



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:04 AM EST

PDB ID : 1GLJ  
Title : ESCHERICHIA COLI GLYCEROL KINASE MUTANT WITH BOUND ATP ANALOG SHOWING SUBSTANTIAL DOMAIN MOTION  
Authors : Bystrom, C.E.; Pettigrew, D.W.; Branchaud, B.P.; Remington, S.J.  
Deposited on : 1998-09-03  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

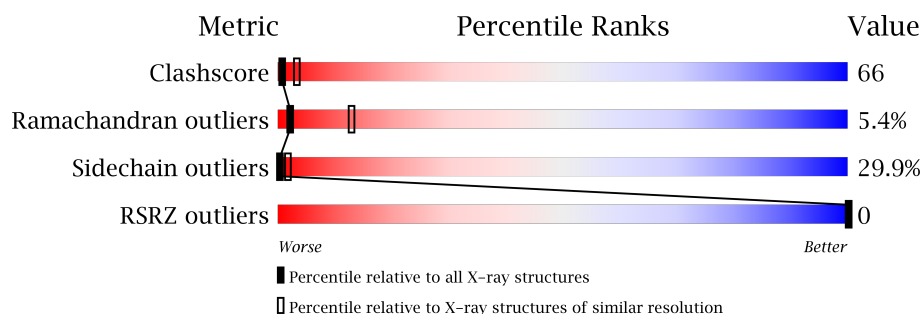
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7895 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLYCEROL KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			
1	O	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			

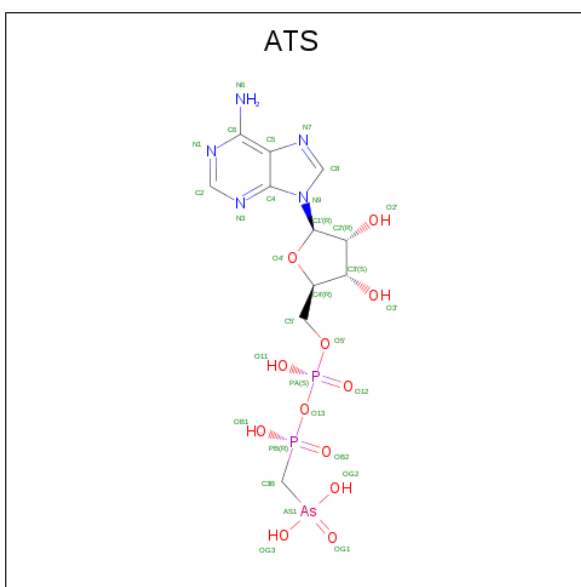
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	58	TRP	SER	ENGINEERED	UNP P0A6F3
O	58	TRP	SER	ENGINEERED MUTATION	UNP P0A6F3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

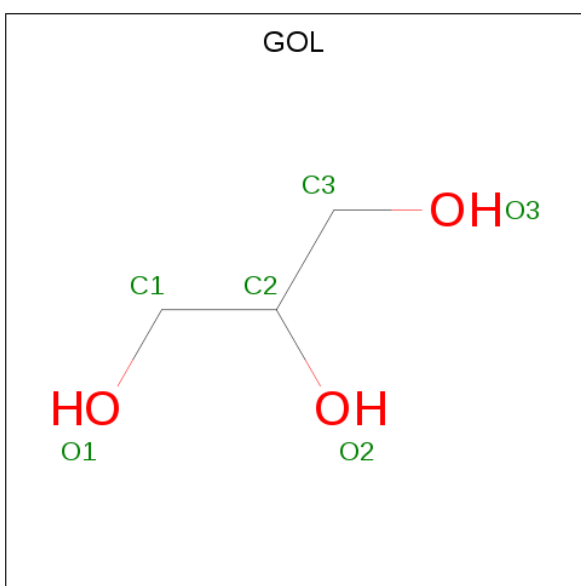
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GAMMA-ARSONO-BETA, GAMMA-METHYLENEADENOSINE-5'-DIPHOSPHATE (three-letter code: ATS) (formula: C<sub>11</sub>H<sub>18</sub>AsN<sub>5</sub>O<sub>12</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	Y	1	Total 31	As 1	C 11	N 5	O 12	P 2	0	0
3	O	1	Total 31	As 1	C 11	N 5	O 12	P 2	0	0

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

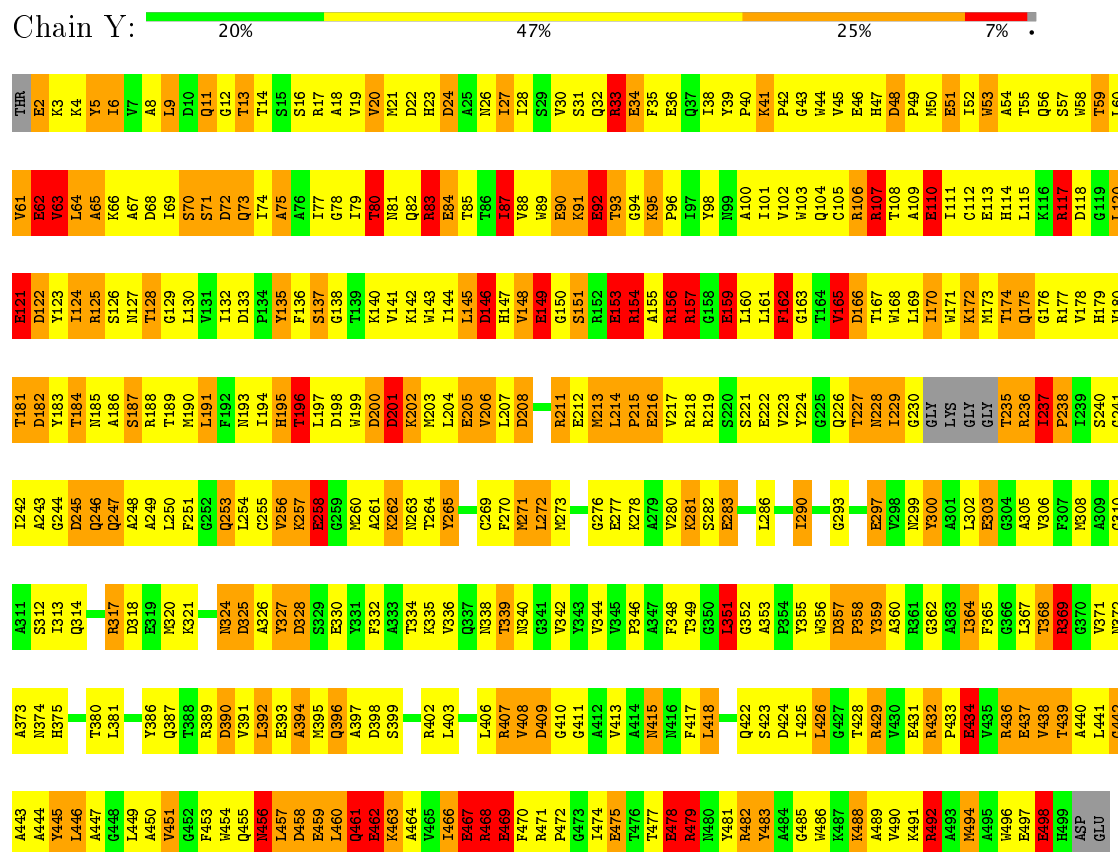


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0

### 3 Residue-property plots

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

#### • Molecule 1: GLYCEROL KINASE



L444	L381	L316	Q246	T184
Y445	E382	R317	Q247	N185
L446	S383	D318	A248	A186
A447		E319	A249	S187
G448	Y386	N320	L250	R188
L449	Q387	K321	P251	T189
A450	T388	L322	G352	N190
V451	R389	L323	Q253	L191
F453	D390	N324	L254	F192
N454	V391	D325	C255	N193
	L392	A326	V256	L194
Q455	E393	Y327	K257	H195
N456	A394	D328	E358	T196
L457	N395	S329		L197
D458	Q396	E330	K262	D198
E459	A397	Y331	N263	N199
L460	D398	F332	T264	D200
Q461	S399	A333	Y265	D201
E462	G400	T334		K202
K463	I401	K335	C269	N203
A464	R402		F270	L204
L466	L403		E271	E205
E467		N338	L272	V206
E468	L406	T339	N273	L207
F470	R407	N340	N274	D208
E471	V408	G343	T275	L209
P472	D409	Y342	G276	P210
G473	G410	T343	E277	R211
L474		V344	K278	E212
E475	V413	V345	A279	N213
T476	A414	P346	V280	L214
T477	N415	A347	K281	P215
E478	I416	F348	S282	E216
R479	F417		E283	V217
N480	L418	L351		R218
Y481	N419	G352	L286	R219
Y483	Q420	P353	L287	S220
A484	P421	Y354	T288	S221
Q485	Q422	N355	T289	E222
N486	S423	D357	L290	
K487	D424	P358	A291	Q226
K488	I425	Y359	C292	T227
A489	L426	A360	G293	N228
K491	Q427	R361	P294	T229
K492	T428	G362	T295	G230
A493	R429	A363	G296	GLY
N494	V430	I364	E297	LYS
N495	E431		V298	GLY
N496	R432	L367	N299	T235
E497	P433	T368	X300	T236
N498	E434	R369	A301	K236
H499	V435		L302	T237
E499	R436	A373	E303	P238
H499	V438	N374		L239
H499	V439	H375	G310	S240
ASP	T439	I376	A311	G241
GLU	A440	I377	S312	T242
	L441	R378	I313	A243
	G442	A379	Q314	G244
	A443	T380	W315	D245

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.67Å 200.70Å 114.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 18.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 90.6 (18.49-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	246.72 (at 2.98Å)	Xtriage
Refinement program	TNT 5F, X-PLOR	Depositor
R, $R_{free}$	0.166 , (Not available) 0.159 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 130.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MG, ATS

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	1.29	39/3991 (1.0%)	1.72	80/5412 (1.5%)
1	Y	1.38	36/3991 (0.9%)	1.86	104/5412 (1.9%)
All	All	1.33	75/7982 (0.9%)	1.79	184/10824 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y	0	1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	258	GLU	CD-OE2	8.77	1.35	1.25
1	Y	283	GLU	CD-OE1	8.74	1.35	1.25
1	Y	462	GLU	CD-OE2	8.57	1.35	1.25
1	O	153	GLU	CD-OE1	8.19	1.34	1.25
1	Y	498	GLU	CD-OE2	8.11	1.34	1.25
1	Y	62	GLU	CD-OE1	8.09	1.34	1.25
1	O	393	GLU	CD-OE1	8.07	1.34	1.25
1	Y	297	GLU	CD-OE2	8.01	1.34	1.25
1	O	84	GLU	CD-OE1	7.97	1.34	1.25
1	O	113	GLU	CD-OE2	7.91	1.34	1.25
1	O	330	GLU	CD-OE1	7.88	1.34	1.25
1	Y	149	GLU	CD-OE1	7.87	1.34	1.25
1	Y	34	GLU	CD-OE1	7.79	1.34	1.25
1	Y	36	GLU	CD-OE2	7.76	1.34	1.25
1	O	36	GLU	CD-OE2	7.72	1.34	1.25
1	Y	431	GLU	CD-OE1	7.65	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	121	GLU	CD-OE2	7.65	1.34	1.25
1	O	159	GLU	CD-OE2	7.64	1.34	1.25
1	O	462	GLU	CD-OE2	7.53	1.33	1.25
1	Y	475	GLU	CD-OE1	7.49	1.33	1.25
1	Y	153	GLU	CD-OE1	7.41	1.33	1.25
1	O	51	GLU	CD-OE1	7.40	1.33	1.25
1	Y	51	GLU	CD-OE1	7.35	1.33	1.25
1	Y	216	GLU	CD-OE2	7.24	1.33	1.25
1	Y	106	ARG	CZ-NH1	7.17	1.42	1.33
1	O	92	GLU	CD-OE2	7.14	1.33	1.25
1	O	205	GLU	CD-OE1	7.14	1.33	1.25
1	O	62	GLU	CD-OE1	7.13	1.33	1.25
1	Y	205	GLU	CD-OE1	7.07	1.33	1.25
1	O	459	GLU	CD-OE1	7.05	1.33	1.25
1	O	498	GLU	CD-OE2	6.97	1.33	1.25
1	O	34	GLU	CD-OE1	6.97	1.33	1.25
1	Y	258	GLU	CD-OE2	6.96	1.33	1.25
1	O	149	GLU	CD-OE2	6.95	1.33	1.25
1	Y	110	GLU	CD-OE2	6.94	1.33	1.25
1	Y	196	THR	CB-CG2	-6.91	1.29	1.52
1	Y	92	GLU	CD-OE2	6.75	1.33	1.25
1	O	2	GLU	CD-OE2	6.70	1.33	1.25
1	O	469	GLU	CD-OE2	6.67	1.32	1.25
1	O	431	GLU	CD-OE1	6.63	1.32	1.25
1	Y	2	GLU	CD-OE2	6.62	1.32	1.25
1	Y	459	GLU	CD-OE1	6.62	1.32	1.25
1	O	216	GLU	CD-OE2	6.60	1.32	1.25
1	Y	212	GLU	CD-OE2	6.56	1.32	1.25
1	Y	456	ASN	C-O	-6.50	1.11	1.23
1	O	277	GLU	CD-OE1	6.49	1.32	1.25
1	O	90	GLU	CD-OE2	6.44	1.32	1.25
1	Y	277	GLU	CD-OE1	6.34	1.32	1.25
1	O	283	GLU	CD-OE1	6.33	1.32	1.25
1	O	110	GLU	CD-OE2	6.28	1.32	1.25
1	O	222	GLU	CD-OE2	6.25	1.32	1.25
1	Y	330	GLU	CD-OE1	5.83	1.32	1.25
1	Y	84	GLU	CD-OE1	5.82	1.32	1.25
1	Y	121	GLU	CD-OE1	5.79	1.32	1.25
1	Y	113	GLU	CD-OE2	5.79	1.32	1.25
1	O	303	GLU	CD-OE2	-5.71	1.19	1.25
1	Y	467	GLU	CD-OE2	5.65	1.31	1.25
1	O	437	GLU	CD-OE1	5.58	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	434	GLU	CD-OE1	5.55	1.31	1.25
1	O	478	GLU	CD-OE2	5.53	1.31	1.25
1	Y	33	ARG	NE-CZ	5.52	1.40	1.33
1	O	497	GLU	CD-OE1	5.50	1.31	1.25
1	O	125	ARG	NE-CZ	5.42	1.40	1.33
1	Y	303	GLU	CD-OE1	5.36	1.31	1.25
1	O	212	GLU	CD-OE2	5.35	1.31	1.25
1	O	475	GLU	CD-OE1	5.33	1.31	1.25
1	Y	469	GLU	CD-OE2	5.28	1.31	1.25
1	O	303	GLU	CD-OE1	5.24	1.31	1.25
1	O	297	GLU	CD-OE2	5.13	1.31	1.25
1	Y	90	GLU	CD-OE2	5.10	1.31	1.25
1	Y	33	ARG	CZ-NH2	5.10	1.39	1.33
1	Y	159	GLU	CD-OE2	5.09	1.31	1.25
1	O	46	GLU	CD-OE2	5.07	1.31	1.25
1	O	359	TYR	CB-CG	-5.05	1.44	1.51
1	O	319	GLU	CD-OE2	5.05	1.31	1.25

