



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:00 AM UTC

PDB ID : 1BOT / pdb_00001bot
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN ESCHERICHIA COLI GLYCEROL KINASE AND THE ALLOSTERIC REGULATOR FRUCTOSE 1,6-BISPHOSPHATE.
Authors : Ormo, M.; Bystrom, C.E.; Remington, S.J.
Deposited on : 1998-08-05
Resolution : 3.05 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
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

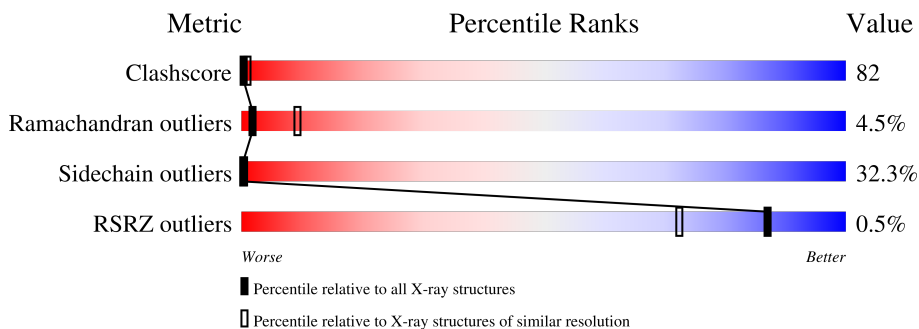
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	% 14% 50% 28% 7% .
1	Z	501	16% 50% 30% ..

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
3	GOL	O	601	-	-	X	-

2 Entry composition [i](#)

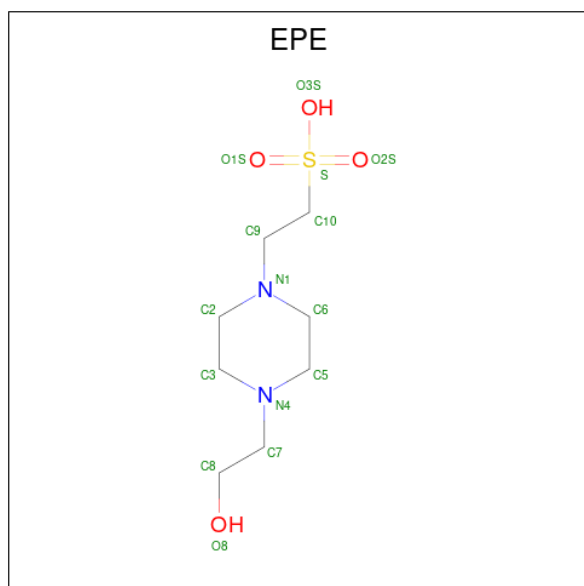
There are 3 unique types of molecules in this entry. The entry contains 7864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GLYCEROL KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	497	Total	C	N	O	S	0	0	0
			3914	2469	686	740	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3923	2474	687	743	19			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

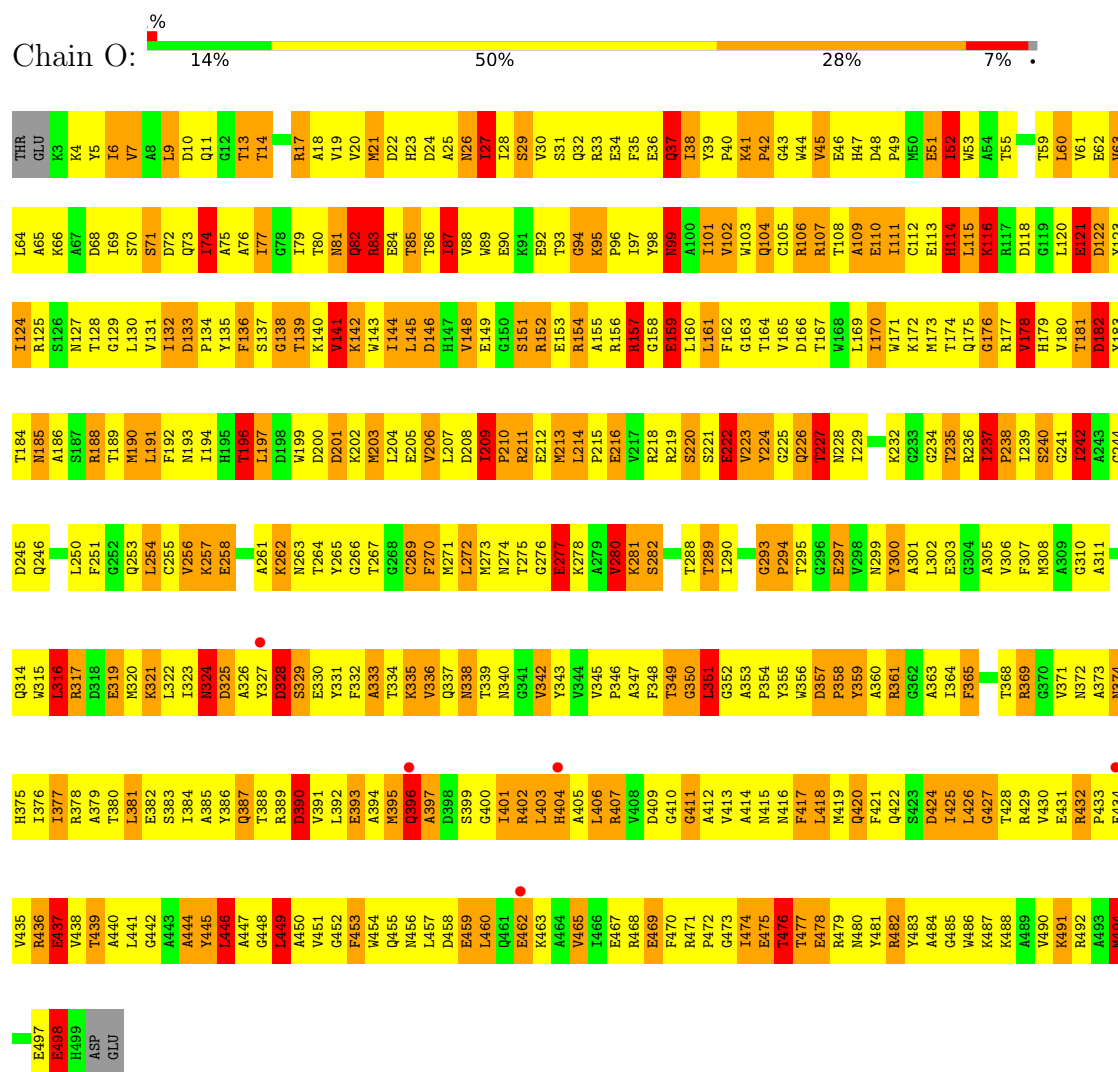


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

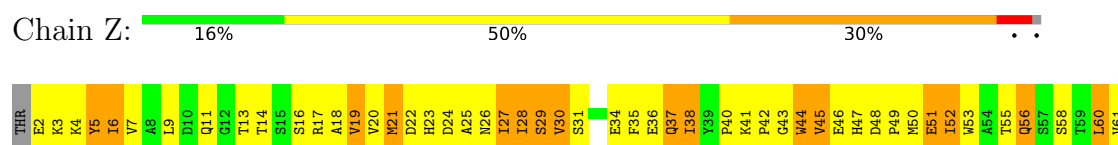
3 Residue-property plots

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: PROTEIN (GLYCEROL KINASE)



• Molecule 1: PROTEIN (GLYCEROL KINASE)



L441	Q442	A443	A444	Y445	L446	L449	A450	V451	G452	F453	W454	Q455	M456	L457	D458	E459	L460	Q461	E462	K463	A464	V465	I466	E467	R468	E469	F470	R471	P472	G473	I474	E475	T476	T477	E478	R479	N480	Y481	Y482	A483	A484	G485	W486	K487	K488	A489	V490	K491	R492	E497	E498	H499	ASP	GLU															
L381	E382	S383	I384	A385	Y386	Q387	T388	R389	D390	V391	L392	E393	A394	M395	Q396	D397	A397	R398	S399	G400	R401	R402	L403	L406	R407	V408	D409	G410	G411	A412	V413	A414	N415	N416	F417	L418	M419	Q420	F421	Q422	S423	D424	L425	L426	G427	T428	R429	V430	E431	R432	P433	E434	V435	R436	E437	V438	T439	A440											
R317	D318	E319	M320	K321	L322	I323	N324	D325	A326	Y327	D328	S329	E330	F331	A332	A333	T334	K335	V336	Q337	N338	T339	N340	G341	V342	Y343	V344	V345	P346	A347	F348	T349	G350	L351	G352	A353	P354	Y355	W356	D357	P358	Y359	A360	R361	G362	I363	F365	T368	R369	G370	V371	N372	A373	N374	H375	I376	I377												
F251	G252	Q253	L254	C255	Y256	K257	M260	A261	K262	M263	T264	Y265	G266	T267	G268	C269	F270	M271	L272	M273	N274	T275	K278	A279	K281	L286	T289	I290	A291	C292	G293	P294	T295	G296	E297	V298	N299	Y300	A301	L302	E303	G304	A305	V306	F307	M308	A309	G310	A311	S312	I313	Q314	W315	L316															
A186	S187	R188	T189	M190	C191	F192	M193	I194	H195	T196	L197	D198	W199	D200	D201	K202	M203	C204	L204	L145	E206	L207	D208	E209	P210	R211	E212	M213	L214	A155	R156	V217	R218	K219	S220	C221	E222	F223	G224	Y224	G225	Q226	T227	W228	R229	I229						T235	R236	I237	P238	Q175	S240	G241	L242	H179	A243	G244	D245	T181	D182	Y183	A249	L250	R185
E62	V63	L64	A65	I69	S70	S71	D72	F73	I74	A75	I79	N80	N81	Q82	R83	E84	T85	T86	I87	V88	W89	E90	K91	E92	T93	G94	K95	P96	I97	Y98	N99	A100	I101	F102	V103	Q104	C105	R106	R107	T108	A109	E110	I111	C112	E113	M173	T174	Q175	G176	R117	V178	H179	G119	L120	T121	D122	Y123	R124	N125										

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.80Å 168.80Å 202.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 20.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-3.05) 80.9 (20.00-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.88Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.219 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 123.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7864	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.46	15/3994 (0.4%)	1.89	109/5414 (2.0%)
1	Z	1.48	10/4003 (0.2%)	1.87	107/5426 (2.0%)
All	All	1.47	25/7997 (0.3%)	1.88	216/10840 (2.0%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	44	TRP	CA-C	-7.10	1.44	1.52
1	Z	34	GLU	CD-OE2	6.65	1.38	1.25
1	O	270	PHE	CA-C	-6.34	1.46	1.53
1	O	216	GLU	CD-OE2	6.29	1.37	1.25
1	O	345	VAL	CA-CB	-6.21	1.48	1.54
1	O	196	THR	N-CA	-6.02	1.39	1.46
1	O	342	VAL	CA-CB	-6.00	1.47	1.54
1	Z	364	ILE	CA-CB	-5.88	1.47	1.54
1	O	280	VAL	CA-CB	-5.86	1.46	1.54
1	O	178	VAL	CA-CB	-5.71	1.47	1.54
1	Z	111	ILE	N-CA	-5.67	1.39	1.46
1	Z	111	ILE	CA-CB	-5.61	1.46	1.54
1	Z	111	ILE	CA-C	-5.53	1.45	1.52
1	O	475	GLU	CA-C	-5.41	1.46	1.52
1	O	238	PRO	N-CA	-5.34	1.40	1.47
1	O	272	LEU	CA-C	-5.27	1.46	1.52
1	Z	165	VAL	CA-CB	-5.26	1.47	1.54
1	O	300	TYR	CA-C	-5.25	1.46	1.52
1	Z	317	ARG	N-CA	-5.23	1.39	1.46
1	Z	34	GLU	CA-C	-5.12	1.46	1.53
1	O	437	GLU	CD-OE1	5.11	1.35	1.25
1	O	424	ASP	C-N	-5.07	1.27	1.33
1	O	74	ILE	CA-C	-5.06	1.48	1.53
1	Z	475	GLU	CD-OE2	5.05	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	462	GLU	CD-OE1	5.02	1.34	1.25

