



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:25 AM UTC

PDB ID : 1R59 / pdb_00001r59
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

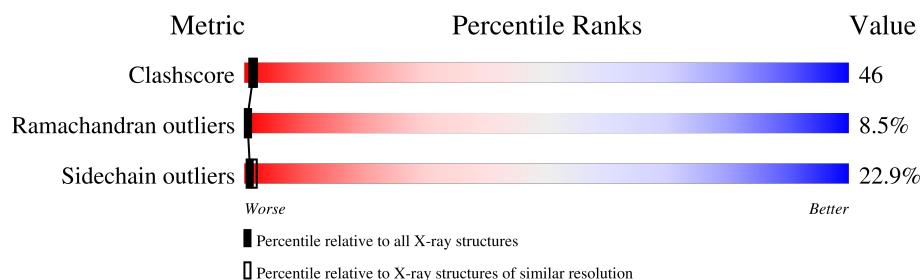
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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.

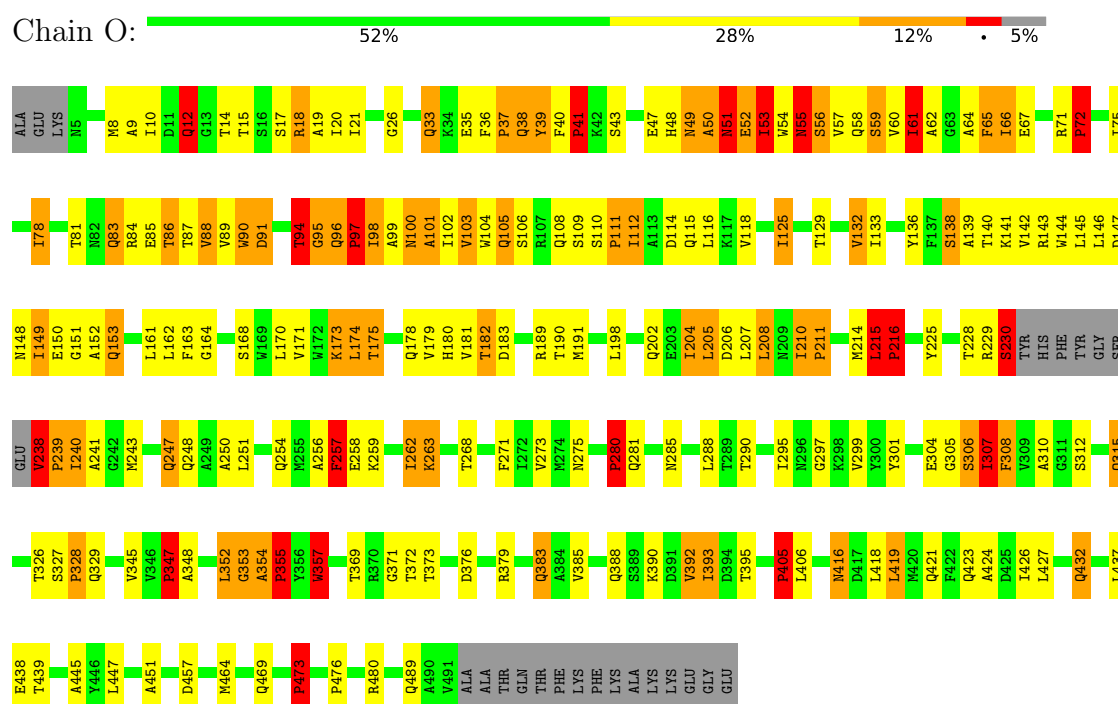
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	51	Total	O	0	0
			51	51		
2	X	51	Total	O	0	0
			51	51		

3 Residue-property plots

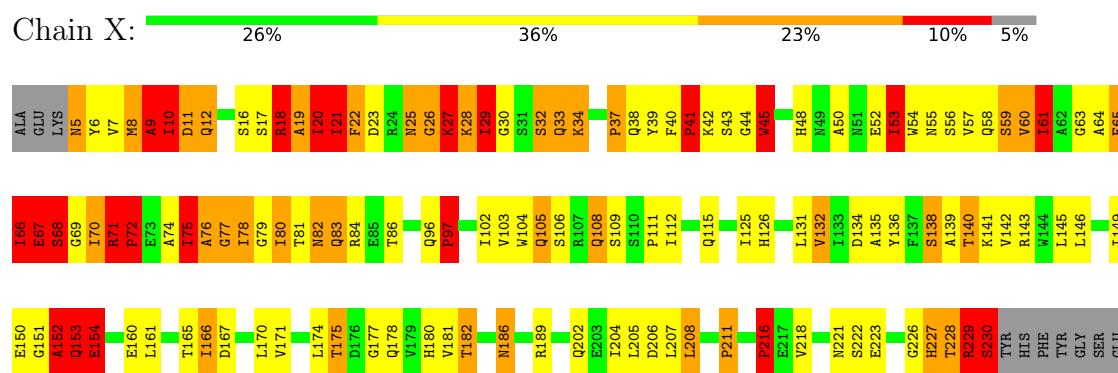
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



K488	V238	L303	V365	I426	K489	V239	E304	F366	F426	K490	E305	F367	L427	Q489	ALA
V491	I240	E306	G368	L428	A490	I241	G306	L368	D428	A491	S307	I369	I429	THR	THR
ALA	M243	I307	T369	D430	ALA	G242	F308	T369	V431	ALA	R370	R371	V432	GLN	GLN
THR	A244	V309	R370	V431	THR	A245	V309	R371	Q432	THR	R372	T372	Q433	THR	THR
GLN	G246	A310	Q432	Q433	GLN	Q247	A311	T373	R434	GLN	T373	T374	R435	PHE	PHE
GLY	Q248	S312	R434	A435	GLY	Q249	S313	K374	A436	GLY	K375	E375	N436	LYS	LYS
GLU	A249	A314	E375	L437	GLU	A250	I314	D376	L437	GLU	D376	F377	E438	LYS	LYS
	A251	F315	F377	E439		A252	W316	V378	T440	ALA	V378	V379	T441	ALA	ALA
	L251	E258	V379	T442		A253	L317	R379	A441	LYS	R379	A380	A442	LYS	LYS
	F252	K259	A380	L443		M254	R318	A381	L443	LYS	A381	T381	L444	GLY	GLY
	G259	G260	T381	A444		M255	D320	L382	G443	GLY	L382	Q383	A444	GLY	GLY
	M261	I262	Q383	A445		A256	L321	Q384	A445	GLY	Q384	A384	A446		
	I263	F267	A384	Y446		E256	R322	V385	Y446	THR	A385	V386	Y447		
	M264	E268	V385	L447		E257	M323	A386	L447	THR	A386	Y387	A448		
	N264	K269	A386	A448		E258	E325	Y387	A448	THR	Y387	Q388	G449		
	Y266	A270	E325	G449		G260	T326	Q388	G449	THR	Q388	S389	L450		
	G267	I271	T326	L450		M261	S327	S389	L450	THR	S327	K390	A451		
	T272	F271	S327	A451		I262	F328	K390	A451	THR	F328	D391			
	V273	I272	K390			K263	Q329	D391			Q329	V392	F454		
	M274	G277	V392			M264	S330	V392			S330	I393	W455		
	N275	G277	I393			N264	E331	I393			E331	T394	K456		
	T276	G277	T394			N264	E332	T394			E332	T395	D457		
	G277	G277	T395			N264	L333	T395			L333	M396	L458		
	P280	Q281	L333			N264	A334	M396			A334	K397	D459		
	Q281	L282	A334			N264	A335	K397			A335	K398	E460		
	S283	D284	K397			N264	K336	K398			K336	D399	L461		
	D285	L286	K336			N264	A337	D399			A337		K462		
	L286	L288	D399			N264	K338				K338	I402	S463		
	L288	L288	I402			N264	G339				G339	D403	M464		
	L288	L288	D403			N264	D340				D340	P404	A465		
	L288	L288	P404			N264	N341				N341	P405	G468		
	L288	L288	E342			N264	E342				E342	L406	Q469		
	L288	L288	V343			N264	V343				V343	L407	M470		
	L288	L288	Y344			N264	V344				Y344	K408	F471		
	L288	L288	V345			N264	V345				V345	V409	T472		
	L288	L288	V346			N264	V346				V346	D410	P473		
	L288	L288	P347			N264	P347				P347	G411	E474		
	L288	L288	A348			N264	A348				A348	G412	M475		
	L288	L288	F349			N264	F349				F349	A413	P476		
	L288	L288	N285			N264	N285				N285	A414	A477		
	L288	L288	T350			N264	T350				T350	K415	E478		
	L288	L288	G351			N264	G351				G351	M416	E479		
	L288	L288	L352			N264	L352				L352	D417	R480		
	L288	L288	G353			N264	G353				G353	L418	D481		
	L288	L288	A354			N264	A354				A354	L419	N482		
	L288	L288	P355			N264	P355				P355	M420	L483		
	L288	L288	Y356			N264	Y356				Y356	G421	Y484		
	L288	L288	W357			N264	W357				W357	F422	E485		
	L288	L288	D358			N264	D358				D358	Q423	G486		
	L288	L288	S359			N264	S359				S359	A424	W487		
	L288	L288	G363			N264	G363				G363	D425			
	L288	L288	A364			N264	A364				A364				

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.83Å 107.11Å 201.12Å 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 ²)	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	1.16	16/3790 (0.4%)	1.92	127/5141 (2.5%)
1	X	1.56	55/3790 (1.5%)	2.26	210/5141 (4.1%)
All	All	1.38	71/7580 (0.9%)	2.10	337/10282 (3.3%)

