



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2017 – 04:23 pm GMT

PDB ID : 4D0A  
Title : 3D EM map of the sodium proton antiporter MjNhaP1 from Methanocaldococcus jannaschii  
Authors : Paulino, C.; Woehlert, D.; Yildiz, O.; Kuhlbrandt, W.  
Deposited on : 2014-04-25  
Resolution : 6.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29102

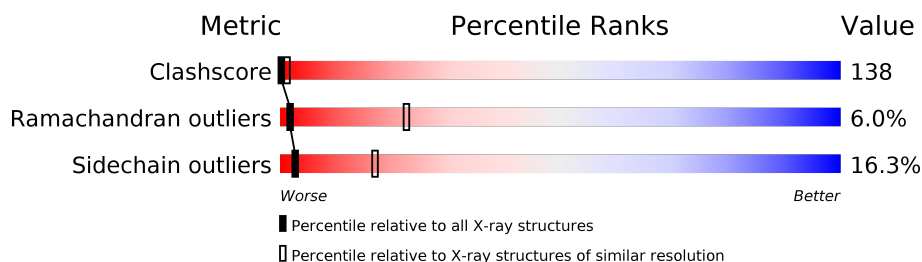
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 6.00 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))
Clashscore	112137	1017 (8.20-3.80)
Ramachandran outliers	110173	1001 (8.20-3.72)
Sidechain outliers	110143	1085 (8.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	426	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3175 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 NA(+)/H(+) ANTIPORTER 1.

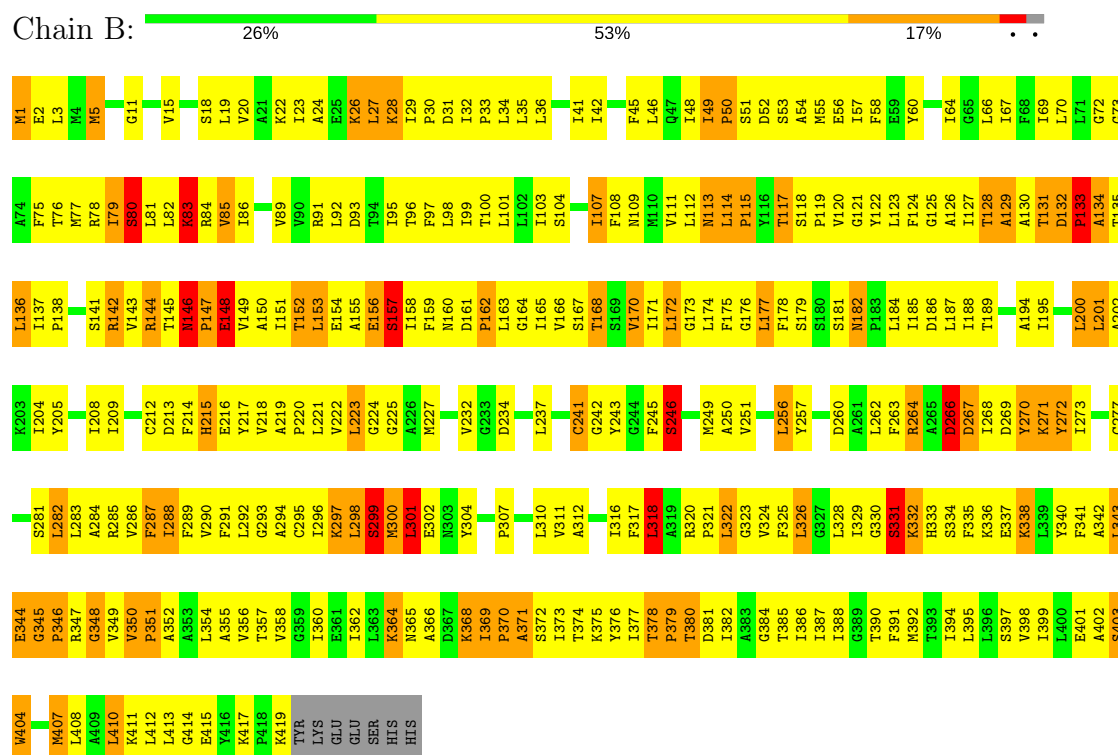
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	419	Total	C	N	O	S	0	0	0
			3175	2129	479	551	16			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

#### • Molecule 1: NA(+)/H(+) ANTIPORTER 1



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.50Å 103.30Å 200.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 6.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-6.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	2DX	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3175	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

## 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	B	1.66	30/3232 (0.9%)	1.21	35/4382 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	SER	C-N	-48.74	0.45	1.33
1	B	148	GLU	C-N	-29.14	0.67	1.34
1	B	83	LYS	C-N	27.12	1.96	1.34
1	B	215	HIS	C-N	-24.76	0.77	1.34
1	B	114	LEU	C-N	23.22	1.78	1.34
1	B	298	LEU	C-N	23.05	1.87	1.34
1	B	131	THR	C-N	21.86	1.84	1.34
1	B	331	SER	C-N	21.37	1.83	1.34
1	B	80	SER	C-N	-16.89	0.95	1.34
1	B	201	LEU	C-N	12.00	1.61	1.34
1	B	133	PRO	C-N	-11.77	1.06	1.34
1	B	299	SER	C-N	11.37	1.60	1.34
1	B	288	ILE	C-N	11.33	1.60	1.34
1	B	391	PHE	C-N	11.05	1.59	1.34
1	B	392	MET	C-N	-10.57	1.09	1.34
1	B	318	LEU	C-N	9.12	1.55	1.34
1	B	157	SER	C-N	-8.75	1.14	1.34
1	B	157	SER	CB-OG	-8.59	1.31	1.42
1	B	282	LEU	C-N	-8.25	1.15	1.34
1	B	188	ILE	C-N	8.07	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	SER	C-O	7.28	1.37	1.23
1	B	143	VAL	C-N	-6.38	1.19	1.34
1	B	195	ILE	C-N	6.38	1.48	1.34
1	B	223	LEU	C-N	-5.37	1.23	1.33
1	B	129	ALA	C-N	5.37	1.46	1.34
1	B	154	GLU	C-N	5.35	1.46	1.34
1	B	115	PRO	N-CD	5.25	1.55	1.47
1	B	379	PRO	N-CD	5.25	1.55	1.47
1	B	142	ARG	C-N	-5.18	1.22	1.34
1	B	162	PRO	N-CD	5.04	1.54	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	THR	O-C-N	25.89	164.13	122.70
1	B	80	SER	O-C-N	24.27	161.53	122.70
1	B	131	THR	CA-C-N	-19.06	75.27	117.20
1	B	131	THR	C-N-CA	-18.19	76.22	121.70
1	B	80	SER	CA-C-N	-18.15	77.28	117.20
1	B	83	LYS	O-C-N	-16.32	96.60	122.70
1	B	80	SER	C-N-CA	-15.34	83.36	121.70
1	B	299	SER	O-C-N	-14.45	99.58	122.70
1	B	246	SER	CA-C-N	-12.89	90.42	116.20
1	B	246	SER	C-N-CA	-12.78	95.47	122.30
1	B	133	PRO	CA-C-N	-10.11	94.96	117.20
1	B	392	MET	O-C-N	9.97	138.65	122.70
1	B	282	LEU	O-C-N	-9.30	107.81	122.70
1	B	392	MET	CA-C-N	-9.18	97.00	117.20
1	B	391	PHE	O-C-N	9.04	137.16	122.70
1	B	133	PRO	O-C-N	8.69	136.60	122.70
1	B	83	LYS	CA-C-N	8.65	136.24	117.20
1	B	392	MET	C-N-CA	-8.09	101.47	121.70
1	B	391	PHE	CA-C-N	-7.29	101.16	117.20
1	B	288	ILE	C-N-CA	-7.14	103.86	121.70
1	B	201	LEU	C-N-CA	-6.58	105.26	121.70
1	B	148	GLU	O-C-N	-6.54	112.24	122.70
1	B	148	GLU	C-N-CA	6.46	137.84	121.70
1	B	188	ILE	O-C-N	6.41	132.96	122.70
1	B	146	ASN	C-N-CD	6.31	141.66	128.40
1	B	182	ASN	C-N-CD	6.10	141.21	128.40
1	B	345	GLY	C-N-CD	6.07	141.15	128.40
1	B	49	ILE	C-N-CD	6.05	141.11	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	LYS	C-N-CD	6.04	141.09	128.40
1	B	369	ILE	C-N-CD	6.03	141.07	128.40
1	B	282	LEU	CA-C-N	5.97	130.33	117.20
1	B	301	LEU	O-C-N	-5.71	113.57	122.70
1	B	318	LEU	C-N-CA	-5.64	107.61	121.70
1	B	378	THR	C-N-CD	5.62	140.20	128.40
1	B	188	ILE	CA-C-N	-5.09	106.00	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	PRO	Mainchain
1	B	246	SER	Mainchain
1	B	299	SER	Mainchain

## 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	B	3175	0	3364	903	43
All	All	3175	0	3364	903	43

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 138.