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	404	HIS	CA-CB-CG	-9.99	103.81	113.80
1	Z	237	ILE	CA-C-N	9.68	129.44	119.76
1	Z	237	ILE	C-N-CA	9.68	129.44	119.76
1	Z	136	PHE	CA-C-N	9.04	132.75	120.54
1	Z	136	PHE	C-N-CA	9.04	132.75	120.54
1	O	206	VAL	N-CA-C	8.93	119.51	110.23
1	Z	351	LEU	CA-C-N	-8.84	108.33	122.65
1	Z	351	LEU	C-N-CA	-8.84	108.33	122.65
1	Z	228	ASN	CA-C-N	-8.83	112.12	122.36
1	Z	228	ASN	C-N-CA	-8.83	112.12	122.36
1	O	133	ASP	N-CA-C	8.78	116.12	108.22
1	Z	137	SER	N-CA-C	8.65	121.50	111.11
1	O	237	ILE	CA-C-O	8.63	124.43	119.94
1	O	357	ASP	C-N-CD	-8.47	90.26	125.00
1	O	185	ASN	CA-CB-CG	-8.29	104.31	112.60
1	O	178	VAL	N-CA-C	7.91	119.87	108.48
1	O	27	ILE	N-CA-CB	7.85	119.95	111.00
1	O	83	ARG	O-C-N	-7.85	111.63	122.46
1	O	351	LEU	N-CA-C	7.84	122.94	111.02
1	O	293	GLY	N-CA-C	-7.83	102.47	112.10
1	Z	133	ASP	N-CA-C	7.72	118.06	108.11
1	Z	83	ARG	CA-C-N	-7.70	109.12	122.36
1	Z	83	ARG	C-N-CA	-7.70	109.12	122.36
1	O	280	VAL	N-CA-C	7.61	118.87	107.75
1	O	206	VAL	CB-CA-C	-7.59	101.98	111.70
1	O	26	ASN	CA-C-N	-7.47	113.03	122.37
1	O	26	ASN	C-N-CA	-7.47	113.03	122.37
1	Z	43	GLY	N-CA-C	-7.45	104.21	114.64
1	Z	307	PHE	N-CA-C	7.35	120.35	111.82
1	Z	81	ASN	N-CA-C	7.35	118.89	108.74
1	O	38	ILE	N-CA-C	7.26	118.60	107.99
1	Z	237	ILE	CA-C-O	7.22	123.98	119.51
1	Z	292	CYS	N-CA-C	7.19	120.49	108.20
1	O	83	ARG	N-CA-C	7.14	121.75	112.89
1	O	325	ASP	N-CA-C	-7.12	104.59	113.28
1	Z	421	PHE	CA-CB-CG	-7.11	106.69	113.80
1	Z	38	ILE	CA-C-N	-7.10	113.87	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	38	ILE	C-N-CA	-7.10	113.87	123.46
1	Z	83	ARG	O-C-N	-7.04	113.00	122.43
1	Z	256	VAL	N-CA-CB	-7.01	103.21	112.26
1	O	405	ALA	CA-C-N	-7.00	113.35	123.00
1	O	405	ALA	C-N-CA	-7.00	113.35	123.00
1	O	159	GLU	N-CA-C	-6.97	104.75	113.18
1	Z	83	ARG	N-CA-C	6.94	121.01	112.54
1	Z	469	GLU	N-CA-CB	6.94	122.94	111.08
1	O	114	HIS	CA-CB-CG	-6.93	106.87	113.80
1	O	5	TYR	N-CA-C	6.90	120.55	108.75
1	Z	167	THR	N-CA-CB	6.86	120.17	109.94
1	Z	178	VAL	N-CA-C	6.82	117.86	107.77
1	O	289	THR	N-CA-CB	6.81	122.69	111.31
1	O	74	ILE	N-CA-CB	6.79	119.40	111.66
1	O	83	ARG	CA-C-N	-6.72	111.80	122.08
1	O	83	ARG	C-N-CA	-6.72	111.80	122.08
1	O	357	ASP	N-CA-C	-6.68	101.65	110.40
1	Z	237	ILE	O-C-N	6.68	127.86	121.11
1	Z	477	THR	N-CA-C	-6.66	100.57	110.23
1	Z	61	VAL	CB-CA-C	-6.64	103.34	112.04
1	O	350	GLY	N-CA-C	-6.58	100.85	112.77
1	Z	87	ILE	N-CA-C	6.53	118.11	108.45
1	Z	38	ILE	N-CA-C	6.50	118.17	108.54
1	Z	293	GLY	CA-C-N	6.49	127.95	119.84
1	Z	293	GLY	C-N-CA	6.49	127.95	119.84
1	Z	220	SER	CA-C-N	-6.44	114.31	123.20
1	Z	220	SER	C-N-CA	-6.44	114.31	123.20
1	O	289	THR	N-CA-C	6.43	117.92	108.86
1	O	82	GLN	N-CA-C	-6.40	100.81	110.28
1	Z	357	ASP	CA-C-N	6.39	126.08	119.82
1	Z	357	ASP	C-N-CA	6.39	126.08	119.82
1	O	307	PHE	N-CA-C	6.38	119.05	111.71
1	Z	94	GLY	N-CA-C	-6.37	105.89	115.32
1	Z	416	ASN	CA-CB-CG	-6.37	106.23	112.60
1	O	182	ASP	CA-CB-CG	-6.34	106.26	112.60
1	O	402	ARG	N-CA-CB	6.34	119.77	109.95
1	Z	320	MET	N-CA-C	-6.32	105.39	113.23
1	Z	351	LEU	N-CA-C	6.31	124.23	110.80
1	O	223	VAL	N-CA-CB	6.30	118.55	110.99
1	Z	122	ASP	CA-CB-CG	-6.29	106.31	112.60
1	O	328	ASP	N-CA-C	6.26	118.87	110.35
1	Z	133	ASP	CA-C-O	6.26	125.83	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	363	ALA	N-CA-C	6.25	118.64	108.76
1	Z	263	ASN	CA-CB-CG	-6.23	106.37	112.60
1	O	282	SER	CA-C-O	6.23	127.17	120.38
1	Z	81	ASN	CA-CB-CG	-6.21	106.39	112.60
1	Z	149	GLU	N-CA-C	6.18	123.97	110.80
1	O	210	PRO	N-CA-CB	6.14	108.63	103.17
1	Z	427	GLY	N-CA-C	-6.12	104.35	114.76
1	O	342	VAL	N-CA-C	6.12	117.94	109.80
1	O	338	ASN	CA-CB-CG	-6.10	106.50	112.60
1	O	14	THR	N-CA-CB	-6.04	102.87	110.90
1	O	325	ASP	CA-CB-CG	6.03	118.63	112.60
1	O	432	ARG	CA-C-N	6.02	126.48	120.52
1	O	432	ARG	C-N-CA	6.02	126.48	120.52
1	Z	390	ASP	N-CA-CB	6.01	118.89	109.94
1	O	465	VAL	N-CA-C	5.99	116.48	107.80
1	O	161	LEU	N-CA-C	5.98	119.45	109.95
1	Z	384	ILE	N-CA-CB	5.96	116.88	110.62
1	O	201	ASP	CA-CB-CG	-5.96	106.64	112.60
1	O	328	ASP	CA-CB-CG	-5.96	106.64	112.60
1	Z	118	ASP	CA-CB-CG	5.95	118.55	112.60
1	O	209	ILE	N-CA-CB	-5.94	104.19	112.27
1	Z	384	ILE	CB-CA-C	-5.93	104.11	111.70
1	O	82	GLN	CB-CA-C	5.90	119.74	109.65
1	Z	297	GLU	CA-C-N	-5.89	112.14	120.75
1	Z	297	GLU	C-N-CA	-5.89	112.14	120.75
1	O	324	ASN	N-CA-C	5.89	116.05	108.34
1	Z	314	GLN	N-CA-C	-5.88	104.95	111.71
1	Z	89	TRP	N-CA-C	5.82	117.81	109.14
1	O	417	PHE	CA-CB-CG	-5.80	108.00	113.80
1	O	209	ILE	CB-CA-C	5.79	116.01	110.16
1	Z	82	GLN	CA-C-O	5.78	127.28	120.58
1	O	38	ILE	CB-CA-C	-5.77	103.08	110.98
1	O	401	ILE	N-CA-C	5.77	116.17	107.75
1	Z	223	VAL	N-CA-CB	5.74	117.19	110.82
1	O	77	ILE	N-CA-C	5.70	116.32	108.12
1	O	206	VAL	N-CA-CB	5.68	116.58	110.62
1	Z	417	PHE	CA-CB-CG	-5.63	108.17	113.80
1	Z	19	VAL	CA-C-N	-5.62	115.77	123.14
1	Z	19	VAL	C-N-CA	-5.62	115.77	123.14
1	O	432	ARG	O-C-N	5.60	127.58	121.36
1	Z	61	VAL	N-CA-CB	5.60	118.58	110.52
1	O	159	GLU	CA-C-N	5.59	130.71	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	159	GLU	C-N-CA	5.59	130.71	123.00
1	O	242	ILE	CB-CA-C	-5.58	102.13	111.29
1	O	293	GLY	CA-C-N	5.58	126.81	119.84
1	O	293	GLY	C-N-CA	5.58	126.81	119.84
1	O	290	ILE	N-CA-C	5.55	116.17	108.84
1	O	240	SER	N-CA-C	5.55	119.30	112.03
1	O	390	ASP	N-CA-CB	5.50	119.79	110.49
1	O	87	ILE	N-CA-C	5.48	116.56	108.45
1	Z	390	ASP	CA-C-N	-5.47	111.32	120.30
1	Z	390	ASP	C-N-CA	-5.47	111.32	120.30
1	Z	182	ASP	CA-CB-CG	-5.47	107.13	112.60
1	O	427	GLY	N-CA-C	-5.46	104.58	114.46
1	O	99	ASN	CA-C-N	-5.44	113.72	121.50
1	O	99	ASN	C-N-CA	-5.44	113.72	121.50
1	O	94	GLY	N-CA-C	-5.43	106.72	115.08
1	Z	279	ALA	CA-C-N	-5.42	116.08	123.12
1	Z	279	ALA	C-N-CA	-5.42	116.08	123.12
1	Z	409	ASP	CA-CB-CG	-5.42	107.18	112.60
1	O	133	ASP	CA-C-O	5.40	125.39	120.26
1	O	498	GLU	CB-CA-C	5.40	118.66	109.53
1	O	227	THR	N-CA-CB	5.40	119.38	110.69
1	O	390	ASP	CA-CB-CG	5.40	118.00	112.60
1	Z	5	TYR	CA-C-N	-5.39	115.62	123.06
1	Z	5	TYR	C-N-CA	-5.39	115.62	123.06
1	O	228	ASN	N-CA-CB	5.39	119.41	110.47
1	O	316	LEU	N-CA-CB	5.33	119.38	110.32
1	Z	60	LEU	CA-C-N	-5.33	113.12	120.74
1	Z	60	LEU	C-N-CA	-5.33	113.12	120.74
1	Z	465	VAL	CB-CA-C	-5.32	102.57	111.29
1	Z	195	HIS	CA-CB-CG	-5.31	108.49	113.80
1	Z	223	VAL	CB-CA-C	-5.31	104.21	111.33
1	Z	390	ASP	CA-CB-CG	5.30	117.91	112.60
1	O	424	ASP	N-CA-CB	5.30	117.88	109.82
1	O	430	VAL	N-CA-CB	-5.30	104.61	111.82
1	O	281	LYS	N-CA-CB	5.30	117.76	109.97
1	Z	223	VAL	N-CA-C	5.29	115.83	108.84
1	Z	219	ARG	CA-C-N	5.28	127.61	120.38
1	Z	219	ARG	C-N-CA	5.28	127.61	120.38
1	O	136	PHE	N-CA-C	5.27	118.41	109.76
1	Z	180	VAL	N-CA-CB	-5.27	104.49	112.35
1	Z	389	ARG	CA-C-N	-5.25	113.45	120.54
1	Z	389	ARG	C-N-CA	-5.25	113.45	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	73	GLN	N-CA-C	-5.24	105.75	113.61
1	O	310	GLY	N-CA-C	-5.24	106.35	113.37
1	Z	37	GLN	CA-C-N	-5.23	114.47	121.80
1	Z	37	GLN	C-N-CA	-5.23	114.47	121.80
1	O	300	TYR	N-CA-CB	5.22	120.08	111.62
1	Z	38	ILE	CB-CA-C	-5.21	104.98	111.08
1	Z	218	ARG	CA-C-N	-5.21	113.16	122.07
1	Z	218	ARG	C-N-CA	-5.21	113.16	122.07
1	Z	267	THR	N-CA-C	-5.20	105.61	111.28
1	O	469	GLU	CA-C-N	-5.19	115.67	122.99
1	O	469	GLU	C-N-CA	-5.19	115.67	122.99
1	O	277	GLU	N-CA-CB	5.19	118.38	110.44
1	Z	398	ASP	N-CA-C	-5.19	105.54	111.14
1	Z	465	VAL	N-CA-C	5.18	120.12	109.34
1	Z	152	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	Z	61	VAL	N-CA-C	5.17	115.84	110.82
1	O	359	TYR	N-CA-C	-5.17	107.99	114.56
1	Z	104	GLN	N-CA-C	5.15	116.98	111.36
1	O	222	GLU	CA-C-N	-5.15	116.44	122.93
1	O	222	GLU	C-N-CA	-5.15	116.44	122.93
1	Z	292	CYS	CB-CA-C	-5.14	102.56	110.78
1	O	494	MET	N-CA-C	5.13	117.30	110.53
1	O	374	ASN	CA-CB-CG	-5.13	107.47	112.60
1	Z	114	HIS	CA-CB-CG	-5.12	108.68	113.80
1	O	424	ASP	CA-CB-CG	-5.12	107.48	112.60
1	O	402	ARG	CA-C-N	-5.11	114.11	121.42
1	O	402	ARG	C-N-CA	-5.11	114.11	121.42
1	Z	51	GLU	N-CA-C	-5.11	105.60	111.07
1	Z	351	LEU	CB-CA-C	-5.11	100.25	110.42
1	Z	83	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	Z	209	ILE	C-N-CD	-5.09	104.13	125.00
1	O	129	GLY	N-CA-C	-5.09	108.59	115.21
1	Z	136	PHE	O-C-N	5.08	128.63	122.94
1	Z	167	THR	CA-CB-OG1	5.08	117.22	109.60
1	O	68	ASP	CA-C-N	-5.07	114.39	122.50
1	O	68	ASP	C-N-CA	-5.07	114.39	122.50
1	O	106	ARG	CA-C-N	-5.07	113.10	120.29
1	O	106	ARG	C-N-CA	-5.07	113.10	120.29
1	Z	36	GLU	N-CA-C	5.07	117.78	110.28
1	Z	384	ILE	N-CA-C	5.06	115.50	110.23
1	Z	30	VAL	N-CA-C	5.06	115.03	108.35
1	O	350	GLY	CA-C-N	-5.05	116.42	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	350	GLY	C-N-CA	-5.05	116.42	122.44
1	O	176	GLY	N-CA-C	-5.05	107.55	114.67
1	Z	80	THR	CA-C-N	-5.05	114.08	122.11
1	Z	80	THR	C-N-CA	-5.05	114.08	122.11
1	O	164	THR	N-CA-CB	5.04	119.20	110.07
1	O	37	GLN	CA-C-N	-5.04	116.45	122.90
1	O	37	GLN	C-N-CA	-5.04	116.45	122.90
1	Z	477	THR	CB-CA-C	5.04	118.08	109.72
1	O	157	ARG	N-CA-C	-5.03	107.30	112.93
1	O	449	LEU	N-CA-CB	5.01	117.40	109.94
1	Z	162	PHE	CA-CB-CG	-5.01	108.79	113.80

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	3914	0	3853	673	0
1	Z	3923	0	3859	606	0
2	O	15	0	18	2	0
3	O	6	0	8	4	0
3	Z	6	0	8	3	0
All	All	7864	0	7746	1278	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 82.

