1:B:371:LEU:CD1	2.41	0.51
1:B:270:GLY:O	1:B:273:GLN:HB3	2.11	0.51
1:B:495:HIS:HD2	1:B:497:ARG:HG3	1.70	0.51
1:B:118:LEU:O	1:B:119:LYS:C	2.53	0.51
1:A:54:PHE:CD1	1:A:214:TYR:CD1	2.99	0.51
1:A:233:ASP:OD2	1:A:234:TYR:N	2.44	0.51
1:A:373:LEU:HB2	1:A:449:LEU:CD1	2.41	0.51
1:A:110:VAL:HG22	1:A:301:VAL:CG1	2.40	0.51
1:A:26:VAL:HG13	1:A:245:ALA:HA	1.93	0.50
1:A:67:VAL:HG11	1:A:401:ARG:N	2.25	0.50
1:A:325:LEU:CB	1:A:326:PRO:HD3	2.40	0.50
1:B:240:LEU:HA	1:B:243:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:PRO:C	1:B:264:GLU:OE1	2.54	0.50
1:A:66:THR:O	1:A:67:VAL:CB	2.59	0.50
1:B:94:PHE:CD2	1:B:380:CYS:CB	2.93	0.50
1:B:42:LEU:O	1:B:46:LEU:HD13	2.11	0.50
1:A:67:VAL:HG21	1:A:400:LYS:CB	2.41	0.50
1:A:304:GLU:O	1:A:307:SER:N	2.44	0.50
1:A:25:MET:CB	1:A:495:HIS:CE1	2.94	0.50
1:A:240:LEU:O	1:A:241:LEU:C	2.55	0.50
1:B:113:ALA:HB2	1:B:272:MET:HE1	1.93	0.50
1:A:66:THR:O	1:A:401:ARG:HA	2.12	0.50
1:A:361:GLY:H	1:A:365:MET:CE	2.23	0.50
1:B:96:TYR:O	1:B:99:ILE:HB	2.11	0.50
1:B:377:ILE:HD11	1:B:456:VAL:HG21	1.93	0.50
1:B:380:CYS:O	1:B:383:PHE:HB2	2.11	0.50
1:A:94:PHE:C	1:A:96:TYR:H	2.20	0.50
1:B:40:PHE:O	1:B:40:PHE:CD1	2.64	0.50
1:B:48:LEU:HD12	1:B:207:PHE:CE2	2.47	0.50
1:B:129:THR:O	1:B:130:LYS:C	2.52	0.50
1:B:204:LEU:C	1:B:206:VAL:N	2.69	0.50
1:B:281:HIS:O	1:B:283:ALA:N	2.44	0.50
1:B:292:VAL:O	1:B:295:ALA:HB3	2.11	0.50
1:B:29:VAL:C	1:B:31:GLU:H	2.20	0.49
1:B:365:MET:CA	1:B:437:ILE:HD11	2.41	0.49
1:A:106:MET:HE1	1:A:308:TRP:CZ3	2.47	0.49
1:A:114:LEU:CD2	1:A:298:LEU:HD13	2.42	0.49
1:A:128:ILE:HD12	1:A:128:ILE:H	1.75	0.49
1:A:208:VAL:HG12	1:A:209:ALA:N	2.27	0.49
1:B:178:TYR:CD2	1:B:178:TYR:C	2.91	0.49
1:A:19:PHE:HE1	1:A:241:LEU:CA	2.23	0.49
1:A:128:ILE:N	1:A:128:ILE:CD1	2.75	0.49
1:A:361:GLY:HA3	1:A:441:SER:CA	2.42	0.49
1:B:51:ILE:O	1:B:56:PRO:HD3	2.12	0.49
1:B:464:TYR:O	1:B:464:TYR:CD2	2.55	0.49
1:A:30:TYR:CE2	1:A:301:VAL:CG2	2.95	0.49
1:A:103:PHE:HE2	1:A:308:TRP:HB2	1.76	0.49
1:A:202:GLY:HA3	1:A:434:PRO:HG3	1.94	0.49
1:A:275:PHE:O	1:A:276:THR:C	2.55	0.49
1:A:393:VAL:HG11	1:A:413:LEU:HD13	1.94	0.49
1:B:240:LEU:HD23	1:B:243:VAL:HG12	1.94	0.49
1:B:163:GLY:O	1:B:164:ILE:CG1	2.60	0.49
1:B:324:LEU:HD13	1:B:467:HIS:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ILE:C	1:B:103:PHE:N	2.69	0.49
1:A:333:ASN:CG	1:A:334:LYS:N	2.70	0.49
1:A:286:ILE:HA	1:A:288:TRP:HD1	1.78	0.49
1:B:306:ALA:HA	1:B:309:ILE:CG1	2.40	0.49
1:A:193:THR:O	1:A:194:PHE:C	2.56	0.49
1:A:218:GLU:H	1:A:218:GLU:HG3	1.31	0.49
1:B:311:GLY:O	1:B:312:PRO:C	2.55	0.49
1:A:317:TYR:O	1:A:319:THR:N	2.45	0.49
1:A:343:ILE:HG22	1:A:344:SER:N	2.28	0.49
1:A:76:PHE:O	1:A:80:SER:HB2	2.13	0.48
1:A:101:ILE:HG22	1:A:374:THR:HG1	1.77	0.48
1:A:124:ASN:HD21	1:A:269:ALA:N	2.10	0.48
1:A:322:LYS:O	1:A:324:LEU:N	2.45	0.48
1:B:92:ILE:CG2	1:B:316:MET:HG3	2.43	0.48
1:A:286:ILE:O	1:A:288:TRP:N	2.36	0.48
1:B:48:LEU:HD12	1:B:207:PHE:CZ	2.48	0.48
1:A:48:LEU:HD12	1:A:207:PHE:CE2	2.48	0.48
1:A:364:ASN:HB2	1:A:440:ASP:OD2	2.13	0.48
1:B:44:PHE:CA	1:B:193:THR:HG22	2.42	0.48
1:B:66:THR:CG2	1:B:224:VAL:HG11	2.43	0.48
1:B:104:ILE:N	1:B:105:PRO:HD2	2.28	0.48
1:B:275:PHE:HB3	1:B:290:VAL:HG22	1.94	0.48
1:B:316:MET:O	1:B:316:MET:HG2	2.13	0.48
