



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:54 PM GMT

PDB ID : 1R59  
Title : Enterococcus casseliflavus glycerol kinase  
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Deposited on : 2003-10-09  
Resolution : 2.50 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

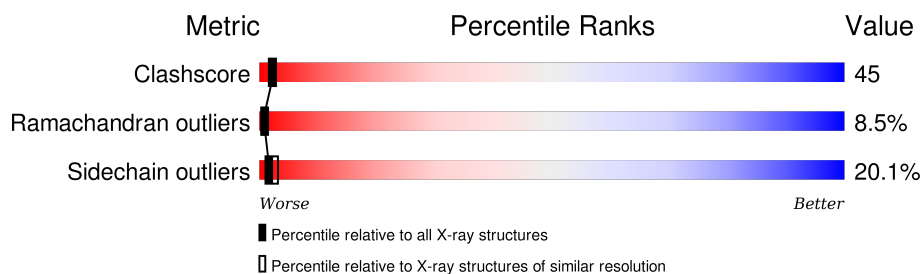
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.


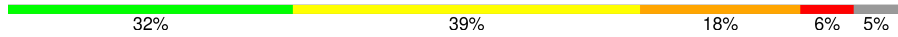
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	O	505	
1	X	505	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7532 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	480	Total	C	N	O	S	0	0	0
			3715	2350	621	730	14			
1	X	480	Total	C	N	O	S	0	0	0
			3715	2350	621	730	14			

- Molecule 2 is water.

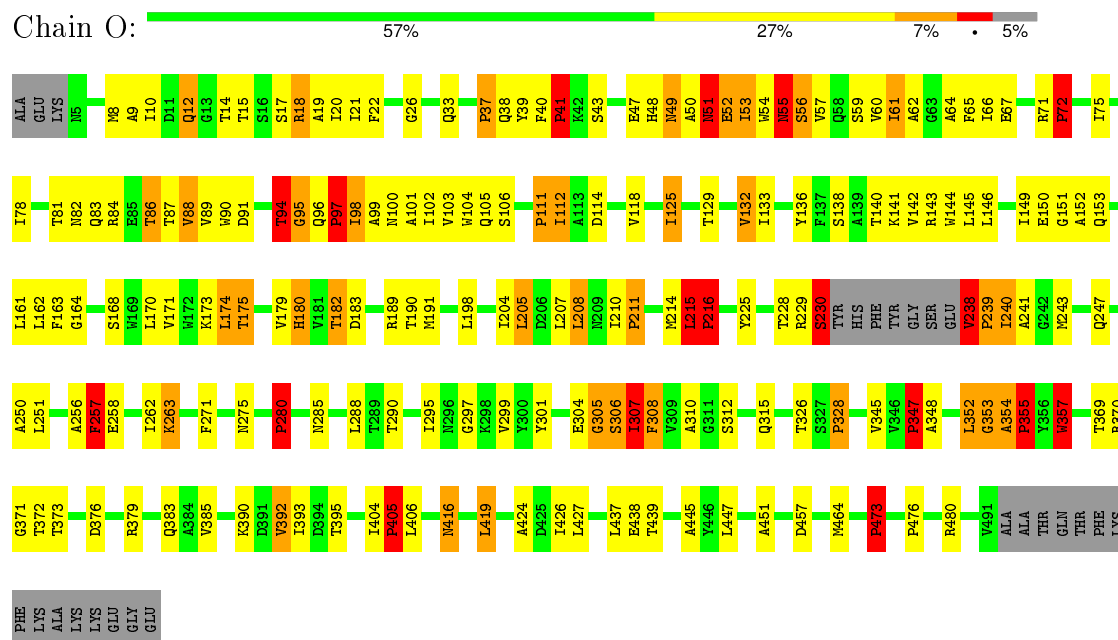
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	51	Total	O	0	0
			51	51		
2	X	51	Total	O	0	0
			51	51		

### 3 Residue-property plots

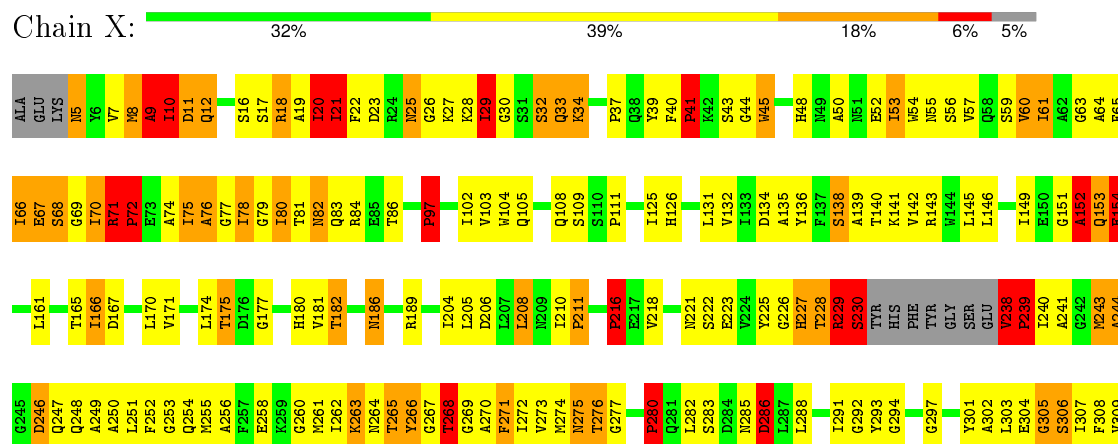
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Glycerol kinase



- Molecule 1: Glycerol kinase



LYS	L437	E375	A310
LYS	E438	D376	G311
GLU	T439	F377	S312
GLY	T440	V378	A313
GLU	A441	R379	I314
	L442	A380	D315
	G443	T381	I316
	A444	L382	L317
	A445	Q383	R318
	Y446	A384	D319
	L447	V385	G320
	A448	A386	L321
	G449	Y387	R322
	L450	Q388	R323
		S389	S324
	F454	K390	
	N455	D391	S327
	K456	V392	P328
	D457	I393	L329
	L458	D394	S330
	D459	T395	E331
	E460	M396	E332
	L461	K397	L333
	K462	K398	A334
	S463	D399	A335
	N464		K336
	A465	I402	A337
	G468	D403	K338
		I404	G339
	F471	P405	D340
	T472	L406	N341
	P473	L407	E342
	E474	K408	V343
	N475	V409	Y344
	P476	D410	V345
		G411	V346
	E479	G412	P347
	R480	A413	
	D481	A414	T350
	N482	K415	G351
	L483	N416	L352
	Y484	D417	G353
	E485	L418	A354
	G486	L419	P355
	N487	M420	Y356
	K488	Q421	P357
	Q489	F422	D358
	A490	Q423	S359
	V491	A424	
	ALA	D425	G363
	ALA	I426	A364
	THR	L427	V365
	GLN	D428	F366
	THR	I429	G367
	PHE	D430	
	LYS	V431	R370
	PHE	Q432	G371
	LYS	R433	T372
	LYS	A434	T373
	ALA		K374

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.83 Å   107.11 Å   201.12 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	O	0.76	7/3790 (0.2%)	1.40	36/5141 (0.7%)
1	X	1.00	15/3790 (0.4%)	1.63	80/5141 (1.6%)
All	All	0.89	22/7580 (0.3%)	1.52	116/10282 (1.1%)

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	X	0	3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	238	VAL	N-CA	13.28	1.73	1.46
1	X	154	GLU	C-N	12.97	1.63	1.34
1	X	238	VAL	C-N	11.36	1.55	1.34
1	X	238	VAL	N-CA	10.89	1.68	1.46
1	O	230	SER	C-N	10.23	1.57	1.34
1	X	228	THR	C-N	-9.73	1.11	1.34
1	X	238	VAL	CA-C	8.86	1.75	1.52
1	O	230	SER	CA-C	8.69	1.75	1.52
1	X	230	SER	C-N	8.51	1.53	1.34
1	O	230	SER	N-CA	8.23	1.62	1.46
1	X	239	PRO	N-CA	7.89	1.60	1.47
1	X	72	PRO	N-CA	7.30	1.59	1.47
1	X	230	SER	CA-C	6.95	1.71	1.52
1	X	70	ILE	N-CA	6.92	1.60	1.46
1	O	229	ARG	C-N	6.88	1.49	1.34
1	X	69	GLY	CA-C	6.38	1.62	1.51
1	X	21	ILE	N-CA	5.34	1.57	1.46
1	O	239	PRO	N-CA	5.25	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	20	ILE	CA-C	5.22	1.66	1.52
1	O	305	GLY	N-CA	-5.15	1.38	1.46
1	X	426	ILE	N-CA	5.14	1.56	1.46
1	X	239	PRO	N-CD	5.13	1.55	1.47

