



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:25 pm BST

PDB ID : 6AC3  
Title : Structure of a natural red emitting luciferase from Phrixothrix hirtus (P3121 crystal form)  
Authors : Carrasco-Lopez, C.; Panjikar, S.; Naumov, P.; Rabeh, W.  
Deposited on : 2018-07-24  
Resolution : 3.60 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

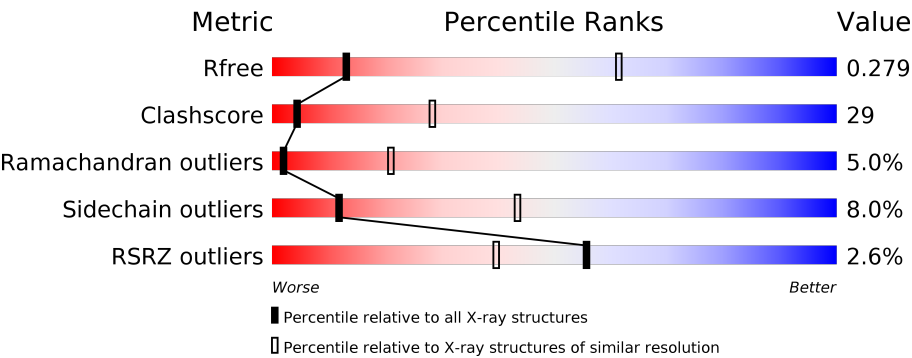
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	546	<div><div>2%</div><div><div></div><div>42%</div><div>31%</div><div>• •</div><div>23%</div></div></div>
1	B	546	<div><div>2%</div><div><div></div><div>44%</div><div>40%</div><div>12%</div><div>• •</div></div></div>
1	C	546	<div><div>%</div><div><div></div><div>43%</div><div>30%</div><div>•</div><div>24%</div></div></div>
1	D	546	<div><div>3%</div><div><div></div><div>46%</div><div>27%</div><div>•</div><div>24%</div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13982 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.

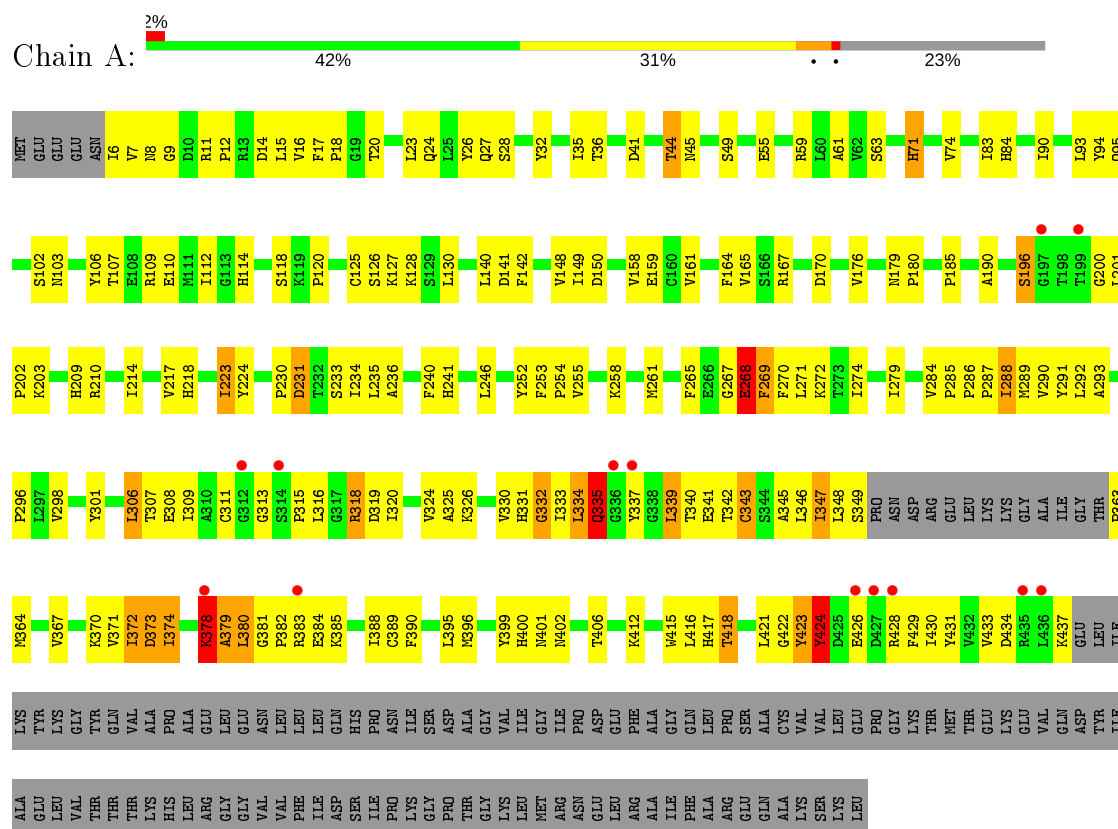
- Molecule 1 is a protein called Red-bioluminescence eliciting luciferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3296	2134	544	599	19			
1	B	528	Total	C	N	O	S	0	0	0
			4135	2667	686	760	22			
1	C	417	Total	C	N	O	S	0	0	0
			3279	2122	541	597	19			
1	D	416	Total	C	N	O	S	0	0	0
			3272	2117	540	596	19			

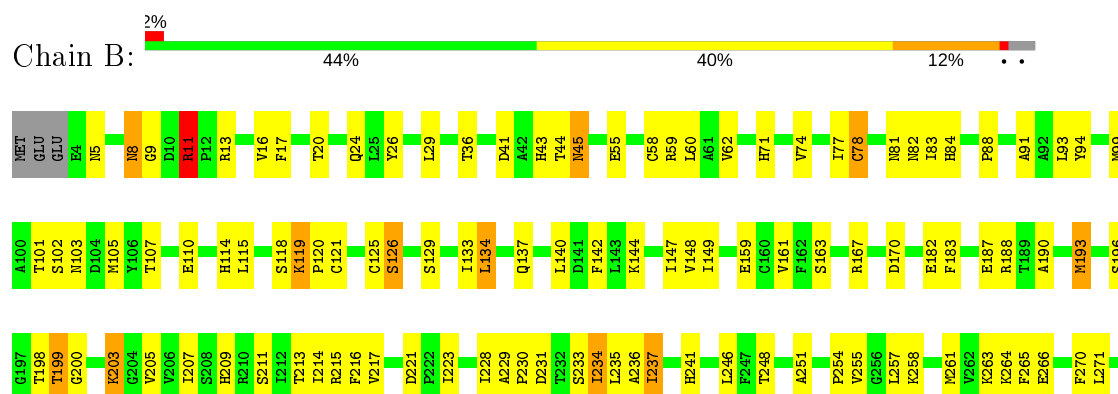
### 3 Residue-property plots

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.

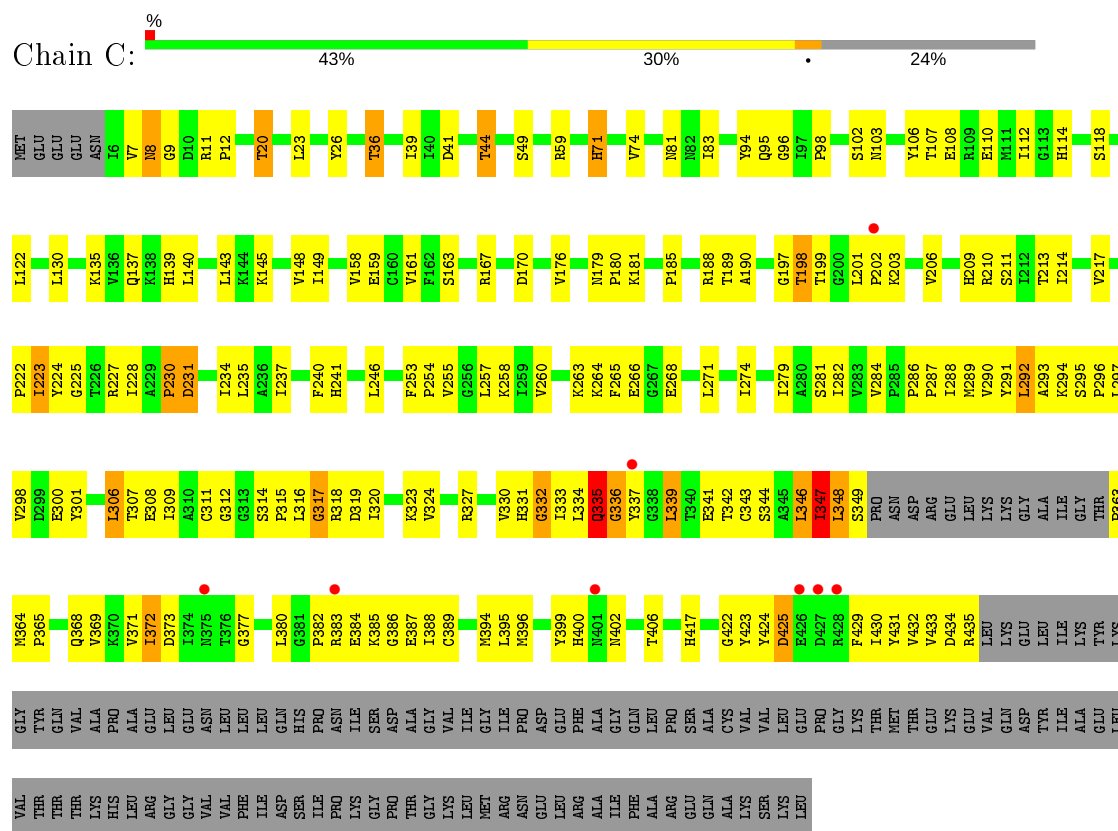
- Molecule 1: Red-bioluminescence eliciting luciferase



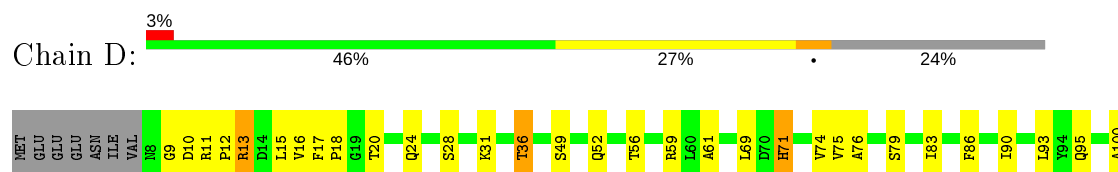
- Molecule 1: Red-bioluminescence eliciting luciferase