All (1278) 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:Z:329:SER:HB2	1:Z:381:LEU:HD11	1.28	1.14
1:Z:84:GLU:HB2	1:Z:103:TRP:HB3	1.15	1.12
1:O:145:LEU:HD12	1:O:151:SER:HB2	1.23	1.11
1:O:271:MET:HE1	1:O:392:LEU:HA	1.14	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:228:ASN:HB2	1:Z:236:ARG:HD2	1.28	1.09
1:O:273:MET:HB2	1:O:395:MET:HE3	1.25	1.09
1:O:17:ARG:HD2	1:O:32:GLN:HE21	1.17	1.07
1:Z:407:ARG:HH12	1:Z:466:ILE:HD11	1.21	1.06
1:O:85:THR:HB	1:O:102:VAL:HA	1.27	1.06
1:O:83:ARG:HG3	1:O:83:ARG:HH11	1.20	1.05
1:O:234:GLY:HA2	1:O:236:ARG:HH21	1.16	1.05
1:Z:187:SER:HB3	1:Z:290:ILE:HD12	1.39	1.03
1:Z:6:ILE:HD11	1:Z:444:ALA:HA	1.39	1.03
1:Z:84:GLU:HB2	1:Z:103:TRP:CB	1.88	1.02
1:O:108:THR:HG21	1:O:139:THR:HB	1.41	1.02
1:O:336:VAL:HG23	1:O:338:ASN:H	1.27	0.98
1:O:86:THR:HG23	1:O:162:PHE:HE1	1.28	0.98
1:O:204:LEU:HD21	1:O:214:LEU:HD11	1.46	0.98
1:O:340:ASN:HB2	1:O:375:HIS:CD2	2.01	0.94
1:Z:385:ALA:HA	1:Z:422:GLN:HE22	1.32	0.94
1:O:74:ILE:HB	1:O:237:ILE:HD13	1.46	0.94
1:Z:419:MET:HA	1:Z:419:MET:HE2	1.50	0.94
1:O:83:ARG:HH11	1:O:83:ARG:CG	1.81	0.93
1:O:161:LEU:HD22	1:O:179:HIS:CE1	2.03	0.93
1:Z:137:SER:HB2	1:Z:189:THR:HA	1.51	0.92
1:O:120:LEU:O	1:O:121:GLU:C	2.10	0.91
1:O:369:ARG:HG3	1:O:369:ARG:HH11	1.33	0.91
1:O:17:ARG:HD2	1:O:32:GLN:NE2	1.83	0.91
1:Z:83:ARG:NE	1:Z:246:GLN:HB2	1.85	0.91
1:O:434:GLU:HB2	1:O:465:VAL:HB	1.53	0.90
1:O:23:HIS:HA	1:O:453:PHE:CE2	2.05	0.90
1:O:108:THR:CG2	1:O:139:THR:HB	2.03	0.89
1:O:7:VAL:HG12	1:O:77:ILE:HG12	1.53	0.88
1:O:293:GLY:HA3	1:O:297:GLU:HG2	1.53	0.88
1:O:88:VAL:HG12	1:O:97:ILE:HG12	1.56	0.87
1:Z:45:VAL:HG23	1:Z:105:CYS:HA	1.56	0.87
1:Z:170:ILE:HA	1:Z:173:MET:HE3	1.54	0.87
1:Z:224:TYR:CZ	1:Z:242:ILE:HD12	2.10	0.87
1:Z:469:GLU:HG3	1:Z:471:ARG:NH2	1.88	0.87
1:O:122:ASP:O	1:O:123:TYR:C	2.18	0.87
1:Z:256:VAL:HG13	1:Z:294:PRO:HD3	1.57	0.87
1:O:89:TRP:HD1	1:O:94:GLY:HA2	1.40	0.86
1:O:224:TYR:CZ	1:O:242:ILE:HD12	2.11	0.86
1:Z:84:GLU:CB	1:Z:103:TRP:HB3	2.02	0.86
1:O:115:LEU:HD22	1:O:115:LEU:H	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:261:ALA:HB2	1:Z:273:MET:HB2	1.56	0.85
1:Z:354:PRO:HD2	1:Z:355:TYR:CE1	2.12	0.85
1:O:402:ARG:HG2	1:O:404:HIS:CD2	2.12	0.85
1:O:265:TYR:HB3	1:O:412:ALA:HB3	1.59	0.84
1:Z:83:ARG:HH11	1:Z:83:ARG:HB2	1.43	0.84
1:O:234:GLY:HA2	1:O:236:ARG:NH2	1.91	0.84
1:O:361:ARG:HG2	1:O:361:ARG:HH11	1.43	0.83
1:O:86:THR:HG23	1:O:162:PHE:CE1	2.12	0.83
1:Z:178:VAL:HG12	1:Z:180:VAL:HG12	1.58	0.83
1:O:331:TYR:HE2	1:O:335:LYS:HE2	1.43	0.82
1:O:112:CYS:HA	1:O:115:LEU:HD23	1.62	0.82
1:Z:256:VAL:HG13	1:Z:294:PRO:CD	2.09	0.82
1:Z:51:GLU:O	1:Z:55:THR:HG23	1.79	0.82
1:Z:385:ALA:HA	1:Z:422:GLN:NE2	1.95	0.81
1:Z:48:ASP:HB3	1:Z:51:GLU:HB2	1.60	0.81
1:O:452:GLY:O	1:O:453:PHE:C	2.22	0.81
1:O:85:THR:HG22	1:O:103:TRP:H	1.46	0.81
1:Z:6:ILE:CD1	1:Z:444:ALA:HA	2.10	0.81
1:Z:85:THR:HG23	1:Z:102:VAL:HA	1.61	0.81
1:O:270:PHE:CZ	3:O:601:GOL:H11	2.16	0.81
1:Z:271:MET:C	1:Z:272:LEU:HD12	2.06	0.81
1:O:137:SER:HB2	1:O:189:THR:HA	1.60	0.80
1:O:365:PHE:CE2	1:O:492:ARG:HB3	2.16	0.80
1:Z:228:ASN:HB2	1:Z:236:ARG:CD	2.11	0.80
1:O:497:GLU:HG3	1:O:498:GLU:N	1.96	0.80
1:Z:351:LEU:HD22	1:Z:360:ALA:CB	2.11	0.80
1:Z:407:ARG:HH12	1:Z:466:ILE:CD1	1.95	0.80
1:O:152:ARG:HG3	1:O:152:ARG:HH11	1.47	0.80
1:O:324:ASN:N	1:O:324:ASN:HD22	1.78	0.80
1:Z:407:ARG:NH1	1:Z:466:ILE:HD11	1.98	0.79
1:Z:202:LYS:O	1:Z:206:VAL:HG23	1.83	0.79
1:Z:354:PRO:HD2	1:Z:355:TYR:CD1	2.17	0.79
1:O:271:MET:HE1	1:O:392:LEU:CA	2.07	0.79
1:O:491:LYS:HA	1:O:494:MET:HE3	1.63	0.79
1:Z:114:HIS:O	1:Z:115:LEU:C	2.23	0.79
1:O:17:ARG:HH22	1:O:437:GLU:CG	1.96	0.78
1:O:406:LEU:HD22	1:O:407:ARG:H	1.48	0.78
1:O:406:LEU:HD22	1:O:407:ARG:N	1.98	0.78
1:Z:108:THR:CB	1:Z:139:THR:HB	2.12	0.78
1:Z:413:VAL:HA	1:Z:419:MET:SD	2.23	0.78
1:Z:460:LEU:H	1:Z:460:LEU:HD22	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:173:MET:HB3	1:O:227:THR:HG23	1.66	0.78
1:Z:387:GLN:HA	1:Z:390:ASP:OD2	1.82	0.78
1:O:428:THR:N	1:O:472:PRO:HG3	1.97	0.78
1:O:438:VAL:HA	1:O:441:LEU:HD12	1.64	0.78
1:O:105:CYS:SG	1:O:107:ARG:HD2	2.24	0.78
1:Z:407:ARG:HG3	1:Z:407:ARG:HH11	1.46	0.78
1:O:456:ASN:O	1:O:459:GLU:HG3	1.84	0.77
1:O:120:LEU:HD12	1:O:120:LEU:H	1.47	0.77
1:O:169:LEU:O	1:O:173:MET:HG3	1.83	0.77
1:Z:86:THR:HG23	1:Z:162:PHE:HE1	1.49	0.77
1:Z:330:GLU:O	1:Z:334:THR:HG23	1.83	0.77
1:O:275:THR:HG23	1:O:301:ALA:HA	1.64	0.77
1:O:142:LYS:O	1:O:143:TRP:C	2.29	0.76
1:Z:187:SER:HB3	1:Z:290:ILE:CD1	2.14	0.76
1:O:324:ASN:N	1:O:324:ASN:ND2	2.28	0.76
1:Z:237:ILE:HG23	1:Z:238:PRO:HD2	1.67	0.76
1:O:438:VAL:CA	1:O:441:LEU:HD12	2.15	0.76
1:O:241:GLY:O	1:O:242:ILE:HG13	1.86	0.76
1:O:347:ALA:HB3	1:O:361:ARG:C	2.11	0.76
1:Z:108:THR:HB	1:Z:139:THR:HB	1.68	0.76
1:O:324:ASN:HD22	1:O:324:ASN:H	1.32	0.76
1:O:388:THR:HB	1:O:422:GLN:HE22	1.50	0.75
1:O:145:LEU:CD1	1:O:151:SER:HB2	2.12	0.75
1:Z:11:GLN:HE21	1:Z:165:VAL:HG11	1.51	0.75
1:Z:457:LEU:HD13	1:Z:460:LEU:HD23	1.69	0.75
1:O:17:ARG:HH22	1:O:437:GLU:HG3	1.51	0.75
1:Z:271:MET:HE1	1:Z:392:LEU:HB2	1.68	0.75
1:Z:250:LEU:CD1	1:Z:255:CYS:HB2	2.16	0.75
1:Z:347:ALA:HB3	1:Z:361:ARG:C	2.12	0.75
1:Z:422:GLN:O	1:Z:426:LEU:HB2	1.86	0.75
1:O:81:ASN:N	1:O:81:ASN:HD22	1.85	0.75
1:O:422:GLN:O	1:O:425:ILE:HG22	1.87	0.74
1:Z:187:SER:CB	1:Z:290:ILE:HD12	2.15	0.74
1:O:204:LEU:CD2	1:O:214:LEU:HD11	2.18	0.74
1:O:350:GLY:HA2	1:O:360:ALA:O	1.88	0.74
1:Z:127:ASN:O	1:Z:194:ILE:HD13	1.87	0.74
1:O:200:ASP:O	1:O:204:LEU:HD12	1.88	0.74
1:O:202:LYS:O	1:O:206:VAL:HG23	1.88	0.73
1:O:332:PHE:O	1:O:333:ALA:C	2.30	0.73
1:Z:81:ASN:ND2	1:Z:166:ASP:HB3	2.03	0.73
1:O:89:TRP:CD1	1:O:94:GLY:HA2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:327:TYR:HB3	1:Z:332:PHE:CZ	2.22	0.73
1:O:256:VAL:HG11	1:O:294:PRO:HA	1.69	0.73
1:O:396:GLN:O	1:O:397:ALA:C	2.30	0.73
1:O:82:GLN:OE1	1:O:85:THR:HG21	1.88	0.73
1:O:490:VAL:HG12	1:O:494:MET:CE	2.19	0.73
1:Z:237:ILE:CG2	1:Z:238:PRO:HD2	2.19	0.73
1:Z:257:LYS:O	1:Z:260:MET:HG3	1.89	0.72
1:Z:115:LEU:H	1:Z:115:LEU:HD22	1.54	0.72
1:Z:295:THR:HG23	1:Z:297:GLU:OE2	1.88	0.72
1:O:79:ILE:HD12	1:O:170:ILE:CD1	2.19	0.72
1:O:224:TYR:CE1	1:O:240:SER:HA	2.24	0.72
1:Z:152:ARG:O	1:Z:156:ARG:HG2	1.89	0.72
1:Z:178:VAL:HG12	1:Z:180:VAL:CG1	2.19	0.72
1:Z:167:THR:HG23	1:Z:180:VAL:O	1.89	0.72
1:O:114:HIS:O	1:O:115:LEU:C	2.32	0.72
1:Z:160:LEU:C	1:Z:161:LEU:HD23	2.14	0.72
1:Z:407:ARG:NH1	1:Z:407:ARG:HG3	2.03	0.72
1:O:180:VAL:HG23	1:O:216:GLU:O	1.90	0.71
1:Z:174:THR:O	1:Z:177:ARG:HB2	1.89	0.71
1:O:120:LEU:HB2	1:O:124:ILE:HD12	1.72	0.71
1:O:221:SER:OG	1:O:450:ALA:HB2	1.90	0.71
1:O:455:GLN:HA	1:O:455:GLN:HE21	1.55	0.71
1:Z:196:THR:HG22	1:Z:198:ASP:N	2.04	0.71
1:O:174:THR:HG21	1:O:178:VAL:HG13	1.73	0.71
1:O:387:GLN:HA	1:O:390:ASP:OD2	1.89	0.71
1:O:438:VAL:N	1:O:441:LEU:HD12	2.05	0.71
1:O:329:SER:OG	1:O:381:LEU:HD11	1.91	0.71
1:Z:202:LYS:O	1:Z:203:MET:C	2.33	0.71
1:O:27:ILE:N	1:O:27:ILE:HD12	2.05	0.70
1:O:179:HIS:CD2	1:O:215:PRO:HB3	2.26	0.70
1:O:473:GLY:O	1:O:474:ILE:HD13	1.91	0.70
1:O:476:THR:HG23	1:O:479:ARG:NH2	2.05	0.70
1:Z:221:SER:HB2	1:Z:446:LEU:HG	1.74	0.70
1:Z:246:GLN:HG3	1:Z:270:PHE:HB3	1.73	0.70
1:O:337:GLN:HA	1:O:337:GLN:HE21	1.56	0.70
1:O:437:GLU:C	1:O:441:LEU:HD12	2.16	0.70
1:Z:45:VAL:HG23	1:Z:105:CYS:CA	2.20	0.70
1:O:83:ARG:HG3	3:O:601:GOL:O2	1.91	0.70
1:O:237:ILE:CG2	1:O:238:PRO:HD2	2.22	0.70
1:O:85:THR:CB	1:O:102:VAL:HA	2.15	0.70
1:Z:83:ARG:HD2	1:Z:244:GLY:HA3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:344:VAL:HG22	1:Z:364:ILE:HG12	1.72	0.70
1:O:232:LYS:O	1:O:235:THR:HB	1.92	0.69
1:Z:246:GLN:OE1	1:Z:246:GLN:HA	1.92	0.69
1:Z:478:GLU:HA	1:Z:481:TYR:HB3	1.73	0.69
1:O:19:VAL:CG1	1:O:27:ILE:HG23	2.22	0.69
1:Z:83:ARG:CZ	1:Z:246:GLN:HB2	2.23	0.69
1:Z:120:LEU:HD12	1:Z:120:LEU:N	2.07	0.69
1:Z:142:LYS:HG3	1:Z:146:ASP:OD1	1.91	0.69
1:Z:219:ARG:HD3	1:Z:222:GLU:HB3	1.75	0.69
1:O:173:MET:HB3	1:O:227:THR:CG2	2.21	0.69
1:O:102:VAL:HG23	1:O:103:TRP:N	2.07	0.69
1:Z:241:GLY:O	1:Z:242:ILE:HG13	1.92	0.69
1:O:237:ILE:HG22	1:O:238:PRO:HD2	1.73	0.69
1:O:352:GLY:HA2	1:O:356:TRP:CE3	2.27	0.68
1:O:258:GLU:HB2	1:O:276:GLY:N	2.07	0.68
1:O:439:THR:HG22	1:O:440:ALA:N	2.08	0.68
1:Z:84:GLU:OE2	1:Z:188:ARG:NH1	2.27	0.68
1:Z:438:VAL:HA	1:Z:441:LEU:HD12	1.75	0.68
1:O:81:ASN:HD22	1:O:81:ASN:H	1.41	0.68
1:O:407:ARG:HD3	1:O:431:GLU:HG3	1.76	0.68
1:Z:409:ASP:CG	1:Z:438:VAL:HG21	2.19	0.68
1:O:273:MET:CB	1:O:395:MET:HE3	2.15	0.68
1:O:441:LEU:O	1:O:442:GLY:C	2.35	0.68
1:Z:19:VAL:HG22	1:Z:30:VAL:HG22	1.74	0.68
1:Z:122:ASP:O	1:Z:123:TYR:C	2.37	0.68
1:Z:272:LEU:HD12	1:Z:272:LEU:N	2.08	0.68
1:Z:365:PHE:CE2	1:Z:492:ARG:HB3	2.29	0.68
1:O:112:CYS:SG	1:O:134:PRO:HD3	2.33	0.68
1:Z:218:ARG:HH21	1:Z:222:GLU:CD	2.01	0.68
1:O:45:VAL:O	1:O:102:VAL:HG13	1.94	0.68
1:Z:86:THR:HG23	1:Z:162:PHE:CE1	2.29	0.68
1:Z:445:TYR:O	1:Z:446:LEU:C	2.36	0.68
1:O:256:VAL:CG1	1:O:294:PRO:HA	2.23	0.67
1:O:120:LEU:HB2	1:O:124:ILE:CD1	2.24	0.67
1:O:418:LEU:HD13	1:O:419:MET:HE3	1.76	0.67
1:O:40:PRO:HG2	1:O:44:TRP:HB3	1.76	0.67
1:O:170:ILE:O	1:O:171:TRP:C	2.35	0.67
1:Z:47:HIS:O	1:Z:49:PRO:HD3	1.94	0.67
1:Z:269:CYS:HB2	1:Z:306:VAL:HB	1.74	0.67
1:Z:456:ASN:O	1:Z:459:GLU:HG3	1.94	0.67
1:O:63:VAL:O	1:O:66:LYS:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:170:ILE:HG22	1:O:171:TRP:N	2.09	0.67
1:O:385:ALA:HA	1:O:422:GLN:NE2	2.09	0.67
1:O:429:ARG:HA	1:O:470:PHE:O	1.93	0.67
1:Z:413:VAL:CG2	1:Z:436:ARG:HD2	2.25	0.67
1:O:7:VAL:CG1	1:O:77:ILE:HG12	2.24	0.67
1:O:23:HIS:NE2	1:O:453:PHE:O	2.28	0.67
1:O:271:MET:CE	1:O:392:LEU:HA	2.08	0.67
1:O:330:GLU:O	1:O:334:THR:HG23	1.95	0.67
1:O:476:THR:O	1:O:477:THR:C	2.36	0.67
1:Z:44:TRP:HA	1:Z:105:CYS:SG	2.35	0.67
1:Z:293:GLY:O	1:Z:295:THR:N	2.28	0.67
1:O:83:ARG:HG3	1:O:83:ARG:NH1	1.95	0.67
1:O:97:ILE:HD11	1:O:144:ILE:HG21	1.76	0.67
1:Z:490:VAL:HG12	1:Z:491:LYS:N	2.07	0.67
1:O:181:THR:HG23	1:O:182:ASP:N	2.10	0.66
1:O:204:LEU:HD12	1:O:204:LEU:H	1.60	0.66
1:O:357:ASP:OD1	1:O:358:PRO:N	2.28	0.66
1:Z:235:THR:C	1:Z:236:ARG:HD3	2.19	0.66
1:O:110:GLU:O	1:O:113:GLU:N	2.28	0.66
1:Z:105:CYS:SG	1:Z:107:ARG:HD2	2.36	0.66
1:O:41:LYS:HB2	1:O:42:PRO:HD2	1.78	0.66
1:O:144:ILE:O	1:O:148:VAL:HG23	1.96	0.66
1:O:111:ILE:O	1:O:115:LEU:HD22	1.94	0.66
1:O:146:ASP:OD1	1:O:146:ASP:N	2.27	0.66
1:Z:419:MET:HA	1:Z:419:MET:CE	2.23	0.66
1:O:46:GLU:OE2	1:O:107:ARG:NH2	2.29	0.66
1:O:315:TRP:CZ3	1:O:316:LEU:HD23	2.29	0.66
1:O:331:TYR:CE2	1:O:335:LYS:HE2	2.29	0.66
1:Z:22:ASP:O	1:Z:25:ALA:N	2.29	0.66
1:Z:144:ILE:O	1:Z:148:VAL:HG22	1.95	0.66
1:Z:360:ALA:O	1:Z:361:ARG:NH1	2.28	0.66
1:Z:152:ARG:O	1:Z:155:ALA:HB3	1.96	0.66
1:Z:199:TRP:CD2	1:Z:214:LEU:HD13	2.30	0.66
1:Z:330:GLU:O	1:Z:331:TYR:C	2.38	0.66
1:O:93:THR:OG1	1:O:95:LYS:HB3	1.96	0.66
1:O:176:GLY:O	1:O:177:ARG:C	2.36	0.66
1:Z:385:ALA:O	1:Z:388:THR:HB	1.95	0.66
1:O:74:ILE:HD13	1:O:74:ILE:N	2.11	0.66
1:O:143:TRP:CE3	1:O:144:ILE:HA	2.31	0.66
1:O:420:GLN:NE2	1:O:424:ASP:OD1	2.29	0.66
1:O:336:VAL:HG23	1:O:337:GLN:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:245:ASP:OD1	1:Z:246:GLN:N	2.29	0.66
1:O:214:LEU:HD23	1:O:214:LEU:N	2.11	0.65
1:Z:295:THR:N	1:Z:297:GLU:OE2	2.29	0.65
1:O:83:ARG:CG	1:O:83:ARG:NH1	2.51	0.65
1:Z:223:VAL:HA	1:Z:240:SER:HB3	1.77	0.65
1:Z:255:CYS:HB3	1:Z:260:MET:HB2	1.77	0.65
1:O:389:ARG:O	1:O:390:ASP:C	2.38	0.65
1:Z:432:ARG:NH1	1:Z:470:PHE:HZ	1.93	0.65
1:O:90:GLU:O	1:O:94:GLY:N	2.29	0.65
1:O:245:ASP:OD1	1:O:246:GLN:N	2.30	0.65
1:Z:332:PHE:HA	1:Z:335:LYS:HG3	1.79	0.65
1:O:388:THR:O	1:O:389:ARG:C	2.39	0.65
1:Z:35:PHE:HB3	1:Z:55:THR:HG21	1.79	0.65
1:Z:456:ASN:ND2	1:Z:458:ASP:HB2	2.11	0.65
1:O:456:ASN:OD1	1:O:458:ASP:HB2	1.97	0.65
1:O:352:GLY:O	1:O:355:TYR:N	2.29	0.65
1:O:473:GLY:C	1:O:474:ILE:HD13	2.21	0.65
1:O:21:MET:HA	1:O:26:ASN:O	1.96	0.64
1:Z:182:ASP:HA	1:Z:218:ARG:O	1.97	0.64
1:O:388:THR:CB	1:O:422:GLN:HE22	2.09	0.64
1:O:382:GLU:HB3	1:O:421:PHE:CE2	2.33	0.64
1:Z:222:GLU:O	1:Z:240:SER:HA	1.98	0.64
1:Z:20:VAL:O	1:Z:28:ILE:N	2.27	0.64
1:Z:452:GLY:O	1:Z:453:PHE:C	2.40	0.64
1:O:13:THR:CG2	1:O:103:TRP:HE1	2.10	0.64
1:O:331:TYR:HD2	1:O:332:PHE:CD1	2.16	0.64
1:O:460:LEU:N	1:O:460:LEU:HD23	2.12	0.64
1:Z:202:LYS:O	1:Z:205:GLU:N	2.31	0.64
1:Z:402:ARG:NH2	1:Z:428:THR:OG1	2.30	0.64
1:O:330:GLU:O	1:O:331:TYR:C	2.40	0.64
1:O:476:THR:O	1:O:480:ASN:N	2.28	0.64
1:O:395:MET:O	1:O:396:GLN:C	2.40	0.64
1:Z:193:ASN:HB3	1:Z:196:THR:HB	1.80	0.64
1:O:108:THR:O	1:O:110:GLU:N	2.31	0.64
1:O:166:ASP:OD1	1:O:167:THR:N	2.29	0.64
1:Z:224:TYR:CE2	1:Z:242:ILE:HD12	2.33	0.63
1:O:145:LEU:HD12	1:O:151:SER:CB	2.15	0.63
1:O:476:THR:HG23	1:O:479:ARG:HH22	1.64	0.63
1:Z:324:ASN:N	1:Z:324:ASN:ND2	2.44	0.63
1:O:293:GLY:HA3	1:O:297:GLU:CG	2.26	0.63
1:O:332:PHE:HA	1:O:335:LYS:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:369:ARG:HG3	1:O:369:ARG:NH1	2.09	0.63
1:O:250:LEU:CD1	1:O:255:CYS:HB2	2.29	0.63
1:Z:286:LEU:HD11	1:Z:394:ALA:HB3	1.78	0.63
1:O:29:SER:OG	1:O:63:VAL:HG12	1.99	0.63
1:O:47:HIS:O	1:O:49:PRO:HD3	1.99	0.63
1:O:76:ALA:HB2	1:O:238:PRO:HG2	1.81	0.63
1:O:108:THR:OG1	1:O:134:PRO:HA	1.99	0.63
1:Z:28:ILE:N	1:Z:28:ILE:HD13	2.13	0.63
1:Z:396:GLN:O	1:Z:400:GLY:N	2.30	0.63
1:Z:468:ARG:HD3	1:Z:470:PHE:CZ	2.33	0.63
1:O:410:GLY:O	1:O:413:VAL:HG13	1.98	0.63
1:O:424:ASP:HB3	1:O:474:ILE:HB	1.80	0.63
1:O:486:TRP:O	1:O:490:VAL:HG23	1.98	0.63
1:O:455:GLN:HA	1:O:455:GLN:NE2	2.13	0.62
1:Z:478:GLU:O	1:Z:482:ARG:HG2	1.99	0.62
1:O:392:LEU:HD23	1:O:392:LEU:C	2.23	0.62
1:O:98:TYR:OH	1:O:107:ARG:NH2	2.32	0.62
1:O:120:LEU:HD12	1:O:120:LEU:N	2.13	0.62
1:Z:40:PRO:HG2	1:Z:44:TRP:CB	2.30	0.62
1:Z:115:LEU:H	1:Z:115:LEU:CD2	2.12	0.62
1:O:120:LEU:CB	1:O:124:ILE:HD12	2.29	0.62
1:Z:40:PRO:HG2	1:Z:44:TRP:HB3	1.80	0.62
1:Z:423:SER:HB2	1:Z:430:VAL:HG23	1.80	0.62
1:O:377:ILE:O	1:O:380:THR:HB	1.99	0.62
1:Z:90:GLU:HB2	1:Z:93:THR:OG1	1.99	0.62
1:O:262:LYS:O	1:O:271:MET:HA	1.99	0.62
1:O:275:THR:OG1	1:O:300:TYR:HB2	1.98	0.62
1:O:332:PHE:O	1:O:335:LYS:N	2.28	0.62
1:Z:203:MET:HE3	1:Z:203:MET:HA	1.80	0.62
1:O:390:ASP:HA	1:O:483:TYR:OH	2.00	0.62
1:Z:108:THR:HG21	1:Z:139:THR:C	2.25	0.62
1:Z:225:GLY:O	1:Z:238:PRO:HA	1.99	0.62
1:Z:171:TRP:CE2	1:Z:176:GLY:HA2	2.35	0.62
1:O:154:ARG:HB3	1:O:159:GLU:OE2	1.99	0.62
1:Z:137:SER:HB2	1:Z:189:THR:CA	2.27	0.62
1:O:293:GLY:CA	1:O:297:GLU:HG2	2.29	0.61
1:O:410:GLY:O	1:O:413:VAL:HG22	2.00	0.61
1:Z:151:SER:O	1:Z:155:ALA:N	2.32	0.61
1:Z:460:LEU:HD22	1:Z:460:LEU:N	2.15	0.61
1:O:20:VAL:HG12	1:O:28:ILE:CG1	2.30	0.61
1:O:452:GLY:O	1:O:454:TRP:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:6:ILE:HD11	1:Z:444:ALA:CA	2.24	0.61
1:Z:201:ASP:OD2	1:Z:211:ARG:NH2	2.33	0.61
1:Z:244:GLY:O	1:Z:245:ASP:C	2.41	0.61
1:Z:142:LYS:O	1:Z:143:TRP:C	2.42	0.61
1:Z:415:ASN:O	1:Z:419:MET:HG2	1.99	0.61
1:O:85:THR:HG22	1:O:103:TRP:N	2.14	0.61
1:Z:74:ILE:HD13	1:Z:74:ILE:N	2.15	0.61
1:Z:106:ARG:HD2	1:Z:349:THR:O	1.99	0.61
1:Z:204:LEU:HD23	1:Z:209:ILE:HB	1.82	0.61
1:O:166:ASP:OD1	1:O:166:ASP:N	2.29	0.61
1:Z:83:ARG:HD3	1:Z:245:ASP:OD1	1.99	0.61
1:Z:458:ASP:N	1:Z:458:ASP:OD1	2.28	0.61
1:O:220:SER:O	1:O:446:LEU:HD23	1.99	0.61
1:Z:202:LYS:C	1:Z:206:VAL:HG23	2.25	0.61
1:Z:275:THR:HG21	1:Z:280:VAL:HG11	1.83	0.61
1:O:315:TRP:CE3	1:O:316:LEU:HD23	2.36	0.61
1:Z:169:LEU:C	1:Z:173:MET:HE2	2.26	0.61
1:O:83:ARG:HH11	1:O:83:ARG:CB	2.13	0.61
1:O:485:GLY:O	1:O:486:TRP:C	2.44	0.61
1:O:338:ASN:O	1:O:375:HIS:HD2	1.84	0.60
1:Z:112:CYS:SG	1:Z:139:THR:HG21	2.41	0.60
1:Z:251:PHE:O	1:Z:254:LEU:N	2.29	0.60
1:O:114:HIS:ND1	1:O:114:HIS:N	2.44	0.60
1:Z:70:SER:O	1:Z:73:GLN:HG3	2.01	0.60
1:Z:406:LEU:HD23	1:Z:407:ARG:N	2.16	0.60
1:O:111:ILE:O	1:O:112:CYS:C	2.44	0.60
1:O:331:TYR:CE2	1:O:335:LYS:HD3	2.35	0.60
1:O:137:SER:O	1:O:141:VAL:HG23	2.01	0.60
1:O:361:ARG:HG2	1:O:361:ARG:NH1	2.13	0.60
1:Z:108:THR:HB	1:Z:139:THR:CB	2.31	0.60
1:Z:153:GLU:HA	1:Z:156:ARG:HG3	1.83	0.60
1:O:386:TYR:HB3	1:O:486:TRP:CE2	2.37	0.60
1:Z:41:LYS:HB2	1:Z:42:PRO:HD2	1.83	0.60
1:Z:52:ILE:HG22	1:Z:53:TRP:N	2.13	0.60
1:Z:83:ARG:NH2	1:Z:303:GLU:OE2	2.35	0.60
1:Z:410:GLY:O	1:Z:413:VAL:HG22	2.02	0.60
1:O:23:HIS:HA	1:O:453:PHE:HE2	1.58	0.60
1:O:74:ILE:CB	1:O:237:ILE:HD13	2.26	0.60
1:O:437:GLU:O	1:O:438:VAL:C	2.44	0.60
1:O:204:LEU:HD21	1:O:214:LEU:CD1	2.28	0.60
1:O:79:ILE:HD12	1:O:170:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:385:ALA:HB1	1:O:425:ILE:HG21	1.83	0.60
1:Z:223:VAL:CG2	1:Z:240:SER:HB3	2.32	0.60
1:Z:351:LEU:HD22	1:Z:360:ALA:HB3	1.82	0.60
1:O:478:GLU:O	1:O:479:ARG:C	2.43	0.59
1:O:18:ALA:HB1	1:O:63:VAL:HG21	1.84	0.59
1:O:109:ALA:HA	1:O:134:PRO:HG3	1.83	0.59
1:O:273:MET:HB2	1:O:395:MET:CE	2.15	0.59
1:Z:109:ALA:O	1:Z:112:CYS:HB2	2.03	0.59
1:Z:265:TYR:HB3	1:Z:412:ALA:HB3	1.85	0.59
1:Z:490:VAL:O	1:Z:491:LYS:C	2.45	0.59
1:O:373:ALA:O	1:O:377:ILE:HG13	2.01	0.59
1:O:432:ARG:NE	1:O:467:GLU:OE1	2.35	0.59
1:Z:110:GLU:O	1:Z:111:ILE:C	2.45	0.59
1:O:152:ARG:HH11	1:O:152:ARG:CG	2.14	0.59
1:O:143:TRP:HE3	1:O:144:ILE:HA	1.68	0.59
1:O:478:GLU:O	1:O:481:TYR:N	2.35	0.59
1:Z:224:TYR:HE2	1:Z:241:GLY:N	2.01	0.59
1:O:19:VAL:HG12	1:O:20:VAL:N	2.17	0.59
1:O:387:GLN:O	1:O:388:THR:C	2.43	0.59
1:O:79:ILE:HD12	1:O:170:ILE:HD12	1.85	0.59
1:O:336:VAL:HG13	1:O:374:ASN:HB3	1.85	0.59
1:O:396:GLN:OE1	1:O:396:GLN:N	2.36	0.59
1:O:314:GLN:HG2	1:O:317:ARG:HH21	1.68	0.59
1:O:104:GLN:NE2	1:O:308:MET:HE2	2.18	0.58
1:O:438:VAL:HG23	1:O:439:THR:N	2.17	0.58
1:Z:97:ILE:HD11	1:Z:144:ILE:HG21	1.84	0.58
1:Z:125:ARG:O	1:Z:129:GLY:HA2	2.02	0.58
1:Z:250:LEU:HD12	1:Z:255:CYS:HB2	1.84	0.58
1:O:13:THR:HG23	1:O:103:TRP:HE1	1.68	0.58
1:O:224:TYR:CE2	1:O:242:ILE:HD12	2.38	0.58
1:Z:350:GLY:HA2	1:Z:360:ALA:O	2.04	0.58
1:Z:389:ARG:O	1:Z:390:ASP:C	2.40	0.58
1:O:37:GLN:NE2	1:O:47:HIS:NE2	2.50	0.58
1:O:251:PHE:CE2	1:O:446:LEU:HD12	2.37	0.58
1:Z:110:GLU:O	1:Z:113:GLU:N	2.36	0.58
1:Z:156:ARG:CG	1:Z:156:ARG:HH11	2.16	0.58
1:Z:5:TYR:HB2	1:Z:74:ILE:HD12	1.85	0.58
1:Z:20:VAL:HG23	1:Z:63:VAL:HG22	1.85	0.58
1:O:28:ILE:N	1:O:28:ILE:HD13	2.17	0.58
1:O:104:GLN:HB3	1:O:349:THR:HG21	1.84	0.58
1:O:445:TYR:CZ	1:O:460:LEU:HD12	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:196:THR:HG22	1:Z:197:LEU:N	2.18	0.58
1:O:110:GLU:OE1	1:O:110:GLU:HA	2.04	0.58
1:Z:23:HIS:HA	1:Z:453:PHE:CE2	2.38	0.58
1:Z:268:GLY:HA2	1:Z:309:ALA:N	2.18	0.58
1:O:428:THR:HG22	1:O:429:ARG:N	2.17	0.58
1:Z:410:GLY:O	1:Z:413:VAL:HG13	2.03	0.58
1:Z:460:LEU:N	1:Z:460:LEU:HD13	2.18	0.58
1:Z:478:GLU:O	1:Z:479:ARG:C	2.44	0.58
