



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:34 PM UTC

PDB ID : 1GLL / pdb_00001gll
Title : ESCHERICHIA COLI GLYCEROL KINASE MUTANT WITH BOUND ATP
ANALOG SHOWING SUBSTANTIAL DOMAIN MOTION
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Deposited on : 1998-09-24
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

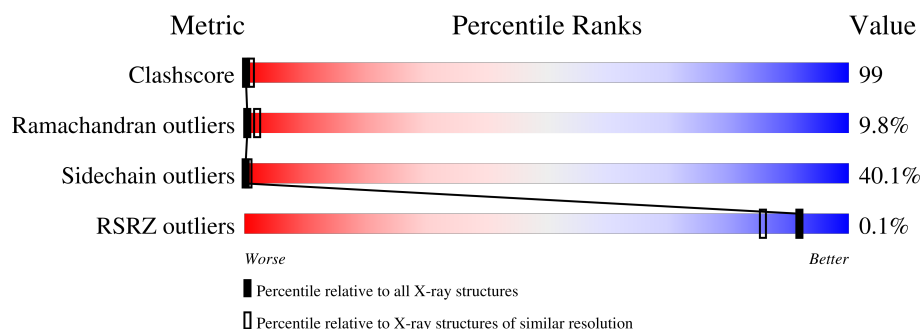
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	501	
1	Y	501	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	O	600	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7896 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	Y	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			
1	O	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			

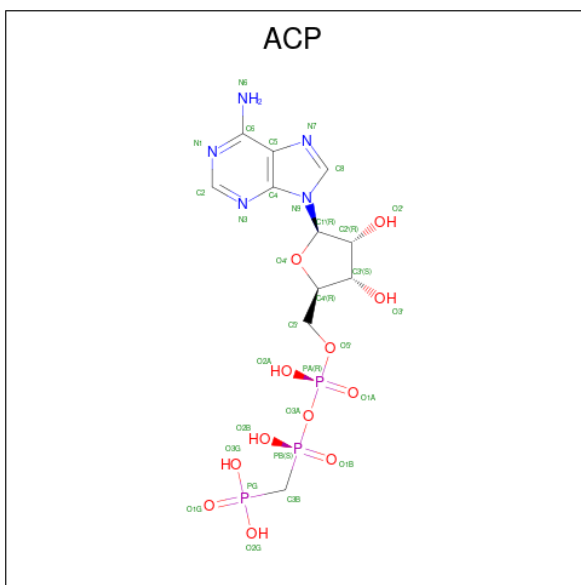
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	58	TRP	SER	engineered mutation	UNP P0A6F3
O	58	TRP	SER	engineered mutation	UNP P0A6F3

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Mg	0	0
			1	1		
2	O	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Y	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	O	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

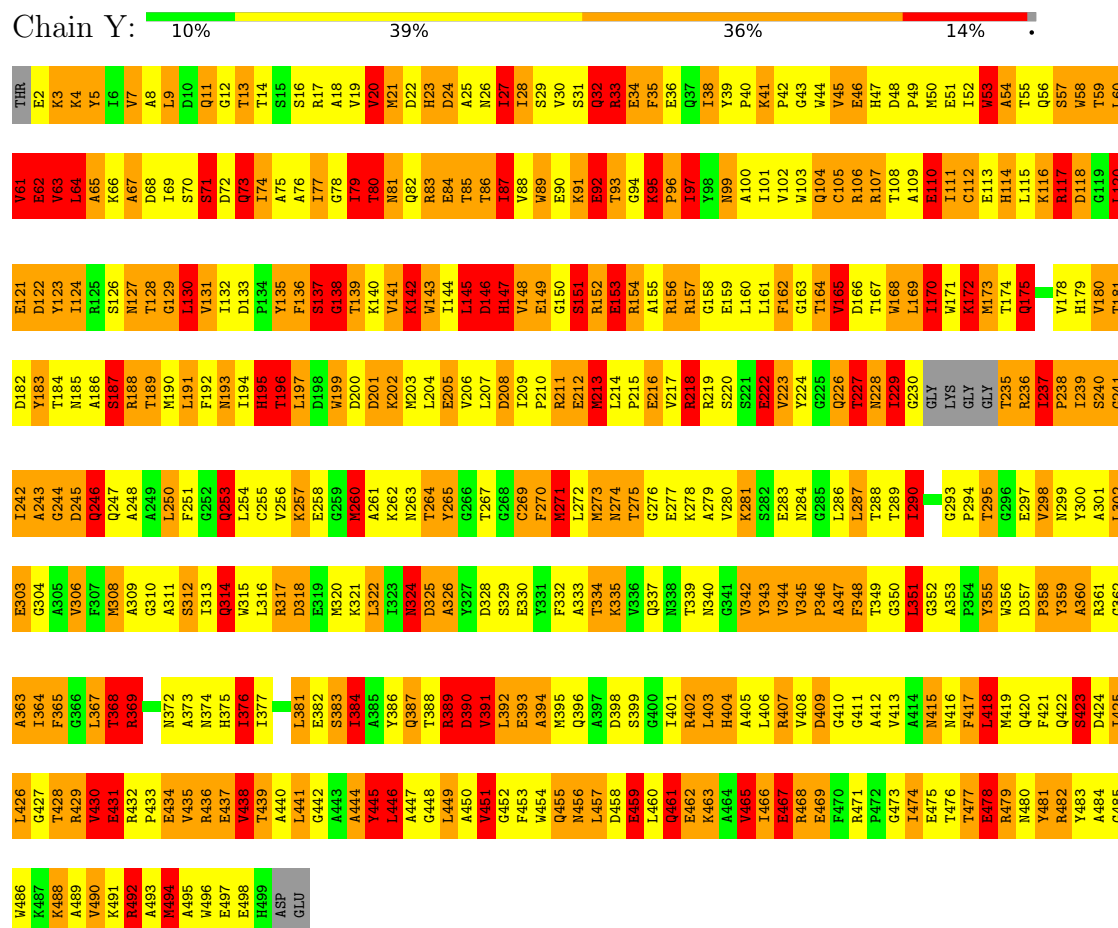


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: GLYCEROL KINASE



V490	K491	A492	A493	A494	A495	A496	A497	A498	A499	ASP	GLU
T428	R429	V430	E431	R432	P433	E434	V435	R436	E437	V438	T439
A440	L441	G442	A443	A444	V445	L446	A447	G448	L449	A450	V451
G452	F453	W454	Q455	N456	Y457	D458	E459	L460	Q461	E462	R463
A464	V465	L466	E467	R468	E469	F470	T474	E475	T476	T477	E478
R479	N480	Y481	R482	Y483	A484	C485	N486	K487	R488	A489	
F385	T386	R389	N372	A373	N374	H375	I376	I377	R378	A379	T380
L381	E382	S383	I384	A385	Y386	T387	T388	R389	D390	Y391	L392
E393	A394	N395	Q396	G397	G398	G400	I401	R402	L403	H404	A405
L406	R407	V408	D409	G410	V413	A414	N415	N416	F417	L418	N419
Q420	F421	Q422	S423	D424	L425	L426	A427				
L302	E303	V306	F307	N308	A309	G310	A311	S312	I313	Q314	V315
L316	R317	D318	K321	L322	I323	N324	D325	R326	Y327	D328	S329
E330	Y331	F332	A333	T334	K335	V336	Q337	L401	R402	L403	H404
Y343	V344	V345	P346	A347	F348	T349	G350	L351	T288	G352	A353
P354	Y355	W356	D357	P358	Y359	A360	R361	G362	A363		
I242	A243	G244	N245	Q246	N247	A248	L249	L250	F251	G252	D253
L254	C255	V256	E258	H259	A261	K262	N263	T264	Y265	G266	T267
G268	C269	F270	P271	M271	L272	M273	N274	T275	G276	E277	K278
A279	V280	K281	E282	E283	N284	C285	L286	L287	T288	T289	I290
A291	C292	G293	P294	T295	G296	E297	V298	N299	Y300	A301	
D182	Y183	T184	N185	A186	S187	R188	T189	M190	L191	F192	N193
D194	H195	T196	L197	D198	W199	D200	K201	K202	M203	W143	L204
E205	L145	D146	H147	V148	E149	P210	G211	S151	R152	E153	R154
A155	R156	R157	G158	E159	L160	L161	F162	G163	T164	V165	D166
T167	W168	L169	I170	W171	K172	M173	T174	Q175	G176	R177	V178
H179	S240	V180	T181								

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.77Å 201.15Å 114.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 82.3 (20.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	93.19 (at 2.97Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.176 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 205.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7896	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, GOL, MG

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	1.55	22/3991 (0.6%)	2.03	142/5412 (2.6%)
1	Y	1.71	49/3991 (1.2%)	2.15	153/5412 (2.8%)
All	All	1.63	71/7982 (0.9%)	2.09	295/10824 (2.7%)

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	300	TYR	CA-C	-7.75	1.43	1.52
1	Y	270	PHE	CA-C	-7.62	1.44	1.53
1	O	325	ASP	CA-C	-7.29	1.43	1.52
1	O	196	THR	CA-C	-6.66	1.44	1.52
1	O	331	TYR	C-O	6.61	1.31	1.24
1	O	193	ASN	CA-C	-6.60	1.44	1.52
1	Y	62	GLU	N-CA	-6.51	1.38	1.46
1	Y	308	MET	CA-C	-6.51	1.44	1.52
1	O	299	ASN	CA-C	-6.45	1.44	1.52
1	Y	146	ASP	CA-C	-6.42	1.46	1.53
1	Y	438	VAL	CA-CB	-6.41	1.46	1.54
1	Y	223	VAL	CA-C	-6.37	1.45	1.52
1	Y	359	TYR	CA-C	-6.23	1.44	1.52
1	Y	418	LEU	N-CA	-6.22	1.38	1.46
1	Y	403	LEU	CA-C	-6.20	1.45	1.52
1	Y	111	ILE	CA-CB	-6.11	1.46	1.54
1	Y	351	LEU	C-N	-6.07	1.26	1.32
1	Y	112	CYS	N-CA	-6.04	1.39	1.46
1	Y	304	GLY	CA-C	5.97	1.58	1.52
1	Y	347	ALA	C-N	-5.94	1.25	1.33
1	Y	195	HIS	CA-C	-5.89	1.44	1.52
1	O	348	PHE	N-CA	-5.86	1.39	1.46
1	O	419	MET	C-N	-5.85	1.26	1.33
1	O	478	GLU	CD-OE2	5.78	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	239	ILE	N-CA	-5.74	1.40	1.46
1	Y	84	GLU	CA-C	-5.73	1.44	1.52
1	Y	68	ASP	CG-OD1	5.68	1.36	1.25
1	Y	147	HIS	CA-C	-5.68	1.45	1.52
1	O	415	ASN	CA-C	5.66	1.60	1.52
1	O	416	ASN	CA-C	-5.66	1.45	1.52
1	Y	135	TYR	C-O	-5.64	1.17	1.24
1	Y	193	ASN	CA-C	-5.63	1.45	1.52
1	Y	351	LEU	C-O	-5.55	1.17	1.24
1	O	391	VAL	N-CA	-5.54	1.40	1.46
1	O	195	HIS	CA-C	-5.53	1.46	1.53
1	Y	153	GLU	CD-OE1	5.53	1.35	1.25
1	Y	306	VAL	CA-C	-5.52	1.46	1.52
1	O	258	GLU	CD-OE2	5.50	1.35	1.25
1	O	405	ALA	CA-C	-5.49	1.46	1.52
1	Y	250	LEU	C-O	5.45	1.30	1.24
1	Y	34	GLU	CD-OE1	5.42	1.35	1.25
1	Y	368	THR	N-CA	-5.42	1.39	1.45
1	O	403	LEU	CA-C	-5.42	1.46	1.52
1	Y	478	GLU	CD-OE2	5.41	1.35	1.25
1	Y	84	GLU	CD-OE1	5.37	1.35	1.25
1	Y	271	MET	CA-C	-5.31	1.46	1.52
1	Y	263	ASN	C-N	-5.30	1.26	1.33
1	O	301	ALA	N-CA	-5.30	1.39	1.46
1	Y	342	VAL	CA-C	-5.27	1.46	1.52
1	Y	333	ALA	N-CA	-5.25	1.40	1.46
1	Y	444	ALA	C-N	5.25	1.41	1.33
1	Y	391	VAL	C-N	-5.24	1.27	1.33
1	Y	290	ILE	N-CA	-5.22	1.40	1.46
1	Y	208	ASP	N-CA	-5.21	1.39	1.46
1	Y	326	ALA	C-N	-5.19	1.27	1.33
1	Y	110	GLU	CD-OE2	5.18	1.35	1.25
1	O	316	LEU	N-CA	-5.17	1.40	1.46
1	Y	351	LEU	CA-C	-5.14	1.45	1.52
1	Y	86	THR	CA-C	-5.13	1.46	1.52
1	Y	260	MET	CA-C	-5.13	1.46	1.52
1	O	420	GLN	N-CA	-5.11	1.40	1.46
1	O	153	GLU	CD-OE1	5.11	1.35	1.25
1	Y	36	GLU	CD-OE2	5.11	1.35	1.25
1	Y	387	GLN	N-CA	-5.10	1.40	1.46
1	Y	216	GLU	CD-OE2	5.09	1.35	1.25
1	Y	462	GLU	CD-OE2	5.09	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	394	ALA	CA-C	-5.08	1.46	1.52
1	O	418	LEU	N-CA	-5.07	1.39	1.46
1	Y	381	LEU	CA-C	-5.06	1.46	1.52
1	Y	389	ARG	NE-CZ	5.06	1.38	1.33
1	Y	438	VAL	CA-C	-5.04	1.46	1.52