1:A:113:ALA:N	1:A:272:MET:HE3	2.28	0.48
1:A:432:LEU:HD23	1:A:432:LEU:N	2.28	0.48
1:B:13:LEU:HB2	1:B:226:GLU:O	2.13	0.48
1:B:42:LEU:CD1	1:B:250:SER:HB2	2.43	0.48
1:A:141:LEU:HA	1:A:144:THR:HG22	1.94	0.48
1:A:204:LEU:HB3	1:A:429:VAL:HG11	1.96	0.48
1:B:31:GLU:O	1:B:34:THR:N	2.47	0.48
1:B:46:LEU:CD1	1:B:210:PHE:CE1	2.97	0.48
1:B:371:LEU:O	1:B:372:ALA:C	2.55	0.48
1:B:392:LEU:HD12	1:B:392:LEU:C	2.39	0.48
1:B:171:LEU:HB2	1:B:275:PHE:CZ	2.49	0.48
1:B:258:MET:O	1:B:259:VAL:CG1	2.58	0.48
1:A:339:VAL:O	1:A:340:THR:C	2.56	0.48
1:B:53:TRP:O	1:B:56:PRO:HD2	2.14	0.48
1:B:167:PRO:CB	1:B:297:LEU:HD21	2.44	0.48
1:B:217:VAL:C	1:B:219:ALA:H	2.22	0.48
1:A:15:LEU:C	1:A:15:LEU:HD12	2.39	0.47
1:A:130:LYS:HZ3	1:A:363:ASN:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ALA:O	1:A:167:PRO:HD3	2.14	0.47
1:A:464:TYR:C	1:A:464:TYR:CD2	2.92	0.47
1:B:101:ILE:C	1:B:103:PHE:H	2.21	0.47
1:B:149:THR:CG2	1:B:314:ARG:HH22	2.26	0.47
1:B:326:PRO:HB2	1:B:329:PHE:CE2	2.48	0.47
1:A:33:PRO:HB2	1:A:267:LEU:HA	1.96	0.47
1:A:53:TRP:CZ2	1:A:57:VAL:HG21	2.50	0.47
1:A:385:LEU:HD23	1:A:386:PHE:N	2.29	0.47
1:B:208:VAL:HG11	1:B:371:LEU:HB3	1.96	0.47
1:B:442:THR:O	1:B:443:ASP:C	2.56	0.47
1:A:193:THR:HG22	1:A:193:THR:O	2.15	0.47
1:B:368:LEU:HD23	1:B:437:ILE:HG21	1.96	0.47
1:B:464:TYR:HE2	1:B:468:ASP:C	2.22	0.47
1:A:30:TYR:CD1	1:A:106:MET:HG2	2.50	0.47
1:A:42:LEU:HD12	1:A:43:VAL:N	2.30	0.47
1:A:297:LEU:HD22	1:A:297:LEU:HA	1.80	0.47
1:B:27:MET:HG2	1:B:164:ILE:HG23	1.95	0.47
1:B:315:GLY:O	1:B:318:VAL:HG23	2.14	0.47
1:A:14:THR:O	1:A:17:GLY:N	2.48	0.47
1:A:53:TRP:O	1:A:56:PRO:HD2	2.14	0.47
1:A:101:ILE:HG21	1:A:373:LEU:HD23	1.96	0.47
1:A:314:ARG:HH22	1:A:336:GLY:HA3	1.79	0.47
1:B:142:ALA:CB	1:B:346:LEU:HD11	2.45	0.47
1:B:212:LEU:HA	1:B:215:MET:SD	2.54	0.47
1:A:123:LEU:O	1:A:130:LYS:HG3	2.14	0.47
1:A:293:ILE:HA	1:A:296:LEU:CD1	2.43	0.47
1:A:397:PRO:HD2	1:A:398:ASP:OD2	2.14	0.47
1:A:496:PRO:C	1:A:498:ALA:N	2.66	0.47
1:B:47:LEU:HD12	1:B:193:THR:CG2	2.44	0.47
1:B:48:LEU:HD22	1:B:52:LEU:HD12	1.96	0.47
1:B:67:VAL:HB	1:B:401:ARG:HA	1.96	0.47
1:B:114:LEU:HD23	1:B:298:LEU:HD22	1.95	0.47
1:B:125:GLU:O	1:B:126:ASP:C	2.58	0.47
1:B:157:LYS:NZ	1:B:491:HIS:N	2.62	0.47
1:B:208:VAL:HG13	1:B:375:VAL:CG2	2.40	0.47
1:B:219:ALA:CB	1:B:220:SER:HB2	2.34	0.47
1:B:257:ALA:C	1:B:261:PRO:HG2	2.40	0.47
1:B:274:THR:O	1:B:278:LEU:CB	2.62	0.47
1:B:317:TYR:CZ	1:B:330:ALA:HB1	2.50	0.47
1:B:321:GLN:OE1	1:B:321:GLN:HA	2.13	0.47
1:B:500:SER:H	1:B:501:PRO:CD	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:C	1:A:167:PRO:HD2	2.40	0.47
1:A:389:TYR:CD2	1:A:416:ALA:HB2	2.49	0.47
1:A:431:PHE:HD1	1:A:446:VAL:HG12	1.79	0.47
1:A:496:PRO:O	1:A:498:ALA:N	2.48	0.47
1:B:101:ILE:HD13	1:B:373:LEU:HD13	1.97	0.47
1:B:464:TYR:CE2	1:B:468:ASP:C	2.93	0.47
1:A:207:PHE:O	1:A:208:VAL:C	2.58	0.47
1:B:47:LEU:HD12	1:B:193:THR:HG23	1.97	0.46
1:B:111:LEU:HD12	1:B:130:LYS:HG3	1.97	0.46
1:B:229:ASN:O	1:B:230:PRO:C	2.59	0.46
1:B:357:THR:HG22	1:B:358:ASN:ND2	2.31	0.46
1:B:398:ASP:CA	1:B:399:LEU:CB	2.92	0.46
1:A:88:GLY:O	1:A:91:ALA:HB3	2.15	0.46
1:A:94:PHE:HE1	1:A:460:PRO:HG2	1.69	0.46
1:A:373:LEU:CD1	1:A:452:SER:HB3	2.44	0.46
1:A:413:LEU:O	1:A:414:VAL:C	2.58	0.46