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	239	PRO	CA-N-CD	-22.07	80.60	111.50
1	O	239	PRO	CA-N-CD	-21.77	81.03	111.50
1	O	328	PRO	CA-N-CD	-20.94	82.18	111.50
1	O	355	PRO	CA-N-CD	-19.62	84.03	111.50
1	X	280	PRO	CA-N-CD	-19.20	84.62	111.50
1	O	211	PRO	CA-N-CD	-18.43	85.69	111.50
1	O	111	PRO	CA-N-CD	-17.58	86.88	111.50
1	O	97	PRO	CA-N-CD	-17.19	87.43	111.50
1	X	355	PRO	CA-N-CD	-16.98	87.73	111.50
1	X	347	PRO	CA-N-CD	-16.36	88.59	111.50
1	X	97	PRO	CA-N-CD	-15.96	89.15	111.50
1	O	41	PRO	CA-N-CD	-15.23	90.17	111.50
1	X	211	PRO	CA-N-CD	-14.97	90.54	111.50
1	O	476	PRO	CA-N-CD	-14.85	90.71	111.50
1	X	476	PRO	CA-N-CD	-13.97	91.94	111.50
1	O	280	PRO	CA-N-CD	-13.73	92.27	111.50
1	O	347	PRO	CA-N-CD	-13.50	92.60	111.50
1	O	473	PRO	CA-N-CD	-13.48	92.63	111.50
1	X	111	PRO	CA-N-CD	-12.25	94.36	111.50
1	X	405	PRO	CA-N-CD	-12.18	94.45	111.50
1	O	229	ARG	C-N-CA	11.31	149.96	121.70
1	O	405	PRO	CA-N-CD	-11.17	95.87	111.50
1	O	37	PRO	CA-N-CD	-10.94	96.19	111.50
1	X	37	PRO	CA-N-CD	-10.70	96.52	111.50
1	X	328	PRO	CA-N-CD	-10.66	96.58	111.50
1	X	229	ARG	C-N-CA	10.63	148.27	121.70
1	X	473	PRO	CA-N-CD	-10.05	97.43	111.50
1	X	25	ASN	CA-C-N	-9.96	96.29	116.20
1	X	72	PRO	CA-N-CD	-9.92	97.61	111.50
1	X	228	THR	C-N-CA	9.84	146.29	121.70
1	O	307	ILE	CA-C-N	-9.82	95.60	117.20
1	X	72	PRO	N-CA-C	9.78	137.54	112.10
1	O	216	PRO	CA-N-CD	-9.71	97.90	111.50
1	X	216	PRO	CA-N-CD	-9.48	98.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	25	ASN	N-CA-C	9.35	136.24	111.00
1	O	307	ILE	N-CA-C	9.24	135.96	111.00
1	X	154	GLU	CA-C-N	-9.07	97.25	117.20
1	X	41	PRO	CA-N-CD	-9.05	98.82	111.50
1	O	230	SER	C-N-CA	8.84	143.80	121.70
1	O	307	ILE	C-N-CA	8.83	143.79	121.70
1	X	456	LYS	C-N-CA	8.82	143.76	121.70
1	X	229	ARG	CA-C-N	-8.60	98.28	117.20
1	X	230	SER	C-N-CA	8.52	143.01	121.70
1	O	40	PHE	C-N-CD	-8.31	102.32	120.60
1	X	32	SER	N-CA-C	8.03	132.69	111.00
1	X	456	LYS	CA-C-N	-7.94	99.74	117.20
1	X	347	PRO	N-CA-CB	7.66	112.49	103.30
1	X	40	PHE	C-N-CD	-7.42	104.28	120.60
1	O	229	ARG	CB-CA-C	7.33	125.06	110.40
1	X	225	TYR	CB-CG-CD1	7.15	125.29	121.00
1	X	32	SER	CA-C-N	-7.09	101.61	117.20
1	X	25	ASN	C-N-CA	6.90	136.80	122.30
1	X	8	MET	C-N-CA	-6.84	104.59	121.70
1	X	33	GLN	N-CA-C	6.81	129.39	111.00
1	X	154	GLU	CB-CA-C	6.77	123.94	110.40
1	O	238	VAL	CA-C-N	6.77	136.05	117.10
1	X	461	LEU	CA-CB-CG	6.72	130.75	115.30
1	X	239	PRO	N-CD-CG	6.69	113.23	103.20
1	X	32	SER	C-N-CA	6.60	138.21	121.70
1	X	229	ARG	CB-CA-C	6.57	123.55	110.40
1	O	307	ILE	O-C-N	6.57	133.21	122.70
1	O	328	PRO	N-CD-CG	6.54	113.01	103.20
1	X	446	TYR	CA-CB-CG	6.50	125.75	113.40
1	X	446	TYR	CB-CG-CD1	6.43	124.86	121.00
1	X	316	TRP	CA-CB-CG	-6.39	101.55	113.70
1	X	61	ILE	CB-CA-C	6.34	124.27	111.60
1	O	357	TRP	CA-C-N	-6.27	103.40	117.20
1	O	306	SER	N-CA-C	6.24	127.85	111.00
1	X	405	PRO	N-CA-C	6.24	128.32	112.10
1	O	72	PRO	CA-N-CD	-6.22	102.79	111.50
1	X	9	ALA	C-N-CA	6.22	137.24	121.70
1	X	25	ASN	CA-CB-CG	-6.14	99.90	113.40
1	X	238	VAL	CA-C-N	6.13	134.27	117.10
1	X	25	ASN	O-C-N	6.12	133.61	123.20
1	X	229	ARG	O-C-N	6.03	132.35	122.70
1	X	472	THR	C-N-CD	-6.01	107.37	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	357	TRP	N-CA-C	-5.94	94.97	111.00
1	O	97	PRO	N-CD-CG	5.92	112.08	103.20
1	O	239	PRO	CB-CA-C	-5.92	97.21	112.00
1	X	152	ALA	C-N-CA	5.88	136.40	121.70
1	X	370	ARG	N-CA-C	5.88	126.87	111.00
1	X	238	VAL	N-CA-C	5.85	126.80	111.00
1	X	228	THR	N-CA-C	5.77	126.58	111.00
1	X	422	PHE	CA-CB-CG	-5.76	100.08	113.90
1	X	69	GLY	N-CA-C	5.74	127.44	113.10
1	X	429	ILE	N-CA-C	-5.67	95.69	111.00
1	O	357	TRP	C-N-CA	5.65	135.82	121.70
1	O	211	PRO	N-CD-CG	5.64	111.67	103.20
1	X	32	SER	CB-CA-C	-5.61	99.43	110.10
1	X	456	LYS	O-C-N	5.60	131.66	122.70
1	O	355	PRO	N-CD-CG	5.56	111.53	103.20
1	O	41	PRO	N-CA-CB	5.54	109.95	103.30
1	X	422	PHE	N-CA-CB	5.50	120.49	110.60
1	O	404	ILE	C-N-CD	-5.49	108.51	120.60
1	X	344	TYR	CA-CB-CG	-5.38	103.18	113.40
1	X	461	LEU	CB-CA-C	5.38	120.42	110.20
1	X	474	GLU	N-CA-C	5.36	125.48	111.00
1	X	343	VAL	CB-CA-C	-5.36	101.22	111.40
1	X	97	PRO	N-CD-CG	5.33	111.20	103.20
1	X	375	GLU	N-CA-C	5.32	125.36	111.00
1	X	357	TRP	CA-CB-CG	5.32	123.80	113.70
1	O	307	ILE	CA-C-O	5.28	131.19	120.10
1	X	416	ASN	CB-CA-C	-5.28	99.84	110.40
1	X	33	GLN	CA-C-N	-5.25	105.64	117.20
1	X	338	LYS	N-CA-C	5.22	125.09	111.00
1	X	72	PRO	N-CA-CB	-5.20	96.88	102.60
1	X	305	GLY	N-CA-C	-5.19	100.12	113.10
1	X	210	ILE	C-N-CD	-5.16	109.25	120.60
1	X	339	GLY	C-N-CA	5.16	134.60	121.70
1	X	446	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	X	32	SER	N-CA-CB	-5.15	102.78	110.50
1	X	227	HIS	C-N-CA	-5.10	108.96	121.70
1	X	487	TRP	CA-CB-CG	5.09	123.38	113.70
1	X	239	PRO	CA-CB-CG	-5.05	94.40	104.00
1	O	211	PRO	N-CA-CB	5.03	109.33	103.30
1	X	355	PRO	N-CD-CG	5.00	110.71	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	154	GLU	Mainchain
1	X	266	TYR	Sidechain
1	X	446	TYR	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	O	3715	0	3626	217	0
1	X	3715	0	3624	454	0
2	O	51	0	0	8	0
2	X	51	0	0	11	0
All	All	7532	0	7250	664	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (664) 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:X:132:VAL:HG11	1:X:357:TRP:CZ2	1.32	1.60
1:X:238:VAL:CA	1:X:238:VAL:N	1.68	1.52
1:X:238:VAL:CA	1:X:238:VAL:C	1.76	1.51
1:O:230:SER:C	1:O:230:SER:CA	1.75	1.51
1:O:238:VAL:N	1:O:238:VAL:CA	1.72	1.50
1:O:257:PHE:CE1	1:O:295:ILE:HD12	1.59	1.36
1:X:10:ILE:CG1	1:X:61:ILE:HD12	1.62	1.28
1:O:307:ILE:HG13	1:O:353:GLY:CA	1.65	1.24
1:X:10:ILE:HG13	1:X:61:ILE:CD1	1.66	1.24
1:X:132:VAL:CG1	1:X:357:TRP:HZ2	1.50	1.23
1:X:356:TYR:CZ	1:X:491:VAL:HG11	1.75	1.21
1:X:132:VAL:CG1	1:X:357:TRP:CZ2	2.23	1.20
1:O:353:GLY:CA	1:O:357:TRP:HB3	1.73	1.17
1:X:356:TYR:CE1	1:X:491:VAL:CG1	2.27	1.16
1:O:307:ILE:CG1	1:O:353:GLY:HA3	1.76	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:306:SER:OG	1:O:354:ALA:HA	1.46	1.15
1:O:62:ALA:O	1:O:66:ILE:HD12	1.47	1.14
1:X:175:THR:HA	1:X:228:THR:CG2	1.76	1.13
1:O:353:GLY:HA2	1:O:357:TRP:HB3	1.12	1.11
1:X:356:TYR:CE1	1:X:491:VAL:HG12	1.85	1.10
1:O:353:GLY:HA2	1:O:357:TRP:CB	1.84	1.07
1:X:78:ILE:HD13	1:X:174:LEU:CD2	1.85	1.06
1:X:230:SER:O	1:X:238:VAL:HG12	1.54	1.06
1:O:307:ILE:HD13	1:O:308:PHE:CG	1.89	1.06
1:X:321:LEU:HD13	1:X:321:LEU:H	1.16	1.05
1:X:74:ALA:O	1:X:75:ILE:O	1.72	1.05
1:O:307:ILE:CD1	1:O:308:PHE:CG	2.42	1.03
1:X:304:GLU:HG2	1:X:305:GLY:O	1.60	1.02
1:X:78:ILE:HD13	1:X:174:LEU:HD21	1.38	1.02
1:O:307:ILE:HD13	1:O:308:PHE:CB	1.90	1.02
1:X:175:THR:HA	1:X:228:THR:HG21	1.05	1.02
1:O:424:ALA:HB1	1:O:473:PRO:HD3	1.42	1.01
1:O:307:ILE:HG13	1:O:353:GLY:HA3	1.28	1.00
1:O:98:ILE:HD13	1:O:98:ILE:N	1.75	1.00
1:X:416:ASN:HB3	1:X:418:LEU:H	1.21	0.99
1:X:25:ASN:CB	1:X:461:LEU:HD11	1.92	0.98
1:X:356:TYR:CE1	1:X:491:VAL:HG11	1.93	0.98
1:O:352:LEU:HD12	1:O:352:LEU:O	1.63	0.97
1:X:345:VAL:HG13	1:X:347:PRO:HD3	1.43	0.97
1:X:45:TRP:HE1	1:X:108:GLN:HE21	1.10	0.96
1:X:45:TRP:CD1	1:X:108:GLN:HB2	2.01	0.96
1:X:20:ILE:HG23	1:X:21:ILE:H	1.30	0.95
1:X:79:GLY:O	1:X:80:ILE:HD12	1.64	0.95
1:X:132:VAL:HG11	1:X:357:TRP:CE2	2.00	0.94
1:X:414:ALA:HB3	1:X:437:LEU:HD22	1.46	0.94
1:X:422:PHE:C	1:X:424:ALA:H	1.66	0.94
1:X:175:THR:CA	1:X:228:THR:HG21	1.97	0.92
1:X:379:ARG:O	1:X:383:GLN:HG2	1.67	0.92
1:O:132:VAL:CG1	1:O:357:TRP:CH2	2.53	0.92
1:O:180:HIS:CE1	1:O:216:PRO:HG3	2.05	0.91
1:O:257:PHE:CE1	1:O:295:ILE:CD1	2.53	0.91
1:O:60:VAL:O	1:O:64:ALA:HB3	1.71	0.91
1:O:12:GLN:NE2	1:O:53:ILE:HG22	1.86	0.90
1:X:227:HIS:O	1:X:228:THR:HB	1.69	0.89
1:X:426:ILE:HG13	1:X:480:ARG:HG3	1.55	0.88
1:X:321:LEU:CD1	1:X:321:LEU:H	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:19:ALA:HB1	1:X:64:ALA:HB3	1.54	0.88
1:O:132:VAL:HG11	1:O:357:TRP:CZ2	2.09	0.88
1:X:10:ILE:HG23	1:X:11:ASP:N	1.89	0.88
1:O:257:PHE:HE1	1:O:295:ILE:CD1	1.87	0.86
1:O:143:ARG:HG2	1:O:208:LEU:HB3	1.54	0.86
1:O:257:PHE:CZ	1:O:295:ILE:HD12	2.09	0.86
1:X:25:ASN:HB2	1:X:461:LEU:HD11	1.54	0.86
1:X:25:ASN:HB2	1:X:461:LEU:CD1	2.06	0.85
1:O:307:ILE:HD11	1:O:308:PHE:CD2	2.12	0.85
1:X:411:GLY:H	1:X:437:LEU:HB3	1.41	0.85
1:X:25:ASN:CB	1:X:461:LEU:CD1	2.55	0.84
1:O:50:ALA:HB2	1:O:101:ALA:H	1.40	0.84
1:O:257:PHE:HE1	1:O:295:ILE:HD12	1.03	0.84
1:O:307:ILE:HG13	1:O:353:GLY:C	1.98	0.83
1:X:25:ASN:ND2	1:X:461:LEU:HD11	1.93	0.83
1:O:307:ILE:CG1	1:O:353:GLY:CA	2.44	0.83
1:X:72:PRO:HA	1:X:75:ILE:HG22	1.58	0.82
1:X:71:ARG:HB3	1:X:72:PRO:HD2	1.60	0.82
1:X:82:ASN:HD21	1:X:186:ASN:HD21	1.28	0.82
1:X:77:GLY:CA	1:X:239:PRO:O	2.28	0.82