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	83	ARG	CA-C-N	-17.81	94.28	122.24
1	Y	83	ARG	C-N-CA	-17.81	94.28	122.24
1	Y	390	ASP	CA-CB-CG	11.94	124.53	112.60
1	O	83	ARG	N-CA-C	10.84	126.84	113.50
1	Y	136	PHE	CA-CB-CG	-10.79	103.02	113.80
1	O	100	ALA	CA-C-N	-10.54	109.41	123.12
1	O	100	ALA	C-N-CA	-10.54	109.41	123.12
1	O	122	ASP	CA-CB-CG	-10.06	102.54	112.60
1	O	453	PHE	N-CA-C	-10.03	100.79	113.23
1	O	38	ILE	CB-CA-C	-9.76	100.69	111.23
1	O	355	TYR	N-CA-C	9.76	121.68	111.14
1	Y	114	HIS	CA-CB-CG	-9.57	104.23	113.80
1	Y	237	ILE	C-N-CD	-9.52	85.98	125.00
1	Y	246	GLN	N-CA-C	9.22	120.93	111.07
1	Y	83	ARG	N-CA-C	9.17	124.73	113.17
1	Y	229	ILE	N-CA-C	-8.90	101.73	110.72
1	Y	253	GLN	N-CA-C	-8.76	101.95	114.12
1	O	83	ARG	CA-C-N	-8.69	107.42	122.36
1	O	83	ARG	C-N-CA	-8.69	107.42	122.36
1	Y	376	ILE	N-CA-CB	8.48	119.92	110.51
1	Y	122	ASP	CA-CB-CG	-8.37	104.23	112.60
1	Y	243	ALA	CA-C-N	-8.01	112.51	120.60
1	Y	243	ALA	C-N-CA	-8.01	112.51	120.60
1	O	465	VAL	CA-C-N	-8.01	112.04	122.37
1	O	465	VAL	C-N-CA	-8.01	112.04	122.37
1	Y	64	LEU	N-CA-CB	7.84	123.75	110.49
1	Y	62	GLU	N-CA-CB	7.79	121.37	110.07
1	Y	390	ASP	N-CA-CB	7.77	123.62	110.49
1	Y	84	GLU	O-C-N	7.74	130.85	122.34
1	Y	5	TYR	N-CA-C	7.73	121.16	109.41
1	Y	83	ARG	O-C-N	-7.63	112.81	122.34
1	O	390	ASP	CA-CB-CG	7.62	120.22	112.60
1	Y	365	PHE	N-CA-C	7.57	120.67	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	147	HIS	CA-CB-CG	-7.53	106.27	113.80
1	Y	32	GLN	N-CA-C	7.49	120.38	107.28
1	O	73	GLN	CA-C-N	-7.46	113.47	123.10
1	O	73	GLN	C-N-CA	-7.46	113.47	123.10
1	Y	222	GLU	CA-C-N	-7.44	112.69	123.10
1	Y	222	GLU	C-N-CA	-7.44	112.69	123.10
1	Y	403	LEU	CA-C-N	-7.39	111.03	122.49
1	Y	403	LEU	C-N-CA	-7.39	111.03	122.49
1	Y	363	ALA	N-CA-C	7.35	120.53	108.99
1	Y	303	GLU	N-CA-C	7.35	120.71	108.73
1	Y	189	THR	N-CA-C	7.33	120.20	111.33
1	Y	38	ILE	CB-CA-C	-7.29	101.57	111.33
1	Y	465	VAL	CA-C-N	-7.27	111.62	121.66
1	Y	465	VAL	C-N-CA	-7.27	111.62	121.66
1	O	38	ILE	N-CA-C	7.27	118.96	107.98
1	Y	20	VAL	N-CA-CB	7.27	124.04	111.39
1	Y	318	ASP	N-CA-C	7.26	118.98	111.14
1	O	81	ASN	N-CA-C	7.24	119.14	108.14
1	O	36	GLU	N-CA-C	7.23	120.22	109.59
1	O	357	ASP	CA-C-N	7.18	126.86	119.82
1	O	357	ASP	C-N-CA	7.18	126.86	119.82
1	O	466	ILE	N-CA-CB	7.16	118.52	110.72
1	Y	250	LEU	CA-C-N	7.14	130.15	120.44
1	Y	250	LEU	C-N-CA	7.14	130.15	120.44
1	Y	137	SER	N-CA-C	7.12	119.04	111.28
1	Y	61	VAL	CA-C-N	-7.09	110.80	120.44
1	Y	61	VAL	C-N-CA	-7.09	110.80	120.44
1	O	20	VAL	CB-CA-C	-7.06	100.11	110.62
1	Y	20	VAL	CB-CA-C	-7.06	100.11	110.62
1	O	32	GLN	N-CA-C	7.04	119.61	107.28
1	O	38	ILE	N-CA-CB	7.02	119.53	111.39
1	Y	38	ILE	N-CA-CB	7.01	118.60	110.82
1	Y	62	GLU	CA-C-N	-6.99	111.59	120.60
1	Y	62	GLU	C-N-CA	-6.99	111.59	120.60
1	O	5	TYR	N-CA-C	6.96	118.67	108.86
1	O	85	THR	CA-C-N	6.95	133.00	122.65
1	O	85	THR	C-N-CA	6.95	133.00	122.65
1	O	494	MET	N-CA-CB	6.89	120.24	109.83
1	Y	123	TYR	CA-C-N	6.89	129.13	120.72
1	Y	123	TYR	C-N-CA	6.89	129.13	120.72
1	Y	348	PHE	N-CA-C	-6.88	104.35	112.89
1	O	97	ILE	N-CA-CB	-6.87	102.05	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	369	ARG	N-CA-C	6.83	118.38	111.07
1	Y	384	ILE	N-CA-C	6.80	116.95	110.42
1	O	195	HIS	N-CA-C	-6.80	103.28	112.26
1	Y	38	ILE	N-CA-C	6.79	117.80	108.84
1	O	348	PHE	N-CA-C	-6.79	103.88	111.28
1	O	480	ASN	CA-CB-CG	-6.69	105.91	112.60
1	O	416	ASN	CA-CB-CG	-6.67	105.93	112.60
1	O	427	GLY	N-CA-C	-6.67	106.11	115.32
1	Y	471	ARG	CA-C-N	6.66	128.16	119.84
1	Y	471	ARG	C-N-CA	6.66	128.16	119.84
1	O	229	ILE	N-CA-C	-6.65	103.75	111.00
1	Y	63	VAL	N-CA-CB	6.62	117.86	110.51
1	Y	459	GLU	CA-C-N	6.60	129.79	120.28
1	Y	459	GLU	C-N-CA	6.60	129.79	120.28
1	O	365	PHE	N-CA-C	6.57	119.70	109.52
1	Y	147	HIS	CA-CB-CG	-6.57	107.23	113.80
1	Y	104	GLN	N-CA-CB	-6.54	100.15	110.28
1	Y	275	THR	CA-C-O	6.54	125.96	118.97
1	Y	127	ASN	O-C-N	6.52	129.84	122.27
1	Y	250	LEU	O-C-N	6.52	129.58	122.15
1	Y	67	ALA	CA-C-O	6.45	125.72	119.08
1	Y	438	VAL	O-C-N	6.44	128.20	121.89
1	Y	269	CYS	CA-C-N	-6.43	112.28	122.76
1	Y	269	CYS	C-N-CA	-6.43	112.28	122.76
1	Y	89	TRP	N-CA-C	6.42	118.93	109.24
1	O	129	GLY	N-CA-C	-6.37	106.12	115.30
1	O	208	ASP	CA-CB-CG	6.37	118.97	112.60
1	O	318	ASP	N-CA-C	6.37	117.88	111.07
1	Y	129	GLY	N-CA-C	-6.36	107.01	115.40
1	Y	100	ALA	CA-C-N	-6.33	114.95	122.93
1	Y	100	ALA	C-N-CA	-6.33	114.95	122.93
1	Y	130	LEU	CA-C-N	6.32	129.19	122.11
1	Y	130	LEU	C-N-CA	6.32	129.19	122.11
1	O	29	SER	N-CA-C	6.32	116.78	107.88
1	Y	117	ARG	N-CA-C	6.29	120.81	113.20
1	Y	80	THR	N-CA-CB	6.29	122.81	111.37
1	Y	183	TYR	CA-CB-CG	-6.27	102.61	113.90
1	O	256	VAL	N-CA-CB	-6.27	100.88	111.23
1	Y	244	GLY	N-CA-C	-6.26	103.61	112.37
1	O	86	THR	N-CA-C	6.18	119.89	109.76
1	Y	494	MET	N-CA-CB	6.17	119.14	109.83
1	Y	471	ARG	O-C-N	6.15	127.44	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	296	GLY	CA-C-O	6.14	125.60	118.96
1	Y	481	TYR	CA-CB-CG	-6.14	102.84	113.90
1	Y	33	ARG	CA-C-N	6.13	129.42	120.71
1	Y	33	ARG	C-N-CA	6.13	129.42	120.71
1	Y	404	HIS	CA-CB-CG	-6.13	107.67	113.80
1	O	415	ASN	CA-CB-CG	-6.09	106.51	112.60
1	Y	412	ALA	N-CA-C	6.08	120.17	112.87
1	O	227	THR	CA-C-N	-6.05	112.66	122.34
1	O	227	THR	C-N-CA	-6.05	112.66	122.34
1	Y	245	ASP	CA-CB-CG	6.04	118.64	112.60
1	O	459	GLU	CA-C-N	6.04	130.35	120.63
1	O	459	GLU	C-N-CA	6.04	130.35	120.63
1	Y	345	VAL	CA-C-N	6.03	127.38	119.84
1	Y	345	VAL	C-N-CA	6.03	127.38	119.84
1	O	332	PHE	CA-CB-CG	-6.02	107.78	113.80
1	Y	73	GLN	CA-C-N	-6.01	114.32	122.91
1	Y	73	GLN	C-N-CA	-6.01	114.32	122.91
1	O	20	VAL	N-CA-CB	6.00	121.83	111.39
1	O	404	HIS	CA-CB-CG	-6.00	107.80	113.80
1	Y	193	ASN	N-CA-CB	5.99	119.64	109.87
1	O	97	ILE	CB-CA-C	5.97	120.06	111.88
1	Y	444	ALA	N-CA-C	-5.97	104.47	110.97
1	O	491	LYS	N-CA-CB	5.96	118.88	109.82
1	O	364	ILE	N-CA-CB	5.96	120.39	110.86
1	Y	85	THR	N-CA-CB	-5.95	100.43	110.49
1	O	79	ILE	N-CA-C	5.95	116.43	108.27
1	O	430	VAL	CA-C-N	5.94	131.11	122.85
1	O	430	VAL	C-N-CA	5.94	131.11	122.85
1	O	423	SER	N-CA-CB	5.94	118.58	109.91
1	O	237	ILE	N-CA-CB	5.93	119.52	111.21
1	O	331	TYR	N-CA-C	5.92	118.49	111.33
1	Y	288	THR	CA-C-N	-5.91	112.91	122.36
1	Y	288	THR	C-N-CA	-5.91	112.91	122.36
1	Y	381	LEU	O-C-N	5.90	128.46	122.09
1	O	403	LEU	CA-C-N	-5.89	112.08	122.26
1	O	403	LEU	C-N-CA	-5.89	112.08	122.26
1	Y	367	LEU	N-CA-CB	5.88	119.07	109.95
1	O	340	ASN	N-CA-C	5.87	119.75	112.24
1	O	239	ILE	N-CA-CB	-5.85	106.80	112.65
1	Y	467	GLU	CA-C-O	5.84	126.93	120.80
1	Y	253	GLN	CA-C-O	5.84	125.32	118.90
1	O	20	VAL	N-CA-C	5.83	116.87	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	431	GLU	N-CA-C	5.80	118.55	107.75
1	O	404	HIS	N-CA-C	-5.79	106.25	113.38
1	Y	55	THR	N-CA-CB	5.79	120.28	110.49
1	O	189	THR	N-CA-C	5.79	119.86	112.34
1	O	468	ARG	CA-C-N	-5.76	115.05	123.00
1	O	468	ARG	C-N-CA	-5.76	115.05	123.00
1	O	350	GLY	N-CA-C	-5.76	101.85	112.62
1	O	355	TYR	CB-CA-C	-5.76	101.81	110.90
1	O	253	GLN	N-CA-C	-5.75	105.92	113.17
1	O	307	PHE	N-CA-C	5.75	117.22	111.07
1	O	359	TYR	CA-CB-CG	-5.74	103.57	113.90
1	O	268	GLY	N-CA-C	-5.73	99.60	113.18
1	O	288	THR	CA-C-N	-5.72	111.85	121.75
1	O	288	THR	C-N-CA	-5.72	111.85	121.75
1	Y	117	ARG	N-CA-CB	5.72	119.69	110.42
1	O	494	MET	N-CA-C	5.70	118.49	110.23
1	Y	430	VAL	N-CA-C	5.69	115.79	107.37
1	Y	7	VAL	N-CA-C	5.68	115.78	107.37
1	Y	227	THR	N-CA-CB	5.68	119.49	110.57
1	O	218	ARG	N-CA-C	5.67	118.11	109.95
1	Y	355	TYR	N-CA-C	5.65	122.83	110.80
1	Y	431	GLU	N-CA-C	5.64	117.92	107.99
1	O	24	ASP	N-CA-C	-5.64	106.44	113.15
1	O	37	GLN	CA-C-O	-5.64	115.06	121.66
1	O	90	GLU	N-CA-CB	5.63	118.31	109.69
1	O	374	ASN	N-CA-CB	5.62	118.11	109.91
1	Y	263	ASN	N-CA-CB	5.61	119.51	110.65
1	O	277	GLU	N-CA-C	5.60	119.29	112.23
1	O	445	TYR	N-CA-CB	5.60	119.95	110.49
1	O	299	ASN	CA-C-N	-5.60	113.41	122.82
1	O	299	ASN	C-N-CA	-5.60	113.41	122.82
1	Y	451	VAL	N-CA-C	5.58	117.57	111.77
1	Y	96	PRO	N-CA-CB	5.57	108.52	103.34
1	O	345	VAL	CA-C-N	5.56	126.79	119.84
1	O	345	VAL	C-N-CA	5.56	126.79	119.84
1	O	494	MET	CB-CA-C	-5.55	100.51	109.72
1	Y	363	ALA	CA-C-N	-5.54	114.37	122.68
1	Y	363	ALA	C-N-CA	-5.54	114.37	122.68
1	Y	117	ARG	CB-CA-C	-5.53	99.60	110.11
1	Y	360	ALA	N-CA-C	-5.53	102.70	110.50
1	Y	23	HIS	CA-CB-CG	-5.53	108.27	113.80
1	Y	417	PHE	CA-CB-CG	-5.53	108.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	324	ASN	CA-C-O	5.52	124.88	118.97
1	Y	465	VAL	N-CA-C	5.52	115.73	107.51
1	Y	95	LYS	CA-C-N	5.51	125.27	119.76
1	Y	95	LYS	C-N-CA	5.51	125.27	119.76
1	O	263	ASN	N-CA-CB	5.51	119.25	110.65
1	Y	138	GLY	CA-C-N	5.51	127.93	120.38
1	Y	138	GLY	C-N-CA	5.51	127.93	120.38
1	O	32	GLN	O-C-N	-5.51	118.43	123.50
1	O	300	TYR	N-CA-CB	5.50	120.17	111.43
1	O	126	SER	CA-C-N	-5.50	113.72	122.29
1	O	126	SER	C-N-CA	-5.50	113.72	122.29
1	O	4	LYS	CA-C-N	-5.49	113.70	122.53
1	O	4	LYS	C-N-CA	-5.49	113.70	122.53
1	Y	218	ARG	N-CA-C	5.48	116.96	109.18
1	Y	404	HIS	N-CA-C	-5.48	105.96	113.30
1	O	481	TYR	CA-CB-CG	-5.47	104.05	113.90
1	Y	314	GLN	N-CA-CB	5.47	118.09	109.94
1	O	250	LEU	CA-C-O	5.47	126.35	120.55
1	O	372	ASN	N-CA-C	5.46	118.17	109.81
1	O	301	ALA	O-C-N	5.44	129.58	123.48
1	Y	106	ARG	N-CA-C	5.43	119.01	112.93
1	Y	318	ASP	CB-CA-C	-5.43	102.32	110.90
1	O	350	GLY	O-C-N	5.43	128.07	122.91
1	Y	386	TYR	O-C-N	5.43	128.77	122.20
1	Y	33	ARG	N-CA-C	5.43	117.74	108.90
1	Y	265	TYR	CB-CA-C	-5.43	104.33	112.09
1	O	90	GLU	CA-C-N	-5.43	114.17	121.71
1	O	90	GLU	C-N-CA	-5.43	114.17	121.71
1	O	275	THR	N-CA-C	-5.42	105.88	112.88
1	O	278	LYS	N-CA-CB	5.40	119.39	110.69
1	O	97	ILE	N-CA-C	-5.38	107.23	112.29
1	O	32	GLN	CA-C-N	-5.38	115.52	123.05
1	O	32	GLN	C-N-CA	-5.38	115.52	123.05
1	Y	334	THR	CA-CB-CG2	-5.37	101.38	110.50
1	O	431	GLU	CB-CA-C	-5.36	102.31	111.31
1	Y	168	TRP	O-C-N	5.35	127.65	122.09
1	Y	423	SER	N-CA-CB	5.33	117.95	110.12
1	Y	80	THR	CA-CB-CG2	-5.33	101.45	110.50
1	O	312	SER	CA-C-O	5.32	126.37	120.63
1	Y	83	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	Y	274	ASN	N-CA-C	5.31	117.39	109.59
1	O	430	VAL	N-CA-C	5.31	115.50	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	237	ILE	N-CA-CB	5.30	118.64	111.21
1	O	279	ALA	CA-C-N	-5.30	114.10	122.64
1	O	279	ALA	C-N-CA	-5.30	114.10	122.64
1	O	61	VAL	N-CA-C	5.30	115.44	110.30
1	O	67	ALA	N-CA-C	-5.30	106.59	114.64
1	O	85	THR	N-CA-CB	-5.28	101.56	110.49
1	O	486	TRP	CA-C-N	-5.28	111.81	121.52
1	O	486	TRP	C-N-CA	-5.28	111.81	121.52
1	O	193	ASN	N-CA-CB	5.25	118.83	110.16
1	Y	390	ASP	CB-CA-C	-5.25	99.97	110.42
1	O	194	ILE	CA-C-N	-5.25	114.83	122.86
1	O	194	ILE	C-N-CA	-5.25	114.83	122.86
1	O	263	ASN	CA-CB-CG	-5.25	107.35	112.60
1	Y	132	ILE	N-CA-CB	5.24	117.75	111.31
1	O	125	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	Y	105	CYS	N-CA-C	5.21	117.26	109.59
1	O	270	PHE	CA-CB-CG	-5.21	108.59	113.80
1	O	408	VAL	N-CA-C	5.21	116.68	109.29
1	Y	304	GLY	O-C-N	-5.20	118.15	123.35
1	O	364	ILE	CA-CB-CG1	5.19	119.23	110.40
1	O	122	ASP	N-CA-C	5.19	119.09	112.34
1	Y	427	GLY	N-CA-C	-5.19	105.07	114.46
1	Y	87	ILE	CB-CA-C	-5.17	101.47	110.71
1	O	137	SER	N-CA-C	5.16	117.30	111.11
1	Y	431	GLU	CA-C-O	-5.16	115.56	120.92
1	O	256	VAL	CB-CA-C	5.15	119.74	111.29
1	O	255	CYS	CA-C-N	-5.13	112.74	121.97
1	O	255	CYS	C-N-CA	-5.13	112.74	121.97
1	O	457	LEU	N-CA-C	-5.13	106.71	113.12
1	O	479	ARG	CA-C-N	-5.13	112.16	120.72
1	O	479	ARG	C-N-CA	-5.13	112.16	120.72
1	Y	35	PHE	CA-C-N	5.13	128.05	120.82
1	Y	35	PHE	C-N-CA	5.13	128.05	120.82
1	Y	36	GLU	N-CA-C	5.12	117.72	110.10
1	O	47	HIS	CA-C-N	-5.11	114.99	121.74
1	O	47	HIS	C-N-CA	-5.11	114.99	121.74
1	O	456	ASN	N-CA-CB	5.10	119.12	110.49
1	Y	79	ILE	N-CA-C	5.10	115.38	107.78
1	O	446	LEU	N-CA-CB	-5.10	101.88	110.49
1	Y	84	GLU	N-CA-CB	5.08	117.65	110.90
1	Y	20	VAL	N-CA-C	5.07	115.78	108.48
1	Y	227	THR	CA-C-N	-5.05	115.29	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	227	THR	C-N-CA	-5.05	115.29	122.41
1	Y	241	GLY	O-C-N	5.05	127.11	123.27
1	O	425	ILE	CB-CA-C	-5.05	104.53	111.65
1	Y	260	MET	N-CA-CB	5.04	118.08	109.87
1	Y	97	ILE	N-CA-C	-5.03	107.39	112.17
1	Y	87	ILE	N-CA-CB	5.02	121.31	111.92
1	O	283	GLU	CA-C-O	5.02	124.88	119.15
1	Y	120	LEU	N-CA-CB	5.02	118.17	110.70
1	Y	343	TYR	CA-C-N	-5.02	115.97	122.94
1	Y	343	TYR	C-N-CA	-5.02	115.97	122.94

There are no chirality outliers.

There are no planarity outliers.

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	3910	0	3841	787	0
1	Y	3910	0	3841	771	0
2	O	1	0	0	0	0
2	Y	1	0	0	0	0
3	O	31	0	14	4	0
3	Y	31	0	14	5	0
4	O	6	0	8	7	0
4	Y	6	0	8	3	0
All	All	7896	0	7726	1550	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 99.