1:O:320:MET:HB3	1:O:322:LEU:HG	1.85	0.58
1:O:357:ASP:OD1	1:O:359:TYR:N	2.30	0.58
1:O:394:ALA:O	1:O:397:ALA:HB3	2.03	0.58
1:Z:275:THR:HG21	1:Z:280:VAL:CG1	2.34	0.58
1:Z:308:MET:HA	1:Z:308:MET:HE2	1.86	0.58
1:O:295:THR:N	1:O:297:GLU:OE2	2.37	0.58
1:O:391:VAL:HG23	1:O:392:LEU:N	2.19	0.58
1:Z:371:VAL:HG13	1:Z:375:HIS:HB2	1.86	0.58
1:Z:361:ARG:O	1:Z:362:GLY:C	2.45	0.58
1:O:103:TRP:CE3	1:O:104:GLN:HG2	2.39	0.57
1:Z:275:THR:N	1:Z:300:TYR:O	2.31	0.57
1:O:386:TYR:O	1:O:387:GLN:C	2.47	0.57
1:Z:174:THR:C	1:Z:175:GLN:HG2	2.29	0.57
1:Z:423:SER:HB2	1:Z:428:THR:O	2.05	0.57
1:O:336:VAL:HG23	1:O:338:ASN:N	2.09	0.57
1:O:481:TYR:O	1:O:484:ALA:HB3	2.05	0.57
1:Z:11:GLN:HE22	1:Z:82:GLN:HE21	1.52	0.57
1:O:43:GLY:C	1:O:44:TRP:HD1	2.13	0.57
1:O:327:TYR:HB3	1:O:332:PHE:CZ	2.39	0.57
1:Z:386:TYR:HB3	1:Z:486:TRP:CE2	2.39	0.57
1:Z:83:ARG:HD2	1:Z:244:GLY:CA	2.34	0.57
1:Z:153:GLU:N	1:Z:156:ARG:NH1	2.53	0.57
1:O:337:GLN:HA	1:O:337:GLN:NE2	2.19	0.57
1:Z:118:ASP:HB2	1:Z:120:LEU:HD11	1.87	0.57
1:Z:180:VAL:HG23	1:Z:216:GLU:O	2.05	0.57
1:Z:261:ALA:HB2	1:Z:273:MET:CB	2.32	0.57
1:Z:6:ILE:HD12	1:Z:7:VAL:N	2.19	0.57
1:Z:246:GLN:HG3	1:Z:270:PHE:CB	2.33	0.57
1:O:428:THR:HG22	1:O:429:ARG:O	2.03	0.57
1:Z:153:GLU:OE1	1:Z:156:ARG:HG3	2.04	0.57
1:Z:162:PHE:HB2	1:Z:213:MET:HE2	1.86	0.57
1:O:374:ASN:O	1:O:375:HIS:C	2.48	0.57
1:Z:51:GLU:O	1:Z:52:ILE:C	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:108:THR:HB	1:Z:139:THR:CG2	2.35	0.57
1:Z:110:GLU:HA	1:Z:110:GLU:OE1	2.05	0.57
1:Z:298:VAL:HG23	1:Z:299:ASN:N	2.19	0.57
1:O:402:ARG:O	1:O:404:HIS:HD2	1.87	0.56
1:O:422:GLN:O	1:O:426:LEU:HD22	2.05	0.56
1:Z:170:ILE:HA	1:Z:173:MET:CE	2.33	0.56
1:O:173:MET:CB	1:O:227:THR:HG23	2.34	0.56
1:O:179:HIS:CD2	1:O:215:PRO:HA	2.40	0.56
1:O:373:ALA:O	1:O:376:ILE:HB	2.06	0.56
1:O:420:GLN:O	1:O:421:PHE:C	2.47	0.56
1:O:438:VAL:HA	1:O:441:LEU:CD1	2.32	0.56
1:Z:473:GLY:O	1:Z:474:ILE:HD13	2.05	0.56
1:Z:498:GLU:OE1	1:Z:498:GLU:HA	2.05	0.56
1:Z:87:ILE:HG22	1:Z:88:VAL:N	2.20	0.56
1:O:113:GLU:O	1:O:114:HIS:C	2.46	0.56
1:O:251:PHE:O	1:O:254:LEU:N	2.29	0.56
1:Z:153:GLU:HA	1:Z:156:ARG:NH1	2.21	0.56
1:Z:436:ARG:NH1	1:Z:436:ARG:HG3	2.20	0.56
1:Z:455:GLN:N	1:Z:459:GLU:OE2	2.29	0.56
1:O:391:VAL:O	1:O:392:LEU:C	2.45	0.56
1:Z:20:VAL:CG2	1:Z:63:VAL:HG22	2.36	0.56
1:Z:189:THR:O	1:Z:190:MET:HB3	2.05	0.56
1:O:20:VAL:HG12	1:O:28:ILE:HG12	1.87	0.56
1:O:324:ASN:HD21	1:O:327:TYR:HB2	1.71	0.56
1:O:490:VAL:HG12	1:O:494:MET:HE2	1.88	0.56
1:Z:332:PHE:HA	1:Z:335:LYS:CG	2.36	0.56
1:O:317:ARG:O	1:O:321:LYS:HA	2.06	0.55
1:O:415:ASN:OD1	1:O:417:PHE:HB3	2.06	0.55
1:O:174:THR:O	1:O:177:ARG:HG3	2.06	0.55
1:O:378:ARG:O	1:O:379:ALA:C	2.48	0.55
1:Z:114:HIS:O	1:Z:117:ARG:N	2.39	0.55
1:Z:266:GLY:O	1:Z:310:GLY:N	2.29	0.55
1:Z:416:ASN:N	1:Z:416:ASN:ND2	2.54	0.55
1:O:130:LEU:HD12	1:O:190:MET:HB2	1.87	0.55
1:Z:457:LEU:O	1:Z:460:LEU:N	2.39	0.55
1:O:110:GLU:O	1:O:111:ILE:C	2.49	0.55
1:O:111:ILE:O	1:O:114:HIS:N	2.39	0.55
1:O:240:SER:O	1:O:447:ALA:HA	2.06	0.55
1:O:210:PRO:O	1:O:213:MET:HG3	2.07	0.55
1:O:274:ASN:OD1	1:O:276:GLY:N	2.28	0.55
1:O:475:GLU:O	1:O:476:THR:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:382:GLU:HG2	1:Z:421:PHE:CZ	2.42	0.55
1:O:133:ASP:CG	1:O:134:PRO:HD2	2.31	0.55
1:O:355:TYR:CE2	1:O:490:VAL:HG11	2.42	0.55
1:Z:63:VAL:HG13	1:Z:64:LEU:N	2.22	0.55
1:Z:98:TYR:HD1	1:Z:99:ASN:O	1.89	0.55
1:Z:442:GLY:O	1:Z:445:TYR:HB2	2.07	0.55
1:O:441:LEU:O	1:O:444:ALA:HB3	2.06	0.55
1:O:22:ASP:O	1:O:25:ALA:N	2.30	0.55
1:O:108:THR:CB	1:O:139:THR:HB	2.36	0.55
1:O:335:LYS:HB2	1:O:374:ASN:HD22	1.71	0.55
1:O:434:GLU:N	1:O:465:VAL:O	2.38	0.55
1:Z:111:ILE:O	1:Z:115:LEU:HD23	2.06	0.55
1:O:86:THR:CG2	1:O:162:PHE:HE1	2.11	0.55
1:O:246:GLN:HA	1:O:246:GLN:OE1	2.01	0.55
1:O:406:LEU:O	1:O:431:GLU:N	2.29	0.55
1:O:115:LEU:O	1:O:116:LYS:C	2.50	0.54
1:O:180:VAL:HG22	1:O:181:THR:N	2.22	0.54
1:O:339:THR:HG21	1:O:379:ALA:HA	1.88	0.54
1:Z:83:ARG:HB2	1:Z:83:ARG:NH1	2.17	0.54
1:Z:262:LYS:O	1:Z:271:MET:HA	2.07	0.54
1:O:112:CYS:HB3	1:O:132:ILE:HG22	1.88	0.54
1:O:137:SER:O	1:O:138:GLY:C	2.49	0.54
1:O:186:ALA:O	1:O:189:THR:HG23	2.07	0.54
1:O:380:THR:HG22	1:O:381:LEU:N	2.22	0.54
1:O:388:THR:O	1:O:391:VAL:HG22	2.07	0.54
1:Z:104:GLN:O	1:Z:106:ARG:NE	2.39	0.54
1:O:21:MET:HG3	1:O:25:ALA:HA	1.90	0.54
1:O:127:ASN:HD22	1:O:193:ASN:HD21	1.55	0.54
1:Z:241:GLY:C	1:Z:242:ILE:HG13	2.32	0.54
1:Z:422:GLN:O	1:Z:425:ILE:HG22	2.07	0.54
1:O:392:LEU:HD23	1:O:393:GLU:N	2.23	0.54
1:O:104:GLN:CB	1:O:349:THR:HG21	2.38	0.54
1:O:402:ARG:HG2	1:O:404:HIS:NE2	2.23	0.54
1:Z:48:ASP:O	1:Z:49:PRO:C	2.47	0.54
1:Z:117:ARG:HG2	1:Z:118:ASP:OD1	2.07	0.54
1:O:115:LEU:HD13	1:O:115:LEU:N	2.22	0.54
1:Z:11:GLN:NE2	1:Z:165:VAL:HG11	2.21	0.54
1:O:20:VAL:HG12	1:O:28:ILE:HB	1.89	0.54
1:O:74:ILE:HB	1:O:237:ILE:CD1	2.29	0.54
1:O:442:GLY:O	1:O:445:TYR:HB2	2.07	0.54
1:Z:145:LEU:HG	1:Z:152:ARG:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:293:GLY:HA2	1:Z:299:ASN:ND2	2.23	0.54
1:O:346:PRO:C	1:O:348:PHE:H	2.15	0.53
1:O:41:LYS:CB	1:O:42:PRO:HD2	2.36	0.53
1:O:101:ILE:HD13	1:O:107:ARG:NE	2.23	0.53
1:O:314:GLN:HG2	1:O:317:ARG:NH2	2.22	0.53
1:Z:56:GLN:O	1:Z:56:GLN:NE2	2.28	0.53
1:Z:108:THR:HG21	1:Z:140:LYS:N	2.23	0.53
1:Z:196:THR:HG22	1:Z:198:ASP:H	1.69	0.53
1:O:269:CYS:HB2	1:O:306:VAL:HB	1.90	0.53
1:Z:9:LEU:HB2	1:Z:79:ILE:HD13	1.89	0.53
1:Z:428:THR:HG22	1:Z:429:ARG:N	2.23	0.53
1:O:244:GLY:O	1:O:245:ASP:C	2.51	0.53
1:O:272:LEU:HG	1:O:303:GLU:HB2	1.89	0.53
1:Z:47:HIS:HD2	1:Z:82:GLN:HE22	1.57	0.53
1:Z:74:ILE:HB	1:Z:237:ILE:HD13	1.91	0.53
1:Z:236:ARG:HD3	1:Z:236:ARG:N	2.22	0.53
1:O:339:THR:CG2	1:O:379:ALA:HA	2.38	0.53
1:O:62:GLU:O	1:O:63:VAL:C	2.51	0.53
1:O:250:LEU:HG	1:O:255:CYS:HB2	1.89	0.53
1:Z:453:PHE:HE2	1:Z:454:TRP:CZ2	2.26	0.53
1:O:51:GLU:O	1:O:55:THR:HG23	2.09	0.53
1:O:106:ARG:HD2	1:O:349:THR:O	2.09	0.53
1:Z:165:VAL:O	1:Z:169:LEU:HG	2.09	0.53
1:O:83:ARG:HG3	1:O:245:ASP:OD1	2.09	0.53
1:Z:89:TRP:HD1	1:Z:94:GLY:HA2	1.73	0.53
1:Z:220:SER:O	1:Z:224:TYR:OH	2.26	0.53
1:Z:419:MET:HB2	1:Z:470:PHE:CE2	2.44	0.53
1:O:204:LEU:O	1:O:205:GLU:C	2.52	0.53
1:O:271:MET:C	1:O:272:LEU:HD12	2.34	0.53
1:O:293:GLY:C	1:O:295:THR:H	2.17	0.53
1:O:436:ARG:N	1:O:436:ARG:HD3	2.24	0.53
1:Z:193:ASN:CG	1:Z:196:THR:HB	2.34	0.52
1:O:414:ALA:HA	1:O:432:ARG:HH11	1.73	0.52
1:Z:120:LEU:O	1:Z:121:GLU:C	2.53	0.52
1:Z:273:MET:O	1:Z:301:ALA:HA	2.09	0.52
1:O:151:SER:O	1:O:155:ALA:N	2.35	0.52
1:O:403:LEU:HD13	1:O:403:LEU:N	2.23	0.52
1:Z:342:VAL:HG12	1:Z:343:TYR:N	2.24	0.52
1:O:157:ARG:O	1:O:158:GLY:C	2.50	0.52
1:O:264:THR:HA	1:O:409:ASP:O	2.08	0.52
1:O:372:ASN:ND2	1:O:375:HIS:CE1	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:85:THR:HA	1:Z:101:ILE:O	2.09	0.52
1:Z:162:PHE:CB	1:Z:213:MET:HE2	2.40	0.52
1:Z:416:ASN:H	1:Z:416:ASN:HD22	1.58	0.52
1:O:41:LYS:O	1:O:44:TRP:HB2	2.09	0.52
1:O:83:ARG:NH1	3:O:601:GOL:O1	2.42	0.52
1:Z:190:MET:O	1:Z:203:MET:HG3	2.10	0.52
1:Z:203:MET:CE	1:Z:207:LEU:HD11	2.40	0.52
1:Z:382:GLU:HG2	1:Z:421:PHE:CE2	2.44	0.52
1:O:94:GLY:HA3	1:O:171:TRP:CH2	2.44	0.52
1:O:143:TRP:HE3	1:O:144:ILE:N	2.08	0.52
1:O:256:VAL:CB	1:O:294:PRO:HA	2.40	0.52
1:O:10:ASP:HB3	1:O:17:ARG:HB3	1.91	0.52
1:O:30:VAL:HG12	1:O:31:SER:N	2.24	0.52
1:O:89:TRP:CB	1:O:96:PRO:HA	2.39	0.52
1:O:143:TRP:HE3	1:O:144:ILE:CA	2.23	0.52
1:O:181:THR:HG23	1:O:182:ASP:O	2.09	0.52
1:O:267:THR:HG23	1:O:311:ALA:HB2	1.91	0.52
1:O:433:PRO:HA	1:O:465:VAL:O	2.10	0.52
1:O:199:TRP:HB2	1:O:211:ARG:NH2	2.25	0.52
1:O:203:MET:O	1:O:204:LEU:C	2.50	0.52
1:O:316:LEU:HA	1:O:320:MET:HB2	1.92	0.52
1:O:20:VAL:CG1	1:O:28:ILE:HB	2.39	0.52
1:O:104:GLN:HE22	1:O:308:MET:HE2	1.75	0.52
1:O:339:THR:O	1:O:342:VAL:HB	2.10	0.52
1:O:396:GLN:O	1:O:400:GLY:N	2.30	0.52
1:Z:262:LYS:HZ3	1:Z:264:THR:HB	1.73	0.52
1:Z:23:HIS:C	1:Z:25:ALA:H	2.15	0.52
1:Z:93:THR:OG1	1:Z:95:LYS:HB3	2.10	0.52
1:O:62:GLU:O	1:O:65:ALA:HB3	2.10	0.51
1:Z:37:GLN:OE1	1:Z:47:HIS:HE1	1.93	0.51
1:Z:331:TYR:O	1:Z:335:LYS:HG2	2.10	0.51
1:Z:344:VAL:O	1:Z:346:PRO:HD3	2.10	0.51
1:O:83:ARG:HD3	1:O:244:GLY:HA3	1.90	0.51
1:O:347:ALA:O	1:O:361:ARG:HA	2.10	0.51
1:Z:143:TRP:CE3	1:Z:144:ILE:HA	2.46	0.51
1:Z:293:GLY:C	1:Z:295:THR:H	2.17	0.51
1:Z:340:ASN:HB2	1:Z:375:HIS:CD2	2.45	0.51
1:Z:342:VAL:HA	1:Z:365:PHE:O	2.10	0.51
1:O:112:CYS:HA	1:O:115:LEU:CD2	2.38	0.51
1:Z:3:LYS:HD2	1:Z:72:ASP:O	2.10	0.51
1:Z:336:VAL:HG23	1:Z:338:ASN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:199:TRP:HA	1:O:199:TRP:CE3	2.45	0.51
1:O:396:GLN:NE2	1:O:403:LEU:H	2.08	0.51
1:Z:111:ILE:HG22	1:Z:115:LEU:HD21	1.93	0.51
1:Z:250:LEU:HD11	1:Z:255:CYS:HB2	1.92	0.51
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.92	0.51
1:O:253:GLN:OE1	1:O:253:GLN:HA	2.11	0.51
1:Z:5:TYR:O	1:Z:75:ALA:N	2.44	0.51
1:Z:29:SER:O	1:Z:30:VAL:HG23	2.10	0.51
1:Z:434:GLU:HB2	1:Z:465:VAL:HB	1.93	0.51
1:O:87:ILE:HG22	1:O:88:VAL:N	2.24	0.51
1:O:101:ILE:HD13	1:O:107:ARG:HD3	1.91	0.51
1:O:196:THR:O	1:O:197:LEU:HB2	2.10	0.51
1:O:368:THR:HG22	1:O:369:ARG:N	2.25	0.51
1:O:485:GLY:O	1:O:488:LYS:N	2.43	0.51
1:Z:217:VAL:O	1:Z:218:ARG:HG2	2.10	0.51
1:Z:355:TYR:CD1	1:Z:355:TYR:N	2.77	0.51
1:O:40:PRO:O	1:O:41:LYS:HB3	2.10	0.51
1:O:46:GLU:HB3	1:O:99:ASN:ND2	2.25	0.51
1:O:395:MET:O	1:O:396:GLN:O	2.29	0.51
1:Z:475:GLU:O	1:Z:477:THR:O	2.29	0.51
1:O:19:VAL:HG13	1:O:27:ILE:HG23	1.93	0.51
1:O:221:SER:HB2	1:O:446:LEU:HG	1.92	0.51
1:O:235:THR:C	1:O:236:ARG:HD3	2.36	0.51
1:Z:251:PHE:CE2	1:Z:446:LEU:HD12	2.46	0.51
1:Z:466:ILE:N	1:Z:466:ILE:HD13	2.25	0.51
1:O:162:PHE:CG	1:O:163:GLY:N	2.79	0.51
1:O:332:PHE:O	1:O:334:THR:N	2.43	0.51
1:O:235:THR:O	1:O:236:ARG:HD3	2.10	0.51
1:O:340:ASN:HB2	1:O:375:HIS:CG	2.45	0.51
1:O:407:ARG:HH11	1:O:407:ARG:CG	2.23	0.51
1:Z:175:GLN:C	1:Z:177:ARG:H	2.19	0.51
1:Z:429:ARG:HD3	1:Z:469:GLU:OE2	2.10	0.51
1:O:103:TRP:CZ3	1:O:104:GLN:HG2	2.46	0.50
1:O:180:VAL:HG22	1:O:181:THR:O	2.11	0.50
1:O:190:MET:O	1:O:190:MET:HG2	2.11	0.50
1:O:324:ASN:HB2	1:O:326:ALA:H	1.75	0.50
1:O:475:GLU:O	1:O:478:GLU:N	2.44	0.50
1:Z:123:TYR:OH	1:Z:200:ASP:OD1	2.28	0.50
1:Z:428:THR:N	1:Z:472:PRO:HG3	2.25	0.50
1:O:46:GLU:HB3	1:O:99:ASN:HD22	1.76	0.50
1:O:118:ASP:HB2	1:O:120:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:200:ASP:C	1:O:204:LEU:HD12	2.36	0.50
1:O:434:GLU:CB	1:O:465:VAL:HB	2.35	0.50
1:O:210:PRO:HB3	1:O:212:GLU:OE1	2.11	0.50
1:Z:19:VAL:HG13	1:Z:27:ILE:HG23	1.92	0.50
1:Z:153:GLU:HA	1:Z:156:ARG:HH11	1.76	0.50
1:Z:327:TYR:HB3	1:Z:332:PHE:CE1	2.47	0.50
1:Z:436:ARG:HG3	1:Z:436:ARG:HH11	1.77	0.50
1:O:347:ALA:HB2	1:O:351:LEU:HD11	1.93	0.50
1:O:360:ALA:CB	1:O:494:MET:HA	2.41	0.50
1:O:448:GLY:HA3	1:O:454:TRP:CZ3	2.46	0.50
1:Z:11:GLN:HG2	1:Z:16:SER:OG	2.12	0.50
1:O:151:SER:O	1:O:152:ARG:C	2.55	0.50
1:Z:261:ALA:HA	1:Z:272:LEU:O	2.12	0.50
1:O:41:LYS:O	1:O:44:TRP:N	2.45	0.50
1:O:388:THR:HG21	1:O:422:GLN:NE2	2.27	0.50
1:Z:98:TYR:CD1	1:Z:99:ASN:N	2.80	0.50
1:Z:143:TRP:O	1:Z:144:ILE:C	2.54	0.50
1:Z:409:ASP:CB	1:Z:438:VAL:HG21	2.40	0.50
1:O:331:TYR:CD2	1:O:332:PHE:CD1	2.97	0.50
1:O:365:PHE:HE2	1:O:492:ARG:HB3	1.67	0.50
1:O:427:GLY:C	1:O:472:PRO:HG3	2.36	0.50
1:Z:22:ASP:HB3	1:Z:28:ILE:HD11	1.93	0.50
1:Z:44:TRP:CD1	1:Z:44:TRP:N	2.79	0.50
1:Z:179:HIS:CG	1:Z:215:PRO:HB3	2.47	0.50
1:O:382:GLU:O	1:O:383:SER:C	2.55	0.50
1:Z:171:TRP:NE1	1:Z:176:GLY:HA2	2.27	0.50
1:Z:355:TYR:H	1:Z:355:TYR:HD1	1.54	0.50
1:O:101:ILE:HD13	1:O:107:ARG:CD	2.42	0.50
1:O:142:LYS:O	1:O:146:ASP:OD1	2.30	0.50
1:O:327:TYR:HH	1:Z:331:TYR:HE2	1.59	0.50
1:Z:48:ASP:O	1:Z:51:GLU:N	2.45	0.50
1:Z:126:SER:O	1:Z:195:HIS:HE1	1.95	0.50
1:Z:223:VAL:HG22	1:Z:240:SER:HB3	1.93	0.50
1:Z:453:PHE:CE2	1:Z:454:TRP:CZ2	3.00	0.50
1:O:36:GLU:HG2	1:O:38:ILE:HG13	1.93	0.49
1:O:324:ASN:ND2	1:O:327:TYR:HB2	2.27	0.49
1:Z:44:TRP:CZ3	1:Z:107:ARG:NH2	2.80	0.49
1:Z:117:ARG:C	1:Z:119:GLY:H	2.19	0.49
1:O:52:ILE:O	1:O:53:TRP:C	2.55	0.49
1:O:293:GLY:O	1:O:295:THR:N	2.45	0.49
1:O:327:TYR:HH	1:Z:331:TYR:HH	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:193:ASN:CB	1:Z:196:THR:HB	2.41	0.49
1:O:35:PHE:HE1	1:O:47:HIS:CE1	2.31	0.49
1:O:98:TYR:CD1	1:O:99:ASN:N	2.81	0.49
1:Z:162:PHE:O	1:Z:179:HIS:HE1	1.96	0.49
1:O:208:ASP:C	1:O:209:ILE:HG12	2.37	0.49
1:Z:347:ALA:O	1:Z:361:ARG:HA	2.11	0.49
1:Z:355:TYR:OH	1:Z:390:ASP:OD1	2.30	0.49
1:Z:359:TYR:CZ	1:Z:499:HIS:CE1	2.99	0.49
1:O:38:ILE:O	1:O:40:PRO:HD3	2.13	0.49
1:O:83:ARG:NH1	1:O:83:ARG:CB	2.74	0.49
1:Z:60:LEU:HD12	1:Z:60:LEU:O	2.11	0.49
1:Z:457:LEU:O	1:Z:458:ASP:C	2.55	0.49
1:O:89:TRP:HB3	1:O:96:PRO:HA	1.93	0.49
1:O:343:TYR:CE2	1:O:486:TRP:N	2.81	0.49
1:O:355:TYR:N	1:O:355:TYR:CD1	2.79	0.49
1:Z:423:SER:CB	1:Z:430:VAL:HG23	2.43	0.49
1:O:335:LYS:HB2	1:O:374:ASN:ND2	2.28	0.49
1:Z:413:VAL:HG22	1:Z:436:ARG:HD2	1.94	0.49
1:O:6:ILE:HD13	1:O:75:ALA:HB3	1.95	0.49
1:O:61:VAL:O	1:O:62:GLU:C	2.56	0.49
1:O:106:ARG:HH22	1:O:135:TYR:HA	1.78	0.49
1:O:241:GLY:C	1:O:242:ILE:HG13	2.37	0.49
1:Z:40:PRO:HG3	1:Z:46:GLU:CD	2.38	0.49
1:Z:151:SER:HA	1:Z:160:LEU:HD11	1.95	0.49
1:O:6:ILE:CD1	1:O:75:ALA:HB3	2.42	0.49
1:O:173:MET:O	1:O:227:THR:HG23	2.13	0.49
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.95	0.49
1:O:97:ILE:HG21	1:O:160:LEU:HD21	1.94	0.49
1:Z:56:GLN:HE21	1:Z:56:GLN:C	2.17	0.49
1:Z:174:THR:HG22	1:Z:226:GLN:O	2.12	0.49
1:Z:228:ASN:ND2	1:Z:229:ILE:N	2.61	0.49
1:Z:256:VAL:HG11	1:Z:294:PRO:HB3	1.94	0.49
1:O:435:VAL:HG12	1:O:437:GLU:H	1.77	0.48
1:Z:151:SER:O	1:Z:152:ARG:C	2.56	0.48
1:Z:396:GLN:HB3	1:Z:401:ILE:O	2.13	0.48
1:Z:416:ASN:O	1:Z:417:PHE:C	2.56	0.48
1:Z:488:LYS:O	1:Z:489:ALA:C	2.56	0.48
1:O:13:THR:CG2	1:O:103:TRP:NE1	2.77	0.48
1:Z:104:GLN:NE2	1:Z:308:MET:CE	2.77	0.48
1:Z:161:LEU:HD23	1:Z:161:LEU:N	2.26	0.48
1:Z:265:TYR:OH	1:Z:422:GLN:NE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:316:LEU:HD23	1:Z:316:LEU:HA	1.61	0.48
1:Z:456:ASN:ND2	1:Z:459:GLU:H	2.11	0.48
1:O:83:ARG:HH11	1:O:83:ARG:HB2	1.78	0.48
1:O:97:ILE:HD11	1:O:144:ILE:CG2	2.43	0.48
1:O:240:SER:HB2	1:O:450:ALA:CB	2.43	0.48
1:Z:166:ASP:O	1:Z:170:ILE:HG12	2.13	0.48
1:Z:14:THR:HG22	1:Z:37:GLN:CD	2.38	0.48
1:Z:89:TRP:N	1:Z:89:TRP:CE3	2.81	0.48
1:O:204:LEU:O	1:O:208:ASP:N	2.46	0.48
1:O:409:ASP:CG	1:O:438:VAL:HG21	2.38	0.48
1:Z:311:ALA:HA	1:Z:314:GLN:HE21	1.77	0.48
1:O:48:ASP:O	1:O:51:GLU:N	2.45	0.48
1:Z:83:ARG:HB2	3:Z:603:GOL:O2	2.13	0.48
1:Z:179:HIS:CD2	1:Z:215:PRO:HA	2.48	0.48
1:Z:196:THR:O	1:Z:197:LEU:HB2	2.13	0.48
1:O:59:THR:O	1:O:60:LEU:C	2.56	0.48
1:O:142:LYS:NZ	1:O:146:ASP:OD2	2.46	0.48
1:Z:114:HIS:O	1:Z:116:LYS:N	2.46	0.48
1:Z:193:ASN:O	1:Z:197:LEU:N	2.43	0.48
1:Z:416:ASN:ND2	1:Z:416:ASN:H	2.12	0.48
1:O:94:GLY:HA3	1:O:171:TRP:CZ3	2.49	0.48
1:O:368:THR:HB	1:O:371:VAL:HG23	1.95	0.48
1:O:425:ILE:HD12	1:O:425:ILE:HA	1.54	0.48
1:Z:152:ARG:C	1:Z:156:ARG:HH11	2.22	0.48
1:Z:286:LEU:CD2	1:Z:304:GLY:HA2	2.44	0.48
1:Z:315:TRP:CZ2	1:Z:320:MET:HG3	2.49	0.48
1:O:13:THR:HG21	1:O:103:TRP:NE1	2.29	0.48
1:O:137:SER:HA	1:O:140:LYS:HD2	1.96	0.48
1:O:256:VAL:HB	1:O:294:PRO:HA	1.96	0.48
1:O:265:TYR:CB	1:O:412:ALA:HB3	2.39	0.48
1:Z:21:MET:HA	1:Z:26:ASN:O	2.14	0.48
1:Z:179:HIS:CD2	1:Z:215:PRO:HB3	2.48	0.48
1:Z:203:MET:HA	1:Z:203:MET:CE	2.35	0.48
1:Z:474:ILE:HG13	1:Z:478:GLU:OE1	2.13	0.48
1:O:175:GLN:C	1:O:177:ARG:H	2.22	0.48
1:Z:89:TRP:HB2	1:Z:95:LYS:O	2.14	0.48
1:Z:104:GLN:HE22	1:Z:308:MET:CE	2.27	0.48
1:Z:142:LYS:O	1:Z:146:ASP:OD1	2.32	0.48
1:Z:420:GLN:NE2	1:Z:424:ASP:OD1	2.46	0.48
1:O:40:PRO:HG2	1:O:44:TRP:CB	2.43	0.47
1:Z:19:VAL:HG12	1:Z:21:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:111:ILE:HB	1:Z:139:THR:HG22	1.96	0.47
1:Z:192:PHE:CZ	1:Z:197:LEU:HA	2.49	0.47
1:Z:2:GLU:HG3	1:Z:3:LYS:N	2.30	0.47
1:Z:133:ASP:CG	1:Z:134:PRO:HD2	2.38	0.47
1:Z:180:VAL:CG2	1:Z:181:THR:N	2.76	0.47
1:O:174:THR:HG21	1:O:178:VAL:CG1	2.43	0.47
1:O:251:PHE:CD2	1:O:446:LEU:CD1	2.97	0.47
1:O:257:LYS:O	1:O:274:ASN:HB3	2.14	0.47
1:Z:104:GLN:NE2	1:Z:308:MET:HE3	2.29	0.47
1:Z:290:ILE:CG2	1:Z:291:ALA:N	2.78	0.47
1:Z:332:PHE:HB3	1:Z:374:ASN:OD1	2.15	0.47
1:Z:438:VAL:O	1:Z:441:LEU:HB2	2.14	0.47
1:Z:445:TYR:CD1	1:Z:445:TYR:N	2.82	0.47
1:O:60:LEU:O	1:O:63:VAL:HG23	2.13	0.47
1:Z:18:ALA:HB1	1:Z:63:VAL:HG11	1.95	0.47
1:Z:136:PHE:HB3	1:Z:188:ARG:O	2.13	0.47
1:Z:209:ILE:HA	1:Z:210:PRO:HD2	1.65	0.47
1:Z:256:VAL:HG11	1:Z:294:PRO:CA	2.45	0.47
1:O:125:ARG:HD3	1:O:281:LYS:HE3	1.96	0.47
1:O:368:THR:CG2	1:O:369:ARG:N	2.78	0.47
1:O:406:LEU:N	1:O:429:ARG:O	2.47	0.47
1:Z:115:LEU:HD22	1:Z:115:LEU:N	2.20	0.47
1:Z:332:PHE:HB2	1:Z:377:ILE:HD12	1.95	0.47
1:Z:463:LYS:HD2	1:Z:463:LYS:HA	1.50	0.47
1:O:174:THR:O	1:O:175:GLN:HB2	2.14	0.47
1:O:347:ALA:HB2	1:O:351:LEU:CD1	2.45	0.47
1:O:364:ILE:HG22	1:O:365:PHE:N	2.28	0.47
1:O:406:LEU:CD2	1:O:407:ARG:H	2.23	0.47
1:O:428:THR:CG2	1:O:429:ARG:N	2.78	0.47
1:O:455:GLN:N	1:O:459:GLU:OE2	2.28	0.47
1:O:497:GLU:HG3	1:O:498:GLU:O	2.15	0.47
1:Z:27:ILE:N	1:Z:27:ILE:HD12	2.28	0.47
1:Z:46:GLU:OE2	1:Z:107:ARG:NH2	2.43	0.47
1:Z:181:THR:O	1:Z:217:VAL:HA	2.14	0.47
1:Z:250:LEU:O	1:Z:253:GLN:HB2	2.14	0.47
1:Z:263:ASN:HB3	1:Z:408:VAL:HG12	1.96	0.47
1:Z:293:GLY:O	1:Z:296:GLY:N	2.44	0.47
1:Z:407:ARG:HH11	1:Z:407:ARG:CG	2.19	0.47
1:Z:432:ARG:O	1:Z:467:GLU:N	2.48	0.47
1:O:13:THR:HG21	1:O:103:TRP:HE1	1.80	0.47
1:O:23:HIS:HA	1:O:453:PHE:CZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:338:ASN:C	1:O:340:ASN:H	2.23	0.47
1:Z:443:ALA:O	1:Z:444:ALA:C	2.57	0.47
1:O:193:ASN:CG	1:O:196:THR:HB	2.40	0.47
1:O:226:GLN:HA	1:O:239:ILE:HG13	1.97	0.47
1:O:445:TYR:CZ	1:O:460:LEU:CD1	2.98	0.47
1:O:456:ASN:O	1:O:458:ASP:N	2.48	0.47
1:Z:109:ALA:O	1:Z:112:CYS:N	2.48	0.47
1:O:20:VAL:HG12	1:O:28:ILE:CB	2.45	0.47
1:O:277:GLU:CD	1:O:277:GLU:H	2.23	0.47
1:O:407:ARG:CG	1:O:407:ARG:NH1	2.78	0.47
1:Z:23:HIS:HA	1:Z:453:PHE:CZ	2.50	0.47
1:Z:256:VAL:HG11	1:Z:294:PRO:HA	1.97	0.47
1:Z:374:ASN:O	1:Z:375:HIS:C	2.58	0.47
1:Z:478:GLU:CA	1:Z:481:TYR:HB3	2.45	0.47
1:O:7:VAL:HG12	1:O:77:ILE:CG1	2.37	0.46
1:O:83:ARG:NH1	1:O:83:ARG:HB2	2.30	0.46
1:O:137:SER:O	1:O:140:LYS:HB2	2.15	0.46
1:Z:457:LEU:HD13	1:Z:457:LEU:HA	1.52	0.46
1:O:59:THR:O	1:O:63:VAL:HG22	2.16	0.46
1:Z:87:ILE:CG2	1:Z:88:VAL:N	2.79	0.46
1:Z:251:PHE:CE2	1:Z:446:LEU:CD1	2.99	0.46
1:Z:332:PHE:O	1:Z:333:ALA:C	2.57	0.46
1:Z:342:VAL:CG1	1:Z:343:TYR:N	2.78	0.46
1:O:162:PHE:O	1:O:179:HIS:HE1	1.98	0.46
1:O:440:ALA:O	1:O:441:LEU:C	2.57	0.46
1:Z:114:HIS:CD2	1:Z:117:ARG:NH2	2.83	0.46
1:Z:256:VAL:HG11	1:Z:294:PRO:CB	2.45	0.46
1:Z:456:ASN:HD22	1:Z:459:GLU:H	1.63	0.46