1:O:228:THR:HG22	1:O:238:VAL:O	1.80	0.81
1:O:132:VAL:HG13	1:O:357:TRP:CH2	2.15	0.81
1:O:306:SER:OG	1:O:354:ALA:CA	2.26	0.81
1:X:78:ILE:CD1	1:X:174:LEU:HD21	2.10	0.81
1:X:252:PHE:HD1	1:X:256:ALA:HB3	1.45	0.81
1:O:55:ASN:C	1:O:57:VAL:H	1.83	0.80
1:X:180:HIS:CE1	1:X:216:PRO:HG3	2.16	0.80
1:X:132:VAL:HG22	1:X:357:TRP:HE1	1.47	0.80
1:O:354:ALA:O	1:O:357:TRP:CD1	2.34	0.80
1:X:75:ILE:HG12	1:X:230:SER:O	1.83	0.79
1:X:321:LEU:HD13	1:X:321:LEU:N	1.97	0.79
1:O:307:ILE:HD11	1:O:308:PHE:CG	2.17	0.79
1:X:356:TYR:CD1	1:X:491:VAL:HG12	2.18	0.79
1:X:33:GLN:O	1:X:34:LYS:HG3	1.83	0.79
1:X:418:LEU:HA	1:X:421:GLN:HB3	1.64	0.78
1:O:424:ALA:O	1:O:473:PRO:HG3	1.82	0.78
1:O:306:SER:HG	1:O:354:ALA:HA	1.47	0.78
1:O:307:ILE:HG12	1:O:353:GLY:HA3	1.64	0.78
1:X:48:HIS:HD2	1:X:83:GLN:HE22	1.31	0.78
1:X:414:ALA:HB3	1:X:437:LEU:CD2	2.14	0.78
1:X:422:PHE:C	1:X:424:ALA:N	2.37	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:132:VAL:CG1	1:X:357:TRP:CE2	2.65	0.78
1:X:77:GLY:HA2	1:X:239:PRO:O	1.84	0.77
1:X:20:ILE:CG2	1:X:21:ILE:H	1.97	0.77
1:X:78:ILE:HD13	1:X:174:LEU:HD23	1.66	0.76
1:O:307:ILE:HD13	1:O:308:PHE:HB2	1.66	0.76
1:X:132:VAL:CG2	1:X:357:TRP:NE1	2.48	0.76
1:X:43:SER:O	1:X:45:TRP:CD1	2.38	0.76
1:X:10:ILE:CG1	1:X:61:ILE:CD1	2.41	0.75
1:X:374:LYS:HG2	1:X:374:LYS:O	1.87	0.75
1:X:132:VAL:HG22	1:X:357:TRP:NE1	2.02	0.75
1:X:56:SER:O	1:X:60:VAL:HG22	1.87	0.75
1:X:10:ILE:CG2	1:X:11:ASP:N	2.49	0.74
1:O:141:LYS:O	1:O:145:LEU:HD13	1.86	0.74
1:X:262:ILE:HG22	1:X:263:LYS:H	1.49	0.74
1:X:78:ILE:HG22	1:X:240:ILE:HG23	1.67	0.74
1:X:343:VAL:O	1:X:344:TYR:CD1	2.40	0.74
1:X:8:MET:O	1:X:9:ALA:HB2	1.87	0.74
1:X:280:PRO:HD3	1:X:301:TYR:CG	2.22	0.74
1:X:19:ALA:HB1	1:X:64:ALA:CB	2.17	0.74
1:X:5:ASN:HD22	1:X:5:ASN:N	1.85	0.74
1:O:369:THR:HG22	1:O:371:GLY:H	1.51	0.73
1:X:286:ASP:HB2	1:X:357:TRP:CZ3	2.24	0.73
1:O:353:GLY:C	1:O:357:TRP:HB3	2.09	0.73
1:X:370:ARG:HD3	2:X:515:HOH:O	1.89	0.73
1:X:167:ASP:O	1:X:171:VAL:HG23	1.88	0.72
1:X:356:TYR:CD1	1:X:491:VAL:CG1	2.72	0.72
1:O:345:VAL:HG12	1:O:347:PRO:HD3	1.71	0.72
1:X:262:ILE:HD11	1:X:274:MET:HE2	1.71	0.72
1:O:98:ILE:H	1:O:98:ILE:HD13	1.49	0.72
1:X:354:ALA:O	1:X:357:TRP:CE3	2.42	0.72
1:O:50:ALA:H	1:O:100:ASN:HB2	1.53	0.72
1:X:25:ASN:HD22	1:X:461:LEU:HD11	1.51	0.72
1:X:280:PRO:HD3	1:X:301:TYR:CD2	2.25	0.71
1:X:64:ALA:HA	1:X:67:GLU:OE1	1.89	0.71
1:X:238:VAL:HA	1:X:238:VAL:C	2.05	0.71
1:X:480:ARG:HG2	1:X:480:ARG:O	1.88	0.71
1:X:20:ILE:HG23	1:X:21:ILE:N	2.03	0.71
1:X:288:LEU:HD12	1:X:305:GLY:O	1.90	0.71
1:X:132:VAL:CG2	1:X:357:TRP:HE1	2.02	0.71
1:X:246:ASP:O	1:X:249:ALA:HB3	1.91	0.71
1:X:20:ILE:CG2	1:X:21:ILE:N	2.52	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:252:PHE:CD1	1:X:256:ALA:HB3	2.26	0.71
1:X:327:SER:HB3	1:X:328:PRO:HD2	1.71	0.71
1:X:431:VAL:CG2	1:X:432:GLN:N	2.54	0.71
1:O:304:GLU:HG2	1:O:305:GLY:O	1.91	0.70
1:X:416:ASN:O	1:X:433:ARG:NH2	2.21	0.70
1:X:10:ILE:HG23	1:X:11:ASP:H	1.56	0.70
1:O:15:THR:HG21	1:O:315:GLN:NE2	2.07	0.69
1:X:355:PRO:HA	1:X:357:TRP:HZ3	1.57	0.69
1:X:383:GLN:HE22	1:X:422:PHE:HE2	1.39	0.69
1:O:12:GLN:HE22	1:O:53:ILE:HG22	1.55	0.69
1:X:307:ILE:HG21	1:X:385:VAL:HG23	1.75	0.69
1:X:32:SER:OG	1:X:33:GLN:HG3	1.93	0.69
1:X:189:ARG:HH12	1:X:288:LEU:HD13	1.58	0.69
1:X:380:ALA:HA	1:X:383:GLN:HB2	1.74	0.69
1:X:238:VAL:HG22	1:X:239:PRO:N	2.08	0.69
1:O:205:LEU:HD21	1:O:215:LEU:HD11	1.75	0.69
1:X:86:THR:HG22	1:X:103:VAL:HA	1.74	0.69
1:X:25:ASN:HD22	1:X:461:LEU:CD1	2.05	0.68
1:O:352:LEU:C	1:O:352:LEU:HD12	2.14	0.68
1:X:327:SER:HB3	1:X:328:PRO:CD	2.22	0.68
1:O:51:ASN:HD22	1:O:51:ASN:N	1.90	0.68
1:X:460:GLU:O	1:X:461:LEU:HB3	1.92	0.68
1:X:71:ARG:HB3	1:X:72:PRO:CD	2.23	0.68
1:X:313:ALA:C	1:X:315:GLN:H	1.94	0.68
1:X:434:ALA:O	1:X:437:LEU:CD1	2.41	0.68
1:X:25:ASN:CG	1:X:461:LEU:HD11	2.14	0.68
1:X:356:TYR:C	1:X:357:TRP:O	2.29	0.68
1:X:10:ILE:HD12	1:X:61:ILE:HD13	1.75	0.68
1:X:10:ILE:HG21	1:X:170:LEU:HD13	1.75	0.67
1:O:352:LEU:O	1:O:352:LEU:CD1	2.42	0.67
1:X:345:VAL:CG1	1:X:347:PRO:HD3	2.22	0.67
1:O:12:GLN:HE22	1:O:53:ILE:CG2	2.07	0.67
1:O:132:VAL:HG11	1:O:357:TRP:CH2	2.26	0.67
1:X:431:VAL:HG22	1:X:432:GLN:N	2.09	0.67
1:X:238:VAL:CG2	1:X:239:PRO:HD2	2.25	0.67
1:X:75:ILE:HG13	1:X:76:ALA:N	2.07	0.67
1:O:256:ALA:O	1:O:257:PHE:C	2.32	0.67
1:O:256:ALA:O	1:O:257:PHE:O	2.13	0.67
1:X:356:TYR:CZ	1:X:491:VAL:CG1	2.57	0.67
1:X:45:TRP:NE1	1:X:108:GLN:HB2	2.09	0.67
1:O:405:PRO:HB2	1:O:406:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:352:LEU:O	1:O:353:GLY:O	2.14	0.66
1:X:434:ALA:O	1:X:437:LEU:HD12	1.96	0.66
1:X:429:ILE:HG22	1:X:430:ASP:N	2.10	0.66
1:O:102:ILE:HG23	1:O:106:SER:OG	1.95	0.65
1:X:251:LEU:HD11	1:X:275:ASN:N	2.11	0.65
1:X:262:ILE:HD11	1:X:274:MET:CE	2.26	0.65
1:X:419:LEU:O	1:X:423:GLN:N	2.24	0.65
1:X:238:VAL:HA	1:X:238:VAL:N	2.03	0.65
1:X:10:ILE:CD1	1:X:61:ILE:CD1	2.75	0.65
1:X:66:ILE:HD11	1:X:71:ARG:HG3	1.79	0.65
1:X:132:VAL:CG1	1:X:357:TRP:NE1	2.60	0.65
1:X:407:LEU:O	1:X:431:VAL:HG23	1.97	0.65
1:X:175:THR:CA	1:X:228:THR:CG2	2.65	0.65
1:X:314:ILE:O	1:X:314:ILE:HG22	1.97	0.65
1:X:293:TYR:CZ	1:X:447:LEU:HD12	2.32	0.64
1:X:175:THR:HG23	1:X:228:THR:HG22	1.79	0.64
1:X:346:VAL:O	1:X:363:GLY:HA2	1.95	0.64
1:X:321:LEU:N	1:X:321:LEU:CD1	2.58	0.64
1:X:262:ILE:HG22	1:X:263:LYS:N	2.13	0.64
1:X:66:ILE:CG2	1:X:66:ILE:O	2.46	0.64
1:X:132:VAL:HG13	1:X:357:TRP:HE1	1.61	0.64
1:X:433:ARG:HD3	1:X:437:LEU:HD11	1.79	0.64
1:X:251:LEU:HD11	1:X:275:ASN:H	1.63	0.64
1:X:378:VAL:O	1:X:382:LEU:HB2	1.99	0.63
1:X:385:VAL:O	1:X:389:SER:HB2	1.99	0.63
1:O:257:PHE:C	1:O:257:PHE:CD2	2.72	0.63
1:O:138:SER:O	1:O:142:VAL:HG23	1.98	0.63
1:O:307:ILE:CD1	1:O:308:PHE:CD1	2.82	0.62
1:X:356:TYR:CE2	1:X:491:VAL:HG11	2.29	0.62
1:X:74:ALA:C	1:X:75:ILE:O	2.37	0.62
1:O:163:PHE:O	1:O:216:PRO:HD2	1.99	0.62
1:O:96:GLN:HB3	1:X:68:SER:O	2.00	0.62
1:X:132:VAL:CG1	1:X:357:TRP:HE1	2.13	0.61
1:X:383:GLN:NE2	1:X:422:PHE:CE2	2.59	0.61
1:O:357:TRP:CD1	1:O:357:TRP:N	2.67	0.61
1:X:383:GLN:O	1:X:384:ALA:HB2	2.00	0.61
1:O:241:ALA:HB1	1:O:451:ALA:HB3	1.81	0.61
1:O:12:GLN:NE2	1:O:53:ILE:CG2	2.61	0.61
1:X:419:LEU:HD23	1:X:420:MET:HE2	1.82	0.61
1:X:171:VAL:HG11	1:X:181:VAL:HG12	1.81	0.61
1:X:72:PRO:C	1:X:74:ALA:H	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:138:SER:O	1:X:142:VAL:HG23	2.00	0.61
1:O:230:SER:N	1:O:230:SER:C	2.54	0.61
1:O:48:HIS:CD2	1:O:83:GLN:HE22	2.19	0.61
1:X:105:GLN:O	1:X:350:THR:HB	2.01	0.61
1:O:49:ASN:HB2	1:O:52:GLU:HB2	1.81	0.61
1:X:265:THR:HG22	1:X:270:ALA:HA	1.83	0.60
1:X:307:ILE:HG12	1:X:388:GLN:HB3	1.83	0.60
1:X:354:ALA:O	1:X:357:TRP:CZ3	2.55	0.60
1:X:386:ALA:O	1:X:390:LYS:HB2	2.00	0.60
1:X:230:SER:C	1:X:238:VAL:HG12	2.22	0.60
1:X:379:ARG:O	1:X:383:GLN:CG	2.47	0.60
1:X:428:ASP:HB2	1:X:480:ARG:HH11	1.66	0.60
1:X:402:ILE:HG22	1:X:403:ASP:H	1.67	0.60
1:X:262:ILE:HG23	1:X:273:VAL:O	2.01	0.60
1:O:238:VAL:N	1:O:238:VAL:HA	2.06	0.60
1:O:189:ARG:HH22	1:O:288:LEU:HD13	1.67	0.60
1:O:60:VAL:O	1:O:64:ALA:CB	2.47	0.60
1:X:20:ILE:O	1:X:21:ILE:HG13	2.01	0.60
1:O:114:ASP:O	1:O:118:VAL:HG23	2.01	0.60
1:X:66:ILE:HG22	1:X:66:ILE:O	2.01	0.60
1:X:143:ARG:HE	1:X:208:LEU:HD13	1.67	0.60
1:X:286:ASP:O	1:X:357:TRP:CH2	2.55	0.60
1:O:54:TRP:CD1	1:O:170:LEU:CD2	2.85	0.60
1:X:355:PRO:HA	1:X:357:TRP:CZ3	2.36	0.59
1:O:379:ARG:O	1:O:383:GLN:HG2	2.02	0.59
1:O:307:ILE:HG13	1:O:354:ALA:N	2.17	0.59
1:X:165:THR:O	1:X:167:ASP:N	2.35	0.59
1:X:416:ASN:HB3	1:X:418:LEU:N	2.05	0.59
1:O:51:ASN:ND2	1:O:51:ASN:N	2.49	0.59
1:X:84:ARG:NH1	2:X:554:HOH:O	2.35	0.59
1:X:386:ALA:HA	1:X:389:SER:HB2	1.84	0.59
1:X:84:ARG:O	1:X:104:TRP:HB3	2.03	0.59
1:X:174:LEU:O	1:X:228:THR:CG2	2.51	0.59
1:O:307:ILE:HG13	1:O:353:GLY:N	2.17	0.59
1:O:14:THR:HG23	1:O:48:HIS:NE2	2.17	0.59
1:X:132:VAL:HG13	1:X:357:TRP:NE1	2.17	0.59
1:O:182:THR:OG1	1:O:216:PRO:HB2	2.02	0.59
1:X:10:ILE:CD1	1:X:61:ILE:HD13	2.32	0.58
1:X:247:GLN:OE1	1:X:263:LYS:NZ	2.36	0.58
1:O:55:ASN:O	1:O:57:VAL:N	2.35	0.58
1:X:345:VAL:HG13	1:X:347:PRO:CD	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:44:GLY:O	1:X:350:THR:HG22	2.03	0.58
1:O:171:VAL:HG21	1:O:243:MET:SD	2.43	0.58
1:X:10:ILE:HG13	1:X:61:ILE:HD12	0.73	0.58
1:X:27:LYS:HB2	1:X:27:LYS:NZ	2.19	0.58
1:X:303:LEU:O	1:X:396:MET:SD	2.62	0.58
1:O:55:ASN:C	1:O:57:VAL:N	2.56	0.58
1:X:321:LEU:O	1:X:322:ARG:C	2.42	0.58
1:X:484:TYR:HE2	1:X:488:LYS:NZ	2.01	0.58
1:X:104:TRP:HA	1:X:141:LYS:HZ3	1.69	0.58
1:O:103:VAL:C	1:O:105:GLN:H	2.07	0.58
1:O:90:TRP:O	1:O:162:LEU:N	2.35	0.58
1:X:286:ASP:C	1:X:357:TRP:CH2	2.77	0.58
