



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:27 am GMT

PDB ID : 4M64  
Title : 3D crystal structure of Na<sup>+</sup>/melibiose symporter of Salmonella typhimurium  
Authors : Ethayathulla, A.S.; Guan, L.  
Deposited on : 2013-08-08  
Resolution : 3.35 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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

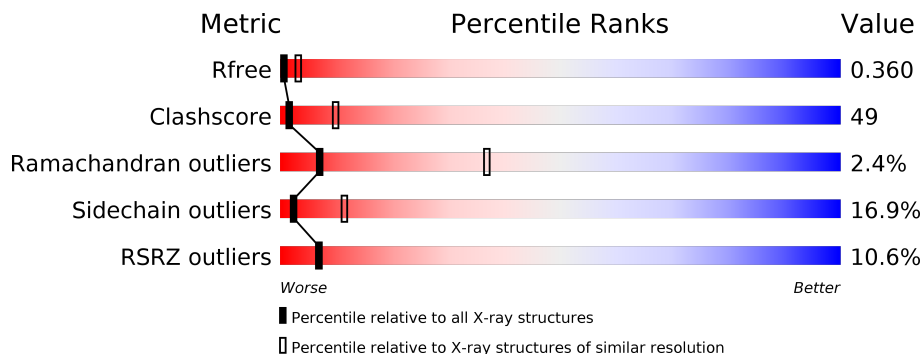
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	100719	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)

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.

Mol	Chain	Length	Quality of chain
1	A	486	
1	B	486	
1	C	486	
1	D	486	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12982 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 Melibiose carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3442	2295	540	585	22			
1	B	426	Total	C	N	O	S	0	0	0
			3258	2176	503	558	21			
1	C	431	Total	C	N	O	S	0	0	0
			3352	2242	520	568	22			
1	D	382	Total	C	N	O	S	0	0	0
			2930	1965	449	497	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
A	477	HIS	-	EXPRESSION TAG	UNP P30878
A	478	HIS	-	EXPRESSION TAG	UNP P30878
A	479	HIS	-	EXPRESSION TAG	UNP P30878
A	480	HIS	-	EXPRESSION TAG	UNP P30878
A	481	HIS	-	EXPRESSION TAG	UNP P30878
A	482	HIS	-	EXPRESSION TAG	UNP P30878
A	483	HIS	-	EXPRESSION TAG	UNP P30878
A	484	HIS	-	EXPRESSION TAG	UNP P30878
A	485	HIS	-	EXPRESSION TAG	UNP P30878
A	486	HIS	-	EXPRESSION TAG	UNP P30878
B	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
B	477	HIS	-	EXPRESSION TAG	UNP P30878
B	478	HIS	-	EXPRESSION TAG	UNP P30878
B	479	HIS	-	EXPRESSION TAG	UNP P30878
B	480	HIS	-	EXPRESSION TAG	UNP P30878
B	481	HIS	-	EXPRESSION TAG	UNP P30878
B	482	HIS	-	EXPRESSION TAG	UNP P30878
B	483	HIS	-	EXPRESSION TAG	UNP P30878
B	484	HIS	-	EXPRESSION TAG	UNP P30878
B	485	HIS	-	EXPRESSION TAG	UNP P30878

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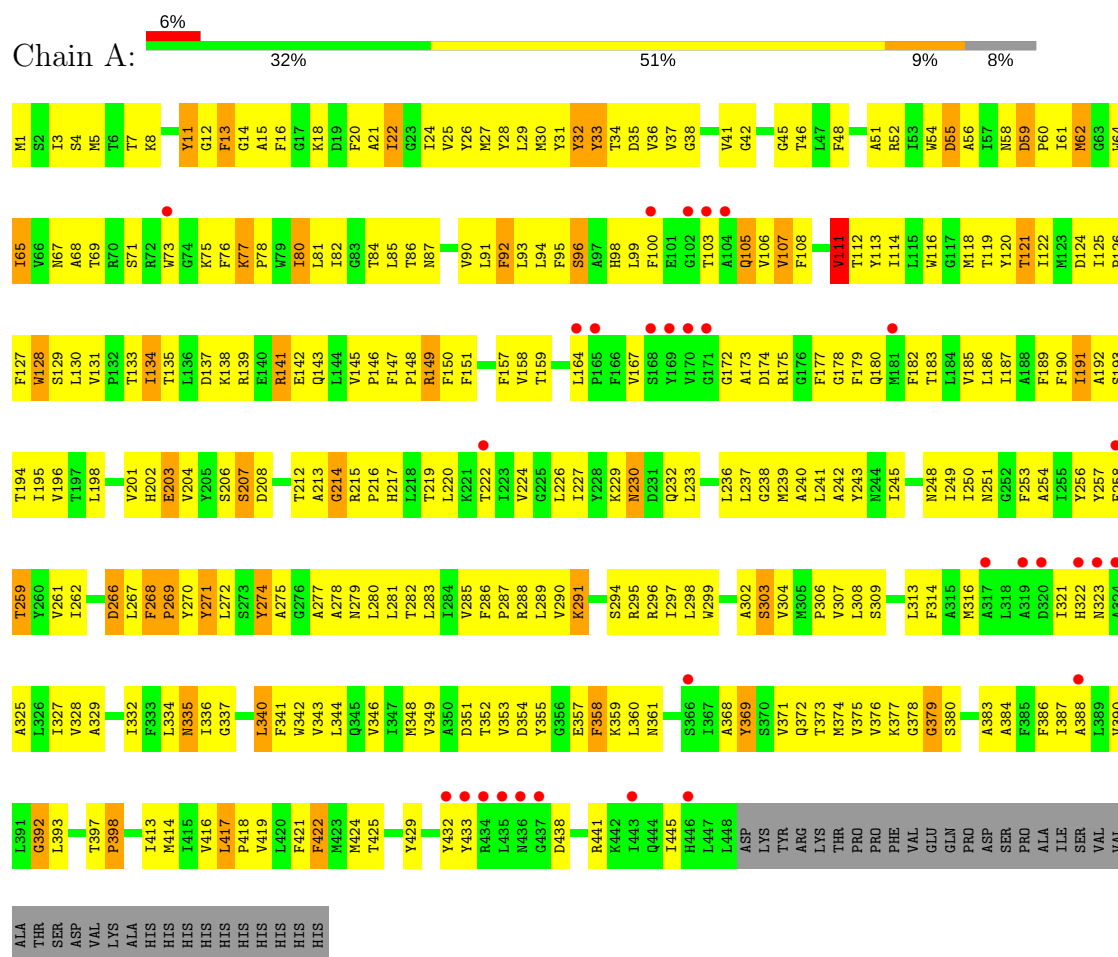
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Chain	Residue	Modelled	Actual	Comment	Reference
B	486	HIS	-	EXPRESSION TAG	UNP P30878
C	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
C	477	HIS	-	EXPRESSION TAG	UNP P30878
C	478	HIS	-	EXPRESSION TAG	UNP P30878
C	479	HIS	-	EXPRESSION TAG	UNP P30878
C	480	HIS	-	EXPRESSION TAG	UNP P30878
C	481	HIS	-	EXPRESSION TAG	UNP P30878
C	482	HIS	-	EXPRESSION TAG	UNP P30878
C	483	HIS	-	EXPRESSION TAG	UNP P30878
C	484	HIS	-	EXPRESSION TAG	UNP P30878
C	485	HIS	-	EXPRESSION TAG	UNP P30878
C	486	HIS	-	EXPRESSION TAG	UNP P30878
D	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
D	477	HIS	-	EXPRESSION TAG	UNP P30878
D	478	HIS	-	EXPRESSION TAG	UNP P30878
D	479	HIS	-	EXPRESSION TAG	UNP P30878
D	480	HIS	-	EXPRESSION TAG	UNP P30878
D	481	HIS	-	EXPRESSION TAG	UNP P30878
D	482	HIS	-	EXPRESSION TAG	UNP P30878
D	483	HIS	-	EXPRESSION TAG	UNP P30878
D	484	HIS	-	EXPRESSION TAG	UNP P30878
D	485	HIS	-	EXPRESSION TAG	UNP P30878
D	486	HIS	-	EXPRESSION TAG	UNP P30878

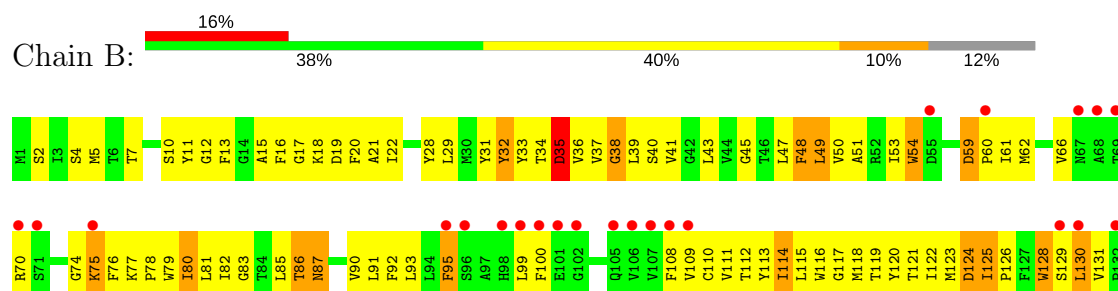
### 3 Residue-property plots

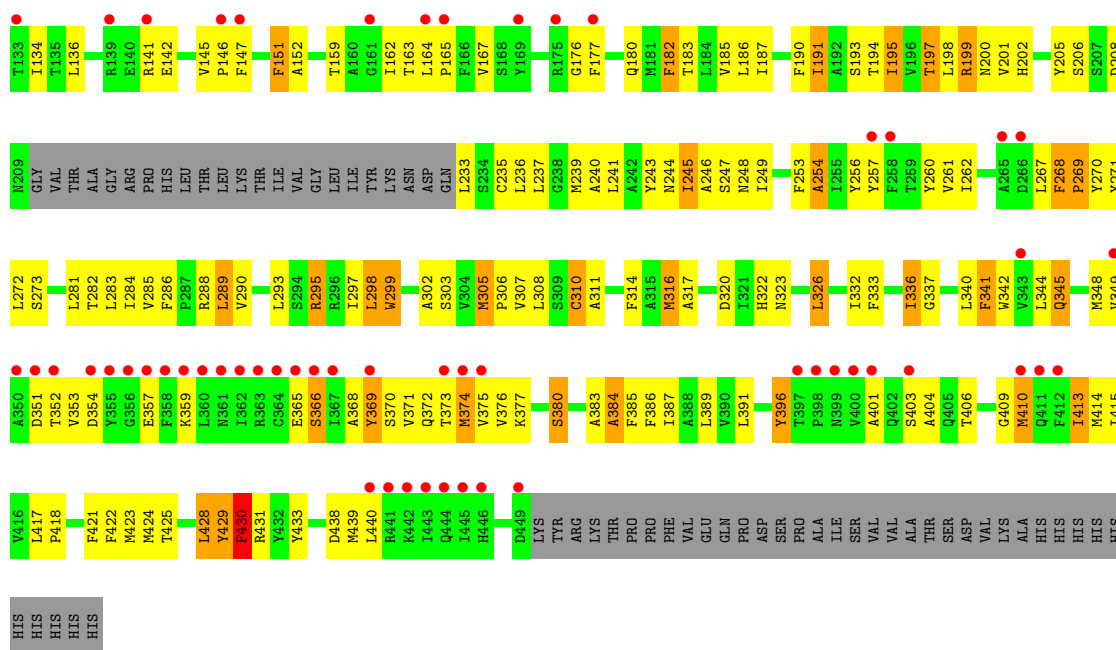
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Melibiose carrier protein

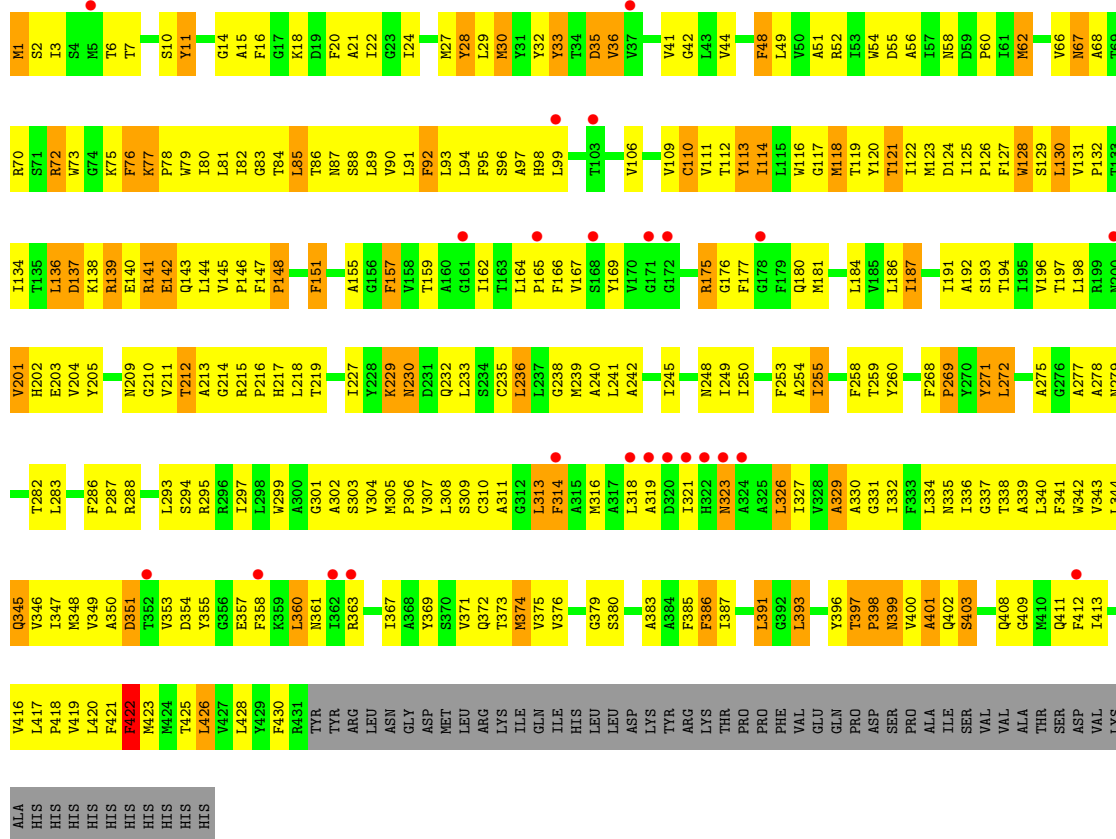


#### • Molecule 1: Melibiose carrier protein

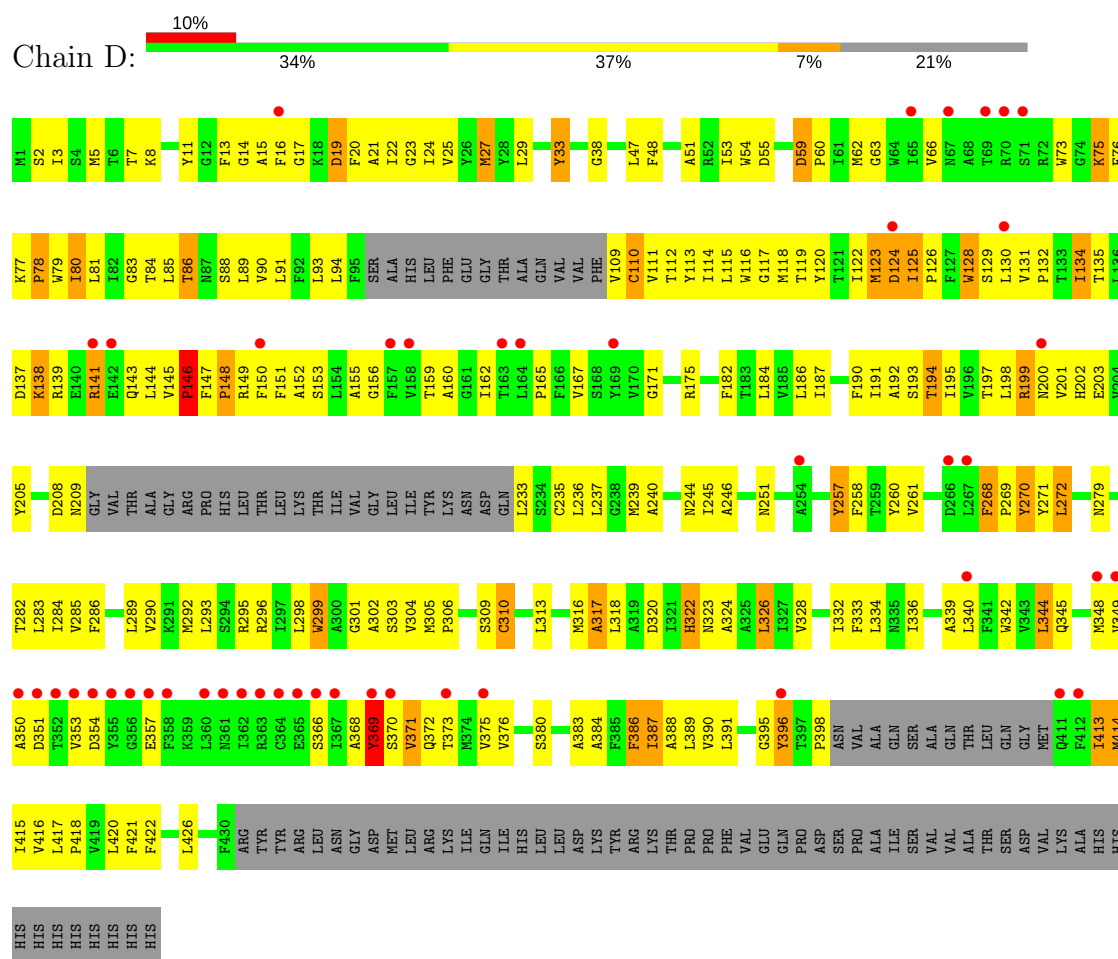




### • Molecule 1: Melibiose carrier protein



### • Molecule 1: Melibiose carrier protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.21Å 127.21Å 206.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.64 – 3.35 38.64 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.64-3.35) 99.5 (38.64-3.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	47.41 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.312 , 0.359 0.311 , 0.360	Depositor DCC
$R_{free}$ test set	2712 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 85.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.039 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.3433e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.63	0/3530	0.87	2/4813 (0.0%)
1	B	0.60	0/3342	0.82	3/4561 (0.1%)
1	C	0.66	0/3440	0.91	1/4689 (0.0%)
1	D	0.59	0/3004	0.81	1/4097 (0.0%)
All	All	0.62	0/13316	0.86	7/18160 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	C	0	4
1	D	0	1
All	All	0	10

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	55	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	55	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	308	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	340	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	B	298	LEU	CA-CB-CG	5.17	127.20	115.30
1	D	272	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ILE	Peptide
1	B	254	ALA	Peptide
1	B	38	GLY	Peptide
1	B	429	TYR	Peptide
1	B	74	GLY	Peptide
1	C	201	VAL	Peptide
1	C	329	ALA	Peptide
1	C	399	ASN	Peptide
1	C	68	ALA	Peptide
1	D	146	PRO	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3479	346	0
1	B	3258	0	3249	299	0
1	C	3352	0	3433	352	0
1	D	2930	0	2965	285	0
All	All	12982	0	13126	1273	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 49.

