



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:48 AM UTC

PDB ID : 1GLJ / pdb_00001glj
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

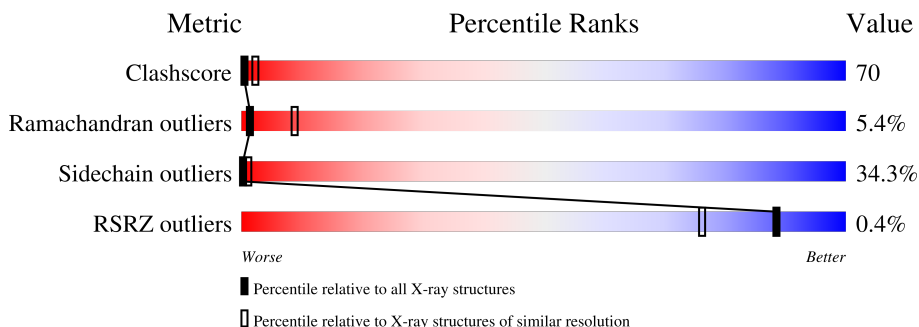
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

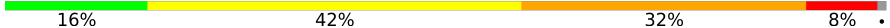
The reported resolution of this entry is 3.00 Å.

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



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

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

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

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			

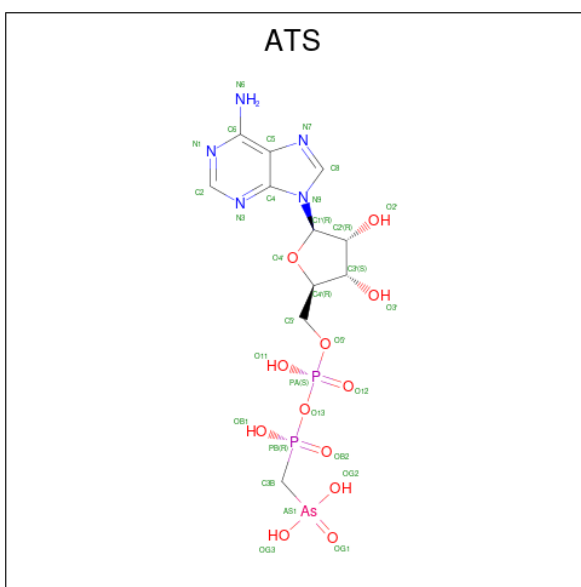
There are 2 discrepancies between the modelled and reference sequences:

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

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

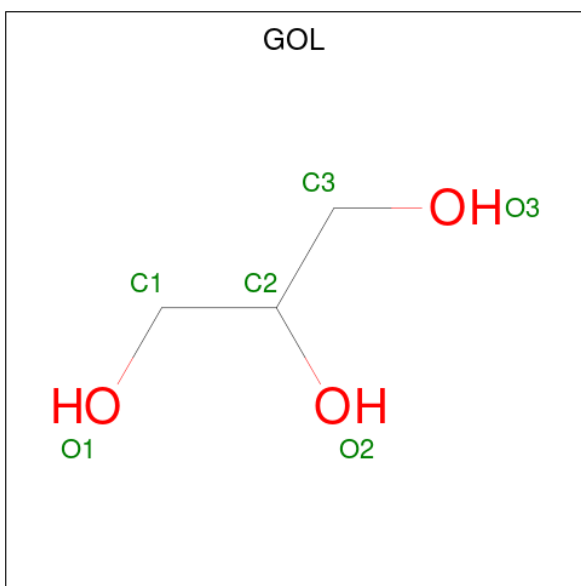
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GAMMA-ARSONO-BETA, GAMMA-METHYLENEADENOSINE-5'-DIPHOSPHATE (CCD ID: ATS) (formula: C₁₁H₁₈AsN₅O₁₂P₂).



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 (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).

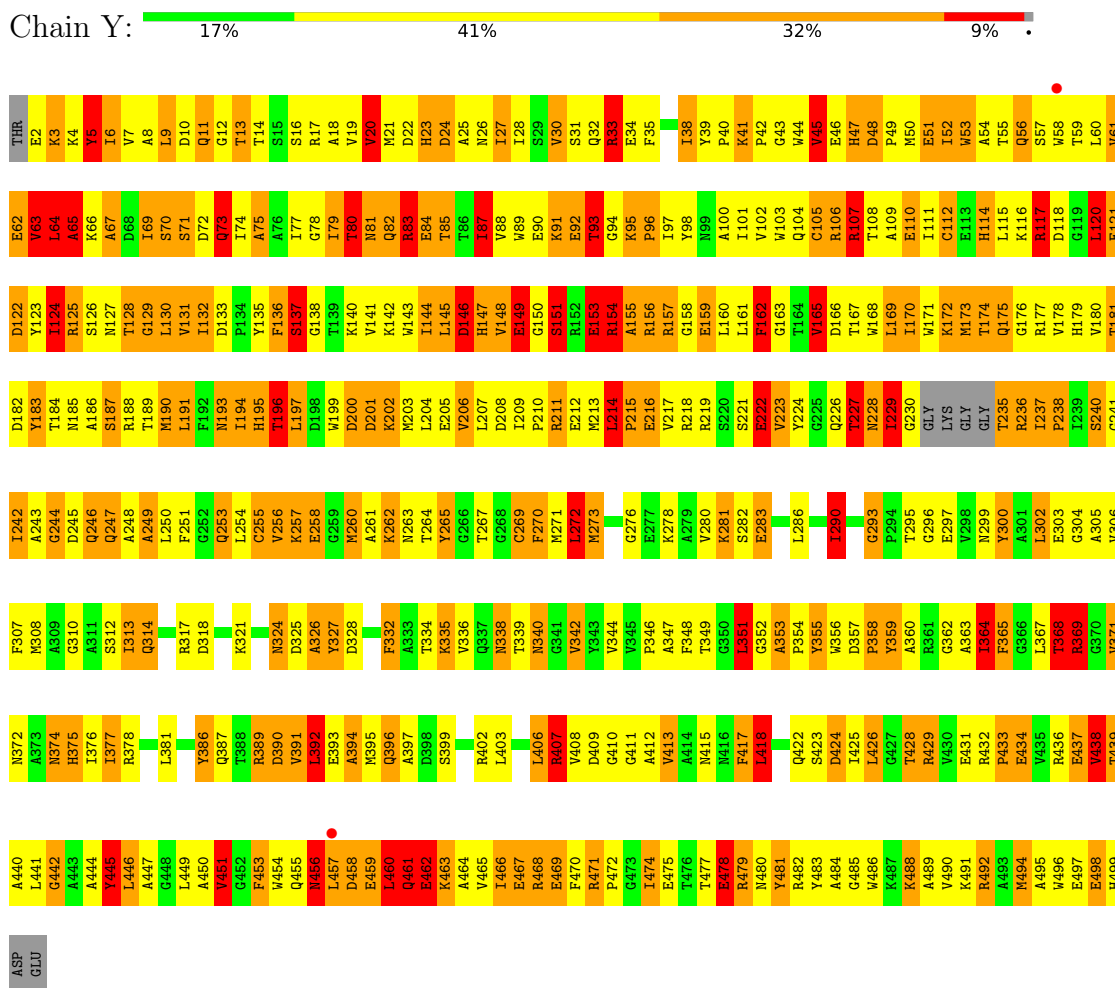


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Y	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0

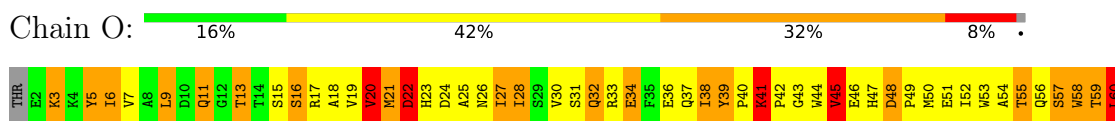
3 Residue-property plots

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

• Molecule 1: GLYCEROL KINASE



• Molecule 1: GLYCEROL KINASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.67Å 200.70Å 114.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 90.1 (20.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 171.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.57	26/3991 (0.7%)	2.07	133/5412 (2.5%)
1	Y	1.74	51/3991 (1.3%)	2.25	192/5412 (3.5%)
All	All	1.66	77/7982 (1.0%)	2.16	325/10824 (3.0%)

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 (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	353	ALA	CA-C	-10.61	1.41	1.53
1	Y	456	ASN	C-O	-10.30	1.11	1.24
1	Y	197	LEU	CA-C	8.61	1.64	1.53
1	Y	195	HIS	C-N	8.32	1.45	1.33
1	Y	196	THR	C-N	7.98	1.43	1.33
1	Y	481	TYR	N-CA	-7.14	1.37	1.46
1	O	353	ALA	CA-C	-7.04	1.44	1.52
1	Y	196	THR	CB-CG2	-6.97	1.29	1.52
1	Y	270	PHE	CA-C	-6.95	1.44	1.52
1	Y	106	ARG	CZ-NH1	6.87	1.42	1.32
1	Y	38	ILE	CA-CB	-6.82	1.46	1.54
1	Y	195	HIS	C-O	6.76	1.32	1.24
1	Y	368	THR	CA-C	-6.72	1.44	1.52
1	Y	33	ARG	NE-CZ	6.52	1.40	1.33
1	O	476	THR	C-N	-6.52	1.25	1.33
1	Y	223	VAL	CA-C	-6.41	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	125	ARG	NE-CZ	6.40	1.40	1.33
1	Y	332	PHE	CA-C	-6.40	1.44	1.52
1	O	300	TYR	CA-C	-6.26	1.45	1.52
1	Y	112	CYS	N-CA	-6.23	1.38	1.46
1	Y	377	ILE	CA-CB	-6.14	1.47	1.54
1	O	455	GLN	CA-CB	6.12	1.61	1.53
1	Y	255	CYS	CA-C	-6.10	1.44	1.52
1	O	355	TYR	CA-C	-6.07	1.45	1.52
1	O	395	MET	N-CA	-6.06	1.38	1.46
1	Y	144	ILE	CA-CB	-6.03	1.47	1.54
1	O	325	ASP	CA-C	-6.00	1.45	1.52
1	Y	371	VAL	CA-C	-5.92	1.46	1.52
1	Y	424	ASP	C-N	-5.83	1.27	1.34
1	O	195	HIS	CA-C	-5.73	1.45	1.52
1	Y	196	THR	CA-C	-5.71	1.44	1.52
1	Y	364	ILE	CA-C	-5.70	1.46	1.52
1	Y	495	ALA	CA-C	-5.67	1.45	1.53
1	Y	480	ASN	C-N	-5.65	1.26	1.33
1	O	353	ALA	C-O	-5.64	1.17	1.24
1	Y	318	ASP	CG-OD2	5.62	1.36	1.25
1	O	292	CYS	CA-C	-5.62	1.46	1.52
1	Y	154	ARG	C-O	-5.62	1.17	1.24
1	Y	326	ALA	C-N	-5.61	1.27	1.33
1	O	303	GLU	C-N	5.61	1.36	1.33
1	O	418	LEU	N-CA	-5.61	1.39	1.46
1	Y	359	TYR	CA-CB	-5.60	1.45	1.54
1	Y	144	ILE	CA-C	-5.57	1.46	1.52
1	Y	327	TYR	N-CA	-5.54	1.39	1.46
1	Y	96	PRO	CA-C	-5.50	1.45	1.52
1	O	438	VAL	CA-CB	-5.48	1.47	1.54
1	O	471	ARG	CD-NE	-5.44	1.38	1.46
1	Y	265	TYR	CA-C	-5.41	1.46	1.52
1	Y	342	VAL	CA-CB	-5.41	1.49	1.54
1	Y	347	ALA	C-N	-5.38	1.26	1.33
1	Y	445	TYR	C-N	-5.36	1.27	1.33
1	O	374	ASN	CA-C	-5.34	1.46	1.52
1	Y	300	TYR	CA-C	-5.30	1.46	1.52
1	O	304	GLY	CA-C	5.30	1.56	1.51
1	Y	197	LEU	C-O	5.28	1.30	1.23
1	Y	418	LEU	CA-C	-5.28	1.46	1.52
1	O	245	ASP	C-N	-5.28	1.26	1.33
1	Y	283	GLU	CA-C	-5.27	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	377	ILE	C-N	-5.24	1.27	1.33
1	O	258	GLU	CD-OE2	5.24	1.35	1.25
1	Y	283	GLU	CD-OE1	5.22	1.35	1.25
1	Y	146	ASP	CA-C	-5.21	1.45	1.52
1	Y	131	VAL	CA-C	5.20	1.58	1.52
1	O	269	CYS	N-CA	-5.19	1.39	1.46
1	Y	47	HIS	CB-CG	-5.17	1.43	1.50
1	O	263	ASN	C-O	5.17	1.30	1.24
1	Y	456	ASN	C-N	-5.16	1.26	1.33
1	O	457	LEU	C-N	-5.16	1.26	1.33
1	Y	438	VAL	CA-CB	-5.14	1.47	1.54
1	O	50	MET	N-CA	-5.12	1.40	1.46
1	Y	462	GLU	CD-OE2	5.12	1.35	1.25
1	Y	262	LYS	CA-C	-5.12	1.46	1.52
1	O	323	ILE	CA-C	-5.12	1.47	1.52
1	Y	242	ILE	C-O	-5.03	1.19	1.24
1	O	348	PHE	N-CA	-5.03	1.40	1.46
1	O	41	LYS	CA-C	-5.02	1.46	1.52
1	Y	394	ALA	CA-C	-5.00	1.46	1.52

