



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 10:10 AM EDT

PDB ID : 1BWF  
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 : 1998-09-23  
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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

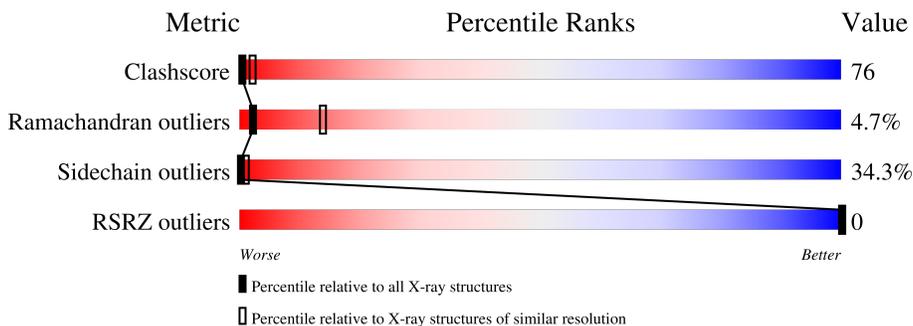
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

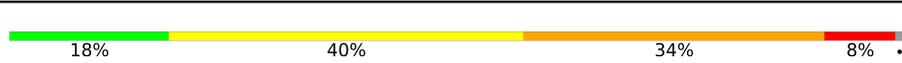
The reported resolution of this entry is 3.00 Å.

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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  $\geq 3$ , 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	 18% 40% 34% 8% .
1	Y	501	 21% 43% 26% 9% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7900 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
			Total	C	N	O	S			
1	Y	494	3910	2470	683	738	19	0	0	0
1	O	494	3910	2470	683	738	19	0	0	0

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHODIFLUOROMETHYLPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ATF) (formula: C<sub>11</sub>H<sub>16</sub>F<sub>2</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).

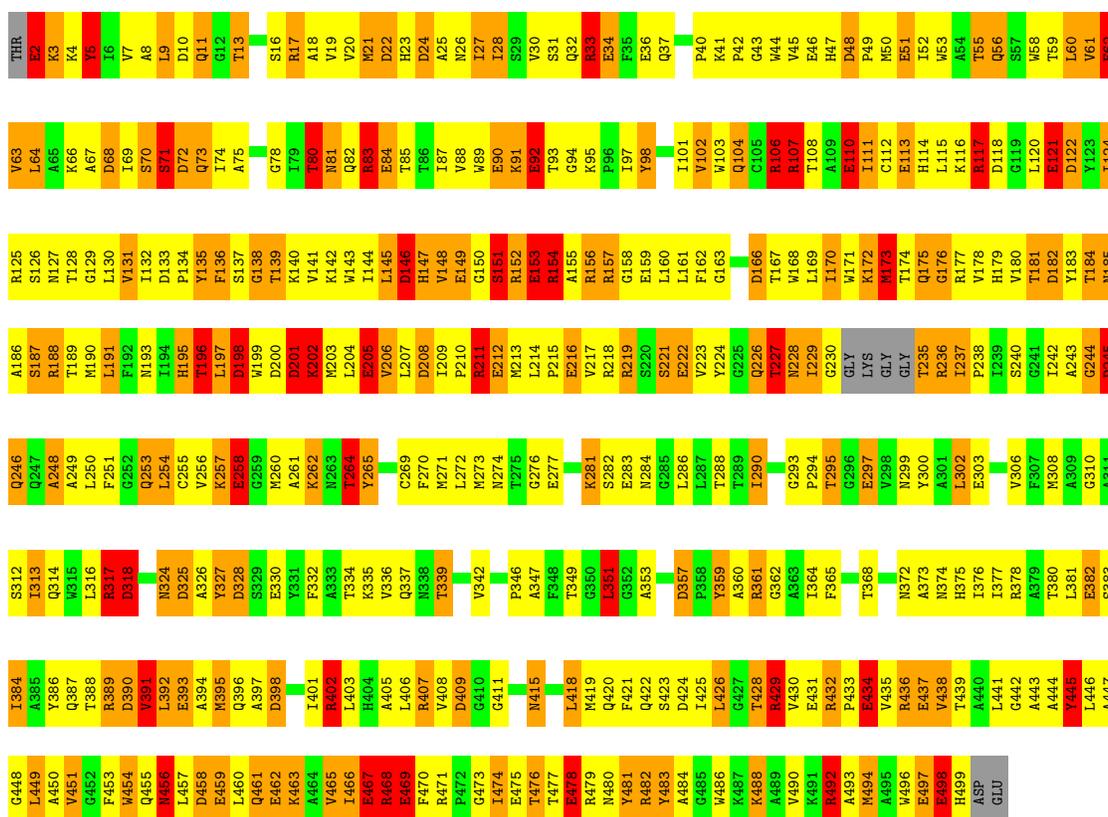


### 3 Residue-property plots

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

Chain Y: 



#### • Molecule 1: GLYCEROL KINASE

Chain O: 



A444	A445	A446	A447	A448	A449	A450	A451	G452	F453	W454	Q455	M456	L457	D458	E459	L460	Q461	E462	K463	A464	V465	I466	E467	R468	E469	F470	G473	I474	E475	I476	T477	E478	R479	M480	Y481	R482	Y483	A484	G485	W486	K487	K488	A489	V490	K491	R492	A493	M494	A495	W496	E497	E498	H499	ASP	GLU					
L381	E382	S383	Y386	Q387	F388	R389	R389	D390	V391	D392	E393	A394	M395	Q396	A397	D398	S399	G400	I401	R402	T394	L403	H404	A405	L406	R407	G408	D409	G410	V413	A414	M415	N416	F417	L418	M419	Q420	F421	Q422	S423	D424	I425	L426	G427	T428	R429	V430	E431	R432	P433	E434	V435	E437	V438	T439	L441				
I313	Q314	W315	L316	R317	D318	E319	L322	I323	M324	D325	A326	Y327	D328	S329	E330	Y331	F332	A333	T334	K335	T339	M340	G341	F342	D343	F344	P346	A347	F348	T349	G350	L351	G352	A353	P354	Y355	W356	D357	P358	Y359	A360	R361	G362	A363	I364	F365	G366	L367	T368	V371	N372	A373	N374	R375	A376	I377				
I242	A243	G244	D245	L246	Q247	A248	A249	L250	F251	G252	Q253	L254	C255	V256	K257	E258	K262	M263	T264	Y265	C269	F270	M271	L272	M273	N274	T275	G276	E277	K278	A279	V280	K281	S282	E283	M284	G285	L286	L287	T288	T289	L290	G293	P294	I299	T295	G296	E297	V298	N299	Y300	A301	L302	E303	G304	G310				
E121	D122	T123	Y124	M125	A126	S127	R128	T129	L130	V131	F132	M133	I134	Y135	F136	G137	G138	T139	K140	V141	K142	W143	I144	E145	D146	H147	V148	E149	G150	R151	E152	E153	R154	A155	R156	R157	G158	E159	L160	F161	F162	T163	T164	V165	D166	T167	W168	L169	I170	W171	K172	M173	T174	Q175	G176	R177	V178	H179	W180	T181
D182	Y183	T184	M185	I186	S187	R188	T189	M190	L191	F192	M193	I194	H195	T196	L197	G198	W199	D200	D201	R202	M203	L204	E205	V206	L207	D208	I209	P210	R211	E212	M213	L214	P215	E216	V217	R218	R219	S220	E221	F222	V223	Y224	G225	Q226	T227	N228	I229	G230	GLY	LYS	GLY	GLY	T235	R236	I237	P238	I239	S240	G241	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.77Å 200.29Å 114.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 18.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 92.3 (18.17-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	200.72 (at 2.92Å)	Xtrriage
Refinement program	TNT 5F	Depositor
R, $R_{free}$	0.168 , (Not available) 0.160 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 123.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	O	1.24	36/3991 (0.9%)	1.72	77/5412 (1.4%)
1	Y	1.30	36/3991 (0.9%)	1.79	98/5412 (1.8%)
All	All	1.27	72/7982 (0.9%)	1.76	175/10824 (1.6%)

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	34	GLU	CD-OE1	9.50	1.36	1.25
1	O	121	GLU	CD-OE2	8.64	1.35	1.25
1	O	34	GLU	CD-OE2	8.52	1.35	1.25
1	O	84	GLU	CD-OE1	8.38	1.34	1.25
1	Y	216	GLU	CD-OE2	8.37	1.34	1.25
1	Y	498	GLU	CD-OE2	8.19	1.34	1.25
1	O	62	GLU	CD-OE1	8.17	1.34	1.25
1	Y	462	GLU	CD-OE2	8.14	1.34	1.25
1	Y	92	GLU	CD-OE2	8.12	1.34	1.25
1	Y	153	GLU	CD-OE1	8.10	1.34	1.25
1	Y	205	GLU	CD-OE1	8.04	1.34	1.25
1	O	92	GLU	CD-OE2	7.76	1.34	1.25
1	Y	283	GLU	CD-OE1	7.68	1.34	1.25
1	O	205	GLU	CD-OE1	7.58	1.33	1.25
1	O	258	GLU	CD-OE2	7.42	1.33	1.25
1	Y	121	GLU	CD-OE1	7.41	1.33	1.25
1	O	330	GLU	CD-OE1	7.38	1.33	1.25
1	Y	149	GLU	CD-OE1	7.30	1.33	1.25
1	O	283	GLU	CD-OE1	7.26	1.33	1.25
1	O	216	GLU	CD-OE2	7.24	1.33	1.25
1	O	113	GLU	CD-OE2	7.24	1.33	1.25
1	O	277	GLU	CD-OE1	7.18	1.33	1.25
1	O	462	GLU	CD-OE1	7.15	1.33	1.25
1	O	153	GLU	CD-OE1	7.09	1.33	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	110	GLU	CD-OE1	7.07	1.33	1.25
1	Y	36	GLU	CD-OE2	7.03	1.33	1.25
1	O	159	GLU	CD-OE2	6.90	1.33	1.25
1	O	51	GLU	CD-OE1	6.90	1.33	1.25
1	Y	84	GLU	CD-OE1	6.85	1.33	1.25
1	O	149	GLU	CD-OE1	6.85	1.33	1.25
1	O	36	GLU	CD-OE2	6.84	1.33	1.25
1	Y	277	GLU	CD-OE2	6.80	1.33	1.25
1	Y	2	GLU	CD-OE1	6.76	1.33	1.25
1	Y	431	GLU	CD-OE1	6.75	1.33	1.25
1	O	393	GLU	CD-OE1	6.75	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	O	353	ALA	C-O	6.62	1.35	1.23
1	O	437	GLU	CD-OE1	6.61	1.32	1.25
1	Y	437	GLU	CD-OE1	6.54	1.32	1.25
1	O	2	GLU	CD-OE2	6.50	1.32	1.25
1	O	212	GLU	CD-OE2	6.40	1.32	1.25
1	Y	330	GLU	CD-OE1	6.36	1.32	1.25
1	Y	258	GLU	CD-OE2	6.30	1.32	1.25
1	O	467	GLU	CD-OE2	6.29	1.32	1.25
1	O	222	GLU	CD-OE2	6.28	1.32	1.25
1	Y	110	GLU	CD-OE1	6.24	1.32	1.25
1	Y	382	GLU	CD-OE2	6.21	1.32	1.25
1	O	459	GLU	CD-OE1	6.14	1.32	1.25
1	O	497	GLU	CD-OE1	5.99	1.32	1.25
1	O	90	GLU	CD-OE2	5.96	1.32	1.25
1	Y	90	GLU	CD-OE2	5.95	1.32	1.25
1	O	319	GLU	CD-OE2	5.88	1.32	1.25
1	Y	467	GLU	CD-OE2	5.84	1.32	1.25
1	Y	62	GLU	CD-OE2	5.79	1.32	1.25
1	Y	459	GLU	CD-OE1	5.79	1.32	1.25
1	O	478	GLU	CD-OE2	5.72	1.31	1.25
1	O	382	GLU	CD-OE2	5.71	1.31	1.25
1	Y	51	GLU	CD-OE2	5.66	1.31	1.25
1	Y	327	TYR	CB-CG	-5.63	1.43	1.51
1	Y	297	GLU	CD-OE2	5.62	1.31	1.25
1	Y	113	GLU	CD-OE2	5.55	1.31	1.25
1	O	498	GLU	CD-OE2	5.51	1.31	1.25
1	Y	212	GLU	CD-OE2	5.49	1.31	1.25
1	Y	469	GLU	CD-OE2	5.38	1.31	1.25
1	Y	497	GLU	CD-OE1	5.38	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	434	GLU	CD-OE1	5.35	1.31	1.25
1	Y	33	ARG	NE-CZ	5.34	1.40	1.33
1	Y	106	ARG	CZ-NH1	5.33	1.40	1.33
1	Y	478	GLU	CD-OE2	5.21	1.31	1.25
1	O	125	ARG	NE-CZ	5.18	1.39	1.33
1	Y	84	GLU	CD-OE2	-5.10	1.20	1.25

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	327	TYR	CB-CG-CD1	-10.81	114.51	121.00
1	O	318	ASP	CB-CG-OD2	-10.45	108.90	118.30
1	Y	361	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	Y	106	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	O	357	ASP	CB-CG-OD2	-10.08	109.23	118.30
1	O	351	LEU	C-N-CA	-9.90	101.51	122.30
1	Y	351	LEU	C-N-CA	-9.60	102.14	122.30
1	Y	83	ARG	C-N-CA	-9.45	98.07	121.70
1	O	409	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	O	146	ASP	CB-CG-OD2	-8.82	110.37	118.30
1	Y	245	ASP	CB-CG-OD2	-8.75	110.42	118.30
1	O	357	ASP	CB-CG-OD1	8.55	126.00	118.30
1	Y	117	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	Y	357	ASP	CB-CG-OD1	8.41	125.87	118.30
1	Y	361	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	O	317	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	O	146	ASP	CB-CG-OD1	8.08	125.57	118.30
1	Y	468	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	O	359	TYR	CA-CB-CG	-8.00	98.20	113.40
1	Y	104	GLN	N-CA-CB	-7.99	96.22	110.60
1	Y	24	ASP	CB-CG-OD1	-7.97	111.12	118.30
1	O	13	THR	CA-CB-CG2	-7.95	101.27	112.40
1	Y	334	THR	CA-CB-CG2	-7.92	101.31	112.40
1	O	106	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	Y	106	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	O	208	ASP	CB-CG-OD2	7.72	125.25	118.30
1	O	24	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	Y	353	ALA	CB-CA-C	-7.66	98.62	110.10
1	O	198	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	O	325	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	Y	188	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	Y	353	ALA	N-CA-CB	7.57	120.69	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	424	ASP	CB-CG-OD1	7.55	125.10	118.30
1	Y	228	ASN	N-CA-CB	7.46	124.03	110.60
1	Y	200	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	O	122	ASP	CB-CG-OD2	-7.38	111.65	118.30
1	O	468	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	Y	68	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	O	133	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	O	33	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	O	200	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	O	182	ASP	CB-CG-OD2	-7.18	111.83	118.30
1	Y	398	ASP	CB-CG-OD2	7.17	124.75	118.30
1	Y	166	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	Y	10	ASP	CB-CG-OD1	-7.08	111.93	118.30
1	Y	122	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	O	107	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	Y	182	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	Y	390	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	Y	325	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	O	424	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	O	334	THR	CA-CB-CG2	-6.95	102.67	112.40
1	Y	152	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	Y	227	THR	CA-CB-CG2	-6.69	103.03	112.40
1	Y	327	TYR	CA-CB-CG	-6.65	100.76	113.40
1	O	228	ASN	N-CA-CB	6.62	122.51	110.60
1	Y	33	ARG	CD-NE-CZ	6.61	132.86	123.60
1	Y	248	ALA	N-CA-CB	6.58	119.32	110.10
1	Y	424	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	O	328	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	Y	80	THR	N-CA-CB	6.53	122.71	110.30
1	O	302	LEU	CA-CB-CG	-6.50	100.36	115.30
1	Y	328	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	O	245	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	Y	390	ASP	N-CA-CB	6.38	122.08	110.60
1	Y	436	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	Y	152	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	Y	17	ARG	N-CA-CB	6.28	121.90	110.60
1	Y	125	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	Y	409	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	Y	359	TYR	CA-CB-CG	-6.26	101.51	113.40
1	Y	468	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	O	208	ASP	CB-CG-OD1	-6.24	112.68	118.30
1	Y	398	ASP	CB-CG-OD1	-6.24	112.69	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	492	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	O	83	ARG	N-CA-C	6.20	127.73	111.00
1	O	289	THR	CA-CB-CG2	-6.19	103.73	112.40
1	Y	211	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	O	83	ARG	C-N-CA	-6.10	106.46	121.70
1	Y	481	TYR	CA-CB-CG	-6.06	101.89	113.40
1	Y	104	GLN	CB-CA-C	6.05	122.50	110.40
1	Y	432	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	O	328	ASP	CB-CG-OD2	6.02	123.72	118.30
1	Y	154	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	Y	432	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	O	147	HIS	CA-CB-CG	-6.00	103.39	113.60
1	Y	245	ASP	CB-CG-OD1	6.00	123.70	118.30
1	O	72	ASP	CB-CG-OD2	5.98	123.68	118.30
1	Y	328	ASP	CB-CG-OD2	5.96	123.67	118.30
1	Y	458	ASP	CB-CG-OD2	5.96	123.66	118.30
1	O	72	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	Y	318	ASP	N-CA-CB	5.94	121.30	110.60
1	O	80	THR	N-CA-CB	5.93	121.57	110.30
1	Y	107	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	O	327	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	Y	135	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	Y	166	ASP	CB-CG-OD1	5.85	123.56	118.30
1	O	481	TYR	CA-CB-CG	-5.82	102.33	113.40
1	O	200	ASP	CB-CG-OD1	5.82	123.53	118.30
1	Y	72	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	Y	5	TYR	CB-CA-C	-5.72	98.97	110.40
1	Y	22	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	O	20	VAL	CB-CA-C	-5.67	100.62	111.40
1	Y	357	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	O	204	LEU	CA-CB-CG	-5.63	102.34	115.30
1	O	33	ARG	CD-NE-CZ	5.62	131.47	123.60
1	O	22	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	O	275	THR	CA-CB-CG2	-5.59	104.58	112.40
1	Y	264	THR	CA-CB-CG2	-5.58	104.59	112.40
1	O	68	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	Y	429	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	O	125	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	Y	10	ASP	CB-CG-OD2	5.53	123.28	118.30
1	Y	318	ASP	CB-CA-C	-5.53	99.35	110.40
1	O	432	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	Y	48	ASP	CB-CG-OD1	-5.50	113.35	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	118	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	O	318	ASP	CB-CG-OD1	5.47	123.23	118.30
1	O	398	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	O	173	MET	N-CA-CB	5.46	120.42	110.60
1	Y	83	ARG	CA-C-N	5.43	129.14	117.20
1	O	201	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	O	211	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	O	242	ILE	CB-CA-C	-5.39	100.82	111.60
1	Y	317	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	O	133	ASP	CB-CG-OD1	5.38	123.14	118.30
1	O	71	SER	N-CA-CB	-5.34	102.49	110.50
1	Y	147	HIS	CA-CB-CG	-5.34	104.52	113.60
1	Y	208	ASP	CB-CG-OD2	5.34	123.11	118.30
1	Y	443	ALA	N-CA-CB	5.34	117.57	110.10
1	O	325	ASP	CB-CG-OD1	5.33	123.09	118.30
1	Y	24	ASP	CB-CG-OD2	5.33	123.09	118.30
1	O	282	SER	N-CA-CB	5.32	118.48	110.50
1	O	386	TYR	CG-CD2-CE2	-5.30	117.06	121.30
1	O	227	THR	C-N-CA	-5.30	108.45	121.70
1	Y	56	GLN	N-CA-CB	5.30	120.13	110.60
1	O	468	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	Y	184	THR	CA-CB-CG2	-5.28	105.01	112.40
1	Y	146	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	Y	118	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	O	45	VAL	CA-CB-CG1	-5.24	103.04	110.90
1	Y	438	VAL	CA-CB-CG2	-5.23	103.05	110.90
1	O	288	THR	CA-CB-CG2	-5.21	105.11	112.40
1	Y	13	THR	CA-CB-CG2	-5.21	105.11	112.40
1	Y	125	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	Y	391	VAL	CA-CB-CG1	-5.19	103.12	110.90
1	Y	445	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	O	48	ASP	N-CA-CB	5.16	119.89	110.60
1	O	86	THR	CA-CB-CG2	-5.15	105.18	112.40
1	Y	7	VAL	CA-CB-CG2	-5.15	103.18	110.90
1	Y	465	VAL	CA-CB-CG1	-5.13	103.20	110.90
1	O	257	LYS	N-CA-CB	5.13	119.84	110.60
1	O	323	ILE	CA-CB-CG1	-5.13	101.25	111.00
1	Y	208	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	Y	471	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	Y	244	GLY	N-CA-C	-5.13	100.28	113.10
1	O	407	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	O	352	GLY	C-N-CA	-5.11	108.93	121.70