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	106	ARG	NE-CZ-NH2	-14.77	112.92	120.30
1	Y	117	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	O	471	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	Y	245	ASP	CB-CG-OD2	-11.70	107.77	118.30
1	Y	196	THR	N-CA-CB	-11.20	89.02	110.30
1	Y	328	ASP	CB-CG-OD1	-10.97	108.43	118.30
1	Y	214	LEU	C-N-CD	-10.40	97.73	120.60
1	Y	351	LEU	C-N-CA	-9.63	102.08	122.30
1	Y	357	ASP	CB-CG-OD1	9.61	126.95	118.30
1	Y	479	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	O	409	ASP	CB-CG-OD1	-9.36	109.88	118.30
1	Y	106	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	Y	327	TYR	CB-CG-CD1	-8.95	115.63	121.00
1	Y	157	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	O	325	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	O	357	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	Y	468	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	O	146	ASP	CB-CG-OD2	-8.34	110.79	118.30
1	O	468	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	Y	479	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	Y	83	ARG	C-N-CA	-8.26	101.04	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	107	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	Y	13	THR	CA-CB-CG2	-8.14	101.00	112.40
1	Y	334	THR	CA-CB-CG2	-8.11	101.04	112.40
1	O	328	ASP	CB-CG-OD1	-8.10	111.02	118.30
1	O	198	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	Y	357	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	O	353	ALA	C-N-CD	8.02	145.25	128.40
1	O	133	ASP	CB-CG-OD2	-7.96	111.13	118.30
1	Y	265	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	O	318	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	O	357	ASP	CB-CG-OD1	7.88	125.39	118.30
1	O	245	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	O	13	THR	CA-CB-CG2	-7.78	101.51	112.40
1	Y	72	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	O	361	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	O	474	ILE	CA-CB-CG1	-7.67	96.44	111.00
1	Y	80	THR	N-CA-CB	7.63	124.80	110.30
1	O	122	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	Y	247	GLN	N-CA-CB	-7.56	97.00	110.60
1	O	369	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	O	327	TYR	CB-CG-CD1	-7.47	116.52	121.00
1	Y	122	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	O	359	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	Y	24	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	O	468	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	O	198	ASP	CB-CG-OD1	7.36	124.92	118.30
1	Y	478	GLU	N-CA-CB	-7.34	97.39	110.60
1	O	68	ASP	CB-CG-OD2	7.28	124.85	118.30
1	Y	328	ASP	CB-CG-OD2	7.27	124.84	118.30
1	Y	436	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	Y	162	PHE	CB-CG-CD1	7.23	125.86	120.80
1	Y	154	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	O	182	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	Y	196	THR	CA-CB-CG2	-7.08	102.49	112.40
1	Y	390	ASP	CB-CG-OD1	-7.06	111.94	118.30
1	O	353	ALA	N-CA-CB	6.97	119.85	110.10
1	O	424	ASP	CB-CG-OD1	6.91	124.51	118.30
1	O	133	ASP	CB-CG-OD1	6.90	124.51	118.30
1	Y	72	ASP	CB-CG-OD1	6.88	124.49	118.30
1	Y	125	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	Y	117	ARG	CD-NE-CZ	6.83	133.16	123.60
1	Y	300	TYR	CB-CG-CD1	-6.82	116.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	200	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	O	351	LEU	C-N-CA	-6.72	108.19	122.30
1	O	68	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	Y	325	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	O	83	ARG	N-CA-C	6.52	128.61	111.00
1	O	436	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	Y	398	ASP	CB-CG-OD2	6.51	124.16	118.30
1	Y	468	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	O	359	TYR	CA-CB-CG	-6.45	101.15	113.40
1	Y	146	ASP	N-CA-CB	6.42	122.15	110.60
1	O	398	ASP	CB-CG-OD2	6.40	124.06	118.30
1	O	201	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	Y	245	ASP	CB-CG-OD1	6.37	124.03	118.30
1	O	318	ASP	CB-CG-OD1	6.36	124.02	118.30
1	Y	24	ASP	CB-CG-OD2	6.35	124.02	118.30
1	O	409	ASP	CB-CG-OD2	6.32	123.98	118.30
1	Y	443	ALA	N-CA-CB	6.25	118.86	110.10
1	Y	305	ALA	N-CA-CB	6.24	118.84	110.10
1	Y	318	ASP	N-CA-CB	6.21	121.78	110.60
1	Y	459	GLU	CG-CD-OE2	6.19	130.68	118.30
1	O	325	ASP	CB-CG-OD1	6.19	123.87	118.30
1	Y	409	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	O	492	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	Y	68	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	Y	351	LEU	O-C-N	-6.15	112.75	123.20
1	Y	135	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	O	146	ASP	CB-CG-OD1	6.11	123.80	118.30
1	O	90	GLU	N-CA-CB	6.09	121.56	110.60
1	O	20	VAL	CB-CA-C	-6.06	99.89	111.40
1	Y	201	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	O	125	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	Y	166	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	Y	482	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	Y	200	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	O	72	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	Y	201	ASP	CB-CG-OD1	5.88	123.59	118.30
1	O	80	THR	N-CA-CB	5.87	121.46	110.30
1	Y	492	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	O	398	ASP	CB-CG-OD1	-5.85	113.03	118.30
1	O	24	ASP	CB-CG-OD1	-5.83	113.06	118.30
1	Y	198	ASP	CB-CG-OD1	5.81	123.53	118.30
1	O	107	ARG	NE-CZ-NH1	5.81	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	117	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	Y	208	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	Y	107	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	O	378	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	Y	184	THR	CA-CB-CG2	-5.75	104.34	112.40
1	Y	117	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	Y	380	THR	CA-CB-CG2	-5.74	104.36	112.40
1	O	292	CYS	N-CA-CB	5.71	120.88	110.60
1	Y	182	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	Y	154	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	Y	87	ILE	CB-CA-C	-5.69	100.22	111.60
1	O	369	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	Y	317	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	Y	118	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	Y	195	HIS	CA-CB-CG	-5.66	103.97	113.60
1	O	122	ASP	CA-CB-CG	-5.65	100.97	113.40
1	O	72	ASP	CB-CG-OD1	5.65	123.38	118.30
1	Y	87	ILE	N-CA-CB	5.65	123.78	110.80
1	O	386	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	Y	174	THR	CA-CB-CG2	-5.62	104.53	112.40
1	O	327	TYR	CB-CG-CD2	5.61	124.37	121.00
1	Y	390	ASP	CB-CG-OD2	5.61	123.35	118.30
1	Y	156	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	O	265	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	Y	20	VAL	CA-CB-CG1	-5.55	102.57	110.90
1	Y	459	GLU	CG-CD-OE1	-5.55	107.20	118.30
1	O	195	HIS	N-CA-CB	5.54	120.58	110.60
1	O	317	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	Y	432	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	Y	458	ASP	CA-CB-CG	5.49	125.48	113.40
1	O	201	ASP	CB-CG-OD1	5.47	123.22	118.30
1	O	156	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	Y	359	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	Y	432	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	Y	443	ALA	CB-CA-C	-5.40	101.99	110.10
1	Y	327	TYR	CA-CB-CG	-5.40	103.14	113.40
1	Y	369	ARG	CB-CA-C	-5.39	99.61	110.40
1	Y	247	GLN	CB-CA-C	5.38	121.15	110.40
1	Y	398	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	Y	359	TYR	CG-CD1-CE1	-5.34	117.03	121.30
1	O	236	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	Y	408	VAL	CA-CB-CG2	-5.30	102.95	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	318	ASP	CB-CA-C	-5.30	99.81	110.40
1	O	118	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	O	105	CYS	CA-CB-SG	-5.29	104.48	114.00
1	O	354	PRO	N-CA-CB	5.29	109.64	103.30
1	O	328	ASP	CB-CG-OD2	5.28	123.05	118.30
1	O	13	THR	CA-CB-OG1	5.28	120.08	109.00
1	O	471	ARG	CD-NE-CZ	5.25	130.96	123.60
1	Y	373	ALA	CB-CA-C	5.24	117.97	110.10
1	Y	394	ALA	N-CA-CB	5.24	117.44	110.10
1	Y	325	ASP	CB-CG-OD1	5.22	123.00	118.30
1	Y	369	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	O	359	TYR	CG-CD2-CE2	-5.20	117.14	121.30
1	Y	59	THR	CA-CB-CG2	-5.19	105.13	112.40
1	Y	213	MET	CA-CB-CG	-5.19	104.48	113.30
1	Y	456	ASN	CA-C-O	5.17	130.96	120.10
1	Y	237	ILE	C-N-CD	-5.17	109.23	120.60
1	Y	196	THR	N-CA-C	5.16	124.92	111.00
1	Y	196	THR	CA-C-N	-5.15	105.88	117.20
1	Y	83	ARG	N-CA-C	5.11	124.79	111.00
1	O	471	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	O	200	ASP	CB-CG-OD1	5.10	122.89	118.30
1	O	361	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	O	196	THR	CA-CB-CG2	-5.09	105.28	112.40
1	O	20	VAL	CA-CB-CG1	-5.08	103.27	110.90
1	Y	48	ASP	N-CA-CB	5.07	119.73	110.60
1	Y	196	THR	C-N-CA	-5.07	109.03	121.70
1	Y	271	MET	CA-CB-CG	-5.07	104.69	113.30
1	O	83	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	O	475	GLU	N-CA-CB	5.04	119.67	110.60
1	Y	55	THR	N-CA-CB	5.02	119.84	110.30
1	O	147	HIS	CA-CB-CG	-5.02	105.07	113.60
1	O	334	THR	CA-CB-CG2	-5.02	105.38	112.40
1	Y	390	ASP	N-CA-CB	5.01	119.62	110.60
1	Y	33	ARG	CD-NE-CZ	5.01	130.61	123.60
1	O	80	THR	CA-CB-CG2	-5.00	105.39	112.40
1	Y	117	ARG	CB-CA-C	-5.00	100.39	110.40
1	O	342	VAL	CA-CB-CG2	-5.00	103.40	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	196	THR	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3910	0	3841	558	0
1	Y	3910	0	3841	486	0
2	Y	1	0	0	0	0
3	O	31	0	12	2	0
3	Y	31	0	12	2	0
4	O	6	0	8	2	0
4	Y	6	0	8	3	0
All	All	7895	0	7722	1036	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 66.