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	83	ARG	CA-C-N	-13.50	101.04	122.24
1	Y	83	ARG	C-N-CA	-13.50	101.04	122.24
1	Y	458	ASP	CA-CB-CG	12.88	125.48	112.60
1	Y	351	LEU	CA-C-N	-12.58	102.08	121.45
1	Y	351	LEU	C-N-CA	-12.58	102.08	121.45
1	O	83	ARG	N-CA-C	12.40	128.61	113.23
1	Y	196	THR	N-CA-CB	-12.21	89.02	110.39
1	O	122	ASP	CA-CB-CG	-11.63	100.97	112.60
1	O	453	PHE	N-CA-C	-11.46	99.41	113.50
1	O	353	ALA	CA-C-N	-11.08	105.99	119.84
1	O	353	ALA	C-N-CA	-11.08	105.99	119.84
1	Y	471	ARG	CA-C-N	10.11	130.75	119.93
1	Y	471	ARG	C-N-CA	10.11	130.75	119.93
1	Y	196	THR	N-CA-C	9.93	124.92	113.01
1	Y	195	HIS	CA-CB-CG	-9.83	103.97	113.80
1	Y	81	ASN	CA-CB-CG	-9.75	102.85	112.60
1	Y	83	ARG	N-CA-C	9.60	124.79	113.18
1	Y	122	ASP	CA-CB-CG	-9.59	103.01	112.60
1	Y	196	THR	CA-C-N	-9.52	109.03	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	196	THR	C-N-CA	-9.52	109.03	122.46
1	Y	137	SER	N-CA-C	9.13	122.37	111.33
1	Y	246	GLN	N-CA-C	9.03	121.95	111.11
1	Y	132	ILE	N-CA-CB	8.92	120.94	110.95
1	O	296	GLY	CA-C-O	8.82	127.07	118.77
1	O	147	HIS	CA-CB-CG	-8.73	105.07	113.80
1	Y	247	GLN	N-CA-CB	-8.69	97.00	109.94
1	O	332	PHE	CA-CB-CG	-8.69	105.11	113.80
1	O	351	LEU	N-CA-C	8.68	124.20	111.96
1	O	194	ILE	N-CA-C	8.62	119.58	111.91
1	Y	458	ASP	N-CA-C	-8.51	102.66	113.72
1	O	449	LEU	N-CA-C	-8.47	101.56	112.23
1	Y	5	TYR	N-CA-C	8.43	121.16	109.18
1	O	304	GLY	O-C-N	-8.36	118.09	123.35
1	Y	210	PRO	N-CA-CB	8.35	108.83	103.23
1	O	20	VAL	N-CA-C	8.29	119.71	108.11
1	O	474	ILE	CA-CB-CG1	-8.21	96.44	110.40
1	Y	262	LYS	CA-C-N	-8.19	111.45	122.99
1	Y	262	LYS	C-N-CA	-8.19	111.45	122.99
1	O	351	LEU	CA-C-N	-8.09	108.19	120.65
1	O	351	LEU	C-N-CA	-8.09	108.19	120.65
1	O	144	ILE	N-CA-CB	8.03	119.38	110.62
1	O	97	ILE	N-CA-CB	-7.91	101.86	112.22
1	Y	244	GLY	N-CA-C	-7.87	101.35	112.37
1	O	90	GLU	N-CA-CB	7.86	121.56	109.85
1	Y	478	GLU	N-CA-CB	-7.75	97.39	110.49
1	Y	318	ASP	N-CA-CB	7.73	121.78	110.26
1	O	345	VAL	O-C-N	7.72	126.23	121.37
1	O	102	VAL	N-CA-C	7.69	119.50	109.58
1	Y	80	THR	N-CA-CB	7.62	124.80	111.00
1	Y	369	ARG	N-CA-C	7.53	122.13	112.34
1	Y	87	ILE	N-CA-CB	7.52	123.78	111.45
1	Y	332	PHE	CA-CB-CG	-7.51	106.28	113.80
1	O	353	ALA	CA-C-O	-7.47	109.92	120.16
1	O	344	VAL	CA-C-N	-7.47	114.33	122.85
1	O	344	VAL	C-N-CA	-7.47	114.33	122.85
1	Y	451	VAL	N-CA-CB	-7.42	102.29	111.94
1	Y	453	PHE	N-CA-C	-7.41	104.22	113.18
1	O	499	HIS	CA-CB-CG	7.41	121.21	113.80
1	Y	293	GLY	N-CA-C	-7.41	102.99	112.10
1	Y	136	PHE	CA-C-N	7.38	130.49	120.38
1	Y	136	PHE	C-N-CA	7.38	130.49	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	84	GLU	O-C-N	7.37	130.45	122.34
1	O	210	PRO	N-CA-CB	7.36	108.16	103.23
1	O	296	GLY	N-CA-C	-7.34	103.97	116.01
1	O	458	ASP	CA-CB-CG	7.33	119.93	112.60
1	Y	456	ASN	CA-C-O	7.31	130.96	120.51
1	O	20	VAL	CB-CA-C	-7.25	99.89	110.63
1	O	270	PHE	CA-CB-CG	-7.23	106.57	113.80
1	O	303	GLU	N-CA-C	7.21	120.94	108.76
1	Y	73	GLN	CA-C-N	-7.18	113.84	123.10
1	Y	73	GLN	C-N-CA	-7.18	113.84	123.10
1	Y	114	HIS	CA-CB-CG	-7.18	106.62	113.80
1	Y	465	VAL	CA-C-N	-7.17	111.76	121.66
1	Y	465	VAL	C-N-CA	-7.17	111.76	121.66
1	Y	195	HIS	CB-CG-ND1	-7.16	111.96	122.70
1	O	170	ILE	N-CA-CB	-7.16	103.10	110.62
1	Y	471	ARG	O-C-N	7.15	128.38	121.66
1	O	359	TYR	CA-CB-CG	-7.08	101.15	113.90
1	O	132	ILE	N-CA-CB	7.06	118.86	110.95
1	Y	499	HIS	CA-CB-CG	7.03	120.83	113.80
1	O	129	GLY	N-CA-C	-7.02	105.19	115.30
1	O	13	THR	CA-CB-OG1	6.99	120.08	109.60
1	Y	106	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	Y	129	GLY	N-CA-C	-6.98	105.68	115.32
1	O	345	VAL	N-CA-CB	6.95	119.51	111.31
1	Y	147	HIS	CA-CB-CG	-6.94	106.86	113.80
1	Y	38	ILE	N-CA-C	6.90	118.06	107.99
1	O	100	ALA	CA-C-N	-6.89	114.08	122.90
1	O	100	ALA	C-N-CA	-6.89	114.08	122.90
1	Y	351	LEU	O-C-N	-6.82	112.75	122.03
1	O	73	GLN	CA-C-N	-6.77	114.79	123.19
1	O	73	GLN	C-N-CA	-6.77	114.79	123.19
1	Y	146	ASP	CA-C-N	-6.73	112.06	122.49
1	Y	146	ASP	C-N-CA	-6.73	112.06	122.49
1	Y	146	ASP	N-CA-CB	6.72	122.15	110.39
1	Y	244	GLY	CA-C-N	-6.71	110.52	121.19
1	Y	244	GLY	C-N-CA	-6.71	110.52	121.19
1	O	144	ILE	CB-CA-C	-6.71	103.42	111.81
1	O	122	ASP	N-CA-C	6.66	119.37	111.71
1	Y	214	LEU	C-N-CD	-6.65	97.73	125.00
1	O	245	ASP	O-C-N	-6.64	115.08	122.12
1	O	426	LEU	O-C-N	6.63	131.22	122.33
1	O	475	GLU	N-CA-CB	6.59	119.67	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	24	ASP	N-CA-C	-6.57	105.14	113.02
1	O	292	CYS	N-CA-CB	6.57	120.88	110.57
1	Y	283	GLU	N-CA-C	-6.57	103.52	113.89
1	O	30	VAL	N-CA-C	6.56	118.23	108.46
1	Y	194	ILE	CA-C-N	-6.55	110.36	122.09
1	Y	194	ILE	C-N-CA	-6.55	110.36	122.09
1	Y	334	THR	N-CA-C	-6.55	105.25	113.18
1	Y	10	ASP	CA-CB-CG	6.55	119.15	112.60
1	O	195	HIS	N-CA-C	-6.53	102.88	113.19
1	Y	363	ALA	N-CA-C	6.48	119.83	108.75
1	Y	47	HIS	CA-C-O	-6.47	113.87	121.44
1	Y	247	GLN	CB-CA-C	6.46	121.15	110.81
1	Y	195	HIS	N-CA-C	-6.44	105.55	113.41
1	Y	48	ASP	N-CA-CB	6.41	119.73	110.11
1	Y	93	THR	N-CA-C	6.41	119.08	111.71
1	Y	30	VAL	N-CA-C	6.33	117.14	107.77
1	Y	63	VAL	N-CA-CB	6.32	121.65	111.23
1	Y	365	PHE	N-CA-C	6.29	118.74	109.24
1	O	349	THR	CA-C-N	-6.29	112.32	121.44
1	O	349	THR	C-N-CA	-6.29	112.32	121.44
1	O	326	ALA	N-CA-C	-6.27	104.36	111.07
1	Y	117	ARG	CD-NE-CZ	6.26	133.16	124.40
1	Y	340	ASN	CA-CB-CG	6.26	118.86	112.60
1	Y	406	LEU	CA-C-N	-6.25	114.45	122.77
1	Y	406	LEU	C-N-CA	-6.25	114.45	122.77
1	Y	456	ASN	CA-CB-CG	6.24	118.84	112.60
1	Y	228	ASN	N-CA-CB	6.22	119.58	110.25
1	O	355	TYR	N-CA-C	6.20	117.72	110.97
1	Y	304	GLY	O-C-N	-6.19	119.45	123.35
1	Y	200	ASP	CB-CA-C	6.13	119.58	110.14
1	Y	376	ILE	N-CA-CB	6.11	117.70	110.55
1	O	354	PRO	N-CA-CB	6.09	109.64	103.25
1	Y	417	PHE	O-C-N	6.08	128.34	122.07
1	Y	87	ILE	CB-CA-C	-6.07	100.22	110.71
1	Y	193	ASN	CA-C-N	-6.07	113.05	122.09
1	Y	193	ASN	C-N-CA	-6.07	113.05	122.09
1	Y	431	GLU	N-CA-C	6.04	118.37	108.52
1	O	23	HIS	CA-CB-CG	-6.04	107.76	113.80
1	Y	67	ALA	CA-C-O	6.04	125.85	119.03
1	O	318	ASP	N-CA-CB	6.02	119.37	110.33
1	O	307	PHE	N-CA-C	6.02	117.51	111.07
1	Y	149	GLU	N-CA-C	6.01	123.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	307	PHE	N-CA-C	5.99	117.50	110.97
1	Y	7	VAL	N-CA-C	5.99	116.55	108.17
1	Y	85	THR	CB-CA-C	5.99	118.03	109.71
1	Y	327	TYR	CA-CB-CG	-5.98	103.14	113.90
1	O	158	GLY	CA-C-N	5.95	128.26	120.28
1	O	158	GLY	C-N-CA	5.95	128.26	120.28
1	O	311	ALA	N-CA-C	5.95	118.55	111.71
1	Y	222	GLU	CA-C-N	-5.94	115.15	122.93
1	Y	222	GLU	C-N-CA	-5.94	115.15	122.93
1	O	431	GLU	N-CA-C	5.94	118.50	107.99
1	Y	246	GLN	CB-CA-C	-5.91	101.36	110.81
1	Y	386	TYR	O-C-N	5.91	128.17	122.03
1	O	22	ASP	CA-CB-CG	5.90	118.50	112.60
1	Y	338	ASN	N-CA-C	5.84	117.13	108.60
1	Y	212	GLU	N-CA-C	5.84	117.31	111.07
1	O	58	TRP	O-C-N	5.83	129.25	122.20
1	O	126	SER	N-CA-C	5.79	117.68	111.36
