



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BOT
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

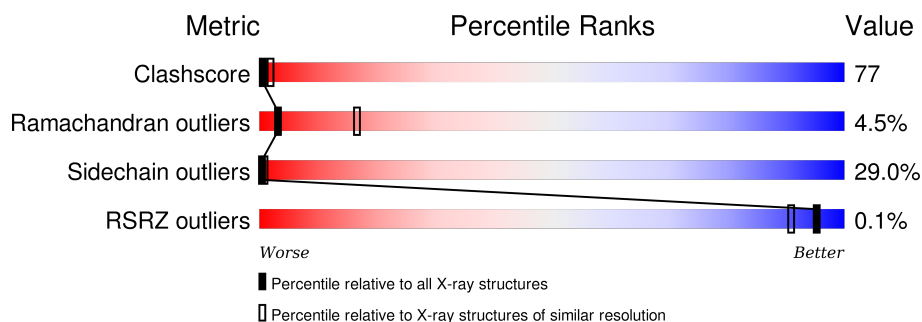
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	501	
1	Z	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
2	EPE	O	602	-	-	-	X
3	GOL	O	601	-	-	X	-

2 Entry composition [i](#)

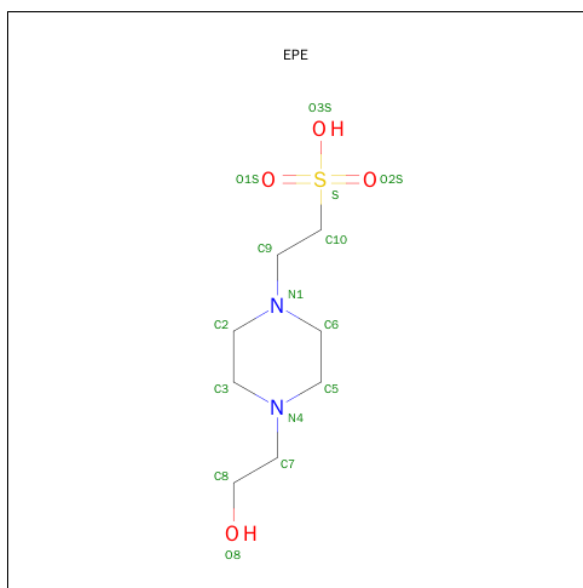
There are 3 unique types of molecules in this entry. The entry contains 7864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).

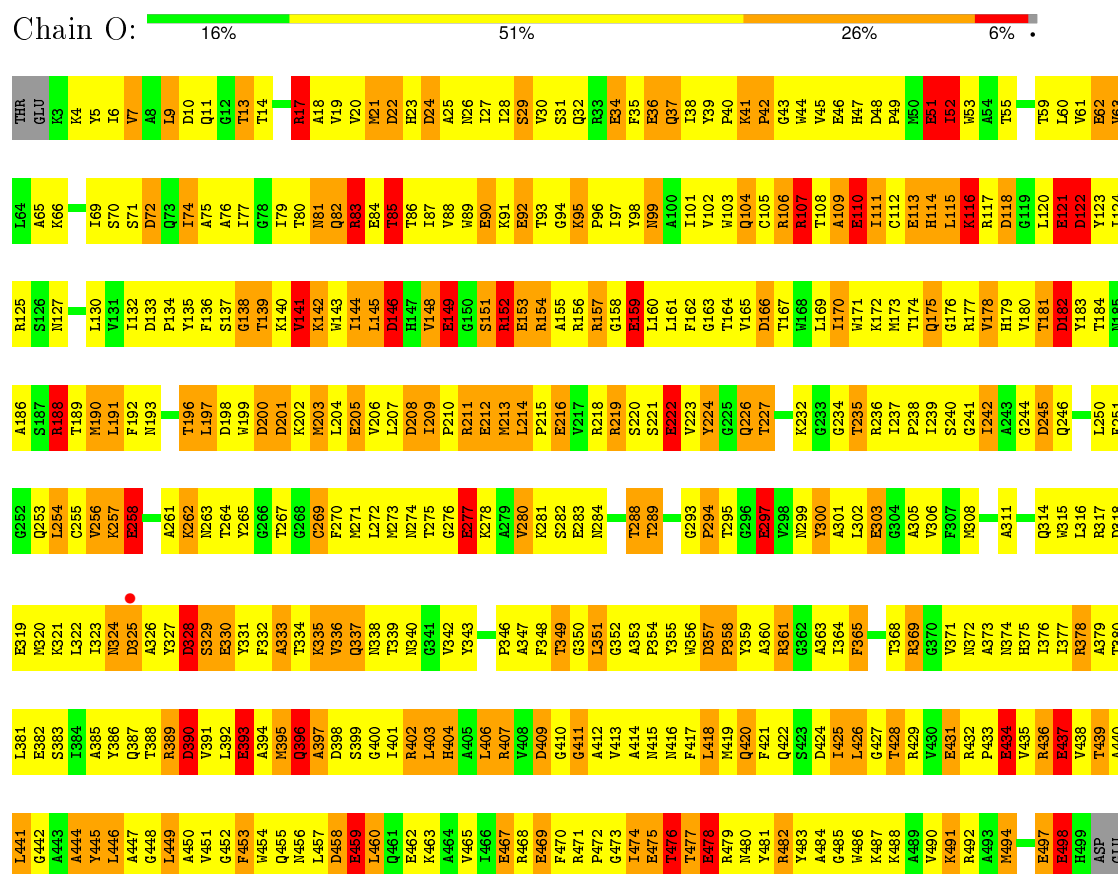


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

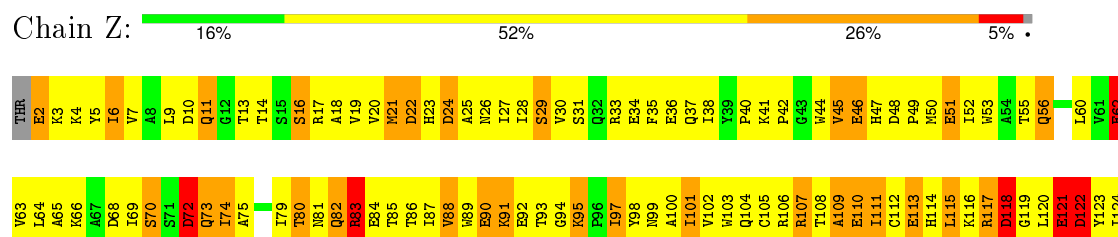
3 Residue-property plots

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

• Molecule 1: PROTEIN (GLYCEROL KINASE)



• Molecule 1: PROTEIN (GLYCEROL KINASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.80 Å 168.80 Å 202.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 19.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-3.05) 73.8 (19.98-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.88 Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, R_{free}	0.219 , (Not available) 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 106.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 48098 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, EPE

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	1.20	34/3994 (0.9%)	1.57	57/5414 (1.1%)
1	Z	1.21	37/4003 (0.9%)	1.56	65/5426 (1.2%)
All	All	1.21	71/7997 (0.9%)	1.56	122/10840 (1.1%)

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	34	GLU	CD-OE2	11.22	1.38	1.25
1	O	216	GLU	CD-OE2	10.60	1.37	1.25
1	O	437	GLU	CD-OE1	8.56	1.35	1.25
1	Z	475	GLU	CD-OE2	8.45	1.34	1.25
1	O	462	GLU	CD-OE1	8.39	1.34	1.25
1	Z	205	GLU	CD-OE2	8.06	1.34	1.25
1	Z	92	GLU	CD-OE2	7.99	1.34	1.25
1	Z	393	GLU	CD-OE1	7.93	1.34	1.25
1	Z	330	GLU	CD-OE1	7.81	1.34	1.25
1	O	205	GLU	CD-OE2	7.79	1.34	1.25
1	O	51	GLU	CD-OE1	7.50	1.33	1.25
1	O	92	GLU	CD-OE1	7.44	1.33	1.25
1	O	62	GLU	CD-OE2	7.44	1.33	1.25
1	Z	110	GLU	CD-OE2	7.38	1.33	1.25
1	Z	62	GLU	CD-OE1	7.22	1.33	1.25
1	Z	51	GLU	CD-OE1	7.19	1.33	1.25
1	Z	258	GLU	CD-OE1	7.15	1.33	1.25
1	O	113	GLU	CD-OE2	7.15	1.33	1.25
1	Z	434	GLU	CD-OE1	7.05	1.33	1.25
1	O	393	GLU	CD-OE1	7.03	1.33	1.25
1	O	467	GLU	CD-OE2	7.00	1.33	1.25
1	O	149	GLU	CD-OE2	6.98	1.33	1.25
1	Z	498	GLU	CD-OE2	6.94	1.33	1.25
1	O	498	GLU	CD-OE2	6.94	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	110	GLU	CD-OE1	6.93	1.33	1.25
1	Z	149	GLU	CD-OE2	6.92	1.33	1.25
1	Z	462	GLU	CD-OE1	6.77	1.33	1.25
1	O	469	GLU	CD-OE1	6.71	1.33	1.25
1	O	434	GLU	CD-OE2	6.70	1.33	1.25
1	O	478	GLU	CD-OE2	6.67	1.32	1.25
1	O	283	GLU	CD-OE2	6.62	1.32	1.25
1	O	90	GLU	CD-OE2	6.58	1.32	1.25
1	O	121	GLU	CD-OE2	6.53	1.32	1.25
1	Z	153	GLU	CD-OE2	6.51	1.32	1.25
1	O	303	GLU	CD-OE1	6.48	1.32	1.25
1	Z	216	GLU	CD-OE1	6.48	1.32	1.25
1	O	159	GLU	CD-OE2	6.46	1.32	1.25
1	Z	437	GLU	CD-OE1	6.36	1.32	1.25
1	O	34	GLU	CD-OE2	6.34	1.32	1.25
1	Z	2	GLU	CD-OE2	6.33	1.32	1.25
1	Z	222	GLU	CD-OE2	6.30	1.32	1.25
1	Z	459	GLU	CD-OE1	6.24	1.32	1.25
1	Z	382	GLU	CD-OE2	6.24	1.32	1.25
1	Z	431	GLU	CD-OE1	6.18	1.32	1.25
1	Z	478	GLU	CD-OE1	6.16	1.32	1.25
1	Z	277	GLU	CD-OE2	6.04	1.32	1.25
1	O	258	GLU	CD-OE2	6.04	1.32	1.25
1	O	431	GLU	CD-OE2	6.03	1.32	1.25
1	Z	297	GLU	CD-OE1	6.00	1.32	1.25
1	O	153	GLU	CD-OE1	5.97	1.32	1.25
1	O	459	GLU	CD-OE1	5.94	1.32	1.25
1	Z	159	GLU	CD-OE2	5.88	1.32	1.25
1	O	497	GLU	CD-OE1	5.86	1.32	1.25
1	O	222	GLU	CD-OE2	5.86	1.32	1.25
1	O	475	GLU	CD-OE2	5.84	1.32	1.25
1	Z	90	GLU	CD-OE2	5.81	1.32	1.25
1	O	330	GLU	CD-OE2	5.71	1.31	1.25
1	Z	212	GLU	CD-OE2	5.70	1.31	1.25
1	Z	469	GLU	CD-OE1	5.69	1.31	1.25
1	O	36	GLU	CD-OE2	5.69	1.31	1.25
1	Z	113	GLU	CD-OE2	5.69	1.31	1.25
1	Z	36	GLU	CD-OE2	5.60	1.31	1.25
1	Z	497	GLU	CD-OE1	5.60	1.31	1.25
1	Z	283	GLU	CD-OE2	5.59	1.31	1.25
1	O	297	GLU	CD-OE2	5.53	1.31	1.25
1	Z	467	GLU	CD-OE2	5.51	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	277	GLU	CD-OE2	5.44	1.31	1.25
1	Z	121	GLU	CD-OE1	5.23	1.31	1.25
1	Z	319	GLU	CD-OE2	5.22	1.31	1.25
1	O	212	GLU	CD-OE1	5.14	1.31	1.25
1	Z	46	GLU	CD-OE2	5.09	1.31	1.25