All (903) 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:135:THR:HG21	1:B:289:PHE:CZ	1.31	1.66
1:B:131:THR:CA	1:B:347:ARG:HB2	1.24	1.59
1:B:301:LEU:CD1	1:B:388:ILE:HD11	1.15	1.59
1:B:89:VAL:CG2	1:B:152:THR:HG22	1.20	1.57
1:B:89:VAL:HG22	1:B:152:THR:CG2	1.18	1.57
1:B:131:THR:HA	1:B:347:ARG:CB	1.32	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLY:HA2	1:B:177:LEU:CD2	1.09	1.53
1:B:332:LYS:HG3	1:B:333:HIS:CD2	1.44	1.52
1:B:320:ARG:CD	1:B:344:GLU:HB2	1.09	1.51
1:B:78:ARG:HD2	1:B:263:PHE:CD1	1.44	1.50
1:B:320:ARG:CD	1:B:344:GLU:CB	1.86	1.50
1:B:120:VAL:CA	1:B:175:PHE:HE2	1.05	1.46
1:B:320:ARG:NE	1:B:344:GLU:HB2	1.30	1.44
1:B:119:PRO:CB	1:B:175:PHE:HA	1.48	1.44
1:B:51:SER:CB	1:B:298:LEU:N	1.74	1.43
1:B:301:LEU:HD11	1:B:388:ILE:CD1	0.93	1.40
1:B:78:ARG:HD2	1:B:263:PHE:CG	1.58	1.39
1:B:114:LEU:C	1:B:115:PRO:N	1.78	1.37
1:B:78:ARG:NE	1:B:263:PHE:CE2	1.93	1.36
1:B:173:GLY:CA	1:B:177:LEU:CD2	2.02	1.36
1:B:85:VAL:CG2	1:B:148:GLU:HG3	1.29	1.35
1:B:51:SER:CB	1:B:298:LEU:H	1.34	1.33
1:B:153:LEU:HD11	1:B:340:TYR:CE2	1.62	1.33
1:B:89:VAL:CG2	1:B:152:THR:CG2	1.81	1.33
1:B:215:HIS:C	1:B:216:GLU:CA	1.95	1.33
1:B:120:VAL:HG11	1:B:382:ILE:CG1	1.44	1.32
1:B:131:THR:C	1:B:347:ARG:HB2	1.50	1.32
1:B:131:THR:C	1:B:132:ASP:N	1.84	1.31
1:B:347:ARG:HD3	1:B:351:PRO:CG	1.58	1.31
1:B:333:HIS:C	1:B:334:SER:HB3	1.50	1.31
1:B:331:SER:C	1:B:332:LYS:N	1.83	1.31
1:B:301:LEU:CD1	1:B:388:ILE:CD1	1.81	1.31
1:B:108:PHE:CD2	1:B:121:GLY:HA2	1.67	1.30
1:B:120:VAL:CG1	1:B:382:ILE:CG1	2.04	1.29
1:B:120:VAL:CG1	1:B:382:ILE:HG12	1.61	1.29
1:B:148:GLU:O	1:B:149:VAL:N	1.62	1.28
1:B:215:HIS:CA	1:B:216:GLU:N	1.95	1.28
1:B:320:ARG:HD3	1:B:344:GLU:CB	1.49	1.28
1:B:212:CYS:HB3	1:B:213:ASP:N	1.48	1.27
1:B:298:LEU:C	1:B:299:SER:N	1.87	1.27
1:B:148:GLU:C	1:B:149:VAL:CA	2.00	1.27
1:B:205:TYR:OH	1:B:221:LEU:HG	1.09	1.26
1:B:85:VAL:HG21	1:B:148:GLU:CG	1.65	1.26
1:B:79:ILE:O	1:B:81:LEU:N	1.69	1.24
1:B:131:THR:C	1:B:132:ASP:HA	1.57	1.24
1:B:131:THR:C	1:B:132:ASP:CA	2.06	1.24
1:B:148:GLU:CA	1:B:149:VAL:N	2.00	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:CZ	1:B:263:PHE:CZ	2.22	1.22
1:B:205:TYR:CZ	1:B:221:LEU:HG	1.75	1.22
1:B:120:VAL:HA	1:B:175:PHE:CE2	1.35	1.22
1:B:296:ILE:CG2	1:B:387:ILE:HD13	1.69	1.22
1:B:320:ARG:CG	1:B:344:GLU:HB2	1.70	1.22
1:B:158:ILE:O	1:B:162:PRO:HD3	1.36	1.22
1:B:343:LEU:O	1:B:344:GLU:O	1.55	1.22
1:B:133:PRO:HB3	1:B:157:SER:CB	1.69	1.21
1:B:153:LEU:HD21	1:B:340:TYR:OH	1.06	1.21
1:B:407:MET:O	1:B:411:LYS:HB3	1.37	1.20
1:B:332:LYS:HG3	1:B:333:HIS:CG	1.66	1.20
1:B:120:VAL:HG13	1:B:382:ILE:CG2	1.71	1.19
1:B:83:LYS:C	1:B:84:ARG:N	1.96	1.19
1:B:133:PRO:HG3	1:B:157:SER:HB2	1.19	1.19
1:B:120:VAL:CA	1:B:175:PHE:CE2	1.81	1.19
1:B:135:THR:CG2	1:B:289:PHE:CZ	2.24	1.18
1:B:89:VAL:HG22	1:B:152:THR:HG21	1.20	1.18
1:B:136:LEU:HD11	1:B:398:VAL:HG13	1.19	1.18
1:B:153:LEU:CD2	1:B:340:TYR:OH	1.92	1.17
1:B:78:ARG:CD	1:B:263:PHE:CG	2.27	1.17
1:B:114:LEU:CD2	1:B:377:ILE:HD12	1.74	1.16
1:B:335:PHE:CZ	1:B:415:GLU:OE2	1.98	1.16
1:B:133:PRO:HB3	1:B:157:SER:HB3	1.23	1.16
1:B:166:VAL:HG13	1:B:187:LEU:HD22	1.16	1.15
1:B:347:ARG:CD	1:B:351:PRO:HG2	1.74	1.15
1:B:332:LYS:CG	1:B:333:HIS:CD2	2.28	1.15
1:B:214:PHE:HB3	1:B:217:TYR:HB2	1.17	1.15
1:B:131:THR:CA	1:B:132:ASP:N	2.07	1.15
1:B:119:PRO:HB2	1:B:175:PHE:CG	1.82	1.15
1:B:119:PRO:CB	1:B:175:PHE:CA	2.24	1.14
1:B:215:HIS:O	1:B:216:GLU:N	1.80	1.14
1:B:162:PRO:HB3	1:B:249:MET:HE1	1.23	1.14
1:B:232:VAL:HG12	1:B:245:PHE:CE2	1.81	1.14
1:B:119:PRO:CG	1:B:175:PHE:HA	1.77	1.14
1:B:132:ASP:HB2	1:B:348:GLY:H	1.10	1.14
1:B:205:TYR:CE1	1:B:221:LEU:HD21	1.82	1.14
1:B:133:PRO:CB	1:B:157:SER:HB3	1.77	1.13
1:B:126:ALA:CB	1:B:171:ILE:HD11	1.76	1.13
1:B:173:GLY:HA2	1:B:177:LEU:HD23	1.14	1.13
1:B:132:ASP:HB2	1:B:348:GLY:N	1.62	1.13
1:B:335:PHE:HZ	1:B:415:GLU:OE2	1.28	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:PHE:CE1	1:B:291:PHE:CD2	2.37	1.12
1:B:119:PRO:CB	1:B:175:PHE:CG	2.32	1.12
1:B:83:LYS:O	1:B:86:ILE:CG2	1.97	1.12
1:B:232:VAL:HG12	1:B:245:PHE:HE2	1.05	1.12
1:B:292:LEU:O	1:B:295:CYS:SG	2.07	1.11
1:B:301:LEU:HD11	1:B:388:ILE:HD12	1.16	1.11
1:B:131:THR:HA	1:B:347:ARG:HB3	1.28	1.10
1:B:79:ILE:HG23	1:B:80:SER:N	1.65	1.10
1:B:300:MET:CB	1:B:301:LEU:HD13	1.71	1.10
1:B:320:ARG:NE	1:B:344:GLU:CB	2.04	1.10
1:B:242:GLY:N	1:B:243:TYR:N	2.00	1.10
1:B:162:PRO:HB3	1:B:249:MET:CE	1.81	1.10
1:B:32:ILE:HD11	1:B:136:LEU:HG	1.33	1.09
1:B:35:LEU:CD2	1:B:286:VAL:HG13	1.81	1.09
1:B:159:PHE:O	1:B:162:PRO:HD2	1.52	1.09
1:B:173:GLY:HA2	1:B:177:LEU:HD22	1.32	1.09
1:B:78:ARG:NE	1:B:263:PHE:CZ	2.19	1.09
1:B:51:SER:HB3	1:B:298:LEU:H	1.01	1.09
1:B:135:THR:HG21	1:B:289:PHE:CE2	1.87	1.09
1:B:205:TYR:OH	1:B:221:LEU:CG	2.01	1.09
1:B:214:PHE:CB	1:B:217:TYR:HB2	1.81	1.09
1:B:104:SER:HB3	1:B:125:GLY:HA2	1.25	1.08
1:B:340:TYR:O	1:B:343:LEU:HD11	1.53	1.08
1:B:120:VAL:HG13	1:B:382:ILE:HG23	1.35	1.08
1:B:296:ILE:HG22	1:B:387:ILE:CD1	1.83	1.08
1:B:237:LEU:HB3	1:B:243:TYR:O	1.54	1.07
1:B:66:LEU:CD1	1:B:349:VAL:HG12	1.84	1.07
1:B:133:PRO:CB	1:B:157:SER:CB	2.31	1.07
1:B:332:LYS:CG	1:B:333:HIS:CG	2.36	1.07
1:B:51:SER:HB2	1:B:298:LEU:N	1.21	1.07
1:B:108:PHE:CD2	1:B:124:PHE:HB3	1.89	1.07
1:B:173:GLY:HA2	1:B:177:LEU:HD21	1.12	1.07
1:B:347:ARG:HD3	1:B:351:PRO:CD	1.85	1.07
1:B:296:ILE:HG21	1:B:387:ILE:HG21	1.35	1.07
1:B:131:THR:CA	1:B:347:ARG:CB	2.03	1.06
1:B:287:PHE:HE1	1:B:291:PHE:CD2	1.72	1.06
1:B:331:SER:HB2	1:B:333:HIS:O	1.53	1.06
1:B:320:ARG:HB3	1:B:321:PRO:HD3	1.37	1.06
1:B:162:PRO:HA	1:B:249:MET:SD	1.94	1.06
1:B:124:PHE:O	1:B:127:ILE:HG12	1.55	1.06
1:B:114:LEU:HD21	1:B:377:ILE:HD12	1.11	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PRO:HG3	1:B:157:SER:CB	1.84	1.05
1:B:132:ASP:HB2	1:B:347:ARG:HG2	1.35	1.05
1:B:78:ARG:CD	1:B:263:PHE:CD1	2.37	1.04
1:B:287:PHE:CE1	1:B:291:PHE:HD2	1.72	1.04
1:B:131:THR:HA	1:B:132:ASP:N	1.68	1.04
1:B:333:HIS:C	1:B:334:SER:CB	2.25	1.04
1:B:69:ILE:HD11	1:B:349:VAL:HG11	1.40	1.04
1:B:153:LEU:HD11	1:B:340:TYR:HE2	0.87	1.04
1:B:133:PRO:CG	1:B:157:SER:CB	2.35	1.03
1:B:78:ARG:NE	1:B:263:PHE:CD2	2.25	1.03
1:B:153:LEU:CD1	1:B:340:TYR:HE2	1.71	1.03
1:B:132:ASP:CB	1:B:347:ARG:HG2	1.89	1.03
1:B:153:LEU:HD21	1:B:340:TYR:CZ	1.94	1.02
1:B:108:PHE:HD2	1:B:121:GLY:HA2	1.00	1.02
1:B:114:LEU:HD21	1:B:377:ILE:CD1	1.88	1.02
1:B:50:PRO:HD2	1:B:53:SER:HB2	1.37	1.02
1:B:89:VAL:HG21	1:B:152:THR:CG2	1.79	1.02
1:B:335:PHE:HZ	1:B:415:GLU:CD	1.62	1.02
1:B:79:ILE:CG2	1:B:80:SER:H	1.70	1.02
1:B:301:LEU:HD13	1:B:388:ILE:HD11	1.33	1.01
1:B:300:MET:HB3	1:B:301:LEU:CD1	1.90	1.01
1:B:296:ILE:HG21	1:B:387:ILE:CG2	1.90	1.01
1:B:32:ILE:HD12	1:B:398:VAL:HG13	1.39	1.01
1:B:132:ASP:CB	1:B:348:GLY:H	1.73	1.00
1:B:200:LEU:O	1:B:204:ILE:HG12	1.58	1.00
1:B:333:HIS:HB2	1:B:334:SER:N	1.77	1.00
1:B:75:PHE:CB	1:B:277:CYS:SG	2.50	1.00
1:B:320:ARG:HG2	1:B:344:GLU:N	1.75	1.00
1:B:332:LYS:HB2	1:B:333:HIS:CG	1.95	1.00
1:B:119:PRO:HB2	1:B:175:PHE:HA	1.43	1.00
1:B:66:LEU:HD11	1:B:349:VAL:HG12	1.43	0.99
1:B:79:ILE:HG23	1:B:80:SER:H	0.85	0.99
1:B:320:ARG:HD3	1:B:344:GLU:HB3	1.42	0.99
1:B:320:ARG:NH2	1:B:344:GLU:OE1	1.95	0.99
1:B:347:ARG:HD3	1:B:351:PRO:HG2	1.00	0.99
1:B:374:THR:HG23	1:B:377:ILE:HG21	1.40	0.99
1:B:32:ILE:HD12	1:B:398:VAL:CG1	1.90	0.99
1:B:301:LEU:CD1	1:B:388:ILE:CG1	2.40	0.99
1:B:166:VAL:HG13	1:B:187:LEU:CD2	1.93	0.99
1:B:241:CYS:CB	1:B:243:TYR:HB3	1.91	0.99
1:B:119:PRO:HB3	1:B:175:PHE:CA	1.90	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASN:ND2	1:B:122:TYR:CE1	2.31	0.98
1:B:114:LEU:CD2	1:B:377:ILE:CD1	2.41	0.98
1:B:135:THR:CG2	1:B:289:PHE:CE2	2.44	0.98
1:B:109:ASN:OD1	1:B:121:GLY:HA3	1.63	0.98
1:B:135:THR:CG2	1:B:285:ARG:HH12	1.75	0.98
1:B:158:ILE:HG21	1:B:256:LEU:CD1	1.92	0.98
1:B:242:GLY:C	1:B:243:TYR:N	2.18	0.98
1:B:271:LYS:O	1:B:272:TYR:HB2	1.61	0.97