All (1036) 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:O:22:ASP:HB3	1:O:28:ILE:HD11	1.30	1.13
1:O:47:HIS:HB3	1:O:52:ILE:HD11	1.32	1.09
1:O:5:TYR:HB2	1:O:74:ILE:HG22	1.37	1.07
1:Y:193:ASN:HB3	1:Y:196:THR:HG21	1.37	1.06
1:Y:458:ASP:HA	1:Y:461:GLN:HG3	1.34	1.06
1:Y:415:ASN:ND2	1:Y:418:LEU:H	1.58	1.02
1:Y:415:ASN:HD22	1:Y:418:LEU:H	1.07	1.02
1:Y:5:TYR:HB2	1:Y:74:ILE:HG22	1.39	1.00
1:Y:250:LEU:HD11	1:Y:255:CYS:HB2	1.43	0.98
1:O:415:ASN:ND2	1:O:418:LEU:H	1.63	0.96
1:O:463:LYS:HA	1:O:463:LYS:HE2	1.44	0.96
1:Y:460:LEU:H	1:Y:460:LEU:HD12	1.27	0.95
1:O:137:SER:HA	1:O:140:LYS:HD3	1.45	0.95
1:Y:117:ARG:HB2	1:Y:117:ARG:NH1	1.82	0.94
1:O:415:ASN:HD22	1:O:418:LEU:H	1.15	0.94
1:O:492:ARG:HH11	1:O:492:ARG:HG2	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:460:LEU:HD12	1:O:460:LEU:H	1.29	0.94
1:Y:117:ARG:HB2	1:Y:117:ARG:HH11	1.32	0.93
1:O:206:VAL:HG12	1:O:207:LEU:HD23	1.51	0.92
1:Y:227:THR:HB	1:Y:229:ILE:HG23	1.51	0.91
1:O:33:ARG:NH2	1:O:58:TRP:HB3	1.84	0.91
1:O:70:SER:H	1:O:73:GLN:HE21	1.11	0.91
1:Y:41:LYS:HG3	1:Y:42:PRO:HD2	1.54	0.90
1:Y:230:GLY:HA2	1:Y:235:THR:HB	1.54	0.89
1:Y:70:SER:H	1:Y:73:GLN:HE21	1.16	0.89
1:O:91:LYS:HB2	1:O:161:LEU:HD12	1.55	0.88
1:Y:180:VAL:HG21	1:Y:218:ARG:HG3	1.54	0.88
1:Y:456:ASN:HD22	1:Y:457:LEU:N	1.71	0.88
1:O:124:ILE:HD13	1:O:203:MET:HE3	1.54	0.88
1:O:47:HIS:CB	1:O:52:ILE:HD11	2.03	0.88
1:Y:91:LYS:O	1:Y:92:GLU:C	2.10	0.87
1:Y:9:LEU:HD21	1:Y:60:LEU:HD13	1.56	0.87
1:Y:70:SER:N	1:Y:73:GLN:HE21	1.73	0.86
1:O:441:LEU:HD22	1:O:445:TYR:CE1	2.09	0.86
1:O:9:LEU:HB2	1:O:79:ILE:HD13	1.58	0.86
1:O:403:LEU:H	1:O:403:LEU:HD12	1.41	0.86
1:Y:19:VAL:HG22	1:Y:30:VAL:HG22	1.56	0.85
1:Y:492:ARG:HG2	1:Y:492:ARG:HH11	1.40	0.84
1:O:22:ASP:HB3	1:O:28:ILE:CD1	2.06	0.84
1:O:41:LYS:HG3	1:O:42:PRO:HD2	1.59	0.84
1:O:80:THR:HG21	1:O:245:ASP:HA	1.59	0.83
1:O:230:GLY:HA2	1:O:235:THR:HB	1.59	0.82
1:Y:84:GLU:HB2	1:Y:103:TRP:HB3	1.61	0.82
1:Y:124:ILE:HD13	1:Y:203:MET:CE	2.09	0.82
1:O:70:SER:N	1:O:73:GLN:HE21	1.77	0.82
1:O:91:LYS:O	1:O:92:GLU:C	2.18	0.82
1:O:313:ILE:HD11	1:O:381:LEU:HD23	1.62	0.81
1:Y:468:ARG:HD2	1:Y:469:GLU:N	1.96	0.81
1:Y:226:GLN:HB2	1:Y:236:ARG:HD3	1.61	0.81
1:O:18:ALA:CB	1:O:59:THR:HG22	2.11	0.80
1:Y:227:THR:HB	1:Y:229:ILE:CG2	2.11	0.80
1:O:180:VAL:HG21	1:O:218:ARG:HG3	1.64	0.80
1:O:466:ILE:HG12	1:O:467:GLU:N	1.96	0.80
1:Y:193:ASN:HB3	1:Y:196:THR:CG2	2.11	0.79
1:Y:463:LYS:HE2	1:Y:463:LYS:HA	1.64	0.79
1:O:206:VAL:CG1	1:O:207:LEU:HD23	2.13	0.79
1:O:144:ILE:O	1:O:148:VAL:HG23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:253:GLN:CG	1:O:407:ARG:HD2	2.13	0.79
1:Y:60:LEU:O	1:Y:63:VAL:HG23	1.82	0.79
1:O:373:ALA:O	1:O:377:ILE:HG13	1.84	0.78
1:Y:458:ASP:HA	1:Y:461:GLN:CG	2.11	0.78
1:Y:5:TYR:CB	1:Y:74:ILE:HG22	2.14	0.78
1:Y:3:LYS:HG2	1:Y:72:ASP:O	1.83	0.78
1:O:48:ASP:C	1:O:52:ILE:HD12	2.04	0.78
1:Y:70:SER:H	1:Y:73:GLN:NE2	1.82	0.78
1:O:95:LYS:HG3	1:O:96:PRO:HD2	1.64	0.77
1:O:415:ASN:HD21	1:O:417:PHE:HB3	1.49	0.77
1:Y:5:TYR:HB2	1:Y:74:ILE:CG2	2.12	0.77
1:O:183:TYR:CE1	1:O:217:VAL:HG12	2.19	0.77
1:Y:183:TYR:CE1	1:Y:217:VAL:HG12	2.20	0.77
1:Y:230:GLY:CA	1:Y:235:THR:HB	2.14	0.77
1:O:5:TYR:CB	1:O:74:ILE:HG22	2.13	0.76
1:Y:250:LEU:CD1	1:Y:255:CYS:HB2	2.15	0.76
1:Y:362:GLY:HA3	1:O:367:LEU:HB2	1.67	0.76
1:O:62:GLU:O	1:O:63:VAL:C	2.23	0.76
1:Y:144:ILE:O	1:Y:148:VAL:HG23	1.86	0.76
1:Y:479:ARG:HG3	1:Y:479:ARG:HH11	1.51	0.76
1:Y:157:ARG:HG3	1:Y:159:GLU:OE1	1.86	0.76
1:O:463:LYS:HA	1:O:463:LYS:CE	2.13	0.75
1:O:184:THR:O	1:O:187:SER:HB3	1.86	0.75
1:O:137:SER:O	1:O:138:GLY:C	2.21	0.75
1:Y:270:PHE:CE1	4:Y:600:GOL:H31	2.22	0.75
1:O:164:THR:H	1:O:167:THR:HB	1.49	0.75
1:O:86:THR:OG1	1:O:137:SER:HB3	1.86	0.75
1:Y:403:LEU:HD12	1:Y:403:LEU:H	1.52	0.75
1:O:486:TRP:O	1:O:490:VAL:HG23	1.86	0.75
1:Y:80:THR:CG2	1:Y:245:ASP:HA	2.16	0.75
1:O:153:GLU:O	1:O:157:ARG:HG2	1.87	0.74
1:O:173:MET:HB3	1:O:227:THR:CG2	2.17	0.74
1:O:226:GLN:HB2	1:O:236:ARG:HD3	1.68	0.74
1:Y:270:PHE:CZ	4:Y:600:GOL:H31	2.21	0.74
1:O:254:LEU:HD11	1:O:445:TYR:HE2	1.51	0.74
1:Y:33:ARG:NH2	1:Y:58:TRP:HB3	2.01	0.74
1:Y:111:ILE:O	1:Y:115:LEU:HD12	1.88	0.74
1:O:272:LEU:HD11	1:O:303:GLU:CG	2.17	0.74
1:O:80:THR:HG21	1:O:248:ALA:CB	2.18	0.73
1:Y:105:CYS:SG	1:Y:107:ARG:HD2	2.28	0.73
1:Y:255:CYS:HB3	1:Y:260:MET:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:181:THR:HG23	1:O:182:ASP:O	1.89	0.73
1:O:410:GLY:O	1:O:413:VAL:HG13	1.89	0.73
1:O:221:SER:OG	1:O:450:ALA:HB2	1.89	0.73
1:Y:229:ILE:HG13	1:Y:230:GLY:N	2.04	0.73
1:Y:3:LYS:HA	1:Y:73:GLN:HA	1.71	0.73
1:Y:261:ALA:HB2	1:Y:273:MET:HG3	1.72	0.72
1:O:253:GLN:HG3	1:O:407:ARG:HD2	1.72	0.72
1:Y:74:ILE:CD1	1:Y:237:ILE:HG21	2.20	0.72
1:Y:61:VAL:O	1:Y:62:GLU:C	2.26	0.72
1:O:85:THR:HG23	1:O:102:VAL:HA	1.71	0.72
1:O:330:GLU:HG3	1:O:417:PHE:HB3	1.71	0.72
1:O:3:LYS:HA	1:O:73:GLN:HA	1.71	0.71
1:O:251:PHE:CE2	1:O:446:LEU:HD13	2.25	0.71
1:O:39:TYR:HA	1:O:44:TRP:O	1.90	0.71
1:Y:129:GLY:C	1:Y:130:LEU:HD23	2.11	0.71
1:O:55:THR:HA	1:O:58:TRP:CD1	2.24	0.71
1:Y:140:LYS:O	1:Y:144:ILE:HD12	1.91	0.71
1:O:80:THR:CG2	1:O:245:ASP:HA	2.21	0.71
1:Y:396:GLN:HA	1:Y:399:SER:OG	1.91	0.71
1:Y:41:LYS:CG	1:Y:42:PRO:HD2	2.20	0.71
1:O:179:HIS:CD2	1:O:215:PRO:HB3	2.26	0.70
1:Y:257:LYS:O	1:Y:260:MET:HG3	1.91	0.70
1:O:254:LEU:HD11	1:O:445:TYR:CE2	2.24	0.70
1:Y:180:VAL:CG2	1:Y:218:ARG:HG3	2.21	0.70
1:Y:33:ARG:HH12	1:Y:62:GLU:HG3	1.55	0.70
1:O:396:GLN:HE21	1:O:403:LEU:HD12	1.56	0.70
1:Y:80:THR:HG21	1:Y:245:ASP:HA	1.73	0.70
1:O:226:GLN:CB	1:O:236:ARG:HD3	2.22	0.70
1:Y:458:ASP:C	1:Y:461:GLN:HB2	2.11	0.70
1:O:202:LYS:O	1:O:206:VAL:HB	1.91	0.70
1:O:90:GLU:HB2	1:O:93:THR:OG1	1.91	0.70
1:O:468:ARG:HD2	1:O:469:GLU:N	2.06	0.70
1:Y:137:SER:HA	1:Y:140:LYS:HD3	1.73	0.70
1:Y:179:HIS:CE1	1:Y:215:PRO:HG3	2.26	0.70
1:O:467:GLU:OE2	1:O:468:ARG:HB2	1.92	0.69
1:Y:137:SER:O	1:Y:141:VAL:HG23	1.92	0.69
1:Y:47:HIS:HB3	1:Y:52:ILE:HD11	1.74	0.69
1:Y:124:ILE:HD13	1:Y:203:MET:HE3	1.73	0.69
1:Y:168:TRP:O	1:Y:172:LYS:HG2	1.93	0.69
1:O:70:SER:H	1:O:73:GLN:NE2	1.87	0.69
1:O:197:LEU:N	1:O:197:LEU:HD22	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:255:CYS:HB3	1:Y:260:MET:HB3	1.74	0.69
1:Y:458:ASP:O	1:Y:461:GLN:HB2	1.92	0.69
1:O:441:LEU:HD22	1:O:445:TYR:CZ	2.27	0.69
1:Y:293:GLY:HA2	1:Y:299:ASN:ND2	2.08	0.69
1:O:182:ASP:OD1	1:O:185:ASN:HB2	1.93	0.68
1:Y:201:ASP:HA	1:Y:204:LEU:HB2	1.75	0.68
1:Y:422:GLN:HE21	1:Y:426:LEU:HD22	1.58	0.68
1:O:48:ASP:O	1:O:52:ILE:HD12	1.94	0.68
1:O:102:VAL:HG12	1:O:103:TRP:CD1	2.29	0.68
1:O:41:LYS:CG	1:O:42:PRO:HD2	2.24	0.68
1:O:74:ILE:HD12	1:O:74:ILE:O	1.94	0.68
1:Y:429:ARG:NH1	1:Y:469:GLU:OE2	2.26	0.68
1:O:236:ARG:HH11	1:O:236:ARG:HG3	1.58	0.68
1:Y:222:GLU:O	1:Y:240:SER:HA	1.94	0.68
1:O:161:LEU:HD23	1:O:179:HIS:CE1	2.29	0.68
1:O:293:GLY:HA2	1:O:299:ASN:ND2	2.08	0.68
1:Y:456:ASN:HD22	1:Y:457:LEU:H	1.41	0.67
1:O:170:ILE:O	1:O:171:TRP:C	2.33	0.67
1:Y:228:ASN:HD21	1:Y:235:THR:N	1.92	0.67
1:O:322:LEU:N	1:O:322:LEU:HD23	2.09	0.67
1:O:85:THR:HA	1:O:101:ILE:O	1.94	0.67
1:O:123:TYR:CD2	1:O:203:MET:HE2	2.29	0.67
1:O:377:ILE:O	1:O:380:THR:HB	1.93	0.67
1:O:17:ARG:HH22	1:O:437:GLU:CG	2.07	0.67
1:Y:467:GLU:OE2	1:Y:468:ARG:HB2	1.95	0.67
1:O:61:VAL:O	1:O:62:GLU:C	2.29	0.67
1:Y:123:TYR:CD1	1:Y:203:MET:HE2	2.29	0.67
1:O:398:ASP:O	1:O:399:SER:C	2.29	0.67
1:O:457:LEU:O	1:O:459:GLU:N	2.28	0.67
1:Y:18:ALA:HB1	1:Y:63:VAL:HG21	1.77	0.67
1:Y:127:ASN:HB3	1:Y:193:ASN:HD22	1.59	0.67
1:Y:456:ASN:ND2	1:Y:457:LEU:N	2.42	0.67
1:O:5:TYR:HB3	1:O:21:MET:O	1.95	0.67
1:O:207:LEU:HB3	1:O:209:ILE:CD1	2.24	0.67
1:Y:130:LEU:HD23	1:Y:130:LEU:N	2.09	0.67
1:Y:27:ILE:N	1:Y:27:ILE:HD12	2.10	0.67
1:O:249:ALA:HB2	1:O:439:THR:OG1	1.96	0.66
1:O:272:LEU:HD11	1:O:303:GLU:OE1	1.95	0.66
1:O:84:GLU:OE1	1:O:84:GLU:N	2.28	0.66
1:O:90:GLU:N	1:O:95:LYS:O	2.28	0.66
1:O:391:VAL:O	1:O:392:LEU:C	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:5:TYR:O	1:O:75:ALA:N	2.28	0.66
1:Y:62:GLU:O	1:Y:63:VAL:C	2.30	0.66
1:O:180:VAL:CG2	1:O:218:ARG:HG3	2.24	0.66
1:Y:91:LYS:HB2	1:Y:161:LEU:HD12	1.76	0.66
1:O:127:ASN:HD22	1:O:193:ASN:HD21	1.43	0.66
1:O:18:ALA:HB3	1:O:59:THR:HG22	1.76	0.66
1:Y:456:ASN:N	1:Y:459:GLU:OE2	2.29	0.66
1:O:358:PRO:HG2	1:O:359:TYR:CE2	2.31	0.66
1:Y:14:THR:N	3:Y:601:ATS:OG2	2.28	0.66
1:Y:174:THR:O	1:Y:176:GLY:N	2.29	0.66
1:O:173:MET:HB3	1:O:227:THR:HG23	1.78	0.66
1:Y:253:GLN:CG	1:Y:407:ARG:HD2	2.25	0.66
1:Y:463:LYS:CE	1:Y:463:LYS:HA	2.26	0.66
1:Y:154:ARG:CB	1:Y:159:GLU:HB3	2.25	0.66
1:Y:17:ARG:HG2	1:Y:32:GLN:HG3	1.78	0.66
1:Y:21:MET:HA	1:Y:28:ILE:HD13	1.79	0.66
1:O:162:PHE:HB3	1:O:213:MET:HG3	1.78	0.65
1:Y:169:LEU:O	1:Y:173:MET:HG2	1.96	0.65
1:Y:189:THR:HB	1:Y:191:LEU:CD1	2.26	0.65
1:Y:155:ALA:HA	1:Y:160:LEU:HB2	1.78	0.65
1:O:124:ILE:HD13	1:O:203:MET:CE	2.26	0.65
1:O:33:ARG:CZ	1:O:58:TRP:HB3	2.25	0.65
1:Y:64:LEU:O	1:Y:66:LYS:N	2.29	0.65
1:O:439:THR:HG22	1:O:440:ALA:N	2.11	0.65
1:O:91:LYS:O	1:O:94:GLY:N	2.30	0.65
1:O:183:TYR:CD1	1:O:217:VAL:HG12	2.30	0.65
1:O:415:ASN:HD22	1:O:418:LEU:N	1.93	0.65
1:O:144:ILE:HG22	1:O:148:VAL:CG2	2.27	0.65
1:O:179:HIS:CE1	1:O:215:PRO:HG3	2.31	0.65
1:Y:177:ARG:NH1	1:Y:226:GLN:O	2.30	0.65
1:O:120:LEU:O	1:O:121:GLU:C	2.28	0.65
1:O:492:ARG:NH1	1:O:492:ARG:HG2	2.05	0.65
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.78	0.65
1:O:184:THR:HG22	1:O:290:ILE:O	1.97	0.64
1:O:41:LYS:CB	1:O:42:PRO:HD2	2.27	0.64
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.78	0.64
1:O:274:ASN:OD1	1:O:276:GLY:N	2.30	0.64
1:O:125:ARG:NH1	1:O:282:SER:O	2.30	0.64
1:O:47:HIS:CD2	1:O:82:GLN:HE22	2.15	0.64
1:Y:180:VAL:HG23	1:Y:216:GLU:O	1.97	0.64
1:Y:70:SER:O	1:Y:73:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:26:ASN:O	1:O:28:ILE:HD13	1.97	0.64
1:O:498:GLU:HA	1:O:498:GLU:OE1	1.96	0.64
1:Y:183:TYR:CD1	1:Y:217:VAL:HG12	2.33	0.64
1:Y:478:GLU:O	1:Y:482:ARG:HG2	1.97	0.64
1:Y:69:ILE:N	1:Y:69:ILE:HD12	2.11	0.64
1:Y:205:GLU:O	1:Y:208:ASP:N	2.30	0.64
1:O:183:TYR:HB3	1:O:290:ILE:HG21	1.78	0.64
1:O:386:TYR:HB3	1:O:486:TRP:CE2	2.32	0.64
1:O:179:HIS:CE1	1:O:215:PRO:HB3	2.33	0.64
1:O:88:VAL:HA	1:O:161:LEU:O	1.98	0.64
1:Y:196:THR:O	1:Y:197:LEU:C	2.34	0.64
1:Y:433:PRO:HA	1:Y:466:ILE:HA	1.80	0.64
1:O:27:ILE:HD12	1:O:27:ILE:N	2.12	0.64
1:O:72:ASP:OD1	1:O:73:GLN:HG2	1.98	0.64
1:Y:124:ILE:HG13	1:Y:132:ILE:HD11	1.79	0.64
1:Y:153:GLU:O	1:Y:156:ARG:N	2.31	0.64
1:O:110:GLU:O	1:O:113:GLU:HB2	1.98	0.63
1:O:22:ASP:OD1	1:O:24:ASP:N	2.32	0.63
1:O:146:ASP:N	1:O:146:ASP:OD1	2.30	0.63
1:O:62:GLU:O	1:O:66:LYS:HG2	1.98	0.63
1:Y:127:ASN:HB3	1:Y:193:ASN:ND2	2.14	0.63
1:O:5:TYR:HB2	1:O:74:ILE:CG2	2.21	0.63
1:Y:117:ARG:CZ	1:Y:117:ARG:HB2	2.29	0.63
1:Y:498:GLU:OE1	1:Y:498:GLU:HA	1.97	0.63
1:O:166:ASP:O	1:O:169:LEU:N	2.30	0.63
1:Y:181:THR:HG23	1:Y:182:ASP:N	2.12	0.63
1:O:95:LYS:HG3	1:O:96:PRO:CD	2.29	0.63
1:Y:182:ASP:HB3	1:Y:242:ILE:HB	1.81	0.63
1:Y:240:SER:HB2	1:Y:450:ALA:CB	2.27	0.63
1:O:254:LEU:CD1	1:O:445:TYR:HE2	2.12	0.62
1:O:70:SER:O	1:O:73:GLN:HG3	1.99	0.62
1:Y:211:ARG:HH11	1:Y:211:ARG:HG3	1.64	0.62
1:O:227:THR:N	1:O:237:ILE:O	2.29	0.62
1:Y:178:VAL:HG12	1:Y:180:VAL:HG12	1.82	0.62
1:O:47:HIS:O	1:O:49:PRO:HD3	1.99	0.62
1:Y:72:ASP:OD1	1:Y:73:GLN:HG2	1.98	0.62
1:Y:4:LYS:N	1:Y:73:GLN:O	2.33	0.62
1:O:123:TYR:HD2	1:O:203:MET:HE2	1.65	0.62
1:Y:340:ASN:HB2	1:Y:375:HIS:CD2	2.34	0.62
1:O:137:SER:HA	1:O:140:LYS:CD	2.24	0.62
1:O:60:LEU:O	1:O:63:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:458:ASP:CA	1:Y:461:GLN:HB2	2.29	0.62
1:Y:32:GLN:HA	1:Y:59:THR:HG21	1.82	0.62
1:Y:24:ASP:HB2	1:Y:26:ASN:ND2	2.13	0.62
1:O:195:HIS:N	1:O:195:HIS:ND1	2.46	0.61
1:Y:114:HIS:O	1:Y:115:LEU:C	2.37	0.61
1:Y:250:LEU:HD12	1:Y:250:LEU:O	1.99	0.61
1:O:199:TRP:CG	1:O:214:LEU:HD23	2.36	0.61
1:O:55:THR:HA	1:O:58:TRP:HD1	1.62	0.61
1:Y:32:GLN:HA	1:Y:59:THR:CG2	2.30	0.61
1:O:227:THR:HB	1:O:229:ILE:CG2	2.30	0.61
1:O:88:VAL:HG12	1:O:97:ILE:HG12	1.83	0.61
1:Y:78:GLY:O	1:Y:79:ILE:HD13	2.00	0.61
1:O:17:ARG:HG2	1:O:32:GLN:HG3	1.82	0.61
1:O:278:LYS:HD2	1:O:280:VAL:HG23	1.82	0.61
1:O:133:ASP:OD1	1:O:135:TYR:N	2.31	0.61
1:O:89:TRP:HB2	1:O:95:LYS:O	2.01	0.61
1:O:181:THR:HG23	1:O:182:ASP:N	2.15	0.60
1:O:173:MET:HB3	1:O:227:THR:HG21	1.82	0.60
1:O:202:LYS:O	1:O:205:GLU:HG2	2.02	0.60
1:O:272:LEU:HD11	1:O:303:GLU:HG3	1.82	0.60
1:O:88:VAL:HG12	1:O:97:ILE:CG1	2.32	0.60
1:Y:61:VAL:HG12	1:Y:62:GLU:N	2.16	0.60
1:O:352:GLY:HA2	1:O:356:TRP:CE3	2.36	0.60
1:O:53:TRP:O	1:O:54:ALA:C	2.39	0.60
1:Y:240:SER:HB2	1:Y:450:ALA:HB3	1.82	0.60
1:O:177:ARG:NH1	1:O:226:GLN:O	2.29	0.60
1:O:478:GLU:O	1:O:482:ARG:HG2	2.02	0.60
1:O:389:ARG:HB2	1:O:426:LEU:CD1	2.32	0.60
1:Y:124:ILE:HD13	1:Y:203:MET:HE1	1.82	0.60
1:O:15:SER:HB2	1:O:33:ARG:O	2.02	0.60
1:Y:422:GLN:O	1:Y:426:LEU:HD22	2.00	0.60
1:O:447:ALA:O	1:O:450:ALA:HB3	2.01	0.59
1:Y:195:HIS:ND1	1:Y:195:HIS:N	2.47	0.59
1:Y:422:GLN:NE2	1:Y:426:LEU:HD22	2.17	0.59
1:O:246:GLN:OE1	1:O:270:PHE:HB2	2.01	0.59
1:Y:173:MET:HB3	1:Y:227:THR:HG23	1.84	0.59
1:Y:24:ASP:HB2	1:Y:26:ASN:HD21	1.67	0.59
1:O:420:GLN:HE21	1:O:424:ASP:CG	2.05	0.59
1:O:24:ASP:HB2	1:O:26:ASN:HD21	1.66	0.59
1:O:497:GLU:HA	1:O:497:GLU:OE1	2.01	0.59
1:Y:87:ILE:HG22	1:Y:88:VAL:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:TRP:HA	1:O:105:CYS:SG	2.42	0.59
1:O:144:ILE:HG22	1:O:148:VAL:HG21	1.84	0.59
1:O:153:GLU:O	1:O:156:ARG:HB3	2.02	0.59
1:Y:120:LEU:O	1:Y:124:ILE:HG12	2.02	0.59
1:Y:262:LYS:O	1:Y:262:LYS:HD2	2.02	0.59
1:Y:468:ARG:CG	1:Y:468:ARG:HH11	2.16	0.59
1:O:201:ASP:HA	1:O:204:LEU:HB2	1.85	0.59
1:O:74:ILE:CD1	1:O:237:ILE:HG21	2.33	0.59
1:O:88:VAL:HG22	1:O:162:PHE:HB2	1.83	0.58
1:Y:166:ASP:O	1:Y:167:THR:C	2.41	0.58
1:Y:313:ILE:N	1:Y:313:ILE:HD13	2.17	0.58
1:Y:5:TYR:C	1:Y:74:ILE:HG22	2.23	0.58
1:O:183:TYR:CD2	1:O:298:VAL:HG23	2.39	0.58
1:O:317:ARG:HB2	1:O:323:ILE:HG13	1.86	0.58
1:Y:170:ILE:HG22	1:Y:171:TRP:N	2.18	0.58
1:O:227:THR:HB	1:O:229:ILE:HG23	1.85	0.58
1:Y:130:LEU:HD13	1:Y:136:PHE:CD1	2.38	0.58
1:Y:271:MET:C	1:Y:272:LEU:HD13	2.24	0.58
1:O:38:ILE:O	1:O:45:VAL:HA	2.04	0.58
1:Y:272:LEU:HD11	1:Y:303:GLU:CG	2.34	0.58
1:Y:172:LYS:O	1:Y:173:MET:C	2.40	0.58
1:O:241:GLY:O	1:O:242:ILE:HG13	2.04	0.58
1:O:245:ASP:O	1:O:248:ALA:HB3	2.02	0.58
1:O:67:ALA:HB3	1:O:69:ILE:CD1	2.33	0.58
1:Y:156:ARG:HG2	1:Y:156:ARG:HH11	1.69	0.58
1:Y:253:GLN:HG3	1:Y:407:ARG:HD2	1.85	0.58
1:O:394:ALA:O	1:O:395:MET:C	2.38	0.58
1:Y:262:LYS:C	1:Y:262:LYS:HD2	2.24	0.58
1:Y:173:MET:HB2	1:Y:174:THR:HG23	1.85	0.57
1:O:219:ARG:HD3	1:O:222:GLU:HB2	1.86	0.57
1:O:460:LEU:HD12	1:O:460:LEU:N	2.11	0.57
1:Y:62:GLU:O	1:Y:66:LYS:HG2	2.04	0.57
1:Y:89:TRP:HD1	1:Y:90:GLU:O	1.87	0.57
1:O:313:ILE:HD11	1:O:381:LEU:CD2	2.34	0.57
1:Y:153:GLU:O	1:Y:154:ARG:C	2.37	0.57
1:Y:154:ARG:HB2	1:Y:159:GLU:HB3	1.85	0.57
1:O:123:TYR:HD2	1:O:203:MET:CE	2.17	0.57
1:O:17:ARG:HH22	1:O:437:GLU:HG2	1.68	0.57
1:O:222:GLU:O	1:O:240:SER:HA	2.04	0.57
1:O:468:ARG:HH11	1:O:468:ARG:CG	2.17	0.57
