



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:34 AM BST

PDB ID : 1BO5  
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN ESCHERICHIA COLI GLYCEROL KINASE AND THE ALLOSTERIC REGULATOR FRUCTOSE 1,6-BISPHOSPHATE.  
Authors : Ormo, M.; Bystrom, C.E.; Remington, S.J.  
Deposited on : 1998-08-10  
Resolution : 3.20 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

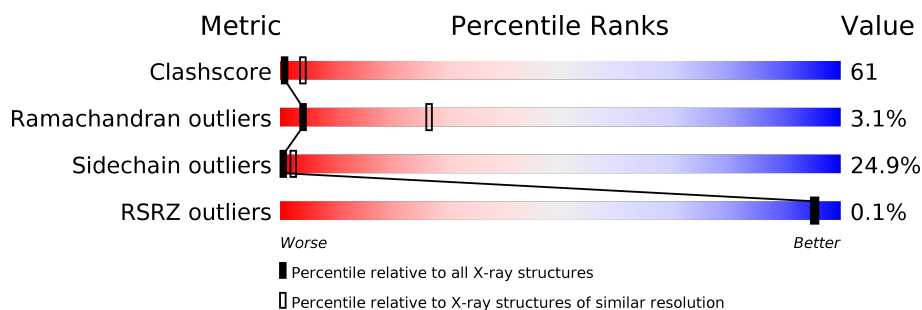
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	Z	501	

## 2 Entry composition [i](#)

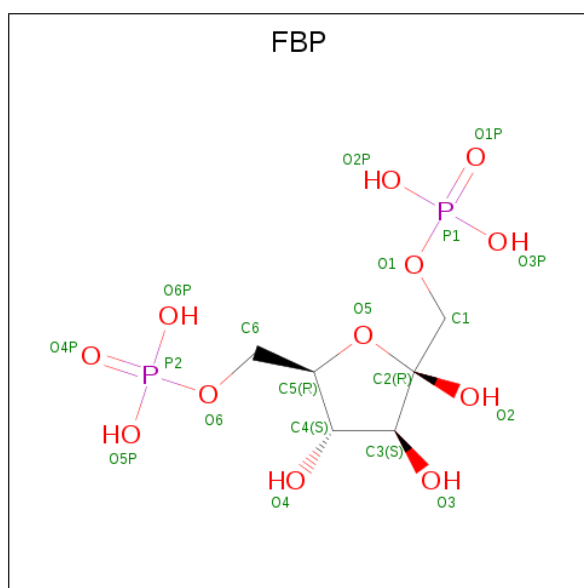
There are 3 unique types of molecules in this entry. The entry contains 7818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEIN (GLYCEROL KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	498	Total	C	N	O	S	0	0	0
			3878	2453	671	735	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3888	2456	674	739	19			

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	O	P	0	1
			40	12	24	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

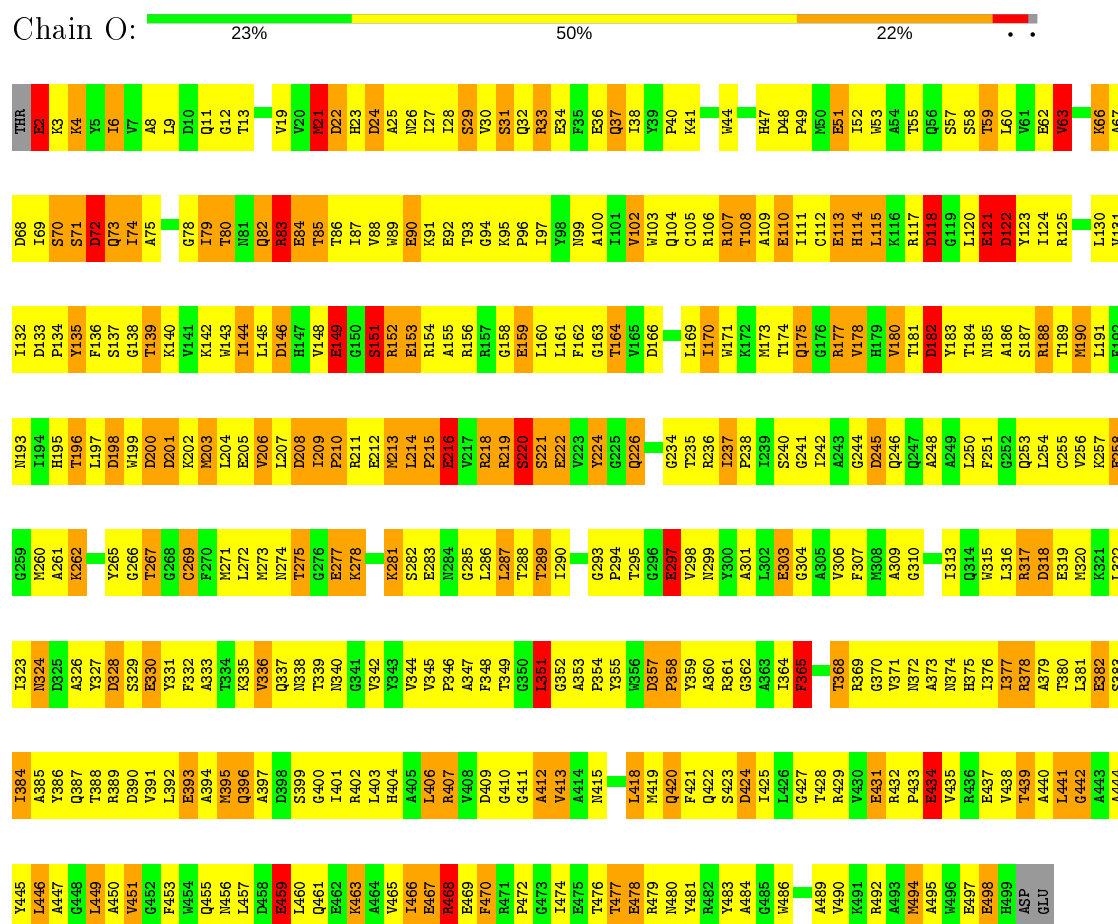


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

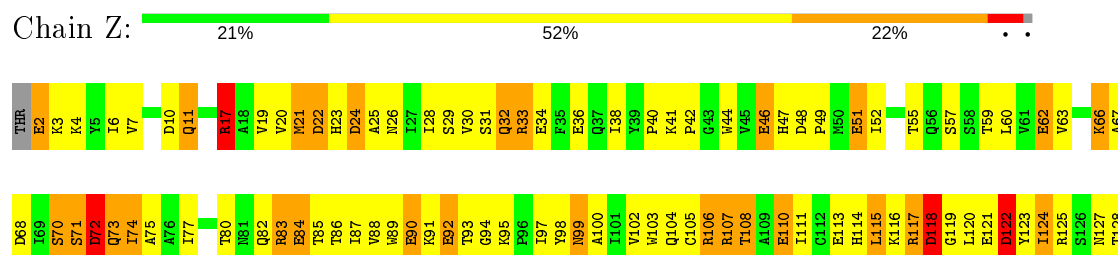
### 3 Residue-property plots

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

#### • Molecule 1: PROTEIN (GLYCEROL KINASE)



#### • Molecule 1: PROTEIN (GLYCEROL KINASE)



L441	G442	A443	A444	Y445	L446	A447	G448	L449	A450	V451	G452	F453	Y454	Q455	Y456	L457	Y458	F459	L460	Q461	F462	K463	A464	Y465	L466	E467	R468	E469	F470	R471	P472	E475	T476	T477	E478	R479	N480	Y481	R482	Y483	A484	G485	Y486	A489	V490	F491	R492	A493	N494	Y495	Y496	F497	F498	H499	ASP	GLU						
A379	T380	L381	E382	S383	L384	A385	T386	Q387	T388	R389	D390	V391	L392	E393	A394	N395	Q396	A397	D398	S399	G400	L401	R402	L403	L406	R407	V408	D409	G410	G411	A412	V413	A414	N415	L418	N419	Q420	F421	Q422	S423	D424	L425	L426	G427	T428	R429	V430	E431	R432	P433	Y434	Y435	R436	E437	V438	T439	A440					
R317	D318	E319	N320	K321	L322	T323	N324	D325	A326	R327	D328	S329	E330	F331	C332	A333	T334	K335	V336	Q337	N338	T339	N340	G341	V342	T343	V344	V345	P346	A347	F348	T349	G350	L351	G352	A353	P354	T355	V356	D357	P358	Y359	A360	R361	G362	I363	I364	F365	T368	V371	N372	A373	N374	R375	I376	I377	R378					
C254	L255	V256	K257	E258	G259	K260	A261	R262	N263	T264	Y265	G266	T267	G268	C269	F270	M271	L272	M273	N274	E277	V280	K281	E282	E283	L286	L287	T288	T289	I290	A291	G292	G293	P294	T295	G296	E297	V298	N299	Y300	A301	L302	E303	G304	A305	V306	F307	M308	G310	A311	S312	I313	Q314	W315	L316							
M190	L191	F192	N193	I194	H195	T196	L197	D198	W199	D200	T201	K202	M203	L204	E205	I144	V206	L207	D208	I209	P210	R211	E212	M213	L214	P215	E216	V217	R218	R219	G158	S220	S221	E222	V223	Y224	G225	Q226	K232	G233	G234	T235	R236	I237	P238	L239	G240	G241	I242	A243	G244	D245	Q246	Q247	T183	A248	A249	L250	F251	G252	R188	T189
G129	L130	V131	I132	D133	P134	Y135	F136	S137	G138	T139	K140	V141	K142	W143	E205	I144	V206	L145	D146	H147	V148	E149	G150	S151	R152	E153	R154	A155	R156	R157	G158	E159	L160	L161	F162	G163	T164	V165	D166	L169	I170	W171	K172	M173	T174	Q175	G176	R177	V178	H179	V180	T181	D182	Y183	T184	N185	A186	S187	R188	T189		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.41Å 169.41Å 204.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.20) 90.3 (19.97-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.98Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, $R_{free}$	0.211 , (Not available) 0.190 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 92.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: GOL, FBP

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	1.17	35/3958 (0.9%)	1.51	55/5373 (1.0%)
1	Z	1.18	32/3968 (0.8%)	1.53	55/5387 (1.0%)
All	All	1.18	67/7926 (0.8%)	1.52	110/10760 (1.0%)

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	O	1	1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	51	GLU	CD-OE1	8.97	1.35	1.25
1	Z	92	GLU	CD-OE1	8.22	1.34	1.25
1	Z	382	GLU	CD-OE2	8.19	1.34	1.25
1	O	51	GLU	CD-OE1	8.05	1.34	1.25
1	Z	212	GLU	CD-OE2	7.96	1.34	1.25
1	O	216	GLU	CD-OE2	7.96	1.34	1.25
1	Z	393	GLU	CD-OE1	7.47	1.33	1.25
1	O	437	GLU	CD-OE2	7.47	1.33	1.25
1	O	149	GLU	CD-OE2	7.37	1.33	1.25
1	Z	216	GLU	CD-OE1	7.37	1.33	1.25
1	O	34	GLU	CD-OE1	7.36	1.33	1.25
1	O	393	GLU	CD-OE1	7.10	1.33	1.25
1	Z	431	GLU	CD-OE1	7.01	1.33	1.25
1	Z	297	GLU	CD-OE1	6.97	1.33	1.25
1	O	277	GLU	CD-OE1	6.92	1.33	1.25
1	Z	277	GLU	CD-OE2	6.91	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	153	GLU	CD-OE2	6.85	1.33	1.25
1	Z	498	GLU	CD-OE1	6.79	1.33	1.25
1	Z	149	GLU	CD-OE2	6.64	1.32	1.25
1	Z	34	GLU	CD-OE1	6.63	1.32	1.25
1	O	110	GLU	CD-OE1	6.62	1.32	1.25
1	Z	205	GLU	CD-OE2	6.60	1.32	1.25
1	Z	478	GLU	CD-OE2	6.57	1.32	1.25
1	Z	467	GLU	CD-OE2	6.49	1.32	1.25
1	O	467	GLU	CD-OE2	6.36	1.32	1.25
1	Z	36	GLU	CD-OE2	6.36	1.32	1.25
1	Z	434	GLU	CD-OE1	6.32	1.32	1.25
1	Z	258	GLU	CD-OE1	6.30	1.32	1.25
1	O	92	GLU	CD-OE1	6.26	1.32	1.25
1	O	222	GLU	CD-OE2	6.24	1.32	1.25
1	O	283	GLU	CD-OE1	6.21	1.32	1.25
1	O	497	GLU	CD-OE1	6.19	1.32	1.25
1	O	431	GLU	CD-OE2	6.08	1.32	1.25
1	O	297	GLU	CD-OE2	6.07	1.32	1.25
1	Z	437	GLU	CD-OE1	6.03	1.32	1.25
1	O	434	GLU	CD-OE1	6.00	1.32	1.25
1	O	2	GLU	CD-OE2	5.96	1.32	1.25
1	O	159	GLU	CD-OE1	5.93	1.32	1.25
1	Z	62	GLU	CD-OE2	5.90	1.32	1.25
1	Z	110	GLU	CD-OE2	5.90	1.32	1.25
1	Z	459	GLU	CD-OE2	5.88	1.32	1.25
1	O	36	GLU	CD-OE2	5.86	1.32	1.25
1	Z	90	GLU	CD-OE2	5.82	1.32	1.25
1	Z	222	GLU	CD-OE2	5.76	1.31	1.25
1	O	113	GLU	CD-OE2	5.74	1.31	1.25
1	Z	469	GLU	CD-OE1	5.72	1.31	1.25
1	Z	153	GLU	CD-OE2	5.72	1.31	1.25
1	O	90	GLU	CD-OE2	5.71	1.31	1.25
1	Z	319	GLU	CD-OE2	5.65	1.31	1.25
1	O	469	GLU	CD-OE1	5.64	1.31	1.25
1	O	62	GLU	CD-OE2	5.59	1.31	1.25
1	O	121	GLU	CD-OE2	5.53	1.31	1.25
1	Z	46	GLU	CD-OE2	5.52	1.31	1.25
1	O	330	GLU	CD-OE2	5.49	1.31	1.25
1	Z	497	GLU	CD-OE1	5.48	1.31	1.25
1	O	459	GLU	CD-OE1	5.46	1.31	1.25
1	O	478	GLU	CD-OE2	5.41	1.31	1.25
1	O	498	GLU	CD-OE2	5.39	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	277	GLU	CD-OE2	-5.26	1.19	1.25
1	Z	2	GLU	CD-OE2	5.25	1.31	1.25
1	O	212	GLU	CD-OE2	5.23	1.31	1.25
1	O	258	GLU	CD-OE2	5.17	1.31	1.25
1	O	219	ARG	NE-CZ	5.12	1.39	1.33
1	Z	283	GLU	CD-OE2	5.11	1.31	1.25
1	O	303	GLU	CD-OE1	5.11	1.31	1.25
1	Z	330	GLU	CD-OE1	5.11	1.31	1.25
1	O	382	GLU	CD-OE2	5.07	1.31	1.25