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

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

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	238	VAL	CA-C	22.00	1.75	1.52
1	X	154	GLU	C-N	21.56	1.63	1.33
1	O	230	SER	C-N	21.42	1.57	1.33
1	O	238	VAL	N-CA	21.41	1.73	1.46
1	X	238	VAL	C-N	18.79	1.55	1.33
1	X	230	SER	C-N	17.93	1.53	1.33
1	X	238	VAL	N-CA	17.53	1.68	1.46
1	O	230	SER	CA-C	16.99	1.75	1.52
1	X	228	THR	C-N	-15.73	1.11	1.33
1	X	230	SER	CA-C	13.62	1.71	1.52
1	O	230	SER	N-CA	12.89	1.62	1.46
1	O	238	VAL	CA-C	11.96	1.65	1.52
1	O	229	ARG	C-N	11.56	1.49	1.33
1	X	239	PRO	N-CA	11.55	1.60	1.47
1	X	20	ILE	CA-C	10.85	1.66	1.52
1	X	72	PRO	N-CA	9.63	1.59	1.47
1	X	70	ILE	N-CA	9.59	1.60	1.45
1	X	425	ASP	CA-C	8.64	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	21	ILE	N-CA	8.54	1.57	1.46
1	O	239	PRO	N-CA	8.28	1.56	1.46
1	O	210	ILE	CA-C	8.27	1.59	1.53
1	X	426	ILE	N-CA	8.22	1.56	1.46
1	O	229	ARG	CA-C	7.72	1.65	1.52
1	O	39	TYR	C-N	7.70	1.39	1.33
1	X	69	GLY	CA-C	7.22	1.62	1.51
1	X	456	LYS	C-N	7.09	1.43	1.33
1	X	425	ASP	C-N	7.04	1.43	1.33
1	X	347	PRO	CA-C	-6.77	1.44	1.53
1	O	238	VAL	C-N	6.72	1.41	1.33
1	X	29	ILE	CA-C	6.70	1.61	1.52
1	X	67	GLU	C-N	6.69	1.43	1.33
1	X	21	ILE	CA-C	6.67	1.61	1.52
1	X	326	THR	N-CA	6.61	1.54	1.46
1	X	474	GLU	CA-C	6.48	1.61	1.52
1	X	20	ILE	C-N	6.38	1.42	1.33
1	X	425	ASP	N-CA	6.35	1.54	1.46
1	X	21	ILE	C-N	6.32	1.42	1.33
1	O	40	PHE	N-CA	6.24	1.52	1.46
1	X	66	ILE	CA-C	6.21	1.60	1.52
1	X	405	PRO	N-CA	6.18	1.55	1.47
1	O	110	SER	C-N	6.18	1.41	1.34
1	X	355	PRO	C-N	-6.17	1.26	1.33
1	X	457	ASP	CA-C	6.10	1.60	1.52
1	O	41	PRO	N-CA	6.00	1.55	1.47
1	X	457	ASP	C-N	5.98	1.40	1.33
1	X	19	ALA	C-N	5.98	1.41	1.33
1	X	457	ASP	N-CA	5.91	1.53	1.46
1	X	337	ALA	N-CA	5.89	1.53	1.46
1	X	475	MET	CA-C	5.86	1.60	1.52
1	X	20	ILE	N-CA	5.84	1.53	1.46
1	X	69	GLY	C-N	5.81	1.41	1.33
1	X	458	LEU	N-CA	5.79	1.53	1.46
1	X	461	LEU	N-CA	5.75	1.53	1.46
1	X	325	GLU	N-CA	5.69	1.53	1.46
1	X	72	PRO	CA-C	5.57	1.60	1.52
1	X	69	GLY	N-CA	5.53	1.53	1.45
1	O	327	SER	C-N	5.51	1.40	1.33
1	X	427	LEU	N-CA	5.51	1.53	1.46
1	X	19	ALA	N-CA	5.48	1.53	1.46
1	X	357	TRP	N-CA	-5.43	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	316	TRP	CA-C	5.43	1.60	1.52
1	X	369	THR	N-CA	5.38	1.52	1.45
1	X	22	PHE	N-CA	5.33	1.52	1.45
1	X	18	ARG	C-N	5.32	1.39	1.33
1	X	228	THR	N-CA	5.28	1.52	1.46
1	X	68	SER	N-CA	5.23	1.52	1.46
1	X	239	PRO	N-CD	5.20	1.55	1.47
1	O	100	ASN	C-N	5.16	1.40	1.33
1	X	28	LYS	C-N	5.13	1.40	1.33
1	X	404	ILE	CA-C	5.11	1.58	1.52
1	X	77	GLY	CA-C	5.08	1.56	1.51