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	357	ASP	C-N-CD	-13.79	90.26	120.60
1	Z	152	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	O	200	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	O	409	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	Z	10	ASP	CB-CG-OD1	-8.85	110.34	118.30
1	O	398	ASP	CB-CG-OD1	-8.43	110.71	118.30
1	Z	146	ASP	CB-CG-OD1	-8.15	110.97	118.30
1	O	201	ASP	CB-CG-OD1	-8.15	110.97	118.30
1	O	24	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	Z	200	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	Z	378	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	O	188	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	Z	328	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	Z	209	ILE	C-N-CD	-7.49	104.13	120.60
1	Z	68	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	O	166	ASP	CB-CG-OD1	-7.44	111.60	118.30
1	Z	167	THR	CA-CB-CG2	-7.28	102.21	112.40
1	Z	152	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	O	85	THR	CA-CB-CG2	-7.19	102.33	112.40
1	Z	378	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	O	328	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	O	402	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	Z	389	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	O	152	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	O	72	ASP	CB-CG-OD1	-7.11	111.91	118.30
1	Z	275	THR	CA-CB-CG2	-7.10	102.46	112.40
1	Z	245	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	Z	188	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	Z	83	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	Z	146	ASP	CB-CG-OD2	6.96	124.56	118.30
1	Z	118	ASP	CB-CG-OD1	6.94	124.55	118.30
1	O	83	ARG	O-C-N	-6.92	111.63	122.70
1	Z	469	GLU	N-CA-CB	6.86	122.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	398	ASP	CB-CG-OD2	6.82	124.44	118.30
1	Z	118	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	O	409	ASP	CB-CG-OD1	6.77	124.39	118.30
1	Z	24	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	O	245	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	Z	208	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	O	24	ASP	CB-CG-OD1	6.67	124.30	118.30
1	Z	351	LEU	C-N-CA	-6.66	108.33	122.30
1	Z	357	ASP	CB-CG-OD1	6.65	124.29	118.30
1	O	117	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	O	390	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	O	200	ASP	CB-CG-OD2	6.63	124.27	118.30
1	O	458	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	Z	424	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	O	289	THR	N-CA-CB	6.52	122.69	110.30
1	O	318	ASP	CB-CG-OD1	6.49	124.14	118.30
1	O	182	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	Z	182	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	Z	10	ASP	CB-CG-OD2	6.39	124.05	118.30
1	O	107	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	O	288	THR	CA-CB-CG2	-6.38	103.46	112.40
1	O	289	THR	CA-CB-CG2	-6.37	103.49	112.40
1	Z	68	ASP	CB-CG-OD2	6.33	124.00	118.30
1	Z	325	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	O	325	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	Z	201	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	Z	432	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	O	118	ASP	CB-CG-OD2	-6.19	112.72	118.30
1	Z	72	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	Z	361	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	Z	183	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	Z	83	ARG	O-C-N	-6.07	113.00	122.70
1	O	188	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	O	245	ASP	CB-CG-OD1	5.99	123.69	118.30
1	Z	389	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	Z	390	ASP	CB-CG-OD1	-5.94	112.96	118.30
1	O	389	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	O	22	ASP	CB-CG-OD1	-5.91	112.99	118.30
1	O	83	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	Z	361	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	Z	165	VAL	CA-CB-CG2	-5.79	102.21	110.90
1	Z	398	ASP	CB-CG-OD2	5.79	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	198	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	O	404	HIS	CA-CB-CG	-5.76	103.81	113.60
1	Z	236	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	O	146	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	Z	357	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	O	378	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	O	122	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	Z	409	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	O	166	ASP	CB-CG-OD2	5.64	123.38	118.30
1	Z	122	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	O	106	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	Z	245	ASP	CB-CG-OD1	5.50	123.25	118.30
1	Z	88	VAL	CA-CB-CG1	-5.47	102.70	110.90
1	O	201	ASP	CB-CG-OD2	5.44	123.20	118.30
1	O	118	ASP	CB-CG-OD1	5.43	123.19	118.30
1	Z	135	TYR	CB-CG-CD1	5.42	124.25	121.00
1	Z	208	ASP	CB-CG-OD2	5.37	123.13	118.30
1	Z	80	THR	CA-CB-CG2	-5.36	104.90	112.40
1	O	441	LEU	CA-CB-CG	-5.34	103.02	115.30
1	Z	201	ASP	CB-CG-OD2	5.33	123.09	118.30
1	Z	200	ASP	CB-CG-OD2	5.32	123.09	118.30
1	O	428	THR	CA-CB-CG2	-5.32	104.95	112.40
1	O	208	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	Z	166	ASP	CB-CG-OD1	-5.27	113.55	118.30
1	O	219	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	O	300	TYR	N-CA-CB	5.27	120.08	110.60
1	Z	351	LEU	CB-CA-C	-5.24	100.25	110.20
1	Z	328	ASP	CB-CG-OD1	5.21	122.99	118.30
1	Z	34	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	Z	468	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	Z	167	THR	N-CA-CB	5.19	120.17	110.30
1	Z	22	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	Z	482	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	Z	429	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	Z	436	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	O	325	ASP	CB-CG-OD1	5.16	122.95	118.30
1	Z	441	LEU	CA-CB-CG	-5.16	103.44	115.30
1	O	107	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	O	390	ASP	N-CA-CB	5.11	119.79	110.60
1	O	402	ARG	N-CA-CB	5.09	119.77	110.60
1	O	363	ALA	CB-CA-C	-5.08	102.48	110.10
1	O	72	ASP	CB-CG-OD2	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	83	ARG	C-N-CA	-5.03	109.12	121.70
1	O	17	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	Z	177	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	O	164	THR	CA-CB-CG2	-5.00	105.40	112.40
1	Z	318	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	631	0
1	Z	3923	0	3859	572	0
2	O	15	0	18	2	0
3	O	6	0	8	4	0
3	Z	6	0	8	2	0
All	All	7864	0	7746	1204	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 77.