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	22	ASP	CB-CG-OD1	8.79	126.21	118.30
1	O	201	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	Z	10	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	Z	409	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	O	24	ASP	CB-CG-OD1	-7.97	111.12	118.30
1	O	378	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	O	133	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	Z	328	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	Z	245	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	Z	22	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	Z	24	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	O	200	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	O	219	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	Z	407	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	O	122	ASP	CB-CG-OD1	-7.67	111.40	118.30
1	O	468	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	Z	200	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	O	72	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	O	328	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	O	188	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	O	351	LEU	C-N-CA	-7.50	106.56	122.30
1	Z	407	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	O	357	ASP	C-N-CD	-7.22	104.71	120.60
1	Z	219	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	Z	200	ASP	CB-CG-OD1	7.18	124.76	118.30
1	Z	390	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	Z	389	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	Z	349	THR	CA-CB-CG2	-7.02	102.57	112.40
1	O	318	ASP	CB-CG-OD1	7.01	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	211	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	Z	83	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	O	245	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	Z	325	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	Z	208	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	O	182	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	O	24	ASP	CB-CG-OD2	6.61	124.25	118.30
1	O	208	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	O	378	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	Z	68	ASP	CB-CG-OD1	-6.49	112.46	118.30
1	Z	72	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	O	118	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	O	289	THR	N-CA-CB	6.39	122.44	110.30
1	Z	245	ASP	CB-CG-OD1	6.38	124.04	118.30
1	Z	211	ARG	N-CA-CB	6.34	122.00	110.60
1	O	318	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	Z	182	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	O	114	HIS	CA-CB-CG	-6.14	103.16	113.60
1	O	198	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	O	468	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	Z	201	ASP	CB-CG-OD2	6.08	123.77	118.30
1	Z	357	ASP	CB-CG-OD1	6.04	123.73	118.30
1	Z	398	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	Z	390	ASP	N-CA-CB	5.97	121.36	110.60
1	O	22	ASP	CB-CG-OD2	5.96	123.67	118.30
1	Z	471	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	O	21	MET	N-CA-CB	5.96	121.33	110.60
1	Z	357	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	O	275	THR	CA-CB-CG2	-5.92	104.11	112.40
1	Z	198	ASP	CB-CG-OD1	5.90	123.61	118.30
1	O	357	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	O	200	ASP	CB-CG-OD1	5.87	123.58	118.30
1	O	245	ASP	CB-CG-OD1	5.86	123.57	118.30
1	O	135	TYR	CB-CG-CD1	5.85	124.51	121.00
1	Z	182	ASP	CB-CG-OD1	5.85	123.56	118.30
1	Z	122	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	Z	118	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	Z	68	ASP	CB-CG-OD2	5.72	123.45	118.30
1	Z	409	ASP	CB-CG-OD1	5.69	123.42	118.30
1	O	164	THR	CA-CB-CG2	-5.67	104.47	112.40
1	O	409	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	Z	471	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	201	ASP	CB-CG-OD2	5.57	123.31	118.30
1	Z	166	ASP	CB-CG-OD2	5.57	123.31	118.30
1	Z	458	ASP	CB-CG-OD1	-5.52	113.34	118.30
1	O	424	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	O	282	SER	N-CA-CB	5.50	118.74	110.50
1	O	83	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	Z	24	ASP	CB-CG-OD1	5.46	123.21	118.30
1	O	118	ASP	CB-CG-OD2	5.43	123.19	118.30
1	Z	118	ASP	CB-CG-OD2	5.43	123.19	118.30
1	O	68	ASP	CB-CG-OD1	-5.43	113.42	118.30
1	Z	10	ASP	CB-CG-OD2	5.42	123.18	118.30
1	O	34	GLU	N-CA-CB	5.39	120.30	110.60
1	O	22	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	O	63	VAL	CB-CA-C	-5.36	101.22	111.40
1	Z	106	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	O	267	THR	CA-CB-CG2	-5.32	104.95	112.40
1	Z	325	ASP	CB-CG-OD1	5.29	123.06	118.30
1	Z	219	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	Z	17	ARG	N-CA-CB	5.24	120.02	110.60
1	Z	198	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	O	208	ASP	CB-CG-OD2	5.22	123.00	118.30
1	Z	201	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	Z	378	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	Z	177	ARG	N-CA-CB	5.19	119.94	110.60
1	O	219	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	Z	124	ILE	CB-CA-C	-5.16	101.28	111.60
1	O	449	LEU	CB-CA-C	-5.16	100.40	110.20
1	Z	264	THR	CA-CB-CG2	-5.15	105.19	112.40
1	O	365	PHE	N-CA-CB	5.14	119.85	110.60
1	O	441	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	Z	161	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	O	72	ASP	CB-CG-OD2	5.12	122.91	118.30
1	Z	181	THR	CA-CB-CG2	-5.11	105.24	112.40
1	O	146	ASP	CB-CG-OD1	5.11	122.90	118.30
1	O	68	ASP	CB-CG-OD2	5.08	122.87	118.30
1	O	441	LEU	CA-CB-CG	-5.07	103.64	115.30
1	O	177	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	O	357	ASP	CB-CG-OD1	5.03	122.83	118.30
1	Z	349	THR	N-CA-CB	-5.02	100.76	110.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	O	21	MET	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	351	LEU	Mainchain

## 5.2 Too-close contacts [i](#)

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	3878	0	3774	472	0
1	Z	3888	0	3778	463	0
2	O	40	0	20	3	0
3	O	6	0	8	2	0
3	Z	6	0	8	0	0
All	All	7818	0	7588	935	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 61.