1	Y	247	GLN	O-C-N	5.79	128.12	122.09
1	O	86	THR	N-CA-C	5.79	118.91	109.59
1	Y	326	ALA	N-CA-C	-5.78	104.33	111.33
1	O	288	THR	CA-C-N	-5.77	112.40	121.87
1	O	288	THR	C-N-CA	-5.77	112.40	121.87
1	O	36	GLU	N-CA-C	5.75	118.56	110.23
1	O	83	ARG	CA-C-N	-5.75	112.48	122.36
1	O	83	ARG	C-N-CA	-5.75	112.48	122.36
1	O	20	VAL	N-CA-CB	5.72	119.30	111.41
1	Y	155	ALA	O-C-N	5.69	128.01	122.09
1	O	350	GLY	O-C-N	5.68	128.17	122.77
1	Y	290	ILE	N-CA-CB	-5.68	102.72	110.56
1	Y	13	THR	OG1-CB-CG2	5.67	120.63	109.30
1	O	7	VAL	N-CA-C	5.65	116.26	108.12
1	O	477	THR	O-C-N	5.65	127.90	122.03
1	O	189	THR	N-CA-C	5.64	117.43	111.28
1	Y	326	ALA	CA-C-O	5.64	126.72	120.63
1	Y	272	LEU	N-CA-CB	5.63	119.86	110.85
1	Y	169	LEU	O-C-N	5.62	128.10	122.03
1	O	48	ASP	N-CA-CB	5.60	118.51	110.11
1	Y	249	ALA	CA-C-N	-5.60	111.22	121.52
1	Y	249	ALA	C-N-CA	-5.60	111.22	121.52
1	O	164	THR	N-CA-C	-5.59	101.02	109.85
1	Y	13	THR	CA-CB-CG2	-5.59	101.00	110.50
1	Y	195	HIS	CB-CG-CD2	5.58	138.45	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	39	TYR	CB-CA-C	5.57	116.45	110.65
1	Y	354	PRO	CA-C-N	5.57	128.01	120.65
1	Y	354	PRO	C-N-CA	5.57	128.01	120.65
1	Y	335	LYS	N-CA-C	-5.57	105.36	111.82
1	Y	334	THR	CA-CB-CG2	-5.56	101.04	110.50
1	O	453	PHE	CA-C-O	5.55	125.25	119.14
1	Y	227	THR	N-CA-CB	5.55	119.26	110.55
1	Y	195	HIS	CA-C-N	5.54	132.15	121.18
1	Y	195	HIS	C-N-CA	5.54	132.15	121.18
1	O	180	VAL	N-CA-CB	-5.54	105.46	112.60
1	Y	117	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	O	348	PHE	CA-C-N	5.53	132.59	123.25
1	O	348	PHE	C-N-CA	5.53	132.59	123.25
1	Y	23	HIS	CA-CB-CG	-5.52	108.28	113.80
1	Y	45	VAL	N-CA-C	5.51	116.00	107.78
1	Y	355	TYR	N-CA-C	5.51	116.98	110.97
1	Y	460	LEU	N-CA-C	-5.51	105.38	111.71
1	O	328	ASP	N-CA-C	5.51	118.80	111.75
1	O	185	ASN	CA-CB-CG	5.50	118.10	112.60
1	O	374	ASN	N-CA-CB	5.50	118.05	110.07
1	O	84	GLU	N-CA-CB	5.49	117.89	110.59
1	Y	155	ALA	CA-C-N	5.48	127.62	120.28
1	Y	155	ALA	C-N-CA	5.48	127.62	120.28
1	Y	458	ASP	N-CA-CB	5.46	118.68	110.65
1	Y	318	ASP	CB-CA-C	-5.45	99.81	110.11
1	O	81	ASN	N-CA-C	5.45	115.74	108.38
1	Y	82	GLN	N-CA-C	-5.45	101.99	110.10
1	Y	158	GLY	CA-C-N	5.44	128.12	120.28
1	Y	158	GLY	C-N-CA	5.44	128.12	120.28
1	O	417	PHE	O-C-N	5.42	127.88	122.08
1	Y	48	ASP	O-C-N	5.42	126.32	120.85
1	Y	374	ASN	CA-CB-CG	-5.40	107.20	112.60
1	Y	390	ASP	N-CA-CB	5.40	119.62	110.49
1	Y	96	PRO	N-CA-CB	5.39	108.11	103.31
1	Y	81	ASN	O-C-N	5.38	129.29	123.10
1	Y	56	GLN	CA-C-N	5.38	127.43	120.44
1	Y	56	GLN	C-N-CA	5.38	127.43	120.44
1	Y	255	CYS	N-CA-C	-5.38	98.98	108.23
1	O	67	ALA	CA-C-N	5.38	130.20	122.35
1	O	67	ALA	C-N-CA	5.38	130.20	122.35
1	O	227	THR	CA-C-N	-5.38	114.02	122.08
1	O	227	THR	C-N-CA	-5.38	114.02	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	197	LEU	CB-CA-C	-5.37	103.89	111.95
1	Y	55	THR	N-CA-CB	5.37	119.84	110.18
1	Y	105	CYS	N-CA-CB	5.36	117.79	109.48
1	O	107	ARG	CA-C-N	5.35	131.75	121.54
1	O	107	ARG	C-N-CA	5.35	131.75	121.54
1	Y	412	ALA	N-CA-C	5.34	119.28	112.87
1	Y	459	GLU	CG-CD-OE2	5.34	130.68	118.40
1	O	80	THR	N-CA-CB	5.34	121.46	111.53
1	O	252	GLY	CA-C-O	5.34	125.95	119.65
1	O	211	ARG	CA-C-N	5.33	127.69	120.38
1	O	211	ARG	C-N-CA	5.33	127.69	120.38
1	O	353	ALA	N-CA-CB	5.33	119.85	110.37
1	Y	183	TYR	N-CA-C	5.33	116.89	111.14
1	Y	81	ASN	N-CA-CB	-5.32	103.15	111.56
1	O	244	GLY	CA-C-N	-5.32	113.09	120.38
1	O	244	GLY	C-N-CA	-5.32	113.09	120.38
1	Y	314	GLN	O-C-N	5.30	127.61	122.09
1	O	471	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	Y	162	PHE	N-CA-C	5.30	118.04	109.40
1	Y	124	ILE	N-CA-CB	5.29	116.39	110.62
1	Y	296	GLY	N-CA-C	-5.29	106.40	115.08
1	O	13	THR	CA-CB-CG2	-5.29	101.51	110.50
1	O	194	ILE	CB-CA-C	-5.29	106.11	112.19
1	Y	79	ILE	N-CA-C	5.28	115.65	107.78
1	Y	51	GLU	CA-C-N	-5.28	112.47	121.97
1	Y	51	GLU	C-N-CA	-5.28	112.47	121.97
1	Y	353	ALA	CA-C-O	-5.28	114.73	120.69
1	Y	117	ARG	CB-CA-C	-5.27	100.39	110.57
1	Y	305	ALA	N-CA-CB	5.27	118.84	110.57
1	O	240	SER	CA-C-N	-5.25	117.57	121.61
1	O	240	SER	C-N-CA	-5.25	117.57	121.61
1	O	38	ILE	N-CA-C	5.25	115.14	107.37
1	O	494	MET	N-CA-CB	5.25	117.75	110.04
1	Y	454	TRP	CA-C-N	-5.24	114.97	122.67
1	Y	454	TRP	C-N-CA	-5.24	114.97	122.67
1	O	466	ILE	N-CA-CB	5.24	117.15	110.13
1	O	30	VAL	CA-C-N	-5.24	114.37	122.59
1	O	30	VAL	C-N-CA	-5.24	114.37	122.59
1	O	131	VAL	N-CA-CB	-5.23	102.60	111.23
1	Y	375	HIS	ND1-CG-CD2	5.22	111.32	106.10
1	O	334	THR	CA-C-N	-5.21	112.78	120.28
1	O	334	THR	C-N-CA	-5.21	112.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	229	ILE	N-CA-C	-5.21	104.58	111.09
1	O	491	LYS	N-CA-CB	5.20	118.25	109.78
1	Y	48	ASP	CB-CA-C	-5.20	105.76	110.44
1	O	323	ILE	CA-CB-CG1	-5.19	101.58	110.40
1	Y	65	ALA	CA-C-N	-5.18	114.36	122.65
1	Y	65	ALA	C-N-CA	-5.18	114.36	122.65
1	Y	84	GLU	N-CA-CB	5.17	117.78	110.90
1	Y	283	GLU	CB-CG-CD	5.17	121.40	112.60
1	O	45	VAL	N-CA-C	5.17	115.57	108.12
1	Y	433	PRO	CA-C-N	5.16	127.65	120.63
1	Y	433	PRO	C-N-CA	5.16	127.65	120.63
1	O	499	HIS	N-CA-CB	5.16	119.27	110.50
1	Y	458	ASP	CA-C-O	5.15	124.71	119.05
1	O	334	THR	N-CA-C	-5.15	106.95	113.18
1	O	88	VAL	CA-C-N	-5.14	113.88	122.21
1	O	88	VAL	C-N-CA	-5.14	113.88	122.21
1	Y	120	LEU	CA-C-N	-5.14	113.60	120.54
1	Y	120	LEU	C-N-CA	-5.14	113.60	120.54
1	O	283	GLU	N-CA-C	-5.14	107.04	113.72
1	Y	228	ASN	CA-CB-CG	-5.13	107.47	112.60
1	O	250	LEU	CA-C-O	5.12	125.98	120.55
1	O	116	LYS	O-C-N	5.12	127.42	122.09
1	O	195	HIS	CA-C-O	5.12	124.35	119.08
1	Y	260	MET	CA-C-N	-5.12	114.56	122.59
1	Y	260	MET	C-N-CA	-5.12	114.56	122.59
1	Y	302	LEU	CA-C-N	-5.12	114.86	122.74
1	Y	302	LEU	C-N-CA	-5.12	114.86	122.74
1	O	228	ASN	N-CA-CB	5.12	116.89	110.45
1	Y	20	VAL	N-CA-C	5.11	115.94	108.53
1	O	307	PHE	N-CA-CB	5.10	117.41	110.01
1	Y	5	TYR	CB-CA-C	-5.10	100.41	111.11
1	Y	82	GLN	CB-CA-C	5.10	117.85	109.90
1	Y	64	LEU	CA-C-O	5.09	127.79	120.51
1	Y	193	ASN	N-CA-CB	5.09	117.45	109.97
1	Y	269	CYS	CA-C-N	-5.09	115.82	123.00
1	Y	269	CYS	C-N-CA	-5.09	115.82	123.00
1	Y	107	ARG	N-CA-CB	5.09	117.69	110.06
1	Y	216	GLU	CA-C-N	-5.09	115.81	122.37
1	Y	216	GLU	C-N-CA	-5.09	115.81	122.37
1	O	481	TYR	CA-CB-CG	-5.09	104.75	113.90
1	O	239	ILE	CB-CA-C	5.07	116.72	111.09
1	O	193	ASN	N-CA-CB	5.07	117.40	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	69	ILE	CA-C-N	-5.06	114.86	122.81
1	Y	69	ILE	C-N-CA	-5.06	114.86	122.81
1	Y	265	TYR	CA-C-O	-5.05	115.09	120.40
1	O	363	ALA	N-CA-C	5.04	116.90	108.99
1	Y	125	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	Y	407	ARG	CA-C-O	5.04	125.75	120.36
1	Y	136	PHE	O-C-N	5.03	128.95	123.01
1	Y	394	ALA	N-CA-CB	5.03	117.44	109.94
1	Y	392	LEU	CA-C-N	-5.02	113.92	120.44
1	Y	392	LEU	C-N-CA	-5.02	113.92	120.44
1	O	39	TYR	O-C-N	5.01	126.14	120.68
1	O	375	HIS	ND1-CE1-NE2	5.00	113.41	108.40