All (1550) 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:Y:458:ASP:HA	1:Y:461:GLN:HG3	1.25	1.13
1:O:48:ASP:HB3	1:O:51:GLU:HB3	1.16	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:415:ASN:ND2	1:O:418:LEU:H	1.48	1.11
1:Y:31:SER:HB2	1:Y:63:VAL:HG22	1.28	1.08
1:O:83:ARG:HB2	4:O:600:GOL:H12	1.11	1.08
1:Y:459:GLU:HB2	1:Y:460:LEU:HD12	1.25	1.07
1:Y:84:GLU:HB2	1:Y:103:TRP:HB3	1.36	1.06
1:Y:31:SER:HB3	1:Y:59:THR:HA	1.39	1.04
1:O:117:ARG:HH11	1:O:117:ARG:HB2	1.16	1.04
1:O:19:VAL:HG12	1:O:21:MET:HE2	1.33	1.03
1:O:413:VAL:HA	1:O:419:MET:HE3	1.07	1.03
1:O:435:VAL:HG21	1:O:441:LEU:HD11	1.41	1.02
1:O:313:ILE:HD11	1:O:381:LEU:HD23	1.42	1.01
1:Y:21:MET:HE1	1:Y:444:ALA:HB2	1.44	1.00
1:O:211:ARG:HG3	1:O:211:ARG:HH11	1.22	1.00
1:O:47:HIS:HB3	1:O:52:ILE:HD11	1.41	0.99
1:O:138:GLY:HA2	1:O:191:LEU:HD21	1.42	0.98
1:O:272:LEU:HD11	1:O:303:GLU:HG3	1.41	0.98
1:Y:413:VAL:HA	1:Y:419:MET:HE3	1.44	0.98
1:O:137:SER:O	1:O:138:GLY:C	2.02	0.97
1:Y:460:LEU:HD12	1:Y:460:LEU:H	1.29	0.97
1:O:144:ILE:HD12	1:O:144:ILE:H	1.28	0.96
1:O:460:LEU:HD12	1:O:460:LEU:H	1.31	0.96
1:Y:27:ILE:HD12	1:Y:27:ILE:H	1.31	0.96
1:Y:117:ARG:HH11	1:Y:117:ARG:HB2	1.31	0.96
1:Y:229:ILE:HG21	1:Y:237:ILE:HG12	1.47	0.96
1:Y:91:LYS:O	1:Y:92:GLU:C	2.05	0.93
1:Y:226:GLN:HB2	1:Y:236:ARG:HD3	1.50	0.93
1:Y:152:ARG:HB3	1:Y:156:ARG:HH22	1.34	0.93
1:O:468:ARG:HG3	1:O:468:ARG:HH11	1.32	0.92
1:O:415:ASN:HD21	1:O:417:PHE:HB3	1.33	0.92
1:Y:117:ARG:HB2	1:Y:117:ARG:NH1	1.84	0.91
1:Y:468:ARG:HD2	1:Y:469:GLU:N	1.85	0.91
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.50	0.91
1:O:415:ASN:HD22	1:O:418:LEU:H	1.01	0.91
1:Y:91:LYS:HB2	1:Y:161:LEU:HD12	1.53	0.91
1:O:27:ILE:H	1:O:27:ILE:HD12	1.35	0.91
1:O:115:LEU:HD12	1:O:115:LEU:H	1.38	0.89
1:Y:459:GLU:HB2	1:Y:460:LEU:CD1	2.03	0.88
1:O:463:LYS:HE2	1:O:463:LYS:HA	1.56	0.88
1:O:164:THR:H	1:O:167:THR:HB	1.39	0.87
1:Y:279:ALA:HB2	1:Y:300:TYR:CD2	2.09	0.87
1:Y:196:THR:H	1:Y:197:LEU:HD22	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:193:ASN:HB3	1:O:196:THR:CG2	2.04	0.87
1:Y:257:LYS:H	1:Y:260:MET:HG3	1.40	0.87
1:O:3:LYS:HG3	1:O:73:GLN:HA	1.57	0.87
1:Y:211:ARG:HG3	1:Y:211:ARG:HH11	1.40	0.87
1:O:203:MET:HA	1:O:206:VAL:HG12	1.57	0.87
1:O:35:PHE:HB2	1:O:51:GLU:HG3	1.56	0.86
1:Y:193:ASN:HB3	1:Y:196:THR:CG2	2.05	0.86
1:Y:31:SER:CB	1:Y:63:VAL:HG22	2.05	0.86
1:O:63:VAL:HA	1:O:66:LYS:HG2	1.55	0.85
1:O:91:LYS:HB2	1:O:161:LEU:HD12	1.57	0.85
1:O:91:LYS:O	1:O:92:GLU:C	2.12	0.85
1:Y:463:LYS:HA	1:Y:463:LYS:HE2	1.56	0.85
1:Y:468:ARG:HD2	1:Y:469:GLU:H	1.37	0.85
1:O:184:THR:HB	1:O:247:GLN:HG2	1.59	0.85
1:Y:183:TYR:CE1	1:Y:217:VAL:HG12	2.12	0.85
1:O:90:GLU:HB3	1:O:93:THR:HG23	1.58	0.84
1:Y:124:ILE:HG12	1:Y:203:MET:HE1	1.60	0.84
1:O:17:ARG:HH22	1:O:437:GLU:HG3	1.40	0.84
1:Y:193:ASN:HB3	1:Y:196:THR:HB	1.58	0.83
1:O:199:TRP:CZ2	1:O:214:LEU:HB3	2.13	0.83
1:Y:84:GLU:HB2	1:Y:103:TRP:CB	2.07	0.83
1:Y:240:SER:HB2	1:Y:450:ALA:CB	2.08	0.83
1:Y:81:ASN:N	1:Y:81:ASN:HD22	1.77	0.83
1:Y:328:ASP:HB3	1:Y:332:PHE:HE2	1.43	0.82
1:O:102:VAL:HG12	1:O:103:TRP:CD1	2.13	0.82
1:O:47:HIS:HB3	1:O:52:ILE:CD1	2.08	0.82
1:O:80:THR:HG21	1:O:245:ASP:HA	1.61	0.82
1:Y:47:HIS:HB3	1:Y:52:ILE:HD11	1.60	0.82
1:Y:458:ASP:HA	1:Y:461:GLN:CG	2.09	0.82
1:O:271:MET:HG2	1:O:395:MET:HE2	1.59	0.82
1:O:415:ASN:HD22	1:O:418:LEU:N	1.78	0.82
1:O:459:GLU:HB2	1:O:460:LEU:HD12	1.62	0.82
1:Y:262:LYS:HZ3	1:Y:264:THR:HB	1.44	0.81
1:O:114:HIS:HA	1:O:117:ARG:NH1	1.95	0.81
1:Y:433:PRO:HA	1:Y:466:ILE:HA	1.61	0.81
1:O:55:THR:HA	1:O:58:TRP:CD1	2.16	0.81
1:Y:286:LEU:C	1:Y:287:LEU:HD23	2.05	0.81
1:Y:58:TRP:O	1:Y:59:THR:C	2.24	0.81
1:O:313:ILE:HD11	1:O:381:LEU:CD2	2.11	0.81
1:O:48:ASP:CB	1:O:51:GLU:HB3	2.08	0.80
1:O:91:LYS:NZ	1:O:91:LYS:HB3	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:189:THR:HB	1:Y:191:LEU:HG	1.63	0.80
1:O:193:ASN:HB3	1:O:196:THR:HB	1.62	0.80
1:O:373:ALA:O	1:O:377:ILE:HG13	1.82	0.80
1:Y:195:HIS:N	1:Y:195:HIS:ND1	2.29	0.80
1:Y:251:PHE:CE2	1:Y:446:LEU:HD12	2.17	0.80
1:Y:457:LEU:HA	1:Y:460:LEU:HD13	1.61	0.80
1:O:253:GLN:HE21	1:O:262:LYS:CB	1.96	0.79
1:O:138:GLY:HA2	1:O:191:LEU:CD2	2.12	0.79
1:O:199:TRP:CE2	1:O:214:LEU:HB3	2.18	0.79
1:Y:106:ARG:HD2	1:Y:349:THR:O	1.82	0.79
1:O:48:ASP:HB3	1:O:51:GLU:CB	2.07	0.79
1:O:153:GLU:C	1:O:157:ARG:HD3	2.08	0.79
1:O:188:ARG:HH21	1:O:289:THR:HG21	1.48	0.79
1:O:272:LEU:CD1	1:O:303:GLU:HG3	2.13	0.78
1:O:463:LYS:HA	1:O:463:LYS:CE	2.13	0.78
1:Y:458:ASP:CA	1:Y:461:GLN:HG3	2.12	0.78
1:O:170:ILE:O	1:O:171:TRP:C	2.25	0.78
1:Y:3:LYS:HA	1:Y:73:GLN:HA	1.64	0.78
1:Y:413:VAL:HA	1:Y:419:MET:CE	2.13	0.78
1:O:438:VAL:HA	1:O:441:LEU:HD12	1.65	0.78
1:Y:230:GLY:HA2	1:Y:235:THR:CB	2.13	0.78
1:O:40:PRO:HG2	1:O:44:TRP:CB	2.14	0.78
1:O:164:THR:O	1:O:165:VAL:C	2.26	0.77
1:Y:415:ASN:HD21	1:Y:417:PHE:HB3	1.47	0.77
1:O:146:ASP:HB3	1:O:152:ARG:HH12	1.49	0.77
1:Y:492:ARG:HG2	1:Y:492:ARG:HH11	1.47	0.77
1:O:253:GLN:HE21	1:O:262:LYS:HB2	1.49	0.77
1:Y:413:VAL:HG12	1:Y:419:MET:CE	2.15	0.77
1:Y:246:GLN:HG3	1:Y:262:LYS:HZ1	1.49	0.77
1:O:17:ARG:HH22	1:O:437:GLU:CG	1.98	0.76
1:O:33:ARG:HH21	1:O:58:TRP:HB3	1.50	0.76
1:O:435:VAL:CG2	1:O:441:LEU:HD11	2.14	0.76
1:O:360:ALA:O	1:O:361:ARG:HD3	1.84	0.76
1:O:155:ALA:HB1	1:O:210:PRO:HG2	1.66	0.76
1:Y:127:ASN:HB3	1:Y:193:ASN:ND2	2.00	0.76
1:Y:162:PHE:HB3	1:Y:213:MET:HG3	1.67	0.76
1:Y:273:MET:HE1	1:Y:401:ILE:HD12	1.67	0.76
1:Y:373:ALA:O	1:Y:377:ILE:HG13	1.84	0.76
1:O:152:ARG:O	1:O:155:ALA:HB3	1.85	0.76
1:Y:142:LYS:O	1:Y:143:TRP:C	2.28	0.76
1:Y:360:ALA:O	1:Y:361:ARG:HD3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:457:LEU:HD22	1:Y:460:LEU:HD13	1.66	0.76
1:Y:137:SER:O	1:Y:138:GLY:C	2.28	0.76
1:O:173:MET:HB3	1:O:227:THR:HG21	1.67	0.76
1:O:123:TYR:CZ	1:O:202:LYS:HG3	2.20	0.76
1:O:164:THR:H	1:O:167:THR:CB	1.98	0.76
1:Y:141:VAL:O	1:Y:145:LEU:HD22	1.86	0.75
1:Y:267:THR:OG1	3:Y:601:ACP:H3B2	1.86	0.75
1:Y:255:CYS:HB3	1:Y:260:MET:HB2	1.68	0.75
1:Y:269:CYS:HB2	1:Y:306:VAL:HB	1.68	0.75
1:O:31:SER:OG	1:O:62:GLU:HB2	1.85	0.75
1:O:195:HIS:ND1	1:O:195:HIS:N	2.29	0.75
1:Y:152:ARG:O	1:Y:155:ALA:HB3	1.87	0.75
1:O:221:SER:CB	1:O:296:GLY:HA3	2.16	0.75
1:Y:447:ALA:O	1:Y:450:ALA:HB3	1.86	0.75
1:O:241:GLY:O	1:O:242:ILE:HG13	1.86	0.75
1:Y:193:ASN:HB3	1:Y:196:THR:CB	2.17	0.75
1:O:141:VAL:O	1:O:145:LEU:HD22	1.85	0.75
1:Y:441:LEU:HD22	1:Y:445:TYR:CE1	2.22	0.74
1:O:156:ARG:HB2	1:O:156:ARG:CZ	2.16	0.74
1:Y:8:ALA:O	1:Y:9:LEU:HD13	1.87	0.74
1:Y:40:PRO:HG3	1:Y:46:GLU:CD	2.12	0.74
1:O:184:THR:CG2	1:O:247:GLN:HG2	2.18	0.74
1:O:137:SER:HA	1:O:140:LYS:HD2	1.67	0.74
1:Y:410:GLY:O	1:Y:413:VAL:HG22	1.87	0.74
1:Y:123:TYR:CD2	1:Y:203:MET:HE2	2.23	0.74
1:Y:85:THR:HA	1:Y:101:ILE:O	1.87	0.74
1:Y:449:LEU:HD12	1:Y:449:LEU:O	1.87	0.74
1:Y:154:ARG:O	1:Y:155:ALA:C	2.28	0.74
1:Y:168:TRP:O	1:Y:172:LYS:HG2	1.88	0.74
1:Y:454:TRP:CD1	1:Y:460:LEU:HD11	2.22	0.74
1:O:33:ARG:HE	1:O:58:TRP:CG	2.06	0.74
1:O:276:GLY:HA2	1:O:299:ASN:ND2	2.03	0.74
1:O:332:PHE:O	1:O:335:LYS:HB2	1.87	0.74
1:Y:183:TYR:CD1	1:Y:217:VAL:HG12	2.22	0.74
1:O:3:LYS:HG3	1:O:73:GLN:CA	2.17	0.74
1:Y:120:LEU:HD12	1:Y:120:LEU:H	1.54	0.73
1:O:193:ASN:HB3	1:O:196:THR:CB	2.18	0.73
1:O:41:LYS:HG3	1:O:42:PRO:HD2	1.70	0.73
1:O:444:ALA:O	1:O:445:TYR:C	2.32	0.73
1:Y:257:LYS:C	1:Y:274:ASN:HD22	1.97	0.73
1:O:80:THR:CG2	1:O:245:ASP:HA	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:LYS:HB3	1:O:91:LYS:HZ3	1.51	0.73
1:Y:44:TRP:CE2	1:Y:107:ARG:HB2	2.23	0.73
1:O:184:THR:CB	1:O:247:GLN:HG2	2.19	0.73
1:O:221:SER:HB3	1:O:296:GLY:HA3	1.70	0.73
1:O:253:GLN:HG3	1:O:407:ARG:HD2	1.71	0.73
1:O:271:MET:C	1:O:272:LEU:HD12	2.13	0.73
1:Y:246:GLN:HG3	1:Y:262:LYS:NZ	2.04	0.72
1:O:226:GLN:CB	1:O:236:ARG:HD3	2.18	0.72
1:Y:151:SER:O	1:Y:152:ARG:C	2.30	0.72
1:Y:415:ASN:ND2	1:Y:418:LEU:H	1.86	0.72
1:O:261:ALA:HB2	1:O:273:MET:HG2	1.71	0.72
1:Y:9:LEU:HD23	1:Y:77:ILE:HG23	1.71	0.72
1:Y:196:THR:N	1:Y:197:LEU:HD22	2.03	0.72
1:Y:262:LYS:HZ3	1:Y:264:THR:CB	2.01	0.72
1:O:200:ASP:OD1	1:O:202:LYS:HB2	1.88	0.72
1:O:358:PRO:HG2	1:O:359:TYR:CE2	2.24	0.72
1:O:83:ARG:HB2	4:O:600:GOL:C1	2.06	0.72
1:O:245:ASP:O	1:O:248:ALA:HB3	1.90	0.72
1:Y:17:ARG:HD3	1:Y:32:GLN:HE21	1.54	0.72
1:O:63:VAL:O	1:O:64:LEU:C	2.32	0.72
1:O:84:GLU:HB2	1:O:103:TRP:CB	2.20	0.72
1:Y:91:LYS:HG2	1:Y:92:GLU:N	2.03	0.71
1:Y:363:ALA:C	1:Y:364:ILE:HD13	2.15	0.71
1:O:256:VAL:HG13	1:O:294:PRO:HG3	1.72	0.71
1:Y:84:GLU:CB	1:Y:103:TRP:HB3	2.19	0.71
1:Y:279:ALA:HB2	1:Y:300:TYR:CG	2.25	0.71
1:O:254:LEU:HD11	1:O:445:TYR:HE2	1.55	0.71
1:Y:88:VAL:CG2	1:Y:162:PHE:HB2	2.20	0.71
1:Y:463:LYS:HA	1:Y:463:LYS:CE	2.16	0.71
1:O:253:GLN:CG	1:O:407:ARG:HD2	2.20	0.71
1:O:9:LEU:HD12	1:O:56:GLN:NE2	2.05	0.71
1:O:90:GLU:OE2	1:O:93:THR:HG21	1.91	0.71
1:O:91:LYS:HB2	1:O:161:LEU:CD1	2.21	0.71
1:Y:27:ILE:H	1:Y:27:ILE:CD1	2.03	0.70
1:Y:328:ASP:HB3	1:Y:332:PHE:CE2	2.25	0.70
1:Y:39:TYR:OH	1:O:369:ARG:HD2	1.91	0.70
1:O:203:MET:HA	1:O:206:VAL:CG1	2.20	0.70
1:O:403:LEU:N	1:O:403:LEU:HD12	2.06	0.70
1:Y:31:SER:HB3	1:Y:59:THR:CA	2.20	0.70
1:Y:403:LEU:N	1:Y:403:LEU:HD12	2.05	0.70
1:O:486:TRP:O	1:O:490:VAL:HG23	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:348:PHE:CE1	1:Y:362:GLY:HA3	2.27	0.70
1:Y:467:GLU:HG2	1:Y:468:ARG:N	2.06	0.70
1:Y:422:GLN:O	1:Y:426:LEU:HD22	1.92	0.70
1:Y:230:GLY:HA2	1:Y:235:THR:HB	1.73	0.70
1:O:33:ARG:NH2	1:O:58:TRP:HB3	2.07	0.70
1:O:117:ARG:HH11	1:O:117:ARG:CB	1.98	0.70
1:Y:11:GLN:O	1:Y:81:ASN:HA	1.92	0.70
1:Y:88:VAL:HG22	1:Y:162:PHE:HB2	1.74	0.70
1:O:78:GLY:C	1:O:79:ILE:HG12	2.16	0.70
1:O:388:THR:O	1:O:391:VAL:HG13	1.92	0.70
1:Y:154:ARG:HA	1:Y:157:ARG:HG2	1.72	0.69
1:O:40:PRO:HG3	1:O:46:GLU:OE2	1.91	0.69
1:O:74:ILE:HD11	1:O:237:ILE:HG21	1.74	0.69
1:O:19:VAL:CG1	1:O:21:MET:HE2	2.16	0.69
1:O:385:ALA:HB1	1:O:422:GLN:NE2	2.06	0.69
1:O:492:ARG:HG2	1:O:492:ARG:HH11	1.56	0.69
1:O:77:ILE:HB	1:O:238:PRO:O	1.92	0.69
1:O:451:VAL:HG12	1:O:453:PHE:HB2	1.74	0.69
1:Y:143:TRP:O	1:Y:147:HIS:HB2	1.93	0.69
1:Y:26:ASN:O	1:Y:28:ILE:HD13	1.92	0.69
1:Y:153:GLU:O	1:Y:154:ARG:C	2.32	0.69
1:Y:246:GLN:HG2	1:Y:270:PHE:CB	2.23	0.69
1:O:117:ARG:HB2	1:O:117:ARG:NH1	2.00	0.69
1:O:322:LEU:N	1:O:322:LEU:HD23	2.07	0.69
1:Y:123:TYR:CZ	1:Y:202:LYS:HG3	2.27	0.69
1:Y:207:LEU:HB3	1:Y:209:ILE:HD12	1.73	0.69
1:O:70:SER:H	1:O:73:GLN:HE21	1.41	0.69
1:Y:35:PHE:HB2	1:Y:51:GLU:HG2	1.75	0.68
1:Y:222:GLU:HG2	1:Y:224:TYR:CE1	2.28	0.68
1:Y:115:LEU:HD12	1:Y:115:LEU:H	1.57	0.68
1:Y:317:ARG:O	1:Y:321:LYS:HA	1.93	0.68
1:Y:170:ILE:HG22	1:Y:171:TRP:N	2.07	0.68
1:O:21:MET:HE1	1:O:444:ALA:HB2	1.76	0.68
1:Y:203:MET:HA	1:Y:206:VAL:HG12	1.75	0.68
1:Y:337:GLN:NE2	1:Y:337:GLN:HA	2.09	0.68
1:Y:413:VAL:CA	1:Y:419:MET:HE3	2.20	0.68
1:O:317:ARG:HG2	1:O:318:ASP:N	2.08	0.68
1:Y:271:MET:HG2	1:Y:395:MET:CE	2.23	0.68
1:O:193:ASN:CB	1:O:196:THR:HB	2.24	0.68
1:Y:153:GLU:C	1:Y:157:ARG:HD3	2.18	0.68
1:Y:156:ARG:CZ	1:Y:156:ARG:HB2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:413:VAL:HG12	1:Y:419:MET:HE3	1.76	0.68
1:O:439:THR:HG22	1:O:440:ALA:N	2.07	0.68
1:Y:62:GLU:O	1:Y:63:VAL:C	2.32	0.68
1:Y:169:LEU:O	1:Y:172:LYS:HB2	1.94	0.68
1:O:182:ASP:HB3	1:O:242:ILE:CG2	2.24	0.68
1:Y:124:ILE:HG12	1:Y:203:MET:CE	2.24	0.67
1:O:20:VAL:HG23	1:O:63:VAL:HG11	1.77	0.67
1:O:31:SER:HB2	1:O:63:VAL:CG2	2.25	0.67
1:Y:193:ASN:CB	1:Y:196:THR:HB	2.24	0.67
1:Y:286:LEU:HD11	1:Y:394:ALA:CB	2.25	0.67
1:O:44:TRP:CE2	1:O:107:ARG:HB2	2.30	0.67
1:O:47:HIS:O	1:O:49:PRO:HD3	1.93	0.67
1:O:227:THR:OG1	1:O:239:ILE:HD11	1.94	0.67
1:Y:20:VAL:HG12	1:Y:21:MET:N	2.09	0.67
1:Y:61:VAL:HG12	1:Y:62:GLU:N	2.08	0.67
1:Y:186:ALA:O	1:Y:187:SER:C	2.38	0.67
1:O:226:GLN:HB2	1:O:236:ARG:HD3	1.76	0.67
1:Y:82:GLN:O	1:Y:165:VAL:HG21	1.94	0.67
1:Y:322:LEU:N	1:Y:322:LEU:HD23	2.09	0.67
1:O:33:ARG:HE	1:O:58:TRP:CD1	2.12	0.67
1:Y:392:LEU:HD23	1:Y:393:GLU:N	2.10	0.67
1:Y:20:VAL:O	1:Y:28:ILE:N	2.28	0.67
1:O:113:GLU:O	1:O:116:LYS:HB2	1.95	0.67
1:Y:276:GLY:O	1:Y:300:TYR:N	2.29	0.66
1:O:229:ILE:HG21	1:O:237:ILE:HG12	1.78	0.66
1:Y:47:HIS:O	1:Y:99:ASN:HB3	1.96	0.66
1:Y:197:LEU:HD22	1:Y:197:LEU:N	2.10	0.66
1:O:20:VAL:O	1:O:28:ILE:N	2.29	0.66
1:O:278:LYS:HE3	1:O:280:VAL:HG23	1.77	0.66
1:Y:345:VAL:O	1:Y:362:GLY:HA2	1.96	0.66
1:O:90:GLU:OE1	1:O:95:LYS:HG2	1.94	0.66
1:O:207:LEU:HB3	1:O:209:ILE:CD1	2.26	0.66
1:O:40:PRO:HG2	1:O:44:TRP:HB3	1.77	0.66
1:O:164:THR:O	1:O:167:THR:N	2.29	0.66
1:Y:22:ASP:OD2	1:Y:26:ASN:HB2	1.96	0.66
1:Y:138:GLY:O	1:Y:141:VAL:HG23	1.95	0.66
1:O:3:LYS:HA	1:O:73:GLN:HA	1.77	0.66
1:O:91:LYS:O	1:O:94:GLY:N	2.29	0.66
1:O:181:THR:HG23	1:O:182:ASP:O	1.95	0.66
1:Y:114:HIS:O	1:Y:115:LEU:C	2.39	0.66
1:O:197:LEU:N	1:O:197:LEU:HD22	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:ASP:N	1:O:118:ASP:OD1	2.29	0.66
1:O:468:ARG:HG3	1:O:468:ARG:NH1	2.00	0.66
1:Y:153:GLU:O	1:Y:156:ARG:N	2.29	0.66
1:Y:128:THR:HG21	1:Y:190:MET:HA	1.79	0.65
1:Y:166:ASP:OD2	1:Y:242:ILE:HG21	1.95	0.65
1:O:271:MET:HG2	1:O:395:MET:CE	2.26	0.65
1:Y:179:HIS:CD2	1:Y:215:PRO:HA	2.30	0.65
1:Y:205:GLU:O	1:Y:208:ASP:N	2.30	0.65
1:O:26:ASN:O	1:O:28:ILE:HD13	1.97	0.65
1:O:125:ARG:NH1	1:O:282:SER:O	2.29	0.65
1:O:144:ILE:H	1:O:144:ILE:CD1	2.06	0.65
1:O:478:GLU:HA	1:O:478:GLU:OE1	1.96	0.65
1:Y:19:VAL:HG22	1:Y:30:VAL:HG22	1.79	0.65
1:Y:85:THR:HG23	1:Y:102:VAL:HA	1.78	0.65
1:O:84:GLU:CB	1:O:103:TRP:HB3	2.26	0.65
1:Y:21:MET:HE1	1:Y:444:ALA:CB	2.25	0.65
1:Y:201:ASP:O	1:Y:202:LYS:C	2.38	0.65
1:O:183:TYR:CD1	1:O:217:VAL:HG12	2.31	0.65
1:O:410:GLY:O	1:O:413:VAL:HG13	1.97	0.65
1:Y:91:LYS:O	1:Y:94:GLY:N	2.30	0.65
1:O:81:ASN:N	1:O:81:ASN:HD22	1.95	0.65
1:O:114:HIS:HA	1:O:117:ARG:CZ	2.26	0.65
1:O:352:GLY:O	1:O:355:TYR:N	2.29	0.65
1:Y:58:TRP:O	1:Y:61:VAL:N	2.30	0.65
1:O:152:ARG:HB3	1:O:156:ARG:HH22	1.61	0.65
1:Y:477:THR:O	1:Y:478:GLU:C	2.39	0.65
1:O:65:ALA:O	1:O:67:ALA:N	2.30	0.65
1:O:205:GLU:O	1:O:208:ASP:N	2.29	0.65
1:O:219:ARG:NH2	1:O:295:THR:OG1	2.29	0.65
1:O:489:ALA:O	1:O:492:ARG:N	2.29	0.65
1:O:84:GLU:N	1:O:84:GLU:OE1	2.29	0.65
1:O:88:VAL:HG22	1:O:162:PHE:HB2	1.78	0.65
1:O:137:SER:O	1:O:140:LYS:N	2.30	0.65
1:O:179:HIS:CD2	1:O:215:PRO:HA	2.32	0.65
1:Y:58:TRP:O	1:Y:60:LEU:N	2.30	0.65
1:Y:212:GLU:O	1:Y:214:LEU:N	2.29	0.65
1:O:40:PRO:HG2	1:O:44:TRP:HB2	1.77	0.65
1:Y:4:LYS:N	1:Y:73:GLN:O	2.30	0.65
1:Y:257:LYS:O	1:Y:258:GLU:C	2.39	0.65
1:O:144:ILE:O	1:O:147:HIS:N	2.30	0.65
1:O:420:GLN:NE2	1:O:424:ASP:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:451:VAL:CG1	1:O:453:PHE:HB2	2.26	0.65
1:Y:237:ILE:HG22	1:Y:238:PRO:N	2.12	0.64
1:O:220:SER:HB3	1:O:242:ILE:O	1.97	0.64
1:Y:137:SER:OG	1:Y:189:THR:HA	1.97	0.64
1:Y:420:GLN:NE2	1:Y:424:ASP:OD1	2.30	0.64
1:O:146:ASP:HB3	1:O:152:ARG:NH1	2.11	0.64
1:Y:63:VAL:HA	1:Y:66:LYS:HD3	1.78	0.64
1:O:120:LEU:O	1:O:124:ILE:HG13	1.97	0.64
1:O:171:TRP:CE2	1:O:176:GLY:HA2	2.32	0.64
1:Y:205:GLU:HG2	1:Y:206:VAL:N	2.12	0.64
1:Y:314:GLN:O	1:Y:318:ASP:N	2.29	0.64
1:Y:364:ILE:HD13	1:Y:364:ILE:N	2.13	0.64
1:O:454:TRP:HD1	1:O:459:GLU:CD	2.06	0.64
1:Y:30:VAL:C	1:Y:63:VAL:HG13	2.22	0.64
1:O:31:SER:HB3	1:O:59:THR:HA	1.79	0.64
1:O:46:GLU:O	1:O:47:HIS:ND1	2.30	0.64
1:O:127:ASN:HD22	1:O:193:ASN:HD21	1.46	0.64
1:O:216:GLU:HG2	1:O:218:ARG:HH11	1.62	0.64
1:O:230:GLY:HA2	1:O:235:THR:CB	2.27	0.64
1:O:33:ARG:HE	1:O:58:TRP:CB	2.11	0.64
1:O:183:TYR:CE1	1:O:217:VAL:HG12	2.33	0.64
1:O:87:ILE:HD13	1:O:168:TRP:HB2	1.79	0.64
1:O:142:LYS:HE3	1:O:146:ASP:CG	2.22	0.64
1:Y:3:LYS:HG3	1:Y:72:ASP:O	1.98	0.64
1:Y:109:ALA:O	1:Y:112:CYS:HB2	1.98	0.64
1:Y:124:ILE:CG1	1:Y:203:MET:HE1	2.28	0.64
1:Y:396:GLN:HA	1:Y:399:SER:OG	1.98	0.64
1:Y:130:LEU:HD23	1:Y:130:LEU:N	2.07	0.63
1:Y:157:ARG:HG3	1:Y:159:GLU:OE1	1.98	0.63
1:O:272:LEU:HD11	1:O:303:GLU:CG	2.22	0.63
1:O:394:ALA:O	1:O:395:MET:C	2.41	0.63
1:O:186:ALA:O	1:O:187:SER:C	2.40	0.63
1:O:143:TRP:O	1:O:147:HIS:HB2	1.98	0.63
1:Y:359:TYR:HB3	1:Y:497:GLU:HB3	1.80	0.63
1:O:353:ALA:HB2	1:O:356:TRP:CZ2	2.34	0.63
1:Y:496:TRP:O	1:O:488:LYS:HE2	1.98	0.63
1:O:286:LEU:HD11	1:O:394:ALA:CB	2.29	0.63
1:O:386:TYR:HB3	1:O:486:TRP:CE2	2.33	0.63
1:Y:9:LEU:HD23	1:Y:77:ILE:CG2	2.29	0.63
1:Y:18:ALA:CB	1:Y:63:VAL:HG21	2.29	0.63
1:Y:48:ASP:C	1:Y:52:ILE:HD13	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:229:ILE:CG2	1:Y:237:ILE:HG12	2.23	0.63
1:O:20:VAL:HG12	1:O:21:MET:N	2.14	0.63
1:O:181:THR:HG23	1:O:182:ASP:N	2.13	0.63
1:Y:40:PRO:HG3	1:Y:46:GLU:OE2	1.99	0.63
1:O:80:THR:HG21	1:O:248:ALA:CB	2.27	0.63
1:O:111:ILE:CD1	1:O:142:LYS:HG2	2.29	0.63
1:Y:29:SER:OG	1:Y:63:VAL:HG12	1.99	0.63
1:Y:182:ASP:HA	1:Y:218:ARG:O	1.99	0.63
1:O:11:GLN:O	1:O:81:ASN:HA	1.98	0.63
1:O:88:VAL:HG13	1:O:161:LEU:O	1.99	0.63
1:O:458:ASP:O	1:O:461:GLN:HB2	1.98	0.63
1:O:267:THR:OG1	3:O:601:ACP:H3B1	1.98	0.62