- Molecule 1: Red-bioluminescence eliciting luciferase



- Molecule 1: Red-bioluminescence eliciting luciferase



LEU	ALA	G377	T307	P222	M103
ARG	GLU	K378	E308	I223	
GLY	LEU	A379	I309		T107
VAL	GLU	L380	A310	I228	E108
VAL	ASN	G381	C311	A229	R109
PHE	LEU	P382	G312	P230	
ILE	LEU	R383	G313	D231	I112
ASP	LEU	E384	S314		G113
SER	GLN	K385	P315	I234	H114
HIS	PRO		L316		
ILE	ASN	I388	G317	I237	S118
PRO	ASN	G389	R318	F240	K119
LYS	ILE	F390	D319	H241	P120
GLY	SER				G121
PRO	ASP	Q393	K323		L122
THR	ALA	M394	V324		S126
GLY	GLY	L395	A325	L246	
LYS	VAL	M396	K326	A251	L134
LEU	ILE	K397	R327		L140
MET	GLY	G398	L328	P254	F142
ARG	ILE	Y399			K145
ASN	PRO	N402	H331	V260	I149
GLU	ASP		G332	M261	E159
LEU	GLU		I333	V262	C160
ARG	PHE	A405	L334	K263	V161
ALA	ALA	T406	Q335	K264	F162
ILE	GLY	R407	G336	F265	S163
PHE	GLN	D408	Y337	E266	F173
ALA	LEU		G338	G267	D174
ARG	PRO	T418	L339	E268	K177
GLU	SER			P269	P185
GLN	ALA	L421	T342	V284	L186
ALA	CYS	G422	C343	P285	A190
LYS	VAL	Y423	S344	P286	T194
SER	VAL	Y424	A345	P287	
LYS	LEU	D425	L346	I288	G197
LEU	GLU	E426	I347	M289	T198
PRO	PRO	D427	L348	V290	T199
GLY	LYS	R428	S349	Y291	G200
LYS	THR	F429	PRO	L292	K203
THR	MET	Y431	ASN	L293	G204
THR	THR	V432	ASP	A293	V298
GLU	GLY	V433	ARG		H209
LYS	LYS	D434	LEU		R210
GLU	VAL	R435	LYS		S211
VAL	GLN	L436	GLY		S304
ASP	ASP		ALA		S305
LEU	LEU	LYS	ILE		L306
ILE	ILE	LEU	GLY		
ALA	ALA	LYS	THR		
GLU	GLU	TYR	P363		
LEU	LEU	LYS	V371		
VAL	VAL	GLY			
THR	THR	TYR	B372		
THR	THR	GLN	D373		
LYS	VAL	VAL	I374		
ALA	LYS	ALA	R375		
PRO	HIS	PRO	T376		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.10Å 119.10Å 351.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 3.60 19.85 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.85-3.60) 99.1 (19.85-3.60)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.207 , 0.271 0.226 , 0.279	Depositor DCC
$R_{free}$ test set	1020 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.3	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	0/3375	0.83	2/4573 (0.0%)
1	B	0.60	0/4229	0.77	2/5730 (0.0%)
1	C	0.56	0/3358	0.78	0/4551
1	D	0.57	0/3351	0.78	0/4541
All	All	0.58	0/14313	0.79	4/19395 (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	B	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	TYR	CA-CB-CG	7.25	127.18	113.40
1	B	134	LEU	CA-CB-CG	-5.30	103.10	115.30
1	B	328	LEU	CA-CB-CG	-5.17	103.40	115.30
1	A	423	TYR	C-N-CA	-5.17	108.78	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	ARG	Sidechain
1	B	511	ARG	Sidechain
1	B	539	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3296	0	3330	209	0
1	B	4135	0	4187	291	0
1	C	3279	0	3306	164	0
1	D	3272	0	3297	157	0
All	All	13982	0	14120	808	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 29.

