



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:15 PM UTC

PDB ID : 1BO5 / pdb_00001bo5
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

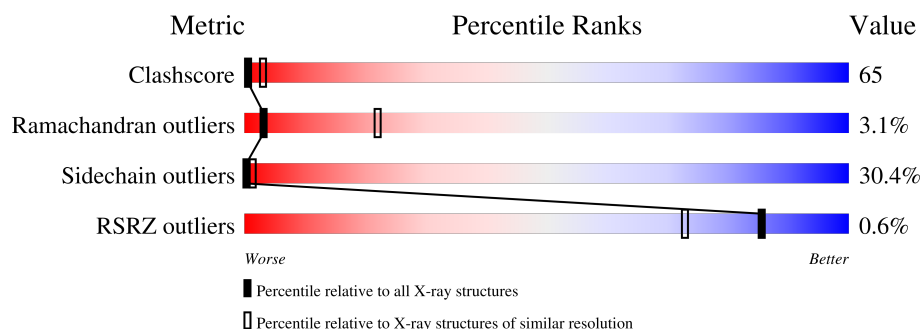
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	501	20% 50% 23% 6% .
1	Z	501	19% 51% 25% 5% .

2 Entry composition [i](#)

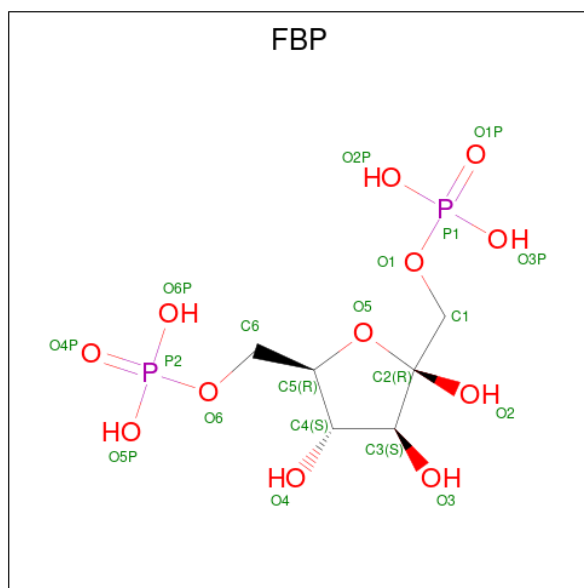
There are 3 unique types of molecules in this entry. The entry contains 7818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).

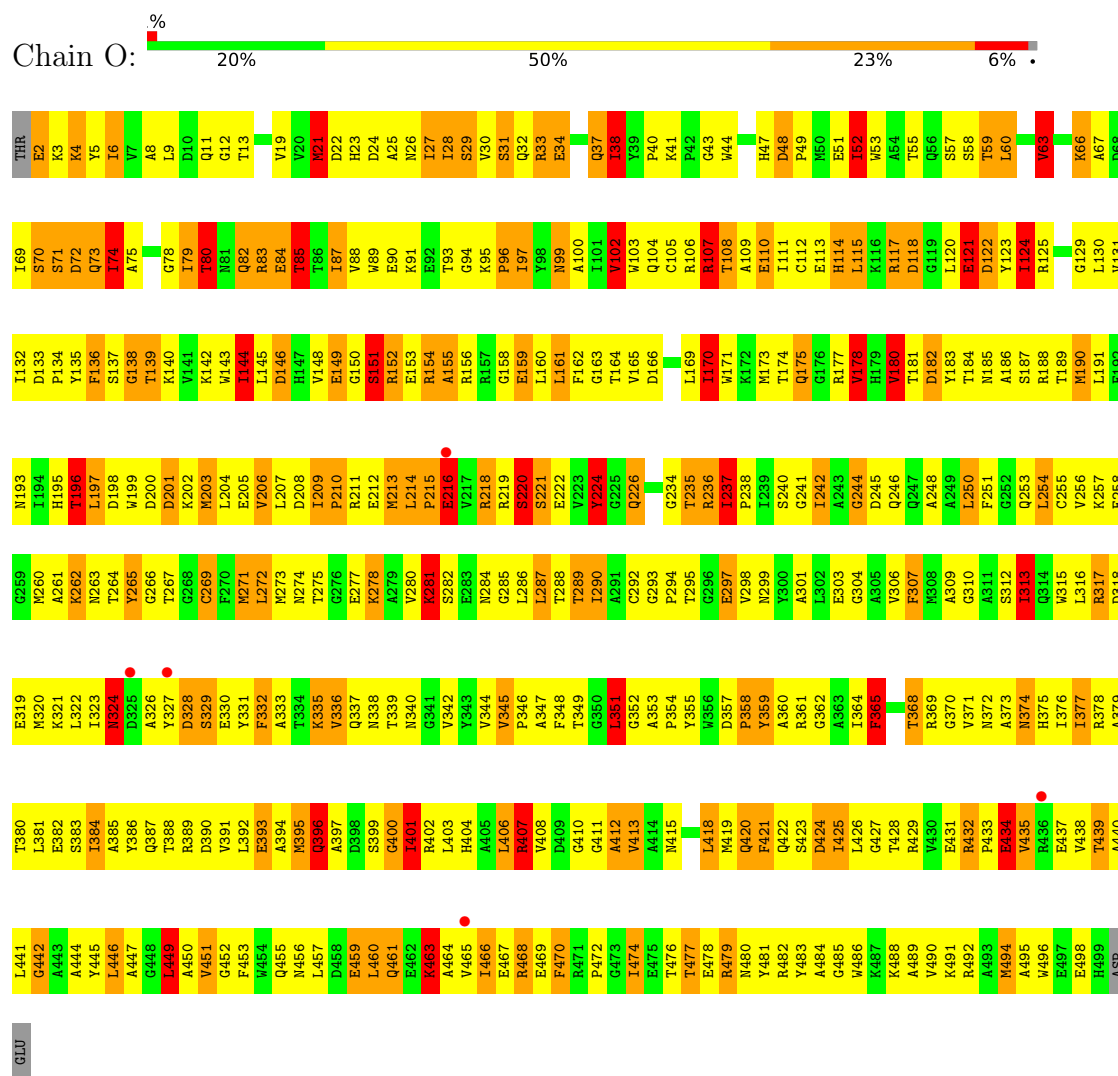


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

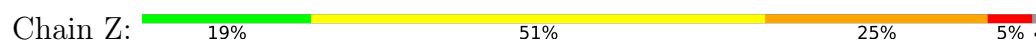
3 Residue-property plots

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)



A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	ASP	GLU					
E382	S383	S384	L384	A385	A386	Q387	T388	R389	D390	Q452	F453	L392	E393	A394	M395	Q396	A397	D398	S399	G400	I401	R402	L403	L406	R407	V408	D409	F470	G410	G411	A412	V413	E475	T476	N415	L418	M419	Q420	F421	Q422	S423	D424	I425	G427	T428	R429	V430	E431	R432	P433	E434	V435	R436	E437	V438	T439	A440	L441	G442	A443
M320	K321	L322	T323	R324	D325	A326	Y327	D328	S329	E330	Y331	F332	A333	T334	K335	V336	Q337	R338	T339	N340	G341	V342	Y343	V344	V345	P346	A347	F348	T349	G350	L351	G352	A353	P354	Y355	K356	D357	F358	Y359	A360	N361	G362	A363	I364	F365	T368	V371	N372	A373	N374	H375	I376	I377	R378	A379	T380	L381			
C255	V256	K257	E258	G259	M260	A261	K262	N263	T264	Y265	G266	T267	G268	C269	F270	M271	L272	D273	M274	A279	V280	M281	K281	S282	E283	L286	L287	T288	T289	I290	A291	C292	G293	G294	P294	T295	G296	E297	Y298	N299	Y300	A301	L302	E303	G304	V306	F307	K308	L309	G310	A311	S312	I313	A249	L250	P251	L316	R317		
L191	F192	N193	I194	H195	T196	L197	D198	W199	D200	D201	K202	M203	L204	E205	V206	L207	D208	I209	P210	R211	E212	M213	L214	P215	E216	V217	R218	L219	S220	S221	E222	V223	Y224	G225	Q226	K232	G233	G234	T235	R236	I237	P238	T239	S240	G241	I242	V243	G244	D245	Q246	A247	A248	I249	L250	P251	G252	Q253	L254		
V131	I132	D133	P134	Y135	F136	L137	G138	T139	K140	V141	K142	W143	I144	L145	H146	V147	E148	E149	G150	S151	R152	E153	R154	A155	R156	R157	E158	L160	L161	F162	G163	T164	V165	D166	T167	H168	L169	I170	W171	K172	M173	T174	Q175	G176	R177	V178	H179	I180	T181	D182	Y183	T184	N185	A186	S187	R188	T189	M190		
S70	S71	D72	Q73	I74	A75	G76	I77	T80	N81	Q82	R83	E84	T85	T86	I87	V88	W89	E90	K91	E92	T93	G94	K95	P96	I97	N98	A99	I100	V101	W102	Y103	Q104	C105	R106	R107	T108	A109	E110	I111	G112	E113	H114	L115	K116	R117	D118	G119	L120	E121	D122	Y123	T124	R125	S126	N127	T128	G129	L130		
THR	E2	K3	K4	Y5	I6	V7	Q11	R17	A18	V19	V20	M21	D22	H23	D24	A25	N26	I27	I28	S29	V30	S31	Q32	R33	E34	F35	E36	Q37	R38	Y39	P40	K41	P42	G43	W44	V45	E46	H47	D48	P49	M50	E51	I52	T55	Q56	S57	S58	T59	L60	V61	E62	V63	K66	A67						

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.41Å 169.41Å 204.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.20) 93.8 (20.00-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	44.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 114.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	1.45	16/3958 (0.4%)	1.85	97/5373 (1.8%)
1	Z	1.45	8/3968 (0.2%)	1.84	92/5387 (1.7%)
All	All	1.45	24/7926 (0.3%)	1.84	189/10760 (1.8%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	396	GLN	CA-C	-6.46	1.44	1.52
1	O	313	ILE	CA-CB	-6.45	1.47	1.54
1	Z	373	ALA	N-CA	-6.36	1.38	1.46
1	O	401	ILE	CA-CB	-6.26	1.46	1.54
1	O	272	LEU	CA-C	-6.09	1.45	1.52
1	O	219	ARG	NE-CZ	6.05	1.39	1.33
1	O	265	TYR	CA-C	-5.75	1.46	1.53
1	O	324	ASN	C-O	5.61	1.31	1.24
1	Z	111	ILE	CA-CB	-5.56	1.48	1.54
1	Z	325	ASP	CG-OD2	5.54	1.35	1.25
1	O	201	ASP	CA-C	-5.47	1.45	1.52
1	Z	96	PRO	C-N	-5.37	1.27	1.33
1	Z	424	ASP	C-N	-5.36	1.28	1.34
1	O	280	VAL	CA-CB	-5.35	1.47	1.54
1	Z	51	GLU	CD-OE1	5.35	1.35	1.25
1	O	146	ASP	N-CA	-5.30	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	38	ILE	CA-CB	-5.30	1.47	1.54
1	O	224	TYR	N-CA	-5.29	1.39	1.46
1	O	5	TYR	CA-C	-5.24	1.46	1.52
1	O	74	ILE	CA-C	-5.21	1.46	1.52
1	O	38	ILE	CA-CB	-5.18	1.47	1.54
1	O	170	ILE	N-CA	-5.11	1.40	1.46
1	O	196	THR	N-CA	-5.06	1.40	1.46
1	Z	357	ASP	C-N	-5.04	1.28	1.34