All (1204) 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:Z:228:ASN:HB2	1:Z:236:ARG:HD2	1.28	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:HH11	1:O:83:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:83:ARG:CG	1:O:83:ARG:HH11	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:273:MET:HB2	1:O:395:MET:HE3	1.50	0.91
1:O:369:ARG:HH11	1:O:369:ARG:HG3	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: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:Z:256:VAL:HG13	1:Z:294:PRO:HD3	1.57	0.87
1:O:120:LEU:O	1:O:121:GLU:C	2.10	0.86
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
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:O:271:MET:CE	1:O:392:LEU:HA	2.08	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:HH11	1:O:361:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:122:ASP:O	1:O:123:TYR:C	2.18	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:170:ILE:HA	1:Z:173:MET:HE3	1.60	0.81
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:324:ASN:ND2	1:O:324:ASN:N	2.28	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:O:137:SER:HB2	1:O:189:THR:HA	1.60	0.80
1:Z:228:ASN:HB2	1:Z:236:ARG:CD	2.11	0.80
1:O:365:PHE:CE2	1:O:492:ARG:HB3	2.16	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:HH11	1:O:152:ARG:HG3	1.47	0.80
1:O:324:ASN:HD22	1:O:324:ASN:N	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:17:ARG:HH22	1:O:437:GLU:CG	1.96	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: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:460:LEU:H	1:Z:460:LEU:HD22	1.46	0.78
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:Z:330:GLU:O	1:Z:334:THR:HG23	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:275:THR:HG23	1:O:301:ALA:HA	1.64	0.77
1:O:273:MET:HB2	1:O:395:MET:CE	2.15	0.77
1:Z:187:SER:HB3	1:Z:290:ILE:CD1	2.14	0.76
1:O:452:GLY:O	1:O:453:PHE:C	2.22	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:Z:271:MET:C	1:Z:272:LEU:HD12	2.06	0.76
1:O:491:LYS:HA	1:O:494:MET:HE3	1.66	0.76
1:Z:108:THR:HB	1:Z:139:THR:HB	1.68	0.76
1:O:324:ASN:H	1:O:324:ASN:HD22	1.32	0.76
1:O:271:MET:HE1	1:O:392:LEU:HA	1.67	0.75
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:250:LEU:CD1	1:Z:255:CYS:HB2	2.16	0.75
1:Z:422:GLN:O	1:Z:426:LEU:HB2	1.86	0.75
1:O:81:ASN:HD22	1:O:81:ASN:N	1.85	0.75
1:Z:187:SER:CB	1:Z:290:ILE:HD12	2.15	0.74
1:O:422:GLN:O	1:O:425:ILE:HG22	1.87	0.74
1:O:204:LEU:CD2	1:O:214:LEU:HD11	2.18	0.74
1:Z:114:HIS:O	1:Z:115:LEU:C	2.23	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Z:407:ARG:NH1	1:Z:407:ARG:HG3	2.03	0.72
1:O:142:LYS:O	1:O:143:TRP:C	2.29	0.71
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:221:SER:OG	1:O:450:ALA:HB2	1.90	0.71
1:O:120:LEU:HB2	1:O:124:ILE:HD12	1.72	0.71
1:O:347:ALA:HB3	1:O:361:ARG:C	2.11	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:438:VAL:N	1:O:441:LEU:HD12	2.05	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:329:SER:OG	1:O:381:LEU:HD11	1.91	0.71
1:O:179:HIS:CD2	1:O:215:PRO:HB3	2.26	0.70
1:O:27:ILE:HD12	1:O:27:ILE:N	2.05	0.70
1:O:473:GLY:O	1:O:474:ILE:HD13	1.91	0.70
1:Z:221:SER:HB2	1:Z:446:LEU:HG	1.74	0.70
1:O:476:THR:HG23	1:O:479:ARG:NH2	2.05	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:Z:45:VAL:HG23	1:Z:105:CYS:CA	2.20	0.70
1:Z:347:ALA:HB3	1:Z:361:ARG:C	2.12	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
1:Z:344:VAL:HG22	1:Z:364:ILE:HG12	1.72	0.70
1:Z:246:GLN:OE1	1:Z:246:GLN:HA	1.92	0.69
1:O:232:LYS:O	1:O:235:THR:HB	1.92	0.69
1:Z:478:GLU:HA	1:Z:481:TYR:HB3	1.73	0.69
1:Z:83:ARG:CZ	1:Z:246:GLN:HB2	2.23	0.69
1:Z:219:ARG:HD3	1:Z:222:GLU:HB3	1.75	0.69
1:O:19:VAL:CG1	1:O:27:ILE:HG23	2.22	0.69
1:Z:120:LEU:N	1:Z:120:LEU:HD12	2.07	0.69
1:Z:142:LYS:HG3	1:Z:146:ASP:OD1	1.91	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:O:332:PHE:O	1:O:333:ALA:C	2.30	0.69
1:Z:241:GLY:O	1:Z:242:ILE:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:419:MET:HA	1:Z:419:MET:CE	2.23	0.69
1:Z:490:VAL:HG12	1:Z:491:LYS:N	2.07	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:439:THR:HG22	1:O:440:ALA:N	2.08	0.68
1:O:258:GLU:HB2	1:O:276:GLY:N	2.07	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:396:GLN:O	1:O:397:ALA:C	2.30	0.68
1:O:407:ARG:HD3	1:O:431:GLU:HG3	1.76	0.68
1:O:81:ASN:H	1:O:81:ASN:HD22	1.41	0.68
1:Z:19:VAL:HG22	1:Z:30:VAL:HG22	1.74	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: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: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:114:HIS:O	1:O:115:LEU:C	2.32	0.67
1:Z:47:HIS:O	1:Z:49:PRO:HD3	1.94	0.67
1:Z:456:ASN:O	1:Z:459:GLU:HG3	1.94	0.67
1:O:40:PRO:HG2	1:O:44:TRP:HB3	1.76	0.67
1:Z:269:CYS:HB2	1:Z:306:VAL:HB	1.74	0.67
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:Z:413:VAL:CG2	1:Z:436:ARG:HD2	2.25	0.67
1:O:429:ARG:HA	1:O:470:PHE:O	1.93	0.67
1:Z:160:LEU:C	1:Z:161:LEU:HD23	2.14	0.67
1:O:63:VAL:O	1:O:66:LYS:HG2	1.94	0.67
1:O:23:HIS:NE2	1:O:453:PHE:O	2.28	0.67
1:O:7:VAL:CG1	1:O:77:ILE:HG12	2.24	0.67
1:Z:169:LEU:C	1:Z:173:MET:HE2	2.15	0.67
1:O:330:GLU:O	1:O:334:THR:HG23	1.95	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:97:ILE:HD11	1:O:144:ILE:HG21	1.76	0.67
1:O:83:ARG:NH1	1:O:83:ARG:HG3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:144:ILE:O	1:O:148:VAL:HG23	1.96	0.66
1:O:41:LYS:HB2	1:O:42:PRO:HD2	1.78	0.66
1:Z:202:LYS:O	1:Z:203:MET:C	2.33	0.66
1:O:111:ILE:O	1:O:115:LEU:HD22	1.94	0.66
1:O:146:ASP:N	1:O:146:ASP:OD1	2.27	0.66
1:O:46:GLU:OE2	1:O:107:ARG:NH2	2.29	0.66
1:O:331:TYR:CE2	1:O:335:LYS:HE2	2.29	0.66
1:Z:360:ALA:O	1:Z:361:ARG:NH1	2.28	0.66
1:Z:144:ILE:O	1:Z:148:VAL:HG22	1.95	0.66
1:Z:22:ASP:O	1:Z:25:ALA:N	2.29	0.66
1:O:315:TRP:CZ3	1:O:316:LEU:HD23	2.29	0.66
1:Z:199:TRP:CD2	1:Z:214:LEU:HD13	2.30	0.66
1:Z:152:ARG:O	1:Z:155:ALA:HB3	1.96	0.66
1:Z:385:ALA:O	1:Z:388:THR:HB	1.95	0.66
1:O:93:THR:OG1	1:O:95:LYS:HB3	1.96	0.66
1:O:143:TRP:CE3	1:O:144:ILE:HA	2.31	0.66
1:O:74:ILE:HD13	1:O:74:ILE:N	2.11	0.66
1:O:420:GLN:NE2	1:O:424:ASP:OD1	2.29	0.66
1:Z:245:ASP:OD1	1:Z:246:GLN:N	2.29	0.66
1:O:336:VAL:HG23	1:O:337:GLN:N	2.09	0.66
1:O:437:GLU:C	1:O:441:LEU:HD12	2.16	0.65
1:Z:203:MET:HA	1:Z:203:MET:HE3	1.78	0.65
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:NH1	1:O:83:ARG:CG	2.51	0.65
1:Z:223:VAL:HA	1:Z:240:SER:HB3	1.77	0.65
1:Z:419:MET:HA	1:Z:419:MET:HE2	1.78	0.65
1:Z:255:CYS:HB3	1:Z:260:MET:HB2	1.77	0.65
1:Z:432:ARG:NH1	1:Z:470:PHE:HZ	1.93	0.65
1:O:245:ASP:OD1	1:O:246:GLN:N	2.30	0.65
1:O:90:GLU:O	1:O:94:GLY:N	2.29	0.65
1:Z:332:PHE:HA	1:Z:335:LYS:HG3	1.79	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:Z:324:ASN:N	1:Z:324:ASN:ND2	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:388:THR:CB	1:O:422:GLN:HE22	2.09	0.64
1:Z:222:GLU:O	1:Z:240:SER:HA	1.98	0.64
1:O:382:GLU:HB3	1:O:421:PHE:CE2	2.33	0.64
1:Z:20:VAL:O	1:Z:28:ILE:N	2.27	0.64
1:O:13:THR:CG2	1:O:103:TRP:HE1	2.10	0.64
1:Z:218:ARG:HH21	1:Z:222:GLU:CD	2.01	0.64
1:O:331:TYR:HD2	1:O:332:PHE:CD1	2.16	0.64
1:Z:202:LYS:O	1:Z:205:GLU:N	2.31	0.64
1:O:460:LEU:HD23	1:O:460:LEU:N	2.12	0.64
1:Z:402:ARG:NH2	1:Z:428:THR:OG1	2.30	0.64
1:O:476:THR:O	1:O:480:ASN:N	2.28	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:Z:409:ASP:CG	1:Z:438:VAL:HG21	2.19	0.63
1:Z:122:ASP:O	1:Z:123:TYR:C	2.37	0.63
1:O:145:LEU:HD12	1:O:151:SER:CB	2.15	0.63
1:O:441:LEU:O	1:O:442:GLY:C	2.35	0.63
1:O:476:THR:HG23	1:O:479:ARG:HH22	1.64	0.63
1:O:332:PHE:HA	1:O:335:LYS:HG3	1.79	0.63
1:O:369:ARG:NH1	1:O:369:ARG:HG3	2.09	0.63
1:O:293:GLY:HA3	1:O:297:GLU:CG	2.26	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:108:THR:OG1	1:O:134:PRO:HA	1.99	0.63
1:Z:445:TYR:O	1:Z:446:LEU:C	2.36	0.63
1:O:76:ALA:HB2	1:O:238:PRO:HG2	1.81	0.63
1:Z:396:GLN:O	1:Z:400:GLY:N	2.30	0.63
1:Z:28:ILE:HD13	1:Z:28:ILE:N	2.13	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: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:170:ILE:O	1:O:171:TRP:C	2.35	0.62
1:O:98:TYR:OH	1:O:107:ARG:NH2	2.32	0.62
1:Z:115:LEU:CD2	1:Z:115:LEU:H	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:40:PRO:HG2	1:Z:44:TRP:CB	2.30	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:HB3	1.80	0.62
1:Z:423:SER:HB2	1:Z:430:VAL:HG23	1.80	0.62
1:O:120:LEU:CB	1:O:124:ILE:HD12	2.29	0.62
1:O:476:THR:O	1:O:477:THR:C	2.36	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:332:PHE:O	1:O:335:LYS:N	2.28	0.62
1:O:275:THR:OG1	1:O:300:TYR:HB2	1.98	0.62
1:O:262:LYS:O	1:O:271:MET:HA	1.99	0.62