1:O:108:THR:O	1:O:109:ALA:C	2.58	0.46
1:Z:20:VAL:HG23	1:Z:63:VAL:CG2	2.45	0.46
1:Z:387:GLN:O	1:Z:388:THR:C	2.57	0.46
1:O:109:ALA:O	1:O:112:CYS:HB2	2.15	0.46
1:Z:130:LEU:HD23	1:Z:190:MET:HB2	1.97	0.46
1:Z:330:GLU:HG3	1:Z:415:ASN:CG	2.40	0.46
1:O:353:ALA:HA	1:O:354:PRO:HA	1.56	0.46
1:Z:6:ILE:HD12	1:Z:6:ILE:C	2.41	0.46
1:Z:19:VAL:HG22	1:Z:30:VAL:CG2	2.43	0.46
1:Z:153:GLU:CA	1:Z:156:ARG:NH1	2.79	0.46
1:Z:240:SER:HB2	1:Z:450:ALA:CB	2.45	0.46
1:Z:392:LEU:O	1:Z:392:LEU:HG	2.11	0.46
1:Z:394:ALA:O	1:Z:398:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:83:ARG:NE	1:O:246:GLN:HB2	2.30	0.46
1:Z:22:ASP:CG	1:Z:28:ILE:HD11	2.40	0.46
1:Z:141:VAL:CG2	1:Z:162:PHE:CD1	2.99	0.46
1:Z:184:THR:O	1:Z:187:SER:OG	2.29	0.46
1:Z:186:ALA:C	1:Z:188:ARG:H	2.23	0.46
1:Z:253:GLN:OE1	1:Z:407:ARG:HD3	2.16	0.46
1:Z:272:LEU:N	1:Z:272:LEU:CD1	2.79	0.46
1:Z:355:TYR:CE2	1:Z:490:VAL:HG11	2.51	0.46
1:O:222:GLU:O	1:O:240:SER:HA	2.16	0.46
1:O:403:LEU:N	1:O:403:LEU:CD1	2.79	0.46
1:O:432:ARG:HA	1:O:433:PRO:HD3	1.68	0.46
1:Z:38:ILE:O	1:Z:40:PRO:HD3	2.16	0.46
1:Z:114:HIS:HD2	1:Z:117:ARG:NH2	2.14	0.46
1:Z:373:ALA:O	1:Z:377:ILE:HG13	2.16	0.46
1:O:74:ILE:HD12	1:O:74:ILE:HA	1.80	0.46
1:O:154:ARG:HB3	1:O:159:GLU:HG3	1.97	0.46
1:O:183:TYR:O	1:O:184:THR:C	2.57	0.46
1:Z:93:THR:HG1	1:Z:95:LYS:HB3	1.80	0.46
1:Z:223:VAL:O	1:Z:223:VAL:HG12	2.10	0.46
1:Z:401:ILE:CG2	1:Z:402:ARG:N	2.79	0.46
1:O:19:VAL:CG1	1:O:20:VAL:N	2.79	0.46
1:O:80:THR:OG1	1:O:245:ASP:HA	2.16	0.46
1:Z:30:VAL:CG1	1:Z:31:SER:N	2.77	0.46
1:Z:212:GLU:OE1	1:Z:212:GLU:N	2.38	0.46
1:O:180:VAL:CG2	1:O:181:THR:N	2.79	0.45
1:Z:153:GLU:HA	1:Z:153:GLU:OE1	2.16	0.45
1:Z:317:ARG:NE	1:Z:318:ASP:OD1	2.49	0.45
1:O:124:ILE:O	1:O:128:THR:OG1	2.29	0.45
1:O:223:VAL:HG22	1:O:240:SER:HB3	1.97	0.45
1:O:274:ASN:HD21	1:O:299:ASN:HD22	1.63	0.45
1:Z:117:ARG:HG2	1:Z:118:ASP:N	2.31	0.45
1:Z:311:ALA:O	1:Z:314:GLN:HG3	2.15	0.45
1:O:94:GLY:CA	1:O:171:TRP:CH2	2.99	0.45
1:O:275:THR:HB	1:O:280:VAL:HG21	1.97	0.45
1:O:289:THR:O	1:O:301:ALA:N	2.47	0.45
1:O:346:PRO:HG3	1:O:383:SER:OG	2.16	0.45
1:O:420:GLN:NE2	1:O:420:GLN:O	2.50	0.45
1:O:436:ARG:N	1:O:436:ARG:CD	2.79	0.45
1:O:482:ARG:O	1:O:483:TYR:C	2.58	0.45
1:Z:401:ILE:HG22	1:Z:402:ARG:N	2.32	0.45
1:O:142:LYS:O	1:O:144:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:155:ALA:CB	1:O:210:PRO:HG2	2.47	0.45
1:O:236:ARG:HD3	1:O:236:ARG:HA	1.76	0.45
1:O:372:ASN:OD1	1:O:374:ASN:HB2	2.16	0.45
1:O:407:ARG:NH1	1:O:407:ARG:HG2	2.30	0.45
1:Z:91:LYS:HB2	1:Z:161:LEU:HD21	1.98	0.45
1:Z:128:THR:OG1	1:Z:130:LEU:HB2	2.17	0.45
1:Z:251:PHE:CD2	1:Z:446:LEU:CD1	3.00	0.45
1:Z:313:ILE:O	1:Z:314:GLN:C	2.56	0.45
1:Z:372:ASN:O	1:Z:373:ALA:C	2.57	0.45
1:Z:417:PHE:C	1:Z:417:PHE:CD2	2.95	0.45
1:Z:428:THR:CG2	1:Z:429:ARG:N	2.79	0.45
1:Z:436:ARG:HH11	1:Z:436:ARG:CG	2.29	0.45
1:O:352:GLY:C	1:O:356:TRP:H	2.20	0.45
1:O:364:ILE:CG2	1:O:365:PHE:N	2.80	0.45
1:O:411:GLY:O	1:O:412:ALA:C	2.59	0.45
1:Z:64:LEU:HD22	1:Z:69:ILE:HG22	1.99	0.45
1:Z:83:ARG:HH11	1:Z:83:ARG:CB	2.22	0.45
1:Z:141:VAL:HG22	1:Z:162:PHE:CD1	2.52	0.45
1:Z:170:ILE:CA	1:Z:173:MET:HE3	2.38	0.45
1:Z:184:THR:HG22	1:Z:290:ILE:O	2.16	0.45
1:Z:406:LEU:HD23	1:Z:407:ARG:H	1.81	0.45
1:Z:456:ASN:ND2	1:Z:458:ASP:CB	2.79	0.45
1:O:83:ARG:NH1	1:O:246:GLN:HG2	2.31	0.45
1:O:138:GLY:HA2	1:O:191:LEU:HD21	1.99	0.45
1:O:251:PHE:CE1	1:O:256:VAL:CG1	3.00	0.45
1:O:272:LEU:HA	1:O:302:LEU:O	2.16	0.45
1:O:337:GLN:NE2	1:O:337:GLN:CA	2.79	0.45
1:Z:457:LEU:HA	1:Z:460:LEU:HD23	1.99	0.45
1:O:201:ASP:O	1:O:202:LYS:C	2.59	0.45
1:O:218:ARG:HB3	1:O:222:GLU:OE2	2.16	0.45
1:O:272:LEU:HD12	1:O:272:LEU:N	2.31	0.45
1:O:385:ALA:O	1:O:388:THR:HB	2.17	0.45
1:O:395:MET:O	1:O:399:SER:N	2.45	0.45
1:Z:324:ASN:HB2	1:Z:325:ASP:H	1.30	0.45
1:O:179:HIS:CD2	1:O:215:PRO:CA	3.00	0.45
1:O:214:LEU:O	2:O:602:EPE:H62	2.17	0.45
1:O:449:LEU:C	1:O:451:VAL:H	2.25	0.45
1:Z:252:GLY:HA2	1:Z:445:TYR:CE2	2.52	0.45
1:Z:286:LEU:HA	1:Z:286:LEU:HD23	1.45	0.45
1:Z:418:LEU:HD23	1:Z:418:LEU:HA	1.63	0.45
1:Z:441:LEU:O	1:Z:442:GLY:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:336:VAL:HG21	1:O:338:ASN:O	2.16	0.45
1:O:352:GLY:HA2	1:O:356:TRP:HA	1.98	0.45
1:Z:27:ILE:N	1:Z:27:ILE:CD1	2.79	0.45
1:Z:115:LEU:CD2	1:Z:115:LEU:N	2.78	0.45
1:Z:224:TYR:CE2	1:Z:242:ILE:CD1	2.99	0.45
1:Z:360:ALA:C	1:Z:361:ARG:HG2	2.41	0.45
1:O:48:ASP:HB3	1:O:51:GLU:HB2	1.97	0.45
1:O:97:ILE:O	1:O:98:TYR:HB2	2.16	0.45
1:O:145:LEU:HB3	1:O:152:ARG:NH1	2.32	0.45
1:O:425:ILE:O	1:O:479:ARG:HD2	2.17	0.45
1:Z:446:LEU:HD12	1:Z:446:LEU:N	2.32	0.45
1:O:27:ILE:N	1:O:27:ILE:CD1	2.79	0.44
1:O:184:THR:O	1:O:185:ASN:C	2.58	0.44
1:O:474:ILE:HG22	1:O:479:ARG:HB2	1.99	0.44
1:Z:111:ILE:HG22	1:Z:115:LEU:CD2	2.47	0.44
1:Z:346:PRO:C	1:Z:348:PHE:H	2.25	0.44
1:Z:414:ALA:O	1:Z:416:ASN:ND2	2.50	0.44
1:O:7:VAL:HG23	1:O:20:VAL:HG22	2.00	0.44
1:O:224:TYR:CD1	1:O:224:TYR:N	2.86	0.44
1:O:281:LYS:HG2	1:O:282:SER:N	2.32	0.44
1:O:331:TYR:CE2	1:O:335:LYS:CE	3.00	0.44
1:O:460:LEU:HD23	1:O:460:LEU:H	1.78	0.44
1:Z:63:VAL:CG1	1:Z:64:LEU:N	2.80	0.44
1:Z:203:MET:HE3	1:Z:207:LEU:HD11	2.00	0.44
1:Z:419:MET:HB2	1:Z:470:PHE:CZ	2.52	0.44
1:O:144:ILE:O	1:O:145:LEU:C	2.59	0.44
1:O:190:MET:HE3	1:O:190:MET:HB3	1.78	0.44
1:O:476:THR:CG2	1:O:479:ARG:NH2	2.79	0.44
1:Z:22:ASP:CB	1:Z:28:ILE:HD11	2.48	0.44
1:Z:88:VAL:HA	1:Z:161:LEU:O	2.18	0.44
1:O:115:LEU:HD22	1:O:115:LEU:N	2.20	0.44
1:O:294:PRO:O	1:O:295:THR:HG22	2.17	0.44
1:O:380:THR:O	1:O:381:LEU:C	2.58	0.44
1:Z:171:TRP:CD1	1:Z:176:GLY:HA2	2.53	0.44
1:Z:186:ALA:O	1:Z:189:THR:HG23	2.18	0.44
1:Z:337:GLN:O	1:Z:338:ASN:HB3	2.17	0.44
1:Z:406:LEU:CD2	1:Z:407:ARG:N	2.80	0.44
1:Z:456:ASN:ND2	1:Z:459:GLU:HG3	2.33	0.44
1:Z:456:ASN:HD22	1:Z:456:ASN:C	2.25	0.44
1:O:200:ASP:O	1:O:201:ASP:C	2.58	0.44
1:O:250:LEU:HD13	1:O:262:LYS:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:361:ARG:NH1	1:O:361:ARG:CG	2.79	0.44
1:O:402:ARG:HG3	1:O:403:LEU:O	2.18	0.44
1:Z:80:THR:OG1	1:Z:245:ASP:HA	2.18	0.44
1:Z:155:ALA:O	1:Z:158:GLY:N	2.51	0.44
1:Z:223:VAL:HA	1:Z:240:SER:CB	2.46	0.44
1:Z:271:MET:HG2	1:Z:395:MET:HE3	1.99	0.44
1:Z:438:VAL:H	1:Z:438:VAL:HG22	1.50	0.44
1:Z:446:LEU:CD1	1:Z:446:LEU:N	2.81	0.44
1:O:69:ILE:CG2	1:O:70:SER:N	2.80	0.44
1:O:145:LEU:O	1:O:146:ASP:C	2.61	0.44
1:O:418:LEU:HD13	1:O:419:MET:CE	2.46	0.44
1:Z:47:HIS:HB3	1:Z:52:ILE:HD11	2.00	0.44
1:Z:180:VAL:HG22	1:Z:181:THR:N	2.33	0.44
1:Z:339:THR:O	1:Z:375:HIS:HB3	2.18	0.44
1:O:41:LYS:O	1:O:42:PRO:C	2.61	0.44
1:O:250:LEU:CG	1:O:255:CYS:HB2	2.47	0.44
1:O:342:VAL:HG12	1:O:379:ALA:CB	2.47	0.44
1:O:420:GLN:C	1:O:420:GLN:HE21	2.26	0.44
1:Z:9:LEU:HB2	1:Z:79:ILE:CD1	2.47	0.44
1:Z:427:GLY:C	1:Z:472:PRO:HG3	2.43	0.44
1:O:69:ILE:HG22	1:O:70:SER:N	2.31	0.44
1:O:170:ILE:O	1:O:174:THR:HG23	2.18	0.44
1:O:224:TYR:HE1	1:O:240:SER:C	2.25	0.44
1:O:365:PHE:CE2	1:O:492:ARG:CB	2.95	0.44
1:O:438:VAL:O	1:O:439:THR:C	2.60	0.44
1:Z:73:GLN:C	1:Z:74:ILE:HD13	2.43	0.44
1:Z:74:ILE:HB	1:Z:237:ILE:CD1	2.47	0.44
1:Z:150:GLY:O	1:Z:152:ARG:N	2.51	0.44
1:Z:203:MET:HE3	1:Z:203:MET:CA	2.48	0.44
1:O:88:VAL:HA	1:O:161:LEU:O	2.17	0.44
1:O:224:TYR:HE1	1:O:241:GLY:N	2.16	0.44
1:Z:84:GLU:OE1	3:Z:603:GOL:O1	2.33	0.44
1:Z:123:TYR:O	1:Z:127:ASN:N	2.48	0.44
1:Z:441:LEU:HD23	1:Z:441:LEU:HA	1.75	0.44
1:O:108:THR:HB	1:O:139:THR:CG2	2.47	0.43
1:O:179:HIS:CD2	1:O:215:PRO:CB	2.97	0.43
1:O:224:TYR:CE1	1:O:240:SER:CA	3.00	0.43
1:Z:390:ASP:HA	1:Z:483:TYR:OH	2.18	0.43
1:O:214:LEU:HA	1:O:215:PRO:HD3	1.85	0.43
1:O:222:GLU:HG3	1:O:223:VAL:N	2.31	0.43
1:Z:127:ASN:HB3	1:Z:193:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:339:THR:HB	1:O:342:VAL:HB	1.99	0.43
1:O:396:GLN:HE22	1:O:403:LEU:HD22	1.82	0.43
1:Z:131:VAL:HG11	1:Z:356:TRP:CD2	2.53	0.43
1:Z:210:PRO:O	1:Z:212:GLU:N	2.51	0.43
1:O:53:TRP:CZ3	1:O:172:LYS:HB2	2.54	0.43
1:O:134:PRO:O	1:O:140:LYS:NZ	2.51	0.43
1:O:152:ARG:CG	1:O:152:ARG:NH1	2.78	0.43
1:O:178:VAL:O	1:O:178:VAL:HG22	2.16	0.43
1:O:200:ASP:O	1:O:203:MET:N	2.51	0.43
1:O:213:MET:HG3	1:O:213:MET:H	1.54	0.43
1:O:225:GLY:C	1:O:226:GLN:HG3	2.40	0.43
1:Z:102:VAL:O	1:Z:103:TRP:C	2.62	0.43
1:Z:182:ASP:OD2	1:Z:184:THR:OG1	2.30	0.43
1:Z:275:THR:HG23	1:Z:301:ALA:HA	2.01	0.43
1:Z:425:ILE:HG23	1:Z:426:LEU:N	2.34	0.43
1:O:120:LEU:O	1:O:121:GLU:O	2.36	0.43
1:O:456:ASN:C	1:O:458:ASP:N	2.74	0.43
1:O:27:ILE:HD12	1:O:27:ILE:H	1.82	0.43
1:O:98:TYR:CE2	1:O:143:TRP:HH2	2.37	0.43
1:O:135:TYR:CD2	1:O:136:PHE:CE1	3.07	0.43
1:O:145:LEU:HG	1:O:152:ARG:HG2	2.01	0.43
1:Z:24:ASP:O	1:Z:463:LYS:HE2	2.19	0.43
1:Z:41:LYS:O	1:Z:44:TRP:N	2.43	0.43
1:Z:143:TRP:HE3	1:Z:144:ILE:HA	1.82	0.43
1:Z:174:THR:HB	1:Z:177:ARG:HB3	1.99	0.43
1:Z:289:THR:HG23	1:Z:290:ILE:N	2.33	0.43
1:O:92:GLU:H	1:O:92:GLU:HG2	1.52	0.43
1:O:328:ASP:O	1:O:331:TYR:HB3	2.18	0.43
1:Z:345:VAL:O	1:Z:362:GLY:HA2	2.18	0.43
1:Z:381:LEU:HA	1:Z:381:LEU:HD23	1.74	0.43
1:Z:479:ARG:HG2	1:Z:480:ASN:OD1	2.19	0.43
1:O:416:ASN:H	1:O:416:ASN:ND2	2.16	0.43
1:O:468:ARG:CG	1:O:469:GLU:N	2.82	0.43
1:Z:23:HIS:C	1:Z:25:ALA:N	2.77	0.43
1:Z:144:ILE:HG22	1:Z:145:LEU:N	2.33	0.43
1:O:197:LEU:N	1:O:197:LEU:HD13	2.33	0.43
1:O:315:TRP:CD1	1:O:319:GLU:HB2	2.53	0.43
1:Z:91:LYS:NZ	1:Z:158:GLY:O	2.43	0.43
1:Z:197:LEU:HA	1:Z:197:LEU:HD12	1.60	0.43
1:O:76:ALA:CB	1:O:238:PRO:HG2	2.48	0.43
1:O:220:SER:O	1:O:241:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:258:GLU:HB2	1:O:275:THR:C	2.43	0.43
1:O:265:TYR:CD1	1:O:265:TYR:N	2.86	0.43
1:Z:210:PRO:C	1:Z:212:GLU:N	2.75	0.43
1:Z:214:LEU:HA	1:Z:215:PRO:HD3	1.76	0.43
1:O:265:TYR:HB2	1:O:413:VAL:HG13	1.99	0.42
1:O:266:GLY:O	1:O:267:THR:C	2.60	0.42
1:O:346:PRO:HA	1:O:348:PHE:CD1	2.54	0.42
1:O:391:VAL:CG2	1:O:392:LEU:N	2.81	0.42
1:Z:103:TRP:CE2	3:Z:603:GOL:H11	2.53	0.42
1:Z:131:VAL:O	1:Z:136:PHE:HE2	2.02	0.42
1:Z:160:LEU:O	1:Z:161:LEU:HD23	2.18	0.42
1:Z:469:GLU:HG3	1:Z:471:ARG:HH21	1.73	0.42
1:O:97:ILE:HD12	1:O:148:VAL:HG21	2.01	0.42
1:O:153:GLU:O	1:O:156:ARG:HB2	2.19	0.42
1:O:165:VAL:O	1:O:166:ASP:C	2.61	0.42
1:O:342:VAL:CG1	1:O:343:TYR:N	2.79	0.42
1:O:388:THR:CB	1:O:422:GLN:NE2	2.78	0.42
1:Z:83:ARG:NH2	1:Z:303:GLU:CD	2.77	0.42
1:Z:263:ASN:ND2	1:Z:265:TYR:CE1	2.87	0.42
1:Z:128:THR:HB	1:Z:130:LEU:HD22	2.00	0.42
1:O:141:VAL:HB	1:O:209:ILE:CD1	2.49	0.42
1:O:151:SER:O	1:O:154:ARG:N	2.52	0.42
1:O:155:ALA:HA	1:O:160:LEU:HB2	2.01	0.42
1:O:297:GLU:HG2	1:O:297:GLU:H	1.50	0.42
1:O:406:LEU:HA	1:O:406:LEU:HD23	1.33	0.42
1:O:452:GLY:C	1:O:454:TRP:N	2.74	0.42
1:O:458:ASP:O	1:O:459:GLU:C	2.62	0.42
1:Z:143:TRP:HE3	1:Z:144:ILE:N	2.17	0.42
1:Z:186:ALA:C	1:Z:188:ARG:N	2.75	0.42
1:Z:340:ASN:HB2	1:Z:375:HIS:NE2	2.35	0.42
1:Z:355:TYR:HH	1:Z:390:ASP:CG	2.26	0.42
1:Z:423:SER:O	1:Z:424:ASP:C	2.62	0.42
1:O:172:LYS:HB3	1:O:172:LYS:HE3	1.85	0.42
1:O:273:MET:O	1:O:301:ALA:HA	2.18	0.42
1:Z:56:GLN:NE2	1:Z:56:GLN:HA	2.34	0.42
1:Z:152:ARG:C	1:Z:156:ARG:NH1	2.77	0.42
1:Z:190:MET:C	1:Z:191:LEU:HD23	2.44	0.42
1:Z:268:GLY:HA2	1:Z:309:ALA:H	1.85	0.42
1:Z:365:PHE:CZ	1:Z:492:ARG:HB3	2.54	0.42
1:Z:497:GLU:HG3	1:Z:498:GLU:N	2.34	0.42
1:O:21:MET:HB3	1:O:21:MET:HE3	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:81:ASN:N	1:O:81:ASN:ND2	2.54	0.42
1:O:305:ALA:O	1:O:353:ALA:HB3	2.20	0.42
1:O:339:THR:HG22	1:O:379:ALA:CA	2.49	0.42
1:Z:310:GLY:O	1:Z:311:ALA:C	2.63	0.42
1:O:70:SER:O	1:O:71:SER:C	2.63	0.42
1:O:82:GLN:HA	1:O:245:ASP:OD2	2.20	0.42
1:O:97:ILE:HG21	1:O:160:LEU:CD2	2.50	0.42
1:Z:62:GLU:O	1:Z:65:ALA:HB3	2.20	0.42
1:Z:74:ILE:HD12	1:Z:74:ILE:HA	1.84	0.42
1:Z:337:GLN:NE2	1:Z:337:GLN:HA	2.34	0.42
1:O:21:MET:CE	1:O:444:ALA:CB	2.98	0.42
1:O:140:LYS:O	1:O:143:TRP:HB3	2.19	0.42
1:O:254:LEU:HA	1:O:254:LEU:HD12	1.64	0.42
1:O:392:LEU:C	1:O:392:LEU:CD2	2.92	0.42
1:O:432:ARG:O	1:O:432:ARG:HG2	2.18	0.42
1:Z:106:ARG:HH22	1:Z:135:TYR:HA	1.85	0.42
1:Z:240:SER:HB2	1:Z:450:ALA:HB3	2.02	0.42
1:Z:281:LYS:HE3	1:Z:281:LYS:HB2	1.71	0.42
1:Z:449:LEU:HD12	1:Z:449:LEU:HA	1.37	0.42
1:Z:468:ARG:HG2	1:Z:470:PHE:CE1	2.55	0.42
1:O:44:TRP:N	1:O:44:TRP:CD1	2.87	0.42
1:O:84:GLU:OE2	1:O:188:ARG:HD3	2.20	0.42
1:O:98:TYR:CD1	1:O:98:TYR:C	2.97	0.42
1:O:188:ARG:HH22	1:O:303:GLU:CD	2.28	0.42
1:O:438:VAL:O	1:O:441:LEU:HB2	2.20	0.42
1:Z:108:THR:OG1	1:Z:134:PRO:HA	2.20	0.42
1:Z:109:ALA:O	1:Z:110:GLU:C	2.60	0.42
1:Z:111:ILE:O	1:Z:114:HIS:N	2.47	0.42
1:Z:272:LEU:C	1:Z:395:MET:HE1	2.45	0.42
1:Z:358:PRO:HG2	1:Z:359:TYR:CE1	2.55	0.42
1:O:138:GLY:O	1:O:139:THR:C	2.61	0.42
1:O:170:ILE:HG21	1:O:178:VAL:HG22	2.01	0.42
1:Z:123:TYR:C	1:Z:123:TYR:CD1	2.98	0.42
1:Z:256:VAL:HG13	1:Z:294:PRO:CG	2.50	0.42
1:Z:328:ASP:O	1:Z:329:SER:C	2.63	0.42
1:Z:336:VAL:HG21	1:Z:375:HIS:CD2	2.55	0.42
1:O:60:LEU:O	1:O:60:LEU:HD12	2.20	0.41
1:O:143:TRP:C	1:O:143:TRP:CE3	2.98	0.41
1:O:224:TYR:HE1	1:O:240:SER:CA	2.33	0.41
1:O:262:LYS:HD2	1:O:262:LYS:C	2.45	0.41
1:O:364:ILE:HD12	1:O:364:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:38:ILE:HG22	1:Z:40:PRO:HD3	2.02	0.41
1:Z:145:LEU:HD12	1:Z:151:SER:HB2	2.00	0.41
1:Z:290:ILE:HG22	1:Z:291:ALA:N	2.32	0.41
1:Z:353:ALA:HA	1:Z:354:PRO:HA	1.65	0.41
1:Z:474:ILE:HA	1:Z:474:ILE:HD12	1.30	0.41
1:O:83:ARG:CZ	1:O:246:GLN:HB2	2.50	0.41
1:Z:64:LEU:HD23	1:Z:69:ILE:HB	2.00	0.41
1:Z:117:ARG:CG	1:Z:118:ASP:N	2.79	0.41
1:Z:154:ARG:O	1:Z:159:GLU:HG3	2.20	0.41
1:Z:162:PHE:CG	1:Z:163:GLY:N	2.87	0.41
1:Z:165:VAL:H	1:Z:165:VAL:HG23	1.43	0.41
1:Z:173:MET:HE3	1:Z:173:MET:HB2	1.70	0.41
1:Z:217:VAL:C	1:Z:218:ARG:HG2	2.45	0.41
1:Z:308:MET:CE	1:Z:311:ALA:CB	2.98	0.41
1:O:64:LEU:O	1:O:65:ALA:C	2.62	0.41
1:O:81:ASN:HB2	1:O:165:VAL:HB	2.03	0.41
1:O:106:ARG:NH2	1:O:135:TYR:HA	2.34	0.41
1:O:130:LEU:HD12	1:O:190:MET:CB	2.49	0.41
1:O:191:LEU:CD2	1:O:207:LEU:HD13	2.50	0.41
1:O:200:ASP:OD2	1:O:203:MET:N	2.44	0.41
1:O:331:TYR:C	1:O:331:TYR:CD2	2.98	0.41
1:Z:89:TRP:CD1	1:Z:94:GLY:HA2	2.53	0.41
1:Z:260:MET:O	1:Z:274:ASN:N	2.51	0.41
1:Z:334:THR:HG23	1:Z:334:THR:H	1.62	0.41
1:Z:352:GLY:H	1:Z:356:TRP:HA	1.85	0.41
1:O:34:GLU:OE1	1:O:34:GLU:N	2.53	0.41
1:O:39:TYR:O	1:O:41:LYS:N	2.53	0.41
1:O:97:ILE:CD1	1:O:144:ILE:CG2	2.99	0.41
1:O:160:LEU:HA	1:O:160:LEU:HD23	1.88	0.41
1:O:171:TRP:NE1	1:O:176:GLY:HA2	2.34	0.41
1:O:251:PHE:CD2	1:O:446:LEU:HD12	2.55	0.41
1:O:343:TYR:CE2	1:O:486:TRP:CA	3.03	0.41
1:O:352:GLY:CA	1:O:356:TRP:HA	2.50	0.41
1:O:385:ALA:HA	1:O:422:GLN:HE22	1.81	0.41
1:Z:41:LYS:HD3	1:Z:44:TRP:CE2	2.55	0.41
1:Z:153:GLU:O	1:Z:156:ARG:N	2.54	0.41
1:Z:164:THR:O	1:Z:165:VAL:C	2.63	0.41
1:Z:256:VAL:CG1	1:Z:294:PRO:CB	2.97	0.41
1:Z:257:LYS:HB2	1:Z:260:MET:SD	2.60	0.41
1:Z:297:GLU:H	1:Z:297:GLU:HG3	1.34	0.41
1:O:211:ARG:O	1:O:214:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:250:LEU:CD1	1:O:255:CYS:CB	2.99	0.41
1:O:338:ASN:C	1:O:340:ASN:N	2.78	0.41
1:O:419:MET:HE2	1:O:419:MET:HA	2.03	0.41
1:Z:81:ASN:HB2	1:Z:165:VAL:HB	2.03	0.41
1:Z:352:GLY:O	1:Z:355:TYR:N	2.54	0.41
1:O:420:GLN:NE2	1:O:420:GLN:C	2.79	0.41
1:O:421:PHE:O	1:O:422:GLN:C	2.63	0.41
1:Z:88:VAL:HB	1:Z:97:ILE:CD1	2.51	0.41
1:Z:253:GLN:O	1:Z:254:LEU:HB2	2.20	0.41
1:Z:368:THR:O	1:Z:369:ARG:C	2.63	0.41
1:Z:421:PHE:O	1:Z:425:ILE:HG22	2.21	0.41
1:Z:484:ALA:O	1:Z:485:GLY:C	2.63	0.41
1:O:19:VAL:HG13	1:O:27:ILE:CG2	2.51	0.41
1:O:226:GLN:HB3	1:O:237:ILE:O	2.20	0.41
1:O:346:PRO:C	1:O:348:PHE:N	2.77	0.41
1:Z:47:HIS:HB2	1:Z:100:ALA:HB3	2.02	0.41
1:Z:111:ILE:C	1:Z:115:LEU:HD23	2.46	0.41
1:Z:124:ILE:C	1:Z:126:SER:N	2.77	0.41
1:Z:191:LEU:CD2	1:Z:207:LEU:HD13	2.50	0.41
1:O:9:LEU:HD12	1:O:9:LEU:HA	1.67	0.41
1:O:39:TYR:C	1:O:41:LYS:N	2.78	0.41
1:O:133:ASP:OD1	1:O:134:PRO:N	2.54	0.41
1:O:360:ALA:O	1:O:361:ARG:HG2	2.21	0.41
1:Z:21:MET:HE3	1:Z:21:MET:HB2	1.50	0.41
1:Z:198:ASP:CG	1:Z:199:TRP:N	2.79	0.41
1:O:125:ARG:HH11	1:O:125:ARG:HD2	1.73	0.41
1:O:174:THR:CG2	1:O:178:VAL:HG13	2.45	0.41
1:O:261:ALA:HA	1:O:272:LEU:O	2.21	0.41
1:O:438:VAL:CG2	1:O:439:THR:N	2.82	0.41
1:Z:45:VAL:CG2	1:Z:105:CYS:HA	2.39	0.41
1:Z:107:ARG:HG2	1:Z:108:THR:N	2.35	0.41
1:Z:152:ARG:HB3	1:Z:156:ARG:NH1	2.36	0.41
1:Z:153:GLU:C	1:Z:155:ALA:N	2.78	0.41
1:Z:175:GLN:C	1:Z:177:ARG:N	2.79	0.41
1:Z:255:CYS:HA	1:Z:260:MET:SD	2.61	0.41
1:Z:334:THR:C	1:Z:336:VAL:N	2.78	0.41
1:Z:377:ILE:HD13	1:Z:377:ILE:HG21	1.84	0.41
1:Z:382:GLU:O	1:Z:383:SER:C	2.63	0.41
1:Z:403:LEU:HD12	1:Z:403:LEU:HA	1.77	0.41
1:Z:446:LEU:O	1:Z:449:LEU:HB2	2.21	0.41
1:O:106:ARG:HH22	1:O:135:TYR:CA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:191:LEU:O	1:O:199:TRP:HE3	2.03	0.41
1:O:192:PHE:HB2	1:O:199:TRP:CZ3	2.56	0.41
1:O:360:ALA:C	1:O:361:ARG:HG2	2.46	0.41
1:O:392:LEU:O	1:O:393:GLU:C	2.63	0.41
1:O:422:GLN:C	1:O:425:ILE:HG22	2.46	0.41
1:Z:244:GLY:C	1:Z:246:GLN:N	2.79	0.41
1:Z:249:ALA:CB	1:Z:262:LYS:HE2	2.51	0.41
1:O:53:TRP:CD1	1:O:172:LYS:HE2	2.56	0.40
1:O:302:LEU:HD23	1:O:302:LEU:HA	1.91	0.40
1:O:487:LYS:O	1:O:491:LYS:HG2	2.21	0.40
1:Z:156:ARG:HG2	1:Z:156:ARG:H	1.72	0.40
1:Z:260:MET:O	1:Z:273:MET:HA	2.21	0.40
1:Z:266:GLY:O	1:Z:267:THR:C	2.61	0.40
1:O:83:ARG:CG	3:O:601:GOL:O2	2.63	0.40
1:O:173:MET:HB3	1:O:227:THR:HG21	2.02	0.40
1:O:347:ALA:CB	1:O:351:LEU:CD1	3.00	0.40
2:O:602:EPE:H52	2:O:602:EPE:H82	1.79	0.40
1:Z:83:ARG:NH1	1:Z:83:ARG:CB	2.81	0.40
1:Z:172:LYS:HE2	1:Z:172:LYS:HB3	1.71	0.40
1:Z:383:SER:O	1:Z:387:GLN:HG3	2.21	0.40
1:Z:388:THR:CB	1:Z:422:GLN:NE2	2.85	0.40
1:O:188:ARG:NH2	1:O:303:GLU:CD	2.79	0.40
1:O:237:ILE:HG23	1:O:238:PRO:HD2	2.03	0.40
1:O:324:ASN:ND2	1:O:327:TYR:H	2.19	0.40
1:O:339:THR:C	1:O:375:HIS:HB3	2.46	0.40
1:O:384:ILE:O	1:O:385:ALA:C	2.64	0.40
1:O:468:ARG:NE	1:O:470:PHE:CE2	2.90	0.40
1:Z:228:ASN:CG	1:Z:236:ARG:NH1	2.79	0.40
1:Z:425:ILE:CG2	1:Z:426:LEU:N	2.84	0.40
1:Z:457:LEU:N	1:Z:457:LEU:HD22	2.35	0.40
1:O:41:LYS:O	1:O:41:LYS:HG2	2.19	0.40
1:O:171:TRP:CE2	1:O:176:GLY:HA2	2.57	0.40
1:Z:20:VAL:O	1:Z:27:ILE:HA	2.22	0.40
1:Z:156:ARG:CG	1:Z:156:ARG:NH1	2.80	0.40
1:Z:220:SER:HB3	1:Z:242:ILE:O	2.22	0.40
1:O:83:ARG:CG	1:O:245:ASP:OD1	2.70	0.40
1:O:189:THR:HG23	1:O:189:THR:H	1.57	0.40
1:O:262:LYS:HD2	1:O:263:ASN:N	2.35	0.40
1:Z:53:TRP:CZ3	1:Z:172:LYS:HB2	2.57	0.40
1:Z:81:ASN:ND2	1:Z:81:ASN:N	2.69	0.40
1:Z:338:ASN:O	1:Z:375:HIS:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:412:ALA:C	1:Z:414:ALA:N	2.75	0.40
1:Z:426:LEU:HD12	1:Z:426:LEU:HA	1.63	0.40
1:Z:433:PRO:HA	1:Z:465:VAL:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	495/501 (99%)	370 (75%)	94 (19%)	31 (6%)	1	5
1	Z	496/501 (99%)	397 (80%)	85 (17%)	14 (3%)	4	16
All	All	991/1002 (99%)	767 (77%)	179 (18%)	45 (4%)	2	9