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	114	HIS	CA-CB-CG	-10.64	103.16	113.80
1	O	463	LYS	N-CA-C	9.48	121.21	111.07
1	O	351	LEU	CA-C-N	-9.37	106.56	122.21
1	O	351	LEU	C-N-CA	-9.37	106.56	122.21
1	Z	424	ASP	CA-CB-CG	-8.42	104.18	112.60
1	O	63	VAL	CB-CA-C	-8.33	101.22	111.88
1	Z	390	ASP	CA-CB-CG	7.89	120.50	112.60
1	Z	289	THR	N-CA-C	7.88	120.88	109.14
1	O	165	VAL	N-CA-C	7.54	118.07	110.23
1	Z	293	GLY	CA-C-N	7.37	129.06	119.84
1	Z	293	GLY	C-N-CA	7.37	129.06	119.84
1	O	284	ASN	CA-CB-CG	-7.33	105.27	112.60
1	O	365	PHE	N-CA-C	7.31	120.86	109.52
1	Z	469	GLU	CA-C-N	-7.21	112.48	122.93
1	Z	469	GLU	C-N-CA	-7.21	112.48	122.93
1	Z	114	HIS	CA-CB-CG	-7.12	106.68	113.80
1	O	432	ARG	O-C-N	7.11	127.87	121.19
1	O	437	GLU	N-CA-C	6.99	118.39	108.54
1	Z	36	GLU	N-CA-C	6.96	120.41	109.96
1	O	201	ASP	CA-CB-CG	-6.87	105.73	112.60
1	O	464	ALA	N-CA-C	6.86	120.67	109.76
1	Z	390	ASP	N-CA-CB	6.84	121.36	109.72
1	O	21	MET	N-CA-C	6.82	120.51	109.40
1	Z	39	TYR	CA-C-N	6.80	128.34	119.84
1	Z	39	TYR	C-N-CA	6.80	128.34	119.84
1	O	180	VAL	N-CA-CB	-6.77	102.26	112.35
1	Z	237	ILE	CA-C-O	6.74	123.97	119.38
1	Z	133	ASP	CA-C-O	6.74	126.30	119.76
1	Z	328	ASP	N-CA-C	6.74	120.00	110.50
1	O	236	ARG	CA-C-N	-6.73	116.85	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	236	ARG	C-N-CA	-6.73	116.85	123.04
1	Z	307	PHE	N-CA-C	6.73	118.61	111.28
1	O	449	LEU	CB-CA-C	-6.67	100.40	110.88
1	O	289	THR	N-CA-CB	6.66	122.44	111.31
1	Z	263	ASN	CA-CB-CG	-6.63	105.97	112.60
1	Z	211	ARG	N-CA-CB	6.57	122.00	110.18
1	Z	147	HIS	CA-C-N	-6.56	114.34	123.13
1	Z	147	HIS	C-N-CA	-6.56	114.34	123.13
1	O	38	ILE	CB-CA-C	-6.50	102.69	111.15
1	Z	27	ILE	N-CA-CB	6.49	118.91	111.39
1	O	34	GLU	N-CA-CB	6.48	120.30	110.45
1	O	400	GLY	N-CA-C	-6.38	106.43	115.30
1	O	124	ILE	CB-CA-C	-6.35	103.57	111.70
1	Z	38	ILE	CB-CA-C	-6.35	102.90	111.15
1	Z	349	THR	N-CA-CB	-6.35	100.76	111.17
1	O	110	GLU	N-CA-CB	6.33	119.38	109.94
1	Z	214	LEU	N-CA-CB	6.32	117.76	109.55
1	O	281	LYS	CA-C-N	-6.32	114.00	122.72
1	O	281	LYS	C-N-CA	-6.32	114.00	122.72
1	Z	499	HIS	CA-CB-CG	-6.30	107.50	113.80
1	O	97	ILE	N-CA-C	-6.29	106.60	112.83
1	O	155	ALA	CA-C-N	6.28	128.97	120.44
1	O	155	ALA	C-N-CA	6.28	128.97	120.44
1	Z	107	ARG	N-CA-C	6.27	117.78	111.07
1	O	159	GLU	N-CA-C	-6.25	105.65	113.28
1	O	289	THR	N-CA-C	6.25	117.68	108.86
1	O	351	LEU	N-CA-C	6.21	124.03	110.80
1	O	155	ALA	O-C-N	6.20	128.46	122.07
1	Z	237	ILE	N-CA-CB	6.20	118.24	111.61
1	Z	104	GLN	N-CA-C	6.19	118.03	111.28
1	O	165	VAL	CB-CA-C	6.15	119.57	111.70
1	Z	432	ARG	N-CA-CB	6.14	118.27	110.23
1	O	307	PHE	N-CA-C	6.11	118.72	111.33
1	Z	124	ILE	CB-CA-C	-6.10	101.28	111.29
1	Z	408	VAL	N-CA-CB	-6.06	105.67	112.45
1	O	408	VAL	N-CA-C	6.04	117.62	108.80
1	O	280	VAL	N-CA-C	6.04	116.56	108.11
1	Z	177	ARG	N-CA-CB	6.04	119.94	110.46
1	O	21	MET	N-CA-CB	6.03	121.33	110.83
1	O	396	GLN	CB-CA-C	-6.03	101.68	110.96
1	Z	43	GLY	N-CA-C	-6.02	106.22	114.64
1	Z	134	PRO	N-CA-C	-6.01	106.03	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	136	PHE	N-CA-C	5.99	119.81	110.17
1	O	401	ILE	CB-CA-C	-5.97	101.61	110.33
1	Z	236	ARG	CA-C-N	-5.96	116.88	123.43
1	Z	236	ARG	C-N-CA	-5.96	116.88	123.43
1	Z	406	LEU	CA-C-N	-5.96	114.50	122.72
1	Z	406	LEU	C-N-CA	-5.96	114.50	122.72
1	O	432	ARG	CA-C-N	5.93	125.91	120.21
1	O	432	ARG	C-N-CA	5.93	125.91	120.21
1	Z	434	GLU	CA-C-N	5.93	129.89	122.48
1	Z	434	GLU	C-N-CA	5.93	129.89	122.48
1	Z	159	GLU	N-CA-C	-5.92	106.10	113.38
1	O	80	THR	CA-C-N	-5.90	112.73	122.11
1	O	80	THR	C-N-CA	-5.90	112.73	122.11
1	O	469	GLU	CA-C-N	-5.90	114.79	123.05
1	O	469	GLU	C-N-CA	-5.90	114.79	123.05
1	O	129	GLY	N-CA-C	-5.88	106.95	114.37
1	O	102	VAL	CB-CA-C	5.86	118.57	111.13
1	O	426	LEU	N-CA-C	-5.85	106.27	113.41
1	O	107	ARG	N-CA-C	5.84	117.65	111.28
1	Z	474	ILE	CA-C-N	5.83	129.11	120.95
1	Z	474	ILE	C-N-CA	5.83	129.11	120.95
1	O	96	PRO	N-CA-CB	5.82	108.41	103.35
1	Z	480	ASN	CA-CB-CG	-5.81	106.79	112.60
1	O	396	GLN	N-CA-CB	5.80	118.37	109.91
1	O	324	ASN	CA-C-N	-5.79	113.57	122.60
1	O	324	ASN	C-N-CA	-5.79	113.57	122.60
1	O	421	PHE	CA-CB-CG	-5.77	108.03	113.80
1	Z	320	MET	N-CA-C	-5.71	105.81	112.89
1	Z	86	THR	N-CA-C	5.70	119.10	109.76
1	Z	136	PHE	N-CA-C	5.70	118.91	110.48
1	O	129	GLY	CA-C-O	5.68	125.01	119.27
1	O	178	VAL	N-CA-C	5.66	116.27	108.12
1	O	292	CYS	N-CA-C	5.66	117.75	108.52
1	O	38	ILE	N-CA-C	5.66	116.36	108.89
1	Z	133	ASP	N-CA-C	5.65	115.40	108.11
1	O	219	ARG	N-CA-CB	5.64	119.47	110.16
1	O	237	ILE	CA-C-O	5.63	122.85	119.19
1	Z	136	PHE	CA-C-N	5.63	129.26	120.82
1	Z	136	PHE	C-N-CA	5.63	129.26	120.82
1	Z	497	GLU	N-CA-C	5.58	118.41	110.10
1	Z	4	LYS	CA-C-N	-5.56	112.81	122.37
1	Z	4	LYS	C-N-CA	-5.56	112.81	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	38	ILE	CA-C-N	-5.56	116.32	123.16
1	Z	38	ILE	C-N-CA	-5.56	116.32	123.16
1	Z	474	ILE	N-CA-CB	5.55	121.05	111.39
1	Z	99	ASN	CA-CB-CG	-5.55	107.05	112.60
1	O	401	ILE	N-CA-C	5.54	116.10	108.12
1	Z	165	VAL	CB-CA-C	5.54	120.38	111.29
1	O	146	ASP	N-CA-C	-5.53	105.16	111.07
1	Z	34	GLU	N-CA-CB	5.51	117.94	110.38
1	O	328	ASP	N-CA-C	5.51	118.64	110.48
1	O	161	LEU	N-CA-C	5.51	118.44	109.24
1	Z	292	CYS	N-CA-C	5.50	117.87	108.90
1	O	144	ILE	CB-CA-C	-5.46	104.98	111.97
1	Z	250	LEU	O-C-N	5.45	127.76	122.09
1	O	332	PHE	CA-CB-CG	-5.45	108.35	113.80
1	O	133	ASP	O-C-N	5.44	126.07	121.83
1	Z	178	VAL	N-CA-C	5.43	115.80	107.77
1	Z	266	GLY	CA-C-N	-5.42	112.95	120.38
1	Z	266	GLY	C-N-CA	-5.42	112.95	120.38
1	O	345	VAL	CA-C-N	5.41	126.61	119.84
1	O	345	VAL	C-N-CA	5.41	126.61	119.84
1	O	407	ARG	CA-C-N	-5.41	115.13	122.92
1	O	407	ARG	C-N-CA	-5.41	115.13	122.92
1	O	182	ASP	CA-CB-CG	-5.40	107.20	112.60
1	Z	177	ARG	CB-CA-C	5.40	120.08	109.72
1	O	242	ILE	CB-CA-C	-5.39	102.45	111.29
1	Z	180	VAL	N-CA-CB	-5.38	104.34	112.35
1	Z	201	ASP	CB-CA-C	5.37	119.75	110.84
1	Z	320	MET	CA-C-N	-5.35	114.42	122.07
1	Z	320	MET	C-N-CA	-5.35	114.42	122.07
1	O	27	ILE	CA-C-N	-5.35	116.04	122.35
1	O	27	ILE	C-N-CA	-5.35	116.04	122.35
1	O	96	PRO	CA-C-N	-5.34	114.13	122.09
1	O	96	PRO	C-N-CA	-5.34	114.13	122.09
1	Z	337	GLN	N-CA-C	5.34	119.64	113.18
1	O	85	THR	CB-CA-C	5.33	117.47	110.06
1	Z	474	ILE	O-C-N	5.33	128.93	123.18
1	Z	327	TYR	CA-C-N	5.32	129.30	120.94
1	Z	327	TYR	C-N-CA	5.32	129.30	120.94
1	O	48	ASP	CA-C-O	5.32	123.25	119.32
1	Z	342	VAL	N-CA-C	5.28	115.81	110.05
1	O	216	GLU	CB-CG-CD	5.27	121.55	112.60
1	Z	279	ALA	CA-C-N	-5.25	116.29	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	279	ALA	C-N-CA	-5.25	116.29	123.12
1	O	99	ASN	CA-CB-CG	-5.24	107.36	112.60
1	Z	324	ASN	N-CA-C	5.23	115.29	108.07
1	Z	298	VAL	N-CA-CB	5.22	119.63	110.49
1	Z	328	ASP	N-CA-CB	-5.22	102.65	110.17
1	Z	215	PRO	CB-CA-C	-5.21	102.97	111.56
1	O	393	GLU	CB-CG-CD	5.20	121.45	112.60
1	O	87	ILE	N-CA-C	5.20	116.14	108.45
1	O	52	ILE	CB-CA-C	-5.15	105.37	111.81
1	O	374	ASN	CA-CB-CG	-5.14	107.45	112.60
1	Z	96	PRO	CA-C-N	-5.14	114.69	122.76
1	Z	96	PRO	C-N-CA	-5.14	114.69	122.76
1	O	244	GLY	N-CA-C	-5.14	104.55	111.54
1	O	488	LYS	O-C-N	5.13	127.43	122.09
1	O	102	VAL	N-CA-C	5.13	117.78	110.09
1	Z	497	GLU	N-CA-CB	5.12	117.53	109.69
1	Z	237	ILE	O-C-N	5.12	126.02	121.41
1	O	282	SER	N-CA-CB	5.10	118.74	110.43
1	Z	451	VAL	CA-C-O	5.09	123.81	119.38
1	Z	350	GLY	N-CA-C	-5.06	103.61	112.77
1	Z	308	MET	N-CA-C	5.05	117.85	107.69
1	O	424	ASP	CB-CA-C	-5.04	102.91	110.92
1	O	197	LEU	N-CA-CB	5.04	119.00	110.49
1	Z	18	ALA	CA-C-N	-5.04	115.46	122.71
1	Z	18	ALA	C-N-CA	-5.04	115.46	122.71
1	Z	148	VAL	N-CA-C	5.04	115.29	107.28
1	O	27	ILE	N-CA-CB	5.03	116.41	110.82
1	O	74	ILE	N-CA-CB	5.03	116.73	111.00
1	O	263	ASN	CA-C-O	5.03	125.79	120.36
1	O	329	SER	N-CA-C	-5.03	105.08	111.11
1	O	359	TYR	N-CA-C	-5.01	107.15	114.12
1	Z	480	ASN	CB-CA-C	5.01	118.72	110.95
1	Z	83	ARG	NE-CZ-NH2	5.01	123.71	119.20