1:O:390:ASP:HA	1:O:483:TYR:OH	2.00	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:Z:137:SER:HB2	1:Z:189:THR:CA	2.27	0.62
1:O:154:ARG:HB3	1:O:159:GLU:OE2	1.99	0.62
1:Z:235:THR:C	1:Z:236:ARG:HD3	2.19	0.61
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:460:LEU:N	1:Z:460:LEU:HD22	2.15	0.61
1:Z:151:SER:O	1:Z:155:ALA:N	2.32	0.61
1:Z:6:ILE:HD11	1:Z:444:ALA:CA	2.24	0.61
1:O:452:GLY:O	1:O:454:TRP:N	2.33	0.61
1:O:20:VAL:HG12	1:O:28:ILE:CG1	2.30	0.61
1:Z:201:ASP:OD2	1:Z:211:ARG:NH2	2.33	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:204:LEU:HD23	1:Z:209:ILE:HB	1.82	0.61
1:Z:106:ARG:HD2	1:Z:349:THR:O	1.99	0.61
1:Z:83:ARG:HD3	1:Z:245:ASP:OD1	1.99	0.61
1:Z:330:GLU:O	1:Z:331:TYR:C	2.38	0.61
1:Z:458:ASP:N	1:Z:458:ASP:OD1	2.28	0.61
1:O:166:ASP:OD1	1:O:166:ASP:N	2.29	0.61
1:O:220:SER:O	1:O:446:LEU:HD23	1.99	0.61
1:O:176:GLY:O	1:O:177:ARG:C	2.36	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:O:83:ARG:CB	1:O:83:ARG:HH11	2.13	0.61
1:Z:251:PHE:O	1:Z:254:LEU:N	2.29	0.60
1:O:338:ASN:O	1:O:375:HIS:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:112:CYS:SG	1:Z:139:THR:HG21	2.41	0.60
1:O:114:HIS:N	1:O:114:HIS:ND1	2.44	0.60
1:Z:406:LEU:HD23	1:Z:407:ARG:N	2.16	0.60
1:Z:70:SER:O	1:Z:73:GLN:HG3	2.01	0.60
1:O:331:TYR:CE2	1:O:335:LYS:HD3	2.35	0.60
1:O:389:ARG:O	1:O:390:ASP:C	2.38	0.60
1:O:137:SER:O	1:O:141:VAL:HG23	2.01	0.60
1:Z:108:THR:HB	1:Z:139:THR:CB	2.31	0.60
1:O:361:ARG:NH1	1:O:361:ARG:HG2	2.13	0.60
1:Z:153:GLU:HA	1:Z:156:ARG:HG3	1.83	0.60
1:Z:83:ARG:NH2	1:Z:303:GLU:OE2	2.35	0.60
1:Z:41:LYS:HB2	1:Z:42:PRO:HD2	1.83	0.60
1:O:386:TYR:HB3	1:O:486:TRP:CE2	2.37	0.60
1:Z:52:ILE:HG22	1:Z:53:TRP:N	2.13	0.60
1:Z:410:GLY:O	1:Z:413:VAL:HG22	2.02	0.60
1:O:74:ILE:CB	1:O:237:ILE:HD13	2.26	0.60
1:O:23:HIS:HA	1:O:453:PHE:HE2	1.58	0.60
1:O:388:THR:O	1:O:389:ARG:C	2.39	0.60
1:O:204:LEU:HD21	1:O:214:LEU:CD1	2.28	0.60
1:O:473:GLY:C	1:O:474:ILE:HD13	2.21	0.60
1:Z:223:VAL:CG2	1:Z:240:SER:HB3	2.32	0.60
1:O:79:ILE:HD12	1:O:170:ILE:HD11	1.84	0.60
1:O:385:ALA:HB1	1:O:425:ILE:HG21	1.83	0.60
1:Z:351:LEU:HD22	1:Z:360:ALA:HB3	1.82	0.60
1:O:109:ALA:HA	1:O:134:PRO:HG3	1.83	0.59
1:Z:109:ALA:O	1:Z:112:CYS:HB2	2.03	0.59
1:O:18:ALA:HB1	1:O:63:VAL:HG21	1.84	0.59
1:Z:265:TYR:HB3	1:Z:412:ALA:HB3	1.85	0.59
1:Z:452:GLY:O	1:Z:453:PHE:C	2.40	0.59
1:O:432:ARG:NE	1:O:467:GLU:OE1	2.35	0.59
1:O:373:ALA:O	1:O:377:ILE:HG13	2.01	0.59
1:O:152:ARG:HH11	1:O:152:ARG:CG	2.14	0.59
1:O:330:GLU:O	1:O:331:TYR:C	2.40	0.59
1:O:143:TRP:HE3	1:O:144:ILE:HA	1.68	0.59
1:O:246:GLN:OE1	1:O:246:GLN:HA	2.01	0.59
1:O:395:MET:O	1:O:396:GLN:C	2.40	0.59
1:Z:224:TYR:HE2	1:Z:241:GLY:N	2.01	0.59
1:O:478:GLU:O	1:O:481:TYR:N	2.35	0.59
1:O:19:VAL:HG12	1:O:20:VAL:N	2.17	0.59
1:O:336:VAL:HG13	1:O:374:ASN:HB3	1.85	0.59
1:O:396:GLN:N	1:O:396:GLN:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:79:ILE:HD12	1:O:170:ILE:HD12	1.85	0.59
1:O:314:GLN:HG2	1:O:317:ARG:HH21	1.68	0.59
1:O:438:VAL:HG23	1:O:439:THR:N	2.17	0.58
1:Z:250:LEU:HD12	1:Z:255:CYS:HB2	1.84	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: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: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:HH11	1:Z:156:ARG:CG	2.16	0.58
1:O:37:GLN:NE2	1:O:47:HIS:NE2	2.50	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:445:TYR:CZ	1:O:460:LEU:HD12	2.38	0.58
1:O:104:GLN:HB3	1:O:349:THR:HG21	1.84	0.58
1:O:28:ILE:HD13	1:O:28:ILE:N	2.17	0.58
1:O:392:LEU:HD23	1:O:392:LEU:C	2.23	0.58
1:Z:196:THR:HG22	1:Z:197:LEU:N	2.18	0.58
1:O:110:GLU:HA	1:O:110:GLU:OE1	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:Z:410:GLY:O	1:Z:413:VAL:HG13	2.03	0.58
1:O:428:THR:HG22	1:O:429:ARG:N	2.17	0.58
1:Z:460:LEU:N	1:Z:460:LEU:HD13	2.18	0.58
1:Z:275:THR:HG21	1:Z:280:VAL:CG1	2.34	0.58
1:O:394:ALA:O	1:O:397:ALA:HB3	2.03	0.58
1:O:357:ASP:OD1	1:O:359:TYR:N	2.30	0.58
1:O:320:MET:HB3	1:O:322:LEU:HG	1.85	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:275:THR:N	1:Z:300:TYR:O	2.31	0.57
1:O:103:TRP:CE3	1:O:104:GLN:HG2	2.39	0.57
1:Z:423:SER:HB2	1:Z:428:THR:O	2.05	0.57
1:Z:389:ARG:O	1:Z:390:ASP:C	2.40	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:327:TYR:HB3	1:O:332:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:108:THR:HG21	1:Z:139:THR:C	2.25	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:Z:261:ALA:HB2	1:Z:273:MET:CB	2.32	0.57
1:Z:180:VAL:HG23	1:Z:216:GLU:O	2.05	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:170:ILE:HA	1:Z:173:MET:CE	2.33	0.57
1:Z:246:GLN:HG3	1:Z:270:PHE:CB	2.33	0.57
1:Z:6:ILE:HD12	1:Z:7:VAL:N	2.19	0.57
1:Z:244:GLY:O	1:Z:245:ASP:C	2.41	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: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:142:LYS:O	1:Z:143:TRP:C	2.42	0.56
1:Z:202:LYS:C	1:Z:206:VAL:HG23	2.25	0.56
1:O:179:HIS:CD2	1:O:215:PRO:HA	2.40	0.56
1:O:438:VAL:HA	1:O:441:LEU:CD1	2.32	0.56
1:O:173:MET:CB	1:O:227:THR:HG23	2.34	0.56
1:O:373:ALA:O	1:O:376:ILE:HB	2.06	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:O:81:ASN:ND2	1:O:81:ASN:N	2.54	0.56
1:Z:87:ILE:HG22	1:Z:88:VAL:N	2.20	0.56
1:O:271:MET:HE2	1:O:392:LEU:HA	1.85	0.56
1:O:485:GLY:O	1:O:486:TRP:C	2.44	0.56
1:O:251:PHE:O	1:O:254:LEU:N	2.29	0.56
1:Z:436:ARG:HG3	1:Z:436:ARG:NH1	2.20	0.56
1:Z:455:GLN:N	1:Z:459:GLU:OE2	2.29	0.56
1:Z:153:GLU:HA	1:Z:156:ARG:NH1	2.21	0.56
1:Z:189:THR:O	1:Z:190:MET:HB3	2.05	0.56
1:O:111:ILE:O	1:O:112:CYS:C	2.44	0.56
1:Z:20:VAL:CG2	1:Z:63:VAL:HG22	2.36	0.56
1:Z:416:ASN:N	1:Z:416:ASN:ND2	2.54	0.56
1:O:324:ASN:HD21	1:O:327:TYR:HB2	1.71	0.56
1:O:20:VAL:HG12	1:O:28:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Z:114:HIS:O	1:Z:117:ARG:N	2.39	0.55
1:O:174:THR:O	1:O:177:ARG:HG3	2.06	0.55
1:O:490:VAL:HG12	1:O:494:MET:HE2	1.87	0.55
1:Z:266:GLY:O	1:Z:310:GLY:N	2.29	0.55
1:O:437:GLU:O	1:O:438:VAL:C	2.44	0.55
1:Z:457:LEU:O	1:Z:460:LEU:N	2.39	0.55
1:O:130:LEU:HD12	1:O:190:MET:HB2	1.87	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:Z:382:GLU:HG2	1:Z:421:PHE:CZ	2.42	0.55
1:Z:442:GLY:O	1:Z:445:TYR:HB2	2.07	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:O:441:LEU:O	1:O:444:ALA:HB3	2.06	0.55
1:O:478:GLU:O	1:O:479:ARG:C	2.43	0.55
1:O:108:THR:CB	1:O:139:THR:HB	2.36	0.55
1:O:22:ASP:O	1:O:25:ALA:N	2.30	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:Z:490:VAL:O	1:Z:491:LYS:C	2.45	0.55
1:O:86:THR:CG2	1:O:162:PHE:HE1	2.11	0.55
1:O:406:LEU:O	1:O:431:GLU:N	2.29	0.55
1:Z:83:ARG:NH1	1:Z:83:ARG:HB2	2.17	0.54
1:Z:262:LYS:O	1:Z:271:MET:HA	2.07	0.54
1:Z:110:GLU:O	1:Z:111:ILE:C	2.45	0.54
1:O:339:THR:HG21	1:O:379:ALA:HA	1.88	0.54
1:O:180:VAL:HG22	1:O:181:THR:N	2.22	0.54
1:O:112:CYS:HB3	1:O:132:ILE:HG22	1.88	0.54
1:O:186:ALA:O	1:O:189:THR:HG23	2.07	0.54
1:O:388:THR:O	1:O:391:VAL:HG22	2.07	0.54
1:O:380:THR:HG22	1:O:381:LEU:N	2.22	0.54
1:Z:104:GLN:O	1:Z:106:ARG:NE	2.39	0.54
1:Z:422:GLN:O	1:Z:425:ILE:HG22	2.07	0.54
1:O:21:MET:HG3	1:O:25:ALA:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:127:ASN:HD22	1:O:193:ASN:HD21	1.55	0.54
1:O:387:GLN:O	1:O:388:THR:C	2.43	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:117:ARG:HG2	1:Z:118:ASP:OD1	2.07	0.54
1:O:115:LEU:N	1:O:115:LEU:HD13	2.22	0.54
1:Z:11:GLN:NE2	1:Z:165:VAL:HG11	2.21	0.54
1:O:442:GLY:O	1:O:445:TYR:HB2	2.07	0.54
1:O:74:ILE:HB	1:O:237:ILE:CD1	2.29	0.54
1:O:20:VAL:HG12	1:O:28:ILE:HB	1.89	0.54
1:Z:293:GLY:HA2	1:Z:299:ASN:ND2	2.23	0.54
1:Z:145:LEU:HG	1:Z:152:ARG:HG2	1.90	0.54
1:O:101:ILE:HD13	1:O:107:ARG:NE	2.23	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:41:LYS:CB	1:O:42:PRO:HD2	2.36	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:428:THR:HG22	1:Z:429:ARG:N	2.23	0.53
1:Z:361:ARG:O	1:Z:362:GLY:C	2.45	0.53
1:Z:478:GLU:O	1:Z:479:ARG:C	2.44	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:236:ARG:N	1:Z:236:ARG:HD3	2.22	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:O:339:THR:CG2	1:O:379:ALA:HA	2.38	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: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:51:GLU:O	1:O:55:THR:HG23	2.09	0.53
1:O:83:ARG:HG3	1:O:245:ASP:OD1	2.09	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:Z:89:TRP:HD1	1:Z:94:GLY:HA2	1.73	0.53
1:O:386:TYR:O	1:O:387:GLN:C	2.47	0.53
1:O:436:ARG:N	1:O:436:ARG:HD3	2.24	0.53
1:Z:271:MET:HE3	1:Z:392:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:273:MET:O	1:Z:301:ALA:HA	2.09	0.52
1:O:414:ALA:HA	1:O:432:ARG:HH11	1.73	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: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
