



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:54 PM UTC

PDB ID : 2VAO / pdb_00002vao
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH ISOEUGENOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

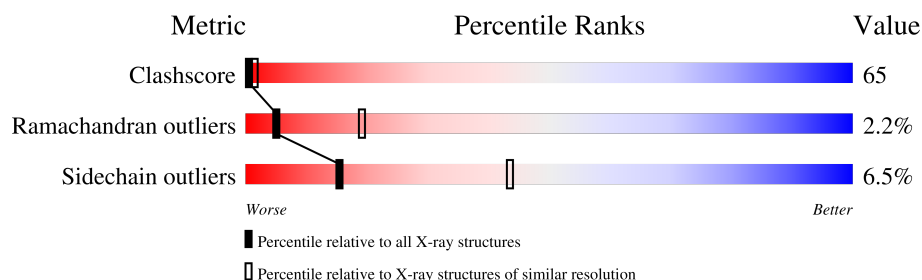
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8948 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 VANILLYL-ALCOHOL OXIDASE.

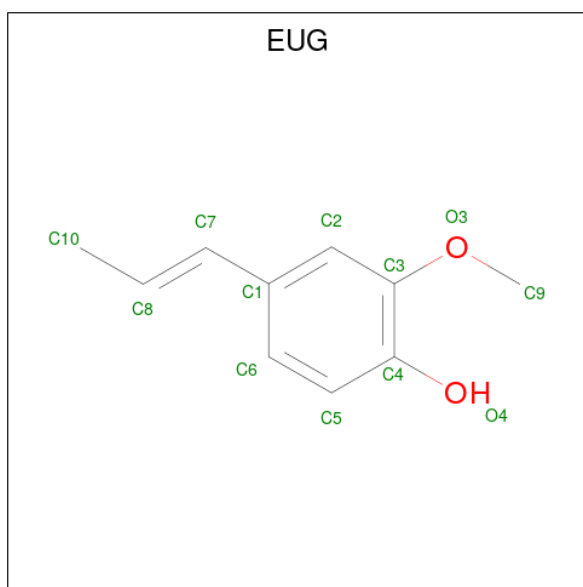
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (CCD ID: EUG) (formula: $C_{10}H_{12}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	24	Total	O	0	0
			24	24		

G499	W500	G501	E502	Y503	R504	T505	H506	L507	A508	F509	E510	M511	Q512	S513	N514	E515	T516	Y517	N518	W519	N520	N521	S522			L525	R526	F527	N528	E529	W530	L531	R532	A533	A534	V535	D536	P537	N538	G539	T540	I541	A542		K545	S546	G547	V548	W549	P550	S551	Q552	Y553	S554	H555	T557	W558	K559	L560																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
Q439	Y440	A441	V442	T443	K444	K445	R446	C447	Q448	E449	A450	G451	L452	D453	F454	I455	G456	T457	F458	T459	V460	G461	M462	R463	E464	M465	H466	H467	I468	Y469	C470	L471	V472	F473	A474	N475	K476	D477	L478	I479	Q480	K481	R482	K483	V484	Q485	V486	L487	M488	R489	T490	L491	I492	D493	D494	C495	A496	M497	N498																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
P379	G380	V381	K382	F383	Y384	F385	P386	E387	D388	T389	P390	E391	N392	S393	V394	L395	R396	V397	R398	D399	K400	T401	M402	Q403	G404	I405	H406	H407	Y408	D409	E410	L411	K412	F413	I414	D415	W416	P417	P418	N419	G420	A421	H422	L423	F424	Q425	S426	P427	I428	A429	K430	V431	S432	G433	A434	D435	A436	M437	N438																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
D317	A318	A319	V320	L321	G322	D323	K324	R325	S326	Y327		R330	T331	E332	P333	L334	S335		E338	L339	D340	K341	I342	A343	K344	Q345	L346	N347	L348	G349	E350	W351	N352	F353	Y354	G355	A356	L357	Y358	G359	P360	E361	P362	I363	R364	R365	V366	L367	V368	E369	T370	I371	K372	D373	A374	F375	S376	A377	I378																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
Q256	S257	N258	M259		V262	T263	K264	L265	G266	T267	W268	L269	M270	P271	N272	P273	R274	G275	Y276	Q277	S278	Y279	L280	I281	T282	L283	P284	K285	D286	G287	D288	L289	K290	Q291	A292	V293	D294	I295	L296	R297	P298	L299	R300	L301	G302	N303	A304	L305	Q306	N307	V308	P309	T310	R311	R312	H313	I314	L315	L316																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
Y190	G191	D192	H193	W194	M195	N196	H197	S198	G199	M200	A138	E201	V202	V203	L204	A205		L210	R211		M214	G215	A216	L217	P218	D219	P220	E221	R222	P223	E224	T225	M226	G227	L228	K229	P230	E231	D232	Q233		S236	K237	L238	A239	H240	L241	S242	P243	Y244		G247	P248	Y249	L250	D251	G252	L253	F254	S255																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
H62	V63	S64	L65	T66	Q67	D68	F69	R70	P71	L72	A73	Y74	M75					R78	N79	V80					T147	Y148	H149	G150	S151	E152	K153	D154	L155	G156	A157	N158	L159	F160	S161	D162	K163	Y164	E165	I166	T167	V168	G169	D170	N171	S172	P173	H174	L175	G176	A177	I178	E179	M180																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	128.38Å 128.38Å 130.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.6 (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.214 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8948	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: FAD, EUG

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	A	1.06	7/4511 (0.2%)	2.49	342/6131 (5.6%)
1	B	1.06	7/4511 (0.2%)	2.49	339/6131 (5.5%)
All	All	1.06	14/9022 (0.2%)	2.49	681/12262 (5.6%)

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	A	2	0
1	B	2	0
All	All	4	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	MET	SD-CE	7.34	1.97	1.79
1	A	303	MET	SD-CE	7.32	1.97	1.79
1	A	64	MET	SD-CE	6.35	1.95	1.79
1	B	64	MET	SD-CE	6.32	1.95	1.79
1	B	120	VAL	CA-CB	-6.22	1.46	1.54
1	A	120	VAL	CA-CB	-6.15	1.47	1.54
1	B	200	MET	CA-C	-5.65	1.45	1.52
1	A	200	MET	CA-C	-5.59	1.45	1.52
1	B	458	PHE	CA-C	-5.50	1.46	1.52
1	A	458	PHE	CA-C	-5.49	1.46	1.52
1	A	74	ILE	CA-CB	-5.42	1.47	1.54
1	B	74	ILE	CA-CB	-5.39	1.48	1.54
1	A	541	ILE	CA-C	-5.38	1.47	1.53
1	B	541	ILE	CA-C	-5.34	1.47	1.53