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	592	0
1	Y	3910	0	3841	511	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	1	0
4	Y	6	0	8	3	0
All	All	7895	0	7722	1096	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 70.

All (1096) 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:HE2	1:O:463:LYS:HA	1.44	0.96
1:Y:460:LEU:HD12	1:Y:460:LEU:H	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:HG2	1:O:492:ARG:HH11	1.30	0.94
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:Y:91:LYS:O	1:Y:92:GLU:C	2.10	0.92
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:Y:173:MET:HE2	1:Y:173:MET:HA	1.50	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:47:HIS:CB	1:O:52:ILE:HD11	2.03	0.88
1:Y:9:LEU:HD21	1:Y:60:LEU:HD13	1.56	0.87
1:O:91:LYS:O	1:O:92:GLU:C	2.18	0.86
1:Y:70:SER:N	1:Y:73:GLN:HE21	1.73	0.86
1:O:9:LEU:HB2	1:O:79:ILE:HD13	1.58	0.86
1:O:441:LEU:HD22	1:O:445:TYR:CE1	2.09	0.86
1:O:403:LEU:HD12	1:O:403:LEU:H	1.41	0.86
1:O:123:TYR:CD2	1:O:203:MET:HE2	2.11	0.85
1:Y:19:VAL:HG22	1:Y:30:VAL:HG22	1.56	0.85
1:O:123:TYR:HD2	1:O:203:MET:HE2	1.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:41:LYS:HG3	1:O:42:PRO:HD2	1.59	0.84
1:Y:271:MET:SD	1:Y:395:MET:HE2	2.18	0.83
1:O:80:THR:HG21	1:O:245:ASP:HA	1.59	0.83
1:Y:124:ILE:HD13	1:Y:203:MET:HE1	1.59	0.83
1:O:48:ASP:C	1:O:52:ILE:HD12	2.04	0.82
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:O:70:SER:N	1:O:73:GLN:HE21	1.77	0.82
1:Y:124:ILE:HD13	1:Y:203:MET:CE	2.09	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:62:GLU:O	1:O:63:VAL:C	2.23	0.81
1:Y:227:THR:HB	1:Y:229:ILE:CG2	2.11	0.80
1:O:18:ALA:CB	1:O:59:THR:HG22	2.11	0.80
1:O:180:VAL:HG21	1:O:218:ARG:HG3	1.64	0.80
1:O:137:SER:O	1:O:138:GLY:C	2.21	0.80
1:Y:193:ASN:HB3	1:Y:196:THR:CG2	2.11	0.79
1:Y:463:LYS:HA	1:Y:463:LYS:HE2	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
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:Y:458:ASP:HA	1:Y:461:GLN:CG	2.11	0.78
1:O:373:ALA:O	1:O:377:ILE:HG13	1.84	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: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:Y:5:TYR:HB2	1:Y:74:ILE:CG2	2.12	0.77
1:O:415:ASN:HD21	1:O:417:PHE:HB3	1.49	0.77
1:O:183:TYR:CE1	1:O:217:VAL:HG12	2.19	0.77
1:Y:61:VAL:O	1:Y:62:GLU:C	2.26	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:466:ILE:HG12	1:O:467:GLU:N	1.96	0.77
1:Y:250:LEU:CD1	1:Y:255:CYS:HB2	2.15	0.76
1:O:5:TYR:CB	1:O:74:ILE:HG22	2.13	0.76
1:Y:362:GLY:HA3	1:O:367:LEU:HB2	1.67	0.76
1:Y:129:GLY:C	1:Y:130:LEU:HD23	2.11	0.76
1:Y:19:VAL:HG12	1:Y:21:MET:HE2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:Y:403:LEU:H	1:Y:403:LEU:HD12	1.52	0.75
1:Y:458:ASP:C	1:Y:461:GLN:HB2	2.11	0.75
1:O:86:THR:OG1	1:O:137:SER:HB3	1.86	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:Y:270:PHE:CZ	4:Y:600:GOL:H31	2.21	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:33:ARG:NH2	1:Y:58:TRP:HB3	2.01	0.74
1:O:254:LEU:HD11	1:O:445:TYR:HE2	1.51	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
1:O:181:THR:HG23	1:O:182:ASP:O	1.89	0.73
1:Y:3:LYS:HA	1:Y:73:GLN:HA	1.71	0.73
1:Y:229:ILE:HG13	1:Y:230:GLY:N	2.04	0.73
1:O:221:SER:OG	1:O:450:ALA:HB2	1.89	0.73
1:O:410:GLY:O	1:O:413:VAL:HG13	1.89	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:O:170:ILE:O	1:O:171:TRP:C	2.33	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:61:VAL:O	1:O:62:GLU:C	2.29	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:398:ASP:O	1:O:399:SER:C	2.29	0.71
1:O:39:TYR:HA	1:O:44:TRP:O	1.90	0.71
1:Y:140:LYS:O	1:Y:144:ILE:HD12	1.91	0.71
1:O:55:THR:HA	1:O:58:TRP:CD1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:396:GLN:HA	1:Y:399:SER:OG	1.91	0.71
1:O:80:THR:CG2	1:O:245:ASP:HA	2.21	0.71
1:O:391:VAL:O	1:O:392:LEU:C	2.29	0.71
1:Y:62:GLU:O	1:Y:63:VAL:C	2.30	0.71
1:Y:41:LYS:CG	1:Y:42:PRO:HD2	2.20	0.71
1:Y:257:LYS:O	1:Y:260:MET:HG3	1.91	0.70
1:O:179:HIS:CD2	1:O:215:PRO:HB3	2.26	0.70
1:Y:33:ARG:HH12	1:Y:62:GLU:HG3	1.55	0.70
1:Y:180:VAL:CG2	1:Y:218:ARG:HG3	2.21	0.70
1:O:254:LEU:HD11	1:O:445:TYR:CE2	2.24	0.70
1:Y:80:THR:HG21	1:Y:245:ASP:HA	1.73	0.70
1:O:396:GLN:HE21	1:O:403:LEU:HD12	1.56	0.70
1:O:226:GLN:CB	1:O:236:ARG:HD3	2.22	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:273:MET:HB2	1:Y:395:MET:HE3	1.74	0.69
1:O:120:LEU:O	1:O:121:GLU:C	2.28	0.69
1:Y:47:HIS:HB3	1:Y:52:ILE:HD11	1.74	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:357:ASP:OD2	1:O:494:MET:HE3	1.93	0.69
1:O:197:LEU:N	1:O:197:LEU:HD22	2.07	0.69
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:Y:293:GLY:HA2	1:Y:299:ASN:ND2	2.08	0.69
1:O:441:LEU:HD22	1:O:445:TYR:CZ	2.27	0.69
1:Y:196:THR:O	1:Y:197:LEU:C	2.34	0.68
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:Y:429:ARG:NH1	1:Y:469:GLU:OE2	2.26	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:O:102:VAL:HG12	1:O:103:TRP:CD1	2.29	0.68
1:Y:222:GLU:O	1:Y:240:SER:HA	1.94	0.68
1:O:236:ARG:HG3	1:O:236:ARG:HH11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:ASP:O	1:O:52:ILE:HD12	1.94	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:377:ILE:O	1:O:380:THR:HB	1.93	0.67
1:Y:467:GLU:OE2	1:Y:468:ARG:HB2	1.95	0.67
1:O:17:ARG:HH22	1:O:437:GLU:CG	2.07	0.67
1:Y:18:ALA:HB1	1:Y:63:VAL:HG21	1.77	0.67
1:O:457:LEU:O	1:O:459:GLU:N	2.28	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:413:VAL:HA	1:O:419:MET:HE3	1.75	0.67
1:O:5:TYR:HB3	1:O:21:MET:O	1.95	0.67
1:Y:27:ILE:HD12	1:Y:27:ILE:N	2.10	0.67
1:Y:130:LEU:HD23	1:Y:130:LEU:N	2.09	0.67
1:O:207:LEU:HB3	1:O:209:ILE:CD1	2.24	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:Y:114:HIS:O	1:Y:115:LEU:C	2.37	0.66
1:O:84:GLU:N	1:O:84:GLU:OE1	2.28	0.66
1:O:90:GLU:N	1:O:95:LYS:O	2.28	0.66
1:O:5:TYR:O	1:O:75:ALA:N	2.28	0.66
1:Y:91:LYS:HB2	1:Y:161:LEU:HD12	1.76	0.66
1:O:180:VAL:CG2	1:O:218:ARG:HG3	2.24	0.66
1:Y:456:ASN:N	1:Y:459:GLU:OE2	2.29	0.66
1:O:18:ALA:HB3	1:O:59:THR:HG22	1.76	0.66
1:O:127:ASN:HD22	1:O:193:ASN:HD21	1.43	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:358:PRO:HG2	1:O:359:TYR:CE2	2.31	0.66
1:Y:253:GLN:CG	1:Y:407:ARG:HD2	2.25	0.66
1:Y:463:LYS:HA	1:Y:463:LYS:CE	2.26	0.66
1:O:173:MET:HB3	1:O:227:THR:HG23	1.78	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:Y:154:ARG:CB	1:Y:159:GLU:HB3	2.25	0.66
1:Y:169:LEU:O	1:Y:173:MET:HG2	1.96	0.65
1:Y:173:MET:HE2	1:Y:173:MET:CA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:189:THR:HB	1:Y:191:LEU:CD1	2.26	0.65
1:O:162:PHE:HB3	1:O:213:MET:HG3	1.78	0.65
1:Y:155:ALA:HA	1:Y:160:LEU:HB2	1.78	0.65
1:Y:64:LEU:O	1:Y:66:LYS:N	2.29	0.65
1:O:33:ARG:CZ	1:O:58:TRP:HB3	2.25	0.65
1:O:124:ILE:HD13	1:O:203:MET:CE	2.26	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:Y:123:TYR:CD1	1:Y:203:MET:HE2	2.31	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:Y:177:ARG:NH1	1:Y:226:GLN:O	2.30	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:O:53:TRP:O	1:O:54:ALA:C	2.39	0.65
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.78	0.65
1:O:492:ARG:HG2	1:O:492:ARG:NH1	2.05	0.65
1:O:41:LYS:CB	1:O:42:PRO:HD2	2.27	0.64
1:O:184:THR:HG22	1:O:290:ILE:O	1.97	0.64
1:O:47:HIS:CD2	1:O:82:GLN:HE22	2.15	0.64
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.78	0.64
1:O:125:ARG:NH1	1:O:282:SER:O	2.30	0.64
1:O:274:ASN:OD1	1:O:276:GLY:N	2.30	0.64
1:Y:70:SER:O	1:Y:73:GLN:HG3	1.97	0.64
1:Y:180:VAL:HG23	1:Y:216:GLU:O	1.97	0.64
1:Y:69:ILE:HD12	1:Y:69:ILE:N	2.11	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:O:26:ASN:O	1:O:28:ILE:HD13	1.97	0.64
1:O:498:GLU:OE1	1:O:498:GLU:HA	1.96	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:420:GLN:HE21	1:O:424:ASP:CG	2.05	0.64
1:O:88:VAL:HA	1:O:161:LEU:O	1.98	0.64
1:O:179:HIS:CE1	1:O:215:PRO:HB3	2.33	0.64
1:Y:433:PRO:HA	1:Y:466:ILE:HA	1.80	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:27:ILE:N	1:O:27:ILE:HD12	2.12	0.64
1:O:72:ASP:OD1	1:O:73:GLN:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:22:ASP:OD1	1:O:24:ASP:N	2.32	0.63
1:O:110:GLU:O	1:O:113:GLU:HB2	1.98	0.63
1:O:146:ASP:OD1	1:O:146:ASP:N	2.30	0.63
1:O:62:GLU:O	1:O:66:LYS:HG2	1.98	0.63
1:Y:5:TYR:C	1:Y:74:ILE:HG22	2.23	0.63
1:Y:127:ASN:HB3	1:Y:193:ASN:ND2	2.14	0.63
1:Y:166:ASP:O	1:Y:167:THR:C	2.41	0.63
1:Y:117:ARG:HB2	1:Y:117:ARG:CZ	2.29	0.63
1:O:5:TYR:HB2	1:O:74:ILE:CG2	2.21	0.63
1:Y:498:GLU:OE1	1:Y:498:GLU:HA	1.97	0.63
1:Y:181:THR:HG23	1:Y:182:ASP:N	2.12	0.63
1:Y:271:MET:C	1:Y:272:LEU:HD13	2.24	0.63
1:O:166:ASP:O	1:O:169:LEU:N	2.30	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:95:LYS:HG3	1:O:96:PRO:CD	2.29	0.63
1:Y:172:LYS:O	1:Y:173:MET:C	2.40	0.62
1:Y:211:ARG:HG3	1:Y:211:ARG:HH11	1.64	0.62
1:O:70:SER:O	1:O:73:GLN:HG3	1.99	0.62
1:O:254:LEU:CD1	1:O:445:TYR:HE2	2.12	0.62
1:Y:262:LYS:HD2	1:Y:262:LYS:C	2.24	0.62
1:O:394:ALA:O	1:O:395:MET:C	2.38	0.62
1:Y:178:VAL:HG12	1:Y:180:VAL:HG12	1.82	0.62
1:O:227:THR:N	1:O:237:ILE:O	2.29	0.62
1:Y:72:ASP:OD1	1:Y:73:GLN:HG2	1.98	0.62
1:O:47:HIS:O	1:O:49:PRO:HD3	1.99	0.62
1:Y:4:LYS:N	1:Y:73:GLN:O	2.33	0.62
1:Y:153:GLU:O	1:Y:154:ARG:C	2.37	0.62
1:Y:340:ASN:HB2	1:Y:375:HIS:CD2	2.34	0.62
1:Y:458:ASP:CA	1:Y:461:GLN:HB2	2.29	0.62
1:O:60:LEU:O	1:O:63:VAL:HG23	2.00	0.62
1:O:137:SER:HA	1:O:140:LYS:CD	2.24	0.62
1:Y:32:GLN:HA	1:Y:59:THR:HG21	1.82	0.62
1:O:164:THR:O	1:O:165:VAL:C	2.43	0.62
1:Y:24:ASP:HB2	1:Y:26:ASN:ND2	2.13	0.62
1:Y:250:LEU:O	1:Y:250:LEU:HD12	1.99	0.61
1:O:195:HIS:ND1	1:O:195:HIS:N	2.46	0.61
1:O:55:THR:HA	1:O:58:TRP:HD1	1.62	0.61
1:O:199:TRP:CG	1:O:214:LEU:HD23	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:GLY:C	1:O:79:ILE:HG12	2.25	0.61
1:Y:78:GLY:O	1:Y:79:ILE:HD13	2.00	0.61
1:O:88:VAL:HG12	1:O:97:ILE:HG12	1.83	0.61
1:O:17:ARG:HG2	1:O:32:GLN:HG3	1.82	0.61