1:O:164:THR:O	1:O:165:VAL:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:48:ASP:O	1:O:51:GLU:N	2.38	0.57
1:O:44:TRP:CZ2	1:O:107:ARG:HB2	2.39	0.57
1:O:127:ASN:HD22	1:O:193:ASN:ND2	2.02	0.57
1:O:207:LEU:HD23	1:O:207:LEU:N	2.20	0.57
1:Y:181:THR:HG23	1:Y:182:ASP:O	2.05	0.57
1:Y:109:ALA:O	1:Y:112:CYS:HB2	2.04	0.57
1:Y:123:TYR:HD1	1:Y:203:MET:HE2	1.69	0.57
1:Y:250:LEU:HD11	1:Y:255:CYS:CB	2.28	0.57
1:O:420:GLN:HG3	1:O:420:GLN:O	2.05	0.56
1:Y:497:GLU:OE1	1:Y:497:GLU:HA	2.04	0.56
1:Y:83:ARG:HH21	4:Y:600:GOL:H2	1.70	0.56
1:O:9:LEU:HG	1:O:56:GLN:NE2	2.20	0.56
1:Y:3:LYS:HB2	1:Y:3:LYS:NZ	2.19	0.56
1:Y:80:THR:HG21	1:Y:248:ALA:CB	2.34	0.56
1:O:18:ALA:HB2	1:O:59:THR:HG22	1.86	0.56
1:O:47:HIS:HD2	1:O:82:GLN:HE22	1.51	0.56
1:Y:269:CYS:HB2	1:Y:306:VAL:HB	1.85	0.56
1:O:179:HIS:CG	1:O:215:PRO:HB3	2.39	0.56
1:Y:111:ILE:HG22	1:Y:115:LEU:CD1	2.36	0.56
1:O:118:ASP:N	1:O:118:ASP:OD1	2.39	0.56
1:O:180:VAL:HG23	1:O:216:GLU:O	2.05	0.56
1:O:183:TYR:CB	1:O:290:ILE:HG21	2.35	0.56
1:O:237:ILE:HG22	1:O:238:PRO:HD2	1.88	0.56
1:O:262:LYS:C	1:O:262:LYS:HD2	2.25	0.56
1:O:420:GLN:NE2	1:O:424:ASP:OD1	2.37	0.56
1:O:78:GLY:C	1:O:79:ILE:HG12	2.25	0.56
1:Y:125:ARG:NH1	1:Y:282:SER:O	2.38	0.56
1:Y:357:ASP:OD2	1:Y:494:MET:HB3	2.05	0.56
1:Y:394:ALA:O	1:Y:395:MET:C	2.44	0.56
1:Y:459:GLU:HB2	1:Y:460:LEU:HD12	1.87	0.56
1:O:178:VAL:HG12	1:O:180:VAL:HG12	1.88	0.56
1:O:3:LYS:HA	1:O:73:GLN:CA	2.34	0.56
1:O:286:LEU:O	1:O:287:LEU:HD23	2.05	0.56
1:Y:432:ARG:HD2	1:Y:436:ARG:NH1	2.19	0.56
1:O:41:LYS:HG3	1:O:42:PRO:CD	2.34	0.56
1:Y:138:GLY:HA2	1:Y:191:LEU:HD21	1.88	0.56
1:Y:280:VAL:HG12	1:Y:281:LYS:N	2.19	0.56
1:Y:58:TRP:O	1:Y:59:THR:C	2.41	0.56
1:O:135:TYR:O	1:O:140:LYS:HE2	2.06	0.56
1:O:206:VAL:HG12	1:O:207:LEU:N	2.21	0.56
1:O:244:GLY:O	1:O:245:ASP:C	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:142:LYS:O	1:O:143:TRP:C	2.42	0.56
1:Y:245:ASP:O	1:Y:248:ALA:HB3	2.06	0.56
1:O:236:ARG:CG	1:O:236:ARG:HH11	2.18	0.55
1:Y:202:LYS:O	1:Y:206:VAL:HB	2.04	0.55
1:O:130:LEU:HD13	1:O:136:PHE:CD1	2.42	0.55
1:Y:165:VAL:O	1:Y:168:TRP:N	2.40	0.55
1:Y:415:ASN:HD22	1:Y:418:LEU:N	1.90	0.55
1:O:80:THR:CG2	1:O:248:ALA:HB2	2.36	0.55
1:Y:478:GLU:OE1	1:Y:478:GLU:HA	2.05	0.55
1:O:166:ASP:O	1:O:167:THR:C	2.44	0.55
1:O:439:THR:HG22	1:O:440:ALA:H	1.71	0.55
1:Y:180:VAL:HG22	1:Y:181:THR:N	2.22	0.55
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.89	0.55
1:Y:35:PHE:HB2	1:Y:51:GLU:HG2	1.89	0.55
1:O:149:GLU:O	1:O:150:GLY:C	2.45	0.55
1:Y:184:THR:O	1:Y:187:SER:HB3	2.07	0.55
1:O:438:VAL:O	1:O:441:LEU:HB2	2.06	0.55
1:Y:488:LYS:HD3	1:O:496:TRP:CZ3	2.41	0.55
1:Y:133:ASP:OD1	1:Y:135:TYR:HB2	2.07	0.55
1:Y:293:GLY:N	1:Y:297:GLU:O	2.31	0.55
1:Y:130:LEU:HD13	1:Y:136:PHE:CE1	2.42	0.54
1:Y:206:VAL:HG12	1:Y:207:LEU:N	2.22	0.54
1:Y:351:LEU:HB3	1:Y:355:TYR:HB2	1.89	0.54
1:O:445:TYR:CD1	1:O:460:LEU:HD22	2.43	0.54
1:O:74:ILE:HD11	1:O:237:ILE:HG21	1.89	0.54
1:O:272:LEU:HD11	1:O:303:GLU:CD	2.28	0.54
1:Y:115:LEU:O	1:Y:120:LEU:HD12	2.06	0.54
1:Y:8:ALA:O	1:Y:9:LEU:HD12	2.07	0.54
1:O:179:HIS:NE2	1:O:215:PRO:HB3	2.22	0.54
1:O:89:TRP:HB2	1:O:95:LYS:C	2.27	0.54
1:Y:22:ASP:OD1	1:Y:24:ASP:N	2.40	0.54
1:O:94:GLY:HA2	1:O:171:TRP:CH2	2.43	0.54
1:O:389:ARG:HB2	1:O:426:LEU:HD13	1.89	0.54
1:Y:221:SER:OG	1:Y:450:ALA:HB2	2.08	0.54
1:O:490:VAL:O	1:O:494:MET:HG2	2.08	0.54
1:Y:28:ILE:HD12	1:Y:28:ILE:N	2.23	0.54
1:Y:491:LYS:O	1:Y:494:MET:HG3	2.07	0.54
1:Y:425:ILE:O	1:Y:479:ARG:HD3	2.08	0.54
1:Y:51:GLU:O	1:Y:52:ILE:C	2.41	0.54
1:O:482:ARG:HG3	1:O:482:ARG:HH11	1.72	0.54
1:Y:492:ARG:CG	1:Y:492:ARG:HH11	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:149:GLU:OE1	1:Y:149:GLU:HA	2.04	0.54
1:Y:393:GLU:O	1:Y:394:ALA:C	2.45	0.54
1:Y:74:ILE:HD11	1:Y:237:ILE:HG21	1.90	0.54
1:O:219:ARG:HG2	1:O:222:GLU:HB3	1.89	0.53
1:O:218:ARG:NE	1:O:222:GLU:OE2	2.33	0.53
1:O:455:GLN:O	1:O:456:ASN:HB2	2.08	0.53
1:O:75:ALA:HB2	1:O:453:PHE:CD2	2.43	0.53
1:O:88:VAL:CG2	1:O:162:PHE:HB2	2.37	0.53
1:O:43:GLY:O	1:O:106:ARG:N	2.40	0.53
1:Y:84:GLU:OE1	1:Y:84:GLU:N	2.41	0.53
1:O:251:PHE:O	1:O:254:LEU:HD12	2.08	0.53
1:O:40:PRO:HD2	1:O:44:TRP:HB2	1.91	0.53
1:Y:5:TYR:HB3	1:Y:21:MET:O	2.08	0.53
1:Y:496:TRP:O	1:O:488:LYS:HE2	2.08	0.53
1:O:332:PHE:O	1:O:335:LYS:HB2	2.08	0.53
1:O:253:GLN:HG2	1:O:407:ARG:HD2	1.87	0.53
1:O:60:LEU:HD12	1:O:60:LEU:O	2.08	0.53
1:O:351:LEU:HB3	1:O:355:TYR:HB2	1.91	0.53
1:O:357:ASP:OD2	1:O:494:MET:HB3	2.07	0.53
1:Y:189:THR:HB	1:Y:191:LEU:HD11	1.89	0.53
1:O:113:GLU:O	1:O:117:ARG:HD3	2.08	0.53
1:O:344:VAL:O	1:O:346:PRO:HD3	2.09	0.53
1:Y:328:ASP:HB3	1:Y:332:PHE:HE2	1.72	0.53
1:O:87:ILE:HD13	1:O:168:TRP:HB2	1.91	0.53
1:O:199:TRP:CD2	1:O:214:LEU:HD23	2.44	0.53
1:O:40:PRO:HG2	1:O:44:TRP:HB3	1.90	0.53
1:Y:165:VAL:O	1:Y:166:ASP:C	2.45	0.53
1:Y:173:MET:HA	1:Y:173:MET:CE	2.39	0.53
1:Y:338:ASN:OD1	1:Y:340:ASN:N	2.42	0.53
1:Y:458:ASP:HA	1:Y:461:GLN:HB2	1.88	0.53
1:O:138:GLY:HA2	1:O:191:LEU:HD21	1.91	0.53
1:O:451:VAL:HG12	1:O:453:PHE:HB2	1.91	0.53
1:O:478:GLU:OE1	1:O:478:GLU:HA	2.09	0.53
1:Y:445:TYR:O	1:Y:446:LEU:C	2.45	0.53
1:O:114:HIS:HA	1:O:117:ARG:NH1	2.24	0.53
1:O:81:ASN:N	1:O:81:ASN:ND2	2.56	0.53
1:O:398:ASP:O	1:O:400:GLY:N	2.42	0.52
1:Y:11:GLN:HE22	1:Y:82:GLN:HE21	1.57	0.52
1:Y:22:ASP:OD2	1:Y:26:ASN:HB2	2.08	0.52
1:Y:458:ASP:HA	1:Y:461:GLN:CB	2.38	0.52
1:O:156:ARG:O	1:O:212:GLU:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:340:ASN:HB2	1:O:375:HIS:CD2	2.44	0.52
1:O:265:TYR:HE1	1:O:408:VAL:CG1	2.22	0.52
1:Y:169:LEU:N	1:Y:169:LEU:HD22	2.25	0.52
1:Y:22:ASP:CG	1:Y:26:ASN:HD22	2.12	0.52
1:Y:367:LEU:HB2	1:O:362:GLY:HA3	1.90	0.52
1:Y:432:ARG:HG2	1:Y:436:ARG:NH1	2.24	0.52
1:O:409:ASP:C	1:O:413:VAL:HG11	2.30	0.52
1:O:74:ILE:O	1:O:75:ALA:O	2.27	0.52
1:Y:146:ASP:OD1	1:Y:146:ASP:N	2.40	0.52
1:Y:261:ALA:HB2	1:Y:273:MET:CG	2.39	0.52
1:O:22:ASP:CB	1:O:28:ILE:HD11	2.21	0.52
1:Y:272:LEU:HD12	1:Y:303:GLU:HA	1.90	0.52
1:Y:276:GLY:O	1:Y:300:TYR:N	2.43	0.52
1:O:115:LEU:O	1:O:120:LEU:HD12	2.10	0.52
1:O:49:PRO:HD3	1:O:100:ALA:H	1.75	0.52
1:Y:110:GLU:O	1:Y:114:HIS:HD2	1.92	0.52
1:Y:150:GLY:O	1:Y:153:GLU:HG2	2.10	0.52
1:Y:39:TYR:HA	1:Y:44:TRP:O	2.09	0.52
1:Y:403:LEU:HD12	1:Y:403:LEU:N	2.24	0.52
1:Y:43:GLY:C	1:Y:44:TRP:HD1	2.13	0.52
1:O:221:SER:HB3	1:O:295:THR:O	2.10	0.52
1:O:40:PRO:HG2	1:O:44:TRP:CB	2.40	0.52
1:O:97:ILE:O	1:O:98:TYR:HB2	2.09	0.52
1:Y:104:GLN:NE2	1:Y:308:MET:HE1	2.25	0.52
1:O:156:ARG:HB2	1:O:156:ARG:CZ	2.39	0.52
1:O:40:PRO:HD2	1:O:44:TRP:CB	2.40	0.52
1:Y:173:MET:HB3	1:Y:227:THR:CG2	2.39	0.52
1:O:163:GLY:HA2	1:O:167:THR:HG21	1.91	0.52
1:O:90:GLU:HB2	1:O:93:THR:HG1	1.74	0.52
1:Y:227:THR:N	1:Y:237:ILE:O	2.31	0.52
1:Y:342:VAL:HA	1:Y:365:PHE:O	2.10	0.52
1:Y:445:TYR:O	1:Y:449:LEU:N	2.29	0.52
1:Y:20:VAL:HG12	1:Y:21:MET:N	2.25	0.52
1:Y:244:GLY:O	1:Y:245:ASP:C	2.46	0.52
1:Y:16:SER:HB3	1:Y:56:GLN:HA	1.92	0.52
1:Y:255:CYS:HB3	1:Y:260:MET:HB2	1.91	0.52
1:Y:32:GLN:N	1:Y:59:THR:HG22	2.24	0.52
1:Y:104:GLN:HG2	1:Y:349:THR:HG21	1.92	0.52
1:Y:47:HIS:O	1:Y:49:PRO:HD3	2.10	0.52
1:Y:468:ARG:HD2	1:Y:468:ARG:C	2.31	0.51
1:O:156:ARG:HH11	1:O:156:ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:200:ASP:OD1	1:O:202:LYS:HB2	2.11	0.51
1:O:390:ASP:HA	1:O:483:TYR:OH	2.10	0.51
1:Y:390:ASP:HA	1:Y:483:TYR:OH	2.10	0.51
1:O:357:ASP:OD2	1:O:494:MET:HE3	2.10	0.51
1:O:394:ALA:O	1:O:397:ALA:N	2.44	0.51
1:O:484:ALA:O	1:O:485:GLY:C	2.49	0.51
1:Y:148:VAL:O	1:Y:151:SER:OG	2.29	0.51
1:O:297:GLU:O	1:O:298:VAL:C	2.48	0.51
1:Y:482:ARG:HG3	1:Y:482:ARG:NH1	2.25	0.51
1:O:286:LEU:C	1:O:287:LEU:HD23	2.31	0.51
1:O:387:GLN:O	1:O:390:ASP:HB2	2.11	0.51
1:Y:137:SER:OG	1:Y:189:THR:HA	2.10	0.51
1:Y:154:ARG:HH21	1:Y:159:GLU:HG2	1.75	0.51
1:Y:16:SER:HB3	1:Y:56:GLN:OE1	2.11	0.51
1:O:84:GLU:HB2	1:O:103:TRP:CB	2.40	0.51
1:Y:153:GLU:O	1:Y:156:ARG:HB3	2.11	0.51
1:Y:226:GLN:HA	1:Y:237:ILE:O	2.11	0.51
1:O:48:ASP:HB3	1:O:51:GLU:HB3	1.91	0.51
1:Y:70:SER:N	1:Y:73:GLN:NE2	2.48	0.51
1:O:415:ASN:HB3	1:O:418:LEU:HB2	1.93	0.51
1:O:9:LEU:HD21	1:O:60:LEU:HD22	1.92	0.51
1:O:90:GLU:OE1	1:O:95:LYS:HE3	2.11	0.51
1:Y:154:ARG:O	1:Y:155:ALA:C	2.49	0.51
1:Y:21:MET:HA	1:Y:26:ASN:O	2.11	0.51
1:O:137:SER:CA	1:O:140:LYS:HD3	2.31	0.50
1:O:162:PHE:O	1:O:179:HIS:HE1	1.94	0.50
1:Y:144:ILE:O	1:Y:145:LEU:C	2.43	0.50
1:Y:328:ASP:HB3	1:Y:332:PHE:CE2	2.46	0.50
1:O:258:GLU:HG3	1:O:276:GLY:HA3	1.93	0.50
1:O:485:GLY:O	1:O:488:LYS:HB3	2.11	0.50
1:Y:205:GLU:HG2	1:Y:206:VAL:H	1.76	0.50
1:O:17:ARG:CA	1:O:59:THR:HG21	2.41	0.50
1:Y:87:ILE:HD12	1:Y:163:GLY:O	2.11	0.50
1:Y:40:PRO:HG3	1:Y:46:GLU:OE2	2.12	0.50
1:Y:486:TRP:O	1:Y:490:VAL:HG23	2.11	0.50
1:O:279:ALA:HB2	1:O:300:TYR:CD2	2.46	0.50
1:O:422:GLN:HG3	1:O:426:LEU:CD2	2.42	0.50
1:Y:52:ILE:HG22	1:Y:53:TRP:N	2.25	0.50
1:O:279:ALA:HB2	1:O:300:TYR:CG	2.45	0.50
1:O:85:THR:OG1	1:O:103:TRP:HD1	1.95	0.50
1:O:9:LEU:HB2	1:O:79:ILE:CD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:272:LEU:CD1	1:Y:303:GLU:HB2	2.42	0.50
1:Y:348:PHE:N	1:Y:348:PHE:CD1	2.79	0.50
1:O:156:ARG:CG	1:O:156:ARG:HH11	2.25	0.50
1:O:40:PRO:HD2	1:O:44:TRP:O	2.10	0.50
1:O:17:ARG:HH22	1:O:437:GLU:HG3	1.77	0.50
1:Y:432:ARG:HD2	1:Y:436:ARG:CZ	2.41	0.50
1:O:114:HIS:HA	1:O:117:ARG:CZ	2.41	0.50
1:O:330:GLU:O	1:O:334:THR:HG23	2.12	0.50
1:O:37:GLN:HE22	1:O:47:HIS:CE1	2.30	0.50
1:Y:85:THR:HG23	1:Y:102:VAL:HA	1.93	0.50
1:Y:237:ILE:HG22	1:Y:238:PRO:HD2	1.92	0.50
1:O:133:ASP:OD1	1:O:135:TYR:HB2	2.11	0.50
1:O:263:ASN:ND2	1:O:265:TYR:CZ	2.79	0.50
1:O:439:THR:O	1:O:442:GLY:N	2.45	0.50
1:O:37:GLN:NE2	1:O:47:HIS:CE1	2.80	0.50
1:Y:391:VAL:HG22	1:Y:392:LEU:N	2.26	0.50
1:O:103:TRP:N	1:O:103:TRP:CD1	2.80	0.49
1:O:211:ARG:HG3	1:O:211:ARG:HH11	1.77	0.49
1:O:228:ASN:HD21	1:O:235:THR:N	2.10	0.49
1:O:27:ILE:H	1:O:27:ILE:HD12	1.77	0.49
1:O:281:LYS:HZ2	1:O:281:LYS:HB2	1.76	0.49
1:O:293:GLY:N	1:O:297:GLU:O	2.41	0.49
1:O:11:GLN:O	1:O:81:ASN:HA	2.12	0.49
1:Y:415:ASN:HD21	1:Y:417:PHE:HB3	1.77	0.49
1:Y:415:ASN:ND2	1:Y:418:LEU:HB2	2.27	0.49
1:O:75:ALA:HB2	1:O:453:PHE:HD2	1.77	0.49
1:Y:468:ARG:HG3	1:Y:468:ARG:HH11	1.76	0.49
1:O:22:ASP:CG	1:O:26:ASN:HD22	2.16	0.49
1:Y:199:TRP:CG	1:Y:214:LEU:HD23	2.47	0.49
1:Y:251:PHE:O	1:Y:254:LEU:HD12	2.11	0.49
1:Y:432:ARG:HG2	1:Y:436:ARG:HH12	1.77	0.49
1:O:256:VAL:HG13	1:O:256:VAL:O	2.11	0.49
1:O:438:VAL:HG12	1:O:439:THR:N	2.27	0.49
1:O:456:ASN:N	1:O:459:GLU:OE2	2.44	0.49
1:Y:256:VAL:O	1:Y:256:VAL:HG13	2.12	0.49
1:Y:411:GLY:HA3	3:Y:601:ATS:O5'	2.12	0.49
1:Y:415:ASN:ND2	1:Y:418:LEU:N	2.43	0.49
1:Y:54:ALA:O	1:Y:57:SER:HB2	2.13	0.49
1:Y:193:ASN:OD1	1:Y:195:HIS:N	2.32	0.49
1:Y:246:GLN:HB3	1:Y:272:LEU:HD21	1.95	0.49
1:Y:486:TRP:O	1:Y:489:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:74:ILE:HD12	1:Y:74:ILE:O	2.12	0.49
1:O:312:SER:O	1:O:315:TRP:HB3	2.12	0.49
1:Y:269:CYS:CB	1:Y:306:VAL:HB	2.42	0.49
1:Y:44:TRP:CD1	1:Y:44:TRP:N	2.80	0.49
1:O:345:VAL:O	1:O:362:GLY:HA2	2.13	0.49
1:O:17:ARG:C	1:O:59:THR:HG21	2.32	0.49
1:Y:137:SER:HA	1:Y:140:LYS:CD	2.41	0.49
1:Y:281:LYS:HE3	1:Y:283:GLU:OE2	2.13	0.49
1:Y:282:SER:HB2	1:Y:286:LEU:HB2	1.94	0.49
1:Y:447:ALA:O	1:Y:450:ALA:HB3	2.13	0.49
1:Y:466:ILE:O	1:Y:466:ILE:HD13	2.13	0.49
1:O:403:LEU:N	1:O:403:LEU:HD12	2.20	0.49
1:Y:205:GLU:HG2	1:Y:206:VAL:N	2.28	0.49
1:Y:3:LYS:HA	1:Y:73:GLN:CA	2.41	0.49
1:O:141:VAL:HA	1:O:144:ILE:CD1	2.43	0.49
1:O:435:VAL:HG22	1:O:436:ARG:N	2.27	0.49
1:O:69:ILE:HA	1:O:73:GLN:NE2	2.28	0.49
1:Y:184:THR:HG22	1:Y:290:ILE:HG22	1.93	0.49
1:Y:429:ARG:HA	1:Y:470:PHE:O	2.13	0.49
1:Y:48:ASP:HB3	1:Y:51:GLU:HB3	1.95	0.49
1:O:293:GLY:HA2	1:O:299:ASN:HD22	1.77	0.48
1:O:44:TRP:N	1:O:44:TRP:CD1	2.80	0.48
1:Y:445:TYR:O	1:Y:449:LEU:HB2	2.14	0.48
1:Y:87:ILE:HD13	1:Y:168:TRP:HB2	1.95	0.48
1:O:440:ALA:O	1:O:441:LEU:C	2.50	0.48
1:Y:182:ASP:HA	1:Y:218:ARG:O	2.14	0.48
1:Y:272:LEU:HD13	1:Y:272:LEU:N	2.28	0.48
1:Y:61:VAL:O	1:Y:62:GLU:O	2.31	0.48
1:O:24:ASP:HB2	1:O:26:ASN:ND2	2.27	0.48
1:O:22:ASP:OD1	1:O:25:ALA:N	2.46	0.48
1:O:347:ALA:HB2	1:O:351:LEU:HD13	1.95	0.48
1:Y:77:ILE:N	1:Y:238:PRO:O	2.46	0.48
1:Y:272:LEU:HD12	1:Y:303:GLU:CB	2.43	0.48
1:Y:441:LEU:HD22	1:Y:445:TYR:OH	2.13	0.48
1:Y:80:THR:HG22	1:Y:245:ASP:HA	1.95	0.48
1:O:165:VAL:O	1:O:166:ASP:C	2.51	0.48
1:Y:154:ARG:HB3	1:Y:154:ARG:HE	1.44	0.48
1:Y:20:VAL:C	1:Y:21:MET:HG3	2.33	0.48
1:Y:360:ALA:HB2	1:Y:494:MET:HA	1.95	0.48
1:O:278:LYS:HD2	1:O:280:VAL:CG2	2.43	0.48
1:O:221:SER:HB2	1:O:296:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:163:GLY:CA	1:O:167:THR:HG21	2.44	0.48
1:Y:23:HIS:HE1	1:Y:453:PHE:O	1.97	0.48
1:O:171:TRP:CE2	1:O:176:GLY:HA2	2.48	0.48
1:O:251:PHE:CD2	1:O:446:LEU:HD13	2.48	0.48
1:Y:143:TRP:O	1:Y:147:HIS:HD2	1.97	0.48
1:Y:150:GLY:O	1:Y:153:GLU:N	2.42	0.48
1:O:219:ARG:HD3	1:O:222:GLU:CB	2.44	0.48
1:O:449:LEU:HD22	1:O:457:LEU:CD2	2.44	0.48
1:Y:30:VAL:HG12	1:Y:30:VAL:O	2.13	0.48
1:Y:38:ILE:O	1:Y:40:PRO:HD3	2.14	0.48
1:O:226:GLN:HB3	1:O:236:ARG:HD3	1.95	0.48
1:Y:80:THR:HG21	1:Y:248:ALA:HB3	1.96	0.48
1:O:45:VAL:HG21	1:O:104:GLN:HB3	1.96	0.47
1:Y:434:GLU:OE2	1:Y:467:GLU:HB2	2.14	0.47
1:Y:471:ARG:HB3	1:Y:472:PRO:HD2	1.96	0.47
1:Y:5:TYR:O	1:Y:75:ALA:N	2.41	0.47
1:O:185:ASN:O	1:O:188:ARG:HB2	2.14	0.47
1:O:3:LYS:HB2	1:O:3:LYS:NZ	2.29	0.47
1:O:442:GLY:O	1:O:443:ALA:C	2.50	0.47
1:Y:78:GLY:HA2	1:Y:447:ALA:HB2	1.95	0.47
1:O:219:ARG:NH2	1:O:295:THR:OG1	2.48	0.47
1:O:424:ASP:OD1	1:O:473:GLY:N	2.45	0.47
1:O:57:SER:O	1:O:58:TRP:C	2.50	0.47
1:Y:161:LEU:HD22	1:Y:179:HIS:CE1	2.49	0.47
1:Y:173:MET:HA	1:Y:173:MET:HE2	1.96	0.47
1:Y:201:ASP:O	1:Y:202:LYS:C	2.52	0.47
1:O:144:ILE:HG22	1:O:148:VAL:HG23	1.95	0.47
1:O:211:ARG:NH1	1:O:211:ARG:HG3	2.30	0.47
1:O:173:MET:CB	1:O:227:THR:HG23	2.44	0.47
1:O:221:SER:CB	1:O:296:GLY:HA3	2.44	0.47
1:O:297:GLU:HG2	1:O:297:GLU:O	2.13	0.47
1:O:475:GLU:O	1:O:476:THR:C	2.52	0.47
1:Y:396:GLN:HE21	1:Y:403:LEU:HD12	1.77	0.47
1:Y:5:TYR:CA	1:Y:74:ILE:HG22	2.44	0.47
1:O:124:ILE:O	1:O:125:ARG:C	2.50	0.47
1:O:158:GLY:HA2	1:O:212:GLU:HB3	1.95	0.47
1:O:433:PRO:HA	1:O:466:ILE:HA	1.95	0.47
1:Y:137:SER:O	1:Y:138:GLY:C	2.53	0.47
1:Y:265:TYR:N	1:Y:265:TYR:CD1	2.83	0.47
1:Y:63:VAL:O	1:Y:64:LEU:O	2.32	0.47
1:O:83:ARG:CZ	1:O:246:GLN:HG3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:246:GLN:HB3	1:Y:272:LEU:CD2	2.44	0.47
1:Y:396:GLN:O	1:Y:397:ALA:C	2.51	0.47
1:Y:263:ASN:O	1:Y:408:VAL:HA	2.14	0.47
1:O:15:SER:CB	1:O:34:GLU:HA	2.45	0.47
1:O:342:VAL:HG12	1:O:343:TYR:N	2.28	0.47
1:Y:255:CYS:CB	1:Y:260:MET:HB3	2.45	0.47
1:Y:326:ALA:O	1:Y:327:TYR:C	2.50	0.47
1:Y:439:THR:HG22	1:Y:440:ALA:N	2.30	0.47
1:Y:359:TYR:HD1	1:Y:497:GLU:HB3	1.80	0.47
1:Y:48:ASP:O	1:Y:51:GLU:N	2.48	0.47
1:O:186:ALA:O	1:O:187:SER:C	2.53	0.47
1:O:314:GLN:OE1	1:O:317:ARG:NH1	2.30	0.47
1:O:65:ALA:O	1:O:67:ALA:N	2.47	0.47
1:Y:162:PHE:HB3	1:Y:213:MET:HG3	1.96	0.47
1:Y:80:THR:HG22	1:Y:243:ALA:O	2.15	0.47
1:O:128:THR:HG21	1:O:190:MET:HA	1.95	0.47
1:O:148:VAL:HB	1:O:151:SER:HB3	1.96	0.47
1:O:21:MET:HA	1:O:26:ASN:O	2.15	0.47
1:O:389:ARG:HG2	1:O:483:TYR:CZ	2.50	0.47
1:O:389:ARG:HA	1:O:426:LEU:HD11	1.97	0.47