All (681) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	SER	N-CA-C	-17.32	91.73	113.55
1	A	72	SER	N-CA-C	-17.27	91.79	113.55
1	A	129	ARG	N-CA-C	15.71	133.53	110.28
1	B	129	ARG	N-CA-C	15.70	133.51	110.28
1	A	304	ALA	N-CA-C	-15.54	94.43	111.36
1	B	304	ALA	N-CA-C	-15.53	94.43	111.36
1	A	410	GLU	N-CA-C	15.13	127.78	111.28
1	B	410	GLU	N-CA-C	15.07	127.70	111.28
1	A	366	VAL	CB-CA-C	-14.38	92.73	112.14
1	B	366	VAL	CB-CA-C	-14.36	92.75	112.14
1	B	518	ASN	N-CA-C	14.25	133.04	113.37
1	A	518	ASN	N-CA-C	14.23	133.01	113.37
1	B	505	THR	CB-CA-C	-13.89	83.30	111.91
1	A	505	THR	CB-CA-C	-13.89	83.31	111.91
1	B	187	TYR	N-CA-C	13.71	130.16	113.16
1	A	187	TYR	N-CA-C	13.67	130.11	113.16
1	B	558	TRP	N-CA-C	13.19	131.03	112.04
1	A	558	TRP	N-CA-C	13.15	130.97	112.04
1	A	164	LEU	N-CA-C	12.04	127.89	109.23
1	B	164	LEU	N-CA-C	12.03	127.88	109.23
1	A	7	PHE	N-CA-C	11.51	125.44	111.40
1	B	7	PHE	N-CA-C	11.48	125.41	111.40
1	B	457	THR	CB-CA-C	-11.44	89.97	114.10
1	A	457	THR	CB-CA-C	-11.43	89.98	114.10
1	B	350	ARG	N-CA-C	-11.36	95.68	112.04
1	A	350	ARG	N-CA-C	-11.35	95.69	112.04
1	A	452	LEU	N-CA-C	11.29	127.34	109.50
1	B	452	LEU	N-CA-C	11.27	127.31	109.50
1	B	306	GLN	N-CA-C	11.27	128.80	111.56
1	A	306	GLN	N-CA-C	11.26	128.79	111.56
1	B	369	GLU	N-CA-C	-11.05	99.23	111.28
1	A	369	GLU	N-CA-C	-11.05	99.24	111.28
1	A	392	ASN	N-CA-C	-10.99	97.89	114.16
1	B	392	ASN	N-CA-C	-10.97	97.92	114.16
1	B	384	TYR	N-CA-C	10.80	125.82	108.76
1	A	384	TYR	N-CA-C	10.79	125.81	108.76
1	B	160	LEU	N-CA-C	10.74	124.28	111.82
1	A	160	LEU	N-CA-C	10.73	124.27	111.82
1	B	395	LEU	N-CA-C	-10.40	99.75	111.82
1	A	395	LEU	N-CA-C	-10.39	99.77	111.82
1	B	312	ARG	N-CA-C	10.36	126.80	110.32
1	A	312	ARG	N-CA-C	10.36	126.78	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ILE	CB-CA-C	10.30	124.69	111.81
1	A	363	ILE	CB-CA-C	10.30	124.68	111.81
1	B	418	PRO	CA-C-N	-10.25	109.29	123.03
1	B	418	PRO	C-N-CA	-10.25	109.29	123.03
1	A	418	PRO	CA-C-N	-10.21	109.34	123.03
1	A	418	PRO	C-N-CA	-10.21	109.34	123.03
1	B	460	VAL	CB-CA-C	10.20	128.02	111.29
1	B	419	ASN	N-CA-C	-10.18	91.70	108.49
1	A	460	VAL	CB-CA-C	10.17	127.96	111.29
1	A	419	ASN	N-CA-C	-10.15	91.74	108.49
1	A	378	ILE	CA-C-O	10.15	125.14	119.15
1	A	353	PHE	N-CA-C	10.13	124.72	108.41
1	B	353	PHE	N-CA-C	10.12	124.71	108.41
1	A	411	LEU	CB-CA-C	-10.08	90.91	110.46
1	B	411	LEU	CB-CA-C	-10.07	90.92	110.46
1	B	290	LYS	N-CA-C	10.06	121.83	111.07
1	B	378	ILE	CA-C-O	10.03	125.07	119.15
1	A	290	LYS	N-CA-C	9.99	121.76	111.07
1	B	342	ILE	N-CA-C	9.94	119.96	110.42
1	A	53	LYS	N-CA-CB	9.93	123.41	111.09
1	A	165	TRP	N-CA-C	9.93	125.94	109.06
1	A	342	ILE	N-CA-C	9.90	119.92	110.42
1	B	53	LYS	N-CA-CB	9.90	123.36	111.09
1	B	165	TRP	N-CA-C	9.88	125.86	109.06
1	B	87	VAL	CB-CA-C	-9.87	99.34	111.97
1	A	87	VAL	CB-CA-C	-9.86	99.35	111.97
1	A	383	PHE	N-CA-C	9.86	126.05	110.17
1	B	383	PHE	N-CA-C	9.85	126.03	110.17
1	B	13	PRO	N-CA-C	-9.84	98.70	110.70
1	B	454	PHE	N-CA-C	-9.83	96.63	110.50
1	A	454	PHE	N-CA-C	-9.81	96.67	110.50
1	A	13	PRO	N-CA-C	-9.79	98.75	110.70
1	A	244	TYR	N-CA-C	9.70	124.37	112.54
1	A	541	ILE	CB-CA-C	-9.70	99.37	111.88
1	B	244	TYR	N-CA-C	9.69	124.36	112.54
1	B	541	ILE	CB-CA-C	-9.66	99.42	111.88
1	B	130	VAL	N-CA-C	-9.65	93.46	108.23
1	A	130	VAL	N-CA-C	-9.64	93.47	108.23
1	B	473	PHE	N-CA-C	-9.34	90.92	110.80
1	A	370	THR	N-CA-C	9.33	121.45	111.28
1	B	370	THR	N-CA-C	9.33	121.45	111.28
1	A	473	PHE	N-CA-C	-9.32	90.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	LEU	N-CA-C	9.22	124.98	112.90
1	A	346	LEU	N-CA-C	9.19	124.94	112.90
1	B	442	VAL	CB-CA-C	-9.09	100.06	111.70
1	A	442	VAL	CB-CA-C	-9.08	100.08	111.70
1	B	202	VAL	CB-CA-C	-9.05	94.56	111.30
1	A	202	VAL	CB-CA-C	-9.05	94.56	111.30
1	B	401	THR	CB-CA-C	8.95	125.12	110.81
1	A	70	LEU	N-CA-C	8.94	122.10	108.52
1	A	401	THR	CB-CA-C	8.93	125.09	110.81
1	B	70	LEU	N-CA-C	8.92	122.08	108.52
1	B	495	CYS	CA-CB-SG	-8.88	93.97	114.40
1	A	495	CYS	CA-CB-SG	-8.88	93.98	114.40
1	A	494	ASP	CB-CA-C	-8.87	97.29	110.96
1	B	494	ASP	CB-CA-C	-8.85	97.33	110.96
1	B	15	LYS	CA-C-N	-8.83	109.74	122.19
1	B	15	LYS	C-N-CA	-8.83	109.74	122.19
1	A	215	GLY	N-CA-C	-8.78	101.74	113.24
1	B	308	VAL	N-CA-C	-8.77	97.73	107.73
1	B	215	GLY	N-CA-C	-8.77	101.75	113.24
1	A	15	LYS	CA-C-N	-8.76	109.83	122.19
1	A	15	LYS	C-N-CA	-8.76	109.83	122.19
1	A	308	VAL	N-CA-C	-8.73	97.77	107.73
1	A	265	ILE	N-CA-C	8.73	119.24	108.06
1	B	265	ILE	N-CA-C	8.73	119.23	108.06
1	A	225	THR	N-CA-C	8.72	124.16	113.17
1	B	225	THR	N-CA-C	8.65	124.07	113.17
1	B	341	LYS	N-CA-C	-8.63	101.84	111.07
1	A	341	LYS	N-CA-C	-8.61	101.86	111.07
1	A	540	ILE	N-CA-C	8.61	119.41	110.72
1	B	142	VAL	CB-CA-C	-8.59	97.03	110.52
1	A	415	ASP	N-CA-C	8.59	123.59	113.20
1	A	320	VAL	N-CA-C	-8.59	102.05	110.72
1	B	540	ILE	N-CA-C	8.59	119.39	110.72
1	B	415	ASP	N-CA-C	8.58	123.58	113.20
1	B	320	VAL	N-CA-C	-8.56	102.07	110.72
1	A	142	VAL	CB-CA-C	-8.56	97.08	110.52
1	B	424	PHE	N-CA-C	8.51	122.39	108.52
1	B	34	SER	N-CA-C	-8.50	101.94	111.71
1	A	291	GLN	N-CA-C	-8.47	101.99	111.14
1	A	424	PHE	N-CA-C	8.47	122.33	108.52
1	A	34	SER	N-CA-C	-8.46	101.98	111.71
1	B	291	GLN	N-CA-C	-8.45	102.01	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ASP	O-C-N	8.45	128.30	121.20
1	B	536	ASP	O-C-N	8.45	128.29	121.20
1	B	272	ASN	N-CA-C	-8.39	99.96	109.60
1	A	272	ASN	N-CA-C	-8.36	99.99	109.60
1	B	267	ILE	CB-CA-C	-8.34	98.40	110.83
1	A	267	ILE	CB-CA-C	-8.33	98.42	110.83
1	A	147	THR	N-CA-C	-8.27	99.86	110.53
1	B	147	THR	N-CA-C	-8.27	99.86	110.53
1	A	62	HIS	N-CA-C	8.21	128.29	110.80
1	B	62	HIS	N-CA-C	8.18	128.22	110.80
1	A	362	PRO	N-CA-C	-8.14	102.22	113.53
1	B	362	PRO	N-CA-C	-8.11	102.25	113.53
1	B	281	ILE	N-CA-CB	-8.00	101.39	110.99
1	B	114	ARG	CB-CG-CD	7.99	129.68	111.30
1	A	114	ARG	CB-CG-CD	7.99	129.68	111.30
1	A	281	ILE	N-CA-CB	-7.95	101.45	110.99
1	A	74	ILE	CA-C-N	-7.90	112.01	122.99
1	A	74	ILE	C-N-CA	-7.90	112.01	122.99
1	B	16	LEU	CA-CB-CG	-7.90	88.66	116.30
1	A	16	LEU	CA-CB-CG	-7.88	88.70	116.30
1	B	74	ILE	CA-C-N	-7.88	112.04	122.99
1	B	74	ILE	C-N-CA	-7.88	112.04	122.99
1	B	478	LEU	CB-CA-C	-7.84	97.77	110.79
1	A	458	PHE	CB-CA-C	-7.84	98.79	110.24
1	A	478	LEU	CB-CA-C	-7.83	97.80	110.79
1	A	250	ILE	N-CA-C	7.81	123.36	112.50
1	B	458	PHE	CB-CA-C	-7.81	98.84	110.24
1	B	59	ASP	CA-C-O	7.80	124.36	119.29
1	B	250	ILE	N-CA-C	7.79	123.32	112.50
1	A	65	ASP	N-CA-C	-7.78	99.76	110.35
1	B	65	ASP	N-CA-C	-7.78	99.77	110.35
1	A	268	TRP	CB-CA-C	-7.75	96.44	109.53
1	B	268	TRP	CB-CA-C	-7.74	96.45	109.53
1	A	44	ASP	CB-CA-C	7.74	124.67	110.36
1	B	22	ASN	N-CA-C	7.73	119.71	111.28
1	A	59	ASP	CA-C-O	7.73	124.31	119.29
1	B	44	ASP	CB-CA-C	7.72	124.65	110.36
1	A	22	ASN	N-CA-C	7.71	119.68	111.28
1	A	386	PRO	CA-C-N	7.61	130.81	120.54
1	A	386	PRO	C-N-CA	7.61	130.81	120.54
1	B	233	GLN	CA-C-N	7.58	128.60	120.11
1	B	233	GLN	C-N-CA	7.58	128.60	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	PHE	CB-CA-C	7.58	122.48	110.19
1	B	386	PRO	CA-C-N	7.58	130.78	120.54
1	B	386	PRO	C-N-CA	7.58	130.78	120.54
1	A	425	PHE	CB-CA-C	7.58	122.46	110.19
1	A	233	GLN	CA-C-N	7.54	128.56	120.11
1	A	233	GLN	C-N-CA	7.54	128.56	120.11
1	A	555	HIS	N-CA-C	-7.46	103.09	111.14
1	A	471	ILE	CB-CA-C	-7.45	101.94	110.96
1	B	471	ILE	CB-CA-C	-7.45	101.95	110.96
1	B	555	HIS	N-CA-C	-7.43	103.11	111.14
1	A	149	HIS	N-CA-C	-7.40	102.23	111.11
1	B	120	VAL	N-CA-CB	7.40	119.86	111.21
1	B	149	HIS	N-CA-C	-7.38	102.26	111.11
1	A	120	VAL	N-CA-CB	7.37	119.83	111.21
1	B	540	ILE	CB-CA-C	-7.36	102.06	112.22
1	A	540	ILE	CB-CA-C	-7.34	102.09	112.22
1	B	93	PHE	N-CA-C	7.31	122.04	113.20
1	B	162	ASP	CB-CA-C	7.26	125.17	109.99
1	A	162	ASP	CB-CA-C	7.26	125.17	109.99
1	A	327	TYR	CA-CB-CG	7.25	126.96	113.90
1	B	327	TYR	CA-CB-CG	7.23	126.91	113.90
1	A	363	ILE	N-CA-C	7.22	117.31	110.30
1	B	15	LYS	N-CA-CB	-7.22	101.53	112.28
1	A	15	LYS	N-CA-CB	-7.21	101.54	112.28
1	A	95	PHE	CA-C-N	-7.20	110.84	119.84
1	A	95	PHE	C-N-CA	-7.20	110.84	119.84
1	B	423	LEU	CA-C-N	-7.20	112.97	123.05
1	B	423	LEU	C-N-CA	-7.20	112.97	123.05
1	A	423	LEU	CA-C-N	-7.20	112.98	123.05
1	A	423	LEU	C-N-CA	-7.20	112.98	123.05
1	A	330	ARG	N-CA-CB	-7.19	98.60	110.68
1	B	95	PHE	CA-C-N	-7.19	110.86	119.84
1	B	95	PHE	C-N-CA	-7.19	110.86	119.84
1	A	344	LYS	N-CA-C	7.18	118.90	111.14
1	B	560	LEU	CB-CG-CD2	-7.18	89.15	110.70
1	B	363	ILE	N-CA-C	7.18	117.26	110.30
1	B	330	ARG	N-CA-CB	-7.18	98.62	110.68
1	A	560	LEU	CB-CG-CD2	-7.17	89.19	110.70
1	A	476	LYS	CB-CA-C	7.17	122.91	110.01
1	B	159	ASN	N-CA-C	7.17	121.36	112.47
1	B	476	LYS	CB-CA-C	7.17	122.91	110.01
1	A	93	PHE	N-CA-C	7.16	122.04	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASN	N-CA-C	7.16	121.35	112.47
1	B	432	SER	N-CA-C	-7.16	95.60	108.48
1	B	244	TYR	CB-CA-C	-7.15	95.38	110.31
1	A	478	LEU	N-CA-C	7.14	119.07	111.28
1	A	432	SER	N-CA-C	-7.14	95.63	108.48
1	B	344	LYS	N-CA-C	7.13	118.84	111.14
1	A	244	TYR	CB-CA-C	-7.12	95.42	110.31
1	A	112	ALA	CA-C-N	7.10	127.66	119.99
1	A	112	ALA	C-N-CA	7.10	127.66	119.99
1	B	478	LEU	N-CA-C	7.08	119.00	111.28
1	A	202	VAL	N-CA-C	7.08	117.69	108.35
1	B	202	VAL	N-CA-C	7.07	117.69	108.35
1	B	112	ALA	CA-C-N	7.06	127.62	119.99
1	B	112	ALA	C-N-CA	7.06	127.62	119.99
1	B	521	ASN	N-CA-C	7.06	121.41	111.52
1	B	276	TYR	CB-CA-C	-7.05	100.99	110.79
1	A	521	ASN	N-CA-C	7.04	121.38	111.52
1	A	195	MET	N-CA-C	7.03	121.45	113.01
1	A	376	SER	N-CA-C	7.03	118.94	111.28
1	A	276	TYR	CB-CA-C	-7.03	101.02	110.79
1	B	195	MET	N-CA-C	7.03	121.44	113.01
1	B	551	SER	CA-C-N	6.99	130.59	120.38
1	B	551	SER	C-N-CA	6.99	130.59	120.38
1	A	551	SER	CA-C-N	6.99	130.59	120.38
1	A	551	SER	C-N-CA	6.99	130.59	120.38
1	A	128	ASN	N-CA-C	6.99	121.64	113.18
1	B	128	ASN	N-CA-C	6.99	121.63	113.18
1	A	536	ASP	CA-C-N	6.98	128.57	119.84
1	A	536	ASP	C-N-CA	6.98	128.57	119.84
1	B	536	ASP	CA-C-N	6.97	128.56	119.84
1	B	536	ASP	C-N-CA	6.97	128.56	119.84
1	B	376	SER	N-CA-C	6.97	118.88	111.28
1	B	231	GLU	CA-CB-CG	-6.97	100.17	114.10
1	A	231	GLU	CA-CB-CG	-6.96	100.19	114.10
1	A	152	HIS	N-CA-C	6.94	118.53	110.97
1	A	44	ASP	CA-C-N	6.93	133.27	121.14
1	A	44	ASP	C-N-CA	6.93	133.27	121.14
1	B	44	ASP	CA-C-N	6.93	133.26	121.14
1	B	44	ASP	C-N-CA	6.93	133.26	121.14
1	A	443	THR	CB-CA-C	-6.90	98.95	110.68
1	B	241	LEU	CB-CA-C	-6.90	97.89	109.75
1	A	241	LEU	CB-CA-C	-6.89	97.90	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	THR	CB-CA-C	-6.89	98.97	110.68
1	B	152	HIS	N-CA-C	6.88	118.47	110.97
1	B	387	GLU	N-CA-CB	-6.87	99.70	109.94
1	B	97	LEU	N-CA-C	6.86	120.67	110.52
1	A	387	GLU	N-CA-CB	-6.86	99.72	109.94
1	B	11	THR	CB-CA-C	-6.85	97.66	109.65
1	A	11	THR	CB-CA-C	-6.83	97.69	109.65
1	A	97	LEU	N-CA-C	6.83	120.63	110.52
1	B	316	LEU	N-CA-C	-6.83	103.76	111.14
1	A	316	LEU	N-CA-C	-6.83	103.77	111.14
1	A	253	LEU	N-CA-C	-6.82	104.22	112.54
1	B	253	LEU	N-CA-C	-6.80	104.24	112.54
1	B	554	SER	CA-C-N	-6.80	111.19	120.44
1	B	554	SER	C-N-CA	-6.80	111.19	120.44
1	B	385	PHE	CB-CA-C	6.80	119.01	108.61
1	A	385	PHE	CB-CA-C	6.78	118.98	108.61
1	A	521	ASN	N-CA-CB	-6.78	101.61	111.91
1	B	521	ASN	N-CA-CB	-6.78	101.61	111.91
1	A	554	SER	CA-C-N	-6.77	111.23	120.44
1	A	554	SER	C-N-CA	-6.77	111.23	120.44
1	B	363	ILE	N-CA-CB	6.73	117.96	110.62
1	A	444	LYS	N-CA-CB	-6.72	100.23	109.98
1	B	444	LYS	N-CA-CB	-6.72	100.23	109.98
1	B	73	ALA	CA-C-N	-6.72	114.46	122.93
1	B	73	ALA	C-N-CA	-6.72	114.46	122.93
1	A	73	ALA	CA-C-N	-6.71	114.47	122.93
1	A	73	ALA	C-N-CA	-6.71	114.47	122.93
1	A	177	LEU	CA-CB-CG	6.71	139.78	116.30
1	A	45	GLN	CA-C-N	6.71	134.04	121.97
1	A	45	GLN	C-N-CA	6.71	134.04	121.97
1	B	177	LEU	CA-CB-CG	6.70	139.74	116.30
1	A	363	ILE	N-CA-CB	6.69	117.92	110.62
1	A	15	LYS	N-CA-C	-6.68	104.19	112.47
1	B	45	GLN	CA-C-N	6.67	133.98	121.97
1	B	45	GLN	C-N-CA	6.67	133.98	121.97
1	B	195	MET	CA-CB-CG	-6.66	100.77	114.10
1	A	195	MET	CA-CB-CG	-6.66	100.78	114.10
1	B	15	LYS	N-CA-C	-6.63	104.25	112.47
1	B	70	LEU	N-CA-CB	-6.62	100.72	111.24
1	A	70	LEU	N-CA-CB	-6.61	100.73	111.24
1	B	312	ARG	CB-CG-CD	-6.61	96.10	111.30
1	A	312	ARG	CB-CG-CD	-6.61	96.10	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	LEU	CA-CB-CG	-6.60	93.19	116.30
1	A	452	LEU	CA-CB-CG	-6.60	93.21	116.30
1	A	262	VAL	N-CA-C	6.51	118.06	109.21
1	B	389	THR	N-CA-C	6.50	118.77	108.23
1	A	389	THR	N-CA-C	6.50	118.75	108.23
1	A	432	SER	N-CA-CB	6.47	121.45	110.71
1	B	358	TYR	N-CA-C	6.46	118.93	108.34
1	B	432	SER	N-CA-CB	6.46	121.43	110.71
1	B	262	VAL	N-CA-C	6.46	117.99	109.21
1	A	264	LYS	CB-CA-C	-6.45	99.60	110.43
1	A	358	TYR	N-CA-C	6.43	118.88	108.34
1	B	264	LYS	CB-CA-C	-6.43	99.63	110.43
1	B	397	VAL	N-CA-C	6.43	116.59	110.42
1	A	74	ILE	N-CA-C	6.42	117.54	108.36
1	B	9	PRO	N-CA-C	-6.41	101.83	111.57
1	B	74	ILE	N-CA-C	6.41	117.53	108.36
1	A	9	PRO	N-CA-C	-6.40	101.85	111.57
1	A	397	VAL	N-CA-C	6.39	116.56	110.42
1	A	40	ILE	CA-C-N	6.38	129.35	120.29
1	A	40	ILE	C-N-CA	6.38	129.35	120.29
1	B	40	ILE	CA-C-N	6.38	129.35	120.29
1	B	40	ILE	C-N-CA	6.38	129.35	120.29
1	B	468	ILE	N-CA-C	6.36	116.88	107.15
1	A	468	ILE	N-CA-C	6.35	116.87	107.15
1	B	360	PRO	N-CA-C	-6.35	101.23	111.14
1	A	360	PRO	N-CA-C	-6.33	101.27	111.14
1	B	198	SER	CB-CA-C	6.32	119.19	110.34
1	A	198	SER	CB-CA-C	6.30	119.15	110.34
1	A	384	TYR	CA-CB-CG	6.29	125.22	113.90
1	A	242	PHE	CA-C-N	6.29	126.03	119.05
1	A	242	PHE	C-N-CA	6.29	126.03	119.05
1	B	242	PHE	CA-C-N	6.29	126.03	119.05
1	B	242	PHE	C-N-CA	6.29	126.03	119.05
1	B	227	GLY	N-CA-C	6.29	123.72	115.36
1	B	384	TYR	CA-CB-CG	6.28	125.21	113.90
1	A	227	GLY	N-CA-C	6.28	123.71	115.36
1	B	139	TYR	CA-C-N	-6.27	112.29	122.82
1	B	139	TYR	C-N-CA	-6.27	112.29	122.82
1	A	139	TYR	CA-C-N	-6.26	112.30	122.82
1	A	139	TYR	C-N-CA	-6.26	112.30	122.82
1	B	217	LEU	N-CA-C	-6.26	95.97	109.81
1	B	177	LEU	CB-CA-C	6.26	121.30	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	MET	CA-C-O	6.26	123.95	119.32
1	B	341	LYS	CB-CA-C	-6.25	101.06	110.88
1	A	217	LEU	N-CA-C	-6.25	96.00	109.81
1	A	28	ILE	N-CA-C	6.25	116.42	110.42
1	A	177	LEU	CB-CA-C	6.25	121.28	110.79
1	B	216	ALA	N-CA-C	6.24	119.06	111.82
1	B	28	ILE	N-CA-C	6.23	116.41	110.42
1	A	341	LYS	CB-CA-C	-6.23	101.10	110.88
1	A	216	ALA	N-CA-C	6.22	119.03	111.82
1	A	270	MET	CA-C-O	6.21	123.92	119.32
1	A	67	ASP	N-CA-CB	-6.19	99.53	110.42
1	B	67	ASP	N-CA-CB	-6.19	99.53	110.42
1	A	400	LYS	N-CA-C	-6.17	104.47	111.07
1	A	241	LEU	N-CA-C	-6.16	104.16	113.89
1	A	507	LEU	CB-CA-C	-6.16	100.21	110.68
1	B	538	ASN	N-CA-C	6.16	120.40	113.01
1	A	185	VAL	CB-CA-C	-6.15	99.70	110.71
1	B	400	LYS	N-CA-C	-6.15	104.49	111.07
1	B	360	PRO	CB-CA-C	-6.14	103.54	111.46
1	B	185	VAL	CB-CA-C	-6.14	99.72	110.71
1	A	10	LEU	CB-CA-C	-6.14	98.89	110.67
1	B	241	LEU	N-CA-C	-6.13	104.20	113.89
1	A	360	PRO	CB-CA-C	-6.13	103.56	111.46
1	B	10	LEU	CB-CA-C	-6.13	98.90	110.67
1	B	507	LEU	CB-CA-C	-6.13	100.27	110.68
1	B	270	MET	CA-C-N	6.11	126.05	119.76
1	B	270	MET	C-N-CA	6.11	126.05	119.76
1	A	185	VAL	CA-C-N	6.10	126.95	121.82
1	A	185	VAL	C-N-CA	6.10	126.95	121.82
1	A	538	ASN	N-CA-C	6.10	120.33	113.01
1	A	398	ARG	N-CA-C	6.09	119.80	112.38
1	A	270	MET	CA-C-N	6.08	126.02	119.76
1	A	270	MET	C-N-CA	6.08	126.02	119.76
1	B	95	PHE	N-CA-C	-6.08	102.41	110.07
1	B	185	VAL	CA-C-N	6.07	126.92	121.82
1	B	185	VAL	C-N-CA	6.07	126.92	121.82
1	A	155	LEU	CB-CA-C	-6.07	98.68	110.46
1	A	502	GLU	N-CA-C	-6.07	99.76	109.96
1	B	502	GLU	N-CA-C	-6.07	99.76	109.96
1	B	155	LEU	CB-CA-C	-6.06	98.70	110.46
1	A	129	ARG	CB-CA-C	-6.05	99.30	109.65
1	B	398	ARG	N-CA-C	6.05	119.76	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	PHE	CB-CA-C	-6.04	100.28	110.19
1	B	129	ARG	CB-CA-C	-6.04	99.32	109.65
1	A	424	PHE	CB-CA-C	-6.04	100.29	110.19
1	B	384	TYR	CB-CA-C	-6.03	99.12	110.16