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 ⓘ

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	495	0
1	Z	3888	0	3778	505	0
2	O	40	0	20	3	0
3	O	6	0	8	2	0
3	Z	6	0	8	1	0
All	All	7818	0	7588	1000	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 65.

All (1000) 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:HG3	1:O:83:ARG:HH11	1.04	1.11
1:O:145:LEU:HD11	1:O:213:MET:HE1	1.33	1.08
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:88:VAL:HG12	1:Z:97:ILE:HG12	1.39	1.01
1:Z:137:SER:HB2	1:Z:189:THR:HA	1.40	1.01
1:Z:419:MET:HA	1:Z:419:MET:HE2	1.45	0.98
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:273:MET:HB3	1:O:395:MET:HE3	1.53	0.90
1:Z:48:ASP:HB3	1:Z:51:GLU:HB2	1.53	0.89
1:O:122:ASP:O	1:O:123:TYR:C	2.14	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:HG3	1:O:83:ARG:NH1	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: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:O:255:CYS:HA	1:O:260:MET:HE2	1.60	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:273:MET:CB	1:O:395:MET:HE3	2.11	0.80
1:O:419:MET:HE2	1:O:419:MET:HA	1.63	0.80
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:HG3	1:O:369:ARG:HH11	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:HA	1:Z:455:GLN:NE2	1.97	0.77
1:O:114:HIS:O	1:O:115:LEU:C	2.22	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:468:ARG:HG3	1:O:468:ARG:HH11	1.50	0.77
1:O:250:LEU:CD1	1:O:255:CYS:HB2	2.15	0.77
1:O:120:LEU:O	1:O:121:GLU:C	2.28	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: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:108:THR:HG21	1:Z:139:THR:C	2.11	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:240:SER:O	1:Z:447:ALA:HA	1.87	0.73
1:Z:410:GLY:O	1:Z:413:VAL:HG13	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:23:HIS:HA	1:O:453:PHE:CE2	2.25	0.72
1:O:178:VAL:HG23	1:O:180:VAL:HG12	1.71	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:418:LEU:HD13	1:O:419:MET:HE3	1.70	0.72
1:O:455:GLN:HA	1:O:455:GLN:NE2	2.02	0.72
1:Z:23:HIS:HA	1:Z:453:PHE:HE2	1.51	0.72
1:Z:250:LEU:HD12	1:Z:255:CYS:HB2	1.71	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:200:ASP:C	1:O:204:LEU:HD12	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:434:GLU:CD	1:O:435:VAL:H	1.98	0.71
1:O:22:ASP:CB	1:O:28:ILE:HD11	2.20	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
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:Z:347:ALA:HB3	1:Z:361:ARG:C	2.16	0.70
1:O:124:ILE:HG13	1:O:203:MET:HE1	1.73	0.70
1:O:240:SER:O	1:O:447:ALA:HA	1.92	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:271:MET:C	1:Z:272:LEU:HD12	2.17	0.70
1:Z:115:LEU:N	1:Z:115:LEU:HD23	2.07	0.69
1:Z:120:LEU:HD12	1:Z:120:LEU:N	2.07	0.69
1:Z:204:LEU:HD12	1:Z:204:LEU:H	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:N	1:O:460:LEU:HD23	2.08	0.69
1:Z:360:ALA:O	1:Z:361:ARG:HG2	1.93	0.69
1:Z:434:GLU:CD	1:Z:435:VAL:H	2.00	0.69
1:O:434:GLU:CB	1:O:465:VAL:HB	2.21	0.69
1:Z:88:VAL:CG1	1:Z:97:ILE:HG12	2.21	0.69
1:Z:103:TRP:CZ3	1:Z:104:GLN:HG2	2.27	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:285:GLY:O	1:O:286:LEU:HD23	1.93	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: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:O:438:VAL:O	1:O:439:THR:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:208:ASP:C	1:O:209:ILE:HG12	2.18	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
1:Z:458:ASP:OD1	1:Z:458:ASP:N	2.28	0.67
1:Z:272:LEU:HG	1:Z:303:GLU:HB2	1.75	0.67
1:O:41:LYS:O	1:O:44:TRP:HB2	1.94	0.67
1:O:323:ILE:HG22	1:O:332:PHE:CD2	2.30	0.67
1:O:110:GLU:O	1:O:113:GLU:HB2	1.94	0.66
1:O:114:HIS:ND1	1:O:114:HIS:N	2.38	0.66
1:Z:114:HIS:O	1:Z:115:LEU:C	2.36	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: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:O:389:ARG:NH1	1:O:425:ILE:O	2.29	0.66
1:O:396:GLN:O	1:O:397:ALA:C	2.38	0.65
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:HG3	1:Z:407:ARG:NH1	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: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: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:407:ARG:HH11	1:Z:407:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:122:ASP:O	1:Z:123:TYR:C	2.39	0.64
1:Z:419:MET:HA	1:Z:419:MET:CE	2.26	0.64
1:Z:498:GLU:O	1:Z:499:HIS:C	2.38	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:O:411:GLY:O	1:O:412:ALA:C	2.39	0.64
1:O:109:ALA:HA	1:O:134:PRO:HG3	1.80	0.64
1:O:145:LEU:CD1	1:O:213:MET:HE1	2.20	0.64
1:O:191:LEU:CD2	1:O:207:LEU:HD12	2.28	0.64
1:O:200:ASP:HB3	1:O:203:MET:HB2	1.79	0.64
1:Z:402:ARG:NH2	1:Z:428:THR:OG1	2.30	0.64
1:O:188:ARG:HH22	1:O:303:GLU:CD	2.05	0.64
1:O:142:LYS:NZ	1:O:146:ASP:OD2	2.30	0.64
1:Z:246:GLN:OE1	1:Z:246:GLN:HA	1.98	0.64
1:Z:415:ASN:O	1:Z:419:MET:HG2	1.98	0.63
1:O:120:LEU:O	1:O:122:ASP:N	2.30	0.63
1:O:336:VAL:HG23	1:O:338:ASN:N	2.07	0.63
1:O:457:LEU:HD23	1:O:457:LEU:N	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: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:80:THR:HG21	1:O:248:ALA:CB	2.29	0.63
1:O:85:THR:CG2	1:O:103:TRP:HD1	2.11	0.63
1:O:481:TYR:O	1:O:484:ALA:HB3	1.99	0.63
1:O:83:ARG:HG3	3:O:601:GOL:O2	1.99	0.63
1:O:360:ALA:O	1:O:361:ARG:HG2	1.99	0.63
1:O:389:ARG:HG2	1:O:483:TYR:CZ	2.33	0.63
1:O:438:VAL:HG23	1:O:439:THR:N	2.14	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:320:MET:HB3	1:O:322:LEU:HG	1.79	0.62
1:O:490:VAL:HG12	1:O:494:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:258:GLU:HA	1:Z:274:ASN:O	1.99	0.62
1:Z:47:HIS:HB3	1:Z:52:ILE:HD11	1.80	0.62
1:Z:457:LEU:H	1:Z:457:LEU:CD2	2.13	0.62
1:Z:458:ASP:O	1:Z:461:GLN:HG2	2.00	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
1:Z:365:PHE:CE2	1:Z:492:ARG:HB2	2.35	0.62
1:Z:442:GLY:O	1:Z:445:TYR:HB2	2.00	0.62
1:O:110:GLU:OE1	1:O:110:GLU:HA	1.99	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:57:SER:O	1:O:60:LEU:HB3	2.00	0.61
1:O:406:LEU:HD22	1:O:407:ARG:N	2.15	0.61
1:Z:480:ASN:N	1:Z:480:ASN:ND2	2.45	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:6:ILE:HD13	1:O:453:PHE:CD2	2.35	0.61
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.81	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:Z:174:THR:C	1:Z:175:GLN:HG2	2.25	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:Z:241:GLY:C	1:Z:242:ILE:HG13	2.25	0.60
1:Z:313:ILE:O	1:Z:314:GLN:C	2.43	0.60
1:O:104:GLN:HB3	1:O:349:THR:HG21	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:209:ILE:O	1:O:210:PRO:C	2.43	0.60
1:O:285:GLY:C	1:O:286:LEU:HD23	2.26	0.60
1:O:422:GLN:O	1:O:425:ILE:HG22	2.02	0.59
1:Z:204:LEU:HD21	1:Z:214:LEU:HD11	1.85	0.59
1:Z:207:LEU:HB2	1:Z:209:ILE:HG13	1.84	0.59
1:Z:330:GLU:O	1:Z:334:THR:HG23	2.02	0.59
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: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:174:THR:O	1:O:175:GLN:C	2.44	0.59
1:Z:240:SER:HB2	1:Z:450:ALA:HB3	1.85	0.59
1:Z:360:ALA:C	1:Z:361:ARG:HG2	2.28	0.59
1:Z:460:LEU:HD22	1:Z:460:LEU:H	1.67	0.59
1:Z:478:GLU:O	1:Z:479:ARG:C	2.46	0.59
1:Z:262:LYS:HD2	1:Z:262:LYS:C	2.27	0.58
1:Z:441:LEU:O	1:Z:442:GLY:C	2.44	0.58
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:Z:120:LEU:O	1:Z:121:GLU:C	2.46	0.58
1:O:8:ALA:O	1:O:9:LEU:HD12	2.03	0.58
1:O:83:ARG:HH11	1:O:83:ARG:CG	1.97	0.58
1:O:26:ASN:O	1:O:28:ILE:HD12	2.03	0.58
1:Z:361:ARG:HG2	1:Z:361:ARG:NH1	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:8:ALA:C	1:O:9:LEU:HD12	2.30	0.57
1:O:220:SER:O	1:O:446:LEU:HD23	2.04	0.57