All (935) 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:83:ARG:HH11	1:O:83:ARG:HG3	1.04	1.11
1:O:145:LEU:HD11	1:O:213:MET:HE1	1.30	1.11
1:Z:438:VAL:HA	1:Z:441:LEU:HD12	1.30	1.06
1:Z:71:SER:HB2	1:Z:235:THR:HG21	1.32	1.05
1:O:255:CYS:HB3	1:O:260:MET:HB3	1.39	1.03
1:Z:137:SER:HB2	1:Z:189:THR:HA	1.40	1.01
1:Z:88:VAL:HG12	1:Z:97:ILE:HG12	1.39	1.01
1:O:85:THR:HB	1:O:102:VAL:HA	1.44	0.96
1:Z:256:VAL:HG22	1:Z:294:PRO:HD3	1.47	0.96
1:O:336:VAL:HG23	1:O:338:ASN:H	1.24	0.96
1:O:137:SER:HB2	1:O:189:THR:HA	1.44	0.96
1:O:261:ALA:HB2	1:O:273:MET:HB2	1.43	0.95
1:O:108:THR:HG21	1:O:139:THR:HB	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:48:ASP:HB3	1:O:51:GLU:HB2	1.48	0.95
1:O:434:GLU:HG2	1:O:465:VAL:H	1.29	0.94
1:O:434:GLU:HB3	1:O:465:VAL:HB	1.48	0.94
1:Z:38:ILE:HG22	1:Z:40:PRO:HD3	1.48	0.94
1:O:22:ASP:HB3	1:O:28:ILE:HD11	1.52	0.92
1:Z:127:ASN:HB3	1:Z:193:ASN:ND2	1.85	0.91
1:Z:48:ASP:HB3	1:Z:51:GLU:HB2	1.53	0.89
1:O:85:THR:HG22	1:O:103:TRP:H	1.37	0.89
1:Z:145:LEU:HD12	1:Z:151:SER:HB2	1.55	0.89
1:Z:71:SER:HB2	1:Z:235:THR:CG2	2.03	0.88
1:O:83:ARG:NH1	1:O:83:ARG:HG3	1.82	0.87
1:Z:354:PRO:HD2	1:Z:355:TYR:CD1	2.09	0.87
1:Z:191:LEU:HD21	1:Z:207:LEU:HD12	1.57	0.85
1:Z:108:THR:HG21	1:Z:139:THR:HB	1.56	0.85
1:O:108:THR:CG2	1:O:139:THR:HB	2.06	0.85
1:O:368:THR:HG22	1:O:370:GLY:H	1.39	0.85
1:O:122:ASP:O	1:O:123:TYR:C	2.14	0.84
1:Z:23:HIS:HA	1:Z:453:PHE:CE2	2.12	0.84
1:Z:407:ARG:HG3	1:Z:407:ARG:HH11	1.41	0.83
1:Z:344:VAL:HG22	1:Z:364:ILE:HG12	1.59	0.83
1:Z:108:THR:CG2	1:Z:139:THR:HB	2.09	0.83
1:Z:329:SER:HB2	1:Z:381:LEU:HD11	1.61	0.83
1:O:38:ILE:HG22	1:O:40:PRO:HD3	1.60	0.82
1:O:115:LEU:HB3	1:O:132:ILE:HD13	1.61	0.82
1:Z:372:ASN:HD22	1:Z:374:ASN:H	1.27	0.82
1:Z:354:PRO:HD2	1:Z:355:TYR:CE1	2.15	0.81
1:Z:256:VAL:HG22	1:Z:294:PRO:CD	2.11	0.81
1:O:293:GLY:HA3	1:O:297:GLU:HG2	1.62	0.81
1:O:124:ILE:HG13	1:O:203:MET:CE	2.11	0.81
1:Z:372:ASN:HD22	1:Z:374:ASN:N	1.79	0.81
1:Z:385:ALA:HA	1:Z:422:GLN:HE22	1.46	0.81
1:O:21:MET:HB2	1:O:26:ASN:O	1.82	0.80
1:O:74:ILE:HB	1:O:237:ILE:HD13	1.63	0.78
1:O:200:ASP:O	1:O:204:LEU:HD12	1.82	0.78
1:O:456:ASN:O	1:O:459:GLU:HG3	1.84	0.78
1:Z:250:LEU:CD1	1:Z:255:CYS:HB2	2.14	0.78
1:O:369:ARG:HH11	1:O:369:ARG:HG3	1.49	0.78
1:Z:108:THR:CB	1:Z:139:THR:HB	2.13	0.78
1:O:424:ASP:HB3	1:O:474:ILE:HG12	1.65	0.78
1:Z:455:GLN:NE2	1:Z:455:GLN:HA	1.97	0.77
1:O:468:ARG:HH11	1:O:468:ARG:HG3	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:250:LEU:CD1	1:O:255:CYS:HB2	2.15	0.77
1:O:105:CYS:SG	1:O:107:ARG:HD2	2.25	0.76
1:Z:480:ASN:N	1:Z:480:ASN:HD22	1.81	0.76
1:O:82:GLN:OE1	1:O:85:THR:HG21	1.86	0.76
1:Z:203:MET:O	1:Z:206:VAL:HG12	1.86	0.76
1:O:250:LEU:HD11	1:O:255:CYS:HB2	1.68	0.75
1:O:169:LEU:O	1:O:173:MET:HG3	1.85	0.75
1:Z:70:SER:O	1:Z:73:GLN:HG3	1.87	0.75
1:Z:423:SER:HB2	1:Z:430:VAL:HG23	1.68	0.75
1:O:261:ALA:HB2	1:O:273:MET:CB	2.16	0.75
1:O:255:CYS:HA	1:O:260:MET:HE2	1.67	0.75
1:O:265:TYR:HB3	1:O:412:ALA:HB3	1.69	0.75
1:O:71:SER:HB2	1:O:235:THR:HG21	1.69	0.74
1:Z:458:ASP:HA	1:Z:461:GLN:HG2	1.69	0.74
1:Z:256:VAL:HG21	1:Z:294:PRO:HA	1.68	0.74
1:O:186:ALA:O	1:O:189:THR:HG23	1.87	0.74
1:O:197:LEU:HD12	1:O:197:LEU:N	2.02	0.73
1:Z:410:GLY:O	1:Z:413:VAL:HG13	1.87	0.73
1:Z:240:SER:O	1:Z:447:ALA:HA	1.87	0.73
1:Z:361:ARG:HG2	1:Z:361:ARG:HH11	1.53	0.73
1:Z:373:ALA:O	1:Z:377:ILE:HG13	1.87	0.73
1:O:486:TRP:O	1:O:490:VAL:HG23	1.88	0.73
1:O:80:THR:CG2	1:O:245:ASP:HA	2.19	0.73
1:Z:385:ALA:HA	1:Z:422:GLN:NE2	2.03	0.73
1:Z:84:GLU:HB2	1:Z:103:TRP:HB3	1.70	0.72
1:O:410:GLY:O	1:O:413:VAL:HG13	1.88	0.72
1:Z:295:THR:OG1	1:Z:297:GLU:HG2	1.90	0.72
1:O:114:HIS:O	1:O:115:LEU:C	2.22	0.72
1:O:178:VAL:HG23	1:O:180:VAL:HG12	1.71	0.72
1:O:23:HIS:HA	1:O:453:PHE:CE2	2.25	0.72
1:Z:406:LEU:HD22	1:Z:407:ARG:N	2.04	0.72
1:Z:235:THR:O	1:Z:236:ARG:HD3	1.90	0.72
1:Z:237:ILE:HG23	1:Z:238:PRO:HD2	1.71	0.72
1:O:120:LEU:O	1:O:121:GLU:C	2.28	0.72
1:O:455:GLN:HA	1:O:455:GLN:NE2	2.02	0.72
1:Z:250:LEU:HD12	1:Z:255:CYS:HB2	1.71	0.72
1:Z:23:HIS:HA	1:Z:453:PHE:HE2	1.51	0.72
1:Z:237:ILE:CG2	1:Z:238:PRO:HD2	2.20	0.71
1:Z:105:CYS:SG	1:Z:107:ARG:HD2	2.29	0.71
1:O:145:LEU:HD11	1:O:213:MET:CE	2.16	0.71
1:O:170:ILE:HG22	1:O:171:TRP:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:22:ASP:CB	1:O:28:ILE:HD11	2.20	0.71
1:O:323:ILE:HG22	1:O:332:PHE:CE2	2.26	0.71
1:O:103:TRP:CZ3	1:O:104:GLN:HG2	2.26	0.70
1:O:240:SER:O	1:O:447:ALA:HA	1.92	0.70
1:Z:108:THR:HG21	1:Z:139:THR:C	2.11	0.70
1:Z:88:VAL:HG12	1:Z:97:ILE:CG1	2.20	0.70
1:Z:460:LEU:N	1:Z:460:LEU:HD22	2.07	0.70
1:Z:115:LEU:N	1:Z:115:LEU:HD23	2.07	0.69
1:Z:120:LEU:N	1:Z:120:LEU:HD12	2.07	0.69
1:Z:204:LEU:H	1:Z:204:LEU:HD12	1.57	0.69
1:O:335:LYS:HB2	1:O:374:ASN:HD22	1.58	0.69
1:O:152:ARG:O	1:O:155:ALA:HB3	1.92	0.69
1:O:460:LEU:HD23	1:O:460:LEU:N	2.08	0.69
1:Z:360:ALA:O	1:Z:361:ARG:HG2	1.93	0.69
1:O:434:GLU:CB	1:O:465:VAL:HB	2.21	0.69
1:Z:103:TRP:CZ3	1:Z:104:GLN:HG2	2.27	0.69
1:Z:88:VAL:CG1	1:Z:97:ILE:HG12	2.21	0.69
1:O:80:THR:HG21	1:O:245:ASP:HA	1.75	0.69
1:Z:204:LEU:HD12	1:Z:204:LEU:N	2.08	0.69
1:O:386:TYR:O	1:O:389:ARG:HB3	1.93	0.69
1:Z:108:THR:HB	1:Z:139:THR:HB	1.74	0.69
1:O:285:GLY:O	1:O:286:LEU:HD23	1.93	0.69
1:Z:434:GLU:HG2	1:Z:465:VAL:H	1.57	0.69
1:Z:196:THR:HG22	1:Z:198:ASP:N	2.08	0.69
1:Z:253:GLN:NE2	1:Z:409:ASP:HB3	2.07	0.69
1:Z:137:SER:O	1:Z:140:LYS:HB2	1.93	0.68
1:O:222:GLU:O	1:O:240:SER:HA	1.93	0.68
1:O:224:TYR:HE1	1:O:241:GLY:N	1.91	0.68
1:O:347:ALA:O	1:O:361:ARG:HA	1.94	0.68
1:O:336:VAL:HG23	1:O:337:GLN:N	2.08	0.68
1:Z:21:MET:HA	1:Z:26:ASN:O	1.93	0.68
1:Z:372:ASN:ND2	1:Z:374:ASN:H	1.91	0.68
1:Z:74:ILE:HD13	1:Z:74:ILE:N	2.07	0.68
1:Z:186:ALA:O	1:Z:189:THR:HG23	1.94	0.67
1:O:461:GLN:HA	1:O:461:GLN:NE2	2.08	0.67
1:O:182:ASP:OD1	1:O:185:ASN:HB2	1.94	0.67
1:O:483:TYR:O	1:O:486:TRP:HB3	1.95	0.67
1:Z:169:LEU:O	1:Z:173:MET:HG3	1.92	0.67
1:Z:136:PHE:HB3	1:Z:188:ARG:O	1.94	0.67
1:Z:156:ARG:HG3	1:Z:156:ARG:HH11	1.58	0.67
1:O:155:ALA:HA	1:O:160:LEU:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:458:ASP:N	1:Z:458:ASP:OD1	2.28	0.67
1:Z:272:LEU:HG	1:Z:303:GLU:HB2	1.75	0.67
1:O:323:ILE:HG22	1:O:332:PHE:CD2	2.30	0.67
1:O:41:LYS:O	1:O:44:TRP:HB2	1.94	0.67
1:O:110:GLU:O	1:O:113:GLU:HB2	1.94	0.66
1:O:114:HIS:N	1:O:114:HIS:ND1	2.38	0.66
1:O:200:ASP:C	1:O:204:LEU:HD12	2.16	0.66
1:O:381:LEU:O	1:O:384:ILE:HG13	1.94	0.66
1:Z:180:VAL:HG23	1:Z:181:THR:N	2.10	0.66
1:O:327:TYR:HB3	1:O:332:PHE:CZ	2.30	0.66
1:O:434:GLU:CD	1:O:435:VAL:H	1.98	0.66
1:Z:457:LEU:HA	1:Z:460:LEU:HD23	1.78	0.66
1:Z:483:TYR:O	1:Z:486:TRP:HB3	1.96	0.66
1:Z:117:ARG:NH1	1:Z:118:ASP:OD2	2.28	0.66
1:Z:298:VAL:HG23	1:Z:299:ASN:N	2.09	0.66
1:Z:347:ALA:HB3	1:Z:361:ARG:C	2.16	0.66
1:O:389:ARG:NH1	1:O:425:ILE:O	2.29	0.66
1:Z:422:GLN:O	1:Z:425:ILE:HG22	1.95	0.65
1:O:31:SER:HB3	1:O:59:THR:HG22	1.79	0.65
1:O:204:LEU:HD21	1:O:214:LEU:HD11	1.77	0.65
1:O:411:GLY:O	1:O:413:VAL:N	2.29	0.65
1:Z:407:ARG:NH1	1:Z:407:ARG:HG3	2.10	0.65
1:O:202:LYS:O	1:O:206:VAL:HG12	1.96	0.65
1:O:365:PHE:CE2	1:O:492:ARG:HB2	2.31	0.65
1:Z:419:MET:HA	1:Z:419:MET:CE	2.26	0.65
1:O:214:LEU:HD23	1:O:214:LEU:N	2.11	0.65
1:Z:174:THR:O	1:Z:177:ARG:HG2	1.95	0.65
1:Z:271:MET:C	1:Z:272:LEU:HD12	2.17	0.65
1:Z:480:ASN:ND2	1:Z:480:ASN:N	2.45	0.65
1:O:145:LEU:HD23	1:O:151:SER:HB2	1.79	0.65
1:O:178:VAL:HG23	1:O:180:VAL:CG1	2.26	0.65
1:O:74:ILE:HD13	1:O:74:ILE:N	2.11	0.65
1:Z:152:ARG:O	1:Z:155:ALA:HB3	1.97	0.65
1:Z:434:GLU:CD	1:Z:435:VAL:H	2.00	0.65
1:Z:407:ARG:CG	1:Z:407:ARG:HH11	2.10	0.64
1:O:295:THR:N	1:O:297:GLU:OE2	2.28	0.64
1:Z:191:LEU:CD2	1:Z:207:LEU:HD12	2.26	0.64
1:Z:198:ASP:OD1	1:Z:199:TRP:N	2.30	0.64
1:O:22:ASP:HB3	1:O:28:ILE:CD1	2.26	0.64
1:Z:196:THR:HG22	1:Z:197:LEU:N	2.12	0.64
1:Z:419:MET:HA	1:Z:419:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:ALA:HA	1:O:134:PRO:HG3	1.80	0.64
1:O:200:ASP:HB3	1:O:203:MET:HB2	1.79	0.64
1:O:191:LEU:CD2	1:O:207:LEU:HD12	2.28	0.64
1:Z:402:ARG:NH2	1:Z:428:THR:OG1	2.30	0.64
1:O:124:ILE:HG13	1:O:203:MET:HE1	1.78	0.64
1:O:142:LYS:NZ	1:O:146:ASP:OD2	2.30	0.64
1:Z:246:GLN:HA	1:Z:246:GLN:OE1	1.98	0.64
1:O:120:LEU:O	1:O:122:ASP:N	2.30	0.63
1:Z:415:ASN:O	1:Z:419:MET:HG2	1.98	0.63
1:O:336:VAL:HG23	1:O:338:ASN:N	2.07	0.63
1:O:457:LEU:N	1:O:457:LEU:HD23	2.13	0.63
1:Z:324:ASN:ND2	1:Z:327:TYR:H	1.96	0.63
1:Z:324:ASN:HD22	1:Z:327:TYR:H	1.46	0.63
1:O:324:ASN:HD22	1:O:326:ALA:HB3	1.63	0.63
1:O:340:ASN:HD22	1:O:371:VAL:HG22	1.64	0.63
1:O:434:GLU:N	1:O:465:VAL:O	2.30	0.63
1:Z:327:TYR:HB3	1:Z:332:PHE:CZ	2.34	0.63
1:Z:389:ARG:HG2	1:Z:483:TYR:CZ	2.34	0.63
1:O:255:CYS:CB	1:O:260:MET:HB3	2.24	0.63
1:Z:148:VAL:HG22	1:Z:151:SER:HB3	1.80	0.63
1:Z:420:GLN:O	1:Z:423:SER:HB3	1.98	0.63
1:O:438:VAL:O	1:O:439:THR:C	2.34	0.63
1:Z:267:THR:HG23	1:Z:311:ALA:HB2	1.80	0.63
1:O:188:ARG:NH2	1:O:303:GLU:OE1	2.31	0.63
1:O:85:THR:CG2	1:O:103:TRP:HD1	2.11	0.63
1:O:80:THR:HG21	1:O:248:ALA:CB	2.29	0.63
1:O:481:TYR:O	1:O:484:ALA:HB3	1.99	0.63
1:O:360:ALA:O	1:O:361:ARG:HG2	1.99	0.63
1:O:438:VAL:HG23	1:O:439:THR:N	2.14	0.63
1:O:389:ARG:HG2	1:O:483:TYR:CZ	2.33	0.63
1:O:83:ARG:HG3	3:O:601:GOL:O2	1.99	0.63
1:O:396:GLN:OE1	1:O:402:ARG:HA	1.97	0.62
1:O:486:TRP:O	1:O:489:ALA:HB3	1.99	0.62
1:O:208:ASP:C	1:O:209:ILE:HG12	2.18	0.62
1:O:320:MET:HB3	1:O:322:LEU:HG	1.79	0.62
1:Z:258:GLU:HA	1:Z:274:ASN:O	1.99	0.62
1:Z:457:LEU:CD2	1:Z:457:LEU:H	2.13	0.62
1:Z:458:ASP:O	1:Z:461:GLN:HG2	2.00	0.62
1:Z:47:HIS:HB3	1:Z:52:ILE:HD11	1.80	0.62
1:O:329:SER:HB2	1:O:381:LEU:HD11	1.81	0.62
1:Z:19:VAL:HG22	1:Z:30:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:442:GLY:O	1:Z:445:TYR:HB2	2.00	0.62
1:Z:365:PHE:CE2	1:Z:492:ARG:HB2	2.35	0.62
1:O:110:GLU:HA	1:O:110:GLU:OE1	1.99	0.62
1:Z:114:HIS:O	1:Z:115:LEU:C	2.36	0.62
1:Z:178:VAL:HG12	1:Z:180:VAL:HG13	1.81	0.62
1:Z:263:ASN:HB2	1:Z:406:LEU:HD11	1.80	0.62
1:O:108:THR:CB	1:O:139:THR:HB	2.30	0.62
1:Z:245:ASP:OD1	1:Z:246:GLN:N	2.29	0.62
1:Z:251:PHE:CE2	1:Z:446:LEU:HD12	2.35	0.62
1:O:245:ASP:OD1	1:O:246:GLN:N	2.28	0.61
1:Z:141:VAL:CG1	1:Z:209:ILE:HD13	2.31	0.61
1:O:406:LEU:HD22	1:O:407:ARG:N	2.15	0.61
1:O:57:SER:O	1:O:60:LEU:HB3	2.00	0.61
1:O:345:VAL:O	1:O:362:GLY:HA2	1.99	0.61
1:Z:41:LYS:O	1:Z:44:TRP:HB2	2.01	0.61
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.81	0.61
1:O:6:ILE:HD13	1:O:453:PHE:CD2	2.35	0.61
1:Z:171:TRP:CE2	1:Z:176:GLY:HA2	2.36	0.61
1:O:331:TYR:HD2	1:O:332:PHE:CE1	2.19	0.61
1:Z:128:THR:HB	1:Z:130:LEU:HD22	1.83	0.61
1:O:396:GLN:O	1:O:397:ALA:C	2.38	0.61
1:O:261:ALA:CB	1:O:273:MET:HB2	2.25	0.61
1:O:468:ARG:HH11	1:O:468:ARG:CG	2.13	0.61
1:O:354:PRO:HD2	1:O:355:TYR:CE1	2.36	0.60
1:O:433:PRO:HA	1:O:465:VAL:O	2.01	0.60
1:Z:272:LEU:HD12	1:Z:272:LEU:N	2.15	0.60
1:Z:110:GLU:O	1:Z:113:GLU:HB2	2.01	0.60
1:Z:200:ASP:O	1:Z:203:MET:HB2	2.01	0.60
1:O:104:GLN:HB3	1:O:349:THR:HG21	1.83	0.60
1:O:419:MET:HE2	1:O:419:MET:HA	1.84	0.60
1:Z:33:ARG:HG2	1:Z:55:THR:HG22	1.83	0.60
1:O:155:ALA:HB1	1:O:210:PRO:HG2	1.84	0.60
1:O:468:ARG:HG3	1:O:468:ARG:NH1	2.13	0.60
1:Z:360:ALA:O	1:Z:361:ARG:NH1	2.34	0.60
1:O:188:ARG:HH22	1:O:303:GLU:CD	2.05	0.60
1:O:422:GLN:O	1:O:425:ILE:HG22	2.02	0.59
1:Z:498:GLU:O	1:Z:499:HIS:C	2.38	0.59
1:Z:122:ASP:O	1:Z:123:TYR:C	2.39	0.59
1:Z:207:LEU:HB2	1:Z:209:ILE:HG13	1.84	0.59
1:Z:204:LEU:HD21	1:Z:214:LEU:HD11	1.85	0.59
1:Z:330:GLU:O	1:Z:334:THR:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:80:THR:HG22	1:O:245:ASP:N	2.16	0.59
1:O:117:ARG:NH1	1:O:118:ASP:OD2	2.34	0.59
1:O:411:GLY:O	1:O:412:ALA:C	2.39	0.59
1:Z:17:ARG:NH1	1:Z:437:GLU:HG2	2.18	0.59
1:O:85:THR:HG22	1:O:103:TRP:N	2.13	0.59
1:Z:171:TRP:CD1	1:Z:176:GLY:HA2	2.37	0.59
1:Z:458:ASP:HA	1:Z:461:GLN:CG	2.33	0.59
1:Z:106:ARG:HD2	1:Z:349:THR:O	2.02	0.59
1:O:255:CYS:HA	1:O:260:MET:CE	2.33	0.59
1:Z:240:SER:HB2	1:Z:450:ALA:HB3	1.85	0.59
1:Z:460:LEU:H	1:Z:460:LEU:HD22	1.67	0.59
1:Z:340:ASN:HD22	1:Z:371:VAL:HG22	1.67	0.58
1:O:153:GLU:HG2	1:O:156:ARG:HH12	1.68	0.58
1:O:23:HIS:HA	1:O:453:PHE:HE2	1.67	0.58
1:O:83:ARG:CG	1:O:83:ARG:HH11	1.97	0.58
1:O:8:ALA:O	1:O:9:LEU:HD12	2.03	0.58
1:O:26:ASN:O	1:O:28:ILE:HD12	2.03	0.58
1:Z:361:ARG:NH1	1:Z:361:ARG:HG2	2.19	0.58
1:O:354:PRO:HD2	1:O:355:TYR:CD1	2.39	0.58
1:O:396:GLN:O	1:O:400:GLY:N	2.25	0.57
1:Z:328:ASP:O	1:Z:331:TYR:HB3	2.03	0.57
1:Z:413:VAL:O	1:Z:432:ARG:HD3	2.04	0.57
1:O:40:PRO:HG2	1:O:44:TRP:HB3	1.86	0.57
1:Z:317:ARG:O	1:Z:321:LYS:HA	2.04	0.57
1:O:220:SER:O	1:O:446:LEU:HD23	2.04	0.57
1:O:352:GLY:O	1:O:355:TYR:N	2.37	0.57
1:O:47:HIS:O	1:O:49:PRO:HD3	2.04	0.57
1:Z:220:SER:O	1:Z:446:LEU:HD23	2.05	0.57
1:O:419:MET:HB2	1:O:470:PHE:CE2	2.40	0.57
1:O:476:THR:HG22	1:O:480:ASN:ND2	2.18	0.57
1:Z:166:ASP:N	1:Z:166:ASP:OD1	2.37	0.57
1:Z:20:VAL:O	1:Z:28:ILE:N	2.30	0.57
1:Z:328:ASP:HB3	1:Z:331:TYR:H	1.70	0.57
1:O:369:ARG:HG3	1:O:369:ARG:NH1	2.20	0.57
1:Z:174:THR:C	1:Z:175:GLN:HG2	2.25	0.57
1:Z:190:MET:O	1:Z:191:LEU:HD23	2.04	0.57
1:Z:331:TYR:CE2	1:Z:335:LYS:HE3	2.40	0.57
1:Z:422:GLN:O	1:Z:426:LEU:HB2	2.05	0.57
1:O:70:SER:HB2	1:O:72:ASP:OD1	2.05	0.56
1:Z:104:GLN:HB3	1:Z:349:THR:OG1	2.05	0.56
1:O:33:ARG:NH1	1:O:58:SER:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:108:THR:OG1	1:O:134:PRO:HA	2.05	0.56
1:O:382:GLU:HB3	1:O:421:PHE:CE2	2.40	0.56
1:O:70:SER:O	1:O:73:GLN:HG3	2.06	0.56
1:Z:115:LEU:HD23	1:Z:115:LEU:H	1.70	0.56
1:Z:154:ARG:O	1:Z:159:GLU:HG3	2.06	0.56
1:Z:475:GLU:O	1:Z:478:GLU:N	2.39	0.56
1:O:196:THR:HG22	1:O:197:LEU:N	2.20	0.56
1:O:272:LEU:HG	1:O:303:GLU:HB2	1.86	0.56
1:Z:241:GLY:O	1:Z:242:ILE:HG13	2.06	0.56
1:Z:433:PRO:HA	1:Z:465:VAL:O	2.05	0.56