All (337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	239	PRO	CA-N-CD	-22.43	80.60	112.00
1	O	239	PRO	CA-N-CD	-22.12	81.03	112.00
1	O	328	PRO	CA-N-CD	-21.30	82.18	112.00
1	O	307	ILE	N-CA-C	20.45	135.96	109.58
1	O	355	PRO	CA-N-CD	-19.98	84.03	112.00
1	X	280	PRO	CA-N-CD	-19.56	84.62	112.00
1	O	211	PRO	CA-N-CD	-18.79	85.69	112.00
1	O	111	PRO	CA-N-CD	-17.94	86.88	112.00
1	O	97	PRO	CA-N-CD	-17.55	87.43	112.00
1	X	355	PRO	CA-N-CD	-17.33	87.73	112.00
1	X	25	ASN	N-CA-C	17.30	136.24	110.64
1	X	347	PRO	CA-N-CD	-16.72	88.59	112.00
1	X	97	PRO	CA-N-CD	-16.32	89.15	112.00
1	O	41	PRO	CA-N-CD	-15.59	90.17	112.00
1	X	211	PRO	CA-N-CD	-15.33	90.54	112.00
1	O	476	PRO	CA-N-CD	-15.21	90.71	112.00
1	O	229	ARG	CA-C-N	14.88	149.96	121.54
1	O	229	ARG	C-N-CA	14.88	149.96	121.54
1	X	347	PRO	N-CA-CB	14.45	112.49	102.81
1	X	476	PRO	CA-N-CD	-14.32	91.94	112.00
1	O	280	PRO	CA-N-CD	-14.09	92.27	112.00
1	X	229	ARG	CA-C-N	13.99	148.27	121.54
1	X	229	ARG	C-N-CA	13.99	148.27	121.54
1	O	347	PRO	CA-N-CD	-13.86	92.60	112.00
1	O	473	PRO	CA-N-CD	-13.84	92.63	112.00
1	X	422	PHE	CA-CB-CG	-13.72	100.08	113.80
1	X	228	THR	CA-C-N	12.96	146.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	228	THR	C-N-CA	12.96	146.29	121.54
1	X	25	ASN	CA-CB-CG	-12.70	99.90	112.60
1	X	111	PRO	CA-N-CD	-12.60	94.36	112.00
1	X	405	PRO	CA-N-CD	-12.54	94.45	112.00
1	X	370	ARG	N-CA-C	12.31	126.87	109.15
1	X	72	PRO	N-CA-C	12.17	137.54	112.47
1	X	228	THR	N-CA-C	12.00	126.58	108.46
1	O	230	SER	CA-C-N	11.71	143.80	122.13
1	O	230	SER	C-N-CA	11.71	143.80	122.13
1	O	307	ILE	CA-C-N	11.65	143.79	121.54
1	O	307	ILE	C-N-CA	11.65	143.79	121.54
1	X	456	LYS	CA-C-N	11.63	143.76	121.54
1	X	456	LYS	C-N-CA	11.63	143.76	121.54
1	O	405	PRO	CA-N-CD	-11.52	95.87	112.00
1	O	37	PRO	CA-N-CD	-11.29	96.19	112.00
1	X	230	SER	CA-C-N	11.29	143.01	122.13
1	X	230	SER	C-N-CA	11.29	143.01	122.13
1	O	229	ARG	CB-CA-C	11.16	125.06	111.22
1	X	37	PRO	CA-N-CD	-11.06	96.52	112.00
1	X	328	PRO	CA-N-CD	-11.01	96.58	112.00
1	O	281	GLN	OE1-CD-NE2	-10.94	111.66	122.60
1	O	83	GLN	OE1-CD-NE2	-10.77	111.83	122.60
1	O	12	GLN	OE1-CD-NE2	-10.68	111.92	122.60
1	O	115	GLN	OE1-CD-NE2	-10.64	111.96	122.60
1	O	388	GLN	OE1-CD-NE2	-10.64	111.96	122.60
1	O	469	GLN	OE1-CD-NE2	-10.54	112.06	122.60
1	X	115	GLN	OE1-CD-NE2	-10.49	112.11	122.60
1	O	489	GLN	OE1-CD-NE2	-10.47	112.13	122.60
1	X	473	PRO	CA-N-CD	-10.40	97.43	112.00
1	O	248	GLN	OE1-CD-NE2	-10.37	112.23	122.60
1	X	38	GLN	OE1-CD-NE2	-10.34	112.26	122.60
1	X	32	SER	N-CA-C	10.28	132.69	110.80
1	X	72	PRO	CA-N-CD	-10.28	97.61	112.00
1	X	96	GLN	OE1-CD-NE2	-10.26	112.34	122.60
1	X	153	GLN	OE1-CD-NE2	-10.20	112.40	122.60
1	X	338	LYS	N-CA-C	10.15	125.09	109.96
1	X	388	GLN	OE1-CD-NE2	-10.15	112.45	122.60
1	O	432	GLN	OE1-CD-NE2	-10.14	112.46	122.60
1	O	216	PRO	CA-N-CD	-10.07	97.90	112.00
1	O	423	GLN	OE1-CD-NE2	-10.06	112.54	122.60
1	X	247	GLN	OE1-CD-NE2	-10.02	112.58	122.60
1	X	423	GLN	OE1-CD-NE2	-10.00	112.60	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	430	ASP	CA-CB-CG	9.96	122.56	112.60
1	X	108	GLN	OE1-CD-NE2	-9.95	112.65	122.60
1	O	202	GLN	OE1-CD-NE2	-9.92	112.68	122.60
1	O	329	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	X	375	GLU	N-CA-C	9.88	125.36	112.12
1	X	432	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	X	12	GLN	OE1-CD-NE2	-9.86	112.74	122.60
1	X	216	PRO	CA-N-CD	-9.84	98.23	112.00
1	O	108	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	X	25	ASN	CA-C-O	9.81	130.10	120.88
1	O	105	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	X	83	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	X	248	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	O	59	SER	N-CA-C	-9.73	100.91	113.17
1	X	33	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	X	469	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	O	307	ILE	O-C-N	9.72	133.21	122.61
1	O	153	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	O	239	PRO	CB-CA-C	-9.70	97.21	110.60
1	X	489	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	X	383	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	O	38	GLN	OE1-CD-NE2	-9.62	112.98	122.60
1	O	383	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	O	96	GLN	OE1-CD-NE2	-9.58	113.02	122.60
1	X	58	GLN	OE1-CD-NE2	-9.58	113.02	122.60
1	X	202	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	O	315	GLN	OE1-CD-NE2	-9.56	113.04	122.60
1	O	247	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	X	25	ASN	CA-C-N	9.54	136.80	122.86
1	X	25	ASN	C-N-CA	9.54	136.80	122.86
1	X	417	ASP	N-CA-C	-9.54	99.49	112.94
1	O	254	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	X	70	ILE	N-CA-C	9.50	120.41	108.82
1	X	281	GLN	OE1-CD-NE2	-9.49	113.11	122.60
1	O	33	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	O	58	GLN	OE1-CD-NE2	-9.42	113.18	122.60
1	X	41	PRO	CA-N-CD	-9.41	98.82	112.00
1	X	421	GLN	OE1-CD-NE2	-9.37	113.23	122.60
1	O	307	ILE	CA-C-O	9.31	131.19	121.23
1	X	378	VAL	N-CA-C	-9.30	99.58	112.50
1	O	178	GLN	OE1-CD-NE2	-9.28	113.32	122.60
1	X	431	VAL	N-CA-C	9.27	120.15	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	329	GLN	OE1-CD-NE2	-9.26	113.34	122.60
1	X	105	GLN	OE1-CD-NE2	-9.25	113.35	122.60
1	X	386	ALA	N-CA-C	-9.24	100.39	112.41
1	O	65	PHE	CA-CB-CG	9.21	123.02	113.80
1	O	421	GLN	OE1-CD-NE2	-9.20	113.40	122.60
1	X	254	GLN	OE1-CD-NE2	-9.14	113.46	122.60
1	X	315	GLN	OE1-CD-NE2	-9.04	113.56	122.60
1	X	71	ARG	CA-C-N	9.02	131.12	119.84
1	X	71	ARG	C-N-CA	9.02	131.12	119.84
1	X	153	GLN	CA-C-N	-8.94	110.00	122.87
1	X	153	GLN	C-N-CA	-8.94	110.00	122.87
1	X	8	MET	CA-C-N	-8.87	104.59	121.54
1	X	8	MET	C-N-CA	-8.87	104.59	121.54
1	O	90	TRP	N-CA-C	8.83	122.31	108.79
1	X	415	LYS	N-CA-C	-8.82	99.11	111.81
1	X	178	GLN	OE1-CD-NE2	-8.76	113.84	122.60
1	X	32	SER	CA-C-N	8.73	138.21	121.54
1	X	32	SER	C-N-CA	8.73	138.21	121.54
1	X	33	GLN	N-CA-C	8.73	129.39	110.80
1	X	404	ILE	CA-C-N	8.69	130.70	119.84
1	X	404	ILE	C-N-CA	8.69	130.70	119.84
1	X	25	ASN	O-C-N	8.65	133.61	122.89
1	X	9	ALA	CA-C-N	8.48	137.24	121.97
1	X	9	ALA	C-N-CA	8.48	137.24	121.97
1	X	238	VAL	N-CA-C	8.30	126.80	108.88
1	X	419	LEU	N-CA-C	-8.28	102.19	111.14
1	X	22	PHE	CA-CB-CG	8.28	122.08	113.80
1	O	50	ALA	N-CA-C	-8.24	102.23	111.71
1	O	96	GLN	N-CA-C	8.19	122.93	109.58
1	X	421	GLN	N-CA-C	-8.15	104.48	114.75
1	O	238	VAL	CA-C-N	-8.11	112.36	120.31
1	O	238	VAL	C-N-CA	-8.11	112.36	120.31
1	X	248	GLN	N-CA-C	-8.03	103.50	112.57
1	O	306	SER	N-CA-C	8.00	127.85	110.80
1	O	61	ILE	N-CA-C	-8.00	103.46	110.74
1	O	238	VAL	N-CA-CB	7.93	122.32	111.21
1	X	250	ALA	N-CA-C	-7.89	103.45	113.23
1	X	228	THR	CA-C-O	7.84	129.16	120.31
1	X	152	ALA	CA-C-N	7.78	136.40	121.54
1	X	152	ALA	C-N-CA	7.78	136.40	121.54
1	X	416	ASN	N-CA-C	7.71	120.88	109.24
1	X	405	PRO	N-CA-C	7.69	128.32	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	477	ALA	N-CA-C	7.65	120.03	109.54
1	X	312	SER	N-CA-C	-7.56	103.78	113.16
1	O	238	VAL	CA-C-O	-7.54	109.85	119.95
1	X	344	TYR	N-CA-C	7.48	119.07	108.74
1	O	357	TRP	CA-C-N	7.48	135.82	121.54
1	O	357	TRP	C-N-CA	7.48	135.82	121.54
1	X	61	ILE	CB-CA-C	7.43	124.27	112.16
1	X	357	TRP	N-CA-C	-7.43	94.97	110.80
1	O	383	GLN	CG-CD-NE2	7.41	127.52	116.40
