



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 AM UTC

PDB ID : 1AHU / pdb_00001ahu
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH P-CRESOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.70 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

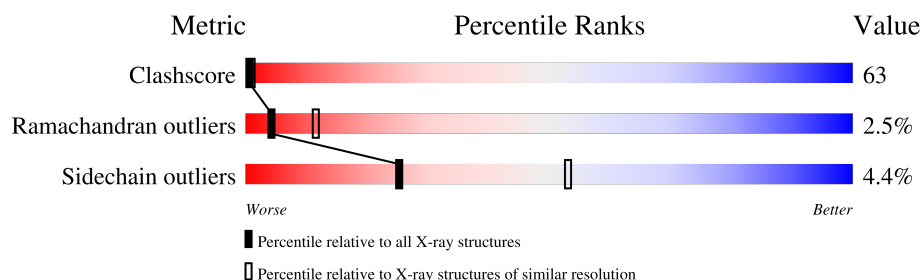
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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](#)

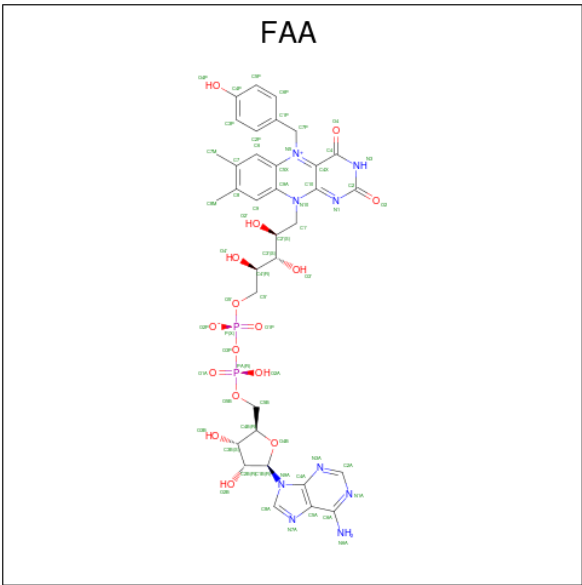
There are 3 unique types of molecules in this entry. The entry contains 9011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	37	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	37	0	0
			4391	2817	751	799	24			

- Molecule 2 is N5-(4-HYDROXYBENZYL)FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAA) (formula: C₃₄H₃₉N₉O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			61	34	9	16	2		
2	B	1	Total	C	N	O	P	0	0
			61	34	9	16	2		

- Molecule 3 is water.

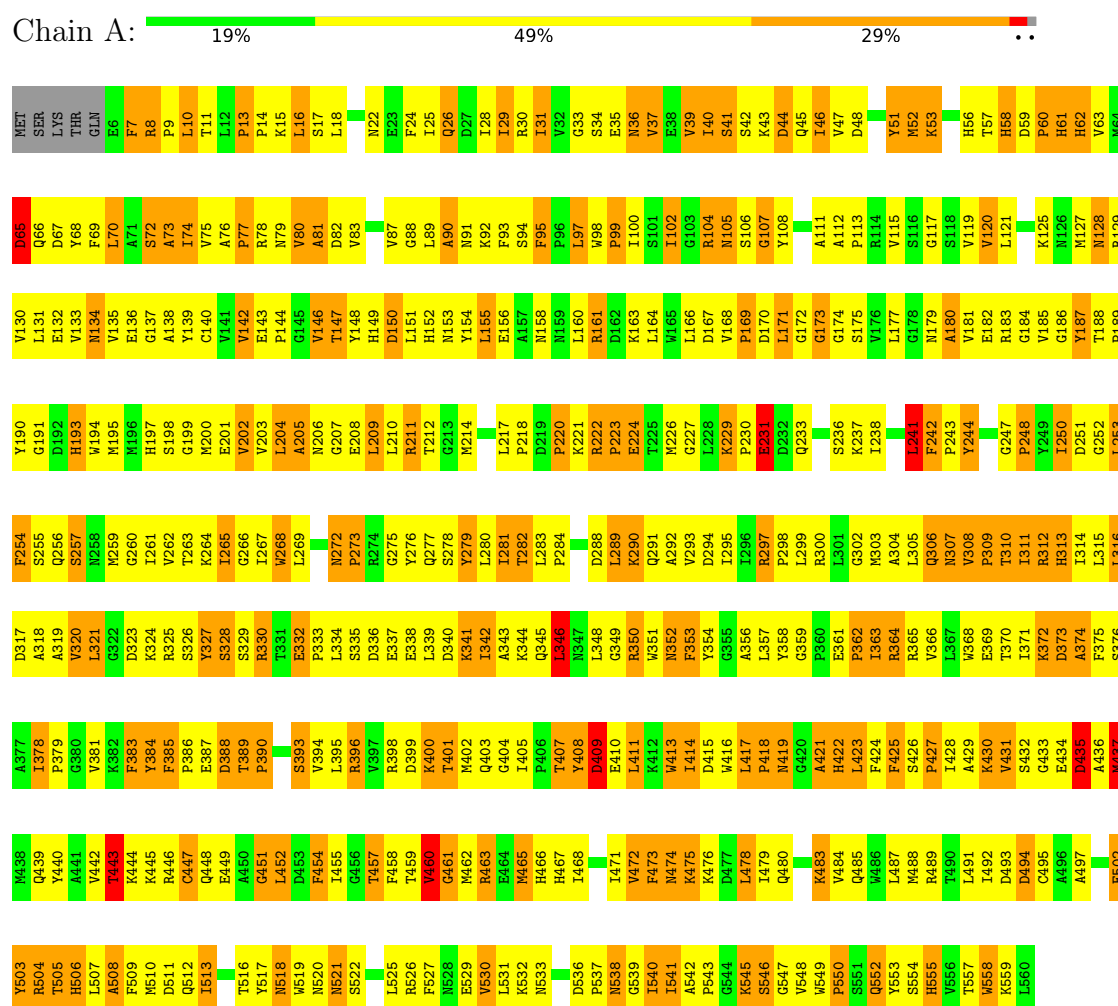
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	52	Total 52	O 52	1	0

3 Residue-property plots

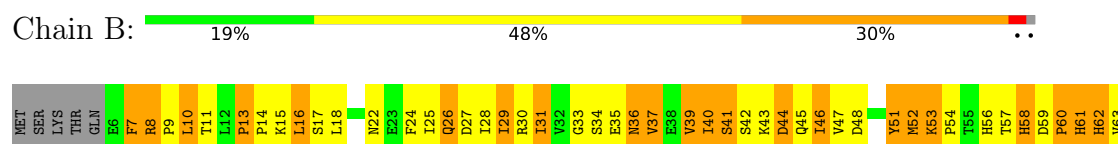
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



A436	F375	L315	L253	P189	R129	W64
M437	S376	L316	F254	Y190	V130	D65
M438	A377	D317	S255	G191	E131	D66
Q439	I378	A318	S256	D192	E132	D67
Y440	P379	A319	S257	H193	V133	F68
A441	G380	V320	M258	W194	M134	F69
V442	V381	L321	M259	M195	V135	L70
T443	K382	G322	G260	M196	E136	A71
K444	F383	D323	L261	H197	S137	S72
K445	Y384	K324	V262	S198	A138	A73
R446	F385	K325	T263	G199	Y139	I74
C447	P386	S326	K264	M200	C140	V75
Q448	E387	Y327	L265	E201	V141	A76
E449	D388	S328	G266	V202	V142	P77
A450	T389	S329	L267	V203	E143	R78
L452	P390	R330	W268	L204	P144	N79
D453	S393	T331	L269	A205	G145	V80
D454	V394	E332	M270	N206	V146	A81
I455	L395	P333	P271	G207	T147	D82
G456	R396	L334	M272	E208	Y148	V83
T457	V397	S335	P273	L209	H149	
F458	R398	D336	R274	L210	D150	V87
T459	D399	E337	G275	R211	L151	G88
Y460	K400	E338	Y276	T212	H152	L89
G461	T401	L339	Q277	G213	N153	A90
M462	M402	D340	S278	M214	Y154	N91
R463	Q403	K341	Y279	L217	L155	R92
E464	G404	L342	L280	P218	E156	F93
M465	I405	A343	T281	D219	A157	S94
H466	K406	K344	T282	P220	N158	F95
H467	T407	Q345	L283	K221	M159	P96
I468	Y408	L346	P284	R222	L160	L97
	D409	M347		K223	R161	W98
I471	E410	L348	D288	P223	D162	P99
V472	L411	R350	K290	E224	K163	I100
F473	K412	W351	Q291	T225	L164	S101
M474	W413	N352	A292	M226	W165	I102
K475	I414	F353	G293	G227	L166	G103
K476	D415	Y354	D294	K228	D167	R104
D477	W416	G355	T295	P230	V168	N105
L478	L417	A356	I296	P231	P169	S106
I479	P418	L357	R297	D232	D170	G107
M419	M419	Y358	P298	L171	G172	Y108
G420	G420	G359	L299	Q233	G173	
K483	A421	P360	R300	S236	G174	A111
V484	H422	E361	L301	K237	S175	A112
Q485	L423	P362	G302	I238	V176	P113
W486	F424	I363	M303		L177	R114
L487	F425	R364	A304	L241	G178	V115
M488	S426	R365	L305	F242	N179	S116
R489	P427	V366	Q306	P243	A180	G117
T490	I428	L367	N307	Y244	V181	S118
S491	A429	W368	V308		E182	V119
Y492	K430	E369	P309	G247	R183	V120
D493	V431	T370	I310	P248	G184	L121
D494	S432	I371	I311	Y249	V185	K125
C495	E433	K372	R312	L250	G186	M126
A496	E434	D373	H313	D251	Y187	N127
A497	D435	A374	I314	G252	T188	N128
W500	G501	E502	Q503	P504	R505	S506
S507	L508	K509	M510	N511	O512	P513
A514	F515	G516	H517	I518	J519	K520
L521	M522	N523	O524	P525	Q526	R527
S528	T529	U530	V531	W532	X533	Y534
Z535	A536	B537	C538	D539	E540	F541
G542	H543	I544	J545	K546	L547	M548
N549	O550	P551	Q552	R553	S554	T555
U556	V557	W558	X559	Y560	Z561	A562
B563	C564	D565	E566	F567	G568	H569
I570	J571	K572	L573	M574	N575	O576
P577	Q578	R579	S580	T581	U582	V583
W584	X585	Y586	Z587	A588	B589	C590
D591	E592	F593	G594	H595	I596	J597
K598	L599	M600	N601	O602	P603	Q604
R605	S606	T607	U608	V609	W610	X611
Y612	Z613	A614	B615	C616	D617	E618
F619	G620	H621	I622	J623	K624	L625
M626	N627	O628	P629	Q630	R631	S632
T633	U634	V635	W636	X637	Y638	Z639
A640	B641	C642	D643	E644	F645	G646
H647	I648	J649	K650	L651	M652	N653
O654	P655	Q656	R657	S658	T659	U660
V661	W662	X663	Y664	Z665	A666	B667
C668	D669	E670	F671	G672	H673	I674
J675	K676	L677	M678	N679	O680	P681
Q682	R683	S684	T685	U686	V687	W688
X689	Y690	Z691	A692	B693	C694	D695
E696	F697	G698	H699	I700	J701	K702
L703	M704	N705	O706	P707	Q708	R709
S710	T711	U712	V713	W714	X715	Y716
Z717	A718	B719	C720	D721	E722	F723
G724	H725	I726	J727	K728	L729	M730
N731	O732	P733	Q734	R735	S736	T737
U738	V739	W740	X741	Y742	Z743	A744
B745	C746	D747	E748	F749	G750	H751
I752	J753	K754	L755	M756	N757	O758
P759	Q760	R761	S762	T763	U764	V765
W766	X767	Y768	Z769	A770	B771	C772
D773	E774	F775	G776	H777	I778	J779
K780	L781	M782	N783	O784	P785	Q786
R787	S788	T789	U790	V791	W792	X793
Y794	Z795	A796	B797	C798	D799	E800
F801	G802	H803	I804	J805	K806	L807
M808	N809	O810	P811	Q812	R813	S814
T815	U816	V817	W818	X819	Y820	Z821
A822	B823	C824	D825	E826	F827	G828
H829	I830	J831	K832	L833	M834	N835
O836	P837	Q838	R839	S840	T841	U842
V843	W844	X845	Y846	Z847	A848	B849
C850	D851	E852	F853	G854	H855	I856
J857	K858	L859	M860	N861	O862	P863
Q864	R865	S866	T867	U868	V869	W870
X871	Y872	Z873	A874	B875	C876	D877
E878	F879	G880	H881	I882	J883	K884
L885	M886	N887	O888	P889	Q890	R891
S892	T893	U894	V895	W896	X897	Y898
Z899	A900	B901	C902	D903	E904	F905
G906	H907	I908	J909	K910	L911	M912
N913	O914	P915	Q916	R917	S918	T919
U920	V921	W922	X923	Y924	Z925	A926
B927	C928	D929	E930	F931	G932	H933
I934	J935	K936	L937	M938	N939	O940
P941	Q942	R943	S944	T945	U946	V947
W948	X949	Y950	Z951	A952	B953	C954
D955	E956	F957	G958	H959	I960	J961
K962	L963	M964	N965	O966	P967	Q968
R969	S970	T971	U972	V973	W974	X975
Y976	Z977	A978	B979	C980	D981	E982
F983	G984	H985	I986	J987	K988	L989
M990	N991	O992	P993	Q994	R995	S996
T997	U998	V999	W1000	X1001	Y1002	Z1003

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	128.82Å 128.82Å 130.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.4 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.97	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.221 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9011	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: FAA

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	0.95	6/4511 (0.1%)	2.33	281/6131 (4.6%)
1	B	0.95	6/4511 (0.1%)	2.33	278/6131 (4.5%)
All	All	0.95	12/9022 (0.1%)	2.33	559/12262 (4.6%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	MET	SD-CE	-6.00	1.64	1.79
1	B	226	MET	SD-CE	-5.99	1.64	1.79
1	B	513	ILE	CA-CB	-5.60	1.47	1.54
1	A	513	ILE	CA-CB	-5.59	1.47	1.54
1	A	264	LYS	CA-C	-5.37	1.46	1.52
1	A	506	HIS	CA-CB	-5.34	1.44	1.53
1	B	506	HIS	CA-CB	-5.30	1.44	1.53
1	B	264	LYS	CA-C	-5.29	1.46	1.52
1	B	267	ILE	CA-CB	-5.20	1.47	1.54
1	A	267	ILE	CA-CB	-5.18	1.47	1.54
1	A	460	VAL	CA-CB	-5.06	1.48	1.54