1:O:385:ALA:HA	1:O:422:GLN:OE1	2.05	0.56
1:O:434:GLU:CG	1:O:465:VAL:H	2.10	0.56
1:Z:241:GLY:C	1:Z:242:ILE:HG13	2.25	0.56
1:Z:190:MET:O	1:Z:203:MET:HG3	2.06	0.56
1:Z:458:ASP:CA	1:Z:461:GLN:HG2	2.36	0.56
1:O:255:CYS:HB3	1:O:260:MET:CB	2.27	0.56
1:O:439:THR:HG22	1:O:440:ALA:N	2.20	0.56
1:Z:155:ALA:HA	1:Z:160:LEU:HB2	1.87	0.56
1:Z:313:ILE:O	1:Z:314:GLN:C	2.43	0.56
1:O:112:CYS:HB3	1:O:132:ILE:HG22	1.89	0.55
1:O:71:SER:HB2	1:O:235:THR:CG2	2.36	0.55
1:O:80:THR:CG2	1:O:248:ALA:HB2	2.36	0.55
1:Z:70:SER:HB2	1:Z:72:ASP:OD1	2.06	0.55
1:O:428:THR:N	1:O:472:PRO:HG3	2.21	0.55
1:O:432:ARG:NE	1:O:467:GLU:OE1	2.39	0.55
1:Z:456:ASN:O	1:Z:459:GLU:HB2	2.05	0.55
1:Z:289:THR:HG23	1:Z:290:ILE:N	2.20	0.55
1:O:115:LEU:O	1:O:120:LEU:HD12	2.06	0.55
1:O:209:ILE:O	1:O:210:PRO:C	2.43	0.55
1:O:155:ALA:CB	1:O:210:PRO:HG2	2.37	0.55
1:Z:269:CYS:HB2	1:Z:306:VAL:HB	1.88	0.55
1:Z:110:GLU:HA	1:Z:110:GLU:OE1	2.06	0.55
1:Z:161:LEU:HD22	1:Z:179:HIS:CE1	2.42	0.55
1:O:344:VAL:O	1:O:346:PRO:HD3	2.05	0.55
1:O:89:TRP:HD1	1:O:94:GLY:HA2	1.72	0.55
1:Z:103:TRP:CE3	1:Z:104:GLN:HG2	2.42	0.55
1:O:419:MET:HA	1:O:419:MET:CE	2.37	0.55
1:Z:147:HIS:HD2	1:Z:148:VAL:HG12	1.70	0.55
1:Z:423:SER:HB2	1:Z:430:VAL:CG2	2.36	0.55
1:Z:424:ASP:O	1:Z:479:ARG:HD3	2.07	0.55
1:O:190:MET:O	1:O:203:MET:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:285:GLY:C	1:O:286:LEU:HD23	2.26	0.55
1:O:293:GLY:HA2	1:O:299:ASN:ND2	2.22	0.55
1:Z:11:GLN:HE21	1:Z:165:VAL:HG11	1.71	0.55
1:Z:196:THR:HG22	1:Z:198:ASP:H	1.72	0.55
1:Z:320:MET:HB3	1:Z:322:LEU:HG	1.88	0.55
1:Z:461:GLN:NE2	1:Z:461:GLN:HA	2.22	0.55
1:Z:60:LEU:O	1:Z:63:VAL:HG12	2.06	0.55
1:O:130:LEU:N	1:O:130:LEU:HD23	2.20	0.55
1:Z:224:TYR:CZ	1:Z:242:ILE:HD12	2.42	0.55
1:O:346:PRO:HG2	1:O:387:GLN:NE2	2.22	0.54
1:O:351:LEU:HD12	1:O:360:ALA:CB	2.36	0.54
1:Z:25:ALA:HB3	1:Z:463:LYS:HD3	1.88	0.54
1:O:191:LEU:O	1:O:199:TRP:HE3	1.90	0.54
1:Z:49:PRO:HD3	1:Z:100:ALA:H	1.73	0.54
1:O:11:GLN:NE2	1:O:12:GLY:O	2.35	0.54
1:O:2:GLU:O	1:O:4:LYS:HG2	2.06	0.54
1:O:424:ASP:HB3	1:O:474:ILE:CG1	2.36	0.54
1:Z:86:THR:HG23	1:Z:162:PHE:HE1	1.73	0.54
1:Z:222:GLU:O	1:Z:240:SER:HA	2.08	0.54
1:Z:497:GLU:HA	1:Z:497:GLU:OE1	2.07	0.54
1:Z:498:GLU:OE1	1:Z:498:GLU:HA	2.05	0.54
1:O:174:THR:O	1:O:175:GLN:C	2.44	0.54
1:Z:445:TYR:CD1	1:Z:445:TYR:N	2.76	0.54
1:Z:48:ASP:O	1:Z:51:GLU:N	2.40	0.54
1:O:191:LEU:HD21	1:O:207:LEU:CD1	2.38	0.54
1:Z:262:LYS:HD2	1:Z:262:LYS:C	2.27	0.54
1:Z:360:ALA:C	1:Z:361:ARG:HG2	2.28	0.54
1:Z:478:GLU:O	1:Z:479:ARG:C	2.46	0.54
1:O:155:ALA:O	1:O:158:GLY:HA2	2.08	0.54
1:O:59:THR:O	1:O:63:VAL:HG22	2.08	0.54
1:Z:256:VAL:HG21	1:Z:294:PRO:CA	2.37	0.54
1:Z:441:LEU:O	1:Z:442:GLY:C	2.44	0.54
1:O:418:LEU:HD13	1:O:419:MET:CE	2.38	0.54
1:Z:47:HIS:HB2	1:Z:100:ALA:HB3	1.89	0.54
1:O:360:ALA:O	1:O:361:ARG:NH1	2.33	0.54
1:Z:208:ASP:C	1:Z:209:ILE:HG12	2.29	0.54
1:Z:253:GLN:HE22	1:Z:409:ASP:HB3	1.73	0.54
1:Z:281:LYS:HE3	1:Z:283:GLU:OE2	2.08	0.54
1:Z:17:ARG:HH12	1:Z:437:GLU:HG2	1.72	0.54
1:Z:419:MET:HB2	1:Z:470:PHE:CZ	2.44	0.54
1:O:180:VAL:HA	1:O:215:PRO:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:331:TYR:CD2	1:O:332:PHE:CE1	2.97	0.53
1:O:37:GLN:NE2	1:O:47:HIS:NE2	2.55	0.53
1:Z:120:LEU:O	1:Z:121:GLU:C	2.46	0.53
1:O:82:GLN:OE1	1:O:85:THR:CG2	2.54	0.53
1:Z:178:VAL:HG12	1:Z:180:VAL:CG1	2.38	0.53
1:Z:396:GLN:O	1:Z:400:GLY:N	2.41	0.53
1:O:211:ARG:O	1:O:214:LEU:HG	2.08	0.53
1:Z:218:ARG:NH1	1:Z:222:GLU:OE2	2.35	0.53
1:Z:340:ASN:HB2	1:Z:375:HIS:CD2	2.44	0.53
1:O:340:ASN:HB2	1:O:375:HIS:CD2	2.43	0.53
1:O:391:VAL:HG23	1:O:392:LEU:N	2.23	0.53
1:O:60:LEU:O	1:O:63:VAL:HG23	2.08	0.53
1:Z:162:PHE:CG	1:Z:163:GLY:N	2.76	0.53
1:Z:428:THR:HG22	1:Z:429:ARG:N	2.23	0.53
1:O:328:ASP:O	1:O:331:TYR:HB3	2.08	0.53
1:O:336:VAL:HG21	1:O:338:ASN:O	2.09	0.53
1:Z:153:GLU:O	1:Z:156:ARG:N	2.41	0.53
1:Z:422:GLN:HG3	1:Z:426:LEU:HD23	1.90	0.53
1:O:49:PRO:HD3	1:O:100:ALA:H	1.74	0.53
1:O:202:LYS:O	1:O:205:GLU:HB3	2.08	0.53
1:O:256:VAL:HG21	1:O:294:PRO:HB3	1.90	0.53
1:Z:312:SER:O	1:Z:315:TRP:HB3	2.09	0.53
1:O:295:THR:OG1	1:O:297:GLU:OE1	2.27	0.53
1:Z:47:HIS:O	1:Z:49:PRO:HD3	2.09	0.53
1:O:191:LEU:HD21	1:O:207:LEU:HD12	1.91	0.53
1:O:78:GLY:O	1:O:79:ILE:HG12	2.09	0.53
1:Z:171:TRP:CD2	1:Z:176:GLY:HA2	2.43	0.53
1:Z:406:LEU:HD22	1:Z:407:ARG:H	1.74	0.53
1:O:328:ASP:HB3	1:O:331:TYR:H	1.73	0.52
1:Z:156:ARG:HG3	1:Z:156:ARG:NH1	2.22	0.52
1:O:8:ALA:C	1:O:9:LEU:HD12	2.30	0.52
1:Z:307:PHE:HB3	1:Z:349:THR:HG21	1.90	0.52
1:Z:386:TYR:O	1:Z:389:ARG:HB3	2.09	0.52
1:O:271:MET:C	1:O:272:LEU:HD12	2.30	0.52
1:Z:123:TYR:O	1:Z:127:ASN:OD1	2.27	0.52
1:O:148:VAL:HG12	1:O:149:GLU:N	2.23	0.52
1:O:218:ARG:NH1	1:O:222:GLU:OE2	2.36	0.52
1:O:41:LYS:O	1:O:41:LYS:HG2	2.08	0.52
1:Z:145:LEU:CD1	1:Z:151:SER:HB2	2.34	0.52
1:Z:344:VAL:O	1:Z:346:PRO:HD3	2.10	0.52
1:Z:46:GLU:OE2	1:Z:107:ARG:NH2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:373:ALA:O	1:O:377:ILE:HD12	2.09	0.52
1:Z:11:GLN:HE22	1:Z:82:GLN:HE21	1.57	0.52
1:Z:428:THR:N	1:Z:472:PRO:HG3	2.25	0.52
1:O:392:LEU:HD23	1:O:392:LEU:C	2.30	0.52
1:Z:187:SER:HB3	1:Z:290:ILE:HG13	1.92	0.52
1:O:19:VAL:HG11	1:O:27:ILE:HD12	1.92	0.52
1:O:273:MET:CE	1:O:401:ILE:HD12	2.40	0.52
1:Z:24:ASP:O	1:Z:463:LYS:HE2	2.10	0.52
1:Z:457:LEU:O	1:Z:458:ASP:C	2.45	0.52
1:Z:48:ASP:O	1:Z:49:PRO:C	2.47	0.52
1:O:339:THR:O	1:O:340:ASN:HB3	2.09	0.51
1:Z:340:ASN:HB2	1:Z:375:HIS:NE2	2.25	0.51
1:Z:89:TRP:HB2	1:Z:95:LYS:O	2.09	0.51
1:O:137:SER:O	1:O:140:LYS:HB2	2.09	0.51
1:O:87:ILE:HG22	1:O:88:VAL:N	2.24	0.51
1:Z:127:ASN:O	1:Z:194:ILE:HG12	2.10	0.51
1:O:418:LEU:HD13	1:O:419:MET:HE3	1.92	0.51
1:Z:293:GLY:C	1:Z:295:THR:H	2.13	0.51
1:Z:407:ARG:HH12	1:Z:466:ILE:HD11	1.75	0.51
1:O:494:MET:O	1:O:495:ALA:HB3	2.11	0.51
1:Z:223:VAL:HG22	1:Z:240:SER:HB3	1.92	0.51
1:Z:421:PHE:O	1:Z:424:ASP:N	2.43	0.51
1:Z:457:LEU:N	1:Z:457:LEU:HD22	2.25	0.51
1:O:125:ARG:HD3	1:O:281:LYS:HD2	1.93	0.51
1:O:3:LYS:HB3	1:O:75:ALA:HA	1.92	0.51
1:Z:345:VAL:O	1:Z:362:GLY:HA2	2.11	0.51
1:Z:445:TYR:O	1:Z:446:LEU:C	2.47	0.51
1:O:166:ASP:OD1	1:O:166:ASP:N	2.44	0.51
1:O:442:GLY:O	1:O:445:TYR:HB2	2.10	0.51
1:O:200:ASP:O	1:O:203:MET:HB2	2.10	0.51
1:O:226:GLN:HA	1:O:237:ILE:O	2.09	0.51
1:O:287:LEU:HD12	1:O:303:GLU:HG2	1.93	0.51
1:Z:134:PRO:O	1:Z:140:LYS:NZ	2.39	0.51
1:O:80:THR:HG22	1:O:245:ASP:HA	1.91	0.51
1:O:357:ASP:OD1	1:O:358:PRO:N	2.43	0.51
1:Z:391:VAL:HG23	1:Z:392:LEU:N	2.25	0.51
1:O:251:PHE:O	1:O:254:LEU:HD12	2.11	0.51
1:O:418:LEU:HB3	1:O:419:MET:HE3	1.93	0.51
1:O:415:ASN:O	1:O:419:MET:HG2	2.11	0.51
1:Z:44:TRP:HA	1:Z:105:CYS:SG	2.51	0.51
1:O:162:PHE:CG	1:O:163:GLY:N	2.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:152:ARG:HH21	1:O:208:ASP:HB3	1.75	0.50
1:Z:180:VAL:HA	1:Z:215:PRO:HB2	1.92	0.50
1:Z:214:LEU:HD23	1:Z:214:LEU:N	2.26	0.50
1:Z:90:GLU:O	1:Z:94:GLY:N	2.37	0.50
1:O:391:VAL:O	1:O:392:LEU:C	2.47	0.50
1:O:85:THR:HG22	1:O:103:TRP:CD1	2.46	0.50
1:Z:164:THR:O	1:Z:165:VAL:C	2.49	0.50
1:Z:114:HIS:O	1:Z:117:ARG:N	2.44	0.50
1:Z:347:ALA:O	1:Z:361:ARG:HA	2.11	0.50
1:Z:457:LEU:HD22	1:Z:457:LEU:H	1.76	0.50
1:O:148:VAL:O	1:O:151:SER:OG	2.28	0.50
1:O:393:GLU:O	1:O:394:ALA:C	2.48	0.50
1:Z:188:ARG:HH11	1:Z:289:THR:HG21	1.77	0.50
1:O:24:ASP:O	1:O:463:LYS:HE2	2.12	0.50
1:O:459:GLU:C	1:O:460:LEU:HD23	2.32	0.50
1:O:490:VAL:HG12	1:O:494:MET:CE	2.41	0.50
1:Z:141:VAL:HG12	1:Z:209:ILE:HD13	1.92	0.50
1:Z:435:VAL:O	1:Z:435:VAL:HG12	2.10	0.50
1:Z:459:GLU:CB	1:Z:460:LEU:HD22	2.40	0.50
1:Z:389:ARG:HH22	1:Z:480:ASN:ND2	2.09	0.50
1:O:88:VAL:O	1:O:97:ILE:HG12	2.12	0.50
1:Z:223:VAL:O	1:Z:223:VAL:HG12	2.09	0.50
1:Z:87:ILE:HG22	1:Z:88:VAL:N	2.26	0.50
1:O:396:GLN:HA	1:O:399:SER:OG	2.11	0.50
1:Z:372:ASN:ND2	1:Z:374:ASN:N	2.52	0.50
1:Z:460:LEU:N	1:Z:460:LEU:CD2	2.74	0.50
1:O:114:HIS:O	1:O:117:ARG:N	2.45	0.49
1:O:120:LEU:HB2	1:O:124:ILE:CD1	2.42	0.49
1:O:451:VAL:HG13	1:O:451:VAL:O	2.12	0.49
1:Z:359:TYR:CZ	1:Z:499:HIS:CE1	2.99	0.49
1:Z:381:LEU:O	1:Z:384:ILE:HG13	2.11	0.49
1:O:315:TRP:CD1	1:O:319:GLU:HB2	2.46	0.49
1:Z:171:TRP:CG	1:Z:176:GLY:HA2	2.47	0.49
1:Z:17:ARG:HD2	1:Z:32:GLN:HG3	1.93	0.49
1:O:317:ARG:HB2	1:O:323:ILE:HG13	1.94	0.49
1:O:221:SER:OG	1:O:450:ALA:HB2	2.11	0.49
1:Z:152:ARG:NH2	1:Z:208:ASP:HB3	2.27	0.49
1:Z:170:ILE:O	1:Z:171:TRP:C	2.50	0.49
1:O:142:LYS:HG3	1:O:152:ARG:HH22	1.78	0.49
1:O:331:TYR:CZ	1:O:335:LYS:HE2	2.47	0.49
1:O:146:ASP:OD1	1:O:152:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:180:VAL:HG23	1:O:216:GLU:O	2.12	0.49
1:O:254:LEU:O	1:O:260:MET:HE1	2.11	0.49
1:O:332:PHE:HA	1:O:335:LYS:CG	2.42	0.49
1:O:368:THR:HG22	1:O:370:GLY:N	2.18	0.49
1:O:84:GLU:O	1:O:85:THR:C	2.50	0.49
1:Z:232:LYS:O	1:Z:233:GLY:C	2.49	0.49
1:Z:359:TYR:CE2	1:Z:499:HIS:CD2	3.00	0.49
1:O:406:LEU:HD22	1:O:407:ARG:H	1.76	0.49
1:Z:481:TYR:O	1:Z:484:ALA:HB3	2.13	0.49
1:O:174:THR:C	1:O:175:GLN:HG2	2.32	0.49
1:O:273:MET:N	1:O:395:MET:HE1	2.28	0.49
1:O:490:VAL:HG12	1:O:494:MET:HE2	1.94	0.49
1:Z:355:TYR:CE2	1:Z:490:VAL:HG11	2.47	0.49
1:Z:387:GLN:HA	1:Z:390:ASP:OD2	2.12	0.49
1:Z:106:ARG:NE	1:Z:106:ARG:HA	2.28	0.49
1:Z:131:VAL:HG12	1:Z:136:PHE:CE1	2.48	0.49
1:Z:23:HIS:HA	1:Z:453:PHE:CZ	2.48	0.49
1:Z:60:LEU:C	1:Z:60:LEU:HD12	2.33	0.49
1:O:386:TYR:HB3	1:O:486:TRP:CE2	2.47	0.49
1:O:394:ALA:O	1:O:397:ALA:HB3	2.13	0.49
1:Z:24:ASP:O	1:Z:25:ALA:HB3	2.13	0.49
1:Z:293:GLY:O	1:Z:295:THR:N	2.46	0.49
1:Z:434:GLU:HG2	1:Z:465:VAL:N	2.25	0.49
1:O:256:VAL:HG11	1:O:294:PRO:HA	1.95	0.48
1:O:428:THR:CG2	1:O:429:ARG:N	2.76	0.48
1:Z:244:GLY:O	1:Z:245:ASP:C	2.50	0.48
1:Z:421:PHE:O	1:Z:422:GLN:C	2.50	0.48
1:O:240:SER:HB2	1:O:450:ALA:CB	2.43	0.48
1:O:108:THR:HG21	1:O:139:THR:C	2.34	0.48
1:O:137:SER:HB2	1:O:189:THR:CA	2.30	0.48
1:O:251:PHE:O	1:O:254:LEU:N	2.35	0.48
1:O:376:ILE:O	1:O:377:ILE:C	2.50	0.48
1:O:438:VAL:CG2	1:O:439:THR:N	2.76	0.48
1:O:476:THR:O	1:O:480:ASN:ND2	2.46	0.48
1:O:90:GLU:HB2	1:O:93:THR:OG1	2.13	0.48
1:O:435:VAL:HG12	1:O:435:VAL:O	2.12	0.48
1:O:407:ARG:NH1	1:O:466:ILE:HD11	2.28	0.48
1:Z:224:TYR:HE1	1:Z:241:GLY:N	2.11	0.48
1:Z:38:ILE:O	1:Z:38:ILE:HG22	2.09	0.48
1:O:213:MET:HB2	1:O:214:LEU:HD23	1.95	0.48
1:Z:250:LEU:HD11	1:Z:255:CYS:HB2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:259:GLY:N	1:Z:274:ASN:O	2.39	0.48
1:O:145:LEU:CD1	1:O:213:MET:HE1	2.22	0.48
1:O:307:PHE:N	1:O:307:PHE:CD1	2.79	0.48
1:Z:71:SER:CB	1:Z:235:THR:HG21	2.23	0.48
1:O:108:THR:HG21	1:O:140:LYS:N	2.27	0.48
1:O:108:THR:HB	1:O:139:THR:HB	1.95	0.48
1:O:83:ARG:CG	3:O:601:GOL:O2	2.61	0.48
1:O:80:THR:HG22	1:O:245:ASP:CA	2.43	0.48
1:O:88:VAL:HG12	1:O:97:ILE:HG12	1.94	0.48
1:Z:377:ILE:O	1:Z:380:THR:HB	2.14	0.48
1:O:241:GLY:C	1:O:242:ILE:HG13	2.34	0.47
1:Z:44:TRP:N	1:Z:44:TRP:CD1	2.81	0.47
1:O:445:TYR:N	1:O:445:TYR:CD1	2.80	0.47
1:Z:468:ARG:HG3	1:Z:470:PHE:CE1	2.49	0.47
1:O:153:GLU:O	1:O:156:ARG:N	2.47	0.47
1:O:29:SER:C	1:O:30:VAL:HG23	2.35	0.47
1:Z:145:LEU:HA	1:Z:145:LEU:HD12	1.59	0.47
1:Z:494:MET:O	1:Z:495:ALA:HB3	2.13	0.47
1:O:273:MET:HB3	1:O:395:MET:CE	2.43	0.47
1:O:83:ARG:CG	1:O:83:ARG:NH1	2.64	0.47
1:Z:153:GLU:O	1:Z:154:ARG:C	2.49	0.47
1:Z:200:ASP:O	1:Z:204:LEU:HD12	2.14	0.47
1:Z:261:ALA:HB2	1:Z:273:MET:HA	1.96	0.47
1:Z:346:PRO:HA	1:Z:348:PHE:CE1	2.50	0.47
1:O:246:GLN:HA	1:O:246:GLN:OE1	2.13	0.47
1:O:303:GLU:HG3	1:O:304:GLY:N	2.29	0.47
1:O:360:ALA:C	1:O:361:ARG:HG2	2.34	0.47
1:Z:313:ILE:O	1:Z:316:LEU:HB2	2.14	0.47
1:O:120:LEU:CB	1:O:124:ILE:HD12	2.45	0.47
1:Z:191:LEU:HD21	1:Z:207:LEU:CD1	2.39	0.47
1:Z:226:GLN:HA	1:Z:237:ILE:O	2.15	0.47
1:O:339:THR:HB	1:O:342:VAL:HB	1.97	0.47
1:O:340:ASN:HB2	1:O:375:HIS:NE2	2.30	0.47
1:O:220:SER:C	1:O:446:LEU:HD23	2.35	0.47
1:Z:303:GLU:CG	1:Z:304:GLY:N	2.77	0.47
1:Z:327:TYR:HB3	1:Z:332:PHE:CE2	2.50	0.47
1:Z:47:HIS:ND1	1:Z:102:VAL:HG22	2.29	0.47
1:Z:98:TYR:HB3	1:Z:144:ILE:HD13	1.96	0.47
1:Z:41:LYS:HB2	1:Z:42:PRO:HD2	1.95	0.47
1:Z:84:GLU:O	1:Z:85:THR:C	2.52	0.47
1:O:118:ASP:HB2	1:O:120:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:22:ASP:OD1	1:O:26:ASN:HB2	2.14	0.47
1:O:234:GLY:N	2:O:502[A]:FBP:O6P	2.41	0.47
1:Z:108:THR:HG22	1:Z:111:ILE:HD12	1.97	0.47
1:Z:118:ASP:N	1:Z:118:ASP:OD1	2.47	0.47
1:Z:254:LEU:HA	1:Z:254:LEU:HD12	1.77	0.47
1:O:80:THR:HG21	1:O:248:ALA:HB3	1.96	0.47
1:O:250:LEU:HD11	1:O:255:CYS:CB	2.42	0.47
1:O:332:PHE:HA	1:O:335:LYS:HG2	1.96	0.47
1:O:429:ARG:HA	1:O:470:PHE:O	2.15	0.47
1:O:428:THR:HG22	1:O:429:ARG:N	2.30	0.47
1:Z:123:TYR:OH	1:Z:200:ASP:OD2	2.29	0.47
1:Z:332:PHE:HB2	1:Z:377:ILE:HD12	1.97	0.47
1:Z:274:ASN:HD21	1:Z:299:ASN:HD22	1.62	0.46
1:Z:342:VAL:CG1	1:Z:343:TYR:N	2.79	0.46
1:Z:390:ASP:OD1	1:Z:486:TRP:NE1	2.39	0.46
1:Z:460:LEU:H	1:Z:460:LEU:CD2	2.28	0.46
1:O:251:PHE:CD2	1:O:446:LEU:CD1	2.98	0.46
1:O:377:ILE:O	1:O:380:THR:HB	2.15	0.46
1:O:251:PHE:CD2	1:O:446:LEU:HD11	2.50	0.46
1:Z:141:VAL:CG2	1:Z:162:PHE:CD1	2.97	0.46
1:Z:30:VAL:HG12	1:Z:31:SER:N	2.29	0.46
1:Z:391:VAL:CG2	1:Z:392:LEU:N	2.79	0.46
1:Z:486:TRP:O	1:Z:490:VAL:HG23	2.15	0.46
1:O:102:VAL:CG2	1:O:103:TRP:N	2.78	0.46
1:O:372:ASN:O	1:O:375:HIS:HB2	2.14	0.46
1:O:90:GLU:O	1:O:94:GLY:N	2.45	0.46
1:Z:118:ASP:HB2	1:Z:120:LEU:HD11	1.98	0.46
1:Z:111:ILE:CG2	1:Z:139:THR:HG22	2.46	0.46
1:Z:201:ASP:O	1:Z:202:LYS:C	2.53	0.46
1:Z:192:PHE:CE1	1:Z:217:VAL:HG21	2.51	0.46
1:Z:361:ARG:O	1:Z:362:GLY:C	2.53	0.46
1:O:115:LEU:N	1:O:115:LEU:HD13	2.29	0.46
1:O:420:GLN:O	1:O:423:SER:HB3	2.15	0.46
1:Z:141:VAL:HG12	1:Z:142:LYS:N	2.27	0.46
1:Z:204:LEU:H	1:Z:204:LEU:CD1	2.27	0.46
1:Z:401:ILE:HG23	1:Z:401:ILE:HD13	1.60	0.46
1:O:196:THR:C	1:O:197:LEU:HD12	2.35	0.46
1:O:468:ARG:HB3	1:O:470:PHE:CE1	2.51	0.46