1	A	384	TYR	CB-CA-C	-6.03	99.13	110.16
1	A	95	PHE	N-CA-C	-6.01	102.49	110.07
1	B	430	LYS	CB-CG-CD	-6.01	97.48	111.30
1	A	430	LYS	CB-CG-CD	-6.00	97.50	111.30
1	A	396	ARG	CG-CD-NE	-5.99	98.81	112.00
1	B	536	ASP	N-CA-CB	5.99	119.13	110.74
1	A	536	ASP	N-CA-CB	5.98	119.12	110.74
1	B	396	ARG	CG-CD-NE	-5.98	98.85	112.00
1	B	430	LYS	CB-CA-C	-5.97	96.29	110.02
1	A	156	GLU	CB-CG-CD	5.97	122.74	112.60
1	B	7	PHE	CB-CA-C	-5.97	100.77	110.79
1	A	7	PHE	CB-CA-C	-5.96	100.78	110.79
1	A	339	LEU	N-CA-C	-5.96	104.71	111.14
1	A	352	ASN	CB-CA-C	-5.95	102.52	110.79
1	B	233	GLN	N-CA-CB	-5.95	100.62	110.02
1	A	233	GLN	N-CA-CB	-5.95	100.62	110.02
1	A	430	LYS	CB-CA-C	-5.95	96.33	110.02
1	B	156	GLU	CB-CG-CD	5.95	122.72	112.60
1	B	364	ARG	N-CA-C	5.95	117.77	111.28
1	B	178	GLY	N-CA-C	-5.94	105.61	112.50
1	A	364	ARG	N-CA-C	5.94	117.75	111.28
1	B	352	ASN	CB-CA-C	-5.93	102.54	110.79
1	B	479	ILE	CB-CA-C	5.93	120.15	112.14
1	A	49	GLY	N-CA-C	5.93	127.23	113.18
1	A	55	THR	N-CA-CB	5.93	120.07	110.41
1	A	73	ALA	N-CA-C	5.93	118.13	108.76
1	A	479	ILE	CB-CA-C	5.92	120.14	112.14
1	B	49	GLY	N-CA-C	5.92	127.21	113.18
1	B	339	LEU	N-CA-C	-5.92	104.75	111.14
1	B	73	ALA	N-CA-C	5.91	118.10	108.76
1	B	502	GLU	CB-CA-C	5.91	119.28	109.53
1	B	55	THR	N-CA-CB	5.90	120.03	110.41
1	B	294	ASP	N-CA-C	-5.90	104.20	111.75
1	A	502	GLU	CB-CA-C	5.90	119.26	109.53
1	A	178	GLY	N-CA-C	-5.90	105.66	112.50
1	B	142	VAL	O-C-N	5.89	129.48	122.95
1	B	97	LEU	CA-CB-CG	-5.88	95.70	116.30
1	A	6	GLU	CA-C-N	5.88	130.53	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	GLU	C-N-CA	5.88	130.53	120.71
1	B	169	PRO	N-CA-C	-5.88	100.36	112.47
1	A	97	LEU	CA-CB-CG	-5.88	95.73	116.30
1	A	169	PRO	N-CA-C	-5.88	100.36	112.47
1	A	100	ILE	CB-CA-C	-5.87	103.12	111.40
1	B	100	ILE	CB-CA-C	-5.87	103.13	111.40
1	B	479	ILE	N-CA-C	-5.86	104.64	110.62
1	B	421	ALA	N-CA-C	-5.86	99.80	108.99
1	A	294	ASP	N-CA-C	-5.85	104.26	111.75
1	B	293	VAL	N-CA-C	5.85	116.03	110.53
1	B	371	ILE	N-CA-CB	-5.85	104.04	110.65
1	A	442	VAL	N-CA-CB	-5.84	104.48	110.62
1	B	6	GLU	CA-C-N	5.84	130.47	120.71
1	B	6	GLU	C-N-CA	5.84	130.47	120.71
1	B	413	TRP	CA-CB-CG	5.84	124.69	113.60
1	A	142	VAL	O-C-N	5.84	129.43	122.95
1	A	371	ILE	N-CA-CB	-5.84	104.05	110.65
1	B	480	GLN	N-CA-C	5.84	117.44	111.14
1	A	293	VAL	N-CA-C	5.83	116.02	110.53
1	B	332	GLU	N-CA-C	5.83	122.69	109.81
1	B	442	VAL	N-CA-CB	-5.82	104.51	110.62
1	A	413	TRP	CA-CB-CG	5.82	124.65	113.60
1	A	332	GLU	N-CA-C	5.82	122.66	109.81
1	A	421	ALA	N-CA-C	-5.82	99.86	108.99
1	B	42	SER	N-CA-C	5.81	117.62	108.96
1	A	42	SER	N-CA-C	5.81	117.62	108.96
1	A	480	GLN	N-CA-C	5.81	117.41	111.14
1	B	385	PHE	CA-C-O	5.80	126.61	120.63
1	A	479	ILE	N-CA-C	-5.79	104.72	110.62
1	A	385	PHE	CA-C-O	5.79	126.59	120.63
1	B	349	GLY	N-CA-C	-5.78	103.45	112.58
1	B	133	VAL	N-CA-C	-5.76	97.22	107.18
1	A	349	GLY	N-CA-C	-5.75	103.50	112.58
1	A	53	LYS	O-C-N	5.75	126.06	121.17
1	A	133	VAL	N-CA-C	-5.75	97.24	107.18
1	B	120	VAL	CA-C-N	-5.74	113.15	122.34
1	B	120	VAL	C-N-CA	-5.74	113.15	122.34
1	A	27	ASP	N-CA-C	-5.73	105.03	111.28
1	A	120	VAL	CA-C-N	-5.73	113.17	122.34
1	A	120	VAL	C-N-CA	-5.73	113.17	122.34
1	A	464	GLU	N-CA-CB	-5.72	102.53	111.56
1	B	53	LYS	O-C-N	5.70	126.02	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	464	GLU	N-CA-CB	-5.69	102.56	111.56
1	B	142	VAL	N-CA-C	5.69	116.90	108.65
1	A	142	VAL	N-CA-C	5.67	116.87	108.65
1	B	536	ASP	CA-C-O	5.67	127.07	121.29
1	B	27	ASP	N-CA-C	-5.65	105.12	111.28
1	B	288	ASP	CB-CA-C	5.63	120.42	110.85
1	A	288	ASP	CB-CA-C	5.61	120.39	110.85
1	A	43	LYS	N-CA-C	-5.61	105.63	113.37
1	A	536	ASP	CA-C-O	5.61	127.01	121.29
1	B	172	GLY	N-CA-C	5.60	122.26	113.86
1	A	172	GLY	N-CA-C	5.60	122.26	113.86
1	A	282	THR	CB-CA-C	-5.60	100.30	109.53
1	B	263	THR	N-CA-CB	-5.58	103.58	111.00
1	B	117	GLY	N-CA-C	-5.58	107.62	115.32
1	A	263	THR	N-CA-CB	-5.58	103.58	111.00
1	B	43	LYS	N-CA-C	-5.57	105.68	113.37
1	B	282	THR	CB-CA-C	-5.57	100.34	109.53
1	B	395	LEU	N-CA-CB	5.57	118.91	110.28
1	A	236	SER	N-CA-C	-5.57	103.14	110.43
1	A	395	LEU	N-CA-CB	5.56	118.90	110.28
1	A	269	LEU	N-CA-C	5.55	118.87	109.76
1	A	117	GLY	N-CA-C	-5.55	107.66	115.32
1	B	236	SER	N-CA-C	-5.55	103.16	110.43
1	B	269	LEU	N-CA-C	5.54	118.85	109.76
1	A	222	ARG	CA-C-N	5.54	126.76	119.84
1	A	222	ARG	C-N-CA	5.54	126.76	119.84
1	B	296	ILE	N-CA-CB	-5.54	99.81	110.78
1	B	237	LYS	N-CA-C	5.54	117.77	111.02
1	A	296	ILE	N-CA-CB	-5.53	99.83	110.78
1	A	288	ASP	O-C-N	5.53	128.45	122.15
1	B	254	PHE	N-CA-C	5.53	119.65	113.02
1	A	51	TYR	N-CA-C	-5.52	105.26	111.28
1	A	237	LYS	N-CA-C	5.52	117.76	111.02
1	B	434	GLU	CB-CA-C	-5.52	102.45	110.96
1	B	51	TYR	N-CA-C	-5.52	105.27	111.28
1	A	434	GLU	CB-CA-C	-5.51	102.47	110.96
1	A	254	PHE	N-CA-C	5.51	119.63	113.02
1	A	514	MET	N-CA-C	-5.51	105.38	111.71
1	A	447	CYS	N-CA-C	-5.50	105.43	111.82
1	B	514	MET	N-CA-C	-5.50	105.38	111.71
1	B	447	CYS	N-CA-C	-5.50	105.44	111.82
1	B	542	ALA	CA-C-N	5.50	125.93	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	542	ALA	C-N-CA	5.50	125.93	119.99
1	A	47	VAL	CA-C-N	5.49	130.01	120.68
1	A	47	VAL	C-N-CA	5.49	130.01	120.68
1	B	222	ARG	CA-C-N	5.49	126.70	119.84
1	B	222	ARG	C-N-CA	5.49	126.70	119.84
1	A	52	MET	CB-CA-C	5.48	120.00	110.68
1	B	68	TYR	CA-C-N	-5.48	114.48	122.65
1	B	68	TYR	C-N-CA	-5.48	114.48	122.65
1	A	98	TRP	CA-CB-CG	-5.48	103.19	113.60
1	A	104	ARG	CA-CB-CG	-5.48	103.15	114.10
1	A	173	GLY	N-CA-C	5.47	122.49	115.32
1	B	104	ARG	CA-CB-CG	-5.47	103.15	114.10
1	B	46	ILE	CA-C-N	5.47	129.78	122.01
1	B	46	ILE	C-N-CA	5.47	129.78	122.01
1	B	52	MET	CB-CA-C	5.47	119.98	110.68
1	A	542	ALA	CA-C-N	5.47	125.90	119.99
1	A	542	ALA	C-N-CA	5.47	125.90	119.99
1	B	98	TRP	CA-CB-CG	-5.47	103.21	113.60
1	A	61	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	83	VAL	N-CA-C	-5.47	104.62	110.36
1	B	53	LYS	CB-CA-C	5.47	120.17	111.15
1	B	61	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	68	TYR	CA-C-N	-5.46	114.51	122.65
1	A	68	TYR	C-N-CA	-5.46	114.51	122.65
1	B	36	ASN	CB-CA-C	5.46	120.09	110.37
1	B	173	GLY	N-CA-C	5.46	122.47	115.32
1	A	47	VAL	N-CA-CB	-5.46	105.06	111.39
1	B	463	ARG	N-CA-C	-5.46	104.57	113.19
1	A	378	ILE	CA-C-N	5.46	125.40	119.78
1	A	378	ILE	C-N-CA	5.46	125.40	119.78
1	B	288	ASP	O-C-N	5.45	128.37	122.15
1	B	83	VAL	N-CA-C	-5.45	104.64	110.36
1	A	236	SER	N-CA-CB	-5.44	102.48	110.26
1	B	378	ILE	CA-C-N	5.44	125.39	119.78
1	B	378	ILE	C-N-CA	5.44	125.39	119.78
1	A	53	LYS	CB-CA-C	5.44	120.12	111.15
1	A	193	HIS	N-CA-C	5.44	120.28	111.37
1	A	463	ARG	N-CA-C	-5.43	104.61	113.19
1	B	193	HIS	N-CA-C	5.42	120.26	111.37
1	A	426	SER	N-CA-CB	-5.42	103.24	111.21
1	A	32	VAL	N-CA-C	5.42	120.04	113.00
1	B	279	TYR	CB-CA-C	-5.42	100.97	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASN	CB-CA-C	5.41	120.00	110.37
1	A	558	TRP	CA-CB-CG	-5.41	103.33	113.60
1	A	279	TYR	CB-CA-C	-5.41	100.99	112.78
1	B	289	LEU	N-CA-C	-5.41	102.45	111.37
1	B	243	PRO	CA-C-N	-5.40	111.70	120.72
1	B	243	PRO	C-N-CA	-5.40	111.70	120.72
1	A	289	LEU	N-CA-C	-5.40	102.46	111.37
1	B	558	TRP	CA-CB-CG	-5.40	103.34	113.60
1	B	236	SER	N-CA-CB	-5.40	102.54	110.26
1	A	21	PHE	N-CA-C	-5.39	105.30	111.07
1	A	243	PRO	CA-C-N	-5.39	111.72	120.72
1	A	243	PRO	C-N-CA	-5.39	111.72	120.72
1	A	46	ILE	CA-C-N	5.38	129.65	122.01
1	A	46	ILE	C-N-CA	5.38	129.65	122.01
1	B	21	PHE	N-CA-C	-5.38	105.32	111.07
1	B	32	VAL	N-CA-C	5.38	119.99	113.00
1	B	426	SER	N-CA-CB	-5.38	103.31	111.21
1	A	64	MET	N-CA-CB	5.37	117.79	110.38
1	B	64	MET	N-CA-CB	5.37	117.80	110.38
1	A	398	ARG	CA-CB-CG	-5.37	103.36	114.10
1	B	541	ILE	O-C-N	5.37	128.90	122.62
1	B	47	VAL	N-CA-CB	-5.36	105.17	111.39
1	A	541	ILE	O-C-N	5.36	128.89	122.62
1	B	114	ARG	N-CA-C	-5.36	105.34	111.07
1	B	398	ARG	CA-CB-CG	-5.35	103.40	114.10
1	B	293	VAL	CB-CA-C	-5.35	105.01	112.02
1	A	112	ALA	N-CA-C	5.33	121.58	109.81
1	A	293	VAL	CB-CA-C	-5.33	105.04	112.02
1	A	114	ARG	N-CA-C	-5.32	105.37	111.07
1	A	399	ASP	CB-CA-C	5.31	119.29	110.90
1	B	399	ASP	CB-CA-C	5.31	119.28	110.90
1	B	112	ALA	N-CA-C	5.29	121.50	109.81
1	B	242	PHE	C-N-CD	-5.29	103.32	125.00
1	A	237	LYS	CB-CA-C	-5.28	102.52	110.92
1	A	242	PHE	C-N-CD	-5.28	103.34	125.00
1	A	344	LYS	CB-CA-C	-5.28	102.56	110.90
1	B	344	LYS	CB-CA-C	-5.28	102.56	110.90
1	B	444	LYS	O-C-N	5.27	127.73	122.03
1	A	119	VAL	CA-C-N	-5.26	116.16	122.90
1	A	119	VAL	C-N-CA	-5.26	116.16	122.90
1	B	37	VAL	CB-CA-C	-5.26	102.27	110.69
1	B	237	LYS	CB-CA-C	-5.26	102.56	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ILE	N-CA-C	-5.26	100.29	107.75
1	A	37	VAL	CB-CA-C	-5.25	102.29	110.69
1	B	119	VAL	CA-C-N	-5.25	116.18	122.90
1	B	119	VAL	C-N-CA	-5.25	116.18	122.90
1	B	313	HIS	N-CA-C	-5.25	101.14	109.96
1	A	313	HIS	N-CA-C	-5.25	101.15	109.96
1	B	100	ILE	N-CA-C	-5.24	100.31	107.75
1	A	443	THR	N-CA-CB	-5.24	102.20	110.06
1	B	405	ILE	CA-C-N	5.23	125.13	119.85
1	B	405	ILE	C-N-CA	5.23	125.13	119.85
1	B	443	THR	N-CA-CB	-5.23	102.22	110.06
1	A	219	ASP	CA-C-N	-5.22	114.57	119.85
1	A	219	ASP	C-N-CA	-5.22	114.57	119.85
1	B	534	ALA	N-CA-C	-5.22	104.84	111.11
1	A	444	LYS	O-C-N	5.22	127.66	122.03
1	B	498	ASN	N-CA-C	-5.21	106.61	113.17
1	B	419	ASN	CB-CA-C	5.20	119.49	111.85
1	A	224	GLU	N-CA-C	5.20	121.86	110.80
1	A	270	MET	CA-CB-CG	-5.20	103.71	114.10
1	A	472	VAL	N-CA-C	-5.20	101.91	109.29
1	B	224	GLU	N-CA-C	5.19	121.86	110.80
1	B	339	LEU	CB-CA-C	-5.19	102.70	110.90
1	A	259	MET	CA-CB-CG	-5.19	103.72	114.10
1	A	473	PHE	O-C-N	5.19	129.49	122.59
1	A	419	ASN	CB-CA-C	5.19	119.47	111.85
1	A	498	ASN	N-CA-C	-5.19	106.63	113.17
1	A	30	ARG	CB-CG-CD	-5.18	99.37	111.30
1	A	339	LEU	CB-CA-C	-5.18	102.71	110.90
1	B	219	ASP	CA-C-N	-5.18	114.61	119.85
1	B	219	ASP	C-N-CA	-5.18	114.61	119.85
1	B	203	VAL	CB-CA-C	-5.18	104.69	110.96
1	B	270	MET	CA-CB-CG	-5.18	103.74	114.10
1	A	165	TRP	N-CA-CB	-5.18	101.86	111.13
1	A	59	ASP	CA-C-N	5.18	124.49	118.85
1	A	59	ASP	C-N-CA	5.18	124.49	118.85
1	B	259	MET	CA-CB-CG	-5.18	103.75	114.10
1	B	348	LEU	O-C-N	5.18	129.02	122.65
1	B	473	PHE	O-C-N	5.18	129.48	122.59
1	B	30	ARG	CB-CG-CD	-5.17	99.40	111.30
1	A	203	VAL	CB-CA-C	-5.17	104.70	110.96
1	A	534	ALA	N-CA-C	-5.17	104.91	111.11
1	B	59	ASP	CA-C-N	5.17	124.48	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASP	C-N-CA	5.17	124.48	118.85
1	A	440	TYR	N-CA-C	5.16	117.58	111.33
1	B	165	TRP	N-CA-CB	-5.16	101.90	111.13
1	B	361	GLU	N-CA-C	5.16	120.62	113.45
1	B	472	VAL	N-CA-C	-5.16	101.97	109.29
1	B	353	PHE	N-CA-CB	-5.16	102.01	110.21
1	B	440	TYR	N-CA-C	5.16	117.57	111.33
1	A	405	ILE	CA-C-N	5.15	125.05	119.85
1	A	405	ILE	C-N-CA	5.15	125.05	119.85
1	B	17	SER	N-CA-C	-5.14	103.14	110.59
1	B	310	THR	N-CA-C	5.13	117.61	109.24
1	A	353	PHE	N-CA-CB	-5.13	102.05	110.21
1	A	348	LEU	O-C-N	5.13	128.96	122.65
1	A	361	GLU	N-CA-C	5.13	120.58	113.45
1	B	267	ILE	CA-C-N	-5.13	114.09	121.42
1	B	267	ILE	C-N-CA	-5.13	114.09	121.42
1	A	182	GLU	CA-CB-CG	-5.12	103.86	114.10
1	A	17	SER	N-CA-C	-5.11	103.17	110.59
1	B	182	GLU	CA-CB-CG	-5.11	103.89	114.10
1	B	272	ASN	CA-C-N	5.10	125.93	120.47
1	B	272	ASN	C-N-CA	5.10	125.93	120.47
1	A	267	ILE	CA-C-N	-5.10	114.13	121.42
1	A	267	ILE	C-N-CA	-5.10	114.13	121.42
1	A	310	THR	N-CA-C	5.09	117.54	109.24
1	B	407	THR	CB-CA-C	-5.09	99.83	111.95
1	B	369	GLU	N-CA-CB	5.09	117.60	110.12
1	A	35	GLU	CA-CB-CG	-5.08	103.93	114.10
1	A	369	GLU	N-CA-CB	5.08	117.59	110.12
1	B	35	GLU	CA-CB-CG	-5.08	103.94	114.10
1	B	155	LEU	CA-CB-CG	-5.08	98.52	116.30
1	A	407	THR	CB-CA-C	-5.08	99.87	111.95
1	A	155	LEU	CA-CB-CG	-5.07	98.54	116.30
1	B	14	PRO	O-C-N	5.07	129.17	123.03
1	A	414	ILE	N-CA-C	-5.06	104.61	111.89
1	A	475	LYS	N-CA-C	5.05	118.21	111.75
1	A	520	ASN	CA-C-N	-5.05	115.32	122.34
1	A	520	ASN	C-N-CA	-5.05	115.32	122.34
1	B	371	ILE	CG1-CB-CG2	5.05	125.85	110.70
1	A	371	ILE	CG1-CB-CG2	5.05	125.84	110.70
1	A	272	ASN	CA-C-N	5.05	125.87	120.47
1	A	272	ASN	C-N-CA	5.05	125.87	120.47
1	B	414	ILE	N-CA-C	-5.04	104.63	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	ALA	CA-C-N	-5.04	114.75	122.87
1	B	421	ALA	C-N-CA	-5.04	114.75	122.87
1	B	520	ASN	CA-C-N	-5.04	115.34	122.34
1	B	520	ASN	C-N-CA	-5.04	115.34	122.34
1	B	475	LYS	N-CA-C	5.03	118.19	111.75
1	A	421	ALA	CA-C-N	-5.03	114.77	122.87
1	A	421	ALA	C-N-CA	-5.03	114.77	122.87
1	A	551	SER	O-C-N	5.03	127.89	122.11
1	A	281	ILE	N-CA-C	-5.02	101.19	108.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	363	ILE	CA
1	A	410	GLU	CA
1	B	363	ILE	CA
1	B	410	GLU	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4391	0	4330	576	0
1	B	4391	0	4330	574	0
2	A	53	0	31	17	0
2	B	53	0	31	16	0
3	A	11	0	7	5	0
3	B	11	0	7	5	0
4	A	14	0	0	2	0
4	B	24	0	0	0	0
All	All	8948	0	8736	1136	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 (1136) 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:A:422:HIS:NE2	2:A:600:FAD:HM83	1.00	1.30
1:B:422:HIS:NE2	2:B:600:FAD:HM83	1.00	1.30
1:A:422:HIS:CE1	2:A:600:FAD:HM83	1.72	1.24
1:B:422:HIS:CE1	2:B:600:FAD:HM83	1.72	1.24
1:A:507:LEU:HA	1:A:510:MET:HE3	1.28	1.12
1:B:507:LEU:HA	1:B:510:MET:HE3	1.28	1.09
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.27	1.08
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.27	1.08
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.18	1.08
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.31	1.07
1:B:177:LEU:HD22	1:B:265:ILE:HG22	1.35	1.07
1:A:177:LEU:HD22	1:A:265:ILE:HG22	1.35	1.05
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.18	1.05
1:B:361:GLU:N	1:B:364:ARG:HH21	1.57	1.02
1:A:361:GLU:N	1:A:364:ARG:HH21	1.57	1.01
1:A:133:VAL:HG21	1:A:154:TYR:CE1	2.00	0.97
1:B:133:VAL:HG21	1:B:154:TYR:CE1	2.00	0.97
1:B:78:ARG:HD3	1:B:82:ASP:OD2	1.69	0.93
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.50	0.92
1:A:478:LEU:HD12	1:A:478:LEU:H	1.35	0.92
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.50	0.91
1:A:78:ARG:HD3	1:A:82:ASP:OD2	1.69	0.91
1:B:419:ASN:O	1:B:474:ASN:HA	1.71	0.90
1:A:419:ASN:O	1:A:474:ASN:HA	1.71	0.90
1:B:478:LEU:HD12	1:B:478:LEU:H	1.35	0.90
1:B:422:HIS:NE2	2:B:600:FAD:HM81	1.87	0.89
1:B:56:HIS:HA	1:B:111:ALA:CB	2.03	0.89
1:A:422:HIS:NE2	2:A:600:FAD:HM81	1.87	0.88
1:A:91:ASN:ND2	1:A:538:ASN:HD22	1.71	0.88
1:A:300:ARG:HH21	1:A:308:VAL:HA	1.37	0.88
1:B:205:ALA:HA	1:B:541:ILE:HD11	1.56	0.88
1:A:205:ALA:HA	1:A:541:ILE:HD11	1.55	0.88
1:A:56:HIS:HA	1:A:111:ALA:CB	2.03	0.87
1:B:91:ASN:ND2	1:B:538:ASN:HD22	1.71	0.87
1:B:555:HIS:CG	1:B:559:LYS:HE3	2.09	0.87
1:A:443:THR:HA	1:A:491:LEU:HD21	1.57	0.86
1:A:555:HIS:CG	1:A:559:LYS:HE3	2.09	0.86
1:B:443:THR:HA	1:B:491:LEU:HD21	1.57	0.86
1:B:300:ARG:HH21	1:B:308:VAL:HA	1.37	0.86
1:B:422:HIS:CE1	2:B:600:FAD:C8M	2.46	0.85
1:A:457:THR:HG22	1:A:458:PHE:H	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:LEU:HD21	1:B:488:MET:HG3	1.57	0.85
1:B:457:THR:HG22	1:B:458:PHE:H	1.39	0.84
1:A:423:LEU:HD21	1:A:488:MET:HG3	1.57	0.84
2:A:600:FAD:H8A	2:A:600:FAD:C5B	2.08	0.84
1:A:431:VAL:HG22	1:A:465:MET:HG3	1.60	0.83
1:A:425:PHE:HB2	1:A:488:MET:CE	2.09	0.83
1:B:550:PRO:HB2	1:B:552:GLN:NE2	1.94	0.82
2:B:600:FAD:H8A	2:B:600:FAD:C5B	2.08	0.82
1:A:40:ILE:CD1	1:A:57:THR:HG22	2.10	0.82
1:B:550:PRO:CB	1:B:552:GLN:HE21	1.93	0.81
1:A:247:GLY:O	1:B:183:ARG:NH2	2.12	0.81
1:B:431:VAL:HG22	1:B:465:MET:HG3	1.60	0.81
1:B:425:PHE:HB2	1:B:488:MET:CE	2.09	0.81
1:A:459:THR:OG1	1:A:466:HIS:HB2	1.81	0.81
1:A:505:THR:HG22	1:A:506:HIS:H	1.45	0.81
1:A:156:GLU:HG3	1:A:161:ARG:CZ	2.10	0.80
1:A:550:PRO:CB	1:A:552:GLN:HE21	1.94	0.80
1:B:40:ILE:CD1	1:B:57:THR:HG22	2.10	0.80
1:B:505:THR:HG22	1:B:506:HIS:H	1.45	0.80
1:A:275:GLY:HA3	1:A:359:GLY:O	1.81	0.80
1:A:295:ILE:O	1:A:298:PRO:HD2	1.81	0.80
1:B:156:GLU:HG3	1:B:161:ARG:CZ	2.11	0.80