1:A:433:PRO:HG3	1:A:445:TYR:HD2	1.79	0.46
1:B:275:PHE:O	1:B:278:LEU:N	2.48	0.46
1:B:362:GLY:C	1:B:364:ASN:H	2.22	0.46
1:A:117:ILE:HG22	1:A:118:LEU:N	2.30	0.46
1:A:491:HIS:O	1:A:494:LEU:CD2	2.57	0.46
1:A:491:HIS:CE1	1:A:492:PHE:CE2	3.04	0.46
1:B:244:ALA:C	1:B:246:ILE:N	2.73	0.46
1:B:323:ASN:O	1:B:324:LEU:C	2.58	0.46
1:A:92:ILE:HD12	1:A:316:MET:HG3	1.97	0.46
1:A:259:VAL:HG21	1:A:278:LEU:CD1	2.45	0.46
1:B:29:VAL:O	1:B:30:TYR:C	2.58	0.46
1:B:67:VAL:HG21	1:B:401:ARG:H	1.80	0.46
1:B:175:ALA:O	1:B:178:TYR:N	2.48	0.46
1:B:337:VAL:N	1:B:338:PRO:CD	2.78	0.46
1:A:94:PHE:CD2	1:A:380:CYS:HB3	2.49	0.46
1:A:215:MET:HE3	1:A:375:VAL:HG13	1.98	0.46
1:A:283:ALA:HB1	1:A:287:GLU:HG2	1.97	0.46
1:B:22:THR:C	1:B:24:SER:N	2.66	0.46
1:B:138:LEU:HD11	1:B:346:LEU:HD22	1.97	0.46
1:B:378:TYR:CE1	1:B:382:TYR:HE2	2.34	0.46
1:A:230:PRO:O	1:A:231:GLY:C	2.58	0.46
1:B:462:ILE:O	1:B:466:VAL:HG13	2.16	0.46
1:A:46:LEU:CD1	1:A:210:PHE:CD1	2.97	0.46
1:A:207:PHE:CE1	1:A:211:ILE:HG13	2.51	0.46
1:A:210:PHE:O	1:A:213:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:VAL:HG23	1:B:227:MET:SD	2.55	0.46
1:A:109:PHE:HZ	1:A:297:LEU:CD1	2.28	0.46
1:A:233:ASP:O	1:A:236:LEU:HB2	2.16	0.46
1:A:419:GLY:O	1:A:420:LEU:C	2.59	0.46
1:A:172:ILE:HG12	1:A:251:VAL:CG1	2.46	0.46
1:A:317:TYR:C	1:A:319:THR:N	2.72	0.46
1:A:415:VAL:HG12	1:A:416:ALA:N	2.28	0.46
1:B:22:THR:HG22	1:B:220:SER:OG	2.15	0.46
1:B:120:TRP:CE3	1:B:123:LEU:HG	2.51	0.46
1:B:162:ALA:O	1:B:166:LEU:HB3	2.16	0.46
1:B:325:LEU:HB2	1:B:326:PRO:HD3	1.97	0.46
1:B:103:PHE:HA	1:B:106:MET:HE2	1.97	0.46
1:B:224:VAL:HG13	1:B:225:ASN:OD1	2.16	0.46
1:B:442:THR:HG21	1:B:444:MET:CE	2.40	0.46
1:A:48:LEU:HD22	1:A:52:LEU:HD12	1.96	0.45
1:A:112:GLY:C	1:A:272:MET:HE3	2.41	0.45
1:A:114:LEU:HA	1:A:114:LEU:HD23	1.73	0.45
1:A:255:SER:O	1:A:256:ILE:C	2.58	0.45
1:B:365:MET:HA	1:B:437:ILE:HD12	1.98	0.45
1:A:46:LEU:CD1	1:A:210:PHE:HD1	2.27	0.45
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.67	0.45
1:B:46:LEU:HD12	1:B:210:PHE:HD1	1.80	0.45
1:A:342:VAL:HG12	1:A:343:ILE:N	2.32	0.45
1:B:94:PHE:C	1:B:96:TYR:N	2.74	0.45
1:B:166:LEU:O	1:B:167:PRO:C	2.56	0.45
1:B:384:MET:O	1:B:385:LEU:C	2.60	0.45
1:A:459:LEU:O	1:A:462:ILE:HG12	2.16	0.45
1:B:26:VAL:HG12	1:B:248:LEU:HG	1.99	0.45
1:B:123:LEU:HD23	1:B:123:LEU:HA	1.56	0.45
1:B:283:ALA:HA	1:B:285:GLU:H	1.81	0.45
1:A:244:ALA:C	1:A:246:ILE:N	2.74	0.45
1:A:491:HIS:O	1:A:494:LEU:N	2.44	0.45
1:B:63:GLU:HA	1:B:403:PHE:HD2	1.81	0.45
1:B:172:ILE:HG12	1:B:251:VAL:CG1	2.46	0.45
1:B:428:ILE:H	1:B:428:ILE:HG13	1.62	0.45
1:B:27:MET:SD	1:B:248:LEU:HD11	2.57	0.45
1:A:118:LEU:O	1:A:118:LEU:CD2	2.64	0.45
1:A:128:ILE:H	1:A:128:ILE:CD1	2.29	0.45
1:A:164:ILE:HG22	1:A:165:LEU:N	2.32	0.45
1:B:142:ALA:HA	1:B:309:ILE:HG21	1.98	0.45
1:B:337:VAL:HG12	1:B:341:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ALA:O	1:A:22:THR:N	2.50	0.45
1:A:124:ASN:ND2	1:A:266:ASN:ND2	2.65	0.45
1:A:345:GLN:O	1:A:345:GLN:HG3	2.15	0.45
1:B:85:PRO:CD	1:B:86:ARG:H	2.30	0.45
1:A:44:PHE:HA	1:A:193:THR:HG21	1.98	0.45
1:B:66:THR:C	1:B:67:VAL:HG12	2.42	0.45
1:B:267:LEU:HB3	1:B:367:PHE:CD2	2.52	0.45
1:A:119:LYS:HE3	1:A:119:LYS:CA	2.44	0.44
1:B:46:LEU:HD22	1:B:250:SER:HB3	1.99	0.44