1:Y:394:ALA:O	1:Y:395:MET:C	2.44	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:262:LYS:HD2	1:O:262:LYS:C	2.25	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:244:GLY:O	1:O:245:ASP:C	2.40	0.60
1:O:142:LYS:O	1:O:143:TRP:C	2.42	0.60
1:Y:61:VAL:HG12	1:Y:62:GLU:N	2.16	0.60
1:O:88:VAL:HG12	1:O:97:ILE:CG1	2.32	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:Y:240:SER:HB2	1:Y:450:ALA:HB3	1.82	0.60
1:O:352:GLY:HA2	1:O:356:TRP:CE3	2.36	0.60
1:Y:58:TRP:O	1:Y:59:THR:C	2.41	0.60
1:O:166:ASP:O	1:O:167:THR:C	2.44	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:422:GLN:O	1:Y:426:LEU:HD22	2.00	0.60
1:O:15:SER:HB2	1:O:33:ARG:O	2.02	0.60
1:O:149:GLU:O	1:O:150:GLY:C	2.45	0.60
1:Y:195:HIS:N	1:Y:195:HIS:ND1	2.47	0.59
1:Y:422:GLN:NE2	1:Y:426:LEU:HD22	2.17	0.59
1:O:447:ALA:O	1:O:450:ALA:HB3	2.01	0.59
1:Y:173:MET:HB3	1:Y:227:THR:HG23	1.84	0.59
1:O:90:GLU:HB2	1:O:93:THR:HG1	1.67	0.59
1:O:246:GLN:OE1	1:O:270:PHE:HB2	2.01	0.59
1:Y:24:ASP:HB2	1:Y:26:ASN:HD21	1.67	0.59
1:Y:87:ILE:HG22	1:Y:88:VAL:N	2.18	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:O:44:TRP:HA	1:O:105:CYS:SG	2.42	0.59
1:Y:120:LEU:O	1:Y:124:ILE:HG12	2.02	0.59
1:O:89:TRP:HB2	1:O:95:LYS:C	2.27	0.59
1:O:144:ILE:HG22	1:O:148:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:153:GLU:O	1:O:156:ARG:HB3	2.02	0.59
1:O:272:LEU:HD11	1:O:303:GLU:CD	2.28	0.59
1:Y:262:LYS:HD2	1:Y:262:LYS:O	2.02	0.59
1:Y:468:ARG:HH11	1:Y:468:ARG:CG	2.16	0.59
1:O:74:ILE:CD1	1:O:237:ILE:HG21	2.33	0.59
1:O:201:ASP:HA	1:O:204:LEU:HB2	1.85	0.59
1:O:88:VAL:HG22	1:O:162:PHE:HB2	1.83	0.58
1:Y:51:GLU:O	1:Y:52:ILE:C	2.41	0.58
1:Y:313:ILE:HD13	1:Y:313:ILE:N	2.17	0.58
1:Y:170:ILE:HG22	1:Y:171:TRP:N	2.18	0.58
1:Y:393:GLU:O	1:Y:394:ALA:C	2.45	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:130:LEU:HD13	1:Y:136:PHE:CD1	2.38	0.58
1:O:227:THR:HB	1:O:229:ILE:HG23	1.85	0.58
1:Y:272:LEU:HD11	1:Y:303:GLU:CG	2.34	0.58
1:O:38:ILE:O	1:O:45:VAL:HA	2.04	0.58
1:Y:156:ARG:HH11	1:Y:156:ARG:HG2	1.69	0.58
1:Y:253:GLN:HG3	1:Y:407:ARG:HD2	1.85	0.58
1:O:67:ALA:HB3	1:O:69:ILE:CD1	2.33	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:Y:165:VAL:O	1:Y:166:ASP:C	2.45	0.57
1:Y:173:MET:HB2	1:Y:174:THR:HG23	1.85	0.57
1:Y:62:GLU:O	1:Y:66:LYS:HG2	2.04	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:89:TRP:HD1	1:Y:90:GLU:O	1.87	0.57
1:Y:154:ARG:HB2	1:Y:159:GLU:HB3	1.85	0.57
1:O:313:ILE:HD11	1:O:381:LEU:CD2	2.34	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:Y:22:ASP:CG	1:Y:26:ASN:HD22	2.12	0.57
1:O:48:ASP:O	1:O:51:GLU:N	2.38	0.57
1:Y:445:TYR:O	1:Y:446:LEU:C	2.45	0.57
1:O:409:ASP:C	1:O:413:VAL:HG11	2.30	0.57
1:O:44:TRP:CZ2	1:O:107:ARG:HB2	2.39	0.57
1:Y:43:GLY:C	1:Y:44:TRP:HD1	2.13	0.57
1:Y:181:THR:HG23	1:Y:182:ASP:O	2.05	0.57
1:O:123:TYR:HD2	1:O:203:MET:CE	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:ALA:O	1:Y:112:CYS:HB2	2.04	0.57
1:Y:250:LEU:HD11	1:Y:255:CYS:CB	2.28	0.57
1:Y:83:ARG:HH21	4:Y:600:GOL:H2	1.70	0.56
1:Y:497:GLU:HA	1:Y:497:GLU:OE1	2.04	0.56
1:Y:3:LYS:NZ	1:Y:3:LYS:HB2	2.19	0.56
1:O:9:LEU:HG	1:O:56:GLN:NE2	2.20	0.56
1:Y:80:THR:HG21	1:Y:248:ALA:CB	2.34	0.56
1:Y:244:GLY:O	1:Y:245:ASP:C	2.46	0.56
1:Y:269:CYS:HB2	1:Y:306:VAL:HB	1.85	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:111:ILE:HG22	1:Y:115:LEU:CD1	2.36	0.56
1:Y:468:ARG:HD2	1:Y:468:ARG:C	2.31	0.56
1:O:179:HIS:CG	1:O:215:PRO:HB3	2.39	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:459:GLU:HB2	1:Y:460:LEU:HD12	1.87	0.56
1:O:19:VAL:HG12	1:O:21:MET:HE2	1.88	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:273:MET:HB2	1:O:395:MET:HE3	1.87	0.56
1:O:420:GLN:NE2	1:O:424:ASP:OD1	2.37	0.56
1:O:3:LYS:HA	1:O:73:GLN:CA	2.34	0.56
1:O:178:VAL:HG12	1:O:180:VAL:HG12	1.88	0.56
1:O:484:ALA:O	1:O:485:GLY:C	2.49	0.56
1:Y:432:ARG:HD2	1:Y:436:ARG:NH1	2.19	0.56
1:O:286:LEU:O	1:O:287:LEU:HD23	2.05	0.56
1:Y:103:TRP:H	1:Y:103:TRP:CD1	2.21	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:O:41:LYS:HG3	1:O:42:PRO:CD	2.34	0.56
1:O:297:GLU:O	1:O:298:VAL:C	2.48	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:286:LEU:C	1:O:287:LEU:HD23	2.31	0.56
1:Y:124:ILE:CD1	1:Y:203:MET:HE1	2.34	0.56
1:Y:245:ASP:O	1:Y:248:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:104:GLN:NE2	1:Y:308:MET:HE1	2.21	0.55
1:Y:202:LYS:O	1:Y:206:VAL:HB	2.04	0.55
1:O:124:ILE:HD13	1:O:203:MET:HE3	1.89	0.55
1:O:236:ARG:HH11	1:O:236:ARG:CG	2.18	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:130:LEU:HD13	1:O:136:PHE:CD1	2.42	0.55
1:Y:154:ARG:O	1:Y:155:ALA:C	2.49	0.55
1:Y:478:GLU:HA	1:Y:478:GLU:OE1	2.05	0.55
1:O:80:THR:CG2	1:O:248:ALA:HB2	2.36	0.55
1:Y:144:ILE:O	1:Y:145:LEU:C	2.43	0.55
1:Y:180:VAL:HG22	1:Y:181:THR:N	2.22	0.55
1:O:439:THR:HG22	1:O:440:ALA:H	1.71	0.55
1:Y:35:PHE:HB2	1:Y:51:GLU:HG2	1.89	0.55
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.89	0.55
1:Y:184:THR:O	1:Y:187:SER:HB3	2.07	0.55
1:Y:488:LYS:HD3	1:O:496:TRP:CZ3	2.41	0.55
1:O:438:VAL:O	1:O:441:LEU:HB2	2.06	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:74:ILE:HD11	1:O:237:ILE:HG21	1.89	0.54
1:O:445:TYR:CD1	1:O:460:LEU:HD22	2.43	0.54
1:Y:8:ALA:O	1:Y:9:LEU:HD12	2.07	0.54
1:Y:115:LEU:O	1:Y:120:LEU:HD12	2.06	0.54
1:Y:262:LYS:HZ3	1:Y:264:THR:CB	2.19	0.54
1:Y:22:ASP:OD1	1:Y:24:ASP:N	2.40	0.54
1:O:179:HIS:NE2	1:O:215:PRO:HB3	2.22	0.54
1:O:22:ASP:CG	1:O:26:ASN:HD22	2.16	0.54
1:O:94:GLY:HA2	1:O:171:TRP:CH2	2.43	0.54
1:Y:221:SER:OG	1:Y:450:ALA:HB2	2.08	0.54
1:O:389:ARG:HB2	1:O:426:LEU:HD13	1.89	0.54
1:Y:28:ILE:N	1:Y:28:ILE:HD12	2.23	0.54
1:Y:491:LYS:O	1:Y:494:MET:HG3	2.07	0.54
1:O:173:MET:HE2	1:O:173:MET:HA	1.88	0.54
1:O:490:VAL:O	1:O:494:MET:HG2	2.08	0.54
1:Y:425:ILE:O	1:Y:479:ARG:HD3	2.08	0.54
1:O:17:ARG:C	1:O:59:THR:HG21	2.32	0.54
1:Y:492:ARG:HH11	1:Y:492:ARG:CG	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:482:ARG:HH11	1:O:482:ARG:HG3	1.72	0.54
1:Y:74:ILE:HD11	1:Y:237:ILE:HG21	1.90	0.54
1:O:420:GLN:HG3	1:O:420:GLN:O	2.05	0.54
1:O:75:ALA:HB2	1:O:453:PHE:CD2	2.43	0.53
1:O:218:ARG:NE	1:O:222:GLU:OE2	2.33	0.53
1:O:219:ARG:HG2	1:O:222:GLU:HB3	1.89	0.53
1:O:455:GLN:O	1:O:456:ASN:HB2	2.08	0.53
1:Y:84:GLU:N	1:Y:84:GLU:OE1	2.41	0.53
1:O:43:GLY:O	1:O:106:ARG:N	2.40	0.53
1:O:88:VAL:CG2	1:O:162:PHE:HB2	2.37	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:40:PRO:HD2	1:O:44:TRP:HB2	1.91	0.53
1:O:251:PHE:O	1:O:254:LEU:HD12	2.08	0.53
1:O:60:LEU:O	1:O:60:LEU:HD12	2.08	0.53
1:O:253:GLN:HG2	1:O:407:ARG:HD2	1.87	0.53
1:O:332:PHE:O	1:O:335:LYS:HB2	2.08	0.53
1:O:440:ALA:O	1:O:441:LEU:C	2.50	0.53
1:Y:189:THR:HB	1:Y:191:LEU:HD11	1.89	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:328:ASP:HB3	1:Y:332:PHE:HE2	1.72	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: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:40:PRO:HG2	1:O:44:TRP:HB3	1.90	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:165:VAL:O	1:O:166:ASP:C	2.51	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:HA	1:O:478:GLU:OE1	2.09	0.53
1:O:81:ASN:N	1:O:81:ASN:ND2	2.56	0.53
1:O:114:HIS:HA	1:O:117:ARG:NH1	2.24	0.53
1:Y:11:GLN:HE22	1:Y:82:GLN:HE21	1.57	0.52
1:Y:20:VAL:C	1:Y:21:MET:HG3	2.33	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:Y:169:LEU:N	1:Y:169:LEU:HD22	2.25	0.52
1:Y:367:LEU:HB2	1:O:362:GLY:HA3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:432:ARG:HG2	1:Y:436:ARG:NH1	2.24	0.52
1:O:156:ARG:O	1:O:212:GLU:HG2	2.08	0.52
1:O:265:TYR:HE1	1:O:408:VAL:CG1	2.22	0.52
1:O:340:ASN:HB2	1:O:375:HIS:CD2	2.44	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:74:ILE:O	1:O:75:ALA:O	2.27	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:22:ASP:CB	1:O:28:ILE:HD11	2.21	0.52
1:Y:39:TYR:HA	1:Y:44:TRP:O	2.09	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:201:ASP:O	1:Y:202:LYS:C	2.52	0.52
1:Y:403:LEU:HD12	1:Y:403:LEU:N	2.24	0.52
1:O:49:PRO:HD3	1:O:100:ALA:H	1.75	0.52
1:O:57:SER:O	1:O:58:TRP:C	2.50	0.52
1:O:115:LEU:O	1:O:120:LEU:HD12	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:O:221:SER:HB3	1:O:295:THR:O	2.10	0.52
1:O:475:GLU:O	1:O:476:THR:C	2.52	0.52
1:Y:137:SER:O	1:Y:138:GLY:C	2.53	0.52
1:Y:173:MET:HB3	1:Y:227:THR:CG2	2.39	0.52
1:O:40:PRO:HD2	1:O:44:TRP:CB	2.40	0.52
1:O:156:ARG:HB2	1:O:156:ARG:CZ	2.39	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:396:GLN:O	1:Y:397:ALA:C	2.51	0.52
1:Y:445:TYR:O	1:Y:449:LEU:N	2.29	0.52
1:O:163:GLY:HA2	1:O:167:THR:HG21	1.91	0.52
1:Y:20:VAL:HG12	1:Y:21:MET:N	2.25	0.52
1:Y:326:ALA:O	1:Y:327:TYR:C	2.50	0.52
1:Y:16:SER:HB3	1:Y:56:GLN:HA	1.92	0.52
1:Y:32:GLN:N	1:Y:59:THR:HG22	2.24	0.52
1:Y:47:HIS:O	1:Y:49:PRO:HD3	2.10	0.52
1:Y:104:GLN:HG2	1:Y:349:THR:HG21	1.92	0.52
1:Y:255:CYS:HB3	1:Y:260:MET:HB2	1.91	0.52
1:O:186:ALA:O	1:O:187:SER:C	2.53	0.52
1:O:398:ASP:O	1:O:400:GLY:N	2.42	0.51
1:Y:53:TRP:O	1:Y:54:ALA:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:390:ASP:HA	1:Y:483:TYR:OH	2.10	0.51
1:O:156:ARG:HG2	1:O:156:ARG:HH11	1.75	0.51
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:148:VAL:O	1:Y:151:SER:OG	2.29	0.51
1:O:394:ALA:O	1:O:397:ALA:N	2.44	0.51
1:O:445:TYR:O	1:O:446:LEU:C	2.51	0.51
1:O:201:ASP:O	1:O:202:LYS:C	2.54	0.51
1:Y:482:ARG:NH1	1:Y:482:ARG:HG3	2.25	0.51
1:Y:16:SER:HB3	1:Y:56:GLN:OE1	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:O:387:GLN:O	1:O:390:ASP:HB2	2.11	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:84:GLU:HB2	1:O:103:TRP:CB	2.40	0.51
1:Y:70:SER:N	1:Y:73:GLN:NE2	2.48	0.51
1:O:48:ASP:HB3	1:O:51:GLU:HB3	1.91	0.51
1:Y:257:LYS:O	1:Y:258:GLU:C	2.54	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:O:415:ASN:HB3	1:O:418:LEU:HB2	1.93	0.51
1:Y:21:MET:HA	1:Y:26:ASN:O	2.11	0.51
1:Y:328:ASP:HB3	1:Y:332:PHE:CE2	2.46	0.50
1:O:123:TYR:CE2	1:O:203:MET:HE2	2.46	0.50