1:B:133:PRO:CG	1:B:157:SER:HB2	1.92	0.97
1:B:69:ILE:HD11	1:B:349:VAL:CG1	1.93	0.97
1:B:374:THR:O	1:B:379:PRO:HD3	1.64	0.97
1:B:241:CYS:HB3	1:B:243:TYR:HB3	1.47	0.96
1:B:104:SER:CB	1:B:125:GLY:HA2	1.94	0.96
1:B:377:ILE:HG13	1:B:378:THR:CA	1.95	0.96
1:B:89:VAL:HG21	1:B:152:THR:HG22	1.32	0.96
1:B:214:PHE:HB3	1:B:217:TYR:CB	1.95	0.96
1:B:345:GLY:O	1:B:397:SER:CB	2.14	0.96
1:B:300:MET:HB3	1:B:301:LEU:HD13	0.96	0.96
1:B:104:SER:CB	1:B:125:GLY:CA	2.43	0.95
1:B:83:LYS:O	1:B:86:ILE:HG21	1.66	0.95
1:B:126:ALA:HB3	1:B:171:ILE:HD11	1.42	0.95
1:B:92:LEU:CD1	1:B:341:PHE:CD2	2.47	0.95
1:B:115:PRO:HG2	1:B:118:SER:HB3	1.48	0.95
1:B:133:PRO:CG	1:B:157:SER:HB3	1.94	0.95
1:B:324:VAL:HG21	1:B:342:ALA:N	1.80	0.95
1:B:205:TYR:CZ	1:B:221:LEU:CG	2.50	0.95
1:B:109:ASN:ND2	1:B:122:TYR:HE1	1.65	0.94
1:B:160:ASN:O	1:B:163:LEU:N	1.98	0.94
1:B:126:ALA:HB3	1:B:171:ILE:CD1	1.97	0.94
1:B:320:ARG:NE	1:B:344:GLU:OE1	2.01	0.94
1:B:137:ILE:O	1:B:141:SER:OG	1.86	0.94
1:B:320:ARG:CG	1:B:344:GLU:CB	2.36	0.94
1:B:345:GLY:O	1:B:397:SER:HB2	1.67	0.93
1:B:333:HIS:CB	1:B:334:SER:N	2.31	0.93
1:B:296:ILE:HG22	1:B:387:ILE:HD13	0.92	0.92
1:B:78:ARG:CD	1:B:263:PHE:CD2	2.52	0.92
1:B:287:PHE:HE1	1:B:291:PHE:HD2	0.98	0.92
1:B:320:ARG:CZ	1:B:344:GLU:OE1	2.18	0.92
1:B:130:ALA:HB3	1:B:351:PRO:CG	2.00	0.92
1:B:70:LEU:HD21	1:B:251:VAL:HG23	1.51	0.92
1:B:70:LEU:CD2	1:B:251:VAL:HG23	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD21	1:B:286:VAL:HG22	1.50	0.92
1:B:79:ILE:O	1:B:81:LEU:CA	2.17	0.92
1:B:108:PHE:HD2	1:B:121:GLY:CA	1.82	0.91
1:B:119:PRO:HG3	1:B:174:LEU:O	1.70	0.91
1:B:332:LYS:CB	1:B:333:HIS:CG	2.53	0.91
1:B:205:TYR:CE1	1:B:221:LEU:CD2	2.53	0.91
1:B:301:LEU:HD12	1:B:388:ILE:HG13	1.52	0.91
1:B:126:ALA:HB1	1:B:171:ILE:HD11	1.50	0.90
1:B:166:VAL:CG1	1:B:187:LEU:HD22	2.00	0.90
1:B:153:LEU:CD1	1:B:340:TYR:CE2	2.49	0.90
1:B:158:ILE:O	1:B:162:PRO:CD	2.19	0.89
1:B:75:PHE:HB3	1:B:277:CYS:SG	2.13	0.89
1:B:104:SER:HB2	1:B:125:GLY:CA	2.03	0.89
1:B:379:PRO:O	1:B:382:ILE:N	2.06	0.89
1:B:332:LYS:HG3	1:B:333:HIS:HD2	1.29	0.89
1:B:135:THR:CG2	1:B:285:ARG:NH1	2.36	0.89
1:B:104:SER:HB3	1:B:125:GLY:CA	2.03	0.89
1:B:119:PRO:HG2	1:B:175:PHE:HA	1.54	0.89
1:B:320:ARG:CZ	1:B:344:GLU:CD	2.41	0.89
1:B:80:SER:N	1:B:260:ASP:OD1	2.02	0.89
1:B:241:CYS:HB3	1:B:243:TYR:CB	2.03	0.88
1:B:126:ALA:CB	1:B:171:ILE:CD1	2.51	0.88
1:B:153:LEU:HD21	1:B:340:TYR:HH	1.15	0.88
1:B:320:ARG:HG2	1:B:344:GLU:CB	2.02	0.88
1:B:232:VAL:CG1	1:B:245:PHE:HE2	1.86	0.88
1:B:158:ILE:HG21	1:B:256:LEU:HD12	1.53	0.88
1:B:212:CYS:CB	1:B:213:ASP:N	2.36	0.88
1:B:324:VAL:HG21	1:B:342:ALA:H	1.33	0.87
1:B:78:ARG:CZ	1:B:263:PHE:CE2	2.51	0.87
1:B:75:PHE:HB2	1:B:277:CYS:SG	2.14	0.87
1:B:320:ARG:HD3	1:B:344:GLU:CG	2.04	0.87
1:B:162:PRO:CA	1:B:249:MET:SD	2.62	0.87
1:B:376:TYR:C	1:B:378:THR:HG22	1.94	0.87
1:B:85:VAL:CG2	1:B:148:GLU:CG	2.18	0.87
1:B:145:THR:N	1:B:146:ASN:HA	1.87	0.86
1:B:320:ARG:NE	1:B:344:GLU:CG	2.37	0.86
1:B:301:LEU:HD11	1:B:388:ILE:CG1	1.99	0.86
1:B:320:ARG:HE	1:B:344:GLU:HB2	1.35	0.86
1:B:262:LEU:HB3	1:B:270:TYR:HE1	1.38	0.86
1:B:50:PRO:CD	1:B:53:SER:HB2	2.04	0.86
1:B:214:PHE:HD2	1:B:217:TYR:HB3	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:HG3	1:B:345:GLY:H	1.39	0.86
1:B:301:LEU:HD12	1:B:388:ILE:CG1	2.05	0.86
1:B:123:LEU:H	1:B:175:PHE:HZ	1.23	0.86
1:B:66:LEU:CD1	1:B:349:VAL:CG1	2.53	0.85
1:B:119:PRO:HB2	1:B:175:PHE:CD2	2.11	0.85
1:B:78:ARG:HD2	1:B:263:PHE:CE1	2.11	0.85
1:B:120:VAL:HG23	1:B:374:THR:HG21	1.57	0.85
1:B:83:LYS:O	1:B:86:ILE:HG22	1.75	0.85
1:B:285:ARG:NH2	1:B:289:PHE:HE2	1.74	0.85
1:B:377:ILE:HG13	1:B:378:THR:C	1.98	0.85
1:B:97:PHE:CE1	1:B:160:ASN:ND2	2.45	0.84
1:B:159:PHE:C	1:B:162:PRO:HD2	1.98	0.84
1:B:92:LEU:HD13	1:B:341:PHE:CD2	2.11	0.84
1:B:296:ILE:CG2	1:B:387:ILE:HG21	2.07	0.84
1:B:120:VAL:HG13	1:B:382:ILE:CG1	2.00	0.84
1:B:379:PRO:O	1:B:381:ASP:N	2.11	0.84
1:B:132:ASP:OD2	1:B:349:VAL:HB	1.76	0.84
1:B:142:ARG:O	1:B:142:ARG:NE	2.10	0.84
1:B:167:SER:O	1:B:170:VAL:HG23	1.77	0.84
1:B:320:ARG:HG2	1:B:344:GLU:H	1.38	0.84
1:B:93:ASP:OD2	1:B:156:GLU:HA	1.76	0.84
1:B:69:ILE:CD1	1:B:349:VAL:HG11	2.08	0.84
1:B:292:LEU:CD1	1:B:352:ALA:HB1	2.08	0.84
1:B:320:ARG:NE	1:B:344:GLU:CD	2.30	0.83
1:B:131:THR:C	1:B:347:ARG:CB	2.33	0.83
1:B:30:PRO:HG3	1:B:402:ALA:HB1	1.59	0.83
1:B:167:SER:O	1:B:171:ILE:HG13	1.78	0.82
1:B:135:THR:HG22	1:B:285:ARG:HH12	1.43	0.82
1:B:32:ILE:HD12	1:B:136:LEU:CD1	2.08	0.82
1:B:130:ALA:CB	1:B:351:PRO:HG3	2.08	0.82
1:B:215:HIS:C	1:B:216:GLU:N	0.77	0.82
1:B:328:LEU:HD22	1:B:338:LYS:HA	1.62	0.82
1:B:119:PRO:CB	1:B:175:PHE:CD1	2.63	0.82
1:B:130:ALA:HB3	1:B:351:PRO:HG2	1.60	0.82
1:B:172:LEU:O	1:B:177:LEU:HD22	1.79	0.82
1:B:70:LEU:CD2	1:B:251:VAL:CG2	2.57	0.82
1:B:119:PRO:HB3	1:B:175:PHE:CD1	2.15	0.81
1:B:232:VAL:CG1	1:B:245:PHE:CE2	2.62	0.81
1:B:32:ILE:HB	1:B:398:VAL:HG11	1.62	0.81
1:B:271:LYS:O	1:B:272:TYR:CB	2.28	0.81
1:B:108:PHE:CD2	1:B:124:PHE:CB	2.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ALA:HB1	1:B:386:ILE:CG2	2.10	0.81
1:B:82:LEU:HA	1:B:151:ILE:HG12	1.60	0.81
1:B:374:THR:HG22	1:B:377:ILE:HG12	1.63	0.81
1:B:32:ILE:HD12	1:B:136:LEU:HD11	1.63	0.81
1:B:205:TYR:CZ	1:B:221:LEU:CD2	2.63	0.81
1:B:120:VAL:HG11	1:B:382:ILE:HG12	0.81	0.81
1:B:136:LEU:CD1	1:B:398:VAL:HG13	2.08	0.81
1:B:377:ILE:N	1:B:378:THR:HA	1.94	0.81
1:B:214:PHE:HD2	1:B:217:TYR:CB	1.93	0.80
1:B:78:ARG:HG2	1:B:263:PHE:CB	2.12	0.80
1:B:89:VAL:CG2	1:B:152:THR:HG23	2.05	0.80
1:B:119:PRO:CG	1:B:174:LEU:O	2.30	0.80
1:B:162:PRO:O	1:B:166:VAL:HG23	1.82	0.80
1:B:168:THR:CG2	1:B:354:LEU:HD13	2.12	0.79
1:B:173:GLY:CA	1:B:177:LEU:HD21	1.93	0.79
1:B:162:PRO:HB3	1:B:249:MET:SD	2.22	0.79
1:B:32:ILE:CB	1:B:398:VAL:HG11	2.13	0.79
1:B:320:ARG:CD	1:B:344:GLU:CG	2.60	0.79
1:B:147:PRO:O	1:B:149:VAL:HG23	1.81	0.79
1:B:58:PHE:CE2	1:B:292:LEU:HA	2.18	0.79
1:B:123:LEU:HD12	1:B:171:ILE:HD13	1.65	0.78
1:B:166:VAL:O	1:B:170:VAL:HG22	1.82	0.78
1:B:119:PRO:HD2	1:B:374:THR:OG1	1.83	0.78
1:B:173:GLY:CA	1:B:177:LEU:HD22	1.91	0.78
1:B:215:HIS:CB	1:B:216:GLU:N	2.46	0.78
1:B:287:PHE:CD1	1:B:291:PHE:CD2	2.70	0.78
1:B:93:ASP:CB	1:B:156:GLU:OE2	2.30	0.78
1:B:119:PRO:HB3	1:B:175:PHE:CG	2.16	0.78
1:B:162:PRO:CB	1:B:249:MET:SD	2.72	0.78
1:B:124:PHE:O	1:B:127:ILE:CG1	2.30	0.78
1:B:32:ILE:HG12	1:B:285:ARG:NH2	1.99	0.78
1:B:335:PHE:CZ	1:B:415:GLU:CD	2.48	0.78
1:B:202:ALA:HB3	1:B:257:TYR:HD2	1.47	0.77
1:B:32:ILE:CD1	1:B:136:LEU:HG	2.12	0.77
1:B:321:PRO:HA	1:B:342:ALA:HB2	1.64	0.77
1:B:89:VAL:CB	1:B:152:THR:HG22	2.12	0.77
1:B:130:ALA:HB3	1:B:351:PRO:HG3	1.64	0.77
1:B:320:ARG:HE	1:B:344:GLU:CB	1.91	0.77
1:B:114:LEU:HG	1:B:377:ILE:HB	1.66	0.77
1:B:119:PRO:HB3	1:B:175:PHE:N	1.99	0.77
1:B:158:ILE:HG21	1:B:256:LEU:HD11	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:THR:HG23	1:B:285:ARG:NH1	1.97	0.77
1:B:119:PRO:HB2	1:B:175:PHE:CB	2.14	0.77
1:B:79:ILE:O	1:B:81:LEU:HB2	1.85	0.77
1:B:135:THR:HG21	1:B:289:PHE:HZ	0.96	0.77
1:B:162:PRO:CB	1:B:249:MET:CE	2.61	0.77
1:B:202:ALA:HB3	1:B:257:TYR:CD2	2.20	0.77
1:B:114:LEU:CD2	1:B:377:ILE:HB	2.14	0.77
1:B:135:THR:CG2	1:B:289:PHE:HZ	1.80	0.76
1:B:376:TYR:O	1:B:378:THR:HG22	1.84	0.76
1:B:130:ALA:CB	1:B:351:PRO:CG	2.63	0.76
1:B:89:VAL:HG21	1:B:152:THR:HG23	1.64	0.76
1:B:133:PRO:HB3	1:B:157:SER:OG	1.86	0.76
1:B:182:ASN:OD1	1:B:185:ILE:HD13	1.86	0.76
1:B:214:PHE:CD2	1:B:217:TYR:CB	2.69	0.76
1:B:335:PHE:CZ	1:B:415:GLU:OE1	2.39	0.76
1:B:293:GLY:O	1:B:296:ILE:HG12	1.86	0.75
1:B:355:ALA:HB1	1:B:386:ILE:HG22	1.67	0.75
1:B:194:ALA:HB1	1:B:250:ALA:HA	1.67	0.75
1:B:97:PHE:CD2	1:B:163:LEU:HD13	2.21	0.75
1:B:135:THR:HG22	1:B:285:ARG:HH22	1.51	0.75
1:B:51:SER:HB2	1:B:298:LEU:CA	2.15	0.75
1:B:186:ASP:HA	1:B:189:THR:HG22	1.68	0.75
1:B:136:LEU:HD12	1:B:398:VAL:HG22	1.66	0.75
1:B:168:THR:HG21	1:B:354:LEU:HD22	1.66	0.75