1	B	460	VAL	CA-CB	-5.04	1.48	1.54

All (559) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	TYR	N-CA-C	20.62	133.84	111.36
1	B	187	TYR	N-CA-C	20.58	133.79	111.36
1	B	404	GLY	CA-C-N	-14.25	112.33	122.59
1	B	404	GLY	C-N-CA	-14.25	112.33	122.59
1	B	129	ARG	N-CA-C	14.23	132.68	110.20
1	A	129	ARG	N-CA-C	14.21	132.65	110.20
1	A	404	GLY	CA-C-N	-14.18	112.38	122.59
1	A	404	GLY	C-N-CA	-14.18	112.38	122.59
1	B	304	ALA	N-CA-C	-13.83	96.28	111.36
1	A	304	ALA	N-CA-C	-13.81	96.31	111.36
1	B	457	THR	CB-CA-C	-13.79	87.78	109.99
1	A	457	THR	CB-CA-C	-13.79	87.80	109.99
1	B	244	TYR	N-CA-C	13.77	126.36	111.36
1	A	244	TYR	N-CA-C	13.75	126.35	111.36
1	A	72	SER	N-CA-C	-13.41	97.05	113.41
1	B	72	SER	N-CA-C	-13.35	97.12	113.41
1	A	8	ARG	CB-CA-C	-12.82	94.53	110.81
1	B	8	ARG	CB-CA-C	-12.81	94.53	110.81
1	A	541	ILE	CB-CA-C	-12.25	98.00	111.23
1	B	541	ILE	CB-CA-C	-12.21	98.04	111.23
1	A	518	ASN	N-CA-C	12.15	126.54	112.93
1	B	518	ASN	N-CA-C	12.13	126.52	112.93
1	A	558	TRP	N-CA-C	12.09	129.25	112.45
1	B	558	TRP	N-CA-C	12.06	129.21	112.45
1	A	452	LEU	N-CA-C	11.96	129.37	109.76
1	B	452	LEU	N-CA-C	11.95	129.36	109.76
1	A	366	VAL	CB-CA-C	-11.51	96.61	112.14
1	B	40	ILE	N-CA-C	11.50	118.52	106.21
1	A	40	ILE	N-CA-C	11.48	118.50	106.21
1	B	366	VAL	CB-CA-C	-11.48	96.64	112.14
1	B	505	THR	CB-CA-C	-11.39	90.45	110.95
1	A	505	THR	CB-CA-C	-11.37	90.48	110.95
1	B	193	HIS	N-CA-C	10.29	123.46	111.11
1	B	290	LYS	N-CA-C	10.25	122.04	111.07
1	A	193	HIS	N-CA-C	10.25	123.41	111.11
1	A	290	LYS	N-CA-C	10.24	122.02	111.07
1	A	297	ARG	N-CA-C	10.05	126.41	112.75
1	B	297	ARG	N-CA-C	10.04	126.40	112.75
1	A	90	ALA	N-CA-C	-9.99	100.39	111.28
1	A	415	ASP	N-CA-C	9.98	125.46	113.28
1	B	415	ASP	N-CA-C	9.98	125.45	113.28
1	B	90	ALA	N-CA-C	-9.97	100.41	111.28
1	A	173	GLY	N-CA-C	9.77	126.46	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	GLY	N-CA-C	9.76	126.44	113.37
1	B	7	PHE	N-CA-C	9.58	121.81	111.36
1	A	7	PHE	N-CA-C	9.56	121.79	111.36
1	B	120	VAL	CB-CA-C	9.51	122.21	111.08
1	B	385	PHE	N-CA-C	-9.48	94.12	109.58
1	A	385	PHE	N-CA-C	-9.47	94.14	109.58
1	B	265	ILE	N-CA-C	9.47	120.18	108.06
1	B	512	GLN	N-CA-C	-9.45	100.98	111.28
1	A	265	ILE	N-CA-C	9.44	120.15	108.06
1	A	120	VAL	CB-CA-C	9.43	122.12	111.08
1	B	31	ILE	CB-CA-C	-9.43	95.82	111.29
1	B	146	VAL	CB-CA-C	-9.43	101.07	111.35
1	A	31	ILE	CB-CA-C	-9.42	95.84	111.29
1	A	512	GLN	N-CA-C	-9.41	101.02	111.28
1	A	146	VAL	CB-CA-C	-9.38	101.13	111.35
1	A	51	TYR	N-CA-C	-9.35	100.66	112.90
1	B	51	TYR	N-CA-C	-9.33	100.68	112.90
1	A	321	LEU	N-CA-C	9.24	121.43	111.36
1	B	321	LEU	N-CA-C	9.23	121.43	111.36
1	A	459	THR	CA-C-N	-9.20	110.87	122.37
1	A	459	THR	C-N-CA	-9.20	110.87	122.37
1	B	459	THR	CA-C-N	-9.19	110.89	122.37
1	B	459	THR	C-N-CA	-9.19	110.89	122.37
1	A	130	VAL	N-CA-C	-9.16	93.44	107.73
1	B	130	VAL	N-CA-C	-9.16	93.44	107.73
1	A	320	VAL	N-CA-C	-9.02	99.78	111.05
1	A	472	VAL	CB-CA-C	-9.01	96.51	111.29
1	B	320	VAL	N-CA-C	-9.01	99.79	111.05
1	B	472	VAL	CB-CA-C	-9.01	96.52	111.29
1	B	473	PHE	N-CA-C	-8.99	93.78	108.07
1	A	473	PHE	N-CA-C	-8.98	93.79	108.07
1	A	13	PRO	N-CA-C	-8.96	99.77	110.70
1	B	13	PRO	N-CA-C	-8.94	99.79	110.70
1	A	250	ILE	N-CA-C	8.84	122.96	112.80
1	A	272	ASN	CA-C-N	8.82	129.04	119.87
1	A	272	ASN	C-N-CA	8.82	129.04	119.87
1	B	250	ILE	N-CA-C	8.79	122.91	112.80
1	B	272	ASN	CA-C-N	8.79	129.01	119.87
1	B	272	ASN	C-N-CA	8.79	129.01	119.87
1	A	372	LYS	N-CA-C	-8.61	100.52	111.02
1	A	444	LYS	N-CA-CB	-8.60	97.61	110.07
1	B	372	LYS	N-CA-C	-8.58	100.55	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	LYS	N-CA-CB	-8.57	97.64	110.07
1	B	289	LEU	N-CA-C	-8.52	101.03	111.33
1	A	289	LEU	N-CA-C	-8.51	101.03	111.33
1	A	190	TYR	N-CA-C	-8.47	103.00	112.57
1	B	190	TYR	N-CA-C	-8.46	103.01	112.57
1	B	540	ILE	CB-CA-C	-8.36	99.21	112.16
1	A	540	ILE	CB-CA-C	-8.34	99.24	112.16
1	B	460	VAL	N-CA-C	8.21	120.79	108.23
1	A	460	VAL	N-CA-C	8.20	120.78	108.23
1	B	311	ILE	N-CA-CB	-8.13	102.67	112.35
1	A	104	ARG	N-CA-C	8.13	122.86	113.19
1	B	53	LYS	O-C-N	8.12	126.92	121.23
1	A	53	LYS	O-C-N	8.12	126.91	121.23
1	A	311	ILE	N-CA-CB	-8.12	102.69	112.35
1	B	227	GLY	N-CA-C	8.12	126.99	115.30
1	B	104	ARG	N-CA-C	8.11	122.84	113.19
1	B	461	GLY	N-CA-C	-8.11	99.80	112.85
1	A	227	GLY	N-CA-C	8.09	126.95	115.30
1	A	461	GLY	N-CA-C	-8.09	99.83	112.85
1	A	353	PHE	N-CA-C	8.01	121.08	108.67
1	B	353	PHE	N-CA-C	8.01	121.08	108.67
1	B	97	LEU	N-CA-C	8.00	122.55	110.14
1	B	451	GLY	N-CA-C	-8.00	104.18	115.30
1	A	97	LEU	N-CA-C	8.00	122.54	110.14
1	A	451	GLY	N-CA-C	-8.00	104.19	115.30
1	A	401	THR	CB-CA-C	7.95	123.35	110.88
1	B	443	THR	CB-CA-C	-7.94	98.11	110.81
1	B	401	THR	CB-CA-C	7.92	123.32	110.88
1	A	443	THR	CB-CA-C	-7.92	98.14	110.81
1	A	65	ASP	N-CA-C	-7.89	98.79	110.23
1	B	65	ASP	N-CA-C	-7.88	98.80	110.23
1	A	294	ASP	N-CA-C	-7.87	102.66	111.71
1	B	294	ASP	N-CA-C	-7.87	102.66	111.71
1	A	418	PRO	CA-C-N	-7.85	111.98	122.42
1	A	418	PRO	C-N-CA	-7.85	111.98	122.42
1	B	418	PRO	CA-C-N	-7.83	112.01	122.42
1	B	418	PRO	C-N-CA	-7.83	112.01	122.42
1	B	8	ARG	N-CA-CB	-7.78	100.64	111.77
1	B	306	GLN	N-CA-C	7.77	127.36	110.80
1	A	8	ARG	N-CA-CB	-7.75	100.69	111.77
1	A	306	GLN	N-CA-C	7.75	127.30	110.80
1	B	468	ILE	N-CA-C	7.72	117.75	106.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	PHE	N-CA-C	-7.72	100.07	109.72
1	A	468	ILE	N-CA-C	7.72	117.74	106.55
1	B	310	THR	N-CA-C	-7.68	97.32	109.23
1	A	310	THR	N-CA-C	-7.67	97.34	109.23
1	A	95	PHE	N-CA-C	-7.67	100.13	109.72
1	A	419	ASN	CB-CA-C	7.61	123.36	110.81
1	B	337	GLU	N-CA-C	7.60	119.35	111.14
1	B	128	ASN	CB-CA-C	-7.60	96.31	110.36
1	B	419	ASN	CB-CA-C	7.58	123.32	110.81
1	A	128	ASN	CB-CA-C	-7.58	96.34	110.36
1	B	555	HIS	N-CA-C	-7.58	103.03	111.82
1	B	465	MET	CB-CA-C	-7.57	98.48	110.14
1	A	454	PHE	N-CA-C	-7.57	99.83	110.50
1	A	465	MET	CB-CA-C	-7.57	98.48	110.14
1	A	494	ASP	CB-CA-C	-7.57	98.95	110.90
1	A	555	HIS	N-CA-C	-7.56	103.05	111.82
1	A	337	GLU	N-CA-C	7.56	119.31	111.14
1	B	494	ASP	CB-CA-C	-7.56	98.95	110.90
1	A	74	ILE	CA-C-N	-7.54	112.51	122.99
1	A	74	ILE	C-N-CA	-7.54	112.51	122.99
1	B	454	PHE	N-CA-C	-7.54	99.88	110.50
1	A	316	LEU	N-CA-C	-7.52	103.02	111.07
1	A	102	ILE	N-CA-C	7.52	124.98	109.34
1	B	316	LEU	N-CA-C	-7.52	103.03	111.07
1	A	26	GLN	N-CA-C	7.51	119.10	111.07
1	B	74	ILE	CA-C-N	-7.50	112.56	122.99
1	B	74	ILE	C-N-CA	-7.50	112.56	122.99
1	B	102	ILE	N-CA-C	7.50	124.94	109.34
1	B	26	GLN	N-CA-C	7.49	119.08	111.07
1	B	264	LYS	CB-CA-C	-7.45	96.76	110.62
1	A	67	ASP	N-CA-CB	-7.45	97.31	110.42
1	A	264	LYS	CB-CA-C	-7.44	96.78	110.62
1	A	77	PRO	N-CA-C	-7.44	99.51	111.19
1	A	129	ARG	CB-CG-CD	-7.44	94.19	111.30
1	B	129	ARG	CB-CG-CD	-7.43	94.20	111.30
1	B	67	ASP	N-CA-CB	-7.42	97.36	110.42
1	B	77	PRO	N-CA-C	-7.42	99.55	111.19
1	A	36	ASN	N-CA-C	7.40	122.33	113.16
1	B	36	ASN	N-CA-C	7.39	122.32	113.16
1	A	34	SER	N-CA-C	-7.33	103.44	112.38