1:X:84:ARG:NH2	1:X:246:ASP:OD1	2.35	0.57
1:X:247:GLN:HA	2:X:535:HOH:O	2.04	0.57
1:X:19:ALA:CB	1:X:64:ALA:CB	2.82	0.57
1:X:321:LEU:O	1:X:323:MET:HG2	2.04	0.57
1:X:10:ILE:CG2	1:X:170:LEU:HD13	2.34	0.57
1:O:10:ILE:HD13	1:O:78:ILE:HG23	1.85	0.57
1:O:348:ALA:HB2	1:O:352:LEU:HD22	1.85	0.57
1:X:383:GLN:O	1:X:384:ALA:CB	2.52	0.57
1:X:421:GLN:NE2	1:X:471:PHE:HB2	2.20	0.57
1:X:252:PHE:CE2	1:X:293:TYR:HD2	2.22	0.56
1:X:355:PRO:O	1:X:357:TRP:CE3	2.58	0.56
1:O:210:ILE:HG23	1:O:214:MET:SD	2.44	0.56
1:O:230:SER:CB	1:O:230:SER:C	2.69	0.56
1:X:419:LEU:O	1:X:423:GLN:HB3	2.06	0.56
1:O:189:ARG:HH21	1:O:290:THR:HB	1.69	0.56
1:X:429:ILE:CG2	1:X:430:ASP:N	2.68	0.56
1:X:371:GLY:HA3	2:X:541:HOH:O	2.05	0.56
1:X:28:LYS:C	1:X:29:ILE:HG12	2.24	0.56
1:X:80:ILE:CG2	1:X:81:THR:N	2.68	0.56
1:X:426:ILE:HG13	1:X:480:ARG:CG	2.32	0.56
1:O:15:THR:HG21	1:O:315:GLN:HE22	1.71	0.56
1:X:293:TYR:CE2	1:X:447:LEU:HD12	2.41	0.56
1:X:327:SER:CB	1:X:328:PRO:CD	2.84	0.56
1:X:238:VAL:CB	1:X:238:VAL:N	2.63	0.56
1:X:250:ALA:HB3	1:X:263:LYS:HD3	1.86	0.56
1:X:8:MET:HE3	1:X:65:PHE:HA	1.86	0.56
1:X:189:ARG:NH1	1:X:288:LEU:HD13	2.20	0.56
1:X:71:ARG:CB	1:X:72:PRO:HD2	2.34	0.56
1:X:385:VAL:O	1:X:389:SER:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:409:VAL:HG21	1:X:420:MET:HE3	1.87	0.56
1:O:132:VAL:CG1	1:O:357:TRP:CZ2	2.81	0.56
1:X:227:HIS:O	1:X:228:THR:CB	2.43	0.56
1:X:238:VAL:HG23	1:X:239:PRO:HD2	1.86	0.56
1:X:74:ALA:O	1:X:75:ILE:C	2.44	0.56
2:O:516:HOH:O	1:X:229:ARG:HB3	2.06	0.56
1:X:344:TYR:C	1:X:365:VAL:HG21	2.25	0.55
1:X:84:ARG:HB2	1:X:104:TRP:CG	2.41	0.55
1:X:247:GLN:HB3	1:X:273:VAL:CG2	2.36	0.55
1:X:274:MET:HB3	1:X:303:LEU:HB2	1.88	0.55
1:O:307:ILE:HD13	1:O:308:PHE:N	2.20	0.55
1:O:17:SER:HB2	1:O:56:SER:HB2	1.89	0.55
1:O:84:ARG:NH1	2:O:550:HOH:O	2.40	0.55
1:X:416:ASN:CB	1:X:419:LEU:H	2.19	0.55
1:X:10:ILE:CD1	1:X:61:ILE:HD12	2.33	0.55
1:O:54:TRP:CD1	1:O:170:LEU:HD21	2.41	0.55
1:X:405:PRO:HB2	1:X:406:LEU:HD12	1.89	0.55
1:X:221:ASN:HB3	1:X:447:LEU:HD11	1.89	0.55
1:O:163:PHE:O	1:O:216:PRO:CD	2.55	0.55
1:X:254:GLN:HG2	1:X:439:THR:HG21	1.88	0.54
1:X:75:ILE:CG1	1:X:76:ALA:N	2.70	0.54
1:O:142:VAL:O	1:O:142:VAL:HG12	2.07	0.54
1:X:238:VAL:CG2	1:X:239:PRO:CD	2.85	0.54
1:X:7:VAL:O	1:X:7:VAL:HG13	2.08	0.54
1:O:19:ALA:HB2	1:O:57:VAL:HG13	1.89	0.54
1:X:428:ASP:OD2	1:X:480:ARG:HD3	2.08	0.54
1:O:143:ARG:C	1:O:145:LEU:H	2.10	0.54
1:X:175:THR:CG2	1:X:228:THR:HG22	2.39	0.53
1:O:372:THR:HG23	1:O:376:ASP:HB2	1.89	0.53
1:O:307:ILE:HD13	1:O:308:PHE:CD1	2.39	0.53
1:X:80:ILE:HG23	1:X:81:THR:N	2.23	0.53
1:O:78:ILE:CD1	1:O:230:SER:CB	2.86	0.53
1:O:78:ILE:HD11	1:O:230:SER:CB	2.37	0.53
1:O:54:TRP:NE1	1:O:170:LEU:HD23	2.24	0.53
1:O:39:TYR:CE2	1:O:41:PRO:HD3	2.43	0.53
1:X:248:GLN:HA	1:X:251:LEU:HD23	1.90	0.53
1:X:273:VAL:HG12	1:X:274:MET:N	2.22	0.53
1:X:486:GLY:HA2	1:X:489:GLN:HE21	1.72	0.53
1:X:78:ILE:O	1:X:240:ILE:HG23	2.09	0.53
1:X:310:ALA:O	1:X:313:ALA:HB3	2.09	0.53
1:O:10:ILE:CD1	1:O:78:ILE:HG23	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:250:ALA:HB3	2:O:534:HOH:O	2.08	0.53
1:X:45:TRP:HE1	1:X:108:GLN:NE2	1.93	0.53
1:X:238:VAL:CG2	1:X:239:PRO:N	2.72	0.53
1:X:26:GLY:HA3	1:X:464:MET:CE	2.39	0.53
1:O:307:ILE:CD1	1:O:353:GLY:N	2.72	0.53
1:X:272:ILE:HG22	1:X:396:MET:CE	2.39	0.53
1:X:344:TYR:HB3	1:X:365:VAL:HG11	1.90	0.53
1:O:163:PHE:CG	1:O:164:GLY:N	2.76	0.53
1:X:352:LEU:HD12	1:X:388:GLN:HE21	1.74	0.52
1:O:173:LYS:HB2	1:X:71:ARG:NH1	2.24	0.52
1:O:54:TRP:NE1	1:O:170:LEU:CD2	2.73	0.52
1:O:66:ILE:HG12	1:X:54:TRP:NE1	2.24	0.52
1:X:275:ASN:HD21	1:X:292:GLY:HA3	1.75	0.52
1:X:390:LYS:HZ3	1:X:427:LEU:HG	1.73	0.52
1:X:230:SER:O	1:X:238:VAL:CG1	2.44	0.52
1:X:78:ILE:N	1:X:239:PRO:O	2.43	0.52
1:X:181:VAL:HG22	1:X:182:THR:N	2.25	0.52
1:X:81:THR:HG22	1:X:82:ASN:N	2.25	0.52
1:X:273:VAL:HG22	1:X:304:GLU:HG3	1.92	0.52
1:X:238:VAL:CA	1:X:238:VAL:O	2.49	0.52
1:O:78:ILE:CD1	1:O:230:SER:HB2	2.40	0.52
1:X:222:SER:HB2	1:X:447:LEU:HG	1.91	0.52
1:X:407:LEU:HD23	1:X:408:LYS:N	2.25	0.52
1:O:354:ALA:O	1:O:357:TRP:NE1	2.42	0.52
1:X:189:ARG:NH1	2:X:554:HOH:O	2.43	0.51
1:X:39:TYR:CE2	1:X:41:PRO:HD3	2.46	0.51
1:X:389:SER:O	1:X:393:ILE:HB	2.11	0.51
1:O:151:GLY:O	1:O:152:ALA:HB3	2.09	0.51
1:X:270:ALA:O	1:X:307:ILE:HD13	2.09	0.51
1:X:480:ARG:O	1:X:481:ASP:HB2	2.10	0.51
1:O:67:GLU:HG2	1:X:55:ASN:HD21	1.75	0.51
1:X:258:GLU:HB2	1:X:261:MET:CE	2.40	0.51
1:X:174:LEU:O	1:X:228:THR:HG21	2.09	0.51
1:O:86:THR:HG23	2:O:528:HOH:O	2.11	0.51
1:O:78:ILE:HD11	1:O:230:SER:HB3	1.93	0.51
1:X:323:MET:HE3	1:X:374:LYS:HE2	1.93	0.51
1:X:286:ASP:O	1:X:357:TRP:CZ3	2.63	0.51
1:O:143:ARG:HE	1:O:208:LEU:HD13	1.76	0.51
1:O:174:LEU:HD13	1:O:240:ILE:HG12	1.91	0.51
1:X:266:TYR:HB2	1:X:411:GLY:HA3	1.92	0.51
1:X:175:THR:HA	1:X:228:THR:HG22	1.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:238:VAL:CG2	1:X:238:VAL:C	2.79	0.51
1:X:238:VAL:HG23	1:X:239:PRO:CD	2.41	0.51
1:O:9:ALA:HB2	1:O:445:ALA:HB2	1.93	0.51
1:O:132:VAL:CG1	1:O:357:TRP:HH2	2.20	0.50
1:O:307:ILE:CD1	1:O:308:PHE:HB2	2.38	0.50
1:X:405:PRO:O	1:X:429:ILE:CG2	2.59	0.50
1:X:75:ILE:HG13	1:X:238:VAL:HG13	1.92	0.50
1:X:45:TRP:N	1:X:45:TRP:CD1	2.80	0.50
1:O:393:ILE:HD13	1:O:427:LEU:HD21	1.92	0.50
1:X:104:TRP:HA	1:X:141:LYS:NZ	2.27	0.50
1:X:386:ALA:O	1:X:390:LYS:HE2	2.12	0.50
1:X:385:VAL:HA	1:X:388:GLN:HB2	1.92	0.50
1:X:78:ILE:H	1:X:240:ILE:HA	1.76	0.50
1:O:57:VAL:O	1:O:61:ILE:N	2.44	0.50
1:X:356:TYR:CB	1:X:357:TRP:O	2.60	0.50
1:X:377:PHE:HD1	1:X:380:ALA:HB3	1.77	0.50
1:O:416:ASN:HD22	1:O:419:LEU:H	1.58	0.50
1:X:377:PHE:CD1	1:X:380:ALA:HB3	2.47	0.50
1:X:19:ALA:CB	1:X:64:ALA:HB2	2.42	0.50
1:O:251:LEU:HD11	1:O:275:ASN:ND2	2.27	0.50
1:X:104:TRP:HZ3	1:X:308:PHE:HA	1.76	0.49
1:X:134:ASP:C	1:X:136:TYR:H	2.15	0.49
1:X:273:VAL:CG1	1:X:302:ALA:HB1	2.42	0.49
1:X:428:ASP:HB2	1:X:480:ARG:NH1	2.27	0.49
1:O:55:ASN:O	1:O:59:SER:HB3	2.12	0.49
1:O:50:ALA:HB2	1:O:101:ALA:N	2.18	0.49
1:X:405:PRO:O	1:X:429:ILE:HG21	2.13	0.49
1:X:246:ASP:OD2	1:X:247:GLN:NE2	2.46	0.49
1:X:354:ALA:HB3	1:X:356:TYR:HD2	1.78	0.49
1:O:307:ILE:HD11	1:O:353:GLY:N	2.28	0.49
1:O:97:PRO:C	1:O:98:ILE:HD13	2.30	0.49
1:O:228:THR:CG2	1:O:238:VAL:O	2.57	0.49
1:X:82:ASN:HB2	1:X:166:ILE:HB	1.93	0.49
1:X:50:ALA:HB3	1:X:97:PRO:HG2	1.93	0.49
1:X:75:ILE:HD12	1:X:76:ALA:H	1.78	0.49
1:O:288:LEU:HD21	1:O:357:TRP:CH2	2.48	0.49
1:O:72:PRO:HB3	1:O:230:SER:O	2.13	0.49
1:O:50:ALA:C	1:O:52:GLU:H	2.15	0.49
1:X:280:PRO:CD	1:X:301:TYR:CD2	2.96	0.49
1:X:267:GLY:C	1:X:269:GLY:H	2.16	0.49
1:O:306:SER:OG	1:O:307:ILE:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:80:ILE:HG23	1:X:81:THR:H	1.77	0.48
1:O:89:VAL:HG22	1:O:163:PHE:HD1	1.78	0.48
1:X:446:TYR:HD2	1:X:458:LEU:HD22	1.77	0.48
1:O:307:ILE:CD1	1:O:308:PHE:CB	2.76	0.48
1:O:180:HIS:CE1	1:O:216:PRO:CG	2.88	0.48
1:X:402:ILE:HG22	1:X:403:ASP:N	2.28	0.48
1:O:102:ILE:HG23	1:O:106:SER:CB	2.43	0.48
1:O:271:PHE:CD1	1:O:306:SER:O	2.67	0.48
1:X:126:HIS:NE2	1:X:283:SER:O	2.28	0.48
1:X:5:ASN:HA	1:X:74:ALA:O	2.13	0.48
1:X:264:ASN:HB2	1:X:407:LEU:HD21	1.95	0.48
1:X:75:ILE:CD1	1:X:76:ALA:H	2.27	0.48
1:X:33:GLN:O	1:X:34:LYS:CG	2.58	0.48
1:O:48:HIS:HD2	1:O:83:GLN:HE22	1.61	0.48
1:X:223:GLU:O	1:X:241:ALA:O	2.31	0.48
1:X:253:GLY:O	1:X:442:LEU:HD12	2.14	0.48
1:X:26:GLY:HA3	1:X:464:MET:HE3	1.95	0.48
1:X:238:VAL:CB	1:X:238:VAL:C	2.73	0.48
1:X:72:PRO:O	1:X:75:ILE:CG2	2.62	0.48
1:O:19:ALA:O	1:O:60:VAL:HG12	2.13	0.48
1:X:305:GLY:O	1:X:306:SER:OG	2.29	0.48
1:X:251:LEU:HD11	1:X:275:ASN:HB2	1.96	0.47
1:X:10:ILE:O	1:X:11:ASP:HB2	2.13	0.47
1:X:263:LYS:HD2	1:X:264:ASN:N	2.30	0.47
1:X:72:PRO:C	1:X:74:ALA:N	2.67	0.47
1:X:356:TYR:O	1:X:357:TRP:HB2	2.13	0.47
1:X:420:MET:HB2	1:X:471:PHE:HE1	1.78	0.47
1:X:78:ILE:HG22	1:X:240:ILE:HG12	1.97	0.47
1:X:82:ASN:OD1	2:X:530:HOH:O	2.20	0.47
1:O:138:SER:HB2	1:O:190:THR:HA	1.96	0.47
1:O:125:ILE:O	1:O:125:ILE:HD13	2.14	0.47
1:X:151:GLY:O	1:X:152:ALA:C	2.50	0.47
1:O:285:ASN:HB3	1:O:395:THR:HG23	1.96	0.47
1:X:226:GLY:H	1:X:240:ILE:HB	1.79	0.47
1:X:174:LEU:O	1:X:228:THR:HG23	2.13	0.47
1:X:455:TRP:HH2	1:X:461:LEU:CD2	2.27	0.47
1:O:75:ILE:HG13	1:O:238:VAL:CG2	2.45	0.47
1:X:343:VAL:O	1:X:344:TYR:CG	2.67	0.47
1:O:21:ILE:HD11	1:O:64:ALA:O	2.14	0.47
1:X:282:LEU:HD12	1:X:282:LEU:N	2.29	0.47
1:X:404:ILE:HG12	1:X:404:ILE:H	1.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:112:ILE:HG13	1:O:112:ILE:H	1.37	0.47
1:X:175:THR:C	1:X:177:GLY:H	2.17	0.47
1:X:25:ASN:HD22	1:X:461:LEU:CG	2.27	0.47
1:X:410:ASP:HB3	1:X:439:THR:OG1	2.15	0.47