1:O:459:GLU:HB2	1:O:460:LEU:CD1	2.28	0.62
1:Y:257:LYS:O	1:Y:260:MET:HG2	1.98	0.62
1:Y:140:LYS:O	1:Y:144:ILE:HD12	1.99	0.62
1:Y:445:TYR:O	1:Y:446:LEU:C	2.42	0.62
1:Y:14:THR:N	3:Y:601:ACP:O2G	2.30	0.62
1:Y:179:HIS:CE1	1:Y:215:PRO:HB3	2.34	0.62
1:O:67:ALA:HB3	1:O:69:ILE:CD1	2.29	0.62
1:O:179:HIS:O	1:O:216:GLU:N	2.29	0.62
1:Y:478:GLU:HA	1:Y:478:GLU:OE1	1.97	0.62
1:O:142:LYS:O	1:O:143:TRP:C	2.41	0.62
1:O:166:ASP:OD1	1:O:167:THR:N	2.31	0.62
1:O:208:ASP:O	1:O:209:ILE:HG13	1.99	0.62
1:O:438:VAL:HA	1:O:441:LEU:CD1	2.29	0.62
1:O:447:ALA:O	1:O:450:ALA:HB3	2.00	0.62
1:Y:53:TRP:CH2	1:Y:172:LYS:HB3	2.34	0.62
1:Y:120:LEU:HD12	1:Y:120:LEU:N	2.13	0.62
1:Y:144:ILE:O	1:Y:145:LEU:C	2.42	0.62
1:O:455:GLN:O	1:O:455:GLN:HG3	1.99	0.62
1:Y:211:ARG:HH11	1:Y:211:ARG:CG	2.12	0.62
1:Y:337:GLN:HA	1:Y:337:GLN:HE21	1.64	0.62
1:O:193:ASN:CG	1:O:196:THR:HB	2.24	0.62
1:Y:272:LEU:HG	1:Y:303:GLU:HB2	1.81	0.62
1:Y:87:ILE:HG22	1:Y:88:VAL:H	1.65	0.62
1:O:117:ARG:O	1:O:119:GLY:N	2.30	0.62
1:O:164:THR:O	1:O:166:ASP:N	2.32	0.62
1:O:350:GLY:HA2	1:O:360:ALA:O	2.00	0.62
1:O:483:TYR:O	1:O:487:LYS:HG3	2.00	0.62
1:Y:20:VAL:C	1:Y:21:MET:HG3	2.24	0.62
1:Y:488:LYS:HD2	1:O:496:TRP:CH2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:140:LYS:O	1:O:143:TRP:N	2.33	0.62
1:O:182:ASP:CG	1:O:242:ILE:HG22	2.23	0.62
1:O:382:GLU:O	1:O:383:SER:C	2.40	0.62
1:Y:16:SER:HB3	1:Y:56:GLN:HA	1.82	0.61
1:Y:344:VAL:HG22	1:Y:364:ILE:HD12	1.81	0.61
1:O:89:TRP:HB2	1:O:95:LYS:C	2.24	0.61
1:Y:141:VAL:O	1:Y:144:ILE:HB	1.99	0.61
1:Y:310:GLY:O	1:Y:313:ILE:N	2.33	0.61
1:O:105:CYS:SG	1:O:107:ARG:HB3	2.40	0.61
1:O:185:ASN:HD21	1:O:244:GLY:CA	2.12	0.61
1:Y:257:LYS:N	1:Y:260:MET:HG3	2.14	0.61
1:Y:286:LEU:HD11	1:Y:394:ALA:HB1	1.81	0.61
1:O:475:GLU:O	1:O:478:GLU:HB2	2.00	0.61
1:Y:330:GLU:O	1:Y:334:THR:HG23	2.00	0.61
1:O:390:ASP:HA	1:O:483:TYR:OH	2.00	0.61
1:Y:38:ILE:O	1:Y:40:PRO:HD3	2.00	0.61
1:Y:127:ASN:HD22	1:Y:193:ASN:HD21	1.47	0.61
1:Y:287:LEU:HD23	1:Y:287:LEU:N	2.15	0.61
1:O:226:GLN:HB3	1:O:236:ARG:HD3	1.81	0.61
1:Y:81:ASN:N	1:Y:81:ASN:ND2	2.42	0.61
1:Y:156:ARG:C	1:Y:158:GLY:H	2.09	0.61
1:O:279:ALA:HB2	1:O:300:TYR:CD2	2.36	0.61
1:Y:138:GLY:HA2	1:Y:191:LEU:CD2	2.31	0.61
1:O:110:GLU:O	1:O:113:GLU:HB2	2.00	0.61
1:Y:442:GLY:O	1:Y:445:TYR:N	2.33	0.61
1:O:202:LYS:O	1:O:206:VAL:HB	2.00	0.61
1:Y:91:LYS:HZ3	1:Y:91:LYS:HB3	1.66	0.61
1:Y:142:LYS:O	1:Y:145:LEU:N	2.34	0.61
1:O:91:LYS:CB	1:O:161:LEU:HD12	2.29	0.61
1:O:196:THR:HG22	1:O:198:ASP:N	2.16	0.61
1:O:387:GLN:O	1:O:390:ASP:HB2	2.01	0.61
1:Y:152:ARG:CB	1:Y:156:ARG:HH22	2.12	0.60
1:O:63:VAL:CA	1:O:66:LYS:HG2	2.30	0.60
1:O:164:THR:N	1:O:167:THR:HB	2.13	0.60
1:O:213:MET:HG2	1:O:214:LEU:HD12	1.83	0.60
1:Y:123:TYR:OH	1:Y:202:LYS:HG3	2.01	0.60
1:Y:222:GLU:HG3	1:Y:223:VAL:N	2.15	0.60
1:O:29:SER:OG	1:O:30:VAL:N	2.29	0.60
1:O:216:GLU:HG2	1:O:218:ARG:NH1	2.17	0.60
1:O:262:LYS:HD2	1:O:262:LYS:O	2.01	0.60
1:Y:118:ASP:HB2	1:Y:120:LEU:HD11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:179:HIS:CG	1:Y:215:PRO:HB3	2.37	0.60
1:Y:283:GLU:HA	1:Y:283:GLU:OE1	2.00	0.60
1:Y:387:GLN:O	1:Y:391:VAL:HG12	2.01	0.60
1:O:405:ALA:HB1	1:O:431:GLU:OE2	2.01	0.60
1:O:442:GLY:O	1:O:443:ALA:C	2.42	0.60
1:O:123:TYR:CD2	1:O:203:MET:HE2	2.36	0.60
1:Y:179:HIS:ND1	1:Y:215:PRO:HB3	2.16	0.60
1:Y:295:THR:N	1:Y:297:GLU:OE1	2.32	0.60
1:O:85:THR:HA	1:O:101:ILE:O	2.01	0.60
1:O:111:ILE:HD13	1:O:142:LYS:HG2	1.82	0.60
1:O:211:ARG:HG3	1:O:211:ARG:NH1	1.98	0.60
1:O:227:THR:N	1:O:237:ILE:O	2.33	0.60
1:O:279:ALA:HB2	1:O:300:TYR:CE2	2.37	0.60
1:O:297:GLU:OE1	1:O:297:GLU:N	2.28	0.60
1:Y:19:VAL:HG12	1:Y:21:MET:HE2	1.84	0.60
1:Y:87:ILE:HD12	1:Y:163:GLY:O	2.02	0.60
1:Y:262:LYS:NZ	1:Y:264:THR:HB	2.15	0.60
1:O:90:GLU:N	1:O:95:LYS:O	2.29	0.60
1:O:203:MET:CA	1:O:206:VAL:HG12	2.30	0.60
1:Y:35:PHE:CB	1:Y:51:GLU:HG2	2.32	0.60
1:Y:81:ASN:HD22	1:Y:81:ASN:H	1.47	0.60
1:Y:271:MET:C	1:Y:272:LEU:HD12	2.26	0.60
1:Y:275:THR:OG1	1:Y:300:TYR:HB2	2.01	0.60
1:Y:388:THR:O	1:Y:391:VAL:HG13	2.01	0.60
1:O:90:GLU:HB3	1:O:93:THR:CG2	2.31	0.60
1:O:278:LYS:CE	1:O:280:VAL:HG23	2.31	0.60
1:Y:255:CYS:CB	1:Y:260:MET:HB2	2.31	0.59
1:O:84:GLU:HG2	1:O:135:TYR:CD1	2.37	0.59
1:O:180:VAL:HG23	1:O:216:GLU:O	2.02	0.59
1:Y:253:GLN:HE21	1:Y:262:LYS:HB2	1.67	0.59
1:O:130:LEU:O	1:O:131:VAL:HG23	2.02	0.59
1:Y:44:TRP:CZ2	1:Y:107:ARG:HB2	2.37	0.59
1:O:286:LEU:O	1:O:287:LEU:HD23	2.02	0.59
1:Y:46:GLU:O	1:Y:47:HIS:ND1	2.32	0.59
1:Y:164:THR:O	1:Y:165:VAL:C	2.45	0.59
1:Y:183:TYR:HE1	1:Y:217:VAL:HG12	1.62	0.59
1:Y:413:VAL:HG12	1:Y:419:MET:HE1	1.84	0.59
1:Y:20:VAL:HB	1:Y:28:ILE:HB	1.84	0.59
1:Y:62:GLU:O	1:Y:66:LYS:HG2	2.02	0.59
1:Y:203:MET:O	1:Y:206:VAL:HG12	2.03	0.59
1:Y:261:ALA:HB2	1:Y:273:MET:CG	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:423:SER:CB	1:Y:430:VAL:HG23	2.32	0.59
1:O:224:TYR:CZ	1:O:242:ILE:HD12	2.37	0.59
1:O:497:GLU:HA	1:O:497:GLU:OE1	2.01	0.59
1:Y:390:ASP:HA	1:Y:483:TYR:OH	2.02	0.59
1:O:78:GLY:O	1:O:79:ILE:HG12	2.03	0.59
1:O:89:TRP:HB2	1:O:95:LYS:O	2.02	0.59
1:O:254:LEU:CD1	1:O:445:TYR:HE2	2.15	0.59
1:Y:70:SER:H	1:Y:73:GLN:HE21	1.51	0.59
1:Y:123:TYR:CE2	1:Y:203:MET:HE2	2.38	0.59
1:Y:141:VAL:C	1:Y:145:LEU:HD22	2.27	0.59
1:Y:144:ILE:HD12	1:Y:144:ILE:H	1.67	0.59
1:O:83:ARG:CB	4:O:600:GOL:H12	2.07	0.59
1:O:246:GLN:NE2	1:O:246:GLN:N	2.50	0.59
1:O:265:TYR:HE1	1:O:408:VAL:CG1	2.16	0.59
1:Y:22:ASP:OD1	1:Y:24:ASP:N	2.35	0.59
1:Y:123:TYR:HD2	1:Y:203:MET:HE2	1.66	0.59
1:Y:188:ARG:HH21	1:Y:289:THR:HG21	1.67	0.59
1:Y:242:ILE:HG22	1:Y:243:ALA:H	1.67	0.59
1:Y:415:ASN:O	1:Y:419:MET:HG2	2.03	0.59
1:O:27:ILE:H	1:O:27:ILE:CD1	2.01	0.59
1:O:59:THR:O	1:O:63:VAL:HG23	2.03	0.59
1:O:173:MET:HB3	1:O:227:THR:CG2	2.32	0.59
1:O:205:GLU:HG2	1:O:206:VAL:N	2.17	0.59
1:O:229:ILE:CG2	1:O:237:ILE:HG12	2.33	0.59
1:Y:48:ASP:O	1:Y:52:ILE:HD13	2.03	0.59
1:Y:148:VAL:HG12	1:Y:151:SER:OG	2.03	0.59
1:O:5:TYR:O	1:O:75:ALA:N	2.29	0.59
1:Y:240:SER:HB2	1:Y:450:ALA:HB3	1.85	0.58
1:Y:432:ARG:HD2	1:Y:436:ARG:NH2	2.17	0.58
1:O:17:ARG:NH2	1:O:437:GLU:HG3	2.15	0.58
1:O:247:GLN:OE1	1:O:247:GLN:N	2.36	0.58
1:Y:317:ARG:HG2	1:Y:318:ASP:N	2.17	0.58
1:O:415:ASN:ND2	1:O:418:LEU:N	2.34	0.58
1:Y:280:VAL:HG12	1:Y:281:LYS:N	2.19	0.58
1:O:47:HIS:CB	1:O:52:ILE:HD11	2.25	0.58
1:O:87:ILE:HD13	1:O:168:TRP:CB	2.33	0.58
1:O:415:ASN:O	1:O:419:MET:HG2	2.02	0.58
1:O:438:VAL:O	1:O:441:LEU:HB2	2.02	0.58
1:O:47:HIS:O	1:O:99:ASN:HB3	2.03	0.58
1:O:345:VAL:O	1:O:362:GLY:HA2	2.03	0.58
1:O:422:GLN:O	1:O:425:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:170:ILE:O	1:Y:171:TRP:C	2.45	0.58
1:Y:372:ASN:O	1:Y:375:HIS:N	2.36	0.58
1:Y:204:LEU:HD22	1:Y:209:ILE:O	2.04	0.58
1:Y:220:SER:O	1:Y:241:GLY:HA2	2.03	0.58
1:Y:416:ASN:O	1:Y:417:PHE:C	2.46	0.58
1:Y:458:ASP:O	1:Y:461:GLN:HB2	2.03	0.58
1:O:81:ASN:N	1:O:81:ASN:ND2	2.51	0.58
1:Y:118:ASP:OD1	1:Y:118:ASP:N	2.35	0.58
1:Y:325:ASP:O	1:Y:326:ALA:C	2.44	0.58
1:Y:86:THR:HG23	1:Y:162:PHE:HE2	1.68	0.58
1:O:50:MET:O	1:O:53:TRP:HB3	2.04	0.58
1:O:237:ILE:N	1:O:237:ILE:HD13	2.19	0.58
1:Y:31:SER:OG	1:Y:63:VAL:N	2.36	0.58
1:Y:70:SER:O	1:Y:73:GLN:HG3	2.04	0.58
1:Y:104:GLN:CG	1:Y:349:THR:HG21	2.33	0.58
1:Y:293:GLY:N	1:Y:297:GLU:O	2.37	0.58
1:Y:432:ARG:O	1:Y:466:ILE:HG12	2.04	0.58
1:O:115:LEU:H	1:O:115:LEU:CD1	2.14	0.58
1:O:179:HIS:CE1	1:O:215:PRO:HB3	2.39	0.58
1:O:203:MET:O	1:O:207:LEU:N	2.30	0.58
1:Y:193:ASN:HB3	1:Y:196:THR:HG21	1.83	0.57
1:Y:103:TRP:HA	1:Y:140:LYS:HE3	1.86	0.57
1:Y:240:SER:HB2	1:Y:450:ALA:HB1	1.82	0.57
1:O:314:GLN:O	1:O:318:ASP:N	2.37	0.57
1:Y:128:THR:HB	1:Y:130:LEU:HB2	1.86	0.57
1:O:463:LYS:HZ3	1:O:465:VAL:HG23	1.69	0.57
1:Y:492:ARG:HH11	1:Y:492:ARG:CG	2.15	0.57
1:O:78:GLY:HA2	1:O:447:ALA:HB2	1.85	0.57
1:O:83:ARG:HE	4:O:600:GOL:C2	2.16	0.57
1:O:184:THR:HG22	1:O:291:ALA:HA	1.85	0.57
1:Y:104:GLN:HG3	1:Y:349:THR:HG21	1.87	0.57
1:Y:172:LYS:O	1:Y:175:GLN:N	2.38	0.57
1:O:156:ARG:C	1:O:158:GLY:H	2.13	0.57
1:O:198:ASP:C	1:O:199:TRP:O	2.43	0.57
1:O:219:ARG:HG3	1:O:296:GLY:O	2.04	0.57
1:Y:71:SER:HB2	1:Y:235:THR:CG2	2.35	0.57
1:O:423:SER:HB2	1:O:430:VAL:HG23	1.87	0.57
1:Y:154:ARG:HB2	1:Y:159:GLU:HB3	1.86	0.57
1:Y:413:VAL:CB	1:Y:419:MET:HE3	2.34	0.57
1:Y:420:GLN:HE21	1:Y:424:ASP:CG	2.12	0.57
1:O:140:LYS:O	1:O:141:VAL:C	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:185:ASN:O	1:O:188:ARG:HB2	2.05	0.57
1:O:445:TYR:O	1:O:448:GLY:N	2.37	0.57
1:Y:88:VAL:HG22	1:Y:162:PHE:HA	1.87	0.57
1:Y:205:GLU:O	1:Y:206:VAL:C	2.43	0.57
1:O:60:LEU:C	1:O:60:LEU:HD12	2.30	0.56
1:O:230:GLY:HA2	1:O:235:THR:OG1	2.05	0.56
1:O:17:ARG:HG2	1:O:32:GLN:HG2	1.86	0.56
1:Y:53:TRP:CZ2	1:Y:172:LYS:HB3	2.39	0.56
1:Y:110:GLU:O	1:Y:113:GLU:N	2.38	0.56
1:Y:194:ILE:HG13	1:Y:195:HIS:CE1	2.40	0.56
1:Y:453:PHE:HD2	1:Y:454:TRP:CE3	2.23	0.56
1:O:103:TRP:CD1	1:O:103:TRP:H	2.22	0.56
1:O:244:GLY:O	1:O:245:ASP:C	2.44	0.56
1:O:253:GLN:HE21	1:O:262:LYS:HB3	1.68	0.56
1:O:442:GLY:O	1:O:444:ALA:N	2.38	0.56
1:O:468:ARG:HD2	1:O:469:GLU:N	2.20	0.56
1:Y:78:GLY:C	1:Y:79:ILE:HG12	2.29	0.56
1:Y:102:VAL:O	1:Y:103:TRP:C	2.47	0.56
1:Y:137:SER:HA	1:Y:140:LYS:HD2	1.87	0.56
1:Y:192:PHE:CZ	1:Y:197:LEU:HA	2.41	0.56
1:Y:246:GLN:HG2	1:Y:270:PHE:HB2	1.85	0.56
1:Y:271:MET:HG2	1:Y:395:MET:HE2	1.87	0.56
1:Y:496:TRP:CH2	1:O:488:LYS:HD2	2.40	0.56
1:O:85:THR:OG1	1:O:103:TRP:HD1	1.89	0.56
1:O:196:THR:N	1:O:197:LEU:HD22	2.21	0.56
1:Y:110:GLU:O	1:Y:113:GLU:HB2	2.06	0.56
1:Y:181:THR:HG23	1:Y:182:ASP:N	2.21	0.56
1:O:203:MET:O	1:O:206:VAL:HG12	2.05	0.56
1:O:256:VAL:HG13	1:O:294:PRO:CG	2.35	0.56
1:O:154:ARG:O	1:O:159:GLU:HB2	2.05	0.56
1:Y:184:THR:HA	1:Y:290:ILE:HG22	1.88	0.56
1:O:83:ARG:HE	4:O:600:GOL:C1	2.19	0.56
1:Y:78:GLY:HA2	1:Y:447:ALA:HB2	1.88	0.56
1:Y:207:LEU:HB3	1:Y:209:ILE:CD1	2.36	0.56
1:Y:357:ASP:O	1:Y:359:TYR:N	2.39	0.56
1:O:83:ARG:HE	4:O:600:GOL:H12	1.70	0.56
1:O:170:ILE:HG22	1:O:171:TRP:N	2.21	0.56
1:O:183:TYR:CB	1:O:290:ILE:HG21	2.36	0.56
1:O:221:SER:HB3	1:O:295:THR:O	2.06	0.56
1:Y:71:SER:HB2	1:Y:235:THR:HG21	1.87	0.56
1:Y:105:CYS:SG	1:Y:107:ARG:HB3	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:41:LYS:HG3	1:O:42:PRO:CD	2.35	0.56
1:O:130:LEU:HD13	1:O:136:PHE:CD1	2.41	0.56
1:O:251:PHE:CE2	1:O:446:LEU:HD13	2.41	0.56
1:O:484:ALA:O	1:O:487:LYS:N	2.36	0.56
1:Y:262:LYS:HD2	1:Y:262:LYS:O	2.06	0.56
1:O:20:VAL:O	1:O:28:ILE:HB	2.05	0.56
1:O:144:ILE:O	1:O:145:LEU:C	2.49	0.56
1:Y:89:TRP:HB2	1:Y:95:LYS:C	2.32	0.55
1:Y:154:ARG:HG3	1:Y:160:LEU:CD1	2.36	0.55
1:Y:246:GLN:HG2	1:Y:270:PHE:HB3	1.87	0.55
1:Y:441:LEU:HD22	1:Y:445:TYR:HE1	1.67	0.55
1:O:258:GLU:N	1:O:274:ASN:HD22	2.04	0.55
1:O:409:ASP:C	1:O:413:VAL:HG11	2.30	0.55
1:Y:340:ASN:HB2	1:Y:375:HIS:CD2	2.42	0.55
1:Y:352:GLY:O	1:Y:353:ALA:C	2.44	0.55
1:O:44:TRP:HA	1:O:105:CYS:SG	2.46	0.55
1:O:448:GLY:O	1:O:453:PHE:N	2.35	0.55
1:Y:21:MET:HA	1:Y:26:ASN:O	2.06	0.55
1:Y:53:TRP:HA	1:Y:53:TRP:CE3	2.41	0.55
1:Y:111:ILE:HG22	1:Y:115:LEU:HD13	1.88	0.55
1:Y:498:GLU:OE1	1:Y:498:GLU:HA	2.06	0.55
1:O:6:ILE:O	1:O:20:VAL:HG13	2.06	0.55
1:O:115:LEU:HD12	1:O:115:LEU:N	2.11	0.55
1:O:389:ARG:HA	1:O:426:LEU:HD11	1.88	0.55
1:O:425:ILE:HG22	1:O:426:LEU:HD22	1.88	0.55
1:O:430:VAL:O	1:O:469:GLU:HA	2.06	0.55
1:O:445:TYR:O	1:O:446:LEU:C	2.48	0.55
1:O:405:ALA:HA	1:O:429:ARG:O	2.07	0.55
1:Y:40:PRO:HG2	1:Y:44:TRP:HB3	1.87	0.55
1:Y:113:GLU:O	1:Y:116:LYS:HB2	2.06	0.55
1:Y:181:THR:O	1:Y:218:ARG:N	2.30	0.55
1:Y:351:LEU:HB2	1:Y:357:ASP:H	1.72	0.55
1:O:97:ILE:O	1:O:98:TYR:HB2	2.07	0.55
1:Y:227:THR:N	1:Y:237:ILE:O	2.28	0.55
1:Y:265:TYR:HE1	1:Y:408:VAL:CG1	2.19	0.55
1:Y:425:ILE:HD12	1:Y:479:ARG:HG2	1.89	0.55
1:O:254:LEU:HD11	1:O:445:TYR:CE2	2.40	0.55
1:Y:286:LEU:HD11	1:Y:395:MET:N	2.22	0.55
1:Y:392:LEU:O	1:Y:395:MET:HB3	2.07	0.55
1:O:137:SER:O	1:O:139:THR:N	2.39	0.55
1:O:286:LEU:HD11	1:O:394:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:279:ALA:HB2	1:Y:300:TYR:CE2	2.40	0.55
1:Y:445:TYR:O	1:Y:448:GLY:N	2.39	0.55
1:O:430:VAL:O	1:O:470:PHE:N	2.29	0.55
1:Y:404:HIS:O	1:Y:429:ARG:HD2	2.07	0.55
1:O:80:THR:HG22	1:O:245:ASP:N	2.22	0.55
1:Y:18:ALA:HB3	1:Y:63:VAL:HG21	1.87	0.54
1:Y:368:THR:HG23	1:Y:369:ARG:N	2.20	0.54
1:Y:415:ASN:HD22	1:Y:418:LEU:H	1.52	0.54
1:O:463:LYS:NZ	1:O:465:VAL:HG23	2.21	0.54
1:Y:85:THR:OG1	1:Y:103:TRP:HD1	1.90	0.54
1:Y:87:ILE:HD13	1:Y:168:TRP:HB2	1.88	0.54
1:Y:189:THR:HB	1:Y:191:LEU:CG	2.35	0.54
1:Y:344:VAL:CG2	1:Y:364:ILE:HG23	2.37	0.54
1:O:170:ILE:HA	1:O:173:MET:HG3	1.89	0.54
1:O:193:ASN:O	1:O:197:LEU:N	2.40	0.54
1:Y:11:GLN:HE22	1:Y:82:GLN:HE21	1.55	0.54
1:Y:63:VAL:HA	1:Y:66:LYS:CD	2.38	0.54
1:Y:228:ASN:HD21	1:Y:235:THR:N	2.05	0.54
1:Y:424:ASP:OD1	1:Y:473:GLY:N	2.29	0.54
1:O:166:ASP:O	1:O:167:THR:C	2.51	0.54
1:O:200:ASP:O	1:O:201:ASP:C	2.50	0.54
1:O:258:GLU:HA	1:O:274:ASN:O	2.07	0.54
1:O:150:GLY:HA3	1:O:154:ARG:HD2	1.89	0.54
1:O:265:TYR:HE1	1:O:408:VAL:HG12	1.72	0.54
1:O:326:ALA:O	1:O:327:TYR:C	2.49	0.54
1:Y:460:LEU:H	1:Y:460:LEU:CD1	1.98	0.54
1:O:271:MET:CG	1:O:395:MET:HE2	2.35	0.54
1:Y:41:LYS:O	1:Y:44:TRP:HB2	2.08	0.54
1:O:35:PHE:HB2	1:O:51:GLU:CG	2.33	0.54
1:O:162:PHE:HB3	1:O:213:MET:HG3	1.90	0.54
1:Y:53:TRP:HA	1:Y:53:TRP:HE3	1.72	0.54
1:Y:218:ARG:HG3	1:Y:218:ARG:NH1	2.23	0.54
1:O:249:ALA:HB2	1:O:439:THR:OG1	2.07	0.54
1:Y:138:GLY:HA2	1:Y:191:LEU:HD21	1.88	0.54
1:Y:454:TRP:HD1	1:Y:459:GLU:CD	2.15	0.54
1:O:101:ILE:HD13	1:O:107:ARG:CZ	2.37	0.54
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.89	0.54
1:O:420:GLN:HE21	1:O:424:ASP:CG	2.16	0.54
1:Y:38:ILE:O	1:Y:45:VAL:HA	2.08	0.54
1:Y:205:GLU:C	1:Y:208:ASP:H	2.16	0.54
1:Y:449:LEU:HD12	1:Y:449:LEU:C	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:20:VAL:HB	1:O:28:ILE:HB	1.89	0.54
1:O:54:ALA:O	1:O:55:THR:C	2.49	0.54
1:O:142:LYS:HE3	1:O:146:ASP:OD2	2.07	0.54
1:Y:286:LEU:HD21	1:Y:394:ALA:CB	2.37	0.54
1:Y:445:TYR:O	1:Y:447:ALA:N	2.41	0.54
1:O:88:VAL:HA	1:O:161:LEU:O	2.08	0.54
1:O:139:THR:OG1	1:O:140:LYS:N	2.41	0.54
1:Y:203:MET:O	1:Y:207:LEU:HB2	2.08	0.53
1:O:41:LYS:CG	1:O:42:PRO:HD2	2.37	0.53
1:Y:28:ILE:HD13	1:Y:28:ILE:N	2.21	0.53
1:Y:80:THR:HG22	1:Y:243:ALA:O	2.08	0.53
1:Y:86:THR:HG23	1:Y:162:PHE:CE2	2.43	0.53
1:Y:227:THR:O	1:Y:236:ARG:HA	2.08	0.53
1:Y:332:PHE:O	1:Y:335:LYS:HB2	2.09	0.53
1:Y:446:LEU:O	1:Y:450:ALA:HB2	2.08	0.53
1:Y:18:ALA:HB3	1:Y:63:VAL:CG2	2.38	0.53
1:Y:498:GLU:OE2	1:O:488:LYS:HE3	2.08	0.53
1:O:141:VAL:C	1:O:145:LEU:HD22	2.34	0.53
1:O:272:LEU:HD12	1:O:272:LEU:N	2.23	0.53
1:O:280:VAL:HG13	1:O:281:LYS:N	2.23	0.53
1:Y:246:GLN:CG	1:Y:270:PHE:HB2	2.38	0.53
1:Y:422:GLN:HE21	1:Y:426:LEU:HD22	1.74	0.53
1:O:193:ASN:HB3	1:O:196:THR:HG21	1.89	0.53
1:Y:137:SER:O	1:Y:140:LYS:N	2.42	0.53
1:Y:17:ARG:HH22	1:Y:437:GLU:HG3	1.72	0.53
1:O:219:ARG:HG2	1:O:221:SER:H	1.74	0.53
1:O:363:ALA:HB3	1:O:365:PHE:CE1	2.43	0.53
1:Y:127:ASN:ND2	1:Y:193:ASN:HD21	2.06	0.53
1:Y:152:ARG:HB3	1:Y:156:ARG:NH2	2.14	0.53
1:Y:201:ASP:HA	1:Y:204:LEU:HB2	1.91	0.53
1:Y:372:ASN:OD1	1:Y:374:ASN:HB2	2.09	0.53
1:Y:405:ALA:HB1	1:Y:431:GLU:OE2	2.07	0.53
1:Y:451:VAL:O	1:Y:451:VAL:HG13	2.07	0.53
1:O:201:ASP:O	1:O:202:LYS:C	2.52	0.53
1:O:207:LEU:HB3	1:O:209:ILE:HD11	1.89	0.53
1:O:220:SER:HB2	1:O:292:CYS:SG	2.48	0.53
1:O:293:GLY:O	1:O:295:THR:N	2.42	0.53
1:O:387:GLN:O	1:O:388:THR:C	2.51	0.53
1:O:401:ILE:HG22	1:O:402:ARG:N	2.23	0.53
1:Y:111:ILE:CG2	1:Y:115:LEU:HD13	2.39	0.53
1:Y:173:MET:C	1:Y:175:GLN:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:413:VAL:CG1	1:Y:419:MET:HE3	2.39	0.53
1:O:63:VAL:HA	1:O:66:LYS:CG	2.33	0.53
1:Y:416:ASN:OD1	1:Y:432:ARG:NH1	2.30	0.53
1:Y:441:LEU:O	1:Y:444:ALA:HB3	2.09	0.53
1:O:460:LEU:H	1:O:460:LEU:CD1	1.96	0.53
1:O:61:VAL:O	1:O:62:GLU:C	2.51	0.53
1:O:434:GLU:OE1	1:O:465:VAL:HB	2.08	0.53
1:O:490:VAL:O	1:O:494:MET:HG2	2.09	0.53
1:Y:67:ALA:HB3	1:Y:69:ILE:CD1	2.38	0.52
1:Y:128:THR:C	1:Y:130:LEU:H	2.17	0.52
1:O:183:TYR:HB3	1:O:290:ILE:HG21	1.91	0.52
1:Y:423:SER:HB2	1:Y:428:THR:O	2.10	0.52
1:O:253:GLN:NE2	1:O:262:LYS:HB2	2.21	0.52
1:O:263:ASN:HB2	1:O:406:LEU:HD11	1.91	0.52
1:O:451:VAL:O	1:O:452:GLY:C	2.46	0.52
1:O:462:GLU:C	1:O:464:ALA:H	2.15	0.52
1:Y:50:MET:O	1:Y:51:GLU:C	2.51	0.52
1:Y:113:GLU:OE1	1:Y:113:GLU:HA	2.08	0.52
1:Y:124:ILE:CD1	1:Y:203:MET:HE1	2.38	0.52
1:O:123:TYR:HD2	1:O:203:MET:CE	2.22	0.52
1:O:142:LYS:O	1:O:145:LEU:N	2.43	0.52
1:Y:146:ASP:HB3	1:Y:152:ARG:HH12	1.74	0.52
1:Y:193:ASN:CG	1:Y:196:THR:HB	2.33	0.52
1:O:422:GLN:O	1:O:426:LEU:HD22	2.10	0.52
1:Y:22:ASP:O	1:Y:25:ALA:N	2.31	0.52
1:Y:295:THR:HG23	1:Y:297:GLU:OE1	2.09	0.52
1:Y:308:MET:HB2	1:Y:346:PRO:HB2	1.91	0.52
1:Y:483:TYR:O	1:Y:486:TRP:HB3	2.09	0.52
1:O:228:ASN:HD21	1:O:235:THR:N	2.07	0.52
1:O:453:PHE:HD2	1:O:454:TRP:CZ3	2.28	0.52
1:Y:50:MET:O	1:Y:53:TRP:HB3	2.09	0.52
1:Y:164:THR:O	1:Y:167:THR:N	2.42	0.52