1:O:271:MET:C	1:O:272:LEU:HD12	2.30	0.57
1:O:47:HIS:O	1:O:49:PRO:HD3	2.04	0.57
1:O:352:GLY:O	1:O:355:TYR:N	2.37	0.57
1:Z:208:ASP:C	1:Z:209:ILE:HG12	2.29	0.57
1:Z:220:SER:O	1:Z:446:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:166:ASP:OD1	1:Z:166:ASP:N	2.37	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
1:O:108:THR:OG1	1:O:134:PRO:HA	2.05	0.56
1:O:255:CYS:HA	1:O:260:MET:CE	2.33	0.56
1:O:382:GLU:HB3	1:O:421:PHE:CE2	2.40	0.56
1:O:392:LEU:HD23	1:O:392:LEU:C	2.30	0.56
1:Z:457:LEU:O	1:Z:458:ASP:C	2.45	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:293:GLY:C	1:Z:295:THR:H	2.13	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:445:TYR:O	1:Z:446:LEU:C	2.47	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: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:O:112:CYS:HB3	1:O:132:ILE:HG22	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:459:GLU:C	1:O:460:LEU:HD23	2.32	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:89:TRP:HD1	1:O:94:GLY:HA2	1.72	0.55
1:O:344:VAL:O	1:O:346:PRO:HD3	2.05	0.55
1:O:391:VAL:O	1:O:392:LEU:C	2.47	0.55
1:Z:84:GLU:OE1	3:Z:601:GOL:O1	2.17	0.55
1:Z:103:TRP:CE3	1:Z:104:GLN:HG2	2.42	0.55
1:Z:164:THR:O	1:Z:165:VAL:C	2.49	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
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:48:ASP:O	1:Z:49:PRO:C	2.47	0.55
1:Z:60:LEU:O	1:Z:63:VAL:HG12	2.06	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:HA	1:Z:461:GLN:NE2	2.22	0.55
1:O:130:LEU:HD23	1:O:130:LEU:N	2.20	0.55
1:Z:224:TYR:CZ	1:Z:242:ILE:HD12	2.42	0.55
1:O:174:THR:C	1:O:175:GLN:HG2	2.32	0.54
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:2:GLU:O	1:O:4:LYS:HG2	2.06	0.54
1:O:11:GLN:NE2	1:O:12:GLY:O	2.35	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:OE1	1:Z:497:GLU:HA	2.07	0.54
1:Z:48:ASP:O	1:Z:51:GLU:N	2.40	0.54
1:Z:170:ILE:O	1:Z:171:TRP:C	2.50	0.54
1:Z:445:TYR:CD1	1:Z:445:TYR:N	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:191:LEU:HD21	1:O:207:LEU:CD1	2.38	0.54
1:O:59:THR:O	1:O:63:VAL:HG22	2.08	0.54
1:O:84:GLU:O	1:O:85:THR:C	2.50	0.54
1:O:155:ALA:O	1:O:158:GLY:HA2	2.08	0.54
1:Z:134:PRO:O	1:Z:140:LYS:NZ	2.39	0.54
1:Z:232:LYS:O	1:Z:233:GLY:C	2.49	0.54
1:Z:256:VAL:HG21	1:Z:294:PRO:CA	2.37	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:253:GLN:HE22	1:Z:409:ASP:HB3	1.73	0.54
1:Z:17:ARG:HH12	1:Z:437:GLU:HG2	1.72	0.54
1:Z:281:LYS:HE3	1:Z:283:GLU:OE2	2.08	0.54
1:Z:419:MET:HB2	1:Z:470:PHE:CZ	2.44	0.54
1:O:37:GLN:NE2	1:O:47:HIS:NE2	2.55	0.53
1:O:180:VAL:HA	1:O:215:PRO:HB2	1.90	0.53
1:O:331:TYR:CD2	1:O:332:PHE:CE1	2.97	0.53
1:Z:60:LEU:HD12	1:Z:60:LEU:C	2.33	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:Z:244:GLY:O	1:Z:245:ASP:C	2.50	0.53
1:Z:421:PHE:O	1:Z:422:GLN:C	2.50	0.53
1:O:211:ARG:O	1:O:214:LEU:HG	2.08	0.53
1:O:376:ILE:O	1:O:377:ILE:C	2.50	0.53
1:O:393:GLU:O	1:O:394:ALA:C	2.48	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:60:LEU:O	1:O:63:VAL:HG23	2.08	0.53
1:O:108:THR:HG21	1:O:139:THR:C	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:312:SER:O	1:Z:315:TRP:HB3	2.09	0.53
1:Z:47:HIS:O	1:Z:49:PRO:HD3	2.09	0.53
1:Z:162:PHE:HB2	1:Z:213:MET:HE2	1.90	0.53
1:O:78:GLY:O	1:O:79:ILE:HG12	2.09	0.53
1:O:191:LEU:HD21	1:O:207:LEU:HD12	1.91	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: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:29:SER:C	1:O:30:VAL:HG23	2.35	0.52
1:Z:498:GLU:OE1	1:Z:498:GLU:HA	2.05	0.52
1:Z:123:TYR:O	1:Z:127:ASN:OD1	2.27	0.52
1:O:41:LYS:O	1:O:41:LYS:HG2	2.08	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:Z:46:GLU:OE2	1:Z:107:ARG:NH2	2.38	0.52
1:Z:145:LEU:CD1	1:Z:151:SER:HB2	2.34	0.52
1:Z:153:GLU:O	1:Z:154:ARG:C	2.49	0.52
1:Z:344:VAL:O	1:Z:346:PRO:HD3	2.10	0.52
1:O:241:GLY:C	1:O:242:ILE:HG13	2.34	0.52
1:O:360:ALA:C	1:O:361:ARG:HG2	2.34	0.52
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:220:SER:C	1:O:446:LEU:HD23	2.35	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:O:339:THR:O	1:O:340:ASN:HB3	2.09	0.51
1:Z:84:GLU:O	1:Z:85:THR:C	2.52	0.51
1:Z:89:TRP:HB2	1:Z:95:LYS:O	2.09	0.51
1:Z:340:ASN:HB2	1:Z:375:HIS:NE2	2.25	0.51
1:O:87:ILE:HG22	1:O:88:VAL:N	2.24	0.51
1:O:137:SER:O	1:O:140:LYS:HB2	2.09	0.51
1:Z:127:ASN:O	1:Z:194:ILE:HG12	2.10	0.51
1:Z:407:ARG:HH12	1:Z:466:ILE:HD11	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:457:LEU:N	1:Z:457:LEU:HD22	2.25	0.51
1:O:3:LYS:HB3	1:O:75:ALA:HA	1.92	0.51
1:O:125:ARG:HD3	1:O:281:LYS:HD2	1.93	0.51
1:O:494:MET:O	1:O:495:ALA:HB3	2.11	0.51
1:Z:345:VAL:O	1:Z:362:GLY:HA2	2.11	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:201:ASP:O	1:Z:202:LYS:C	2.53	0.51
1:Z:361:ARG:O	1:Z:362:GLY:C	2.53	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:196:THR:C	1:O:197:LEU:HD12	2.35	0.51
1:O:251:PHE:O	1:O:254:LEU:HD12	2.11	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
1:O:152:ARG:HH21	1:O:208:ASP:HB3	1.75	0.50
1:Z:90:GLU:O	1:Z:94:GLY:N	2.37	0.50
1:Z:180:VAL:HA	1:Z:215:PRO:HB2	1.92	0.50
1:Z:214:LEU:N	1:Z:214:LEU:HD23	2.26	0.50
1:O:85:THR:HG22	1:O:103:TRP:CD1	2.46	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:H	1:Z:457:LEU:HD22	1.76	0.50
1:O:148:VAL:O	1:O:151:SER:OG	2.28	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: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:389:ARG:HH22	1:Z:480:ASN:ND2	2.09	0.50
1:Z:435:VAL:HG12	1:Z:435:VAL:O	2.10	0.50
1:Z:459:GLU:CB	1:Z:460:LEU:HD22	2.40	0.50
1:O:88:VAL:O	1:O:97:ILE:HG12	2.12	0.50
1:O:332:PHE:O	1:O:333:ALA:C	2.52	0.50
1:O:444:ALA:O	1:O:445:TYR:C	2.53	0.50
1:Z:87:ILE:HG22	1:Z:88:VAL:N	2.26	0.50
1:Z:223:VAL:O	1:Z:223:VAL:HG12	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:389:ARG:O	1:O:390:ASP:C	2.51	0.49
1:Z:359:TYR:CZ	1:Z:499:HIS:CE1	2.99	0.49
1:Z:372:ASN:HD22	1:Z:372:ASN:C	2.19	0.49
1:Z:381:LEU:O	1:Z:384:ILE:HG13	2.11	0.49
1:O:195:HIS:C	1:O:197:LEU:HD12	2.36	0.49
1:O:315:TRP:CD1	1:O:319:GLU:HB2	2.46	0.49
1:Z:17:ARG:HD2	1:Z:32:GLN:HG3	1.93	0.49
1:Z:171:TRP:CG	1:Z:176:GLY:HA2	2.47	0.49
1:O:104:GLN:O	1:O:105:CYS:C	2.52	0.49
1:O:200:ASP:O	1:O:201:ASP:C	2.55	0.49
1:O:221:SER:OG	1:O:450:ALA:HB2	2.11	0.49
1:O:317:ARG:HB2	1:O:323:ILE:HG13	1.94	0.49
1:Z:152:ARG:NH2	1:Z:208:ASP:HB3	2.27	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
1:O:180:VAL:HG23	1:O:216:GLU:O	2.12	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:Z:330:GLU:O	1:Z:331:TYR:C	2.54	0.49
1:Z:346:PRO:C	1:Z:348:PHE:H	2.20	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:295:THR:OG1	1:O:297:GLU:OE1	2.27	0.49
1:O:478:GLU:O	1:O:479:ARG:C	2.55	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:23:HIS:HA	1:Z:453:PHE:CZ	2.48	0.49
1:Z:106:ARG:HA	1:Z:106:ARG:NE	2.28	0.49
1:Z:131:VAL:HG12	1:Z:136:PHE:CE1	2.48	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:347:ALA:O	1:Z:348:PHE:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:419:MET:HA	1:O:419:MET:CE	2.37	0.48
1:O:428:THR:CG2	1:O:429:ARG:N	2.76	0.48
1:O:240:SER:HB2	1:O:450:ALA:CB	2.43	0.48
1:O:90:GLU:HB2	1:O:93:THR:OG1	2.13	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: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:Z:133:ASP:CG	1:Z:134:PRO:HD2	2.38	0.48
1:Z:138:GLY:O	1:Z:139:THR:C	2.56	0.48
1:Z:257:LYS:O	1:Z:258:GLU:C	2.55	0.48
1:O:435:VAL:HG12	1:O:435:VAL:O	2.12	0.48
1:Z:142:LYS:O	1:Z:143:TRP:C	2.55	0.48
1:O:244:GLY:O	1:O:245:ASP:C	2.56	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:O:451:VAL:O	1:O:451:VAL:HG13	2.12	0.48