1:B:120:VAL:CG2	1:B:374:THR:HG21	2.16	0.75
1:B:214:PHE:CD2	1:B:217:TYR:HB2	2.22	0.74
1:B:182:ASN:CG	1:B:185:ILE:HD13	2.05	0.74
1:B:194:ALA:HB1	1:B:250:ALA:CA	2.16	0.74
1:B:215:HIS:O	1:B:216:GLU:CA	2.24	0.74
1:B:93:ASP:HA	1:B:156:GLU:OE2	1.87	0.74
1:B:130:ALA:O	1:B:347:ARG:HB3	1.88	0.74
1:B:347:ARG:HD3	1:B:351:PRO:HD2	1.70	0.74
1:B:410:LEU:HD12	1:B:411:LYS:N	2.03	0.74
1:B:78:ARG:CG	1:B:263:PHE:CG	2.70	0.74
1:B:201:LEU:HD11	1:B:205:TYR:CE1	2.23	0.74
1:B:35:LEU:HD23	1:B:286:VAL:HG13	1.70	0.74
1:B:153:LEU:HD11	1:B:340:TYR:CZ	2.23	0.73
1:B:330:GLY:O	1:B:331:SER:O	2.05	0.73
1:B:335:PHE:CE2	1:B:415:GLU:OE2	2.42	0.73
1:B:27:LEU:HD22	1:B:29:ILE:CD1	2.19	0.73
1:B:120:VAL:C	1:B:175:PHE:CZ	2.61	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:O	1:B:81:LEU:CB	2.36	0.73
1:B:123:LEU:N	1:B:175:PHE:CZ	2.56	0.73
1:B:328:LEU:O	1:B:330:GLY:N	2.22	0.73
1:B:32:ILE:CD1	1:B:136:LEU:CD1	2.67	0.72
1:B:215:HIS:CE1	1:B:269:ASP:OD1	2.42	0.72
1:B:70:LEU:HD23	1:B:251:VAL:CG2	2.19	0.72
1:B:123:LEU:HD12	1:B:171:ILE:CD1	2.18	0.72
1:B:407:MET:O	1:B:411:LYS:CB	2.29	0.72
1:B:132:ASP:OD1	1:B:347:ARG:HG2	1.89	0.72
1:B:114:LEU:HD23	1:B:377:ILE:CD1	2.19	0.72
1:B:97:PHE:CD1	1:B:160:ASN:ND2	2.57	0.72
1:B:148:GLU:C	1:B:149:VAL:N	0.67	0.72
1:B:135:THR:O	1:B:285:ARG:NH1	2.22	0.72
1:B:205:TYR:HE2	1:B:222:VAL:HG12	1.55	0.72
1:B:292:LEU:HD11	1:B:352:ALA:HB1	1.71	0.72
1:B:379:PRO:HA	1:B:382:ILE:HG13	1.71	0.71
1:B:148:GLU:O	1:B:149:VAL:CA	2.23	0.71
1:B:237:LEU:HD22	1:B:245:PHE:CD2	2.25	0.71
1:B:324:VAL:CG2	1:B:342:ALA:N	2.53	0.71
1:B:123:LEU:HB2	1:B:175:PHE:CZ	2.26	0.71
1:B:127:ILE:O	1:B:347:ARG:NH2	2.23	0.71
1:B:93:ASP:HB2	1:B:156:GLU:OE2	1.89	0.71
1:B:69:ILE:CD1	1:B:349:VAL:CG1	2.68	0.71
1:B:135:THR:HG22	1:B:285:ARG:NH1	2.04	0.71
1:B:160:ASN:O	1:B:164:GLY:N	2.23	0.71
1:B:345:GLY:O	1:B:397:SER:OG	2.07	0.71
1:B:132:ASP:CG	1:B:347:ARG:HG2	2.10	0.70
1:B:78:ARG:HG2	1:B:263:PHE:CG	2.26	0.70
1:B:97:PHE:CE2	1:B:163:LEU:HB3	2.25	0.70
1:B:375:LYS:O	1:B:379:PRO:HD2	1.91	0.70
1:B:85:VAL:HG21	1:B:148:GLU:HG3	0.71	0.70
1:B:241:CYS:C	1:B:243:TYR:N	2.44	0.70
1:B:167:SER:HA	1:B:170:VAL:CG2	2.22	0.70
1:B:114:LEU:CG	1:B:377:ILE:HB	2.21	0.70
1:B:115:PRO:O	1:B:118:SER:OG	2.09	0.70
1:B:364:LYS:HG3	1:B:365:ASN:H	1.56	0.70
1:B:120:VAL:HG13	1:B:382:ILE:HG21	1.74	0.70
1:B:35:LEU:HD22	1:B:286:VAL:HA	1.73	0.70
1:B:269:ASP:C	1:B:270:TYR:N	2.45	0.69
1:B:66:LEU:HD11	1:B:349:VAL:CG1	2.21	0.69
1:B:127:ILE:HD13	1:B:386:ILE:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:OG1	1:B:150:ALA:HB2	1.92	0.69
1:B:78:ARG:CD	1:B:263:PHE:CE1	2.72	0.69
1:B:120:VAL:HG13	1:B:382:ILE:CB	2.21	0.69
1:B:132:ASP:OD1	1:B:350:VAL:HG12	1.92	0.69
1:B:35:LEU:HD13	1:B:289:PHE:HD2	1.58	0.69
1:B:99:ILE:O	1:B:103:ILE:HG13	1.90	0.69
1:B:215:HIS:HE1	1:B:269:ASP:OD1	1.74	0.69
1:B:214:PHE:CG	1:B:217:TYR:HB2	2.27	0.69
1:B:120:VAL:C	1:B:175:PHE:CE2	2.66	0.69
1:B:132:ASP:CB	1:B:347:ARG:CG	2.63	0.69
1:B:55:MET:HE3	1:B:356:VAL:CG1	2.22	0.69
1:B:32:ILE:HD11	1:B:136:LEU:CG	2.16	0.69
1:B:394:ILE:O	1:B:398:VAL:HG23	1.92	0.69
1:B:23:ILE:O	1:B:27:LEU:HB2	1.93	0.68
1:B:262:LEU:HB3	1:B:270:TYR:CE1	2.24	0.68
1:B:377:ILE:HG13	1:B:378:THR:HA	1.73	0.68
1:B:119:PRO:CB	1:B:175:PHE:CB	2.70	0.68
1:B:335:PHE:O	1:B:336:LYS:HG2	1.94	0.68
1:B:108:PHE:CE2	1:B:124:PHE:HB2	2.29	0.68
1:B:31:ASP:OD2	1:B:285:ARG:NE	2.27	0.68
1:B:119:PRO:HB2	1:B:175:PHE:CA	2.07	0.68
1:B:298:LEU:C	1:B:298:LEU:HD13	2.14	0.68
1:B:234:ASP:OD1	1:B:246:SER:HA	1.94	0.68
1:B:168:THR:HG23	1:B:354:LEU:HD13	1.75	0.68
1:B:93:ASP:CA	1:B:156:GLU:OE2	2.42	0.67
1:B:335:PHE:HZ	1:B:415:GLU:OE1	1.72	0.67
1:B:32:ILE:HD12	1:B:398:VAL:HG11	1.76	0.67
1:B:35:LEU:HD22	1:B:286:VAL:HG13	1.76	0.67
1:B:346:PRO:HD2	1:B:347:ARG:H	1.59	0.67
1:B:292:LEU:HD13	1:B:352:ALA:HB1	1.76	0.67
1:B:135:THR:HG22	1:B:285:ARG:NH2	2.10	0.67
1:B:66:LEU:HD13	1:B:349:VAL:HG12	1.73	0.67
1:B:347:ARG:CD	1:B:351:PRO:CD	2.69	0.67
1:B:95:ILE:O	1:B:99:ILE:HG12	1.93	0.67
1:B:242:GLY:CA	1:B:243:TYR:N	2.57	0.67
1:B:112:LEU:HB3	1:B:114:LEU:HD13	1.77	0.66
1:B:109:ASN:HD22	1:B:122:TYR:HE1	1.38	0.66
1:B:347:ARG:CD	1:B:351:PRO:HD2	2.25	0.66
1:B:410:LEU:C	1:B:410:LEU:HD12	2.15	0.66
1:B:155:ALA:O	1:B:159:PHE:HB2	1.95	0.66
1:B:78:ARG:NH2	1:B:263:PHE:CZ	2.64	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:LYS:HG3	1:B:365:ASN:N	2.10	0.66
1:B:135:THR:CA	1:B:285:ARG:HH12	2.09	0.66
1:B:296:ILE:HG21	1:B:387:ILE:HG23	1.77	0.66
1:B:132:ASP:OD1	1:B:347:ARG:CG	2.44	0.66
1:B:137:ILE:HG21	1:B:153:LEU:HB3	1.77	0.66
1:B:35:LEU:CD2	1:B:286:VAL:CG1	2.68	0.66
1:B:35:LEU:HD21	1:B:286:VAL:HG13	1.77	0.65
1:B:370:PRO:O	1:B:372:SER:N	2.29	0.65
1:B:133:PRO:O	1:B:138:PRO:HD2	1.97	0.65
1:B:92:LEU:HD11	1:B:341:PHE:CD2	2.29	0.65
1:B:114:LEU:HD23	1:B:377:ILE:HD13	1.79	0.65
1:B:35:LEU:HD21	1:B:286:VAL:CG2	2.24	0.65
1:B:160:ASN:HA	1:B:163:LEU:HB2	1.78	0.65
1:B:214:PHE:C	1:B:217:TYR:H	2.00	0.65
1:B:382:ILE:O	1:B:386:ILE:HD13	1.97	0.65
1:B:108:PHE:HB2	1:B:124:PHE:CD1	2.32	0.64
1:B:31:ASP:N	1:B:31:ASP:OD1	2.28	0.64
1:B:104:SER:HB2	1:B:125:GLY:HA3	1.80	0.64
1:B:321:PRO:HA	1:B:342:ALA:CB	2.28	0.64
1:B:212:CYS:HB3	1:B:213:ASP:CA	2.25	0.64
1:B:205:TYR:HE2	1:B:222:VAL:CG1	2.10	0.64
1:B:144:ARG:NH2	1:B:144:ARG:HG3	2.11	0.64
1:B:108:PHE:CE2	1:B:124:PHE:CB	2.80	0.64
1:B:335:PHE:O	1:B:412:LEU:HD21	1.98	0.64
1:B:162:PRO:O	1:B:166:VAL:CG2	2.46	0.64
1:B:173:GLY:CA	1:B:177:LEU:HD23	1.95	0.63
1:B:320:ARG:HG2	1:B:344:GLU:CA	2.27	0.63
1:B:379:PRO:O	1:B:380:THR:C	2.36	0.63
1:B:160:ASN:C	1:B:163:LEU:H	2.01	0.63
1:B:108:PHE:O	1:B:112:LEU:HD23	1.97	0.63
1:B:27:LEU:HD23	1:B:29:ILE:HG12	1.78	0.63
1:B:347:ARG:NE	1:B:351:PRO:HG2	2.14	0.63
1:B:162:PRO:CB	1:B:249:MET:HE1	2.13	0.63
1:B:328:LEU:HD21	1:B:337:GLU:HG2	1.81	0.63
1:B:237:LEU:HD22	1:B:245:PHE:HD2	1.62	0.62
1:B:32:ILE:CD1	1:B:398:VAL:CG1	2.74	0.62
1:B:214:PHE:HB3	1:B:217:TYR:CA	2.30	0.62
1:B:271:LYS:O	1:B:272:TYR:CD1	2.52	0.62
1:B:55:MET:HE2	1:B:360:ILE:CG2	2.30	0.62
1:B:89:VAL:HG22	1:B:152:THR:HG22	0.81	0.62
1:B:108:PHE:CG	1:B:124:PHE:HB3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HD3	1:B:344:GLU:HG2	1.82	0.62
1:B:36:LEU:HD13	1:B:395:LEU:HD13	1.82	0.62
1:B:153:LEU:CG	1:B:340:TYR:OH	2.48	0.62
1:B:80:SER:CB	1:B:260:ASP:OD1	2.48	0.62
1:B:20:VAL:HG13	1:B:34:LEU:HD23	1.80	0.62
1:B:372:SER:O	1:B:373:ILE:HG13	2.00	0.62
1:B:50:PRO:HD2	1:B:53:SER:CB	2.22	0.62
1:B:132:ASP:CB	1:B:348:GLY:N	2.43	0.62
1:B:144:ARG:HH21	1:B:144:ARG:HG3	1.63	0.61
1:B:133:PRO:CD	1:B:157:SER:HB3	2.29	0.61
1:B:168:THR:HG21	1:B:354:LEU:CD2	2.30	0.61
1:B:241:CYS:CB	1:B:243:TYR:N	2.63	0.61
1:B:27:LEU:O	1:B:28:LYS:HB2	1.99	0.61
1:B:93:ASP:OD2	1:B:156:GLU:HG3	1.99	0.61
1:B:120:VAL:HA	1:B:175:PHE:HE2	0.45	0.61
1:B:370:PRO:C	1:B:372:SER:H	2.02	0.61
1:B:104:SER:HB2	1:B:125:GLY:C	2.21	0.61
1:B:93:ASP:OD1	1:B:159:PHE:HB3	2.01	0.61
1:B:374:THR:HG23	1:B:377:ILE:CG2	2.24	0.61
1:B:20:VAL:CG1	1:B:34:LEU:HD23	2.31	0.61
1:B:320:ARG:CG	1:B:344:GLU:H	2.11	0.61
1:B:35:LEU:CD2	1:B:286:VAL:HA	2.30	0.61
1:B:114:LEU:HD21	1:B:377:ILE:HB	1.83	0.61
1:B:48:ILE:C	1:B:49:ILE:HG13	2.19	0.61
1:B:172:LEU:O	1:B:176:GLY:O	2.17	0.61
1:B:79:ILE:HD12	1:B:256:LEU:CD2	2.31	0.61
1:B:114:LEU:HD11	1:B:377:ILE:O	2.01	0.61
1:B:320:ARG:CD	1:B:344:GLU:HB3	2.06	0.61
1:B:127:ILE:O	1:B:347:ARG:CZ	2.49	0.60
1:B:149:VAL:HA	1:B:152:THR:OG1	2.00	0.60
1:B:123:LEU:N	1:B:175:PHE:CE1	2.69	0.60
1:B:182:ASN:OD1	1:B:185:ILE:CD1	2.48	0.60
1:B:343:LEU:C	1:B:344:GLU:O	2.38	0.60
1:B:182:ASN:CG	1:B:185:ILE:CD1	2.55	0.60
1:B:320:ARG:HB3	1:B:321:PRO:CD	2.21	0.60
1:B:332:LYS:CB	1:B:333:HIS:CD2	2.80	0.60
1:B:194:ALA:HB1	1:B:250:ALA:N	2.15	0.60
1:B:78:ARG:NE	1:B:263:PHE:CE1	2.69	0.60
1:B:271:LYS:O	1:B:272:TYR:HD1	1.84	0.60
1:B:32:ILE:CG2	1:B:398:VAL:HG11	2.32	0.60