1	X	472	THR	N-CA-C	7.35	120.79	110.20
1	X	229	ARG	O-C-N	7.34	132.35	122.59
1	X	331	GLU	N-CA-C	-7.32	104.35	113.28
1	X	377	PHE	CA-CB-CG	7.27	121.07	113.80
1	X	340	ASP	CA-CB-CG	-7.23	105.37	112.60
1	X	381	THR	N-CA-C	-7.14	103.83	112.54
1	O	108	GLN	CG-CD-NE2	7.11	127.07	116.40
1	O	33	GLN	CG-CD-NE2	7.09	127.03	116.40
1	X	202	GLN	CG-CD-NE2	7.06	127.00	116.40
1	X	65	PHE	N-CA-C	-7.04	103.80	112.38
1	O	111	PRO	CB-CA-C	-7.00	102.06	112.55
1	X	247	GLN	CG-CD-NE2	6.99	126.89	116.40
1	X	248	GLN	CG-CD-NE2	6.98	126.88	116.40
1	X	388	GLN	N-CA-C	-6.96	104.92	113.41
1	O	328	PRO	CB-CA-C	-6.96	101.97	111.85
1	X	489	GLN	CG-CD-NE2	6.94	126.81	116.40
1	O	115	GLN	CG-CD-NE2	6.94	126.81	116.40
1	O	105	GLN	CG-CD-NE2	6.93	126.80	116.40
1	O	489	GLN	CG-CD-NE2	6.92	126.79	116.40
1	O	248	GLN	CG-CD-NE2	6.91	126.77	116.40
1	O	96	GLN	CG-CD-NE2	6.91	126.76	116.40
1	X	12	GLN	CG-CD-NE2	6.89	126.74	116.40
1	X	474	GLU	N-CA-C	6.89	125.48	110.80
1	O	423	GLN	CG-CD-NE2	6.89	126.74	116.40
1	X	339	GLY	CA-C-N	6.84	134.60	121.54
1	X	339	GLY	C-N-CA	6.84	134.60	121.54
1	X	440	THR	N-CA-C	-6.83	103.92	111.36
1	X	456	LYS	O-C-N	6.82	131.66	122.59
1	O	58	GLN	CG-CD-NE2	6.81	126.62	116.40
1	O	83	GLN	CG-CD-NE2	6.81	126.62	116.40
1	O	38	GLN	CG-CD-NE2	6.81	126.61	116.40
1	O	281	GLN	CG-CD-NE2	6.81	126.61	116.40
1	X	388	GLN	CG-CD-NE2	6.79	126.59	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	33	GLN	CG-CD-NE2	6.79	126.58	116.40
1	X	239	PRO	CB-CA-C	-6.77	103.04	111.64
1	X	329	GLN	CG-CD-NE2	6.76	126.55	116.40
1	O	12	GLN	CG-CD-NE2	6.75	126.53	116.40
1	X	238	VAL	O-C-N	-6.75	113.40	121.10
1	X	346	VAL	CA-C-N	-6.75	114.83	121.65
1	X	346	VAL	C-N-CA	-6.75	114.83	121.65
1	O	315	GLN	CG-CD-NE2	6.73	126.50	116.40
1	X	115	GLN	CG-CD-NE2	6.73	126.49	116.40
1	X	108	GLN	CG-CD-NE2	6.72	126.48	116.40
1	O	469	GLN	CG-CD-NE2	6.71	126.47	116.40
1	O	254	GLN	CG-CD-NE2	6.69	126.43	116.40
1	X	239	PRO	N-CD-CG	6.69	113.23	103.20
1	O	257	PHE	CA-CB-CG	-6.67	107.13	113.80
1	O	153	GLN	CG-CD-NE2	6.66	126.38	116.40
1	O	388	GLN	CG-CD-NE2	6.65	126.38	116.40
1	O	432	GLN	CG-CD-NE2	6.63	126.35	116.40
1	X	281	GLN	CG-CD-NE2	6.62	126.33	116.40
1	O	210	ILE	N-CA-C	6.60	114.31	108.63
1	X	229	ARG	CB-CA-C	6.60	123.55	110.42
1	X	153	GLN	CG-CD-NE2	6.59	126.28	116.40
1	O	72	PRO	CA-N-CD	-6.58	102.79	112.00
1	X	446	TYR	CA-CB-CG	6.58	125.75	113.90
1	O	202	GLN	CG-CD-NE2	6.57	126.25	116.40
1	X	429	ILE	N-CA-C	-6.56	95.69	109.34
1	X	432	GLN	CG-CD-NE2	6.54	126.21	116.40
1	O	247	GLN	CG-CD-NE2	6.54	126.21	116.40
1	O	328	PRO	N-CD-CG	6.54	113.01	103.20
1	X	19	ALA	N-CA-C	6.53	118.46	108.07
1	X	469	GLN	CG-CD-NE2	6.53	126.20	116.40
1	X	254	GLN	CG-CD-NE2	6.53	126.19	116.40
1	X	59	SER	N-CA-C	-6.52	104.36	112.90
1	X	83	GLN	CG-CD-NE2	6.52	126.18	116.40
1	O	268	THR	N-CA-C	-6.47	105.92	113.88
1	X	178	GLN	CG-CD-NE2	6.43	126.04	116.40
1	X	27	LYS	N-CA-C	6.42	119.58	109.96
1	X	96	GLN	CG-CD-NE2	6.41	126.01	116.40
1	O	41	PRO	N-CA-CB	6.38	109.95	103.25
1	O	35	GLU	N-CA-C	6.36	119.11	109.95
1	X	316	TRP	CA-CB-CG	-6.34	101.55	113.60
1	X	53	ILE	N-CA-C	-6.33	104.87	111.58
1	O	147	ASP	N-CA-C	-6.33	105.72	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	315	GLN	CG-CD-NE2	6.31	125.87	116.40
1	O	178	GLN	CG-CD-NE2	6.29	125.83	116.40
1	X	479	GLU	N-CA-C	6.29	121.87	107.48
1	X	244	ALA	N-CA-C	6.28	124.19	110.80
1	O	421	GLN	CG-CD-NE2	6.28	125.82	116.40
1	X	239	PRO	N-CA-C	6.24	121.44	111.26
1	X	333	LEU	N-CA-C	-6.23	106.04	113.21
1	X	58	GLN	CG-CD-NE2	6.22	125.73	116.40
1	X	228	THR	O-C-N	-6.20	116.70	123.52
1	O	91	ASP	N-CA-C	6.19	120.30	112.87
1	O	230	SER	N-CA-C	-6.19	97.61	110.80
1	X	229	ARG	CA-C-O	6.19	129.35	120.51
1	O	329	GLN	CG-CD-NE2	6.18	125.66	116.40
1	X	389	SER	N-CA-C	-6.16	104.64	111.36
1	O	238	VAL	O-C-N	-6.16	114.08	121.10
1	O	206	ASP	CA-C-N	6.15	128.81	120.38
1	O	206	ASP	C-N-CA	6.15	128.81	120.38
1	X	421	GLN	CG-CD-NE2	6.15	125.62	116.40
1	O	181	VAL	N-CA-C	6.13	118.29	108.85
1	X	423	GLN	CG-CD-NE2	6.12	125.58	116.40
1	X	460	GLU	N-CA-C	6.08	121.11	108.53
1	X	38	GLN	CG-CD-NE2	6.07	125.51	116.40
1	X	376	ASP	N-CA-C	6.07	118.86	111.82
1	X	72	PRO	N-CA-CB	-6.07	96.88	103.25
1	X	105	GLN	CG-CD-NE2	6.05	125.48	116.40
1	X	343	VAL	CB-CA-C	-6.05	101.22	110.95
1	X	69	GLY	N-CA-C	6.02	127.44	113.18
1	O	204	ILE	N-CA-C	-5.99	106.41	111.56
1	X	347	PRO	CB-CA-C	-5.97	102.61	112.10
1	X	344	TYR	CA-CB-CG	-5.96	103.18	113.90
1	X	227	HIS	CA-C-N	-5.95	108.96	121.81
1	X	227	HIS	C-N-CA	-5.95	108.96	121.81
1	O	355	PRO	CB-CA-C	-5.94	102.47	111.44
1	O	97	PRO	N-CD-CG	5.92	112.08	103.20
1	O	109	SER	N-CA-C	-5.92	105.88	112.57
1	X	242	GLY	N-CA-C	5.89	121.86	110.66
1	X	422	PHE	N-CA-C	-5.89	106.01	113.43
1	X	422	PHE	N-CA-CB	5.87	120.49	110.51
1	O	211	PRO	CB-CA-C	-5.87	101.88	111.56
1	X	383	GLN	CG-CD-NE2	5.86	125.19	116.40
1	O	357	TRP	O-C-N	5.86	130.38	122.59
1	X	9	ALA	N-CA-C	5.84	123.23	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	6	TYR	N-CA-C	5.83	119.05	109.72
1	X	32	SER	O-C-N	5.80	130.30	122.59
1	O	211	PRO	N-CA-CB	5.79	109.33	103.25
1	X	45	TRP	N-CA-C	5.79	119.07	109.46
1	O	36	PHE	CA-CB-CG	5.77	119.57	113.80
1	X	67	GLU	N-CA-C	5.76	117.99	108.49
1	X	409	VAL	N-CA-C	5.73	116.68	110.21
1	X	271	PHE	CA-CB-CG	5.71	119.51	113.80
1	X	22	PHE	N-CA-C	5.70	118.53	109.81
1	X	462	LYS	N-CA-C	5.69	118.43	107.44
1	X	238	VAL	CA-C-O	-5.69	112.33	119.95
1	O	41	PRO	CB-CA-C	-5.67	102.20	111.56
1	X	313	ALA	N-CA-C	-5.67	106.50	113.41
1	X	456	LYS	CA-C-O	5.65	128.59	120.51
1	O	211	PRO	N-CD-CG	5.64	111.67	103.20
1	O	138	SER	N-CA-C	5.64	117.42	111.28
1	X	428	ASP	CA-C-N	5.56	131.97	121.97
1	X	428	ASP	C-N-CA	5.56	131.97	121.97
1	O	355	PRO	N-CD-CG	5.56	111.53	103.20
1	O	40	PHE	C-N-CD	-5.53	102.32	125.00
1	X	106	SER	N-CA-C	5.53	118.03	110.24
1	X	476	PRO	N-CA-C	5.52	119.14	110.80
1	X	32	SER	CB-CA-C	-5.52	99.43	110.42
1	X	305	GLY	N-CA-C	-5.51	100.12	113.18
1	O	103	VAL	CB-CA-C	-5.48	105.32	111.45
1	O	476	PRO	N-CA-C	-5.44	109.03	114.68
1	X	446	TYR	CB-CA-C	-5.42	104.02	112.31
1	O	148	ASN	CA-C-N	-5.38	114.61	122.58
1	O	148	ASN	C-N-CA	-5.38	114.61	122.58
1	X	357	TRP	CA-CB-CG	5.37	123.80	113.60
1	X	97	PRO	N-CD-CG	5.33	111.20	103.20
1	X	239	PRO	CA-CB-CG	-5.32	94.40	104.50
1	O	259	LYS	N-CA-C	5.29	116.77	109.15
1	X	32	SER	CA-C-O	5.29	128.08	120.51
1	O	53	ILE	N-CA-C	5.28	120.33	109.34
1	X	325	GLU	N-CA-C	5.26	122.01	110.80
1	X	451	ALA	N-CA-C	5.26	119.42	112.89
1	X	262	ILE	N-CA-C	5.21	116.41	108.80
1	X	154	GLU	CB-CA-C	5.20	123.94	111.83
1	X	431	VAL	CB-CA-C	-5.19	105.88	111.59
1	X	309	VAL	N-CA-C	5.18	115.58	108.12
1	X	327	SER	N-CA-C	5.17	121.24	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	26	GLY	N-CA-C	5.17	120.84	114.69
1	X	61	ILE	N-CA-C	-5.16	104.53	111.44
1	X	487	TRP	CA-CB-CG	5.15	123.38	113.60
1	X	70	ILE	CB-CA-C	-5.14	104.14	111.34
1	X	490	ALA	N-CA-C	-5.11	106.20	112.90
1	X	269	GLY	N-CA-C	-5.11	101.08	113.18
1	O	101	ALA	N-CA-C	5.10	117.87	109.76
1	X	150	GLU	N-CA-C	5.06	116.48	110.97
1	X	40	PHE	C-N-CD	-5.05	104.28	125.00
1	O	476	PRO	N-CA-CB	5.05	108.50	102.60
1	O	239	PRO	N-CA-C	5.04	119.23	111.57
1	X	285	ASN	CA-C-N	5.03	131.16	121.54
1	X	285	ASN	C-N-CA	5.03	131.16	121.54
1	X	461	LEU	CB-CA-C	5.03	120.42	110.42
1	X	355	PRO	N-CD-CG	5.00	110.71	103.20
1	O	239	PRO	N-CA-CB	5.00	108.88	103.23