All (1273) 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:D:299:TRP:CB	1:D:344:LEU:HD13	1.63	1.26
1:D:86:THR:CG2	1:D:115:LEU:HG	1.65	1.26
1:C:75:LYS:HG3	1:C:205:TYR:CB	1.77	1.15
1:D:299:TRP:HB2	1:D:344:LEU:CD1	1.77	1.15
1:C:128:TRP:CH2	1:C:373:THR:HG21	1.83	1.13
1:A:3:ILE:HG23	1:A:203:GLU:HG3	1.28	1.11
1:B:93:LEU:HD13	1:B:112:THR:HG21	1.32	1.11
1:D:86:THR:HG21	1:D:115:LEU:HG	1.24	1.09
1:C:250:ILE:O	1:C:254:ALA:HB2	1.52	1.07
1:C:93:LEU:CD2	1:C:112:THR:HB	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HG23	1:A:191:ILE:HG13	1.36	1.06
1:B:352:THR:HA	1:B:433:TYR:OH	1.55	1.06
1:B:306:PRO:HG2	1:B:422:PHE:CD2	1.90	1.05
1:D:80:ILE:HG22	1:D:126:PRO:HB2	1.32	1.05
1:A:24:ILE:HD12	1:A:186:LEU:HD13	1.38	1.05
1:D:75:LYS:HE3	1:D:76:PHE:H	1.18	1.05
1:B:141:ARG:NH1	1:B:354:ASP:HB2	1.72	1.04
1:A:183:THR:HG22	1:A:187:ILE:HD12	1.36	1.04
1:C:175:ARG:HG3	1:C:175:ARG:HH11	1.22	1.03
1:D:353:VAL:HG12	1:D:357:GLU:CB	1.88	1.03
1:D:75:LYS:HG3	1:D:202:HIS:HA	1.38	1.02
1:A:417:LEU:HD23	1:A:418:PRO:HD3	1.37	1.01
1:D:75:LYS:HE3	1:D:76:PHE:N	1.76	1.01
1:D:302:ALA:HA	1:D:305:MET:SD	2.01	1.01
1:D:349:VAL:O	1:D:353:VAL:HG23	1.63	0.99
1:B:352:THR:HA	1:B:433:TYR:CZ	1.97	0.99
1:D:313:LEU:O	1:D:313:LEU:HD12	1.63	0.98
1:C:397:THR:OG1	1:C:398:PRO:HD2	1.61	0.98
1:B:306:PRO:HG2	1:B:422:PHE:CE2	1.99	0.97
1:C:282:THR:HG21	1:C:337:GLY:O	1.63	0.97
1:A:3:ILE:HG23	1:A:203:GLU:CG	1.94	0.97
1:D:79:TRP:CE3	1:D:126:PRO:HB3	1.98	0.97
1:D:137:ASP:O	1:D:138:LYS:HG3	1.61	0.97
1:A:58:ASN:CG	1:A:121:THR:HG21	1.83	0.97
1:D:141:ARG:HG2	1:D:141:ARG:O	1.63	0.97
1:C:142:GLU:O	1:C:146:PRO:HG3	1.65	0.96
1:B:141:ARG:HH12	1:B:354:ASP:HB2	1.27	0.96
1:C:106:VAL:O	1:C:110:CYS:HB2	1.65	0.96
1:B:77:LYS:HA	1:B:201:VAL:HG11	1.45	0.96
1:B:414:MET:O	1:B:418:PRO:HD2	1.67	0.95
1:D:299:TRP:O	1:D:303:SER:HB2	1.67	0.95
1:D:310:CYS:O	1:D:310:CYS:SG	2.25	0.94
1:C:128:TRP:CZ2	1:C:373:THR:HG21	2.02	0.94
1:A:105:GLN:HE21	1:A:105:GLN:N	1.65	0.94
1:D:296:ARG:HA	1:D:344:LEU:HD11	1.45	0.94
1:C:11:TYR:CE2	1:C:130:LEU:HB3	2.03	0.94
1:A:417:LEU:HD23	1:A:418:PRO:CD	1.98	0.93
1:A:283:LEU:O	1:A:287:PRO:HG2	1.69	0.93
1:C:139:ARG:HD2	1:C:139:ARG:N	1.82	0.93
1:C:82:ILE:O	1:C:86:THR:HG23	1.69	0.93
1:A:1:MET:SD	1:A:3:ILE:HB	2.08	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:VAL:HG11	1:B:295:ARG:HG2	1.50	0.93
1:A:3:ILE:CG2	1:A:203:GLU:HG3	1.98	0.92
1:A:7:THR:HG23	1:A:201:VAL:HG13	1.46	0.92
1:D:86:THR:HG22	1:D:90:VAL:CG2	1.99	0.91
1:B:47:LEU:O	1:B:50:VAL:HG12	1.70	0.91
1:C:139:ARG:HH22	1:C:358:PHE:HB2	1.35	0.91
1:C:24:ILE:HD12	1:C:186:LEU:HD13	1.49	0.91
1:B:302:ALA:HA	1:B:305:MET:SD	2.09	0.91
1:A:77:LYS:HG3	1:A:201:VAL:HB	1.53	0.91
1:B:320:ASP:HB2	1:B:323:ASN:CB	2.01	0.91
1:C:78:PRO:HA	1:C:81:LEU:HD23	1.52	0.91
1:C:387:ILE:HG23	1:C:417:LEU:HD11	1.54	0.90
1:C:75:LYS:HG2	1:C:76:PHE:H	1.37	0.90
1:B:112:THR:O	1:B:115:LEU:HB3	1.70	0.89
1:D:236:LEU:HD22	1:D:348:MET:HB3	1.51	0.89
1:C:7:THR:O	1:C:11:TYR:HB2	1.73	0.88
1:D:150:PHE:HD1	1:D:283:LEU:CD2	1.86	0.88
1:B:62:MET:CE	1:B:122:ILE:HD11	2.03	0.88
1:C:93:LEU:HD21	1:C:112:THR:HB	1.54	0.88
1:B:32:TYR:CD1	1:B:32:TYR:O	2.27	0.88
1:D:236:LEU:HD23	1:D:349:VAL:HG23	1.56	0.88
1:B:32:TYR:HD1	1:B:32:TYR:O	1.56	0.87
1:C:21:ALA:HA	1:C:186:LEU:HD11	1.56	0.87
1:A:241:LEU:HD23	1:A:379:GLY:HA3	1.55	0.87
1:D:86:THR:HG21	1:D:115:LEU:CG	2.04	0.87
1:B:352:THR:HA	1:B:433:TYR:CE2	2.10	0.86
1:D:86:THR:HG22	1:D:90:VAL:HG21	1.56	0.86
1:A:261:VAL:HG21	1:A:328:VAL:HG23	1.57	0.86
1:A:397:THR:CG2	1:A:398:PRO:HD2	2.06	0.86
1:C:215:ARG:N	1:C:216:PRO:HD2	1.91	0.86
1:D:414:MET:O	1:D:418:PRO:HD2	1.75	0.86
1:C:75:LYS:CG	1:C:205:TYR:CB	2.53	0.85
1:A:417:LEU:CD2	1:A:418:PRO:HD3	2.05	0.85
1:B:254:ALA:O	1:B:257:TYR:HB3	1.74	0.85
1:D:301:GLY:O	1:D:305:MET:HG3	1.77	0.85
1:C:287:PRO:HG3	1:C:340:LEU:HD22	1.59	0.85
1:A:250:ILE:O	1:A:254:ALA:HB2	1.77	0.85
1:B:32:TYR:CD1	1:B:176:GLY:HA2	2.12	0.85
1:A:87:ASN:HB2	1:A:119:THR:HG21	1.59	0.84
1:B:299:TRP:CE3	1:B:429:TYR:CE2	2.65	0.84
1:B:245:ILE:HG21	1:B:421:PHE:CD2	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:HD3	1:B:201:VAL:HB	1.60	0.84
1:A:344:LEU:O	1:A:348:MET:HG2	1.78	0.84
1:A:76:PHE:O	1:A:80:ILE:HG23	1.78	0.84
1:A:3:ILE:HG22	1:A:203:GLU:HB3	1.58	0.84
1:C:3:ILE:HG22	1:C:204:VAL:HG22	1.58	0.84
1:D:296:ARG:HG3	1:D:344:LEU:HD21	1.60	0.83
1:A:202:HIS:O	1:A:203:GLU:OE1	1.97	0.83
1:D:299:TRP:CB	1:D:344:LEU:CD1	2.45	0.83
1:D:244:ASN:CB	1:D:376:VAL:HG11	2.08	0.83
1:C:240:ALA:HB3	1:C:376:VAL:HG21	1.58	0.83
1:C:387:ILE:HG23	1:C:417:LEU:CD1	2.08	0.83
1:A:58:ASN:ND2	1:A:121:THR:HG21	1.93	0.82
1:A:325:ALA:O	1:A:328:VAL:HG12	1.80	0.82
1:C:175:ARG:HD2	1:C:175:ARG:O	1.80	0.82
1:C:239:MET:HG2	1:C:425:THR:HA	1.62	0.82
1:A:86:THR:HG22	1:A:119:THR:OG1	1.80	0.81
1:A:167:VAL:HG23	1:A:182:PHE:CE2	2.14	0.81
1:B:307:VAL:O	1:B:311:ALA:HB2	1.80	0.81
1:A:189:PHE:O	1:A:192:ALA:HB3	1.80	0.81
1:C:15:ALA:HB2	1:C:127:PHE:CE2	2.15	0.81
1:C:140:GLU:HG2	1:C:143:GLN:HB2	1.60	0.81
1:C:212:THR:O	1:C:213:ALA:C	2.18	0.81
1:B:35:ASP:HA	1:B:38:GLY:HA2	1.63	0.80
1:B:39:LEU:HD22	1:B:41:VAL:HG23	1.63	0.80
1:C:387:ILE:CG2	1:C:417:LEU:HD21	2.12	0.80
1:D:125:ILE:HG23	1:D:369:TYR:CD1	2.16	0.80
1:B:87:ASN:HB2	1:B:119:THR:HG21	1.63	0.80
1:D:386:PHE:O	1:D:390:VAL:HG22	1.82	0.80
1:C:387:ILE:O	1:C:391:LEU:HD23	1.81	0.79
1:D:244:ASN:HB3	1:D:376:VAL:HG11	1.64	0.79
1:D:384:ALA:O	1:D:387:ILE:HG13	1.82	0.79
1:C:240:ALA:CB	1:C:376:VAL:HG21	2.12	0.79
1:C:144:LEU:O	1:C:148:PRO:HD2	1.82	0.79
1:C:85:LEU:HD11	1:C:194:THR:OG1	1.82	0.79
1:D:129:SER:HB3	1:D:369:TYR:OH	1.83	0.79
1:A:15:ALA:HB2	1:A:127:PHE:CZ	2.16	0.78
1:C:139:ARG:NH2	1:C:358:PHE:HB2	1.97	0.78
1:C:283:LEU:O	1:C:287:PRO:CD	2.32	0.78
1:D:299:TRP:HB2	1:D:344:LEU:HD13	0.82	0.78
1:C:307:VAL:O	1:C:310:CYS:HB3	1.83	0.78
1:C:77:LYS:HA	1:C:80:ILE:HG12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ASP:HB2	1:B:323:ASN:HB2	1.66	0.78
1:A:78:PRO:HA	1:A:81:LEU:HB3	1.66	0.78
1:C:93:LEU:CD2	1:C:112:THR:CB	2.62	0.78
1:D:150:PHE:CD1	1:D:283:LEU:HD23	2.18	0.78
1:C:139:ARG:CD	1:C:139:ARG:N	2.46	0.77
1:C:250:ILE:O	1:C:254:ALA:CB	2.30	0.77
1:A:8:LYS:HA	1:A:11:TYR:HB2	1.65	0.77
1:D:3:ILE:O	1:D:7:THR:HG23	1.84	0.77
1:A:141:ARG:HG3	1:A:142:GLU:N	1.98	0.77
1:D:25:VAL:O	1:D:29:LEU:HG	1.85	0.77
1:A:270:TYR:O	1:A:274:TYR:HB2	1.83	0.77
1:A:15:ALA:HB2	1:A:127:PHE:HZ	1.49	0.76
1:C:236:LEU:HD13	1:C:349:VAL:HA	1.65	0.76
1:A:257:TYR:O	1:A:261:VAL:HG12	1.85	0.76
1:B:320:ASP:HB2	1:B:323:ASN:HB3	1.65	0.76
1:A:183:THR:HG22	1:A:187:ILE:CD1	2.15	0.76
1:C:142:GLU:O	1:C:146:PRO:CG	2.33	0.76
1:A:128:TRP:CD1	1:A:369:TYR:HE1	2.02	0.76
1:B:122:ILE:O	1:B:126:PRO:HD2	1.86	0.76
1:D:150:PHE:HD1	1:D:283:LEU:HD23	1.47	0.76
1:A:90:VAL:HG21	1:A:116:TRP:HB2	1.69	0.75
1:B:75:LYS:O	1:B:78:PRO:HD2	1.87	0.75
1:B:163:THR:HG22	1:B:182:PHE:CZ	2.22	0.75
1:B:299:TRP:CD1	1:B:344:LEU:HB2	2.22	0.75
1:C:387:ILE:HG21	1:C:417:LEU:HD21	1.68	0.75
1:C:387:ILE:HD12	1:C:417:LEU:HD21	1.68	0.74
1:C:78:PRO:HA	1:C:81:LEU:CD2	2.15	0.74
1:C:88:SER:O	1:C:92:PHE:HB2	1.86	0.74
1:C:75:LYS:HD2	1:C:202:HIS:O	1.88	0.74
1:D:245:ILE:HG12	1:D:376:VAL:HG23	1.68	0.74
1:D:129:SER:CB	1:D:369:TYR:OH	2.35	0.74
1:C:58:ASN:CG	1:C:121:THR:HG21	2.08	0.74
1:A:149:ARG:CB	1:A:283:LEU:HD21	2.18	0.74
1:C:374:MET:HE1	1:C:375:VAL:HG12	1.69	0.74
1:C:397:THR:OG1	1:C:398:PRO:CD	2.35	0.73
1:C:95:PHE:O	1:C:180:GLN:HG2	1.87	0.73
1:D:125:ILE:HG23	1:D:369:TYR:CE1	2.22	0.73
1:A:7:THR:O	1:A:11:TYR:HB2	1.88	0.73
1:B:39:LEU:HD23	1:B:39:LEU:O	1.87	0.73
1:C:282:THR:HG23	1:C:286:PHE:CD1	2.22	0.73
1:C:33:TYR:O	1:C:33:TYR:CD1	2.42	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLN:HA	1:C:295:ARG:HH21	1.54	0.73
1:A:92:PHE:CD1	1:A:187:ILE:HD13	2.23	0.73
1:C:283:LEU:O	1:C:287:PRO:HD2	1.88	0.73
1:B:417:LEU:O	1:B:421:PHE:N	2.21	0.72
1:C:56:ALA:O	1:C:374:MET:HE3	1.89	0.72
1:C:44:VAL:O	1:C:48:PHE:N	2.22	0.72
1:D:246:ALA:HB1	1:D:422:PHE:CE1	2.24	0.72
1:A:28:TYR:CZ	1:A:179:PHE:HB2	2.25	0.72
1:A:268:PHE:N	1:A:269:PRO:HD3	2.05	0.72
1:A:80:ILE:HG22	1:A:126:PRO:HB3	1.71	0.72
1:D:75:LYS:O	1:D:78:PRO:HD2	1.90	0.72
1:C:211:VAL:HG12	1:C:212:THR:H	1.53	0.72
1:A:286:PHE:HA	1:A:289:LEU:HD12	1.70	0.72
1:B:299:TRP:CE3	1:B:429:TYR:CD2	2.78	0.72
1:C:3:ILE:HG22	1:C:204:VAL:CG2	2.19	0.72
1:D:244:ASN:HD22	1:D:376:VAL:HG11	1.54	0.72
1:D:86:THR:CG2	1:D:115:LEU:CG	2.57	0.71
1:A:3:ILE:CG2	1:A:203:GLU:CG	2.63	0.71
1:B:244:ASN:ND2	1:B:376:VAL:HG11	2.04	0.71
1:A:215:ARG:N	1:A:216:PRO:HD2	2.04	0.71
1:C:316:MET:O	1:C:319:ALA:HB3	1.89	0.71
1:B:77:LYS:HB2	1:B:201:VAL:HG12	1.71	0.71
1:C:308:LEU:O	1:C:309:SER:C	2.29	0.71
1:D:138:LYS:HD2	1:D:138:LYS:O	1.91	0.71
1:D:380:SER:HA	1:D:383:ALA:HB3	1.72	0.71
1:B:10:SER:O	1:B:13:PHE:HB2	1.91	0.71
1:C:145:VAL:N	1:C:146:PRO:HD2	2.06	0.71
1:D:86:THR:HG22	1:D:90:VAL:HG23	1.71	0.71
1:B:77:LYS:HA	1:B:201:VAL:CG1	2.21	0.71
1:B:298:LEU:HD12	1:B:340:LEU:HD22	1.73	0.71
1:D:353:VAL:CG1	1:D:357:GLU:CB	2.68	0.71
1:A:249:ILE:O	1:A:253:PHE:HB2	1.91	0.70
1:A:282:THR:HG23	1:A:286:PHE:CD1	2.26	0.70
1:A:397:THR:HG23	1:A:398:PRO:HD2	1.72	0.70
1:B:320:ASP:CB	1:B:323:ASN:HB2	2.20	0.70
1:D:271:TYR:CD1	1:D:332:ILE:HD11	2.24	0.70
1:C:391:LEU:HD13	1:C:413:ILE:HD13	1.73	0.70
1:C:30:MET:O	1:C:33:TYR:HB3	1.92	0.70
1:C:128:TRP:CE2	1:C:346:VAL:HG11	2.26	0.70
1:B:142:GLU:HA	1:B:145:VAL:HG23	1.74	0.70
1:D:125:ILE:CG2	1:D:369:TYR:CE1	2.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:O	1:A:65:ILE:HG12	1.92	0.70
1:C:143:GLN:O	1:C:147:PHE:CD1	2.44	0.70
1:B:131:VAL:O	1:B:134:ILE:HG12	1.92	0.69
1:B:77:LYS:HB2	1:B:201:VAL:CG1	2.21	0.69
1:A:397:THR:HG22	1:A:398:PRO:HD2	1.74	0.69
1:B:141:ARG:NH1	1:B:354:ASP:CB	2.52	0.69
1:C:334:LEU:HD23	1:C:334:LEU:O	1.92	0.69
1:D:153:SER:CB	1:D:283:LEU:HD22	2.22	0.69
1:A:77:LYS:HG3	1:A:201:VAL:CB	2.20	0.69
1:C:301:GLY:O	1:C:305:MET:N	2.25	0.69
1:A:187:ILE:HG23	1:A:191:ILE:CG1	2.19	0.69
1:D:246:ALA:HB1	1:D:422:PHE:CZ	2.27	0.69
1:A:67:ASN:HB3	1:A:217:HIS:CD2	2.28	0.69
1:C:175:ARG:O	1:C:177:PHE:N	2.25	0.69
1:C:128:TRP:CE3	1:C:346:VAL:HG21	2.27	0.69
1:D:391:LEU:HD22	1:D:413:ILE:HD12	1.75	0.69
1:B:51:ALA:HA	1:B:54:TRP:CE3	2.27	0.69
1:A:243:TYR:CE1	1:A:341:PHE:HD2	2.11	0.68
1:C:240:ALA:HB3	1:C:376:VAL:CG2	2.23	0.68
1:C:162:ILE:C	1:C:165:PRO:HD2	2.13	0.68
1:C:77:LYS:HB2	1:C:201:VAL:HG21	1.76	0.68
1:D:380:SER:O	1:D:384:ALA:N	2.26	0.68
1:D:77:LYS:O	1:D:81:LEU:CB	2.42	0.68
1:B:376:VAL:HG23	1:B:377:LYS:HG3	1.75	0.68
1:A:283:LEU:O	1:A:287:PRO:CG	2.41	0.68
1:C:241:LEU:HD23	1:C:376:VAL:O	1.94	0.68
1:C:90:VAL:HG11	1:C:116:TRP:N	2.09	0.68
1:A:346:VAL:HG12	1:A:369:TYR:CE1	2.29	0.68
1:B:122:ILE:HG23	1:B:126:PRO:HG2	1.74	0.68
1:C:27:MET:SD	1:C:159:THR:HG22	2.34	0.68
1:D:147:PHE:HD1	1:D:150:PHE:HD2	1.42	0.68
1:A:95:PHE:O	1:A:180:GLN:CG	2.42	0.68
1:B:320:ASP:CB	1:B:323:ASN:CB	2.72	0.68
1:B:62:MET:HE1	1:B:122:ILE:HD11	1.72	0.68
1:C:93:LEU:HD23	1:C:112:THR:CB	2.23	0.68
1:D:75:LYS:HD2	1:D:201:VAL:HG12	1.75	0.68
1:A:124:ASP:O	1:A:128:TRP:NE1	2.27	0.68