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	99	ASN
1	O	109	ALA
1	O	149	GLU
1	O	151	SER
1	O	358	PRO
1	O	476	THR
1	O	477	THR
1	Z	151	SER
1	Z	294	PRO
1	Z	478	GLU
1	O	72	ASP
1	O	138	GLY
1	O	390	ASP
1	O	397	ALA
1	O	446	LEU

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Mol	Chain	Res	Type
1	Z	445	TYR
1	Z	446	LEU
1	Z	450	ALA
1	O	121	GLU
1	O	222	GLU
1	O	294	PRO
1	O	333	ALA
1	O	396	GLN
1	O	444	ALA
1	Z	149	GLU
1	Z	215	PRO
1	O	116	LYS
1	O	141	VAL
1	O	453	PHE
1	Z	111	ILE
1	Z	331	TYR
1	Z	476	THR
1	O	42	PRO
1	O	52	ILE
1	O	110	GLU
1	O	142	LYS
1	O	411	GLY
1	O	445	TYR
1	Z	202	LYS
1	Z	203	MET
1	O	457	LEU
1	O	478	GLU
1	Z	109	ALA
1	O	111	ILE
1	O	242	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%)	276 (68%)	132 (32%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Z	409/412 (99%)	277 (68%)	132 (32%)	0 0
All	All	817/824 (99%)	553 (68%)	264 (32%)	0 0