1:B:153:LEU:O	1:B:157:SER:OG	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:THR:O	1:B:374:THR:HG22	2.01	0.60
1:B:320:ARG:NH2	1:B:344:GLU:CD	2.52	0.60
1:B:390:THR:O	1:B:394:ILE:HG12	2.01	0.60
1:B:112:LEU:O	1:B:113:ASN:HB2	2.00	0.59
1:B:343:LEU:HD12	1:B:344:GLU:N	2.17	0.59
1:B:131:THR:C	1:B:347:ARG:CG	2.71	0.59
1:B:301:LEU:HD11	1:B:388:ILE:HD11	0.62	0.59
1:B:332:LYS:N	1:B:333:HIS:O	2.34	0.59
1:B:104:SER:HB3	1:B:128:THR:OG1	2.01	0.59
1:B:241:CYS:HB2	1:B:243:TYR:HB3	1.80	0.59
1:B:333:HIS:O	1:B:334:SER:HB3	1.98	0.59
1:B:374:THR:O	1:B:377:ILE:HG12	2.03	0.59
1:B:32:ILE:CD1	1:B:398:VAL:HG11	2.32	0.59
1:B:333:HIS:HB3	1:B:334:SER:N	2.17	0.59
1:B:213:ASP:C	1:B:214:PHE:N	2.56	0.59
1:B:78:ARG:HG2	1:B:263:PHE:HB2	1.85	0.59
1:B:186:ASP:HA	1:B:189:THR:CG2	2.33	0.58
1:B:267:ASP:OD1	1:B:268:ILE:N	2.37	0.58
1:B:366:ALA:HA	1:B:370:PRO:HB3	1.85	0.58
1:B:335:PHE:O	1:B:412:LEU:CD2	2.50	0.58
1:B:115:PRO:O	1:B:118:SER:CB	2.50	0.58
1:B:155:ALA:O	1:B:159:PHE:HD2	1.86	0.58
1:B:70:LEU:HD23	1:B:251:VAL:HG23	1.77	0.58
1:B:374:THR:HG22	1:B:377:ILE:CG1	2.33	0.58
1:B:73:GLY:O	1:B:76:THR:HG22	2.04	0.58
1:B:304:TYR:CE2	1:B:381:ASP:O	2.55	0.58
1:B:70:LEU:HD21	1:B:251:VAL:CG2	2.23	0.58
1:B:321:PRO:HG3	1:B:342:ALA:HB1	1.85	0.57
1:B:377:ILE:HD11	1:B:382:ILE:HD11	1.85	0.57
1:B:136:LEU:HD11	1:B:398:VAL:CG1	2.13	0.57
1:B:120:VAL:C	1:B:175:PHE:HZ	2.05	0.57
1:B:304:TYR:CD2	1:B:381:ASP:O	2.58	0.57
1:B:335:PHE:H	1:B:338:LYS:CD	2.17	0.57
1:B:131:THR:HG21	1:B:344:GLU:OE2	2.05	0.57
1:B:172:LEU:C	1:B:177:LEU:HD22	2.24	0.57
1:B:79:ILE:HD12	1:B:256:LEU:HD23	1.85	0.57
1:B:333:HIS:C	1:B:334:SER:CA	2.72	0.57
1:B:79:ILE:CG2	1:B:80:SER:N	2.41	0.57
1:B:123:LEU:HD21	1:B:358:VAL:HG11	1.86	0.57
1:B:155:ALA:O	1:B:159:PHE:CD2	2.58	0.57
1:B:335:PHE:H	1:B:338:LYS:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HD13	1:B:395:LEU:CD1	2.35	0.56
1:B:399:ILE:O	1:B:403:SER:OG	2.23	0.56
1:B:202:ALA:CB	1:B:257:TYR:CD2	2.87	0.56
1:B:137:ILE:CG2	1:B:153:LEU:HB3	2.34	0.56
1:B:346:PRO:CD	1:B:347:ARG:H	2.18	0.56
1:B:119:PRO:CG	1:B:175:PHE:CA	2.69	0.56
1:B:55:MET:CE	1:B:356:VAL:CG1	2.83	0.56
1:B:26:LYS:O	1:B:26:LYS:HG2	2.06	0.56
1:B:370:PRO:C	1:B:372:SER:N	2.59	0.56
1:B:304:TYR:CD2	1:B:385:THR:OG1	2.58	0.56
1:B:166:VAL:CG1	1:B:187:LEU:CD2	2.72	0.56
1:B:126:ALA:HB3	1:B:171:ILE:HD13	1.84	0.56
1:B:32:ILE:HG21	1:B:398:VAL:HG21	1.88	0.56
1:B:347:ARG:CD	1:B:351:PRO:CG	2.49	0.56
1:B:155:ALA:HB1	1:B:159:PHE:CE2	2.41	0.56
1:B:160:ASN:O	1:B:163:LEU:CA	2.53	0.56
1:B:237:LEU:CD2	1:B:245:PHE:HD2	2.18	0.56
1:B:307:PRO:O	1:B:311:VAL:HG23	2.07	0.55
1:B:332:LYS:HB2	1:B:333:HIS:ND1	2.20	0.55
1:B:355:ALA:HB1	1:B:386:ILE:HG21	1.86	0.55
1:B:83:LYS:HA	1:B:86:ILE:HD13	1.87	0.55
1:B:135:THR:HG22	1:B:285:ARG:CZ	2.36	0.55
1:B:317:PHE:O	1:B:321:PRO:HG2	2.07	0.55
1:B:296:ILE:CG2	1:B:387:ILE:CG2	2.72	0.55
1:B:348:GLY:HA3	1:B:394:ILE:HD11	1.88	0.55
1:B:132:ASP:OD2	1:B:349:VAL:CB	2.50	0.55
1:B:214:PHE:CD2	1:B:217:TYR:HB3	2.29	0.55
1:B:32:ILE:HG12	1:B:285:ARG:HH22	1.71	0.55
1:B:27:LEU:CD2	1:B:29:ILE:HG12	2.37	0.55
1:B:54:ALA:C	1:B:295:CYS:HA	2.27	0.55
1:B:242:GLY:C	1:B:243:TYR:CA	2.74	0.55
1:B:144:ARG:HH21	1:B:144:ARG:CG	2.20	0.55
1:B:267:ASP:CG	1:B:268:ILE:H	2.09	0.54
1:B:213:ASP:C	1:B:214:PHE:HA	2.28	0.54
1:B:320:ARG:CG	1:B:344:GLU:HB3	2.31	0.54
1:B:80:SER:CA	1:B:260:ASP:OD1	2.55	0.54
1:B:408:LEU:HA	1:B:412:LEU:HD12	1.89	0.54
1:B:32:ILE:HG21	1:B:398:VAL:HG11	1.90	0.54
1:B:2:GLU:OE1	1:B:2:GLU:N	2.37	0.54
1:B:377:ILE:CD1	1:B:382:ILE:HD11	2.37	0.54
1:B:412:LEU:C	1:B:414:GLY:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASN:N	1:B:147:PRO:HD3	2.23	0.54
1:B:215:HIS:HB3	1:B:216:GLU:N	2.23	0.54
1:B:70:LEU:HD23	1:B:251:VAL:HG21	1.89	0.54
1:B:78:ARG:CG	1:B:263:PHE:CB	2.85	0.54
1:B:78:ARG:NH2	1:B:263:PHE:CE2	2.76	0.54
1:B:374:THR:CG2	1:B:377:ILE:HD13	2.38	0.54
1:B:30:PRO:HG3	1:B:402:ALA:CB	2.34	0.54
1:B:50:PRO:CG	1:B:53:SER:HB2	2.37	0.54
1:B:53:SER:O	1:B:57:ILE:HG13	2.08	0.54
1:B:80:SER:OG	1:B:260:ASP:OD1	2.23	0.53
1:B:78:ARG:CG	1:B:263:PHE:CD2	2.90	0.53
1:B:292:LEU:C	1:B:295:CYS:SG	2.85	0.53
1:B:89:VAL:CG1	1:B:152:THR:HG22	2.37	0.53
1:B:333:HIS:C	1:B:334:SER:N	2.62	0.53
1:B:375:LYS:O	1:B:378:THR:HB	2.08	0.53
1:B:177:LEU:HG	1:B:179:SER:O	2.09	0.53
1:B:27:LEU:HD22	1:B:29:ILE:HD13	1.90	0.53
1:B:324:VAL:HG21	1:B:338:LYS:O	2.09	0.53
1:B:32:ILE:CD1	1:B:136:LEU:CG	2.80	0.53
1:B:97:PHE:HE1	1:B:160:ASN:HD22	1.54	0.53
1:B:108:PHE:CE2	1:B:121:GLY:HA2	2.36	0.53
1:B:132:ASP:HB2	1:B:347:ARG:CG	2.08	0.53
1:B:372:SER:C	1:B:373:ILE:HG13	2.29	0.53
1:B:69:ILE:HD11	1:B:349:VAL:HG13	1.86	0.53
1:B:131:THR:CA	1:B:347:ARG:CG	2.83	0.53
1:B:300:MET:CB	1:B:301:LEU:CD1	2.62	0.52
1:B:92:LEU:HD11	1:B:341:PHE:CG	2.43	0.52
1:B:153:LEU:CD2	1:B:340:TYR:CZ	2.80	0.52
1:B:120:VAL:CG1	1:B:382:ILE:HG23	2.25	0.52
1:B:58:PHE:HE2	1:B:292:LEU:N	2.07	0.52
1:B:324:VAL:CG2	1:B:338:LYS:O	2.57	0.52
1:B:336:LYS:NZ	1:B:411:LYS:O	2.42	0.52
1:B:92:LEU:O	1:B:96:THR:HB	2.10	0.52
1:B:343:LEU:HB2	1:B:404:TRP:HZ2	1.75	0.52
1:B:108:PHE:CD1	1:B:124:PHE:CG	2.98	0.52
1:B:27:LEU:CD2	1:B:29:ILE:CD1	2.86	0.52
1:B:96:THR:HG23	1:B:323:GLY:HA3	1.92	0.52
1:B:365:ASN:OD1	1:B:368:LYS:HB3	2.10	0.52
1:B:364:LYS:CG	1:B:365:ASN:N	2.73	0.52
1:B:215:HIS:O	1:B:216:GLU:C	2.48	0.52
1:B:149:VAL:HA	1:B:152:THR:HG1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:TYR:CE2	1:B:222:VAL:HG12	2.42	0.52
1:B:58:PHE:HE2	1:B:292:LEU:HA	1.74	0.52
1:B:262:LEU:C	1:B:270:TYR:CE1	2.81	0.51
1:B:96:THR:HG23	1:B:323:GLY:CA	2.41	0.51
1:B:119:PRO:CB	1:B:175:PHE:CD2	2.83	0.51
1:B:260:ASP:O	1:B:264:ARG:HB2	2.11	0.51
1:B:335:PHE:H	1:B:338:LYS:CE	2.23	0.51
1:B:36:LEU:CD1	1:B:395:LEU:HD12	2.40	0.51
1:B:328:LEU:HD22	1:B:338:LYS:CA	2.38	0.51
1:B:83:LYS:HA	1:B:86:ILE:CD1	2.40	0.51
1:B:108:PHE:CG	1:B:124:PHE:CD1	2.99	0.51
1:B:155:ALA:HB1	1:B:159:PHE:CD2	2.46	0.51
1:B:331:SER:C	1:B:332:LYS:CA	2.77	0.51
1:B:379:PRO:C	1:B:381:ASP:N	2.62	0.51
1:B:78:ARG:CZ	1:B:263:PHE:CE1	2.90	0.51
1:B:135:THR:HA	1:B:285:ARG:NH1	2.26	0.51
1:B:119:PRO:CA	1:B:175:PHE:CD1	2.90	0.50
1:B:66:LEU:HD12	1:B:69:ILE:HD11	1.92	0.50
1:B:178:PHE:CD1	1:B:179:SER:N	2.79	0.50
1:B:108:PHE:CG	1:B:124:PHE:CG	3.00	0.50
1:B:369:ILE:O	1:B:369:ILE:HG23	2.12	0.50
1:B:162:PRO:CG	1:B:249:MET:CE	2.89	0.50
1:B:133:PRO:CB	1:B:157:SER:HB2	2.24	0.50
1:B:159:PHE:O	1:B:163:LEU:HG	2.12	0.50
1:B:167:SER:HA	1:B:170:VAL:HG23	1.94	0.50
1:B:42:ILE:O	1:B:48:ILE:HB	2.12	0.50
1:B:42:ILE:HD11	1:B:290:VAL:HG11	1.94	0.49
1:B:158:ILE:CG2	1:B:256:LEU:HD12	2.34	0.49
1:B:410:LEU:CD1	1:B:411:LYS:N	2.74	0.49
1:B:109:ASN:ND2	1:B:122:TYR:CD1	2.68	0.49
1:B:27:LEU:CD2	1:B:29:ILE:HD13	2.42	0.49
1:B:318:LEU:O	1:B:322:LEU:HB2	2.13	0.49
1:B:374:THR:CG2	1:B:377:ILE:HG21	2.28	0.49
1:B:82:LEU:HD21	1:B:151:ILE:O	2.12	0.49
1:B:162:PRO:HG3	1:B:249:MET:HE3	1.93	0.49
1:B:135:THR:CG2	1:B:285:ARG:CZ	2.90	0.49
1:B:124:PHE:C	1:B:127:ILE:HG12	2.30	0.49
1:B:167:SER:C	1:B:170:VAL:HG23	2.33	0.49
1:B:241:CYS:CB	1:B:243:TYR:CB	2.72	0.49
1:B:104:SER:CB	1:B:125:GLY:O	2.61	0.49
1:B:205:TYR:CE1	1:B:221:LEU:CG	2.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PHE:CG	1:B:295:CYS:HB3	2.48	0.49
1:B:78:ARG:HG2	1:B:263:PHE:CD2	2.47	0.49
1:B:107:ILE:O	1:B:111:VAL:HG23	2.13	0.49
1:B:131:THR:O	1:B:132:ASP:HA	2.06	0.49
1:B:285:ARG:NH2	1:B:289:PHE:CE2	2.66	0.49
1:B:78:ARG:CG	1:B:263:PHE:HB2	2.41	0.49
1:B:32:ILE:CD1	1:B:136:LEU:HD12	2.44	0.48
1:B:186:ASP:CA	1:B:189:THR:HG22	2.40	0.48
1:B:357:THR:O	1:B:360:ILE:HG13	2.14	0.48
1:B:377:ILE:N	1:B:378:THR:CA	2.73	0.48
1:B:93:ASP:OD2	1:B:156:GLU:CG	2.61	0.48
1:B:131:THR:C	1:B:347:ARG:HG3	2.33	0.48
1:B:108:PHE:HB2	1:B:124:PHE:HD1	1.76	0.48
1:B:58:PHE:CD2	1:B:291:PHE:O	2.66	0.48
1:B:58:PHE:HE2	1:B:292:LEU:CA	2.26	0.48
1:B:104:SER:C	1:B:125:GLY:HA3	2.33	0.48
1:B:300:MET:CG	1:B:301:LEU:HD13	2.39	0.48