1:O:20:VAL:C	1:O:21:MET:HG3	2.34	0.52
1:Y:154:ARG:HA	1:Y:157:ARG:CG	2.40	0.52
1:O:9:LEU:HB2	1:O:79:ILE:HD13	1.91	0.52
1:O:65:ALA:O	1:O:68:ASP:N	2.40	0.52
1:O:154:ARG:HA	1:O:159:GLU:OE1	2.10	0.52
1:Y:151:SER:O	1:Y:153:GLU:N	2.43	0.52
1:Y:172:LYS:O	1:Y:173:MET:C	2.49	0.52
1:O:172:LYS:HD2	1:O:172:LYS:N	2.25	0.52
1:O:415:ASN:HB3	1:O:418:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:108:THR:HG1	1:Y:139:THR:HG1	1.55	0.52
1:O:67:ALA:HB3	1:O:69:ILE:HD12	1.91	0.52
1:Y:87:ILE:HG22	1:Y:88:VAL:N	2.25	0.51
1:Y:130:LEU:HD13	1:Y:136:PHE:CD1	2.45	0.51
1:Y:12:GLY:HA3	3:Y:601:ACP:O3G	2.11	0.51
1:Y:272:LEU:HD11	1:Y:303:GLU:HG3	1.92	0.51
1:O:14:THR:N	3:O:601:ACP:O3G	2.43	0.51
1:O:116:LYS:HG2	1:O:132:ILE:HG21	1.92	0.51
1:O:330:GLU:O	1:O:334:THR:HG23	2.09	0.51
1:Y:16:SER:HB3	1:Y:56:GLN:OE1	2.10	0.51
1:O:80:THR:CG2	1:O:248:ALA:HB2	2.41	0.51
1:O:188:ARG:NH2	1:O:289:THR:HG21	2.21	0.51
1:O:298:VAL:HG12	1:O:299:ASN:N	2.25	0.51
1:Y:423:SER:HB2	1:Y:430:VAL:HG23	1.91	0.51
1:O:38:ILE:O	1:O:40:PRO:HD3	2.11	0.51
1:O:261:ALA:HB2	1:O:273:MET:CG	2.39	0.51
1:O:271:MET:O	1:O:272:LEU:HD12	2.11	0.51
1:Y:130:LEU:HD12	1:Y:190:MET:HB2	1.91	0.51
1:Y:235:THR:O	1:Y:237:ILE:HD13	2.11	0.51
1:O:39:TYR:O	1:O:40:PRO:C	2.53	0.51
1:Y:152:ARG:C	1:Y:155:ALA:HB3	2.36	0.51
1:O:193:ASN:OD1	1:O:196:THR:HB	2.10	0.51
1:O:455:GLN:O	1:O:456:ASN:HB2	2.09	0.51
1:O:484:ALA:O	1:O:485:GLY:C	2.53	0.51
1:Y:33:ARG:NE	1:Y:58:TRP:CE3	2.79	0.51
1:O:218:ARG:HH11	1:O:218:ARG:CG	2.24	0.51
1:O:375:HIS:O	1:O:376:ILE:C	2.50	0.51
1:O:438:VAL:HG12	1:O:439:THR:N	2.24	0.51
1:O:482:ARG:HH11	1:O:482:ARG:CG	2.24	0.51
1:Y:22:ASP:O	1:Y:23:HIS:C	2.51	0.51
1:Y:89:TRP:HB2	1:Y:95:LYS:O	2.10	0.51
1:Y:89:TRP:HD1	1:Y:90:GLU:O	1.93	0.51
1:Y:432:ARG:HB3	1:Y:468:ARG:HB3	1.93	0.51
1:O:154:ARG:O	1:O:159:GLU:N	2.30	0.51
1:Y:115:LEU:HD12	1:Y:115:LEU:N	2.24	0.51
1:Y:179:HIS:CE1	1:Y:215:PRO:HG3	2.46	0.51
1:O:38:ILE:O	1:O:45:VAL:HA	2.10	0.51
1:O:77:ILE:HG22	1:O:239:ILE:HG23	1.93	0.51
1:O:476:THR:O	1:O:477:THR:C	2.51	0.51
1:Y:422:GLN:NE2	1:Y:426:LEU:HD22	2.25	0.51
1:O:41:LYS:CB	1:O:42:PRO:HD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:56:GLN:O	1:O:59:THR:HB	2.11	0.51
1:Y:222:GLU:O	1:Y:240:SER:HA	2.11	0.50
1:O:359:TYR:CZ	1:O:499:HIS:CE1	2.99	0.50
1:Y:91:LYS:HB2	1:Y:161:LEU:CD1	2.34	0.50
1:Y:237:ILE:HD13	1:Y:237:ILE:N	2.26	0.50
1:Y:262:LYS:HD2	1:Y:262:LYS:C	2.36	0.50
1:Y:389:ARG:O	1:Y:390:ASP:C	2.52	0.50
1:Y:456:ASN:O	1:Y:459:GLU:OE2	2.29	0.50
1:Y:491:LYS:O	1:Y:493:ALA:N	2.44	0.50
1:O:114:HIS:CD2	1:O:117:ARG:NH2	2.79	0.50
1:O:137:SER:O	1:O:138:GLY:O	2.29	0.50
1:O:142:LYS:O	1:O:146:ASP:OD1	2.29	0.50
1:O:185:ASN:ND2	1:O:244:GLY:N	2.59	0.50
1:O:283:GLU:HA	1:O:283:GLU:OE1	2.10	0.50
1:O:453:PHE:HD2	1:O:454:TRP:CE3	2.29	0.50
1:Y:242:ILE:HG22	1:Y:243:ALA:N	2.25	0.50
1:O:163:GLY:HA3	1:O:167:THR:HB	1.94	0.50
1:O:182:ASP:OD1	1:O:185:ASN:HB2	2.12	0.50
1:O:428:THR:HG23	1:O:429:ARG:N	2.26	0.50
1:Y:5:TYR:O	1:Y:75:ALA:N	2.33	0.50
1:Y:170:ILE:HA	1:Y:173:MET:HG3	1.93	0.50
1:Y:244:GLY:O	1:Y:245:ASP:C	2.52	0.50
1:Y:253:GLN:HE21	1:Y:262:LYS:CB	2.23	0.50
1:Y:267:THR:CB	3:Y:601:ACP:H3B2	2.42	0.50
1:Y:394:ALA:O	1:Y:395:MET:C	2.52	0.50
1:Y:453:PHE:CD2	1:Y:454:TRP:CZ3	2.99	0.50
1:O:184:THR:HA	1:O:290:ILE:HG22	1.94	0.50
1:O:196:THR:C	1:O:197:LEU:HD22	2.37	0.50
1:Y:12:GLY:O	1:Y:35:PHE:HZ	1.95	0.50
1:Y:63:VAL:O	1:Y:64:LEU:O	2.29	0.50
1:Y:211:ARG:HG3	1:Y:211:ARG:NH1	2.15	0.50
1:Y:257:LYS:CA	1:Y:274:ASN:HD22	2.24	0.50
1:O:95:LYS:HG3	1:O:96:PRO:N	2.25	0.50
1:O:103:TRP:CD1	1:O:103:TRP:N	2.80	0.50
1:O:37:GLN:NE2	1:O:47:HIS:CE1	2.80	0.50
1:O:44:TRP:CE3	1:O:107:ARG:NH2	2.80	0.50
1:O:101:ILE:HD13	1:O:107:ARG:NE	2.26	0.50
1:O:163:GLY:CA	1:O:167:THR:HB	2.42	0.50
1:O:263:ASN:ND2	1:O:265:TYR:CE1	2.80	0.50
1:Y:3:LYS:HG3	1:Y:73:GLN:CA	2.41	0.50
1:Y:3:LYS:HG3	1:Y:73:GLN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:114:HIS:O	1:Y:117:ARG:N	2.44	0.50
1:Y:183:TYR:O	1:Y:184:THR:C	2.55	0.50
1:Y:444:ALA:O	1:Y:445:TYR:O	2.30	0.50
1:O:153:GLU:O	1:O:157:ARG:HD3	2.12	0.50
1:O:310:GLY:HA3	3:O:601:ACP:O3'	2.10	0.50
1:Y:74:ILE:HD11	1:Y:237:ILE:HG21	1.94	0.50
1:Y:257:LYS:H	1:Y:260:MET:CG	2.19	0.50
1:Y:343:TYR:CD2	1:Y:486:TRP:HA	2.47	0.50
1:O:144:ILE:HD12	1:O:144:ILE:N	2.10	0.50
1:O:278:LYS:HD2	1:O:280:VAL:HG23	1.93	0.50
1:O:348:PHE:CD1	1:O:348:PHE:N	2.79	0.50
1:O:386:TYR:HB3	1:O:486:TRP:CD2	2.45	0.50
1:Y:87:ILE:O	1:Y:88:VAL:HG23	2.11	0.50
1:Y:90:GLU:N	1:Y:95:LYS:O	2.36	0.50
1:Y:188:ARG:NH2	1:Y:289:THR:HG21	2.26	0.50
1:Y:212:GLU:C	1:Y:214:LEU:H	2.19	0.50
1:Y:328:ASP:O	1:Y:329:SER:C	2.53	0.50
1:O:44:TRP:N	1:O:44:TRP:CD1	2.79	0.50
1:O:148:VAL:HG12	1:O:151:SER:HB3	1.92	0.50
1:O:198:ASP:O	1:O:199:TRP:O	2.30	0.50
1:Y:44:TRP:CD1	1:Y:44:TRP:N	2.78	0.49
1:Y:114:HIS:N	1:Y:114:HIS:CD2	2.78	0.49
1:Y:121:GLU:O	1:Y:122:ASP:C	2.53	0.49
1:Y:203:MET:CA	1:Y:206:VAL:HG12	2.42	0.49
1:Y:253:GLN:HG3	1:Y:407:ARG:HD2	1.94	0.49
1:O:11:GLN:NE2	1:O:82:GLN:HG2	2.27	0.49
1:O:138:GLY:O	1:O:141:VAL:HG23	2.12	0.49
1:O:237:ILE:CG2	1:O:238:PRO:HD2	2.42	0.49
1:O:457:LEU:HD22	1:O:460:LEU:HD13	1.93	0.49
1:Y:77:ILE:N	1:Y:238:PRO:O	2.45	0.49
1:Y:88:VAL:HG22	1:Y:162:PHE:CB	2.43	0.49
1:Y:298:VAL:O	1:Y:299:ASN:OD1	2.30	0.49
1:Y:344:VAL:HG22	1:Y:364:ILE:HG23	1.94	0.49
1:O:202:LYS:HA	1:O:205:GLU:OE2	2.12	0.49
1:O:275:THR:OG1	1:O:300:TYR:HB2	2.12	0.49
1:O:352:GLY:O	1:O:353:ALA:C	2.51	0.49
1:Y:70:SER:N	1:Y:73:GLN:HE21	2.08	0.49
1:Y:445:TYR:CD2	1:Y:457:LEU:HD11	2.48	0.49
1:O:153:GLU:HA	1:O:156:ARG:NH1	2.27	0.49
1:O:325:ASP:O	1:O:328:ASP:HB2	2.12	0.49
1:O:488:LYS:O	1:O:492:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:229:ILE:HG23	1:Y:237:ILE:CD1	2.43	0.49
1:Y:271:MET:O	1:Y:272:LEU:HD12	2.12	0.49
1:Y:455:GLN:O	1:Y:456:ASN:OD1	2.30	0.49
1:O:22:ASP:OD2	1:O:26:ASN:HB2	2.11	0.49
1:O:83:ARG:HE	4:O:600:GOL:H2	1.78	0.49
1:O:142:LYS:HG3	1:O:143:TRP:N	2.24	0.49
1:O:155:ALA:CB	1:O:210:PRO:HG2	2.38	0.49
1:O:199:TRP:CG	1:O:214:LEU:HD23	2.47	0.49
1:O:389:ARG:O	1:O:390:ASP:C	2.56	0.49
1:Y:29:SER:OG	1:Y:30:VAL:N	2.42	0.49
1:Y:59:THR:O	1:Y:60:LEU:C	2.56	0.49
1:Y:91:LYS:O	1:Y:93:THR:N	2.43	0.49
1:Y:182:ASP:CG	1:Y:242:ILE:HB	2.37	0.49
1:Y:220:SER:O	1:Y:446:LEU:HD23	2.12	0.49
1:Y:256:VAL:CG1	1:Y:294:PRO:HG3	2.42	0.49
1:Y:441:LEU:CD2	1:Y:445:TYR:HE1	2.26	0.49
1:O:123:TYR:CE2	1:O:203:MET:HE2	2.47	0.49
1:Y:31:SER:CB	1:Y:59:THR:HA	2.28	0.49
1:Y:86:THR:HG22	1:Y:87:ILE:N	2.27	0.49
1:Y:324:ASN:N	1:Y:324:ASN:ND2	2.61	0.49
1:O:7:VAL:HG12	1:O:9:LEU:HD22	1.95	0.49
1:O:21:MET:HB3	1:O:26:ASN:O	2.13	0.49
1:O:53:TRP:O	1:O:54:ALA:C	2.56	0.49
1:O:80:THR:C	1:O:81:ASN:HD22	2.20	0.49
1:O:272:LEU:HG	1:O:303:GLU:HB2	1.94	0.49
1:O:422:GLN:NE2	1:O:426:LEU:HD21	2.28	0.49
1:Y:3:LYS:HG3	1:Y:72:ASP:C	2.37	0.49
1:Y:111:ILE:O	1:Y:112:CYS:C	2.50	0.49
1:O:91:LYS:O	1:O:92:GLU:O	2.30	0.49
1:O:108:THR:HG21	1:O:140:LYS:HA	1.95	0.49
1:O:264:THR:HA	1:O:409:ASP:O	2.13	0.49
1:Y:7:VAL:O	1:Y:77:ILE:HA	2.13	0.49
1:Y:8:ALA:HB2	1:Y:21:MET:HE1	1.95	0.49
1:Y:123:TYR:HD2	1:Y:203:MET:CE	2.26	0.49
1:Y:261:ALA:HB2	1:Y:273:MET:HG3	1.94	0.49
1:O:39:TYR:HA	1:O:44:TRP:O	2.12	0.49
1:Y:43:GLY:C	1:Y:44:TRP:HD1	2.20	0.49
1:Y:133:ASP:OD1	1:Y:135:TYR:HB2	2.12	0.49
1:O:48:ASP:O	1:O:51:GLU:N	2.46	0.49
1:Y:69:ILE:HG22	1:Y:70:SER:N	2.28	0.48
1:Y:218:ARG:HH11	1:Y:218:ARG:CG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:261:ALA:HB2	1:Y:273:MET:HG2	1.95	0.48
1:O:91:LYS:HG2	1:O:92:GLU:N	2.26	0.48
1:O:117:ARG:C	1:O:119:GLY:H	2.18	0.48
1:O:196:THR:HG22	1:O:198:ASP:H	1.77	0.48
1:O:219:ARG:HG2	1:O:220:SER:N	2.28	0.48
1:O:451:VAL:O	1:O:451:VAL:HG13	2.11	0.48
1:Y:166:ASP:OD2	1:Y:185:ASN:OD1	2.31	0.48
1:Y:391:VAL:O	1:Y:394:ALA:HB3	2.12	0.48
1:O:122:ASP:O	1:O:126:SER:OG	2.30	0.48
1:Y:185:ASN:O	1:Y:188:ARG:HB2	2.13	0.48
1:O:199:TRP:CD2	1:O:214:LEU:HD23	2.48	0.48
1:O:389:ARG:O	1:O:392:LEU:N	2.46	0.48
1:Y:9:LEU:CD2	1:Y:77:ILE:HG23	2.41	0.48
1:Y:74:ILE:C	1:Y:74:ILE:HD12	2.38	0.48
1:Y:146:ASP:OD1	1:Y:146:ASP:N	2.39	0.48
1:Y:348:PHE:CD1	1:Y:348:PHE:N	2.78	0.48
1:O:65:ALA:C	1:O:67:ALA:H	2.21	0.48
1:O:113:GLU:O	1:O:117:ARG:HD3	2.13	0.48
1:O:481:TYR:O	1:O:484:ALA:HB3	2.13	0.48
1:Y:54:ALA:O	1:Y:57:SER:HB2	2.13	0.48
1:Y:142:LYS:HG3	1:Y:143:TRP:N	2.27	0.48
1:Y:476:THR:O	1:Y:477:THR:C	2.56	0.48
1:O:74:ILE:C	1:O:74:ILE:HD12	2.38	0.48
1:O:93:THR:OG1	1:O:95:LYS:HB3	2.12	0.48
1:O:221:SER:HB2	1:O:296:GLY:HA3	1.92	0.48
1:O:40:PRO:HD2	1:O:44:TRP:O	2.14	0.48
1:O:124:ILE:HG12	1:O:203:MET:CE	2.43	0.48
1:Y:17:ARG:HD3	1:Y:32:GLN:NE2	2.26	0.48
1:Y:17:ARG:HG2	1:Y:32:GLN:HG2	1.95	0.48
1:Y:64:LEU:O	1:Y:65:ALA:C	2.56	0.48
1:Y:110:GLU:O	1:Y:111:ILE:C	2.55	0.48
1:Y:271:MET:HE1	1:Y:392:LEU:HB2	1.95	0.48
1:Y:436:ARG:C	1:Y:438:VAL:H	2.20	0.48
1:Y:484:ALA:O	1:Y:485:GLY:C	2.54	0.48
1:O:132:ILE:O	1:O:133:ASP:HB2	2.11	0.48
1:O:141:VAL:O	1:O:142:LYS:C	2.57	0.48
1:O:150:GLY:HA3	1:O:154:ARG:CD	2.43	0.48
1:O:263:ASN:ND2	1:O:265:TYR:CZ	2.80	0.48
1:Y:8:ALA:C	1:Y:9:LEU:HD22	2.39	0.48
1:Y:489:ALA:O	1:Y:490:VAL:C	2.57	0.48
1:O:257:LYS:O	1:O:258:GLU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:273:MET:HB2	1:O:395:MET:HE3	1.95	0.48
1:Y:222:GLU:HG3	1:Y:223:VAL:H	1.79	0.48
1:Y:439:THR:O	1:Y:440:ALA:C	2.56	0.48
1:O:90:GLU:HB2	1:O:93:THR:OG1	2.14	0.48
1:O:276:GLY:HA2	1:O:299:ASN:HD22	1.77	0.48
1:Y:71:SER:OG	1:Y:230:GLY:O	2.29	0.48
1:Y:227:THR:O	1:Y:237:ILE:N	2.34	0.48
1:O:278:LYS:HG3	1:O:279:ALA:N	2.27	0.48
1:Y:20:VAL:HG12	1:Y:21:MET:H	1.77	0.47
1:Y:91:LYS:HB3	1:Y:91:LYS:NZ	2.16	0.47
1:Y:115:LEU:H	1:Y:115:LEU:CD1	2.26	0.47
1:Y:289:THR:O	1:Y:301:ALA:N	2.43	0.47
1:Y:479:ARG:CG	1:Y:479:ARG:HH11	2.27	0.47
1:O:129:GLY:HA3	1:O:288:THR:HB	1.94	0.47
1:O:140:LYS:O	1:O:144:ILE:HD12	2.14	0.47
1:O:154:ARG:CA	1:O:159:GLU:HB2	2.44	0.47
1:Y:50:MET:O	1:Y:53:TRP:N	2.47	0.47
1:Y:207:LEU:O	1:Y:208:ASP:HB3	2.13	0.47
1:Y:247:GLN:NE2	1:Y:290:ILE:O	2.47	0.47
1:Y:357:ASP:OD2	1:Y:494:MET:HB3	2.14	0.47
1:O:9:LEU:HD13	1:O:9:LEU:HA	1.43	0.47
1:O:118:ASP:HB2	1:O:120:LEU:HD11	1.95	0.47
1:O:257:LYS:C	1:O:274:ASN:HD22	2.21	0.47
1:Y:80:THR:HG21	1:Y:248:ALA:HB2	1.95	0.47
1:Y:140:LYS:O	1:Y:143:TRP:HB3	2.13	0.47
1:Y:179:HIS:O	1:Y:216:GLU:N	2.42	0.47
1:Y:251:PHE:C	1:Y:254:LEU:H	2.21	0.47
1:Y:367:LEU:HD11	1:O:364:ILE:HD13	1.96	0.47
1:Y:408:VAL:O	1:Y:409:ASP:HB3	2.13	0.47
1:Y:468:ARG:HH11	1:Y:468:ARG:HG2	1.78	0.47
1:Y:482:ARG:O	1:Y:483:TYR:C	2.53	0.47
1:O:273:MET:HB2	1:O:395:MET:CE	2.44	0.47
1:O:451:VAL:HG12	1:O:453:PHE:CB	2.44	0.47
1:O:458:ASP:HA	1:O:461:GLN:HB2	1.95	0.47
1:O:460:LEU:C	1:O:462:GLU:H	2.22	0.47
1:Y:203:MET:C	1:Y:206:VAL:HG12	2.40	0.47
1:Y:350:GLY:HA2	1:Y:360:ALA:O	2.14	0.47
1:O:477:THR:O	1:O:478:GLU:C	2.57	0.47
1:Y:40:PRO:HD2	1:Y:44:TRP:C	2.38	0.47
1:O:22:ASP:O	1:O:25:ALA:N	2.43	0.47
1:O:24:ASP:HB3	1:O:26:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.96	0.47
1:O:247:GLN:O	1:O:250:LEU:HB3	2.15	0.47
1:Y:9:LEU:HD13	1:Y:9:LEU:HA	1.67	0.47
1:Y:329:SER:HB2	1:Y:381:LEU:HD11	1.95	0.47
1:Y:421:PHE:O	1:Y:422:GLN:C	2.57	0.47
1:O:31:SER:HB2	1:O:63:VAL:HG23	1.96	0.47
1:O:278:LYS:CD	1:O:280:VAL:HG23	2.44	0.47
1:Y:69:ILE:HD12	1:Y:69:ILE:H	1.80	0.47
1:Y:117:ARG:HB2	1:Y:117:ARG:CZ	2.42	0.47
1:Y:154:ARG:HG3	1:Y:160:LEU:HD11	1.96	0.47
1:Y:174:THR:O	1:Y:175:GLN:C	2.55	0.47
1:Y:310:GLY:O	1:Y:313:ILE:HB	2.15	0.47
1:Y:342:VAL:HA	1:Y:365:PHE:O	2.15	0.47
1:Y:343:TYR:CE2	1:Y:486:TRP:CA	2.98	0.47
1:Y:356:TRP:O	1:Y:358:PRO:HD3	2.15	0.47
1:Y:415:ASN:ND2	1:Y:417:PHE:HB3	2.25	0.47
1:Y:415:ASN:HD22	1:Y:415:ASN:C	2.23	0.47
1:Y:418:LEU:HA	1:Y:418:LEU:HD23	1.73	0.47
1:Y:438:VAL:HA	1:Y:441:LEU:HD12	1.96	0.47
1:O:24:ASP:O	1:O:25:ALA:HB3	2.15	0.47
1:O:77:ILE:CG2	1:O:79:ILE:HD11	2.44	0.47
1:O:103:TRP:HB2	1:O:135:TYR:CE1	2.50	0.47
1:O:127:ASN:HB3	1:O:193:ASN:ND2	2.30	0.47
1:O:130:LEU:HD12	1:O:190:MET:HB2	1.97	0.47
1:O:152:ARG:C	1:O:155:ALA:HB3	2.39	0.47
1:O:257:LYS:O	1:O:258:GLU:O	2.32	0.47
1:O:382:GLU:O	1:O:384:ILE:N	2.48	0.47
1:O:419:MET:O	1:O:420:GLN:C	2.52	0.47
1:Y:169:LEU:O	1:Y:173:MET:HG2	2.14	0.47
1:Y:201:ASP:O	1:Y:204:LEU:N	2.48	0.47
1:Y:428:THR:HG23	1:Y:429:ARG:N	2.30	0.47
1:O:40:PRO:HD2	1:O:44:TRP:C	2.40	0.47
1:O:158:GLY:H	1:O:212:GLU:HG2	1.78	0.47
1:O:404:HIS:O	1:O:429:ARG:HD2	2.15	0.47
1:O:466:ILE:HD13	1:O:466:ILE:C	2.39	0.47
1:Y:24:ASP:O	1:Y:25:ALA:HB3	2.14	0.47
1:O:95:LYS:HG3	1:O:96:PRO:O	2.14	0.47
1:O:120:LEU:O	1:O:121:GLU:C	2.57	0.47
1:O:482:ARG:NH1	1:O:482:ARG:HG3	2.30	0.47
1:O:185:ASN:HD21	1:O:244:GLY:HA2	1.79	0.47
1:O:468:ARG:HH11	1:O:468:ARG:CG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:84:GLU:OE1	4:Y:600:GOL:O1	2.30	0.46
1:Y:403:LEU:N	1:Y:403:LEU:CD1	2.78	0.46
1:O:148:VAL:CG1	1:O:151:SER:HB3	2.45	0.46
1:O:185:ASN:HD21	1:O:244:GLY:N	2.13	0.46
1:O:351:LEU:HD12	1:O:351:LEU:HA	1.74	0.46
1:Y:70:SER:O	1:Y:71:SER:C	2.59	0.46
1:Y:180:VAL:CG2	1:Y:181:THR:N	2.78	0.46
1:Y:253:GLN:O	1:Y:254:LEU:HB2	2.15	0.46
1:Y:392:LEU:HD23	1:Y:393:GLU:HG2	1.96	0.46
1:O:74:ILE:HD12	1:O:76:ALA:N	2.30	0.46
1:O:117:ARG:HD3	1:O:117:ARG:H	1.81	0.46
1:O:378:ARG:O	1:O:379:ALA:C	2.57	0.46
1:O:439:THR:O	1:O:442:GLY:N	2.48	0.46
1:Y:18:ALA:HB1	1:Y:63:VAL:HG21	1.97	0.46
1:Y:343:TYR:CE2	1:Y:486:TRP:HA	2.51	0.46
1:Y:351:LEU:HB3	1:Y:355:TYR:HB2	1.97	0.46
1:O:184:THR:O	1:O:187:SER:HB3	2.16	0.46
1:O:374:ASN:O	1:O:375:HIS:C	2.58	0.46
1:O:487:LYS:O	1:O:488:LYS:C	2.58	0.46
1:Y:5:TYR:O	1:Y:74:ILE:HA	2.15	0.46
1:Y:104:GLN:HG2	1:Y:349:THR:HG21	1.97	0.46
1:Y:203:MET:HA	1:Y:206:VAL:CG1	2.42	0.46
1:Y:237:ILE:N	1:Y:237:ILE:CD1	2.78	0.46
1:Y:256:VAL:HG12	1:Y:294:PRO:HG3	1.98	0.46
1:Y:438:VAL:O	1:Y:441:LEU:HB2	2.16	0.46
1:Y:457:LEU:HA	1:Y:460:LEU:CD1	2.39	0.46
1:O:158:GLY:N	1:O:212:GLU:HG2	2.30	0.46
1:O:284:ASN:OD1	1:O:398:ASP:OD1	2.34	0.46
1:Y:170:ILE:CD1	1:Y:170:ILE:N	2.79	0.46
1:Y:422:GLN:NE2	1:Y:426:LEU:CD2	2.78	0.46
1:Y:453:PHE:HD2	1:Y:454:TRP:CZ3	2.34	0.46
1:Y:468:ARG:HH11	1:Y:468:ARG:CG	2.27	0.46
1:O:124:ILE:HG12	1:O:203:MET:HE1	1.96	0.46
1:O:145:LEU:N	1:O:145:LEU:HD13	2.26	0.46
1:O:224:TYR:CE2	1:O:242:ILE:HD12	2.51	0.46
1:O:245:ASP:OD1	1:O:246:GLN:NE2	2.48	0.46
1:O:311:ALA:O	1:O:312:SER:C	2.59	0.46
1:O:435:VAL:CG2	1:O:436:ARG:N	2.79	0.46
1:Y:88:VAL:HG22	1:Y:162:PHE:CA	2.46	0.46
1:Y:114:HIS:O	1:Y:116:LYS:N	2.48	0.46
1:Y:435:VAL:HG21	1:Y:441:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:TYR:N	1:O:73:GLN:O	2.44	0.46
1:O:77:ILE:CG2	1:O:239:ILE:HG23	2.45	0.46
1:O:78:GLY:HA3	1:O:443:ALA:O	2.15	0.46
1:O:85:THR:HG23	1:O:102:VAL:HA	1.97	0.46
1:O:86:THR:C	1:O:87:ILE:HG13	2.40	0.46
1:O:154:ARG:HA	1:O:159:GLU:HB2	1.97	0.46
1:O:163:GLY:HA2	1:O:167:THR:HG21	1.98	0.46
1:O:172:LYS:O	1:O:175:GLN:N	2.40	0.46
1:O:269:CYS:HB2	1:O:306:VAL:HB	1.96	0.46
1:O:316:LEU:HA	1:O:316:LEU:HD23	1.26	0.46
1:O:347:ALA:O	1:O:361:ARG:HA	2.16	0.46
1:O:489:ALA:O	1:O:490:VAL:C	2.59	0.46
1:Y:181:THR:CG2	1:Y:182:ASP:N	2.79	0.46
1:O:52:ILE:O	1:O:55:THR:OG1	2.34	0.46
1:O:70:SER:O	1:O:73:GLN:HG3	2.16	0.46
1:O:142:LYS:CG	1:O:143:TRP:N	2.79	0.46
1:Y:22:ASP:OD1	1:Y:25:ALA:N	2.49	0.46
1:Y:47:HIS:O	1:Y:49:PRO:HD3	2.16	0.46
1:Y:64:LEU:HB2	1:Y:65:ALA:H	1.54	0.46
1:Y:104:GLN:NE2	1:Y:308:MET:CE	2.79	0.46
1:Y:466:ILE:HD13	1:Y:466:ILE:C	2.41	0.46
1:O:5:TYR:O	1:O:74:ILE:HA	2.16	0.46
1:O:11:GLN:NE2	1:O:82:GLN:HE21	2.14	0.46
1:O:33:ARG:HE	1:O:58:TRP:HB3	1.80	0.46
1:O:111:ILE:O	1:O:112:CYS:C	2.58	0.46
1:O:113:GLU:OE1	1:O:113:GLU:HA	2.14	0.46
1:O:317:ARG:O	1:O:321:LYS:HA	2.15	0.46
1:Y:50:MET:O	1:Y:52:ILE:N	2.49	0.46
1:Y:120:LEU:O	1:Y:124:ILE:HG13	2.16	0.46
1:Y:254:LEU:O	1:Y:256:VAL:N	2.48	0.46
1:O:88:VAL:CG2	1:O:162:PHE:HB2	2.46	0.46
1:O:145:LEU:HB3	1:O:152:ARG:CZ	2.46	0.46
1:O:347:ALA:O	1:O:348:PHE:C	2.58	0.46
1:Y:57:SER:O	1:Y:60:LEU:HD23	2.16	0.45
1:Y:222:GLU:HG2	1:Y:224:TYR:CD1	2.52	0.45
1:Y:441:LEU:HA	1:Y:441:LEU:HD23	1.67	0.45
1:Y:482:ARG:NH1	1:Y:482:ARG:HG3	2.30	0.45
1:O:161:LEU:CD2	1:O:179:HIS:CE1	2.99	0.45
1:O:179:HIS:CD2	1:O:215:PRO:CA	2.99	0.45
1:O:467:GLU:OE2	1:O:468:ARG:HB2	2.15	0.45
1:Y:101:ILE:HD13	1:Y:107:ARG:NE	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:193:ASN:OD1	1:Y:196:THR:HB	2.16	0.45
1:Y:284:ASN:OD1	1:Y:398:ASP:OD1	2.34	0.45
1:Y:375:HIS:O	1:Y:376:ILE:C	2.57	0.45
1:O:78:GLY:HA2	1:O:241:GLY:HA3	1.97	0.45
1:O:179:HIS:CG	1:O:215:PRO:HB3	2.52	0.45
1:O:199:TRP:HB3	1:O:204:LEU:HD11	1.98	0.45
1:O:251:PHE:CE2	1:O:446:LEU:CD1	2.98	0.45
1:O:117:ARG:HD3	1:O:117:ARG:N	2.31	0.45
1:O:191:LEU:HD23	1:O:207:LEU:CD1	2.46	0.45
1:O:230:GLY:HA2	1:O:235:THR:HB	1.98	0.45
1:O:285:GLY:O	1:O:356:TRP:NE1	2.39	0.45
1:O:309:ALA:O	1:O:312:SER:OG	2.30	0.45
1:O:310:GLY:O	1:O:313:ILE:N	2.49	0.45
1:O:401:ILE:CG2	1:O:402:ARG:N	2.79	0.45