1:B:277:GLN:HB3	1:B:357:LEU:HD12	1.62	0.80
1:A:277:GLN:HB3	1:A:357:LEU:HD12	1.62	0.80
1:B:295:ILE:O	1:B:298:PRO:HD2	1.81	0.80
1:B:459:THR:OG1	1:B:466:HIS:HB2	1.81	0.80
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.94	0.79
2:A:600:FAD:H51A	2:A:600:FAD:C8A	2.11	0.79
1:B:10:LEU:HD11	1:B:42:SER:HA	1.64	0.79
1:A:422:HIS:CE1	2:A:600:FAD:C8M	2.46	0.79
1:A:57:THR:O	1:A:70:LEU:HD12	1.83	0.79
1:A:378:ILE:O	1:A:381:VAL:HB	1.83	0.79
1:B:361:GLU:O	1:B:361:GLU:HG3	1.77	0.79
1:B:275:GLY:HA3	1:B:359:GLY:O	1.81	0.79
1:A:94:SER:HA	1:A:540:ILE:HD11	1.66	0.78
1:B:57:THR:O	1:B:70:LEU:HD12	1.83	0.78
1:B:378:ILE:O	1:B:381:VAL:HB	1.83	0.78
1:B:48:ASP:OD1	1:B:60:PRO:HA	1.84	0.78
1:A:377:ALA:O	1:A:379:PRO:HD3	1.84	0.78
1:A:132:GLU:HG2	1:A:133:VAL:N	1.99	0.78
1:A:10:LEU:HD11	1:A:42:SER:HA	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:O	1:A:89:LEU:HD13	1.85	0.77
1:A:479:ILE:O	1:A:483:LYS:HG3	1.84	0.77
1:B:377:ALA:O	1:B:379:PRO:HD3	1.84	0.77
1:A:431:VAL:HA	1:A:465:MET:HE2	1.64	0.77
1:B:134:ASN:OD1	1:B:137:GLY:N	2.17	0.77
1:A:361:GLU:O	1:A:361:GLU:HG3	1.77	0.77
1:B:132:GLU:HG2	1:B:133:VAL:N	1.99	0.77
1:A:32:VAL:HA	1:A:78:ARG:HD2	1.67	0.77
1:B:56:HIS:HA	1:B:111:ALA:HB1	1.67	0.77
1:B:479:ILE:O	1:B:483:LYS:HG3	1.84	0.77
1:B:85:SER:O	1:B:89:LEU:HD13	1.85	0.77
1:B:431:VAL:HA	1:B:465:MET:HE2	1.65	0.77
1:B:312:ARG:HH22	1:B:410:GLU:CD	1.93	0.76
2:B:600:FAD:H51A	2:B:600:FAD:C8A	2.11	0.76
1:A:357:LEU:HB3	1:A:364:ARG:HG2	1.66	0.76
1:A:48:ASP:OD1	1:A:60:PRO:HA	1.84	0.76
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.68	0.76
1:B:357:LEU:HB3	1:B:364:ARG:HG2	1.66	0.76
1:B:94:SER:HA	1:B:540:ILE:HD11	1.66	0.76
1:A:56:HIS:HA	1:A:111:ALA:HB1	1.66	0.76
1:A:134:ASN:OD1	1:A:137:GLY:N	2.17	0.75
1:A:183:ARG:NH2	1:B:247:GLY:O	2.20	0.75
1:A:443:THR:HA	1:A:491:LEU:CD2	2.17	0.75
1:B:32:VAL:HA	1:B:78:ARG:HD2	1.67	0.75
1:B:443:THR:HA	1:B:491:LEU:CD2	2.17	0.75
1:A:248:PRO:HD3	1:B:256:GLN:O	1.87	0.74
1:A:423:LEU:HD21	1:A:488:MET:CG	2.16	0.74
1:A:244:TYR:OH	1:B:195:MET:HG3	1.86	0.74
1:A:312:ARG:HH22	1:A:410:GLU:CD	1.93	0.74
1:B:423:LEU:HD21	1:B:488:MET:CG	2.16	0.74
1:A:79:ASN:HD21	1:A:81:ALA:HB3	1.52	0.74
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.23	0.74
1:B:79:ASN:HD21	1:B:81:ALA:HB3	1.52	0.74
1:B:527:PHE:CE2	1:B:531:LEU:HD11	2.23	0.74
2:B:600:FAD:N5	3:B:601:EUG:H7	2.02	0.74
2:A:600:FAD:N5	3:A:601:EUG:H7	2.02	0.74
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.70	0.74
1:A:284:PRO:HD2	1:A:288:ASP:OD2	1.87	0.73
1:B:361:GLU:N	1:B:364:ARG:NH2	2.36	0.73
1:B:284:PRO:HD2	1:B:288:ASP:OD2	1.87	0.73
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ASN:H	1:B:474:ASN:ND2	1.86	0.73
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.68	0.73
1:A:339:LEU:HD12	1:A:350:ARG:CZ	2.19	0.73
1:A:205:ALA:CA	1:A:541:ILE:HD11	2.19	0.73
1:A:487:LEU:HD11	1:A:491:LEU:HD11	1.70	0.73
1:B:102:ILE:CG1	1:B:175:SER:HB2	2.19	0.73
1:A:102:ILE:CG1	1:A:175:SER:HB2	2.19	0.72
1:A:419:ASN:H	1:A:474:ASN:ND2	1.86	0.72
1:B:52:MET:O	1:B:53:LYS:HG3	1.90	0.72
1:A:187:TYR:O	1:A:307:ASN:HB2	1.89	0.72
1:B:187:TYR:O	1:B:307:ASN:HB2	1.89	0.72
1:A:487:LEU:HG	1:A:491:LEU:HD12	1.72	0.72
1:B:96:PRO:O	1:B:97:LEU:HD23	1.89	0.72
1:B:425:PHE:CZ	1:B:427:PRO:HG3	2.25	0.72
1:A:418:PRO:HD2	1:A:474:ASN:HD22	1.53	0.72
1:B:223:PRO:HG2	1:B:224:GLU:OE2	1.89	0.72
1:B:418:PRO:HD2	1:B:474:ASN:HD22	1.53	0.72
1:B:487:LEU:HD11	1:B:491:LEU:HD11	1.71	0.72
1:A:425:PHE:CZ	1:A:427:PRO:HG3	2.25	0.72
1:B:339:LEU:HD12	1:B:350:ARG:CZ	2.19	0.72
1:A:223:PRO:HG2	1:A:224:GLU:OE2	1.89	0.71
1:A:550:PRO:HG2	1:A:553:TYR:CD1	2.26	0.71
1:B:205:ALA:CA	1:B:541:ILE:HD11	2.19	0.71
1:B:13:PRO:HG2	1:B:16:LEU:HB2	1.72	0.71
1:A:183:ARG:HD2	1:B:244:TYR:CD2	2.26	0.71
1:B:425:PHE:HB2	1:B:488:MET:HE3	1.72	0.71
2:B:600:FAD:C5X	3:B:601:EUG:H7	2.21	0.71
1:B:217:LEU:O	1:B:236:SER:HB2	1.91	0.71
1:A:52:MET:O	1:A:53:LYS:HG3	1.90	0.71
1:A:425:PHE:HB2	1:A:488:MET:HE3	1.72	0.71
1:A:96:PRO:O	1:A:97:LEU:HD23	1.89	0.71
1:A:217:LEU:O	1:A:236:SER:HB2	1.91	0.71
1:A:238:ILE:HG21	1:B:428:ILE:HG21	1.72	0.71
1:A:299:LEU:HB2	1:A:305:LEU:HD12	1.72	0.71
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.70	0.71
1:B:18:LEU:HD12	1:B:21:PHE:HB3	1.73	0.71
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.73	0.71
2:A:600:FAD:C5X	3:A:601:EUG:H7	2.21	0.71
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.26	0.71
1:B:61:HIS:ND1	1:B:422:HIS:ND1	2.39	0.71
1:A:21:PHE:O	1:A:25:ILE:HG22	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.73	0.70
1:B:487:LEU:HG	1:B:491:LEU:HD12	1.72	0.70
1:B:21:PHE:O	1:B:25:ILE:HG22	1.91	0.70
1:B:391:GLU:HA	1:B:396:ARG:HD2	1.73	0.70
1:B:550:PRO:HG2	1:B:553:TYR:CD1	2.26	0.70
1:B:292:ALA:O	1:B:296:ILE:HG13	1.91	0.70
1:B:299:LEU:HB2	1:B:305:LEU:HD12	1.72	0.70
1:A:391:GLU:HA	1:A:396:ARG:HD2	1.73	0.70
1:A:61:HIS:ND1	1:A:422:HIS:ND1	2.39	0.69
1:A:292:ALA:O	1:A:296:ILE:HG13	1.91	0.69
1:A:361:GLU:N	1:A:364:ARG:NH2	2.35	0.69
1:A:13:PRO:HG2	1:A:16:LEU:HB2	1.72	0.69
1:A:59:ASP:N	1:A:112:ALA:HB2	2.07	0.69
1:A:419:ASN:N	1:A:474:ASN:ND2	2.40	0.69
1:B:59:ASP:N	1:B:112:ALA:HB2	2.07	0.69
1:B:425:PHE:C	1:B:427:PRO:HD3	2.17	0.69
1:A:55:THR:HG21	1:A:58:HIS:CE1	2.26	0.69
1:B:214:MET:HB2	1:B:239:ALA:HA	1.74	0.69
1:A:164:LEU:HD23	1:A:271:PRO:HA	1.74	0.69
1:B:224:GLU:CD	1:B:224:GLU:H	2.01	0.69
1:B:426:SER:N	1:B:427:PRO:HD3	2.08	0.69
1:B:464:GLU:HG2	1:B:465:MET:N	2.08	0.69
1:A:18:LEU:HD12	1:A:21:PHE:HB3	1.73	0.69
1:A:195:MET:HG3	1:B:244:TYR:OH	1.93	0.68
1:B:419:ASN:N	1:B:474:ASN:ND2	2.40	0.68
1:A:222:ARG:HB2	1:A:223:PRO:HD2	1.74	0.68
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.75	0.68
1:A:224:GLU:CD	1:A:224:GLU:H	2.01	0.68
1:B:494:ASP:O	1:B:498:ASN:ND2	2.26	0.68
1:A:61:HIS:CE1	1:A:422:HIS:HD1	2.11	0.68
1:A:464:GLU:HG2	1:A:465:MET:N	2.08	0.68
1:B:48:ASP:OD1	1:B:58:HIS:NE2	2.24	0.68
1:B:61:HIS:CE1	1:B:422:HIS:HD1	2.11	0.68
1:B:502:GLU:N	1:B:502:GLU:OE1	2.26	0.68
1:A:425:PHE:C	1:A:427:PRO:HD3	2.17	0.68
1:B:222:ARG:HB2	1:B:223:PRO:HD2	1.74	0.68
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.75	0.68
1:B:316:LEU:O	1:B:320:VAL:HG23	1.94	0.68
1:A:214:MET:HB2	1:A:239:ALA:HA	1.74	0.68
1:A:427:PRO:HD2	1:A:467:HIS:O	1.93	0.68
1:B:164:LEU:HD23	1:B:271:PRO:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:PRO:HD2	1:B:467:HIS:O	1.93	0.68
1:A:316:LEU:O	1:A:320:VAL:HG23	1.94	0.68
1:A:494:ASP:O	1:A:498:ASN:ND2	2.26	0.68
1:A:502:GLU:N	1:A:502:GLU:OE1	2.26	0.68
1:A:324:LYS:HA	1:A:416:TRP:CH2	2.29	0.68
1:B:112:ALA:O	1:B:507:LEU:HD11	1.94	0.67
1:A:506:HIS:CE1	1:A:508:ALA:H	2.13	0.67
1:A:147:THR:O	1:A:150:ASP:HB2	1.95	0.67
1:A:200:MET:CE	1:A:251:ASP:HB3	2.25	0.67
1:A:426:SER:N	1:A:427:PRO:HD3	2.08	0.67
1:B:147:THR:O	1:B:150:ASP:HB2	1.95	0.67
1:B:324:LYS:HA	1:B:416:TRP:CH2	2.29	0.67
1:B:422:HIS:CD2	2:B:600:FAD:C8M	2.73	0.67
1:A:422:HIS:CD2	2:A:600:FAD:C8M	2.73	0.67
1:A:112:ALA:O	1:A:507:LEU:HD11	1.94	0.67
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.30	0.67
1:A:522:SER:O	1:A:526:ARG:HG2	1.95	0.66
1:B:152:HIS:CE1	1:B:161:ARG:HH21	2.13	0.66
1:A:238:ILE:HG21	1:B:428:ILE:CG2	2.25	0.66
1:B:205:ALA:HB2	1:B:541:ILE:HD12	1.77	0.66
1:B:295:ILE:HD12	1:B:378:ILE:HD11	1.77	0.66
1:B:486:TRP:O	1:B:490:THR:OG1	2.14	0.66
1:B:506:HIS:CE1	1:B:508:ALA:H	2.12	0.66
1:B:522:SER:O	1:B:526:ARG:HG2	1.95	0.66
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.30	0.66
1:A:95:PHE:HD1	1:A:96:PRO:CD	2.09	0.66
1:A:457:THR:CG2	1:A:458:PHE:H	2.01	0.66
1:B:351:TRP:O	1:B:352:ASN:ND2	2.29	0.66
1:B:200:MET:CE	1:B:251:ASP:HB3	2.25	0.66
1:B:95:PHE:HD1	1:B:96:PRO:CD	2.09	0.66
1:B:95:PHE:O	1:B:540:ILE:HD12	1.96	0.66
1:B:270:MET:CG	1:B:271:PRO:HD2	2.26	0.66
1:B:283:LEU:HB2	1:B:351:TRP:HB2	1.78	0.66
1:A:205:ALA:HB2	1:A:541:ILE:HD12	1.77	0.65
1:A:230:PRO:HA	1:A:233:GLN:CD	2.21	0.65
1:A:486:TRP:O	1:A:490:THR:OG1	2.14	0.65
1:A:425:PHE:CD1	1:A:488:MET:HE1	2.31	0.65
1:A:479:ILE:HG22	1:A:483:LYS:CE	2.27	0.65
1:B:289:LEU:HD23	1:B:437:MET:SD	2.37	0.65
1:A:95:PHE:O	1:A:540:ILE:HD12	1.96	0.65
1:A:270:MET:CG	1:A:271:PRO:HD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:HIS:CE1	1:A:161:ARG:HH21	2.13	0.65
1:A:200:MET:HE2	1:A:251:ASP:HB3	1.77	0.65
1:A:289:LEU:HD23	1:A:437:MET:SD	2.37	0.65
1:B:200:MET:HE2	1:B:251:ASP:HB3	1.77	0.65
1:A:479:ILE:HG22	1:A:483:LYS:HE3	1.77	0.65
1:A:295:ILE:HD12	1:A:378:ILE:HD11	1.77	0.65
1:A:351:TRP:O	1:A:352:ASN:ND2	2.29	0.65
1:B:149:HIS:O	1:B:153:ASN:ND2	2.29	0.65
1:A:136:GLU:CD	1:A:136:GLU:H	2.05	0.65
1:B:507:LEU:HA	1:B:510:MET:CE	2.18	0.65
1:B:230:PRO:HA	1:B:233:GLN:CD	2.21	0.64
1:A:312:ARG:NH2	1:A:410:GLU:OE2	2.30	0.64
1:A:555:HIS:CB	1:A:559:LYS:HE3	2.27	0.64
1:B:312:ARG:NH2	1:B:410:GLU:OE2	2.30	0.64
1:B:479:ILE:HG22	1:B:483:LYS:CE	2.27	0.64
1:B:91:ASN:HD22	1:B:538:ASN:HD22	1.45	0.64
1:B:96:PRO:C	1:B:97:LEU:HD23	2.22	0.64
1:A:96:PRO:C	1:A:97:LEU:HD23	2.22	0.64
1:A:95:PHE:HD1	1:A:96:PRO:N	1.96	0.64
1:B:425:PHE:CD1	1:B:488:MET:HE1	2.32	0.64
1:A:108:TYR:O	1:A:506:HIS:HA	1.98	0.64
1:A:283:LEU:HB2	1:A:351:TRP:HB2	1.78	0.64
1:B:506:HIS:ND1	1:B:508:ALA:N	2.39	0.64
1:B:550:PRO:HG2	1:B:553:TYR:HD1	1.62	0.64
1:B:95:PHE:HD1	1:B:96:PRO:N	1.96	0.64
1:B:151:LEU:HD12	1:B:151:LEU:O	1.98	0.64
1:B:555:HIS:CB	1:B:559:LYS:HE3	2.27	0.64
1:A:91:ASN:HD22	1:A:538:ASN:HD22	1.45	0.64
1:B:136:GLU:H	1:B:136:GLU:CD	2.05	0.64
1:A:149:HIS:O	1:A:153:ASN:ND2	2.30	0.63
1:A:269:LEU:O	1:B:463:ARG:NH2	2.31	0.63
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.80	0.63
1:B:309:PRO:HB2	1:B:353:PHE:CE1	2.33	0.63
1:B:479:ILE:HG22	1:B:483:LYS:HE3	1.77	0.63
1:A:309:PRO:HB2	1:A:353:PHE:CE1	2.33	0.63
1:B:349:GLY:H	1:B:352:ASN:HD21	1.47	0.63
1:B:411:LEU:O	1:B:414:ILE:HB	1.99	0.63
1:A:48:ASP:OD1	1:A:58:HIS:NE2	2.24	0.63
1:A:151:LEU:HD12	1:A:151:LEU:O	1.98	0.63
1:A:559:LYS:O	1:A:560:LEU:HG	1.99	0.63
1:B:393:SER:OG	1:B:396:ARG:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:HIS:HB2	1:A:265:ILE:HD11	1.81	0.63
1:A:349:GLY:H	1:A:352:ASN:HD21	1.47	0.63
1:A:185:VAL:HG12	1:A:186:GLY:N	2.15	0.62
1:A:425:PHE:HB2	1:A:488:MET:HE1	1.80	0.62
1:B:79:ASN:HD22	1:B:81:ALA:H	1.46	0.62
1:A:507:LEU:HA	1:A:510:MET:CE	2.18	0.62
1:A:79:ASN:HD22	1:A:81:ALA:H	1.46	0.62
1:A:256:GLN:O	1:B:248:PRO:HD3	1.98	0.62
1:A:393:SER:OG	1:A:396:ARG:HG3	1.99	0.62
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.80	0.62
1:B:108:TYR:O	1:B:506:HIS:HA	1.98	0.62
1:A:411:LEU:O	1:A:414:ILE:HB	1.99	0.62
1:B:324:LYS:HA	1:B:416:TRP:CZ3	2.34	0.62
1:B:559:LYS:O	1:B:560:LEU:HG	1.99	0.62
1:B:10:LEU:HD11	1:B:42:SER:CA	2.30	0.62
1:B:24:PHE:CE1	1:B:28:ILE:HD12	2.34	0.62
1:B:280:LEU:HB2	1:B:395:LEU:HD13	1.81	0.62
1:A:24:PHE:CE1	1:A:28:ILE:HD12	2.34	0.62
1:A:148:TYR:HB2	1:A:172:GLY:O	2.00	0.62
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.00	0.62
1:B:425:PHE:HB2	1:B:488:MET:HE1	1.80	0.62
1:A:315:LEU:HA	1:A:318:ALA:HB3	1.82	0.62
1:A:550:PRO:HG2	1:A:553:TYR:HD1	1.62	0.62
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.35	0.62
1:B:148:TYR:HB2	1:B:172:GLY:O	2.00	0.62
1:B:197:HIS:HB2	1:B:265:ILE:HD11	1.81	0.62
1:A:280:LEU:HB2	1:A:395:LEU:HD13	1.81	0.61
1:A:506:HIS:ND1	1:A:508:ALA:N	2.39	0.61
1:B:6:GLU:N	1:B:39:VAL:HG21	2.15	0.61
1:B:189:PRO:HA	1:B:307:ASN:HA	1.82	0.61
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.35	0.61
1:A:485:GLN:O	1:A:489:ARG:HG3	2.00	0.61
1:B:285:LYS:O	1:B:288:ASP:HB2	2.00	0.61
1:A:6:GLU:N	1:A:39:VAL:HG21	2.15	0.61
1:B:485:GLN:O	1:B:489:ARG:HG3	2.00	0.61
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.00	0.61
1:A:189:PRO:HA	1:A:307:ASN:HA	1.82	0.61
1:A:505:THR:HG22	1:A:506:HIS:N	2.15	0.61
1:B:61:HIS:CE1	1:B:422:HIS:ND1	2.69	0.61
1:B:149:HIS:O	1:B:152:HIS:HB3	2.01	0.61
1:B:505:THR:HG22	1:B:506:HIS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD11	1:A:42:SER:CA	2.30	0.61
1:A:61:HIS:CE1	1:A:422:HIS:ND1	2.69	0.61
1:A:285:LYS:O	1:A:288:ASP:HB2	2.00	0.61
1:A:316:LEU:HD11	1:A:413:TRP:NE1	2.16	0.61
1:A:503:TYR:OH	3:A:601:EUG:O4	2.15	0.61
1:B:185:VAL:HG12	1:B:186:GLY:N	2.15	0.61
1:B:416:TRP:HA	1:B:416:TRP:CE3	2.36	0.61
1:A:39:VAL:HG12	1:A:40:ILE:H	1.66	0.61
1:A:324:LYS:HA	1:A:416:TRP:CZ3	2.34	0.61
1:A:156:GLU:C	1:A:158:ASN:H	2.09	0.61
1:A:426:SER:O	1:A:502:GLU:HA	2.01	0.61
1:B:315:LEU:HA	1:B:318:ALA:HB3	1.82	0.60
1:B:39:VAL:HG12	1:B:40:ILE:H	1.66	0.60
1:B:156:GLU:C	1:B:158:ASN:H	2.09	0.60
1:B:316:LEU:HD11	1:B:413:TRP:NE1	2.16	0.60
1:A:24:PHE:CD2	1:A:95:PHE:HD2	2.20	0.60
1:B:82:ASP:O	1:B:86:ILE:HG13	2.01	0.60
1:B:129:ARG:HB2	1:B:131:LEU:HD21	1.83	0.60
1:A:149:HIS:O	1:A:152:HIS:HB3	2.01	0.60
1:A:549:TRP:CZ2	1:A:558:TRP:HB3	2.37	0.60
1:A:445:LYS:O	1:A:449:GLU:HG3	2.02	0.60
1:B:24:PHE:CD2	1:B:95:PHE:HD2	2.20	0.60
1:B:37:VAL:HG12	1:B:38:GLU:N	2.17	0.60
1:B:164:LEU:C	1:B:165:TRP:HD1	2.10	0.60
1:B:549:TRP:CZ2	1:B:558:TRP:HB3	2.37	0.60
1:B:426:SER:O	1:B:502:GLU:HA	2.01	0.60
1:A:37:VAL:HG12	1:A:38:GLU:N	2.17	0.59
1:A:478:LEU:H	1:A:478:LEU:CD1	2.12	0.59
1:B:445:LYS:O	1:B:449:GLU:HG3	2.02	0.59
1:A:129:ARG:HB2	1:A:131:LEU:HD21	1.83	0.59
1:A:554:SER:HB3	1:A:557:THR:HB	1.84	0.59
1:A:82:ASP:O	1:A:86:ILE:HG13	2.01	0.59
1:A:242:PHE:CD1	1:A:243:PRO:HD2	2.37	0.59
1:A:416:TRP:HA	1:A:416:TRP:CE3	2.36	0.59
1:A:39:VAL:HG12	1:A:40:ILE:N	2.17	0.59
1:A:164:LEU:C	1:A:165:TRP:HD1	2.10	0.59
1:A:299:LEU:HB2	1:A:305:LEU:CD1	2.33	0.59
1:A:243:PRO:HD2	1:A:244:TYR:H	1.68	0.59
1:B:242:PHE:CD1	1:B:243:PRO:HD2	2.37	0.59
1:A:217:LEU:HD13	1:A:217:LEU:C	2.28	0.58
1:B:217:LEU:C	1:B:217:LEU:HD13	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:HD12	1:B:351:TRP:HB3	1.85	0.58
1:A:332:GLU:CB	1:A:333:PRO:HD2	2.33	0.58
1:B:243:PRO:HD2	1:B:244:TYR:H	1.68	0.58
1:B:554:SER:HB3	1:B:557:THR:HB	1.84	0.58
1:A:230:PRO:HD2	1:A:231:GLU:H	1.68	0.58
1:A:411:LEU:HA	1:A:414:ILE:HD12	1.86	0.58
1:B:154:TYR:HD1	1:B:155:LEU:HD23	1.68	0.58
1:B:222:ARG:CB	1:B:223:PRO:HD2	2.30	0.58
1:B:299:LEU:HB2	1:B:305:LEU:CD1	2.33	0.58
1:A:525:LEU:HD12	1:A:525:LEU:O	2.04	0.58
1:B:230:PRO:HD2	1:B:231:GLU:H	1.68	0.58
1:B:475:LYS:O	1:B:481:LYS:HD2	2.04	0.58
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.04	0.58
1:A:154:TYR:HD1	1:A:155:LEU:HD23	1.68	0.58
1:B:35:GLU:HA	1:B:35:GLU:OE1	2.04	0.58
1:B:51:TYR:CZ	1:B:104:ARG:HD3	2.39	0.58
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.33	0.58
1:A:272:ASN:OD1	1:A:273:PRO:HD2	2.04	0.57
1:A:475:LYS:O	1:A:481:LYS:HD2	2.04	0.57
1:B:503:TYR:OH	3:B:601:EUG:O4	2.15	0.57
1:A:24:PHE:CE1	1:A:28:ILE:CD1	2.87	0.57
1:A:51:TYR:CZ	1:A:104:ARG:HD3	2.39	0.57
1:A:61:HIS:CE1	1:A:422:HIS:CE1	2.93	0.57
1:B:13:PRO:HD3	1:B:117:GLY:O	2.04	0.57
1:B:383:PHE:C	1:B:384:TYR:CD1	2.82	0.57
1:A:65:ASP:N	1:A:65:ASP:OD1	2.37	0.57
1:A:283:LEU:HD12	1:A:351:TRP:HB3	1.85	0.57
1:B:39:VAL:HG12	1:B:40:ILE:N	2.17	0.57
1:B:83:VAL:O	1:B:87:VAL:HG23	2.04	0.57
1:A:13:PRO:HD3	1:A:117:GLY:O	2.04	0.57
1:B:411:LEU:HA	1:B:414:ILE:HD12	1.86	0.57
1:B:24:PHE:CE1	1:B:28:ILE:CD1	2.88	0.57
1:B:393:SER:O	1:B:396:ARG:HB2	2.05	0.57
1:B:421:ALA:O	1:B:472:VAL:HA	2.05	0.57
1:A:83:VAL:O	1:A:87:VAL:HG23	2.04	0.57
1:A:332:GLU:CG	1:A:333:PRO:HD2	2.35	0.57
1:A:383:PHE:C	1:A:384:TYR:CD1	2.82	0.57
1:A:222:ARG:CB	1:A:223:PRO:HD2	2.30	0.56
1:A:280:LEU:O	1:A:280:LEU:HG	2.05	0.56
1:B:165:TRP:HB2	1:B:270:MET:O	2.05	0.56
1:B:525:LEU:HD12	1:B:525:LEU:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:HA	1:A:58:HIS:CE1	2.40	0.56
1:A:165:TRP:HB2	1:A:270:MET:O	2.05	0.56
1:A:393:SER:O	1:A:396:ARG:HB2	2.05	0.56
1:A:421:ALA:O	1:A:472:VAL:HA	2.05	0.56
1:A:448:GLN:O	1:A:451:GLY:N	2.33	0.56
1:B:444:LYS:O	1:B:447:CYS:N	2.39	0.56
1:B:48:ASP:HA	1:B:58:HIS:CE1	2.40	0.56
1:B:61:HIS:CE1	1:B:422:HIS:CE1	2.93	0.56