1:X:286:ASP:C	1:X:357:TRP:HH2	2.18	0.47
1:X:286:ASP:HB2	1:X:357:TRP:CH2	2.50	0.47
1:X:310:ALA:HB2	1:X:385:VAL:HG21	1.97	0.47
1:X:79:GLY:O	1:X:80:ILE:CD1	2.51	0.47
1:O:280:PRO:HD3	1:O:301:TYR:CD2	2.50	0.47
1:X:238:VAL:HG22	1:X:239:PRO:CD	2.44	0.46
1:X:238:VAL:CA	1:X:238:VAL:H	2.06	0.46
1:O:129:THR:HG21	1:O:191:MET:HA	1.97	0.46
1:X:247:GLN:HB2	2:X:557:HOH:O	2.15	0.46
1:X:434:ALA:O	1:X:437:LEU:HD11	2.15	0.46
1:X:82:ASN:ND2	1:X:167:ASP:HB3	2.31	0.46
1:X:352:LEU:HD21	1:X:491:VAL:HG13	1.96	0.46
1:X:268:THR:N	2:X:553:HOH:O	2.48	0.46
1:X:357:TRP:O	1:X:358:ASP:CB	2.63	0.46
1:X:314:ILE:HD11	1:X:413:ALA:HB2	1.96	0.46
1:X:52:GLU:HA	1:X:55:ASN:HB2	1.97	0.46
1:O:352:LEU:O	1:O:353:GLY:C	2.54	0.46
1:O:390:LYS:HD2	1:O:426:ILE:HG23	1.96	0.46
1:X:419:LEU:C	1:X:421:GLN:H	2.18	0.46
1:X:84:ARG:NE	2:X:552:HOH:O	2.49	0.46
1:X:484:TYR:HE2	1:X:488:LYS:HZ3	1.64	0.46
1:X:267:GLY:O	1:X:269:GLY:N	2.49	0.46
1:X:5:ASN:ND2	1:X:5:ASN:N	2.57	0.46
1:O:173:LYS:HE2	1:X:71:ARG:HD3	1.98	0.46
1:X:390:LYS:NZ	1:X:427:LEU:HA	2.30	0.46
1:X:345:VAL:HG12	1:X:384:ALA:HB2	1.98	0.46
1:X:267:GLY:O	1:X:311:GLY:N	2.49	0.46
1:O:94:THR:HB	1:O:95:GLY:H	1.63	0.46
1:X:272:ILE:O	1:X:396:MET:HE3	2.16	0.45
1:X:204:ILE:O	1:X:208:LEU:HG	2.17	0.45
1:X:252:PHE:CE2	1:X:293:TYR:CD2	3.03	0.45
1:O:38:GLN:HE22	1:O:48:HIS:CE1	2.35	0.45
1:O:98:ILE:CD1	1:O:98:ILE:N	2.47	0.45
1:X:181:VAL:HG22	1:X:182:THR:H	1.82	0.45
1:O:39:TYR:HE2	1:O:41:PRO:HG3	1.81	0.45
1:X:55:ASN:O	1:X:59:SER:HB3	2.15	0.45
1:O:306:SER:OG	1:O:354:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:102:ILE:HD12	1:X:145:LEU:HD11	1.99	0.45
1:X:134:ASP:HB2	1:X:357:TRP:CD1	2.51	0.45
1:X:252:PHE:CZ	1:X:294:GLY:O	2.70	0.45
1:X:258:GLU:HB2	1:X:261:MET:HE2	1.98	0.45
1:O:262:ILE:HG22	1:O:263:LYS:H	1.82	0.45
1:O:26:GLY:HA3	1:O:464:MET:HG3	1.99	0.45
1:X:251:LEU:HD22	1:X:273:VAL:CG1	2.46	0.45
1:X:20:ILE:HG12	1:X:30:GLY:O	2.16	0.45
1:X:332:GLU:C	1:X:334:ALA:H	2.20	0.45
1:O:357:TRP:N	1:O:357:TRP:HD1	2.15	0.44
1:O:88:VAL:O	1:O:164:GLY:O	2.35	0.44
1:O:98:ILE:H	1:O:98:ILE:CD1	2.14	0.44
1:X:475:MET:HB3	1:X:476:PRO:HD2	1.99	0.44
1:X:307:ILE:HG22	1:X:309:VAL:H	1.81	0.44
1:X:377:PHE:HA	1:X:380:ALA:H	1.82	0.44
1:O:102:ILE:HG22	1:O:103:VAL:O	2.17	0.44
1:O:369:THR:HG22	1:O:371:GLY:N	2.27	0.44
1:X:75:ILE:O	1:X:76:ALA:HB2	2.18	0.44
1:X:274:MET:HG2	1:X:276:THR:HG23	1.98	0.44
1:X:16:SER:OG	1:X:18:ARG:HG2	2.18	0.44
1:X:77:GLY:HA2	1:X:239:PRO:N	2.33	0.44
1:X:45:TRP:CE2	1:X:108:GLN:HG2	2.53	0.44
1:X:48:HIS:CD2	1:X:83:GLN:HE22	2.22	0.44
1:X:126:HIS:ND1	1:X:131:LEU:O	2.50	0.44
1:X:253:GLY:HA2	1:X:442:LEU:HD13	2.00	0.44
1:O:132:VAL:CG2	1:O:133:ILE:N	2.81	0.44
1:X:440:THR:HG22	1:X:441:ALA:N	2.33	0.44
1:O:198:LEU:HD21	1:O:299:VAL:HG21	1.98	0.44
1:X:409:VAL:CG2	1:X:420:MET:HE3	2.48	0.44
1:X:238:VAL:HG22	1:X:239:PRO:HD2	1.98	0.44
1:O:146:LEU:HG	1:O:152:ALA:HB1	2.00	0.44
1:X:247:GLN:HB3	1:X:273:VAL:HG21	2.00	0.43
1:X:414:ALA:C	1:X:416:ASN:H	2.21	0.43
1:X:221:ASN:CB	1:X:447:LEU:HD11	2.47	0.43
1:O:182:THR:HG22	1:O:183:ASP:H	1.83	0.43
1:O:47:GLU:HA	1:O:103:VAL:HG23	1.99	0.43
1:X:109:SER:HB3	1:X:140:THR:HB	2.00	0.43
1:X:354:ALA:HA	1:X:392:VAL:CG1	2.48	0.43
1:X:418:LEU:HA	1:X:421:GLN:CB	2.41	0.43
1:O:173:LYS:C	1:O:175:THR:H	2.22	0.43
1:X:345:VAL:CG1	1:X:347:PRO:CD	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:51:ASN:H	1:O:51:ASN:ND2	2.16	0.43
1:O:78:ILE:HD12	1:O:230:SER:HB2	2.00	0.43
1:O:62:ALA:C	1:O:66:ILE:HD12	2.31	0.43
1:X:344:TYR:O	1:X:365:VAL:HG21	2.18	0.43
1:X:387:TYR:OH	1:X:483:LEU:O	2.26	0.43
1:X:8:MET:HE3	1:X:65:PHE:CD1	2.53	0.43
1:X:260:GLY:H	1:X:276:THR:HA	1.83	0.43
1:X:75:ILE:CG1	1:X:76:ALA:H	2.32	0.43
1:X:16:SER:OG	1:X:17:SER:N	2.51	0.43
1:X:145:LEU:O	1:X:149:ILE:HD12	2.19	0.43
1:X:134:ASP:OD1	1:X:359:SER:OG	2.34	0.43
1:X:389:SER:O	1:X:393:ILE:N	2.51	0.43
1:O:307:ILE:HD13	1:O:308:PHE:H	1.83	0.43
1:X:422:PHE:O	1:X:424:ALA:N	2.50	0.43
1:X:262:ILE:CD1	1:X:274:MET:HE3	2.49	0.43
1:X:392:VAL:O	1:X:396:MET:HB2	2.19	0.43
1:O:94:THR:O	1:X:70:ILE:HG22	2.18	0.43
1:X:153:GLN:HB3	1:X:154:GLU:OE2	2.18	0.43
1:X:274:MET:CE	1:X:396:MET:HG3	2.48	0.43
1:X:132:VAL:HG21	1:X:357:TRP:NE1	2.29	0.43
1:X:253:GLY:HA2	1:X:442:LEU:CD1	2.48	0.43
1:O:307:ILE:HG12	1:O:308:PHE:CD1	2.53	0.43
1:O:90:TRP:N	1:O:162:LEU:O	2.51	0.43
1:X:272:ILE:HG22	1:X:396:MET:HE2	1.99	0.43
1:X:227:HIS:CE1	1:X:239:PRO:HD3	2.54	0.43
1:O:352:LEU:CG	1:O:352:LEU:O	2.67	0.43
1:X:331:GLU:HG3	1:X:416:ASN:HD22	1.83	0.43
1:X:79:GLY:C	1:X:80:ILE:HD12	2.36	0.43
1:O:164:GLY:HA2	2:O:544:HOH:O	2.19	0.43
1:O:204:ILE:O	1:O:208:LEU:HG	2.19	0.43
1:O:67:GLU:HG2	1:X:55:ASN:ND2	2.33	0.42
1:X:132:VAL:HG11	1:X:357:TRP:HZ2	0.68	0.42
1:X:71:ARG:CB	1:X:72:PRO:CD	2.89	0.42
1:O:104:TRP:O	1:O:136:TYR:HD1	2.02	0.42
1:O:247:GLN:HA	2:O:534:HOH:O	2.18	0.42
1:X:84:ARG:CZ	2:X:552:HOH:O	2.67	0.42
1:X:8:MET:O	1:X:9:ALA:CB	2.46	0.42
1:X:189:ARG:HH22	1:X:288:LEU:HD13	1.85	0.42
1:X:262:ILE:CD1	1:X:274:MET:CE	2.95	0.42
1:X:429:ILE:CG2	1:X:430:ASP:H	2.33	0.42
1:O:310:ALA:HB1	1:O:385:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:416:ASN:HB3	1:X:419:LEU:H	1.85	0.42
1:O:190:THR:HG21	2:O:542:HOH:O	2.19	0.42
1:X:266:TYR:N	1:X:410:ASP:O	2.52	0.42
1:O:47:GLU:HG2	1:O:100:ASN:ND2	2.34	0.42
1:X:32:SER:HB2	1:X:33:GLN:H	0.98	0.42
1:X:428:ASP:CB	1:X:480:ARG:NH1	2.83	0.42
1:O:18:ARG:HH12	1:O:20:ILE:HD11	1.85	0.42
1:X:254:GLN:N	2:X:517:HOH:O	2.44	0.42
1:X:323:MET:HB2	1:X:324:ILE:CD1	2.50	0.42
1:O:103:VAL:C	1:O:105:GLN:N	2.71	0.42
1:O:146:LEU:HB3	1:O:153:GLN:HE21	1.84	0.42
1:X:386:ALA:HB1	1:X:423:GLN:HE22	1.85	0.42
1:X:75:ILE:HG13	1:X:238:VAL:CG1	2.50	0.42
1:X:56:SER:O	1:X:60:VAL:CG2	2.65	0.42
1:O:18:ARG:NH2	1:O:438:GLU:HB3	2.35	0.42
1:X:273:VAL:HG22	1:X:304:GLU:HB2	2.02	0.41
1:X:431:VAL:CG2	1:X:432:GLN:H	2.32	0.41
1:X:72:PRO:O	1:X:75:ILE:HG22	2.19	0.41
1:O:307:ILE:HD13	1:O:308:PHE:CA	2.49	0.41
1:O:437:LEU:H	1:O:437:LEU:HD12	1.84	0.41
1:X:248:GLN:NE2	1:X:291:ILE:O	2.54	0.41
1:X:25:ASN:HB3	1:X:461:LEU:HD12	2.01	0.41
1:X:18:ARG:O	1:X:19:ALA:HB2	2.19	0.41
1:O:161:LEU:O	1:O:214:MET:HA	2.20	0.41
1:X:475:MET:HB3	1:X:476:PRO:CD	2.50	0.41
1:X:273:VAL:HG22	1:X:304:GLU:CB	2.51	0.41
1:O:132:VAL:HG13	1:O:357:TRP:HH2	1.79	0.41
1:X:12:GLN:HG3	1:X:53:ILE:HG23	2.02	0.41
1:X:439:THR:O	1:X:442:LEU:HB2	2.20	0.41
1:X:428:ASP:CB	1:X:480:ARG:HH11	2.30	0.41
1:X:218:VAL:HG13	1:X:218:VAL:O	2.21	0.41
1:O:355:PRO:HD2	1:O:392:VAL:HG13	2.02	0.41
1:X:275:ASN:ND2	1:X:292:GLY:HA3	2.34	0.41
1:O:39:TYR:CE2	1:O:41:PRO:CD	3.04	0.41
1:X:12:GLN:CG	1:X:53:ILE:HG23	2.50	0.41
1:O:149:ILE:HA	1:O:149:ILE:HD12	1.82	0.41
1:X:251:LEU:O	1:X:256:ALA:HB2	2.21	0.41
1:O:247:GLN:OE1	1:O:271:PHE:HB2	2.20	0.41
1:X:165:THR:O	1:X:167:ASP:OD1	2.39	0.41
1:X:19:ALA:HB3	1:X:64:ALA:HB2	2.03	0.41
1:X:438:GLU:HG2	1:X:441:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:146:LEU:HD23	1:X:153:GLN:HE21	1.85	0.41
1:X:274:MET:HE3	1:X:274:MET:HB2	1.93	0.41
1:O:8:MET:HB2	1:O:78:ILE:HG12	2.02	0.41
1:O:257:PHE:CG	1:O:257:PHE:O	2.73	0.41
1:O:424:ALA:HB1	1:O:473:PRO:CD	2.31	0.41
1:X:139:ALA:O	1:X:143:ARG:HG3	2.21	0.41
1:X:247:GLN:HG3	1:X:271:PHE:HB2	2.02	0.41
1:X:249:ALA:O	1:X:253:GLY:N	2.54	0.41
1:O:78:ILE:HD12	1:O:230:SER:CB	2.51	0.41
1:O:288:LEU:HD21	1:O:357:TRP:HH2	1.84	0.41
1:X:345:VAL:HG12	1:X:383:GLN:O	2.21	0.41
1:O:84:ARG:HH22	1:O:304:GLU:CD	2.23	0.41
1:X:243:MET:O	1:X:244:ALA:HB2	2.21	0.41
1:X:407:LEU:HD23	1:X:408:LYS:H	1.85	0.41
1:O:104:TRP:HZ3	1:O:308:PHE:HA	1.86	0.41
1:X:318:ARG:O	1:X:322:ARG:HA	2.21	0.41
1:X:344:TYR:O	1:X:345:VAL:HG23	2.20	0.41
1:X:27:LYS:HB2	1:X:27:LYS:HZ3	1.86	0.41
1:X:409:VAL:HG11	1:X:420:MET:HE1	2.03	0.40
1:O:369:THR:HG22	1:O:370:ARG:N	2.36	0.40
1:O:225:TYR:CE2	1:O:243:MET:HG2	2.57	0.40
1:X:366:PHE:HB2	1:X:367:GLY:H	1.57	0.40
1:O:230:SER:O	1:O:230:SER:CA	2.53	0.40
1:O:61:ILE:HG22	1:O:62:ALA:N	2.37	0.40
1:X:132:VAL:HG12	1:X:288:LEU:HD23	2.02	0.40
1:X:134:ASP:O	1:X:136:TYR:N	2.54	0.40
1:X:409:VAL:HG11	1:X:420:MET:CE	2.52	0.40
1:X:77:GLY:HA3	1:X:239:PRO:O	2.16	0.40
1:X:67:GLU:O	1:X:68:SER:HB2	2.22	0.40
1:O:84:ARG:NH2	2:O:511:HOH:O	2.54	0.40
1:X:247:GLN:C	1:X:249:ALA:H	2.25	0.40
1:X:256:ALA:HA	1:X:261:MET:SD	2.61	0.40
1:X:274:MET:HE1	1:X:396:MET:HG3	2.04	0.40
1:O:142:VAL:HA	1:O:145:LEU:HD22	2.04	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	O	478/505 (95%)	393 (82%)	63 (13%)	22 (5%)	3	3
1	X	478/505 (95%)	320 (67%)	99 (21%)	59 (12%)	0	0
All	All	956/1010 (95%)	713 (75%)	162 (17%)	81 (8%)	1	1