1:B:58:PHE:CD2	1:B:295:CYS:HB3	2.48	0.48
1:B:104:SER:CB	1:B:125:GLY:HA3	2.34	0.48
1:B:322:LEU:O	1:B:326:LEU:HB2	2.14	0.48
1:B:284:ALA:O	1:B:288:ILE:HG13	2.14	0.48
1:B:377:ILE:HG13	1:B:378:THR:N	2.24	0.48
1:B:93:ASP:O	1:B:97:PHE:HB2	2.14	0.48
1:B:133:PRO:O	1:B:138:PRO:CD	2.63	0.47
1:B:343:LEU:O	1:B:344:GLU:C	2.41	0.47
1:B:30:PRO:O	1:B:33:PRO:HD2	2.15	0.47
1:B:50:PRO:HG2	1:B:53:SER:HB2	1.97	0.47
1:B:123:LEU:HA	1:B:171:ILE:HD13	1.95	0.47
1:B:209:ILE:HD11	1:B:218:VAL:CG2	2.45	0.47
1:B:287:PHE:O	1:B:291:PHE:HB2	2.14	0.47
1:B:36:LEU:CD1	1:B:395:LEU:CD1	2.92	0.47
1:B:215:HIS:C	1:B:216:GLU:C	2.71	0.47
1:B:158:ILE:CG2	1:B:256:LEU:CD1	2.80	0.47
1:B:69:ILE:HD13	1:B:288:ILE:HD12	1.95	0.47
1:B:51:SER:OG	1:B:296:ILE:O	2.26	0.47
1:B:343:LEU:CB	1:B:404:TRP:HZ2	2.28	0.47
1:B:35:LEU:HD21	1:B:286:VAL:CG1	2.43	0.47
1:B:144:ARG:HB3	1:B:145:THR:N	2.30	0.47
1:B:151:ILE:HG23	1:B:152:THR:N	2.30	0.47
1:B:78:ARG:HD2	1:B:270:TYR:CE2	2.35	0.47
1:B:89:VAL:CG2	1:B:152:THR:HG21	2.00	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PRO:HG2	1:B:175:PHE:CA	2.36	0.47
1:B:301:LEU:CD1	1:B:388:ILE:HG13	2.18	0.47
1:B:83:LYS:O	1:B:86:ILE:CB	2.62	0.47
1:B:97:PHE:CD2	1:B:163:LEU:CD1	2.95	0.46
1:B:108:PHE:CG	1:B:124:PHE:CB	2.96	0.46
1:B:168:THR:HG21	1:B:354:LEU:HD13	1.93	0.46
1:B:374:THR:HA	1:B:377:ILE:HG23	1.97	0.46
1:B:132:ASP:OD1	1:B:347:ARG:HG3	2.16	0.46
1:B:237:LEU:HD22	1:B:245:PHE:CE2	2.50	0.46
1:B:300:MET:N	1:B:301:LEU:HB2	1.80	0.46
1:B:2:GLU:HG2	1:B:5:MET:HB3	1.98	0.46
1:B:144:ARG:CA	1:B:145:THR:N	2.78	0.46
1:B:209:ILE:HD11	1:B:218:VAL:HG21	1.97	0.46
1:B:316:ILE:O	1:B:321:PRO:HD3	2.15	0.46
1:B:340:TYR:HA	1:B:343:LEU:HD21	1.97	0.46
1:B:75:PHE:CG	1:B:277:CYS:SG	3.09	0.46
1:B:54:ALA:CB	1:B:294:ALA:HB1	2.46	0.46
1:B:58:PHE:CB	1:B:295:CYS:HB3	2.46	0.46
1:B:173:GLY:N	1:B:177:LEU:CD2	2.73	0.46
1:B:241:CYS:HB2	1:B:243:TYR:N	2.29	0.46
1:B:373:ILE:O	1:B:374:THR:HB	2.15	0.46
1:B:377:ILE:CG1	1:B:378:THR:HA	2.42	0.46
1:B:41:ILE:O	1:B:46:LEU:HB2	2.16	0.46
1:B:122:TYR:HB2	1:B:175:PHE:HE1	1.81	0.46
1:B:35:LEU:HD22	1:B:286:VAL:CA	2.43	0.46
1:B:72:GLY:HA3	1:B:281:SER:HB3	1.98	0.46
1:B:173:GLY:N	1:B:177:LEU:HD22	2.31	0.46
1:B:182:ASN:CG	1:B:185:ILE:HD12	2.33	0.46
1:B:83:LYS:O	1:B:84:ARG:N	2.43	0.46
1:B:135:THR:CA	1:B:285:ARG:NH1	2.79	0.46
1:B:217:TYR:O	1:B:220:PRO:HD2	2.16	0.46
1:B:312:ALA:O	1:B:316:ILE:HG13	2.15	0.46
1:B:153:LEU:CD2	1:B:340:TYR:HH	2.02	0.46
1:B:127:ILE:HG13	1:B:128:THR:N	2.30	0.45
1:B:119:PRO:C	1:B:175:PHE:CG	2.72	0.45
1:B:300:MET:SD	1:B:384:GLY:HA2	2.55	0.45
1:B:58:PHE:HD2	1:B:291:PHE:O	1.99	0.45
1:B:161:ASP:O	1:B:165:ILE:HG13	2.16	0.45
1:B:54:ALA:HB1	1:B:294:ALA:CB	2.42	0.45
1:B:69:ILE:CD1	1:B:349:VAL:HG13	2.46	0.45
1:B:137:ILE:HG12	1:B:153:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASP:O	1:B:267:ASP:HB3	2.17	0.45
1:B:55:MET:N	1:B:295:CYS:HA	2.32	0.45
1:B:155:ALA:O	1:B:159:PHE:CB	2.62	0.45
1:B:285:ARG:HG3	1:B:286:VAL:N	2.31	0.45
1:B:35:LEU:CD1	1:B:289:PHE:HD2	2.28	0.45
1:B:48:ILE:HG22	1:B:48:ILE:O	2.16	0.45
1:B:104:SER:CB	1:B:125:GLY:C	2.84	0.45
1:B:148:GLU:O	1:B:151:ILE:HG22	2.16	0.45
1:B:118:SER:HA	1:B:119:PRO:HD3	1.43	0.45
1:B:395:LEU:O	1:B:399:ILE:HG13	2.17	0.45
1:B:32:ILE:HG12	1:B:285:ARG:HH21	1.76	0.45
1:B:344:GLU:HG3	1:B:345:GLY:N	2.19	0.45
1:B:136:LEU:CD1	1:B:398:VAL:HG22	2.42	0.45
1:B:173:GLY:C	1:B:177:LEU:CD2	2.80	0.44
1:B:320:ARG:CB	1:B:321:PRO:HD3	2.20	0.44
1:B:334:SER:O	1:B:335:PHE:CG	2.70	0.44
1:B:135:THR:CG2	1:B:289:PHE:HE2	2.18	0.44
1:B:219:ALA:HB3	1:B:220:PRO:HD3	1.99	0.44
1:B:27:LEU:HD22	1:B:29:ILE:HD11	1.95	0.44
1:B:96:THR:O	1:B:100:THR:OG1	2.32	0.44
1:B:155:ALA:C	1:B:159:PHE:HD2	2.20	0.44
1:B:194:ALA:HA	1:B:250:ALA:HB2	1.99	0.44
1:B:135:THR:C	1:B:285:ARG:HH12	2.19	0.44
1:B:133:PRO:O	1:B:134:ALA:C	2.55	0.44
1:B:335:PHE:CD1	1:B:335:PHE:O	2.70	0.44
1:B:355:ALA:CB	1:B:386:ILE:CG2	2.90	0.44
1:B:122:TYR:HB2	1:B:175:PHE:CE1	2.52	0.44
1:B:205:TYR:OH	1:B:221:LEU:CD1	2.64	0.44
1:B:205:TYR:HA	1:B:208:ILE:HG22	2.00	0.44
1:B:135:THR:HA	1:B:285:ARG:HH12	1.80	0.44
1:B:376:TYR:O	1:B:376:TYR:CG	2.70	0.44
1:B:377:ILE:HD11	1:B:382:ILE:CD1	2.48	0.44
1:B:64:ILE:O	1:B:67:ILE:HG22	2.17	0.44
1:B:104:SER:HB2	1:B:125:GLY:O	2.18	0.44
1:B:108:PHE:CD2	1:B:121:GLY:CA	2.61	0.44
1:B:125:GLY:O	1:B:128:THR:OG1	2.36	0.44
1:B:334:SER:O	1:B:335:PHE:CD2	2.71	0.44
1:B:123:LEU:CB	1:B:175:PHE:CZ	2.96	0.44
1:B:35:LEU:HD21	1:B:286:VAL:CB	2.48	0.44
1:B:55:MET:SD	1:B:297:LYS:HG2	2.57	0.44
1:B:104:SER:CB	1:B:128:THR:OG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:CG2	1:B:256:LEU:HD11	2.41	0.44
1:B:117:THR:O	1:B:118:SER:C	2.55	0.43
1:B:28:LYS:CE	1:B:28:LYS:HA	2.48	0.43
1:B:36:LEU:HD12	1:B:395:LEU:HD12	2.00	0.43
1:B:340:TYR:O	1:B:343:LEU:CD1	2.44	0.43
1:B:374:THR:CG2	1:B:377:ILE:CD1	2.96	0.43
1:B:101:LEU:C	1:B:101:LEU:HD23	2.38	0.43
1:B:178:PHE:CG	1:B:179:SER:N	2.86	0.43
1:B:205:TYR:O	1:B:209:ILE:HG13	2.19	0.43
1:B:264:ARG:HD2	1:B:264:ARG:HA	1.60	0.43
1:B:362:ILE:O	1:B:366:ALA:HB2	2.18	0.43
1:B:58:PHE:CE2	1:B:292:LEU:CA	2.93	0.43
1:B:134:ALA:HA	1:B:138:PRO:HG2	2.00	0.43
1:B:32:ILE:HB	1:B:398:VAL:CG1	2.43	0.43
1:B:394:ILE:O	1:B:398:VAL:CG2	2.64	0.43
1:B:55:MET:HE3	1:B:356:VAL:HG12	1.96	0.43
1:B:79:ILE:O	1:B:82:LEU:N	2.51	0.43
1:B:115:PRO:O	1:B:118:SER:HB3	2.17	0.43
1:B:177:LEU:HD12	1:B:179:SER:H	1.84	0.43
1:B:173:GLY:C	1:B:177:LEU:HD23	2.37	0.43
1:B:79:ILE:HD12	1:B:256:LEU:HD22	2.01	0.43
1:B:119:PRO:HB3	1:B:175:PHE:CB	2.40	0.43
1:B:162:PRO:HG3	1:B:249:MET:CE	2.49	0.43
1:B:173:GLY:O	1:B:177:LEU:HD23	2.20	0.42
1:B:331:SER:CA	1:B:332:LYS:N	2.77	0.42
1:B:91:ARG:HD3	1:B:91:ARG:HA	1.81	0.42
1:B:146:ASN:N	1:B:147:PRO:CD	2.82	0.42
1:B:145:THR:HG22	1:B:147:PRO:HD2	2.02	0.42
1:B:156:GLU:O	1:B:160:ASN:OD1	2.38	0.42
1:B:213:ASP:C	1:B:214:PHE:CA	2.88	0.42
1:B:335:PHE:N	1:B:338:LYS:CD	2.82	0.42
1:B:232:VAL:CG1	1:B:245:PHE:CZ	3.01	0.42
1:B:374:THR:CG2	1:B:377:ILE:HG12	2.42	0.42
1:B:267:ASP:CG	1:B:268:ILE:N	2.73	0.42
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.83	0.42
1:B:114:LEU:HD21	1:B:377:ILE:CB	2.48	0.41
1:B:347:ARG:HH11	1:B:351:PRO:HB2	1.84	0.41
1:B:414:GLY:O	1:B:415:GLU:HG2	2.20	0.41
1:B:93:ASP:OD2	1:B:156:GLU:OE2	2.38	0.41
1:B:97:PHE:HD1	1:B:160:ASN:HD21	1.67	0.41
1:B:119:PRO:CA	1:B:175:PHE:CG	3.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ALA:O	1:B:373:ILE:HG13	2.20	0.41
1:B:412:LEU:C	1:B:414:GLY:N	2.74	0.41
1:B:168:THR:HG21	1:B:354:LEU:CD1	2.49	0.41
1:B:144:ARG:HA	1:B:145:THR:N	2.36	0.41
1:B:332:LYS:CD	1:B:333:HIS:CD2	3.00	0.41
1:B:330:GLY:C	1:B:331:SER:O	2.59	0.41
1:B:410:LEU:CG	1:B:411:LYS:N	2.84	0.41
1:B:19:LEU:O	1:B:23:ILE:HG12	2.21	0.41
1:B:24:ALA:O	1:B:28:LYS:N	2.54	0.41
1:B:346:PRO:CD	1:B:347:ARG:N	2.82	0.41
1:B:350:VAL:O	1:B:352:ALA:N	2.53	0.41
1:B:374:THR:HG22	1:B:377:ILE:CD1	2.50	0.41
1:B:401:GLU:HA	1:B:404:TRP:NE1	2.36	0.41
1:B:114:LEU:HD21	1:B:377:ILE:CG1	2.45	0.41
1:B:133:PRO:CG	1:B:134:ALA:N	2.78	0.41
1:B:241:CYS:HB3	1:B:243:TYR:N	2.34	0.41
1:B:101:LEU:HA	1:B:129:ALA:HB2	2.02	0.41
1:B:133:PRO:C	1:B:135:THR:N	2.70	0.41
1:B:27:LEU:HD23	1:B:29:ILE:CG1	2.46	0.41
1:B:345:GLY:C	1:B:397:SER:HB2	2.38	0.41
1:B:214:PHE:CA	1:B:217:TYR:HB2	2.46	0.41
1:B:360:ILE:O	1:B:364:LYS:CG	2.69	0.41
1:B:223:LEU:O	1:B:227:MET:HG3	2.21	0.40
1:B:282:LEU:O	1:B:283:LEU:C	2.55	0.40
1:B:168:THR:CG2	1:B:354:LEU:HD22	2.46	0.40
1:B:51:SER:O	1:B:55:MET:HG3	2.21	0.40
1:B:177:LEU:HD13	1:B:177:LEU:HA	1.91	0.40
1:B:241:CYS:HB3	1:B:243:TYR:HB2	1.96	0.40
1:B:151:ILE:CG2	1:B:152:THR:N	2.84	0.40
1:B:332:LYS:HB2	1:B:333:HIS:CD2	2.44	0.40
1:B:335:PHE:CE1	1:B:415:GLU:OE1	2.74	0.40
1:B:335:PHE:C	1:B:336:LYS:HG2	2.41	0.40
1:B:27:LEU:CD2	1:B:29:ILE:CG1	3.00	0.40
1:B:375:LYS:HA	1:B:379:PRO:HD3	2.03	0.40
1:B:374:THR:CG2	1:B:377:ILE:CG1	2.99	0.40
1:B:51:SER:HA	1:B:296:ILE:O	2.22	0.40