1:O:89:TRP:HB3	1:O:96:PRO:HA	1.97	0.46
1:Z:253:GLN:O	1:Z:254:LEU:HB2	2.15	0.46
1:O:180:VAL:CG2	1:O:181:THR:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:281:LYS:HB3	1:O:281:LYS:HE2	1.58	0.46
1:O:336:VAL:CG2	1:O:338:ASN:H	2.12	0.46
1:Z:97:ILE:HD12	1:Z:148:VAL:HG21	1.98	0.46
1:O:200:ASP:O	1:O:203:MET:N	2.49	0.46
1:O:22:ASP:N	1:O:28:ILE:CD1	2.79	0.46
1:O:335:LYS:HB2	1:O:374:ASN:ND2	2.28	0.46
1:O:6:ILE:CD1	1:O:453:PHE:CG	2.98	0.46
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.97	0.46
1:Z:171:TRP:NE1	1:Z:176:GLY:HA2	2.30	0.46
1:Z:204:LEU:CD1	1:Z:204:LEU:N	2.79	0.46
1:Z:413:VAL:HA	1:Z:419:MET:SD	2.56	0.46
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.98	0.46
1:O:237:ILE:CG2	1:O:238:PRO:HD2	2.46	0.46
1:O:21:MET:HG3	1:O:25:ALA:HA	1.97	0.46
1:O:278:LYS:HE2	1:O:278:LYS:HB2	1.55	0.46
1:O:389:ARG:HG2	1:O:483:TYR:CE1	2.50	0.46
1:Z:209:ILE:HA	1:Z:210:PRO:HD2	1.65	0.46
1:Z:111:ILE:HG21	1:Z:139:THR:HG22	1.97	0.46
1:Z:155:ALA:O	1:Z:158:GLY:HA2	2.16	0.46
1:O:182:ASP:HB3	1:O:242:ILE:HB	1.96	0.45
1:O:269:CYS:HB2	1:O:306:VAL:HB	1.98	0.45
1:O:63:VAL:HA	1:O:66:LYS:HD3	1.97	0.45
1:Z:406:LEU:HD23	1:Z:406:LEU:HA	1.51	0.45
1:Z:98:TYR:CD1	1:Z:99:ASN:N	2.83	0.45
1:O:257:LYS:O	1:O:260:MET:HB2	2.16	0.45
1:Z:425:ILE:HA	1:Z:425:ILE:HD12	1.67	0.45
1:Z:446:LEU:HD12	1:Z:446:LEU:H	1.81	0.45
1:O:196:THR:HG22	1:O:198:ASP:H	1.82	0.45
1:Z:149:GLU:OE1	1:Z:149:GLU:HA	2.16	0.45
1:Z:272:LEU:CD1	1:Z:272:LEU:N	2.79	0.45
1:Z:425:ILE:HD12	1:Z:479:ARG:HG3	1.98	0.45
1:Z:80:THR:OG1	1:Z:245:ASP:HA	2.16	0.45
1:O:140:LYS:O	1:O:143:TRP:HB3	2.16	0.45
1:O:275:THR:HG23	1:O:301:ALA:HA	1.97	0.45
1:O:425:ILE:HD12	1:O:479:ARG:HG2	1.98	0.45
1:Z:144:ILE:O	1:Z:148:VAL:HG13	2.16	0.45
1:Z:331:TYR:OH	1:Z:335:LYS:HE2	2.17	0.45
1:O:112:CYS:SG	1:O:134:PRO:HD3	2.56	0.45
1:O:182:ASP:OD2	1:O:184:THR:OG1	2.31	0.45
1:O:234:GLY:H	2:O:502[A]:FBP:P2	2.39	0.45
1:O:332:PHE:O	1:O:333:ALA:C	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:444:ALA:O	1:O:445:TYR:C	2.53	0.45
1:Z:166:ASP:O	1:Z:170:ILE:HD12	2.16	0.45
1:Z:372:ASN:C	1:Z:372:ASN:HD22	2.19	0.45
1:O:104:GLN:O	1:O:105:CYS:C	2.52	0.45
1:O:89:TRP:CB	1:O:96:PRO:HA	2.47	0.45
1:O:93:THR:OG1	1:O:95:LYS:HB3	2.17	0.45
1:Z:171:TRP:CE2	1:Z:176:GLY:CA	3.00	0.45
1:O:368:THR:CG2	1:O:369:ARG:N	2.79	0.45
1:O:389:ARG:O	1:O:390:ASP:C	2.51	0.45
1:O:195:HIS:C	1:O:197:LEU:HD12	2.36	0.45
1:O:197:LEU:N	1:O:197:LEU:CD1	2.77	0.45
1:Z:162:PHE:O	1:Z:179:HIS:HE1	2.00	0.45
1:Z:30:VAL:CG1	1:Z:31:SER:N	2.80	0.45
1:Z:407:ARG:NH1	1:Z:407:ARG:CG	2.76	0.45
1:O:441:LEU:HA	1:O:441:LEU:HD23	1.55	0.45
1:O:80:THR:HG23	1:O:248:ALA:HB2	1.98	0.45
1:Z:41:LYS:HD3	1:Z:44:TRP:CE2	2.51	0.45
1:Z:251:PHE:CD2	1:Z:446:LEU:CD1	3.00	0.45
1:O:107:ARG:O	1:O:109:ALA:N	2.50	0.45
1:O:115:LEU:HA	1:O:115:LEU:HD12	1.45	0.45
1:O:200:ASP:O	1:O:201:ASP:C	2.55	0.45
1:Z:108:THR:HG21	1:Z:140:LYS:N	2.31	0.45
1:Z:413:VAL:HG23	1:Z:432:ARG:HD2	1.99	0.45
1:Z:60:LEU:O	1:Z:60:LEU:HD12	2.16	0.45
1:O:134:PRO:O	1:O:140:LYS:NZ	2.49	0.44
1:O:253:GLN:O	1:O:254:LEU:HB2	2.17	0.44
1:Z:330:GLU:O	1:Z:331:TYR:C	2.54	0.44
1:Z:428:THR:CG2	1:Z:429:ARG:N	2.80	0.44
1:Z:451:VAL:HG13	1:Z:451:VAL:O	2.17	0.44
1:Z:7:VAL:O	1:Z:77:ILE:HA	2.16	0.44
1:O:102:VAL:HG23	1:O:103:TRP:H	1.80	0.44
1:O:196:THR:CG2	1:O:197:LEU:N	2.79	0.44
1:Z:221:SER:OG	1:Z:450:ALA:HB2	2.17	0.44
1:Z:346:PRO:C	1:Z:348:PHE:H	2.20	0.44
1:O:111:ILE:O	1:O:112:CYS:C	2.55	0.44
1:O:209:ILE:HA	1:O:210:PRO:HD2	1.86	0.44
1:O:19:VAL:CG1	1:O:27:ILE:HG23	2.48	0.44
1:O:344:VAL:HG23	1:O:379:ALA:HB1	1.98	0.44
1:O:478:GLU:O	1:O:479:ARG:C	2.55	0.44
1:Z:104:GLN:HE22	1:Z:308:MET:CE	2.30	0.44
1:Z:143:TRP:CE3	1:Z:144:ILE:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:124:ILE:HG22	1:O:125:ARG:N	2.29	0.44
1:O:266:GLY:O	1:O:267:THR:C	2.55	0.44
1:O:389:ARG:HH12	1:O:479:ARG:HG2	1.82	0.44
1:Z:6:ILE:CD1	1:Z:75:ALA:HB3	2.46	0.44
1:O:235:THR:O	1:O:236:ARG:HD3	2.18	0.44
1:O:351:LEU:HD12	1:O:360:ALA:HB1	1.98	0.44
1:O:420:GLN:NE2	1:O:420:GLN:CA	2.81	0.44
1:Z:108:THR:HG21	1:Z:139:THR:CB	2.38	0.44
1:Z:245:ASP:O	1:Z:248:ALA:HB3	2.17	0.44
1:Z:339:THR:O	1:Z:340:ASN:HB3	2.16	0.44
1:Z:347:ALA:O	1:Z:348:PHE:C	2.56	0.44
1:O:174:THR:HB	1:O:177:ARG:HB2	1.98	0.44
1:O:85:THR:CG2	1:O:103:TRP:CD1	2.95	0.44
1:Z:131:VAL:HG12	1:Z:136:PHE:HE1	1.82	0.44
1:Z:66:LYS:HG3	1:Z:67:ALA:H	1.83	0.44
1:O:52:ILE:O	1:O:53:TRP:C	2.55	0.44
1:Z:169:LEU:HA	1:Z:169:LEU:HD23	1.57	0.44
1:Z:246:GLN:O	1:Z:249:ALA:HB3	2.18	0.44
1:Z:290:ILE:HG22	1:Z:291:ALA:N	2.33	0.44
1:Z:86:THR:HG22	1:Z:87:ILE:N	2.30	0.44
1:Z:133:ASP:CG	1:Z:134:PRO:HD2	2.38	0.44
1:Z:138:GLY:O	1:Z:139:THR:C	2.56	0.44
1:Z:257:LYS:O	1:Z:258:GLU:C	2.55	0.44
1:Z:340:ASN:CB	1:Z:375:HIS:CD2	3.01	0.44
1:Z:389:ARG:HH12	1:Z:479:ARG:CG	2.31	0.44
1:Z:419:MET:HB2	1:Z:470:PHE:CE2	2.52	0.44
1:Z:90:GLU:HB2	1:Z:93:THR:OG1	2.18	0.44
1:O:441:LEU:O	1:O:444:ALA:HB3	2.17	0.43
1:O:55:THR:O	1:O:59:THR:OG1	2.28	0.43
1:Z:142:LYS:O	1:Z:143:TRP:C	2.55	0.43
1:Z:154:ARG:O	1:Z:158:GLY:N	2.51	0.43
1:Z:337:GLN:HE21	1:Z:337:GLN:N	2.16	0.43
1:Z:469:GLU:HG2	1:Z:471:ARG:HD3	2.01	0.43
1:Z:365:PHE:CZ	1:Z:492:ARG:HB2	2.53	0.43
1:O:186:ALA:C	1:O:188:ARG:H	2.22	0.43
1:O:244:GLY:O	1:O:245:ASP:C	2.56	0.43
1:O:422:GLN:HA	1:O:422:GLN:NE2	2.33	0.43
1:Z:160:LEU:HD23	1:Z:160:LEU:HA	1.55	0.43
1:Z:457:LEU:CA	1:Z:460:LEU:HD23	2.46	0.43
1:Z:74:ILE:CG2	1:Z:237:ILE:HG21	2.48	0.43
1:O:123:TYR:CE1	1:O:202:LYS:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:423:SER:O	1:O:427:GLY:N	2.45	0.43
1:O:438:VAL:O	1:O:441:LEU:N	2.50	0.43
1:O:86:THR:CG2	1:O:87:ILE:N	2.79	0.43
1:Z:193:ASN:CG	1:Z:196:THR:HB	2.38	0.43
1:O:274:ASN:HD21	1:O:299:ASN:HD22	1.65	0.43
1:Z:114:HIS:O	1:Z:116:LYS:N	2.50	0.43
1:Z:184:THR:O	1:Z:187:SER:OG	2.35	0.43
1:Z:256:VAL:HG22	1:Z:294:PRO:N	2.33	0.43
1:Z:265:TYR:HB3	1:Z:412:ALA:HB3	2.01	0.43
1:Z:266:GLY:O	1:Z:267:THR:C	2.54	0.43
1:O:199:TRP:CD1	1:O:214:LEU:HD12	2.53	0.43
1:O:250:LEU:HD12	1:O:255:CYS:HB2	1.95	0.43
1:O:298:VAL:CG1	1:O:299:ASN:N	2.78	0.43
1:O:29:SER:OG	1:O:63:VAL:HG12	2.19	0.43
1:O:338:ASN:O	1:O:375:HIS:HD2	2.02	0.43
1:O:386:TYR:HB3	1:O:486:TRP:CD2	2.53	0.43
1:O:234:GLY:HA2	2:O:502[B]:FBP:O5P	2.19	0.43
1:Z:102:VAL:HG12	1:Z:104:GLN:H	1.83	0.43
1:Z:110:GLU:O	1:Z:113:GLU:N	2.51	0.43
1:Z:170:ILE:HG22	1:Z:171:TRP:N	2.32	0.43
1:Z:41:LYS:HG2	1:Z:41:LYS:O	2.18	0.43
1:O:330:GLU:O	1:O:331:TYR:C	2.55	0.43
1:O:346:PRO:HG2	1:O:387:GLN:HE22	1.81	0.43
1:O:376:ILE:O	1:O:379:ALA:HB3	2.19	0.43
1:O:48:ASP:O	1:O:52:ILE:HG13	2.19	0.43
1:Z:90:GLU:HG2	1:Z:154:ARG:HH22	1.84	0.43
1:Z:261:ALA:HB2	1:Z:273:MET:CB	2.49	0.43
1:O:102:VAL:HG23	1:O:103:TRP:N	2.34	0.42
1:O:23:HIS:C	1:O:25:ALA:H	2.22	0.42
1:O:340:ASN:HD22	1:O:371:VAL:CG2	2.31	0.42
1:O:83:ARG:NE	1:O:246:GLN:HB2	2.34	0.42
1:Z:297:GLU:H	1:Z:297:GLU:HG3	1.04	0.42
1:Z:350:GLY:HA2	1:Z:360:ALA:O	2.19	0.42
1:O:107:ARG:HG2	1:O:108:THR:N	2.34	0.42
1:O:160:LEU:HD23	1:O:160:LEU:HA	1.59	0.42
1:O:187:SER:CB	1:O:290:ILE:HG13	2.49	0.42
1:O:353:ALA:HA	1:O:354:PRO:HA	1.79	0.42
1:Z:116:LYS:O	1:Z:119:GLY:HA2	2.18	0.42
1:Z:196:THR:O	1:Z:197:LEU:HB2	2.19	0.42
1:Z:316:LEU:HD23	1:Z:316:LEU:HA	1.49	0.42
1:Z:372:ASN:C	1:Z:372:ASN:ND2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:3:LYS:HB3	1:Z:75:ALA:HA	2.00	0.42
1:O:84:GLU:OE2	1:O:188:ARG:HD2	2.19	0.42
1:O:258:GLU:HA	1:O:274:ASN:OD1	2.19	0.42
1:O:438:VAL:HA	1:O:441:LEU:HD12	2.01	0.42
1:Z:22:ASP:O	1:Z:25:ALA:N	2.45	0.42
1:Z:226:GLN:HB2	1:Z:236:ARG:HB3	2.01	0.42
1:Z:251:PHE:CE2	1:Z:446:LEU:CD1	3.01	0.42
1:Z:411:GLY:O	1:Z:412:ALA:C	2.56	0.42
1:O:151:SER:O	1:O:155:ALA:N	2.44	0.42
1:O:199:TRP:CG	1:O:214:LEU:HD12	2.55	0.42
1:O:261:ALA:HB2	1:O:273:MET:HA	2.01	0.42
1:O:386:TYR:O	1:O:387:GLN:C	2.55	0.42
1:Z:104:GLN:NE2	1:Z:308:MET:CE	2.82	0.42
1:Z:489:ALA:O	1:Z:490:VAL:C	2.57	0.42
1:O:145:LEU:HD23	1:O:151:SER:CB	2.48	0.42
1:O:183:TYR:O	1:O:184:THR:C	2.58	0.42
1:O:204:LEU:CD2	1:O:214:LEU:HD11	2.47	0.42
1:O:378:ARG:O	1:O:379:ALA:C	2.55	0.42
1:Z:432:ARG:NE	1:Z:467:GLU:OE1	2.48	0.42
1:O:120:LEU:O	1:O:123:TYR:N	2.52	0.42
1:O:161:LEU:HA	1:O:161:LEU:HD23	1.28	0.42
1:Z:182:ASP:OD1	1:Z:185:ASN:N	2.38	0.42
1:Z:19:VAL:HG12	1:Z:20:VAL:N	2.34	0.42
1:Z:432:ARG:O	1:Z:467:GLU:N	2.53	0.42
1:Z:445:TYR:O	1:Z:449:LEU:N	2.38	0.42
1:O:387:GLN:O	1:O:388:THR:C	2.58	0.42
1:O:428:THR:HG22	1:O:429:ARG:O	2.20	0.42
1:O:89:TRP:CE3	1:O:89:TRP:N	2.88	0.42
1:Z:114:HIS:HA	1:Z:117:ARG:HG2	2.02	0.42
1:Z:219:ARG:HG2	1:Z:222:GLU:OE1	2.20	0.42
1:O:108:THR:OG1	1:O:134:PRO:HB3	2.20	0.42
1:O:420:GLN:O	1:O:421:PHE:C	2.55	0.42
1:Z:397:ALA:O	1:Z:398:ASP:C	2.55	0.42
1:Z:457:LEU:O	1:Z:460:LEU:N	2.48	0.42
1:Z:459:GLU:HB3	1:Z:460:LEU:HD22	2.01	0.42
1:O:254:LEU:HA	1:O:254:LEU:HD12	1.69	0.42
1:Z:302:LEU:HA	1:Z:302:LEU:HD23	1.88	0.42
1:Z:434:GLU:H	1:Z:434:GLU:HG3	1.40	0.42
1:O:124:ILE:HG13	1:O:203:MET:HE3	1.99	0.42
1:O:153:GLU:HA	1:O:156:ARG:NH1	2.35	0.42
1:Z:110:GLU:O	1:Z:111:ILE:C	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:117:ARG:C	1:Z:119:GLY:H	2.23	0.42
1:Z:130:LEU:HA	1:Z:130:LEU:HD12	1.63	0.42
1:Z:359:TYR:CD2	1:Z:499:HIS:CD2	3.08	0.42
1:Z:86:THR:HG23	1:Z:162:PHE:CE1	2.53	0.42
1:O:109:ALA:CA	1:O:134:PRO:HG3	2.49	0.41
1:O:262:LYS:O	1:O:271:MET:HA	2.20	0.41
1:O:309:ALA:O	1:O:310:GLY:C	2.56	0.41
1:O:316:LEU:HD23	1:O:316:LEU:HA	1.79	0.41
1:Z:124:ILE:HB	1:Z:125:ARG:H	1.68	0.41
1:Z:372:ASN:HB2	1:Z:373:ALA:H	1.63	0.41
1:Z:382:GLU:O	1:Z:383:SER:C	2.58	0.41
1:O:273:MET:CB	1:O:395:MET:HE3	2.51	0.41
1:O:310:GLY:O	1:O:313:ILE:HB	2.20	0.41
1:O:419:MET:O	1:O:420:GLN:C	2.58	0.41
1:O:413:VAL:HA	1:O:419:MET:SD	2.60	0.41
1:Z:85:THR:OG1	1:Z:102:VAL:HA	2.21	0.41
1:Z:347:ALA:HB3	1:Z:362:GLY:N	2.35	0.41
1:Z:403:LEU:HD12	1:Z:403:LEU:HA	1.77	0.41
1:Z:406:LEU:CD2	1:Z:407:ARG:N	2.78	0.41
1:Z:6:ILE:HA	1:Z:6:ILE:HD13	1.34	0.41
1:O:151:SER:O	1:O:152:ARG:C	2.58	0.41
1:O:130:LEU:HD13	1:O:136:PHE:CD1	2.54	0.41
1:O:144:ILE:O	1:O:148:VAL:HG23	2.19	0.41
1:Z:146:ASP:OD1	1:Z:152:ARG:NH1	2.40	0.41
1:Z:250:LEU:HD13	1:Z:262:LYS:HG3	2.01	0.41
1:Z:389:ARG:O	1:Z:390:ASP:C	2.55	0.41
1:Z:286:LEU:HD11	1:Z:395:MET:N	2.35	0.41
1:O:434:GLU:H	1:O:434:GLU:HG3	1.27	0.41
1:O:83:ARG:CZ	1:O:246:GLN:HB2	2.50	0.41
1:Z:289:THR:O	1:Z:300:TYR:HA	2.20	0.41
1:O:153:GLU:HG2	1:O:156:ARG:NH1	2.35	0.41
1:O:152:ARG:O	1:O:156:ARG:HG3	2.20	0.41
1:O:468:ARG:HB3	1:O:470:PHE:HE1	1.86	0.41
1:O:476:THR:HG22	1:O:480:ASN:HD21	1.82	0.41
1:Z:203:MET:HA	1:Z:206:VAL:HG12	2.03	0.41
1:Z:320:MET:O	1:Z:321:LYS:C	2.58	0.41
1:Z:331:TYR:CZ	1:Z:335:LYS:HE3	2.56	0.41
1:Z:393:GLU:O	1:Z:394:ALA:C	2.57	0.41
1:O:344:VAL:HG22	1:O:364:ILE:HG12	2.03	0.41
1:Z:251:PHE:O	1:Z:254:LEU:N	2.50	0.41
1:Z:349:THR:H	1:Z:349:THR:HG22	1.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:445:TYR:HD1	1:Z:445:TYR:N	2.18	0.41
1:Z:87:ILE:CG2	1:Z:88:VAL:N	2.84	0.41
1:Z:89:TRP:HA	1:Z:97:ILE:HG23	2.02	0.41
1:O:107:ARG:C	1:O:109:ALA:H	2.24	0.41
1:O:120:LEU:HB3	1:O:124:ILE:HD12	2.01	0.41
1:O:250:LEU:HD22	1:O:272:LEU:HB2	2.03	0.41
1:O:385:ALA:O	1:O:386:TYR:C	2.58	0.41
1:O:406:LEU:HA	1:O:406:LEU:HD23	1.37	0.41
1:Z:161:LEU:HD22	1:Z:179:HIS:NE2	2.36	0.41
1:Z:217:VAL:O	1:Z:218:ARG:HG2	2.21	0.41
1:Z:381:LEU:O	1:Z:382:GLU:C	2.58	0.41
1:O:396:GLN:CD	1:O:402:ARG:HA	2.41	0.41
1:O:106:ARG:NE	1:O:106:ARG:HA	2.35	0.41
1:O:120:LEU:CB	1:O:124:ILE:CD1	2.98	0.41
1:O:142:LYS:O	1:O:143:TRP:C	2.59	0.41
1:O:346:PRO:HA	1:O:348:PHE:CE1	2.56	0.41
1:Z:106:ARG:CA	1:Z:106:ARG:NE	2.83	0.41
1:Z:120:LEU:O	1:Z:124:ILE:HG12	2.21	0.41
1:Z:153:GLU:HA	1:Z:156:ARG:NH1	2.36	0.41
1:Z:174:THR:O	1:Z:175:GLN:C	2.58	0.41
1:Z:392:LEU:O	1:Z:392:LEU:HG	2.17	0.41
1:Z:418:LEU:HD23	1:Z:418:LEU:HA	1.91	0.41
1:O:97:ILE:HD12	1:O:148:VAL:HG21	2.03	0.41
1:O:88:VAL:HA	1:O:161:LEU:O	2.21	0.41
1:O:181:THR:OG1	1:O:182:ASP:N	2.53	0.41
1:O:382:GLU:O	1:O:383:SER:C	2.58	0.41
1:O:439:THR:CG2	1:O:440:ALA:N	2.81	0.41
1:Z:202:LYS:O	1:Z:206:VAL:HB	2.21	0.41
1:Z:315:TRP:O	1:Z:316:LEU:C	2.55	0.41
1:Z:452:GLY:O	1:Z:453:PHE:C	2.58	0.41
1:O:357:ASP:OD1	1:O:359:TYR:N	2.45	0.40
1:O:466:ILE:O	1:O:466:ILE:HG22	2.20	0.40
1:O:476:THR:O	1:O:477:THR:C	2.59	0.40
1:Z:213:MET:HB2	1:Z:213:MET:HE2	1.57	0.40
1:Z:310:GLY:O	1:Z:311:ALA:C	2.58	0.40
1:O:254:LEU:CD1	1:O:254:LEU:N	2.81	0.40
1:O:261:ALA:HB2	1:O:273:MET:CA	2.50	0.40
1:O:391:VAL:HG23	1:O:392:LEU:H	1.86	0.40
1:Z:108:THR:HB	1:Z:139:THR:CB	2.46	0.40
1:Z:353:ALA:HA	1:Z:354:PRO:HA	1.76	0.40
1:Z:372:ASN:ND2	1:Z:375:HIS:H	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:122:ASP:O	1:O:123:TYR:O	2.36	0.40
1:O:289:THR:HB	1:O:290:ILE:H	1.51	0.40
1:O:389:ARG:HH12	1:O:479:ARG:HD2	1.86	0.40
1:Z:272:LEU:HA	1:Z:302:LEU:O	2.21	0.40
1:Z:389:ARG:NH1	1:Z:479:ARG:CG	2.84	0.40
1:O:106:ARG:HH22	1:O:135:TYR:HA	1.86	0.40
1:O:67:ALA:CB	1:O:69:ILE:HD12	2.52	0.40
1:Z:152:ARG:O	1:Z:153:GLU:C	2.59	0.40
1:Z:183:TYR:O	1:Z:184:THR:C	2.60	0.40
1:Z:194:ILE:HG22	1:Z:290:ILE:HD11	2.03	0.40
1:Z:261:ALA:HB2	1:Z:273:MET:HB2	2.03	0.40
1:Z:268:GLY:HA3	1:Z:306:VAL:O	2.22	0.40
1:Z:339:THR:HB	1:Z:342:VAL:HB	2.03	0.40
1:Z:443:ALA:O	1:Z:444:ALA:C	2.59	0.40
1:O:193:ASN:OD1	1:O:196:THR:HB	2.21	0.40
1:O:245:ASP:O	1:O:246:GLN:C	2.60	0.40
1:O:273:MET:O	1:O:301:ALA:HB1	2.22	0.40
1:O:387:GLN:O	1:O:390:ASP:N	2.55	0.40
1:O:432:ARG:HA	1:O:433:PRO:HD3	1.78	0.40
1:Z:141:VAL:HG11	1:Z:209:ILE:HD13	2.01	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	496/501 (99%)	406 (82%)	74 (15%)	16 (3%)	4	26
1	Z	496/501 (99%)	414 (84%)	67 (14%)	15 (3%)	4	28
All	All	992/1002 (99%)	820 (83%)	141 (14%)	31 (3%)	4	26