1:B:332:GLU:CG	1:B:333:PRO:HD2	2.35	0.56
1:B:389:THR:HB	1:B:390:PRO:HD2	1.86	0.56
1:B:418:PRO:HB2	1:B:474:ASN:ND2	2.21	0.56
1:B:478:LEU:H	1:B:478:LEU:CD1	2.12	0.56
1:A:223:PRO:O	1:A:226:MET:HG2	2.06	0.56
1:A:389:THR:HB	1:A:390:PRO:CD	2.36	0.56
1:B:389:THR:HB	1:B:390:PRO:CD	2.36	0.56
1:A:237:LYS:NZ	1:B:500:TRP:CZ2	2.73	0.56
1:A:389:THR:HB	1:A:390:PRO:HD2	1.86	0.56
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.87	0.56
1:B:223:PRO:O	1:B:226:MET:HG2	2.06	0.56
1:A:10:LEU:HD13	1:A:40:ILE:O	2.06	0.56
1:A:545:LYS:HG3	1:A:546:SER:N	2.20	0.56
1:A:27:ASP:N	1:A:27:ASP:OD1	2.39	0.56
1:B:229:LYS:HB3	1:B:230:PRO:CD	2.36	0.56
1:A:444:LYS:O	1:A:447:CYS:N	2.39	0.56
1:A:494:ASP:O	1:A:497:ALA:HB3	2.06	0.56
1:B:10:LEU:HD13	1:B:40:ILE:O	2.06	0.56
1:A:270:MET:HG3	1:A:271:PRO:HD2	1.87	0.55
1:B:59:ASP:O	1:B:62:HIS:HB3	2.07	0.55
1:B:65:ASP:OD1	1:B:65:ASP:N	2.37	0.55
1:B:494:ASP:O	1:B:497:ALA:HB3	2.06	0.55
1:B:555:HIS:HB3	1:B:559:LYS:CE	2.37	0.55
1:A:201:GLU:HG2	1:A:202:VAL:N	2.20	0.55
1:B:270:MET:HG3	1:B:271:PRO:HD2	1.87	0.55
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.41	0.55
1:A:59:ASP:O	1:A:62:HIS:HB3	2.07	0.55
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.41	0.55
1:A:35:GLU:OE1	1:A:35:GLU:HA	2.04	0.55
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.89	0.55
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.42	0.55
1:B:171:LEU:HD21	2:B:600:FAD:HM72	1.88	0.55
1:B:403:GLN:HG3	1:B:405:ILE:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:LYS:HG3	1:B:546:SER:N	2.20	0.55
1:A:223:PRO:HG2	1:A:224:GLU:CD	2.32	0.55
1:A:418:PRO:HB2	1:A:474:ASN:ND2	2.21	0.55
1:B:276:TYR:OH	1:B:399:ASP:O	2.19	0.55
1:A:229:LYS:HB3	1:A:230:PRO:CD	2.36	0.55
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.42	0.55
1:A:75:VAL:O	1:A:122:ASP:N	2.37	0.55
1:A:361:GLU:N	1:A:362:PRO:HD2	2.22	0.55
1:A:18:LEU:HD12	1:A:18:LEU:O	2.07	0.55
1:A:270:MET:HG2	1:A:271:PRO:HD2	1.88	0.54
1:A:317:ASP:O	1:A:321:LEU:HG	2.08	0.54
1:A:463:ARG:NH2	1:B:269:LEU:O	2.40	0.54
1:B:201:GLU:HG2	1:B:202:VAL:N	2.19	0.54
1:B:270:MET:HG2	1:B:271:PRO:HD2	1.88	0.54
1:B:280:LEU:O	1:B:280:LEU:HG	2.05	0.54
1:A:422:HIS:CD2	1:A:424:PHE:CZ	2.95	0.54
1:A:554:SER:HB3	1:A:557:THR:CB	2.37	0.54
1:B:97:LEU:CD2	1:B:119:VAL:HB	2.37	0.54
1:A:555:HIS:HB3	1:A:559:LYS:CE	2.37	0.54
1:B:223:PRO:HG2	1:B:224:GLU:CD	2.32	0.54
1:B:312:ARG:NH1	1:B:317:ASP:OD1	2.40	0.54
1:B:422:HIS:CD2	1:B:424:PHE:CZ	2.95	0.54
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.42	0.54
1:B:89:LEU:N	1:B:89:LEU:CD1	2.71	0.54
1:B:361:GLU:N	1:B:362:PRO:HD2	2.22	0.54
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.87	0.54
1:B:478:LEU:O	1:B:482:ARG:HG3	2.08	0.54
1:A:7:PHE:HB3	1:A:8:ARG:HG3	1.89	0.54
1:A:171:LEU:HD21	2:A:600:FAD:HM72	1.88	0.54
1:A:229:LYS:O	1:A:233:GLN:HG3	2.08	0.54
1:B:7:PHE:HB3	1:B:8:ARG:HG3	1.89	0.54
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.42	0.54
1:B:312:ARG:HD2	1:B:354:TYR:CE1	2.43	0.54
1:B:506:HIS:ND1	1:B:507:LEU:N	2.56	0.54
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.89	0.54
1:B:58:HIS:C	1:B:112:ALA:HB2	2.32	0.54
1:A:312:ARG:HD2	1:A:354:TYR:CE1	2.43	0.54
1:A:506:HIS:ND1	1:A:507:LEU:N	2.56	0.54
1:B:229:LYS:O	1:B:233:GLN:HG3	2.08	0.54
1:B:317:ASP:O	1:B:321:LEU:HG	2.08	0.54
1:B:533:ASN:OD1	1:B:552:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:CD2	1:A:119:VAL:HB	2.37	0.54
1:B:221:LYS:O	1:B:222:ARG:HB3	2.08	0.54
1:A:505:THR:CG2	1:A:506:HIS:N	2.71	0.54
1:B:18:LEU:HD12	1:B:18:LEU:O	2.07	0.54
1:B:103:GLY:C	1:B:105:ASN:H	2.16	0.54
1:A:58:HIS:C	1:A:112:ALA:HB2	2.32	0.53
1:A:296:ILE:HG21	1:A:460:VAL:HG11	1.90	0.53
1:A:221:LYS:O	1:A:222:ARG:HB3	2.08	0.53
1:A:403:GLN:HG3	1:A:405:ILE:HG13	1.89	0.53
1:B:554:SER:HB3	1:B:557:THR:CB	2.37	0.53
1:A:79:ASN:ND2	1:A:81:ALA:H	2.06	0.53
1:A:464:GLU:OE2	1:A:466:HIS:ND1	2.41	0.53
1:A:103:GLY:C	1:A:105:ASN:H	2.16	0.53
1:A:533:ASN:OD1	1:A:552:GLN:NE2	2.41	0.53
1:A:205:ALA:CB	1:A:536:ASP:HB2	2.39	0.53
1:A:478:LEU:O	1:A:482:ARG:HG3	2.08	0.53
1:B:27:ASP:OD1	1:B:27:ASP:N	2.39	0.53
1:B:149:HIS:C	1:B:153:ASN:HD22	2.17	0.53
1:B:194:TRP:O	1:B:197:HIS:CD2	2.62	0.53
1:B:253:LEU:O	1:B:257:SER:OG	2.25	0.53
1:A:89:LEU:N	1:A:89:LEU:CD1	2.71	0.53
1:A:136:GLU:OE1	1:A:136:GLU:N	2.34	0.53
1:B:23:GLU:O	1:B:27:ASP:OD1	2.27	0.53
1:B:422:HIS:NE2	2:B:600:FAD:C8	2.64	0.53
1:B:422:HIS:HD2	1:B:424:PHE:CZ	2.27	0.53
1:A:7:PHE:HA	1:A:22:ASN:OD1	2.09	0.53
1:A:23:GLU:O	1:A:27:ASP:OD1	2.27	0.53
1:A:495:CYS:HB2	4:A:605:HOH:O	2.07	0.53
1:A:509:PHE:O	1:A:513:ILE:HG13	2.09	0.53
1:B:205:ALA:CB	1:B:536:ASP:HB2	2.39	0.53
1:A:194:TRP:O	1:A:197:HIS:CD2	2.62	0.53
1:A:422:HIS:HD2	1:A:424:PHE:CZ	2.27	0.53
1:B:390:PRO:O	1:B:393:SER:HB3	2.09	0.53
1:B:509:PHE:O	1:B:513:ILE:HG13	2.09	0.53
1:A:390:PRO:O	1:A:393:SER:HB3	2.09	0.53
1:B:79:ASN:ND2	1:B:81:ALA:H	2.06	0.53
1:A:160:LEU:O	1:A:163:LYS:N	2.37	0.53
1:A:419:ASN:O	1:A:475:LYS:N	2.38	0.53
1:A:472:VAL:HG12	1:A:473:PHE:N	2.24	0.53
1:B:62:HIS:O	1:B:62:HIS:ND1	2.39	0.53
1:B:194:TRP:O	1:B:197:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:C	1:A:153:ASN:HD22	2.17	0.52
1:A:165:TRP:N	1:A:270:MET:O	2.39	0.52
1:A:247:GLY:HA2	1:B:546:SER:OG	2.09	0.52
1:B:7:PHE:HA	1:B:22:ASN:OD1	2.09	0.52
1:B:349:GLY:N	1:B:352:ASN:HD21	2.07	0.52
1:B:419:ASN:O	1:B:475:LYS:N	2.38	0.52
1:A:55:THR:HG21	1:A:58:HIS:ND1	2.25	0.52
1:A:62:HIS:O	1:A:62:HIS:ND1	2.39	0.52
1:A:194:TRP:O	1:A:197:HIS:HD2	1.91	0.52
1:A:349:GLY:N	1:A:352:ASN:HD21	2.07	0.52
1:B:108:TYR:HD1	1:B:505:THR:C	2.17	0.52
1:B:457:THR:CG2	1:B:458:PHE:H	2.01	0.52
1:B:464:GLU:OE2	1:B:466:HIS:ND1	2.41	0.52
1:B:165:TRP:N	1:B:270:MET:O	2.39	0.52
1:B:296:ILE:HG21	1:B:460:VAL:HG11	1.90	0.52
1:A:369:GLU:O	1:A:373:ASP:HB3	2.10	0.52
1:B:369:GLU:O	1:B:373:ASP:HB3	2.10	0.52
1:A:108:TYR:HD1	1:A:505:THR:C	2.17	0.52
1:B:371:ILE:O	1:B:374:ALA:HB3	2.10	0.52
1:B:243:PRO:CD	1:B:244:TYR:H	2.23	0.52
1:A:243:PRO:CD	1:A:244:TYR:H	2.23	0.52
1:A:312:ARG:NH1	1:A:317:ASP:OD1	2.40	0.52
1:A:371:ILE:O	1:A:374:ALA:HB3	2.10	0.52
1:B:156:GLU:O	1:B:158:ASN:N	2.43	0.52
1:B:55:THR:HG21	1:B:58:HIS:ND1	2.25	0.52
1:A:132:GLU:HG2	1:A:133:VAL:H	1.75	0.51
1:A:323:ASP:OD1	1:A:326:SER:HB3	2.10	0.51
1:B:515:GLU:OE1	1:B:515:GLU:HA	2.11	0.51
1:B:494:ASP:C	1:B:498:ASN:HD22	2.18	0.51
1:B:323:ASP:OD1	1:B:326:SER:HB3	2.10	0.51
1:A:409:ASP:HA	1:A:412:LYS:HE3	1.92	0.51
1:A:505:THR:HG21	1:A:509:PHE:HB2	1.91	0.51
1:B:472:VAL:HG12	1:B:473:PHE:N	2.24	0.51
1:A:414:ILE:HD11	2:A:600:FAD:HM73	1.93	0.51
1:B:442:VAL:O	1:B:445:LYS:HB3	2.11	0.51
1:B:200:MET:O	1:B:211:ARG:HA	2.11	0.51
1:B:409:ASP:N	1:B:409:ASP:OD1	2.44	0.51
1:B:433:GLY:O	1:B:437:MET:HB2	2.11	0.51
1:A:411:LEU:HA	1:A:414:ILE:CD1	2.41	0.51
1:A:533:ASN:HD21	1:A:551:SER:H	1.59	0.51
1:B:95:PHE:CD1	1:B:96:PRO:CD	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:C	1:B:165:TRP:CD1	2.89	0.51
1:B:300:ARG:NH2	1:B:308:VAL:HA	2.18	0.51
1:B:418:PRO:CD	1:B:474:ASN:HD22	2.22	0.51
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.91	0.51
1:A:425:PHE:CE1	1:A:502:GLU:CG	2.94	0.51
1:A:433:GLY:O	1:A:437:MET:HB2	2.11	0.51
1:A:484:VAL:O	1:A:487:LEU:HB3	2.11	0.51
1:B:107:GLY:HA2	1:B:422:HIS:O	2.11	0.51
1:B:136:GLU:OE1	1:B:136:GLU:N	2.34	0.51
1:B:289:LEU:HB2	1:B:351:TRP:NE1	2.26	0.51
1:B:388:ASP:N	1:B:388:ASP:OD1	2.41	0.51
1:B:409:ASP:HA	1:B:412:LYS:HE3	1.92	0.51
1:B:425:PHE:CE1	1:B:502:GLU:CG	2.94	0.51
1:A:156:GLU:O	1:A:158:ASN:N	2.43	0.50
1:A:277:GLN:O	1:A:357:LEU:N	2.29	0.50
1:A:388:ASP:OD1	1:A:388:ASP:N	2.41	0.50
1:A:133:VAL:HG21	1:A:154:TYR:CZ	2.44	0.50
1:A:139:TYR:CD1	1:A:139:TYR:C	2.90	0.50
1:A:289:LEU:HB2	1:A:351:TRP:NE1	2.26	0.50
1:A:351:TRP:HA	1:A:351:TRP:CE3	2.47	0.50
1:A:164:LEU:C	1:A:165:TRP:CD1	2.89	0.50
1:A:300:ARG:HE	1:A:309:PRO:HD2	1.76	0.50
1:A:355:GLY:O	1:A:402:MET:HE1	2.12	0.50
1:A:442:VAL:O	1:A:445:LYS:HB3	2.11	0.50
1:A:459:THR:HG1	1:A:466:HIS:HB2	1.76	0.50
1:B:533:ASN:HD21	1:B:551:SER:H	1.59	0.50
1:A:371:ILE:O	1:A:374:ALA:N	2.44	0.50
1:B:179:ASN:OD1	1:B:184:GLY:HA3	2.11	0.50
1:B:414:ILE:HD11	2:B:600:FAD:HM73	1.93	0.50
1:A:22:ASN:HA	1:A:25:ILE:HG22	1.94	0.50
1:A:144:PRO:HA	1:A:177:LEU:HG	1.93	0.50
1:B:28:ILE:O	1:B:32:VAL:HG22	2.12	0.50
1:B:411:LEU:HA	1:B:414:ILE:CD1	2.41	0.50
1:B:448:GLN:O	1:B:451:GLY:N	2.33	0.50
1:A:24:PHE:CE2	1:A:95:PHE:CD2	3.00	0.50
1:A:349:GLY:CA	1:A:352:ASN:HD21	2.25	0.50
1:A:385:PHE:HB2	1:A:387:GLU:OE1	2.11	0.50
1:B:24:PHE:CE2	1:B:95:PHE:CD2	3.00	0.50
1:B:277:GLN:O	1:B:357:LEU:N	2.29	0.50
1:A:200:MET:O	1:A:211:ARG:HA	2.11	0.50
1:B:75:VAL:O	1:B:122:ASP:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LYS:HE2	1:B:334:LEU:HD21	1.94	0.50
1:B:351:TRP:CE3	1:B:351:TRP:HA	2.47	0.50
1:B:371:ILE:O	1:B:374:ALA:N	2.44	0.50
1:B:51:TYR:CE1	1:B:171:LEU:HD13	2.47	0.50
1:A:425:PHE:HE1	1:A:502:GLU:CG	2.25	0.50
1:B:144:PRO:HA	1:B:177:LEU:HG	1.93	0.50
1:B:385:PHE:HB2	1:B:387:GLU:OE1	2.11	0.50
1:B:484:VAL:O	1:B:487:LEU:HB3	2.11	0.50
1:A:107:GLY:HA2	1:A:422:HIS:O	2.11	0.49
1:A:179:ASN:OD1	1:A:184:GLY:HA3	2.11	0.49
1:B:139:TYR:CD1	1:B:139:TYR:C	2.90	0.49
1:B:205:ALA:HB2	1:B:541:ILE:CD1	2.42	0.49
1:A:205:ALA:HB2	1:A:541:ILE:CD1	2.42	0.49
1:B:132:GLU:HG2	1:B:133:VAL:H	1.75	0.49
1:B:155:LEU:O	1:B:160:LEU:N	2.40	0.49
1:B:279:TYR:HB3	1:B:385:PHE:CE1	2.47	0.49
1:A:152:HIS:CE1	1:A:161:ARG:NH2	2.79	0.49
1:A:279:TYR:HB3	1:A:385:PHE:CE1	2.47	0.49
1:A:409:ASP:OD1	1:A:409:ASP:N	2.44	0.49
1:A:10:LEU:HD11	1:A:41:SER:C	2.37	0.49
1:A:514:MET:HE2	1:A:546:SER:O	2.12	0.49
1:A:51:TYR:CE1	1:A:171:LEU:HD13	2.47	0.49
1:B:10:LEU:HD11	1:B:41:SER:C	2.37	0.49
1:B:133:VAL:HG21	1:B:154:TYR:CZ	2.44	0.49
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.42	0.49
1:B:349:GLY:CA	1:B:352:ASN:HD21	2.25	0.49
1:B:355:GLY:O	1:B:402:MET:HE1	2.12	0.49
1:B:22:ASN:HA	1:B:25:ILE:HG22	1.94	0.49
1:B:293:VAL:C	1:B:295:ILE:N	2.68	0.49
1:B:459:THR:HG1	1:B:466:HIS:HB2	1.76	0.49
1:A:28:ILE:O	1:A:32:VAL:HG22	2.12	0.49
1:A:428:ILE:HG21	1:B:238:ILE:HG21	1.93	0.49
1:B:217:LEU:HA	1:B:217:LEU:HD22	1.41	0.49
1:B:454:PHE:CD1	1:B:455:ILE:N	2.81	0.49
1:B:309:PRO:HB2	1:B:353:PHE:HE1	1.78	0.49
1:B:514:MET:HE2	1:B:546:SER:O	2.12	0.49
1:A:244:TYR:CD1	1:A:244:TYR:N	2.77	0.49
1:A:422:HIS:CD2	2:A:600:FAD:HM81	2.46	0.49
1:A:515:GLU:HA	1:A:515:GLU:OE1	2.11	0.49
1:A:526:ARG:NH1	1:A:529:GLU:OE1	2.46	0.49
1:B:186:GLY:O	1:B:191:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ARG:HE	1:B:309:PRO:HD2	1.76	0.49
1:B:526:ARG:NH1	1:B:529:GLU:OE1	2.46	0.49
1:A:324:LYS:HE2	1:A:334:LEU:HD21	1.94	0.49
1:A:243:PRO:CD	1:A:244:TYR:N	2.76	0.48
1:A:361:GLU:CA	1:A:364:ARG:NH2	2.76	0.48
1:A:454:PHE:CD1	1:A:455:ILE:N	2.81	0.48
1:A:478:LEU:HB2	1:A:479:ILE:HD12	1.95	0.48
1:B:14:PRO:C	1:B:16:LEU:N	2.68	0.48
1:B:147:THR:HG23	1:B:150:ASP:OD2	2.13	0.48
1:B:360:PRO:C	1:B:364:ARG:HH21	2.20	0.48
1:B:425:PHE:HE1	1:B:502:GLU:CG	2.25	0.48
1:A:186:GLY:O	1:A:191:GLY:HA3	2.13	0.48
1:A:535:VAL:C	1:A:537:PRO:HD3	2.38	0.48
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.48	0.48
1:A:321:LEU:HD12	1:A:346:LEU:CD2	2.43	0.48
1:A:422:HIS:NE2	2:A:600:FAD:C8	2.64	0.48
1:A:6:GLU:N	1:A:39:VAL:CG2	2.76	0.48
1:A:72:SER:HB3	1:A:117:GLY:C	2.39	0.48
1:A:147:THR:HG23	1:A:150:ASP:OD2	2.13	0.48
1:A:229:LYS:O	1:A:232:ASP:N	2.43	0.48
1:A:414:ILE:HD11	2:A:600:FAD:HM81	1.95	0.48
1:A:270:MET:HA	1:A:271:PRO:HD3	1.72	0.48
1:A:494:ASP:C	1:A:498:ASN:HD22	2.18	0.48
1:A:552:GLN:CD	1:A:552:GLN:H	2.22	0.48
1:B:167:ASP:OD2	1:B:191:GLY:N	2.47	0.48
1:B:321:LEU:HD12	1:B:346:LEU:CD2	2.43	0.48
1:B:361:GLU:CA	1:B:364:ARG:NH2	2.76	0.48
1:B:535:VAL:C	1:B:537:PRO:HD3	2.38	0.48
1:A:87:VAL:O	1:A:91:ASN:N	2.44	0.48
1:A:238:ILE:HD13	1:A:238:ILE:N	2.28	0.48
1:A:253:LEU:O	1:A:257:SER:OG	2.25	0.48
1:B:72:SER:HB3	1:B:117:GLY:C	2.39	0.48
1:B:158:ASN:O	1:B:160:LEU:HG	2.13	0.48
1:B:160:LEU:O	1:B:163:LYS:N	2.37	0.48
1:A:69:PHE:HB3	1:A:113:PRO:O	2.14	0.48
1:A:324:LYS:CE	1:A:334:LEU:HD21	2.44	0.48
1:A:463:ARG:HH21	1:B:138:ALA:CB	2.27	0.48
1:B:6:GLU:N	1:B:39:VAL:CG2	2.76	0.48
1:B:148:TYR:O	1:B:152:HIS:N	2.45	0.48
1:B:244:TYR:N	1:B:244:TYR:CD1	2.77	0.48
1:A:158:ASN:O	1:A:160:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:TYR:CE1	1:B:270:MET:HG3	2.48	0.48
1:A:472:VAL:HG12	1:A:473:PHE:H	1.79	0.48
1:A:53:LYS:HA	1:A:54:PRO:HD3	1.70	0.48
1:A:496:ALA:N	4:A:605:HOH:O	2.46	0.48
1:B:87:VAL:O	1:B:91:ASN:N	2.44	0.48
1:B:279:TYR:CD2	1:B:280:LEU:N	2.82	0.48
1:B:478:LEU:HB2	1:B:479:ILE:HD12	1.95	0.48
1:A:148:TYR:O	1:A:152:HIS:N	2.44	0.47
1:A:167:ASP:OD2	1:A:191:GLY:N	2.47	0.47
1:A:201:GLU:HA	1:A:210:LEU:O	2.14	0.47
1:A:217:LEU:HB2	1:B:517:TYR:CE1	2.50	0.47
1:A:268:TRP:O	1:A:269:LEU:HD23	2.13	0.47
1:B:24:PHE:CD2	1:B:95:PHE:CD2	3.01	0.47
1:B:201:GLU:HA	1:B:210:LEU:O	2.14	0.47
1:B:383:PHE:N	1:B:383:PHE:CD1	2.82	0.47
1:B:484:VAL:O	1:B:488:MET:N	2.31	0.47
1:B:99:PRO:HA	1:B:121:LEU:HB3	1.97	0.47
1:B:243:PRO:CD	1:B:244:TYR:N	2.76	0.47
1:B:268:TRP:O	1:B:269:LEU:HD23	2.14	0.47
1:B:414:ILE:HD11	2:B:600:FAD:HM81	1.95	0.47
1:A:9:PRO:HA	1:A:40:ILE:O	2.15	0.47
1:B:59:ASP:HA	1:B:60:PRO:HD2	1.67	0.47
1:B:324:LYS:CE	1:B:334:LEU:HD21	2.43	0.47
1:B:468:ILE:HG22	1:B:470:CYS:SG	2.54	0.47
1:A:95:PHE:CD1	1:A:96:PRO:CD	2.94	0.47
1:A:99:PRO:HA	1:A:121:LEU:HB3	1.96	0.47
1:A:545:LYS:C	1:A:547:GLY:N	2.71	0.47
1:B:413:TRP:C	1:B:413:TRP:HE3	2.22	0.47
1:B:545:LYS:C	1:B:547:GLY:N	2.71	0.47
1:A:61:HIS:N	1:A:61:HIS:CD2	2.82	0.47
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.72	0.47
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.65	0.47
1:A:300:ARG:NH2	1:A:308:VAL:HA	2.18	0.47
1:A:383:PHE:CD1	1:A:383:PHE:N	2.82	0.47
1:B:104:ARG:C	1:B:106:SER:H	2.23	0.47
1:A:8:ARG:O	1:A:41:SER:HA	2.15	0.47
1:A:425:PHE:CB	1:A:488:MET:HE1	2.44	0.47
1:A:494:ASP:O	1:A:497:ALA:N	2.48	0.47
1:B:148:TYR:O	1:B:151:LEU:N	2.48	0.47
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.65	0.47
1:A:249:TYR:CE1	1:A:251:ASP:CG	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:CD2	1:A:280:LEU:N	2.82	0.47
1:A:290:LYS:HG3	1:A:433:GLY:HA3	1.97	0.47
1:A:489:ARG:NE	1:A:512:GLN:OE1	2.46	0.47
1:B:8:ARG:O	1:B:41:SER:HA	2.15	0.47
1:B:37:VAL:CG1	1:B:38:GLU:N	2.78	0.47
1:B:69:PHE:HB3	1:B:113:PRO:O	2.14	0.47
1:B:108:TYR:CD1	1:B:505:THR:C	2.93	0.47
1:B:229:LYS:O	1:B:232:ASP:N	2.43	0.47
1:B:238:ILE:N	1:B:238:ILE:HD13	2.28	0.47
1:B:507:LEU:HD23	1:B:510:MET:HE3	1.96	0.47
1:B:552:GLN:CD	1:B:552:GLN:H	2.22	0.47
1:A:24:PHE:CD2	1:A:95:PHE:CD2	3.01	0.47
1:A:323:ASP:OD1	1:A:323:ASP:N	2.46	0.47
1:A:327:TYR:HB3	1:A:342:ILE:HD11	1.97	0.47
1:A:413:TRP:HE3	1:A:413:TRP:C	2.22	0.47
1:A:418:PRO:CD	1:A:474:ASN:HD22	2.22	0.47
1:A:468:ILE:HG22	1:A:470:CYS:SG	2.54	0.47
1:A:520:ASN:O	1:A:521:ASN:HB2	2.15	0.47
1:B:152:HIS:CE1	1:B:161:ARG:NH2	2.80	0.47
1:B:454:PHE:CD1	1:B:454:PHE:C	2.93	0.47
1:A:342:ILE:HA	1:A:345:GLN:HG3	1.97	0.47
1:A:79:ASN:ND2	1:A:81:ALA:N	2.63	0.47
1:B:290:LYS:HG3	1:B:433:GLY:HA3	1.97	0.47
1:B:472:VAL:HG12	1:B:473:PHE:H	1.79	0.47
1:B:479:ILE:C	1:B:483:LYS:HE3	2.40	0.47
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.49	0.46
1:A:293:VAL:C	1:A:295:ILE:N	2.68	0.46
1:B:99:PRO:HD3	1:B:542:ALA:HB2	1.97	0.46
1:B:314:ILE:HB	1:B:350:ARG:O	2.15	0.46
1:B:441:ALA:O	1:B:444:LYS:HB3	2.15	0.46
1:A:104:ARG:C	1:A:106:SER:H	2.23	0.46
1:A:143:GLU:HB3	1:A:144:PRO:CD	2.45	0.46
1:A:173:GLY:N	1:A:408:TYR:HE1	2.13	0.46
1:A:222:ARG:HG2	1:A:225:THR:OG1	2.16	0.46
1:B:79:ASN:HD22	1:B:81:ALA:N	2.14	0.46
1:B:249:TYR:CE1	1:B:251:ASP:CG	2.93	0.46
1:A:108:TYR:CD1	1:A:505:THR:C	2.93	0.46
1:A:148:TYR:O	1:A:151:LEU:N	2.48	0.46
1:A:301:LEU:HA	1:A:462:MET:HE3	1.97	0.46
1:B:189:PRO:CA	1:B:307:ASN:HA	2.45	0.46
1:B:278:SER:HA	1:B:356:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLU:N	1:B:362:PRO:CD	2.78	0.46