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	43	SER
1	O	238	VAL
1	O	257	PHE
1	O	258	GLU
1	O	308	PHE
1	O	353	GLY
1	O	354	ALA
1	X	10	ILE
1	X	20	ILE
1	X	21	ILE
1	X	29	ILE
1	X	68	SER
1	X	75	ILE
1	X	135	ALA
1	X	166	ILE
1	X	229	ARG
1	X	238	VAL
1	X	318	ARG
1	X	335	ALA
1	X	342	GLU
1	X	358	ASP
1	X	366	PHE
1	X	384	ALA
1	X	429	ILE
1	X	444	ALA

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Mol	Chain	Res	Type
1	X	456	LYS
1	X	461	LEU
1	X	463	SER
1	X	465	ALA
1	O	52	GLU
1	O	357	TRP
1	X	9	ALA
1	X	11	ASP
1	X	76	ALA
1	X	153	GLN
1	X	230	SER
1	X	244	ALA
1	X	268	THR
1	X	277	GLY
1	X	286	ASP
1	X	330	SER
1	X	340	ASP
1	X	354	ALA
1	X	428	ASP
1	X	457	ASP
1	X	475	MET
1	X	481	ASP
1	O	55	ASN
1	O	56	SER
1	O	99	ALA
1	O	150	GLU
1	O	174	LEU
1	X	23	ASP
1	X	371	GLY
1	X	412	GLY
1	O	72	PRO
1	O	94	THR
1	X	34	LYS
1	X	41	PRO
1	X	152	ALA
1	X	255	MET
1	X	306	SER
1	X	336	LYS
1	X	395	THR
1	X	449	GLY
1	O	41	PRO
1	O	51	ASN