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	99	ASN
1	O	121	GLU
1	O	151	SER
1	Z	149	GLU
1	O	72	ASP
1	O	220	SER
1	O	412	ALA
1	O	434	GLU
1	Z	151	SER
1	Z	294	PRO
1	O	108	THR
1	O	149	GLU
1	Z	72	ASP
1	Z	99	ASN
1	Z	108	THR
1	Z	445	TYR
1	O	358	PRO
1	Z	210	PRO
1	Z	434	GLU
1	Z	456	ASN
1	Z	476	THR
1	O	84	GLU
1	O	138	GLY
1	O	210	PRO
1	O	215	PRO
1	Z	84	GLU
1	Z	215	PRO
1	O	446	LEU
1	Z	197	LEU
1	Z	138	GLY
1	O	442	GLY

### 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	396/412 (96%)	301 (76%)	95 (24%)	<b>0</b> <b>3</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	398/412 (97%)	295 (74%)	103 (26%)	0	2
All	All	794/824 (96%)	596 (75%)	198 (25%)	0	2

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	2	GLU
1	O	4	LYS
1	O	6	ILE
1	O	13	THR
1	O	21	MET
1	O	29	SER
1	O	31	SER
1	O	32	GLN
1	O	33	ARG
1	O	37	GLN
1	O	59	THR
1	O	63	VAL
1	O	66	LYS
1	O	70	SER
1	O	71	SER
1	O	73	GLN
1	O	74	ILE
1	O	79	ILE
1	O	80	THR
1	O	82	GLN
1	O	83	ARG
1	O	85	THR
1	O	91	LYS
1	O	102	VAL
1	O	107	ARG
1	O	115	LEU
1	O	118	ASP
1	O	121	GLU
1	O	122	ASP
1	O	131	VAL
1	O	139	THR
1	O	144	ILE
1	O	151	SER
1	O	152	ARG
1	O	154	ARG
1	O	159	GLU