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:123:TYR:HD1	1:Y:203:MET:HE2	1.72	0.50
1:Y:205:GLU:HG2	1:Y:206:VAL:H	1.76	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:40:PRO:HG3	1:Y:46:GLU:OE2	2.12	0.50
1:Y:87:ILE:HD12	1:Y:163:GLY:O	2.11	0.50
1:Y:486:TRP:O	1:Y:490:VAL:HG23	2.11	0.50
1:O:17:ARG:CA	1:O:59:THR:HG21	2.41	0.50
1:O:54:ALA:O	1:O:55:THR:C	2.53	0.50
1:O:103:TRP:CD1	1:O:103:TRP:H	2.30	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:272:LEU:CD1	1:Y:303:GLU:HB2	2.42	0.50
1:Y:348:PHE:CD1	1:Y:348:PHE:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:9:LEU:HB2	1:O:79:ILE:CD1	2.38	0.50
1:O:85:THR:OG1	1:O:103:TRP:HD1	1.95	0.50
1:O:279:ALA:HB2	1:O:300:TYR:CG	2.45	0.50
1:Y:3:LYS:HB2	1:Y:3:LYS:HZ3	1.77	0.50
1:Y:120:LEU:O	1:Y:121:GLU:C	2.51	0.50
1:Y:432:ARG:HD2	1:Y:436:ARG:CZ	2.41	0.50
1:O:17:ARG:HH22	1:O:437:GLU:HG3	1.77	0.50
1:O:40:PRO:HD2	1:O:44:TRP:O	2.10	0.50
1:O:156:ARG:HH11	1:O:156:ARG:CG	2.25	0.50
1:Y:52:ILE:HG22	1:Y:53:TRP:N	2.25	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:37:GLN:HE22	1:O:47:HIS:CE1	2.30	0.50
1:O:60:LEU:C	1:O:63:VAL:HG23	2.37	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:133:ASP:OD1	1:O:135:TYR:HB2	2.11	0.50
1:O:166:ASP:CG	1:O:167:THR:H	2.18	0.50
1:O:263:ASN:ND2	1:O:265:TYR:CZ	2.79	0.50
1:Y:391:VAL:HG22	1:Y:392:LEU:N	2.26	0.50
1:O:37:GLN:NE2	1:O:47:HIS:CE1	2.80	0.50
1:O:439:THR:O	1:O:442:GLY:N	2.45	0.50
1:Y:205:GLU:O	1:Y:206:VAL:C	2.53	0.49
1:Y:415:ASN:ND2	1:Y:418:LEU:HB2	2.27	0.49
1:Y:415:ASN:HD21	1:Y:417:PHE:HB3	1.77	0.49
1:O:11:GLN:O	1:O:81:ASN:HA	2.12	0.49
1:O:27:ILE:HD12	1:O:27:ILE:H	1.77	0.49
1:O:103:TRP:CD1	1:O:103:TRP:N	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: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:Y:468:ARG:HH11	1:Y:468:ARG:HG3	1.76	0.49
1:O:75:ALA:HB2	1:O:453:PHE:HD2	1.77	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:90:GLU:CD	1:O:93:THR:HG21	2.37	0.49
1:Y:54:ALA:O	1:Y:57:SER:HB2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:415:ASN:ND2	1:Y:418:LEU:N	2.43	0.49
1:O:256:VAL:O	1:O:256:VAL:HG13	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:74:ILE:HD12	1:Y:74:ILE:O	2.12	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
1:O:124:ILE:O	1:O:125:ARG:C	2.50	0.49
1:Y:44:TRP:CD1	1:Y:44:TRP:N	2.80	0.49
1:Y:269:CYS:CB	1:Y:306:VAL:HB	2.42	0.49
1:O:312:SER:O	1:O:315:TRP:HB3	2.12	0.49
1:O:457:LEU:C	1:O:459:GLU:H	2.20	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:HD13	1:Y:466:ILE:O	2.13	0.49
1:O:345:VAL:O	1:O:362:GLY:HA2	2.13	0.49
1:Y:3:LYS:HA	1:Y:73:GLN:CA	2.41	0.49
1:Y:205:GLU:HG2	1:Y:206:VAL:N	2.28	0.49
1:O:403:LEU:HD12	1:O:403:LEU:N	2.20	0.49
1:O:33:ARG:HH12	1:O:62:GLU:CD	2.21	0.49
1:Y:48:ASP:HB3	1:Y:51:GLU:HB3	1.95	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:O:69:ILE:HA	1:O:73:GLN:NE2	2.28	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:Y:87:ILE:HD13	1:Y:168:TRP:HB2	1.95	0.48
1:Y:445:TYR:O	1:Y:449:LEU:HB2	2.14	0.48
1:O:44:TRP:N	1:O:44:TRP:CD1	2.80	0.48
1:O:293:GLY:HA2	1:O:299:ASN:HD22	1.77	0.48
1:O:468:ARG:HD2	1:O:468:ARG:C	2.38	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:Y:77:ILE:N	1:Y:238:PRO:O	2.46	0.48
1:Y:80:THR:HG22	1:Y:245:ASP:HA	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:22:ASP:OD1	1:O:25:ALA:N	2.46	0.48
1:O:24:ASP:HB2	1:O:26:ASN:ND2	2.27	0.48
1:O:347:ALA:HB2	1:O:351:LEU:HD13	1.95	0.48
1:Y:154:ARG:HE	1:Y:154:ARG:HB3	1.44	0.48
1:Y:272:LEU:HD11	1:Y:303:GLU:CD	2.39	0.48
1:O:389:ARG:O	1:O:390:ASP:C	2.57	0.48
1:O:460:LEU:C	1:O:462:GLU:H	2.21	0.48
1:Y:325:ASP:O	1:Y:326:ALA:C	2.57	0.48
1:Y:360:ALA:HB2	1:Y:494:MET:HA	1.95	0.48
1:O:221:SER:HB2	1:O:296:GLY:HA3	1.95	0.48
1:O:278:LYS:HD2	1:O:280:VAL:CG2	2.43	0.48
1:Y:23:HIS:HE1	1:Y:453:PHE:O	1.97	0.48
1:O:40:PRO:HD2	1:O:44:TRP:C	2.38	0.48
1:O:114:HIS:O	1:O:115:LEU:C	2.55	0.48
1:O:163:GLY:CA	1:O:167:THR:HG21	2.44	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: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:38:ILE:O	1:Y:40:PRO:HD3	2.14	0.48
1:Y:313:ILE:O	1:Y:314:GLN:C	2.55	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:80:THR:HG21	1:Y:248:ALA:HB3	1.96	0.48
1:Y:186:ALA:O	1:Y:187:SER:C	2.57	0.48
1:O:226:GLN:HB3	1:O:236:ARG:HD3	1.95	0.48
1:Y:5:TYR:O	1:Y:75:ALA:N	2.41	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:O:45:VAL:HG21	1:O:104:GLN:HB3	1.96	0.47
1:Y:67:ALA:C	1:Y:69:ILE:HD12	2.38	0.47
1:Y:78:GLY:HA2	1:Y:447:ALA:HB2	1.95	0.47
1:Y:477:THR:O	1:Y:478:GLU:C	2.57	0.47
1:O:3:LYS:HB2	1:O:3:LYS:NZ	2.29	0.47
1:O:185:ASN:O	1:O:188:ARG:HB2	2.14	0.47
1:Y:50:MET:O	1:Y:51:GLU:C	2.56	0.47
1:Y:161:LEU:HD22	1:Y:179:HIS:CE1	2.49	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:Y:5:TYR:CA	1:Y:74:ILE:HG22	2.44	0.47
1:Y:250:LEU:HD12	1:Y:250:LEU:C	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:396:GLN:HE21	1:Y:403:LEU:HD12	1.77	0.47
1:O:144:ILE:HG22	1:O:148:VAL:HG23	1.95	0.47
1:O:173:MET:CB	1:O:227:THR:HG23	2.44	0.47
1:O:211:ARG:HG3	1:O:211:ARG:NH1	2.30	0.47
1:O:221:SER:CB	1:O:296:GLY:HA3	2.44	0.47
1:Y:63:VAL:O	1:Y:64:LEU:O	2.32	0.47
1:Y:265:TYR:CD1	1:Y:265:TYR:N	2.83	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:O:442:GLY:O	1:O:443:ALA:C	2.50	0.47
1:Y:246:GLN:HB3	1:Y:272:LEU:CD2	2.44	0.47
1:Y:263:ASN:O	1:Y:408:VAL:HA	2.14	0.47
1:O:83:ARG:CZ	1:O:246:GLN:HG3	2.45	0.47
1:Y:48:ASP:O	1:Y:51:GLU:N	2.48	0.47
1:Y:80:THR:HG22	1:Y:243:ALA:O	2.15	0.47
1:Y:162:PHE:HB3	1:Y:213:MET:HG3	1.96	0.47
1:Y:255:CYS:CB	1:Y:260:MET:HB3	2.45	0.47
1:Y:359:TYR:HD1	1:Y:497:GLU:HB3	1.80	0.47
1:O:15:SER:CB	1:O:34:GLU:HA	2.45	0.47
1:O:65:ALA:O	1:O:67:ALA:N	2.47	0.47
1:O:314:GLN:OE1	1:O:317:ARG:NH1	2.30	0.47
1:O:342:VAL:HG12	1:O:343:TYR:N	2.28	0.47
1:O:21:MET:HA	1:O:26:ASN: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:389:ARG:HG2	1:O:483:TYR:CZ	2.50	0.47
1:Y:23:HIS:ND1	1:Y:453:PHE:CE1	2.81	0.47
1:O:389:ARG:HA	1:O:426:LEU:HD11	1.97	0.47
1:Y:386:TYR:OH	1:Y:482:ARG:HB3	2.15	0.47
1:O:9:LEU:HA	1:O:9:LEU:HD12	1.39	0.47
1:Y:67:ALA:HB3	1:Y:69:ILE:CD1	2.45	0.46
1:Y:336:VAL:HG21	1:Y:338:ASN:O	2.15	0.46
1:O:3:LYS:HG2	1:O:73:GLN:HA	1.97	0.46
1:Y:372:ASN:O	1:Y:375:HIS:N	2.48	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:HG3	1:O:482:ARG:NH1	2.30	0.46
1:Y:128:THR:HG21	1:Y:190:MET:HA	1.97	0.46
1:Y:236:ARG:HG3	1:Y:236:ARG:HH11	1.81	0.46
1:Y:280:VAL:CG1	1:Y:281:LYS:N	2.79	0.46
1:O:160:LEU:O	1:O:213:MET:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:183:TYR:CD2	1:O:298:VAL:CG2	2.99	0.46
1:Y:180:VAL:CG2	1:Y:181:THR:N	2.78	0.46
1:O:3:LYS:HA	1:O:73:GLN:C	2.40	0.46
1:O:38:ILE:O	1:O:46:GLU:N	2.45	0.46
1:O:173:MET:HB2	1:O:174:THR:HG23	1.96	0.46
1:O:251:PHE:CZ	1:O:446:LEU:HD13	2.50	0.46
1:O:297:GLU:O	1:O:297:GLU:HG2	2.13	0.46
1:Y:48:ASP:O	1:Y:52:ILE:N	2.38	0.46
1:Y:142:LYS:O	1:Y:143:TRP:C	2.59	0.46
1:Y:161:LEU:CD2	1:Y:179:HIS:CE1	2.99	0.46
1:Y:221:SER:HG	1:Y:450:ALA:HB2	1.80	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: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:64:LEU:O	1:Y:65:ALA:C	2.56	0.46
1:O:381:LEU:O	1:O:382:GLU:C	2.56	0.46
1:O:442:GLY:O	1:O:445:TYR:N	2.49	0.46
1:Y:206:VAL:CG1	1:Y:207:LEU:N	2.78	0.46
1:Y:439:THR:HG22	1:Y:440:ALA:N	2.30	0.46
1:Y:457:LEU:O	1:Y:461:GLN:HG3	2.16	0.46
1:O:193:ASN:HB3	1:O:196:THR:CG2	2.46	0.46
1:O:203:MET:O	1:O:204:LEU:C	2.59	0.46
1:O:339:THR:OG1	1:O:342:VAL:O	2.33	0.46
1:O:460:LEU:N	1:O:460:LEU:CD1	2.77	0.46
1:Y:28:ILE:N	1:Y:28:ILE:CD1	2.79	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:O:193:ASN:CG	1:O:196:THR:HB	2.40	0.46
1:O:251:PHE:CZ	1:O:446:LEU:CD1	2.99	0.46
1:O:297:GLU:OE1	1:O:297:GLU:N	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:O:20:VAL:HG12	1:O:21:MET:N	2.31	0.45
1:O:169:LEU:N	1:O:169:LEU:HD22	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:Y:18:ALA:HB1	1:Y:63:VAL:CG2	2.44	0.45
1:Y:180:VAL:CG2	1:Y:181:THR:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:487:LYS:O	1:O:488:LYS:C	2.59	0.45
1:Y:61:VAL:O	1:Y:64:LEU:N	2.49	0.45
1:Y:236:ARG:HH11	1:Y:236:ARG:CG	2.28	0.45
1:Y:422:GLN:NE2	1:Y:426:LEU:CD2	2.80	0.45
1:Y:456:ASN:ND2	1:Y:456:ASN:C	2.74	0.45
1:O:13:THR:HB	3:O:601:ATS:OG3	2.16	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:480:ASN:O	1:O:481:TYR:C	2.58	0.45
1:Y:3:LYS:NZ	1:Y:3:LYS:CB	2.80	0.45
1:Y:110:GLU:O	1:Y:111:ILE:C	2.58	0.45
1:Y:302:LEU:HD23	1:Y:302:LEU:HA	1.41	0.45
1:O:17:ARG:HA	1:O:59:THR:HG21	1.99	0.45
1:O:320:MET:HE3	1:O:320:MET:HB3	1.89	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:3:LYS:NZ	1:O:3:LYS:CB	2.80	0.45
1:O:90:GLU:OE2	1:O:93:THR:HG21	2.16	0.45
1:O:101:ILE:HG12	1:O:107:ARG:NH1	2.31	0.45
1:O:124:ILE:HD13	1:O:203:MET:HE1	1.99	0.45
1:O:156:ARG:NH1	1:O:156:ARG:CB	2.79	0.45
1:O:270:PHE:CD1	1:O:270:PHE:N	2.85	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:86:THR:HG22	1:O:87:ILE:N	2.31	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:33:ARG:HH21	1:O:58:TRP:HB3	1.76	0.45
1:O:179:HIS:CD2	1:O:215:PRO:HA	2.52	0.45
1:Y:94:GLY:HA2	1:Y:171:TRP:CH2	2.52	0.45
1:Y:103:TRP:CD1	1:Y:103:TRP:N	2.85	0.45
1:Y:362:GLY:CA	1:O:367:LEU:HB2	2.42	0.45
1:O:114:HIS:O	1:O:117:ARG:HB2	2.16	0.45
1:O:141:VAL:O	1:O:142:LYS:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:451:VAL:O	1:O:451:VAL:HG13	2.17	0.45
1:Y:67:ALA:HB3	1:Y:69:ILE:HD13	1.99	0.45
1:Y:156:ARG:HH11	1:Y:156:ARG:CG	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: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:367:LEU:HB2	1:O:362:GLY:CA	2.47	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:310:GLY:HA3	3:O:601:ATS:O3'	2.17	0.45
1:O:457:LEU:C	1:O:459:GLU:N	2.75	0.45
1:O:468:ARG:HD2	1:O:469:GLU:H	1.80	0.45