1:Z:85:THR:HA	1:Z:101:ILE:O	2.09	0.52
1:Z:416:ASN:HD22	1:Z:416:ASN:H	1.58	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:83:ARG:NH1	3:O:601:GOL:O1	2.42	0.52
1:O:41:LYS:O	1:O:44:TRP:HB2	2.09	0.52
1:O:143:TRP:HE3	1:O:144:ILE:N	2.08	0.52
1:O:374:ASN:O	1:O:375:HIS:C	2.48	0.52
1:O:256:VAL:CB	1:O:294:PRO:HA	2.40	0.52
1:O:94:GLY:HA3	1:O:171:TRP:CH2	2.44	0.52
1:Z:51:GLU:O	1:Z:52:ILE:C	2.48	0.52
1:Z:174:THR:C	1:Z:175:GLN:HG2	2.29	0.52
1:O:143:TRP:HE3	1:O:144:ILE:CA	2.23	0.52
1:O:10:ASP:HB3	1:O:17:ARG:HB3	1.91	0.52
1:O:433:PRO:HA	1:O:465:VAL:O	2.10	0.52
1:O:89:TRP:CB	1:O:96:PRO:HA	2.39	0.52
1:Z:48:ASP:O	1:Z:49:PRO:C	2.47	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:30:VAL:HG12	1:O:31:SER:N	2.24	0.52
1:O:199:TRP:HB2	1:O:211:ARG:NH2	2.25	0.52
1:O:316:LEU:HA	1:O:320:MET:HB2	1.92	0.52
1:O:396:GLN:O	1:O:400:GLY:N	2.30	0.52
1:O:20:VAL:CG1	1:O:28:ILE:HB	2.39	0.52
1:O:339:THR:O	1:O:342:VAL:HB	2.10	0.52
1:O:420:GLN:O	1:O:421:PHE:C	2.47	0.52
1:Z:93:THR:OG1	1:Z:95:LYS:HB3	2.10	0.52
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:62:GLU:O	1:O:65:ALA:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:340:ASN:HB2	1:Z:375:HIS:CD2	2.45	0.51
1:Z:143:TRP:CE3	1:Z:144:ILE:HA	2.46	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:336:VAL:HG23	1:Z:338:ASN:H	1.75	0.51
1:Z:3:LYS:HD2	1:Z:72:ASP:O	2.10	0.51
1:O:199:TRP:CE3	1:O:199:TRP:HA	2.45	0.51
1:Z:250:LEU:HD11	1:Z:255:CYS:HB2	1.92	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:O:113:GLU:O	1:O:114:HIS:C	2.46	0.51
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.92	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:O:43:GLY:C	1:O:44:TRP:HD1	2.13	0.51
1:O:253:GLN:HA	1:O:253:GLN:OE1	2.11	0.51
1:Z:434:GLU:HB2	1:Z:465:VAL:HB	1.93	0.51
1:Z:355:TYR:CD1	1:Z:355:TYR:N	2.77	0.51
1:O:101:ILE:HD13	1:O:107:ARG:HD3	1.91	0.51
1:O:87:ILE:HG22	1:O:88:VAL:N	2.24	0.51
1:Z:217:VAL:O	1:Z:218:ARG:HG2	2.10	0.51
1:O:368:THR:HG22	1:O:369:ARG:N	2.25	0.51
1:O:391:VAL:O	1:O:392:LEU:C	2.45	0.51
1:O:485:GLY:O	1:O:488:LYS:N	2.43	0.51
1:Z:161:LEU:N	1:Z:161:LEU:HD23	2.26	0.51
1:O:196:THR:O	1:O:197:LEU:HB2	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:O:40:PRO:O	1:O:41:LYS:HB3	2.10	0.51
1:Z:475:GLU:O	1:Z:477:THR:O	2.29	0.51
1:Z:251:PHE:CE2	1:Z:446:LEU:HD12	2.46	0.51
1:Z:466:ILE:HD13	1:Z:466:ILE:N	2.25	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:133:ASP:CG	1:O:134:PRO:HD2	2.31	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:Z:429:ARG:HD3	1:Z:469:GLU:OE2	2.10	0.51
1:O:378:ARG:O	1:O:379:ALA:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:407:ARG:HH11	1:O:407:ARG:CG	2.23	0.51
1:O:110:GLU:O	1:O:111:ILE:C	2.49	0.50
1:O:103:TRP:CZ3	1:O:104:GLN:HG2	2.46	0.50
1:O:324:ASN:HB2	1:O:326:ALA:H	1.75	0.50
1:Z:428:THR:N	1:Z:472:PRO:HG3	2.25	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:O:180:VAL:HG22	1:O:181:THR:O	2.11	0.50
1:O:190:MET:HG2	1:O:190:MET:O	2.11	0.50
1:O:46:GLU:HB3	1:O:99:ASN:HD22	1.76	0.50
1:Z:262:LYS:HZ1	1:Z:272:LEU:HD13	1.75	0.50
1:Z:409:ASP:CB	1:Z:438:VAL:HG21	2.40	0.50
1:O:434:GLU:CB	1:O:465:VAL:HB	2.35	0.50
1:O:118:ASP:HB2	1:O:120:LEU:HD11	1.93	0.50
1:O:475:GLU:O	1:O:476:THR:C	2.48	0.50
1:O:210:PRO:HB3	1:O:212:GLU:OE1	2.11	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:Z:153:GLU:HA	1:Z:156:ARG:HH11	1.76	0.50
1:Z:19:VAL:HG13	1:Z:27:ILE:HG23	1.92	0.50
1:O:448:GLY:HA3	1:O:454:TRP:CZ3	2.46	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:Z:11:GLN:HG2	1:Z:16:SER:OG	2.12	0.50
1:Z:261:ALA:HA	1:Z:272:LEU:O	2.12	0.50
1:O:388:THR:HG21	1:O:422:GLN:NE2	2.27	0.50
1:O:41:LYS:O	1:O:44:TRP:N	2.45	0.50
1:Z:98:TYR:CD1	1:Z:99:ASN:N	2.80	0.50
1:O:331:TYR:CD2	1:O:332:PHE:CD1	2.97	0.50
1:Z:44:TRP:N	1:Z:44:TRP:CD1	2.79	0.50
1:O:365:PHE:HE2	1:O:492:ARG:HB3	1.67	0.50
1:Z:179:HIS:CG	1:Z:215:PRO:HB3	2.47	0.50
1:Z:22:ASP:HB3	1:Z:28:ILE:HD11	1.93	0.50
1:Z:355:TYR:HD1	1:Z:355:TYR:H	1.54	0.50
1:O:115:LEU:O	1:O:116:LYS:C	2.50	0.50
1:Z:171:TRP:NE1	1:Z:176:GLY:HA2	2.27	0.50
1:O:101:ILE:HD13	1:O:107:ARG:CD	2.42	0.50
1:O:137:SER:O	1:O:138:GLY:C	2.49	0.50
1:O:142:LYS:O	1:O:146:ASP:OD1	2.30	0.50
1:Z:223:VAL:HG22	1:Z:240:SER:HB3	1.93	0.50
1:Z:48:ASP:O	1:Z:51:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:453:PHE:CE2	1:Z:454:TRP:CZ2	3.00	0.50
1:Z:126:SER:O	1:Z:195:HIS:HE1	1.95	0.50
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:241:GLY:C	1:Z:242:ILE:HG13	2.32	0.49
1:O:36:GLU:HG2	1:O:38:ILE:HG13	1.93	0.49
1:O:293:GLY:O	1:O:295:THR:N	2.45	0.49
1:Z:193:ASN:CB	1:Z:196:THR:HB	2.41	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:35:PHE:HE1	1:O:47:HIS:CE1	2.31	0.49
1:Z:355:TYR:OH	1:Z:390:ASP:OD1	2.30	0.49
1:Z:347:ALA:O	1:Z:361:ARG:HA	2.11	0.49
1:Z:359:TYR:CZ	1:Z:499:HIS:CE1	2.99	0.49
1:O:83:ARG:NH1	1:O:83:ARG:CB	2.74	0.49
1:O:38:ILE:O	1:O:40:PRO:HD3	2.13	0.49
1:Z:60:LEU:O	1:Z:60:LEU:HD12	2.11	0.49
1:Z:423:SER:CB	1:Z:430:VAL:HG23	2.43	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:CD1	1:O:355:TYR:N	2.79	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:106:ARG:HH22	1:O:135:TYR:HA	1.78	0.49
1:Z:151:SER:HA	1:Z:160:LEU:HD11	1.95	0.49
1:O:6:ILE:HD13	1:O:75:ALA:HB3	1.95	0.49
1:Z:392:LEU:O	1:Z:392:LEU:HG	2.11	0.49
1:O:346:PRO:C	1:O:348:PHE:H	2.15	0.49
1:O:173:MET:O	1:O:227:THR:HG23	2.13	0.49
1:O:6:ILE:CD1	1:O:75:ALA:HB3	2.42	0.49
1:O:97:ILE:HG21	1:O:160:LEU:HD21	1.94	0.49
1:Z:228:ASN:ND2	1:Z:229:ILE:N	2.61	0.49
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.95	0.49
1:Z:256:VAL:HG11	1:Z:294:PRO:HB3	1.94	0.49
1:Z:174:THR:HG22	1:Z:226:GLN:O	2.12	0.49
1:O:435:VAL:HG12	1:O:437:GLU:H	1.77	0.48
1:Z:396:GLN:HB3	1:Z:401:ILE:O	2.13	0.48
1:Z:265:TYR:OH	1:Z:422:GLN:NE2	2.45	0.48
1:O:13:THR:CG2	1:O:103:TRP:NE1	2.77	0.48
1:O:244:GLY:O	1:O:245:ASP:C	2.51	0.48
1:Z:456:ASN:ND2	1:Z:459:GLU:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:104:GLN:NE2	1:Z:308:MET:CE	2.77	0.48
1:Z:316:LEU:HD23	1:Z:316:LEU:HA	1.61	0.48
1:O:97:ILE:HD11	1:O:144:ILE:CG2	2.43	0.48
1:O:83:ARG:HH11	1:O:83:ARG:HB2	1.78	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:23:HIS:C	1:Z:25:ALA:H	2.15	0.48
1:O:62:GLU:O	1:O:63:VAL:C	2.51	0.48
1:Z:89:TRP:CE3	1:Z:89:TRP:N	2.81	0.48
1:O:204:LEU:O	1:O:208:ASP:N	2.46	0.48
1:Z:311:ALA:HA	1:Z:314:GLN:HE21	1.77	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:48:ASP:O	1:O:51:GLU:N	2.45	0.48
1:O:142:LYS:NZ	1:O:146:ASP:OD2	2.46	0.48
1:O:204:LEU:O	1:O:205:GLU:C	2.52	0.48
1:Z:114:HIS:O	1:Z:116:LYS:N	2.46	0.48
1:O:271:MET:C	1:O:272:LEU:HD12	2.34	0.48
1:O:364:ILE:HG22	1:O:365:PHE:N	2.28	0.48
1:Z:193:ASN:CG	1:Z:196:THR:HB	2.34	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:368:THR:HB	1:O:371:VAL:HG23	1.95	0.48
1:O:94:GLY:HA3	1:O:171:TRP:CZ3	2.49	0.48
1:O:425:ILE:HD12	1:O:425:ILE:HA	1.54	0.48
1:Z:286:LEU:CD2	1:Z:304:GLY:HA2	2.44	0.48
1:O:190:MET:HB3	1:O:190:MET:HE3	1.69	0.48
1:Z:315:TRP:CZ2	1:Z:320:MET:HG3	2.49	0.48
1:O:137:SER:HA	1:O:140:LYS:HD2	1.96	0.48
1:O:13:THR:HG21	1:O:103:TRP:NE1	2.29	0.48
1:O:256:VAL:HB	1:O:294:PRO:HA	1.96	0.48
1:O:293:GLY:C	1:O:295:THR:H	2.17	0.48
1:O:265:TYR:CB	1:O:412:ALA:HB3	2.39	0.48
1:Z:179:HIS:CD2	1:Z:215:PRO:HB3	2.48	0.48
1:Z:474:ILE:HG13	1:Z:478:GLU:OE1	2.13	0.48
1:Z:21:MET:HA	1:Z:26:ASN:O	2.14	0.48
1:Z:120:LEU:O	1:Z:121:GLU:C	2.53	0.48
1:Z:169:LEU:O	1:Z:173:MET:HE2	2.13	0.48
1:Z:142:LYS:O	1:Z:146:ASP:OD1	2.32	0.48
1:Z:89:TRP:HB2	1:Z:95:LYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:104:GLN:HE22	1:Z:308:MET:CE	2.27	0.48
1:Z:420:GLN:NE2	1:Z:424:ASP:OD1	2.46	0.48
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:19:VAL:HG12	1:Z:21:MET:CE	2.44	0.47
1:O:40:PRO:HG2	1:O:44:TRP:CB	2.43	0.47
1:Z:180:VAL:CG2	1:Z:181:THR:N	2.76	0.47
1:Z:2:GLU:HG3	1:Z:3:LYS:N	2.30	0.47
1:O:157:ARG:O	1:O:158:GLY:C	2.50	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:Z:290:ILE:CG2	1:Z:291:ALA:N	2.78	0.47
1:O:251:PHE:CD2	1:O:446:LEU:CD1	2.97	0.47
1:O:174:THR:HG21	1:O:178:VAL:CG1	2.43	0.47
1:Z:332:PHE:HB3	1:Z:374:ASN:OD1	2.15	0.47
1:O:257:LYS:O	1:O:274:ASN:HB3	2.14	0.47
1:Z:136:PHE:HB3	1:Z:188:ARG:O	2.13	0.47
1:Z:256:VAL:HG11	1:Z:294:PRO:CA	2.45	0.47
1:Z:18:ALA:HB1	1:Z:63:VAL:HG11	1.95	0.47
1:O:60:LEU:O	1:O:63:VAL:HG23	2.13	0.47
1:Z:209:ILE:HA	1:Z:210:PRO:HD2	1.65	0.47
1:O:368:THR:CG2	1:O:369:ARG:N	2.78	0.47
1:Z:115:LEU:N	1:Z:115:LEU:HD22	2.20	0.47
1:Z:332:PHE:HB2	1:Z:377:ILE:HD12	1.95	0.47
1:O:406:LEU:N	1:O:429:ARG:O	2.47	0.47
1:O:125:ARG:HD3	1:O:281:LYS:HE3	1.96	0.47