1	B	212	THR	N-CA-C	7.32	121.36	110.52
1	B	34	SER	N-CA-C	-7.29	103.49	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ALA	N-CA-C	-7.29	96.37	108.32
1	A	513	ILE	N-CA-C	7.28	117.41	110.42
1	A	212	THR	N-CA-C	7.28	121.30	110.52
1	B	513	ILE	N-CA-C	7.27	117.40	110.42
1	A	267	ILE	CB-CA-C	-7.27	100.45	110.77
1	B	421	ALA	N-CA-C	-7.27	96.40	108.32
1	B	536	ASP	O-C-N	7.23	127.28	121.20
1	A	536	ASP	O-C-N	7.22	127.27	121.20
1	B	267	ILE	CB-CA-C	-7.22	100.51	110.77
1	A	205	ALA	N-CA-C	7.19	119.12	111.28
1	A	107	GLY	N-CA-C	-7.19	105.40	115.32
1	A	411	LEU	CB-CA-C	-7.18	98.48	110.68
1	B	107	GLY	N-CA-C	-7.18	105.42	115.32
1	A	312	ARG	N-CA-C	7.16	121.51	110.20
1	B	205	ALA	N-CA-C	7.16	119.08	111.28
1	B	312	ARG	N-CA-C	7.14	121.48	110.20
1	B	411	LEU	CB-CA-C	-7.14	98.55	110.68
1	A	70	LEU	N-CA-C	7.13	120.94	108.75
1	B	70	LEU	N-CA-C	7.12	120.93	108.75
1	A	425	PHE	CB-CA-C	7.11	121.42	109.48
1	A	374	ALA	N-CA-C	7.07	118.64	111.07
1	A	211	ARG	N-CA-C	-7.06	97.06	109.06
1	B	374	ALA	N-CA-C	7.06	118.62	111.07
1	B	211	ARG	N-CA-C	-7.04	97.10	109.06
1	A	521	ASN	N-CA-C	6.93	121.47	111.56
1	B	437	MET	N-CA-CB	-6.93	100.02	110.07
1	B	521	ASN	N-CA-C	6.91	121.45	111.56
1	A	437	MET	N-CA-CB	-6.89	100.08	110.07
1	B	536	ASP	CA-C-N	6.88	128.44	119.84
1	B	536	ASP	C-N-CA	6.88	128.44	119.84
1	A	74	ILE	CB-CA-C	-6.87	99.92	110.50
1	A	330	ARG	NE-CZ-NH1	-6.87	114.63	121.50
1	B	447	CYS	N-CA-C	-6.87	103.79	111.28
1	A	536	ASP	CA-C-N	6.86	128.41	119.84
1	A	536	ASP	C-N-CA	6.86	128.41	119.84
1	B	74	ILE	CB-CA-C	-6.85	99.96	110.50
1	A	447	CYS	N-CA-C	-6.84	103.82	111.28
1	B	330	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	B	204	LEU	N-CA-C	-6.80	101.76	110.19
1	B	273	PRO	N-CA-C	6.79	122.38	114.03
1	A	204	LEU	N-CA-C	-6.77	101.79	110.19
1	A	273	PRO	N-CA-C	6.76	122.35	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	VAL	CB-CA-C	-6.76	103.19	112.04
1	B	80	VAL	CB-CA-C	-6.74	103.22	112.04
1	B	352	ASN	N-CA-C	6.73	120.44	107.44
1	B	425	PHE	CB-CA-C	6.70	121.44	109.38
1	A	352	ASN	N-CA-C	6.69	120.34	107.44
1	B	309	PRO	CB-CA-C	-6.66	102.26	110.98
1	A	309	PRO	CB-CA-C	-6.66	102.26	110.98
1	B	546	SER	N-CA-C	-6.64	104.76	112.86
1	B	511	ASP	N-CA-C	6.63	118.30	111.14
1	B	553	TYR	N-CA-C	6.62	119.52	108.73
1	B	538	ASN	N-CA-C	6.61	121.35	113.28
1	A	546	SER	N-CA-C	-6.60	104.80	112.86
1	A	553	TYR	N-CA-C	6.59	119.47	108.73
1	A	538	ASN	N-CA-C	6.59	121.31	113.28
1	A	180	ALA	N-CA-C	6.57	119.44	111.82
1	A	511	ASP	N-CA-C	6.56	118.23	111.14
1	B	62	HIS	N-CA-C	6.56	119.39	108.96
1	B	202	VAL	N-CA-C	6.56	117.80	108.42
1	A	202	VAL	N-CA-C	6.55	117.78	108.42
1	A	471	ILE	CB-CA-C	-6.55	102.14	111.31
1	A	41	SER	N-CA-C	6.53	120.45	112.23
1	B	341	LYS	N-CA-C	-6.52	104.09	111.07
1	B	471	ILE	CB-CA-C	-6.52	102.18	111.31
1	B	41	SER	N-CA-C	6.52	120.45	112.23
1	A	62	HIS	N-CA-C	6.51	119.32	108.96
1	B	180	ALA	N-CA-C	6.51	119.37	111.82
1	B	474	ASN	N-CA-CB	-6.49	100.82	110.24
1	A	341	LYS	N-CA-C	-6.47	104.15	111.07
1	A	174	GLY	N-CA-C	6.46	119.44	112.33
1	A	474	ASN	N-CA-CB	-6.46	100.87	110.24
1	B	174	GLY	N-CA-C	6.44	119.42	112.33
1	A	80	VAL	N-CA-C	6.44	117.96	110.62
1	A	462	MET	CB-CA-C	-6.42	98.33	110.67
1	B	417	LEU	CA-CB-CG	-6.42	93.83	116.30
1	A	417	LEU	CA-CB-CG	-6.41	93.88	116.30
1	B	462	MET	CB-CA-C	-6.41	98.37	110.67
1	B	80	VAL	N-CA-C	6.40	117.92	110.62
1	A	400	LYS	N-CA-C	-6.39	104.23	111.07
1	B	401	THR	N-CA-C	6.39	117.91	111.07
1	A	502	GLU	CA-CB-CG	-6.38	101.35	114.10
1	B	400	LYS	N-CA-C	-6.37	104.25	111.07
1	A	401	THR	N-CA-C	6.37	117.88	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ASP	N-CA-C	6.37	118.22	111.28
1	B	493	ASP	N-CA-C	6.37	118.22	111.28
1	B	502	GLU	CA-CB-CG	-6.37	101.37	114.10
1	A	536	ASP	C-N-CD	-6.36	98.92	125.00
1	B	536	ASP	C-N-CD	-6.36	98.93	125.00
1	A	169	PRO	N-CA-C	-6.34	99.41	112.47
1	B	342	ILE	CB-CA-C	-6.34	103.48	112.22
1	B	169	PRO	N-CA-C	-6.33	99.44	112.47
1	B	115	VAL	CB-CA-C	-6.32	103.07	110.91
1	A	87	VAL	N-CA-C	-6.32	104.17	110.62
1	A	468	ILE	CB-CA-C	-6.31	105.48	112.68
1	A	115	VAL	CB-CA-C	-6.31	103.09	110.91
1	B	87	VAL	N-CA-C	-6.30	104.19	110.62
1	B	260	GLY	N-CA-C	6.29	120.00	110.18
1	A	342	ILE	CB-CA-C	-6.29	103.54	112.22
1	A	260	GLY	N-CA-C	6.28	119.98	110.18
1	B	468	ILE	CB-CA-C	-6.28	105.52	112.68
1	A	409	ASP	N-CA-C	6.25	119.07	111.82
1	B	341	LYS	CB-CA-C	-6.24	101.08	110.88
1	B	409	ASP	N-CA-C	6.24	119.06	111.82
1	B	502	GLU	N-CA-C	-6.23	101.55	110.59
1	A	341	LYS	CB-CA-C	-6.23	101.11	110.88
1	A	502	GLU	N-CA-C	-6.23	101.56	110.59
1	B	39	VAL	N-CA-CB	6.21	117.48	110.72
1	B	332	GLU	N-CA-CB	6.21	121.42	110.37
1	A	332	GLU	N-CA-CB	6.20	121.41	110.37
1	A	39	VAL	N-CA-CB	6.18	117.46	110.72
1	A	73	ALA	CA-C-N	-6.18	114.35	122.94
1	A	73	ALA	C-N-CA	-6.18	114.35	122.94
1	B	73	ALA	CA-C-N	-6.17	114.36	122.94
1	B	73	ALA	C-N-CA	-6.17	114.36	122.94
1	B	540	ILE	CA-C-N	-6.17	113.25	122.01
1	B	540	ILE	C-N-CA	-6.17	113.25	122.01
1	A	272	ASN	N-CA-C	-6.16	100.97	109.71
1	B	272	ASN	N-CA-C	-6.16	100.97	109.71
1	B	383	PHE	N-CA-C	6.14	119.82	109.76
1	A	427	PRO	N-CA-C	-6.13	101.83	111.34
1	A	383	PHE	N-CA-C	6.13	119.81	109.76
1	A	540	ILE	CA-C-N	-6.12	113.32	122.01
1	A	540	ILE	C-N-CA	-6.12	113.32	122.01
1	A	462	MET	CA-C-N	-6.11	111.15	121.18
1	A	462	MET	C-N-CA	-6.11	111.15	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	MET	CA-C-N	-6.11	111.16	121.18
1	B	462	MET	C-N-CA	-6.11	111.16	121.18
1	B	407	THR	CB-CA-C	-6.11	101.35	113.45
1	B	427	PRO	N-CA-C	-6.11	101.88	111.34
1	B	268	TRP	N-CA-C	6.10	119.12	109.96
1	A	407	THR	CB-CA-C	-6.10	101.37	113.45
1	A	428	ILE	N-CA-C	-6.10	99.70	108.48
1	B	425	PHE	N-CA-C	-6.09	99.78	109.59
1	B	428	ILE	N-CA-C	-6.08	99.72	108.48
1	A	268	TRP	N-CA-C	6.08	119.08	109.96
1	A	425	PHE	N-CA-C	-6.06	99.82	109.76
1	A	29	ILE	N-CA-C	-6.04	104.46	110.62
1	B	530	VAL	CB-CA-C	-6.03	104.16	111.88
1	B	153	ASN	N-CA-C	-6.03	104.78	111.71
1	A	530	VAL	CB-CA-C	-6.02	104.18	111.88
1	B	29	ILE	N-CA-C	-6.01	104.49	110.62
1	A	153	ASN	N-CA-C	-6.01	104.80	111.71
1	A	260	GLY	CA-C-N	-6.00	114.94	123.11
1	A	260	GLY	C-N-CA	-6.00	114.94	123.11
1	A	267	ILE	N-CA-C	5.99	116.50	107.75
1	A	533	ASN	N-CA-CB	5.99	118.65	109.91
1	B	267	ILE	N-CA-C	5.99	116.49	107.75
1	B	533	ASN	N-CA-CB	5.98	118.65	109.91
1	B	384	TYR	N-CA-C	5.97	118.15	109.07
1	A	472	VAL	N-CA-C	-5.97	96.92	109.34
1	B	260	GLY	CA-C-N	-5.97	114.99	123.11
1	B	260	GLY	C-N-CA	-5.97	114.99	123.11
1	B	61	HIS	N-CA-C	-5.96	98.11	110.80
1	B	171	LEU	N-CA-C	5.96	119.76	110.17
1	A	542	ALA	N-CA-C	5.95	122.97	109.81
1	A	171	LEU	N-CA-C	5.95	119.75	110.17
1	B	452	LEU	CA-CB-CG	-5.95	95.47	116.30
1	A	61	HIS	N-CA-C	-5.95	98.13	110.80
1	B	472	VAL	N-CA-C	-5.95	96.97	109.34
1	A	70	LEU	N-CA-CB	-5.94	100.37	111.13
1	A	396	ARG	CA-CB-CG	-5.94	102.22	114.10
1	B	362	PRO	N-CA-C	-5.94	105.63	113.65
1	A	362	PRO	N-CA-C	-5.94	105.63	113.65
1	A	384	TYR	N-CA-C	5.94	118.10	109.07
1	B	396	ARG	CA-CB-CG	-5.94	102.22	114.10