1:A:51:ALA:HA	1:A:54:TRP:CG	2.29	0.68
1:D:83:GLY:HA3	1:D:122:ILE:HD11	1.74	0.68
1:D:147:PHE:CD1	1:D:150:PHE:HD2	2.12	0.68
1:A:21:ALA:HA	1:A:186:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:HA	1:A:122:ILE:HG22	1.74	0.67
1:B:295:ARG:HB3	1:B:344:LEU:HD11	1.76	0.67
1:B:414:MET:O	1:B:417:LEU:HB2	1.94	0.67
1:D:415:ILE:O	1:D:418:PRO:HG2	1.94	0.67
1:D:75:LYS:CE	1:D:76:PHE:H	2.02	0.67
1:B:77:LYS:CA	1:B:201:VAL:HG11	2.21	0.67
1:B:99:LEU:HD11	1:B:177:PHE:HB2	1.76	0.67
1:C:347:ILE:HA	1:C:369:TYR:OH	1.94	0.67
1:A:92:PHE:CE1	1:A:187:ILE:HD13	2.29	0.67
1:A:32:TYR:O	1:A:36:VAL:HG23	1.93	0.67
1:D:296:ARG:CG	1:D:344:LEU:HD21	2.24	0.67
1:C:347:ILE:HD13	1:C:369:TYR:OH	1.94	0.67
1:A:28:TYR:CE1	1:A:179:PHE:HB2	2.30	0.67
1:C:32:TYR:HA	1:C:35:ASP:HB2	1.75	0.67
1:C:346:VAL:HG12	1:C:369:TYR:CD2	2.30	0.67
1:C:72:ARG:HD3	1:D:109:VAL:HG13	1.74	0.67
1:B:244:ASN:HB3	1:B:376:VAL:HB	1.76	0.67
1:A:192:ALA:HA	1:A:195:ILE:HG22	1.77	0.67
1:B:244:ASN:HD22	1:B:376:VAL:CB	2.07	0.67
1:D:77:LYS:HD3	1:D:77:LYS:O	1.95	0.67
1:A:149:ARG:HB3	1:A:283:LEU:HD21	1.77	0.67
1:B:352:THR:CA	1:B:433:TYR:OH	2.39	0.67
1:C:128:TRP:CZ3	1:C:346:VAL:HG21	2.30	0.67
1:D:77:LYS:O	1:D:81:LEU:HB3	1.95	0.67
1:B:86:THR:HG21	1:B:115:LEU:HD11	1.77	0.67
1:D:122:ILE:O	1:D:126:PRO:HD2	1.95	0.67
1:A:278:ALA:HB1	1:A:336:ILE:HG22	1.77	0.66
1:D:244:ASN:HD22	1:D:376:VAL:CG1	2.07	0.66
1:D:391:LEU:HB2	1:D:413:ILE:HG13	1.78	0.66
1:C:80:ILE:O	1:C:84:THR:HG23	1.95	0.66
1:B:417:LEU:O	1:B:421:PHE:HB2	1.95	0.66
1:D:236:LEU:CD2	1:D:348:MET:HB3	2.22	0.66
1:B:353:VAL:HG21	1:B:366:SER:HB3	1.77	0.66
1:C:211:VAL:HG12	1:C:212:THR:N	2.10	0.66
1:C:215:ARG:N	1:C:216:PRO:CD	2.59	0.66
1:D:86:THR:CG2	1:D:90:VAL:CG2	2.72	0.66
1:B:125:ILE:HD11	1:B:369:TYR:CG	2.31	0.66
1:D:75:LYS:CD	1:D:201:VAL:HG12	2.26	0.66
1:A:321:ILE:H	1:A:321:ILE:HD12	1.60	0.65
1:C:175:ARG:CG	1:C:175:ARG:HH11	2.05	0.65
1:C:76:PHE:O	1:C:79:TRP:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PHE:O	1:A:180:GLN:HB3	1.96	0.65
1:B:4:SER:HB2	1:B:134:ILE:HG21	1.79	0.65
1:D:296:ARG:O	1:D:299:TRP:HB3	1.96	0.65
1:B:77:LYS:O	1:B:81:LEU:HB3	1.97	0.65
1:C:282:THR:HB	1:C:336:ILE:O	1.96	0.65
1:C:342:TRP:O	1:C:346:VAL:HG23	1.97	0.65
1:C:176:GLY:O	1:C:180:GLN:N	2.30	0.65
1:C:85:LEU:CD1	1:C:194:THR:OG1	2.45	0.65
1:D:413:ILE:O	1:D:416:VAL:HG12	1.97	0.65
1:B:85:LEU:HD11	1:B:194:THR:HG21	1.79	0.65
1:A:374:MET:SD	1:A:375:VAL:HG23	2.36	0.64
1:B:125:ILE:HG22	1:B:126:PRO:HD3	1.79	0.64
1:D:292:MET:O	1:D:293:LEU:HG	1.97	0.64
1:B:268:PHE:N	1:B:269:PRO:CD	2.60	0.64
1:B:316:MET:O	1:B:316:MET:HE3	1.96	0.64
1:B:114:ILE:O	1:B:118:MET:N	2.30	0.64
1:B:187:ILE:O	1:B:191:ILE:N	2.30	0.64
1:D:244:ASN:HB3	1:D:376:VAL:CG1	2.26	0.64
1:D:240:ALA:HA	1:D:345:GLN:OE1	1.98	0.64
1:A:93:LEU:HD13	1:A:112:THR:HB	1.79	0.64
1:B:19:ASP:HA	1:B:22:ILE:HG22	1.80	0.64
1:D:306:PRO:HG2	1:D:422:PHE:CD2	2.32	0.64
1:A:127:PHE:C	1:A:127:PHE:CD1	2.70	0.64
1:B:374:MET:H	1:B:374:MET:HE2	1.63	0.64
1:B:241:LEU:HD22	1:B:375:VAL:HG21	1.79	0.64
1:C:116:TRP:O	1:C:117:GLY:C	2.32	0.64
1:C:75:LYS:HB2	1:C:205:TYR:CB	2.28	0.64
1:C:91:LEU:HD13	1:C:116:TRP:HZ3	1.63	0.64
1:D:366:SER:HB2	1:D:369:TYR:CD2	2.33	0.64
1:C:371:VAL:O	1:C:375:VAL:HG22	1.98	0.64
1:D:351:ASP:HA	1:D:354:ASP:HB2	1.80	0.64
1:D:75:LYS:HE3	1:D:76:PHE:HB2	1.80	0.64
1:A:78:PRO:O	1:A:82:ILE:HG12	1.97	0.64
1:C:229:LYS:HG2	1:C:233:LEU:HB2	1.80	0.64
1:C:299:TRP:O	1:C:302:ALA:HB3	1.97	0.64
1:C:96:SER:OG	1:D:198:LEU:HD13	1.98	0.64
1:B:383:ALA:O	1:B:386:PHE:N	2.30	0.64
1:C:304:VAL:O	1:C:307:VAL:HB	1.96	0.64
1:C:387:ILE:HD12	1:C:417:LEU:CD2	2.28	0.64
1:C:82:ILE:O	1:C:86:THR:CG2	2.46	0.64
1:D:7:THR:HG22	1:D:200:ASN:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ALA:HB1	1:B:87:ASN:HD21	1.63	0.63
1:A:98:HIS:CD2	1:A:99:LEU:HB2	2.33	0.63
1:C:242:ALA:HA	1:C:245:ILE:HG12	1.79	0.63
1:A:58:ASN:CG	1:A:121:THR:CG2	2.63	0.63
1:B:391:LEU:HA	1:B:413:ILE:HG21	1.81	0.63
1:C:142:GLU:O	1:C:295:ARG:CZ	2.46	0.63
1:C:14:GLY:O	1:C:18:LYS:N	2.24	0.63
1:D:83:GLY:HA3	1:D:122:ILE:CD1	2.27	0.63
1:D:167:VAL:O	1:D:171:GLY:N	2.31	0.63
1:D:59:ASP:CG	1:D:60:PRO:HD3	2.19	0.63
1:A:236:LEU:HD11	1:A:348:MET:HB3	1.80	0.63
1:A:245:ILE:CG2	1:A:417:LEU:HD21	2.28	0.63
1:A:438:ASP:O	1:A:441:ARG:N	2.31	0.63
1:A:91:LEU:HG	1:A:183:THR:HG23	1.79	0.63
1:B:306:PRO:CG	1:B:422:PHE:CE2	2.77	0.63
1:C:109:VAL:O	1:C:113:TYR:HB2	1.98	0.63
1:D:86:THR:HG23	1:D:115:LEU:HG	1.71	0.63
1:D:366:SER:HB2	1:D:369:TYR:HD2	1.64	0.63
1:B:124:ASP:HB2	1:B:373:THR:HG23	1.81	0.63
1:D:313:LEU:CD1	1:D:313:LEU:O	2.44	0.63
1:C:87:ASN:O	1:C:90:VAL:HG22	1.99	0.63
1:D:282:THR:HA	1:D:285:VAL:HG22	1.80	0.63
1:B:32:TYR:CE1	1:B:176:GLY:HA2	2.34	0.63
1:C:33:TYR:C	1:C:33:TYR:CD1	2.72	0.63
1:C:128:TRP:CD2	1:C:346:VAL:HG11	2.33	0.63
1:D:353:VAL:O	1:D:357:GLU:N	2.29	0.63
1:D:77:LYS:N	1:D:78:PRO:CD	2.62	0.63
1:A:212:THR:O	1:A:212:THR:HG22	1.98	0.63
1:A:250:ILE:O	1:A:254:ALA:CB	2.46	0.63
1:C:128:TRP:CH2	1:C:373:THR:CG2	2.74	0.63
1:D:115:LEU:O	1:D:118:MET:HB3	1.97	0.62
1:B:16:PHE:HB2	1:B:151:PHE:CD2	2.34	0.62
1:C:93:LEU:HD23	1:C:112:THR:OG1	1.99	0.62
1:D:391:LEU:HB2	1:D:413:ILE:CD1	2.29	0.62
1:C:308:LEU:HD23	1:C:334:LEU:HD11	1.82	0.62
1:C:387:ILE:CG2	1:C:417:LEU:CD2	2.77	0.62
1:C:91:LEU:HD13	1:C:116:TRP:CZ3	2.34	0.62
1:C:77:LYS:HE2	1:C:197:THR:O	1.99	0.62
1:C:346:VAL:HG12	1:C:369:TYR:CE2	2.33	0.62
1:A:243:TYR:CZ	1:A:341:PHE:HD2	2.17	0.62
1:D:15:ALA:HB1	1:D:152:ALA:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:MET:HB2	1:D:306:PRO:HD3	1.81	0.62
1:D:340:LEU:HG	1:D:340:LEU:O	2.00	0.62
1:A:342:TRP:O	1:A:346:VAL:HG23	1.98	0.62
1:D:59:ASP:OD1	1:D:59:ASP:N	2.33	0.62
1:D:20:PHE:CD2	1:D:186:LEU:HA	2.35	0.62
1:B:268:PHE:N	1:B:269:PRO:HD2	2.15	0.61
1:C:143:GLN:O	1:C:147:PHE:CE1	2.53	0.61
1:C:51:ALA:O	1:C:54:TRP:HB2	2.00	0.61
1:D:20:PHE:HD2	1:D:186:LEU:HA	1.65	0.61
1:A:18:LYS:NZ	1:A:127:PHE:HB2	2.14	0.61
1:B:86:THR:HG21	1:B:115:LEU:CD1	2.30	0.61
1:D:5:MET:SD	1:D:144:LEU:HD22	2.40	0.61
1:A:349:VAL:HG21	1:A:372:GLN:CB	2.30	0.61
1:B:374:MET:H	1:B:374:MET:CE	2.12	0.61
1:C:164:LEU:O	1:C:167:VAL:HG12	1.99	0.61
1:D:47:LEU:HD13	1:D:113:TYR:OH	2.00	0.61
1:D:156:GLY:O	1:D:160:ALA:CB	2.48	0.61
1:D:194:THR:O	1:D:198:LEU:HG	1.99	0.61
1:B:117:GLY:O	1:B:120:TYR:N	2.31	0.61
1:B:142:GLU:HA	1:B:145:VAL:CG2	2.31	0.61
1:D:86:THR:HG21	1:D:115:LEU:CD1	2.30	0.61
1:D:76:PHE:O	1:D:80:ILE:HG23	2.00	0.61
1:A:236:LEU:HD23	1:A:236:LEU:O	2.01	0.61
1:A:8:LYS:HD2	1:A:134:ILE:HD13	1.82	0.61
1:B:112:THR:O	1:B:115:LEU:CB	2.48	0.61
1:C:340:LEU:O	1:C:340:LEU:HG	2.01	0.61
1:B:51:ALA:HA	1:B:54:TRP:CD2	2.35	0.61
1:C:87:ASN:ND2	1:C:119:THR:HG21	2.15	0.61
1:A:58:ASN:ND2	1:A:121:THR:CG2	2.62	0.61
1:B:380:SER:O	1:B:383:ALA:HB3	2.01	0.61
1:C:56:ALA:O	1:C:60:PRO:HD2	2.01	0.61
1:A:240:ALA:HB1	1:A:376:VAL:HG11	1.82	0.61
1:B:417:LEU:O	1:B:421:PHE:CB	2.49	0.61
1:C:14:GLY:O	1:C:18:LYS:HG3	2.01	0.61
1:C:353:VAL:O	1:C:357:GLU:N	2.32	0.61
1:A:73:TRP:CZ2	1:B:109:VAL:HB	2.34	0.60
1:B:21:ALA:HB1	1:B:87:ASN:ND2	2.16	0.60
1:C:216:PRO:HA	1:C:219:THR:HG1	1.66	0.60
1:A:91:LEU:HD13	1:A:116:TRP:HZ3	1.65	0.60
1:D:80:ILE:HG13	1:D:81:LEU:N	2.14	0.60
1:A:5:MET:CG	1:A:135:THR:HG23	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:THR:CG2	1:D:90:VAL:HG23	2.32	0.60
1:B:351:ASP:C	1:B:433:TYR:HE2	2.04	0.60
1:B:115:LEU:HA	1:B:118:MET:HB2	1.82	0.60
1:B:239:MET:HE1	1:B:429:TYR:HB2	1.82	0.60
1:B:80:ILE:HG13	1:B:81:LEU:N	2.16	0.60
1:A:105:GLN:HE21	1:A:105:GLN:CA	2.15	0.60
1:A:219:THR:CG2	1:A:360:LEU:HD11	2.32	0.60
1:B:78:PRO:O	1:B:82:ILE:HG12	2.01	0.60
1:D:14:GLY:HA2	1:D:193:SER:OG	2.00	0.60
1:A:24:ILE:CD1	1:A:186:LEU:HD13	2.24	0.60
1:B:373:THR:N	1:B:374:MET:HE2	2.17	0.60
1:C:175:ARG:HG3	1:C:175:ARG:NH1	2.01	0.60
1:C:323:ASN:O	1:C:323:ASN:ND2	2.32	0.60
1:C:380:SER:O	1:C:383:ALA:HB3	2.02	0.60
1:D:156:GLY:O	1:D:160:ALA:HB2	2.02	0.60
1:B:117:GLY:O	1:B:118:MET:C	2.40	0.59
1:B:163:THR:CG2	1:B:182:PHE:CZ	2.85	0.59
1:B:246:ALA:HB1	1:B:422:PHE:CE1	2.37	0.59
1:B:387:ILE:HG21	1:B:414:MET:SD	2.42	0.59
1:B:244:ASN:HD22	1:B:376:VAL:CG1	2.15	0.59
1:C:321:ILE:HB	1:C:326:LEU:HD13	1.84	0.59
1:C:51:ALA:HA	1:C:54:TRP:CG	2.36	0.59
1:D:62:MET:SD	1:D:122:ILE:HG22	2.42	0.59
1:A:138:LYS:HG3	1:A:139:ARG:HG2	1.84	0.59
1:A:77:LYS:CG	1:A:201:VAL:HB	2.31	0.59
1:C:3:ILE:CG2	1:C:204:VAL:HG22	2.32	0.59
1:B:244:ASN:HD22	1:B:376:VAL:HB	1.68	0.59
1:C:143:GLN:HA	1:C:295:ARG:NH2	2.18	0.59
1:B:110:CYS:O	1:B:114:ILE:HG13	2.02	0.59
1:B:285:VAL:O	1:B:288:ARG:HB2	2.02	0.59
1:D:290:VAL:CG1	1:D:298:LEU:HD22	2.32	0.59
1:B:342:TRP:HA	1:B:345:GLN:HG3	1.85	0.59
1:C:343:VAL:O	1:C:347:ILE:HG12	2.03	0.59
1:D:299:TRP:HB3	1:D:344:LEU:CD1	2.31	0.59
1:D:391:LEU:HB2	1:D:413:ILE:CG1	2.33	0.59
1:A:233:LEU:O	1:A:237:LEU:HG	2.02	0.59
1:C:391:LEU:HD13	1:C:413:ILE:HG21	1.83	0.59
1:D:77:LYS:HB3	1:D:78:PRO:HD3	1.85	0.59
1:B:340:LEU:O	1:B:340:LEU:HD23	2.03	0.59
1:B:141:ARG:NH1	1:B:351:ASP:HA	2.17	0.59
1:A:384:ALA:O	1:A:387:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:SER:O	1:C:92:PHE:CB	2.50	0.58
1:A:232:GLN:HB2	1:A:352:THR:CG2	2.33	0.58
1:C:91:LEU:HD12	1:C:94:LEU:HD23	1.85	0.58
1:D:75:LYS:HE3	1:D:76:PHE:CB	2.34	0.58
1:A:95:PHE:O	1:A:180:GLN:HG3	2.02	0.58
1:B:195:ILE:HA	1:B:198:LEU:HD12	1.85	0.58
1:C:387:ILE:HG21	1:C:417:LEU:CD2	2.32	0.58
1:D:33:TYR:HD1	1:D:33:TYR:O	1.87	0.58
1:A:195:ILE:HG23	1:A:196:VAL:N	2.19	0.58
1:B:34:THR:CG2	1:B:43:LEU:HG	2.33	0.58
1:C:75:LYS:CB	1:C:205:TYR:CB	2.81	0.58
1:B:77:LYS:CA	1:B:201:VAL:CG1	2.81	0.58
1:D:150:PHE:CD1	1:D:283:LEU:CD2	2.75	0.58
1:A:212:THR:O	1:A:213:ALA:HB3	2.04	0.58
1:D:86:THR:CG2	1:D:90:VAL:HG21	2.31	0.58
1:D:162:ILE:HG13	1:D:165:PRO:HG2	1.85	0.57
1:C:62:MET:HE3	1:C:122:ILE:HD12	1.85	0.57
1:D:236:LEU:HD21	1:D:345:GLN:O	2.04	0.57
1:A:239:MET:HB2	1:A:425:THR:HA	1.87	0.57
1:C:129:SER:C	1:C:132:PRO:HD2	2.25	0.57
1:C:140:GLU:HG2	1:C:143:GLN:CB	2.34	0.57
1:D:290:VAL:HG21	1:D:295:ARG:CZ	2.34	0.57
1:D:244:ASN:ND2	1:D:376:VAL:HG11	2.17	0.57
1:A:118:MET:O	1:A:121:THR:HG23	2.04	0.57
1:B:187:ILE:O	1:B:191:ILE:HB	2.03	0.57
1:B:17:GLY:HA3	1:B:190:PHE:HD1	1.69	0.57
1:C:242:ALA:HB1	1:C:422:PHE:HA	1.85	0.57
1:A:313:LEU:HA	1:A:316:MET:HG2	1.87	0.57
1:B:272:LEU:HA	1:B:332:ILE:HD13	1.86	0.57
1:C:75:LYS:HG2	1:C:76:PHE:N	2.13	0.57
1:D:271:TYR:CD1	1:D:332:ILE:CD1	2.88	0.57
1:A:187:ILE:O	1:A:191:ILE:N	2.32	0.57
1:C:399:ASN:N	1:C:399:ASN:OD1	2.38	0.57
1:A:75:LYS:HG2	1:A:76:PHE:N	2.19	0.57
1:B:49:LEU:O	1:B:53:ILE:HG13	2.05	0.57
1:C:342:TRP:O	1:C:345:GLN:HB2	2.05	0.57
1:C:372:GLN:O	1:C:376:VAL:CG2	2.53	0.57
1:D:290:VAL:HG13	1:D:298:LEU:HD22	1.86	0.57
1:A:73:TRP:HZ2	1:B:109:VAL:HB	1.70	0.57
1:B:180:GLN:HA	1:B:183:THR:HG22	1.87	0.57
1:C:235:CYS:O	1:C:428:LEU:HD21	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:MET:CE	1:C:122:ILE:HD12	2.34	0.57
1:A:332:ILE:O	1:A:335:ASN:N	2.36	0.57
1:B:239:MET:SD	1:B:428:LEU:HB3	2.45	0.57
1:C:275:ALA:HB1	1:C:335:ASN:ND2	2.20	0.57
1:A:30:MET:O	1:A:33:TYR:HB3	2.03	0.57