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3715	0	3626	220	0
1	X	3715	0	3625	467	0
2	O	51	0	0	8	0
2	X	51	0	0	11	0
All	All	7532	0	7251	680	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 46.

All (680) 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:O:230:SER:C	1:O:230:SER:CA	1.75	1.56
1:X:238:VAL:C	1:X:238:VAL:CA	1.76	1.55
1:X:238:VAL:CA	1:X:238:VAL:N	1.68	1.52
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
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:O:307:ILE:HD13	1:O:308:PHE:CB	1.90	1.02
1:X:78:ILE:HD13	1:X:174:LEU:HD21	1.38	1.02
1:X:304:GLU:HG2	1:X:305:GLY:O	1.60	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:258:GLU:HB2	1:X:261:MET:HE3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:272:ILE:HG22	1:X:396:MET:HE3	1.45	0.95
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:262:ILE:HD11	1:X:274:MET:HE2	1.50	0.93
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:O:307:ILE:HG13	1:O:353:GLY:C	1.98	0.88
1:X:321:LEU:H	1:X:321:LEU:CD1	1.85	0.88
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:143:ARG:HG2	1:O:208:LEU:HB3	1.54	0.86
1:O:257:PHE:HE1	1:O:295:ILE:CD1	1.87	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:O:55:ASN:C	1:O:57:VAL:H	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:274:MET:HE3	1:X:396:MET:HG3	1.61	0.81
1:X:180:HIS:CE1	1:X:216:PRO:HG3	2.16	0.80
1:X:422:PHE:C	1:X:424:ALA:N	2.37	0.80
1:X:8:MET:HE1	1:X:65:PHE:CD1	2.17	0.80
1:O:354:ALA:O	1:O:357:TRP:CD1	2.34	0.80
1:X:132:VAL:HG22	1:X:357:TRP:HE1	1.47	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: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:238:VAL:C	1:X:238:VAL:HA	2.05	0.78
1:X:414:ALA:HB3	1:X:437:LEU:CD2	2.14	0.78
1:X:132:VAL:CG1	1:X:357:TRP:CE2	2.65	0.78
1:O:353:GLY:C	1:O:357:TRP:HB3	2.09	0.78
1:X:26:GLY:HA3	1:X:464:MET:HE1	1.64	0.77
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:8:MET:HE1	1:X:65:PHE:HD1	1.48	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:56:SER:O	1:X:60:VAL:HG22	1.87	0.75
1:X:132:VAL:HG22	1:X:357:TRP:NE1	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:313:ALA:C	1:X:315:GLN:H	1.94	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:352:LEU:HD12	1:O:352:LEU:C	2.14	0.73
1:X:25:ASN:CG	1:X:461:LEU:HD11	2.14	0.73
1:X:45:TRP:NE1	1:X:108:GLN:HE21	1.84	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:X:356:TYR:C	1:X:357:TRP:O	2.29	0.72
1:O:345:VAL:HG12	1:O:347:PRO:HD3	1.71	0.72
1:O:98:ILE:HD13	1:O:98:ILE:H	1.49	0.72
1:O:50:ALA:H	1:O:100:ASN:HB2	1.53	0.72
1:O:256:ALA:O	1:O:257:PHE:C	2.32	0.72
1:X:354:ALA:O	1:X:357:TRP:CE3	2.42	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:480:ARG:O	1:X:480:ARG:HG2	1.88	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:20:ILE:CG2	1:X:21:ILE:N	2.52	0.71
1:X:246:ASP:O	1:X:249:ALA:HB3	1.91	0.71
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:O:12:GLN:HE22	1:O:53:ILE:HG22	1.55	0.69
1:X:383:GLN:HE22	1:X:422:PHE:HE2	1.39	0.69
1:X:307:ILE:HG21	1:X:385:VAL:HG23	1.75	0.69
1:O:306:SER:HG	1:O:354:ALA:HA	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:238:VAL:HG22	1:X:239:PRO:N	2.08	0.69
1:X:25:ASN:HD22	1:X:461:LEU:CD1	2.05	0.68
1:O:51:ASN:HD22	1:O:51:ASN:N	1.90	0.68
1:X:327:SER:HB3	1:X:328:PRO:CD	2.22	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:434:ALA:O	1:X:437:LEU:CD1	2.41	0.68
1:X:10:ILE:HD12	1:X:61:ILE:HD13	1.75	0.68
1:O:12:GLN:HE22	1:O:53:ILE:CG2	2.07	0.67
1:O:257:PHE:C	1:O:257:PHE:CD2	2.72	0.67
1:O:352:LEU:O	1:O:352:LEU:CD1	2.42	0.67
1:X:10:ILE:HG21	1:X:170:LEU:HD13	1.75	0.67
1:X:345:VAL:CG1	1:X:347:PRO:HD3	2.22	0.67
1:O:132:VAL:HG11	1:O:357:TRP:CH2	2.26	0.67
1:X:75:ILE:HG13	1:X:76:ALA:N	2.07	0.67
1:X:238:VAL:CG2	1:X:239:PRO:HD2	2.25	0.67
1:X:431:VAL:HG22	1:X:432:GLN:N	2.09	0.67
1:O:256:ALA:O	1:O:257:PHE:O	2.13	0.67
1:X:74:ALA:C	1:X:75:ILE:O	2.37	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
1:O:352:LEU:O	1:O:353:GLY:O	2.14	0.66
1:X:429:ILE:HG22	1:X:430:ASP:N	2.10	0.66
1:X:434:ALA:O	1:X:437:LEU:HD12	1.96	0.66
1:O:102:ILE:HG23	1:O:106:SER:OG	1.95	0.65
1:X:72:PRO:C	1:X:74:ALA:H	2.03	0.65
1:X:251:LEU:HD11	1:X:275:ASN:N	2.11	0.65
1:X:419:LEU:O	1:X:423:GLN:N	2.24	0.65
1:X:238:VAL:N	1:X:238:VAL:HA	2.03	0.65
1:X:230:SER:C	1:X:238:VAL:HG12	2.22	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:HG22	1:X:314:ILE:O	1.97	0.65
1:O:230:SER:C	1:O:230:SER:N	2.54	0.64
1:X:175:THR:HG23	1:X:228:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:293:TYR:CZ	1:X:447:LEU:HD12	2.32	0.64
1:X:346:VAL:O	1:X:363:GLY:HA2	1.95	0.64
1:X:321:LEU:CD1	1:X:321:LEU:N	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:262:ILE:CD1	1:X:274:MET:HE2	2.25	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:262:ILE:HD11	1:X:274:MET:CE	2.26	0.63
1:X:385:VAL:O	1:X:389:SER:HB2	1.99	0.63
1:O:138:SER:O	1:O:142:VAL:HG23	1.98	0.63
1:X:321:LEU:O	1:X:322:ARG:C	2.42	0.63
1:O:103:VAL:C	1:O:105:GLN:H	2.07	0.62
1:O:307:ILE:CD1	1:O:308:PHE:CD1	2.82	0.62
1:X:286:ASP:C	1:X:357:TRP:CH2	2.77	0.62
1:X:356:TYR:CE2	1:X:491:VAL:HG11	2.29	0.62
1:X:26:GLY:CA	1:X:464:MET:HE1	2.29	0.62
1:O:163:PHE:O	1:O:216:PRO:HD2	1.99	0.62
1:X:28:LYS:C	1:X:29:ILE:HG12	2.24	0.62
1:O:230:SER:C	1:O:230:SER:CB	2.69	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:241:ALA:HB1	1:O:451:ALA:HB3	1.81	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:12:GLN:NE2	1:O:53:ILE:CG2	2.61	0.61
1:X:171:VAL:HG11	1:X:181:VAL:HG12	1.81	0.61
1:X:138:SER:O	1:X:142:VAL:HG23	2.00	0.61
1:X:409:VAL:HG21	1:X:420:MET:HE3	1.82	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:74:ALA:O	1:X:75:ILE:C	2.44	0.60
1:X:379:ARG:O	1:X:383:GLN:CG	2.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:402:ILE:HG22	1:X:403:ASP:H	1.67	0.60
1:X:428:ASP:HB2	1:X:480:ARG:HH11	1.66	0.60
1:X:262:ILE:HG23	1:X:273:VAL:O	2.01	0.60
1:X:344:TYR:C	1:X:365:VAL:HG21	2.25	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:O:114:ASP:O	1:O:118:VAL:HG23	2.01	0.60
1:X:20:ILE:O	1:X:21:ILE:HG13	2.01	0.60
1:X:66:ILE:O	1:X:66:ILE:HG22	2.01	0.60
1:X:143:ARG:HE	1:X:208:LEU:HD13	1.67	0.60
1:O:54:TRP:CD1	1:O:170:LEU:CD2	2.85	0.60
1:X:286:ASP:O	1:X:357:TRP:CH2	2.55	0.60
1:O:379:ARG:O	1:O:383:GLN:HG2	2.02	0.59
1:X:355:PRO:HA	1:X:357:TRP:CZ3	2.36	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:O:51:ASN:N	1:O:51:ASN:ND2	2.49	0.59
1:X:416:ASN:HB3	1:X:418:LEU:N	2.05	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:O:14:THR:HG23	1:O:48:HIS:NE2	2.17	0.59
1:O:307:ILE:HG13	1:O:353:GLY:N	2.17	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:182:THR:OG1	1:O:216:PRO:HB2	2.02	0.59
1:X:132:VAL:HG13	1:X:357:TRP:NE1	2.17	0.59
1:X:10:ILE:CD1	1:X:61:ILE:HD13	2.32	0.58
1:O:55:ASN:O	1:O:57:VAL:N	2.35	0.58
1:X:44:GLY:O	1:X:350:THR:HG22	2.03	0.58
1:X:247:GLN:OE1	1:X:263:LYS:NZ	2.36	0.58
1:X:345:VAL:HG13	1:X:347:PRO:CD	2.26	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:O:143:ARG:C	1:O:145:LEU:H	2.10	0.58
1:X:303:LEU:O	1:X:396:MET:SD	2.62	0.58
1:X:484:TYR:HE2	1:X:488:LYS:NZ	2.01	0.58
1:O:90:TRP:O	1:O:162:LEU:N	2.35	0.58
1:X:19:ALA:CB	1:X:64:ALA:CB	2.82	0.57
1:X:84:ARG:NH2	1:X:246:ASP:OD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:247:GLN:HA	2:X:535:HOH:O	2.04	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:390:LYS:HZ3	1:X:427:LEU:HG	1.69	0.57