All (808) 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:336:GLY:CA	1:B:348:LEU:HB3	1.41	1.46
1:A:9:GLY:CA	1:A:363:PRO:HG2	1.57	1.34
1:B:347:ILE:HD12	1:B:390:PHE:CE2	1.68	1.28
1:B:347:ILE:CD1	1:B:390:PHE:HE2	1.48	1.26
1:C:339:LEU:HD23	1:C:344:SER:CB	1.69	1.23
1:C:339:LEU:CD2	1:C:344:SER:HB3	1.72	1.20
1:D:372:ILE:O	1:D:380:LEU:HD23	1.36	1.19
1:B:342:THR:CG2	1:B:396:MET:HB3	1.74	1.17
1:C:364:MET:CG	1:C:365:PRO:HD2	1.74	1.16
1:B:342:THR:HG21	1:B:396:MET:HB3	1.29	1.14
1:C:364:MET:HG2	1:C:365:PRO:HD2	1.15	1.13
1:B:342:THR:HG21	1:B:396:MET:CB	1.78	1.13
1:B:336:GLY:HA2	1:B:348:LEU:CB	1.78	1.12
1:B:468:ILE:HG21	1:B:533:LEU:HB2	1.27	1.12
1:B:517:ILE:HG13	1:B:518:ASP:H	1.01	1.11
1:A:9:GLY:HA2	1:A:363:PRO:CG	1.81	1.10
1:A:9:GLY:CA	1:A:363:PRO:CG	2.28	1.10
1:C:339:LEU:HD23	1:C:344:SER:HB3	1.12	1.09
1:A:378:LYS:HA	1:A:378:LYS:HE2	1.32	1.07
1:C:364:MET:CG	1:C:365:PRO:CD	2.32	1.07
1:C:347:ILE:HB	1:C:363:PRO:N	1.68	1.06
1:C:364:MET:HG2	1:C:365:PRO:CD	1.85	1.05
1:B:336:GLY:CA	1:B:348:LEU:CB	2.33	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLY:HA3	1:B:348:LEU:HB3	1.35	1.02
1:B:347:ILE:HD12	1:B:390:PHE:HE2	0.85	1.02
1:B:336:GLY:HA2	1:B:348:LEU:HB3	1.03	1.01
1:A:347:ILE:HG12	1:A:363:PRO:HA	1.44	0.99
1:B:470:ILE:HD12	1:B:478:LEU:HB3	1.44	0.99
1:A:9:GLY:HA2	1:A:363:PRO:HG2	1.00	0.98
1:A:380:LEU:HD23	1:A:385:LYS:O	1.63	0.98
1:B:347:ILE:O	1:B:347:ILE:HG22	1.61	0.98
1:B:497:GLN:HG3	1:B:510:LEU:HD11	1.43	0.98
1:B:510:LEU:HD13	1:B:514:VAL:HG23	1.47	0.97
1:D:13:ARG:NH1	1:D:221:ASP:OD2	1.97	0.96
1:D:399:TYR:H	1:D:406:THR:HG22	1.28	0.96
1:B:346:LEU:O	1:B:347:ILE:HB	1.66	0.96
1:A:311:CYS:H	1:A:335:GLN:HG2	1.27	0.96
1:B:470:ILE:HD11	1:B:480:SER:HB2	1.47	0.96
1:B:497:GLN:HG3	1:B:510:LEU:CD1	1.94	0.96
1:B:510:LEU:CD1	1:B:514:VAL:HG23	1.96	0.96
1:B:342:THR:HG21	1:B:396:MET:CA	1.96	0.95
1:B:347:ILE:CD1	1:B:390:PHE:CE2	2.38	0.94
1:B:517:ILE:HG13	1:B:518:ASP:N	1.83	0.94
1:A:334:LEU:O	1:A:335:GLN:HG3	1.66	0.94
1:B:472:ASP:O	1:B:478:LEU:HD13	1.67	0.93
1:B:479:PRO:HD2	1:B:511:ARG:HB2	1.51	0.92
1:C:237:ILE:HD11	1:C:265:PHE:HA	1.54	0.90
1:C:364:MET:HG3	1:C:365:PRO:CD	2.02	0.89
1:A:9:GLY:HA3	1:A:363:PRO:HG2	1.53	0.89
1:A:339:LEU:HB3	1:A:345:ALA:H	1.38	0.89
1:A:382:PRO:HA	1:A:424:TYR:HD1	1.35	0.89
1:B:480:SER:OG	1:B:537:PHE:CZ	2.27	0.88
1:D:347:ILE:HG12	1:D:363:PRO:HA	1.56	0.87
1:B:517:ILE:CG1	1:B:518:ASP:H	1.88	0.87
1:B:468:ILE:CG2	1:B:533:LEU:HB2	2.04	0.87
1:C:107:THR:HG23	1:C:110:GLU:H	1.40	0.87
1:C:347:ILE:CB	1:C:363:PRO:N	2.37	0.87
1:C:399:TYR:H	1:C:406:THR:HG22	1.40	0.86
1:A:423:TYR:O	1:A:424:TYR:CB	2.19	0.86
1:B:517:ILE:HD13	1:B:540:GLU:OE2	1.75	0.86
1:A:9:GLY:HA3	1:A:363:PRO:CG	2.04	0.84
1:B:496:VAL:HB	1:B:514:VAL:HG21	1.59	0.84
1:C:347:ILE:HA	1:C:363:PRO:N	1.91	0.84
1:D:372:ILE:O	1:D:380:LEU:CD2	2.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:VAL:HB	1:B:508:LYS:HD3	1.60	0.84
1:A:385:LYS:HA	1:A:422:GLY:O	1.77	0.84
1:A:342:THR:HG22	1:A:343:CYS:H	1.44	0.82
1:A:423:TYR:O	1:A:424:TYR:O	1.98	0.81
1:D:347:ILE:O	1:D:347:ILE:HG22	1.79	0.81
1:D:337:TYR:CE2	1:D:348:LEU:HA	2.15	0.81
1:B:335:GLN:O	1:B:348:LEU:HB2	1.80	0.81
1:A:311:CYS:N	1:A:335:GLN:HG2	1.95	0.81
1:D:346:LEU:O	1:D:347:ILE:HB	1.81	0.80
1:C:348:LEU:HD12	1:C:364:MET:CE	2.11	0.80
1:C:348:LEU:HD12	1:C:364:MET:HE1	1.62	0.80
1:D:13:ARG:HG3	1:D:221:ASP:OD2	1.82	0.80
1:A:382:PRO:HA	1:A:424:TYR:CD1	2.15	0.80
1:A:423:TYR:O	1:A:424:TYR:HB3	1.80	0.80
1:B:342:THR:CG2	1:B:396:MET:CB	2.47	0.79
1:A:380:LEU:CD2	1:A:385:LYS:O	2.31	0.79
1:A:372:ILE:O	1:A:380:LEU:HD13	1.84	0.78
1:A:399:TYR:H	1:A:406:THR:HG22	1.47	0.78
1:D:13:ARG:HD2	1:D:222:PRO:HD2	1.65	0.78
1:B:441:LYS:HE2	1:B:530:ARG:HB3	1.66	0.77
1:B:429:PHE:O	1:B:431:TYR:N	2.18	0.77
1:C:364:MET:HG3	1:C:365:PRO:HD3	1.66	0.77
1:B:436:LEU:CD1	1:B:450:ALA:H	1.97	0.77
1:D:347:ILE:CD1	1:D:390:PHE:CE1	2.67	0.77
1:C:342:THR:HG22	1:C:343:CYS:H	1.50	0.77
1:A:347:ILE:HG23	1:A:363:PRO:N	2.00	0.76
1:A:307:THR:HG22	1:A:308:GLU:HG3	1.66	0.76
1:C:347:ILE:HG12	1:C:347:ILE:O	1.83	0.76
1:C:429:PHE:HB3	1:C:431:TYR:CE2	2.20	0.76
1:B:346:LEU:O	1:B:347:ILE:CB	2.33	0.76
1:A:378:LYS:CE	1:A:378:LYS:HA	2.03	0.76
1:A:103:ASN:HD22	1:A:241:HIS:CE1	2.04	0.75
1:B:529:MET:HB2	1:B:532:GLU:HB2	1.67	0.75
1:B:453:GLU:O	1:B:457:LEU:HB2	1.86	0.75
1:D:347:ILE:CG2	1:D:432:VAL:HG21	2.16	0.75
1:B:478:LEU:HG	1:B:511:ARG:HB3	1.70	0.74
1:A:334:LEU:C	1:A:335:GLN:HG3	2.07	0.74
1:A:337:TYR:HD2	1:A:348:LEU:HA	1.52	0.74
1:C:364:MET:HG3	1:C:365:PRO:HD2	1.66	0.74
1:D:174:ASP:HB3	1:D:177:LYS:HD3	1.70	0.74
1:D:13:ARG:HH11	1:D:221:ASP:CG	1.91	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:CYS:SG	1:B:129:SER:HB2	2.28	0.73
1:B:335:GLN:C	1:B:348:LEU:HB2	2.09	0.73
1:A:9:GLY:HA3	1:A:363:PRO:CB	2.18	0.73
1:C:347:ILE:HG22	1:C:363:PRO:HA	1.69	0.73
1:A:268:GLU:HA	1:A:271:LEU:HD23	1.71	0.73
1:A:334:LEU:HB3	1:A:349:SER:HB3	1.70	0.73
1:A:9:GLY:HA3	1:A:363:PRO:HB2	1.69	0.73
1:D:268:GLU:OE1	1:D:268:GLU:N	2.20	0.73
1:D:140:LEU:HB3	1:D:142:PHE:CE1	2.24	0.72
1:B:342:THR:HG23	1:B:396:MET:HB3	1.67	0.72
1:A:378:LYS:HE2	1:A:378:LYS:CA	2.18	0.72
1:D:268:GLU:O	1:D:270:PHE:N	2.21	0.72
1:A:268:GLU:C	1:A:270:PHE:H	1.91	0.72
1:B:458:GLN:O	1:B:459:HIS:ND1	2.18	0.72
1:B:480:SER:OG	1:B:537:PHE:CE1	2.41	0.72
1:B:347:ILE:H	1:B:364:MET:HG3	1.53	0.71
1:B:255:VAL:HG23	1:B:257:LEU:HG	1.72	0.71
1:C:224:TYR:CD2	1:C:364:MET:HE2	2.26	0.71
1:A:236:ALA:HB2	1:A:252:TYR:HE2	1.56	0.71
1:A:285:PRO:HD2	1:A:288:ILE:HD11	1.73	0.71
1:B:451:GLU:OE2	1:B:467:VAL:HG23	1.91	0.71
1:B:468:ILE:HG21	1:B:533:LEU:CB	2.15	0.71
1:B:497:GLN:CG	1:B:510:LEU:CD1	2.67	0.71
1:C:348:LEU:CD1	1:C:364:MET:CE	2.69	0.71
1:B:347:ILE:O	1:B:347:ILE:CG2	2.35	0.70
1:C:348:LEU:CD1	1:C:364:MET:HE1	2.20	0.70
1:A:372:ILE:O	1:A:373:ASP:CB	2.38	0.70
1:B:463:SER:HB3	1:B:483:VAL:HG13	1.73	0.70
1:C:342:THR:HG21	1:C:395:LEU:HA	1.73	0.70
1:C:339:LEU:HD21	1:C:344:SER:HB3	1.72	0.70
1:B:11:ARG:CG	1:B:11:ARG:HH11	2.05	0.69
1:B:451:GLU:OE2	1:B:467:VAL:CG2	2.41	0.69
1:D:337:TYR:HE2	1:D:348:LEU:HA	1.55	0.69
1:A:389:CYS:HA	1:A:418:THR:OG1	1.92	0.69
1:B:235:LEU:HB3	1:B:282:ILE:HG22	1.75	0.68
1:A:334:LEU:O	1:A:335:GLN:CG	2.42	0.68
1:C:429:PHE:O	1:C:431:TYR:N	2.25	0.68
1:B:479:PRO:HD2	1:B:511:ARG:CB	2.22	0.68
1:B:510:LEU:HD13	1:B:514:VAL:H	1.59	0.68
1:A:55:GLU:OE2	1:A:59:ARG:HD2	1.93	0.68
1:B:497:GLN:HG3	1:B:510:LEU:HD12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HB3	1:B:142:PHE:CE1	2.29	0.67
1:C:103:ASN:HD22	1:C:241:HIS:CE1	2.12	0.67
1:A:6:ILE:O	1:A:6:ILE:HG22	1.94	0.67
1:A:383:ARG:HA	1:A:423:TYR:HD2	1.58	0.67
1:B:190:ALA:HB2	1:B:209:HIS:CD2	2.30	0.67
1:A:311:CYS:H	1:A:335:GLN:CG	2.02	0.67
1:B:149:ILE:HA	1:B:161:VAL:HG23	1.77	0.67
1:B:500:ILE:HG22	1:B:503:LEU:HD13	1.75	0.67
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.60	0.67
1:C:425:ASP:O	1:C:429:PHE:HB2	1.95	0.67
1:B:510:LEU:HD11	1:B:514:VAL:HG23	1.75	0.67
1:D:17:PHE:CD2	1:D:24:GLN:HB2	2.30	0.67
1:D:268:GLU:C	1:D:270:PHE:H	1.98	0.67
1:C:422:GLY:HA2	1:C:435:ARG:H	1.60	0.66
1:B:436:LEU:HD13	1:B:450:ALA:H	1.59	0.66
1:C:294:LYS:HE3	1:C:323:LYS:NZ	2.11	0.66
1:C:371:VAL:HG13	1:C:380:LEU:HB2	1.76	0.66
1:D:234:ILE:HD12	1:D:281:SER:HB3	1.77	0.66
1:B:286:PRO:HA	1:B:289:MET:HB2	1.75	0.66
1:B:464:ASP:HB2	1:B:484:VAL:HG13	1.77	0.66
1:D:347:ILE:HG22	1:D:432:VAL:HG21	1.76	0.66
1:C:7:VAL:O	1:C:9:GLY:N	2.27	0.66
1:B:472:ASP:C	1:B:478:LEU:HD13	2.16	0.66
1:D:372:ILE:HG22	1:D:379:ALA:N	2.11	0.66
1:A:429:PHE:O	1:A:431:TYR:N	2.26	0.65
1:B:316:LEU:HD21	1:B:525:THR:HG21	1.76	0.65
1:C:74:VAL:HG12	1:C:98:PRO:HB2	1.76	0.65
1:D:347:ILE:CG1	1:D:363:PRO:HA	2.25	0.65
1:D:380:LEU:HD12	1:D:384:GLU:OE2	1.95	0.65
1:D:429:PHE:O	1:D:431:TYR:N	2.28	0.65
1:A:342:THR:HG21	1:A:395:LEU:HA	1.79	0.65
1:A:318:ARG:O	1:A:320:ILE:N	2.30	0.65
1:C:317:GLY:O	1:C:320:ILE:N	2.29	0.65
1:A:230:PRO:O	1:A:231:ASP:HB2	1.96	0.65
1:A:347:ILE:HD12	1:A:390:PHE:CE1	2.31	0.65
1:C:197:GLY:O	1:C:199:THR:N	2.29	0.65
1:C:268:GLU:HA	1:C:271:LEU:HD23	1.78	0.65
1:C:316:LEU:O	1:C:318:ARG:N	2.29	0.65
1:B:455:LEU:HD23	1:B:467:VAL:HG22	1.78	0.65
1:A:311:CYS:O	1:A:335:GLN:HB2	1.97	0.64
1:B:285:PRO:HD2	1:B:288:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LEU:HD12	1:C:202:PRO:HD2	1.80	0.64
1:C:339:LEU:CD2	1:C:344:SER:CB	2.48	0.64
1:B:505:THR:HG22	1:B:506:THR:H	1.62	0.64
1:C:230:PRO:O	1:C:231:ASP:HB2	1.96	0.63
1:B:472:ASP:OD1	1:B:478:LEU:HD22	1.98	0.63
1:B:497:GLN:CG	1:B:510:LEU:HD12	2.27	0.63
1:D:347:ILE:HA	1:D:363:PRO:CA	2.28	0.63
1:D:429:PHE:HB3	1:D:431:TYR:CE2	2.34	0.63
1:B:342:THR:HG21	1:B:396:MET:HA	1.79	0.63
1:B:435:ARG:HH22	1:B:457:LEU:CD2	2.11	0.63
1:B:533:LEU:HD12	1:B:533:LEU:H	1.64	0.63
1:A:59:ARG:NH2	1:A:170:ASP:O	2.31	0.63
1:C:159:GLU:OE1	1:C:167:ARG:NH1	2.32	0.63
1:A:44:THR:O	1:A:45:ASN:HB2	1.99	0.62
1:B:59:ARG:NH2	1:B:170:ASP:O	2.31	0.62