1:A:282:THR:CB	1:A:337:GLY:HA2	2.35	0.57
1:B:80:ILE:HG21	1:B:130:LEU:HD13	1.87	0.57
1:C:374:MET:CE	1:C:375:VAL:HG12	2.35	0.57
1:C:72:ARG:HG2	1:C:73:TRP:O	2.05	0.57
1:A:232:GLN:HB2	1:A:352:THR:HG21	1.86	0.56
1:A:349:VAL:HG21	1:A:372:GLN:HB2	1.86	0.56
1:D:279:ASN:HA	1:D:282:THR:HG22	1.87	0.56
1:D:33:TYR:HE2	1:D:94:LEU:HD21	1.69	0.56
1:C:87:ASN:CG	1:C:119:THR:HG21	2.26	0.56
1:C:140:GLU:O	1:C:143:GLN:HB2	2.06	0.56
1:A:164:LEU:O	1:A:167:VAL:HG12	2.05	0.56
1:A:368:ALA:O	1:A:371:VAL:HG22	2.03	0.56
1:C:310:CYS:O	1:C:311:ALA:C	2.44	0.56
1:A:84:THR:HB	1:A:194:THR:HB	1.87	0.56
1:B:401:ALA:HB3	1:B:406:THR:HA	1.87	0.56
1:C:275:ALA:HB1	1:C:335:ASN:HD22	1.70	0.56
1:D:79:TRP:CE3	1:D:126:PRO:CB	2.81	0.56
1:A:92:PHE:HD1	1:A:187:ILE:CD1	2.18	0.56
1:B:39:LEU:O	1:B:40:SER:HB3	2.04	0.56
1:C:202:HIS:ND1	1:C:202:HIS:O	2.38	0.56
1:C:302:ALA:O	1:C:306:PRO:HD2	2.05	0.56
1:D:125:ILE:CG2	1:D:369:TYR:CD1	2.87	0.56
1:C:323:ASN:C	1:C:323:ASN:ND2	2.59	0.56
1:C:83:GLY:HA2	1:C:122:ILE:HG23	1.87	0.56
1:A:220:LEU:O	1:A:224:VAL:HG23	2.06	0.56
1:B:122:ILE:O	1:B:126:PRO:CD	2.54	0.56
1:B:194:THR:O	1:B:198:LEU:HG	2.06	0.56
1:B:293:LEU:HD21	1:C:321:ILE:HG12	1.88	0.56
1:B:93:LEU:HD13	1:B:112:THR:CG2	2.22	0.56
1:A:147:PHE:O	1:A:149:ARG:N	2.39	0.56
1:B:18:LYS:HZ3	1:B:123:MET:HA	1.71	0.56
1:D:90:VAL:CG1	1:D:116:TRP:HB2	2.36	0.56
1:A:243:TYR:HE2	1:A:342:TRP:HA	1.70	0.56
1:C:209:ASN:O	1:C:211:VAL:O	2.24	0.56
1:C:416:VAL:O	1:C:419:VAL:HB	2.06	0.56
1:D:124:ASP:HB2	1:D:373:THR:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PRO:HB3	1:A:343:VAL:HG11	1.87	0.55
1:B:17:GLY:CA	1:B:190:PHE:HD1	2.19	0.55
1:D:124:ASP:HB2	1:D:373:THR:HG21	1.87	0.55
1:D:29:LEU:HD22	1:D:33:TYR:CZ	2.41	0.55
1:D:112:THR:O	1:D:115:LEU:HB3	2.06	0.55
1:A:92:PHE:HD1	1:A:187:ILE:HD13	1.71	0.55
1:A:147:PHE:CZ	1:A:288:ARG:HG2	2.41	0.55
1:C:217:HIS:NE2	1:C:218:LEU:HG	2.22	0.55
1:C:242:ALA:CB	1:C:422:PHE:HA	2.37	0.55
1:A:215:ARG:N	1:A:216:PRO:CD	2.70	0.55
1:A:219:THR:HG21	1:A:360:LEU:HD11	1.89	0.55
1:B:99:LEU:HD22	1:B:180:GLN:CD	2.27	0.55
1:B:7:THR:O	1:B:11:TYR:N	2.37	0.55
1:C:143:GLN:O	1:C:147:PHE:HD1	1.90	0.55
1:C:282:THR:OG1	1:C:337:GLY:HA2	2.07	0.55
1:D:48:PHE:CD1	1:D:51:ALA:HB3	2.41	0.55
1:A:25:VAL:HG11	1:A:116:TRP:HH2	1.71	0.55
1:A:11:TYR:CE2	1:A:130:LEU:HB3	2.42	0.55
1:A:125:ILE:CG2	1:A:126:PRO:HD3	2.37	0.55
1:A:294:SER:O	1:A:297:ILE:HG12	2.06	0.55
1:D:391:LEU:HD22	1:D:413:ILE:CD1	2.37	0.55
1:D:387:ILE:CG2	1:D:414:MET:SD	2.94	0.55
1:D:77:LYS:O	1:D:81:LEU:HB2	2.05	0.55
1:A:250:ILE:O	1:A:254:ALA:N	2.40	0.55
1:B:86:THR:CG2	1:B:115:LEU:HG	2.37	0.55
1:C:241:LEU:HA	1:C:376:VAL:HG13	1.88	0.55
1:D:387:ILE:HG22	1:D:417:LEU:HD12	1.87	0.55
1:D:75:LYS:CE	1:D:76:PHE:HB2	2.36	0.55
1:A:299:TRP:O	1:A:303:SER:N	2.39	0.55
1:A:236:LEU:HD13	1:A:349:VAL:HA	1.88	0.55
1:C:140:GLU:O	1:C:143:GLN:N	2.40	0.55
1:D:415:ILE:HA	1:D:418:PRO:CG	2.37	0.55
1:C:175:ARG:NH1	1:C:175:ARG:CG	2.69	0.55
1:D:391:LEU:HB2	1:D:413:ILE:HD12	1.89	0.55
1:C:77:LYS:N	1:C:78:PRO:HD2	2.21	0.55
1:D:62:MET:O	1:D:79:TRP:HZ2	1.90	0.55
1:C:282:THR:CG2	1:C:282:THR:O	2.55	0.54
1:D:125:ILE:HB	1:D:126:PRO:HD3	1.89	0.54
1:A:51:ALA:O	1:A:54:TRP:HB2	2.07	0.54
1:C:119:THR:HA	1:C:122:ILE:HG22	1.90	0.54
1:B:163:THR:HG22	1:B:182:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ILE:HG21	1:B:421:PHE:CE2	2.43	0.54
1:B:48:PHE:O	1:B:51:ALA:HB3	2.07	0.54
1:C:419:VAL:HA	1:C:422:PHE:HB3	1.90	0.54
1:A:13:PHE:CZ	1:A:192:ALA:HB1	2.43	0.54
1:C:386:PHE:C	1:C:386:PHE:CD1	2.81	0.54
1:A:149:ARG:HB2	1:A:283:LEU:HD21	1.90	0.54
1:B:244:ASN:HD22	1:B:376:VAL:HG11	1.68	0.54
1:C:232:GLN:HG2	1:C:232:GLN:O	2.08	0.54
1:C:233:LEU:O	1:C:236:LEU:N	2.31	0.54
1:D:16:PHE:HB2	1:D:151:PHE:CD2	2.42	0.54
1:D:324:ALA:O	1:D:328:VAL:HG23	2.08	0.54
1:D:245:ILE:HG12	1:D:376:VAL:CG2	2.36	0.54
1:C:139:ARG:HH22	1:C:358:PHE:CB	2.15	0.54
1:C:287:PRO:HG3	1:C:340:LEU:CD2	2.35	0.54
1:C:72:ARG:HG2	1:C:73:TRP:N	2.19	0.54
1:D:420:LEU:O	1:D:420:LEU:HD23	2.08	0.54
1:A:125:ILE:HG23	1:A:126:PRO:HD3	1.89	0.54
1:A:8:LYS:HA	1:A:11:TYR:CB	2.34	0.54
1:B:32:TYR:CE1	1:B:176:GLY:CA	2.90	0.54
1:B:285:VAL:HG12	1:B:289:LEU:HD13	1.90	0.54
1:C:387:ILE:HD12	1:C:417:LEU:CG	2.38	0.54
1:A:59:ASP:HB3	1:A:374:MET:HG2	1.89	0.54
1:C:122:ILE:O	1:C:126:PRO:HG2	2.07	0.54
1:D:11:TYR:CD1	1:D:130:LEU:HD22	2.43	0.54
1:C:123:MET:O	1:C:126:PRO:HD2	2.08	0.53
1:D:124:ASP:OD2	1:D:373:THR:CG2	2.56	0.53
1:A:240:ALA:HB1	1:A:376:VAL:CG1	2.38	0.53
1:C:110:CYS:O	1:C:114:ILE:HG12	2.08	0.53
1:C:162:ILE:O	1:C:165:PRO:HD2	2.08	0.53
1:D:125:ILE:HG22	1:D:369:TYR:CE1	2.43	0.53
1:A:236:LEU:CD2	1:A:372:GLN:NE2	2.71	0.53
1:C:310:CYS:SG	1:C:416:VAL:HA	2.49	0.53
1:A:81:LEU:CD1	1:A:85:LEU:HD12	2.39	0.53
1:B:15:ALA:HB1	1:B:152:ALA:HB2	1.89	0.53
1:B:374:MET:N	1:B:374:MET:HE2	2.24	0.53
1:C:177:PHE:O	1:C:180:GLN:HB2	2.08	0.53
1:C:387:ILE:HG23	1:C:417:LEU:HD21	1.90	0.53
1:A:67:ASN:OD1	1:A:220:LEU:HD23	2.08	0.53
1:B:322:HIS:O	1:B:326:LEU:N	2.33	0.53
1:D:285:VAL:O	1:D:289:LEU:HG	2.08	0.53
1:B:286:PHE:O	1:B:290:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ASP:O	1:B:433:TYR:HE2	1.92	0.53
1:C:139:ARG:O	1:C:140:GLU:CB	2.54	0.53
1:C:391:LEU:CD1	1:C:413:ILE:HD13	2.37	0.53
1:A:295:ARG:O	1:A:298:LEU:HB3	2.09	0.53
1:D:135:THR:HB	1:D:141:ARG:HG3	1.89	0.53
1:B:39:LEU:HD22	1:B:41:VAL:CG2	2.38	0.53
1:C:360:LEU:HD22	1:C:361:ASN:OD1	2.07	0.53
1:A:18:LYS:O	1:A:22:ILE:HG22	2.09	0.53
1:A:285:VAL:O	1:A:289:LEU:HG	2.08	0.53
1:A:67:ASN:HB3	1:A:217:HIS:HD2	1.71	0.53
1:A:7:THR:HG23	1:A:201:VAL:CG1	2.30	0.53
1:D:349:VAL:HG11	1:D:366:SER:HB3	1.91	0.53
1:A:62:MET:HE3	1:A:122:ILE:HD12	1.90	0.53
1:B:233:LEU:HG	1:B:368:ALA:HB3	1.90	0.53
1:B:384:ALA:O	1:B:387:ILE:HG13	2.09	0.53
1:B:430:PHE:O	1:B:431:ARG:C	2.47	0.53
1:C:1:MET:SD	1:C:3:ILE:HB	2.49	0.53
1:D:111:VAL:HG23	1:D:112:THR:N	2.24	0.53
1:D:19:ASP:HA	1:D:22:ILE:HG22	1.91	0.53
1:D:268:PHE:N	1:D:269:PRO:CD	2.72	0.52
1:A:352:THR:HA	1:A:355:TYR:CE2	2.44	0.52
1:C:229:LYS:HD2	1:C:229:LYS:O	2.09	0.52
1:D:153:SER:CB	1:D:283:LEU:CD2	2.86	0.52
1:A:59:ASP:CB	1:A:374:MET:HG2	2.39	0.52
1:B:59:ASP:CB	1:B:60:PRO:HD3	2.40	0.52
1:C:141:ARG:HH21	1:C:351:ASP:CG	2.13	0.52
1:C:78:PRO:O	1:C:81:LEU:HG	2.10	0.52
1:C:79:TRP:CZ2	1:C:125:ILE:HG23	2.44	0.52
1:D:128:TRP:HD1	1:D:129:SER:N	2.08	0.52
1:D:153:SER:HB2	1:D:283:LEU:CD2	2.38	0.52
1:B:440:LEU:HD12	1:B:440:LEU:N	2.25	0.52
1:C:124:ASP:OD2	1:C:128:TRP:CZ2	2.63	0.52
1:C:146:PRO:HG3	1:C:295:ARG:NH1	2.24	0.52
1:C:387:ILE:HG23	1:C:417:LEU:CD2	2.38	0.52
1:A:75:LYS:O	1:A:78:PRO:HD2	2.10	0.52
1:B:81:LEU:HD21	1:B:198:LEU:HD23	1.91	0.52
1:B:83:GLY:O	1:B:86:THR:OG1	2.28	0.52
1:C:138:LYS:HA	1:C:139:ARG:HD3	1.90	0.52
1:D:120:TYR:HA	1:D:123:MET:HB2	1.90	0.52
1:A:76:PHE:HB3	1:A:130:LEU:HD22	1.91	0.52
1:A:3:ILE:CG2	1:A:203:GLU:HB3	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:HB2	1:B:43:LEU:HD21	1.92	0.52
1:C:235:CYS:O	1:C:428:LEU:CD2	2.58	0.52
1:D:138:LYS:HE3	1:D:139:ARG:HG3	1.90	0.52
1:B:62:MET:HE2	1:B:122:ILE:HD11	1.91	0.52
1:C:144:LEU:O	1:C:148:PRO:CD	2.54	0.52
1:C:192:ALA:O	1:C:196:VAL:HG23	2.09	0.52
1:A:11:TYR:CZ	1:A:130:LEU:HD23	2.44	0.52
1:A:183:THR:CG2	1:A:187:ILE:HD12	2.26	0.52
1:A:90:VAL:HG21	1:A:116:TRP:CB	2.40	0.52
1:D:370:SER:O	1:D:372:GLN:N	2.42	0.52
1:A:125:ILE:O	1:A:129:SER:HB3	2.09	0.52
1:A:346:VAL:CG1	1:A:369:TYR:CE1	2.91	0.52
1:B:243:TYR:O	1:B:247:SER:N	2.38	0.52
1:C:138:LYS:C	1:C:139:ARG:CD	2.77	0.52
1:C:32:TYR:O	1:C:36:VAL:N	2.42	0.52
1:A:87:ASN:CB	1:A:119:THR:HG21	2.36	0.51
1:A:127:PHE:HD1	1:A:127:PHE:C	2.13	0.51
1:C:78:PRO:HD3	1:C:202:HIS:CD2	2.45	0.51
1:A:91:LEU:HD13	1:A:116:TRP:CZ3	2.44	0.51
1:A:13:PHE:CD2	1:A:196:VAL:HG21	2.45	0.51
1:A:241:LEU:O	1:A:245:ILE:HG13	2.11	0.51
1:A:271:TYR:OH	1:A:329:ALA:HA	2.10	0.51
1:B:267:LEU:C	1:B:269:PRO:HD2	2.31	0.51
1:B:28:TYR:CE2	1:B:32:TYR:HB2	2.45	0.51
1:C:91:LEU:CD1	1:C:94:LEU:HD23	2.39	0.51
1:D:396:TYR:O	1:D:398:PRO:HD3	2.10	0.51
1:A:150:PHE:O	1:A:150:PHE:CD1	2.64	0.51
1:B:77:LYS:CD	1:B:201:VAL:HB	2.35	0.51
1:D:384:ALA:O	1:D:387:ILE:CG1	2.55	0.51
1:A:441:ARG:O	1:A:445:ILE:N	2.43	0.51
1:A:441:ARG:O	1:A:445:ILE:CB	2.59	0.51
1:B:81:LEU:CD2	1:B:198:LEU:HD23	2.40	0.51
1:D:79:TRP:CZ3	1:D:126:PRO:HB3	2.42	0.51
1:A:25:VAL:HG23	1:A:26:TYR:N	2.25	0.51
1:A:3:ILE:HG22	1:A:203:GLU:CB	2.35	0.51
1:C:323:ASN:HA	1:C:327:ILE:HG12	1.91	0.51
1:D:8:LYS:HD2	1:D:134:ILE:HG21	1.92	0.51
1:A:236:LEU:HD11	1:A:348:MET:C	2.31	0.51
1:B:342:TRP:O	1:B:345:GLN:HB2	2.10	0.51
1:C:349:VAL:HG11	1:C:369:TYR:HA	1.93	0.51
1:C:383:ALA:O	1:C:387:ILE:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:THR:HA	1:C:201:VAL:HB	1.93	0.51
1:D:387:ILE:HG21	1:D:414:MET:SD	2.51	0.51
1:A:73:TRP:HZ2	1:B:109:VAL:CB	2.23	0.51
1:C:110:CYS:O	1:C:111:VAL:C	2.47	0.51
1:B:77:LYS:HB2	1:B:201:VAL:CB	2.40	0.51
1:B:36:VAL:HG13	1:B:37:VAL:H	1.76	0.51
1:A:18:LYS:HZ1	1:A:127:PHE:HB2	1.76	0.51
1:A:353:VAL:O	1:A:357:GLU:N	2.34	0.51
1:C:125:ILE:HG22	1:C:126:PRO:HD3	1.93	0.51
1:D:122:ILE:O	1:D:126:PRO:CD	2.59	0.51
1:A:230:ASN:N	1:A:230:ASN:OD1	2.41	0.50
1:A:58:ASN:CB	1:A:121:THR:HG21	2.40	0.50
1:B:373:THR:O	1:B:376:VAL:HG13	2.11	0.50
1:C:11:TYR:CZ	1:C:130:LEU:HB3	2.45	0.50
1:A:272:LEU:HA	1:A:275:ALA:HB3	1.92	0.50
1:A:296:ARG:O	1:A:299:TRP:HB3	2.12	0.50
1:A:61:ILE:HA	1:A:64:TRP:HB3	1.93	0.50
1:B:17:GLY:CA	1:B:190:PHE:CD1	2.94	0.50
1:B:34:THR:O	1:B:36:VAL:N	2.44	0.50
1:C:99:LEU:HD12	1:C:177:PHE:HB2	1.93	0.50
1:C:399:ASN:O	1:C:401:ALA:N	2.44	0.50
1:D:75:LYS:C	1:D:77:LYS:H	2.12	0.50
1:A:131:VAL:O	1:A:134:ILE:HG12	2.11	0.50
1:A:238:GLY:HA3	1:A:424:MET:SD	2.51	0.50
1:B:413:ILE:H	1:B:413:ILE:HD13	1.77	0.50
1:C:41:VAL:HG13	1:C:42:GLY:H	1.76	0.50
1:A:27:MET:HE2	1:A:159:THR:HB	1.92	0.50
1:A:195:ILE:HG23	1:A:196:VAL:H	1.75	0.50
1:B:77:LYS:CB	1:B:201:VAL:CG1	2.90	0.50
1:B:299:TRP:CD2	1:B:429:TYR:CE2	3.00	0.50
1:C:66:VAL:HG12	1:C:67:ASN:N	2.27	0.50
1:A:282:THR:CG2	1:A:282:THR:O	2.58	0.50
1:A:351:ASP:HA	1:A:354:ASP:CB	2.42	0.50
1:A:355:TYR:HA	1:A:358:PHE:HB2	1.94	0.50
1:B:159:THR:O	1:B:159:THR:HG22	2.10	0.50
1:C:351:ASP:O	1:C:354:ASP:N	2.44	0.50
1:D:153:SER:HB2	1:D:283:LEU:HD21	1.93	0.50
1:A:378:GLY:O	1:A:380:SER:N	2.45	0.50
1:A:92:PHE:CD1	1:A:187:ILE:CD1	2.93	0.50
1:A:380:SER:O	1:A:383:ALA:HB3	2.12	0.50
1:B:182:PHE:O	1:B:185:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ARG:HD2	1:C:139:ARG:H	1.71	0.50
1:D:197:THR:O	1:D:201:VAL:HG23	2.12	0.50
1:A:240:ALA:CB	1:A:376:VAL:CG1	2.90	0.50
1:A:322:HIS:O	1:A:323:ASN:HB2	2.12	0.50
1:A:332:ILE:O	1:A:335:ASN:CB	2.60	0.50
1:B:124:ASP:HB2	1:B:373:THR:CG2	2.42	0.50
1:A:290:VAL:O	1:A:290:VAL:HG23	2.12	0.49
1:A:390:VAL:HG12	1:A:413:ILE:HG23	1.94	0.49
1:B:237:LEU:HA	1:B:372:GLN:HE21	1.76	0.49
1:B:391:LEU:HB2	1:B:413:ILE:HD12	1.93	0.49
1:C:349:VAL:CG1	1:C:369:TYR:HA	2.42	0.49
1:B:241:LEU:O	1:B:245:ILE:HG13	2.12	0.49
1:B:383:ALA:O	1:B:385:PHE:N	2.45	0.49
1:B:76:PHE:HA	1:B:79:TRP:CB	2.42	0.49
1:D:77:LYS:CE	1:D:81:LEU:HD22	2.42	0.49