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	198	ASP	CB-CG-OD1	5.10	122.89	118.30
1	O	17	ARG	N-CA-CB	5.10	119.78	110.60
1	Y	402	ARG	CD-NE-CZ	5.09	130.73	123.60
1	Y	390	ASP	CB-CA-C	-5.08	100.23	110.40
1	Y	265	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	O	458	ASP	CB-CG-OD2	5.08	122.87	118.30
1	O	55	THR	CA-CB-CG2	-5.08	105.29	112.40
1	O	198	ASP	CB-CG-OD1	5.07	122.86	118.30
1	O	376	ILE	CB-CA-C	-5.06	101.47	111.60
1	Y	107	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	Y	83	ARG	O-C-N	-5.05	114.62	122.70
1	Y	454	TRP	C-N-CA	-5.05	109.08	121.70
1	Y	173	MET	CG-SD-CE	-5.05	92.12	100.20
1	Y	351	LEU	CA-C-N	5.04	126.29	116.20
1	Y	55	THR	CA-CB-CG2	-5.02	105.38	112.40
1	Y	201	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	O	85	THR	N-CA-CB	-5.00	100.79	110.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3910	0	3841	661	0
1	Y	3910	0	3841	537	1
2	O	1	0	0	0	0
2	Y	1	0	0	0	0
3	O	33	0	12	2	0
3	Y	33	0	12	3	0
4	O	6	0	8	2	0
4	Y	6	0	8	1	0
All	All	7900	0	7722	1195	1

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 76.