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Mol	Chain	Res	Type
1	O	164	THR
1	O	170	ILE
1	O	175	GLN
1	O	178	VAL
1	O	180	VAL
1	O	182	ASP
1	O	190	MET
1	O	196	THR
1	O	203	MET
1	O	206	VAL
1	O	209	ILE
1	O	213	MET
1	O	214	LEU
1	O	216	GLU
1	O	218	ARG
1	O	219	ARG
1	O	220	SER
1	O	221	SER
1	O	224	TYR
1	O	226	GLN
1	O	237	ILE
1	O	262	LYS
1	O	269	CYS
1	O	277	GLU
1	O	278	LYS
1	O	281	LYS
1	O	287	LEU
1	O	288	THR
1	O	297	GLU
1	O	317	ARG
1	O	318	ASP
1	O	324	ASN
1	O	336	VAL
1	O	365	PHE
1	O	368	THR
1	O	377	ILE
1	O	384	ILE
1	O	395	MET
1	O	396	GLN
1	O	403	LEU
1	O	404	HIS
1	O	406	LEU

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Mol	Chain	Res	Type
1	O	407	ARG
1	O	413	VAL
1	O	418	LEU
1	O	420	GLN
1	O	431	GLU
1	O	434	GLU
1	O	439	THR
1	O	449	LEU
1	O	451	VAL
1	O	459	GLU
1	O	463	LYS
1	O	466	ILE
1	O	468	ARG
1	O	470	PHE
1	O	477	THR
1	O	494	MET
1	O	498	GLU
1	Z	2	GLU
1	Z	4	LYS
1	Z	11	GLN
1	Z	17	ARG
1	Z	21	MET
1	Z	29	SER
1	Z	32	GLN
1	Z	33	ARG
1	Z	57	SER
1	Z	59	THR
1	Z	62	GLU
1	Z	66	LYS
1	Z	70	SER
1	Z	71	SER
1	Z	73	GLN
1	Z	74	ILE
1	Z	83	ARG
1	Z	91	LYS
1	Z	92	GLU
1	Z	107	ARG
1	Z	115	LEU
1	Z	117	ARG
1	Z	118	ASP
1	Z	122	ASP
1	Z	130	LEU

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Mol	Chain	Res	Type
1	Z	133	ASP
1	Z	136	PHE
1	Z	139	THR
1	Z	142	LYS
1	Z	145	LEU
1	Z	149	GLU
1	Z	152	ARG
1	Z	153	GLU
1	Z	154	ARG
1	Z	156	ARG
1	Z	159	GLU
1	Z	170	ILE
1	Z	175	GLN
1	Z	182	ASP
1	Z	190	MET
1	Z	196	THR
1	Z	203	MET
1	Z	209	ILE
1	Z	213	MET
1	Z	214	LEU
1	Z	216	GLU
1	Z	218	ARG
1	Z	222	GLU
1	Z	224	TYR
1	Z	226	GLN
1	Z	254	LEU
1	Z	262	LYS
1	Z	280	VAL
1	Z	281	LYS
1	Z	283	GLU
1	Z	287	LEU
1	Z	289	THR
1	Z	297	GLU
1	Z	312	SER
1	Z	314	GLN
1	Z	319	GLU
1	Z	321	LYS
1	Z	324	ASN
1	Z	329	SER
1	Z	336	VAL
1	Z	337	GLN
1	Z	351	LEU

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Mol	Chain	Res	Type
1	Z	361	ARG
1	Z	368	THR
1	Z	372	ASN
1	Z	384	ILE
1	Z	390	ASP
1	Z	392	LEU
1	Z	401	ILE
1	Z	402	ARG
1	Z	403	LEU
1	Z	406	LEU
1	Z	407	ARG
1	Z	418	LEU
1	Z	420	GLN
1	Z	425	ILE
1	Z	426	LEU
1	Z	434	GLU
1	Z	436	ARG
1	Z	437	GLU
1	Z	439	THR
1	Z	451	VAL
1	Z	455	GLN
1	Z	456	ASN
1	Z	458	ASP
1	Z	459	GLU
1	Z	460	LEU
1	Z	463	LYS
1	Z	466	ILE
1	Z	468	ARG
1	Z	470	PHE
1	Z	471	ARG
1	Z	476	THR
1	Z	477	THR
1	Z	482	ARG
1	Z	494	MET
1	Z	497	GLU
1	Z	498	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	32	GLN
1	O	37	GLN