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	4	LYS
1	O	6	ILE
1	O	7	VAL
1	O	9	LEU
1	O	11	GLN
1	O	13	THR
1	O	14	THR
1	O	17	ARG
1	O	21	MET
1	O	24	ASP
1	O	27	ILE
1	O	29	SER
1	O	33	ARG
1	O	37	GLN
1	O	41	LYS
1	O	45	VAL
1	O	51	GLU
1	O	52	ILE
1	O	60	LEU
1	O	63	VAL
1	O	71	SER
1	O	74	ILE
1	O	81	ASN
1	O	82	GLN
1	O	83	ARG
1	O	85	THR
1	O	87	ILE
1	O	95	LYS
1	O	101	ILE
1	O	102	VAL
1	O	104	GLN
1	O	107	ARG
1	O	114	HIS
1	O	115	LEU
1	O	116	LYS
1	O	121	GLU

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Mol	Chain	Res	Type
1	O	122	ASP
1	O	124	ILE
1	O	131	VAL
1	O	132	ILE
1	O	139	THR
1	O	141	VAL
1	O	144	ILE
1	O	145	LEU
1	O	146	ASP
1	O	148	VAL
1	O	152	ARG
1	O	154	ARG
1	O	157	ARG
1	O	159	GLU
1	O	170	ILE
1	O	178	VAL
1	O	181	THR
1	O	182	ASP
1	O	188	ARG
1	O	190	MET
1	O	191	LEU
1	O	194	ILE
1	O	196	THR
1	O	197	LEU
1	O	203	MET
1	O	209	ILE
1	O	211	ARG
1	O	213	MET
1	O	214	LEU
1	O	219	ARG
1	O	220	SER
1	O	222	GLU
1	O	224	TYR
1	O	226	GLN
1	O	227	THR
1	O	229	ILE
1	O	235	THR
1	O	237	ILE
1	O	254	LEU
1	O	256	VAL
1	O	257	LYS
1	O	258	GLU