1	A	452	LEU	CA-CB-CG	-5.93	95.53	116.30
1	B	542	ALA	N-CA-C	5.92	122.90	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	LYS	CB-CA-C	5.91	119.16	109.46
1	B	70	LEU	N-CA-CB	-5.91	100.44	111.13
1	A	254	PHE	N-CA-C	5.90	120.48	113.28
1	A	229	LYS	CB-CA-C	5.90	119.13	109.46
1	A	423	LEU	N-CA-C	-5.89	99.75	108.99
1	B	423	LEU	N-CA-C	-5.88	99.75	108.99
1	B	254	PHE	N-CA-C	5.88	120.46	113.28
1	A	378	ILE	CA-C-O	5.84	123.47	119.20
1	A	476	LYS	N-CA-C	5.84	121.31	113.72
1	B	476	LYS	N-CA-C	5.83	121.30	113.72
1	B	430	LYS	CB-CA-C	-5.82	97.60	109.65
1	A	142	VAL	N-CA-C	5.81	118.54	108.90
1	B	281	ILE	N-CA-C	-5.81	97.26	109.34
1	B	378	ILE	CA-C-O	5.80	123.44	119.20
1	A	281	ILE	N-CA-C	-5.79	97.29	109.34
1	B	142	VAL	N-CA-C	5.79	118.51	108.90
1	A	430	LYS	CB-CA-C	-5.78	97.69	109.65
1	B	15	LYS	CA-C-N	-5.77	113.55	122.09
1	B	15	LYS	C-N-CA	-5.77	113.55	122.09
1	A	15	LYS	CA-C-N	-5.74	113.60	122.09
1	A	15	LYS	C-N-CA	-5.74	113.60	122.09
1	B	511	ASP	O-C-N	5.73	128.28	122.09
1	A	424	PHE	CB-CA-C	-5.71	97.79	109.38
1	A	130	VAL	CB-CA-C	-5.71	104.00	111.25
1	B	307	ASN	N-CA-C	-5.70	101.22	109.31
1	A	52	MET	CB-CA-C	5.70	120.24	110.79
1	A	308	VAL	CA-C-O	5.69	122.51	119.15
1	B	130	VAL	CB-CA-C	-5.69	104.03	111.25
1	B	58	HIS	N-CA-C	5.69	115.75	108.24
1	B	424	PHE	CB-CA-C	-5.68	97.84	109.38
1	A	135	VAL	N-CA-C	5.67	117.19	111.00
1	B	313	HIS	CB-CA-C	5.67	118.89	109.53
1	A	307	ASN	N-CA-C	-5.67	101.26	109.31
1	B	147	THR	N-CA-C	-5.67	103.22	110.53
1	B	52	MET	CB-CA-C	5.67	120.20	110.79
1	B	272	ASN	O-C-N	5.67	125.89	121.47
1	A	313	HIS	CB-CA-C	5.66	118.86	109.53
1	B	135	VAL	N-CA-C	5.65	117.16	111.00
1	A	147	THR	N-CA-C	-5.65	103.24	110.53
1	A	58	HIS	N-CA-C	5.63	115.68	108.24
1	B	158	ASN	N-CA-C	-5.63	104.65	112.30
1	B	308	VAL	CA-C-O	5.62	122.47	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ALA	CA-C-N	-5.62	112.31	120.29
1	B	90	ALA	C-N-CA	-5.62	112.31	120.29
1	A	272	ASN	O-C-N	5.61	125.85	121.47
1	A	511	ASP	O-C-N	5.61	128.15	122.09
1	A	158	ASN	N-CA-C	-5.59	104.69	112.30
1	A	90	ALA	CA-C-N	-5.58	112.37	120.29
1	A	90	ALA	C-N-CA	-5.58	112.37	120.29
1	B	330	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	475	LYS	N-CA-C	5.55	119.53	112.87
1	B	341	LYS	CA-C-N	-5.55	112.55	120.42
1	B	341	LYS	C-N-CA	-5.55	112.55	120.42
1	A	330	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	A	341	LYS	CA-C-N	-5.53	112.57	120.42
1	A	341	LYS	C-N-CA	-5.53	112.57	120.42
1	B	475	LYS	N-CA-C	5.53	119.51	112.87
1	A	431	VAL	N-CA-C	-5.51	98.56	106.55
1	B	241	LEU	N-CA-C	-5.50	105.20	113.89
1	B	327	TYR	CA-CB-CG	5.48	123.77	113.90
1	A	241	LEU	N-CA-C	-5.48	105.23	113.89
1	B	336	ASP	N-CA-C	-5.48	105.41	111.71
1	B	376	SER	N-CA-C	5.48	119.22	112.54
1	A	376	SER	N-CA-C	5.47	119.22	112.54
1	A	236	SER	N-CA-C	-5.46	103.32	110.53
1	A	444	LYS	CB-CG-CD	-5.46	98.75	111.30
1	B	431	VAL	N-CA-C	-5.46	98.64	106.55
1	B	236	SER	N-CA-C	-5.45	103.33	110.53
1	B	444	LYS	CB-CG-CD	-5.45	98.76	111.30
1	A	327	TYR	CA-CB-CG	5.45	123.70	113.90
1	A	336	ASP	N-CA-C	-5.45	105.45	111.71
1	B	279	TYR	N-CA-C	5.44	115.55	107.88
1	B	264	LYS	O-C-N	5.43	129.23	123.42
1	B	332	GLU	CB-CA-C	5.42	120.85	110.17
1	B	105	ASN	CA-C-N	5.42	128.40	120.71
1	B	105	ASN	C-N-CA	5.42	128.40	120.71
1	B	504	ARG	CA-C-N	-5.42	112.02	122.09
1	B	504	ARG	C-N-CA	-5.42	112.02	122.09
1	A	279	TYR	N-CA-C	5.41	115.51	107.88
1	B	16	LEU	CA-CB-CG	-5.41	97.36	116.30
1	A	16	LEU	CA-CB-CG	-5.41	97.36	116.30
1	A	105	ASN	CA-C-N	5.41	128.39	120.71
1	A	105	ASN	C-N-CA	5.41	128.39	120.71
1	A	504	ARG	CA-C-N	-5.41	112.03	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ARG	C-N-CA	-5.41	112.03	122.09
1	A	548	VAL	CB-CA-C	5.41	118.20	110.84
1	A	332	GLU	CB-CA-C	5.40	120.82	110.17
1	B	334	LEU	N-CA-C	5.40	118.27	110.28
1	A	334	LEU	N-CA-C	5.39	118.26	110.28
1	B	502	GLU	N-CA-CB	5.39	118.62	110.42
1	B	548	VAL	CB-CA-C	5.39	118.17	110.84
1	B	396	ARG	CG-CD-NE	-5.39	100.14	112.00
1	A	502	GLU	N-CA-CB	5.38	118.60	110.42
1	B	533	ASN	N-CA-C	5.37	116.82	110.97
1	A	396	ARG	CG-CD-NE	-5.36	100.22	112.00
1	B	81	ALA	N-CA-C	-5.36	105.44	111.28
1	B	44	ASP	CA-C-N	5.35	132.02	121.58
1	B	44	ASP	C-N-CA	5.35	132.02	121.58
1	A	394	VAL	N-CA-C	-5.35	105.29	110.42
1	A	340	ASP	N-CA-C	-5.34	104.70	111.11
1	A	545	LYS	CB-CA-C	-5.34	101.56	109.90
1	A	533	ASN	N-CA-C	5.34	116.79	110.97
1	A	330	ARG	N-CA-CB	-5.34	102.58	110.37
1	A	81	ALA	N-CA-C	-5.33	105.47	111.28
1	A	44	ASP	CA-C-N	5.33	131.97	121.58
1	A	44	ASP	C-N-CA	5.33	131.97	121.58
1	A	264	LYS	O-C-N	5.33	129.12	123.42
1	B	545	LYS	CB-CA-C	-5.33	101.59	109.90
1	B	394	VAL	N-CA-C	-5.32	105.31	110.42
1	B	340	ASP	N-CA-C	-5.32	104.73	111.11
1	A	37	VAL	CB-CA-C	-5.31	102.32	110.50
1	B	37	VAL	CB-CA-C	-5.31	102.32	110.50
1	B	330	ARG	N-CA-CB	-5.31	102.61	110.37
1	B	259	MET	CA-CB-CG	-5.30	103.49	114.10
1	B	422	HIS	CB-CA-C	5.30	118.55	109.80
1	A	259	MET	CA-CB-CG	-5.30	103.50	114.10
1	A	422	HIS	CB-CA-C	5.28	118.51	109.80
1	A	423	LEU	CA-C-N	-5.27	113.30	122.37
1	A	423	LEU	C-N-CA	-5.27	113.30	122.37
1	B	125	LYS	N-CA-C	5.27	117.45	111.02
1	B	155	LEU	N-CA-C	5.27	117.03	111.28
1	B	203	VAL	N-CA-C	-5.27	99.50	107.73
1	A	161	ARG	CB-CA-C	-5.27	100.24	110.46
1	A	203	VAL	N-CA-C	-5.27	99.51	107.73
1	A	125	LYS	N-CA-C	5.26	117.44	111.02
1	B	161	ARG	CB-CA-C	-5.26	100.25	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	LEU	CA-C-N	-5.26	113.33	122.37
1	B	423	LEU	C-N-CA	-5.26	113.33	122.37
1	A	242	PHE	CA-C-N	5.26	126.41	119.84
1	A	242	PHE	C-N-CA	5.26	126.41	119.84
1	A	290	LYS	CA-CB-CG	-5.26	103.58	114.10
1	B	290	LYS	CA-CB-CG	-5.26	103.59	114.10
1	A	155	LEU	N-CA-C	5.25	117.00	111.28
1	B	430	LYS	CB-CG-CD	-5.25	99.23	111.30
1	B	533	ASN	CB-CA-C	5.23	119.02	110.96
1	A	430	LYS	CB-CG-CD	-5.23	99.28	111.30
1	B	495	CYS	CA-CB-SG	-5.23	102.38	114.40
1	B	40	ILE	O-C-N	5.22	126.35	121.96
1	A	389	THR	N-CA-C	5.22	116.70	108.55
1	B	389	THR	N-CA-C	5.22	116.69	108.55
1	A	533	ASN	CB-CA-C	5.22	118.99	110.96
1	A	495	CYS	CA-CB-SG	-5.21	102.41	114.40
1	B	242	PHE	CA-C-N	5.21	126.35	119.84
1	B	242	PHE	C-N-CA	5.21	126.35	119.84
1	B	435	ASP	N-CA-C	-5.21	105.61	111.28
1	A	550	PRO	N-CA-C	-5.20	103.02	111.14
1	B	222	ARG	CA-C-N	5.20	126.34	119.84
1	B	222	ARG	C-N-CA	5.20	126.34	119.84
1	B	550	PRO	N-CA-C	-5.20	103.03	111.14
1	B	36	ASN	CB-CA-C	5.19	119.36	110.01
1	A	36	ASN	CB-CA-C	5.19	119.35	110.01
1	B	257	SER	N-CA-C	-5.19	101.55	108.34
1	B	253	LEU	N-CA-C	-5.18	106.06	112.38
1	A	222	ARG	CA-C-N	5.17	126.31	119.84
1	A	222	ARG	C-N-CA	5.17	126.31	119.84
1	A	253	LEU	N-CA-C	-5.17	106.07	112.38
1	A	40	ILE	O-C-N	5.16	126.30	121.96
1	A	546	SER	CB-CA-C	5.16	119.77	111.36
1	A	422	HIS	CA-C-N	-5.16	112.72	121.85
1	A	422	HIS	C-N-CA	-5.16	112.72	121.85
1	B	422	HIS	CA-C-N	-5.16	112.72	121.85
1	B	422	HIS	C-N-CA	-5.16	112.72	121.85
1	B	546	SER	CB-CA-C	5.16	119.76	111.36
1	A	257	SER	N-CA-C	-5.15	101.59	108.34
1	A	393	SER	N-CA-C	5.14	117.92	110.42
1	A	364	ARG	CG-CD-NE	-5.13	100.72	112.00