1:B:494:ASP:O	1:B:497:ALA:N	2.48	0.46
1:A:155:LEU:O	1:A:160:LEU:N	2.40	0.46
1:A:276:TYR:OH	1:A:399:ASP:O	2.19	0.46
1:A:367:LEU:O	1:A:370:THR:HB	2.15	0.46
1:A:416:TRP:HA	1:A:416:TRP:HE3	1.79	0.46
1:A:479:ILE:C	1:A:483:LYS:HE3	2.40	0.46
1:B:8:ARG:HA	1:B:9:PRO:HD3	1.78	0.46
1:B:507:LEU:HD23	1:B:510:MET:CE	2.46	0.46
1:B:541:ILE:O	1:B:541:ILE:HG22	2.16	0.46
1:A:21:PHE:CE2	1:A:25:ILE:HG21	2.50	0.46
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.43	0.46
1:A:321:LEU:HD12	1:A:346:LEU:HD23	1.97	0.46
1:B:21:PHE:CE2	1:B:25:ILE:HG21	2.50	0.46
1:B:399:ASP:O	1:B:403:GLN:HG2	2.15	0.46
1:A:399:ASP:O	1:A:403:GLN:HG2	2.15	0.46
1:A:454:PHE:CD1	1:A:454:PHE:C	2.93	0.46
1:A:505:THR:OG1	1:A:513:ILE:HD12	2.16	0.46
1:A:507:LEU:HD23	1:A:510:MET:HE3	1.96	0.46
1:B:61:HIS:N	1:B:61:HIS:CD2	2.82	0.46
1:B:137:GLY:O	1:B:138:ALA:HB3	2.16	0.46
1:B:321:LEU:HD12	1:B:346:LEU:HD23	1.96	0.46
1:B:428:ILE:HD13	1:B:428:ILE:HA	1.62	0.46
1:B:79:ASN:ND2	1:B:81:ALA:N	2.63	0.46
1:A:99:PRO:HD3	1:A:542:ALA:HB2	1.97	0.46
1:A:217:LEU:HA	1:A:217:LEU:HD22	1.41	0.46
1:A:309:PRO:HB2	1:A:353:PHE:HE1	1.78	0.46
1:A:484:VAL:O	1:A:488:MET:N	2.31	0.46
1:B:222:ARG:HG2	1:B:225:THR:OG1	2.16	0.46
1:B:533:ASN:HD21	1:B:551:SER:N	2.14	0.46
1:A:332:GLU:CB	1:A:333:PRO:CD	2.94	0.46
1:B:327:TYR:HB3	1:B:342:ILE:HD11	1.97	0.46
1:A:441:ALA:O	1:A:444:LYS:HB3	2.15	0.46
1:B:173:GLY:N	1:B:408:TYR:HE1	2.13	0.46
1:B:280:LEU:HD12	1:B:281:ILE:N	2.31	0.46
1:B:367:LEU:O	1:B:370:THR:HB	2.15	0.46
1:B:560:LEU:HA	1:B:560:LEU:HD23	1.50	0.46
1:A:14:PRO:C	1:A:16:LEU:N	2.69	0.45
1:A:37:VAL:CG1	1:A:38:GLU:N	2.78	0.45
1:A:137:GLY:O	1:A:138:ALA:HB3	2.16	0.45
1:A:230:PRO:HD2	1:A:231:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:PHE:CE1	1:A:502:GLU:HG3	2.52	0.45
1:A:428:ILE:CG2	1:B:238:ILE:HG21	2.46	0.45
1:A:533:ASN:HD21	1:A:551:SER:N	2.14	0.45
1:B:60:PRO:C	1:B:62:HIS:H	2.24	0.45
1:B:489:ARG:NE	1:B:512:GLN:OE1	2.46	0.45
1:A:60:PRO:C	1:A:62:HIS:H	2.24	0.45
1:A:189:PRO:CA	1:A:307:ASN:HA	2.45	0.45
1:A:507:LEU:HD23	1:A:510:MET:CE	2.46	0.45
1:B:9:PRO:HA	1:B:40:ILE:O	2.15	0.45
1:B:68:TYR:CD1	1:B:68:TYR:C	2.94	0.45
1:B:143:GLU:HB3	1:B:144:PRO:CD	2.45	0.45
1:B:342:ILE:HA	1:B:345:GLN:HG3	1.97	0.45
1:B:413:TRP:C	1:B:415:ASP:N	2.72	0.45
1:B:425:PHE:CB	1:B:488:MET:HE1	2.44	0.45
1:A:419:ASN:C	1:A:474:ASN:HA	2.39	0.45
1:B:424:PHE:HD2	1:B:468:ILE:HG23	1.82	0.45
1:A:141:VAL:HG21	1:A:240:HIS:CE1	2.52	0.45
1:A:361:GLU:N	1:A:362:PRO:CD	2.78	0.45
1:A:502:GLU:N	1:A:502:GLU:CD	2.75	0.45
1:B:141:VAL:HG21	1:B:240:HIS:CE1	2.52	0.45
1:B:301:LEU:HA	1:B:462:MET:HE3	1.97	0.45
1:B:425:PHE:CE1	1:B:502:GLU:HG3	2.52	0.45
1:A:14:PRO:HB2	1:A:15:LYS:HE3	1.99	0.45
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.51	0.45
1:A:278:SER:HA	1:A:356:ALA:HA	1.97	0.45
1:A:280:LEU:HD12	1:A:281:ILE:N	2.31	0.45
1:A:314:ILE:HB	1:A:350:ARG:O	2.15	0.45
1:B:243:PRO:CG	1:B:244:TYR:N	2.79	0.45
1:B:416:TRP:HA	1:B:416:TRP:HE3	1.79	0.45
1:A:68:TYR:CD1	1:A:68:TYR:C	2.94	0.45
1:A:243:PRO:CG	1:A:244:TYR:N	2.79	0.45
1:A:487:LEU:HD11	1:A:491:LEU:CD1	2.44	0.45
1:B:323:ASP:OD1	1:B:323:ASP:N	2.46	0.45
1:B:419:ASN:C	1:B:474:ASN:HA	2.39	0.45
1:B:422:HIS:CD2	2:B:600:FAD:HM81	2.46	0.45
1:B:424:PHE:CE2	3:B:601:EUG:H6	2.51	0.45
1:A:10:LEU:CD1	1:A:41:SER:C	2.90	0.45
1:A:56:HIS:O	1:A:111:ALA:HB1	2.17	0.45
1:A:154:TYR:CD1	1:A:154:TYR:C	2.95	0.45
1:A:413:TRP:C	1:A:415:ASP:N	2.72	0.45
1:B:25:ILE:HD12	1:B:25:ILE:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.81	0.45
1:B:502:GLU:N	1:B:502:GLU:CD	2.75	0.45
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.69	0.45
1:A:149:HIS:HB2	1:A:408:TYR:OH	2.17	0.45
1:A:284:PRO:HG2	1:A:379:PRO:O	2.17	0.45
1:A:287:GLY:HA2	1:A:437:MET:CE	2.47	0.45
1:A:424:PHE:CE2	3:A:601:EUG:H6	2.51	0.45
1:A:487:LEU:CD1	1:A:491:LEU:CD1	2.95	0.45
1:A:513:ILE:HA	1:A:516:THR:HG23	1.98	0.45
1:B:33:GLY:C	1:B:35:GLU:N	2.73	0.45
1:B:56:HIS:O	1:B:111:ALA:HB1	2.17	0.45
1:B:413:TRP:C	1:B:413:TRP:CE3	2.95	0.45
1:B:487:LEU:CD1	1:B:491:LEU:CD1	2.95	0.45
1:A:79:ASN:HD22	1:A:81:ALA:N	2.14	0.45
1:A:405:ILE:HA	1:A:406:PRO:HD2	1.79	0.45
1:B:89:LEU:C	1:B:91:ASN:N	2.74	0.45
1:B:149:HIS:HB2	1:B:408:TYR:OH	2.17	0.45
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.65	0.45
1:B:287:GLY:HA2	1:B:437:MET:CE	2.47	0.45
1:B:348:LEU:HA	1:B:348:LEU:HD23	1.69	0.45
1:B:438:MET:O	1:B:442:VAL:HG23	2.17	0.45
1:B:505:THR:OG1	1:B:513:ILE:HD12	2.16	0.45
1:B:513:ILE:HA	1:B:516:THR:HG23	1.98	0.45
1:B:520:ASN:O	1:B:521:ASN:HB2	2.15	0.45
1:B:550:PRO:HB2	1:B:552:GLN:HG2	1.99	0.45
1:A:185:VAL:CG1	1:A:186:GLY:N	2.80	0.44
1:A:89:LEU:N	1:A:89:LEU:HD12	2.33	0.44
1:A:339:LEU:O	1:A:342:ILE:N	2.51	0.44
1:B:40:ILE:O	1:B:40:ILE:HG22	2.18	0.44
1:B:230:PRO:HD2	1:B:231:GLU:OE2	2.18	0.44
1:B:267:ILE:HD13	1:B:267:ILE:HA	1.57	0.44
1:B:279:TYR:O	1:B:395:LEU:HD11	2.17	0.44
1:B:385:PHE:HA	1:B:386:PRO:HD3	1.68	0.44
1:A:103:GLY:C	1:A:105:ASN:N	2.75	0.44
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.63	0.44
1:A:279:TYR:O	1:A:395:LEU:HD11	2.17	0.44
1:A:283:LEU:HD12	1:A:351:TRP:CB	2.47	0.44
1:A:372:LYS:HA	1:A:383:PHE:CE2	2.52	0.44
1:B:53:LYS:HA	1:B:54:PRO:HD3	1.70	0.44
1:B:72:SER:HB3	1:B:117:GLY:O	2.17	0.44
1:B:89:LEU:O	1:B:92:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PRO:HD2	1:B:231:GLU:HG2	1.98	0.44
1:B:283:LEU:HA	1:B:284:PRO:HD3	1.65	0.44
1:B:372:LYS:HA	1:B:383:PHE:CE2	2.52	0.44
1:A:214:MET:CB	1:A:239:ALA:HA	2.46	0.44
1:B:97:LEU:O	1:B:542:ALA:HA	2.17	0.44
1:B:284:PRO:HG2	1:B:379:PRO:O	2.17	0.44
1:B:487:LEU:CD1	1:B:491:LEU:HD11	2.44	0.44
1:A:541:ILE:O	1:A:541:ILE:HG22	2.16	0.44
1:B:103:GLY:C	1:B:105:ASN:N	2.75	0.44
1:B:154:TYR:CD1	1:B:154:TYR:C	2.95	0.44
1:B:188:THR:HB	1:B:189:PRO:HD2	1.99	0.44
1:B:387:GLU:H	1:B:387:GLU:HG3	1.22	0.44
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.48	0.44
1:A:424:PHE:HD2	1:A:468:ILE:HG23	1.82	0.44
1:A:438:MET:O	1:A:442:VAL:HG23	2.17	0.44
1:B:72:SER:HB3	1:B:117:GLY:HA2	1.99	0.44
1:A:72:SER:HB3	1:A:117:GLY:HA2	1.99	0.44
1:A:89:LEU:C	1:A:91:ASN:N	2.74	0.44
1:A:90:ALA:HB2	1:A:97:LEU:HD11	2.00	0.44
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.98	0.44
1:B:89:LEU:N	1:B:89:LEU:HD12	2.33	0.44
1:B:270:MET:HA	1:B:271:PRO:HD3	1.72	0.44
1:B:283:LEU:HD12	1:B:351:TRP:CB	2.48	0.44
1:B:487:LEU:HD11	1:B:491:LEU:CD1	2.44	0.44
1:A:467:HIS:ND1	1:A:467:HIS:C	2.76	0.44
1:A:550:PRO:HB2	1:A:552:GLN:HG2	1.99	0.44
1:B:10:LEU:CD1	1:B:41:SER:C	2.90	0.44
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.98	0.44
1:A:80:VAL:O	1:A:83:VAL:HB	2.17	0.44
1:A:97:LEU:O	1:A:542:ALA:HA	2.17	0.44
1:A:330:ARG:HH22	1:A:335:SER:HB3	1.83	0.44
1:A:378:ILE:HA	1:A:379:PRO:HD2	1.83	0.44
1:A:389:THR:CB	1:A:390:PRO:CD	2.95	0.44
1:A:413:TRP:C	1:A:413:TRP:CE3	2.95	0.44
1:B:102:ILE:HG13	1:B:175:SER:HB2	1.99	0.44
1:B:525:LEU:HD12	1:B:525:LEU:C	2.39	0.44
1:A:177:LEU:HD22	1:A:265:ILE:CG2	2.26	0.43
1:A:546:SER:OG	1:B:247:GLY:HA2	2.17	0.43
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.51	0.43
1:B:90:ALA:HB2	1:B:97:LEU:HD11	2.00	0.43
1:B:23:GLU:O	1:B:26:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:VAL:O	1:B:83:VAL:HB	2.17	0.43
1:B:330:ARG:HH22	1:B:335:SER:HB3	1.83	0.43
1:B:339:LEU:O	1:B:342:ILE:N	2.51	0.43
1:A:27:ASP:O	1:A:30:ARG:HB3	2.18	0.43
1:A:72:SER:HB3	1:A:117:GLY:O	2.17	0.43
1:A:346:LEU:O	1:A:347:ASN:HB2	2.19	0.43
1:A:487:LEU:CD1	1:A:491:LEU:HD11	2.44	0.43
1:B:27:ASP:O	1:B:30:ARG:HB3	2.18	0.43
1:B:272:ASN:HA	1:B:273:PRO:HD3	1.64	0.43
1:B:287:GLY:HA2	1:B:437:MET:HE1	2.01	0.43
1:B:432:SER:OG	1:B:435:ASP:HB2	2.19	0.43
1:A:344:LYS:C	1:A:346:LEU:N	2.75	0.43
1:A:417:LEU:HD22	1:A:473:PHE:HA	2.00	0.43
1:A:537:PRO:O	1:A:552:GLN:NE2	2.51	0.43
1:A:560:LEU:HA	1:A:560:LEU:HD23	1.50	0.43
1:B:440:TYR:O	1:B:444:LYS:HB2	2.19	0.43
1:A:33:GLY:C	1:A:35:GLU:N	2.73	0.43
1:A:58:HIS:HA	1:A:112:ALA:HB2	2.01	0.43
1:A:188:THR:HB	1:A:189:PRO:CD	2.49	0.43
1:A:323:ASP:OD2	1:A:325:ARG:HB3	2.18	0.43
1:A:379:PRO:C	1:A:381:VAL:N	2.77	0.43
1:B:14:PRO:HB2	1:B:15:LYS:HE3	1.99	0.43
1:A:10:LEU:N	1:A:10:LEU:HD12	2.34	0.43
1:A:134:ASN:HB3	1:A:139:TYR:CZ	2.54	0.43
1:A:230:PRO:HD2	1:A:231:GLU:OE2	2.18	0.43
1:A:428:ILE:HD13	1:A:428:ILE:HA	1.62	0.43
1:B:417:LEU:HD22	1:B:473:PHE:HA	2.00	0.43
1:B:537:PRO:O	1:B:552:GLN:NE2	2.52	0.43
1:A:89:LEU:O	1:A:92:LYS:N	2.51	0.43
1:A:188:THR:HB	1:A:189:PRO:HD2	1.99	0.43
1:A:241:LEU:HB3	1:B:463:ARG:O	2.19	0.43
1:B:56:HIS:HA	1:B:111:ALA:HB2	1.97	0.43
1:B:464:GLU:CG	1:B:465:MET:N	2.80	0.43
1:A:195:MET:O	1:A:196:MET:HE2	2.19	0.43
1:A:379:PRO:C	1:A:381:VAL:H	2.26	0.43
1:A:418:PRO:HB2	1:A:474:ASN:HD21	1.84	0.43
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.18	0.43
1:A:40:ILE:O	1:A:40:ILE:HG22	2.17	0.43
1:A:360:PRO:C	1:A:364:ARG:HH21	2.20	0.43
1:A:545:LYS:C	1:A:547:GLY:H	2.26	0.43
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HB	1:B:189:PRO:CD	2.49	0.43
1:B:202:VAL:HG12	1:B:203:VAL:C	2.44	0.43
1:B:395:LEU:HD12	1:B:395:LEU:HA	1.93	0.43
1:A:51:TYR:CE1	1:A:104:ARG:HD3	2.54	0.42
1:A:202:VAL:HG12	1:A:203:VAL:C	2.44	0.42
1:A:233:GLN:HG3	1:A:233:GLN:H	1.32	0.42
1:B:14:PRO:CB	1:B:15:LYS:HE3	2.49	0.42
1:B:323:ASP:OD2	1:B:325:ARG:HB3	2.18	0.42
1:A:160:LEU:C	1:A:162:ASP:N	2.76	0.42
1:A:177:LEU:CD2	1:A:265:ILE:HG22	2.26	0.42
1:B:134:ASN:HB3	1:B:139:TYR:CZ	2.54	0.42
1:B:252:GLY:C	1:B:254:PHE:N	2.76	0.42
1:B:332:GLU:HB3	1:B:333:PRO:CD	2.50	0.42
1:B:335:SER:OG	1:B:338:GLU:N	2.42	0.42
1:B:346:LEU:O	1:B:347:ASN:HB2	2.19	0.42
1:B:386:PRO:N	1:B:395:LEU:HD23	2.34	0.42
1:B:387:GLU:C	1:B:389:THR:H	2.27	0.42
1:A:14:PRO:CB	1:A:15:LYS:HE3	2.49	0.42
1:A:312:ARG:O	1:A:352:ASN:N	2.53	0.42
1:B:224:GLU:CD	1:B:224:GLU:N	2.75	0.42
1:B:379:PRO:C	1:B:381:VAL:N	2.77	0.42
1:A:386:PRO:N	1:A:395:LEU:HD23	2.34	0.42
1:B:344:LYS:C	1:B:346:LEU:N	2.75	0.42
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.50	0.42
1:A:440:TYR:O	1:A:444:LYS:HB2	2.19	0.42
1:A:463:ARG:NH2	1:B:138:ALA:HB3	2.34	0.42
1:B:152:HIS:CE1	1:B:156:GLU:OE1	2.73	0.42
1:B:177:LEU:HD22	1:B:265:ILE:CG2	2.26	0.42
1:B:330:ARG:CZ	1:B:338:GLU:OE1	2.68	0.42
1:B:379:PRO:C	1:B:381:VAL:H	2.26	0.42
1:A:196:MET:HE2	1:A:196:MET:HA	2.02	0.42
1:A:200:MET:CE	1:A:251:ASP:CB	2.97	0.42
1:B:102:ILE:HA	1:B:102:ILE:HD13	1.87	0.42
1:B:195:MET:O	1:B:196:MET:HE2	2.19	0.42
1:B:280:LEU:HD12	1:B:280:LEU:C	2.45	0.42
1:B:324:LYS:N	1:B:416:TRP:CE3	2.88	0.42
1:A:156:GLU:O	1:A:159:ASN:N	2.43	0.42
1:A:295:ILE:HD12	1:A:378:ILE:CD1	2.48	0.42
1:B:10:LEU:N	1:B:10:LEU:HD12	2.33	0.42
1:B:58:HIS:HA	1:B:112:ALA:HB2	2.01	0.42
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:O	1:A:26:GLN:N	2.51	0.42
1:A:296:ILE:HG13	1:A:296:ILE:H	1.57	0.42
1:A:432:SER:OG	1:A:435:ASP:HB2	2.19	0.42
2:A:600:FAD:C4	3:A:601:EUG:C2	2.97	0.42
1:B:279:TYR:CD2	1:B:279:TYR:C	2.97	0.42
1:B:332:GLU:CB	1:B:333:PRO:CD	2.94	0.42
1:A:58:HIS:CA	1:A:112:ALA:HB2	2.50	0.42
1:A:387:GLU:C	1:A:389:THR:H	2.27	0.42
1:B:202:VAL:HG12	1:B:203:VAL:N	2.34	0.42
1:B:299:LEU:HB3	1:B:305:LEU:HG	2.02	0.42
2:B:600:FAD:C4	3:B:601:EUG:C2	2.97	0.42
1:A:324:LYS:N	1:A:416:TRP:CE3	2.88	0.42
1:B:418:PRO:HB2	1:B:474:ASN:HD21	1.84	0.42
1:B:493:ASP:O	1:B:496:ALA:HB3	2.20	0.42
1:A:12:LEU:HD13	1:A:16:LEU:O	2.20	0.41
1:A:201:GLU:HB3	1:A:264:LYS:HB2	2.02	0.41
1:A:287:GLY:HA2	1:A:437:MET:HE1	2.01	0.41
1:A:332:GLU:HB3	1:A:333:PRO:CD	2.50	0.41
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.50	0.41
1:A:516:THR:C	1:A:518:ASN:H	2.28	0.41
1:B:229:LYS:CB	1:B:230:PRO:CD	2.98	0.41
1:B:242:PHE:HA	1:B:243:PRO:HD3	1.49	0.41
1:A:422:HIS:HD1	1:A:422:HIS:H	1.68	0.41
1:A:463:ARG:HH21	1:B:138:ALA:HB3	1.85	0.41
1:B:367:LEU:O	1:B:370:THR:N	2.53	0.41
1:B:411:LEU:O	1:B:414:ILE:N	2.46	0.41
1:B:422:HIS:HD1	1:B:422:HIS:H	1.68	0.41
1:A:330:ARG:NH1	1:A:338:GLU:CD	2.79	0.41
1:B:185:VAL:CG1	1:B:186:GLY:N	2.80	0.41
1:B:378:ILE:HA	1:B:379:PRO:HD2	1.83	0.41
1:A:168:VAL:HA	1:A:169:PRO:HD3	1.75	0.41
1:A:493:ASP:O	1:A:496:ALA:HB3	2.20	0.41
1:B:10:LEU:HD11	1:B:42:SER:N	2.35	0.41
1:B:278:SER:OG	1:B:399:ASP:OD2	2.30	0.41
1:B:545:LYS:C	1:B:547:GLY:H	2.26	0.41
1:A:10:LEU:HD11	1:A:42:SER:N	2.35	0.41
1:A:152:HIS:CE1	1:A:156:GLU:OE1	2.73	0.41
1:A:280:LEU:HD12	1:A:280:LEU:C	2.45	0.41
1:A:330:ARG:CZ	1:A:338:GLU:OE1	2.68	0.41
1:A:363:ILE:HG12	1:B:363:ILE:HG12	2.02	0.41
1:A:411:LEU:O	1:A:414:ILE:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:CG1	1:B:531:LEU:HD21	2.50	0.41
1:B:12:LEU:HD13	1:B:16:LEU:O	2.20	0.41
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.75	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.72	0.41
1:A:139:TYR:HA	1:A:269:LEU:H	1.86	0.41
1:A:202:VAL:HG12	1:A:203:VAL:N	2.34	0.41
1:A:367:LEU:O	1:A:370:THR:N	2.53	0.41
1:A:413:TRP:C	1:A:415:ASP:H	2.27	0.41
1:B:196:MET:HE2	1:B:196:MET:HA	2.01	0.41
1:B:281:ILE:HG21	1:B:375:PHE:CD2	2.56	0.41
1:B:385:PHE:O	1:B:388:ASP:N	2.54	0.41
1:A:385:PHE:HA	1:A:386:PRO:HD3	1.68	0.41
1:B:58:HIS:CA	1:B:112:ALA:HB2	2.50	0.41
1:B:112:ALA:HA	1:B:113:PRO:HD3	1.69	0.41
1:B:201:GLU:HB3	1:B:264:LYS:HB2	2.02	0.41
1:B:316:LEU:HD11	1:B:413:TRP:CE2	2.55	0.41
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.18	0.41
1:A:316:LEU:HD11	1:A:413:TRP:CE2	2.55	0.41
1:A:387:GLU:H	1:A:387:GLU:HG3	1.22	0.41
1:B:39:VAL:CG1	1:B:40:ILE:N	2.84	0.41
1:B:51:TYR:CE1	1:B:104:ARG:HD3	2.54	0.41
1:B:330:ARG:NH1	1:B:338:GLU:CD	2.79	0.41
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.67	0.41
1:A:230:PRO:O	1:B:519:TRP:HZ2	2.02	0.41
1:A:281:ILE:HG21	1:A:375:PHE:CD2	2.56	0.41
1:A:409:ASP:O	1:A:412:LYS:HG3	2.21	0.41
1:A:505:THR:CG2	1:A:513:ILE:CD1	2.99	0.41
1:A:540:ILE:HD13	1:A:540:ILE:HA	1.71	0.41
1:A:542:ALA:HA	1:A:543:PRO:HD2	1.78	0.41
1:B:258:ASN:HB3	1:B:542:ALA:O	2.21	0.41
1:B:283:LEU:O	1:B:349:GLY:CA	2.69	0.41
1:B:444:LYS:HB3	1:B:445:LYS:H	1.66	0.41
1:B:467:HIS:ND1	1:B:467:HIS:C	2.76	0.41
1:B:516:THR:C	1:B:518:ASN:H	2.28	0.41
1:A:79:ASN:ND2	1:A:79:ASN:C	2.79	0.41
1:A:164:LEU:O	1:A:165:TRP:HD1	2.04	0.41
1:A:283:LEU:O	1:A:349:GLY:CA	2.69	0.41
1:A:495:CYS:HA	1:A:500:TRP:HE3	1.86	0.41
1:B:139:TYR:HA	1:B:269:LEU:H	1.86	0.41
1:B:200:MET:CE	1:B:251:ASP:CB	2.97	0.41
1:B:312:ARG:O	1:B:352:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ARG:NH1	1:B:338:GLU:OE1	2.54	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.82	0.40
1:B:214:MET:CB	1:B:239:ALA:HA	2.46	0.40
1:B:425:PHE:CG	1:B:488:MET:HE1	2.56	0.40
1:A:104:ARG:N	2:A:600:FAD:O2P	2.55	0.40
1:A:279:TYR:CD2	1:A:279:TYR:C	2.97	0.40
1:A:339:LEU:O	1:A:343:ALA:N	2.49	0.40
1:B:214:MET:C	1:B:216:ALA:N	2.78	0.40
1:A:279:TYR:HB2	1:A:280:LEU:H	1.60	0.40
1:A:302:GLY:O	1:A:303:MET:HB2	2.21	0.40
1:A:330:ARG:NH1	1:A:338:GLU:OE1	2.54	0.40
1:A:525:LEU:HD12	1:A:525:LEU:C	2.39	0.40
1:B:129:ARG:HB2	1:B:131:LEU:CD2	2.51	0.40
1:B:198:SER:O	1:B:240:HIS:HD2	2.04	0.40
1:A:151:LEU:HD12	1:A:151:LEU:C	2.37	0.40
1:A:198:SER:O	1:A:240:HIS:HD2	2.04	0.40
1:A:258:ASN:HB3	1:A:542:ALA:O	2.21	0.40
1:A:385:PHE:O	1:A:388:ASP:N	2.54	0.40
1:B:302:GLY:O	1:B:303:MET:HB2	2.21	0.40
1:B:388:ASP:C	1:B:389:THR:CG2	2.94	0.40
1:B:400:LYS:O	1:B:403:GLN:HG2	2.21	0.40
1:B:477:ASP:OD2	1:B:480:GLN:HB2	2.21	0.40
1:A:24:PHE:CE1	1:A:28:ILE:HD11	2.56	0.40
1:A:119:VAL:HG12	1:A:120:VAL:N	2.37	0.40
1:A:385:PHE:CB	1:A:386:PRO:CD	2.97	0.40
1:A:477:ASP:OD2	1:A:480:GLN:HB2	2.21	0.40
1:B:119:VAL:HG12	1:B:120:VAL:N	2.37	0.40
1:B:164:LEU:O	1:B:165:TRP:HD1	2.04	0.40
1:B:314:ILE:HG23	1:B:315:LEU:N	2.36	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	A	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	5	19
1	B	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	5	19
All	All	1106/1120 (99%)	944 (85%)	138 (12%)	24 (2%)	5	19