1:X:421:GLN:NE2	1:X:471:PHE:HB2	2.20	0.57
1:X:432:GLN:OE1	1:X:470:MET:HE2	2.05	0.57
1:O:210:ILE:HG23	1:O:214:MET:SD	2.44	0.56
1:X:238:VAL:C	1:X:238:VAL:CB	2.73	0.56
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:97:PRO:C	1:O:98:ILE:HD13	2.30	0.56
1:X:20:ILE:HG23	1:X:21:ILE:N	2.03	0.56
1:O:189:ARG:HH21	1:O:290:THR:HB	1.69	0.56
1:X:8:MET:HE3	1:X:65:PHE:HA	1.87	0.56
1:X:272:ILE:CG2	1:X:396:MET:HE3	2.27	0.56
1:X:371:GLY:HA3	2:X:541:HOH:O	2.05	0.56
1:X:419:LEU:O	1:X:423:GLN:HB3	2.06	0.56
1:X:429:ILE:CG2	1:X:430:ASP:N	2.68	0.56
1:O:15:THR:HG21	1:O:315:GLN:HE22	1.71	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: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:N	1:X:238:VAL:CB	2.63	0.56
1:X:250:ALA:HB3	1:X:263:LYS:HD3	1.86	0.56
1:X:71:ARG:CB	1:X:72:PRO:HD2	2.34	0.56
1:X:189:ARG:NH1	1:X:288:LEU:HD13	2.20	0.56
1:O:132:VAL:CG1	1:O:357:TRP:CZ2	2.81	0.56
1:X:385:VAL:O	1:X:389:SER:CB	2.53	0.56
2:O:516:HOH:O	1:X:229:ARG:HB3	2.06	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: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:O:17:SER:HB2	1:O:56:SER:HB2	1.89	0.55
1:O:307:ILE:HD13	1:O:308:PHE:N	2.20	0.55
1:X:274:MET:HB3	1:X:303:LEU:HB2	1.88	0.55
1:O:84:ARG:NH1	2:O:550:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:TRP:CD1	1:O:170:LEU:HD21	2.41	0.55
1:X:10:ILE:CD1	1:X:61:ILE:HD12	2.33	0.55
1:X:416:ASN:CB	1:X:419:LEU:H	2.19	0.55
1:X:405:PRO:HB2	1:X:406:LEU:HD12	1.89	0.55
1:O:163:PHE:O	1:O:216:PRO:CD	2.55	0.55
1:X:221:ASN:HB3	1:X:447:LEU:HD11	1.89	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:HG12	1:O:142:VAL:O	2.07	0.54
1:X:134:ASP:C	1:X:136:TYR:H	2.15	0.54
1:X:238:VAL:CG2	1:X:239:PRO:CD	2.85	0.54
1:X:238:VAL:C	1:X:238:VAL:CG2	2.79	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:50:ALA:C	1:O:52:GLU:H	2.15	0.53
1:O:372:THR:HG23	1:O:376:ASP:HB2	1.89	0.53
1:X:175:THR:CG2	1:X:228:THR:HG22	2.39	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:39:TYR:CE2	1:O:41:PRO:HD3	2.43	0.53
1:O:54:TRP:NE1	1:O:170:LEU:HD23	2.24	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:X:267:GLY:C	1:X:269:GLY:H	2.16	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:O:10:ILE:CD1	1:O:78:ILE:HG23	2.38	0.53
1:X:310:ALA:O	1:X:313:ALA:HB3	2.09	0.53
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:O:307:ILE:CD1	1:O:353:GLY:N	2.72	0.53
1:O:163:PHE:CG	1:O:164:GLY:N	2.76	0.53
1:X:344:TYR:HB3	1:X:365:VAL:HG11	1.90	0.53
1:O:173:LYS:HB2	1:X:71:ARG:NH1	2.24	0.52
1:X:352:LEU:HD12	1:X:388:GLN:HE21	1.74	0.52
1:X:475:MET:HE2	1:X:475:MET:HA	1.90	0.52
1:O:54:TRP:NE1	1:O:170:LEU:CD2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:ILE:HG12	1:X:54:TRP:NE1	2.24	0.52
1:X:72:PRO:C	1:X:74:ALA:N	2.67	0.52
1:X:151:GLY:O	1:X:152:ALA:C	2.50	0.52
1:X:419:LEU:HD23	1:X:420:MET:HE2	1.90	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:230:SER:O	1:X:238:VAL:CG1	2.44	0.52
1:X:275:ASN:HD21	1:X:292:GLY:HA3	1.75	0.52
1:X:81:THR:HG22	1:X:82:ASN:N	2.25	0.52
1:O:78:ILE:CD1	1:O:230:SER:HB2	2.40	0.52
1:X:273:VAL:HG22	1:X:304:GLU:HG3	1.92	0.52
1:O:354:ALA:O	1:O:357:TRP:NE1	2.42	0.52
1:X:175:THR:C	1:X:177:GLY:H	2.17	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:X:39:TYR:CE2	1:X:41:PRO:HD3	2.46	0.51
1:X:189:ARG:NH1	2:X:554:HOH:O	2.43	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:286:ASP:C	1:X:357:TRP:HH2	2.18	0.51
1:O:67:GLU:HG2	1:X:55:ASN:HD21	1.75	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:86:THR:HG23	2:O:528:HOH:O	2.11	0.51
1:X:174:LEU:O	1:X:228:THR:HG21	2.09	0.51
1:O:78:ILE:HD11	1:O:230:SER:HB3	1.93	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:286:ASP:O	1:X:357:TRP:CZ3	2.63	0.51
1:O:352:LEU:O	1:O:353:GLY:C	2.54	0.51
1:X:266:TYR:HB2	1:X:411:GLY:HA3	1.92	0.51
1:O:9:ALA:HB2	1:O:445:ALA:HB2	1.93	0.51
1:X:175:THR:HA	1:X:228:THR:HG22	1.84	0.51
1:X:238:VAL:HG23	1:X:239:PRO:CD	2.41	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:419:LEU:C	1:X:421:GLN:H	2.18	0.50
1:O:89:VAL:HG11	1:O:214:MET:HE3	1.92	0.50
1:X:104:TRP:HA	1:X:141:LYS:NZ	2.27	0.50
1:X:405:PRO:O	1:X:429:ILE:CG2	2.59	0.50
1:O:393:ILE:HD13	1:O:427:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:45:TRP:CD1	1:X:45:TRP:N	2.80	0.50
1:X:75:ILE:HG13	1:X:238:VAL:HG13	1.92	0.50
1:X:386:ALA:O	1:X:390:LYS:HE2	2.12	0.50
1:X:409:VAL:CG2	1:X:420:MET:HE3	2.42	0.50
1:O:57:VAL:O	1:O:61:ILE:N	2.44	0.50
1:X:78:ILE:H	1:X:240:ILE:HA	1.76	0.50
1:X:385:VAL:HA	1:X:388:GLN:HB2	1.92	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:45:TRP:CD1	1:X:45:TRP:H	2.29	0.50
1:O:251:LEU:HD11	1:O:275:ASN:ND2	2.27	0.50
1:X:19:ALA:CB	1:X:64:ALA:HB2	2.42	0.50
1:X:377:PHE:CD1	1:X:380:ALA:HB3	2.47	0.50
1:X:104:TRP:HZ3	1:X:308:PHE:HA	1.76	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:50:ALA:HB2	1:O:101:ALA:N	2.18	0.49
1:O:55:ASN:O	1:O:59:SER:HB3	2.12	0.49
1:X:332:GLU:C	1:X:334:ALA:H	2.20	0.49
1:X:405:PRO:O	1:X:429:ILE:HG21	2.13	0.49
1:O:307:ILE:HD11	1:O:353:GLY:N	2.28	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:228:THR:CG2	1:O:238:VAL:O	2.57	0.49
1:X:50:ALA:HB3	1:X:97:PRO:HG2	1.93	0.49
1:X:82:ASN:HB2	1:X:166:ILE:HB	1.93	0.49
1:O:288:LEU:HD21	1:O:357:TRP:CH2	2.48	0.49
1:X:75:ILE:HD12	1:X:76:ALA:H	1.78	0.49
1:O:72:PRO:HB3	1:O:230:SER:O	2.13	0.49
1:X:280:PRO:CD	1:X:301:TYR:CD2	2.96	0.49
1:O:89:VAL:HG22	1:O:163:PHE:HD1	1.78	0.48
1:O:306:SER:OG	1:O:307:ILE:N	2.42	0.48
1:X:80:ILE:HG23	1:X:81:THR:H	1.77	0.48
1:X:446:TYR:HD2	1:X:458:LEU:HD22	1.77	0.48
1:O:180:HIS:CE1	1:O:216:PRO:CG	2.88	0.48
1:O:307:ILE:CD1	1:O:308:PHE:CB	2.76	0.48
1:X:323:MET:HE3	1:X:374:LYS:HE2	1.96	0.48
1:X:402:ILE:HG22	1:X:403:ASP:N	2.28	0.48
1:X:414:ALA:C	1:X:416:ASN:H	2.21	0.48
1:O:102:ILE:HG23	1:O:106:SER:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:62:ALA:C	1:O:66:ILE:HD12	2.31	0.48
1:O:48:HIS:HD2	1:O:83:GLN:HE22	1.61	0.48
1:X:33:GLN:O	1:X:34:LYS:CG	2.58	0.48
1:X:75:ILE:CD1	1:X:76:ALA:H	2.27	0.48
1:X:223:GLU:O	1:X:241:ALA:O	2.31	0.48
1:X:264:ASN:HB2	1:X:407:LEU:HD21	1.95	0.48
1:X:253:GLY:O	1:X:442:LEU:HD12	2.14	0.48
1:O:19:ALA:O	1:O:60:VAL:HG12	2.13	0.48
1:X:72:PRO:O	1:X:75:ILE:CG2	2.62	0.48
1:X:10:ILE:O	1:X:11:ASP:HB2	2.13	0.47
1:X:251:LEU:HD11	1:X:275:ASN:HB2	1.96	0.47
1:O:173:LYS:C	1:O:175:THR:H	2.22	0.47
1:X:263:LYS:HD2	1:X:264:ASN:N	2.30	0.47
1:O:125:ILE:HD13	1:O:125:ILE:O	2.14	0.47
1:O:138:SER:HB2	1:O:190:THR:HA	1.96	0.47
1:O:285:ASN:HB3	1:O:395:THR:HG23	1.96	0.47
1:X:78:ILE:HG22	1:X:240:ILE:HG12	1.97	0.47
1:X:79:GLY:C	1:X:80:ILE:HD12	2.36	0.47
1:X:82:ASN:OD1	2:X:530:HOH:O	2.20	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: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:O:112:ILE:H	1:O:112:ILE:HG13	1.37	0.47
1:X:104:TRP:HA	1:X:141:LYS:HZ1	1.80	0.47
1:X:282:LEU:N	1:X:282:LEU:HD12	2.29	0.47
1:X:404:ILE:H	1:X:404:ILE:HG12	1.49	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:O:280:PRO:HD3	1:O:301:TYR:CD2	2.50	0.47
1:X:79:GLY:O	1:X:80:ILE:CD1	2.51	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:26:GLY:HA3	1:X:464:MET:CE	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:238:VAL:HG22	1:X:239:PRO:CD	2.44	0.46
1:O:129:THR:HG21	1:O:191:MET:HA	1.97	0.46
1:X:238:VAL:CA	1:X:238:VAL:H	2.06	0.46
1:X:82:ASN:ND2	1:X:167:ASP:HB3	2.31	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:268:THR:N	2:X:553:HOH:O	2.48	0.46