1:B:44:THR:O	1:B:45:ASN:HB2	1.98	0.62
1:B:335:GLN:OE1	1:B:335:GLN:N	2.32	0.62
1:D:103:ASN:HD22	1:D:241:HIS:CE1	2.17	0.62
1:B:205:VAL:HG11	1:B:342:THR:HG23	1.80	0.62
1:B:347:ILE:HD11	1:B:390:PHE:CE2	2.34	0.62
1:A:400:HIS:C	1:A:402:ASN:H	2.03	0.62
1:A:7:VAL:O	1:A:9:GLY:N	2.33	0.62
1:B:510:LEU:HD13	1:B:514:VAL:CG2	2.26	0.62
1:A:125:CYS:O	1:A:149:ILE:HG12	2.00	0.61
1:C:339:LEU:HD23	1:C:344:SER:OG	1.99	0.61
1:A:26:TYR:HB2	1:A:94:TYR:CE1	2.35	0.61
1:B:470:ILE:N	1:B:478:LEU:O	2.31	0.61
1:B:439:LEU:HG	1:B:442:TYR:OH	2.00	0.61
1:C:312:GLY:HA2	1:C:339:LEU:HD11	1.82	0.61
1:B:296:PRO:HB2	1:B:297:LEU:HG	1.81	0.61
1:B:321:ALA:HA	1:B:333:ILE:HD11	1.80	0.61
1:D:325:ALA:HB2	1:D:333:ILE:HG22	1.83	0.61
1:A:27:GLN:HG2	1:D:15:LEU:HD12	1.83	0.61
1:B:521:PRO:HG3	1:B:533:LEU:HD11	1.82	0.61
1:C:347:ILE:CA	1:C:363:PRO:N	2.62	0.61
1:D:346:LEU:O	1:D:347:ILE:CB	2.48	0.61
1:A:334:LEU:C	1:A:335:GLN:CG	2.69	0.61
1:C:264:LYS:HD3	1:C:266:GLU:OE2	2.00	0.61
1:B:383:ARG:HA	1:B:423:TYR:CD2	2.35	0.60
1:B:26:TYR:HB2	1:B:94:TYR:CE1	2.36	0.60
1:B:293:ALA:HB2	1:B:324:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:TYR:O	1:D:295:SER:HB3	2.01	0.60
1:D:287:PRO:O	1:D:290:VAL:HG22	2.01	0.60
1:D:307:THR:HG22	1:D:308:GLU:HG3	1.82	0.60
1:D:74:VAL:HG11	1:D:118:SER:HB2	1.83	0.60
1:B:103:ASN:OD1	1:B:105:MET:N	2.34	0.60
1:B:529:MET:O	1:B:531:ASN:N	2.34	0.60
1:D:194:THR:HA	1:D:204:GLY:HA2	1.83	0.60
1:D:372:ILE:HG22	1:D:379:ALA:HA	1.82	0.60
1:B:347:ILE:HG21	1:B:432:VAL:CG2	2.31	0.60
1:D:9:GLY:HA3	1:D:363:PRO:HB2	1.84	0.60
1:C:425:ASP:OD2	1:C:433:VAL:HG13	2.00	0.60
1:A:400:HIS:O	1:A:402:ASN:N	2.34	0.60
1:B:458:GLN:O	1:B:458:GLN:NE2	2.35	0.59
1:D:372:ILE:HG22	1:D:379:ALA:CA	2.31	0.59
1:A:371:VAL:C	1:A:372:ILE:HG13	2.22	0.59
1:D:385:LYS:HA	1:D:422:GLY:O	2.03	0.59
1:A:371:VAL:HG11	1:A:384:GLU:O	2.02	0.59
1:D:274:ILE:HG13	1:D:279:ILE:HB	1.84	0.59
1:A:130:LEU:HD21	1:A:158:VAL:HG21	1.84	0.59
1:A:102:SER:HA	1:A:114:HIS:CE1	2.38	0.59
1:A:149:ILE:HA	1:A:161:VAL:HG23	1.85	0.59
1:A:293:ALA:HB2	1:A:324:VAL:HG13	1.84	0.59
1:B:11:ARG:NE	1:C:176:VAL:O	2.36	0.59
1:D:422:GLY:HA3	1:D:434:ASP:HA	1.85	0.59
1:D:237:ILE:HG12	1:D:262:VAL:HB	1.84	0.59
1:A:339:LEU:O	1:A:340:THR:HG23	2.03	0.59
1:B:333:ILE:O	1:B:333:ILE:HG13	2.02	0.59
1:B:207:ILE:CD1	1:B:342:THR:HG22	2.32	0.59
1:B:325:ALA:HA	1:B:330:VAL:HG12	1.85	0.59
1:D:338:GLY:O	1:D:339:LEU:O	2.21	0.58
1:D:399:TYR:N	1:D:406:THR:HG22	2.10	0.58
1:B:340:THR:HG21	1:B:395:LEU:HD22	1.85	0.58
1:A:342:THR:HG22	1:A:343:CYS:N	2.14	0.58
1:B:455:LEU:HD11	1:B:465:ALA:HA	1.84	0.58
1:C:106:TYR:HE2	1:C:114:HIS:ND1	2.00	0.58
1:C:348:LEU:CD1	1:C:364:MET:HE3	2.33	0.58
1:B:347:ILE:HG12	1:B:363:PRO:HA	1.85	0.58
1:B:320:ILE:O	1:B:324:VAL:HG22	2.04	0.58
1:B:26:TYR:HB2	1:B:94:TYR:HE1	1.68	0.58
1:D:347:ILE:HD12	1:D:390:PHE:CE1	2.38	0.58
1:B:510:LEU:HD13	1:B:514:VAL:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:THR:HG21	1:B:395:LEU:CD2	2.34	0.58
1:C:311:CYS:O	1:C:335:GLN:NE2	2.32	0.58
1:B:340:THR:O	1:B:340:THR:HG22	2.04	0.57
1:A:372:ILE:O	1:A:373:ASP:HB3	2.03	0.57
1:A:337:TYR:HD2	1:A:348:LEU:CA	2.17	0.57
1:C:11:ARG:HG3	1:C:12:PRO:HD2	1.86	0.57
1:C:228:ILE:HD11	1:C:307:THR:HG21	1.84	0.57
1:B:120:PRO:HD2	1:B:142:PHE:HE2	1.68	0.57
1:D:271:LEU:HD21	1:D:291:TYR:HE2	1.70	0.57
1:B:483:VAL:O	1:B:516:PHE:HA	2.04	0.57
1:C:383:ARG:HA	1:C:423:TYR:CD2	2.40	0.57
1:C:425:ASP:OD2	1:C:433:VAL:HG22	2.05	0.57
1:B:373:ASP:HB3	1:B:375:ASN:H	1.69	0.57
1:D:339:LEU:HD23	1:D:344:SER:HB3	1.85	0.57
1:D:425:ASP:O	1:D:429:PHE:HB2	2.05	0.57
1:A:63:SER:HB3	1:A:164:PHE:CE2	2.40	0.57
1:C:287:PRO:O	1:C:290:VAL:HG22	2.05	0.57
1:C:307:THR:HG22	1:C:308:GLU:HG3	1.87	0.57
1:B:459:HIS:N	1:B:460:PRO:HD3	2.21	0.56
1:B:493:GLU:HA	1:B:514:VAL:HB	1.86	0.56
1:D:342:THR:HG22	1:D:343:CYS:H	1.68	0.56
1:A:27:GLN:HG3	1:D:13:ARG:O	2.05	0.56
1:A:311:CYS:HB3	1:A:335:GLN:NE2	2.20	0.56
1:C:274:ILE:HG13	1:C:279:ILE:HB	1.86	0.56
1:A:148:VAL:O	1:A:161:VAL:HG23	2.06	0.56
1:B:74:VAL:HG12	1:B:120:PRO:HB3	1.88	0.56
1:D:294:LYS:HD3	1:D:323:LYS:HD2	1.87	0.56
1:A:28:SER:OG	1:A:254:PRO:HA	2.05	0.56
1:B:470:ILE:O	1:B:478:LEU:N	2.38	0.56
1:C:293:ALA:HB2	1:C:324:VAL:HG13	1.87	0.56
1:B:399:TYR:H	1:B:406:THR:HG22	1.69	0.56
1:A:268:GLU:O	1:A:270:PHE:N	2.33	0.56
1:A:384:GLU:N	1:A:423:TYR:HB2	2.21	0.56
1:A:429:PHE:HB3	1:A:431:TYR:CE1	2.41	0.56
1:B:373:ASP:HB2	1:B:377:GLY:H	1.71	0.56
1:C:296:PRO:O	1:C:298:VAL:HG13	2.05	0.56
1:B:207:ILE:HD11	1:B:342:THR:HG22	1.88	0.56
1:C:347:ILE:HG22	1:C:363:PRO:CA	2.36	0.56
1:D:59:ARG:NH1	1:D:173:PHE:HB3	2.20	0.56
1:A:346:LEU:C	1:A:347:ILE:HG13	2.27	0.55
1:B:309:ILE:HB	1:B:333:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLN:HB2	1:C:143:LEU:HD23	1.89	0.55
1:A:337:TYR:CD2	1:A:348:LEU:HA	2.38	0.55
1:A:423:TYR:O	1:A:424:TYR:HB2	2.05	0.55
1:B:456:LEU:O	1:B:456:LEU:HG	2.06	0.55
1:C:148:VAL:O	1:C:161:VAL:HG23	2.06	0.55
1:C:314:SER:O	1:C:314:SER:OG	2.22	0.55
1:B:140:LEU:HD13	1:B:142:PHE:CZ	2.41	0.55
1:A:313:GLY:O	1:A:339:LEU:HD11	2.07	0.55
1:B:484:VAL:HG21	1:B:518:ASP:O	2.06	0.55
1:A:326:LYS:HE2	1:C:301:TYR:CE2	2.42	0.55
1:B:313:GLY:O	1:B:339:LEU:HD21	2.07	0.55
1:A:333:ILE:C	1:A:334:LEU:HD13	2.27	0.55
1:B:436:LEU:HD11	1:B:451:GLU:N	2.22	0.54
1:C:284:VAL:HB	1:C:288:ILE:HG13	1.89	0.54
1:D:316:LEU:HD23	1:D:317:GLY:H	1.71	0.54
1:B:473:GLU:N	1:B:478:LEU:HD13	2.22	0.54
1:A:309:ILE:HG12	1:A:330:VAL:HG21	1.90	0.54
1:C:240:PHE:O	1:C:246:LEU:HB2	2.07	0.54
1:C:286:PRO:HA	1:C:289:MET:HB2	1.89	0.54
1:C:347:ILE:HG13	1:C:432:VAL:HG21	1.90	0.54
1:D:399:TYR:H	1:D:406:THR:CG2	2.13	0.54
1:A:11:ARG:HG3	1:A:12:PRO:HD2	1.90	0.54
1:B:198:THR:O	1:B:203:LYS:NZ	2.40	0.54
1:C:203:LYS:HB3	1:C:399:TYR:HD2	1.73	0.54
1:C:422:GLY:HA3	1:C:434:ASP:HA	1.90	0.54
1:B:336:GLY:HA2	1:B:348:LEU:CA	2.38	0.54
1:D:71:HIS:H	1:D:71:HIS:CD2	2.24	0.54
1:A:126:SER:O	1:A:148:VAL:HG13	2.08	0.54
1:B:504:VAL:CB	1:B:508:LYS:HD3	2.36	0.54
1:B:121:CYS:HB2	1:B:144:LYS:HG2	1.89	0.54
1:B:214:ILE:HG21	1:B:394:MET:HB2	1.90	0.54
1:B:435:ARG:NH2	1:B:457:LEU:HD23	2.23	0.54
1:B:519:SER:OG	1:B:520:ILE:N	2.37	0.54
1:D:289:MET:HE3	1:D:333:ILE:HD11	1.89	0.54
1:B:479:PRO:CD	1:B:511:ARG:HG2	2.38	0.54
1:A:388:ILE:HD12	1:A:422:GLY:CA	2.38	0.53
1:C:108:GLU:OE1	1:C:135:LYS:HE3	2.08	0.53
1:B:479:PRO:HD2	1:B:511:ARG:CG	2.38	0.53
1:A:27:GLN:CD	1:D:15:LEU:CD1	2.76	0.53
1:D:425:ASP:HB2	1:D:431:TYR:O	2.08	0.53
1:A:106:TYR:HE2	1:A:114:HIS:ND1	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ASN:O	1:C:263:LYS:HD3	2.08	0.53
1:B:190:ALA:HB2	1:B:209:HIS:HD2	1.73	0.53
1:C:342:THR:HG22	1:C:343:CYS:N	2.22	0.53
1:B:521:PRO:HG2	1:B:528:LEU:HA	1.91	0.53
1:C:253:PHE:HB2	1:C:254:PRO:HD3	1.91	0.53
1:A:159:GLU:CD	1:A:167:ARG:HH11	2.12	0.53
1:A:333:ILE:O	1:A:334:LEU:HD13	2.09	0.53
1:B:449:PRO:HB2	1:B:453:GLU:HB3	1.90	0.53
1:C:222:PRO:O	1:C:227:ARG:HD3	2.09	0.53
1:A:372:ILE:O	1:A:380:LEU:CD1	2.56	0.53
1:A:382:PRO:CA	1:A:424:TYR:CD1	2.90	0.53
1:A:337:TYR:HE2	1:A:349:SER:HB2	1.74	0.53
1:C:286:PRO:O	1:C:289:MET:HB2	2.09	0.53
1:A:429:PHE:HB3	1:A:431:TYR:HE1	1.73	0.53
1:D:11:ARG:HG3	1:D:12:PRO:HD2	1.90	0.53
1:D:347:ILE:HD12	1:D:390:PHE:CZ	2.44	0.53
1:B:436:LEU:HD22	1:B:442:TYR:HD2	1.73	0.53
1:B:470:ILE:CD1	1:B:478:LEU:HB3	2.28	0.53
1:B:479:PRO:HD2	1:B:511:ARG:HG2	1.91	0.53
1:B:335:GLN:C	1:B:348:LEU:CB	2.78	0.52
1:D:342:THR:HG21	1:D:396:MET:N	2.24	0.52
1:A:347:ILE:CD1	1:A:390:PHE:CE1	2.92	0.52
1:D:149:ILE:HA	1:D:161:VAL:HG23	1.90	0.52
1:D:221:ASP:OD1	1:D:223:ILE:HG22	2.10	0.52
1:B:148:VAL:O	1:B:161:VAL:HG23	2.10	0.52
1:A:17:PHE:HZ	1:A:23:LEU:HD23	1.74	0.52
1:B:233:SER:HA	1:B:258:LYS:O	2.10	0.52
1:B:442:TYR:HB2	1:B:448:ALA:O	2.10	0.52
1:D:90:ILE:HA	1:D:93:LEU:HD12	1.92	0.52
1:D:240:PHE:O	1:D:246:LEU:HB2	2.10	0.52
1:D:336:GLY:HA3	1:D:339:LEU:HD11	1.91	0.52
1:A:274:ILE:HG23	1:A:279:ILE:HB	1.91	0.52
1:B:470:ILE:HD12	1:B:478:LEU:CB	2.29	0.52
1:C:189:THR:HG23	1:C:206:VAL:HG13	1.92	0.52
1:D:421:LEU:HG	1:D:436:LEU:HB2	1.92	0.52
1:B:336:GLY:N	1:B:348:LEU:HB3	2.18	0.52
1:B:149:ILE:HA	1:B:161:VAL:CG2	2.40	0.51
1:C:335:GLN:NE2	1:C:336:GLY:N	2.57	0.51
1:B:515:VAL:HB	1:B:537:PHE:CE1	2.44	0.51
1:C:380:LEU:HD12	1:C:384:GLU:OE2	2.11	0.51
1:D:286:PRO:O	1:D:289:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HB3	1:A:142:PHE:CZ	2.45	0.51
1:D:347:ILE:HA	1:D:363:PRO:N	2.25	0.51
1:B:11:ARG:CD	1:C:176:VAL:O	2.58	0.51
1:B:347:ILE:HG21	1:B:432:VAL:HG21	1.93	0.51
1:D:347:ILE:CG2	1:D:347:ILE:O	2.52	0.51
1:A:114:HIS:C	1:A:114:HIS:CD2	2.84	0.51
1:B:119:LYS:HG2	1:B:142:PHE:CD2	2.45	0.51
1:C:26:TYR:HB2	1:C:94:TYR:CE1	2.46	0.51
1:D:347:ILE:HG21	1:D:432:VAL:HG11	1.92	0.51
1:D:372:ILE:CG2	1:D:379:ALA:HA	2.41	0.51
1:B:326:LYS:NZ	1:B:329:LYS:HZ3	2.08	0.51
1:C:130:LEU:HD21	1:C:158:VAL:HG21	1.91	0.51
1:D:13:ARG:NH1	1:D:13:ARG:CG	2.74	0.51
1:D:347:ILE:HG12	1:D:363:PRO:CA	2.36	0.51
1:A:149:ILE:HA	1:A:161:VAL:CG2	2.39	0.51