1:Z:463:LYS:HD2	1:Z:463:LYS:HA	1.50	0.47
1:O:203:MET:O	1:O:204:LEU:C	2.50	0.47
1:Z:219:ARG:HG2	1:Z:219:ARG:O	2.10	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:Z:263:ASN:HB3	1:Z:408:VAL:HG12	1.96	0.47
1:Z:250:LEU:O	1:Z:253:GLN:HB2	2.14	0.47
1:Z:407:ARG:CG	1:Z:407:ARG:HH11	2.19	0.47
1:Z:181:THR:O	1:Z:217:VAL:HA	2.14	0.47
1:Z:46:GLU:OE2	1:Z:107:ARG:NH2	2.43	0.47
1:O:497:GLU:HG3	1:O:498:GLU:O	2.15	0.47
1:Z:432:ARG:O	1:Z:467:GLU:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:293:GLY:O	1:Z:296:GLY:N	2.44	0.47
1:Z:27:ILE:N	1:Z:27:ILE:HD12	2.28	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
1:O:445:TYR:CZ	1:O:460:LEU:CD1	2.98	0.47
1:O:226:GLN:HA	1:O:239:ILE:HG13	1.97	0.47
1:Z:109:ALA:O	1:Z:112:CYS:N	2.48	0.47
1:O:456:ASN:O	1:O:458:ASP:N	2.48	0.47
1:O:20:VAL:HG12	1:O:28:ILE:CB	2.45	0.47
1:Z:256:VAL:HG11	1:Z:294:PRO:HA	1.97	0.47
1:O:407:ARG:CG	1:O:407:ARG:NH1	2.78	0.47
1:Z:293:GLY:C	1:Z:295:THR:H	2.17	0.47
1:Z:478:GLU:CA	1:Z:481:TYR:HB3	2.45	0.47
1:Z:23:HIS:HA	1:Z:453:PHE:CZ	2.50	0.47
1:Z:203:MET:HE2	1:Z:207:LEU:HD11	1.97	0.46
1:O:137:SER:O	1:O:140:LYS:HB2	2.15	0.46
1:O:83:ARG:NH1	1:O:83:ARG:HB2	2.30	0.46
1:O:7:VAL:HG12	1:O:77:ILE:CG1	2.37	0.46
1:Z:457:LEU:HA	1:Z:457:LEU:HD13	1.52	0.46
1:Z:251:PHE:CE2	1:Z:446:LEU:CD1	2.99	0.46
1:Z:87:ILE:CG2	1:Z:88:VAL:N	2.79	0.46
1:Z:342:VAL:CG1	1:Z:343:TYR:N	2.78	0.46
1:O:59:THR:O	1:O:63:VAL:HG22	2.16	0.46
1:O:418:LEU:HD13	1:O:419:MET:HE2	1.96	0.46
1:O:162:PHE:O	1:O:179:HIS:HE1	1.98	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:Z:20:VAL:HG23	1:Z:63:VAL:CG2	2.45	0.46
1:Z:130:LEU:HD23	1:Z:190:MET:HB2	1.97	0.46
1:O:109:ALA:O	1:O:112:CYS:HB2	2.15	0.46
1:O:235:THR:C	1:O:236:ARG:HD3	2.36	0.46
1:Z:240:SER:HB2	1:Z:450:ALA:CB	2.45	0.46
1:Z:153:GLU:CA	1:Z:156:ARG:NH1	2.79	0.46
1:Z:19:VAL:HG22	1:Z:30:VAL:CG2	2.43	0.46
1:Z:394:ALA:O	1:Z:398:ASP:N	2.45	0.46
1:O:353:ALA:HA	1:O:354:PRO:HA	1.56	0.46
1:Z:355:TYR:CE2	1:Z:490:VAL:HG11	2.51	0.46
1:Z:272:LEU:CD1	1:Z:272:LEU:N	2.79	0.46
1:Z:253:GLN:OE1	1:Z:407:ARG:HD3	2.16	0.46
1:O:83:ARG:NE	1:O:246:GLN:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:184:THR:O	1:Z:187:SER:OG	2.29	0.46
1:Z:141:VAL:CG2	1:Z:162:PHE:CD1	2.99	0.46
1:Z:175:GLN:C	1:Z:177:ARG:H	2.19	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:O:222:GLU:HG3	1:O:223:VAL:N	2.31	0.46
1:O:222:GLU:O	1:O:240:SER:HA	2.16	0.46
1:Z:114:HIS:HD2	1:Z:117:ARG:NH2	2.14	0.46
1:Z:38:ILE:O	1:Z:40:PRO:HD3	2.16	0.46
1:Z:373:ALA:O	1:Z:377:ILE:HG13	2.16	0.46
1:Z:21:MET:HE3	1:Z:21:MET:HB2	1.62	0.46
1:O:154:ARG:HB3	1:O:159:GLU:HG3	1.97	0.46
1:O:200:ASP:C	1:O:204:LEU:HD12	2.36	0.46
1:Z:223:VAL:O	1:Z:223:VAL:HG12	2.10	0.46
1:O:74:ILE:HA	1:O:74:ILE:HD12	1.80	0.46
1:Z:401:ILE:CG2	1:Z:402:ARG:N	2.79	0.46
1:O:80:THR:OG1	1:O:245:ASP:HA	2.16	0.46
1:O:337:GLN:CA	1:O:337:GLN:NE2	2.79	0.46
1:O:19:VAL:CG1	1:O:20:VAL:N	2.79	0.46
1:Z:30:VAL:CG1	1:Z:31:SER:N	2.77	0.46
1:Z:212:GLU:N	1:Z:212:GLU:OE1	2.38	0.46
1:Z:153:GLU:OE1	1:Z:153:GLU:HA	2.16	0.45
1:O:180:VAL:CG2	1:O:181:THR:N	2.79	0.45
1:Z:317:ARG:NE	1:Z:318:ASP:OD1	2.49	0.45
1:O:151:SER:O	1:O:152:ARG:C	2.55	0.45
1:O:223:VAL:HG22	1:O:240:SER:HB3	1.97	0.45
1:Z:117:ARG:HG2	1:Z:118:ASP:N	2.31	0.45
1:O:274:ASN:HD21	1:O:299:ASN:HD22	1.63	0.45
1:Z:311:ALA:O	1:Z:314:GLN:HG3	2.15	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:Z:401:ILE:HG22	1:Z:402:ARG:N	2.32	0.45
1:O:94:GLY:CA	1:O:171:TRP:CH2	2.99	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:Z:143:TRP:O	1:Z:144:ILE:C	2.54	0.45
1:O:436:ARG:N	1:O:436:ARG:CD	2.79	0.45
1:Z:128:THR:OG1	1:Z:130:LEU:HB2	2.17	0.45
1:O:142:LYS:O	1:O:144:ILE:N	2.49	0.45
1:O:155:ALA:CB	1:O:210:PRO:HG2	2.47	0.45
1:Z:251:PHE:CD2	1:Z:446:LEU:CD1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:236:ARG:HA	1:O:236:ARG:HD3	1.76	0.45
1:O:372:ASN:OD1	1:O:374:ASN:HB2	2.16	0.45
1:Z:428:THR:CG2	1:Z:429:ARG:N	2.79	0.45
1:Z:436:ARG:CG	1:Z:436:ARG:HH11	2.29	0.45
1:O:407:ARG:HG2	1:O:407:ARG:NH1	2.30	0.45
1:O:427:GLY:C	1:O:472:PRO:HG3	2.36	0.45
1:Z:91:LYS:HB2	1:Z:161:LEU:HD21	1.98	0.45
1:Z:19:VAL:CG1	1:Z:21:MET:HE1	2.46	0.45
1:Z:83:ARG:HH11	1:Z:83:ARG:CB	2.22	0.45
1:Z:406:LEU:HD23	1:Z:407:ARG:H	1.81	0.45
1:Z:184:THR:HG22	1:Z:290:ILE:O	2.16	0.45
1:O:382:GLU:O	1:O:383:SER:C	2.55	0.45
1:O:364:ILE:CG2	1:O:365:PHE:N	2.80	0.45
1:Z:456:ASN:ND2	1:Z:458:ASP:CB	2.79	0.45
1:Z:141:VAL:HG22	1:Z:162:PHE:CD1	2.52	0.45
1:Z:64:LEU:HD22	1:Z:69:ILE:HG22	1.99	0.45
1:O:138:GLY:HA2	1:O:191:LEU:HD21	1.99	0.45
1:O:83:ARG:NH1	1:O:246:GLN:HG2	2.31	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:Z:457:LEU:HA	1:Z:460:LEU:HD23	1.99	0.45
1:O:395:MET:O	1:O:399:SER:N	2.45	0.45
1:O:218:ARG:HB3	1:O:222:GLU:OE2	2.16	0.45
1:O:272:LEU:N	1:O:272:LEU:HD12	2.31	0.45
1:O:385:ALA:O	1:O:388:THR:HB	2.17	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:Z:252:GLY:HA2	1:Z:445:TYR:CE2	2.52	0.45
1:Z:117:ARG:C	1:Z:119:GLY:H	2.19	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:O:336:VAL:HG21	1:O:338:ASN:O	2.16	0.45
1:Z:115:LEU:N	1:Z:115:LEU:CD2	2.78	0.45
1:Z:224:TYR:CE2	1:Z:242:ILE:CD1	2.99	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:O:52:ILE:O	1:O:53:TRP:C	2.55	0.45
1:O:145:LEU:HB3	1:O:152:ARG:NH1	2.32	0.45
1:O:208:ASP:C	1:O:209:ILE:HG12	2.37	0.45
1:O:97:ILE:O	1:O:98:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:446:LEU:HD12	1:Z:446:LEU:N	2.32	0.45
1:O:425:ILE:O	1:O:479:ARG:HD2	2.17	0.45
1:O:48:ASP:HB3	1:O:51:GLU:HB2	1.97	0.45
1:O:27:ILE:CD1	1:O:27:ILE:N	2.79	0.44
1:Z:111:ILE:HG22	1:Z:115:LEU:CD2	2.47	0.44
1:O:474:ILE:HG22	1:O:479:ARG:HB2	1.99	0.44
1:Z:457:LEU:O	1:Z:458:ASP:C	2.55	0.44
1:Z:414:ALA:O	1:Z:416:ASN:ND2	2.50	0.44
1:O:418:LEU:HD13	1:O:419:MET:CE	2.46	0.44
1:O:460:LEU:HD23	1:O:460:LEU:H	1.78	0.44
1:O:331:TYR:CE2	1:O:335:LYS:CE	3.00	0.44
1:O:7:VAL:HG23	1:O:20:VAL:HG22	2.00	0.44
1:O:224:TYR:N	1:O:224:TYR:CD1	2.86	0.44
1:Z:419:MET:HB2	1:Z:470:PHE:CZ	2.52	0.44
1:Z:63:VAL:CG1	1:Z:64:LEU:N	2.80	0.44
1:O:281:LYS:HG2	1:O:282:SER:N	2.32	0.44
1:O:476:THR:CG2	1:O:479:ARG:NH2	2.79	0.44
1:Z:88:VAL:HA	1:Z:161:LEU:O	2.18	0.44
1:Z:22:ASP:CB	1:Z:28:ILE:HD11	2.48	0.44
1:Z:186:ALA:O	1:Z:189:THR:HG23	2.18	0.44
1:O:115:LEU:HD22	1:O:115:LEU:N	2.20	0.44
1:Z:406:LEU:CD2	1:Z:407:ARG:N	2.80	0.44
1:O:241:GLY:C	1:O:242:ILE:HG13	2.37	0.44
1:O:294:PRO:O	1:O:295:THR:HG22	2.17	0.44
1:Z:40:PRO:HG3	1:Z:46:GLU:CD	2.38	0.44
1:Z:337:GLN:O	1:Z:338:ASN:HB3	2.17	0.44
1:Z:456:ASN:ND2	1:Z:459:GLU:HG3	2.33	0.44
1:Z:213:MET:HB2	1:Z:213:MET:HE2	1.69	0.44
1:O:61:VAL:O	1:O:62:GLU:C	2.56	0.44
1:Z:171:TRP:CD1	1:Z:176:GLY:HA2	2.53	0.44
1:Z:80:THR:OG1	1:Z:245:ASP:HA	2.18	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:Z:223:VAL:HA	1:Z:240:SER:CB	2.46	0.44
1:O:402:ARG:HG3	1:O:403:LEU:O	2.18	0.44
1:O:250:LEU:HD13	1:O:262:LYS:HG3	1.98	0.44
1:O:361:ARG:NH1	1:O:361:ARG:CG	2.79	0.44
1:Z:155:ALA:O	1:Z:158:GLY:N	2.51	0.44
1:Z:180:VAL:HG22	1:Z:181:THR:N	2.33	0.44
1:Z:47:HIS:HB3	1:Z:52:ILE:HD11	2.00	0.44
1:Z:339:THR:O	1:Z:375:HIS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:56:GLN:HE21	1:Z:56:GLN:C	2.17	0.44
1:O:69:ILE:CG2	1:O:70:SER:N	2.80	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:Z:9:LEU:HB2	1:Z:79:ILE:CD1	2.47	0.44
1:Z:488:LYS:O	1:Z:489:ALA:C	2.56	0.44
1:O:170:ILE:O	1:O:174:THR:HG23	2.18	0.44
1:O:365:PHE:CE2	1:O:492:ARG:CB	2.95	0.44
1:Z:74:ILE:HB	1:Z:237:ILE:CD1	2.47	0.44
1:Z:151:SER:O	1:Z:152:ARG:C	2.56	0.44
1:Z:150:GLY:O	1:Z:152:ARG:N	2.51	0.44
1:Z:416:ASN:O	1:Z:417:PHE:C	2.56	0.44
1:O:69:ILE:HG22	1:O:70:SER:N	2.31	0.44
1:O:88:VAL:HA	1:O:161:LEU:O	2.17	0.44
1:Z:441:LEU:HA	1:Z:441:LEU:HD23	1.75	0.44
1:O:224:TYR:HE1	1:O:241:GLY:N	2.16	0.44
1:Z:123:TYR:O	1:Z:127:ASN:N	2.48	0.44
1:Z:390:ASP:HA	1:Z:483:TYR:OH	2.18	0.43
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:Z:290:ILE:HG22	1:Z:291:ALA:N	2.32	0.43
1:O:224:TYR:CE1	1:O:240:SER:CA	3.00	0.43
1:Z:14:THR:HG22	1:Z:37:GLN:CD	2.38	0.43
1:O:214:LEU:HA	1:O:215:PRO:HD3	1.85	0.43
1:O:409:ASP:CG	1:O:438:VAL:HG21	2.38	0.43
1:Z:127:ASN:HB3	1:Z:193:ASN:ND2	2.33	0.43
1:Z:131:VAL:HG11	1:Z:356:TRP:CD2	2.53	0.43
1:O:396:GLN:HE22	1:O:403:LEU:HD22	1.82	0.43
1:O:339:THR:HB	1:O:342:VAL:HB	1.99	0.43
1:Z:90:GLU:HB2	1:Z:93:THR:HG1	1.81	0.43
1:Z:210:PRO:O	1:Z:212:GLU:N	2.51	0.43
1:Z:425:ILE:HG23	1:Z:426:LEU:N	2.34	0.43
1:O:152:ARG:NH1	1:O:152:ARG:CG	2.78	0.43
1:O:200:ASP:O	1:O:203:MET:N	2.51	0.43
1:O:213:MET:H	1:O:213:MET:HG3	1.54	0.43
1:Z:275:THR:HG23	1:Z:301:ALA:HA	2.01	0.43