1:X:352:LEU:HD21	1:X:491:VAL:HG13	1.96	0.46
1:X:52:GLU:HA	1:X:55:ASN:HB2	1.97	0.46
1:X:314:ILE:HD11	1:X:413:ALA:HB2	1.96	0.46
1:X:357:TRP:O	1:X:358:ASP:CB	2.63	0.46
1:O:390:LYS:HD2	1:O:426:ILE:HG23	1.96	0.46
1:X:104:TRP:H	1:X:104:TRP:CD1	2.32	0.46
1:X:473:PRO:C	1:X:474:GLU:HG2	2.40	0.46
1:X:84:ARG:NE	2:X:552:HOH:O	2.49	0.46
1:X:267:GLY:O	1:X:269:GLY:N	2.49	0.46
1:X:484:TYR:HE2	1:X:488:LYS:HZ3	1.64	0.46
1:O:103:VAL:C	1:O:105:GLN:N	2.71	0.46
1:O:173:LYS:HE2	1:X:71:ARG:HD3	1.98	0.46
1:X:5:ASN:N	1:X:5:ASN:ND2	2.57	0.46
1:O:94:THR:HB	1:O:95:GLY:H	1.63	0.46
1:X:267:GLY:O	1:X:311:GLY:N	2.49	0.46
1:X:345:VAL:HG12	1:X:384:ALA:HB2	1.98	0.46
1:X:390:LYS:NZ	1:X:427:LEU:HA	2.30	0.46
1:O:84:ARG:HH22	1:O:304:GLU:CD	2.23	0.45
1:X:323:MET:HE2	1:X:323:MET:HB3	1.67	0.45
1:X:204:ILE:O	1:X:208:LEU:HG	2.17	0.45
1:O:38:GLN:HE22	1:O:48:HIS:CE1	2.35	0.45
1:X:252:PHE:CE2	1:X:293:TYR:CD2	3.03	0.45
1:O:98:ILE:N	1:O:98:ILE:CD1	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:O:352:LEU:C	1:O:352:LEU:CD1	2.86	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
1:X:102:ILE:HD12	1:X:145:LEU:HD11	1.99	0.45
1:O:139:ALA:HB3	1:O:191:MET:HE2	1.99	0.45
1:X:134:ASP:HB2	1:X:357:TRP:CD1	2.51	0.45
1:O:26:GLY:HA3	1:O:464:MET:HG3	1.99	0.45
1:O:262:ILE:HG22	1:O:263:LYS:H	1.82	0.45
1:X:252:PHE:CZ	1:X:294:GLY:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:20:ILE:HG12	1:X:30:GLY:O	2.16	0.45
1:X:251:LEU:HD22	1:X:273:VAL:CG1	2.46	0.45
1:O:88:VAL:O	1:O:164:GLY:O	2.35	0.44
1:O:357:TRP:N	1:O:357:TRP:HD1	2.15	0.44
1:X:440:THR:C	1:X:442:LEU:H	2.25	0.44
1:O:55:ASN:C	1:O:57:VAL:N	2.56	0.44
1:O:98:ILE:H	1:O:98:ILE:CD1	2.14	0.44
1:X:355:PRO:C	1:X:357:TRP:CE3	2.95	0.44
1:X:475:MET:HB3	1:X:476:PRO:HD2	1.99	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: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:X:75:ILE:O	1:X:76:ALA:HB2	2.18	0.44
1:X:414:ALA:C	1:X:416:ASN:N	2.75	0.44
1:X:16:SER:OG	1:X:18:ARG:HG2	2.18	0.44
1:X:274:MET:HG2	1:X:276:THR:HG23	1.98	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:77:GLY:HA2	1:X:239:PRO:N	2.33	0.44
1:X:126:HIS:ND1	1:X:131:LEU:O	2.50	0.44
1:O:132:VAL:CG2	1:O:133:ILE:N	2.81	0.44
1:O:198:LEU:HD21	1:O:299:VAL:HG21	1.98	0.44
1:X:253:GLY:HA2	1:X:442:LEU:HD13	2.00	0.44
1:X:376:ASP:C	1:X:378:VAL:H	2.24	0.44
1:O:146:LEU:HG	1:O:152:ALA:HB1	2.00	0.44
1:X:238:VAL:HG22	1:X:239:PRO:HD2	1.98	0.44
1:O:47:GLU:HA	1:O:103:VAL:HG23	1.99	0.43
1:O:182:THR:HG22	1:O:183:ASP:H	1.83	0.43
1:X:28:LYS:HZ1	1:X:436:ASN:CG	2.26	0.43
1:X:109:SER:HB3	1:X:140:THR:HB	2.00	0.43
1:X:221:ASN:CB	1:X:447:LEU:HD11	2.47	0.43
1:X:247:GLN:HB3	1:X:273:VAL:HG21	2.00	0.43
1:O:51:ASN:ND2	1:O:51:ASN:H	2.16	0.43
1:X:345:VAL:CG1	1:X:347:PRO:CD	2.90	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:78:ILE:HD12	1:O:230:SER:HB2	2.00	0.43
1:X:344:TYR:O	1:X:365:VAL:HG21	2.18	0.43
1:X:75:ILE:CG1	1:X:76:ALA:H	2.32	0.43
1:X:145:LEU:O	1:X:149:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:247:GLN:C	1:X:249:ALA:H	2.25	0.43
1:X:260:GLY:H	1:X:276:THR:HA	1.83	0.43
1:O:307:ILE:HD13	1:O:308:PHE:H	1.83	0.43
1:X:389:SER:O	1:X:393:ILE:N	2.51	0.43
1:X:422:PHE:O	1:X:424:ALA:N	2.50	0.43
1:O:94:THR:O	1:X:70:ILE:HG22	2.18	0.43
1:X:16:SER:OG	1:X:17:SER:N	2.51	0.43
1:X:153:GLN:HB3	1:X:154:GLU:OE2	2.18	0.43
1:X:392:VAL:O	1:X:396:MET:HB2	2.19	0.43
1:O:90:TRP:N	1:O:162:LEU:O	2.51	0.43
1:O:307:ILE:HG12	1:O:308:PHE:CD1	2.53	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:304:GLU:C	1:O:305:GLY:O	2.59	0.43
1:O:352:LEU:O	1:O:352:LEU:CG	2.67	0.43
1:X:227:HIS:CE1	1:X:239:PRO:HD3	2.54	0.43
1:X:440:THR:HG22	1:X:441:ALA:N	2.33	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:X:331:GLU:HG3	1:X:416:ASN:HD22	1.83	0.43
1:O:67:GLU:HG2	1:X:55:ASN:ND2	2.33	0.42
1:X:409:VAL:CB	1:X:420:MET:HE3	2.48	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:71:ARG:CB	1:X:72:PRO:CD	2.89	0.42
1:X:132:VAL:HG11	1:X:357:TRP:HZ2	0.68	0.42
1:X:8:MET:O	1:X:9:ALA:CB	2.46	0.42
1:X:84:ARG:CZ	2:X:552:HOH:O	2.67	0.42
1:O:310:ALA:HB1	1:O:385:VAL:HG13	2.01	0.42
1:X:189:ARG:HH22	1:X:288:LEU:HD13	1.85	0.42
1:X:429:ILE:CG2	1:X:430:ASP:H	2.33	0.42
1:X:305:GLY:N	1:X:396:MET:HE1	2.34	0.42
1:O:190:THR:HG21	2:O:542:HOH:O	2.19	0.42
1:X:322:ARG:C	1:X:323:MET:HG2	2.41	0.42
1:X:416:ASN:HB3	1:X:419:LEU:H	1.85	0.42
1:O:47:GLU:HG2	1:O:100:ASN:ND2	2.34	0.42
1:O:228:THR:C	1:O:230:SER:H	2.27	0.42
1:X:32:SER:HB2	1:X:33:GLN:H	0.98	0.42
1:X:266:TYR:N	1:X:410:ASP:O	2.52	0.42
1:O:18:ARG:HH12	1:O:20:ILE:HD11	1.85	0.42
1:X:428:ASP:CB	1:X:480:ARG:NH1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:146:LEU:HB3	1:O:153:GLN:HE21	1.84	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:18:ARG:NH2	1:O:438:GLU:HB3	2.35	0.42
1:X:56:SER:O	1:X:60:VAL:CG2	2.65	0.42
1:X:75:ILE:HG13	1:X:238:VAL:CG1	2.50	0.42
1:X:386:ALA:HB1	1:X:423:GLN:HE22	1.85	0.42
1:O:307:ILE:HD13	1:O:308:PHE:CA	2.49	0.41
1:O:437:LEU:HD12	1:O:437:LEU:H	1.84	0.41
1:X:72:PRO:O	1:X:75:ILE:HG22	2.19	0.41
1:X:273:VAL:HG22	1:X:304:GLU:HB2	2.02	0.41
1:X:348:ALA:O	1:X:349:PHE:C	2.62	0.41
1:X:431:VAL:CG2	1:X:432:GLN:H	2.32	0.41
1:O:161:LEU:O	1:O:214:MET:HA	2.20	0.41
1:X:18:ARG:O	1:X:19:ALA:HB2	2.19	0.41
1:X:25:ASN:HB3	1:X:461:LEU:HD12	2.01	0.41
1:X:238:VAL:CA	1:X:238:VAL:O	2.49	0.41
1:X:248:GLN:NE2	1:X:291:ILE:O	2.54	0.41
1:X:475:MET:HB3	1:X:476:PRO:CD	2.50	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:273:VAL:HG22	1:X:304:GLU:CB	2.51	0.41
1:X:434:ALA:C	1:X:436:ASN:H	2.28	0.41
1:O:355:PRO:HD2	1:O:392:VAL:HG13	2.02	0.41
1:X:218:VAL:O	1:X:218:VAL:HG13	2.21	0.41
1:X:428:ASP:CB	1:X:480:ARG:HH11	2.30	0.41
1:X:439:THR:O	1:X:442:LEU:HB2	2.20	0.41
1:O:39:TYR:CE2	1:O:41:PRO:CD	3.04	0.41
1:O:149:ILE:HD12	1:O:149:ILE:HA	1.82	0.41
1:X:12:GLN:CG	1:X:53:ILE:HG23	2.50	0.41
1:X:275:ASN:ND2	1:X:292:GLY:HA3	2.34	0.41
1:O:247:GLN:OE1	1:O:271:PHE:HB2	2.20	0.41
1:X:19:ALA:HB3	1:X:64:ALA:HB2	2.03	0.41
1:X:146:LEU:HD23	1:X:153:GLN:HE21	1.85	0.41
1:X:165:THR:O	1:X:167:ASP:OD1	2.39	0.41
1:X:251:LEU:O	1:X:256:ALA:HB2	2.21	0.41
1:X:438:GLU:HG2	1:X:441:ALA:HB3	2.02	0.41
1:X:134:ASP:OD1	1:X:359:SER:OG	2.34	0.41
1:O:8:MET:HB2	1:O:78:ILE:HG12	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:355:PRO:C	1:X:357:TRP:HE3	2.29	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:O:424:ALA:C	1:O:473:PRO:HG3	2.45	0.41
1:X:243:MET:O	1:X:244:ALA:HB2	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:X:345:VAL:HG12	1:X:383:GLN:O	2.21	0.41
1:O:104:TRP:HZ3	1:O:308:PHE:HA	1.86	0.41
1:X:27:LYS:HB2	1:X:27:LYS:HZ3	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:407:LEU:HD23	1:X:408:LYS:H	1.85	0.41
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:61:ILE:HG22	1:O:62:ALA:N	2.37	0.40
1:O:84:ARG:NH2	2:O:511:HOH:O	2.54	0.40
1:X:77:GLY:HA3	1:X:239:PRO:O	2.16	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:O:142:VAL:HA	1:O:145:LEU:HD22	2.04	0.40
1:X:64:ALA:C	1:X:66:ILE:N	2.79	0.40
1:X:67:GLU:O	1:X:68:SER:HB2	2.22	0.40
1:X:256:ALA:HA	1:X:261:MET:SD	2.61	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	O	478/505 (95%)	393 (82%)	63 (13%)	22 (5%)	2 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	478/505 (95%)	320 (67%)	99 (21%)	59 (12%)	0	0
All	All	956/1010 (95%)	713 (75%)	162 (17%)	81 (8%)	0	0