1:Y:310:GLY:O	1:Y:313:ILE:HB	2.17	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:O:137:SER:O	1:O:141:VAL:HG23	2.17	0.44
1:O:174:THR:O	1:O:175:GLN:C	2.60	0.44
1:O:251:PHE:O	1:O:254:LEU:N	2.49	0.44
1:O:271:MET:C	1:O:272:LEU:HD13	2.42	0.44
1:O:428:THR:CG2	1:O:429:ARG:N	2.79	0.44
1:Y:23:HIS:C	1:Y:25:ALA:H	2.23	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:Y:27:ILE:N	1:Y:27:ILE:CD1	2.79	0.44
1:Y:389:ARG:O	1:Y:390:ASP:C	2.60	0.44
1:Y:432:ARG:CD	1:Y:436:ARG:NH1	2.80	0.44
1:O:60:LEU:HD12	1:O:60:LEU:C	2.42	0.44
1:O:183:TYR:CD1	1:O:217:VAL:CG1	3.00	0.44
1:O:190:MET:HE3	1:O:190:MET:HB3	1.79	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:457:LEU:HD13	1:O:457:LEU:HA	1.73	0.44
1:Y:148:VAL:HB	1:Y:151:SER:HB3	1.98	0.44
1:Y:149:GLU:OE1	1:Y:149:GLU:HA	2.04	0.44
1:O:80:THR:HG22	1:O:245:ASP:N	2.32	0.44
1:O:347:ALA:O	1:O:348:PHE:C	2.60	0.44
1:O:439:THR:CG2	1:O:440:ALA:N	2.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:38:ILE:O	1:Y:45:VAL:HA	2.18	0.44
1:O:179:HIS:CD2	1:O:215:PRO:CB	3.00	0.44
1:Y:205:GLU:C	1:Y:208:ASP:H	2.25	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:251:PHE:CE2	1:O:446:LEU:CD1	2.99	0.44
1:O:144:ILE:O	1:O:145:LEU:C	2.60	0.44
1:Y:211:ARG:HG3	1:Y:211:ARG:NH1	2.30	0.44
1:Y:377:ILE:O	1:Y:378:ARG:C	2.58	0.44
1:Y:424:ASP:HB3	1:Y:474:ILE:HB	1.98	0.44
1:Y:439:THR:O	1:Y:442:GLY:N	2.51	0.44
1:O:140:LYS:O	1:O:144:ILE:HD12	2.17	0.44
1:Y:457:LEU:HD13	1:Y:457:LEU:HA	1.58	0.44
1:Y:483:TYR:O	1:Y:484:ALA:C	2.58	0.44
1:O:40:PRO:CG	1:O:44:TRP:HB3	2.47	0.43
1:O:86:THR:HG1	1:O:137:SER:HB3	1.82	0.43
1:O:179:HIS:CE1	1:O:215:PRO:CG	3.00	0.43
1:O:391:VAL:CG2	1:O:392:LEU:N	2.81	0.43
1:Y:91:LYS:O	1:Y:92:GLU:O	2.34	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:436:ARG:C	1:Y:438:VAL:H	2.25	0.43
1:Y:490:VAL:O	1:Y:491:LYS:C	2.61	0.43
1:O:137:SER:O	1:O:138:GLY:O	2.37	0.43
1:O:157:ARG:C	1:O:159:GLU:H	2.26	0.43
1:O:271:MET:SD	1:O:395:MET:HE2	2.57	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:246:GLN:CG	1:Y:270:PHE:HB2	2.47	0.43
1:Y:369:ARG:HG2	1:O:348:PHE:HB3	2.00	0.43
1:O:6:ILE:HD11	1:O:447:ALA:HB3	2.00	0.43
1:O:44:TRP:CE2	1:O:107:ARG:HB2	2.53	0.43
1:O:62:GLU:H	1:O:62:GLU:HG3	1.33	0.43
1:O:103:TRP:HB2	1:O:135:TYR:CE1	2.54	0.43
1:O:129:GLY:HA3	1:O:288:THR:HB	2.00	0.43
1:Y:124:ILE:C	1:Y:128:THR:HG1	2.24	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:204:LEU:HD23	1:O:204:LEU:HA	1.45	0.43
1:O:372:ASN:O	1:O:373:ALA:C	2.60	0.43
1:O:455:GLN:O	1:O:455:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:3:LYS:HZ3	1:Y:3:LYS:CB	2.31	0.43
1:Y:6:ILE:HD13	1:Y:444:ALA:HB1	2.00	0.43
1:Y:81:ASN:ND2	1:Y:81:ASN:N	2.67	0.43
1:Y:478:GLU:O	1:Y:481:TYR:HB3	2.18	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:222:GLU:CG	1:Y:223:VAL:N	2.80	0.43
1:Y:484:ALA:O	1:Y:485:GLY:C	2.60	0.43
1:O:46:GLU:OE2	1:O:107:ARG:NH2	2.50	0.43
1:O:145:LEU:N	1:O:145:LEU:HD13	2.33	0.43
1:Y:124:ILE:HG13	1:Y:132:ILE:CD1	2.46	0.43
1:Y:451:VAL:O	1:Y:451:VAL:HG13	2.17	0.43
1:O:13:THR:O	1:O:13:THR:HG22	2.15	0.43
1:O:122:ASP:O	1:O:126:SER:OG	2.29	0.43
1:Y:58:TRP:CE3	1:Y:58:TRP:HA	2.54	0.43
1:O:31:SER:O	1:O:32:GLN:HB2	2.19	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:185:ASN:O	1:O:186:ALA:C	2.61	0.43
1:Y:12:GLY:O	1:Y:35:PHE:HZ	2.01	0.43
1:Y:18:ALA:CB	1:Y:63:VAL:HG21	2.47	0.43
1:Y:111:ILE:CG2	1:Y:115:LEU:HD11	2.49	0.43
1:Y:166:ASP:OD2	1:Y:185:ASN:OD1	2.37	0.43
1:Y:271:MET:HE1	1:Y:392:LEU:HB2	2.01	0.43
1:Y:346:PRO:HG2	1:Y:387:GLN:NE2	2.32	0.43
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:O:272:LEU:N	1:O:272:LEU:CD1	2.80	0.43
1:O:197:LEU:N	1:O:197:LEU:CD2	2.80	0.43
1:O:229:ILE:HG13	1:O:230:GLY:N	2.34	0.43
1:O:272:LEU:CD1	1:O:303:GLU:HG3	2.48	0.43
1:O:302:LEU:HD23	1:O:302:LEU:HA	1.30	0.43
1:O:422:GLN:HE21	1:O:426:LEU:HD22	1.84	0.43
1:Y:9:LEU:HD11	1:Y:60:LEU:CD1	2.49	0.42
1:Y:16:SER:CB	1:Y:56:GLN:HA	2.48	0.42
1:Y:249:ALA:HB1	1:Y:438:VAL:CG1	2.49	0.42
1:Y:338:ASN:O	1:Y:375:HIS:HD2	2.01	0.42
1:Y:449:LEU:HD12	1:Y:449:LEU:HA	1.93	0.42
1:O:184:THR:CG2	1:O:290:ILE:HG22	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:18:ALA:CB	1:Y:59:THR:HB	2.49	0.42
1:Y:56:GLN:O	1:Y:56:GLN:HG3	2.18	0.42
1:Y:63:VAL:O	1:Y:64:LEU:C	2.62	0.42
1:Y:150:GLY:O	1:Y:151:SER:C	2.62	0.42
1:O:43:GLY:C	1:O:44:TRP:HD1	2.27	0.42
1:O:113:GLU:O	1:O:114:HIS:C	2.62	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: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:Y:466:ILE:HD13	1:Y:466:ILE:C	2.45	0.42
1:O:418:LEU:HA	1:O:418:LEU:HD23	1.70	0.42
1:Y:17:ARG:HH22	1:Y:437:GLU:HG3	1.84	0.42
1:Y:31:SER:O	1:Y:32:GLN:HB2	2.18	0.42
1:Y:204:LEU:HA	1:Y:204:LEU:HD23	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:422:GLN:HG3	1:O:426:LEU:HD23	2.01	0.42
1:O:476:THR:O	1:O:477:THR:C	2.59	0.42
1:Y:41:LYS:HA	1:Y:42:PRO:HD3	1.80	0.42
1:Y:185:ASN:O	1:Y:186:ALA:C	2.60	0.42
1:Y:353:ALA:HA	1:Y:356:TRP:NE1	2.34	0.42
1:Y:482:ARG:HG3	1:Y:482:ARG:HH11	1.83	0.42
1:Y:482:ARG:CG	1:Y:482:ARG:HH11	2.33	0.42
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:O:87:ILE:HD13	1:O:168:TRP:CB	2.49	0.42
1:O:157:ARG:HG2	1:O:157:ARG:H	1.62	0.42
1:O:245:ASP:C	1:O:248:ALA:HB3	2.43	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
1:Y:41:LYS:O	1:Y:44:TRP:HB2	2.19	0.42
1:Y:106:ARG:O	1:Y:107:ARG:C	2.61	0.42
1:Y:410:GLY:O	1:Y:411:GLY:C	2.63	0.42
1:O:124:ILE:CD1	1:O:203:MET:HE1	2.49	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:O:436:ARG:C	1:O:438:VAL:H	2.26	0.42
1:Y:52:ILE:O	1:Y:53:TRP:C	2.62	0.42
1:O:240:SER:HB2	1:O:450:ALA:CB	2.49	0.42
1:O:415:ASN:CG	1:O:418:LEU:HB2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:466:ILE:HD13	1:O:466:ILE:O	2.19	0.42
1:Y:9:LEU:HD12	1:Y:9:LEU:HA	1.65	0.42
1:Y:103:TRP:HB2	1:Y:135:TYR:CD1	2.55	0.42
1:Y:293:GLY:HA3	1:Y:297:GLU:CD	2.44	0.42
1:Y:31:SER:HB2	1:Y:63:VAL:H	1.84	0.42
1:Y:35:PHE:HE2	1:Y:47:HIS:CD2	2.38	0.42
1:O:3:LYS:HG2	1:O:72:ASP:O	2.20	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:Y:11:GLN:NE2	1:Y:82:GLN:HE21	2.16	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:O:468:ARG:CG	1:O:468:ARG:NH1	2.80	0.42
1:Y:242:ILE:HG22	1:Y:243:ALA:N	2.35	0.41
1:O:127:ASN:ND2	1:O:193:ASN:ND2	2.67	0.41
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:199:TRP:HZ2	1:O:215:PRO:O	2.02	0.41
1:Y:18:ALA:CB	1:Y:63:VAL:CG2	2.99	0.41
1:Y:166:ASP:O	1:Y:169:LEU:N	2.50	0.41
1:Y:190:MET:HE2	1:Y:190:MET:HB3	1.88	0.41
1:Y:217:VAL:C	1:Y:218:ARG:HG2	2.45	0.41
1:Y:324:ASN:ND2	1:Y:324:ASN:N	2.67	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:3:LYS:HA	1:Y:73:GLN:C	2.45	0.41
1:Y:47:HIS:HB2	1:Y:100:ALA:HB3	2.02	0.41
1:Y:70:SER:C	1:Y:72:ASP:N	2.78	0.41
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: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:321:LYS:C	1:O:322:LEU:HD23	2.46	0.41
1:O:359:TYR:HB2	1:O:495:ALA:HA	2.02	0.41
1:Y:103:TRP:HB2	1:Y:135:TYR:CE1	2.55	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:Y:32:GLN:HA	1:Y:59:THR:HG22	2.02	0.41
1:Y:48:ASP:C	1:Y:52:ILE:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:108:THR:HG22	1:Y:111:ILE:HD12	2.02	0.41
1:Y:246:GLN:HG2	1:Y:270:PHE:CB	2.50	0.41
1:Y:381:LEU:HD23	1:Y:381:LEU:HA	1.78	0.41
1:Y:479:ARG:NH1	1:Y:479:ARG:CG	2.83	0.41
1:Y:81:ASN:HB2	1:Y:165:VAL:HB	2.03	0.41
1:Y:250:LEU:HD22	1:Y:272:LEU:HB2	2.02	0.41
1:O:52:ILE:O	1:O:55:THR:OG1	2.38	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:492:ARG:NH1	1:O:492:ARG:CG	2.80	0.41
1:Y:169:LEU:HD13	1:Y:169:LEU:HA	1.87	0.41
1:Y:468:ARG:HG3	1:Y:468:ARG:NH1	2.36	0.41
1:O:33:ARG:NH1	1:O:62:GLU:CD	2.79	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: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:O:84:GLU:CD	1:O:135:TYR:CE1	2.99	0.41
1:O:166:ASP:OD2	1:O:185:ASN:OD1	2.39	0.41
1:O:183:TYR:O	1:O:184:THR:C	2.63	0.41
1:O:256:VAL:O	1:O:294:PRO:HD3	2.21	0.41
1:Y:90:GLU:HB3	1:Y:93:THR:HG23	2.02	0.41
1:Y:95:LYS:HA	1:Y:96:PRO:HD3	1.97	0.41
1:Y:127:ASN:HD22	1:Y:193:ASN:HD21	1.68	0.41
1:Y:154:ARG:H	1:Y:154:ARG:HG2	1.09	0.41
1:Y:261:ALA:HB2	1:Y:273:MET:CB	2.50	0.41
1:Y:457:LEU:HD13	1:Y:460:LEU:HD13	2.02	0.41
1:O:24:ASP:O	1:O:25:ALA:HB3	2.21	0.41
1:O:138:GLY:N	1:O:189:THR:O	2.52	0.41
1:O:139:THR:O	1:O:140:LYS:C	2.62	0.41
1:O:354:PRO:CD	1:O:355:TYR:H	2.34	0.41
1:O:451:VAL:CG1	1:O:453:PHE:HB2	2.50	0.41
1:O:460:LEU:C	1:O:462:GLU:N	2.79	0.41
1:Y:30:VAL:O	1:Y:30:VAL:HG12	2.13	0.41
1:Y:111:ILE:O	1:Y:112:CYS:C	2.60	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:O:27:ILE:N	1:O:27:ILE:CD1	2.79	0.41
1:O:81:ASN:N	1:O:81:ASN:HD22	2.18	0.41
1:O:102:VAL:C	1:O:104:GLN:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:180:VAL:HA	1:O:216:GLU:O	2.21	0.41
1:Y:48:ASP:O	1:Y:49:PRO:C	2.64	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: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:O:113:GLU:O	1:O:116:LYS:HB2	2.20	0.40
1:O:229:ILE:O	1:O:230:GLY:C	2.64	0.40
1:O:237:ILE:H	1:O:237:ILE:HG12	1.77	0.40
1:O:345:VAL:HA	1:O:346:PRO:HD3	1.66	0.40
1:O:382:GLU:O	1:O:383:SER:C	2.62	0.40
1:O:428:THR:HG23	1:O:429:ARG:N	2.36	0.40
1:Y:32:GLN:CA	1:Y:59:THR:HG22	2.52	0.40
1:O:295:THR:N	1:O:297:GLU:OE1	2.43	0.40
1:Y:47:HIS:CB	1:Y:52:ILE:HD11	2.47	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:O:90:GLU:HB3	1:O:93:THR:HG23	2.03	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:Y:127:ASN:CB	1:Y:193:ASN:HD22	2.31	0.40
1:Y:272:LEU:CD1	1:Y:303:GLU:CG	3.00	0.40
1:O:344:VAL:HG22	1:O:364:ILE:HD13	2.03	0.40
1:Y:199:TRP:CD1	1:Y:214:LEU:HD23	2.56	0.40
1:O:130:LEU:HD23	1:O:130:LEU:HA	1.71	0.40
1:O:194:ILE:O	1:O:300:TYR:OH	2.29	0.40
1:O:221:SER:HG	1:O:450:ALA:HB2	1.81	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%)	1	7
1	Y	490/501 (98%)	391 (80%)	76 (16%)	23 (5%)	2	11
All	All	980/1002 (98%)	766 (78%)	161 (16%)	53 (5%)	1	9