1:Z:38:ILE:HG22	1:Z:38:ILE:O	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
1:Z:259:GLY:N	1:Z:274:ASN:O	2.39	0.48
1:O:186:ALA:C	1:O:188:ARG:H	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:Z:193:ASN:CG	1:Z:196:THR:HB	2.38	0.48
1:O:108:THR:HG21	1:O:140:LYS:N	2.27	0.48
1:O:80:THR:HG22	1:O:245:ASP:CA	2.43	0.48
1:O:83:ARG:CG	3:O:601:GOL:O2	2.61	0.48
1:O:88:VAL:HG12	1:O:97:ILE:HG12	1.94	0.48
1:O:108:THR:HB	1:O:139:THR:HB	1.95	0.48
1:Z:377:ILE:O	1:Z:380:THR:HB	2.14	0.48
1:Z:44:TRP:CD1	1:Z:44:TRP:N	2.81	0.47
1:O:330:GLU:O	1:O:331:TYR:C	2.55	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:Z:145:LEU:HD12	1:Z:145:LEU:HA	1.59	0.47
1:Z:494:MET:O	1:Z:495:ALA:HB3	2.13	0.47
1:O:23:HIS:C	1:O:25:ALA:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:83:ARG:NH1	1:O:83:ARG:CG	2.64	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:303:GLU:HG3	1:O:304:GLY:N	2.29	0.47
1:O:390:ASP:OD1	1:O:483:TYR:OH	2.28	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:489:ALA:O	1:Z:490:VAL:C	2.57	0.47
1:O:183:TYR:O	1:O:184:THR:C	2.58	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:378:ARG:O	1:O:379:ALA:C	2.55	0.47
1:O:386:TYR:O	1:O:387:GLN:C	2.55	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: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:41:LYS:HB2	1:Z:42:PRO:HD2	1.95	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:479:ARG:C	1:Z:480:ASN:HD22	2.23	0.47
1:O:22:ASP:OD1	1:O:26:ASN:HB2	2.14	0.47
1:O:111:ILE:O	1:O:112:CYS:C	2.55	0.47
1:O:118:ASP:HB2	1:O:120:LEU:HD11	1.95	0.47
1:O:234:GLY:N	2:O:502[A]:FBP:O6P	2.41	0.47
1:O:387:GLN:O	1:O:388:THR:C	2.58	0.47
1:O:419:MET:HE2	1:O:419:MET:CA	2.39	0.47
1:O:420:GLN:O	1:O:421:PHE:C	2.55	0.47
1:Z:108:THR:HG22	1:Z:111:ILE:HD12	1.97	0.47
1:Z:118:ASP:OD1	1:Z:118:ASP:N	2.47	0.47
1:Z:254:LEU:HD12	1:Z:254:LEU:HA	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:428:THR:HG22	1:O:429:ARG:N	2.30	0.47
1:O:429:ARG:HA	1:O:470:PHE:O	2.15	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:397:ALA:O	1:Z:398:ASP:C	2.55	0.47
1:Z:274:ASN:HD21	1:Z:299:ASN:HD22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:342:VAL:CG1	1:Z:343:TYR:N	2.79	0.46
1:Z:372:ASN:ND2	1:Z:372:ASN:C	2.72	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:52:ILE:O	1:O:53:TRP:C	2.55	0.46
1:O:251:PHE:CD2	1:O:446:LEU:CD1	2.98	0.46
1:O:251:PHE:CD2	1:O:446:LEU:HD11	2.50	0.46
1:O:377:ILE:O	1:O:380:THR:HB	2.15	0.46
1:Z:30:VAL:HG12	1:Z:31:SER:N	2.29	0.46
1:Z:141:VAL:CG2	1:Z:162:PHE:CD1	2.97	0.46
1:Z:382:GLU:O	1:Z:383:SER:C	2.58	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:90:GLU:O	1:O:94:GLY:N	2.45	0.46
1:O:102:VAL:CG2	1:O:103:TRP:N	2.78	0.46
1:O:151:SER:O	1:O:152:ARG:C	2.58	0.46
1:O:372:ASN:O	1:O:375:HIS:HB2	2.14	0.46
1:O:419:MET:O	1:O:420:GLN:C	2.58	0.46
1:Z:111:ILE:CG2	1:Z:139:THR:HG22	2.46	0.46
1:Z:118:ASP:HB2	1:Z:120:LEU:HD11	1.98	0.46
1:Z:192:PHE:CE1	1:Z:217:VAL:HG21	2.51	0.46
1:O:115:LEU:HD13	1:O:115:LEU:N	2.29	0.46
1:O:420:GLN:O	1:O:423:SER:HB3	2.15	0.46
1:Z:110:GLU:O	1:Z:111:ILE:C	2.55	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:89:TRP:HB3	1:O:96:PRO:HA	1.97	0.46
1:O:468:ARG:HB3	1:O:470:PHE:CE1	2.51	0.46
1:Z:253:GLN:O	1:Z:254:LEU:HB2	2.15	0.46
1:Z:389:ARG:O	1:Z:390:ASP:C	2.55	0.46
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:Z:266:GLY:O	1:Z:267:THR:C	2.54	0.46
1:O:6:ILE:CD1	1:O:453:PHE:CG	2.98	0.46
1:O:22:ASP:N	1:O:28:ILE:CD1	2.79	0.46
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.97	0.46
1:O:200:ASP:O	1:O:203:MET:N	2.49	0.46
1:O:335:LYS:HB2	1:O:374:ASN:ND2	2.28	0.46
1:Z:117:ARG:C	1:Z:119:GLY:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:171:TRP:NE1	1:Z:176:GLY:HA2	2.30	0.46
1:Z:204:LEU:N	1:Z:204:LEU:CD1	2.79	0.46
1:Z:320:MET:O	1:Z:321:LYS:C	2.58	0.46
1:Z:413:VAL:HA	1:Z:419:MET:SD	2.56	0.46
1:O:21:MET:HG3	1:O:25:ALA:HA	1.97	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:278:LYS:HB2	1:O:278:LYS:HE2	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:O:107:ARG:C	1:O:109:ALA:H	2.24	0.46
1:O:385:ALA:O	1:O:386:TYR:C	2.58	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:Z:381:LEU:O	1:Z:382:GLU:C	2.58	0.46
1:Z:411:GLY:O	1:Z:412:ALA:C	2.56	0.46
1:O:63:VAL:HA	1:O:66:LYS:HD3	1.97	0.45
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:396:GLN:CD	1:O:402:ARG:HA	2.41	0.45
1:Z:98:TYR:CD1	1:Z:99:ASN:N	2.83	0.45
1:Z:406:LEU:HD23	1:Z:406:LEU:HA	1.51	0.45
1:O:142:LYS:O	1:O:143:TRP:C	2.59	0.45
1:O:180:VAL:CG2	1:O:181:THR:N	2.78	0.45
1:O:257:LYS:O	1:O:260:MET:HB2	2.16	0.45
1:Z:174:THR:O	1:Z:175:GLN:C	2.58	0.45
1:Z:203:MET:C	1:Z:206:VAL:HG12	2.41	0.45
1:Z:425:ILE:HD12	1:Z:425:ILE:HA	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:O:382:GLU:O	1:O:383:SER:C	2.58	0.45
1:Z:80:THR:OG1	1:Z:245:ASP:HA	2.16	0.45
1:Z:272:LEU:N	1:Z:272:LEU:CD1	2.79	0.45
1:Z:315:TRP:O	1:Z:316:LEU:C	2.55	0.45
1:Z:425:ILE:HD12	1:Z:479:ARG:HG3	1.98	0.45
1:Z:452:GLY:O	1:Z:453:PHE:C	2.58	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:O:476:THR:O	1:O:477:THR:C	2.59	0.45
1:Z:144:ILE:O	1:Z:148:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:310:GLY:O	1:Z:311:ALA:C	2.58	0.45
1:Z:331:TYR:OH	1:Z:335:LYS:HE2	2.17	0.45
1:Z:393:GLU:O	1:Z:394:ALA:C	2.57	0.45
1:O:112:CYS:SG	1:O:134:PRO:HD3	2.56	0.45
1:O:234:GLY:H	2:O:502[A]:FBP:P2	2.39	0.45
1:Z:166:ASP:O	1:Z:170:ILE:HD12	2.16	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:23:HIS:C	1:Z:25:ALA:H	2.25	0.45
1:Z:152:ARG:O	1:Z:153:GLU:C	2.59	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:Z:149:GLU:OE1	1:Z:149:GLU:HA	2.16	0.45
1:Z:183:TYR:O	1:Z:184:THR:C	2.60	0.45
1:O:197:LEU:N	1:O:197:LEU:CD1	2.77	0.45
1:O:245:ASP:O	1:O:246:GLN:C	2.60	0.45
1:O:273:MET:HB2	1:O:395:MET:HE3	1.96	0.45
1:Z:30:VAL:CG1	1:Z:31:SER:N	2.80	0.45
1:Z:162:PHE:O	1:Z:179:HIS:HE1	2.00	0.45
1:Z:407:ARG:NH1	1:Z:407:ARG:CG	2.76	0.45
1:Z:440:ALA:O	1:Z:441:LEU:C	2.60	0.45
1:O:80:THR:HG23	1:O:248:ALA:HB2	1.98	0.45
1:O:309:ALA:O	1:O:310:GLY:C	2.56	0.45
1:O:441:LEU:HA	1:O:441:LEU:HD23	1.55	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:HD12	1:O:115:LEU:HA	1.45	0.45
1:Z:60:LEU:O	1:Z:60:LEU:HD12	2.16	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: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:7:VAL:O	1:Z:77:ILE:HA	2.16	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: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:O:19:VAL:CG1	1:O:27:ILE:HG23	2.48	0.44
1:O:209:ILE:HA	1:O:210:PRO:HD2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:344:VAL:HG23	1:O:379:ALA:HB1	1.98	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
1:O:21:MET:HB3	1:O:21:MET:HE2	1.55	0.44
1:Z:443:ALA:O	1:Z:444:ALA:C	2.59	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:Z:490:VAL:O	1:Z:491:LYS:C	2.60	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:CA	1:O:420:GLN:NE2	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:O:85:THR:CG2	1:O:103:TRP:CD1	2.95	0.44
1:O:174:THR:HB	1:O:177:ARG:HB2	1.98	0.44
1:O:372:ASN:O	1:O:373:ALA:C	2.61	0.44
1:O:452:GLY:O	1:O:453:PHE:C	2.60	0.44
1:Z:66:LYS:HG3	1:Z:67:ALA:H	1.83	0.44
1:Z:131:VAL:HG12	1:Z:136:PHE:HE1	1.82	0.44
1:Z:86:THR:HG22	1:Z:87:ILE:N	2.30	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:O:449:LEU:C	1:O:451:VAL:H	2.25	0.44
1:O:461:GLN:C	1:O:463:LYS:H	2.24	0.44
1:Z:90:GLU:HB2	1:Z:93:THR:OG1	2.18	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:O:55:THR:O	1:O:59:THR:OG1	2.28	0.43
1:O:153:GLU:O	1:O:154:ARG:C	2.60	0.43
1:O:441:LEU:O	1:O:444:ALA:HB3	2.17	0.43