1:Z:182:ASP:OD2	1:Z:184:THR:OG1	2.30	0.43
1:Z:133:ASP:CG	1:Z:134:PRO:HD2	2.38	0.43
1:O:178:VAL:O	1:O:178:VAL:HG22	2.16	0.43
1:O:59:THR:O	1:O:60:LEU:C	2.56	0.43
1:O:53:TRP:CZ3	1:O:172:LYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:120:LEU:O	1:O:121:GLU:O	2.36	0.43
1:Z:152:ARG:C	1:Z:156:ARG:HH11	2.22	0.43
1:Z:104:GLN:HE22	1:Z:308:MET:HE1	1.83	0.43
1:O:145:LEU:HG	1:O:152:ARG:HG2	2.01	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:Z:289:THR:HG23	1:Z:290:ILE:N	2.33	0.43
1:O:27:ILE:H	1:O:27:ILE:HD12	1.82	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:24:ASP:O	1:Z:463:LYS:HE2	2.19	0.43
1:Z:381:LEU:HD23	1:Z:381:LEU:HA	1.74	0.43
1:O:328:ASP:O	1:O:331:TYR:HB3	2.18	0.43
1:O:175:GLN:C	1:O:177:ARG:H	2.22	0.43
1:Z:345:VAL:O	1:Z:362:GLY:HA2	2.18	0.43
1:Z:479:ARG:HG2	1:Z:480:ASN:OD1	2.19	0.43
1:O:92:GLU:H	1:O:92:GLU:HG2	1.52	0.43
1:O:468:ARG:CG	1:O:469:GLU:N	2.82	0.43
1:Z:144:ILE:HG22	1:Z:145:LEU:N	2.33	0.43
1:O:416:ASN:ND2	1:O:416:ASN:H	2.16	0.43
1:Z:197:LEU:HD12	1:Z:197:LEU:HA	1.60	0.43
1:O:315:TRP:CD1	1:O:319:GLU:HB2	2.53	0.43
1:O:197:LEU:HD13	1:O:197:LEU:N	2.33	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
1:O:265:TYR:CD1	1:O:265:TYR:N	2.86	0.43
1:Z:214:LEU:HA	1:Z:215:PRO:HD3	1.76	0.43
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:469:GLU:HG3	1:Z:471:ARG:HH21	1.73	0.42
1:O:265:TYR:HB2	1:O:413:VAL:HG13	1.99	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:162:PHE:CB	1:Z:213:MET:HE2	2.49	0.42
1:Z:160:LEU:O	1:Z:161:LEU:HD23	2.18	0.42
1:Z:263:ASN:ND2	1:Z:265:TYR:CE1	2.87	0.42
1:O:97:ILE:HD12	1:O:148:VAL:HG21	2.01	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:O:153:GLU:O	1:O:156:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:O:297:GLU:HG2	1.50	0.42
1:Z:330:GLU:HG3	1:Z:415:ASN:CG	2.40	0.42
1:Z:340:ASN:HB2	1:Z:375:HIS:NE2	2.35	0.42
1:O:406:LEU:HA	1:O:406:LEU:HD23	1.33	0.42
1:Z:143:TRP:HE3	1:Z:144:ILE:N	2.17	0.42
1:Z:97:ILE:O	1:Z:97:ILE:HG12	2.19	0.42
1:O:338:ASN:C	1:O:340:ASN:H	2.23	0.42
1:O:273:MET:O	1:O:301:ALA:HA	2.18	0.42
1:Z:365:PHE:CZ	1:Z:492:ARG:HB3	2.54	0.42
1:Z:268:GLY:HA2	1:Z:309:ALA:H	1.85	0.42
1:Z:497:GLU:HG3	1:Z:498:GLU:N	2.34	0.42
1:Z:56:GLN:NE2	1:Z:56:GLN:HA	2.34	0.42
1:O:172:LYS:HE3	1:O:172:LYS:HB3	1.85	0.42
1:O:183:TYR:O	1:O:184:THR:C	2.57	0.42
1:Z:443:ALA:O	1:Z:444:ALA:C	2.57	0.42
1:O:339:THR:HG22	1:O:379:ALA:CA	2.49	0.42
1:Z:364:ILE:HG22	1:Z:365:PHE:N	2.35	0.42
1:O:305:ALA:O	1:O:353:ALA:HB3	2.20	0.42
1:O:97:ILE:HG21	1:O:160:LEU:CD2	2.50	0.42
1:O:104:GLN:HE22	1:O:308:MET:HE1	1.85	0.42
1:O:82:GLN:HA	1:O:245:ASP:OD2	2.20	0.42
1:Z:337:GLN:NE2	1:Z:337:GLN:HA	2.34	0.42
1:Z:74:ILE:HA	1:Z:74:ILE:HD12	1.84	0.42
1:O:193:ASN:CG	1:O:196:THR:HB	2.40	0.42
1:Z:62:GLU:O	1:Z:65:ALA:HB3	2.20	0.42
1:O:140:LYS:O	1:O:143:TRP:HB3	2.19	0.42
1:O:21:MET:CE	1:O:444:ALA:CB	2.98	0.42
1:Z:449:LEU:HD12	1:Z:449:LEU:HA	1.37	0.42
1:Z:240:SER:HB2	1:Z:450:ALA:HB3	2.02	0.42
1:O:432:ARG:HG2	1:O:432:ARG:O	2.18	0.42
1:O:254:LEU:HA	1:O:254:LEU:HD12	1.64	0.42
1:Z:374:ASN:O	1:Z:375:HIS:C	2.58	0.42
1:Z:468:ARG:HG2	1:Z:470:PHE:CE1	2.55	0.42
1:Z:106:ARG:HH22	1:Z:135:TYR:HA	1.85	0.42
1:Z:281:LYS:HE3	1:Z:281:LYS:HB2	1.71	0.42
1:O:277:GLU:CD	1:O:277:GLU:H	2.23	0.42
1:O:438:VAL:O	1:O:441:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:84:GLU:OE2	1:O:188:ARG:HD3	2.20	0.42
1:Z:108:THR:OG1	1:Z:134:PRO:HA	2.20	0.42
1:Z:111:ILE:O	1:Z:114:HIS:N	2.47	0.42
1:Z:372:ASN:O	1:Z:373:ALA:C	2.57	0.42
1:Z:162:PHE:HB2	1:Z:213:MET:HE2	2.02	0.42
1:O:44:TRP:N	1:O:44:TRP:CD1	2.87	0.42
1:Z:358:PRO:HG2	1:Z:359:TYR:CE1	2.55	0.42
1:Z:256:VAL:HG13	1:Z:294:PRO:CG	2.50	0.42
1:O:170:ILE:HG21	1:O:178:VAL:HG22	2.01	0.42
1:Z:332:PHE:O	1:Z:333:ALA:C	2.57	0.42
1:Z:336:VAL:HG21	1:Z:375:HIS:CD2	2.55	0.42
1:Z:353:ALA:HA	1:Z:354:PRO:HA	1.65	0.41
1:O:440:ALA:O	1:O:441:LEU:C	2.57	0.41
1:O:224:TYR:HE1	1:O:240:SER:CA	2.33	0.41
1:Z:38:ILE:HG22	1:Z:40:PRO:HD3	2.02	0.41
1:O:364:ILE:N	1:O:364:ILE:HD12	2.35	0.41
1:Z:145:LEU:HD12	1:Z:151:SER:HB2	2.00	0.41
1:Z:474:ILE:HD12	1:Z:474:ILE:HA	1.30	0.41
1:O:60:LEU:HD12	1:O:60:LEU:O	2.20	0.41
1:Z:387:GLN:O	1:Z:388:THR:C	2.57	0.41
1:O:108:THR:O	1:O:109:ALA:C	2.58	0.41
1:O:83:ARG:CZ	1:O:246:GLN:HB2	2.50	0.41
1:Z:117:ARG:CG	1:Z:118:ASP:N	2.79	0.41
1:Z:165:VAL:HG23	1:Z:165:VAL:H	1.43	0.41
1:Z:162:PHE:CG	1:Z:163:GLY:N	2.87	0.41
1:Z:64:LEU:HD23	1:Z:69:ILE:HB	2.00	0.41
1:Z:308:MET:CE	1:Z:311:ALA:CB	2.98	0.41
1:Z:154:ARG:O	1:Z:159:GLU:HG3	2.20	0.41
1:Z:352:GLY:H	1:Z:356:TRP:HA	1.85	0.41
1:O:200:ASP:OD2	1:O:203:MET:N	2.44	0.41
1:O:191:LEU:CD2	1:O:207:LEU:HD13	2.50	0.41
1:Z:260:MET:O	1:Z:274:ASN:N	2.51	0.41
1:O:106:ARG:NH2	1:O:135:TYR:HA	2.34	0.41
1:O:482:ARG:O	1:O:483:TYR:C	2.58	0.41
1:Z:334:THR:H	1:Z:334:THR:HG23	1.62	0.41
1:O:81:ASN:HB2	1:O:165:VAL:HB	2.03	0.41
1:Z:89:TRP:CD1	1:Z:94:GLY:HA2	2.53	0.41
1:O:130:LEU:HD12	1:O:190:MET:CB	2.49	0.41
1:Z:186:ALA:C	1:Z:188:ARG:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:257:LYS:HB2	1:Z:260:MET:SD	2.60	0.41
1:Z:6:ILE:C	1:Z:6:ILE:HD12	2.41	0.41
1:O:251:PHE:CD2	1:O:446:LEU:HD12	2.55	0.41
1:Z:41:LYS:HD3	1:Z:44:TRP:CE2	2.55	0.41
1:Z:256:VAL:CG1	1:Z:294:PRO:CB	2.97	0.41
1:O:171:TRP:NE1	1:O:176:GLY:HA2	2.34	0.41
1:O:411:GLY:O	1:O:412:ALA:C	2.59	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:297:GLU:HG3	1:Z:297:GLU:H	1.34	0.41
1:Z:153:GLU:O	1:Z:156:ARG:N	2.54	0.41
1:Z:19:VAL:HG12	1:Z:21:MET:HE1	2.01	0.41
1:O:39:TYR:O	1:O:41:LYS:N	2.53	0.41
1:O:41:LYS:O	1:O:41:LYS:HG2	2.19	0.41
1:O:34:GLU:N	1:O:34:GLU:OE1	2.53	0.41
1:Z:352:GLY:O	1:Z:355:TYR:N	2.54	0.41
1:O:211:ARG:O	1:O:214:LEU:HG	2.20	0.41
1:O:250:LEU:CD1	1:O:255:CYS:CB	2.99	0.41
1:Z:81:ASN:HB2	1:Z:165:VAL:HB	2.03	0.41
1:Z:421:PHE:O	1:Z:425:ILE:HG22	2.21	0.41
1:Z:253:GLN:O	1:Z:254:LEU:HB2	2.20	0.41
1:Z:88:VAL:HB	1:Z:97:ILE:CD1	2.51	0.41
1:Z:22:ASP:CG	1:Z:28:ILE:HD11	2.40	0.41
1:Z:308:MET:HE2	1:Z:311:ALA:CB	2.50	0.41
1:Z:191:LEU:CD2	1:Z:207:LEU:HD13	2.50	0.41
1:O:226:GLN:HB3	1:O:237:ILE:O	2.20	0.41
1:O:19:VAL:HG13	1:O:27:ILE:CG2	2.51	0.41
1:Z:47:HIS:HB2	1:Z:100:ALA:HB3	2.02	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:O:9:LEU:HA	1:O:9:LEU:HD12	1.67	0.41
1:O:134:PRO:O	1:O:140:LYS:NZ	2.51	0.41
1:O:438:VAL:CG2	1:O:439:THR:N	2.82	0.41
1:Z:255:CYS:HA	1:Z:260:MET:SD	2.61	0.41
1:Z:446:LEU:O	1:Z:449:LEU:HB2	2.21	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: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:Z:377:ILE:HD13	1:Z:377:ILE:HG21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:152:ARG:HB3	1:Z:156:ARG:NH1	2.36	0.41
1:O:125:ARG:HD2	1:O:125:ARG:HH11	1.73	0.41
1:Z:403:LEU:HD12	1:Z:403:LEU:HA	1.77	0.41
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:Z:249:ALA:CB	1:Z:262:LYS:HE2	2.51	0.41
1:O:106:ARG:HH22	1:O:135:TYR:CA	2.33	0.41
1:Z:260:MET:O	1:Z:273:MET:HA	2.21	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:313:ILE:O	1:Z:314:GLN:C	2.56	0.40
1:O:53:TRP:CD1	1:O:172:LYS:HE2	2.56	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:Z:83:ARG:CB	1:Z:83:ARG:NH1	2.81	0.40
2:O:602:EPE:H82	2:O:602:EPE:H52	1.79	0.40
1:O:83:ARG:CG	3:O:601:GOL:O2	2.63	0.40
1:O:347:ALA:CB	1:O:351:LEU:CD1	3.00	0.40
1:O:352:GLY:C	1:O:356:TRP:H	2.20	0.40
1:Z:172:LYS:HE2	1:Z:172:LYS:HB3	1.71	0.40
1:Z:81:ASN:ND2	1:Z:81:ASN:N	2.69	0.40
1:O:173:MET:HB3	1:O:227:THR:HG21	2.02	0.40
1:O:380:THR:O	1:O:381:LEU:C	2.58	0.40
1:Z:417:PHE:CD2	1:Z:417:PHE:C	2.95	0.40
1:Z:425:ILE:CG2	1:Z:426:LEU:N	2.84	0.40
1:O:324:ASN:ND2	1:O:327:TYR:H	2.19	0.40
1:O:237:ILE:HG23	1:O:238:PRO:HD2	2.03	0.40
1:O:468:ARG:NE	1:O:470:PHE:CE2	2.90	0.40
1:Z:457:LEU:N	1:Z:457:LEU:HD22	2.35	0.40
1:Z:220:SER:HB3	1:Z:242:ILE:O	2.22	0.40
1:O:171:TRP:CE2	1:O:176:GLY:HA2	2.57	0.40
1:O:201:ASP:O	1:O:202:LYS:C	2.59	0.40
1:Z:156:ARG:CG	1:Z:156:ARG:NH1	2.80	0.40
1:Z:20:VAL:O	1:Z:27:ILE:HA	2.22	0.40
1:Z:186:ALA:C	1:Z:188:ARG:N	2.75	0.40
1:Z:426:LEU:HA	1:Z:426:LEU:HD12	1.63	0.40
1:O:189:THR:HG23	1:O:189:THR:H	1.57	0.40
1:Z:441:LEU:O	1:Z:442:GLY:C	2.60	0.40
1:O:83:ARG:CG	1:O:245:ASP:OD1	2.70	0.40
1:O:262:LYS:HD2	1:O:263:ASN:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:53:TRP:CZ3	1:Z:172:LYS:HB2	2.57	0.40
1:Z:360:ALA:C	1:Z:361:ARG:HG2	2.41	0.40
1:Z:338:ASN:O	1:Z:375:HIS:HD2	2.04	0.40
1:Z:433:PRO:HA	1:Z:465:VAL:O	2.20	0.40
1:O:449:LEU:C	1:O:451:VAL:H	2.25	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%)	2	9
1	Z	496/501 (99%)	397 (80%)	85 (17%)	14 (3%)	6	28
All	All	991/1002 (99%)	767 (77%)	179 (18%)	45 (4%)	3	17