1:Y:23:HIS:ND1	1:Y:453:PHE:CE1	2.81	0.47
1:O:445:TYR:O	1:O:446:LEU:C	2.51	0.47
1:O:9:LEU:HA	1:O:9:LEU:HD12	1.39	0.47
1:Y:386:TYR:OH	1:Y:482:ARG:HB3	2.15	0.47
1:Y:53:TRP:O	1:Y:54:ALA:C	2.53	0.47
1:O:201:ASP:O	1:O:202:LYS:C	2.54	0.46
1:Y:67:ALA:HB3	1:Y:69:ILE:CD1	2.45	0.46
1:O:3:LYS:HG2	1:O:73:GLN:HA	1.97	0.46
1:Y:336:VAL:HG21	1:Y:338:ASN:O	2.15	0.46
1:O:346:PRO:HG2	1:O:387:GLN:HE22	1.80	0.46
1:O:468:ARG:HH11	1:O:468:ARG:HG3	1.79	0.46
1:O:482:ARG:NH1	1:O:482:ARG:HG3	2.30	0.46
1:Y:372:ASN:O	1:Y:375:HIS:N	2.48	0.46
1:O:160:LEU:O	1:O:213:MET:HB3	2.15	0.46
1:O:183:TYR:CD2	1:O:298:VAL:CG2	2.99	0.46
1:O:494:MET:HB3	1:O:494:MET:HE3	1.63	0.46
1:Y:128:THR:HG21	1:Y:190:MET:HA	1.97	0.46
1:Y:236:ARG:HH11	1:Y:236:ARG:HG3	1.81	0.46
1:Y:271:MET:SD	1:Y:395:MET:HE2	2.56	0.46
1:Y:280:VAL:CG1	1:Y:281:LYS:N	2.79	0.46
1:O:173:MET:HB2	1:O:174:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:38:ILE:O	1:O:46:GLU:N	2.45	0.46
1:O:251:PHE:CZ	1:O:446:LEU:HD13	2.50	0.46
1:Y:180:VAL:CG2	1:Y:181:THR:N	2.78	0.46
1:Y:257:LYS:O	1:Y:258:GLU:C	2.54	0.46
1:O:253:GLN:HE21	1:O:253:GLN:HB2	1.44	0.46
1:O:272:LEU:N	1:O:272:LEU:HD13	2.30	0.46
1:O:281:LYS:HB2	1:O:281:LYS:NZ	2.31	0.46
1:O:346:PRO:HG2	1:O:387:GLN:NE2	2.31	0.46
1:Y:161:LEU:CD2	1:Y:179:HIS:CE1	2.99	0.46
1:Y:344:VAL:HG22	1:Y:364:ILE:HD13	1.98	0.46
1:Y:438:VAL:HG12	1:Y:439:THR:N	2.29	0.46
1:Y:48:ASP:O	1:Y:52:ILE:N	2.38	0.46
1:O:442:GLY:O	1:O:445:TYR:N	2.49	0.46
1:O:193:ASN:HB3	1:O:196:THR:CG2	2.46	0.46
1:O:460:LEU:CD1	1:O:460:LEU:N	2.77	0.46
1:Y:206:VAL:CG1	1:Y:207:LEU:N	2.78	0.46
1:Y:457:LEU:O	1:Y:461:GLN:HG3	2.16	0.46
1:O:251:PHE:CZ	1:O:446:LEU:CD1	2.99	0.46
1:O:297:GLU:N	1:O:297:GLU:OE1	2.43	0.46
1:O:415:ASN:ND2	1:O:418:LEU:HB2	2.30	0.46
1:O:434:GLU:HB2	1:O:465:VAL:O	2.16	0.46
1:Y:85:THR:HA	1:Y:101:ILE:O	2.16	0.46
1:Y:205:GLU:CG	1:Y:206:VAL:N	2.79	0.46
1:Y:28:ILE:CD1	1:Y:28:ILE:N	2.79	0.46
1:O:169:LEU:HD22	1:O:169:LEU:N	2.31	0.45
1:O:20:VAL:HG12	1:O:21:MET:N	2.31	0.45
1:O:179:HIS:NE2	1:O:215:PRO:CB	2.79	0.45
1:O:386:TYR:HB3	1:O:486:TRP:CD2	2.50	0.45
1:O:54:ALA:O	1:O:55:THR:C	2.53	0.45
1:O:171:TRP:NE1	1:O:176:GLY:HA2	2.31	0.45
1:O:278:LYS:O	1:O:300:TYR:HB2	2.16	0.45
1:Y:180:VAL:CG2	1:Y:181:THR:H	2.30	0.45
1:Y:196:THR:O	1:Y:196:THR:HG23	2.13	0.45
1:Y:426:LEU:HD12	1:Y:426:LEU:HA	1.65	0.45
1:Y:18:ALA:HB1	1:Y:63:VAL:CG2	2.44	0.45
1:O:105:CYS:SG	1:O:107:ARG:NH1	2.89	0.45
1:O:289:THR:O	1:O:301:ALA:N	2.48	0.45
1:O:13:THR:HB	3:O:601:ATS:OG3	2.16	0.45
1:Y:120:LEU:O	1:Y:121:GLU:C	2.51	0.45
1:Y:236:ARG:CG	1:Y:236:ARG:HH11	2.28	0.45
1:Y:422:GLN:NE2	1:Y:426:LEU:CD2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:61:VAL:O	1:Y:64:LEU:N	2.49	0.45
1:O:17:ARG:HA	1:O:59:THR:HG21	1.99	0.45
1:Y:302:LEU:HD23	1:Y:302:LEU:HA	1.41	0.45
1:Y:320:MET:HE1	1:O:376:ILE:HG13	1.97	0.45
1:Y:3:LYS:NZ	1:Y:3:LYS:CB	2.80	0.45
1:O:101:ILE:HG12	1:O:107:ARG:NH1	2.31	0.45
1:O:156:ARG:CB	1:O:156:ARG:NH1	2.79	0.45
1:O:166:ASP:CG	1:O:167:THR:H	2.18	0.45
1:O:270:PHE:N	1:O:270:PHE:CD1	2.85	0.45
1:O:3:LYS:CB	1:O:3:LYS:NZ	2.80	0.45
1:O:90:GLU:OE2	1:O:93:THR:HG21	2.16	0.45
1:Y:108:THR:CG2	1:Y:143:TRP:HB2	2.47	0.45
1:Y:161:LEU:CD2	1:Y:179:HIS:NE2	2.80	0.45
1:Y:183:TYR:CD1	1:Y:217:VAL:CG1	2.98	0.45
1:O:137:SER:O	1:O:140:LYS:N	2.50	0.45
1:O:280:VAL:CG1	1:O:281:LYS:N	2.79	0.45
1:O:86:THR:HG22	1:O:87:ILE:N	2.31	0.45
1:Y:145:LEU:HD12	1:Y:145:LEU:HA	1.65	0.45
1:Y:154:ARG:NH2	1:Y:159:GLU:HG2	2.31	0.45
1:O:179:HIS:CD2	1:O:215:PRO:HA	2.52	0.45
1:O:33:ARG:HH21	1:O:58:TRP:HB3	1.76	0.45
1:Y:205:GLU:O	1:Y:206:VAL:C	2.53	0.45
1:Y:494:MET:HB3	1:Y:494:MET:HE3	1.71	0.45
1:O:114:HIS:O	1:O:117:ARG:HB2	2.16	0.45
1:O:205:GLU:CG	1:O:206:VAL:N	2.80	0.45
1:O:293:GLY:CA	1:O:299:ASN:ND2	2.79	0.45
1:Y:362:GLY:CA	1:O:367:LEU:HB2	2.42	0.45
1:O:451:VAL:HG13	1:O:451:VAL:O	2.17	0.45
1:Y:103:TRP:N	1:Y:103:TRP:CD1	2.85	0.45
1:Y:94:GLY:HA2	1:Y:171:TRP:CH2	2.52	0.45
1:O:161:LEU:CD2	1:O:179:HIS:CE1	2.99	0.45
1:O:281:LYS:NZ	1:O:281:LYS:CB	2.80	0.45
1:Y:156:ARG:CG	1:Y:156:ARG:HH11	2.29	0.45
1:Y:272:LEU:CD1	1:Y:303:GLU:CB	2.95	0.45
1:Y:368:THR:O	1:Y:371:VAL:HG23	2.17	0.45
1:Y:372:ASN:OD1	1:Y:374:ASN:N	2.47	0.45
1:Y:459:GLU:HB2	1:Y:460:LEU:CD1	2.47	0.45
1:Y:67:ALA:HB3	1:Y:69:ILE:HD13	1.99	0.45
1:O:115:LEU:HD23	1:O:120:LEU:HD13	1.98	0.45
1:O:278:LYS:CD	1:O:280:VAL:HG23	2.47	0.45
1:O:468:ARG:HD2	1:O:469:GLU:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:310:GLY:HA3	3:O:601:ATS:O3'	2.17	0.45
1:Y:367:LEU:HB2	1:O:362:GLY:CA	2.47	0.45
1:O:137:SER:O	1:O:141:VAL:HG23	2.17	0.44
1:O:251:PHE:O	1:O:254:LEU:N	2.49	0.44
1:O:428:THR:CG2	1:O:429:ARG:N	2.79	0.44
1:O:48:ASP:OD1	1:O:49:PRO:HD2	2.17	0.44
1:O:83:ARG:H	4:O:600:GOL:H12	1.80	0.44
1:Y:310:GLY:O	1:Y:313:ILE:HB	2.17	0.44
1:Y:339:THR:O	1:Y:339:THR:OG1	2.34	0.44
1:O:457:LEU:C	1:O:459:GLU:H	2.20	0.44
1:O:90:GLU:CD	1:O:93:THR:HG21	2.37	0.44
1:Y:104:GLN:NE2	1:Y:308:MET:CE	2.79	0.44
1:Y:432:ARG:CG	1:Y:436:ARG:NH1	2.80	0.44
1:O:183:TYR:CD1	1:O:217:VAL:CG1	3.00	0.44
1:O:207:LEU:HB3	1:O:209:ILE:HD12	1.95	0.44
1:O:279:ALA:HB2	1:O:300:TYR:CE2	2.52	0.44
1:O:293:GLY:O	1:O:295:THR:N	2.51	0.44
1:O:392:LEU:O	1:O:392:LEU:HG	2.16	0.44
1:O:457:LEU:HA	1:O:457:LEU:HD13	1.73	0.44
1:Y:222:GLU:CG	1:Y:223:VAL:N	2.80	0.44
1:Y:262:LYS:HZ3	1:Y:264:THR:CB	2.30	0.44
1:Y:27:ILE:N	1:Y:27:ILE:CD1	2.79	0.44
1:Y:432:ARG:CD	1:Y:436:ARG:NH1	2.80	0.44
1:O:80:THR:HG22	1:O:245:ASP:N	2.32	0.44
1:O:439:THR:CG2	1:O:440:ALA:N	2.78	0.44
1:Y:148:VAL:HB	1:Y:151:SER:HB3	1.98	0.44
1:O:179:HIS:CD2	1:O:215:PRO:CB	3.00	0.44
1:O:33:ARG:HH12	1:O:62:GLU:CD	2.21	0.44
1:Y:38:ILE:O	1:Y:45:VAL:HA	2.18	0.44
1:O:251:PHE:CE2	1:O:446:LEU:CD1	2.99	0.44
1:Y:272:LEU:HD11	1:Y:303:GLU:HG3	2.00	0.44
1:Y:485:GLY:O	1:Y:488:LYS:HB3	2.18	0.44
1:O:140:LYS:O	1:O:144:ILE:HD12	2.17	0.44
1:O:60:LEU:C	1:O:63:VAL:HG23	2.37	0.44
1:Y:211:ARG:NH1	1:Y:211:ARG:HG3	2.30	0.44
1:Y:439:THR:O	1:Y:442:GLY:N	2.51	0.44
1:Y:424:ASP:HB3	1:Y:474:ILE:HB	1.98	0.44
1:Y:457:LEU:HD13	1:Y:457:LEU:HA	1.58	0.44
1:O:179:HIS:CE1	1:O:215:PRO:CG	3.00	0.43
1:O:389:ARG:O	1:O:390:ASP:C	2.57	0.43
1:O:391:VAL:CG2	1:O:392:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:40:PRO:CG	1:O:44:TRP:HB3	2.47	0.43
1:Y:272:LEU:HD11	1:Y:303:GLU:CD	2.39	0.43
1:O:137:SER:O	1:O:138:GLY:O	2.37	0.43
1:O:449:LEU:CD2	1:O:457:LEU:CD2	2.96	0.43
1:O:488:LYS:O	1:O:492:ARG:HD3	2.18	0.43
1:Y:127:ASN:CB	1:Y:193:ASN:ND2	2.81	0.43
1:Y:214:LEU:HD12	1:Y:214:LEU:HA	1.69	0.43
1:Y:325:ASP:O	1:Y:326:ALA:C	2.57	0.43
1:Y:91:LYS:O	1:Y:92:GLU:O	2.34	0.43
1:O:103:TRP:HB2	1:O:135:TYR:CE1	2.54	0.43
1:O:44:TRP:CE2	1:O:107:ARG:HB2	2.53	0.43
1:O:129:GLY:HA3	1:O:288:THR:HB	2.00	0.43
1:O:6:ILE:HD11	1:O:447:ALA:HB3	2.00	0.43
1:O:62:GLU:H	1:O:62:GLU:HG3	1.33	0.43
1:Y:246:GLN:CG	1:Y:270:PHE:HB2	2.47	0.43
1:Y:313:ILE:O	1:Y:314:GLN:C	2.55	0.43
1:Y:369:ARG:HG2	1:O:348:PHE:HB3	2.00	0.43
1:O:114:HIS:O	1:O:115:LEU:C	2.55	0.43
1:O:204:LEU:HA	1:O:204:LEU:HD23	1.45	0.43
1:O:40:PRO:HD2	1:O:44:TRP:C	2.38	0.43
1:O:455:GLN:O	1:O:455:GLN:HG3	2.18	0.43
1:Y:272:LEU:HD12	1:Y:303:GLU:CA	2.48	0.43
1:Y:351:LEU:HD12	1:Y:351:LEU:HA	1.65	0.43
1:O:415:ASN:ND2	1:O:417:PHE:HB3	2.25	0.43
1:O:421:PHE:O	1:O:424:ASP:HB2	2.19	0.43
1:Y:478:GLU:O	1:Y:481:TYR:HB3	2.18	0.43
1:Y:6:ILE:HD13	1:Y:444:ALA:HB1	2.00	0.43
1:Y:81:ASN:N	1:Y:81:ASN:ND2	2.67	0.43
1:O:145:LEU:N	1:O:145:LEU:HD13	2.33	0.43
1:O:46:GLU:OE2	1:O:107:ARG:NH2	2.50	0.43
1:O:13:THR:HG22	1:O:13:THR:O	2.15	0.43
1:Y:124:ILE:HG13	1:Y:132:ILE:CD1	2.46	0.43
1:Y:186:ALA:O	1:Y:187:SER:C	2.57	0.43
1:Y:451:VAL:O	1:Y:451:VAL:HG13	2.17	0.43
1:O:123:TYR:OH	1:O:202:LYS:HB2	2.18	0.43
1:O:143:TRP:O	1:O:147:HIS:HB2	2.18	0.43
1:O:31:SER:O	1:O:32:GLN:HB2	2.19	0.43
1:Y:31:SER:O	1:Y:32:GLN:HB2	2.18	0.43
1:Y:58:TRP:HA	1:Y:58:TRP:CE3	2.54	0.43
1:O:272:LEU:N	1:O:272:LEU:CD1	2.80	0.43
1:O:460:LEU:C	1:O:462:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:55:THR:CA	1:O:58:TRP:CD1	2.99	0.43
1:O:91:LYS:O	1:O:93:THR:N	2.51	0.43
1:Y:111:ILE:CG2	1:Y:115:LEU:HD11	2.49	0.43
1:Y:12:GLY:O	1:Y:35:PHE:HZ	2.01	0.43
1:Y:166:ASP:OD2	1:Y:185:ASN:OD1	2.37	0.43
1:Y:346:PRO:HG2	1:Y:387:GLN:NE2	2.32	0.43
1:Y:18:ALA:CB	1:Y:63:VAL:HG21	2.47	0.43
1:Y:67:ALA:C	1:Y:69:ILE:HD12	2.38	0.43
1:O:197:LEU:CD2	1:O:197:LEU:N	2.80	0.43
1:O:229:ILE:HG13	1:O:230:GLY:N	2.34	0.43
1:O:302:LEU:HD23	1:O:302:LEU:HA	1.30	0.43
1:O:272:LEU:CD1	1:O:303:GLU:HG3	2.48	0.43
1:O:422:GLN:HE21	1:O:426:LEU:HD22	1.84	0.43
1:Y:477:THR:O	1:Y:478:GLU:C	2.57	0.43
1:Y:50:MET:O	1:Y:51:GLU:C	2.56	0.43
1:O:184:THR:CG2	1:O:290:ILE:HG22	2.49	0.42
1:O:206:VAL:CG1	1:O:207:LEU:N	2.82	0.42
1:O:214:LEU:HA	1:O:215:PRO:HD3	1.73	0.42
1:O:468:ARG:HG3	1:O:468:ARG:NH1	2.34	0.42
1:Y:338:ASN:O	1:Y:375:HIS:HD2	2.01	0.42
1:Y:249:ALA:HB1	1:Y:438:VAL:CG1	2.49	0.42
1:Y:449:LEU:HD12	1:Y:449:LEU:HA	1.93	0.42
1:Y:16:SER:CB	1:Y:56:GLN:HA	2.48	0.42
1:Y:9:LEU:HD11	1:Y:60:LEU:CD1	2.49	0.42
1:O:184:THR:HA	1:O:290:ILE:HG22	2.01	0.42
1:O:279:ALA:HB2	1:O:300:TYR:CD1	2.55	0.42
1:Y:18:ALA:CB	1:Y:59:THR:HB	2.49	0.42
1:Y:3:LYS:HB2	1:Y:3:LYS:HZ3	1.83	0.42
1:Y:56:GLN:HG3	1:Y:56:GLN:O	2.18	0.42
1:O:418:LEU:HD23	1:O:418:LEU:HA	1.70	0.42
1:Y:410:GLY:O	1:Y:413:VAL:HG13	2.19	0.42
1:Y:441:LEU:HD22	1:Y:445:TYR:CE1	2.54	0.42
1:O:422:GLN:HG3	1:O:426:LEU:HD23	2.01	0.42
1:Y:17:ARG:HH22	1:Y:437:GLU:HG3	1.84	0.42
1:Y:204:LEU:HD23	1:Y:204:LEU:HA	1.44	0.42
1:Y:264:THR:HA	1:Y:409:ASP:O	2.18	0.42
1:Y:460:LEU:O	1:Y:462:GLU:N	2.53	0.42
1:O:157:ARG:H	1:O:157:ARG:HG2	1.62	0.42
1:O:87:ILE:HD13	1:O:168:TRP:CB	2.49	0.42
1:O:251:PHE:O	1:O:254:LEU:HA	2.19	0.42
1:O:338:ASN:OD1	1:O:340:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:83:ARG:CZ	1:O:246:GLN:CG	2.97	0.42
1:O:84:GLU:OE1	1:O:103:TRP:HB3	2.19	0.42
1:Y:353:ALA:HA	1:Y:356:TRP:NE1	2.34	0.42
1:Y:41:LYS:HA	1:Y:42:PRO:HD3	1.80	0.42
1:Y:482:ARG:CG	1:Y:482:ARG:HH11	2.33	0.42
1:Y:482:ARG:HG3	1:Y:482:ARG:HH11	1.83	0.42
1:O:144:ILE:CG2	1:O:148:VAL:HG21	2.48	0.42
1:O:395:MET:O	1:O:399:SER:N	2.52	0.42
1:Y:41:LYS:O	1:Y:44:TRP:HB2	2.19	0.42
1:O:193:ASN:CG	1:O:196:THR:HB	2.40	0.42
1:O:240:SER:HB2	1:O:450:ALA:CB	2.49	0.42
1:O:438:VAL:CG1	1:O:439:THR:N	2.80	0.42
1:O:466:ILE:HD13	1:O:466:ILE:O	2.19	0.42
1:Y:103:TRP:HB2	1:Y:135:TYR:CD1	2.55	0.42
1:Y:9:LEU:HD12	1:Y:9:LEU:HA	1.65	0.42
1:O:123:TYR:CE2	1:O:203:MET:HE2	2.54	0.42
1:O:165:VAL:O	1:O:169:LEU:HD23	2.20	0.42
1:O:193:ASN:OD1	1:O:196:THR:HB	2.20	0.42
1:O:272:LEU:HD21	1:O:303:GLU:OE1	2.20	0.42
1:O:434:GLU:N	1:O:465:VAL:O	2.50	0.42
1:O:3:LYS:HG2	1:O:72:ASP:O	2.20	0.42
1:Y:35:PHE:HE2	1:Y:47:HIS:CD2	2.38	0.42
1:Y:31:SER:HB2	1:Y:63:VAL:H	1.84	0.42
1:O:468:ARG:NH1	1:O:468:ARG:CG	2.80	0.42
1:O:135:TYR:OH	4:O:600:GOL:O1	2.31	0.42
1:Y:142:LYS:O	1:Y:146:ASP:OD1	2.37	0.42
1:Y:428:THR:CG2	1:Y:429:ARG:N	2.81	0.42
1:Y:11:GLN:NE2	1:Y:82:GLN:HE21	2.16	0.42
1:O:137:SER:HA	1:O:140:LYS:HB2	2.02	0.41
1:O:179:HIS:CE1	1:O:215:PRO:CB	3.02	0.41
1:O:127:ASN:ND2	1:O:193:ASN:ND2	2.67	0.41
1:O:199:TRP:HZ2	1:O:215:PRO:O	2.02	0.41
1:Y:242:ILE:HG22	1:Y:243:ALA:N	2.35	0.41
1:O:297:GLU:O	1:O:298:VAL:O	2.38	0.41
1:O:432:ARG:O	1:O:467:GLU:N	2.50	0.41
1:Y:166:ASP:O	1:Y:169:LEU:N	2.50	0.41
1:Y:324:ASN:ND2	1:Y:324:ASN:N	2.67	0.41
1:Y:18:ALA:CB	1:Y:63:VAL:CG2	2.99	0.41
1:O:199:TRP:CE2	1:O:214:LEU:HB3	2.54	0.41
1:O:216:GLU:HG2	1:O:218:ARG:HH11	1.85	0.41
1:O:359:TYR:HB2	1:O:495:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:358:PRO:HG2	1:Y:359:TYR:CE2	2.56	0.41
1:Y:441:LEU:HD23	1:Y:441:LEU:HA	1.79	0.41
1:Y:47:HIS:HB2	1:Y:100:ALA:HB3	2.02	0.41
1:O:141:VAL:HA	1:O:144:ILE:HD12	2.02	0.41
1:O:317:ARG:HG2	1:O:318:ASP:N	2.34	0.41
1:O:3:LYS:HA	1:O:73:GLN:C	2.40	0.41
1:Y:103:TRP:HB2	1:Y:135:TYR:CE1	2.55	0.41
1:Y:108:THR:HG22	1:Y:111:ILE:HD12	2.02	0.41
1:Y:142:LYS:O	1:Y:143:TRP:C	2.59	0.41
1:Y:246:GLN:HG2	1:Y:270:PHE:CB	2.50	0.41
1:Y:250:LEU:HD12	1:Y:250:LEU:C	2.38	0.41
1:Y:32:GLN:HA	1:Y:59:THR:HG22	2.02	0.41
1:Y:381:LEU:HA	1:Y:381:LEU:HD23	1.78	0.41
1:Y:479:ARG:CG	1:Y:479:ARG:NH1	2.83	0.41
1:O:264:THR:HA	1:O:409:ASP:O	2.20	0.41
1:O:353:ALA:HB1	1:O:354:PRO:HD3	2.03	0.41
1:O:381:LEU:O	1:O:382:GLU:C	2.56	0.41
1:O:492:ARG:CG	1:O:492:ARG:NH1	2.80	0.41
1:O:52:ILE:O	1:O:55:THR:OG1	2.38	0.41
1:Y:250:LEU:HD22	1:Y:272:LEU:HB2	2.02	0.41
1:Y:64:LEU:O	1:Y:65:ALA:C	2.56	0.41
1:Y:81:ASN:HB2	1:Y:165:VAL:HB	2.03	0.41
1:O:102:VAL:HG12	1:O:103:TRP:N	2.35	0.41
1:O:107:ARG:HG3	1:O:143:TRP:CD1	2.55	0.41
1:O:203:MET:O	1:O:204:LEU:C	2.59	0.41
1:O:236:ARG:CG	1:O:236:ARG:NH1	2.80	0.41
1:O:346:PRO:HG3	1:O:383:SER:OG	2.20	0.41
1:O:353:ALA:CB	1:O:354:PRO:CD	2.98	0.41
1:Y:169:LEU:HD13	1:Y:169:LEU:HA	1.87	0.41
1:Y:468:ARG:NH1	1:Y:468:ARG:HG3	2.36	0.41
1:O:166:ASP:OD2	1:O:185:ASN:OD1	2.39	0.41
1:O:256:VAL:O	1:O:294:PRO:HD3	2.21	0.41
1:O:354:PRO:CD	1:O:355:TYR:H	2.34	0.41
1:Y:154:ARG:HG2	1:Y:154:ARG:H	1.09	0.41
1:Y:95:LYS:HA	1:Y:96:PRO:HD3	1.97	0.41
1:O:138:GLY:N	1:O:189:THR:O	2.52	0.41
1:O:24:ASP:O	1:O:25:ALA:HB3	2.21	0.41
1:O:451:VAL:CG1	1:O:453:PHE:HB2	2.50	0.41
1:O:487:LYS:O	1:O:488:LYS:C	2.59	0.41
1:Y:127:ASN:HD22	1:Y:193:ASN:HD21	1.68	0.41
1:Y:261:ALA:HB2	1:Y:273:MET:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:457:LEU:HD13	1:Y:460:LEU:HD13	2.02	0.41
1:Y:90:GLU:HB3	1:Y:93:THR:HG23	2.02	0.41
1:O:180:VAL:HA	1:O:216:GLU:O	2.21	0.41
1:O:27:ILE:CD1	1:O:27:ILE:N	2.79	0.41
1:O:81:ASN:N	1:O:81:ASN:HD22	2.18	0.41
1:Y:224:TYR:HE2	1:Y:241:GLY:N	2.19	0.41
1:Y:352:GLY:HA2	1:Y:356:TRP:CE3	2.56	0.41
1:Y:456:ASN:ND2	1:Y:456:ASN:C	2.74	0.41
1:O:113:GLU:O	1:O:116:LYS:HB2	2.20	0.40
1:O:237:ILE:HG12	1:O:237:ILE:H	1.77	0.40
1:O:345:VAL:HA	1:O:346:PRO:HD3	1.66	0.40
1:O:428:THR:HG23	1:O:429:ARG:N	2.36	0.40
1:O:480:ASN:O	1:O:481:TYR:C	2.58	0.40
1:O:16:SER:OG	1:O:55:THR:OG1	2.30	0.40
1:O:55:THR:O	1:O:58:TRP:N	2.54	0.40
1:O:81:ASN:HB2	1:O:165:VAL:HB	2.03	0.40
1:Y:110:GLU:O	1:Y:111:ILE:C	2.58	0.40
1:Y:122:ASP:O	1:Y:126:SER:N	2.40	0.40
1:Y:272:LEU:HD11	1:Y:303:GLU:OE1	2.21	0.40
1:O:295:THR:N	1:O:297:GLU:OE1	2.43	0.40
1:Y:32:GLN:CA	1:Y:59:THR:HG22	2.52	0.40
1:O:250:LEU:CD1	1:O:255:CYS:HB2	2.51	0.40
1:O:353:ALA:CB	1:O:354:PRO:HD3	2.51	0.40
1:O:359:TYR:HD1	1:O:497:GLU:HB3	1.86	0.40
1:O:90:GLU:HB3	1:O:93:THR:HG23	2.03	0.40
1:Y:123:TYR:HD1	1:Y:203:MET:CE	2.32	0.40
1:Y:180:VAL:HG22	1:Y:181:THR:H	1.85	0.40
1:Y:47:HIS:CB	1:Y:52:ILE:HD11	2.47	0.40
1:O:344:VAL:HG22	1:O:364:ILE:HD13	2.03	0.40
1:Y:173:MET:CE	1:Y:173:MET:CA	2.99	0.40
1:Y:127:ASN:CB	1:Y:193:ASN:HD22	2.31	0.40
1:Y:273:MET:HB2	1:Y:395:MET:CE	2.52	0.40
1:Y:272:LEU:CD1	1:Y:303:GLU:CG	3.00	0.40
1:O:130:LEU:HD23	1:O:130:LEU:HA	1.71	0.40
1:O:141:VAL:O	1:O:142:LYS:C	2.59	0.40
1:Y:199:TRP:CD1	1:Y:214:LEU:HD23	2.56	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	490/501 (98%)	375 (76%)	85 (17%)	30 (6%)	2	10
1	Y	490/501 (98%)	391 (80%)	76 (16%)	23 (5%)	3	16
All	All	980/1002 (98%)	766 (78%)	161 (16%)	53 (5%)	2	13