1:B:436:LEU:HD11	1:B:451:GLU:H	1.76	0.51
1:C:372:ILE:C	1:C:380:LEU:HD23	2.31	0.51
1:A:346:LEU:HD11	1:A:390:PHE:CD2	2.46	0.51
1:D:119:LYS:HA	1:D:142:PHE:CE2	2.46	0.51
1:D:422:GLY:HA2	1:D:435:ARG:H	1.75	0.51
1:A:223:ILE:HG22	1:A:224:TYR:CD1	2.46	0.51
1:A:388:ILE:CD1	1:A:422:GLY:HA3	2.41	0.51
1:B:264:LYS:HD3	1:B:266:GLU:OE1	2.11	0.51
1:B:472:ASP:O	1:B:478:LEU:HB2	2.11	0.51
1:C:102:SER:HA	1:C:114:HIS:CE1	2.46	0.51
1:C:112:ILE:HG23	1:C:140:LEU:HD21	1.93	0.51
1:A:370:LYS:O	1:A:388:ILE:HA	2.11	0.50
1:A:389:CYS:HB2	1:A:416:LEU:O	2.12	0.50
1:C:95:GLN:O	1:C:181:LYS:HE3	2.12	0.50
1:C:334:LEU:HB3	1:C:349:SER:HB3	1.93	0.50
1:B:264:LYS:HE2	1:B:265:PHE:CZ	2.47	0.50
1:B:455:LEU:CD2	1:B:467:VAL:HG22	2.42	0.50
1:B:472:ASP:O	1:B:478:LEU:CD1	2.51	0.50
1:A:17:PHE:CD2	1:A:24:GLN:HB2	2.47	0.50
1:B:234:ILE:HG13	1:B:235:LEU:N	2.27	0.50
1:B:318:ARG:HG2	1:B:319:ASP:OD1	2.12	0.50
1:A:311:CYS:HB3	1:A:335:GLN:HE21	1.75	0.50
1:B:497:GLN:O	1:B:501:ALA:HB2	2.11	0.50
1:B:507:THR:HB	1:B:511:ARG:NH1	2.27	0.50
1:B:482:CYS:HA	1:B:515:VAL:HG12	1.94	0.50
1:C:271:LEU:O	1:C:274:ILE:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HB3	1:A:142:PHE:CE1	2.47	0.50
1:B:371:VAL:HG23	1:B:380:LEU:HB2	1.93	0.50
1:A:325:ALA:HB2	1:A:333:ILE:HG22	1.94	0.50
1:B:426:GLU:O	1:B:430:ILE:N	2.45	0.50
1:C:293:ALA:O	1:C:327:ARG:NH1	2.34	0.50
1:A:313:GLY:O	1:A:339:LEU:CD1	2.59	0.50
1:A:313:GLY:O	1:A:315:PRO:HD3	2.12	0.50
1:B:449:PRO:HB2	1:B:453:GLU:CB	2.40	0.50
1:A:334:LEU:HG	1:A:349:SER:OG	2.12	0.49
1:D:405:ALA:HA	1:D:408:ASP:HB3	1.92	0.49
1:A:125:CYS:SG	1:A:126:SER:N	2.85	0.49
1:B:283:VAL:HG22	1:B:310:ALA:HB3	1.92	0.49
1:B:309:ILE:HG12	1:B:330:VAL:HG21	1.93	0.49
1:D:347:ILE:HD11	1:D:390:PHE:CE1	2.47	0.49
1:D:86:PHE:HB3	1:D:90:ILE:HD12	1.94	0.49
1:A:27:GLN:CD	1:D:15:LEU:HD12	2.33	0.49
1:B:446:GLN:O	1:B:447:VAL:O	2.30	0.49
1:D:388:ILE:O	1:D:418:THR:HB	2.13	0.49
1:A:27:GLN:CG	1:D:15:LEU:HD12	2.43	0.49
1:A:334:LEU:O	1:A:335:GLN:CB	2.60	0.49
1:A:288:ILE:O	1:A:292:LEU:HG	2.12	0.49
1:B:297:LEU:HB3	1:B:300:GLU:HG3	1.95	0.49
1:D:264:LYS:HD3	1:D:266:GLU:OE1	2.12	0.49
1:B:531:ASN:ND2	1:B:531:ASN:H	2.11	0.49
1:C:373:ASP:HB3	1:C:377:GLY:H	1.77	0.49
1:D:107:THR:HG23	1:D:109:ARG:HB3	1.94	0.49
1:A:286:PRO:HA	1:A:289:MET:HB2	1.94	0.49
1:A:364:MET:O	1:A:367:VAL:HB	2.11	0.49
1:B:159:GLU:OE1	1:B:167:ARG:NH1	2.42	0.49
1:B:462:ILE:HG13	1:B:462:ILE:O	2.10	0.49
1:A:14:ASP:OD2	1:D:31:LYS:HE3	2.12	0.49
1:A:61:ALA:HB1	1:A:95:GLN:HE21	1.78	0.49
1:B:367:VAL:HA	1:B:392:SER:HB2	1.94	0.49
1:C:402:ASN:O	1:C:406:THR:HG23	2.12	0.49
1:C:382:PRO:HA	1:C:424:TYR:CB	2.43	0.49
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.78	0.49
1:D:372:ILE:HA	1:D:379:ALA:HA	1.94	0.49
1:C:294:LYS:HE3	1:C:323:LYS:HZ2	1.75	0.48
1:B:335:GLN:H	1:B:335:GLN:CD	2.12	0.48
1:B:455:LEU:HD21	1:B:466:GLY:N	2.28	0.48
1:A:306:LEU:HG	1:A:309:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:HG13	1:B:279:ILE:HB	1.96	0.48
1:B:234:ILE:HD12	1:B:281:SER:HB3	1.95	0.48
1:B:8:ASN:O	1:B:367:VAL:O	2.30	0.48
1:B:11:ARG:HD3	1:C:176:VAL:O	2.13	0.48
1:D:294:LYS:HD3	1:D:323:LYS:HE3	1.94	0.48
1:D:347:ILE:CG2	1:D:432:VAL:CG2	2.90	0.48
1:B:426:GLU:HB3	1:B:429:PHE:HD2	1.76	0.48
1:C:292:LEU:HB3	1:C:324:VAL:HG11	1.94	0.48
1:A:234:ILE:HG13	1:A:235:LEU:N	2.29	0.48
1:A:218:HIS:HB3	1:A:364:MET:HE1	1.96	0.48
1:A:396:MET:HE2	1:A:416:LEU:HD11	1.95	0.48
1:B:435:ARG:NH2	1:B:457:LEU:CD2	2.76	0.48
1:B:77:ILE:HG22	1:B:99:MET:SD	2.54	0.48
1:A:374:ILE:H	1:A:374:ILE:HG13	1.49	0.48
1:B:478:LEU:HG	1:B:511:ARG:CB	2.40	0.48
1:A:388:ILE:HD12	1:A:422:GLY:HA3	1.96	0.48
1:D:114:HIS:CD2	1:D:114:HIS:C	2.85	0.48
1:D:13:ARG:CG	1:D:13:ARG:HH11	2.25	0.48
1:D:190:ALA:HB2	1:D:209:HIS:CD2	2.48	0.48
1:D:211:SER:HA	1:D:394:MET:HA	1.96	0.48
1:A:382:PRO:CA	1:A:424:TYR:HD1	2.16	0.48
1:B:199:THR:OG1	1:B:203:LYS:NZ	2.45	0.48
1:B:342:THR:HB	1:B:343:CYS:H	1.43	0.48
1:C:197:GLY:HA3	1:C:341:GLU:OE1	2.14	0.48
1:A:240:PHE:O	1:A:246:LEU:HB2	2.14	0.48
1:A:268:GLU:C	1:A:270:PHE:N	2.62	0.48
1:C:235:LEU:HD21	1:C:237:ILE:HB	1.96	0.48
1:D:271:LEU:H	1:D:271:LEU:HD22	1.79	0.48
1:B:9:GLY:HA2	1:B:363:PRO:HB2	1.95	0.47
1:C:185:PRO:HG2	1:C:210:ARG:NH2	2.29	0.47
1:A:176:VAL:O	1:D:11:ARG:NH1	2.47	0.47
1:B:336:GLY:N	1:B:348:LEU:CB	2.75	0.47
1:C:114:HIS:C	1:C:114:HIS:CD2	2.88	0.47
1:D:315:PRO:HG3	1:D:335:GLN:HE22	1.80	0.47
1:B:137:GLN:HG2	1:B:137:GLN:O	2.15	0.47
1:B:496:VAL:CB	1:B:514:VAL:HG21	2.39	0.47
1:A:236:ALA:HB2	1:A:252:TYR:CE2	2.44	0.47
1:C:372:ILE:HD11	1:C:387:GLU:HB3	1.96	0.47
1:D:251:ALA:O	1:D:254:PRO:HD2	2.14	0.47
1:D:36:THR:HA	1:D:49:SER:HB2	1.97	0.47
1:D:230:PRO:O	1:D:231:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:HD12	1:A:422:GLY:N	2.30	0.47
1:B:119:LYS:HA	1:B:142:PHE:CE2	2.50	0.47
1:D:371:VAL:O	1:D:371:VAL:HG13	2.15	0.47
1:D:372:ILE:HG22	1:D:378:LYS:C	2.35	0.47
1:D:422:GLY:CA	1:D:435:ARG:H	2.28	0.47
1:A:63:SER:OG	1:A:165:VAL:HA	2.15	0.47
1:A:399:TYR:CD1	1:A:399:TYR:N	2.83	0.46
1:C:284:VAL:O	1:C:311:CYS:HA	2.16	0.46
1:D:28:SER:OG	1:D:254:PRO:HA	2.15	0.46
1:D:334:LEU:HB3	1:D:349:SER:HB3	1.96	0.46
1:A:159:GLU:OE1	1:A:167:ARG:NH1	2.49	0.46
1:A:342:THR:CG2	1:A:343:CYS:H	2.23	0.46
1:B:506:THR:O	1:B:507:THR:HG23	2.15	0.46
1:C:214:ILE:O	1:C:217:VAL:HB	2.16	0.46
1:C:211:SER:HA	1:C:394:MET:HA	1.96	0.46
1:D:203:LYS:HD3	1:D:399:TYR:HE2	1.80	0.46
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.81	0.46
1:C:382:PRO:HA	1:C:424:TYR:CG	2.50	0.46
1:B:147:ILE:HA	1:B:159:GLU:O	2.14	0.46
1:B:481:ALA:CB	1:B:510:LEU:HD22	2.45	0.46
1:C:318:ARG:HA	1:C:319:ASP:HA	1.60	0.46
1:B:13:ARG:NH1	1:B:221:ASP:OD2	2.48	0.46
1:D:13:ARG:NH1	1:D:221:ASP:CG	2.61	0.46
1:A:230:PRO:HB3	1:A:255:VAL:O	2.15	0.46
1:B:271:LEU:CD1	1:B:303:LEU:HD11	2.46	0.46
1:B:288:ILE:O	1:B:292:LEU:HB2	2.15	0.46
1:B:84:HIS:O	1:B:88:PRO:HD2	2.16	0.46
1:C:399:TYR:N	1:C:399:TYR:CD1	2.84	0.46
1:C:385:LYS:HA	1:C:422:GLY:O	2.15	0.46
1:D:293:ALA:HB2	1:D:324:VAL:HG13	1.97	0.46
1:B:446:GLN:O	1:B:446:GLN:HG3	2.16	0.46
1:B:8:ASN:O	1:B:368:GLN:HA	2.15	0.46
1:B:91:ALA:HA	1:B:94:TYR:CD2	2.51	0.46
1:C:213:THR:O	1:C:217:VAL:HG23	2.15	0.46
1:A:372:ILE:O	1:A:373:ASP:HB2	2.16	0.46
1:D:112:ILE:HG23	1:D:140:LEU:HD21	1.97	0.46
1:B:274:ILE:HG23	1:B:303:LEU:HD22	1.97	0.46
1:C:364:MET:CG	1:C:365:PRO:HD3	2.29	0.46
1:C:341:GLU:HB2	1:C:396:MET:HE1	1.98	0.46
1:C:41:ASP:CG	1:C:44:THR:HG23	2.35	0.46
1:A:253:PHE:HB2	1:A:254:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PHE:O	1:B:213:THR:HG21	2.16	0.46
1:B:306:LEU:HD12	1:B:306:LEU:HA	1.71	0.46
1:B:373:ASP:HB2	1:B:377:GLY:N	2.31	0.46
1:B:492:THR:O	1:B:496:VAL:HG23	2.15	0.46
1:C:96:GLY:HA3	1:C:188:ARG:NH1	2.31	0.46
1:A:318:ARG:O	1:A:318:ARG:HG3	2.16	0.45
1:B:319:ASP:N	1:B:319:ASP:OD1	2.49	0.45
1:B:484:VAL:HG11	1:B:519:SER:O	2.16	0.45
1:A:90:ILE:HA	1:A:93:LEU:HD12	1.98	0.45
1:C:389:CYS:HB3	1:C:417:HIS:HA	1.97	0.45
1:A:190:ALA:HB2	1:A:209:HIS:CD2	2.51	0.45
1:A:16:VAL:HA	1:A:217:VAL:CG2	2.47	0.45
1:B:313:GLY:O	1:B:315:PRO:HD3	2.17	0.45
1:C:231:ASP:OD1	1:C:258:LYS:HE2	2.16	0.45
1:C:286:PRO:HG2	1:C:287:PRO:HD3	1.97	0.45
1:C:371:VAL:HG21	1:C:384:GLU:O	2.16	0.45
1:D:210:ARG:NH1	1:D:393:GLN:OE1	2.49	0.45
1:A:269:PHE:HA	1:A:272:LYS:HB3	1.98	0.45
1:A:381:GLY:C	1:A:424:TYR:CD1	2.90	0.45
1:C:159:GLU:HG2	1:C:163:SER:HB2	1.97	0.45
1:C:346:LEU:O	1:C:346:LEU:HD12	2.16	0.45
1:D:16:VAL:O	1:D:16:VAL:HG13	2.15	0.45
1:A:84:HIS:HB2	1:A:149:ILE:HD12	1.98	0.45
1:B:319:ASP:O	1:B:323:LYS:HG3	2.16	0.45
1:B:205:VAL:CG1	1:B:342:THR:HG23	2.46	0.45
1:B:78:CYS:HB3	1:B:133:ILE:HD11	1.99	0.45
1:C:291:TYR:O	1:C:295:SER:HB3	2.16	0.45
1:A:370:LYS:HG2	1:A:415:TRP:CZ3	2.52	0.45
1:A:372:ILE:HD12	1:A:373:ASP:O	2.16	0.45
1:A:71:HIS:CD2	1:A:71:HIS:H	2.33	0.45
1:B:280:ALA:O	1:B:306:LEU:HD12	2.17	0.45
1:C:83:ILE:H	1:C:83:ILE:HG12	1.52	0.45
1:A:296:PRO:O	1:A:298:VAL:HG13	2.17	0.45
1:B:307:THR:HG22	1:B:308:GLU:HG3	1.99	0.45
1:B:511:ARG:HA	1:B:511:ARG:HD3	1.37	0.45
1:A:74:VAL:HG12	1:A:120:PRO:HB3	1.98	0.45
1:B:102:SER:HA	1:B:114:HIS:HE1	1.81	0.45
1:B:454:ASN:OD1	1:B:455:LEU:N	2.50	0.45
1:C:139:HIS:O	1:C:140:LEU:HD23	2.16	0.45
1:C:296:PRO:HB2	1:C:297:LEU:HG	1.99	0.45
1:D:9:GLY:HA2	1:D:363:PRO:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:HD1	1:A:399:TYR:N	2.15	0.45
1:B:402:ASN:O	1:B:406:THR:HG23	2.17	0.45
1:C:234:ILE:HG13	1:C:235:LEU:N	2.32	0.45
1:C:59:ARG:NH2	1:C:170:ASP:O	2.50	0.45
1:A:268:GLU:HB2	1:A:269:PHE:H	1.38	0.44
1:B:439:LEU:HA	1:B:442:TYR:CE2	2.52	0.44
1:B:501:ALA:HA	1:B:509:HIS:CD2	2.52	0.44
1:B:510:LEU:HD22	1:B:514:VAL:HG22	1.98	0.44
1:C:372:ILE:HB	1:C:373:ASP:H	1.60	0.44
1:D:303:LEU:HD12	1:D:328:LEU:HD21	1.99	0.44
1:D:75:VAL:HG12	1:D:122:LEU:HB3	1.98	0.44
1:A:271:LEU:HD21	1:A:291:TYR:HE2	1.81	0.44
1:D:268:GLU:C	1:D:270:PHE:N	2.65	0.44
1:D:286:PRO:HD3	1:D:311:CYS:SG	2.57	0.44
1:A:107:THR:HG23	1:A:109:ARG:HB3	2.00	0.44