1:C:272:LEU:HA	1:C:275:ALA:HB3	1.94	0.49
1:D:88:SER:HB2	1:D:190:PHE:CD2	2.46	0.49
1:B:130:LEU:O	1:B:134:ILE:HD11	2.13	0.49
1:C:11:TYR:CE2	1:C:127:PHE:HA	2.47	0.49
1:C:16:PHE:O	1:C:20:PHE:HB2	2.11	0.49
1:C:310:CYS:HG	1:C:314:PHE:HD2	1.60	0.49
1:D:110:CYS:O	1:D:111:VAL:C	2.50	0.49
1:D:17:GLY:HA3	1:D:190:PHE:HD1	1.78	0.49
1:D:85:LEU:HD21	1:D:194:THR:HG21	1.94	0.49
1:A:20:PHE:O	1:A:24:ILE:HG13	2.12	0.49
1:A:236:LEU:HD11	1:A:348:MET:CB	2.42	0.49
1:B:17:GLY:HA3	1:B:190:PHE:CD1	2.48	0.49
1:C:236:LEU:HD11	1:C:348:MET:HB3	1.94	0.49
1:D:416:VAL:O	1:D:420:LEU:HB2	2.13	0.49
1:A:242:ALA:HA	1:A:245:ILE:HD12	1.94	0.49
1:B:244:ASN:ND2	1:B:376:VAL:CG1	2.71	0.49
1:B:387:ILE:HG22	1:B:417:LEU:HD22	1.95	0.49
1:C:122:ILE:O	1:C:126:PRO:CG	2.61	0.49
1:D:270:TYR:C	1:D:270:TYR:CD1	2.85	0.49
1:A:11:TYR:CE2	1:A:127:PHE:HA	2.48	0.49
1:A:133:THR:O	1:A:134:ILE:O	2.31	0.49
1:A:397:THR:HG22	1:A:398:PRO:CD	2.42	0.49
1:A:413:ILE:O	1:A:416:VAL:HG12	2.12	0.49
1:B:59:ASP:HB2	1:B:60:PRO:HD3	1.95	0.49
1:B:77:LYS:CB	1:B:78:PRO:HD3	2.42	0.49
1:C:129:SER:O	1:C:132:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PHE:CE1	1:C:277:ALA:HB1	2.48	0.49
1:C:349:VAL:HG13	1:C:350:ALA:N	2.27	0.49
1:C:79:TRP:CD1	1:C:122:ILE:HG13	2.47	0.49
1:A:120:TYR:OH	1:A:377:LYS:NZ	2.46	0.49
1:A:216:PRO:O	1:A:219:THR:HB	2.13	0.49
1:B:34:THR:HG23	1:B:43:LEU:HG	1.94	0.49
1:B:77:LYS:HB2	1:B:201:VAL:HB	1.94	0.49
1:C:33:TYR:HA	1:C:36:VAL:CG1	2.43	0.49
1:D:2:SER:O	1:D:5:MET:N	2.44	0.49
1:A:29:LEU:O	1:A:32:TYR:N	2.43	0.49
1:C:125:ILE:HA	1:C:128:TRP:HE1	1.76	0.49
1:C:10:SER:HB2	1:C:196:VAL:HG12	1.94	0.49
1:D:75:LYS:HG3	1:D:202:HIS:CA	2.27	0.49
1:C:351:ASP:O	1:C:354:ASP:HB2	2.13	0.49
1:D:23:GLY:O	1:D:27:MET:HG2	2.13	0.49
1:A:58:ASN:HD21	1:A:118:MET:HA	1.77	0.48
1:A:11:TYR:CE1	1:A:130:LEU:HD23	2.48	0.48
1:A:271:TYR:O	1:A:275:ALA:N	2.44	0.48
1:A:243:TYR:OH	1:A:341:PHE:HB3	2.13	0.48
1:B:145:VAL:N	1:B:146:PRO:CD	2.76	0.48
1:D:51:ALA:HA	1:D:54:TRP:CD2	2.48	0.48
1:A:222:THR:O	1:A:226:LEU:N	2.38	0.48
1:B:80:ILE:HD13	1:B:130:LEU:HD13	1.95	0.48
1:A:321:ILE:HD12	1:A:321:ILE:N	2.25	0.48
1:A:76:PHE:CE2	1:A:126:PRO:HA	2.48	0.48
1:C:110:CYS:O	1:C:112:THR:N	2.46	0.48
1:C:240:ALA:HB1	1:C:376:VAL:HG21	1.92	0.48
1:A:203:GLU:O	1:A:206:SER:N	2.46	0.48
1:A:37:VAL:HG13	1:A:38:GLY:N	2.29	0.48
1:C:78:PRO:O	1:C:82:ILE:HG12	2.13	0.48
1:C:97:ALA:HA	1:D:199:ARG:HB3	1.95	0.48
1:D:236:LEU:CD2	1:D:349:VAL:HG23	2.37	0.48
1:D:387:ILE:HA	1:D:390:VAL:HG22	1.96	0.48
1:D:76:PHE:HB3	1:D:80:ILE:HG23	1.95	0.48
1:A:227:ILE:O	1:A:227:ILE:HD12	2.14	0.48
1:A:268:PHE:N	1:A:269:PRO:CD	2.74	0.48
1:A:4:SER:OG	1:A:134:ILE:HA	2.12	0.48
1:B:349:VAL:O	1:B:352:THR:HG22	2.13	0.48
1:C:211:VAL:CG1	1:C:212:THR:H	2.23	0.48
1:D:146:PRO:O	1:D:149:ARG:HB2	2.13	0.48
1:D:306:PRO:O	1:D:309:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:CG2	1:A:191:ILE:HG13	2.25	0.48
1:A:22:ILE:O	1:A:22:ILE:HG13	2.13	0.48
1:A:5:MET:HG3	1:A:135:THR:HG23	1.95	0.48
1:B:121:THR:HG22	1:B:374:MET:HB3	1.95	0.48
1:C:236:LEU:HD23	1:C:236:LEU:O	2.12	0.48
1:C:240:ALA:O	1:C:241:LEU:C	2.50	0.48
1:D:417:LEU:O	1:D:421:PHE:N	2.47	0.48
1:D:77:LYS:HD3	1:D:77:LYS:C	2.34	0.48
1:D:80:ILE:CG1	1:D:81:LEU:N	2.77	0.48
1:A:419:VAL:HA	1:A:422:PHE:HB2	1.94	0.48
1:C:175:ARG:C	1:C:177:PHE:N	2.67	0.48
1:D:3:ILE:HG21	1:D:203:GLU:HG3	1.95	0.48
1:D:415:ILE:HA	1:D:418:PRO:HG2	1.96	0.48
1:A:286:PHE:N	1:A:287:PRO:CD	2.76	0.48
1:B:352:THR:CA	1:B:433:TYR:CE2	2.89	0.48
1:B:354:ASP:O	1:B:359:LYS:N	2.47	0.48
1:C:117:GLY:O	1:C:120:TYR:HB3	2.14	0.48
1:C:127:PHE:C	1:C:127:PHE:CD1	2.88	0.48
1:C:15:ALA:HB2	1:C:127:PHE:CZ	2.48	0.48
1:C:191:ILE:HA	1:C:194:THR:HG22	1.95	0.48
1:C:260:TYR:CG	1:C:260:TYR:O	2.66	0.48
1:C:98:HIS:O	1:C:99:LEU:C	2.52	0.48
1:D:286:PHE:CE2	1:D:339:ALA:CB	2.97	0.48
1:A:182:PHE:O	1:A:185:VAL:HB	2.14	0.48
1:B:36:VAL:HG13	1:B:37:VAL:N	2.28	0.48
1:D:350:ALA:O	1:D:354:ASP:HB2	2.14	0.48
1:A:92:PHE:HE1	1:A:187:ILE:HG21	1.79	0.48
1:C:214:GLY:O	1:C:217:HIS:ND1	2.45	0.48
1:D:75:LYS:HD3	1:D:201:VAL:HG12	1.96	0.48
1:A:122:ILE:O	1:A:126:PRO:HG2	2.14	0.47
1:A:145:VAL:CG1	1:A:146:PRO:HD3	2.43	0.47
1:D:21:ALA:O	1:D:25:VAL:HB	2.14	0.47
1:A:282:THR:HB	1:A:336:ILE:O	2.14	0.47
1:C:84:THR:OG1	1:C:85:LEU:HD13	2.14	0.47
1:D:125:ILE:H	1:D:126:PRO:HD2	1.79	0.47
1:D:59:ASP:CG	1:D:60:PRO:CD	2.82	0.47
1:A:191:ILE:HA	1:A:194:THR:HG22	1.95	0.47
1:A:245:ILE:CG2	1:A:417:LEU:CD2	2.92	0.47
1:A:309:SER:HB3	1:A:334:LEU:HD22	1.96	0.47
1:C:245:ILE:O	1:C:249:ILE:HD13	2.14	0.47
1:A:59:ASP:HA	1:A:62:MET:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:CB	1:D:368:ALA:HB3	2.44	0.47
1:A:25:VAL:HG11	1:A:116:TRP:CH2	2.49	0.47
1:B:162:ILE:O	1:B:162:ILE:HG22	2.14	0.47
1:B:81:LEU:HD21	1:B:198:LEU:CD2	2.44	0.47
1:B:333:PHE:CE1	1:B:336:ILE:HD12	2.50	0.47
1:C:313:LEU:HB2	1:C:331:GLY:HA3	1.97	0.47
1:C:80:ILE:CD1	1:C:126:PRO:HB3	2.44	0.47
1:D:369:TYR:O	1:D:372:GLN:HG2	2.14	0.47
1:D:244:ASN:CB	1:D:376:VAL:HG21	2.45	0.47
1:B:128:TRP:HD1	1:B:129:SER:N	2.12	0.47
1:B:282:THR:O	1:B:286:PHE:CD2	2.68	0.47
1:B:29:LEU:HD23	1:B:33:TYR:CZ	2.50	0.47
1:C:239:MET:HA	1:C:425:THR:OG1	2.15	0.47
1:D:83:GLY:O	1:D:119:THR:HB	2.14	0.47
1:A:3:ILE:CG2	1:A:203:GLU:CB	2.93	0.47
1:B:108:PHE:CD1	1:B:108:PHE:N	2.83	0.47
1:B:90:VAL:CG1	1:B:116:TRP:HB2	2.45	0.47
1:C:422:PHE:CG	1:C:422:PHE:O	2.68	0.47
1:A:304:VAL:O	1:A:308:LEU:N	2.47	0.47
1:A:332:ILE:O	1:A:335:ASN:HB2	2.15	0.47
1:A:37:VAL:CG1	1:A:38:GLY:N	2.77	0.47
1:B:240:ALA:HA	1:B:345:GLN:HE22	1.80	0.47
1:B:370:SER:O	1:B:374:MET:HE3	2.15	0.47
1:B:245:ILE:CG2	1:B:421:PHE:CD2	2.94	0.47
1:D:320:ASP:OD1	1:D:320:ASP:N	2.48	0.47
1:A:240:ALA:HB2	1:A:372:GLN:HE21	1.80	0.47
1:C:211:VAL:CG1	1:C:212:THR:N	2.78	0.47
1:C:272:LEU:HG	1:C:275:ALA:HB3	1.95	0.47
1:D:124:ASP:CB	1:D:373:THR:HG21	2.45	0.47
1:A:16:PHE:O	1:A:20:PHE:HB2	2.14	0.47
1:B:141:ARG:HH12	1:B:351:ASP:HA	1.80	0.47
1:B:373:THR:HB	1:B:374:MET:HE1	1.96	0.47
1:C:123:MET:C	1:C:126:PRO:HD2	2.35	0.47
1:D:90:VAL:O	1:D:90:VAL:HG12	2.15	0.47
1:A:291:LYS:O	1:A:291:LYS:HD2	2.14	0.46
1:B:236:LEU:HD13	1:B:348:MET:HG2	1.97	0.46
1:C:14:GLY:HA2	1:C:193:SER:OG	2.14	0.46
1:C:216:PRO:HA	1:C:219:THR:OG1	2.14	0.46
1:D:119:THR:HA	1:D:122:ILE:HG13	1.96	0.46
1:A:128:TRP:CD1	1:A:369:TYR:CE1	2.93	0.46
1:A:376:VAL:HG23	1:A:377:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ALA:O	1:A:392:GLY:HA3	2.15	0.46
1:A:68:ALA:O	1:A:71:SER:O	2.32	0.46
1:C:166:PHE:HA	1:C:169:TYR:CD2	2.50	0.46
1:D:184:LEU:O	1:D:187:ILE:HG13	2.14	0.46
1:A:257:TYR:OH	1:A:327:ILE:O	2.34	0.46
1:A:240:ALA:CB	1:A:376:VAL:HG12	2.45	0.46
1:C:268:PHE:N	1:C:269:PRO:HD3	2.30	0.46
1:D:47:LEU:HD13	1:D:113:TYR:CZ	2.51	0.46
1:D:420:LEU:HD22	1:D:421:PHE:CE1	2.51	0.46
1:A:8:LYS:O	1:A:12:GLY:N	2.44	0.46
1:B:136:LEU:O	1:B:136:LEU:HD23	2.15	0.46
1:B:81:LEU:HD11	1:B:198:LEU:CD2	2.46	0.46
1:C:20:PHE:HD1	1:C:155:ALA:HB1	1.79	0.46
1:C:294:SER:O	1:C:297:ILE:HG13	2.16	0.46
1:D:239:MET:SD	1:D:299:TRP:HH2	2.38	0.46
1:A:111:VAL:HG12	1:A:112:THR:N	2.31	0.46
1:A:208:ASP:OD1	1:A:208:ASP:C	2.54	0.46
1:A:239:MET:CB	1:A:425:THR:HA	2.46	0.46
1:A:304:VAL:O	1:A:307:VAL:HB	2.15	0.46
1:B:341:PHE:CE2	1:B:425:THR:HG21	2.50	0.46
1:B:303:SER:HA	1:B:341:PHE:CZ	2.50	0.46
1:B:233:LEU:HG	1:B:368:ALA:CB	2.46	0.46
1:B:76:PHE:HA	1:B:79:TRP:HB2	1.98	0.46
1:C:387:ILE:HD12	1:C:417:LEU:HG	1.97	0.46
1:C:77:LYS:CB	1:C:201:VAL:CG2	2.94	0.46
1:D:380:SER:CA	1:D:383:ALA:HB3	2.45	0.46
1:D:387:ILE:HA	1:D:390:VAL:CG2	2.46	0.46
1:A:282:THR:HB	1:A:337:GLY:HA2	1.97	0.46
1:C:142:GLU:H	1:C:142:GLU:HG2	1.54	0.46
1:C:426:LEU:O	1:C:430:PHE:N	2.36	0.46
1:C:58:ASN:CG	1:C:121:THR:CG2	2.82	0.46
1:D:80:ILE:O	1:D:84:THR:HG23	2.16	0.46
1:A:287:PRO:HA	1:A:340:LEU:HD21	1.98	0.46
1:B:86:THR:HG22	1:B:115:LEU:HG	1.97	0.46
1:D:416:VAL:HG13	1:D:417:LEU:N	2.31	0.46
1:A:14:GLY:O	1:A:18:LYS:N	2.42	0.46
1:B:202:HIS:O	1:B:206:SER:HB2	2.15	0.46
1:B:2:SER:O	1:B:5:MET:N	2.48	0.46
1:C:421:PHE:C	1:C:423:MET:H	2.19	0.46
1:C:90:VAL:HG23	1:C:91:LEU:N	2.31	0.46
1:C:98:HIS:HB2	1:D:199:ARG:HE	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ILE:HG12	1:D:159:THR:HB	1.98	0.46
1:B:77:LYS:CB	1:B:201:VAL:HG12	2.44	0.46
1:B:373:THR:N	1:B:374:MET:CE	2.78	0.46
1:B:421:PHE:O	1:B:424:MET:HB3	2.15	0.46
1:C:318:LEU:HD21	1:C:409:GLY:HA2	1.98	0.46
1:D:236:LEU:HD11	1:D:345:GLN:HA	1.98	0.46
1:B:167:VAL:HB	1:B:182:PHE:CE2	2.51	0.46
1:C:80:ILE:CD1	1:C:126:PRO:CB	2.94	0.46
1:C:18:LYS:O	1:C:22:ILE:HG22	2.16	0.46
1:A:75:LYS:CG	1:A:76:PHE:N	2.80	0.45
1:B:295:ARG:HH21	1:B:340:LEU:HD11	1.80	0.45
1:B:124:ASP:CB	1:B:373:THR:HG23	2.45	0.45
1:C:340:LEU:CG	1:C:340:LEU:O	2.61	0.45
1:C:393:LEU:HA	1:C:396:TYR:HB3	1.98	0.45
1:D:135:THR:CB	1:D:141:ARG:HG3	2.46	0.45
1:A:216:PRO:HA	1:A:219:THR:OG1	2.16	0.45
1:D:239:MET:SD	1:D:299:TRP:CH2	3.09	0.45
1:D:233:LEU:CB	1:D:349:VAL:HG13	2.46	0.45
1:D:351:ASP:HA	1:D:354:ASP:CB	2.45	0.45
1:A:212:THR:C	1:A:214:GLY:H	2.19	0.45
1:B:28:TYR:CE1	1:B:31:TYR:HB2	2.52	0.45
1:B:370:SER:O	1:B:374:MET:CE	2.64	0.45
1:B:83:GLY:HA3	1:B:122:ILE:HG21	1.97	0.45
1:C:11:TYR:CZ	1:C:130:LEU:HD23	2.52	0.45
1:C:16:PHE:O	1:C:20:PHE:CB	2.65	0.45
1:C:77:LYS:HB2	1:C:201:VAL:CG2	2.43	0.45
1:C:7:THR:HG23	1:C:201:VAL:HB	1.98	0.45
1:D:117:GLY:O	1:D:118:MET:C	2.53	0.45
1:D:387:ILE:HB	1:D:414:MET:SD	2.57	0.45
1:D:75:LYS:HE3	1:D:76:PHE:CA	2.43	0.45
1:A:261:VAL:CG2	1:A:328:VAL:HG23	2.39	0.45
1:B:32:TYR:C	1:B:32:TYR:CD1	2.85	0.45
1:C:279:ASN:HD21	1:C:338:THR:HG23	1.81	0.45
1:C:241:LEU:HD22	1:C:379:GLY:HA3	1.97	0.45
1:D:110:CYS:O	1:D:114:ILE:HB	2.17	0.45
1:D:304:VAL:O	1:D:305:MET:C	2.55	0.45
1:A:172:GLY:O	1:A:173:ALA:HB3	2.17	0.45
1:A:240:ALA:O	1:A:243:TYR:N	2.50	0.45
1:A:372:GLN:O	1:A:376:VAL:HG13	2.15	0.45
1:D:286:PHE:O	1:D:290:VAL:HG22	2.16	0.45
1:D:386:PHE:HA	1:D:389:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:PRO:CA	1:A:340:LEU:HD21	2.46	0.45
1:D:301:GLY:C	1:D:305:MET:HG3	2.35	0.45
1:B:120:TYR:HA	1:B:123:MET:HB2	1.98	0.45
1:B:403:SER:OG	1:B:404:ALA:N	2.50	0.45
1:C:279:ASN:HA	1:C:336:ILE:HA	1.98	0.45
1:C:49:LEU:O	1:C:52:ARG:HG2	2.17	0.45
1:D:375:VAL:HG23	1:D:376:VAL:N	2.32	0.45
1:A:190:PHE:O	1:A:193:SER:N	2.47	0.45
1:A:41:VAL:HG11	1:A:105:GLN:HG2	1.98	0.45
1:B:351:ASP:O	1:B:433:TYR:CE2	2.69	0.45
1:B:428:LEU:HA	1:B:428:LEU:HD12	1.84	0.45
1:D:114:ILE:O	1:D:118:MET:N	2.47	0.45
1:B:261:VAL:HG22	1:B:262:ILE:H	1.82	0.45
1:A:35:ASP:OD2	1:A:175:ARG:NE	2.50	0.45
1:B:13:PHE:O	1:B:193:SER:OG	2.32	0.45
1:B:16:PHE:HB2	1:B:151:PHE:CE2	2.52	0.45
1:B:86:THR:O	1:B:90:VAL:HG23	2.17	0.45
1:C:125:ILE:N	1:C:126:PRO:CD	2.80	0.45
1:C:24:ILE:O	1:C:28:TYR:N	2.37	0.45
1:C:329:ALA:O	1:C:332:ILE:HG12	2.17	0.45
1:D:131:VAL:N	1:D:132:PRO:CD	2.80	0.45
1:A:147:PHE:N	1:A:148:PRO:CD	2.80	0.44
1:A:148:PRO:C	1:A:150:PHE:H	2.21	0.44
1:A:253:PHE:CE2	1:A:414:MET:SD	3.10	0.44
1:B:299:TRP:HD1	1:B:344:LEU:HD13	1.81	0.44
1:B:83:GLY:O	1:B:119:THR:OG1	2.27	0.44
1:D:332:ILE:C	1:D:334:LEU:H	2.19	0.44
1:A:128:TRP:NE1	1:A:346:VAL:HG11	2.31	0.44