All (1195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:458:ASP:HA	1:Y:461:GLN:HG3	1.24	1.17
1:Y:74:ILE:HD11	1:Y:237:ILE:HG13	1.21	1.13
1:Y:229:ILE:HG21	1:Y:237:ILE:HG12	1.31	1.11
1:Y:459:GLU:HB2	1:Y:460:LEU:HD12	1.32	1.07
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.37	1.05
1:Y:476:THR:O	1:Y:480:ASN:ND2	1.88	1.04
1:O:74:ILE:HD11	1:O:237:ILE:HG13	1.39	1.03
1:O:313:ILE:HD11	1:O:381:LEU:HD23	1.40	1.02
1:O:229:ILE:HG21	1:O:237:ILE:HG12	1.41	1.00
1:Y:24:ASP:HB2	1:Y:26:ASN:HD21	1.27	0.99
1:Y:250:LEU:HD11	1:Y:255:CYS:HB2	1.43	0.99
1:Y:230:GLY:HA2	1:Y:235:THR:HB	1.43	0.99
1:O:137:SER:HA	1:O:140:LYS:HD2	1.44	0.97
1:Y:104:GLN:HG3	1:Y:349:THR:HG21	1.45	0.97
1:O:155:ALA:HB1	1:O:210:PRO:HG2	1.46	0.96
1:Y:325:ASP:HB3	1:Y:327:TYR:HB3	1.47	0.95
1:Y:154:ARG:HA	1:Y:157:ARG:HG2	1.49	0.94
1:O:476:THR:O	1:O:480:ASN:ND2	2.01	0.93
1:O:114:HIS:HA	1:O:117:ARG:NH1	1.84	0.92
1:Y:211:ARG:HG3	1:Y:211:ARG:HH11	1.34	0.92
1:O:314:GLN:HG2	1:O:317:ARG:HH12	1.32	0.92
1:Y:492:ARG:HG2	1:Y:492:ARG:HH11	1.34	0.92
1:O:180:VAL:HG23	1:O:216:GLU:HB3	1.50	0.91
1:Y:24:ASP:HB2	1:Y:26:ASN:ND2	1.85	0.91
1:O:251:PHE:CE2	1:O:446:LEU:HD13	2.06	0.90
1:O:480:ASN:ND2	1:O:480:ASN:H	1.64	0.90
1:O:95:LYS:HG3	1:O:96:PRO:HD2	1.53	0.89
1:Y:230:GLY:HA2	1:Y:235:THR:CB	2.03	0.89
1:O:278:LYS:HZ1	1:O:280:VAL:HB	1.38	0.89
1:O:278:LYS:NZ	1:O:280:VAL:HB	1.87	0.89
1:O:314:GLN:HG2	1:O:317:ARG:NH1	1.88	0.88
1:O:228:ASN:HD21	1:O:235:THR:N	1.71	0.88
1:O:253:GLN:HG3	1:O:407:ARG:HD2	1.56	0.88
1:O:5:TYR:HB2	1:O:74:ILE:HG22	1.53	0.88
1:Y:69:ILE:HG23	1:Y:73:GLN:HG3	1.56	0.88
1:O:193:ASN:HB3	1:O:196:THR:HG21	1.56	0.88
1:Y:468:ARG:HD2	1:Y:469:GLU:N	1.89	0.87
1:Y:124:ILE:HD13	1:Y:203:MET:CE	2.03	0.87
1:O:47:HIS:CB	1:O:52:ILE:HD11	2.04	0.87
1:O:17:ARG:HH22	1:O:437:GLU:HG2	1.39	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:250:LEU:CD1	1:Y:255:CYS:HB2	2.05	0.86
1:O:193:ASN:HB3	1:O:196:THR:CG2	2.03	0.86
1:O:415:ASN:ND2	1:O:418:LEU:H	1.73	0.86
1:Y:460:LEU:HD12	1:Y:460:LEU:H	1.41	0.86
1:Y:229:ILE:HG21	1:Y:237:ILE:CG1	2.06	0.85
1:O:183:TYR:HB3	1:O:290:ILE:HG21	1.57	0.85
1:Y:293:GLY:HA2	1:Y:299:ASN:ND2	1.91	0.85
1:Y:314:GLN:HG2	1:Y:317:ARG:HH12	1.41	0.84
1:O:402:ARG:HB3	1:O:402:ARG:HH11	1.41	0.84
1:Y:458:ASP:HA	1:Y:461:GLN:CG	2.05	0.84
1:O:115:LEU:HD12	1:O:115:LEU:H	1.43	0.84
1:O:313:ILE:HD11	1:O:381:LEU:CD2	2.07	0.84
1:O:47:HIS:HB2	1:O:52:ILE:HD11	1.60	0.83
1:O:221:SER:HB3	1:O:296:GLY:HA3	1.61	0.83
1:O:240:SER:HB2	1:O:450:ALA:CB	2.07	0.83
1:O:155:ALA:CB	1:O:210:PRO:HG2	2.07	0.83
1:O:254:LEU:HD11	1:O:445:TYR:HE2	1.41	0.83
1:O:137:SER:O	1:O:138:GLY:C	2.12	0.83
1:O:389:ARG:HB2	1:O:426:LEU:CD1	2.08	0.83
1:O:17:ARG:HA	1:O:59:THR:HG21	1.59	0.83
1:O:83:ARG:HB2	4:O:600:GOL:H12	1.59	0.82
1:Y:415:ASN:ND2	1:Y:418:LEU:H	1.78	0.82
1:O:351:LEU:HD22	1:O:360:ALA:CB	2.09	0.82
1:O:455:GLN:O	1:O:456:ASN:HB2	1.79	0.81
1:Y:124:ILE:HD13	1:Y:203:MET:HE3	1.62	0.80
1:Y:74:ILE:CD1	1:Y:237:ILE:HG13	2.05	0.80
1:O:33:ARG:CZ	1:O:58:TRP:HB3	2.11	0.80
1:Y:434:GLU:HB2	1:Y:465:VAL:HB	1.63	0.80
1:Y:17:ARG:HG2	1:Y:32:GLN:HG3	1.64	0.79
1:O:59:THR:O	1:O:63:VAL:HG23	1.82	0.79
1:O:120:LEU:O	1:O:121:GLU:C	2.17	0.79
1:O:211:ARG:HG3	1:O:211:ARG:HH11	1.45	0.79
1:Y:48:ASP:O	1:Y:52:ILE:HD12	1.83	0.79
1:Y:246:GLN:HG3	1:Y:262:LYS:NZ	1.98	0.79
1:O:19:VAL:CG1	1:O:27:ILE:HD13	2.12	0.79
1:O:206:VAL:HG12	1:O:207:LEU:CD2	2.12	0.79
1:O:199:TRP:CE2	1:O:214:LEU:HD23	2.16	0.79
1:O:70:SER:HB2	1:O:72:ASP:OD1	1.83	0.79
1:Y:60:LEU:O	1:Y:63:VAL:HG23	1.84	0.78
1:O:463:LYS:HE2	1:O:463:LYS:HA	1.65	0.78
1:Y:61:VAL:O	1:Y:62:GLU:C	2.20	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:199:TRP:CD1	1:O:214:LEU:HD23	2.17	0.78
1:O:86:THR:OG1	1:O:137:SER:HB3	1.84	0.78
1:O:250:LEU:HD11	1:O:255:CYS:HB2	1.66	0.78
1:Y:463:LYS:HA	1:Y:463:LYS:CE	2.13	0.78
1:Y:137:SER:O	1:Y:141:VAL:HG23	1.83	0.77
1:Y:31:SER:OG	1:Y:59:THR:HA	1.84	0.77
1:Y:261:ALA:HB2	1:Y:273:MET:HB2	1.66	0.77
1:O:253:GLN:CG	1:O:407:ARG:HD2	2.14	0.77
1:O:360:ALA:O	1:O:361:ARG:HD3	1.84	0.77
1:O:463:LYS:HA	1:O:463:LYS:CE	2.12	0.77
1:O:183:TYR:CE1	1:O:217:VAL:HG12	2.19	0.77
1:O:3:LYS:HA	1:O:73:GLN:HA	1.65	0.77
1:Y:84:GLU:HB2	1:Y:103:TRP:HB3	1.66	0.76
1:O:55:THR:HA	1:O:58:TRP:CD1	2.19	0.76
1:Y:58:TRP:O	1:Y:59:THR:C	2.24	0.76
1:Y:69:ILE:HG23	1:Y:73:GLN:CG	2.15	0.76
1:Y:246:GLN:HG2	1:Y:270:PHE:HB2	1.68	0.76
1:Y:229:ILE:HG23	1:Y:235:THR:O	1.85	0.76
1:O:186:ALA:O	1:O:189:THR:HG23	1.85	0.76
1:Y:154:ARG:CB	1:Y:159:GLU:HB3	2.16	0.76
1:Y:432:ARG:HG2	1:Y:436:ARG:HH12	1.51	0.75
1:O:226:GLN:NE2	1:O:236:ARG:HB3	2.02	0.75
1:Y:185:ASN:HD21	1:Y:244:GLY:N	1.83	0.75
1:O:184:THR:HG22	1:O:290:ILE:O	1.87	0.75
1:Y:117:ARG:CB	1:Y:117:ARG:HH11	2.00	0.75
1:Y:70:SER:HB2	1:Y:72:ASP:OD1	1.87	0.74
1:Y:104:GLN:CG	1:Y:349:THR:HG21	2.16	0.74
1:Y:193:ASN:HB3	1:Y:196:THR:HG21	1.69	0.74
1:O:24:ASP:HB2	1:O:26:ASN:ND2	2.02	0.74
1:O:373:ALA:O	1:O:377:ILE:HG13	1.87	0.74
1:O:17:ARG:CA	1:O:59:THR:HG21	2.16	0.74
1:O:185:ASN:O	1:O:188:ARG:HB2	1.88	0.74
1:Y:271:MET:C	1:Y:272:LEU:HD12	2.07	0.74
1:Y:186:ALA:O	1:Y:189:THR:HG23	1.87	0.74
1:Y:221:SER:HB3	1:Y:446:LEU:HD12	1.69	0.74
1:O:206:VAL:HG12	1:O:207:LEU:HD22	1.68	0.73
1:Y:392:LEU:HD23	1:Y:393:GLU:N	2.02	0.73
1:O:219:ARG:HG2	1:O:222:GLU:HB3	1.69	0.73
1:O:279:ALA:HB2	1:O:300:TYR:CD1	2.23	0.73
1:O:24:ASP:HB2	1:O:26:ASN:HD21	1.53	0.73
1:O:181:THR:HG23	1:O:182:ASP:O	1.89	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:271:MET:C	1:O:272:LEU:HD12	2.09	0.73
1:Y:183:TYR:CD1	1:Y:217:VAL:HG12	2.24	0.73
1:Y:183:TYR:CE1	1:Y:217:VAL:HG12	2.24	0.73
1:O:102:VAL:HG12	1:O:103:TRP:CD1	2.23	0.72
1:O:325:ASP:HB3	1:O:327:TYR:HB3	1.71	0.72
1:O:44:TRP:CE2	1:O:107:ARG:HB2	2.24	0.72
1:Y:145:LEU:HD12	1:Y:151:SER:HB2	1.71	0.72
1:Y:130:LEU:HD13	1:Y:136:PHE:CD1	2.25	0.72
1:O:250:LEU:CD1	1:O:255:CYS:HB2	2.18	0.72
1:O:144:ILE:HD12	1:O:144:ILE:H	1.55	0.72
1:Y:478:GLU:O	1:Y:481:TYR:HB3	1.90	0.72
1:O:152:ARG:O	1:O:155:ALA:HB3	1.91	0.71
1:Y:106:ARG:HD2	1:Y:349:THR:O	1.91	0.71
1:O:434:GLU:HB2	1:O:465:VAL:HB	1.72	0.71
1:Y:180:VAL:HG23	1:Y:216:GLU:HB3	1.72	0.71
1:Y:451:VAL:HG13	1:Y:453:PHE:H	1.55	0.71
1:Y:324:ASN:N	1:Y:324:ASN:ND2	2.38	0.71
1:Y:456:ASN:OD1	1:Y:459:GLU:HG3	1.90	0.71
1:O:332:PHE:O	1:O:335:LYS:HB2	1.90	0.71
1:Y:458:ASP:CA	1:Y:461:GLN:HG3	2.14	0.71
1:O:87:ILE:HD13	1:O:168:TRP:HB2	1.73	0.71
1:Y:193:ASN:HB3	1:Y:196:THR:CG2	2.20	0.71
1:O:254:LEU:HD11	1:O:445:TYR:CE2	2.25	0.71
1:O:435:VAL:HG22	1:O:436:ARG:H	1.56	0.71
1:Y:180:VAL:CG2	1:Y:218:ARG:HG2	2.21	0.70
1:Y:459:GLU:HB2	1:Y:460:LEU:CD1	2.18	0.70
1:O:179:HIS:CE1	1:O:215:PRO:HB3	2.26	0.70
1:Y:51:GLU:O	1:Y:55:THR:HG23	1.90	0.70
1:O:158:GLY:HA2	1:O:212:GLU:HB3	1.71	0.70
1:O:80:THR:HG21	1:O:248:ALA:CB	2.22	0.70
1:O:354:PRO:HD2	1:O:355:TYR:CD2	2.27	0.70
1:Y:2:GLU:O	1:Y:73:GLN:HA	1.90	0.70
1:O:200:ASP:OD1	1:O:202:LYS:HB2	1.91	0.70
1:Y:45:VAL:O	1:Y:102:VAL:HG23	1.92	0.70
1:Y:74:ILE:HD12	1:Y:74:ILE:O	1.91	0.70
1:Y:140:LYS:O	1:Y:144:ILE:HD12	1.92	0.70
1:Y:269:CYS:HB2	1:Y:306:VAL:HB	1.74	0.70
1:O:227:THR:O	1:O:229:ILE:HG22	1.92	0.70
1:Y:27:ILE:HD11	1:Y:30:VAL:HG23	1.73	0.70
1:O:95:LYS:HG3	1:O:96:PRO:CD	2.20	0.70
1:O:199:TRP:CD2	1:O:214:LEU:HD23	2.25	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:435:VAL:HG22	1:O:436:ARG:N	2.07	0.70
1:Y:253:GLN:HG3	1:Y:407:ARG:HD2	1.73	0.70
1:O:47:HIS:HB3	1:O:52:ILE:HD11	1.72	0.70
1:O:87:ILE:HD13	1:O:168:TRP:CB	2.22	0.69
1:Y:22:ASP:OD2	1:Y:26:ASN:HB2	1.90	0.69
1:Y:180:VAL:HG21	1:Y:218:ARG:HG2	1.73	0.69
1:Y:415:ASN:HD22	1:Y:418:LEU:H	1.40	0.69
1:O:211:ARG:HG3	1:O:211:ARG:NH1	2.03	0.69
1:O:196:THR:O	1:O:197:LEU:C	2.27	0.69
1:O:415:ASN:HD21	1:O:417:PHE:HB3	1.58	0.69
1:O:251:PHE:CE1	1:O:256:VAL:HG21	2.26	0.69
1:O:17:ARG:HH22	1:O:437:GLU:CG	2.05	0.69
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.75	0.69
1:O:210:PRO:O	1:O:213:MET:HG2	1.91	0.69
1:O:222:GLU:O	1:O:240:SER:HA	1.93	0.69
1:O:20:VAL:CG2	1:O:63:VAL:HG11	2.23	0.69
1:O:293:GLY:HA2	1:O:299:ASN:ND2	2.08	0.69
1:O:389:ARG:HB2	1:O:426:LEU:HD11	1.75	0.69
1:Y:111:ILE:HG22	1:Y:115:LEU:CD1	2.23	0.69
1:O:441:LEU:HD22	1:O:445:TYR:OH	1.92	0.69
1:O:463:LYS:HZ3	1:O:465:VAL:HG23	1.57	0.69
1:Y:250:LEU:O	1:Y:250:LEU:HD12	1.93	0.69
1:O:179:HIS:CD2	1:O:215:PRO:HB3	2.28	0.68
1:Y:48:ASP:C	1:Y:52:ILE:HD12	2.13	0.68
1:Y:127:ASN:HB3	1:Y:193:ASN:ND2	2.07	0.68
1:Y:210:PRO:O	1:Y:213:MET:HG2	1.94	0.68
1:O:26:ASN:O	1:O:28:ILE:HD13	1.93	0.68
1:O:227:THR:OG1	1:O:239:ILE:HD11	1.94	0.68
1:O:340:ASN:ND2	1:O:371:VAL:HG22	2.09	0.68
1:Y:253:GLN:CG	1:Y:407:ARG:HD2	2.24	0.68
1:Y:448:GLY:O	1:Y:451:VAL:HG12	1.93	0.68
1:Y:115:LEU:HD12	1:Y:115:LEU:H	1.59	0.68
1:Y:5:TYR:HB2	1:Y:74:ILE:HG22	1.75	0.67
1:Y:155:ALA:HA	1:Y:160:LEU:HB2	1.76	0.67
1:Y:180:VAL:HG22	1:Y:181:THR:H	1.58	0.67
1:O:20:VAL:HG12	1:O:21:MET:N	2.09	0.67
1:Y:202:LYS:O	1:Y:205:GLU:HG3	1.93	0.67
1:Y:468:ARG:HD2	1:Y:469:GLU:H	1.60	0.67
1:Y:144:ILE:O	1:Y:148:VAL:HG23	1.95	0.67
1:O:230:GLY:HA2	1:O:235:THR:OG1	1.95	0.67
1:Y:47:HIS:HB3	1:Y:52:ILE:HD11	1.77	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:390:ASP:HA	1:Y:483:TYR:OH	1.94	0.67
1:O:140:LYS:O	1:O:144:ILE:HD12	1.95	0.67
1:O:47:HIS:O	1:O:49:PRO:HD3	1.94	0.67
1:O:88:VAL:O	1:O:97:ILE:HG12	1.94	0.67
1:Y:130:LEU:HD23	1:Y:130:LEU:N	2.07	0.67
1:O:5:TYR:HE2	1:O:73:GLN:HG3	1.60	0.67
1:Y:422:GLN:NE2	1:Y:426:LEU:HD22	2.10	0.66
1:Y:170:ILE:HA	1:Y:173:MET:HG3	1.76	0.66
1:Y:463:LYS:HA	1:Y:463:LYS:HE2	1.75	0.66
1:Y:480:ASN:ND2	1:Y:480:ASN:H	1.94	0.66
1:Y:221:SER:CB	1:Y:450:ALA:HB2	2.25	0.66
1:O:90:GLU:N	1:O:95:LYS:O	2.29	0.66
1:O:154:ARG:HA	1:O:157:ARG:CG	2.25	0.66
1:O:435:VAL:HG11	1:O:441:LEU:HD11	1.76	0.66
1:Y:388:THR:O	1:Y:391:VAL:HG13	1.95	0.66
1:O:169:LEU:O	1:O:172:LYS:HB2	1.94	0.66
1:O:199:TRP:CG	1:O:214:LEU:HD23	2.30	0.66
1:Y:9:LEU:HG	1:Y:56:GLN:HE21	1.60	0.66
1:Y:222:GLU:O	1:Y:240:SER:HA	1.95	0.66
1:Y:127:ASN:HB3	1:Y:193:ASN:HD22	1.58	0.66
1:O:476:THR:O	1:O:477:THR:C	2.31	0.66
1:Y:84:GLU:OE2	1:Y:188:ARG:HD2	1.96	0.66
1:Y:449:LEU:HD12	1:Y:449:LEU:O	1.95	0.66
1:O:279:ALA:HB2	1:O:300:TYR:CE1	2.31	0.66
1:O:286:LEU:C	1:O:287:LEU:HD23	2.15	0.66
1:Y:314:GLN:HG2	1:Y:317:ARG:NH1	2.11	0.66
1:O:74:ILE:HD12	1:O:74:ILE:O	1.96	0.66
1:Y:197:LEU:HD13	1:Y:197:LEU:H	1.60	0.66
1:O:460:LEU:HD12	1:O:460:LEU:N	2.11	0.66
1:O:463:LYS:NZ	1:O:465:VAL:HG23	2.10	0.66
1:Y:81:ASN:N	1:Y:81:ASN:HD22	1.94	0.65
1:O:396:GLN:O	1:O:400:GLY:N	2.29	0.65
1:O:480:ASN:ND2	1:O:480:ASN:N	2.40	0.65
1:Y:33:ARG:HG3	1:Y:33:ARG:HH11	1.60	0.65
1:Y:467:GLU:HG2	1:Y:468:ARG:N	2.07	0.65
1:O:48:ASP:HB3	1:O:51:GLU:HB3	1.78	0.65
1:O:106:ARG:NH2	1:O:133:ASP:OD1	2.30	0.65
1:O:229:ILE:CG2	1:O:237:ILE:HG12	2.22	0.65
1:Y:184:THR:O	1:Y:187:SER:HB3	1.97	0.65
1:Y:212:GLU:N	1:Y:212:GLU:OE1	2.29	0.65
1:Y:373:ALA:O	1:Y:377:ILE:HG13	1.96	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:146:ASP:OD1	1:O:146:ASP:N	2.29	0.65
1:O:275:THR:HG21	1:O:280:VAL:CG1	2.27	0.65
1:Y:496:TRP:HZ3	1:O:492:ARG:HD3	1.62	0.65
1:O:144:ILE:O	1:O:148:VAL:HG23	1.97	0.65
1:Y:142:LYS:NZ	1:Y:146:ASP:OD2	2.30	0.65
1:Y:152:ARG:O	1:Y:155:ALA:HB3	1.97	0.65
1:O:487:LYS:HA	1:O:490:VAL:HG23	1.79	0.65
1:O:177:ARG:NH1	1:O:226:GLN:O	2.29	0.65
1:O:415:ASN:O	1:O:419:MET:HG2	1.97	0.65
1:Y:180:VAL:HG21	1:Y:218:ARG:CG	2.27	0.65
1:O:69:ILE:HD13	1:O:69:ILE:N	2.12	0.65
1:O:124:ILE:HD13	1:O:203:MET:CE	2.27	0.65
1:O:476:THR:HG22	1:O:477:THR:H	1.60	0.65
1:Y:20:VAL:C	1:Y:21:MET:HG3	2.17	0.65
1:Y:435:VAL:HG22	1:Y:436:ARG:N	2.11	0.65
1:O:35:PHE:HB2	1:O:51:GLU:CG	2.26	0.65
1:O:170:ILE:O	1:O:171:TRP:C	2.35	0.65
1:O:161:LEU:HD21	1:O:179:HIS:NE2	2.12	0.64
1:O:429:ARG:HD3	1:O:469:GLU:OE1	1.97	0.64
1:Y:161:LEU:HD22	1:Y:179:HIS:CE1	2.32	0.64
1:Y:262:LYS:HE3	1:Y:270:PHE:O	1.96	0.64
1:Y:460:LEU:H	1:Y:460:LEU:CD1	2.11	0.64
1:O:40:PRO:HG2	1:O:44:TRP:CB	2.27	0.64
1:Y:111:ILE:HG21	1:Y:139:THR:HG22	1.77	0.64
1:Y:460:LEU:HD12	1:Y:460:LEU:N	2.11	0.64
1:O:89:TRP:HB2	1:O:95:LYS:C	2.17	0.64
1:Y:19:VAL:HG13	1:Y:27:ILE:HD13	1.78	0.64
1:O:201:ASP:O	1:O:205:GLU:HG2	1.96	0.64
1:Y:227:THR:O	1:Y:229:ILE:HG22	1.96	0.64
1:O:193:ASN:N	1:O:198:ASP:O	2.29	0.64
1:O:439:THR:HG22	1:O:440:ALA:N	2.12	0.64
1:Y:68:ASP:C	1:Y:69:ILE:HD13	2.17	0.64
1:Y:81:ASN:N	1:Y:81:ASN:ND2	2.46	0.64
1:Y:246:GLN:HG3	1:Y:262:LYS:HZ3	1.61	0.64
1:O:61:VAL:HA	1:O:64:LEU:HD13	1.80	0.64
1:O:84:GLU:N	1:O:84:GLU:OE1	2.31	0.64
1:O:228:ASN:HB2	1:O:236:ARG:HE	1.62	0.64
1:Y:419:MET:HA	1:Y:419:MET:CE	2.28	0.64
1:O:391:VAL:O	1:O:392:LEU:C	2.33	0.64
1:O:474:ILE:HG23	1:O:478:GLU:HB3	1.79	0.64
1:Y:61:VAL:HG12	1:Y:62:GLU:N	2.13	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:262:LYS:NZ	1:Y:264:THR:HB	2.13	0.64
1:Y:382:GLU:HG2	1:Y:421:PHE:CE2	2.32	0.64
1:Y:432:ARG:HD2	1:Y:436:ARG:NH2	2.13	0.64
1:O:156:ARG:HB2	1:O:156:ARG:CZ	2.27	0.64
1:O:354:PRO:HD2	1:O:355:TYR:CE2	2.33	0.64
1:O:432:ARG:O	1:O:467:GLU:N	2.31	0.64
1:O:455:GLN:O	1:O:456:ASN:CB	2.45	0.64
1:O:63:VAL:O	1:O:66:LYS:HG2	1.99	0.63