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Mol	Chain	Res	Type
1	O	81	ASN
1	O	104	GLN
1	O	185	ASN
1	O	226	GLN
1	O	299	ASN
1	O	324	ASN
1	O	340	ASN
1	O	420	GLN
1	O	455	GLN
1	O	461	GLN
1	O	480	ASN
1	Z	11	GLN
1	Z	104	GLN
1	Z	147	HIS
1	Z	179	HIS
1	Z	228	ASN
1	Z	284	ASN
1	Z	299	ASN
1	Z	324	ASN
1	Z	337	GLN
1	Z	340	ASN
1	Z	372	ASN
1	Z	420	GLN
1	Z	455	GLN
1	Z	456	ASN
1	Z	461	GLN
1	Z	480	ASN
1	Z	499	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	O	601	-	5,5,5	0.38	0	5,5,5	0.51	0
2	FBP	O	502[B]	-	18,20,20	0.96	0	23,32,32	1.21	2 (8%)
2	FBP	O	502[A]	-	18,20,20	1.04	0	23,32,32	1.44	2 (8%)
3	GOL	Z	601	-	5,5,5	0.34	0	5,5,5	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	O	601	-	-	2/4/4/4	-
2	FBP	O	502[B]	-	-	9/13/32/32	0/1/1/1
2	FBP	O	502[A]	-	-	10/13/32/32	0/1/1/1
3	GOL	Z	601	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	O	502[A]	FBP	O3P-P1-O2P	4.86	126.22	107.64
2	O	502[A]	FBP	O6P-P2-O5P	3.11	119.54	107.64
2	O	502[B]	FBP	O6P-P2-O5P	3.06	119.34	107.64
2	O	502[B]	FBP	O3P-P1-O2P	2.96	118.94	107.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	601	GOL	O1-C1-C2-C3
2	O	502[B]	FBP	C1-O1-P1-O1P
2	O	502[B]	FBP	C1-O1-P1-O2P
2	O	502[B]	FBP	C1-O1-P1-O3P
2	O	502[B]	FBP	O1-C1-C2-O2
2	O	502[B]	FBP	O1-C1-C2-O5
2	O	502[B]	FBP	C4-C5-C6-O6
2	O	502[B]	FBP	O5-C5-C6-O6
2	O	502[B]	FBP	C6-O6-P2-O6P
2	O	502[A]	FBP	O1-C1-C2-O2
2	O	502[A]	FBP	O1-C1-C2-O5
2	O	502[A]	FBP	C4-C5-C6-O6
2	O	502[A]	FBP	O5-C5-C6-O6
2	O	502[A]	FBP	C6-O6-P2-O5P
2	O	502[A]	FBP	C6-O6-P2-O6P
3	O	601	GOL	O1-C1-C2-O2
2	O	502[A]	FBP	C1-O1-P1-O1P
2	O	502[A]	FBP	C6-O6-P2-O4P
2	O	502[B]	FBP	O1-C1-C2-C3
2	O	502[A]	FBP	C1-O1-P1-O2P
2	O	502[A]	FBP	C5-C6-O6-P2

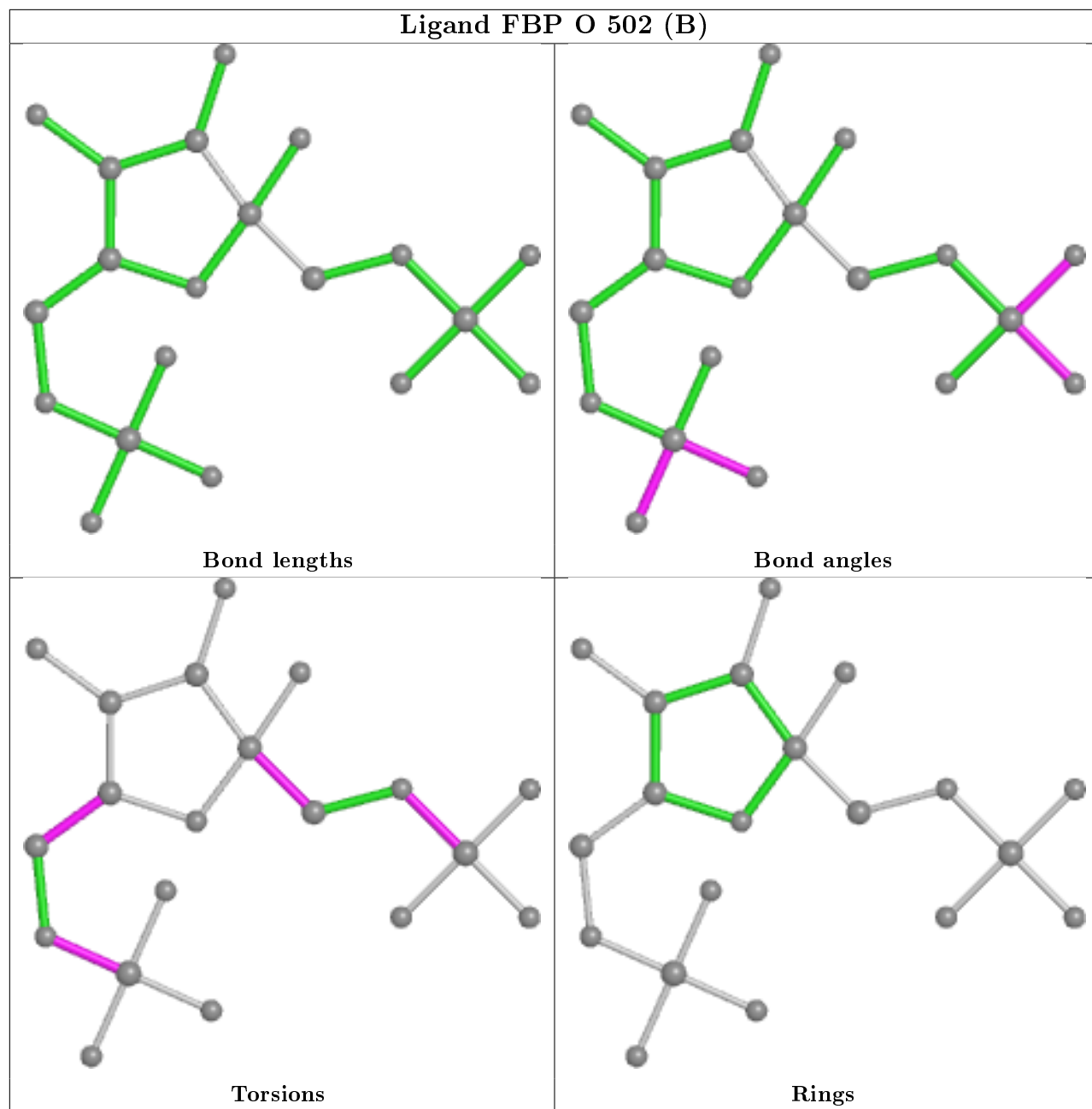
There are no ring outliers.

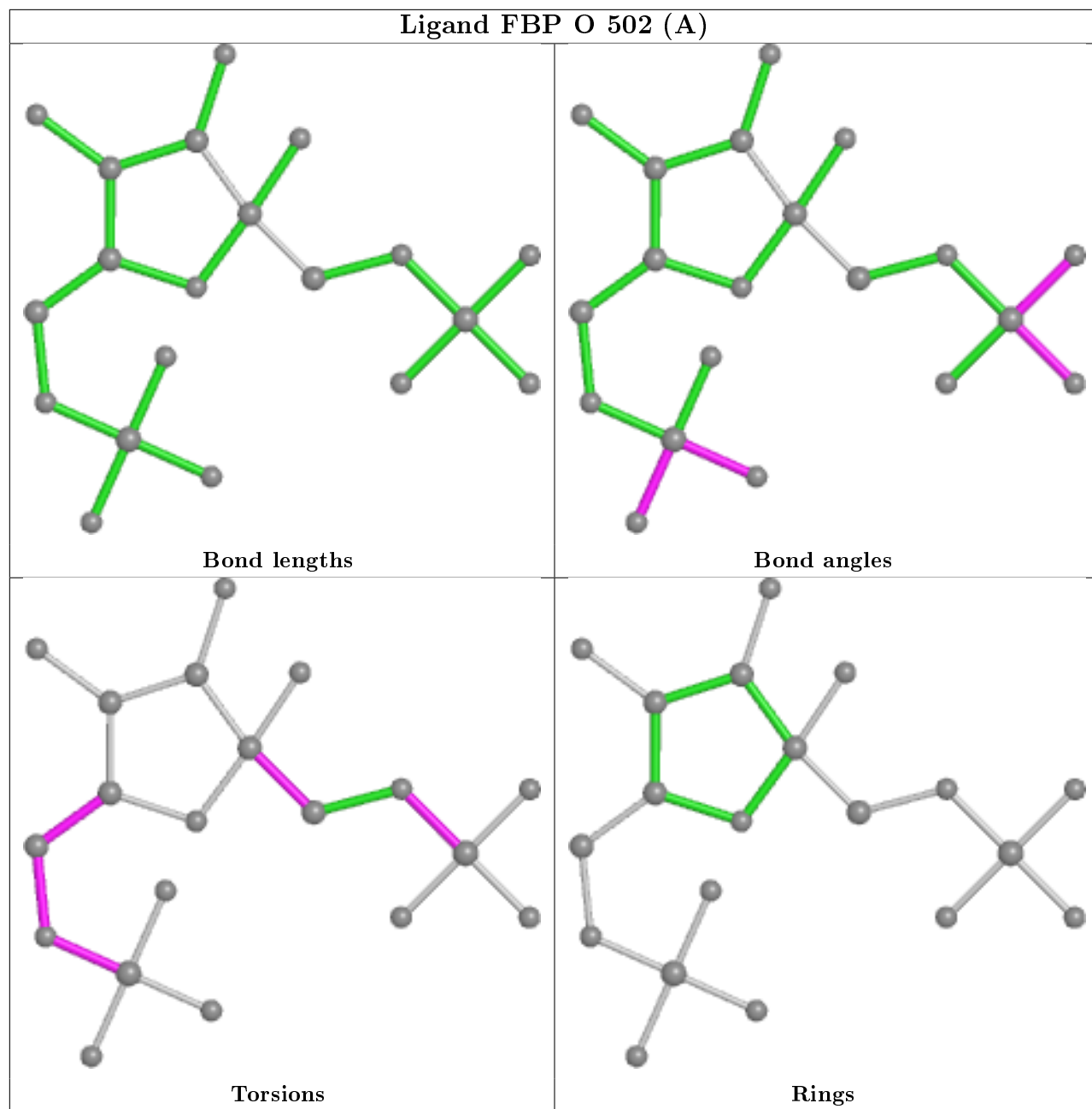
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	601	GOL	2	0
2	O	502[B]	FBP	1	0
2	O	502[A]	FBP	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.

## Ligand FBP O 502 (B)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	O	498/501 (99%)	-0.85	0 <a href="#">100</a> <a href="#">100</a>	12, 28, 62, 90	0
1	Z	498/501 (99%)	-0.89	1 (0%) <a href="#">95</a> <a href="#">94</a>	10, 26, 60, 89	0
All	All	996/1002 (99%)	-0.87	1 (0%) <a href="#">95</a> <a href="#">95</a>	10, 27, 61, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	325	ASP	2.3

### 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.

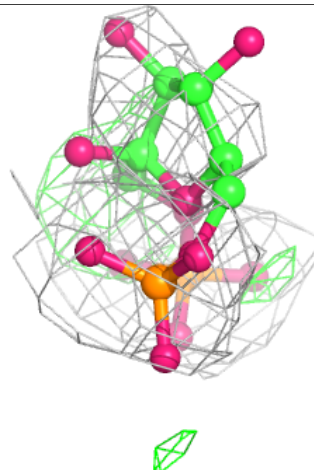
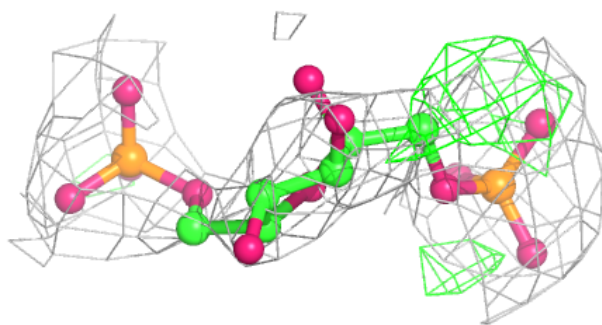
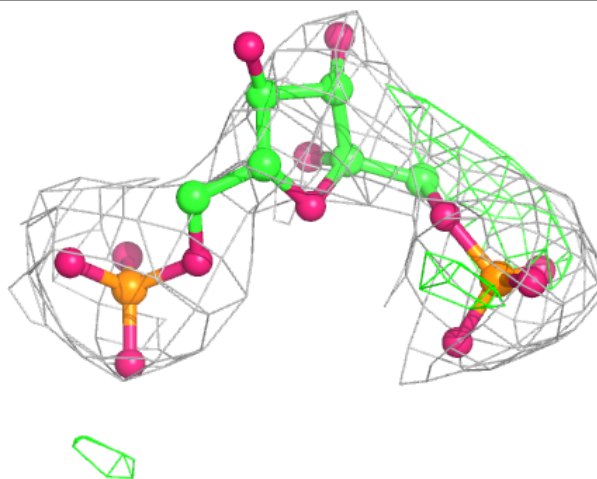
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FBP	O	502[B]	20/20	0.87	0.26	49,49,49,49	20
2	FBP	O	502[A]	20/20	0.87	0.26	49,49,49,49	20
3	GOL	O	601	6/6	0.97	0.15	10,18,32,41	0
3	GOL	Z	601	6/6	0.97	0.14	10,11,15,34	0



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.

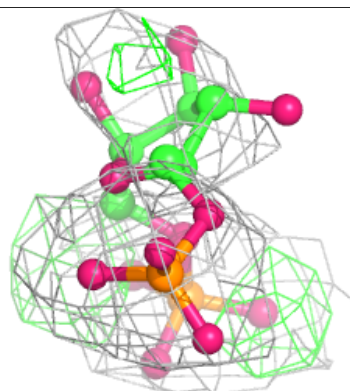
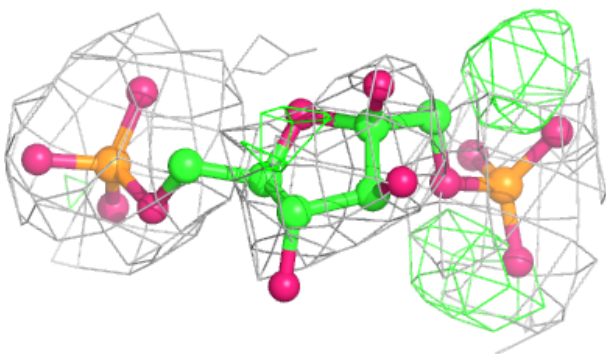
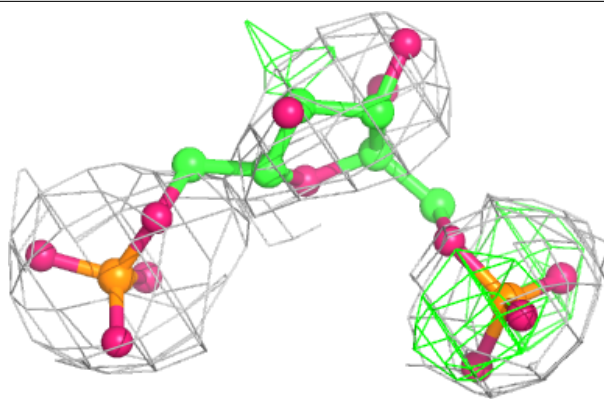
**Electron density around FBP O 502 (B):**

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



**Electron density around FBP O 502 (A):**

$2mF_o - DF_c$  (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.