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	61	VAL
1	Y	64	LEU
1	Y	65	ALA
1	Y	75	ALA
1	Y	151	SER
1	Y	175	GLN
1	Y	188	ARG
1	Y	456	ASN
1	O	75	ALA
1	O	118	ASP
1	O	149	GLU
1	O	258	GLU
1	O	353	ALA
1	O	458	ASP
1	Y	62	GLU
1	Y	98	TYR
1	Y	149	GLU
1	Y	258	GLU
1	Y	442	GLY
1	Y	461	GLN
1	O	63	VAL
1	O	98	TYR
1	O	165	VAL
1	O	187	SER
1	O	294	PRO

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Mol	Chain	Res	Type
1	O	298	VAL
1	Y	71	SER
1	Y	215	PRO
1	O	59	THR
1	O	66	LYS
1	O	151	SER
1	O	175	GLN
1	O	456	ASN
1	Y	53	TRP
1	Y	63	VAL
1	Y	153	GLU
1	Y	464	ALA
1	O	55	THR
1	O	60	LEU
1	O	108	THR
1	O	119	GLY
1	O	166	ASP
1	O	91	LYS
1	O	92	GLU
1	O	138	GLY
1	O	215	PRO
1	O	242	ILE
1	Y	358	PRO
1	O	399	SER
1	Y	165	VAL
1	O	111	ILE
1	Y	238	PRO
1	O	451	VAL