1:O:405:ALA:HB1	1:O:431:GLU:CD	2.42	0.45
1:Y:80:THR:HG21	1:Y:248:ALA:CB	2.47	0.45
1:Y:264:THR:CG2	1:Y:265:TYR:N	2.79	0.45
1:Y:423:SER:HB3	1:Y:430:VAL:HG23	1.98	0.45
1:Y:461:GLN:HE21	1:Y:461:GLN:HB3	1.56	0.45
1:O:145:LEU:HD12	1:O:145:LEU:HA	1.54	0.45
1:O:214:LEU:N	1:O:214:LEU:CD1	2.79	0.45
1:O:251:PHE:O	1:O:254:LEU:HD12	2.16	0.45
1:O:298:VAL:O	1:O:299:ASN:OD1	2.35	0.45
1:O:372:ASN:O	1:O:373:ALA:C	2.59	0.45
1:Y:161:LEU:CD2	1:Y:179:HIS:NE2	2.80	0.45
1:Y:206:VAL:CG1	1:Y:207:LEU:N	2.79	0.45
1:Y:295:THR:HG23	1:Y:297:GLU:CD	2.42	0.45
1:Y:425:ILE:HD12	1:Y:425:ILE:HA	1.53	0.45
1:O:218:ARG:NH1	1:O:218:ARG:CG	2.79	0.45
1:O:438:VAL:CA	1:O:441:LEU:HD12	2.41	0.45
1:O:494:MET:O	1:O:495:ALA:HB3	2.15	0.45
1:Y:53:TRP:CE3	1:Y:53:TRP:CA	3.00	0.45
1:Y:179:HIS:CE1	1:Y:215:PRO:CB	3.00	0.45
1:Y:256:VAL:N	1:Y:260:MET:HG3	2.31	0.45
1:Y:428:THR:CG2	1:Y:429:ARG:N	2.80	0.45
1:O:8:ALA:O	1:O:9:LEU:HD13	2.16	0.45
1:O:13:THR:HB	3:O:601:ACP:O3G	2.16	0.45
1:O:86:THR:CG2	1:O:162:PHE:CE2	2.99	0.45
1:O:153:GLU:O	1:O:156:ARG:N	2.49	0.45
1:O:183:TYR:CD2	1:O:298:VAL:CG2	2.99	0.45
1:Y:3:LYS:HA	1:Y:73:GLN:CA	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:466:ILE:HD13	1:Y:466:ILE:O	2.17	0.45
1:O:33:ARG:NE	1:O:58:TRP:HB3	2.32	0.45
1:O:105:CYS:SG	1:O:107:ARG:NH1	2.89	0.45
1:O:184:THR:OG1	1:O:243:ALA:HA	2.17	0.45
1:O:406:LEU:CD2	1:O:407:ARG:N	2.79	0.45
1:O:480:ASN:O	1:O:481:TYR:C	2.58	0.45
1:Y:130:LEU:HB3	1:Y:131:VAL:H	1.41	0.45
1:Y:435:VAL:CG2	1:Y:436:ARG:N	2.79	0.45
1:O:71:SER:OG	1:O:230:GLY:O	2.30	0.45
1:O:180:VAL:CG2	1:O:181:THR:N	2.80	0.45
1:O:257:LYS:CA	1:O:274:ASN:HD22	2.30	0.45
1:Y:230:GLY:CA	1:Y:235:THR:HB	2.44	0.45
1:Y:426:LEU:HD12	1:Y:426:LEU:HA	1.71	0.45
1:O:33:ARG:CZ	1:O:58:TRP:HB3	2.47	0.45
1:O:428:THR:CG2	1:O:429:ARG:N	2.79	0.45
1:Y:79:ILE:HD11	1:Y:239:ILE:HG23	1.98	0.45
1:Y:142:LYS:O	1:Y:145:LEU:HB2	2.17	0.45
1:Y:312:SER:O	1:Y:315:TRP:HB3	2.17	0.45
1:O:11:GLN:HE22	1:O:82:GLN:HG2	1.82	0.45
1:O:265:TYR:CE1	1:O:408:VAL:CG1	2.99	0.45
1:Y:102:VAL:O	1:Y:104:GLN:N	2.50	0.44
1:Y:149:GLU:OE1	1:Y:149:GLU:HA	2.17	0.44
1:Y:309:ALA:O	1:Y:312:SER:OG	2.32	0.44
1:Y:478:GLU:O	1:Y:481:TYR:N	2.50	0.44
1:Y:488:LYS:O	1:Y:492:ARG:HD3	2.17	0.44
1:O:208:ASP:C	1:O:209:ILE:HG13	2.41	0.44
1:O:237:ILE:N	1:O:237:ILE:CD1	2.80	0.44
1:O:422:GLN:NE2	1:O:426:LEU:CD2	2.79	0.44
1:O:463:LYS:NZ	1:O:465:VAL:CG2	2.80	0.44
1:Y:214:LEU:N	1:Y:214:LEU:CD1	2.79	0.44
1:Y:495:ALA:O	1:O:492:ARG:NH2	2.50	0.44
1:O:3:LYS:HG3	1:O:72:ASP:O	2.17	0.44
1:O:146:ASP:OD1	1:O:146:ASP:N	2.38	0.44
1:Y:70:SER:H	1:Y:73:GLN:HG3	1.82	0.44
1:Y:142:LYS:O	1:Y:146:ASP:OD1	2.35	0.44
1:Y:148:VAL:CG1	1:Y:149:GLU:N	2.80	0.44
1:Y:222:GLU:CG	1:Y:223:VAL:N	2.80	0.44
1:O:20:VAL:C	1:O:28:ILE:HB	2.43	0.44
1:O:37:GLN:HB3	1:O:39:TYR:CZ	2.52	0.44
1:O:37:GLN:HE22	1:O:47:HIS:CE1	2.34	0.44
1:O:186:ALA:HB2	1:O:217:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:357:ASP:OD1	1:O:358:PRO:HD2	2.17	0.44
1:Y:31:SER:HB2	1:Y:63:VAL:CG2	2.20	0.44
1:Y:56:GLN:HG3	1:Y:56:GLN:O	2.18	0.44
1:Y:130:LEU:HD13	1:Y:136:PHE:CE1	2.52	0.44
1:O:41:LYS:CG	1:O:42:PRO:N	2.81	0.44
1:O:60:LEU:HD12	1:O:60:LEU:O	2.16	0.44
1:O:83:ARG:NH1	1:O:246:GLN:HB2	2.33	0.44
1:O:173:MET:HB3	1:O:173:MET:HE2	1.79	0.44
1:Y:228:ASN:HD22	1:Y:230:GLY:N	2.16	0.44
1:O:203:MET:C	1:O:206:VAL:HG12	2.43	0.44
1:O:302:LEU:HD23	1:O:302:LEU:HA	1.62	0.44
1:O:415:ASN:ND2	1:O:417:PHE:HB3	2.15	0.44
1:Y:41:LYS:HB2	1:Y:42:PRO:HD2	2.00	0.44
1:Y:154:ARG:CA	1:Y:159:GLU:HB2	2.47	0.44
1:Y:255:CYS:HA	1:Y:260:MET:CB	2.47	0.44
1:Y:265:TYR:N	1:Y:409:ASP:O	2.51	0.44
1:Y:434:GLU:HB2	1:Y:465:VAL:O	2.17	0.44
1:Y:480:ASN:O	1:Y:481:TYR:C	2.60	0.44
1:O:23:HIS:C	1:O:25:ALA:H	2.26	0.44
1:O:298:VAL:CG1	1:O:299:ASN:N	2.81	0.44
1:O:400:GLY:C	1:O:401:ILE:HG13	2.42	0.44
1:Y:150:GLY:O	1:Y:151:SER:C	2.60	0.44
1:Y:200:ASP:OD1	1:Y:202:LYS:HB2	2.18	0.44
1:Y:253:GLN:CG	1:Y:407:ARG:HD2	2.47	0.44
1:Y:257:LYS:CA	1:Y:274:ASN:ND2	2.81	0.44
1:Y:272:LEU:N	1:Y:272:LEU:CD1	2.80	0.44
1:O:21:MET:HA	1:O:26:ASN:O	2.18	0.44
1:O:124:ILE:O	1:O:125:ARG:C	2.61	0.44
1:O:130:LEU:HD13	1:O:136:PHE:CG	2.52	0.44
1:O:205:GLU:O	1:O:206:VAL:C	2.60	0.44
1:O:278:LYS:O	1:O:278:LYS:HG2	2.09	0.44
1:Y:52:ILE:O	1:Y:53:TRP:C	2.61	0.44
1:Y:74:ILE:HD12	1:Y:75:ALA:N	2.32	0.44
1:Y:97:ILE:H	1:Y:97:ILE:HG13	1.66	0.44
1:Y:218:ARG:NH1	1:Y:218:ARG:CG	2.79	0.44
1:Y:271:MET:HG2	1:Y:271:MET:O	2.13	0.44
1:Y:279:ALA:CB	1:Y:300:TYR:CG	2.99	0.44
1:O:183:TYR:O	1:O:187:SER:N	2.37	0.44
1:Y:111:ILE:O	1:Y:115:LEU:HD13	2.18	0.44
1:Y:120:LEU:O	1:Y:121:GLU:C	2.61	0.44
1:Y:172:LYS:HA	1:Y:172:LYS:HD2	1.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:TYR:CE2	1:O:28:ILE:HG13	2.53	0.44
1:O:148:VAL:CG1	1:O:149:GLU:N	2.80	0.44
1:O:185:ASN:ND2	1:O:244:GLY:CA	2.79	0.44
1:O:354:PRO:HD2	1:O:355:TYR:CE2	2.53	0.44
1:O:442:GLY:O	1:O:445:TYR:N	2.51	0.44
1:O:474:ILE:HD12	1:O:474:ILE:HA	1.79	0.44
1:Y:166:ASP:O	1:Y:167:THR:C	2.58	0.43
1:Y:270:PHE:CZ	4:Y:600:GOL:H11	2.53	0.43
1:Y:348:PHE:N	1:Y:348:PHE:HD1	2.14	0.43
1:Y:445:TYR:HD2	1:Y:457:LEU:HD11	1.81	0.43
1:O:169:LEU:HD13	1:O:169:LEU:HA	1.39	0.43
1:O:278:LYS:HG3	1:O:279:ALA:C	2.43	0.43
1:O:416:ASN:O	1:O:417:PHE:C	2.61	0.43
1:O:453:PHE:CD2	1:O:454:TRP:CZ3	3.05	0.43
1:O:482:ARG:CG	1:O:482:ARG:NH1	2.79	0.43
1:Y:16:SER:CB	1:Y:56:GLN:HA	2.48	0.43
1:Y:48:ASP:O	1:Y:49:PRO:C	2.62	0.43
1:Y:88:VAL:HA	1:Y:161:LEU:O	2.17	0.43
1:O:192:PHE:CZ	1:O:197:LEU:HA	2.53	0.43
1:O:246:GLN:H	1:O:246:GLN:HE21	1.65	0.43
1:O:394:ALA:O	1:O:397:ALA:N	2.51	0.43
1:Y:91:LYS:NZ	1:Y:91:LYS:CB	2.79	0.43
1:Y:161:LEU:HD22	1:Y:179:HIS:CE1	2.52	0.43
1:Y:286:LEU:O	1:Y:287:LEU:HD23	2.17	0.43
1:O:84:GLU:HG2	1:O:135:TYR:O	2.19	0.43
1:O:109:ALA:HA	1:O:134:PRO:HG3	2.01	0.43
1:O:114:HIS:O	1:O:117:ARG:N	2.51	0.43
1:O:123:TYR:OH	1:O:200:ASP:OD2	2.31	0.43
1:O:182:ASP:OD1	1:O:242:ILE:HG22	2.17	0.43
1:O:185:ASN:O	1:O:186:ALA:C	2.60	0.43
1:Y:482:ARG:HH11	1:Y:482:ARG:CG	2.30	0.43
1:O:28:ILE:N	1:O:28:ILE:HD13	2.32	0.43
1:O:129:GLY:C	1:O:130:LEU:HD23	2.43	0.43
1:O:219:ARG:HD3	1:O:221:SER:O	2.18	0.43
1:Y:41:LYS:CB	1:Y:42:PRO:HD2	2.48	0.43
1:Y:83:ARG:HE	1:Y:83:ARG:HB2	1.64	0.43
1:Y:199:TRP:CE2	1:Y:214:LEU:HD23	2.53	0.43
1:Y:302:LEU:HD23	1:Y:302:LEU:HA	1.33	0.43
1:Y:468:ARG:CG	1:Y:468:ARG:NH1	2.80	0.43
1:O:363:ALA:HB3	1:O:365:PHE:HE1	1.81	0.43
1:O:385:ALA:CB	1:O:422:GLN:NE2	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:443:ALA:O	1:O:444:ALA:O	2.35	0.43
1:Y:91:LYS:HZ3	1:Y:91:LYS:CB	2.29	0.43
1:Y:151:SER:O	1:Y:155:ALA:N	2.46	0.43
1:O:21:MET:C	1:O:28:ILE:HG12	2.43	0.43
1:O:33:ARG:NE	1:O:58:TRP:CB	2.80	0.43
1:O:84:GLU:OE1	1:O:103:TRP:HB3	2.19	0.43
1:O:182:ASP:HB3	1:O:242:ILE:HG21	1.99	0.43
1:Y:13:THR:N	3:Y:601:ACP:O2G	2.52	0.43
1:Y:343:TYR:HE2	1:Y:486:TRP:HB2	1.83	0.43
1:Y:478:GLU:O	1:Y:479:ARG:C	2.61	0.43
1:O:204:LEU:HD23	1:O:204:LEU:HA	1.48	0.43
1:O:251:PHE:CD1	1:O:256:VAL:HG21	2.54	0.43
1:O:310:GLY:O	1:O:311:ALA:C	2.61	0.43
1:Y:74:ILE:HD12	1:Y:76:ALA:N	2.33	0.43
1:Y:475:GLU:O	1:Y:478:GLU:HB2	2.19	0.43
1:O:171:TRP:NE1	1:O:176:GLY:HA2	2.33	0.43
1:O:409:ASP:CA	1:O:413:VAL:HG11	2.49	0.43
1:O:457:LEU:HD22	1:O:457:LEU:HA	1.39	0.43
1:O:460:LEU:O	1:O:462:GLU:N	2.52	0.43
1:Y:179:HIS:CD2	1:Y:215:PRO:CA	2.99	0.43
1:Y:286:LEU:HD21	1:Y:394:ALA:HB3	2.01	0.43
1:Y:293:GLY:O	1:Y:295:THR:N	2.52	0.43
1:Y:433:PRO:O	1:Y:436:ARG:NH1	2.52	0.43
1:Y:35:PHE:HB2	1:Y:51:GLU:CG	2.47	0.43
1:Y:38:ILE:HG22	1:Y:40:PRO:HD3	2.01	0.43
1:Y:154:ARG:HA	1:Y:159:GLU:HB2	2.01	0.43
1:Y:179:HIS:CE1	1:Y:215:PRO:CG	3.02	0.43
1:Y:193:ASN:O	1:Y:197:LEU:N	2.52	0.43
1:Y:199:TRP:HZ2	1:Y:215:PRO:O	2.01	0.43
1:Y:45:VAL:O	1:Y:102:VAL:HG23	2.19	0.42
1:Y:144:ILE:HG22	1:Y:145:LEU:N	2.24	0.42
1:Y:153:GLU:H	1:Y:153:GLU:HG2	1.68	0.42
1:Y:251:PHE:CD2	1:Y:446:LEU:HD12	2.54	0.42
1:Y:325:ASP:O	1:Y:328:ASP:N	2.51	0.42
1:Y:420:GLN:O	1:Y:421:PHE:C	2.61	0.42
1:Y:467:GLU:OE2	1:Y:468:ARG:HB2	2.18	0.42
1:Y:478:GLU:O	1:Y:481:TYR:HB3	2.19	0.42
1:O:144:ILE:O	1:O:147:HIS:HB2	2.19	0.42
1:O:228:ASN:HB2	1:O:236:ARG:CZ	2.49	0.42
1:O:276:GLY:O	1:O:300:TYR:N	2.52	0.42
1:Y:128:THR:C	1:Y:130:LEU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:130:LEU:CD1	1:Y:136:PHE:CD1	3.01	0.42
1:Y:401:ILE:HG22	1:Y:402:ARG:N	2.34	0.42
1:O:86:THR:HG23	1:O:162:PHE:CE2	2.54	0.42
1:O:154:ARG:H	1:O:154:ARG:HG2	1.34	0.42
1:O:415:ASN:ND2	1:O:418:LEU:HB2	2.33	0.42
1:O:457:LEU:O	1:O:458:ASP:C	2.60	0.42
1:O:460:LEU:C	1:O:462:GLU:N	2.78	0.42
1:Y:229:ILE:HG23	1:Y:237:ILE:HD13	2.01	0.42
1:O:183:TYR:CD2	1:O:298:VAL:HG22	2.55	0.42
1:O:251:PHE:CE1	1:O:256:VAL:HG21	2.55	0.42
1:Y:3:LYS:HZ2	1:Y:75:ALA:HA	1.85	0.42
1:Y:63:VAL:O	1:Y:64:LEU:C	2.62	0.42
1:Y:129:GLY:C	1:Y:130:LEU:HD23	2.44	0.42
1:Y:372:ASN:OD1	1:Y:374:ASN:N	2.52	0.42
1:Y:440:ALA:O	1:Y:441:LEU:C	2.62	0.42
1:Y:479:ARG:HH11	1:Y:479:ARG:HG3	1.83	0.42
1:O:7:VAL:HG12	1:O:9:LEU:CD2	2.49	0.42
1:O:114:HIS:O	1:O:115:LEU:C	2.61	0.42
1:O:154:ARG:C	1:O:159:GLU:HB2	2.45	0.42
1:O:228:ASN:C	1:O:228:ASN:HD22	2.28	0.42
1:O:262:LYS:HA	1:O:407:ARG:O	2.19	0.42
1:O:487:LYS:O	1:O:491:LYS:HG3	2.20	0.42
1:Y:79:ILE:HD11	1:Y:239:ILE:CG2	2.49	0.42
1:Y:204:LEU:O	1:Y:209:ILE:N	2.39	0.42
1:Y:242:ILE:O	1:Y:243:ALA:HB2	2.19	0.42
1:O:173:MET:C	1:O:227:THR:HG23	2.44	0.42
1:O:205:GLU:C	1:O:208:ASP:H	2.25	0.42
1:O:286:LEU:HD11	1:O:395:MET:N	2.35	0.42
1:O:436:ARG:C	1:O:438:VAL:H	2.27	0.42
1:Y:28:ILE:HD12	1:Y:28:ILE:HA	1.79	0.42
1:Y:273:MET:HB2	1:Y:395:MET:CE	2.50	0.42
1:O:102:VAL:H	1:O:102:VAL:HG23	1.50	0.42
1:O:265:TYR:CE1	1:O:408:VAL:HG11	2.55	0.42
1:O:308:MET:HB2	1:O:346:PRO:HB2	2.00	0.42
1:Y:133:ASP:C	1:Y:135:TYR:H	2.28	0.42
1:Y:154:ARG:O	1:Y:155:ALA:O	2.38	0.42
1:Y:169:LEU:HA	1:Y:169:LEU:HD12	1.57	0.42
1:Y:280:VAL:HG12	1:Y:281:LYS:H	1.83	0.42
1:O:70:SER:O	1:O:72:ASP:N	2.53	0.42
1:O:84:GLU:HG2	1:O:135:TYR:CE1	2.55	0.42
1:O:84:GLU:CD	1:O:135:TYR:CE1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:246:GLN:NE2	1:O:246:GLN:H	2.16	0.42
1:O:486:TRP:CD1	1:O:487:LYS:HG2	2.54	0.42
1:Y:67:ALA:CB	1:Y:69:ILE:CD1	2.98	0.42
1:Y:214:LEU:N	1:Y:214:LEU:HD12	2.33	0.42
1:Y:347:ALA:O	1:Y:362:GLY:N	2.52	0.42
1:O:87:ILE:HD11	1:O:165:VAL:N	2.34	0.42
1:O:101:ILE:HD13	1:O:107:ARG:CD	2.50	0.42
1:O:432:ARG:HA	1:O:433:PRO:HD2	1.84	0.42
1:O:445:TYR:O	1:O:447:ALA:N	2.53	0.42
1:O:457:LEU:HA	1:O:460:LEU:HD13	2.00	0.42
1:Y:81:ASN:ND2	1:Y:81:ASN:H	2.12	0.42
1:Y:95:LYS:HA	1:Y:96:PRO:HD3	1.92	0.42
1:Y:155:ALA:HB1	1:Y:210:PRO:HG2	2.01	0.42
1:O:13:THR:O	1:O:13:THR:HG22	2.19	0.42
1:O:50:MET:O	1:O:53:TRP:N	2.53	0.42
1:O:193:ASN:HB3	1:O:196:THR:HG22	1.95	0.42
1:O:338:ASN:OD1	1:O:340:ASN:N	2.43	0.42
1:Y:251:PHE:C	1:Y:253:GLN:H	2.26	0.42
1:Y:309:ALA:HA	1:Y:384:ILE:HD13	2.02	0.42
1:O:109:ALA:O	1:O:112:CYS:HB2	2.20	0.42
1:O:114:HIS:CD2	1:O:117:ARG:HH22	2.38	0.42
1:O:262:LYS:HD2	1:O:262:LYS:C	2.45	0.42
1:O:422:GLN:HG3	1:O:426:LEU:HD23	2.00	0.42
1:Y:20:VAL:CG1	1:Y:21:MET:N	2.80	0.41
1:Y:154:ARG:H	1:Y:154:ARG:HG2	1.41	0.41
1:Y:173:MET:HB3	1:Y:173:MET:HE2	1.69	0.41
1:Y:364:ILE:N	1:Y:364:ILE:CD1	2.83	0.41
1:O:84:GLU:N	1:O:84:GLU:CD	2.78	0.41
1:O:246:GLN:NE2	1:O:246:GLN:CA	2.80	0.41
1:Y:21:MET:CE	1:Y:444:ALA:HB2	2.32	0.41
1:Y:355:TYR:O	1:Y:356:TRP:HB2	2.20	0.41
1:Y:453:PHE:CE2	1:Y:454:TRP:CZ3	3.08	0.41
1:Y:482:ARG:NH1	1:Y:482:ARG:CG	2.80	0.41
1:O:3:LYS:HD2	1:O:72:ASP:O	2.20	0.41
1:O:154:ARG:HA	1:O:157:ARG:HG2	2.02	0.41
1:O:272:LEU:CD1	1:O:272:LEU:N	2.82	0.41
1:Y:128:THR:HB	1:Y:130:LEU:H	1.85	0.41
1:Y:180:VAL:HA	1:Y:216:GLU:O	2.20	0.41
1:Y:237:ILE:CG2	1:Y:238:PRO:N	2.80	0.41
1:O:82:GLN:OE1	1:O:102:VAL:HG13	2.21	0.41
1:O:207:LEU:HB3	1:O:209:ILE:HD12	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:494:MET:HE3	1:O:494:MET:HB3	1.62	0.41
1:Y:32:GLN:C	1:Y:33:ARG:HG2	2.44	0.41
1:Y:328:ASP:O	1:Y:332:PHE:HD2	2.03	0.41
1:Y:492:ARG:CG	1:Y:492:ARG:NH1	2.80	0.41
1:O:124:ILE:CD1	1:O:203:MET:CE	2.98	0.41
1:O:406:LEU:HD22	1:O:407:ARG:N	2.35	0.41
1:Y:286:LEU:CD1	1:Y:394:ALA:HB1	2.47	0.41
1:Y:313:ILE:O	1:Y:314:GLN:C	2.61	0.41
1:Y:348:PHE:CD1	1:Y:362:GLY:HA3	2.55	0.41
1:O:199:TRP:HZ2	1:O:215:PRO:O	2.02	0.41
1:O:245:ASP:OD1	1:O:246:GLN:N	2.54	0.41
1:O:251:PHE:CE2	1:O:446:LEU:HB2	2.55	0.41
1:Y:144:ILE:O	1:Y:147:HIS:N	2.53	0.41
1:Y:272:LEU:CD1	1:Y:303:GLU:HG3	2.50	0.41
1:Y:376:ILE:HD12	1:Y:376:ILE:HA	1.69	0.41
1:Y:449:LEU:HD13	1:Y:449:LEU:HA	1.55	0.41
1:O:21:MET:HE1	1:O:444:ALA:CB	2.48	0.41
1:O:44:TRP:CE3	1:O:107:ARG:CZ	3.04	0.41
1:O:150:GLY:O	1:O:151:SER:C	2.63	0.41
1:O:183:TYR:HA	1:O:186:ALA:HB3	2.03	0.41
1:O:203:MET:O	1:O:204:LEU:C	2.63	0.41
1:O:286:LEU:HD11	1:O:394:ALA:HB1	2.00	0.41
1:O:372:ASN:OD1	1:O:374:ASN:N	2.54	0.41
1:O:389:ARG:HB2	1:O:426:LEU:HD13	2.03	0.41
1:Y:124:ILE:C	1:Y:126:SER:N	2.78	0.41
1:Y:250:LEU:CD1	1:Y:255:CYS:HB2	2.51	0.41
1:Y:251:PHE:O	1:Y:254:LEU:HD12	2.20	0.41
1:Y:320:MET:O	1:Y:321:LYS:HB2	2.20	0.41
1:Y:488:LYS:HD3	1:O:496:TRP:CZ3	2.56	0.41
1:O:123:TYR:CE2	1:O:202:LYS:CB	3.04	0.41
1:O:343:TYR:CE1	1:O:486:TRP:HB2	2.55	0.41
1:O:410:GLY:O	1:O:413:VAL:HG22	2.20	0.41
1:Y:77:ILE:O	1:Y:239:ILE:HA	2.21	0.41
1:Y:142:LYS:HE3	1:Y:146:ASP:OD2	2.21	0.41
1:Y:256:VAL:CG1	1:Y:294:PRO:CG	2.99	0.41
1:Y:436:ARG:C	1:Y:438:VAL:N	2.78	0.41
1:Y:452:GLY:C	1:Y:454:TRP:N	2.78	0.41
1:O:65:ALA:C	1:O:67:ALA:N	2.78	0.41
1:O:296:GLY:N	1:O:297:GLU:OE1	2.53	0.41
1:Y:22:ASP:CG	1:Y:26:ASN:HD22	2.28	0.41
1:Y:83:ARG:N	4:Y:600:GOL:O2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:127:ASN:CB	1:Y:193:ASN:ND2	2.79	0.41
1:Y:154:ARG:HG3	1:Y:160:LEU:HD12	2.02	0.41
1:Y:154:ARG:CB	1:Y:159:GLU:CB	2.99	0.41
1:Y:183:TYR:CD1	1:Y:183:TYR:N	2.79	0.41
1:Y:183:TYR:CD1	1:Y:217:VAL:CG1	3.00	0.41
1:Y:188:ARG:HH21	1:Y:289:THR:CG2	2.33	0.41
1:Y:219:ARG:O	1:Y:224:TYR:OH	2.27	0.41
1:Y:310:GLY:O	1:Y:311:ALA:C	2.63	0.41
1:Y:401:ILE:CG2	1:Y:402:ARG:N	2.84	0.41
1:Y:434:GLU:N	1:Y:465:VAL:O	2.54	0.41
1:Y:457:LEU:C	1:Y:459:GLU:N	2.77	0.41
1:Y:474:ILE:HA	1:Y:474:ILE:HD12	1.73	0.41
1:O:20:VAL:HG23	1:O:63:VAL:CG1	2.50	0.41
1:O:98:TYR:CD1	1:O:99:ASN:N	2.89	0.41
1:O:133:ASP:OD1	1:O:135:TYR:N	2.43	0.41
1:O:151:SER:HA	1:O:160:LEU:CD1	2.51	0.41
1:O:213:MET:HG2	1:O:214:LEU:CD1	2.49	0.41
1:O:255:CYS:SG	1:O:260:MET:HB3	2.61	0.41
1:O:270:PHE:CD1	1:O:270:PHE:N	2.89	0.41
1:O:290:ILE:CG2	1:O:291:ALA:N	2.80	0.41
1:O:315:TRP:O	1:O:316:LEU:C	2.63	0.41
1:O:394:ALA:O	1:O:398:ASP:N	2.41	0.41
1:Y:23:HIS:C	1:Y:25:ALA:N	2.77	0.41
1:Y:133:ASP:C	1:Y:135:TYR:N	2.79	0.41
1:Y:142:LYS:O	1:Y:144:ILE:N	2.54	0.41
1:Y:152:ARG:CB	1:Y:156:ARG:NH2	2.80	0.41
1:O:9:LEU:CD1	1:O:18:ALA:CB	2.99	0.41
1:O:102:VAL:C	1:O:104:GLN:N	2.79	0.41
1:O:168:TRP:O	1:O:172:LYS:HG2	2.20	0.41
1:O:173:MET:HE2	1:O:227:THR:HG21	2.03	0.41
1:O:254:LEU:O	1:O:256:VAL:N	2.54	0.41
1:O:348:PHE:CE1	1:O:362:GLY:HA3	2.56	0.41
1:Y:269:CYS:C	1:Y:270:PHE:CG	3.00	0.40
1:Y:334:THR:HG23	1:Y:334:THR:H	1.49	0.40
1:Y:357:ASP:C	1:Y:359:TYR:N	2.79	0.40
1:Y:382:GLU:O	1:Y:383:SER:C	2.63	0.40
1:O:257:LYS:H	1:O:260:MET:HG3	1.86	0.40
1:O:271:MET:HE2	1:O:271:MET:HB2	1.70	0.40
1:Y:277:GLU:O	1:Y:300:TYR:HE2	2.04	0.40
1:O:222:GLU:HG3	1:O:223:VAL:N	2.36	0.40
1:O:314:GLN:O	1:O:315:TRP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:344:VAL:O	1:O:346:PRO:HD3	2.20	0.40
1:Y:48:ASP:O	1:Y:52:ILE:N	2.41	0.40
1:Y:54:ALA:O	1:Y:57:SER:N	2.49	0.40
1:Y:123:TYR:CD2	1:Y:203:MET:CE	3.00	0.40
1:Y:316:LEU:HA	1:Y:316:LEU:HD23	1.27	0.40
1:Y:351:LEU:HD22	1:Y:360:ALA:CB	2.52	0.40
1:Y:439:THR:O	1:Y:442:GLY:N	2.55	0.40
1:O:38:ILE:HG22	1:O:40:PRO:N	2.36	0.40
1:O:115:LEU:O	1:O:120:LEU:HD12	2.22	0.40
1:O:135:TYR:CD1	1:O:135:TYR:C	3.00	0.40
1:O:194:ILE:C	1:O:196:THR:H	2.30	0.40
1:Y:381:LEU:HD23	1:Y:381:LEU:HA	1.85	0.40
1:Y:422:GLN:NE2	1:Y:422:GLN:HA	2.37	0.40
1:Y:453:PHE:CD2	1:Y:454:TRP:CE3	3.07	0.40
1:Y:458:ASP:C	1:Y:461:GLN:HB2	2.46	0.40
1:O:41:LYS:CB	1:O:42:PRO:CD	2.99	0.40
1:O:166:ASP:CG	1:O:167:THR:N	2.80	0.40
1:O:181:THR:HG22	1:O:217:VAL:HG13	2.02	0.40
1:O:462:GLU:C	1:O:464:ALA:N	2.79	0.40
1:Y:121:GLU:O	1:Y:124:ILE:N	2.55	0.40
1:Y:124:ILE:CD1	1:Y:203:MET:CE	3.00	0.40
1:Y:162:PHE:O	1:Y:215:PRO:HD3	2.21	0.40
1:Y:251:PHE:O	1:Y:254:LEU:HA	2.22	0.40
1:Y:324:ASN:ND2	1:Y:324:ASN:H	2.19	0.40
1:Y:432:ARG:HG2	1:Y:436:ARG:NH1	2.37	0.40
1:O:44:TRP:CD2	1:O:107:ARG:HB2	2.56	0.40
1:O:228:ASN:HB2	1:O:236:ARG:NH2	2.37	0.40
1:O:336:VAL:HG11	1:O:375:HIS:CD2	2.56	0.40
1:O:347:ALA:HB2	1:O:351:LEU:HD13	2.03	0.40
1:O:389:ARG:HB2	1:O:426:LEU:CD1	2.50	0.40
1:O:422:GLN:HG3	1:O:426:LEU:CD2	2.51	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	490/501 (98%)	341 (70%)	102 (21%)	47 (10%)	0	2
1	Y	490/501 (98%)	354 (72%)	87 (18%)	49 (10%)	0	2
All	All	980/1002 (98%)	695 (71%)	189 (19%)	96 (10%)	0	2