1:O:485:GLY:O	1:O:486:TRP:C	2.61	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:365:PHE:CZ	1:Z:492:ARG:HB2	2.53	0.43
1:Z:469:GLU:HG2	1:Z:471:ARG:HD3	2.01	0.43
1:Z:160:LEU:HD23	1:Z:160:LEU:HA	1.55	0.43
1:O:201:ASP:O	1:O:202:LYS:C	2.62	0.43
1:O:422:GLN:HA	1:O:422:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:74:ILE:CG2	1:Z:237:ILE:HG21	2.48	0.43
1:Z:456:ASN:C	1:Z:456:ASN:HD22	2.25	0.43
1:Z:457:LEU:CA	1:Z:460:LEU:HD23	2.46	0.43
1:O:43:GLY:C	1:O:44:TRP:HD1	2.26	0.43
1:O:123:TYR:CE1	1:O:202:LYS:HD2	2.53	0.43
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:Z:184:THR:O	1:Z:187:SER:OG	2.35	0.43
1:Z:438:VAL:O	1:Z:439:THR:C	2.59	0.43
1:O:124:ILE:HG22	1:O:125:ARG:N	2.29	0.43
1:O:274:ASN:HD21	1:O:299:ASN:HD22	1.65	0.43
1:O:420:GLN:C	1:O:420:GLN:HE21	2.26	0.43
1:Z:114:HIS:O	1:Z:116:LYS:N	2.50	0.43
1:O:347:ALA:HB3	1:O:361:ARG:C	2.44	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:328:ASP:O	1:Z:329:SER:C	2.61	0.43
1:O:29:SER:OG	1:O:63:VAL:HG12	2.19	0.43
1:O:150:GLY:O	1:O:151:SER:C	2.61	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:Z:29:SER:C	1:Z:30:VAL:HG23	2.43	0.43
1:O:234:GLY:HA2	2:O:502[B]:FBP:O5P	2.19	0.43
1:O:240:SER:C	1:O:447:ALA:HA	2.44	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:Z:41:LYS:O	1:Z:41:LYS:HG2	2.18	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:O:48:ASP:O	1:O:52:ILE:HG13	2.19	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:Z:84:GLU:CD	1:Z:135:TYR:CE1	2.97	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:83:ARG:NE	1:O:246:GLN:HB2	2.34	0.42
1:O:102:VAL:HG23	1:O:103:TRP:N	2.34	0.42
1:O:137:SER:O	1:O:138:GLY:C	2.61	0.42
1:O:340:ASN:HD22	1:O:371:VAL:CG2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:441:LEU:O	1:O:442:GLY:C	2.61	0.42
1:Z:166:ASP:CG	1:Z:167:THR:H	2.26	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:HA	1:O:160:LEU:HD23	1.59	0.42
1:O:187:SER:CB	1:O:290:ILE:HG13	2.49	0.42
1:O:266:GLY:O	1:O:267:THR:C	2.55	0.42
1:O:353:ALA:HA	1:O:354:PRO:HA	1.79	0.42
1:Z:3:LYS:HB3	1:Z:75:ALA:HA	2.00	0.42
1:Z:116:LYS:O	1:Z:119:GLY:HA2	2.18	0.42
1:Z:117:ARG:NH1	1:Z:118:ASP:CG	2.78	0.42
1:Z:316:LEU:HD23	1:Z:316:LEU:HA	1.49	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:213:MET:HE2	1:Z:213:MET:HB2	1.72	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: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:Z:104:GLN:NE2	1:Z:308:MET:CE	2.82	0.42
1:O:145:LEU:HD23	1:O:151:SER:CB	2.48	0.42
1:O:204:LEU:CD2	1:O:214:LEU:HD11	2.47	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:19:VAL:HG12	1:Z:20:VAL:N	2.34	0.42
1:Z:182:ASP:OD1	1:Z:185:ASN:N	2.38	0.42
1:Z:213:MET:HE3	1:Z:213:MET:HB3	1.74	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:89:TRP:CE3	1:O:89:TRP:N	2.88	0.42
1:O:428:THR:HG22	1:O:429:ARG:O	2.20	0.42
1:Z:114:HIS:HA	1:Z:117:ARG:HG2	2.02	0.42
1:Z:147:HIS:CD2	1:Z:147:HIS:C	2.98	0.42
1:Z:150:GLY:O	1:Z:151:SER:C	2.63	0.42
1:Z:219:ARG:HG2	1:Z:222:GLU:OE1	2.20	0.42
1:Z:293:GLY:C	1:Z:295:THR:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:385:ALA:HA	1:Z:422:GLN:CD	2.45	0.42
1:Z:458:ASP:C	1:Z:461:GLN:HG2	2.45	0.42
1:O:108:THR:OG1	1:O:134:PRO:HB3	2.20	0.42
1:O:491:LYS:HA	1:O:494:MET:HE3	2.02	0.42
1:Z:155:ALA:C	1:Z:158:GLY:H	2.27	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:156:ARG:C	1:O:158:GLY:N	2.77	0.42
1:O:254:LEU:HD12	1:O:254:LEU:HA	1.69	0.42
1:Z:43:GLY:C	1:Z:44:TRP:HD1	2.28	0.42
1:Z:302:LEU:HD23	1:Z:302:LEU:HA	1.88	0.42
1:Z:434:GLU:H	1:Z:434:GLU:HG3	1.40	0.42
1:O:153:GLU:HA	1:O:156:ARG:NH1	2.35	0.42
1:Z:48:ASP:C	1:Z:50:MET:N	2.78	0.42
1:Z:86:THR:HG23	1:Z:162:PHE:CE1	2.53	0.42
1:Z:130:LEU:HD12	1:Z:130:LEU:HA	1.63	0.42
1:Z:359:TYR:CD2	1:Z:499:HIS:CD2	3.08	0.42
1:Z:387:GLN:O	1:Z:388:THR:C	2.60	0.42
1:Z:458:ASP:O	1:Z:459:GLU:C	2.63	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:316:LEU:HA	1:O:316:LEU:HD23	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:O:310:GLY:O	1:O:313:ILE:HB	2.20	0.41
1:O:413:VAL:HA	1:O:419:MET:SD	2.60	0.41
1:Z:6:ILE:HD13	1:Z:6:ILE:HA	1.34	0.41
1:Z:85:THR:OG1	1:Z:102:VAL:HA	2.21	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:334:THR:C	1:Z:336:VAL:N	2.76	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:196:THR:O	1:Z:197:LEU:HB2	2.19	0.41
1:Z:250:LEU:HD13	1:Z:262:LYS:HG3	2.01	0.41
1:Z:286:LEU:HD11	1:Z:395:MET:N	2.35	0.41
1:O:71:SER:C	1:O:73:GLN:H	2.27	0.41
1:O:83:ARG:CZ	1:O:246:GLN:HB2	2.50	0.41
1:O:434:GLU:H	1:O:434:GLU:HG3	1.27	0.41
1:Z:162:PHE:CB	1:Z:213:MET:HE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:240:SER:C	1:Z:447:ALA:HA	2.44	0.41
1:Z:289:THR:O	1:Z:300:TYR:HA	2.20	0.41
1:O:152:ARG:O	1:O:156:ARG:HG3	2.20	0.41
1:O:153:GLU:HG2	1:O:156:ARG:NH1	2.35	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:O:495:ALA:O	1:O:496:TRP:C	2.63	0.41
1:Z:203:MET:HA	1:Z:206:VAL:HG12	2.03	0.41
1:Z:243:ALA:O	1:Z:244:GLY:C	2.62	0.41
1:Z:331:TYR:CZ	1:Z:335:LYS:HE3	2.56	0.41
1:Z:378:ARG:O	1:Z:379:ALA:C	2.60	0.41
1:O:59:THR:O	1:O:60:LEU:C	2.61	0.41
1:O:210:PRO:C	1:O:212:GLU:N	2.79	0.41
1:O:344:VAL:HG22	1:O:364:ILE:HG12	2.03	0.41
1:O:440:ALA:O	1:O:441:LEU:C	2.63	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: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
1:Z:445:TYR:N	1:Z:445:TYR:HD1	2.18	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:406:LEU:HD23	1:O:406:LEU:HA	1.37	0.41
1:Z:22:ASP:CG	1:Z:26:ASN:HB2	2.46	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:O:106:ARG:HA	1:O:106:ARG:NE	2.35	0.41
1:O:120:LEU:CB	1:O:124:ILE:CD1	2.98	0.41
1:O:346:PRO:HA	1:O:348:PHE:CE1	2.56	0.41
1:O:420:GLN:C	1:O:420:GLN:NE2	2.79	0.41
1:Z:106:ARG:NE	1:Z:106:ARG:CA	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:179:HIS:C	1:Z:180:VAL:HG12	2.45	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:88:VAL:HA	1:O:161:LEU:O	2.21	0.41
1:O:97:ILE:HD12	1:O:148:VAL:HG21	2.03	0.41
1:O:181:THR:OG1	1:O:182:ASP:N	2.53	0.41
1:O:273:MET:HE1	1:O:401:ILE:HD12	2.03	0.41
1:O:439:THR:CG2	1:O:440:ALA:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:202:LYS:O	1:Z:206:VAL:HB	2.21	0.41
1:Z:395:MET:HE3	1:Z:395:MET:HB2	2.00	0.41
1:O:357:ASP:OD1	1:O:359:TYR:N	2.45	0.40
1:Z:347:ALA:HB3	1:Z:362:GLY:N	2.35	0.40
1:O:123:TYR:C	1:O:123:TYR:CD2	3.00	0.40
1:O:254:LEU:N	1:O:254:LEU:CD1	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:198:ASP:CG	1:Z:199:TRP:N	2.78	0.40
1:Z:210:PRO:C	1:Z:212:GLU:N	2.78	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
1:O:122:ASP:O	1:O:123:TYR:O	2.36	0.40
1:O:203:MET:O	1:O:204:LEU:C	2.63	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:102:VAL:O	1:Z:103:TRP:C	2.64	0.40
1:Z:143:TRP:C	1:Z:143:TRP:CE3	3.00	0.40
1:Z:151:SER:O	1:Z:152:ARG:C	2.64	0.40
1:Z:153:GLU:C	1:Z:155:ALA:N	2.78	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:67:ALA:CB	1:O:69:ILE:HD12	2.52	0.40
1:O:106:ARG:HH22	1:O:135:TYR:HA	1.86	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:419:MET:HE2	1:Z:419:MET:CA	2.32	0.40
1:O:193:ASN:OD1	1:O:196:THR:HB	2.21	0.40
1:O:254:LEU:O	1:O:260:MET:HE1	2.21	0.40
1:O:273:MET:O	1:O:301:ALA:HB1	2.22	0.40
1:O:338:ASN:C	1:O:340:ASN:N	2.79	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:80:THR:OG1	1:Z:243:ALA:O	2.37	0.40
1:Z:133:ASP:C	1:Z:135:TYR:N	2.77	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	496/501 (99%)	406 (82%)	74 (15%)	16 (3%)	3	21
1	Z	496/501 (99%)	414 (84%)	67 (14%)	15 (3%)	3	23
All	All	992/1002 (99%)	820 (83%)	141 (14%)	31 (3%)	3	22