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	321 (82%)	69 (18%)	2	3
1	X	390/409 (95%)	280 (72%)	110 (28%)	0	0
All	All	780/818 (95%)	601 (77%)	179 (23%)	1	1

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	O	18	ARG
1	O	33	GLN
1	O	37	PRO
1	O	49	ASN
1	O	51	ASN
1	O	53	ILE
1	O	55	ASN
1	O	61	ILE
1	O	65	PHE
1	O	66	ILE
1	O	71	ARG
1	O	72	PRO
1	O	78	ILE
1	O	81	THR
1	O	85	GLU
1	O	86	THR
1	O	87	THR
1	O	88	VAL
1	O	91	ASP

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Mol	Chain	Res	Type
1	O	94	THR
1	O	97	PRO
1	O	98	ILE
1	O	111	PRO
1	O	112	ILE
1	O	116	LEU
1	O	125	ILE
1	O	132	VAL
1	O	140	THR
1	O	144	TRP
1	O	149	ILE
1	O	168	SER
1	O	173	LYS
1	O	175	THR
1	O	179	VAL
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	262	ILE
1	O	263	LYS
1	O	273	VAL
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
1	O	355	PRO
1	O	373	THR
1	O	392	VAL
1	O	393	ILE
1	O	416	ASN
1	O	418	LEU

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Mol	Chain	Res	Type
1	O	419	LEU
1	O	432	GLN
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	18	ARG
1	X	20	ILE
1	X	21	ILE
1	X	22	PHE
1	X	27	LYS
1	X	29	ILE
1	X	37	PRO
1	X	42	LYS
1	X	45	TRP
1	X	53	ILE
1	X	57	VAL
1	X	60	VAL
1	X	61	ILE
1	X	66	ILE
1	X	67	GLU
1	X	71	ARG
1	X	72	PRO
1	X	75	ILE
1	X	78	ILE
1	X	80	ILE
1	X	82	ASN
1	X	97	PRO
1	X	112	ILE
1	X	125	ILE
1	X	132	VAL
1	X	138	SER
1	X	140	THR
1	X	154	GLU
1	X	160	GLU
1	X	161	LEU
1	X	175	THR
1	X	182	THR
1	X	186	ASN

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Mol	Chain	Res	Type
1	X	205	LEU
1	X	206	ASP
1	X	207	LEU
1	X	208	LEU
1	X	211	PRO
1	X	216	PRO
1	X	238	VAL
1	X	239	PRO
1	X	243	MET
1	X	246	ASP
1	X	251	LEU
1	X	265	THR
1	X	268	THR
1	X	271	PHE
1	X	272	ILE
1	X	275	ASN
1	X	276	THR
1	X	280	PRO
1	X	282	LEU
1	X	286	ASP
1	X	287	LEU
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	377	PHE
1	X	379	ARG
1	X	382	LEU
1	X	385	VAL

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Mol	Chain	Res	Type
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
1	X	421	GLN
1	X	425	ASP
1	X	427	LEU
1	X	429	ILE
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	475	MET
1	X	476	PRO
1	X	479	GLU
1	X	480	ARG
1	X	483	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	48	HIS
1	O	51	ASN
1	O	82	ASN
1	O	105	GLN
1	O	108	GLN

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Mol	Chain	Res	Type
1	O	153	GLN
1	O	158	ASN
1	O	202	GLN
1	O	221	ASN
1	O	227	HIS
1	O	248	GLN
1	O	275	ASN
1	O	315	GLN
1	O	383	GLN
1	O	416	ASN
1	O	482	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
1	X	186	ASN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	X	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	154:GLU	C	155:LYS	N	1.63
1	X	228:THR	C	229:ARG	N	1.11

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.