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	58	TRP
1	Y	59	THR
1	Y	64	LEU
1	Y	151	SER
1	Y	165	VAL
1	Y	212	GLU
1	Y	213	MET
1	Y	445	TYR
1	Y	446	LEU
1	Y	456	ASN
1	O	66	LYS
1	O	165	VAL
1	O	187	SER
1	O	199	TRP
1	O	258	GLU
1	O	443	ALA
1	O	445	TYR
1	O	446	LEU
1	Y	53	TRP
1	Y	65	ALA
1	Y	92	GLU
1	Y	172	LYS
1	Y	187	SER
1	Y	188	ARG
1	Y	196	THR
1	Y	202	LYS
1	Y	358	PRO
1	Y	439	THR
1	Y	461	GLN
1	Y	477	THR
1	O	64	LEU
1	O	71	SER
1	O	99	ASN

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Mol	Chain	Res	Type
1	O	118	ASP
1	O	119	GLY
1	O	138	GLY
1	O	141	VAL
1	O	172	LYS
1	O	188	ARG
1	O	276	GLY
1	O	294	PRO
1	O	444	ALA
1	O	456	ASN
1	Y	54	ALA
1	Y	61	VAL
1	Y	121	GLU
1	Y	130	LEU
1	Y	138	GLY
1	Y	143	TRP
1	Y	153	GLU
1	Y	199	TRP
1	Y	441	LEU
1	Y	459	GLU
1	Y	478	GLU
1	Y	492	ARG
1	O	143	TRP
1	O	201	ASP
1	O	212	GLU
1	O	213	MET
1	O	390	ASP
1	O	442	GLY
1	O	461	GLN
1	Y	71	SER
1	Y	99	ASN
1	Y	147	HIS
1	Y	175	GLN
1	Y	418	LEU
1	O	55	THR
1	O	140	LYS
1	O	151	SER
1	O	202	LYS
1	Y	110	GLU
1	Y	142	LYS
1	Y	145	LEU
1	Y	298	VAL