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

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Mol	Chain	Res	Type
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%)	278 (70%)	118 (30%)	0	1
1	Z	398/412 (97%)	275 (69%)	123 (31%)	0	1
All	All	794/824 (96%)	553 (70%)	241 (30%)	0	1

All (241) 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	28	ILE
1	O	29	SER
1	O	31	SER
1	O	32	GLN
1	O	33	ARG
1	O	34	GLU
1	O	37	GLN
1	O	38	ILE
1	O	52	ILE
1	O	59	THR
1	O	60	LEU
1	O	63	VAL

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Mol	Chain	Res	Type
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	117	ARG
1	O	118	ASP
1	O	121	GLU
1	O	122	ASP
1	O	124	ILE
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
1	O	164	THR
1	O	170	ILE
1	O	175	GLN
1	O	178	VAL
1	O	180	VAL
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	220	SER
1	O	221	SER

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Mol	Chain	Res	Type
1	O	224	TYR
1	O	226	GLN
1	O	235	THR
1	O	237	ILE
1	O	250	LEU
1	O	254	LEU
1	O	262	LYS
1	O	264	THR
1	O	269	CYS
1	O	271	MET
1	O	277	GLU
1	O	278	LYS
1	O	281	LYS
1	O	287	LEU
1	O	288	THR
1	O	290	ILE
1	O	297	GLU
1	O	312	SER
1	O	313	ILE
1	O	317	ARG
1	O	318	ASP
1	O	321	LYS
1	O	324	ASN
1	O	335	LYS
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	401	ILE
1	O	403	LEU
1	O	404	HIS
1	O	406	LEU
1	O	407	ARG
1	O	413	VAL
1	O	418	LEU
1	O	420	GLN
1	O	425	ILE
1	O	431	GLU
1	O	434	GLU

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Mol	Chain	Res	Type
1	O	435	VAL
1	O	439	THR
1	O	449	LEU
1	O	451	VAL
1	O	459	GLU
1	O	460	LEU
1	O	461	GLN
1	O	463	LYS
1	O	466	ILE
1	O	468	ARG
1	O	470	PHE
1	O	474	ILE
1	O	477	THR
1	O	479	ARG
1	O	482	ARG
1	O	494	MET
1	O	498	GLU
1	Z	2	GLU
1	Z	3	LYS
1	Z	4	LYS
1	Z	6	ILE
1	Z	21	MET
1	Z	27	ILE
1	Z	29	SER
1	Z	32	GLN
1	Z	33	ARG
1	Z	34	GLU
1	Z	38	ILE
1	Z	57	SER
1	Z	59	THR
1	Z	60	LEU
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	80	THR
1	Z	88	VAL
1	Z	91	LYS
1	Z	92	GLU
1	Z	107	ARG

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Mol	Chain	Res	Type
1	Z	115	LEU
1	Z	117	ARG
1	Z	118	ASP
1	Z	122	ASP
1	Z	130	LEU
1	Z	132	ILE
1	Z	133	ASP
1	Z	136	PHE
1	Z	139	THR
1	Z	140	LYS
1	Z	142	LYS
1	Z	144	ILE
1	Z	145	LEU
1	Z	147	HIS
1	Z	148	VAL
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	180	VAL
1	Z	182	ASP
1	Z	190	MET
1	Z	196	THR
1	Z	203	MET
1	Z	205	GLU
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	250	LEU
1	Z	254	LEU
1	Z	280	VAL
1	Z	281	LYS
1	Z	283	GLU

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Mol	Chain	Res	Type
1	Z	287	LEU
1	Z	289	THR
1	Z	290	ILE
1	Z	292	CYS
1	Z	297	GLU
1	Z	298	VAL
1	Z	312	SER
1	Z	313	ILE
1	Z	314	GLN
1	Z	316	LEU
1	Z	321	LYS
1	Z	324	ASN
1	Z	329	SER
1	Z	335	LYS
1	Z	336	VAL
1	Z	337	GLN
1	Z	351	LEU
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	413	VAL
1	Z	418	LEU
1	Z	419	MET
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	449	LEU
1	Z	451	VAL
1	Z	455	GLN
1	Z	456	ASN
1	Z	458	ASP

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Mol	Chain	Res	Type
1	Z	459	GLU
1	Z	460	LEU
1	Z	466	ILE
1	Z	468	ARG
1	Z	469	GLU
1	Z	470	PHE
1	Z	471	ARG
1	Z	474	ILE
1	Z	476	THR
1	Z	477	THR
1	Z	482	ARG
1	Z	494	MET
1	Z	497	GLU
1	Z	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	32	GLN
1	O	37	GLN
1	O	81	ASN
1	O	127	ASN
1	O	179	HIS
1	O	185	ASN
1	O	226	GLN
1	O	284	ASN
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

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Mol	Chain	Res	Type
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 [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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	Z	601	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	O	601	-	5,5,5	0.40	0	5,5,5	0.55	0
2	FBP	O	502[B]	-	18,20,20	0.96	0	21,32,32	1.19	2 (9%)
2	FBP	O	502[A]	-	18,20,20	1.04	0	21,32,32	1.49	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	Z	601	-	-	0/4/4/4	-
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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	502[A]	FBP	O3P-P1-O2P	4.91	126.22	107.80
2	O	502[A]	FBP	O6P-P2-O5P	3.13	119.54	107.80
2	O	502[B]	FBP	O6P-P2-O5P	3.08	119.34	107.80
2	O	502[B]	FBP	O3P-P1-O2P	2.97	118.94	107.80

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	502[A]	FBP	O1-C1-C2-O2
2	O	502[A]	FBP	O1-C1-C2-O5
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
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
3	O	601	GOL	O1-C1-C2-C3
2	O	502[A]	FBP	C4-C5-C6-O6
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

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Mol	Chain	Res	Type	Atoms
2	O	502[A]	FBP	C1-O1-P1-O2P
2	O	502[A]	FBP	C5-C6-O6-P2

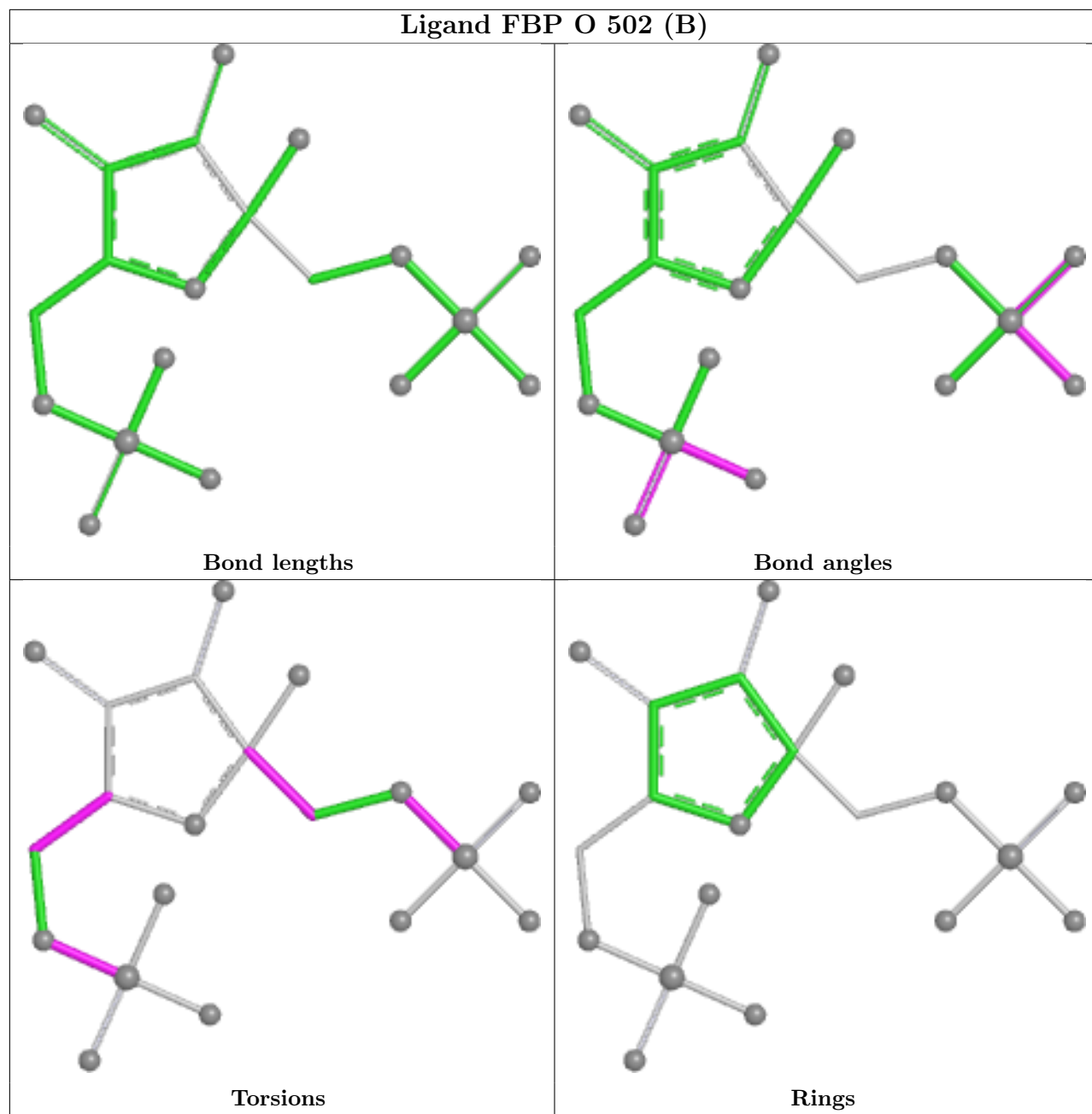
There are no ring outliers.