### 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%)	283 (69%)	125 (31%)	0	2
1	Y	408/412 (99%)	289 (71%)	119 (29%)	0	2
All	All	816/824 (99%)	572 (70%)	244 (30%)	0	2

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	2	GLU
1	Y	5	TYR
1	Y	6	ILE
1	Y	9	LEU
1	Y	11	GLN
1	Y	13	THR
1	Y	27	ILE
1	Y	33	ARG
1	Y	34	GLU
1	Y	41	LYS
1	Y	63	VAL
1	Y	70	SER
1	Y	71	SER
1	Y	73	GLN
1	Y	80	THR
1	Y	83	ARG
1	Y	87	ILE
1	Y	91	LYS
1	Y	92	GLU
1	Y	93	THR
1	Y	95	LYS
1	Y	106	ARG
1	Y	107	ARG
1	Y	110	GLU
1	Y	117	ARG
1	Y	120	LEU
1	Y	121	GLU
1	Y	124	ILE
1	Y	128	THR
1	Y	137	SER
1	Y	145	LEU
1	Y	146	ASP
1	Y	148	VAL
1	Y	149	GLU
1	Y	153	GLU
1	Y	154	ARG
1	Y	156	ARG
1	Y	157	ARG
1	Y	159	GLU
1	Y	162	PHE
1	Y	165	VAL
1	Y	170	ILE