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Mol	Chain	Res	Type
1	O	405	PRO
1	X	310	ALA
1	X	319	ASP
1	X	320	GLY
1	X	324	ILE
1	X	337	ALA
1	O	95	GLY
1	X	297	GLY
1	O	215	LEU
1	O	297	GLY
1	X	63	GLY
1	X	71	ARG
1	X	328	PRO
1	X	468	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	O	390/409 (95%)	328 (84%)	62 (16%)	3	5
1	X	390/409 (95%)	295 (76%)	95 (24%)	1	1
All	All	780/818 (95%)	623 (80%)	157 (20%)	1	3

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	O	18	ARG
1	O	22	PHE
1	O	33	GLN
1	O	37	PRO
1	O	49	ASN
1	O	51	ASN
1	O	53	ILE
1	O	55	ASN

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Mol	Chain	Res	Type
1	O	61	ILE
1	O	65	PHE
1	O	71	ARG
1	O	72	PRO
1	O	81	THR
1	O	82	ASN
1	O	86	THR
1	O	87	THR
1	O	88	VAL
1	O	91	ASP
1	O	94	THR
1	O	97	PRO
1	O	98	ILE
1	O	111	PRO
1	O	112	ILE
1	O	125	ILE
1	O	132	VAL
1	O	140	THR
1	O	144	TRP
1	O	168	SER
1	O	175	THR
1	O	179	VAL
1	O	180	HIS
1	O	182	THR
1	O	205	LEU
1	O	207	LEU
1	O	208	LEU
1	O	211	PRO
1	O	215	LEU
1	O	216	PRO
1	O	230	SER
1	O	239	PRO
1	O	240	ILE
1	O	257	PHE
1	O	263	LYS
1	O	280	PRO
1	O	307	ILE
1	O	312	SER
1	O	326	THR
1	O	328	PRO
1	O	347	PRO
1	O	352	LEU