All (43) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PHE:CD1	1:B:91:ARG:CZ[4_555]	0.47	1.73
1:B:83:LYS:CE	1:B:302:GLU:OE1[4_455]	0.69	1.51
1:B:45:PHE:CG	1:B:91:ARG:NH1[4_555]	0.88	1.32
1:B:45:PHE:CD2	1:B:91:ARG:NH1[4_555]	1.11	1.09
1:B:45:PHE:CG	1:B:91:ARG:CZ[4_555]	1.19	1.01
1:B:19:LEU:CD2	1:B:214:PHE:CZ[2_655]	1.19	1.01
1:B:45:PHE:CD1	1:B:91:ARG:NE[4_555]	1.21	0.99
1:B:22:LYS:CD	1:B:213:ASP:O[2_655]	1.37	0.83
1:B:45:PHE:CD1	1:B:91:ARG:NH2[4_555]	1.44	0.76
1:B:83:LYS:CE	1:B:302:GLU:CD[4_455]	1.49	0.71
1:B:45:PHE:CD1	1:B:91:ARG:NH1[4_555]	1.55	0.65
1:B:1:MET:SD	1:B:60:TYR:OH[2_655]	1.62	0.58
1:B:45:PHE:CG	1:B:91:ARG:NE[4_555]	1.64	0.56
1:B:45:PHE:CE1	1:B:91:ARG:CZ[4_555]	1.71	0.49
1:B:83:LYS:NZ	1:B:302:GLU:CG[4_455]	1.71	0.49
1:B:18:SER:OG	1:B:217:TYR:O[2_655]	1.73	0.47
1:B:83:LYS:CD	1:B:302:GLU:OE1[4_455]	1.74	0.46
1:B:22:LYS:CG	1:B:214:PHE:O[2_655]	1.77	0.43
1:B:22:LYS:CD	1:B:213:ASP:C[2_655]	1.80	0.40
1:B:1:MET:CE	1:B:60:TYR:CE1[2_655]	1.80	0.40
1:B:22:LYS:CG	1:B:214:PHE:CA[2_655]	1.81	0.39
1:B:83:LYS:NZ	1:B:302:GLU:OE1[4_455]	1.81	0.39
1:B:45:PHE:CE2	1:B:91:ARG:NH1[4_555]	1.84	0.36
1:B:45:PHE:CE1	1:B:91:ARG:NH2[4_555]	1.86	0.34
1:B:29:ILE:CG2	1:B:184:LEU:CD1[4_555]	1.90	0.30
1:B:45:PHE:CB	1:B:91:ARG:CD[4_555]	1.97	0.23
1:B:45:PHE:CG	1:B:91:ARG:CD[4_555]	1.97	0.23
1:B:45:PHE:CA	1:B:91:ARG:NE[4_555]	1.98	0.22
1:B:83:LYS:NZ	1:B:302:GLU:CD[4_455]	1.98	0.22
1:B:1:MET:SD	1:B:60:TYR:CZ[2_655]	1.99	0.21
1:B:22:LYS:CG	1:B:217:TYR:CD1[2_655]	1.99	0.21
1:B:22:LYS:CG	1:B:214:PHE:C[2_655]	2.00	0.20
1:B:22:LYS:CE	1:B:213:ASP:O[2_655]	2.02	0.18
1:B:22:LYS:NZ	1:B:213:ASP:O[2_655]	2.04	0.16
1:B:11:GLY:O	1:B:224:GLY:CA[2_655]	2.07	0.13
1:B:45:PHE:CB	1:B:91:ARG:NE[4_555]	2.07	0.13
1:B:19:LEU:CD2	1:B:214:PHE:CE2[2_655]	2.07	0.13
1:B:18:SER:CB	1:B:220:PRO:CB[2_655]	2.10	0.10
1:B:22:LYS:NZ	1:B:213:ASP:CB[2_655]	2.13	0.07
1:B:19:LEU:CA	1:B:214:PHE:CE2[2_655]	2.14	0.06
1:B:15:VAL:CG2	1:B:225:GLY:N[2_655]	2.14	0.06
1:B:22:LYS:CD	1:B:214:PHE:CA[2_655]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PHE:CE1	1:B:91:ARG:NH1[4_555]	2.14	0.06