1:A:284:VAL:HB	1:A:288:ILE:HG13	1.99	0.44
1:B:251:ALA:O	1:B:254:PRO:HD2	2.17	0.44
1:B:435:ARG:HH22	1:B:457:LEU:HD23	1.79	0.44
1:D:323:LYS:O	1:D:327:ARG:HG3	2.17	0.44
1:D:49:SER:N	1:D:52:GLN:OE1	2.42	0.44
1:A:286:PRO:HG2	1:A:287:PRO:HD3	1.98	0.44
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.86	0.44
1:B:215:ARG:NH2	1:B:248:THR:HG22	2.32	0.44
1:B:207:ILE:HD13	1:B:342:THR:HG22	1.99	0.44
1:D:228:ILE:HG12	1:D:229:ALA:N	2.32	0.44
1:A:210:ARG:O	1:A:214:ILE:HG13	2.18	0.44
1:B:215:ARG:HH21	1:B:248:THR:HG22	1.82	0.44
1:D:402:ASN:O	1:D:406:THR:HG23	2.18	0.44
1:A:422:GLY:CA	1:A:434:ASP:HA	2.48	0.44
1:B:336:GLY:HA3	1:B:348:LEU:HD23	1.99	0.44
1:B:454:ASN:O	1:B:456:LEU:N	2.51	0.44
1:B:457:LEU:HA	1:B:457:LEU:HD13	1.75	0.44
1:A:102:SER:HA	1:A:114:HIS:HE1	1.83	0.44
1:A:382:PRO:HB3	1:A:426:GLU:HA	2.00	0.44
1:A:18:PRO:O	1:A:185:PRO:HG3	2.17	0.44
1:B:102:SER:HA	1:B:114:HIS:CE1	2.52	0.44
1:D:9:GLY:HA2	1:D:363:PRO:HG2	2.00	0.44
1:B:211:SER:O	1:B:215:ARG:HB2	2.18	0.44
1:B:441:LYS:HE2	1:B:530:ARG:CB	2.41	0.44
1:C:36:THR:HA	1:C:49:SER:HB2	1.99	0.44
1:D:380:LEU:HD12	1:D:384:GLU:CD	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.80	0.43
1:A:326:LYS:HA	1:A:326:LYS:NZ	2.32	0.43
1:A:41:ASP:HB3	1:A:44:THR:HG23	2.00	0.43
1:C:399:TYR:N	1:C:399:TYR:HD1	2.15	0.43
1:B:13:ARG:HH11	1:B:13:ARG:HG3	1.83	0.43
1:C:364:MET:HG2	1:C:365:PRO:N	2.29	0.43
1:C:7:VAL:HB	1:C:369:VAL:HG13	2.00	0.43
1:D:338:GLY:O	1:D:339:LEU:C	2.56	0.43
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.73	0.43
1:B:16:VAL:HA	1:B:217:VAL:HG21	2.01	0.43
1:B:493:GLU:HG3	1:B:513:GLY:CA	2.49	0.43
1:D:79:SER:OG	1:D:126:SER:HB2	2.18	0.43
1:A:224:TYR:CD2	1:A:364:MET:HE3	2.53	0.43
1:D:186:LEU:O	1:D:186:LEU:HD23	2.18	0.43
1:A:348:LEU:CD1	1:A:348:LEU:N	2.82	0.43
1:B:103:ASN:HD22	1:B:241:HIS:CE1	2.37	0.43
1:C:297:LEU:HB3	1:C:300:GLU:CD	2.38	0.43
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.71	0.43
1:C:274:ILE:HD11	1:C:306:LEU:CD2	2.48	0.43
1:C:315:PRO:CB	1:C:335:GLN:HE22	2.31	0.43
1:C:337:TYR:O	1:C:347:ILE:HG12	2.18	0.43
1:D:313:GLY:O	1:D:315:PRO:HD3	2.18	0.43
1:A:27:GLN:CD	1:D:15:LEU:HD11	2.39	0.43
1:A:378:LYS:HB3	1:A:379:ALA:H	1.69	0.43
1:A:341:GLU:HB2	1:A:396:MET:HE1	1.99	0.43
1:C:288:ILE:O	1:C:292:LEU:HB2	2.19	0.43
1:D:372:ILE:HD12	1:D:373:ASP:N	2.33	0.43
1:D:396:MET:C	1:D:398:GLY:H	2.22	0.43
1:A:83:ILE:HD13	1:A:261:MET:HE1	2.00	0.43
1:C:8:ASN:HA	1:C:368:GLN:HG2	1.99	0.43
1:A:311:CYS:H	1:A:335:GLN:CB	2.31	0.43
1:A:346:LEU:HD11	1:A:390:PHE:CE2	2.54	0.43
1:B:114:HIS:C	1:B:114:HIS:CD2	2.91	0.43
1:B:125:CYS:SG	1:B:126:SER:N	2.92	0.43
1:C:198:THR:HG22	1:C:199:THR:HG23	2.01	0.43
1:D:382:PRO:HA	1:D:424:TYR:HB3	1.99	0.43
1:B:296:PRO:O	1:B:298:VAL:HG13	2.19	0.42
1:B:330:VAL:O	1:B:332:GLY:N	2.52	0.42
1:B:336:GLY:HA3	1:B:348:LEU:CB	2.26	0.42
1:B:41:ASP:OD1	1:B:43:HIS:HB2	2.19	0.42
1:B:481:ALA:HB2	1:B:510:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:VAL:HG21	1:D:288:ILE:HG22	2.01	0.42
1:D:339:LEU:H	1:D:339:LEU:HD12	1.84	0.42
1:B:24:GLN:OE1	1:B:216:PHE:HD2	2.01	0.42
1:C:234:ILE:HD12	1:C:281:SER:HB3	2.01	0.42
1:B:335:GLN:O	1:B:348:LEU:CB	2.58	0.42
1:A:201:LEU:HD12	1:A:202:PRO:HD2	2.02	0.42
1:C:274:ILE:HD12	1:C:282:ILE:HG21	2.01	0.42
1:C:39:ILE:HB	1:C:83:ILE:HG23	2.00	0.42
1:D:286:PRO:HA	1:D:289:MET:HB2	2.00	0.42
1:D:309:ILE:HB	1:D:333:ILE:HD12	2.00	0.42
1:A:203:LYS:HD2	1:A:399:TYR:CD2	2.55	0.42
1:A:337:TYR:HD2	1:A:348:LEU:C	2.22	0.42
1:B:107:THR:HG22	1:B:110:GLU:HG3	2.01	0.42
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.50	0.42
1:B:436:LEU:HD22	1:B:442:TYR:CD2	2.51	0.42
1:B:9:GLY:CA	1:B:363:PRO:HB2	2.49	0.42
1:D:268:GLU:HG2	1:D:269:PHE:N	2.35	0.42
1:A:179:ASN:HA	1:A:180:PRO:HD3	1.91	0.42
1:A:32:TYR:HB3	1:A:35:ILE:HD12	2.01	0.42
1:B:229:ALA:HA	1:B:230:PRO:HD2	1.76	0.42
1:A:271:LEU:HB3	1:A:301:TYR:CD1	2.55	0.42
1:B:215:ARG:HA	1:B:215:ARG:HD2	1.78	0.42
1:B:322:ASP:OD1	1:B:322:ASP:N	2.52	0.42
1:B:470:ILE:H	1:B:470:ILE:HG13	1.52	0.42
1:C:309:ILE:HG12	1:C:330:VAL:HG21	2.02	0.42
1:C:71:HIS:CD2	1:C:71:HIS:H	2.36	0.42
1:A:107:THR:HG23	1:A:110:GLU:H	1.84	0.42
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.90	0.42
1:B:101:THR:HG21	1:B:246:LEU:CD1	2.50	0.42
1:B:326:LYS:HA	1:B:326:LYS:HD2	1.69	0.42
1:B:485:LEU:HD13	1:B:489:LYS:O	2.20	0.42
1:C:185:PRO:O	1:C:210:ARG:N	2.48	0.42
1:C:330:VAL:O	1:C:332:GLY:N	2.44	0.42
1:A:127:LYS:HB2	1:A:150:ASP:OD1	2.19	0.41
1:A:233:SER:HA	1:A:258:LYS:O	2.19	0.41
1:A:389:CYS:HB3	1:A:417:HIS:HA	2.01	0.41
1:A:203:LYS:HD2	1:A:399:TYR:CE2	2.55	0.41
1:A:59:ARG:HB3	1:A:165:VAL:CG1	2.50	0.41
1:B:479:PRO:HG2	1:B:480:SER:H	1.85	0.41
1:C:335:GLN:HB2	1:C:336:GLY:H	1.66	0.41
1:C:423:TYR:HD2	1:C:424:TYR:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:LEU:C	1:D:305:SER:H	2.23	0.41
1:A:289:MET:HE3	1:A:333:ILE:CD1	2.50	0.41
1:A:347:ILE:HD12	1:A:390:PHE:HE1	1.83	0.41
1:B:183:PHE:CE2	1:B:188:ARG:HG2	2.55	0.41
1:B:439:LEU:HA	1:B:442:TYR:HE2	1.85	0.41
1:B:460:PRO:HA	1:B:461:ASN:HA	1.75	0.41
1:B:466:GLY:HA3	1:B:482:CYS:H	1.85	0.41
1:B:82:ASN:O	1:B:84:HIS:N	2.52	0.41
1:B:11:ARG:HD3	1:C:176:VAL:HG12	2.01	0.41
1:C:347:ILE:HG13	1:C:432:VAL:CG2	2.50	0.41
1:D:271:LEU:O	1:D:274:ILE:HG22	2.20	0.41
1:D:348:LEU:HB2	1:D:349:SER:H	1.68	0.41
1:A:339:LEU:O	1:A:340:THR:CG2	2.66	0.41
1:B:198:THR:O	1:B:200:GLY:N	2.49	0.41
1:B:284:VAL:HB	1:B:288:ILE:HD11	2.02	0.41
1:B:349:SER:OG	1:B:349:SER:O	2.29	0.41
1:A:287:PRO:O	1:A:290:VAL:HG22	2.20	0.41
1:B:337:TYR:C	1:B:337:TYR:CD2	2.93	0.41
1:C:372:ILE:O	1:C:386:GLY:HA3	2.21	0.41
1:D:382:PRO:HA	1:D:424:TYR:CB	2.51	0.41
1:A:112:ILE:HG23	1:A:140:LEU:CD2	2.51	0.41
1:A:41:ASP:HB2	1:A:83:ILE:HD11	2.01	0.41
1:A:385:LYS:HB3	1:A:421:LEU:HD13	2.01	0.41
1:B:453:GLU:O	1:B:457:LEU:HD23	2.20	0.41
1:D:134:LEU:HA	1:D:134:LEU:HD23	1.85	0.41
1:A:431:TYR:HE2	1:A:433:VAL:HG23	1.86	0.41
1:B:236:ALA:O	1:B:261:MET:HA	2.21	0.41
1:B:473:GLU:H	1:B:478:LEU:HD13	1.85	0.41
1:B:497:GLN:CG	1:B:510:LEU:HD11	2.29	0.41
1:C:20:THR:HG23	1:C:23:LEU:CB	2.50	0.41
1:C:315:PRO:CG	1:C:336:GLY:HA3	2.51	0.41
1:A:383:ARG:HA	1:A:423:TYR:CD2	2.48	0.41
1:B:383:ARG:HA	1:B:423:TYR:HD2	1.80	0.41
1:C:149:ILE:HA	1:C:161:VAL:HG23	2.01	0.41
1:C:339:LEU:CD2	1:C:344:SER:OG	2.66	0.41
1:D:186:LEU:HD11	1:D:393:GLN:HG2	2.03	0.41
1:D:199:THR:OG1	1:D:200:GLY:N	2.51	0.41
1:D:59:ARG:HH12	1:D:173:PHE:HB3	1.84	0.41
1:D:69:LEU:HD23	1:D:69:LEU:HA	1.82	0.41
1:A:370:LYS:HE2	1:A:415:TRP:CD2	2.56	0.41
1:B:486:GLU:HB2	1:B:487:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLU:CD	1:C:135:LYS:HE3	2.41	0.41
1:C:179:ASN:HA	1:C:180:PRO:HD3	1.89	0.41
1:C:190:ALA:HB2	1:C:209:HIS:CD2	2.56	0.41
1:D:347:ILE:HA	1:D:363:PRO:HA	2.01	0.41
1:A:36:THR:HA	1:A:49:SER:HB2	2.03	0.41
1:B:235:LEU:HD21	1:B:237:ILE:HB	2.03	0.41
1:B:81:ASN:HB2	1:B:263:LYS:HA	2.02	0.41
1:B:420:ASP:N	1:B:420:ASP:OD1	2.54	0.41
1:C:149:ILE:HA	1:C:161:VAL:CG2	2.50	0.41
1:D:120:PRO:HD2	1:D:142:PHE:HE2	1.85	0.41
1:D:271:LEU:HA	1:D:274:ILE:HG22	2.02	0.41
1:D:425:ASP:OD1	1:D:433:VAL:HG22	2.20	0.41
1:D:83:ILE:HG12	1:D:83:ILE:H	1.64	0.41
1:D:61:ALA:HB1	1:D:95:GLN:NE2	2.36	0.41
1:A:330:VAL:O	1:A:332:GLY:N	2.47	0.41
1:A:347:ILE:C	1:A:348:LEU:HD12	2.42	0.41
1:C:122:LEU:HD12	1:C:145:LYS:O	2.21	0.41
1:D:296:PRO:O	1:D:298:VAL:HG13	2.21	0.41
1:D:395:LEU:HD23	1:D:395:LEU:HA	1.79	0.41
1:A:185:PRO:O	1:A:210:ARG:N	2.52	0.40
1:A:196:SER:O	1:A:200:GLY:HA2	2.21	0.40
1:A:284:VAL:HB	1:A:288:ILE:CD1	2.51	0.40
1:B:388:ILE:HG22	1:B:418:THR:HG21	2.02	0.40
1:B:455:LEU:HD23	1:B:467:VAL:CG2	2.50	0.40
1:B:493:GLU:HG3	1:B:514:VAL:N	2.37	0.40
1:D:145:LYS:HE2	1:D:159:GLU:OE1	2.20	0.40
1:D:268:GLU:HA	1:D:271:LEU:HD23	2.03	0.40
1:A:346:LEU:HD12	1:A:347:ILE:HG13	2.03	0.40
1:A:423:TYR:C	1:A:424:TYR:O	2.59	0.40
1:B:270:PHE:O	1:B:274:ILE:HG22	2.20	0.40
1:A:422:GLY:HA2	1:A:434:ASP:HA	2.03	0.40
1:B:335:GLN:OE1	1:B:335:GLN:CA	2.70	0.40
1:B:347:ILE:CG1	1:B:363:PRO:HA	2.50	0.40
1:B:380:LEU:HB3	1:B:381:GLY:H	1.60	0.40
1:B:479:PRO:O	1:B:480:SER:HB3	2.21	0.40
1:B:58:CYS:O	1:B:62:VAL:HG23	2.21	0.40
1:B:71:HIS:HB3	1:B:188:ARG:NH1	2.36	0.40
1:D:76:ALA:HA	1:D:100:ALA:O	2.21	0.40
1:A:306:LEU:HA	1:A:306:LEU:HD12	1.87	0.40
1:B:193:MET:HE1	1:B:246:LEU:HD13	2.03	0.40
1:C:103:ASN:ND2	1:C:241:HIS:CE1	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ILE:HD12	1:C:284:VAL:HG11	2.04	0.40
1:D:18:PRO:O	1:D:185:PRO:HG3	2.20	0.40
1:B:372:ILE:O	1:B:386:GLY:HA3	2.21	0.40
1:C:223:ILE:HG22	1:C:224:TYR:CD1	2.56	0.40
1:C:20:THR:HG23	1:C:23:LEU:HB2	2.02	0.40
1:C:255:VAL:HG23	1:C:257:LEU:HG	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/546 (76%)	342 (82%)	54 (13%)	19 (5%)	2	23
1	B	524/546 (96%)	397 (76%)	88 (17%)	39 (7%)	1	13
1	C	413/546 (76%)	355 (86%)	43 (10%)	15 (4%)	3	29
1	D	412/546 (76%)	343 (83%)	54 (13%)	15 (4%)	3	29
All	All	1764/2184 (81%)	1437 (82%)	239 (14%)	88 (5%)	2	21