1:B:163:THR:CG2	1:B:182:PHE:HZ	2.27	0.44
1:C:131:VAL:HG12	1:C:145:VAL:HG22	1.99	0.44
1:D:258:PHE:HA	1:D:261:VAL:HG22	1.99	0.44
1:D:396:TYR:C	1:D:398:PRO:HD3	2.37	0.44
1:A:127:PHE:O	1:A:127:PHE:CD1	2.71	0.44
1:A:286:PHE:O	1:A:298:LEU:HD21	2.17	0.44
1:A:351:ASP:HA	1:A:354:ASP:HB2	1.98	0.44
1:A:383:ALA:HA	1:A:386:PHE:HB3	2.00	0.44
1:B:353:VAL:O	1:B:357:GLU:N	2.42	0.44
1:B:76:PHE:O	1:B:80:ILE:HG23	2.18	0.44
1:C:235:CYS:SG	1:C:428:LEU:HD11	2.58	0.44
1:C:299:TRP:HA	1:C:302:ALA:HB3	1.99	0.44
1:D:233:LEU:HA	1:D:349:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:PHE:O	1:D:336:ILE:HG13	2.18	0.44
1:B:270:TYR:HD2	1:B:271:TYR:CD1	2.36	0.44
1:C:86:THR:HA	1:C:89:LEU:HD12	1.98	0.44
1:A:105:GLN:HE21	1:A:105:GLN:H	1.59	0.44
1:B:145:VAL:N	1:B:146:PRO:HD3	2.32	0.44
1:B:353:VAL:HG11	1:B:365:GLU:O	2.18	0.44
1:B:59:ASP:HA	1:B:374:MET:SD	2.57	0.44
1:B:415:ILE:C	1:B:417:LEU:N	2.70	0.44
1:B:387:ILE:CG2	1:B:417:LEU:HD22	2.48	0.44
1:B:77:LYS:HB3	1:B:78:PRO:HD3	1.99	0.44
1:A:266:ASP:N	1:A:266:ASP:OD1	2.48	0.44
1:B:373:THR:HB	1:B:374:MET:CE	2.48	0.44
1:D:182:PHE:O	1:D:186:LEU:HD13	2.18	0.44
1:D:244:ASN:HB3	1:D:376:VAL:HG21	2.00	0.44
1:D:90:VAL:HG11	1:D:116:TRP:HB2	1.99	0.44
1:A:287:PRO:O	1:A:295:ARG:NH1	2.51	0.44
1:B:35:ASP:HA	1:B:38:GLY:CA	2.42	0.44
1:C:353:VAL:O	1:C:357:GLU:HB2	2.17	0.44
1:D:129:SER:HB2	1:D:369:TYR:OH	2.13	0.44
1:B:439:MET:CB	1:B:440:LEU:HD12	2.47	0.44
1:C:95:PHE:CE1	1:C:184:LEU:HD11	2.52	0.44
1:D:83:GLY:O	1:D:119:THR:CB	2.66	0.44
1:A:75:LYS:HD3	1:A:202:HIS:HA	1.99	0.44
1:A:32:TYR:CD1	1:A:35:ASP:HB3	2.53	0.44
1:A:388:ALA:O	1:A:392:GLY:CA	2.66	0.44
1:C:16:PHE:CE2	1:C:151:PHE:HD2	2.35	0.44
1:C:77:LYS:CE	1:C:201:VAL:HG22	2.47	0.44
1:C:230:ASN:C	1:C:230:ASN:HD22	2.22	0.44
1:D:387:ILE:HG13	1:D:388:ALA:N	2.32	0.44
1:A:148:PRO:O	1:A:150:PHE:N	2.50	0.43
1:A:157:PHE:HB3	1:A:158:VAL:HG23	2.00	0.43
1:A:282:THR:HG21	1:A:337:GLY:HA2	1.99	0.43
1:B:240:ALA:HA	1:B:345:GLN:NE2	2.32	0.43
1:C:142:GLU:HB3	1:C:344:LEU:CD2	2.48	0.43
1:D:383:ALA:O	1:D:387:ILE:HG23	2.18	0.43
1:D:75:LYS:HB3	1:D:77:LYS:H	1.83	0.43
1:A:105:GLN:O	1:A:106:VAL:C	2.56	0.43
1:A:243:TYR:CZ	1:A:341:PHE:CD2	3.02	0.43
1:C:127:PHE:CZ	1:C:131:VAL:HG21	2.52	0.43
1:A:157:PHE:CE1	1:A:277:ALA:HB1	2.54	0.43
1:A:204:VAL:HA	1:A:207:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLY:O	1:A:393:LEU:HD22	2.18	0.43
1:B:197:THR:O	1:B:201:VAL:HG23	2.19	0.43
1:A:383:ALA:O	1:A:386:PHE:HB3	2.19	0.43
1:C:72:ARG:CG	1:C:73:TRP:N	2.81	0.43
1:D:145:VAL:N	1:D:146:PRO:CD	2.81	0.43
1:D:147:PHE:HD1	1:D:150:PHE:CD2	2.28	0.43
1:D:33:TYR:CD1	1:D:33:TYR:O	2.70	0.43
1:D:75:LYS:C	1:D:77:LYS:N	2.72	0.43
1:B:164:LEU:N	1:B:165:PRO:HD2	2.34	0.43
1:B:20:PHE:CD2	1:B:186:LEU:HA	2.53	0.43
1:B:271:TYR:C	1:B:273:SER:H	2.22	0.43
1:C:79:TRP:HZ2	1:C:125:ILE:HG23	1.83	0.43
1:C:2:SER:O	1:C:6:THR:OG1	2.35	0.43
1:A:195:ILE:HG23	1:A:196:VAL:HG23	2.00	0.43
1:A:429:TYR:O	1:A:429:TYR:CD2	2.71	0.43
1:B:290:VAL:CG1	1:B:295:ARG:HG2	2.35	0.43
1:B:413:ILE:C	1:B:415:ILE:N	2.72	0.43
1:D:125:ILE:O	1:D:128:TRP:CD1	2.72	0.43
1:D:245:ILE:CG1	1:D:376:VAL:HG23	2.43	0.43
1:A:390:VAL:CG1	1:A:413:ILE:HG23	2.49	0.43
1:A:87:ASN:O	1:A:90:VAL:HB	2.18	0.43
1:B:93:LEU:CD1	1:B:112:THR:HG21	2.24	0.43
1:C:139:ARG:HB3	1:C:141:ARG:HH11	1.83	0.43
1:C:255:ILE:O	1:C:258:PHE:HB3	2.19	0.43
1:A:56:ALA:O	1:A:60:PRO:HD2	2.19	0.43
1:B:352:THR:N	1:B:433:TYR:HE2	2.16	0.43
1:B:61:ILE:HA	1:B:61:ILE:HD12	1.87	0.43
1:A:105:GLN:NE2	1:A:105:GLN:CA	2.80	0.43
1:A:302:ALA:O	1:A:306:PRO:HD3	2.19	0.43
1:B:62:MET:SD	1:B:122:ILE:HD11	2.58	0.43
1:B:256:TYR:O	1:B:260:TYR:N	2.52	0.43
1:B:290:VAL:O	1:B:290:VAL:HG12	2.19	0.43
1:B:383:ALA:C	1:B:385:PHE:N	2.71	0.43
1:C:209:ASN:O	1:C:210:GLY:C	2.55	0.43
1:D:117:GLY:O	1:D:120:TYR:N	2.52	0.43
1:A:5:MET:SD	1:A:135:THR:HG23	2.59	0.43
1:A:145:VAL:HG13	1:A:146:PRO:HD3	2.01	0.43
1:A:240:ALA:O	1:A:241:LEU:C	2.56	0.43
1:A:77:LYS:N	1:A:78:PRO:HD2	2.34	0.43
1:B:341:PHE:CZ	1:B:425:THR:HG21	2.53	0.43
1:B:59:ASP:OD1	1:B:374:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:CG1	1:B:81:LEU:N	2.82	0.43
1:C:58:ASN:CB	1:C:121:THR:HG21	2.48	0.43
1:C:332:ILE:O	1:C:335:ASN:HB2	2.18	0.43
1:D:237:LEU:HD22	1:D:371:VAL:HB	2.01	0.43
1:A:128:TRP:HD1	1:A:369:TYR:HE1	1.62	0.42
1:A:245:ILE:HG21	1:A:417:LEU:HD21	1.99	0.42
1:C:313:LEU:HD13	1:C:330:ALA:O	2.18	0.42
1:C:241:LEU:CA	1:C:376:VAL:HG13	2.48	0.42
1:D:420:LEU:HD22	1:D:421:PHE:CD1	2.54	0.42
1:D:76:PHE:HB3	1:D:80:ILE:CG2	2.49	0.42
1:A:164:LEU:HA	1:A:167:VAL:HG12	2.01	0.42
1:A:377:LYS:O	1:A:378:GLY:C	2.58	0.42
1:B:417:LEU:O	1:B:421:PHE:CG	2.72	0.42
1:C:278:ALA:O	1:C:336:ILE:HG22	2.19	0.42
1:A:351:ASP:HA	1:A:354:ASP:HB3	2.02	0.42
1:A:81:LEU:HD12	1:A:85:LEU:HD12	2.01	0.42
1:B:124:ASP:CG	1:B:373:THR:HG23	2.39	0.42
1:C:249:ILE:O	1:C:253:PHE:HB2	2.18	0.42
1:C:349:VAL:HB	1:C:372:GLN:CB	2.49	0.42
1:D:137:ASP:O	1:D:138:LYS:CG	2.50	0.42
1:D:386:PHE:CD1	1:D:389:LEU:HD12	2.54	0.42
1:A:278:ALA:HB1	1:A:336:ILE:CG2	2.45	0.42
1:A:91:LEU:HD12	1:A:94:LEU:HD13	2.01	0.42
1:C:279:ASN:OD1	1:C:338:THR:O	2.36	0.42
1:C:88:SER:O	1:C:92:PHE:N	2.51	0.42
1:D:55:ASP:OD1	1:D:375:VAL:HB	2.20	0.42
1:D:73:TRP:CB	1:D:209:ASN:HB2	2.50	0.42
1:B:12:GLY:O	1:B:15:ALA:HB3	2.19	0.42
1:A:98:HIS:HB2	1:B:199:ARG:HD2	2.02	0.42
1:B:248:ASN:OD1	1:B:377:LYS:HG2	2.19	0.42
1:C:116:TRP:O	1:C:119:THR:HB	2.20	0.42
1:D:320:ASP:HB2	1:D:323:ASN:HB3	2.01	0.42
1:A:334:LEU:O	1:A:336:ILE:N	2.52	0.42
1:B:236:LEU:HD21	1:B:345:GLN:O	2.19	0.42
1:B:415:ILE:CD1	1:B:415:ILE:N	2.83	0.42
1:C:92:PHE:HD1	1:C:187:ILE:HD13	1.85	0.42
1:A:1:MET:SD	1:A:4:SER:N	2.90	0.42
1:A:254:ALA:HB1	1:A:272:LEU:HD21	2.01	0.42
1:A:31:TYR:O	1:A:34:THR:HB	2.19	0.42
1:A:241:LEU:HD11	1:A:375:VAL:HG12	2.01	0.42
1:A:417:LEU:HD23	1:A:418:PRO:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HD11	1:B:369:TYR:CD1	2.54	0.42
1:B:167:VAL:HB	1:B:182:PHE:HE2	1.85	0.42
1:B:235:CYS:SG	1:B:236:LEU:N	2.92	0.42
1:B:239:MET:HE3	1:B:239:MET:HB3	1.79	0.42
1:B:281:LEU:HD23	1:B:284:ILE:HD11	2.00	0.42
1:B:383:ALA:O	1:B:384:ALA:C	2.58	0.42
1:D:391:LEU:HD12	1:D:395:GLY:HA3	2.02	0.42
1:A:100:PHE:CE1	1:A:108:PHE:HB2	2.55	0.42
1:A:143:GLN:HA	1:A:295:ARG:HH21	1.84	0.42
1:B:237:LEU:HD13	1:B:371:VAL:HG21	2.01	0.42
1:D:413:ILE:H	1:D:413:ILE:HD13	1.85	0.42
1:A:45:GLY:O	1:A:48:PHE:HB2	2.20	0.42
1:B:86:THR:OG1	1:B:119:THR:OG1	2.33	0.42
1:B:237:LEU:O	1:B:241:LEU:HG	2.19	0.42
1:B:81:LEU:CD1	1:B:198:LEU:HD23	2.50	0.42
1:B:91:LEU:HD13	1:B:186:LEU:HD22	2.02	0.42
1:C:33:TYR:HA	1:C:36:VAL:HG13	2.02	0.42
1:C:413:ILE:HA	1:C:416:VAL:HG12	2.02	0.42
1:A:107:VAL:HB	1:A:108:PHE:H	1.67	0.42
1:A:299:TRP:CZ2	1:A:341:PHE:CZ	3.08	0.42
1:A:342:TRP:CD1	1:A:346:VAL:HG22	2.55	0.42
1:A:81:LEU:HD11	1:A:85:LEU:CD1	2.49	0.42
1:C:118:MET:O	1:C:122:ILE:HG22	2.20	0.42
1:C:233:LEU:HA	1:C:233:LEU:HD12	1.87	0.42
1:D:380:SER:O	1:D:384:ALA:HB2	2.19	0.42
1:A:76:PHE:HE2	1:A:126:PRO:HA	1.84	0.41
1:A:279:ASN:HA	1:A:335:ASN:O	2.19	0.41
1:A:287:PRO:CB	1:A:340:LEU:HD21	2.50	0.41
1:B:310:CYS:SG	1:B:311:ALA:N	2.89	0.41
1:B:32:TYR:CD1	1:B:176:GLY:CA	2.95	0.41
1:A:18:LYS:HZ3	1:A:127:PHE:HB2	1.83	0.41
1:A:282:THR:HG23	1:A:286:PHE:HD1	1.79	0.41
1:B:333:PHE:CZ	1:B:336:ILE:HD12	2.56	0.41
1:C:216:PRO:O	1:C:219:THR:OG1	2.38	0.41
1:D:17:GLY:CA	1:D:190:PHE:HD1	2.33	0.41
1:D:21:ALA:O	1:D:25:VAL:CG2	2.68	0.41
1:D:320:ASP:CB	1:D:323:ASN:HB2	2.50	0.41
1:A:8:LYS:HG3	1:A:131:VAL:HG22	2.01	0.41
1:A:98:HIS:HD2	1:A:99:LEU:HB2	1.80	0.41
1:B:95:PHE:O	1:B:180:GLN:NE2	2.46	0.41
1:C:128:TRP:O	1:C:132:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:LEU:HD23	1:C:418:PRO:HD3	2.02	0.41
1:D:77:LYS:HE3	1:D:81:LEU:HD22	2.03	0.41
1:B:162:ILE:O	1:B:162:ILE:CG2	2.68	0.41
1:B:305:MET:HB2	1:B:306:PRO:HD3	2.02	0.41
1:B:396:TYR:O	1:B:396:TYR:HD1	2.03	0.41
1:C:32:TYR:O	1:C:36:VAL:HG12	2.20	0.41
1:C:76:PHE:CE1	1:C:79:TRP:CE3	3.09	0.41
1:A:194:THR:O	1:A:198:LEU:HG	2.21	0.41
1:A:81:LEU:CD1	1:A:85:LEU:CD1	2.98	0.41
1:B:34:THR:HG23	1:B:43:LEU:CD2	2.50	0.41
1:C:372:GLN:O	1:C:376:VAL:HG23	2.19	0.41
1:D:316:MET:O	1:D:317:ALA:HB2	2.19	0.41
1:A:346:VAL:HG12	1:A:369:TYR:CD1	2.56	0.41
1:C:83:GLY:CA	1:C:122:ILE:HG23	2.51	0.41
1:C:16:PHE:CE2	1:C:151:PHE:CD2	3.09	0.41
1:C:299:TRP:CZ2	1:C:341:PHE:CZ	3.08	0.41
1:D:147:PHE:N	1:D:148:PRO:HD2	2.36	0.41
1:A:174:ASP:O	1:A:178:GLY:N	2.53	0.41
1:A:256:TYR:HA	1:A:259:THR:HB	2.02	0.41
1:A:307:VAL:CG2	1:A:422:PHE:CD2	3.04	0.41
1:B:77:LYS:O	1:B:81:LEU:CB	2.65	0.41
1:C:242:ALA:HA	1:C:245:ILE:CG1	2.49	0.41
1:C:417:LEU:HA	1:C:420:LEU:HB2	2.02	0.41
1:C:77:LYS:HA	1:C:80:ILE:CG1	2.42	0.41
1:D:342:TRP:O	1:D:345:GLN:HB2	2.21	0.41
1:D:418:PRO:O	1:D:422:PHE:HD1	2.03	0.41
1:A:214:GLY:C	1:A:216:PRO:HD2	2.40	0.41
1:A:240:ALA:O	1:A:243:TYR:HB3	2.21	0.41
1:A:271:TYR:OH	1:A:329:ALA:CB	2.69	0.41
1:B:99:LEU:CD1	1:B:177:PHE:HB2	2.47	0.41
1:C:240:ALA:HA	1:C:345:GLN:HE22	1.86	0.41
1:C:302:ALA:O	1:C:303:SER:C	2.58	0.41
1:D:426:LEU:O	1:D:426:LEU:HD23	2.20	0.41
1:D:91:LEU:HD12	1:D:94:LEU:HB3	2.01	0.41
1:A:75:LYS:HG2	1:A:77:LYS:H	1.86	0.41
1:B:76:PHE:HA	1:B:79:TRP:HB3	2.02	0.41
1:C:58:ASN:ND2	1:C:121:THR:HG21	2.36	0.41
1:C:27:MET:O	1:C:27:MET:HG2	2.21	0.41
1:C:141:ARG:NH2	1:C:351:ASP:OD1	2.53	0.41
1:B:81:LEU:HD11	1:B:198:LEU:HD23	2.03	0.41
1:C:127:PHE:CE1	1:C:131:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:N	1:C:376:VAL:HG13	2.36	0.41
1:D:192:ALA:O	1:D:195:ILE:HG22	2.21	0.41
1:D:19:ASP:HB3	1:D:155:ALA:HB3	2.03	0.41
1:D:269:PRO:O	1:D:272:LEU:HB3	2.20	0.41
1:A:90:VAL:HG21	1:A:116:TRP:CA	2.51	0.41
1:A:28:TYR:O	1:A:29:LEU:C	2.58	0.41
1:B:10:SER:O	1:B:13:PHE:N	2.54	0.41
1:B:21:ALA:CB	1:B:87:ASN:ND2	2.83	0.41
1:C:175:ARG:CD	1:C:175:ARG:O	2.62	0.41
1:C:215:ARG:H	1:C:216:PRO:HD2	1.80	0.41
1:B:76:PHE:O	1:B:79:TRP:N	2.54	0.40
1:D:145:VAL:N	1:D:146:PRO:HD3	2.36	0.40
1:A:32:TYR:HA	1:A:35:ASP:HB3	2.02	0.40
1:A:78:PRO:O	1:A:82:ILE:N	2.55	0.40
1:A:77:LYS:O	1:A:80:ILE:HG13	2.22	0.40
1:A:82:ILE:O	1:A:86:THR:CB	2.70	0.40
1:C:136:LEU:O	1:C:138:LYS:N	2.53	0.40
1:C:397:THR:HG1	1:C:398:PRO:HD2	1.78	0.40
1:C:402:GLN:HG3	1:C:403:SER:N	2.35	0.40
1:D:257:TYR:O	1:D:260:TYR:HB3	2.21	0.40
1:B:99:LEU:CD2	1:B:180:GLN:CD	2.90	0.40
1:B:260:TYR:OH	1:B:317:ALA:CB	2.69	0.40
1:B:410:MET:HB3	1:B:413:ILE:HD11	2.04	0.40
1:C:56:ALA:O	1:C:60:PRO:CD	2.68	0.40
1:C:72:ARG:HE	1:C:72:ARG:HB3	1.61	0.40
1:D:150:PHE:HD1	1:D:283:LEU:HD21	1.78	0.40
1:D:236:LEU:HA	1:D:236:LEU:HD12	1.90	0.40
1:B:241:LEU:O	1:B:245:ILE:CG1	2.69	0.40
1:C:238:GLY:HA2	1:C:241:LEU:HD12	2.03	0.40
1:D:322:HIS:O	1:D:326:LEU:HD13	2.22	0.40
1:A:14:GLY:O	1:A:18:LYS:HB2	2.21	0.40
1:C:75:LYS:CD	1:C:202:HIS:O	2.66	0.40
1:D:63:GLY:N	1:D:370:SER:HB3	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	446/486 (92%)	365 (82%)	65 (15%)	16 (4%)	4	28
1	B	422/486 (87%)	360 (85%)	54 (13%)	8 (2%)	9	42
1	C	429/486 (88%)	358 (83%)	63 (15%)	8 (2%)	9	42
1	D	374/486 (77%)	314 (84%)	52 (14%)	8 (2%)	8	40
All	All	1671/1944 (86%)	1397 (84%)	234 (14%)	40 (2%)	7	37