1:B:442:THR:CG2	1:B:444:MET:HG3	2.47	0.44
1:A:26:VAL:HG13	1:A:245:ALA:CA	2.47	0.44
1:A:29:VAL:C	1:A:31:GLU:H	2.25	0.44
1:A:157:LYS:CE	1:A:491:HIS:N	2.72	0.44
1:B:67:VAL:CG2	1:B:401:ARG:H	2.31	0.44
1:B:202:GLY:HA3	1:B:434:PRO:CB	2.47	0.44
1:B:216:GLY:HA3	1:B:497:ARG:HG2	1.99	0.44
1:A:63:GLU:HA	1:A:403:PHE:HD2	1.82	0.44
1:A:229:ASN:N	1:A:230:PRO:CD	2.81	0.44
1:A:288:TRP:C	1:A:290:VAL:N	2.74	0.44
1:B:66:THR:O	1:B:66:THR:OG1	2.33	0.44
1:B:98:GLN:HG3	1:B:378:TYR:CG	2.52	0.44
1:B:114:LEU:CD2	1:B:298:LEU:HD22	2.46	0.44
1:B:346:LEU:O	1:B:349:THR:HG22	2.18	0.44
1:B:377:ILE:CG1	1:B:456:VAL:HG11	2.47	0.44
1:A:377:ILE:HD11	1:A:456:VAL:HG11	2.00	0.44
1:A:431:PHE:CD1	1:A:449:LEU:HD23	2.52	0.44
1:B:30:TYR:CD1	1:B:106:MET:HG2	2.51	0.44
1:B:141:LEU:O	1:B:144:THR:HG22	2.17	0.44
1:A:15:LEU:HD12	1:A:15:LEU:O	2.17	0.44
1:A:365:MET:CB	1:A:437:ILE:HD11	2.48	0.44
1:A:369:ILE:CG2	1:A:370:ALA:N	2.80	0.44
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.69	0.44
1:B:57:VAL:HG12	1:B:58:GLY:N	2.33	0.44
1:B:177:ILE:C	1:B:179:LEU:N	2.74	0.44
1:B:215:MET:HE2	1:B:378:TYR:HB3	1.99	0.44
1:B:314:ARG:N	1:B:337:VAL:HG11	2.33	0.44
1:A:101:ILE:HG21	1:A:373:LEU:CD2	2.48	0.44
1:A:317:TYR:O	1:A:318:VAL:C	2.60	0.44
1:A:364:ASN:HD22	1:A:438:GLN:CB	2.25	0.44
1:B:194:PHE:O	1:B:195:PHE:C	2.60	0.44
1:B:433:PRO:HB3	1:B:445:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:O	1:A:46:LEU:HD13	2.18	0.44
1:A:407:GLY:HA3	1:A:411:VAL:HB	1.99	0.44
1:B:47:LEU:CD1	1:B:193:THR:HG23	2.48	0.44
1:B:75:VAL:O	1:B:76:PHE:C	2.61	0.44
1:B:279:MET:CE	1:B:289:THR:HG21	2.47	0.44
1:B:443:ASP:C	1:B:445:TYR:H	2.26	0.44
1:A:40:PHE:CD2	1:A:194:PHE:CB	2.97	0.44
1:A:141:LEU:HA	1:A:141:LEU:HD23	1.74	0.44
1:A:154:ARG:O	1:A:155:ILE:C	2.59	0.44
1:A:342:VAL:O	1:A:346:LEU:HG	2.18	0.44
1:A:364:ASN:ND2	1:A:438:GLN:HB2	2.24	0.44
1:B:238:MET:HE3	1:B:238:MET:HB3	1.87	0.44
1:B:254:LEU:HA	1:B:257:ALA:CB	2.33	0.44
1:B:346:LEU:HD23	1:B:346:LEU:HA	1.79	0.44
1:A:58:GLY:O	1:A:59:LEU:C	2.61	0.44
1:A:101:ILE:CD1	1:A:373:LEU:HD21	2.29	0.44
1:A:128:ILE:O	1:A:129:THR:C	2.59	0.44
1:A:285:GLU:O	1:A:288:TRP:HB3	2.18	0.44
1:A:198:PHE:O	1:B:395:LYS:HE2	2.18	0.43
1:A:314:ARG:NH2	1:A:337:VAL:HA	2.23	0.43
1:B:92:ILE:HG21	1:B:319:THR:CG2	2.48	0.43
1:B:149:THR:HG21	1:B:314:ARG:NH2	2.33	0.43
1:A:198:PHE:CD2	1:A:198:PHE:N	2.83	0.43
1:A:436:ASN:ND2	1:A:436:ASN:C	2.73	0.43
1:A:450:VAL:O	1:A:451:VAL:C	2.60	0.43
1:B:104:ILE:C	1:B:106:MET:N	2.75	0.43
1:B:141:LEU:HA	1:B:144:THR:HG22	1.99	0.43
1:B:111:LEU:HD12	1:B:130:LYS:CG	2.49	0.43
1:B:222:THR:O	1:B:224:VAL:HG12	2.18	0.43
1:A:166:LEU:O	1:A:170:ILE:HD13	2.17	0.43
1:A:347:VAL:O	1:A:351:ILE:HG12	2.18	0.43
1:A:495:HIS:CG	1:A:496:PRO:HD2	2.54	0.43
1:B:62:ALA:HB2	1:B:234:TYR:OH	2.18	0.43
1:B:420:LEU:HD12	1:B:420:LEU:HA	1.75	0.43
1:A:145:GLN:O	1:A:146:PHE:C	2.62	0.43
1:A:230:PRO:O	1:A:231:GLY:O	2.37	0.43
1:B:65:ALA:HB2	1:B:78:TRP:CZ2	2.54	0.43
1:B:94:PHE:CE2	1:B:380:CYS:HB3	2.53	0.43
1:B:99:ILE:O	1:B:100:ALA:C	2.62	0.43
1:A:13:LEU:HB3	1:A:227:MET:HA	2.00	0.43
1:A:376:VAL:HB	1:A:427:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:CD1	1:B:204:LEU:HD12	2.28	0.43
1:B:46:LEU:CD2	1:B:250:SER:HB3	2.48	0.43