1:O:386:TYR:HB3	1:O:486:TRP:CE2	2.33	0.63
1:Y:69:ILE:HD13	1:Y:69:ILE:N	2.11	0.63
1:Y:498:GLU:OE1	1:Y:498:GLU:HA	1.99	0.63
1:O:497:GLU:HA	1:O:497:GLU:OE1	1.98	0.63
1:Y:31:SER:HB2	1:Y:62:GLU:HB3	1.80	0.63
1:O:183:TYR:CD1	1:O:217:VAL:HG12	2.33	0.63
1:Y:4:LYS:N	1:Y:73:GLN:O	2.31	0.63
1:O:5:TYR:O	1:O:75:ALA:N	2.29	0.63
1:O:310:GLY:HA3	3:O:601:ATF:O3'	1.99	0.63
1:Y:85:THR:HA	1:Y:101:ILE:O	1.98	0.63
1:Y:157:ARG:HG3	1:Y:159:GLU:OE1	1.98	0.63
1:O:123:TYR:CD2	1:O:203:MET:HE2	2.33	0.63
1:Y:463:LYS:HZ3	1:Y:465:VAL:HG23	1.63	0.63
1:O:199:TRP:NE1	1:O:214:LEU:HD23	2.13	0.63
1:O:390:ASP:HA	1:O:483:TYR:OH	1.98	0.63
1:Y:170:ILE:HA	1:Y:173:MET:CG	2.29	0.63
1:O:50:MET:O	1:O:54:ALA:N	2.28	0.63
1:Y:80:THR:HG21	1:Y:248:ALA:CB	2.28	0.63
1:Y:197:LEU:HD13	1:Y:197:LEU:N	2.11	0.63
1:Y:207:LEU:HB3	1:Y:209:ILE:HD12	1.80	0.63
1:Y:196:THR:HG22	1:Y:198:ASP:H	1.64	0.62
1:Y:205:GLU:O	1:Y:208:ASP:N	2.31	0.62
1:O:113:GLU:O	1:O:116:LYS:HB2	1.98	0.62
1:O:184:THR:HA	1:O:290:ILE:HG22	1.81	0.62
1:O:456:ASN:OD1	1:O:458:ASP:HB2	2.00	0.62
1:Y:146:ASP:OD1	1:Y:146:ASP:N	2.29	0.62
1:O:84:GLU:HB2	1:O:103:TRP:CB	2.29	0.62
1:O:419:MET:HE2	1:O:419:MET:HA	1.79	0.62
1:O:32:GLN:HA	1:O:59:THR:HG23	1.82	0.62
1:O:183:TYR:CB	1:O:290:ILE:HG21	2.29	0.62
1:O:272:LEU:HD21	1:O:303:GLU:OE1	1.99	0.62
1:O:133:ASP:OD1	1:O:135:TYR:N	2.31	0.62
1:Y:22:ASP:O	1:Y:25:ALA:N	2.31	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:433:PRO:HA	1:Y:466:ILE:HD13	1.80	0.62
1:Y:451:VAL:CG1	1:Y:453:PHE:H	2.12	0.62
1:Y:156:ARG:CZ	1:Y:156:ARG:HB2	2.28	0.62
1:Y:179:HIS:CD2	1:Y:215:PRO:HA	2.35	0.62
1:O:19:VAL:HG13	1:O:27:ILE:HD13	1.82	0.62
1:O:202:LYS:O	1:O:205:GLU:HG3	2.00	0.62
1:O:3:LYS:HA	1:O:73:GLN:CA	2.29	0.62
1:O:114:HIS:O	1:O:117:ARG:N	2.32	0.62
1:O:351:LEU:HD22	1:O:360:ALA:HB1	1.82	0.62
1:Y:47:HIS:O	1:Y:49:PRO:HD3	2.00	0.61
1:O:81:ASN:N	1:O:81:ASN:HD22	1.97	0.61
1:O:287:LEU:O	1:O:302:LEU:HD23	2.00	0.61
1:Y:67:ALA:CB	1:Y:69:ILE:HG12	2.30	0.61
1:Y:154:ARG:O	1:Y:155:ALA:C	2.33	0.61
1:Y:174:THR:O	1:Y:176:GLY:N	2.30	0.61
1:O:69:ILE:HG23	1:O:73:GLN:HG3	1.81	0.61
1:O:110:GLU:O	1:O:113:GLU:HB2	2.00	0.61
1:O:17:ARG:NH2	1:O:437:GLU:HG2	2.13	0.61
1:O:207:LEU:HB3	1:O:209:ILE:CD1	2.30	0.61
1:Y:181:THR:HG23	1:Y:182:ASP:O	2.00	0.61
1:O:185:ASN:HD21	1:O:244:GLY:CA	2.12	0.61
1:O:322:LEU:N	1:O:322:LEU:HD23	2.14	0.61
1:O:478:GLU:HA	1:O:478:GLU:OE1	2.00	0.61
1:O:20:VAL:C	1:O:21:MET:HG3	2.20	0.61
1:O:47:HIS:CD2	1:O:82:GLN:HE22	2.18	0.61
1:O:113:GLU:O	1:O:114:HIS:C	2.38	0.61
1:Y:478:GLU:HA	1:Y:478:GLU:OE1	1.98	0.61
1:O:297:GLU:OE1	1:O:297:GLU:N	2.30	0.61
1:O:498:GLU:OE1	1:O:498:GLU:HA	2.00	0.61
1:Y:71:SER:HB2	1:Y:235:THR:HG21	1.83	0.61
1:Y:211:ARG:HG3	1:Y:211:ARG:NH1	2.10	0.61
1:O:74:ILE:CD1	1:O:237:ILE:HG13	2.25	0.61
1:Y:222:GLU:HG3	1:Y:223:VAL:N	2.15	0.61
1:Y:402:ARG:HB3	1:Y:402:ARG:HH11	1.66	0.61
1:O:90:GLU:HB3	1:O:93:THR:HG23	1.83	0.61
1:Y:149:GLU:HA	1:Y:149:GLU:OE1	2.00	0.60
1:Y:310:GLY:O	1:Y:313:ILE:HB	2.01	0.60
1:O:41:LYS:CG	1:O:42:PRO:HD2	2.31	0.60
1:O:143:TRP:CE3	1:O:144:ILE:HA	2.36	0.60
1:O:359:TYR:HB2	1:O:495:ALA:HA	1.83	0.60
1:Y:196:THR:O	1:Y:197:LEU:C	2.38	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:425:ILE:O	1:Y:479:ARG:HD2	2.02	0.60
1:Y:432:ARG:HG2	1:Y:436:ARG:NH1	2.16	0.60
1:Y:482:ARG:O	1:Y:483:TYR:C	2.39	0.60
1:O:108:THR:HB	1:O:139:THR:HB	1.83	0.60
1:O:193:ASN:OD1	1:O:196:THR:HB	2.00	0.60
1:Y:196:THR:HG22	1:Y:198:ASP:N	2.16	0.60
1:O:124:ILE:HD13	1:O:203:MET:HE1	1.83	0.60
1:Y:237:ILE:HG23	1:Y:238:PRO:HD2	1.83	0.60
1:Y:362:GLY:HA3	1:O:367:LEU:HB2	1.83	0.60
1:O:68:ASP:C	1:O:69:ILE:HD13	2.22	0.60
1:O:154:ARG:HA	1:O:157:ARG:HG2	1.84	0.60
1:Y:456:ASN:N	1:Y:459:GLU:OE2	2.35	0.60
1:O:90:GLU:HB3	1:O:93:THR:CG2	2.30	0.60
1:O:353:ALA:HB2	1:O:356:TRP:CZ2	2.37	0.60
1:O:88:VAL:HA	1:O:161:LEU:O	2.02	0.60
1:Y:432:ARG:NE	1:Y:467:GLU:OE2	2.34	0.60
1:O:78:GLY:HA2	1:O:447:ALA:HB2	1.83	0.60
1:Y:154:ARG:HB2	1:Y:159:GLU:HB3	1.83	0.59
1:Y:422:GLN:HE21	1:Y:426:LEU:HD22	1.66	0.59
1:O:251:PHE:O	1:O:254:LEU:N	2.32	0.59
1:Y:430:VAL:HB	1:Y:470:PHE:HB2	1.84	0.59
1:O:69:ILE:HG23	1:O:73:GLN:CG	2.32	0.59
1:Y:94:GLY:HA2	1:Y:171:TRP:CH2	2.38	0.59
1:Y:246:GLN:HG3	1:Y:262:LYS:HZ1	1.67	0.59
1:Y:433:PRO:O	1:Y:436:ARG:NH1	2.35	0.59
1:Y:246:GLN:H	1:Y:246:GLN:NE2	1.99	0.59
1:O:222:GLU:HG3	1:O:223:VAL:N	2.17	0.59
1:Y:101:ILE:HD12	1:Y:144:ILE:HD11	1.85	0.59
1:O:179:HIS:NE2	1:O:215:PRO:HB3	2.17	0.59
1:O:179:HIS:CG	1:O:215:PRO:HB3	2.38	0.59
1:Y:80:THR:HG22	1:Y:243:ALA:O	2.03	0.59
1:Y:237:ILE:HG22	1:Y:238:PRO:N	2.18	0.59
1:Y:419:MET:HA	1:Y:419:MET:HE2	1.83	0.59
1:O:103:TRP:HB2	1:O:135:TYR:HE1	1.67	0.59
1:O:108:THR:OG1	1:O:134:PRO:HB3	2.02	0.59
1:O:147:HIS:ND1	1:O:147:HIS:N	2.46	0.59
1:O:170:ILE:HG22	1:O:171:TRP:N	2.16	0.59
1:O:237:ILE:HG23	1:O:238:PRO:HD2	1.85	0.59
1:O:251:PHE:HE1	1:O:256:VAL:HG21	1.68	0.59
1:O:61:VAL:HA	1:O:64:LEU:CD1	2.33	0.59
1:Y:87:ILE:HG22	1:Y:88:VAL:N	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:111:ILE:O	1:Y:115:LEU:HD12	2.03	0.58
1:O:88:VAL:HG22	1:O:162:PHE:HB2	1.85	0.58
1:Y:87:ILE:HD12	1:Y:163:GLY:O	2.03	0.58
1:Y:124:ILE:HD13	1:Y:203:MET:HE1	1.84	0.58
1:O:477:THR:O	1:O:478:GLU:C	2.41	0.58
1:O:166:ASP:O	1:O:167:THR:C	2.42	0.58
1:O:422:GLN:HE21	1:O:426:LEU:HD22	1.67	0.58
1:O:149:GLU:OE1	1:O:149:GLU:HA	2.03	0.58
1:O:387:GLN:O	1:O:390:ASP:HB2	2.04	0.58
1:O:410:GLY:O	1:O:413:VAL:HG13	2.03	0.58
1:O:475:GLU:O	1:O:478:GLU:HB2	2.04	0.58
1:Y:221:SER:OG	1:Y:450:ALA:HB2	2.03	0.58
1:Y:435:VAL:HG22	1:Y:436:ARG:H	1.68	0.58
1:O:81:ASN:N	1:O:81:ASN:ND2	2.51	0.58
1:O:281:LYS:HB2	1:O:281:LYS:NZ	2.19	0.58
1:O:401:ILE:HG22	1:O:402:ARG:N	2.19	0.58
1:O:445:TYR:O	1:O:447:ALA:N	2.37	0.58
1:O:41:LYS:CB	1:O:42:PRO:HD2	2.34	0.58
1:O:153:GLU:O	1:O:157:ARG:HG2	2.03	0.58
1:Y:31:SER:H	1:Y:63:VAL:HG13	1.68	0.58
1:O:140:LYS:O	1:O:143:TRP:HB3	2.04	0.58
1:O:207:LEU:CB	1:O:209:ILE:HD12	2.34	0.58
1:O:389:ARG:HB2	1:O:426:LEU:HD13	1.84	0.58
1:O:476:THR:CG2	1:O:477:THR:N	2.67	0.58
1:Y:206:VAL:HG12	1:Y:207:LEU:N	2.19	0.58
1:Y:310:GLY:HA3	3:Y:601:ATF:O3'	2.04	0.58
1:O:5:TYR:CE2	1:O:73:GLN:HG3	2.38	0.58
1:O:41:LYS:HG3	1:O:42:PRO:HD2	1.84	0.58
1:Y:3:LYS:HA	1:Y:73:GLN:HA	1.84	0.57
1:Y:22:ASP:OD1	1:Y:24:ASP:N	2.36	0.57
1:Y:67:ALA:HB3	1:Y:69:ILE:HG12	1.86	0.57
1:Y:497:GLU:HA	1:Y:497:GLU:OE1	2.03	0.57
1:Y:18:ALA:HB1	1:Y:63:VAL:HG21	1.85	0.57
1:Y:226:GLN:NE2	1:Y:236:ARG:HB3	2.19	0.57
1:O:207:LEU:HB3	1:O:209:ILE:HD12	1.85	0.57
1:O:40:PRO:HD2	1:O:44:TRP:O	2.05	0.57
1:O:230:GLY:HA2	1:O:235:THR:CB	2.33	0.57
1:O:402:ARG:HB3	1:O:402:ARG:NH1	2.15	0.57
1:O:44:TRP:HA	1:O:105:CYS:SG	2.44	0.57
1:Y:104:GLN:NE2	1:Y:308:MET:HE2	2.19	0.57
1:Y:133:ASP:OD1	1:Y:135:TYR:HB2	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:ILE:HD11	1:O:30:VAL:HG23	1.87	0.57
1:Y:482:ARG:NH1	1:Y:482:ARG:HG3	2.20	0.57
1:O:480:ASN:H	1:O:480:ASN:HD22	1.49	0.57
1:O:273:MET:HB2	1:O:395:MET:HE2	1.86	0.57
1:O:473:GLY:C	1:O:474:ILE:HD13	2.25	0.57
1:O:490:VAL:O	1:O:494:MET:HG2	2.05	0.57
1:Y:193:ASN:OD1	1:Y:196:THR:HB	2.04	0.57
1:O:395:MET:O	1:O:396:GLN:C	2.43	0.57
1:Y:117:ARG:HH11	1:Y:117:ARG:CG	2.16	0.57
1:Y:153:GLU:HA	1:Y:153:GLU:OE1	2.04	0.57
1:O:120:LEU:O	1:O:124:ILE:HG12	2.05	0.57
1:O:143:TRP:O	1:O:147:HIS:ND1	2.38	0.57
1:O:85:THR:HG23	1:O:102:VAL:HA	1.86	0.57
1:Y:190:MET:HG2	1:Y:190:MET:O	2.05	0.56
1:Y:483:TYR:O	1:Y:486:TRP:HB3	2.04	0.56
1:O:137:SER:O	1:O:141:VAL:HG23	2.04	0.56
1:O:153:GLU:O	1:O:156:ARG:HB3	2.05	0.56
1:O:348:PHE:HD1	1:O:348:PHE:H	1.52	0.56
1:Y:182:ASP:HB3	1:Y:242:ILE:HB	1.87	0.56
1:O:123:TYR:CE2	1:O:203:MET:HE2	2.40	0.56
1:Y:237:ILE:N	1:Y:237:ILE:HD13	2.20	0.56
1:O:173:MET:O	1:O:227:THR:HG23	2.06	0.56
1:O:218:ARG:HG3	1:O:218:ARG:NH1	2.20	0.56
1:Y:5:TYR:O	1:Y:74:ILE:HA	2.05	0.56
1:Y:444:ALA:O	1:Y:447:ALA:N	2.38	0.56
1:O:17:ARG:HG2	1:O:32:GLN:HG3	1.88	0.56
1:O:40:PRO:HG2	1:O:44:TRP:HB3	1.87	0.56
1:O:90:GLU:O	1:O:94:GLY:N	2.38	0.56
1:O:419:MET:HA	1:O:419:MET:CE	2.35	0.56
1:O:487:LYS:HA	1:O:490:VAL:CG2	2.35	0.56
1:Y:108:THR:OG1	1:Y:134:PRO:HB3	2.05	0.56
1:O:340:ASN:HD22	1:O:371:VAL:HG22	1.70	0.56
1:Y:27:ILE:HD12	1:Y:27:ILE:C	2.27	0.56
1:O:154:ARG:HA	1:O:157:ARG:HG3	1.87	0.56
1:Y:250:LEU:HD11	1:Y:255:CYS:CB	2.27	0.56
1:O:240:SER:O	1:O:447:ALA:HA	2.06	0.56
1:O:254:LEU:CD1	1:O:445:TYR:HE2	2.14	0.56
1:Y:246:GLN:NE2	1:Y:246:GLN:N	2.54	0.56
1:O:433:PRO:O	1:O:436:ARG:NH1	2.38	0.56
1:O:476:THR:HG22	1:O:477:THR:N	2.21	0.56
1:Y:359:TYR:HD2	1:Y:497:GLU:HB3	1.70	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:445:TYR:O	1:Y:449:LEU:HB2	2.05	0.56
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.87	0.56
1:O:154:ARG:CA	1:O:157:ARG:HG2	2.36	0.56
1:Y:20:VAL:HG12	1:Y:21:MET:N	2.20	0.55
1:O:245:ASP:OD1	1:O:246:GLN:N	2.39	0.55
1:O:408:VAL:HG23	1:O:409:ASP:N	2.21	0.55
1:Y:70:SER:O	1:Y:72:ASP:N	2.40	0.55
1:Y:153:GLU:O	1:Y:156:ARG:N	2.39	0.55
1:O:114:HIS:O	1:O:117:ARG:HB2	2.06	0.55
1:O:142:LYS:O	1:O:143:TRP:C	2.44	0.55
1:Y:83:ARG:HB2	4:Y:600:GOL:O2	2.05	0.55
1:Y:492:ARG:HG2	1:Y:492:ARG:NH1	2.11	0.55
1:O:55:THR:HA	1:O:58:TRP:HD1	1.68	0.55
1:O:64:LEU:HD12	1:O:64:LEU:H	1.70	0.55
1:O:115:LEU:H	1:O:115:LEU:CD1	2.16	0.55
1:O:219:ARG:HD3	1:O:222:GLU:HB2	1.88	0.55
1:O:179:HIS:CD2	1:O:215:PRO:HA	2.42	0.55
1:Y:188:ARG:HH22	1:Y:303:GLU:CD	2.10	0.55
1:Y:463:LYS:NZ	1:Y:465:VAL:HG23	2.22	0.55
1:Y:488:LYS:HD2	1:O:496:TRP:CH2	2.41	0.55
1:O:63:VAL:O	1:O:66:LYS:N	2.40	0.55
1:O:275:THR:HB	1:O:278:LYS:O	2.07	0.55
1:O:441:LEU:HD23	1:O:445:TYR:HE1	1.71	0.55
1:Y:150:GLY:O	1:Y:153:GLU:N	2.39	0.55
1:Y:272:LEU:HD21	1:Y:303:GLU:OE1	2.07	0.55
1:Y:396:GLN:O	1:Y:397:ALA:C	2.45	0.55
1:O:103:TRP:HB2	1:O:135:TYR:CE1	2.41	0.55
1:Y:420:GLN:O	1:Y:420:GLN:NE2	2.39	0.55
1:O:144:ILE:O	1:O:145:LEU:C	2.44	0.55
1:O:482:ARG:NH1	1:O:482:ARG:HG3	2.21	0.55
1:Y:308:MET:HB2	1:Y:346:PRO:HB2	1.88	0.55
1:Y:325:ASP:O	1:Y:326:ALA:C	2.42	0.55
1:Y:405:ALA:HB2	1:Y:429:ARG:HD2	1.88	0.55
1:O:14:THR:O	1:O:34:GLU:HG2	2.07	0.55
1:O:180:VAL:CG2	1:O:218:ARG:HG2	2.37	0.55
1:O:340:ASN:HB2	1:O:375:HIS:CD2	2.40	0.55
1:Y:130:LEU:HD13	1:Y:136:PHE:CE1	2.41	0.54
1:Y:282:SER:HA	1:Y:398:ASP:OD2	2.06	0.54
1:Y:325:ASP:HB3	1:Y:327:TYR:CB	2.29	0.54
1:O:206:VAL:HG12	1:O:207:LEU:HD23	1.89	0.54
1:Y:80:THR:HG21	1:Y:248:ALA:HB3	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:219:ARG:HG2	1:Y:222:GLU:HB3	1.89	0.54
1:O:41:LYS:HG3	1:O:42:PRO:CD	2.38	0.54
1:Y:463:LYS:HA	1:Y:463:LYS:HZ3	1.72	0.54
1:O:3:LYS:HG2	1:O:72:ASP:O	2.07	0.54
1:O:6:ILE:HG13	1:O:7:VAL:H	1.71	0.54
1:O:473:GLY:O	1:O:474:ILE:HD13	2.08	0.54
1:O:164:THR:H	1:O:167:THR:HB	1.72	0.54
1:O:219:ARG:NH2	1:O:295:THR:OG1	2.40	0.54
1:O:424:ASP:OD1	1:O:473:GLY:N	2.36	0.54
1:O:4:LYS:N	1:O:73:GLN:O	2.40	0.54
1:Y:20:VAL:O	1:Y:28:ILE:N	2.30	0.54
1:Y:120:LEU:O	1:Y:124:ILE:HG12	2.06	0.54
1:Y:251:PHE:CE2	1:Y:446:LEU:HD22	2.43	0.54
1:Y:480:ASN:O	1:Y:481:TYR:C	2.44	0.54
1:O:166:ASP:OD1	1:O:166:ASP:N	2.38	0.54
1:Y:113:GLU:O	1:Y:116:LYS:HB2	2.08	0.54
1:Y:227:THR:N	1:Y:237:ILE:O	2.29	0.54
1:O:80:THR:CG2	1:O:248:ALA:HB2	2.38	0.54
1:O:180:VAL:HG21	1:O:218:ARG:HG3	1.90	0.54
1:Y:31:SER:N	1:Y:63:VAL:HG13	2.23	0.54
1:O:244:GLY:O	1:O:245:ASP:C	2.41	0.54
1:Y:201:ASP:O	1:Y:202:LYS:C	2.46	0.54
1:O:468:ARG:HG3	1:O:468:ARG:HH11	1.73	0.54
1:Y:221:SER:HB3	1:Y:446:LEU:CD1	2.36	0.53
1:O:90:GLU:OE1	1:O:95:LYS:NZ	2.38	0.53
1:O:193:ASN:HB3	1:O:196:THR:CB	2.38	0.53
1:O:422:GLN:NE2	1:O:426:LEU:HD22	2.23	0.53
1:Y:18:ALA:HB1	1:Y:63:VAL:CG2	2.38	0.53
1:Y:117:ARG:HH11	1:Y:117:ARG:CA	2.21	0.53
1:O:229:ILE:O	1:O:230:GLY:C	2.46	0.53
1:Y:40:PRO:HG3	1:Y:46:GLU:OE2	2.09	0.53
1:Y:468:ARG:HH11	1:Y:468:ARG:CG	2.21	0.53
1:O:20:VAL:HG23	1:O:63:VAL:HG11	1.90	0.53
1:O:40:PRO:HD2	1:O:44:TRP:HB2	1.91	0.53
1:Y:31:SER:CB	1:Y:62:GLU:HB3	2.39	0.53
1:Y:63:VAL:O	1:Y:64:LEU:C	2.46	0.53
1:Y:360:ALA:HB2	1:Y:494:MET:HA	1.91	0.53
1:O:118:ASP:N	1:O:118:ASP:OD1	2.40	0.53
1:Y:74:ILE:CD1	1:Y:237:ILE:HG21	2.39	0.53
1:Y:272:LEU:HD12	1:Y:272:LEU:N	2.24	0.53
1:O:398:ASP:O	1:O:399:SER:C	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:415:ASN:HD22	1:O:418:LEU:H	1.50	0.53
1:O:71:SER:O	1:O:237:ILE:HD11	2.09	0.53
1:O:451:VAL:O	1:O:451:VAL:HG13	2.09	0.53
1:Y:473:GLY:O	1:Y:474:ILE:HD13	2.09	0.53
1:Y:481:TYR:O	1:Y:484:ALA:HB3	2.09	0.53
1:Y:114:HIS:O	1:Y:115:LEU:C	2.47	0.53
1:O:192:PHE:CE2	1:O:217:VAL:HG11	2.44	0.53
1:O:249:ALA:HB2	1:O:439:THR:OG1	2.09	0.53
1:O:346:PRO:HA	1:O:348:PHE:CE1	2.44	0.53
1:O:180:VAL:HG21	1:O:218:ARG:CG	2.39	0.52
1:Y:61:VAL:O	1:Y:63:VAL:N	2.43	0.52
1:Y:387:GLN:O	1:Y:391:VAL:HG12	2.09	0.52
1:Y:463:LYS:HA	1:Y:463:LYS:NZ	2.25	0.52
1:O:21:MET:HB3	1:O:26:ASN:O	2.09	0.52
1:O:188:ARG:HH22	1:O:303:GLU:CD	2.12	0.52
1:O:488:LYS:O	1:O:492:ARG:HD2	2.09	0.52
1:O:35:PHE:HB2	1:O:51:GLU:HG3	1.91	0.52
1:O:123:TYR:HD2	1:O:203:MET:CE	2.23	0.52
1:O:330:GLU:O	1:O:334:THR:HG23	2.10	0.52
1:O:108:THR:HG21	1:O:140:LYS:N	2.25	0.52
1:O:181:THR:HG23	1:O:182:ASP:N	2.25	0.52
1:Y:236:ARG:C	1:Y:237:ILE:HD13	2.29	0.52