1	A	95	PHE	CA-C-N	-5.11	115.09	120.66
1	A	95	PHE	C-N-CA	-5.11	115.09	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	SER	N-CA-C	5.11	117.87	110.42
1	A	40	ILE	CA-C-N	5.10	129.35	120.68
1	A	40	ILE	C-N-CA	5.10	129.35	120.68
1	B	311	ILE	CB-CA-C	-5.10	105.43	111.09
1	A	282	THR	N-CA-CB	5.10	117.75	110.06
1	B	282	THR	N-CA-CB	5.09	117.75	110.06
1	B	364	ARG	CG-CD-NE	-5.09	100.80	112.00
1	A	503	TYR	N-CA-C	-5.09	105.85	113.89
1	B	244	TYR	CB-CA-C	-5.09	102.19	110.85
1	A	244	TYR	CB-CA-C	-5.09	102.20	110.85
1	A	435	ASP	N-CA-C	-5.09	105.74	111.28
1	B	503	TYR	N-CA-C	-5.08	105.87	113.89
1	A	434	GLU	CB-CA-C	-5.07	103.15	110.96
1	B	95	PHE	CA-C-N	-5.07	115.14	120.66
1	B	95	PHE	C-N-CA	-5.07	115.14	120.66
1	B	350	ARG	N-CA-C	-5.06	105.85	112.23
1	B	434	GLU	CB-CA-C	-5.06	103.16	110.96
1	B	187	TYR	CB-CA-C	5.06	119.46	110.85
1	A	187	TYR	CB-CA-C	5.06	119.45	110.85
1	A	311	ILE	CB-CA-C	-5.06	105.47	111.09
1	B	466	HIS	CB-CA-C	-5.06	102.50	111.05
1	A	346	LEU	N-CA-C	5.05	119.72	113.50
1	A	350	ARG	N-CA-C	-5.05	105.86	112.23
1	B	40	ILE	CA-C-N	5.05	129.27	120.68
1	B	40	ILE	C-N-CA	5.05	129.27	120.68
1	A	77	PRO	CA-C-N	5.05	129.27	120.68
1	A	77	PRO	C-N-CA	5.05	129.27	120.68
1	A	99	PRO	CA-C-N	-5.05	114.95	122.23
1	A	99	PRO	C-N-CA	-5.05	114.95	122.23
1	A	272	ASN	CA-C-O	5.05	123.98	119.59
1	B	553	TYR	CA-CB-CG	-5.05	104.81	113.90
1	A	414	ILE	N-CA-C	-5.05	106.44	113.00
1	A	553	TYR	CA-CB-CG	-5.05	104.81	113.90
1	B	77	PRO	CA-C-N	5.05	129.26	120.68
1	B	77	PRO	C-N-CA	5.05	129.26	120.68
1	B	463	ARG	N-CA-C	-5.04	105.22	113.19
1	A	466	HIS	CB-CA-C	-5.04	102.53	111.05
1	A	65	ASP	CA-C-O	-5.04	115.65	121.19
1	A	463	ARG	N-CA-C	-5.04	105.23	113.19
1	A	483	LYS	N-CA-C	-5.03	105.80	111.28
1	B	99	PRO	CA-C-N	-5.03	114.99	122.23
1	B	99	PRO	C-N-CA	-5.03	114.99	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ILE	N-CA-C	-5.02	106.48	113.00
1	B	346	LEU	N-CA-C	5.02	119.67	113.50
1	A	150	ASP	CB-CA-C	-5.01	103.24	110.96
1	B	209	LEU	CA-CB-CG	5.01	133.84	116.30
1	A	231	GLU	CA-CB-CG	-5.01	104.08	114.10
1	A	289	LEU	CA-C-N	-5.01	113.93	120.44
1	A	289	LEU	C-N-CA	-5.01	113.93	120.44
1	B	289	LEU	CA-C-N	-5.01	113.93	120.44
1	B	289	LEU	C-N-CA	-5.01	113.93	120.44
1	B	231	GLU	CA-CB-CG	-5.01	104.08	114.10
1	A	209	LEU	CA-CB-CG	5.01	133.82	116.30
1	B	65	ASP	CA-C-O	-5.01	115.68	121.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	187	TYR	CA
1	A	332	GLU	CA
1	B	187	TYR	CA
1	B	332	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	547	0
1	B	4391	0	4330	565	0
2	A	61	0	35	12	0
2	B	61	0	35	13	0
3	A	55	0	0	9	0
3	B	52	0	0	9	0
All	All	9011	0	8730	1090	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 63.

All (1090) 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:507:LEU:HA	1:A:510:MET:HE3	1.18	1.18
1:B:507:LEU:HA	1:B:510:MET:HE3	1.18	1.16
2:A:600:FAA:H51A	2:A:600:FAA:H8A	1.21	1.13
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.32	1.11
2:B:600:FAA:H51A	2:B:600:FAA:H8A	1.21	1.10
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.32	1.07
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.32	1.05
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.32	1.05
1:A:56:HIS:HA	1:A:111:ALA:HB3	1.44	0.97
1:B:56:HIS:HA	1:B:111:ALA:HB3	1.44	0.96
1:B:280:LEU:HD12	1:B:281:ILE:H	1.31	0.95
1:A:280:LEU:HD12	1:A:281:ILE:H	1.31	0.95
1:B:61:HIS:HB3	1:B:421:ALA:HB1	1.49	0.94
1:A:61:HIS:HB3	1:A:421:ALA:HB1	1.49	0.92
1:A:253:LEU:HD11	1:B:253:LEU:HD21	1.51	0.91
1:A:200:MET:HE2	1:A:251:ASP:HB3	1.52	0.91
1:B:200:MET:HE2	1:B:251:ASP:HB3	1.52	0.90
1:A:61:HIS:HE1	3:A:641:HOH:O	1.54	0.90
1:B:419:ASN:O	1:B:474:ASN:HA	1.72	0.89
1:B:555:HIS:CB	1:B:559:LYS:HE3	2.02	0.88
1:A:555:HIS:CB	1:A:559:LYS:HE3	2.02	0.88
1:A:480:GLN:HA	1:A:483:LYS:CD	2.04	0.88
1:B:554:SER:HB3	1:B:557:THR:HB	1.56	0.88
1:A:309:PRO:HG2	1:A:460:VAL:CB	2.04	0.88
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.09	0.88
1:B:133:VAL:HG21	1:B:154:TYR:CE1	2.09	0.87
1:A:419:ASN:O	1:A:474:ASN:HA	1.72	0.87
1:B:480:GLN:HA	1:B:483:LYS:CD	2.04	0.87
1:A:133:VAL:HG21	1:A:154:TYR:CE1	2.09	0.87
1:B:507:LEU:HA	1:B:510:MET:CE	2.05	0.87
1:A:507:LEU:HA	1:A:510:MET:CE	2.05	0.87
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.09	0.87
1:B:309:PRO:HG2	1:B:460:VAL:CB	2.04	0.86
1:A:554:SER:HB3	1:A:557:THR:HB	1.56	0.85
1:B:480:GLN:HA	1:B:483:LYS:HD2	1.58	0.85
1:B:463:ARG:HD2	3:B:630:HOH:O	1.76	0.84
1:A:56:HIS:HA	1:A:111:ALA:CB	2.09	0.83
1:A:80:VAL:HG11	1:A:209:LEU:HD21	1.61	0.82
1:A:61:HIS:NE2	1:A:422:HIS:ND1	2.28	0.82
1:A:369:GLU:O	1:A:373:ASP:HB3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ILE:HB	1:A:381:VAL:HG21	1.62	0.82
1:A:425:PHE:CZ	1:A:427:PRO:HG3	2.14	0.82
1:A:480:GLN:HA	1:A:483:LYS:HD2	1.59	0.82
1:A:247:GLY:O	1:B:183:ARG:NH2	2.11	0.82
1:B:56:HIS:HA	1:B:111:ALA:CB	2.09	0.82
1:B:369:GLU:O	1:B:373:ASP:HB3	1.79	0.82
2:B:600:FAA:H8A	2:B:600:FAA:C5B	2.07	0.82
1:B:425:PHE:CZ	1:B:427:PRO:HG3	2.14	0.81
1:A:132:GLU:HG2	1:A:133:VAL:N	1.95	0.81
1:B:61:HIS:NE2	1:B:422:HIS:ND1	2.28	0.81
1:B:80:VAL:HG11	1:B:209:LEU:HD21	1.61	0.81
1:A:309:PRO:CG	1:A:460:VAL:HB	2.10	0.81
1:B:378:ILE:HB	1:B:381:VAL:HG21	1.62	0.81
1:A:187:TYR:O	1:A:307:ASN:HB2	1.82	0.80
2:A:600:FAA:H8A	2:A:600:FAA:C5B	2.07	0.80
1:B:156:GLU:HB2	1:B:161:ARG:HH21	1.46	0.80
2:B:600:FAA:H51A	2:B:600:FAA:C8A	2.09	0.80
1:B:316:LEU:O	1:B:320:VAL:HG23	1.81	0.80
1:A:316:LEU:O	1:A:320:VAL:HG23	1.81	0.80
1:B:187:TYR:O	1:B:307:ASN:HB2	1.82	0.80
1:A:479:ILE:O	1:A:483:LYS:HG3	1.81	0.79
1:A:156:GLU:HB2	1:A:161:ARG:HH21	1.46	0.79
1:A:445:LYS:O	1:A:449:GLU:HG3	1.82	0.79
1:B:479:ILE:O	1:B:483:LYS:HG3	1.81	0.79
1:B:132:GLU:HG2	1:B:133:VAL:N	1.95	0.79
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.64	0.79
1:B:445:LYS:O	1:B:449:GLU:HG3	1.82	0.79
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.64	0.79
1:B:309:PRO:CG	1:B:460:VAL:HB	2.10	0.78
1:B:480:GLN:O	1:B:484:VAL:HG23	1.84	0.78
1:A:341:LYS:O	1:A:345:GLN:HG3	1.83	0.78
1:A:177:LEU:HD12	1:A:265:ILE:HG22	1.66	0.78
1:B:45:GLN:HA	3:B:642:HOH:O	1.83	0.78
1:B:289:LEU:HB2	1:B:351:TRP:NE1	1.98	0.78
1:A:480:GLN:O	1:A:484:VAL:HG23	1.84	0.78
1:B:91:ASN:ND2	1:B:538:ASN:HD22	1.82	0.78
1:A:289:LEU:HB2	1:A:351:TRP:NE1	1.98	0.78
1:B:550:PRO:HB2	1:B:552:GLN:HG2	1.66	0.78
1:A:202:VAL:HG23	1:A:261:ILE:C	2.09	0.77
1:B:177:LEU:HD12	1:B:265:ILE:HG22	1.65	0.77
1:B:341:LYS:O	1:B:345:GLN:HG3	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:ND2	1:B:81:ALA:HB3	2.00	0.77
1:A:91:ASN:ND2	1:A:538:ASN:HD22	1.82	0.77
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.67	0.77
1:B:202:VAL:HG23	1:B:261:ILE:C	2.09	0.77
1:B:300:ARG:HA	1:B:305:LEU:HB2	1.67	0.77
1:A:300:ARG:HA	1:A:305:LEU:HB2	1.67	0.76
1:A:77:PRO:HB2	1:A:127:MET:CE	2.15	0.76
2:A:600:FAA:H51A	2:A:600:FAA:C8A	2.09	0.76
1:B:51:TYR:CE1	1:B:171:LEU:HD13	2.21	0.76
1:B:98:TRP:HB3	1:B:120:VAL:HG22	1.67	0.76