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ILE
1	A	269	PRO
1	A	271	TYR
1	B	430	PHE
1	C	134	ILE
1	C	269	PRO
1	C	271	TYR
1	D	369	TYR
1	A	96	SER
1	A	107	VAL
1	A	214	GLY
1	A	369	TYR
1	A	392	GLY
1	A	398	PRO
1	B	384	ALA
1	C	137	ASP
1	C	339	ALA
1	C	401	ALA
1	C	422	PHE
1	D	38	GLY
1	D	78	PRO
1	D	371	VAL

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Mol	Chain	Res	Type
1	A	433	TYR
1	D	125	ILE
1	D	317	ALA
1	A	111	VAL
1	A	373	THR
1	A	379	GLY
1	A	432	TYR
1	B	35	ASP
1	A	335	ASN
1	D	268	PHE
1	A	42	GLY
1	B	245	ILE
1	B	337	GLY
1	C	397	THR
1	D	146	PRO
1	B	45	GLY
1	B	249	ILE
1	B	409	GLY

### 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	354/406 (87%)	303 (86%)	51 (14%)	4	17
1	B	331/406 (82%)	272 (82%)	59 (18%)	2	9
1	C	353/406 (87%)	281 (80%)	72 (20%)	1	5
1	D	302/406 (74%)	258 (85%)	44 (15%)	3	17
All	All	1340/1624 (82%)	1114 (83%)	226 (17%)	2	11