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Mol	Chain	Res	Type
1	Y	172	LYS
1	Y	175	GLN
1	Y	181	THR
1	Y	187	SER
1	Y	191	LEU
1	Y	194	ILE
1	Y	196	THR
1	Y	200	ASP
1	Y	201	ASP
1	Y	202	LYS
1	Y	206	VAL
1	Y	211	ARG
1	Y	219	ARG
1	Y	227	THR
1	Y	228	ASN
1	Y	229	ILE
1	Y	235	THR
1	Y	236	ARG
1	Y	237	ILE
1	Y	246	GLN
1	Y	247	GLN
1	Y	253	GLN
1	Y	256	VAL
1	Y	257	LYS
1	Y	262	LYS
1	Y	272	LEU
1	Y	278	LYS
1	Y	281	LYS
1	Y	290	ILE
1	Y	312	SER
1	Y	317	ARG
1	Y	321	LYS
1	Y	324	ASN
1	Y	335	LYS
1	Y	339	THR
1	Y	351	LEU
1	Y	364	ILE
1	Y	368	THR
1	Y	369	ARG
1	Y	389	ARG
1	Y	392	LEU
1	Y	396	GLN

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Mol	Chain	Res	Type
1	Y	402	ARG
1	Y	406	LEU
1	Y	407	ARG
1	Y	415	ASN
1	Y	418	LEU
1	Y	423	SER
1	Y	426	LEU
1	Y	429	ARG
1	Y	434	GLU
1	Y	437	GLU
1	Y	438	VAL
1	Y	439	THR
1	Y	445	TYR
1	Y	446	LEU
1	Y	451	VAL
1	Y	454	TRP
1	Y	455	GLN
1	Y	456	ASN
1	Y	457	LEU
1	Y	460	LEU
1	Y	461	GLN
1	Y	462	GLU
1	Y	463	LYS
1	Y	466	ILE
1	Y	467	GLU
1	Y	468	ARG
1	Y	469	GLU
1	Y	475	GLU
1	Y	478	GLU
1	Y	479	ARG
1	Y	483	TYR
1	Y	488	LYS
1	Y	492	ARG
1	Y	494	MET
1	Y	498	GLU
1	O	5	TYR
1	O	9	LEU
1	O	11	GLN
1	O	16	SER
1	O	20	VAL
1	O	22	ASP
1	O	32	GLN

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Mol	Chain	Res	Type
1	O	34	GLU
1	O	41	LYS
1	O	57	SER
1	O	62	GLU
1	O	63	VAL
1	O	64	LEU
1	O	70	SER
1	O	71	SER
1	O	73	GLN
1	O	80	THR
1	O	82	GLN
1	O	87	ILE
1	O	91	LYS
1	O	92	GLU
1	O	93	THR
1	O	95	LYS
1	O	106	ARG
1	O	107	ARG
1	O	115	LEU
1	O	117	ARG
1	O	118	ASP
1	O	120	LEU
1	O	124	ILE
1	O	125	ARG
1	O	128	THR
1	O	131	VAL
1	O	132	ILE
1	O	137	SER
1	O	145	LEU
1	O	146	ASP
1	O	148	VAL
1	O	149	GLU
1	O	153	GLU
1	O	154	ARG
1	O	156	ARG
1	O	157	ARG
1	O	161	LEU
1	O	162	PHE
1	O	164	THR
1	O	165	VAL
1	O	172	LYS
1	O	175	GLN

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Mol	Chain	Res	Type
1	O	181	THR
1	O	182	ASP
1	O	185	ASN
1	O	190	MET
1	O	191	LEU
1	O	195	HIS
1	O	196	THR
1	O	201	ASP
1	O	202	LYS
1	O	206	VAL
1	O	207	LEU
1	O	211	ARG
1	O	213	MET
1	O	219	ARG
1	O	222	GLU
1	O	227	THR
1	O	228	ASN
1	O	229	ILE
1	O	235	THR
1	O	236	ARG
1	O	237	ILE
1	O	253	GLN
1	O	256	VAL
1	O	257	LYS
1	O	262	LYS
1	O	269	CYS
1	O	272	LEU
1	O	278	LYS
1	O	281	LYS
1	O	290	ILE
1	O	317	ARG
1	O	321	LYS
1	O	324	ASN
1	O	335	LYS
1	O	339	THR
1	O	351	LEU
1	O	364	ILE
1	O	368	THR
1	O	389	ARG
1	O	391	VAL
1	O	392	LEU
1	O	402	ARG

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Mol	Chain	Res	Type
1	O	403	LEU
1	O	406	LEU
1	O	407	ARG
1	O	415	ASN
1	O	418	LEU
1	O	423	SER
1	O	426	LEU
1	O	428	THR
1	O	429	ARG
1	O	434	GLU
1	O	436	ARG
1	O	437	GLU
1	O	438	VAL
1	O	439	THR
1	O	451	VAL
1	O	454	TRP
1	O	455	GLN
1	O	456	ASN
1	O	460	LEU
1	O	461	GLN
1	O	462	GLU
1	O	463	LYS
1	O	466	ILE
1	O	467	GLU
1	O	468	ARG
1	O	474	ILE
1	O	478	GLU
1	O	479	ARG
1	O	482	ARG
1	O	488	LYS
1	O	492	ARG
1	O	494	MET
1	O	498	GLU
1	O	499	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	11	GLN
1	Y	26	ASN
1	Y	73	GLN
1	Y	81	ASN

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Mol	Chain	Res	Type
1	Y	99	ASN
1	Y	104	GLN
1	Y	114	HIS
1	Y	127	ASN
1	Y	147	HIS
1	Y	175	GLN
1	Y	185	ASN
1	Y	226	GLN
1	Y	228	ASN
1	Y	299	ASN
1	Y	324	ASN
1	Y	387	GLN
1	Y	396	GLN
1	Y	415	ASN
1	Y	456	ASN
1	Y	461	GLN
1	O	11	GLN
1	O	26	ASN
1	O	37	GLN
1	O	47	HIS
1	O	73	GLN
1	O	81	ASN
1	O	99	ASN
1	O	114	HIS
1	O	127	ASN
1	O	147	HIS
1	O	179	HIS
1	O	185	ASN
1	O	226	GLN
1	O	228	ASN
1	O	253	GLN
1	O	387	GLN
1	O	396	GLN
1	O	415	ASN
1	O	420	GLN
1	O	455	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GOL	O	600	-	5,5,5	0.46	0	5,5,5	0.26	0
3	ATS	O	601	-	25,33,33	1.35	4 (16%)	27,52,52	1.16	2 (7%)
4	GOL	Y	600	-	5,5,5	0.58	0	5,5,5	0.80	0
3	ATS	Y	601	2	25,33,33	1.08	2 (8%)	27,52,52	1.34	3 (11%)

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
4	GOL	O	600	-	-	0/4/4/4	0/0/0/0
3	ATS	O	601	-	-	0/9/38/38	0/3/3/3
4	GOL	Y	600	-	-	0/4/4/4	0/0/0/0
3	ATS	Y	601	2	-	0/9/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	ATS	C4-N3	-3.08	1.31	1.35
3	O	601	ATS	C8-N7	-2.56	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	601	ATS	O2'-C2'	-2.31	1.37	1.43
3	Y	601	ATS	O3'-C3'	-2.22	1.37	1.43
3	O	601	ATS	C5-C4	-2.14	1.35	1.40
3	O	601	ATS	PB-O13	3.27	1.62	1.58

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	601	ATS	PA-O13-PB	-3.34	121.61	132.39
3	O	601	ATS	PA-O13-PB	-2.28	125.03	132.39
3	Y	601	ATS	N6-C6-N1	-2.10	114.59	118.77
3	O	601	ATS	C1'-N9-C4	3.55	132.77	126.64
3	Y	601	ATS	C5-C6-N6	3.78	128.17	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	600	GOL	2	0
3	O	601	ATS	2	0
4	Y	600	GOL	3	0
3	Y	601	ATS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	O	494/501 (98%)	-0.73	0 100 100	7, 52, 91, 100	0
1	Y	494/501 (98%)	-0.94	0 100 100	5, 38, 78, 100	0
All	All	988/1002 (98%)	-0.83	0 100 100	5, 45, 86, 100	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ATS	Y	601	31/31	0.97	0.12	0.72	50,50,50,50	0
3	ATS	O	601	31/31	0.95	0.14	0.61	64,64,64,64	0
4	GOL	Y	600	6/6	0.98	0.11	-0.48	17,17,17,17	0
4	GOL	O	600	6/6	0.98	0.12	-0.49	45,45,45,45	0
2	MG	Y	602	1/1	0.95	0.16	-	27,27,27,27	0

## 6.5 Other polymers

There are no such residues in this entry.