## 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	B	402/426 (94%)	348 (87%)	30 (8%)	24 (6%)	2	22

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	SER
1	B	272	TYR
1	B	299	SER
1	B	329	ILE
1	B	331	SER
1	B	344	GLU
1	B	371	ALA
1	B	380	THR
1	B	134	ALA
1	B	79	ILE
1	B	346	PRO
1	B	413	LEU
1	B	148	GLU
1	B	241	CYS
1	B	267	ASP
1	B	348	GLY
1	B	133	PRO
1	B	266	ASP
1	B	350	VAL
1	B	147	PRO
1	B	370	PRO
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	50	PRO
1	B	351	PRO

### 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	B	344/351 (98%)	288 (84%)	56 (16%)	<b>3</b> <b>17</b>

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	3	LEU
1	B	5	MET
1	B	26	LYS
1	B	27	LEU
1	B	28	LYS
1	B	52	ASP
1	B	56	GLU
1	B	77	MET
1	B	80	SER
1	B	83	LYS
1	B	85	VAL
1	B	98	LEU
1	B	107	ILE
1	B	113	ASN
1	B	117	THR
1	B	128	THR
1	B	132	ASP
1	B	136	LEU
1	B	144	ARG
1	B	152	THR
1	B	153	LEU
1	B	156	GLU
1	B	157	SER

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Mol	Chain	Res	Type
1	B	168	THR
1	B	170	VAL
1	B	172	LEU
1	B	177	LEU
1	B	181	SER
1	B	200	LEU
1	B	256	LEU
1	B	264	ARG
1	B	266	ASP
1	B	270	TYR
1	B	271	LYS
1	B	273	ILE
1	B	287	PHE
1	B	297	LYS
1	B	300	MET
1	B	301	LEU
1	B	310	LEU
1	B	318	LEU
1	B	322	LEU
1	B	325	PHE
1	B	326	LEU
1	B	331	SER
1	B	332	LYS
1	B	338	LYS
1	B	343	LEU
1	B	364	LYS
1	B	368	LYS
1	B	403	SER
1	B	404	TRP
1	B	407	MET
1	B	410	LEU
1	B	419	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	160	ASN
1	B	215	HIS
1	B	333	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 carbohydrates 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.