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Mol	Chain	Res	Type
1	O	355	PRO
1	O	357	TRP
1	O	373	THR
1	O	392	VAL
1	O	416	ASN
1	O	419	LEU
1	O	439	THR
1	O	447	LEU
1	O	457	ASP
1	O	473	PRO
1	O	480	ARG
1	X	5	ASN
1	X	10	ILE
1	X	12	GLN
1	X	18	ARG
1	X	20	ILE
1	X	22	PHE
1	X	29	ILE
1	X	45	TRP
1	X	53	ILE
1	X	57	VAL
1	X	60	VAL
1	X	66	ILE
1	X	67	GLU
1	X	71	ARG
1	X	72	PRO
1	X	78	ILE
1	X	80	ILE
1	X	82	ASN
1	X	97	PRO
1	X	125	ILE
1	X	138	SER
1	X	154	GLU
1	X	161	LEU
1	X	175	THR
1	X	182	THR
1	X	186	ASN
1	X	205	LEU
1	X	206	ASP
1	X	208	LEU
1	X	211	PRO
1	X	216	PRO

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Mol	Chain	Res	Type
1	X	239	PRO
1	X	243	MET
1	X	246	ASP
1	X	263	LYS
1	X	265	THR
1	X	268	THR
1	X	271	PHE
1	X	275	ASN
1	X	276	THR
1	X	280	PRO
1	X	285	ASN
1	X	286	ASP
1	X	315	GLN
1	X	321	LEU
1	X	323	MET
1	X	324	ILE
1	X	328	PRO
1	X	333	LEU
1	X	336	LYS
1	X	338	LYS
1	X	342	GLU
1	X	345	VAL
1	X	352	LEU
1	X	355	PRO
1	X	357	TRP
1	X	365	VAL
1	X	366	PHE
1	X	372	THR
1	X	373	THR
1	X	376	ASP
1	X	377	PHE
1	X	379	ARG
1	X	382	LEU
1	X	387	TYR
1	X	393	ILE
1	X	397	LYS
1	X	399	ASP
1	X	404	ILE
1	X	405	PRO
1	X	406	LEU
1	X	407	LEU
1	X	408	LYS

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Mol	Chain	Res	Type
1	X	421	GLN
1	X	425	ASP
1	X	427	LEU
1	X	430	ASP
1	X	433	ARG
1	X	438	GLU
1	X	439	THR
1	X	440	THR
1	X	442	LEU
1	X	447	LEU
1	X	450	LEU
1	X	454	PHE
1	X	456	LYS
1	X	459	ASP
1	X	464	MET
1	X	471	PHE
1	X	473	PRO
1	X	474	GLU
1	X	476	PRO
1	X	479	GLU
1	X	480	ARG
1	X	483	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	48	HIS
1	O	51	ASN
1	O	82	ASN
1	O	153	GLN
1	O	186	ASN
1	O	275	ASN
1	O	315	GLN
1	O	383	GLN
1	O	388	GLN
1	O	416	ASN
1	X	48	HIS
1	X	55	ASN
1	X	82	ASN
1	X	108	GLN
1	X	148	ASN
1	X	153	GLN

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Mol	Chain	Res	Type
1	X	221	ASN
1	X	227	HIS
1	X	264	ASN
1	X	275	ASN
1	X	315	GLN
1	X	383	GLN
1	X	388	GLN
1	X	421	GLN
1	X	489	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.