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	559	LYS
1	B	46	ILE
1	B	559	LYS
1	A	157	ALA
1	B	157	ALA
1	A	391	GLU
1	A	517	TYR
1	B	391	GLU
1	B	517	TYR
1	A	127	MET
1	A	166	LEU
1	B	127	MET
1	B	166	LEU
1	A	104	ARG
1	A	388	ASP
1	B	104	ARG
1	B	388	ASP
1	A	199	GLY
1	A	284	PRO
1	B	199	GLY
1	B	284	PRO
1	A	542	ALA
1	B	542	ALA

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	A	475/482 (98%)	444 (94%)	31 (6%)	15	43
1	B	475/482 (98%)	444 (94%)	31 (6%)	15	43
All	All	950/964 (98%)	888 (94%)	62 (6%)	15	43

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	63	VAL
1	A	64	MET
1	A	65	ASP
1	A	78	ARG
1	A	79	ASN
1	A	91	ASN
1	A	114	ARG
1	A	128	ASN
1	A	133	VAL
1	A	136	GLU
1	A	177	LEU
1	A	224	GLU
1	A	243	PRO
1	A	248	PRO
1	A	267	ILE
1	A	314	ILE
1	A	350	ARG
1	A	361	GLU
1	A	373	ASP
1	A	384	TYR
1	A	407	THR
1	A	409	ASP
1	A	413	TRP
1	A	464	GLU
1	A	478	LEU
1	A	488	MET
1	A	505	THR
1	A	520	ASN
1	A	535	VAL
1	A	552	GLN
1	B	27	ASP
1	B	63	VAL
1	B	64	MET
1	B	65	ASP