1:Y:364:ILE:O	1:O:363:ALA:HB1	2.09	0.52
1:Y:8:ALA:O	1:Y:9:LEU:HD12	2.09	0.52
1:Y:80:THR:CG2	1:Y:248:ALA:HB2	2.39	0.52
1:Y:18:ALA:CB	1:Y:59:THR:HB	2.40	0.52
1:Y:129:GLY:C	1:Y:130:LEU:HD23	2.29	0.52
1:O:33:ARG:NH1	1:O:62:GLU:OE1	2.43	0.52
1:Y:143:TRP:CD2	1:Y:147:HIS:HD2	2.27	0.52
1:Y:177:ARG:NH1	1:Y:226:GLN:O	2.43	0.52
1:O:39:TYR:HA	1:O:44:TRP:O	2.10	0.52
1:O:97:ILE:O	1:O:98:TYR:HB2	2.08	0.52
1:O:445:TYR:O	1:O:448:GLY:N	2.43	0.52
1:Y:74:ILE:HD12	1:Y:74:ILE:C	2.30	0.51
1:Y:246:GLN:HG2	1:Y:270:PHE:CB	2.40	0.51
1:Y:44:TRP:CE2	1:Y:107:ARG:HB2	2.45	0.51
1:Y:240:SER:HB2	1:Y:450:ALA:HB3	1.92	0.51
1:Y:293:GLY:HA3	1:Y:297:GLU:CD	2.30	0.51
1:O:237:ILE:CG2	1:O:238:PRO:HD2	2.40	0.51
1:O:351:LEU:HD22	1:O:360:ALA:HB2	1.92	0.51
1:Y:480:ASN:H	1:Y:480:ASN:HD22	1.57	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:59:THR:O	1:Y:63:VAL:HG22	2.10	0.51
1:Y:49:PRO:HA	1:Y:52:ILE:HD13	1.93	0.51
1:Y:78:GLY:HA2	1:Y:447:ALA:HB2	1.92	0.51
1:Y:271:MET:HE1	1:Y:392:LEU:HB2	1.92	0.51
1:Y:401:ILE:HG22	1:Y:402:ARG:N	2.24	0.51
1:O:173:MET:HB3	1:O:227:THR:HG21	1.93	0.51
1:O:286:LEU:O	1:O:287:LEU:HD23	2.11	0.51
1:O:445:TYR:O	1:O:446:LEU:C	2.48	0.51
1:O:476:THR:O	1:O:477:THR:O	2.28	0.51
1:Y:142:LYS:O	1:Y:145:LEU:N	2.44	0.51
1:Y:143:TRP:CE2	1:Y:147:HIS:CD2	2.99	0.51
1:O:154:ARG:CA	1:O:159:GLU:HB3	2.41	0.51
1:Y:26:ASN:O	1:Y:28:ILE:HD13	2.10	0.51
1:Y:43:GLY:C	1:Y:44:TRP:HD1	2.14	0.51
1:O:125:ARG:HG2	1:O:130:LEU:O	2.11	0.51
1:O:183:TYR:O	1:O:187:SER:HB3	2.11	0.51
1:O:278:LYS:HG2	1:O:279:ALA:N	2.25	0.51
1:Y:395:MET:O	1:Y:396:GLN:C	2.48	0.51
1:O:281:LYS:HB2	1:O:281:LYS:HZ2	1.75	0.51
1:O:406:LEU:HD23	1:O:407:ARG:N	2.25	0.51
1:Y:56:GLN:HG3	1:Y:56:GLN:O	2.11	0.51
1:Y:75:ALA:O	1:Y:238:PRO:HD2	2.11	0.51
1:Y:137:SER:O	1:Y:138:GLY:C	2.49	0.51
1:Y:185:ASN:ND2	1:Y:244:GLY:N	2.55	0.51
1:O:53:TRP:HE3	1:O:169:LEU:CD1	2.24	0.51
1:O:220:SER:O	1:O:224:TYR:OH	2.29	0.51
1:O:251:PHE:CZ	1:O:446:LEU:HD13	2.46	0.51
1:O:346:PRO:HA	1:O:348:PHE:HE1	1.75	0.51
1:Y:71:SER:HB2	1:Y:235:THR:CG2	2.40	0.50
1:O:352:GLY:O	1:O:356:TRP:N	2.34	0.50
1:O:466:ILE:O	1:O:466:ILE:HG22	2.08	0.50
1:Y:117:ARG:HH11	1:Y:117:ARG:HB2	1.77	0.50
1:Y:273:MET:CB	1:Y:395:MET:HE3	2.41	0.50
1:Y:389:ARG:O	1:Y:390:ASP:C	2.48	0.50
1:Y:466:ILE:HG22	1:Y:466:ILE:O	2.11	0.50
1:O:158:GLY:CA	1:O:212:GLU:HB3	2.39	0.50
1:O:395:MET:O	1:O:399:SER:N	2.44	0.50
1:Y:40:PRO:HG3	1:Y:46:GLU:CD	2.32	0.50
1:O:196:THR:HG22	1:O:198:ASP:H	1.77	0.50
1:Y:314:GLN:O	1:Y:318:ASP:N	2.35	0.50
1:O:137:SER:O	1:O:138:GLY:O	2.29	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:228:ASN:HB2	1:O:236:ARG:NE	2.26	0.50
1:O:477:THR:O	1:O:480:ASN:N	2.44	0.50
1:Y:47:HIS:CD2	1:Y:82:GLN:HE22	2.30	0.50
1:O:144:ILE:CG2	1:O:148:VAL:HG21	2.41	0.50
1:O:174:THR:HB	1:O:177:ARG:HB2	1.93	0.50
1:O:317:ARG:HB2	1:O:323:ILE:HG13	1.94	0.50
1:O:408:VAL:O	1:O:409:ASP:HB3	2.11	0.50
1:Y:242:ILE:HG22	1:Y:243:ALA:N	2.26	0.50
1:O:35:PHE:HB2	1:O:51:GLU:CD	2.32	0.50
1:O:113:GLU:O	1:O:114:HIS:O	2.30	0.50
1:O:15:SER:CB	1:O:34:GLU:HA	2.41	0.50
1:O:28:ILE:HG22	1:O:29:SER:N	2.27	0.50
1:Y:94:GLY:CA	1:Y:171:TRP:HH2	2.25	0.50
1:Y:393:GLU:O	1:Y:394:ALA:C	2.50	0.50
1:O:129:GLY:C	1:O:130:LEU:HD23	2.32	0.50
1:O:418:LEU:O	1:O:419:MET:C	2.50	0.50
1:O:444:ALA:O	1:O:445:TYR:O	2.29	0.50
1:O:218:ARG:CG	1:O:218:ARG:HH11	2.25	0.49
1:O:342:VAL:HA	1:O:365:PHE:O	2.12	0.49
1:Y:197:LEU:N	1:Y:197:LEU:HD22	2.27	0.49
1:O:201:ASP:O	1:O:202:LYS:C	2.48	0.49
1:O:216:GLU:OE2	1:O:218:ARG:HD3	2.11	0.49
1:O:303:GLU:HG3	1:O:304:GLY:N	2.28	0.49
1:Y:33:ARG:NH2	1:Y:58:TRP:HB3	2.27	0.49
1:Y:156:ARG:C	1:Y:158:GLY:H	2.15	0.49
1:O:89:TRP:HB2	1:O:95:LYS:O	2.12	0.49
1:Y:89:TRP:HD1	1:Y:90:GLU:O	1.95	0.49
1:O:166:ASP:CG	1:O:167:THR:H	2.14	0.49
1:O:273:MET:HB2	1:O:395:MET:CE	2.42	0.49
1:O:431:GLU:HB3	1:O:466:ILE:HG13	1.93	0.49
1:O:438:VAL:HA	1:O:441:LEU:HD12	1.93	0.49
1:Y:124:ILE:HG21	1:Y:190:MET:CE	2.43	0.49
1:Y:170:ILE:HG22	1:Y:171:TRP:N	2.27	0.49
1:O:44:TRP:N	1:O:44:TRP:CD1	2.80	0.49
1:O:103:TRP:CD1	1:O:103:TRP:N	2.80	0.49
1:O:284:ASN:OD1	1:O:398:ASP:OD1	2.30	0.49
1:Y:71:SER:HB3	1:Y:229:ILE:HG13	1.95	0.49
1:Y:389:ARG:HB2	1:Y:426:LEU:CD1	2.42	0.49
1:O:3:LYS:HA	1:O:73:GLN:C	2.32	0.49
1:O:154:ARG:O	1:O:155:ALA:C	2.51	0.49
1:O:196:THR:HG22	1:O:198:ASP:N	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:324:ASN:ND2	1:O:324:ASN:N	2.61	0.49
1:O:478:GLU:O	1:O:482:ARG:HG2	2.12	0.49
1:Y:80:THR:HG21	1:Y:248:ALA:HB2	1.94	0.49
1:O:50:MET:O	1:O:53:TRP:HB3	2.12	0.49
1:O:111:ILE:O	1:O:112:CYS:C	2.51	0.49
1:O:413:VAL:HA	1:O:419:MET:SD	2.53	0.49
1:O:415:ASN:HD22	1:O:415:ASN:C	2.15	0.49
1:Y:237:ILE:CG2	1:Y:238:PRO:HD2	2.42	0.49
1:Y:253:GLN:CD	1:Y:407:ARG:HD2	2.33	0.49
1:O:80:THR:HG21	1:O:245:ASP:HA	1.94	0.49
1:O:137:SER:HA	1:O:140:LYS:HB2	1.94	0.49
1:O:389:ARG:O	1:O:393:GLU:HG2	2.11	0.49
1:Y:262:LYS:HZ1	1:Y:264:THR:HB	1.77	0.49
1:O:182:ASP:OD2	1:O:184:THR:OG1	2.29	0.49
1:O:185:ASN:HD21	1:O:244:GLY:HA2	1.77	0.49
1:O:415:ASN:ND2	1:O:418:LEU:HB2	2.28	0.49
1:Y:221:SER:HB2	1:Y:450:ALA:HB2	1.93	0.49
1:Y:249:ALA:HB2	1:Y:439:THR:OG1	2.13	0.49
1:Y:339:THR:O	1:Y:339:THR:OG1	2.31	0.49
1:Y:415:ASN:O	1:Y:419:MET:HG2	2.13	0.49
1:O:143:TRP:HE3	1:O:144:ILE:HA	1.75	0.49
1:O:402:ARG:HH12	1:O:403:LEU:C	2.15	0.49
1:O:448:GLY:O	1:O:451:VAL:HG12	2.13	0.49
1:Y:445:TYR:O	1:Y:446:LEU:C	2.49	0.48
1:O:162:PHE:O	1:O:179:HIS:HE1	1.96	0.48
1:O:272:LEU:HG	1:O:303:GLU:HB2	1.94	0.48
1:O:348:PHE:CD1	1:O:348:PHE:N	2.78	0.48
1:Y:143:TRP:CD2	1:Y:147:HIS:CD2	3.01	0.48
1:Y:174:THR:C	1:Y:176:GLY:H	2.16	0.48
1:Y:221:SER:HB2	1:Y:446:LEU:O	2.13	0.48
1:Y:392:LEU:HD23	1:Y:393:GLU:HG2	1.94	0.48
1:O:61:VAL:O	1:O:62:GLU:C	2.52	0.48
1:O:154:ARG:HA	1:O:159:GLU:HB3	1.95	0.48
1:O:173:MET:HB3	1:O:227:THR:CG2	2.43	0.48
1:Y:250:LEU:HD12	1:Y:250:LEU:C	2.28	0.48
1:O:132:ILE:O	1:O:133:ASP:HB2	2.13	0.48
1:O:199:TRP:CZ2	1:O:215:PRO:HD2	2.48	0.48
1:Y:18:ALA:HB2	1:Y:59:THR:HB	1.95	0.48
1:Y:185:ASN:HD21	1:Y:244:GLY:CA	2.25	0.48
1:O:17:ARG:C	1:O:59:THR:HG21	2.34	0.48
1:O:144:ILE:HG22	1:O:148:VAL:CG2	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:229:ILE:HG23	1:O:235:THR:O	2.13	0.48
1:O:440:ALA:O	1:O:441:LEU:C	2.51	0.48
1:Y:167:THR:HG21	1:Y:215:PRO:HG3	1.94	0.48
1:Y:245:ASP:O	1:Y:249:ALA:N	2.41	0.48
1:O:457:LEU:C	1:O:459:GLU:H	2.17	0.48
1:Y:172:LYS:HD2	1:Y:172:LYS:HA	1.58	0.48
1:Y:328:ASP:HB3	1:Y:332:PHE:HE2	1.79	0.48
1:O:75:ALA:CB	1:O:453:PHE:HD2	2.26	0.48
1:O:156:ARG:C	1:O:158:GLY:H	2.17	0.48
1:O:172:LYS:HD2	1:O:172:LYS:HA	1.45	0.48
1:Y:91:LYS:O	1:Y:92:GLU:C	2.51	0.48
1:Y:153:GLU:O	1:Y:154:ARG:C	2.49	0.48
1:Y:184:THR:HA	1:Y:290:ILE:HG22	1.94	0.48
1:O:441:LEU:HD23	1:O:445:TYR:CE1	2.48	0.48
1:Y:193:ASN:OD1	1:Y:195:HIS:N	2.44	0.48
1:O:151:SER:O	1:O:154:ARG:HG3	2.13	0.48
1:O:161:LEU:CD2	1:O:162:PHE:H	2.27	0.48
1:O:184:THR:CA	1:O:290:ILE:HG22	2.43	0.48
1:O:293:GLY:HA2	1:O:299:ASN:HD22	1.78	0.48
1:Y:3:LYS:HA	1:Y:73:GLN:C	2.33	0.48
1:Y:154:ARG:CA	1:Y:159:GLU:HB3	2.44	0.48
1:Y:246:GLN:CG	1:Y:270:PHE:HB2	2.41	0.48
1:O:24:ASP:O	1:O:25:ALA:HB3	2.14	0.48
1:O:193:ASN:HB3	1:O:196:THR:HB	1.95	0.48
1:O:241:GLY:HA3	1:O:447:ALA:HB2	1.96	0.48
1:O:406:LEU:HD23	1:O:407:ARG:H	1.79	0.48
1:O:462:GLU:O	1:O:465:VAL:HG22	2.14	0.48
1:Y:3:LYS:HA	1:Y:73:GLN:CA	2.43	0.48
1:Y:205:GLU:O	1:Y:206:VAL:C	2.50	0.48
1:O:5:TYR:CB	1:O:74:ILE:HG22	2.35	0.48
1:O:191:LEU:O	1:O:199:TRP:HE3	1.97	0.48
1:O:60:LEU:C	1:O:60:LEU:HD12	2.33	0.47
1:O:408:VAL:HG23	1:O:413:VAL:HG11	1.95	0.47
1:Y:33:ARG:CZ	1:Y:58:TRP:HB3	2.44	0.47
1:Y:124:ILE:O	1:Y:128:THR:OG1	2.29	0.47
1:O:437:GLU:N	1:O:437:GLU:OE1	2.48	0.47
1:O:449:LEU:HD12	1:O:449:LEU:HA	1.72	0.47
1:Y:152:ARG:O	1:Y:153:GLU:C	2.53	0.47
1:Y:169:LEU:O	1:Y:173:MET:HG2	2.14	0.47
1:Y:425:ILE:HA	1:Y:479:ARG:HG2	1.96	0.47
1:Y:32:GLN:HA	1:Y:59:THR:CG2	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:199:TRP:HZ2	1:O:215:PRO:HD2	1.79	0.47
1:O:392:LEU:O	1:O:392:LEU:HG	2.15	0.47
1:Y:207:LEU:CB	1:Y:209:ILE:HD12	2.44	0.47
1:O:141:VAL:O	1:O:142:LYS:C	2.53	0.47
1:O:359:TYR:CD2	1:O:359:TYR:N	2.79	0.47
1:O:405:ALA:HB2	1:O:429:ARG:HD2	1.96	0.47
1:O:468:ARG:HG3	1:O:468:ARG:NH1	2.28	0.47
1:Y:37:GLN:OE1	1:Y:47:HIS:HE1	1.97	0.47
1:O:41:LYS:HG3	1:O:42:PRO:N	2.28	0.47
1:Y:144:ILE:O	1:Y:145:LEU:C	2.52	0.47
1:Y:264:THR:HG23	1:Y:265:TYR:N	2.28	0.47
1:Y:313:ILE:CD1	1:Y:380:THR:HG22	2.44	0.47
1:Y:336:VAL:HG11	1:Y:375:HIS:CD2	2.49	0.47
1:Y:429:ARG:HA	1:Y:470:PHE:O	2.15	0.47
1:Y:477:THR:O	1:Y:478:GLU:C	2.52	0.47
1:O:5:TYR:O	1:O:74:ILE:HA	2.14	0.47
1:O:137:SER:CA	1:O:140:LYS:HD2	2.32	0.47
1:O:250:LEU:HD11	1:O:255:CYS:CB	2.42	0.47
1:O:287:LEU:HD23	1:O:287:LEU:N	2.28	0.47
1:O:354:PRO:O	1:O:356:TRP:HD1	1.97	0.47
1:O:420:GLN:HE21	1:O:424:ASP:CG	2.18	0.47
1:Y:222:GLU:HG2	1:Y:224:TYR:CE1	2.49	0.47
1:O:94:GLY:HA2	1:O:171:TRP:CH2	2.49	0.47
1:O:281:LYS:O	1:O:281:LYS:HG3	2.15	0.47
1:Y:21:MET:HB3	1:Y:26:ASN:O	2.14	0.47
1:O:105:CYS:SG	1:O:107:ARG:NH1	2.87	0.47
1:O:123:TYR:CD2	1:O:203:MET:CE	2.98	0.47
1:O:193:ASN:CG	1:O:196:THR:HB	2.35	0.47
1:O:482:ARG:HH11	1:O:482:ARG:CG	2.27	0.47
1:Y:13:THR:N	3:Y:601:ATF:O2G	2.39	0.47
1:Y:48:ASP:O	1:Y:52:ILE:N	2.44	0.47
3:Y:601:ATF:O3G	3:Y:601:ATF:O2B	2.33	0.47
1:O:20:VAL:HG21	1:O:63:VAL:HG11	1.96	0.47
1:O:124:ILE:HG21	1:O:190:MET:CE	2.44	0.47
1:O:340:ASN:ND2	1:O:371:VAL:CG2	2.77	0.47
1:Y:253:GLN:HE22	1:Y:409:ASP:HB3	1.80	0.46
1:Y:454:TRP:CD1	1:Y:460:LEU:HD11	2.50	0.46
1:O:186:ALA:C	1:O:188:ARG:H	2.17	0.46
1:O:272:LEU:HD12	1:O:272:LEU:N	2.30	0.46
1:O:386:TYR:HB3	1:O:486:TRP:CD2	2.49	0.46
1:O:156:ARG:NH1	1:O:156:ARG:CB	2.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:197:LEU:HD13	1:O:197:LEU:H	1.80	0.46
1:O:197:LEU:HD13	1:O:197:LEU:N	2.30	0.46
1:O:218:ARG:HG3	1:O:218:ARG:HH11	1.81	0.46
1:Y:41:LYS:HG3	1:Y:42:PRO:HD2	1.97	0.46
1:Y:44:TRP:CD1	1:Y:44:TRP:N	2.80	0.46
1:Y:434:GLU:CB	1:Y:465:VAL:HB	2.41	0.46
1:O:124:ILE:HG12	1:O:124:ILE:H	1.37	0.46
1:O:161:LEU:HD23	1:O:162:PHE:H	1.80	0.46
1:O:263:ASN:HB2	1:O:271:MET:HG3	1.96	0.46
1:Y:16:SER:HB3	1:Y:56:GLN:HA	1.98	0.46
1:Y:47:HIS:CB	1:Y:52:ILE:HD11	2.45	0.46
1:Y:74:ILE:HD11	1:Y:237:ILE:CG1	2.15	0.46
1:Y:115:LEU:HD21	1:Y:207:LEU:HD21	1.97	0.46
1:O:183:TYR:CD2	1:O:298:VAL:CG2	2.98	0.46
1:Y:87:ILE:HD13	1:Y:168:TRP:HB2	1.98	0.46
1:Y:293:GLY:N	1:Y:297:GLU:O	2.36	0.46
1:O:403:LEU:N	1:O:403:LEU:CD1	2.79	0.46
1:Y:151:SER:O	1:Y:155:ALA:N	2.37	0.46
1:Y:458:ASP:HA	1:Y:461:GLN:CB	2.44	0.46
1:O:144:ILE:HD12	1:O:144:ILE:N	2.27	0.46
1:O:264:THR:CG2	1:O:265:TYR:N	2.78	0.46
1:Y:281:LYS:O	1:Y:281:LYS:HG3	2.16	0.46
1:Y:284:ASN:OD1	1:Y:398:ASP:OD1	2.33	0.46
1:O:113:GLU:O	1:O:117:ARG:HD3	2.15	0.46
1:O:214:LEU:N	1:O:214:LEU:CD1	2.78	0.46
1:Y:11:GLN:HE22	1:Y:82:GLN:HE21	1.62	0.46
1:Y:313:ILE:HD11	1:Y:381:LEU:HD23	1.98	0.46
1:O:4:LYS:HB3	1:O:4:LYS:HE2	1.68	0.46
1:O:161:LEU:CD2	1:O:162:PHE:N	2.79	0.46
1:Y:142:LYS:O	1:Y:145:LEU:HB2	2.16	0.46
1:Y:201:ASP:O	1:Y:204:LEU:HB2	2.16	0.46
1:Y:401:ILE:CG2	1:Y:402:ARG:N	2.79	0.46
1:O:6:ILE:HG13	1:O:7:VAL:N	2.30	0.46
1:O:53:TRP:HZ3	1:O:173:MET:CE	2.29	0.46
1:O:81:ASN:OD1	1:O:165:VAL:HB	2.15	0.46
1:O:293:GLY:CA	1:O:299:ASN:ND2	2.78	0.46
1:Y:111:ILE:HG22	1:Y:115:LEU:HD11	1.96	0.46
1:Y:150:GLY:O	1:Y:151:SER:C	2.54	0.46
1:O:145:LEU:HD12	1:O:145:LEU:HA	1.78	0.46
1:O:161:LEU:CD2	1:O:179:HIS:CE1	2.99	0.46
1:O:194:ILE:HB	1:O:290:ILE:HD11	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:457:LEU:HD12	1:O:457:LEU:HA	1.82	0.46
1:Y:41:LYS:O	1:Y:44:TRP:HB2	2.16	0.45
1:Y:156:ARG:NH1	1:Y:156:ARG:CB	2.79	0.45
1:O:53:TRP:CE3	1:O:169:LEU:CD1	3.00	0.45
1:O:401:ILE:CG2	1:O:402:ARG:N	2.79	0.45
1:Y:94:GLY:CA	1:Y:171:TRP:CH2	2.99	0.45
1:Y:104:GLN:NE2	1:Y:308:MET:CE	2.79	0.45
1:Y:110:GLU:O	1:Y:113:GLU:N	2.49	0.45
1:O:6:ILE:HD12	1:O:76:ALA:HB3	1.97	0.45
1:O:460:LEU:C	1:O:462:GLU:H	2.19	0.45
1:Y:48:ASP:HB3	1:Y:51:GLU:HB3	1.98	0.45
1:Y:111:ILE:O	1:Y:112:CYS:C	2.51	0.45
1:Y:237:ILE:CG2	1:Y:238:PRO:N	2.79	0.45
1:Y:372:ASN:OD1	1:Y:374:ASN:HB2	2.16	0.45
1:Y:422:GLN:NE2	1:Y:426:LEU:CD2	2.79	0.45
1:O:69:ILE:N	1:O:69:ILE:CD1	2.80	0.45
1:O:144:ILE:HG22	1:O:148:VAL:HG21	1.97	0.45
1:Y:199:TRP:CD2	1:Y:214:LEU:HD23	2.52	0.45
1:Y:214:LEU:N	1:Y:214:LEU:CD1	2.79	0.45
1:Y:316:LEU:HD23	1:Y:316:LEU:HA	1.49	0.45
1:Y:382:GLU:HG2	1:Y:421:PHE:CZ	2.51	0.45
1:Y:391:VAL:O	1:Y:392:LEU:C	2.55	0.45
1:Y:433:PRO:HA	1:Y:466:ILE:CD1	2.44	0.45
1:Y:449:LEU:HD13	1:Y:454:TRP:O	2.15	0.45
1:O:6:ILE:CD1	1:O:76:ALA:HB3	2.46	0.45
1:O:40:PRO:HG2	1:O:44:TRP:HB2	1.95	0.45
1:O:44:TRP:CZ2	1:O:107:ARG:HB2	2.49	0.45
1:O:325:ASP:HB3	1:O:327:TYR:CB	2.45	0.45
1:Y:226:GLN:HB3	1:Y:237:ILE:O	2.17	0.45
1:O:230:GLY:HA2	1:O:235:THR:HB	1.96	0.45
1:Y:161:LEU:CD2	1:Y:179:HIS:NE2	2.80	0.45
1:O:108:THR:HG21	1:O:139:THR:C	2.37	0.45
1:O:125:ARG:NH2	1:O:285:GLY:H	2.15	0.45
1:O:207:LEU:CD2	1:O:207:LEU:N	2.79	0.45
1:O:226:GLN:HE21	1:O:236:ARG:HG2	1.80	0.45
1:O:482:ARG:HG3	1:O:482:ARG:HH11	1.81	0.45
1:Y:351:LEU:HD22	1:Y:360:ALA:CB	2.47	0.45