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Mol	Chain	Res	Type
1	O	63	VAL
1	O	92	GLU
1	O	111	ILE
1	O	121	GLU
1	O	145	LEU
1	O	242	ILE
1	O	298	VAL
1	O	418	LEU
1	O	459	GLU
1	O	110	GLU
1	O	114	HIS
1	O	131	VAL
1	O	157	ARG
1	Y	27	ILE
1	Y	238	PRO
1	Y	346	PRO
1	Y	411	GLY
1	O	490	VAL
1	Y	170	ILE
1	Y	490	VAL
1	O	144	ILE

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	408/412 (99%)	245 (60%)	163 (40%)	0	1
1	Y	408/412 (99%)	244 (60%)	164 (40%)	0	1
All	All	816/824 (99%)	489 (60%)	327 (40%)	0	1

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	2	GLU
1	Y	3	LYS

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Mol	Chain	Res	Type
1	Y	4	LYS
1	Y	9	LEU
1	Y	11	GLN
1	Y	13	THR
1	Y	20	VAL
1	Y	21	MET
1	Y	24	ASP
1	Y	27	ILE
1	Y	28	ILE
1	Y	32	GLN
1	Y	33	ARG
1	Y	34	GLU
1	Y	41	LYS
1	Y	45	VAL
1	Y	46	GLU
1	Y	53	TRP
1	Y	57	SER
1	Y	60	LEU
1	Y	62	GLU
1	Y	63	VAL
1	Y	64	LEU
1	Y	71	SER
1	Y	73	GLN
1	Y	74	ILE
1	Y	77	ILE
1	Y	79	ILE
1	Y	80	THR
1	Y	81	ASN
1	Y	87	ILE
1	Y	91	LYS
1	Y	92	GLU
1	Y	93	THR
1	Y	95	LYS
1	Y	97	ILE
1	Y	107	ARG
1	Y	116	LYS
1	Y	117	ARG
1	Y	118	ASP
1	Y	120	LEU
1	Y	124	ILE
1	Y	128	THR
1	Y	130	LEU

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Mol	Chain	Res	Type
1	Y	131	VAL
1	Y	137	SER
1	Y	139	THR
1	Y	141	VAL
1	Y	142	LYS
1	Y	145	LEU
1	Y	146	ASP
1	Y	147	HIS
1	Y	148	VAL
1	Y	149	GLU
1	Y	151	SER
1	Y	152	ARG
1	Y	153	GLU
1	Y	154	ARG
1	Y	156	ARG
1	Y	157	ARG
1	Y	162	PHE
1	Y	164	THR
1	Y	165	VAL
1	Y	169	LEU
1	Y	170	ILE
1	Y	172	LYS
1	Y	173	MET
1	Y	175	GLN
1	Y	178	VAL
1	Y	180	VAL
1	Y	181	THR
1	Y	187	SER
1	Y	191	LEU
1	Y	195	HIS
1	Y	196	THR
1	Y	197	LEU
1	Y	201	ASP
1	Y	205	GLU
1	Y	211	ARG
1	Y	213	MET
1	Y	218	ARG
1	Y	222	GLU
1	Y	226	GLN
1	Y	227	THR
1	Y	228	ASN
1	Y	229	ILE

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Mol	Chain	Res	Type
1	Y	235	THR
1	Y	236	ARG
1	Y	237	ILE
1	Y	239	ILE
1	Y	240	SER
1	Y	242	ILE
1	Y	246	GLN
1	Y	253	GLN
1	Y	257	LYS
1	Y	260	MET
1	Y	264	THR
1	Y	271	MET
1	Y	273	MET
1	Y	278	LYS
1	Y	281	LYS
1	Y	287	LEU
1	Y	290	ILE
1	Y	295	THR
1	Y	302	LEU
1	Y	312	SER
1	Y	314	GLN
1	Y	317	ARG
1	Y	322	LEU
1	Y	324	ASN
1	Y	325	ASP
1	Y	335	LYS
1	Y	339	THR
1	Y	344	VAL
1	Y	351	LEU
1	Y	364	ILE
1	Y	368	THR
1	Y	369	ARG
1	Y	376	ILE
1	Y	383	SER
1	Y	384	ILE
1	Y	389	ARG
1	Y	390	ASP
1	Y	391	VAL
1	Y	392	LEU
1	Y	393	GLU
1	Y	402	ARG
1	Y	406	LEU

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Mol	Chain	Res	Type
1	Y	407	ARG
1	Y	409	ASP
1	Y	415	ASN
1	Y	418	LEU
1	Y	423	SER
1	Y	425	ILE
1	Y	426	LEU
1	Y	428	THR
1	Y	429	ARG
1	Y	430	VAL
1	Y	431	GLU
1	Y	434	GLU
1	Y	435	VAL
1	Y	436	ARG
1	Y	437	GLU
1	Y	438	VAL
1	Y	445	TYR
1	Y	446	LEU
1	Y	449	LEU
1	Y	451	VAL
1	Y	455	GLN
1	Y	457	LEU
1	Y	461	GLN
1	Y	462	GLU
1	Y	463	LYS
1	Y	465	VAL
1	Y	466	ILE
1	Y	467	GLU
1	Y	468	ARG
1	Y	469	GLU
1	Y	474	ILE
1	Y	479	ARG
1	Y	482	ARG
1	Y	488	LYS
1	Y	492	ARG
1	Y	494	MET
1	O	3	LYS
1	O	4	LYS
1	O	5	TYR
1	O	9	LEU
1	O	11	GLN
1	O	20	VAL

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Mol	Chain	Res	Type
1	O	21	MET
1	O	24	ASP
1	O	27	ILE
1	O	28	ILE
1	O	29	SER
1	O	31	SER
1	O	32	GLN
1	O	33	ARG
1	O	34	GLU
1	O	41	LYS
1	O	45	VAL
1	O	51	GLU
1	O	52	ILE
1	O	57	SER
1	O	60	LEU
1	O	64	LEU
1	O	70	SER
1	O	71	SER
1	O	73	GLN
1	O	74	ILE
1	O	77	ILE
1	O	79	ILE
1	O	80	THR
1	O	81	ASN
1	O	82	GLN
1	O	86	THR
1	O	87	ILE
1	O	91	LYS
1	O	92	GLU
1	O	93	THR
1	O	95	LYS
1	O	102	VAL
1	O	106	ARG
1	O	107	ARG
1	O	117	ARG
1	O	118	ASP
1	O	124	ILE
1	O	125	ARG
1	O	128	THR
1	O	130	LEU
1	O	131	VAL
1	O	137	SER

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Mol	Chain	Res	Type
1	O	139	THR
1	O	141	VAL
1	O	142	LYS
1	O	144	ILE
1	O	145	LEU
1	O	147	HIS
1	O	149	GLU
1	O	152	ARG
1	O	153	GLU
1	O	154	ARG
1	O	156	ARG
1	O	157	ARG
1	O	161	LEU
1	O	162	PHE
1	O	164	THR
1	O	165	VAL
1	O	169	LEU
1	O	170	ILE
1	O	172	LYS
1	O	173	MET
1	O	178	VAL
1	O	180	VAL
1	O	181	THR
1	O	182	ASP
1	O	191	LEU
1	O	195	HIS
1	O	196	THR
1	O	201	ASP
1	O	205	GLU
1	O	206	VAL
1	O	211	ARG
1	O	213	MET
1	O	214	LEU
1	O	218	ARG
1	O	219	ARG
1	O	222	GLU
1	O	223	VAL
1	O	227	THR
1	O	228	ASN
1	O	229	ILE
1	O	235	THR
1	O	236	ARG

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Mol	Chain	Res	Type
1	O	237	ILE
1	O	239	ILE
1	O	240	SER
1	O	246	GLN
1	O	247	GLN
1	O	253	GLN
1	O	256	VAL
1	O	260	MET
1	O	269	CYS
1	O	271	MET
1	O	273	MET
1	O	278	LYS
1	O	280	VAL
1	O	281	LYS
1	O	290	ILE
1	O	295	THR
1	O	314	GLN
1	O	316	LEU
1	O	317	ARG
1	O	322	LEU
1	O	324	ASN
1	O	325	ASP
1	O	335	LYS
1	O	339	THR
1	O	351	LEU
1	O	364	ILE
1	O	368	THR
1	O	369	ARG
1	O	378	ARG
1	O	380	THR
1	O	383	SER
1	O	389	ARG
1	O	391	VAL
1	O	392	LEU
1	O	393	GLU
1	O	402	ARG
1	O	406	LEU
1	O	407	ARG
1	O	413	VAL
1	O	418	LEU
1	O	423	SER
1	O	425	ILE

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Mol	Chain	Res	Type
1	O	426	LEU
1	O	428	THR
1	O	429	ARG
1	O	430	VAL
1	O	434	GLU
1	O	435	VAL
1	O	436	ARG
1	O	437	GLU
1	O	438	VAL
1	O	439	THR
1	O	441	LEU
1	O	451	VAL
1	O	455	GLN
1	O	457	LEU
1	O	460	LEU
1	O	461	GLN
1	O	462	GLU
1	O	463	LYS
1	O	465	VAL
1	O	466	ILE
1	O	467	GLU
1	O	468	ARG
1	O	469	GLU
1	O	474	ILE
1	O	476	THR
1	O	478	GLU
1	O	482	ARG
1	O	486	TRP
1	O	488	LYS
1	O	492	ARG
1	O	494	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	11	GLN
1	Y	23	HIS
1	Y	26	ASN
1	Y	32	GLN
1	Y	73	GLN
1	Y	81	ASN
1	Y	104	GLN

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Mol	Chain	Res	Type
1	Y	114	HIS
1	Y	127	ASN
1	Y	147	HIS
1	Y	185	ASN
1	Y	228	ASN
1	Y	246	GLN
1	Y	253	GLN
1	Y	274	ASN
1	Y	284	ASN
1	Y	299	ASN
1	Y	324	ASN
1	Y	337	GLN
1	Y	415	ASN
1	Y	420	GLN
1	Y	422	GLN
1	Y	456	ASN
1	Y	461	GLN
1	O	11	GLN
1	O	23	HIS
1	O	26	ASN
1	O	32	GLN
1	O	37	GLN
1	O	73	GLN
1	O	81	ASN
1	O	99	ASN
1	O	114	HIS
1	O	127	ASN
1	O	147	HIS
1	O	179	HIS
1	O	185	ASN
1	O	228	ASN
1	O	246	GLN
1	O	253	GLN
1	O	274	ASN
1	O	284	ASN
1	O	299	ASN
1	O	337	GLN
1	O	387	GLN
1	O	415	ASN

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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACP	O	601	2	31,33,33	2.76	6 (19%)	47,52,52	2.25	5 (10%)
3	ACP	Y	601	2	31,33,33	2.76	5 (16%)	47,52,52	1.54	5 (10%)
4	GOL	O	600	-	5,5,5	0.64	0	5,5,5	0.38	0
4	GOL	Y	600	-	5,5,5	0.50	0	5,5,5	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	O	601	2	-	0/19/38/38	0/3/3/3
3	ACP	Y	601	2	-	4/19/38/38	0/3/3/3
4	GOL	O	600	-	-	2/4/4/4	-
4	GOL	Y	600	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	ACP	PG-O2G	9.66	1.76	1.55
3	Y	601	ACP	PA-O3A	9.25	1.69	1.59
3	O	601	ACP	PG-O3G	7.89	1.72	1.55
3	Y	601	ACP	PG-O3G	7.66	1.72	1.55
3	O	601	ACP	PG-O1G	6.50	1.63	1.50
3	Y	601	ACP	PG-O2G	5.65	1.67	1.55
3	Y	601	ACP	PB-O3A	5.15	1.64	1.58
3	Y	601	ACP	PG-O1G	4.65	1.59	1.50
3	O	601	ACP	PB-O3A	3.94	1.62	1.58
3	O	601	ACP	PA-O3A	2.64	1.62	1.59
3	O	601	ACP	PB-O1B	2.43	1.57	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	601	ACP	C1'-N9-C8	-9.97	104.97	127.09
3	O	601	ACP	C4-N9-C1'	9.70	149.31	126.63
3	Y	601	ACP	C4-N9-C1'	5.44	139.36	126.63
3	Y	601	ACP	C1'-N9-C8	-4.40	117.32	127.09
3	Y	601	ACP	PB-O3A-PA	-3.43	121.17	132.37
3	Y	601	ACP	O1G-PG-C3B	-3.38	104.00	111.37
3	O	601	ACP	PB-O3A-PA	-3.10	122.25	132.37
3	O	601	ACP	O1G-PG-C3B	-2.55	105.80	111.37
3	Y	601	ACP	C4-N9-C8	-2.43	103.18	105.74
3	O	601	ACP	O3G-PG-O2G	2.04	113.77	107.96

There are no chirality outliers.

All (8) torsion outliers are listed below:

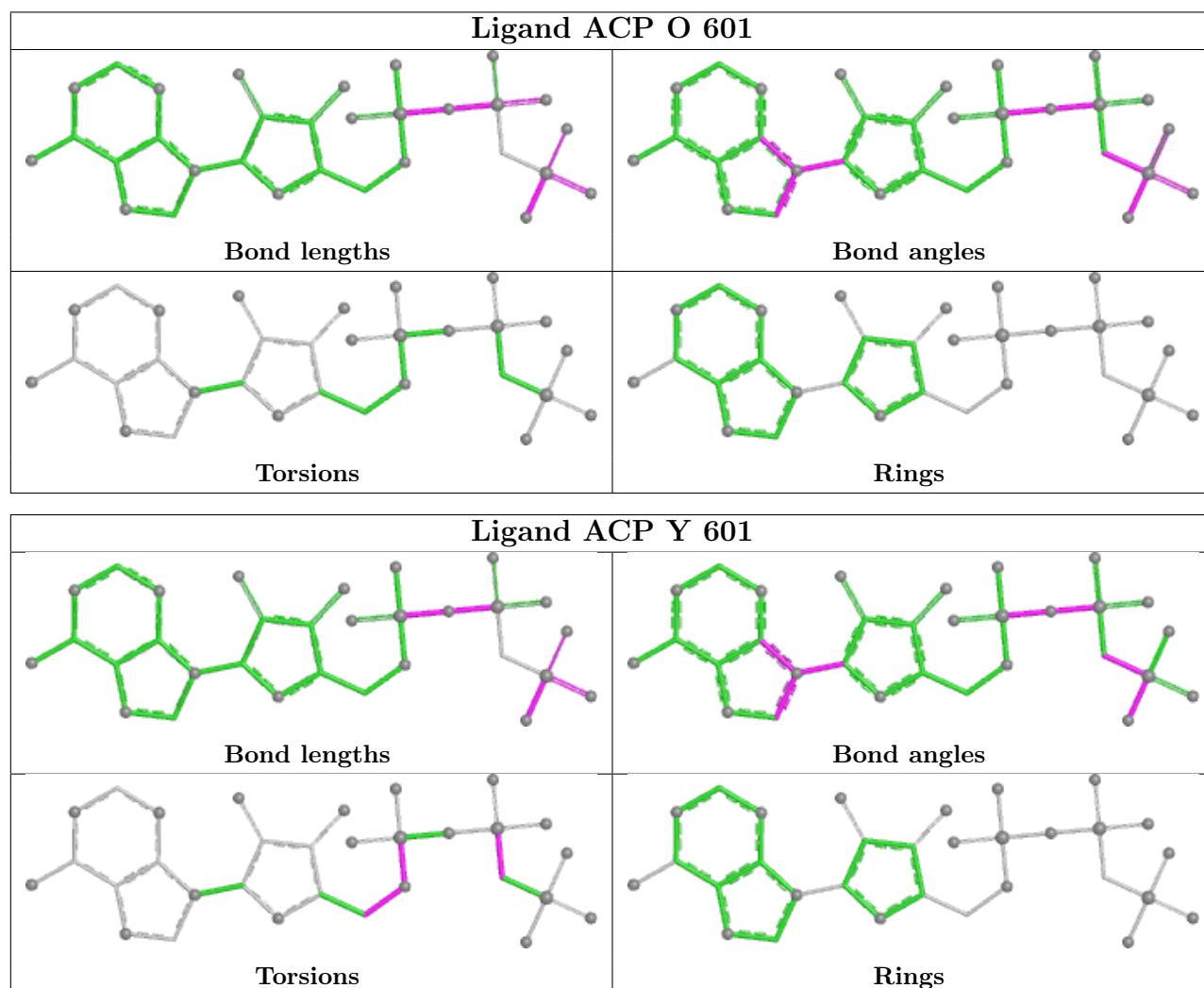
Mol	Chain	Res	Type	Atoms
3	Y	601	ACP	C5'-O5'-PA-O1A
3	Y	601	ACP	C5'-O5'-PA-O3A
4	Y	600	GOL	C1-C2-C3-O3
4	Y	600	GOL	O2-C2-C3-O3
4	O	600	GOL	C1-C2-C3-O3
4	O	600	GOL	O2-C2-C3-O3
3	Y	601	ACP	C4'-C5'-O5'-PA
3	Y	601	ACP	PG-C3B-PB-O1B

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	601	ACP	4	0
3	Y	601	ACP	5	0
4	O	600	GOL	7	0
4	Y	600	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	O	494/501 (98%)	-0.53	1 (0%) 91 83	13, 61, 94, 100	0
1	Y	494/501 (98%)	-0.76	0 100 100	7, 48, 81, 98	0
All	All	988/1002 (98%)	-0.65	1 (0%) 92 86	7, 54, 88, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	160	LEU	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

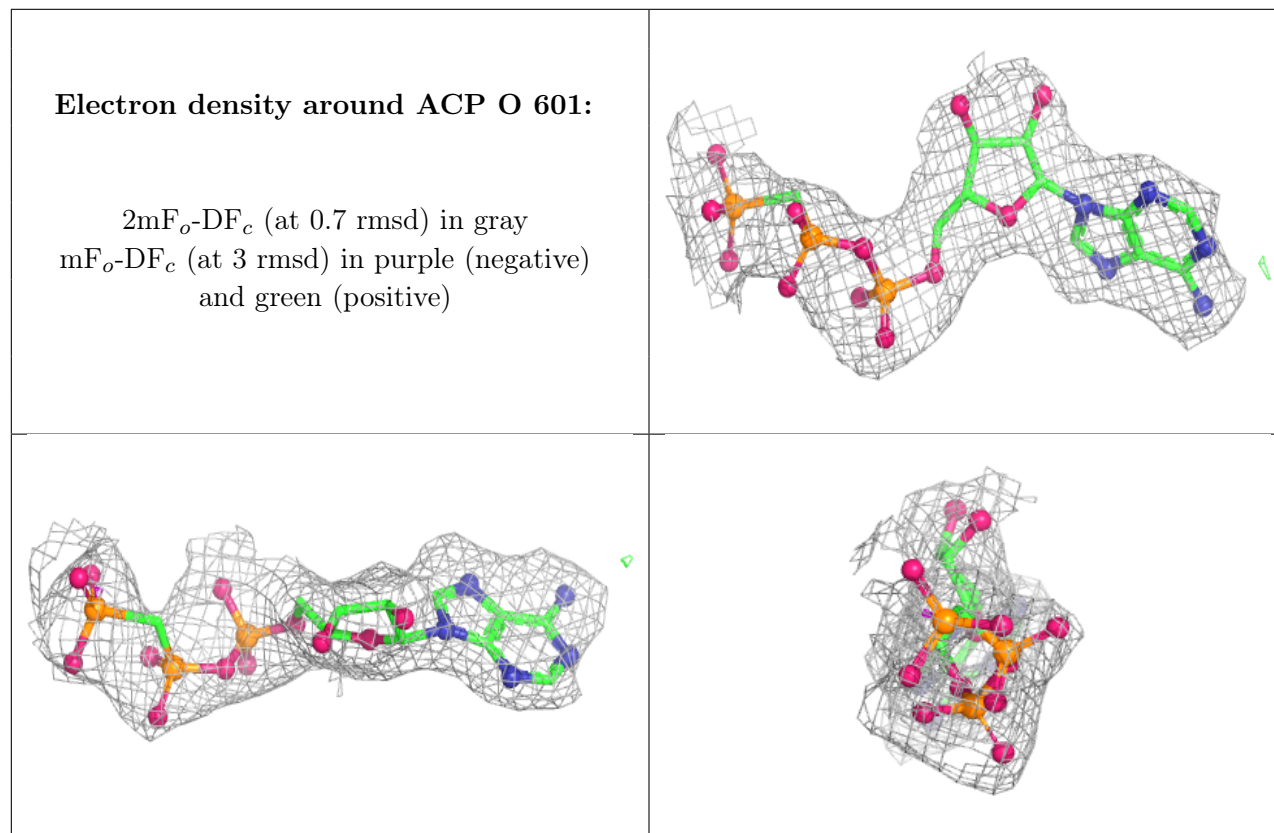
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACP	O	601	31/31	0.94	0.09	60,60,60,60	0
3	ACP	Y	601	31/31	0.96	0.07	47,47,47,47	0
2	MG	O	602	1/1	0.96	0.12	65,65,65,65	0
4	GOL	Y	600	6/6	0.97	0.06	32,32,32,32	0

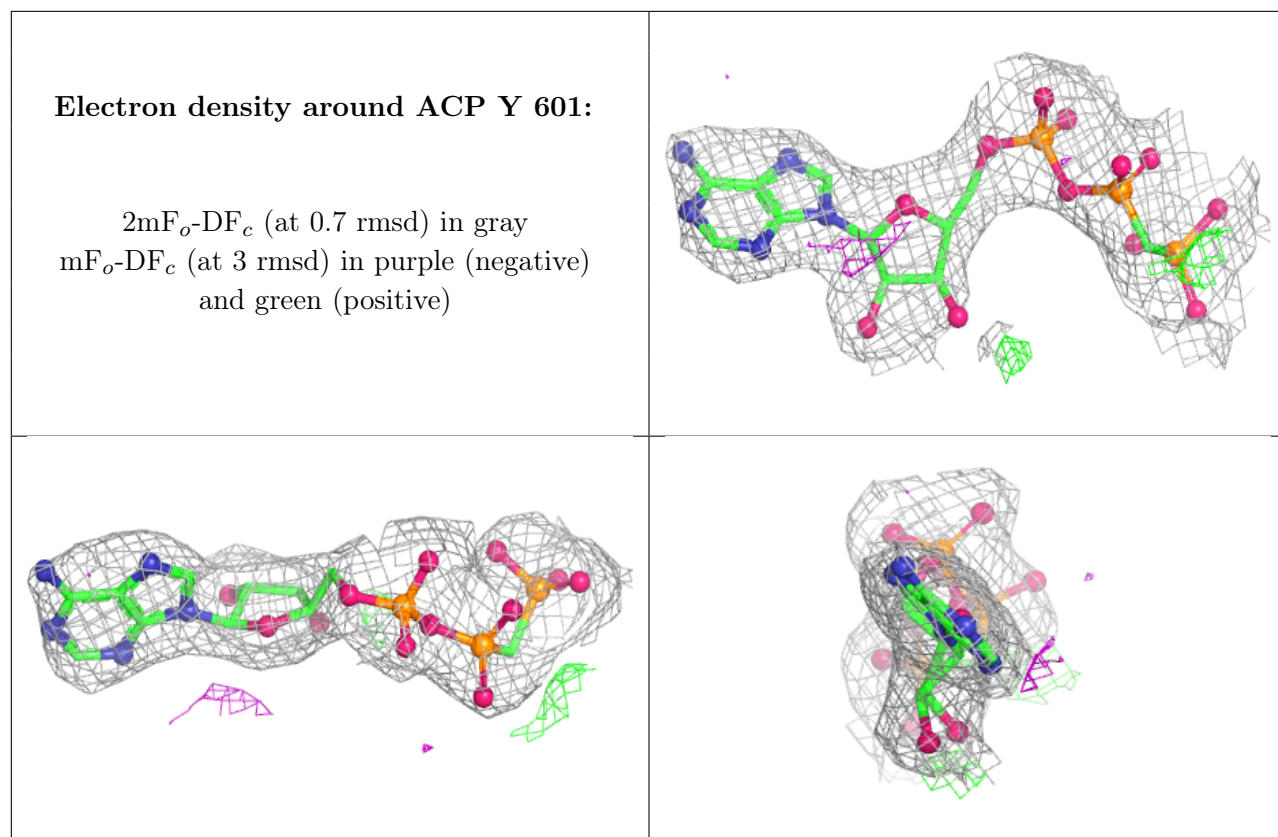
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	Y	602	1/1	0.98	0.03	40,40,40,40	0
4	GOL	O	600	6/6	0.98	0.04	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.