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	13	PHE
1	A	22	ILE

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Mol	Chain	Res	Type
1	A	32	TYR
1	A	33	TYR
1	A	46	THR
1	A	52	ARG
1	A	55	ASP
1	A	59	ASP
1	A	62	MET
1	A	69	THR
1	A	77	LYS
1	A	80	ILE
1	A	92	PHE
1	A	96	SER
1	A	103	THR
1	A	105	GLN
1	A	111	VAL
1	A	113	TYR
1	A	114	ILE
1	A	121	THR
1	A	128	TRP
1	A	137	ASP
1	A	141	ARG
1	A	149	ARG
1	A	151	PHE
1	A	191	ILE
1	A	203	GLU
1	A	207	SER
1	A	229	LYS
1	A	230	ASN
1	A	248	ASN
1	A	251	ASN
1	A	258	PHE
1	A	259	THR
1	A	262	ILE
1	A	266	ASP
1	A	267	LEU
1	A	268	PHE
1	A	274	TYR
1	A	280	LEU
1	A	281	LEU
1	A	291	LYS
1	A	303	SER
1	A	314	PHE

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Mol	Chain	Res	Type
1	A	358	PHE
1	A	359	LYS
1	A	361	ASN
1	A	417	LEU
1	A	421	PHE
1	A	422	PHE
1	B	32	TYR
1	B	35	ASP
1	B	48	PHE
1	B	49	LEU
1	B	54	TRP
1	B	59	ASP
1	B	66	VAL
1	B	70	ARG
1	B	75	LYS
1	B	80	ILE
1	B	86	THR
1	B	87	ASN
1	B	92	PHE
1	B	95	PHE
1	B	100	PHE
1	B	111	VAL
1	B	113	TYR
1	B	114	ILE
1	B	124	ASP
1	B	125	ILE
1	B	128	TRP
1	B	130	LEU
1	B	147	PHE
1	B	151	PHE
1	B	182	PHE
1	B	191	ILE
1	B	195	ILE
1	B	197	THR
1	B	200	ASN
1	B	205	TYR
1	B	208	ASP
1	B	253	PHE
1	B	268	PHE
1	B	269	PRO
1	B	283	LEU
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	295	ARG
1	B	297	ILE
1	B	299	TRP
1	B	305	MET
1	B	310	CYS
1	B	314	PHE
1	B	316	MET
1	B	326	LEU
1	B	336	ILE
1	B	341	PHE
1	B	345	GLN
1	B	366	SER
1	B	369	TYR
1	B	374	MET
1	B	380	SER
1	B	389	LEU
1	B	396	TYR
1	B	410	MET
1	B	413	ILE
1	B	423	MET
1	B	428	LEU
1	B	430	PHE
1	B	438	ASP
1	C	1	MET
1	C	11	TYR
1	C	28	TYR
1	C	29	LEU
1	C	30	MET
1	C	33	TYR
1	C	35	ASP
1	C	36	VAL
1	C	48	PHE
1	C	62	MET
1	C	67	ASN
1	C	70	ARG
1	C	72	ARG
1	C	76	PHE
1	C	77	LYS
1	C	85	LEU
1	C	92	PHE
1	C	110	CYS
1	C	113	TYR

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Mol	Chain	Res	Type
1	C	114	ILE
1	C	118	MET
1	C	121	THR
1	C	128	TRP
1	C	130	LEU
1	C	136	LEU
1	C	137	ASP
1	C	139	ARG
1	C	141	ARG
1	C	142	GLU
1	C	148	PRO
1	C	151	PHE
1	C	157	PHE
1	C	175	ARG
1	C	181	MET
1	C	187	ILE
1	C	198	LEU
1	C	203	GLU
1	C	212	THR
1	C	227	ILE
1	C	229	LYS
1	C	230	ASN
1	C	236	LEU
1	C	248	ASN
1	C	255	ILE
1	C	259	THR
1	C	271	TYR
1	C	272	LEU
1	C	288	ARG
1	C	293	LEU
1	C	313	LEU
1	C	314	PHE
1	C	323	ASN
1	C	326	LEU
1	C	345	GLN
1	C	351	ASP
1	C	355	TYR
1	C	360	LEU
1	C	363	ARG
1	C	367	ILE
1	C	374	MET
1	C	385	PHE

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Mol	Chain	Res	Type
1	C	386	PHE
1	C	391	LEU
1	C	393	LEU
1	C	398	PRO
1	C	400	VAL
1	C	403	SER
1	C	408	GLN
1	C	411	GLN
1	C	412	PHE
1	C	422	PHE
1	C	426	LEU
1	D	13	PHE
1	D	19	ASP
1	D	27	MET
1	D	33	TYR
1	D	53	ILE
1	D	59	ASP
1	D	66	VAL
1	D	75	LYS
1	D	80	ILE
1	D	86	THR
1	D	89	LEU
1	D	93	LEU
1	D	110	CYS
1	D	123	MET
1	D	124	ASP
1	D	128	TRP
1	D	134	ILE
1	D	138	LYS
1	D	141	ARG
1	D	143	GLN
1	D	148	PRO
1	D	175	ARG
1	D	191	ILE
1	D	194	THR
1	D	199	ARG
1	D	205	TYR
1	D	208	ASP
1	D	235	CYS
1	D	251	ASN
1	D	257	TYR
1	D	270	TYR

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Mol	Chain	Res	Type
1	D	284	ILE
1	D	299	TRP
1	D	310	CYS
1	D	318	LEU
1	D	322	HIS
1	D	326	LEU
1	D	344	LEU
1	D	369	TYR
1	D	386	PHE
1	D	387	ILE
1	D	396	TYR
1	D	413	ILE
1	D	414	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	98	HIS
1	A	105	GLN
1	A	217	HIS
1	A	323	ASN
1	A	335	ASN
1	A	345	GLN
1	A	361	ASN
1	B	67	ASN
1	B	244	ASN
1	B	279	ASN
1	B	335	ASN
1	B	372	GLN
1	C	67	ASN
1	C	105	GLN
1	C	230	ASN
1	C	402	GLN
1	C	411	GLN
1	D	244	ASN

### 5.3.3 RNA ⓘ

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	448/486 (92%)	0.04	30 (6%) 19 20	27, 80, 183, 265	25 (5%)
1	B	426/486 (87%)	0.77	78 (18%) 1 2	28, 89, 247, 360	9 (2%)
1	C	431/486 (88%)	0.03	24 (5%) 25 25	24, 76, 168, 340	0
1	D	382/486 (78%)	0.51	47 (12%) 5 4	31, 85, 220, 331	1 (0%)
All	All	1687/1944 (86%)	0.33	179 (10%) 7 7	24, 82, 213, 360	35 (2%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	362	ILE	21.4
1	B	350	ALA	19.7
1	C	321	ILE	16.4
1	B	351	ASP	15.7
1	D	412	PHE	15.5
1	D	364	CYS	14.2
1	C	320	ASP	14.1
1	A	436	ASN	14.0
1	B	411	GLN	13.1
1	D	366	SER	13.1
1	B	101	GLU	13.0
1	B	364	CYS	11.7
1	B	352	THR	11.1
1	B	129	SER	10.2
1	D	363	ARG	10.1
1	A	320	ASP	10.1
1	B	365	GLU	9.6
1	B	108	PHE	9.5
1	A	433	TYR	9.4
1	C	319	ALA	9.1
1	C	322	HIS	9.0

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Mol	Chain	Res	Type	RSRZ
1	B	363	ARG	9.0
1	D	351	ASP	8.8
1	A	323	ASN	8.7
1	B	354	ASP	8.4
1	D	361	ASN	8.2
1	D	169	TYR	8.2
1	D	267	LEU	7.7
1	B	349	VAL	7.6
1	D	350	ALA	7.5
1	B	265	ALA	7.1
1	B	366	SER	7.1
1	D	411	GLN	6.9
1	A	434	ARG	6.9
1	B	374	MET	6.6
1	C	318	LEU	6.5
1	B	165	PRO	6.4
1	D	354	ASP	6.4
1	C	323	ASN	6.3
1	B	362	ILE	6.0
1	B	399	ASN	6.0
1	A	324	ALA	5.9
1	B	355	TYR	5.8
1	D	70	ARG	5.8
1	D	266	ASP	5.6
1	D	157	PHE	5.6
1	D	357	GLU	5.4
1	D	355	TYR	5.4
1	D	349	VAL	5.3
1	B	100	PHE	5.3
1	B	102	GLY	5.3
1	B	106	VAL	5.2
1	B	105	GLN	5.1
1	B	69	THR	5.0
1	B	164	LEU	5.0
1	B	359	LYS	4.8
1	B	99	LEU	4.7
1	B	410	MET	4.7
1	D	69	THR	4.7
1	A	181	MET	4.6
1	A	171	GLY	4.6
1	A	100	PHE	4.5
1	A	435	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	401	ALA	4.5
1	C	358	PHE	4.4
1	B	70	ARG	4.3
1	D	365	GLU	4.3
1	C	171	GLY	4.2
1	D	141	ARG	4.2
1	C	200	ASN	4.2
1	B	445	ILE	4.1
1	C	412	PHE	4.1
1	D	360	LEU	4.1
1	A	73	TRP	4.1
1	D	67	ASN	4.0
1	B	397	THR	3.9
1	C	5	MET	3.9
1	D	164	LEU	3.8
1	B	141	ARG	3.8
1	B	442	LYS	3.7
1	D	370	SER	3.7
1	A	165	PRO	3.7
1	B	96	SER	3.7
1	D	16	PHE	3.7
1	B	107	VAL	3.6
1	D	352	THR	3.6
1	B	357	GLU	3.5
1	D	158	VAL	3.5
1	C	103	THR	3.5
1	C	178	GLY	3.5
1	B	266	ASP	3.4
1	C	324	ALA	3.4
1	A	437	GLY	3.4
1	D	142	GLU	3.4
1	D	367	ILE	3.3
1	B	67	ASN	3.2
1	A	446	HIS	3.2
1	D	369	TYR	3.2
1	A	319	ALA	3.2
1	B	360	LEU	3.2
1	B	446	HIS	3.1
1	B	369	TYR	3.1
1	B	177	PHE	3.1
1	B	444	GLN	3.1
1	B	449	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	388	ALA	3.0
1	A	322	HIS	3.0
1	B	367	ILE	3.0
1	B	95	PHE	3.0
1	B	412	PHE	2.9
1	B	443	ILE	2.9
1	D	150	PHE	2.9
1	B	133	THR	2.9
1	B	398	PRO	2.8
1	B	361	ASN	2.8
1	C	37	VAL	2.8
1	A	103	THR	2.8
1	B	161	GLY	2.8
1	A	164	LEU	2.7
1	B	146	PRO	2.7
1	B	440	LEU	2.6
1	A	443	ILE	2.6
1	B	175	ARG	2.6
1	B	132	PRO	2.6
1	C	161	GLY	2.6
1	B	71	SER	2.6
1	B	400	VAL	2.6
1	C	172	GLY	2.6
1	B	109	VAL	2.6
1	A	258	PHE	2.5
1	B	147	PHE	2.5
1	B	373	THR	2.5
1	B	343	VAL	2.5
1	C	314	PHE	2.5
1	A	317	ALA	2.5
1	A	366	SER	2.5
1	C	99	LEU	2.5
1	C	363	ARG	2.4
1	B	55	ASP	2.4
1	D	65	ILE	2.4
1	A	169	TYR	2.4
1	A	432	TYR	2.4
1	D	396	TYR	2.4
1	B	257	TYR	2.4
1	B	375	VAL	2.4
1	B	403	SER	2.4
1	D	358	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	362	ILE	2.4
1	B	130	LEU	2.4
1	A	102	GLY	2.3
1	D	163	THR	2.3
1	B	441	ARG	2.3
1	B	356	GLY	2.3
1	C	352	THR	2.3
1	D	353	VAL	2.3
1	D	356	GLY	2.3
1	D	375	VAL	2.3
1	D	348	MET	2.2
1	D	373	THR	2.2
1	D	71	SER	2.2
1	D	124	ASP	2.2
1	B	75	LYS	2.2
1	B	139	ARG	2.2
1	A	222	THR	2.2
1	A	104	ALA	2.1
1	B	169	TYR	2.1
1	C	168	SER	2.1
1	A	168	SER	2.1
1	B	258	PHE	2.1
1	B	68	ALA	2.1
1	B	358	PHE	2.1
1	D	130	LEU	2.1
1	D	340	LEU	2.1
1	D	200	ASN	2.1
1	C	165	PRO	2.1
1	A	170	VAL	2.1
1	B	98	HIS	2.1
1	D	254	ALA	2.0
1	B	60	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.