1:O:20:VAL:O	1:O:28:ILE:HB	2.17	0.45
1:O:58:TRP:CE3	1:O:58:TRP:CA	2.99	0.45
1:O:218:ARG:NH1	1:O:218:ARG:CG	2.80	0.45
1:O:428:THR:HG23	1:O:429:ARG:N	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:53:TRP:CZ3	1:O:173:MET:CE	3.00	0.45
1:O:188:ARG:HD3	1:O:188:ARG:HA	1.28	0.45
1:O:204:LEU:HD23	1:O:204:LEU:HA	1.51	0.45
1:O:422:GLN:NE2	1:O:426:LEU:CD2	2.80	0.45
1:Y:108:THR:HB	1:Y:139:THR:HB	1.99	0.45
1:Y:189:THR:OG1	1:Y:191:LEU:HD12	2.17	0.45
1:O:170:ILE:CG2	1:O:171:TRP:N	2.80	0.45
1:O:179:HIS:CD2	1:O:215:PRO:CA	3.00	0.45
1:O:191:LEU:O	1:O:192:PHE:HB2	2.17	0.45
1:O:430:VAL:HB	1:O:470:PHE:HB2	1.97	0.45
1:Y:17:ARG:HH22	1:Y:437:GLU:HG2	1.81	0.45
1:Y:211:ARG:NH1	1:Y:211:ARG:CG	2.80	0.45
1:Y:251:PHE:CD2	1:Y:446:LEU:CD2	3.00	0.45
1:Y:498:GLU:OE2	1:O:488:LYS:HE2	2.17	0.45
1:O:58:TRP:CD2	1:O:58:TRP:N	2.80	0.45
1:O:58:TRP:O	1:O:62:GLU:N	2.42	0.45
1:O:170:ILE:HA	1:O:173:MET:CG	2.47	0.45
1:Y:193:ASN:HB3	1:Y:196:THR:HB	1.99	0.44
1:Y:256:VAL:HG12	1:Y:294:PRO:HG3	1.97	0.44
1:Y:468:ARG:CG	1:Y:468:ARG:NH1	2.80	0.44
1:O:13:THR:O	1:O:13:THR:HG22	2.15	0.44
1:O:168:TRP:O	1:O:169:LEU:C	2.54	0.44
1:O:179:HIS:CD2	1:O:215:PRO:CB	2.99	0.44
1:O:264:THR:HG23	1:O:265:TYR:N	2.32	0.44
1:O:350:GLY:HA2	1:O:360:ALA:HB3	1.99	0.44
1:O:372:ASN:OD1	1:O:374:ASN:N	2.50	0.44
1:O:403:LEU:N	1:O:403:LEU:HD12	2.31	0.44
1:Y:108:THR:CB	1:Y:139:THR:HB	2.47	0.44
1:Y:195:HIS:N	1:Y:195:HIS:ND1	2.65	0.44
1:Y:342:VAL:HA	1:Y:365:PHE:O	2.18	0.44
1:Y:403:LEU:N	1:Y:403:LEU:CD1	2.80	0.44
1:O:37:GLN:OE1	1:O:47:HIS:HE1	1.99	0.44
1:O:41:LYS:HB3	1:O:41:LYS:HE2	1.78	0.44
1:O:58:TRP:CE3	1:O:58:TRP:N	2.85	0.44
1:O:70:SER:O	1:O:72:ASP:N	2.50	0.44
1:O:90:GLU:CD	1:O:93:THR:HG21	2.37	0.44
1:O:199:TRP:CZ2	1:O:214:LEU:HB3	2.52	0.44
3:O:601:ATF:O1G	3:O:601:ATF:O2B	2.35	0.44
1:Y:361:ARG:HD3	1:Y:361:ARG:HA	1.74	0.44
1:Y:480:ASN:ND2	1:Y:480:ASN:N	2.64	0.44
1:O:409:ASP:CA	1:O:413:VAL:HG11	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:115:LEU:O	1:O:116:LYS:C	2.56	0.44
1:Y:24:ASP:CB	1:Y:26:ASN:HD21	2.14	0.44
1:Y:142:LYS:O	1:Y:143:TRP:C	2.55	0.44
1:Y:185:ASN:O	1:Y:188:ARG:HB2	2.16	0.44
1:O:251:PHE:CE1	1:O:256:VAL:CG2	2.99	0.44
1:O:394:ALA:O	1:O:397:ALA:HB3	2.16	0.44
1:O:444:ALA:O	1:O:445:TYR:C	2.53	0.44
1:O:494:MET:HE3	1:O:494:MET:HB3	1.48	0.44
1:Y:117:ARG:H	1:Y:117:ARG:HG3	1.68	0.44
1:Y:150:GLY:O	1:Y:153:GLU:HB2	2.18	0.44
1:Y:191:LEU:O	1:Y:199:TRP:HE3	2.01	0.44
1:Y:393:GLU:HG2	1:Y:393:GLU:H	1.21	0.44
1:O:199:TRP:HB3	1:O:204:LEU:HD11	2.00	0.44
1:O:78:GLY:CA	1:O:447:ALA:HB2	2.48	0.44
1:O:183:TYR:CD1	1:O:217:VAL:CG1	3.00	0.44
1:O:237:ILE:HG22	1:O:238:PRO:N	2.33	0.44
1:Y:67:ALA:HB1	1:Y:69:ILE:HG12	1.99	0.44
1:Y:142:LYS:O	1:Y:146:ASP:OD1	2.36	0.44
1:Y:466:ILE:HD13	1:Y:466:ILE:HA	1.51	0.44
1:O:179:HIS:NE2	1:O:215:PRO:CB	2.80	0.44
1:O:192:PHE:HE2	1:O:217:VAL:HG11	1.83	0.44
1:O:278:LYS:HZ2	1:O:280:VAL:HB	1.77	0.44
1:Y:9:LEU:HD12	1:Y:9:LEU:HA	1.87	0.44
1:Y:27:ILE:HD11	1:Y:30:VAL:CG2	2.45	0.44
1:Y:166:ASP:O	1:Y:167:THR:C	2.56	0.44
1:O:20:VAL:CG1	1:O:21:MET:N	2.80	0.44
1:O:166:ASP:O	1:O:169:LEU:N	2.51	0.44
1:O:219:ARG:HG2	1:O:222:GLU:CB	2.44	0.44
1:Y:40:PRO:HD2	1:Y:44:TRP:HB2	1.99	0.43
1:Y:383:SER:O	1:Y:384:ILE:C	2.52	0.43
1:O:316:LEU:HD23	1:O:316:LEU:HA	1.43	0.43
1:O:428:THR:CG2	1:O:429:ARG:N	2.80	0.43
1:Y:44:TRP:CZ2	1:Y:107:ARG:HB2	2.52	0.43
1:Y:221:SER:OG	1:Y:221:SER:O	2.34	0.43
1:O:156:ARG:O	1:O:212:GLU:HG2	2.18	0.43
1:Y:324:ASN:N	1:Y:324:ASN:HD22	2.14	0.43
1:Y:328:ASP:HB3	1:Y:332:PHE:CE2	2.53	0.43
1:Y:347:ALA:HB2	1:Y:351:LEU:HD13	2.01	0.43
1:Y:482:ARG:NH1	1:Y:482:ARG:CG	2.79	0.43
1:O:339:THR:O	1:O:339:THR:OG1	2.34	0.43
1:Y:32:GLN:N	1:Y:59:THR:HG22	2.34	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:240:SER:HB2	1:Y:450:ALA:CB	2.47	0.43
1:Y:308:MET:HE3	1:Y:349:THR:HG23	2.00	0.43
1:O:148:VAL:HB	1:O:151:SER:HB3	1.99	0.43
1:O:251:PHE:CD2	1:O:446:LEU:HD13	2.51	0.43
1:Y:170:ILE:O	1:Y:171:TRP:C	2.55	0.43
1:Y:286:LEU:HD11	1:Y:394:ALA:CB	2.48	0.43
1:Y:435:VAL:HG21	1:Y:441:LEU:HD11	2.01	0.43
1:O:183:TYR:CD2	1:O:298:VAL:HG22	2.53	0.43
1:Y:264:THR:CG2	1:Y:265:TYR:N	2.80	0.43
1:Y:276:GLY:O	1:Y:300:TYR:N	2.51	0.43
1:Y:386:TYR:HB3	1:Y:486:TRP:CE2	2.53	0.43
1:O:11:GLN:NE2	1:O:82:GLN:HE21	2.17	0.43
1:O:33:ARG:NH2	1:O:58:TRP:HB3	2.31	0.43
1:O:84:GLU:OE1	1:O:103:TRP:HB3	2.19	0.43
1:O:88:VAL:HG12	1:O:97:ILE:HG12	2.01	0.43
1:O:130:LEU:HD13	1:O:136:PHE:CD1	2.54	0.43
1:O:137:SER:O	1:O:140:LYS:N	2.52	0.43
1:Y:156:ARG:HH11	1:Y:156:ARG:CG	2.31	0.43
1:Y:169:LEU:O	1:Y:172:LYS:HB2	2.18	0.43
1:Y:408:VAL:HG23	1:Y:409:ASP:N	2.33	0.43
1:Y:432:ARG:CG	1:Y:436:ARG:NH1	2.81	0.43
1:O:108:THR:CB	1:O:139:THR:HB	2.48	0.43
1:O:142:LYS:O	1:O:145:LEU:N	2.52	0.43
1:O:271:MET:O	1:O:272:LEU:HD12	2.19	0.43
1:O:463:LYS:NZ	1:O:465:VAL:CG2	2.80	0.43
1:Y:91:LYS:HE3	1:Y:91:LYS:HB3	1.80	0.43
1:Y:228:ASN:HD21	1:Y:235:THR:N	2.16	0.43
1:Y:250:LEU:HD12	1:Y:255:CYS:HB2	1.97	0.43
1:Y:326:ALA:O	1:Y:327:TYR:C	2.57	0.43
1:O:49:PRO:HA	1:O:52:ILE:HD12	2.00	0.43
1:O:83:ARG:CZ	1:O:246:GLN:HG2	2.49	0.43
1:O:180:VAL:HG21	1:O:218:ARG:HH11	1.84	0.43
1:O:386:TYR:CB	1:O:486:TRP:CD2	3.01	0.43
1:O:406:LEU:CD2	1:O:407:ARG:N	2.82	0.43
1:O:87:ILE:O	1:O:88:VAL:HG23	2.19	0.43
1:O:95:LYS:HG3	1:O:96:PRO:N	2.33	0.43
1:O:170:ILE:HA	1:O:173:MET:HG2	2.01	0.43
1:O:185:ASN:HD21	1:O:244:GLY:N	2.17	0.43
1:Y:468:ARG:HD2	1:Y:468:ARG:C	2.37	0.43
1:O:78:GLY:HA2	1:O:241:GLY:HA3	2.00	0.43
1:O:263:ASN:HB2	1:O:271:MET:CG	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:389:ARG:O	1:O:389:ARG:HG3	2.19	0.43
1:O:475:GLU:O	1:O:478:GLU:CB	2.67	0.43
1:Y:170:ILE:HA	1:Y:173:MET:HG2	2.01	0.42
1:Y:262:LYS:HZ2	1:Y:264:THR:HB	1.84	0.42
1:Y:302:LEU:HA	1:Y:302:LEU:HD23	1.10	0.42
1:O:136:PHE:HB3	1:O:188:ARG:O	2.19	0.42
1:O:250:LEU:HD12	1:O:255:CYS:HB2	2.01	0.42
1:O:278:LYS:HD3	1:O:279:ALA:C	2.40	0.42
1:O:466:ILE:HD13	1:O:466:ILE:HA	1.61	0.42
1:O:491:LYS:O	1:O:494:MET:HG3	2.19	0.42
1:Y:81:ASN:ND2	1:Y:81:ASN:H	2.16	0.42
1:Y:144:ILE:O	1:Y:147:HIS:N	2.33	0.42
1:Y:357:ASP:OD2	1:Y:494:MET:HB3	2.19	0.42
1:Y:415:ASN:ND2	1:Y:418:LEU:HB2	2.34	0.42
1:O:40:PRO:CG	1:O:44:TRP:HB3	2.49	0.42
1:O:161:LEU:HD23	1:O:161:LEU:HA	1.67	0.42
1:O:240:SER:C	1:O:447:ALA:HA	2.40	0.42
1:O:413:VAL:HG23	1:O:432:ARG:HD2	2.01	0.42
1:Y:23:HIS:ND1	1:Y:453:PHE:CE1	2.88	0.42
1:O:48:ASP:O	1:O:51:GLU:HB3	2.19	0.42
1:O:53:TRP:CH2	1:O:172:LYS:HB3	2.54	0.42
1:O:359:TYR:HD1	1:O:497:GLU:HB3	1.85	0.42
1:O:383:SER:O	1:O:387:GLN:HB2	2.19	0.42
1:O:482:ARG:O	1:O:483:TYR:C	2.58	0.42
1:Y:144:ILE:HG23	1:Y:148:VAL:CG2	2.49	0.42
1:Y:184:THR:HG22	1:Y:290:ILE:HG22	2.00	0.42
1:Y:467:GLU:OE2	1:Y:468:ARG:HB2	2.20	0.42
1:O:90:GLU:HB3	1:O:93:THR:OG1	2.19	0.42
1:O:102:VAL:O	1:O:103:TRP:C	2.57	0.42
1:O:278:LYS:O	1:O:278:LYS:HD2	2.18	0.42
1:O:381:LEU:O	1:O:382:GLU:C	2.55	0.42
1:Y:40:PRO:HD2	1:Y:44:TRP:CB	2.49	0.42
1:Y:50:MET:O	1:Y:53:TRP:HB3	2.19	0.42
1:Y:124:ILE:HG12	1:Y:124:ILE:H	1.68	0.42
1:Y:359:TYR:CD1	1:Y:359:TYR:N	2.87	0.42
1:O:108:THR:CG2	1:O:139:THR:HB	2.50	0.42
1:O:144:ILE:CG2	1:O:148:VAL:CG2	2.97	0.42
1:O:389:ARG:HD2	1:O:393:GLU:OE2	2.20	0.42
1:O:398:ASP:O	1:O:400:GLY:N	2.52	0.42
1:Y:122:ASP:O	1:Y:126:SER:N	2.47	0.42
1:Y:435:VAL:CG2	1:Y:436:ARG:N	2.80	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:441:LEU:HD23	1:Y:441:LEU:HA	1.89	0.42
1:O:5:TYR:N	1:O:73:GLN:O	2.35	0.42
1:O:130:LEU:HD23	1:O:130:LEU:N	2.33	0.42
1:O:157:ARG:HG2	1:O:157:ARG:H	1.61	0.42
1:Y:124:ILE:HG21	1:Y:190:MET:HE1	2.01	0.42
1:Y:151:SER:O	1:Y:152:ARG:C	2.55	0.42
1:Y:325:ASP:CB	1:Y:327:TYR:HB3	2.33	0.42
1:Y:375:HIS:O	1:Y:376:ILE:C	2.56	0.42
1:O:5:TYR:HE2	1:O:69:ILE:HG23	1.84	0.42
1:O:11:GLN:HE22	1:O:82:GLN:HE21	1.66	0.42
1:O:83:ARG:HE	4:O:600:GOL:H2	1.85	0.42
1:O:193:ASN:CB	1:O:196:THR:HB	2.50	0.42
1:O:262:LYS:HA	1:O:407:ARG:O	2.19	0.42
1:O:382:GLU:O	1:O:383:SER:C	2.55	0.42
1:Y:47:HIS:HD2	1:Y:82:GLN:HE22	1.68	0.42
1:Y:111:ILE:CG2	1:Y:115:LEU:HD11	2.50	0.42
1:Y:111:ILE:CG2	1:Y:139:THR:HG22	2.46	0.42
1:O:5:TYR:HB3	1:O:21:MET:O	2.20	0.42
1:O:77:ILE:HB	1:O:238:PRO:O	2.20	0.42
1:O:161:LEU:HD22	1:O:162:PHE:N	2.35	0.42
1:O:161:LEU:HD22	1:O:179:HIS:CE1	2.55	0.42
1:O:188:ARG:HH11	1:O:188:ARG:HD2	1.60	0.42
1:Y:253:GLN:OE1	1:Y:407:ARG:HD2	2.20	0.42
1:Y:408:VAL:O	1:Y:409:ASP:HB3	2.20	0.42
1:O:64:LEU:HD12	1:O:64:LEU:N	2.35	0.42
1:O:137:SER:O	1:O:140:LYS:HB2	2.20	0.42
1:O:229:ILE:HG21	1:O:237:ILE:CG1	2.31	0.42
1:O:351:LEU:HD13	1:O:351:LEU:HA	1.74	0.42
1:Y:17:ARG:HH22	1:Y:437:GLU:CG	2.32	0.42
1:Y:60:LEU:HD12	1:Y:60:LEU:HA	1.80	0.42
1:Y:117:ARG:HH11	1:Y:117:ARG:HG3	1.85	0.42
1:Y:127:ASN:CB	1:Y:193:ASN:ND2	2.80	0.42
1:O:187:SER:CB	1:O:290:ILE:HB	2.50	0.42
1:Y:103:TRP:HA	1:Y:140:LYS:HE3	2.02	0.41
1:Y:254:LEU:C	1:Y:256:VAL:H	2.23	0.41
1:Y:360:ALA:HA	1:Y:493:ALA:O	2.19	0.41
1:O:32:GLN:HA	1:O:59:THR:CG2	2.50	0.41
1:O:46:GLU:HB3	1:O:100:ALA:O	2.20	0.41
1:O:60:LEU:O	1:O:63:VAL:HB	2.20	0.41
1:O:393:GLU:HG2	1:O:393:GLU:H	1.63	0.41
1:Y:87:ILE:HD13	1:Y:168:TRP:CB	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:132:ILE:HD13	1:Y:132:ILE:HG21	1.86	0.41
1:Y:251:PHE:CD2	1:Y:446:LEU:HD22	2.55	0.41
1:Y:458:ASP:HA	1:Y:461:GLN:HB2	2.01	0.41
1:O:133:ASP:HA	1:O:134:PRO:HD3	1.92	0.41
1:O:416:ASN:O	1:O:417:PHE:C	2.59	0.41
1:O:441:LEU:CD2	1:O:445:TYR:CE1	3.03	0.41
1:O:487:LYS:O	1:O:488:LYS:C	2.56	0.41
1:Y:97:ILE:O	1:Y:98:TYR:HB2	2.21	0.41
1:Y:103:TRP:CD1	1:Y:103:TRP:N	2.88	0.41
1:Y:130:LEU:HB3	1:Y:131:VAL:H	1.51	0.41
1:Y:490:VAL:H	1:Y:490:VAL:HG23	1.60	0.41
1:O:38:ILE:O	1:O:45:VAL:HA	2.20	0.41
1:O:128:THR:HG21	1:O:190:MET:HA	2.02	0.41
1:O:263:ASN:ND2	1:O:265:TYR:CZ	2.88	0.41
1:O:376:ILE:O	1:O:376:ILE:HG22	2.20	0.41
1:Y:114:HIS:CD2	1:Y:114:HIS:H	2.38	0.41
1:Y:120:LEU:O	1:Y:121:GLU:C	2.54	0.41
1:Y:145:LEU:HD12	1:Y:145:LEU:HA	1.59	0.41
1:Y:244:GLY:O	1:Y:245:ASP:C	2.59	0.41
1:Y:377:ILE:O	1:Y:378:ARG:C	2.58	0.41
1:O:28:ILE:HA	1:O:28:ILE:HD12	1.85	0.41
1:O:64:LEU:O	1:O:65:ALA:C	2.57	0.41
1:O:113:GLU:OE1	1:O:113:GLU:HA	2.20	0.41
1:Y:16:SER:HB3	1:Y:56:GLN:OE1	2.21	0.41
1:Y:23:HIS:HA	1:Y:453:PHE:HE1	1.86	0.41
1:Y:185:ASN:HD21	1:Y:243:ALA:C	2.24	0.41
1:Y:189:THR:O	1:Y:190:MET:HB3	2.21	0.41
1:Y:256:VAL:HG11	1:Y:294:PRO:HB3	2.02	0.41
1:Y:428:THR:HG23	1:Y:429:ARG:N	2.36	0.41
1:O:55:THR:O	1:O:58:TRP:HB2	2.21	0.41
1:O:89:TRP:CZ2	1:O:161:LEU:HD13	2.56	0.41
1:O:174:THR:HG21	1:O:178:VAL:HG23	2.02	0.41
1:O:273:MET:CB	1:O:395:MET:CE	2.99	0.41
1:O:458:ASP:HA	1:O:461:GLN:HB2	2.01	0.41
1:O:484:ALA:O	1:O:487:LYS:N	2.54	0.41
1:Y:445:TYR:O	1:Y:449:LEU:N	2.39	0.41
1:O:441:LEU:HD22	1:O:445:TYR:CZ	2.55	0.41
1:Y:257:LYS:HG3	1:Y:260:MET:SD	2.61	0.41
1:Y:258:GLU:N	1:Y:274:ASN:OD1	2.54	0.41
1:O:156:ARG:CG	1:O:156:ARG:HH11	2.34	0.41
1:Y:3:LYS:HG2	1:Y:72:ASP:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:23:HIS:HE1	1:Y:453:PHE:O	2.04	0.41
1:Y:117:ARG:CG	1:Y:117:ARG:NH1	2.80	0.41
1:Y:130:LEU:HD13	1:Y:136:PHE:CG	2.56	0.41
1:Y:169:LEU:N	1:Y:169:LEU:HD22	2.36	0.41
1:Y:222:GLU:HG2	1:Y:224:TYR:CD1	2.56	0.41
1:Y:250:LEU:HD13	1:Y:262:LYS:HG2	2.03	0.41
1:Y:251:PHE:O	1:Y:254:LEU:HD12	2.21	0.41
1:O:53:TRP:O	1:O:54:ALA:C	2.58	0.41
1:O:192:PHE:CE1	1:O:197:LEU:HA	2.56	0.41
1:O:195:HIS:HD1	1:O:195:HIS:N	2.19	0.41
1:O:226:GLN:NE2	1:O:236:ARG:CB	2.79	0.41
1:O:487:LYS:O	1:O:490:VAL:HG23	2.21	0.41
1:Y:183:TYR:CD1	1:Y:217:VAL:CG1	2.98	0.41
1:Y:11:GLN:NE2	1:Y:82:GLN:HG2	2.36	0.40
1:Y:84:GLU:HB2	1:Y:103:TRP:CB	2.42	0.40
1:Y:237:ILE:CG2	1:Y:238:PRO:CD	2.99	0.40
1:O:6:ILE:CG1	1:O:7:VAL:N	2.84	0.40
1:O:86:THR:HG1	1:O:137:SER:HB3	1.83	0.40
1:O:262:LYS:HD2	1:O:262:LYS:C	2.42	0.40
1:O:419:MET:CE	1:O:419:MET:CA	2.99	0.40
1:Y:180:VAL:HG21	1:Y:218:ARG:HG3	2.03	0.40
1:O:45:VAL:HG12	1:O:46:GLU:N	2.36	0.40
1:O:155:ALA:O	1:O:212:GLU:HB2	2.20	0.40
1:O:180:VAL:CG2	1:O:218:ARG:CG	2.99	0.40
1:O:439:THR:CG2	1:O:440:ALA:N	2.82	0.40
1:O:480:ASN:O	1:O:481:TYR:C	2.58	0.40
1:Y:226:GLN:HE21	1:Y:236:ARG:HB3	1.85	0.40
1:Y:256:VAL:CG1	1:Y:294:PRO:CB	3.00	0.40
1:Y:295:THR:N	1:Y:297:GLU:OE1	2.50	0.40
1:Y:481:TYR:HD2	1:Y:482:ARG:HD2	1.86	0.40
1:O:41:LYS:CB	1:O:42:PRO:CD	2.99	0.40
1:O:251:PHE:CD1	1:O:256:VAL:CG2	3.04	0.40
1:O:457:LEU:O	1:O:459:GLU:N	2.54	0.40
1:O:474:ILE:HA	1:O:474:ILE:HD12	1.60	0.40
1:Y:41:LYS:CB	1:Y:42:PRO:CD	3.00	0.40
1:Y:74:ILE:HD13	1:Y:237:ILE:HG21	2.02	0.40
1:Y:169:LEU:HA	1:Y:169:LEU:HD13	1.50	0.40
1:Y:256:VAL:CG1	1:Y:294:PRO:CG	2.99	0.40
1:Y:457:LEU:C	1:Y:459:GLU:H	2.24	0.40
1:O:477:THR:O	1:O:479:ARG:N	2.55	0.40
1:Y:87:ILE:CG2	1:Y:88:VAL:N	2.83	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:133:ASP:HA	1:Y:134:PRO:HD3	1.91	0.40
1:Y:201:ASP:O	1:Y:205:GLU:HG2	2.21	0.40
1:Y:229:ILE:HG13	1:Y:230:GLY:N	2.37	0.40
1:Y:432:ARG:CD	1:Y:436:ARG:NH2	2.82	0.40
1:O:160:LEU:O	1:O:213:MET:HB3	2.22	0.40
1:O:326:ALA:O	1:O:327:TYR:C	2.57	0.40
1:O:409:ASP:HB2	1:O:438:VAL:HG21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:58:TRP:CZ2	1:Y:58:TRP:CZ2[3_655]	2.10	0.10