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

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Mol	Chain	Res	Type
1	O	397	ALA
1	O	446	LEU
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%)	293 (72%)	115 (28%)	0	1
1	Z	409/412 (99%)	287 (70%)	122 (30%)	0	1
All	All	817/824 (99%)	580 (71%)	237 (29%)	0	1

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	4	LYS
1	O	5	TYR
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	29	SER
1	O	37	GLN
1	O	41	LYS
1	O	51	GLU
1	O	52	ILE
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	91	LYS
1	O	95	LYS
1	O	104	GLN
1	O	107	ARG
1	O	114	HIS
1	O	115	LEU
1	O	116	LYS
1	O	121	GLU
1	O	122	ASP
1	O	139	THR
1	O	141	VAL
1	O	144	ILE
1	O	145	LEU

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Mol	Chain	Res	Type
1	O	146	ASP
1	O	148	VAL
1	O	149	GLU
1	O	152	ARG
1	O	154	ARG
1	O	157	ARG
1	O	159	GLU
1	O	170	ILE
1	O	175	GLN
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	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	222	GLU
1	O	224	TYR
1	O	226	GLN
1	O	227	THR
1	O	235	THR
1	O	254	LEU
1	O	256	VAL
1	O	257	LYS
1	O	258	GLU
1	O	262	LYS
1	O	269	CYS
1	O	277	GLU
1	O	278	LYS
1	O	280	VAL
1	O	284	ASN
1	O	288	THR
1	O	297	GLU
1	O	323	ILE
1	O	324	ASN

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Mol	Chain	Res	Type
1	O	325	ASP
1	O	328	ASP
1	O	329	SER
1	O	335	LYS
1	O	336	VAL
1	O	337	GLN
1	O	349	THR
1	O	351	LEU
1	O	361	ARG
1	O	365	PHE
1	O	369	ARG
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	434	GLU
1	O	436	ARG
1	O	437	GLU
1	O	439	THR
1	O	449	LEU
1	O	459	GLU
1	O	460	LEU
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	11	GLN
1	Z	13	THR

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Mol	Chain	Res	Type
1	Z	16	SER
1	Z	17	ARG
1	Z	21	MET
1	Z	29	SER
1	Z	33	ARG
1	Z	45	VAL
1	Z	50	MET
1	Z	56	GLN
1	Z	62	GLU
1	Z	66	LYS
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	115	LEU
1	Z	117	ARG
1	Z	118	ASP
1	Z	121	GLU
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	152	ARG
1	Z	153	GLU
1	Z	154	ARG
1	Z	156	ARG
1	Z	159	GLU
1	Z	161	LEU
1	Z	164	THR

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Mol	Chain	Res	Type
1	Z	172	LYS
1	Z	175	GLN
1	Z	177	ARG
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	211	ARG
1	Z	213	MET
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	246	GLN
1	Z	254	LEU
1	Z	256	VAL
1	Z	262	LYS
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	314	GLN
1	Z	317	ARG
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

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Mol	Chain	Res	Type
1	Z	392	LEU
1	Z	395	MET
1	Z	398	ASP
1	Z	403	LEU
1	Z	406	LEU
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
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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

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Mol	Chain	Res	Type
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	81	ASN
1	Z	104	GLN
1	Z	114	HIS
1	Z	127	ASN
1	Z	185	ASN
1	Z	195	HIS
1	Z	228	ASN
1	Z	299	ASN
1	Z	324	ASN
1	Z	404	HIS
1	Z	420	GLN
1	Z	422	GLN
1	Z	455	GLN
1	Z	456	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 carbohydrates in this entry.

5.6 Ligand geometry

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$
3	GOL	O	601	-	5,5,5	0.87	0	5,5,5	0.62	0
2	EPE	O	602	-	14,15,15	2.50	2 (14%)	18,20,20	2.28	6 (33%)
3	GOL	Z	603	-	5,5,5	0.41	0	5,5,5	0.52	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	GOL	O	601	-	-	0/4/4/4	0/0/0/0
2	EPE	O	602	-	-	0/9/19/19	0/1/1/1
3	GOL	Z	603	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	602	EPE	C5-N4	2.09	1.52	1.46
2	O	602	EPE	O3S-S	8.31	1.67	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	602	EPE	O3S-S-O1S	-4.74	100.58	111.61
2	O	602	EPE	C6-N1-C2	2.03	113.29	108.90
2	O	602	EPE	C5-C6-N1	2.14	114.47	110.63
2	O	602	EPE	O2S-S-O1S	2.45	122.41	113.48
2	O	602	EPE	C2-C3-N4	3.36	116.65	110.63
2	O	602	EPE	O2S-S-C10	5.75	111.81	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	601	GOL	4	0
2	O	602	EPE	2	0
3	Z	603	GOL	2	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%)	-0.92	1 (0%) 95 89	12, 33, 66, 90	0
1	Z	498/501 (99%)	-0.95	0 100 100	11, 32, 66, 87	0
All	All	995/1002 (99%)	-0.93	1 (0%) 95 91	11, 32, 66, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	325	ASP	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	EPE	O	602	15/15	0.91	0.28	5.65	84,84,84,84	0
3	GOL	O	601	6/6	0.97	0.11	-0.22	10,11,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	Z	603	6/6	0.98	0.11	-0.45	10,10,10,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.