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	231	ASP
1	A	319	ASP
1	A	378	LYS
1	A	379	ALA
1	A	401	ASN
1	A	430	ILE
1	B	83	ILE
1	B	344	SER

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Mol	Chain	Res	Type
1	B	347	ILE
1	B	430	ILE
1	B	437	LYS
1	B	446	GLN
1	B	447	VAL
1	B	460	PRO
1	B	479	PRO
1	B	530	ARG
1	C	198	THR
1	C	231	ASP
1	C	317	GLY
1	C	372	ILE
1	C	430	ILE
1	D	203	LYS
1	D	231	ASP
1	D	268	GLU
1	D	336	GLY
1	D	339	LEU
1	D	347	ILE
1	D	430	ILE
1	A	71	HIS
1	A	265	PHE
1	A	267	GLY
1	A	268	GLU
1	A	332	GLY
1	A	335	GLN
1	A	347	ILE
1	A	372	ILE
1	A	373	ASP
1	B	5	ASN
1	B	199	THR
1	B	319	ASP
1	B	442	TYR
1	B	465	ALA
1	B	514	VAL
1	B	522	LYS
1	B	543	LYS
1	C	8	ASN
1	C	71	HIS
1	C	332	GLY
1	D	71	HIS
1	D	332	GLY

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Mol	Chain	Res	Type
1	B	231	ASP
1	B	342	THR
1	B	400	HIS
1	B	467	VAL
1	B	525	THR
1	C	335	GLN
1	C	336	GLY
1	D	269	PHE
1	D	372	ILE
1	A	331	HIS
1	A	424	TYR
1	B	45	ASN
1	B	425	ASP
1	B	511	ARG
1	B	520	ILE
1	B	538	ALA
1	C	331	HIS
1	C	400	HIS
1	D	318	ARG
1	A	269	PHE
1	B	8	ASN
1	B	55	GLU
1	B	318	ARG
1	B	345	ALA
1	B	458	GLN
1	B	486	GLU
1	B	521	PRO
1	B	523	GLY
1	D	10	ASP
1	B	376	THR
1	B	528	LEU
1	C	347	ILE
1	D	200	GLY
1	D	230	PRO
1	B	237	ILE
1	C	225	GLY
1	C	230	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	A	365/471 (78%)	341 (93%)	24 (7%)	16	51
1	B	456/471 (97%)	389 (85%)	67 (15%)	3	20
1	C	363/471 (77%)	347 (96%)	16 (4%)	28	63
1	D	362/471 (77%)	345 (95%)	17 (5%)	26	61
All	All	1546/1884 (82%)	1422 (92%)	124 (8%)	12	43