1:A:51:TYR:CE1	1:A:171:LEU:HD13	2.21	0.76
1:B:77:PRO:HB2	1:B:127:MET:CE	2.15	0.76
1:A:61:HIS:HA	1:A:475:LYS:HE2	1.68	0.75
1:A:550:PRO:HB2	1:A:552:GLN:HG2	1.66	0.75
1:A:555:HIS:CG	1:A:559:LYS:HE3	2.22	0.75
1:A:79:ASN:ND2	1:A:81:ALA:HB3	2.00	0.75
1:B:61:HIS:HA	1:B:475:LYS:HE2	1.68	0.75
1:B:414:ILE:HG23	3:B:636:HOH:O	1.85	0.75
1:A:43:LYS:O	1:A:45:GLN:HG2	1.87	0.75
1:B:485:GLN:O	1:B:489:ARG:HG3	1.86	0.75
1:B:555:HIS:CG	1:B:559:LYS:HE3	2.21	0.75
1:A:229:LYS:O	1:A:233:GLN:HG3	1.86	0.75
1:B:341:LYS:O	1:B:344:LYS:HG2	1.87	0.75
1:B:229:LYS:O	1:B:233:GLN:HG3	1.86	0.75
1:B:47:VAL:HG11	3:B:640:HOH:O	1.86	0.75
1:A:289:LEU:HB2	1:A:351:TRP:CD1	2.22	0.74
1:B:280:LEU:HD12	1:B:281:ILE:N	2.02	0.74
1:B:10:LEU:HD21	1:B:42:SER:CA	2.18	0.74
1:B:555:HIS:HB3	1:B:559:LYS:CE	2.15	0.74
1:A:98:TRP:HB3	1:A:120:VAL:HG22	1.67	0.74
1:B:43:LYS:O	1:B:45:GLN:HG2	1.86	0.74
1:A:485:GLN:O	1:A:489:ARG:HG3	1.86	0.74
1:B:289:LEU:HB2	1:B:351:TRP:CD1	2.22	0.74
1:A:247:GLY:C	1:B:183:ARG:HH22	1.95	0.74
1:A:280:LEU:HD12	1:A:281:ILE:N	2.02	0.73
1:A:10:LEU:HD21	1:A:42:SER:CA	2.18	0.73
1:B:399:ASP:O	1:B:403:GLN:HG2	1.88	0.73
1:B:505:THR:OG1	1:B:513:ILE:HD12	1.88	0.73
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.69	0.73
1:A:399:ASP:O	1:A:403:GLN:HG2	1.88	0.73
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:O	1:A:344:LYS:HG2	1.87	0.73
1:B:202:VAL:HG23	1:B:261:ILE:O	1.88	0.73
1:A:505:THR:HG21	1:A:509:PHE:HB2	1.69	0.73
1:A:217:LEU:HB2	1:B:517:TYR:CE1	2.24	0.72
1:A:416:TRP:C	1:A:417:LEU:HD23	2.13	0.72
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.24	0.72
1:B:537:PRO:HD2	1:B:538:ASN:H	1.54	0.72
1:A:170:ASP:OD2	2:A:600:FAA:H7P1	1.89	0.72
1:A:505:THR:OG1	1:A:513:ILE:HD12	1.88	0.72
1:B:460:VAL:HG13	1:B:465:MET:HG2	1.72	0.72
1:A:445:LYS:O	1:A:448:GLN:HB3	1.89	0.72
1:A:361:GLU:O	1:A:361:GLU:HG2	1.90	0.72
1:A:202:VAL:HG23	1:A:261:ILE:O	1.88	0.72
1:A:284:PRO:HD2	1:A:288:ASP:OD2	1.89	0.72
1:B:363:ILE:HD12	1:B:363:ILE:N	2.05	0.72
1:B:170:ASP:OD2	2:B:600:FAA:H7P1	1.88	0.72
1:B:284:PRO:HD2	1:B:288:ASP:OD2	1.89	0.72
1:B:332:GLU:HB3	1:B:333:PRO:CD	2.19	0.72
1:B:416:TRP:C	1:B:417:LEU:HD23	2.13	0.72
1:A:437:MET:HA	1:A:437:MET:HE3	1.72	0.71
1:B:292:ALA:O	1:B:295:ILE:HB	1.90	0.71
1:A:332:GLU:HB3	1:A:333:PRO:CD	2.19	0.71
1:A:537:PRO:HD2	1:A:538:ASN:H	1.54	0.71
1:A:460:VAL:HG13	1:A:465:MET:HG2	1.72	0.71
1:B:433:GLY:O	1:B:437:MET:HB2	1.91	0.71
1:A:79:ASN:HD21	1:A:81:ALA:HB3	1.55	0.71
1:A:537:PRO:HD2	3:A:612:HOH:O	1.89	0.71
1:B:445:LYS:O	1:B:448:GLN:HB3	1.89	0.71
1:B:550:PRO:CB	1:B:552:GLN:HE21	2.03	0.71
1:A:313:HIS:HB2	1:A:351:TRP:CZ3	2.26	0.71
1:A:363:ILE:N	1:A:363:ILE:HD12	2.05	0.71
1:A:433:GLY:O	1:A:437:MET:HB2	1.91	0.71
1:B:61:HIS:NE2	1:B:422:HIS:CE1	2.59	0.71
1:A:519:TRP:CZ3	1:B:211:ARG:HG3	2.26	0.70
1:B:79:ASN:HD21	1:B:81:ALA:HB3	1.55	0.70
1:A:68:TYR:HA	3:A:645:HOH:O	1.91	0.70
1:B:351:TRP:CE3	1:B:351:TRP:HA	2.26	0.70
1:B:361:GLU:O	1:B:361:GLU:HG2	1.90	0.70
1:B:200:MET:CE	1:B:251:ASP:HB3	2.22	0.70
1:A:292:ALA:O	1:A:295:ILE:HB	1.90	0.70
1:A:555:HIS:HB3	1:A:559:LYS:CE	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:MET:HE3	1:B:437:MET:HA	1.72	0.70
1:A:60:PRO:O	1:A:62:HIS:ND1	2.24	0.70
1:A:550:PRO:CB	1:A:552:GLN:HE21	2.04	0.70
1:A:43:LYS:C	1:A:45:GLN:H	1.99	0.69
1:A:58:HIS:HD2	1:A:59:ASP:C	2.00	0.69
1:A:61:HIS:NE2	1:A:422:HIS:CE1	2.59	0.69
1:A:134:ASN:OD1	1:A:137:GLY:N	2.23	0.69
1:A:351:TRP:HA	1:A:351:TRP:CE3	2.26	0.69
1:A:91:ASN:HD22	1:A:538:ASN:HD22	1.40	0.69
1:B:313:HIS:HB2	1:B:351:TRP:CZ3	2.26	0.69
1:B:324:LYS:HB2	1:B:416:TRP:CE2	2.28	0.69
1:B:58:HIS:HD2	1:B:59:ASP:C	2.00	0.68
1:B:43:LYS:C	1:B:45:GLN:H	1.99	0.68
1:B:378:ILE:HB	1:B:381:VAL:CG2	2.23	0.68
1:B:312:ARG:NH1	1:B:317:ASP:OD1	2.27	0.68
1:B:156:GLU:OE1	1:B:161:ARG:NH2	2.27	0.68
1:B:505:THR:HG22	1:B:506:HIS:N	2.08	0.68
1:A:312:ARG:NH1	1:A:317:ASP:OD1	2.27	0.68
1:A:324:LYS:HB2	1:A:416:TRP:CE2	2.28	0.68
1:A:156:GLU:OE1	1:A:161:ARG:NH2	2.27	0.68
1:B:10:LEU:HD21	1:B:42:SER:HA	1.75	0.68
1:B:83:VAL:HG23	1:B:127:MET:HE1	1.76	0.68
1:B:363:ILE:HD12	1:B:363:ILE:H	1.58	0.68
1:B:217:LEU:HD12	1:B:218:PRO:CD	2.23	0.68
1:B:177:LEU:HG	1:B:265:ILE:CG2	2.24	0.67
1:A:177:LEU:HG	1:A:265:ILE:CG2	2.24	0.67
1:A:339:LEU:O	1:A:343:ALA:N	2.24	0.67
1:A:517:TYR:OH	1:B:214:MET:HE1	1.93	0.67
1:A:505:THR:HG22	1:A:506:HIS:N	2.08	0.67
1:A:10:LEU:HD21	1:A:42:SER:HA	1.75	0.67
1:A:217:LEU:HD12	1:A:218:PRO:CD	2.24	0.67
1:A:378:ILE:HB	1:A:381:VAL:CG2	2.24	0.67
1:B:91:ASN:HD22	1:B:538:ASN:HD22	1.40	0.67
1:A:200:MET:CE	1:A:251:ASP:HB3	2.22	0.67
1:A:237:LYS:HD2	1:B:500:TRP:NE1	2.10	0.67
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.77	0.67
1:A:211:ARG:HG3	1:B:519:TRP:CZ3	2.30	0.67
1:B:48:ASP:OD1	1:B:66:GLN:NE2	2.28	0.67
1:A:97:LEU:CD2	1:A:119:VAL:HB	2.25	0.67
1:A:83:VAL:HG23	1:A:127:MET:HE1	1.76	0.66
1:B:97:LEU:CD2	1:B:119:VAL:HB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:HD12	1:A:363:ILE:H	1.58	0.66
1:B:505:THR:HG22	1:B:506:HIS:H	1.61	0.66
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.77	0.66
1:A:505:THR:HG22	1:A:506:HIS:H	1.60	0.66
1:A:48:ASP:OD1	1:A:66:GLN:NE2	2.28	0.66
1:A:283:LEU:HB2	1:A:351:TRP:HB2	1.77	0.66
1:A:531:LEU:HD22	1:B:531:LEU:HD22	1.78	0.66
1:B:283:LEU:HB2	1:B:351:TRP:HB2	1.78	0.65
1:B:312:ARG:NH2	1:B:410:GLU:OE1	2.29	0.65
1:A:312:ARG:NH2	1:A:410:GLU:OE1	2.29	0.65
1:A:503:TYR:HD2	3:A:654:HOH:O	1.78	0.65
1:B:65:ASP:OD1	1:B:65:ASP:N	2.29	0.65
1:A:339:LEU:O	1:A:342:ILE:N	2.30	0.65
1:B:339:LEU:O	1:B:343:ALA:N	2.24	0.65
1:A:429:ALA:HB2	1:A:439:GLN:NE2	2.11	0.65
1:A:446:ARG:NH1	1:A:449:GLU:OE1	2.30	0.65
1:B:339:LEU:O	1:B:342:ILE:N	2.30	0.65
1:B:445:LYS:HD3	3:B:620:HOH:O	1.96	0.65
1:B:134:ASN:OD1	1:B:137:GLY:N	2.23	0.65
1:A:108:TYR:HD1	1:A:505:THR:C	2.05	0.65
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.11	0.65
1:A:62:HIS:HE1	1:A:475:LYS:HD3	1.61	0.64
1:B:177:LEU:CD1	1:B:265:ILE:HG22	2.28	0.64
1:B:324:LYS:HA	1:B:416:TRP:CH2	2.32	0.64
1:B:108:TYR:HD1	1:B:505:THR:C	2.05	0.64
1:A:299:LEU:HB3	1:A:305:LEU:HG	1.79	0.64
1:A:65:ASP:N	1:A:65:ASP:OD1	2.29	0.64
1:A:160:LEU:O	1:A:163:LYS:N	2.30	0.64
1:A:457:THR:HG22	1:A:458:PHE:N	2.11	0.64
1:B:550:PRO:HB3	1:B:552:GLN:HE21	1.62	0.64
1:A:183:ARG:NH2	1:A:256:GLN:HB2	2.13	0.64
1:A:277:GLN:HB3	1:A:357:LEU:HD12	1.78	0.64
1:A:324:LYS:HA	1:A:416:TRP:CH2	2.32	0.64
1:B:277:GLN:HB3	1:B:357:LEU:HD12	1.78	0.64
1:B:60:PRO:O	1:B:62:HIS:ND1	2.24	0.64
1:A:35:GLU:OE1	1:A:35:GLU:HA	1.96	0.64
1:A:414:ILE:HD11	2:A:600:FAA:HM71	1.80	0.64
1:B:446:ARG:NH1	1:B:449:GLU:OE1	2.30	0.64
1:A:62:HIS:CE1	1:A:475:LYS:HD3	2.33	0.64
1:B:62:HIS:HE1	1:B:475:LYS:HD3	1.61	0.64
1:B:166:LEU:HD23	1:B:269:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:NH2	1:B:256:GLN:HB2	2.13	0.64
1:B:62:HIS:CE1	1:B:475:LYS:HD3	2.33	0.64
1:B:299:LEU:HB3	1:B:305:LEU:HG	1.80	0.63
1:B:439:GLN:O	1:B:442:VAL:HB	1.98	0.63
2:B:600:FAA:C2P	2:B:600:FAA:C4	2.76	0.63