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
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

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Mol	Chain	Res	Type
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%)	264 (65%)	144 (35%)	0	1
1	Y	408/412 (99%)	272 (67%)	136 (33%)	0	1
All	All	816/824 (99%)	536 (66%)	280 (34%)	0	1

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	2	GLU
1	Y	3	LYS
1	Y	5	TYR
1	Y	6	ILE
1	Y	9	LEU

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Mol	Chain	Res	Type
1	Y	11	GLN
1	Y	13	THR
1	Y	20	VAL
1	Y	27	ILE
1	Y	33	ARG
1	Y	34	GLU
1	Y	41	LYS
1	Y	45	VAL
1	Y	52	ILE
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	97	ILE
1	Y	107	ARG
1	Y	110	GLU
1	Y	116	LYS
1	Y	117	ARG
1	Y	118	ASP
1	Y	120	LEU
1	Y	121	GLU
1	Y	124	ILE
1	Y	128	THR
1	Y	130	LEU
1	Y	131	VAL
1	Y	137	SER
1	Y	145	LEU
1	Y	146	ASP
1	Y	148	VAL
1	Y	149	GLU
1	Y	151	SER
1	Y	153	GLU
1	Y	154	ARG
1	Y	156	ARG
1	Y	157	ARG

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Mol	Chain	Res	Type
1	Y	159	GLU
1	Y	162	PHE
1	Y	165	VAL
1	Y	170	ILE
1	Y	172	LYS
1	Y	173	MET
1	Y	174	THR
1	Y	175	GLN
1	Y	181	THR
1	Y	187	SER
1	Y	190	MET
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	209	ILE
1	Y	211	ARG
1	Y	214	LEU
1	Y	219	ARG
1	Y	222	GLU
1	Y	227	THR
1	Y	229	ILE
1	Y	235	THR
1	Y	236	ARG
1	Y	237	ILE
1	Y	240	SER
1	Y	247	GLN
1	Y	253	GLN
1	Y	256	VAL
1	Y	257	LYS
1	Y	267	THR
1	Y	272	LEU
1	Y	273	MET
1	Y	278	LYS
1	Y	281	LYS
1	Y	290	ILE
1	Y	295	THR
1	Y	312	SER
1	Y	313	ILE

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Mol	Chain	Res	Type
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	391	VAL
1	Y	392	LEU
1	Y	396	GLN
1	Y	402	ARG
1	Y	406	LEU
1	Y	407	ARG
1	Y	413	VAL
1	Y	418	LEU
1	Y	423	SER
1	Y	426	LEU
1	Y	428	THR
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	455	GLN
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	474	ILE
1	Y	475	GLU
1	Y	478	GLU

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Mol	Chain	Res	Type
1	Y	479	ARG
1	Y	488	LYS
1	Y	492	ARG
1	Y	494	MET
1	Y	498	GLU
1	O	3	LYS
1	O	5	TYR
1	O	6	ILE
1	O	9	LEU
1	O	11	GLN
1	O	16	SER
1	O	20	VAL
1	O	21	MET
1	O	22	ASP
1	O	27	ILE
1	O	28	ILE
1	O	32	GLN
1	O	34	GLU
1	O	41	LYS
1	O	45	VAL
1	O	57	SER
1	O	60	LEU
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	87	ILE
1	O	91	LYS
1	O	92	GLU
1	O	93	THR
1	O	95	LYS
1	O	97	ILE
1	O	102	VAL
1	O	106	ARG
1	O	107	ARG
1	O	108	THR
1	O	116	LYS
1	O	117	ARG
1	O	118	ASP

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Mol	Chain	Res	Type
1	O	120	LEU
1	O	121	GLU
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	140	LYS
1	O	141	VAL
1	O	142	LYS
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	170	ILE
1	O	172	LYS
1	O	173	MET
1	O	175	GLN
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	209	ILE
1	O	211	ARG
1	O	213	MET
1	O	219	ARG

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Mol	Chain	Res	Type
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	267	THR
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	380	THR
1	O	389	ARG
1	O	391	VAL
1	O	392	LEU
1	O	395	MET
1	O	402	ARG
1	O	403	LEU
1	O	406	LEU
1	O	407	ARG
1	O	413	VAL
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

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Mol	Chain	Res	Type
1	O	437	GLU
1	O	438	VAL
1	O	439	THR
1	O	451	VAL
1	O	455	GLN
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	475	GLU
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	497	GLU
1	O	498	GLU
1	O	499	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	11	GLN
1	Y	26	ASN
1	Y	47	HIS
1	Y	56	GLN
1	Y	73	GLN
1	Y	81	ASN
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

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Mol	Chain	Res	Type
1	Y	299	ASN
1	Y	324	ASN
1	Y	387	GLN
1	Y	396	GLN
1	Y	415	ASN
1	Y	455	GLN
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	56	GLN
1	O	73	GLN
1	O	81	ASN
1	O	99	ASN
1	O	114	HIS
1	O	127	ASN
1	O	147	HIS
1	O	185	ASN
1	O	228	ASN
1	O	253	GLN
1	O	299	ASN
1	O	387	GLN
1	O	396	GLN
1	O	415	ASN
1	O	416	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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
3	ATS	Y	601	2	29,33,33	1.03	2 (6%)	42,52,52	1.30	4 (9%)
4	GOL	O	600	-	5,5,5	0.50	0	5,5,5	0.33	0
4	GOL	Y	600	-	5,5,5	0.62	0	5,5,5	0.89	0
3	ATS	O	601	-	29,33,33	1.15	1 (3%)	42,52,52	1.08	4 (9%)

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	ATS	Y	601	2	-	2/13/38/38	0/3/3/3
4	GOL	O	600	-	-	4/4/4/4	-
4	GOL	Y	600	-	-	4/4/4/4	-
3	ATS	O	601	-	-	1/13/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	ATS	PB-O13	3.32	1.62	1.58
3	Y	601	ATS	O2'-C2'	-2.15	1.37	1.43
3	Y	601	ATS	O3'-C3'	-2.06	1.37	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	601	ATS	PB-O13-PA	-3.30	121.61	132.37
3	Y	601	ATS	C2'-C1'-N9	3.19	121.23	113.30
3	O	601	ATS	C1'-N9-C8	-2.88	120.70	127.09
3	O	601	ATS	C4-N9-C1'	2.62	132.77	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	601	ATS	C2'-C1'-N9	2.54	119.62	113.30
3	O	601	ATS	PB-O13-PA	-2.25	125.03	132.37
3	Y	601	ATS	C5-C4-N9	2.24	108.25	105.81
3	Y	601	ATS	C4-N9-C8	-2.22	103.40	105.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

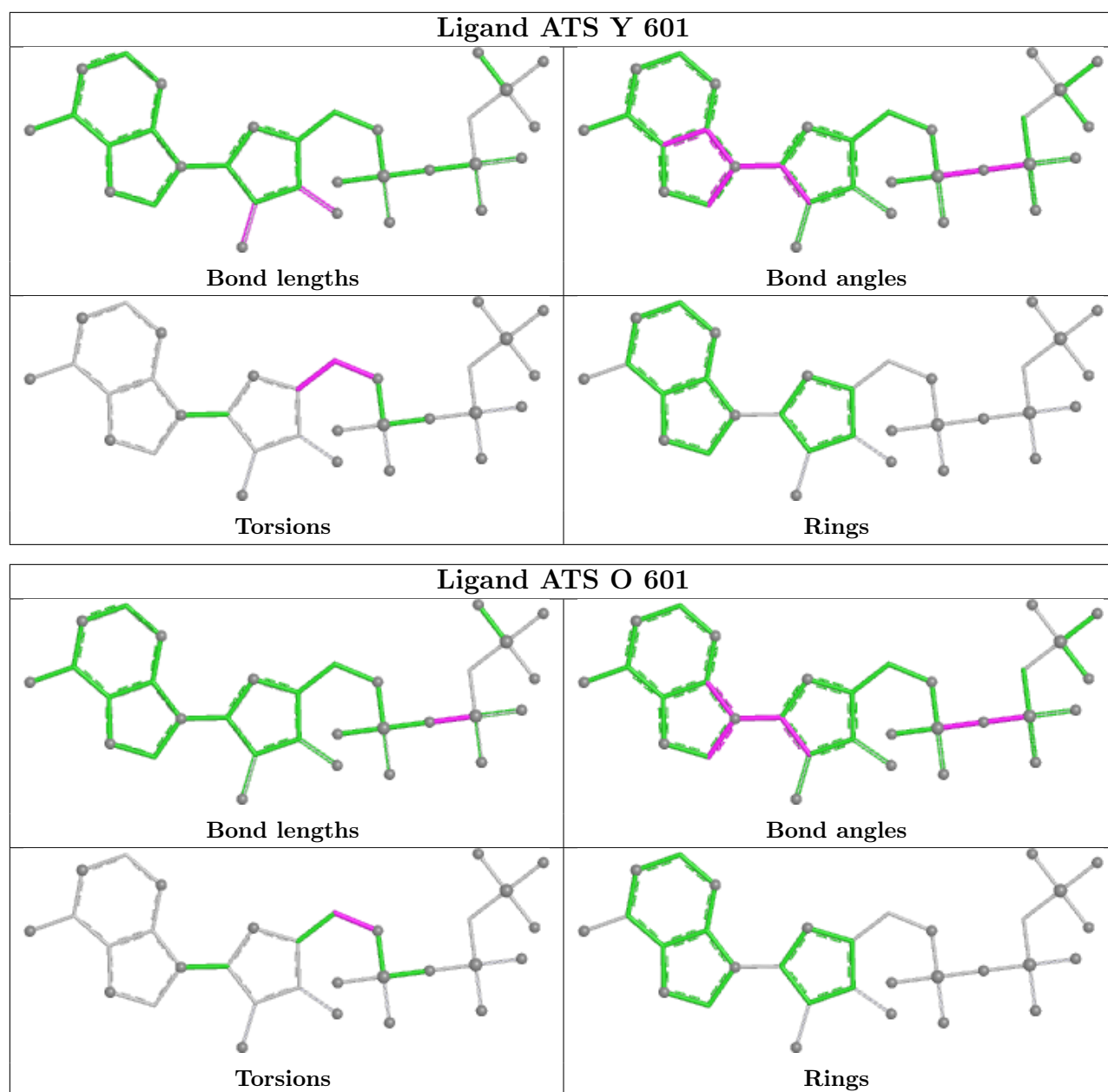
Mol	Chain	Res	Type	Atoms
4	Y	600	GOL	O1-C1-C2-C3
4	Y	600	GOL	C1-C2-C3-O3
4	O	600	GOL	O1-C1-C2-C3
4	O	600	GOL	C1-C2-C3-O3
4	Y	600	GOL	O1-C1-C2-O2
4	Y	600	GOL	O2-C2-C3-O3
4	O	600	GOL	O1-C1-C2-O2
4	O	600	GOL	O2-C2-C3-O3
3	Y	601	ATS	C4'-C5'-O5'-PA
3	Y	601	ATS	C3'-C4'-C5'-O5'
3	O	601	ATS	C4'-C5'-O5'-PA

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	601	ATS	2	0
4	O	600	GOL	1	0
4	Y	600	GOL	3	0
3	O	601	ATS	2	0

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



5.7 Other polymers [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	494/501 (98%)	-0.54	2 (0%) 88 76	7, 52, 91, 100	0
1	Y	494/501 (98%)	-0.79	2 (0%) 88 76	5, 38, 78, 100	0
All	All	988/1002 (98%)	-0.67	4 (0%) 88 76	5, 45, 86, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	296	GLY	2.3
1	O	225	GLY	2.2
1	Y	58	TRP	2.1
1	Y	457	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ATS	O	601	31/31	0.94	0.10	64,64,64,64	0

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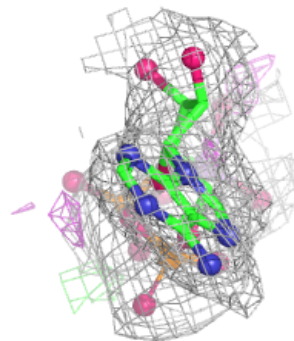
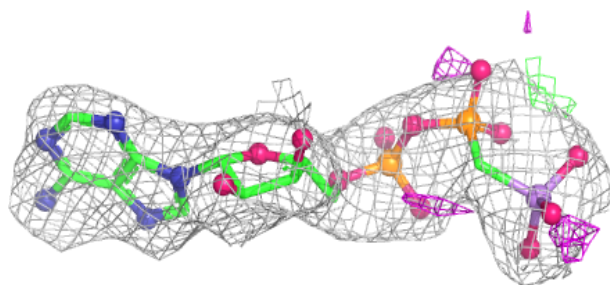
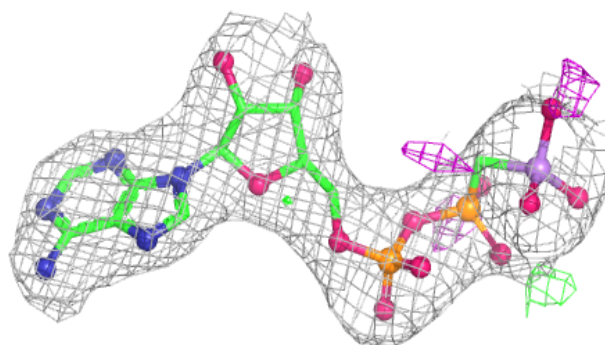
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	O	600	6/6	0.96	0.08	45,45,45,45	0
2	MG	Y	602	1/1	0.97	0.05	27,27,27,27	0
3	ATS	Y	601	31/31	0.97	0.08	50,50,50,50	0
4	GOL	Y	600	6/6	0.98	0.06	17,17,17,17	0

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

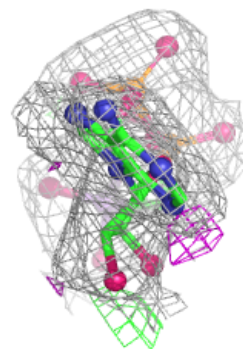
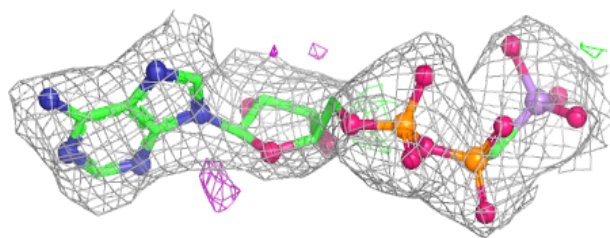
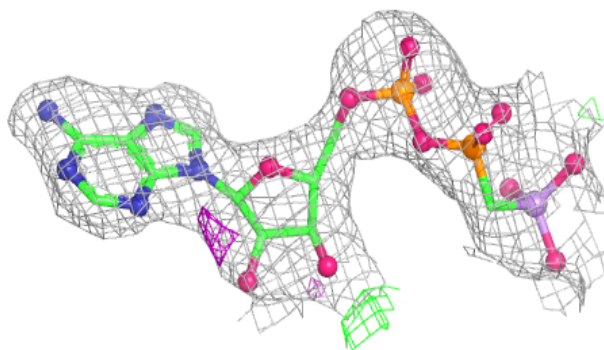
Electron density around ATS O 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATS Y 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.