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	490/501 (98%)	375 (76%)	87 (18%)	28 (6%)	1	10
1	Y	490/501 (98%)	404 (82%)	68 (14%)	18 (4%)	3	19
All	All	980/1002 (98%)	779 (80%)	155 (16%)	46 (5%)	2	14

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	71	SER
1	Y	151	SER
1	Y	153	GLU
1	Y	175	GLN
1	O	60	LEU
1	O	445	TYR

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	446	LEU
1	O	456	ASN
1	Y	61	VAL
1	Y	196	THR
1	O	63	VAL
1	O	75	ALA
1	O	111	ILE
1	O	118	ASP
1	O	151	SER
1	O	199	TRP
1	O	477	THR
1	O	478	GLU
1	Y	111	ILE
1	Y	456	ASN
1	O	71	SER
1	O	98	TYR
1	Y	60	LEU
1	Y	62	GLU
1	Y	64	LEU
1	Y	98	TYR
1	O	110	GLU
1	O	114	HIS
1	O	138	GLY
1	O	176	GLY
1	O	202	LYS
1	O	441	LEU
1	Y	202	LYS
1	Y	258	GLU
1	O	99	ASN
1	O	149	GLU
1	O	196	THR
1	O	479	ARG
1	Y	138	GLY
1	Y	411	GLY
1	O	187	SER
1	O	242	ILE
1	O	258	GLU
1	O	458	ASP
1	Y	176	GLY
1	Y	442	GLY