1:B:286:ILE:C	1:B:288:TRP:N	2.76	0.43
1:B:365:MET:O	1:B:367:PHE:N	2.52	0.43
1:A:124:ASN:OD1	1:A:268:SER:HB2	2.18	0.43
1:A:260:ILE:HG22	1:A:265:ILE:HG12	1.99	0.43
1:B:64:MET:SD	1:B:389:TYR:HB2	2.59	0.43
1:B:386:PHE:O	1:B:387:ILE:C	2.61	0.43
1:B:463:LEU:O	1:B:464:TYR:C	2.62	0.43
1:A:23:ALA:O	1:A:24:SER:C	2.62	0.43
1:A:50:GLY:HA2	1:A:54:PHE:HB3	2.00	0.43
1:B:29:VAL:O	1:B:32:TYR:N	2.51	0.43
1:B:44:PHE:CB	1:B:193:THR:HG22	2.48	0.43
1:B:413:LEU:HD12	1:B:413:LEU:HA	1.89	0.43
1:A:125:GLU:O	1:A:127:PRO:CD	2.67	0.43
1:A:454:LEU:O	1:A:455:VAL:C	2.61	0.43
1:B:333:ASN:O	1:B:333:ASN:ND2	2.52	0.43
1:A:94:PHE:O	1:A:98:GLN:HB3	2.18	0.42
1:A:107:LEU:HA	1:A:107:LEU:HD12	1.66	0.42
1:A:109:PHE:HZ	1:A:297:LEU:HD13	1.84	0.42
1:A:356:LEU:CD2	1:A:370:ALA:HB2	2.49	0.42
1:A:435:ASP:N	1:A:435:ASP:OD1	2.50	0.42
1:A:445:TYR:O	1:A:448:LEU:N	2.52	0.42
1:B:240:LEU:C	1:B:242:MET:N	2.77	0.42
1:B:336:GLY:O	1:B:337:VAL:HB	2.19	0.42
1:A:27:MET:HE3	1:A:165:LEU:HD22	2.01	0.42
1:A:62:ALA:O	1:A:63:GLU:C	2.61	0.42
1:B:369:ILE:CD1	1:B:448:LEU:HD22	2.49	0.42
1:B:500:SER:N	1:B:501:PRO:CD	2.82	0.42
1:A:224:VAL:HG22	1:A:227:MET:SD	2.59	0.42
1:A:376:VAL:HG23	1:A:453:PHE:CD1	2.54	0.42
1:A:386:PHE:CZ	1:A:419:GLY:HA3	2.54	0.42
1:B:317:TYR:O	1:B:318:VAL:C	2.62	0.42
1:B:436:ASN:OD1	1:B:436:ASN:O	2.37	0.42
1:A:389:TYR:CE2	1:A:416:ALA:HB2	2.54	0.42
1:A:500:SER:N	1:A:501:PRO:HD2	2.34	0.42
1:B:24:SER:OG	1:B:495:HIS:HA	2.19	0.42
1:B:326:PRO:HB2	1:B:329:PHE:CZ	2.53	0.42
1:A:240:LEU:O	1:A:242:MET:N	2.53	0.42
1:A:309:ILE:O	1:A:342:VAL:HG22	2.19	0.42
1:A:331:LYS:O	1:A:332:MET:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:N	1:B:167:PRO:HD2	2.35	0.42
1:A:32:TYR:OH	1:A:249:SER:HA	2.20	0.42
1:A:68:ASP:CB	1:A:69:GLY:HA2	2.48	0.42
1:A:98:GLN:O	1:A:98:GLN:HG2	2.20	0.42
1:A:128:ILE:O	1:A:132:ILE:HG22	2.20	0.42
1:A:229:ASN:N	1:A:230:PRO:HD3	2.35	0.42
1:A:280:SER:O	1:A:281:HIS:HB2	2.20	0.42
1:A:334:LYS:HA	1:A:335:ASN:C	2.45	0.42
1:A:365:MET:CA	1:A:437:ILE:HD11	2.45	0.42
1:B:283:ALA:CB	1:B:284:PRO:HA	2.32	0.42
1:B:311:GLY:O	1:B:313:SER:N	2.53	0.42
1:B:329:PHE:O	1:B:329:PHE:CG	2.71	0.42
1:A:54:PHE:CG	1:A:214:TYR:CD1	3.08	0.42
1:A:372:ALA:O	1:A:375:VAL:HB	2.19	0.42
1:A:498:ALA:C	1:A:499:ARG:O	2.63	0.42
1:B:75:VAL:HA	1:B:78:TRP:CE3	2.54	0.42
1:A:161:PHE:CE2	1:A:493:PHE:CE1	3.06	0.42
1:A:211:ILE:HG22	1:A:215:MET:HE3	2.02	0.42
1:A:20:ALA:O	1:A:21:ILE:C	2.62	0.42
1:B:92:ILE:HG23	1:B:316:MET:SD	2.60	0.42
1:B:51:ILE:HD13	1:B:242:MET:SD	2.60	0.41
1:B:54:PHE:CE2	1:B:242:MET:HB2	2.55	0.41
1:B:110:VAL:CG1	1:B:137:ILE:HD13	2.42	0.41
1:B:242:MET:O	1:B:246:ILE:HG13	2.20	0.41
1:B:326:PRO:O	1:B:327:ALA:C	2.62	0.41
1:B:148:GLY:C	1:B:150:LYS:H	2.28	0.41
1:B:322:LYS:O	1:B:323:ASN:C	2.64	0.41
1:A:269:ALA:HA	1:A:272:MET:HE2	2.01	0.41
1:B:240:LEU:HD23	1:B:243:VAL:CG1	2.50	0.41
1:B:260:ILE:HB	1:B:261:PRO:HD3	2.02	0.41
1:B:447:GLU:O	1:B:451:VAL:HG23	2.20	0.41
1:B:48:LEU:CD2	1:B:52:LEU:HD12	2.51	0.41
1:B:261:PRO:HB3	1:B:262:GLY:HA2	2.02	0.41
1:B:373:LEU:HD23	1:B:373:LEU:C	2.46	0.41
1:B:431:PHE:C	1:B:433:PRO:HD3	2.46	0.41
1:A:68:ASP:HB2	1:A:69:GLY:CA	2.50	0.41
1:A:279:MET:HG3	1:A:283:ALA:HB2	2.02	0.41
1:A:456:VAL:O	1:A:459:LEU:N	2.46	0.41