1:A:188:THR:HB	1:A:189:PRO:HD2	1.81	0.63
1:B:222:ARG:HB2	1:B:223:PRO:HD2	1.79	0.63
1:B:416:TRP:O	1:B:417:LEU:HD23	1.99	0.63
1:A:166:LEU:HD23	1:A:269:LEU:HD22	1.79	0.63
1:A:451:GLY:O	1:A:452:LEU:HD23	1.98	0.63
1:A:138:ALA:O	1:B:463:ARG:NH2	2.27	0.63
1:B:457:THR:HG22	1:B:458:PHE:N	2.11	0.63
1:B:506:HIS:ND1	1:B:507:LEU:N	2.46	0.63
2:A:600:FAA:C2P	2:A:600:FAA:C4	2.76	0.63
1:B:78:ARG:HD3	1:B:82:ASP:OD2	1.98	0.63
1:A:104:ARG:C	1:A:106:SER:H	2.07	0.62
1:A:302:GLY:O	1:A:303:MET:HB2	1.98	0.62
1:B:201:GLU:HG2	1:B:263:THR:OG1	1.99	0.62
1:B:302:GLY:O	1:B:303:MET:HB2	1.98	0.62
1:B:411:LEU:O	1:B:414:ILE:HB	1.99	0.62
1:B:451:GLY:O	1:B:452:LEU:HD23	1.98	0.62
1:A:194:TRP:O	1:A:197:HIS:HD2	1.81	0.62
1:A:550:PRO:HB3	1:A:552:GLN:HE21	1.62	0.62
1:B:399:ASP:OD1	1:B:403:GLN:NE2	2.32	0.62
1:A:222:ARG:HB2	1:A:223:PRO:HD2	1.79	0.62
1:A:506:HIS:ND1	1:A:507:LEU:N	2.46	0.62
1:A:62:HIS:ND1	1:A:62:HIS:N	2.47	0.62
1:A:201:GLU:HG2	1:A:263:THR:OG1	1.99	0.62
1:A:210:LEU:C	1:A:210:LEU:HD23	2.25	0.62
1:A:506:HIS:CE1	1:A:508:ALA:H	2.18	0.62
1:A:532:LYS:NZ	1:A:541:ILE:O	2.32	0.62
1:B:200:MET:O	1:B:211:ARG:HA	1.99	0.62
1:B:210:LEU:C	1:B:210:LEU:HD23	2.25	0.62
1:A:399:ASP:OD1	1:A:403:GLN:NE2	2.32	0.62
1:B:194:TRP:O	1:B:197:HIS:HD2	1.81	0.62
1:A:177:LEU:CD1	1:A:265:ILE:HG22	2.28	0.62
1:A:295:ILE:O	1:A:298:PRO:HD2	2.00	0.62
1:A:480:GLN:O	1:A:483:LYS:HB2	1.99	0.62
1:A:78:ARG:HD3	1:A:82:ASP:OD2	1.99	0.62
1:B:149:HIS:O	1:B:152:HIS:HB3	2.00	0.62
1:B:224:GLU:CD	1:B:224:GLU:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ILE:HD11	2:B:600:FAA:HM71	1.80	0.62
1:B:480:GLN:O	1:B:483:LYS:HB2	1.99	0.62
1:A:197:HIS:HA	1:A:266:GLY:O	2.00	0.62
1:B:309:PRO:HG2	1:B:460:VAL:CG2	2.30	0.62
1:B:389:THR:HB	1:B:390:PRO:HD2	1.82	0.62
1:A:200:MET:O	1:A:211:ARG:HA	1.99	0.62
1:B:506:HIS:CE1	1:B:508:ALA:H	2.17	0.62
1:A:439:GLN:O	1:A:442:VAL:HB	1.98	0.61
1:A:309:PRO:HG2	1:A:460:VAL:CG2	2.30	0.61
1:A:416:TRP:O	1:A:417:LEU:HD23	1.99	0.61
1:B:552:GLN:CD	1:B:552:GLN:H	2.08	0.61
1:A:253:LEU:CD1	1:B:253:LEU:HD21	2.29	0.61
1:A:325:ARG:C	1:A:327:TYR:H	2.08	0.61
1:A:411:LEU:O	1:A:414:ILE:HB	1.99	0.61
1:B:35:GLU:HA	1:B:35:GLU:OE1	1.96	0.61
1:A:149:HIS:O	1:A:152:HIS:HB3	2.00	0.61
1:A:552:GLN:CD	1:A:552:GLN:H	2.08	0.61
1:B:104:ARG:C	1:B:106:SER:H	2.07	0.61
1:B:197:HIS:HA	1:B:266:GLY:O	2.00	0.61
1:B:295:ILE:O	1:B:298:PRO:HD2	2.00	0.61
1:A:389:THR:HB	1:A:390:PRO:HD2	1.82	0.61
1:A:283:LEU:O	1:A:349:GLY:HA3	2.01	0.61
1:A:77:PRO:HB2	1:A:127:MET:HE3	1.82	0.61
1:B:74:ILE:HG22	1:B:75:VAL:N	2.16	0.61
1:B:306:GLN:OE1	1:B:357:LEU:HA	2.01	0.61
1:A:51:TYR:CZ	1:A:171:LEU:HD13	2.36	0.61
1:A:306:GLN:OE1	1:A:357:LEU:HA	2.01	0.61
1:B:283:LEU:O	1:B:349:GLY:HA3	2.01	0.61
1:A:43:LYS:O	1:A:45:GLN:N	2.33	0.60
1:B:77:PRO:HB2	1:B:127:MET:HE3	1.82	0.60
1:A:206:ASN:OD1	1:A:208:GLU:N	2.30	0.60
1:A:224:GLU:CD	1:A:224:GLU:H	2.08	0.60
1:A:279:TYR:HA	1:A:395:LEU:HD21	1.83	0.60
1:B:188:THR:HB	1:B:189:PRO:HD2	1.81	0.60
1:B:43:LYS:O	1:B:45:GLN:N	2.33	0.60
1:B:51:TYR:CZ	1:B:171:LEU:HD13	2.36	0.60
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.83	0.60
1:B:532:LYS:NZ	1:B:541:ILE:O	2.32	0.60
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.83	0.60
1:A:414:ILE:HD11	2:A:600:FAA:C8M	2.31	0.60
1:B:62:HIS:ND1	1:B:62:HIS:N	2.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:CD1	1:A:57:THR:HG22	2.31	0.60
1:A:517:TYR:CE1	1:B:217:LEU:HB2	2.37	0.60
1:B:506:HIS:ND1	1:B:508:ALA:N	2.48	0.60
1:B:279:TYR:HA	1:B:395:LEU:HD21	1.83	0.60
1:A:79:ASN:O	1:A:82:ASP:HB2	2.02	0.59
1:B:282:THR:C	1:B:283:LEU:HD23	2.27	0.59
1:A:74:ILE:HG22	1:A:75:VAL:N	2.16	0.59
1:B:79:ASN:O	1:B:82:ASP:HB2	2.02	0.59
1:B:94:SER:HA	1:B:540:ILE:HD11	1.85	0.59
1:B:24:PHE:O	1:B:28:ILE:HG13	2.02	0.59
1:B:160:LEU:O	1:B:163:LYS:N	2.30	0.59
1:B:177:LEU:HG	1:B:265:ILE:HG21	1.85	0.59
1:B:539:GLY:O	1:B:543:PRO:HG3	2.03	0.59
1:B:210:LEU:HD23	1:B:211:ARG:N	2.18	0.59
1:A:237:LYS:HD2	1:B:500:TRP:HE1	1.68	0.59
1:B:189:PRO:HD3	1:B:307:ASN:HB3	1.84	0.59
1:B:273:PRO:O	1:B:359:GLY:HA2	2.03	0.59
1:B:414:ILE:HD11	2:B:600:FAA:C8M	2.32	0.59
1:A:24:PHE:O	1:A:28:ILE:HG13	2.02	0.59
1:A:189:PRO:HD3	1:A:307:ASN:HB3	1.84	0.59
1:A:10:LEU:CD2	1:A:42:SER:HA	2.32	0.59
1:A:173:GLY:N	1:A:408:TYR:HE1	2.01	0.59
1:A:210:LEU:HD23	1:A:211:ARG:N	2.18	0.59
1:A:282:THR:C	1:A:283:LEU:HD23	2.27	0.59
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.85	0.59
1:A:539:GLY:O	1:A:543:PRO:HG3	2.03	0.59
1:B:361:GLU:HB3	1:B:362:PRO:HD3	1.85	0.59
1:A:183:ARG:NH2	1:B:247:GLY:O	2.35	0.58
1:A:309:PRO:HB2	1:A:353:PHE:HE1	1.68	0.58
1:B:325:ARG:C	1:B:327:TYR:H	2.08	0.58
1:A:94:SER:HA	1:A:540:ILE:HD11	1.84	0.58
1:A:156:GLU:HB2	1:A:161:ARG:NH2	2.17	0.58
1:B:223:PRO:HD2	1:B:224:GLU:OE2	2.04	0.58
1:B:309:PRO:HB2	1:B:353:PHE:HE1	1.68	0.58
1:A:273:PRO:O	1:A:359:GLY:HA2	2.03	0.58
1:A:502:GLU:HG2	1:A:503:TYR:N	2.17	0.58
1:B:502:GLU:HG2	1:B:503:TYR:H	1.69	0.58
1:A:95:PHE:O	1:A:540:ILE:HD12	2.03	0.58
1:A:324:LYS:HB2	1:A:416:TRP:CD2	2.39	0.58
1:A:502:GLU:HG2	1:A:503:TYR:H	1.69	0.58
1:B:502:GLU:HG2	1:B:503:TYR:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HD2	1:A:224:GLU:OE2	2.04	0.58
1:B:324:LYS:HB2	1:B:416:TRP:CD2	2.39	0.58
1:A:194:TRP:HH2	1:A:200:MET:HE1	1.69	0.58
1:A:330:ARG:NH1	1:A:338:GLU:OE1	2.37	0.58
1:B:10:LEU:CD2	1:B:42:SER:HA	2.32	0.58
1:B:62:HIS:CG	1:B:66:GLN:HG3	2.39	0.58
1:B:330:ARG:NH1	1:B:338:GLU:OE1	2.37	0.58
1:B:173:GLY:N	1:B:408:TYR:HE1	2.01	0.58
1:B:487:LEU:HD11	1:B:491:LEU:HD11	1.86	0.58
1:B:95:PHE:O	1:B:540:ILE:HD12	2.03	0.58
1:A:58:HIS:C	1:A:112:ALA:HB2	2.29	0.57
1:A:62:HIS:CG	1:A:66:GLN:HG3	2.39	0.57
1:A:241:LEU:HB3	1:B:463:ARG:O	2.04	0.57
1:A:177:LEU:HG	1:A:265:ILE:HG21	1.85	0.57
1:B:156:GLU:HB2	1:B:161:ARG:NH2	2.17	0.57
1:B:40:ILE:CD1	1:B:57:THR:HG22	2.31	0.57
1:B:78:ARG:HB2	1:B:82:ASP:OD2	2.04	0.57
1:A:354:TYR:CD2	1:A:395:LEU:HD13	2.40	0.57
1:B:480:GLN:HA	1:B:483:LYS:CG	2.34	0.57
1:B:488:MET:O	1:B:492:ILE:HG13	2.05	0.57
1:A:338:GLU:O	1:A:342:ILE:HG13	2.04	0.57
1:B:276:TYR:HE2	1:B:403:GLN:NE2	2.02	0.57
1:B:338:GLU:O	1:B:342:ILE:HG13	2.04	0.57
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.04	0.57
1:A:289:LEU:HD23	1:A:437:MET:HE3	1.85	0.57
1:A:480:GLN:HA	1:A:483:LYS:CG	2.34	0.57
1:A:248:PRO:HG3	1:B:257:SER:CB	2.34	0.57
1:A:276:TYR:HE2	1:A:403:GLN:NE2	2.02	0.57
1:A:359:GLY:O	1:A:364:ARG:NE	2.38	0.57
1:B:58:HIS:C	1:B:112:ALA:HB2	2.29	0.57
1:B:289:LEU:HD23	1:B:437:MET:HE3	1.85	0.57
1:B:359:GLY:O	1:B:364:ARG:NE	2.38	0.57
1:B:429:ALA:O	1:B:465:MET:N	2.37	0.57
1:A:312:ARG:NH1	1:A:316:LEU:HG	2.20	0.56
1:A:506:HIS:ND1	1:A:508:ALA:N	2.48	0.56
1:A:238:ILE:HD11	1:B:429:ALA:HA	1.87	0.56
1:A:478:LEU:CD1	1:A:478:LEU:H	2.19	0.56
1:A:423:LEU:HD21	1:A:488:MET:HE3	1.88	0.56
1:A:488:MET:O	1:A:492:ILE:HG13	2.05	0.56
1:A:324:LYS:HA	1:A:416:TRP:CZ3	2.41	0.56
1:A:407:THR:OG1	1:A:408:TYR:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:HD11	1:A:491:LEU:HD11	1.86	0.56