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Mol	Chain	Res	Type
1	B	78	ARG
1	B	79	ASN
1	B	91	ASN
1	B	114	ARG
1	B	128	ASN
1	B	133	VAL
1	B	136	GLU
1	B	177	LEU
1	B	224	GLU
1	B	243	PRO
1	B	248	PRO
1	B	267	ILE
1	B	314	ILE
1	B	350	ARG
1	B	361	GLU
1	B	373	ASP
1	B	384	TYR
1	B	407	THR
1	B	409	ASP
1	B	413	TRP
1	B	464	GLU
1	B	478	LEU
1	B	488	MET
1	B	505	THR
1	B	520	ASN
1	B	535	VAL
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	91	ASN
1	A	152	HIS
1	A	153	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	467	HIS
1	A	474	ASN
1	A	520	ASN
1	A	533	ASN

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Mol	Chain	Res	Type
1	A	552	GLN
1	B	79	ASN
1	B	91	ASN
1	B	152	HIS
1	B	153	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	467	HIS
1	B	474	ASN
1	B	533	ASN
1	B	552	GLN

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	$\# Z > 2$
2	FAD	A	600	1	58,58,58	1.00	5 (8%)	85,89,89	0.89	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	600	1	58,58,58	1.00	5 (8%)	85,89,89	0.89	4 (4%)
3	EUG	A	601	-	11,11,12	0.46	0	14,14,15	1.51	2 (14%)
3	EUG	B	601	-	11,11,12	0.47	0	14,14,15	1.52	2 (14%)

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
2	FAD	A	600	1	-	10/34/50/50	0/6/6/6
2	FAD	B	600	1	-	10/34/50/50	0/6/6/6
3	EUG	A	601	-	-	4/4/4/5	0/1/1/1
3	EUG	B	601	-	-	4/4/4/5	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	PA-O3P	3.42	1.63	1.59
2	B	600	FAD	PA-O3P	3.39	1.63	1.59
2	B	600	FAD	P-O3P	3.27	1.63	1.59
2	A	600	FAD	P-O3P	3.22	1.63	1.59
2	A	600	FAD	C5X-N5	-2.68	1.34	1.39
2	B	600	FAD	C5X-N5	-2.64	1.34	1.39
2	B	600	FAD	O5B-C5B	-2.40	1.35	1.44
2	A	600	FAD	O5B-C5B	-2.38	1.35	1.44
2	A	600	FAD	C9A-N10	-2.10	1.37	1.41
2	B	600	FAD	C9A-N10	-2.08	1.37	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	EUG	O3-C3-C4	3.89	120.38	114.55
3	A	601	EUG	O3-C3-C4	3.85	120.33	114.55
2	B	600	FAD	PA-O5B-C5B	2.60	136.23	121.35
2	A	600	FAD	PA-O5B-C5B	2.59	136.17	121.35
3	B	601	EUG	C9-O3-C3	2.45	121.11	117.51
3	A	601	EUG	C9-O3-C3	2.44	121.10	117.51
2	A	600	FAD	C4-N3-C2	-2.38	121.42	125.64
2	B	600	FAD	C4-N3-C2	-2.37	121.43	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4X-C10-N10	2.14	119.55	116.48
2	A	600	FAD	C4X-C10-N10	2.09	119.48	116.48
2	B	600	FAD	O4B-C1B-N9A	2.09	112.10	108.09
2	A	600	FAD	O4B-C1B-N9A	2.07	112.06	108.09

There are no chirality outliers.

All (28) torsion outliers are listed below:

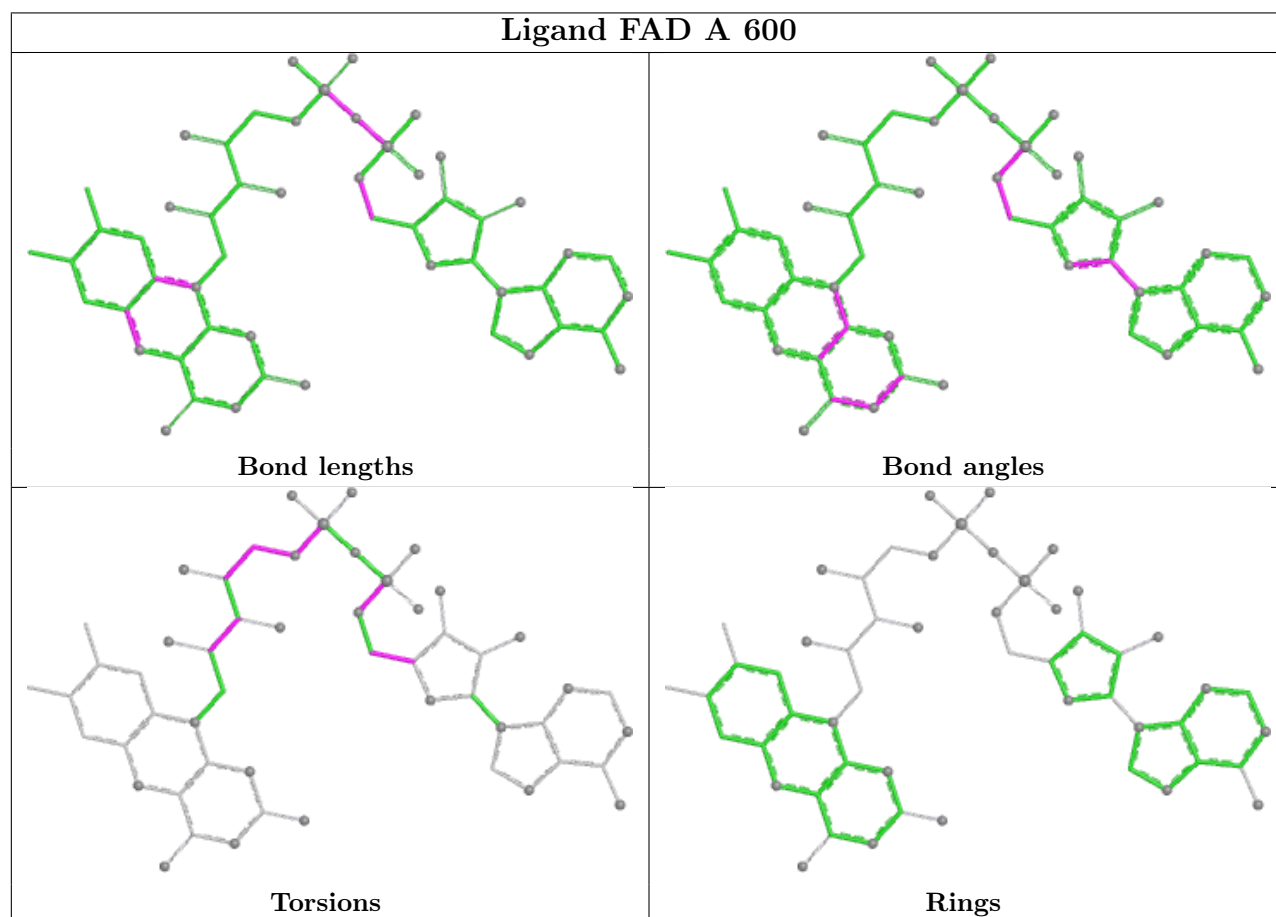
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	C5B-O5B-PA-O3P
2	B	600	FAD	C5'-O5'-P-O1P
3	A	601	EUG	C6-C1-C7-C8
3	B	601	EUG	C6-C1-C7-C8
3	A	601	EUG	C2-C1-C7-C8
3	B	601	EUG	C2-C1-C7-C8
3	A	601	EUG	C2-C3-O3-C9
3	B	601	EUG	C2-C3-O3-C9
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	O4'-C4'-C5'-O5'
2	B	600	FAD	O4'-C4'-C5'-O5'
3	B	601	EUG	C4-C3-O3-C9
2	A	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	C3'-C4'-C5'-O5'
3	A	601	EUG	C4-C3-O3-C9
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	C5B-O5B-PA-O1A
2	A	600	FAD	C5'-O5'-P-O2P
2	A	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C5B-O5B-PA-O1A
2	B	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C5'-O5'-P-O3P
2	A	600	FAD	C1'-C2'-C3'-O3'
2	B	600	FAD	C1'-C2'-C3'-O3'

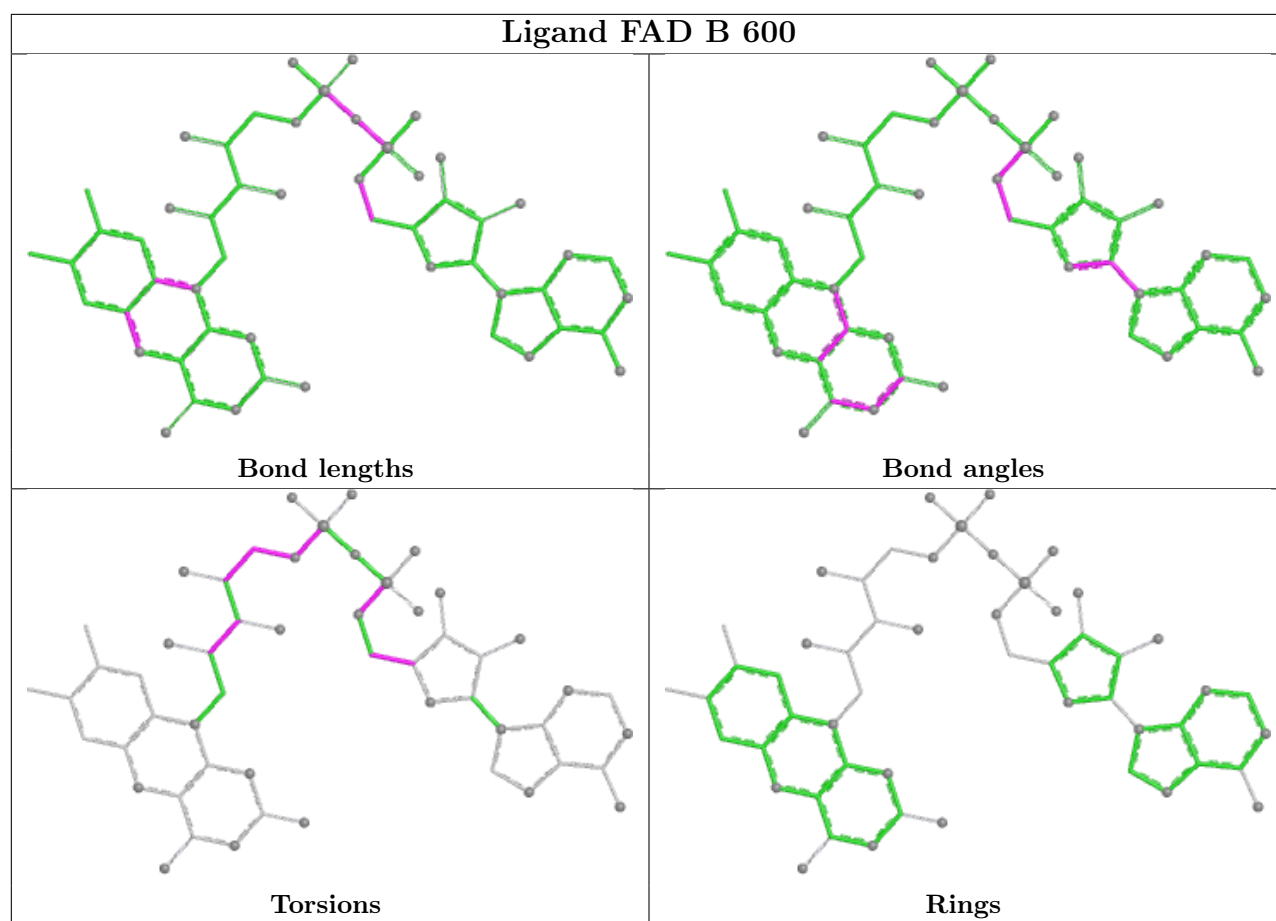
There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	17	0
2	B	600	FAD	16	0
3	A	601	EUG	5	0
3	B	601	EUG	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.