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Mol	Chain	Res	Type
1	O	262	LYS
1	O	269	CYS
1	O	277	GLU
1	O	278	LYS
1	O	280	VAL
1	O	288	THR
1	O	297	GLU
1	O	316	LEU
1	O	317	ARG
1	O	319	GLU
1	O	321	LYS
1	O	323	ILE
1	O	324	ASN
1	O	325	ASP
1	O	328	ASP
1	O	329	SER
1	O	335	LYS
1	O	336	VAL
1	O	349	THR
1	O	351	LEU
1	O	361	ARG
1	O	365	PHE
1	O	369	ARG
1	O	377	ILE
1	O	381	LEU
1	O	387	GLN
1	O	390	ASP
1	O	393	GLU
1	O	395	MET
1	O	396	GLN
1	O	401	ILE
1	O	403	LEU
1	O	406	LEU
1	O	407	ARG
1	O	418	LEU
1	O	420	GLN
1	O	425	ILE
1	O	426	LEU
1	O	436	ARG
1	O	437	GLU
1	O	439	THR
1	O	446	LEU

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Mol	Chain	Res	Type
1	O	449	LEU
1	O	459	GLU
1	O	460	LEU
1	O	462	GLU
1	O	463	LYS
1	O	471	ARG
1	O	474	ILE
1	O	476	THR
1	O	482	ARG
1	O	491	LYS
1	O	494	MET
1	O	498	GLU
1	Z	4	LYS
1	Z	6	ILE
1	Z	13	THR
1	Z	17	ARG
1	Z	21	MET
1	Z	27	ILE
1	Z	28	ILE
1	Z	29	SER
1	Z	45	VAL
1	Z	50	MET
1	Z	52	ILE
1	Z	56	GLN
1	Z	58	SER
1	Z	62	GLU
1	Z	70	SER
1	Z	72	ASP
1	Z	73	GLN
1	Z	74	ILE
1	Z	82	GLN
1	Z	83	ARG
1	Z	91	LYS
1	Z	95	LYS
1	Z	97	ILE
1	Z	101	ILE
1	Z	107	ARG
1	Z	110	GLU
1	Z	115	LEU
1	Z	117	ARG
1	Z	118	ASP
1	Z	121	GLU

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Mol	Chain	Res	Type
1	Z	122	ASP
1	Z	124	ILE
1	Z	125	ARG
1	Z	130	LEU
1	Z	131	VAL
1	Z	132	ILE
1	Z	133	ASP
1	Z	139	THR
1	Z	145	LEU
1	Z	149	GLU
1	Z	153	GLU
1	Z	154	ARG
1	Z	156	ARG
1	Z	159	GLU
1	Z	161	LEU
1	Z	164	THR
1	Z	167	THR
1	Z	172	LYS
1	Z	175	GLN
1	Z	177	ARG
1	Z	180	VAL
1	Z	181	THR
1	Z	182	ASP
1	Z	188	ARG
1	Z	194	ILE
1	Z	196	THR
1	Z	197	LEU
1	Z	205	GLU
1	Z	206	VAL
1	Z	211	ARG
1	Z	213	MET
1	Z	214	LEU
1	Z	217	VAL
1	Z	219	ARG
1	Z	220	SER
1	Z	224	TYR
1	Z	226	GLN
1	Z	228	ASN
1	Z	229	ILE
1	Z	235	THR
1	Z	246	GLN
1	Z	254	LEU

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Mol	Chain	Res	Type
1	Z	256	VAL
1	Z	262	LYS
1	Z	264	THR
1	Z	278	LYS
1	Z	280	VAL
1	Z	281	LYS
1	Z	289	THR
1	Z	295	THR
1	Z	297	GLU
1	Z	298	VAL
1	Z	313	ILE
1	Z	314	GLN
1	Z	321	LYS
1	Z	323	ILE
1	Z	324	ASN
1	Z	325	ASP
1	Z	329	SER
1	Z	336	VAL
1	Z	337	GLN
1	Z	349	THR
1	Z	351	LEU
1	Z	355	TYR
1	Z	368	THR
1	Z	390	ASP
1	Z	391	VAL
1	Z	392	LEU
1	Z	395	MET
1	Z	398	ASP
1	Z	403	LEU
1	Z	406	LEU
1	Z	407	ARG
1	Z	418	LEU
1	Z	419	MET
1	Z	420	GLN
1	Z	423	SER
1	Z	426	LEU
1	Z	431	GLU
1	Z	434	GLU
1	Z	436	ARG
1	Z	439	THR
1	Z	449	LEU
1	Z	455	GLN

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Mol	Chain	Res	Type
1	Z	456	ASN
1	Z	458	ASP
1	Z	460	LEU
1	Z	461	GLN
1	Z	462	GLU
1	Z	463	LYS
1	Z	466	ILE
1	Z	468	ARG
1	Z	469	GLU
1	Z	470	PHE
1	Z	471	ARG
1	Z	474	ILE
1	Z	476	THR
1	Z	478	GLU
1	Z	479	ARG
1	Z	482	ARG
1	Z	492	ARG
1	Z	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	32	GLN
1	O	37	GLN
1	O	104	GLN
1	O	127	ASN
1	O	179	HIS
1	O	299	ASN
1	O	324	ASN
1	O	337	GLN
1	O	375	HIS
1	O	404	HIS
1	O	420	GLN
1	O	422	GLN
1	O	455	GLN
1	Z	11	GLN
1	Z	47	HIS
1	Z	56	GLN
1	Z	81	ASN
1	Z	104	GLN
1	Z	114	HIS
1	Z	185	ASN

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Mol	Chain	Res	Type
1	Z	195	HIS
1	Z	228	ASN
1	Z	299	ASN
1	Z	324	ASN
1	Z	337	GLN
1	Z	387	GLN
1	Z	404	HIS
1	Z	420	GLN
1	Z	422	GLN
1	Z	455	GLN
1	Z	456	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z > 2$
2	EPE	O	602	-	15,15,15	2.07	3 (20%)	19,20,20	1.87	5 (26%)
3	GOL	O	601	-	5,5,5	0.92	0	5,5,5	0.65	0
3	GOL	Z	603	-	5,5,5	0.49	0	5,5,5	0.54	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
2	EPE	O	602	-	-	3/9/19/19	0/1/1/1
3	GOL	O	601	-	-	2/4/4/4	-
3	GOL	Z	603	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	602	EPE	O3S-S	5.49	1.67	1.47
2	O	602	EPE	C10-S	3.70	1.82	1.77
2	O	602	EPE	C5-N4	2.13	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	602	EPE	O3S-S-O1S	-4.32	100.58	111.40
2	O	602	EPE	O2S-S-C10	3.36	111.81	106.73
2	O	602	EPE	C2-C3-N4	2.97	116.65	110.65
2	O	602	EPE	O2S-S-O1S	2.64	122.41	113.82
2	O	602	EPE	C6-N1-C2	2.07	113.29	108.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	601	GOL	C1-C2-C3-O3
2	O	602	EPE	C8-C7-N4-C5
3	O	601	GOL	O2-C2-C3-O3
2	O	602	EPE	C8-C7-N4-C3
2	O	602	EPE	N4-C7-C8-O8

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	602	EPE	2	0
3	O	601	GOL	4	0
3	Z	603	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	497/501 (99%)	-0.37	5 (1%) 79 59	12, 33, 66, 90	0
1	Z	498/501 (99%)	-0.44	0 100 100	11, 32, 66, 87	0
All	All	995/1002 (99%)	-0.41	5 (0%) 87 72	11, 32, 66, 90	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	404	HIS	3.0
1	O	327	TYR	2.7
1	O	396	GLN	2.6
1	O	462	GLU	2.1
1	O	434	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	EPE	O	602	15/15	0.88	0.18	84,84,84,84	0
3	GOL	O	601	6/6	0.98	0.06	10,11,69,71	0
3	GOL	Z	603	6/6	0.98	0.06	10,10,10,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.