1:B:330:ALA:O	1:B:331:LYS:HB2	2.19	0.41
1:B:434:PRO:O	1:B:443:ASP:OD2	2.37	0.41
1:A:52:LEU:O	1:A:56:PRO:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ALA:O	1:B:298:LEU:HB3	2.21	0.41
1:B:376:VAL:CG2	1:B:453:PHE:HD1	2.32	0.41
1:A:55:ILE:HA	1:A:238:MET:HE2	2.01	0.41
1:A:361:GLY:C	1:A:440:ASP:HB3	2.46	0.41
1:A:429:VAL:C	1:A:431:PHE:H	2.29	0.41
1:B:283:ALA:C	1:B:285:GLU:H	2.28	0.41
1:B:318:VAL:O	1:B:322:LYS:HB2	2.20	0.41
1:A:52:LEU:HB3	1:A:422:THR:CG2	2.44	0.41
1:A:67:VAL:CG1	1:A:401:ARG:H	2.30	0.41
1:A:68:ASP:CB	1:A:69:GLY:CA	2.98	0.41
1:A:272:MET:O	1:A:276:THR:HG23	2.20	0.41
1:A:319:THR:O	1:A:320:ALA:C	2.62	0.41
1:B:25:MET:HB3	1:B:495:HIS:CE1	2.56	0.41
1:B:54:PHE:CD1	1:B:214:TYR:HD1	2.38	0.41
1:A:44:PHE:HA	1:A:47:LEU:HD12	2.02	0.41
1:A:50:GLY:C	1:A:242:MET:SD	3.04	0.41
1:A:62:ALA:O	1:A:64:MET:N	2.54	0.41
1:A:102:GLY:HA2	1:A:374:THR:OG1	2.20	0.41
1:A:154:ARG:HA	1:A:157:LYS:HB2	2.03	0.41
1:A:366:SER:O	1:A:367:PHE:C	2.62	0.41
1:A:421:LEU:O	1:A:422:THR:C	2.62	0.41
1:A:441:SER:C	1:A:443:ASP:H	2.25	0.41
1:A:495:HIS:CD2	1:A:497:ARG:H	2.39	0.41
1:B:299:LEU:HA	1:B:299:LEU:HD23	1.78	0.41
1:B:345:GLN:O	1:B:345:GLN:HG3	2.20	0.41
1:B:348:ILE:HG22	1:B:349:THR:N	2.36	0.41
1:B:351:ILE:HG22	1:B:355:ILE:CD1	2.51	0.41
1:B:387:ILE:O	1:B:390:ILE:HG12	2.21	0.41
1:B:459:LEU:CB	1:B:460:PRO:HD3	2.51	0.41
1:A:273:GLN:O	1:A:277:VAL:HG22	2.21	0.41
1:B:104:ILE:O	1:B:105:PRO:C	2.63	0.41
1:A:131:THR:HG22	1:A:357:THR:CG2	2.50	0.40
1:A:171:LEU:HD13	1:A:275:PHE:CE1	2.56	0.40
1:A:282:VAL:HG12	1:A:282:VAL:O	2.21	0.40
1:A:317:TYR:O	1:A:320:ALA:N	2.54	0.40
1:A:336:GLY:HA3	1:A:337:VAL:CB	2.23	0.40
1:A:456:VAL:C	1:A:458:ALA:N	2.77	0.40
1:B:88:GLY:O	1:B:91:ALA:HB3	2.20	0.40
1:B:230:PRO:HB2	1:B:231:GLY:H	1.72	0.40
1:B:254:LEU:CA	1:B:257:ALA:HB3	2.36	0.40
1:B:347:VAL:O	1:B:351:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LEU:HD13	1:B:459:LEU:HA	1.61	0.40
1:A:96:TYR:O	1:A:99:ILE:HB	2.20	0.40
1:B:49:GLY:O	1:B:53:TRP:HB3	2.22	0.40
1:B:93:SER:HB3	1:B:460:PRO:HG3	2.02	0.40
1:B:167:PRO:HB2	1:B:297:LEU:HD21	2.02	0.40
1:A:25:MET:HE1	1:A:217:VAL:HG13	2.02	0.40
1:A:30:TYR:CZ	1:A:301:VAL:CG2	3.05	0.40
1:A:99:ILE:HG22	1:A:100:ALA:N	2.36	0.40
1:A:244:ALA:O	1:A:245:ALA:C	2.64	0.40
1:A:491:HIS:CE1	1:A:492:PHE:HE2	2.39	0.40
1:B:19:PHE:O	1:B:19:PHE:CG	2.75	0.40
1:B:40:PHE:CD1	1:B:40:PHE:C	2.97	0.40
1:B:339:VAL:O	1:B:340:THR:O	2.40	0.40
1:B:361:GLY:O	1:B:440:ASP:HB3	2.21	0.40
1:A:33:PRO:HG3	1:A:267:LEU:O	2.22	0.40
1:A:55:ILE:HB	1:A:56:PRO:HD3	2.03	0.40
1:A:167:PRO:CB	1:A:297:LEU:HD21	2.52	0.40
1:B:70:TRP:N	1:B:70:TRP:CD2	2.75	0.40
1:B:107:LEU:HB3	1:B:134:ALA:HB1	2.03	0.40
1:B:259:VAL:O	1:B:260:ILE:HG12	2.22	0.40
1:A:401:ARG:HB3	1:A:403:PHE:O	2.22	0.40
1:B:415:VAL:HG12	1:B:416:ALA:N	2.35	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	443/511 (87%)	307 (69%)	82 (18%)	54 (12%)	0	1
1	B	443/511 (87%)	304 (69%)	84 (19%)	55 (12%)	0	1
All	All	886/1022 (87%)	611 (69%)	166 (19%)	109 (12%)	0	1

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	100	ALA
1	A	118	LEU
1	A	152	THR
1	A	223	HIS
1	A	241	LEU
1	A	269	ALA
1	A	280	SER
1	A	281	HIS
1	A	287	GLU
1	A	323	ASN
1	A	328	ALA
1	A	339	VAL
1	A	406	PRO
1	A	407	GLY
1	A	442	THR