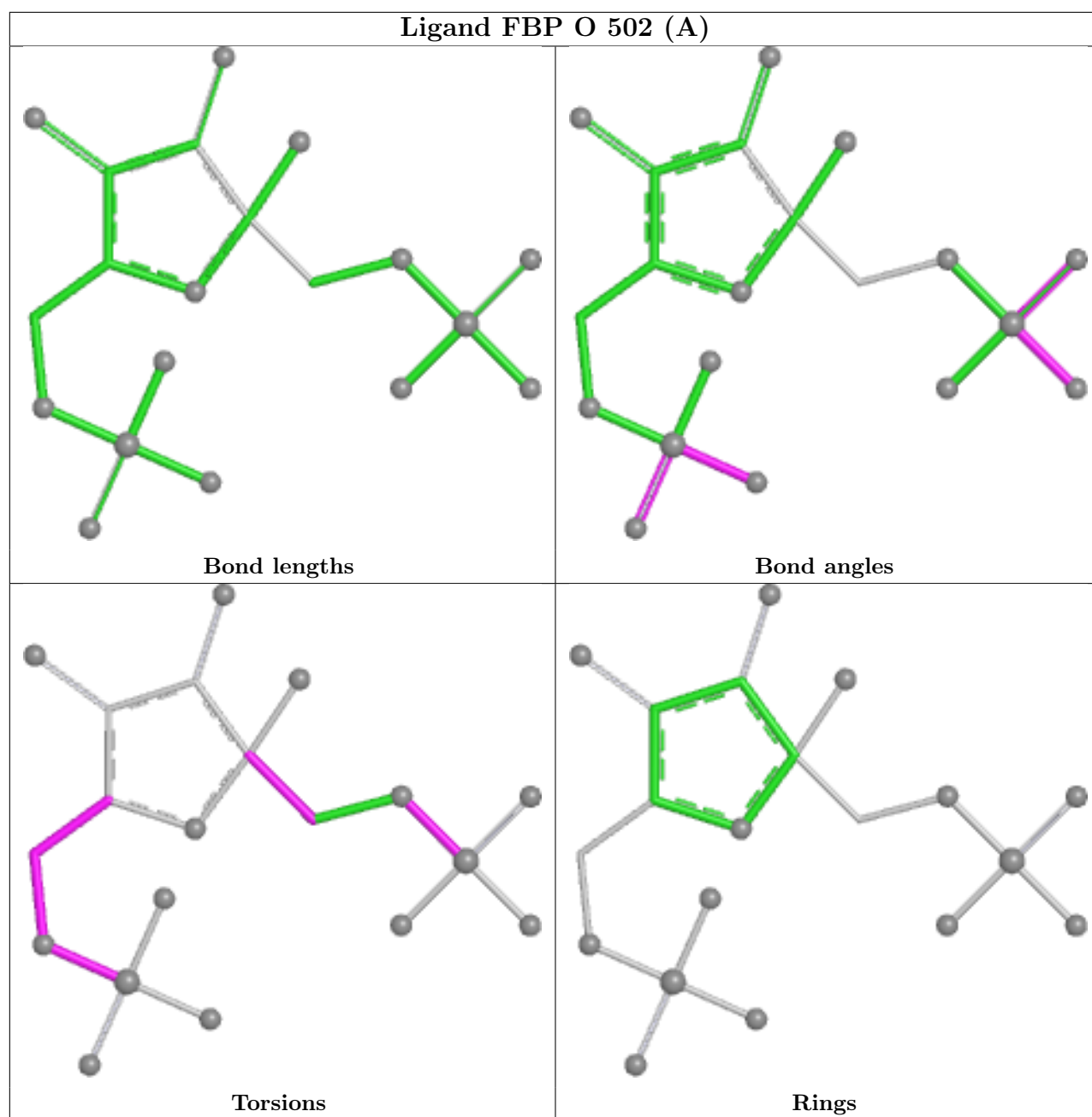
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Z	601	GOL	1	0
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	O	498/501 (99%)	-0.38	5 (1%) 79 63	12, 28, 62, 90	0
1	Z	498/501 (99%)	-0.49	1 (0%) 91 85	10, 26, 60, 89	0
All	All	996/1002 (99%)	-0.44	6 (0%) 85 73	10, 27, 61, 90	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	325	ASP	3.1
1	O	216	GLU	3.0
1	O	465	VAL	2.8
1	Z	437	GLU	2.7
1	O	327	TYR	2.6
1	O	436	ARG	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

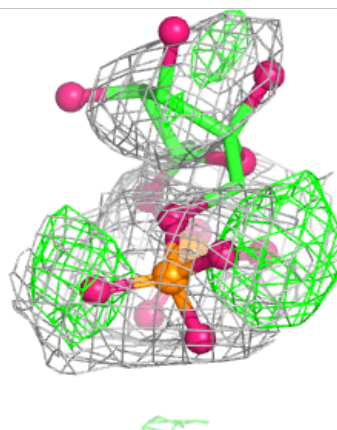
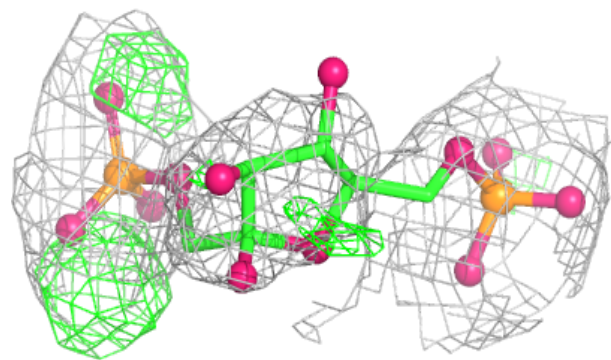
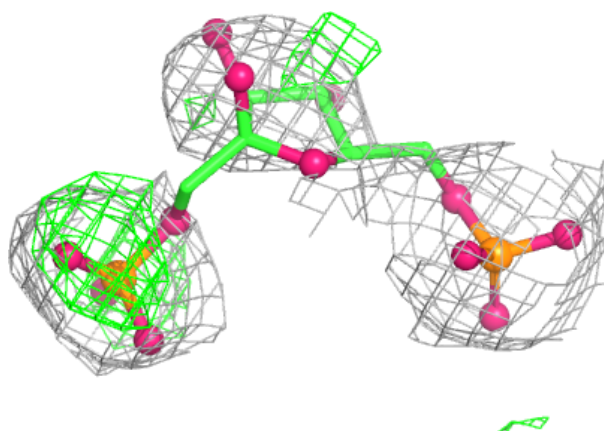
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	O	502[A]	20/20	0.86	0.21	49,49,49,49	20
2	FBP	O	502[B]	20/20	0.86	0.21	49,49,49,49	20
3	GOL	Z	601	6/6	0.98	0.07	10,11,15,34	0
3	GOL	O	601	6/6	0.99	0.07	10,18,32,41	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.

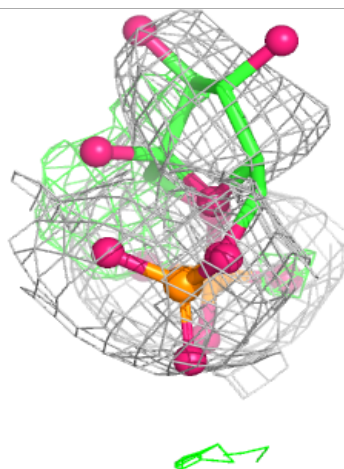
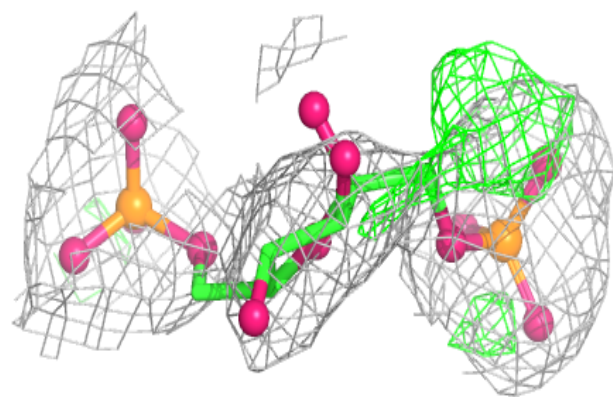
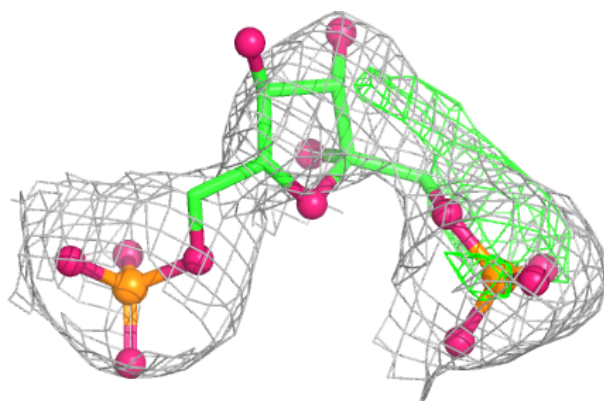
Electron density around FBP O 502 (A):

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 (B):

$2mF_o-DF_c$ (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.