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	44	THR
1	A	118	SER
1	A	128	LYS
1	A	141	ASP
1	A	196	SER
1	A	223	ILE
1	A	268	GLU
1	A	288	ILE
1	A	306	LEU
1	A	316	LEU
1	A	318	ARG
1	A	334	LEU
1	A	335	GLN
1	A	339	LEU
1	A	343	CYS
1	A	374	ILE
1	A	378	LYS
1	A	380	LEU
1	A	412	LYS
1	A	418	THR
1	A	424	TYR
1	A	428	ARG
1	A	437	LYS
1	B	11	ARG
1	B	20	THR
1	B	36	THR
1	B	60	LEU

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Mol	Chain	Res	Type
1	B	78	CYS
1	B	93	LEU
1	B	118	SER
1	B	119	LYS
1	B	126	SER
1	B	163	SER
1	B	182	GLU
1	B	187	GLU
1	B	193	MET
1	B	196	SER
1	B	203	LYS
1	B	223	ILE
1	B	228	ILE
1	B	234	ILE
1	B	288	ILE
1	B	292	LEU
1	B	294	LYS
1	B	309	ILE
1	B	316	LEU
1	B	320	ILE
1	B	322	ASP
1	B	326	LYS
1	B	335	GLN
1	B	337	TYR
1	B	342	THR
1	B	343	CYS
1	B	368	GLN
1	B	369	VAL
1	B	378	LYS
1	B	389	CYS
1	B	420	ASP
1	B	421	LEU
1	B	428	ARG
1	B	433	VAL
1	B	434	ASP
1	B	436	LEU
1	B	439	LEU
1	B	445	TYR
1	B	451	GLU
1	B	452	LEU
1	B	455	LEU
1	B	456	LEU

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Mol	Chain	Res	Type
1	B	457	LEU
1	B	459	HIS
1	B	462	ILE
1	B	467	VAL
1	B	468	ILE
1	B	470	ILE
1	B	472	ASP
1	B	474	PHE
1	B	477	GLN
1	B	484	VAL
1	B	485	LEU
1	B	492	THR
1	B	506	THR
1	B	508	LYS
1	B	510	LEU
1	B	511	ARG
1	B	515	VAL
1	B	518	ASP
1	B	531	ASN
1	B	532	GLU
1	B	543	LYS
1	C	20	THR
1	C	36	THR
1	C	44	THR
1	C	118	SER
1	C	223	ILE
1	C	260	VAL
1	C	292	LEU
1	C	306	LEU
1	C	333	ILE
1	C	335	GLN
1	C	339	LEU
1	C	346	LEU
1	C	347	ILE
1	C	348	LEU
1	C	388	ILE
1	C	425	ASP
1	D	13	ARG
1	D	20	THR
1	D	36	THR
1	D	56	THR
1	D	163	SER

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Mol	Chain	Res	Type
1	D	228	ILE
1	D	237	ILE
1	D	260	VAL
1	D	306	LEU
1	D	335	GLN
1	D	337	TYR
1	D	342	THR
1	D	343	CYS
1	D	348	LEU
1	D	372	ILE
1	D	418	THR
1	D	431	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	71	HIS
1	A	95	GLN
1	A	241	HIS
1	B	71	HIS
1	B	73	ASN
1	B	114	HIS
1	B	139	HIS
1	B	171	HIS
1	B	241	HIS
1	B	393	GLN
1	B	458	GLN
1	B	531	ASN
1	C	27	GLN
1	C	71	HIS
1	C	116	ASN
1	C	241	HIS
1	C	331	HIS
1	C	335	GLN
1	C	375	ASN
1	D	27	GLN
1	D	71	HIS
1	D	95	GLN
1	D	241	HIS
1	D	275	GLN
1	D	335	GLN

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Mol	Chain	Res	Type
1	D	375	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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	419/546 (76%)	-0.29	13 (3%) 49 33	30, 84, 159, 208	0
1	B	528/546 (96%)	-0.30	11 (2%) 63 48	46, 85, 145, 200	0
1	C	417/546 (76%)	-0.32	8 (1%) 66 51	49, 92, 160, 207	0
1	D	416/546 (76%)	-0.35	15 (3%) 42 28	51, 87, 160, 191	0
All	All	1780/2184 (81%)	-0.32	47 (2%) 56 40	30, 87, 157, 208	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	427	ASP	5.7
1	D	198	THR	4.7
1	D	331	HIS	4.5
1	A	426	GLU	4.0
1	C	426	GLU	3.9
1	A	436	LEU	3.7
1	A	435	ARG	3.6
1	B	526	GLY	3.5
1	D	383	ARG	3.5
1	B	525	THR	3.5
1	A	428	ARG	3.3
1	A	312	GLY	3.3
1	A	427	ASP	3.1
1	D	199	THR	3.1
1	D	319	ASP	2.9
1	D	197	GLY	2.8
1	D	377	GLY	2.8
1	B	524	PRO	2.8
1	D	314	SER	2.8
1	D	337	TYR	2.8
1	B	480	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	336	GLY	2.6
1	A	336	GLY	2.6
1	B	509	HIS	2.6
1	D	376	THR	2.6
1	C	383	ARG	2.6
1	D	313	GLY	2.6
1	C	428	ARG	2.6
1	D	427	ASP	2.5
1	C	337	TYR	2.5
1	A	314	SER	2.5
1	B	437	LYS	2.5
1	B	472	ASP	2.4
1	B	314	SER	2.4
1	B	527	LYS	2.3
1	D	385	LYS	2.3
1	A	197	GLY	2.2
1	C	401	ASN	2.2
1	A	337	TYR	2.2
1	A	378	LYS	2.2
1	C	375	ASN	2.2
1	C	202	PRO	2.1
1	D	435	ARG	2.1
1	A	199	THR	2.1
1	A	383	ARG	2.1
1	B	427	ASP	2.0
1	D	375	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.