1	A	492	PHE
1	A	499	ARG
1	A	500	SER
1	B	23	ALA
1	B	67	VAL
1	B	223	HIS
1	B	230	PRO
1	B	233	ASP
1	B	241	LEU
1	B	259	VAL
1	B	261	PRO
1	B	263	ASN
1	B	275	PHE
1	B	280	SER
1	B	286	ILE
1	B	336	GLY
1	B	337	VAL
1	B	339	VAL
1	B	340	THR
1	B	399	LEU
1	B	401	ARG
1	B	441	SER
1	B	492	PHE
1	B	499	ARG
1	B	500	SER
1	A	21	ILE

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Mol	Chain	Res	Type
1	A	102	GLY
1	A	164	ILE
1	A	226	GLU
1	A	231	GLY
1	A	233	ASP
1	A	244	ALA
1	A	245	ALA
1	A	270	GLY
1	A	282	VAL
1	A	332	MET
1	A	336	GLY
1	A	409	LYS
1	A	441	SER
1	A	445	TYR
1	B	30	TYR
1	B	68	ASP
1	B	100	ALA
1	B	119	LYS
1	B	149	THR
1	B	164	ILE
1	B	205	VAL
1	B	208	VAL
1	B	240	LEU
1	B	245	ALA
1	B	257	ALA
1	B	338	PRO
1	B	367	PHE
1	A	30	TYR
1	A	119	LYS
1	A	194	PHE
1	B	218	GLU
1	B	260	ILE
1	B	326	PRO
1	A	24	SER
1	A	169	PHE
1	A	262	GLY
1	A	329	PHE
1	A	399	LEU
1	A	425	MET
1	A	497	ARG
1	B	21	ILE
1	B	195	PHE

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Mol	Chain	Res	Type
1	B	199	SER
1	B	244	ALA
1	B	276	THR
1	B	285	GLU
1	B	409	LYS
1	A	168	ALA
1	A	240	LEU
1	A	337	VAL
1	A	401	ARG
1	B	32	TYR
1	B	85	PRO
1	B	118	LEU
1	B	287	GLU
1	B	322	LYS
1	B	361	GLY
1	A	208	VAL
1	A	58	GLY
1	A	408	GLY
1	B	282	VAL
1	A	271	VAL
1	B	33	PRO
1	A	95	GLY
1	A	361	GLY
1	B	95	GLY
1	B	246	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/414 (88%)	258 (71%)	107 (29%)	0	1
1	B	368/414 (89%)	276 (75%)	92 (25%)	0	2
All	All	733/828 (88%)	534 (73%)	199 (27%)	0	2

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	LEU
1	A	21	ILE
1	A	22	THR
1	A	30	TYR
1	A	34	THR
1	A	42	LEU
1	A	43	VAL
1	A	47	LEU
1	A	48	LEU
1	A	66	THR
1	A	83	LEU
1	A	92	ILE
1	A	98	GLN
1	A	99	ILE
1	A	103	PHE
1	A	107	LEU
1	A	115	SER
1	A	125	GLU
1	A	128	ILE
1	A	131	THR
1	A	132	ILE
1	A	135	LEU
1	A	143	LEU
1	A	144	THR
1	A	149	THR
1	A	151	TYR
1	A	152	THR
1	A	164	ILE
1	A	197	ASP
1	A	198	PHE
1	A	208	VAL
1	A	211	ILE
1	A	217	VAL
1	A	218	GLU
1	A	220	SER
1	A	224	VAL
1	A	225	ASN
1	A	227	MET
1	A	233	ASP
1	A	236	LEU
1	A	239	LEU
1	A	240	LEU

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	243	VAL
1	A	247	CYS
1	A	248	LEU
1	A	258	MET
1	A	259	VAL
1	A	264	GLU
1	A	267	LEU
1	A	268	SER
1	A	272	MET
1	A	274	THR
1	A	278	LEU
1	A	279	MET
1	A	281	HIS
1	A	288	TRP
1	A	289	THR
1	A	290	VAL
1	A	292	VAL
1	A	297	LEU
1	A	298	LEU
1	A	299	LEU
1	A	301	VAL
1	A	309	ILE
1	A	310	VAL
1	A	318	VAL
1	A	321	GLN
1	A	329	PHE
1	A	332	MET
1	A	340	THR
1	A	342	VAL
1	A	343	ILE
1	A	345	GLN
1	A	349	THR
1	A	351	ILE
1	A	353	LEU
1	A	359	THR
1	A	365	MET
1	A	369	ILE
1	A	371	LEU
1	A	373	LEU
1	A	374	THR
1	A	377	ILE

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Mol	Chain	Res	Type
1	A	378	TYR
1	A	390	ILE
1	A	392	LEU
1	A	400	LYS
1	A	404	ASN
1	A	413	LEU
1	A	415	VAL
1	A	424	ILE
1	A	425	MET
1	A	428	ILE
1	A	432	LEU
1	A	436	ASN
1	A	437	ILE
1	A	446	VAL
1	A	447	GLU
1	A	448	LEU
1	A	453	PHE
1	A	454	LEU
1	A	457	LEU
1	A	459	LEU
1	A	466	VAL
1	A	492	PHE
1	B	12	GLN
1	B	13	LEU
1	B	29	VAL
1	B	31	GLU
1	B	34	THR
1	B	57	VAL
1	B	67	VAL
1	B	70	TRP
1	B	92	ILE
1	B	98	GLN
1	B	101	ILE
1	B	103	PHE
1	B	104	ILE
1	B	107	LEU
1	B	111	LEU
1	B	114	LEU
1	B	115	SER
1	B	123	LEU
1	B	125	GLU
1	B	131	THR