### 5.3.2 Protein sidechains [i](#)

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%)	259 (64%)	149 (36%)	0	1
1	Y	408/412 (99%)	277 (68%)	131 (32%)	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	9	LEU
1	Y	11	GLN
1	Y	21	MET
1	Y	27	ILE
1	Y	28	ILE
1	Y	33	ARG
1	Y	34	GLU
1	Y	62	GLU
1	Y	63	VAL
1	Y	66	LYS
1	Y	70	SER
1	Y	71	SER
1	Y	73	GLN
1	Y	80	THR
1	Y	81	ASN
1	Y	83	ARG
1	Y	91	LYS
1	Y	92	GLU
1	Y	93	THR
1	Y	95	LYS
1	Y	102	VAL
1	Y	106	ARG
1	Y	107	ARG
1	Y	110	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Y	117	ARG
1	Y	121	GLU
1	Y	124	ILE
1	Y	131	VAL
1	Y	136	PHE
1	Y	139	THR
1	Y	145	LEU
1	Y	146	ASP
1	Y	148	VAL
1	Y	151	SER
1	Y	154	ARG
1	Y	156	ARG
1	Y	157	ARG
1	Y	162	PHE
1	Y	170	ILE
1	Y	172	LYS
1	Y	173	MET
1	Y	175	GLN
1	Y	178	VAL
1	Y	181	THR
1	Y	185	ASN
1	Y	187	SER
1	Y	191	LEU
1	Y	195	HIS
1	Y	196	THR
1	Y	197	LEU
1	Y	198	ASP
1	Y	201	ASP
1	Y	202	LYS
1	Y	205	GLU
1	Y	206	VAL
1	Y	211	ARG
1	Y	219	ARG
1	Y	221	SER
1	Y	222	GLU
1	Y	226	GLN
1	Y	227	THR
1	Y	229	ILE
1	Y	235	THR
1	Y	236	ARG
1	Y	237	ILE
1	Y	245	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Y	246	GLN
1	Y	253	GLN
1	Y	254	LEU
1	Y	257	LYS
1	Y	258	GLU
1	Y	262	LYS
1	Y	264	THR
1	Y	281	LYS
1	Y	288	THR
1	Y	290	ILE
1	Y	295	THR
1	Y	302	LEU
1	Y	312	SER
1	Y	313	ILE
1	Y	317	ARG
1	Y	318	ASP
1	Y	324	ASN
1	Y	335	LYS
1	Y	337	GLN
1	Y	339	THR
1	Y	351	LEU
1	Y	368	THR
1	Y	384	ILE
1	Y	389	ARG
1	Y	391	VAL
1	Y	392	LEU
1	Y	393	GLU
1	Y	395	MET
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	428	THR
1	Y	429	ARG
1	Y	434	GLU
1	Y	438	VAL
1	Y	445	TYR
1	Y	449	LEU
1	Y	451	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Y	455	GLN
1	Y	456	ASN
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	476	THR
1	Y	478	GLU
1	Y	482	ARG
1	Y	483	TYR
1	Y	488	LYS
1	Y	492	ARG
1	Y	494	MET
1	Y	498	GLU
1	Y	499	HIS
1	O	2	GLU
1	O	3	LYS
1	O	5	TYR
1	O	9	LEU
1	O	11	GLN
1	O	21	MET
1	O	27	ILE
1	O	28	ILE
1	O	33	ARG
1	O	34	GLU
1	O	41	LYS
1	O	46	GLU
1	O	51	GLU
1	O	57	SER
1	O	59	THR
1	O	60	LEU
1	O	64	LEU
1	O	69	ILE
1	O	70	SER
1	O	71	SER
1	O	80	THR
1	O	81	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	82	GLN
1	O	83	ARG
1	O	87	ILE
1	O	91	LYS
1	O	92	GLU
1	O	93	THR
1	O	102	VAL
1	O	104	GLN
1	O	106	ARG
1	O	107	ARG
1	O	110	GLU
1	O	117	ARG
1	O	124	ILE
1	O	125	ARG
1	O	136	PHE
1	O	137	SER
1	O	140	LYS
1	O	141	VAL
1	O	145	LEU
1	O	146	ASP
1	O	148	VAL
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	169	LEU
1	O	170	ILE
1	O	172	LYS
1	O	173	MET
1	O	175	GLN
1	O	178	VAL
1	O	180	VAL
1	O	181	THR
1	O	187	SER
1	O	188	ARG
1	O	191	LEU
1	O	195	HIS
1	O	196	THR
1	O	197	LEU
1	O	198	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	201	ASP
1	O	202	LYS
1	O	207	LEU
1	O	211	ARG
1	O	214	LEU
1	O	218	ARG
1	O	219	ARG
1	O	221	SER
1	O	222	GLU
1	O	226	GLN
1	O	227	THR
1	O	229	ILE
1	O	235	THR
1	O	236	ARG
1	O	253	GLN
1	O	254	LEU
1	O	256	VAL
1	O	257	LYS
1	O	258	GLU
1	O	262	LYS
1	O	264	THR
1	O	269	CYS
1	O	271	MET
1	O	278	LYS
1	O	280	VAL
1	O	281	LYS
1	O	284	ASN
1	O	287	LEU
1	O	288	THR
1	O	290	ILE
1	O	313	ILE
1	O	317	ARG
1	O	324	ASN
1	O	335	LYS
1	O	339	THR
1	O	346	PRO
1	O	351	LEU
1	O	368	THR
1	O	389	ARG
1	O	391	VAL
1	O	392	LEU
1	O	393	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	395	MET
1	O	399	SER
1	O	402	ARG
1	O	406	LEU
1	O	407	ARG
1	O	408	VAL
1	O	409	ASP
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	438	VAL
1	O	439	THR
1	O	451	VAL
1	O	453	PHE
1	O	455	GLN
1	O	457	LEU
1	O	459	GLU
1	O	460	LEU
1	O	461	GLN
1	O	462	GLU
1	O	463	LYS
1	O	465	VAL
1	O	466	ILE
1	O	468	ARG
1	O	469	GLU
1	O	474	ILE
1	O	475	GLU
1	O	476	THR
1	O	477	THR
1	O	478	GLU
1	O	479	ARG
1	O	482	ARG
1	O	483	TYR
1	O	487	LYS
1	O	488	LYS
1	O	490	VAL
1	O	492	ARG
1	O	494	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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	81	ASN
1	Y	104	GLN
1	Y	114	HIS
1	Y	127	ASN
1	Y	147	HIS
1	Y	185	ASN
1	Y	226	GLN
1	Y	246	GLN
1	Y	253	GLN
1	Y	324	ASN
1	Y	340	ASN
1	Y	396	GLN
1	Y	404	HIS
1	Y	415	ASN
1	Y	461	GLN
1	Y	480	ASN
1	Y	499	HIS
1	O	11	GLN
1	O	26	ASN
1	O	47	HIS
1	O	81	ASN
1	O	114	HIS
1	O	179	HIS
1	O	185	ASN
1	O	226	GLN
1	O	314	GLN
1	O	324	ASN
1	O	340	ASN
1	O	396	GLN
1	O	404	HIS
1	O	415	ASN
1	O	420	GLN
1	O	461	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	480	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATF	Y	601	2	27,35,35	2.69	6 (22%)	28,57,57	2.21	6 (21%)
3	ATF	O	601	2	27,35,35	2.66	8 (29%)	28,57,57	1.66	6 (21%)
4	GOL	Y	600	-	5,5,5	0.62	0	5,5,5	0.90	0
4	GOL	O	600	-	5,5,5	0.62	0	5,5,5	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATF	Y	601	2	-	6/13/50/50	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATF	O	601	2	-	4/13/50/50	0/3/3/3
4	GOL	Y	600	-	-	2/4/4/4	-
4	GOL	O	600	-	-	4/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	601	ATF	PG-O3G	8.07	1.69	1.54
3	O	601	ATF	PG-O2G	7.69	1.68	1.54
3	Y	601	ATF	PG-O2G	7.30	1.68	1.54
3	Y	601	ATF	PB-O2B	6.51	1.69	1.56
3	O	601	ATF	PG-O3G	5.75	1.65	1.54
3	O	601	ATF	PB-O2B	5.54	1.67	1.56
3	O	601	ATF	C4-N3	-3.75	1.30	1.35
3	O	601	ATF	PB-O1B	-3.55	1.44	1.51
3	Y	601	ATF	PB-O3A	2.92	1.61	1.58
3	O	601	ATF	O4'-C1'	2.63	1.44	1.41
3	O	601	ATF	O2'-C2'	2.51	1.48	1.43
3	Y	601	ATF	O4'-C1'	2.36	1.44	1.41
3	O	601	ATF	PA-O2A	2.21	1.65	1.55
3	Y	601	ATF	PA-O1A	-2.04	1.43	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	601	ATF	PA-O3A-PB	-6.16	113.82	132.41
3	Y	601	ATF	O2'-C2'-C1'	-5.33	91.17	110.85
3	Y	601	ATF	C5-C6-N6	4.97	127.91	120.35
3	O	601	ATF	PA-O3A-PB	-3.95	120.49	132.41
3	O	601	ATF	O2'-C2'-C1'	-3.51	97.89	110.85
3	O	601	ATF	C1'-N9-C4	3.43	132.67	126.64
3	Y	601	ATF	O5'-C5'-C4'	3.17	119.91	108.99
3	Y	601	ATF	C5'-C4'-C3'	-2.62	105.36	115.18
3	O	601	ATF	C4-C5-N7	2.42	111.92	109.40
3	Y	601	ATF	O3G-PG-O2G	2.31	114.51	107.99
3	O	601	ATF	O3'-C3'-C2'	2.28	119.20	111.82
3	O	601	ATF	N6-C6-N1	2.02	122.76	118.57

There are no chirality outliers.

All (16) torsion outliers are listed below:

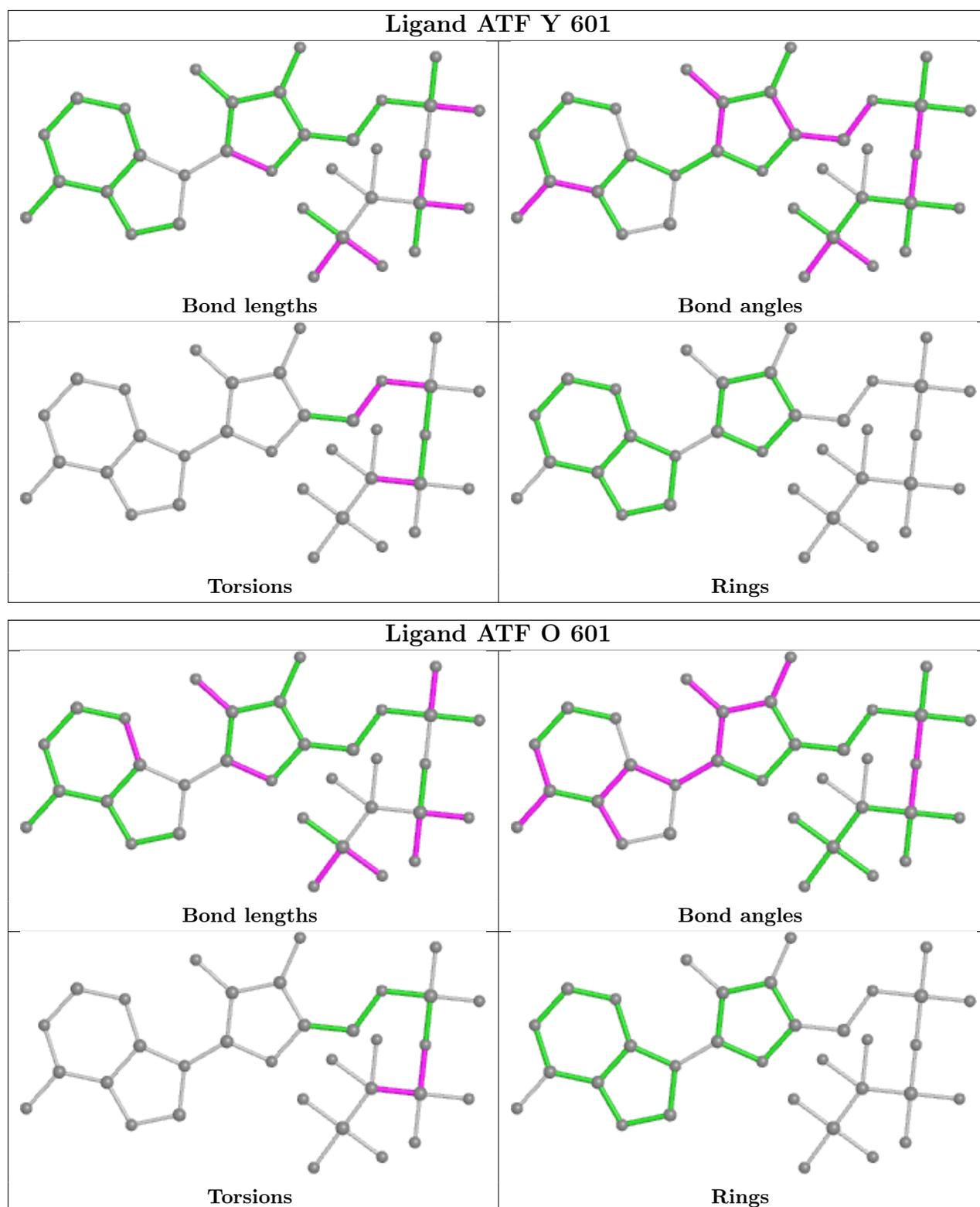
Mol	Chain	Res	Type	Atoms
3	Y	601	ATF	F1B-C3B-PB-O1B
3	Y	601	ATF	F2B-C3B-PB-O1B
3	Y	601	ATF	C5'-O5'-PA-O3A
3	Y	601	ATF	C4'-C5'-O5'-PA
3	O	601	ATF	F1B-C3B-PB-O1B
3	O	601	ATF	F2B-C3B-PB-O1B
4	Y	600	GOL	C1-C2-C3-O3
4	O	600	GOL	O1-C1-C2-C3
4	O	600	GOL	C1-C2-C3-O3
4	O	600	GOL	O2-C2-C3-O3
4	Y	600	GOL	O2-C2-C3-O3
4	O	600	GOL	O1-C1-C2-O2
3	Y	601	ATF	C5'-O5'-PA-O2A
3	O	601	ATF	PA-O3A-PB-O1B
3	Y	601	ATF	C5'-O5'-PA-O1A
3	O	601	ATF	PA-O3A-PB-O2B

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

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%)	-0.75	0 100 100	9, 52, 92, 100	0
1	Y	494/501 (98%)	-0.93	0 100 100	7, 41, 80, 100	0
All	All	988/1002 (98%)	-0.84	0 100 100	7, 47, 88, 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](#)

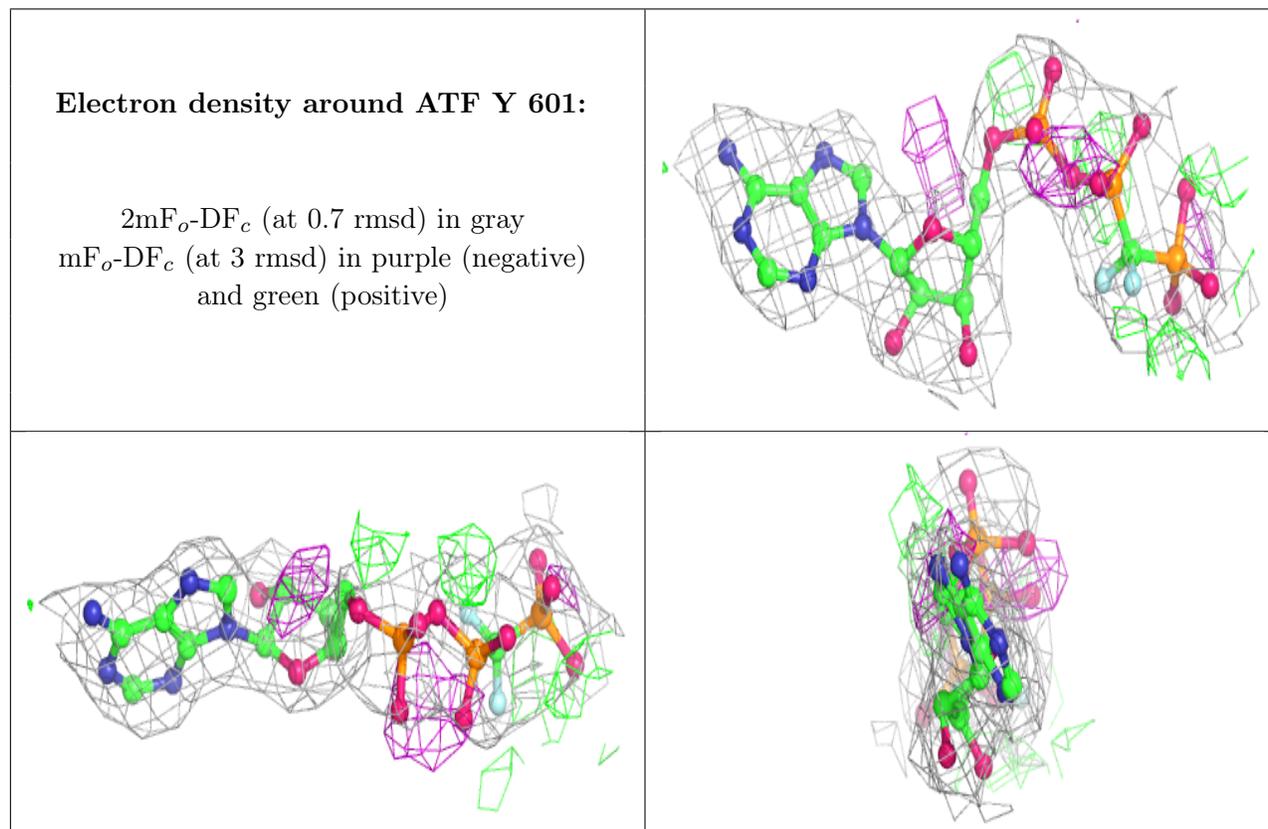
There are no monosaccharides in this entry.

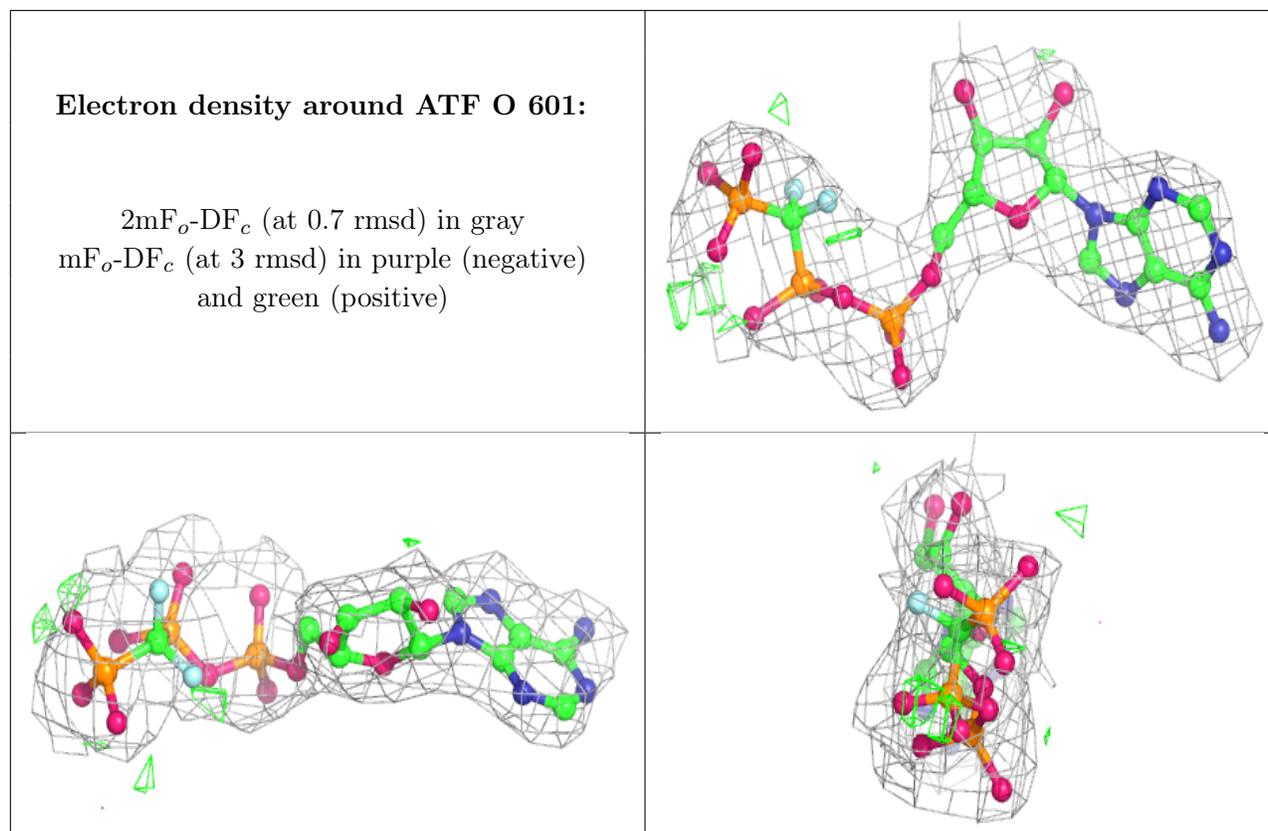
### 6.4 Ligands [i](#)

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	O	602	1/1	0.92	0.38	56,56,56,56	0
3	ATF	Y	601	33/33	0.94	0.15	42,42,42,42	0
2	MG	Y	602	1/1	0.95	0.43	43,43,43,43	0
3	ATF	O	601	33/33	0.96	0.12	56,56,56,56	0
4	GOL	O	600	6/6	0.97	0.10	31,31,31,31	0
4	GOL	Y	600	6/6	0.98	0.10	14,14,14,14	0

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.