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Mol	Chain	Res	Type
1	B	132	ILE
1	B	135	LEU
1	B	136	ILE
1	B	149	THR
1	B	151	TYR
1	B	154	ARG
1	B	158	VAL
1	B	164	ILE
1	B	165	LEU
1	B	177	ILE
1	B	178	TYR
1	B	193	THR
1	B	194	PHE
1	B	201	VAL
1	B	206	VAL
1	B	208	VAL
1	B	211	ILE
1	B	217	VAL
1	B	218	GLU
1	B	222	THR
1	B	233	ASP
1	B	234	TYR
1	B	239	LEU
1	B	240	LEU
1	B	241	LEU
1	B	248	LEU
1	B	251	VAL
1	B	258	MET
1	B	260	ILE
1	B	267	LEU
1	B	268	SER
1	B	272	MET
1	B	277	VAL
1	B	282	VAL
1	B	288	TRP
1	B	290	VAL
1	B	299	LEU
1	B	310	VAL
1	B	321	GLN
1	B	323	ASN
1	B	324	LEU
1	B	329	PHE

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Mol	Chain	Res	Type
1	B	331	LYS
1	B	343	ILE
1	B	345	GLN
1	B	348	ILE
1	B	351	ILE
1	B	355	ILE
1	B	366	SER
1	B	369	ILE
1	B	371	LEU
1	B	373	LEU
1	B	377	ILE
1	B	384	MET
1	B	390	ILE
1	B	391	VAL
1	B	392	LEU
1	B	400	LYS
1	B	401	ARG
1	B	413	LEU
1	B	415	VAL
1	B	425	MET
1	B	428	ILE
1	B	435	ASP
1	B	437	ILE
1	B	441	SER
1	B	447	GLU
1	B	452	SER
1	B	453	PHE
1	B	456	VAL
1	B	459	LEU
1	B	493	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
1	A	495	HIS
1	B	12	GLN
1	B	145	GLN
1	B	363	ASN
1	B	364	ASN
1	B	404	ASN
1	B	467	HIS

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Mol	Chain	Res	Type
1	B	495	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	451/511 (88%)	0.81	56 (12%) 8 5	88, 136, 198, 249	0
1	B	453/511 (88%)	0.65	40 (8%) 15 9	86, 137, 212, 265	0
All	All	904/1022 (88%)	0.73	96 (10%) 11 6	86, 137, 205, 265	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	TYR	5.7
1	B	146	PHE	5.6
1	A	338	PRO	5.4
1	A	64	MET	5.0
1	B	228	SER	4.9
1	B	392	LEU	4.4
1	A	341	LEU	4.3
1	A	316	MET	4.1
1	A	226	GLU	4.1
1	A	123	LEU	4.0
1	A	389	TYR	4.0
1	B	68	ASP	3.9
1	A	118	LEU	3.8
1	A	339	VAL	3.7
1	A	146	PHE	3.7
1	A	63	GLU	3.6
1	B	147	GLY	3.4
1	B	408	GLY	3.4
1	A	82	THR	3.3
1	B	308	TRP	3.3
1	A	193	THR	3.2
1	A	314	ARG	3.1
1	A	267	LEU	3.1
1	A	61	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	430	SER	3.0
1	B	257	ALA	3.0
1	B	356	LEU	3.0
1	B	389	TYR	2.9
1	B	198	PHE	2.9
1	B	79	VAL	2.9
1	B	501	PRO	2.8
1	A	164	ILE	2.8
1	A	213	SER	2.8
1	B	453	PHE	2.8
1	B	206	VAL	2.8
1	A	432	LEU	2.7
1	B	265	ILE	2.7
1	A	501	PRO	2.7
1	A	34	THR	2.7
1	A	121	PRO	2.6
1	A	223	HIS	2.6
1	B	226	GLU	2.6
1	B	448	LEU	2.6
1	B	310	VAL	2.6
1	B	45	PHE	2.5
1	A	89	PHE	2.5
1	A	359	THR	2.5
1	A	254	LEU	2.5
1	B	273	GLN	2.5
1	A	313	SER	2.5
1	A	122	ALA	2.4
1	A	152	THR	2.4
1	B	125	GLU	2.4
1	B	218	GLU	2.4
1	A	30	TYR	2.4
1	A	309	ILE	2.3
1	A	329	PHE	2.3
1	A	137	ILE	2.3
1	A	199	SER	2.3
1	A	116	TYR	2.3
1	B	267	LEU	2.3
1	B	314	ARG	2.3
1	B	432	LEU	2.2
1	A	18	PHE	2.2
1	B	81	ASN	2.2
1	A	340	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	ILE	2.2
1	A	108	TYR	2.2
1	A	297	LEU	2.2
1	A	392	LEU	2.2
1	A	323	ASN	2.2
1	B	386	PHE	2.2
1	B	468	ASP	2.2
1	A	420	LEU	2.1
1	A	163	GLY	2.1
1	A	315	GLY	2.1
1	A	114	LEU	2.1
1	A	386	PHE	2.1
1	A	342	VAL	2.1
1	B	385	LEU	2.1
1	B	430	SER	2.1
1	A	81	ASN	2.1
1	A	394	LEU	2.1
1	A	457	LEU	2.1
1	B	305	ILE	2.1
1	B	457	LEU	2.1
1	B	203	THR	2.1
1	B	258	MET	2.1
1	B	121	PRO	2.1
1	A	455	VAL	2.0
1	B	103	PHE	2.0
1	A	206	VAL	2.0
1	A	281	HIS	2.0
1	B	425	MET	2.0
1	B	156	ALA	2.0
1	A	119	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.