1:B:289:LEU:HD23	1:B:437:MET:CE	2.36	0.56
1:B:324:LYS:HA	1:B:416:TRP:CZ3	2.41	0.56
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.05	0.56
1:B:52:MET:O	1:B:53:LYS:HG3	2.06	0.56
1:B:312:ARG:NH1	1:B:316:LEU:HG	2.20	0.56
1:B:354:TYR:CD2	1:B:395:LEU:HD13	2.40	0.56
1:A:52:MET:O	1:A:53:LYS:HG3	2.06	0.56
1:A:177:LEU:HG	1:A:265:ILE:HG22	1.86	0.56
1:B:177:LEU:HG	1:B:265:ILE:HG22	1.86	0.56
1:B:194:TRP:HH2	1:B:200:MET:HE1	1.69	0.56
1:B:423:LEU:HD21	1:B:488:MET:HE3	1.88	0.56
1:B:169:PRO:HG3	1:B:193:HIS:HE1	1.71	0.56
1:B:430:LYS:O	1:B:465:MET:HE2	2.05	0.56
1:A:430:LYS:O	1:A:465:MET:HE2	2.05	0.55
1:A:169:PRO:HG3	1:A:193:HIS:HE1	1.71	0.55
1:B:62:HIS:H	1:B:62:HIS:HD1	1.51	0.55
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.05	0.55
1:A:39:VAL:HG22	1:A:73:ALA:HB2	1.89	0.55
1:B:9:PRO:HA	1:B:40:ILE:O	2.07	0.55
1:B:478:LEU:H	1:B:478:LEU:CD1	2.19	0.55
1:A:300:ARG:HE	1:A:309:PRO:HD2	1.72	0.55
1:A:383:PHE:C	1:A:384:TYR:CD1	2.85	0.55
1:A:132:GLU:HG2	1:A:133:VAL:H	1.71	0.55
1:A:426:SER:C	1:A:502:GLU:HG3	2.32	0.55
1:A:494:ASP:O	1:A:497:ALA:HB3	2.06	0.55
1:B:108:TYR:CD1	1:B:505:THR:C	2.85	0.55
1:B:383:PHE:C	1:B:384:TYR:CD1	2.85	0.55
1:B:300:ARG:HE	1:B:309:PRO:HD2	1.72	0.55
1:B:385:PHE:O	1:B:388:ASP:N	2.40	0.55
1:A:62:HIS:H	1:A:62:HIS:HD1	1.51	0.55
1:A:152:HIS:CE1	1:A:161:ARG:NH2	2.75	0.55
1:A:289:LEU:HD23	1:A:437:MET:CE	2.36	0.55
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.89	0.55
1:B:494:ASP:O	1:B:497:ALA:HB3	2.06	0.55
1:B:407:THR:OG1	1:B:408:TYR:N	2.37	0.54
1:A:237:LYS:HD2	1:B:500:TRP:CD1	2.42	0.54
1:A:429:ALA:O	1:A:465:MET:N	2.37	0.54
1:A:522:SER:O	1:A:526:ARG:HG2	2.08	0.54
1:A:104:ARG:O	1:A:106:SER:N	2.38	0.54
1:B:206:ASN:OD1	1:B:208:GLU:N	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:SER:C	1:B:502:GLU:HG3	2.32	0.54
1:B:458:PHE:N	1:B:458:PHE:CD1	2.74	0.54
1:B:45:GLN:C	1:B:47:VAL:N	2.65	0.54
1:A:9:PRO:HA	1:A:40:ILE:O	2.07	0.54
1:A:97:LEU:HD23	1:A:119:VAL:HB	1.90	0.54
1:A:429:ALA:HB2	1:A:439:GLN:HE22	1.73	0.54
1:B:426:SER:H	1:B:502:GLU:CD	2.16	0.54
1:B:522:SER:O	1:B:526:ARG:HG2	2.08	0.54
1:A:458:PHE:N	1:A:458:PHE:CD1	2.75	0.54
1:B:97:LEU:HD23	1:B:119:VAL:HB	1.90	0.54
1:B:152:HIS:CE1	1:B:161:ARG:NH2	2.75	0.54
1:B:39:VAL:HG22	1:B:73:ALA:HB2	1.89	0.54
1:B:61:HIS:CB	1:B:421:ALA:HB1	2.31	0.54
1:A:59:ASP:N	1:A:112:ALA:HB2	2.23	0.53
1:A:200:MET:HE2	1:A:251:ASP:CB	2.34	0.53
1:A:385:PHE:O	1:A:388:ASP:N	2.40	0.53
1:B:142:VAL:HB	1:B:146:VAL:HG21	1.90	0.53
1:A:181:VAL:O	1:A:255:SER:HB2	2.08	0.53
1:A:315:LEU:HA	1:A:318:ALA:HB3	1.90	0.53
1:A:426:SER:H	1:A:502:GLU:CD	2.16	0.53
1:A:229:LYS:HB3	1:A:231:GLU:CD	2.34	0.53
1:A:102:ILE:HG21	1:A:104:ARG:HD2	1.90	0.53
1:B:156:GLU:CB	1:B:161:ARG:HE	2.21	0.53
1:A:185:VAL:HG12	1:A:186:GLY:N	2.24	0.53
1:A:422:HIS:HD1	1:A:422:HIS:H	1.57	0.53
1:B:185:VAL:HG12	1:B:186:GLY:N	2.24	0.53
1:B:300:ARG:CA	1:B:305:LEU:HB2	2.37	0.53
1:B:315:LEU:O	1:B:319:ALA:N	2.29	0.53
1:B:315:LEU:HA	1:B:318:ALA:HB3	1.90	0.53
1:B:36:ASN:HB3	1:B:76:ALA:HB3	1.91	0.53
1:B:351:TRP:O	1:B:352:ASN:OD1	2.27	0.53
1:B:59:ASP:N	1:B:112:ALA:HB2	2.23	0.53
1:B:181:VAL:O	1:B:255:SER:HB2	2.08	0.53
1:B:429:ALA:HB2	1:B:439:GLN:HE22	1.73	0.53
2:A:600:FAA:C6P	2:A:600:FAA:C10	2.87	0.53
1:A:36:ASN:HB3	1:A:76:ALA:HB3	1.90	0.53
1:A:177:LEU:C	1:A:177:LEU:HD23	2.33	0.53
1:A:504:ARG:NH2	2:A:600:FAA:O3'	2.41	0.53
1:B:229:LYS:HB3	1:B:231:GLU:CD	2.34	0.53
1:B:422:HIS:HD1	1:B:422:HIS:H	1.57	0.53
1:B:543:PRO:HB3	1:B:550:PRO:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:CE1	1:A:28:ILE:HD12	2.44	0.52
1:A:202:VAL:HG23	1:A:261:ILE:N	2.24	0.52
1:A:156:GLU:CB	1:A:161:ARG:HE	2.21	0.52
1:A:363:ILE:HD11	1:B:366:VAL:HG11	1.90	0.52
1:B:99:PRO:HA	1:B:121:LEU:HB3	1.91	0.52
1:B:238:ILE:HG22	1:B:238:ILE:O	2.09	0.52
1:A:238:ILE:O	1:A:238:ILE:HG22	2.09	0.52
1:A:171:LEU:HD12	3:A:602:HOH:O	2.09	0.52
1:B:177:LEU:HD23	1:B:177:LEU:C	2.33	0.52
1:B:348:LEU:HB3	1:B:352:ASN:HD21	1.74	0.52
1:B:504:ARG:NH2	2:B:600:FAA:O3'	2.41	0.52
1:A:108:TYR:CD1	1:A:505:THR:C	2.85	0.52
1:A:142:VAL:HB	1:A:146:VAL:HG21	1.90	0.52
1:A:316:LEU:HD11	1:A:413:TRP:CD1	2.44	0.52
1:A:463:ARG:NH2	1:B:138:ALA:O	2.38	0.52
1:B:297:ARG:HB2	1:B:431:VAL:HG12	1.91	0.52
2:B:600:FAA:C10	2:B:600:FAA:C6P	2.87	0.52
1:A:45:GLN:C	1:A:47:VAL:N	2.65	0.52
1:A:99:PRO:HA	1:A:121:LEU:HB3	1.92	0.52
1:A:348:LEU:HB3	1:A:352:ASN:HD21	1.74	0.52
1:A:543:PRO:HB3	1:A:550:PRO:CG	2.39	0.52
1:B:202:VAL:HG23	1:B:261:ILE:N	2.24	0.52
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.89	0.52
1:B:426:SER:O	1:B:502:GLU:HG3	2.10	0.52
1:A:95:PHE:CD1	1:A:119:VAL:HG23	2.45	0.52
1:A:401:THR:C	1:A:403:GLN:H	2.17	0.52
1:B:401:THR:C	1:B:403:GLN:H	2.18	0.52
1:B:426:SER:N	1:B:427:PRO:HD3	2.22	0.52
1:A:107:GLY:HA2	1:A:422:HIS:O	2.10	0.52
1:A:297:ARG:HB2	1:A:431:VAL:HG12	1.91	0.52
1:B:520:ASN:O	1:B:521:ASN:HB2	2.09	0.52
1:A:57:THR:O	1:A:70:LEU:HD12	2.10	0.52
1:A:409:ASP:OD1	1:A:409:ASP:N	2.43	0.52
1:A:426:SER:N	1:A:427:PRO:HD3	2.22	0.52
1:B:316:LEU:HD11	1:B:413:TRP:CD1	2.44	0.52
1:A:300:ARG:CA	1:A:305:LEU:HB2	2.37	0.52
1:A:253:LEU:HD21	1:B:253:LEU:CD1	2.39	0.51
1:A:330:ARG:NH1	1:A:338:GLU:CD	2.68	0.51
1:B:24:PHE:CE1	1:B:28:ILE:HD12	2.44	0.51
1:B:409:ASP:N	1:B:409:ASP:OD1	2.43	0.51
1:A:351:TRP:O	1:A:352:ASN:OD1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:O	1:B:106:SER:N	2.38	0.51
1:B:317:ASP:O	1:B:321:LEU:HG	2.10	0.51
1:A:108:TYR:HE1	1:A:505:THR:HA	1.75	0.51
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.92	0.51
1:B:57:THR:O	1:B:70:LEU:HD12	2.10	0.51
1:B:107:GLY:HA2	1:B:422:HIS:O	2.10	0.51
1:B:108:TYR:HE1	1:B:505:THR:HA	1.75	0.51
1:B:275:GLY:HA3	1:B:359:GLY:O	2.11	0.51
1:A:269:LEU:O	1:B:463:ARG:NH2	2.44	0.51
1:A:317:ASP:O	1:A:321:LEU:HG	2.10	0.51
1:B:102:ILE:HG21	1:B:104:ARG:HD2	1.90	0.51
1:B:132:GLU:HG2	1:B:133:VAL:H	1.71	0.51
1:B:217:LEU:HD12	1:B:218:PRO:HD2	1.92	0.51
1:B:330:ARG:NH1	1:B:338:GLU:CD	2.68	0.51
1:B:444:LYS:HE3	3:B:608:HOH:O	2.10	0.51
1:B:511:ASP:HB2	3:B:612:HOH:O	2.11	0.51
1:A:315:LEU:O	1:A:319:ALA:N	2.29	0.51
1:A:520:ASN:O	1:A:521:ASN:HB2	2.09	0.51
1:B:160:LEU:HD23	1:B:163:LYS:HD2	1.93	0.51
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.92	0.51
1:B:543:PRO:HB3	1:B:550:PRO:HG2	1.93	0.51
1:A:160:LEU:HD23	1:A:163:LYS:HD2	1.93	0.51
1:A:214:MET:HE1	1:B:517:TYR:OH	2.11	0.51
1:A:275:GLY:HA3	1:A:359:GLY:O	2.11	0.51
1:A:323:ASP:OD1	1:A:326:SER:N	2.34	0.51
1:B:45:GLN:HG2	1:B:46:ILE:N	2.25	0.51
1:B:95:PHE:CD1	1:B:119:VAL:HG23	2.45	0.51
1:B:502:GLU:HG2	1:B:504:ARG:H	1.75	0.51
1:A:61:HIS:CB	1:A:421:ALA:HB1	2.31	0.51
1:A:527:PHE:O	1:A:530:VAL:HB	2.11	0.51
1:A:479:ILE:HD12	1:A:479:ILE:N	2.26	0.51
1:B:45:GLN:C	1:B:47:VAL:H	2.18	0.51
1:B:479:ILE:N	1:B:479:ILE:HD12	2.26	0.50
1:A:45:GLN:HG2	1:A:46:ILE:N	2.25	0.50
1:A:45:GLN:C	1:A:47:VAL:H	2.18	0.50
1:A:443:THR:HB	1:A:454:PHE:HE2	1.76	0.50
1:B:155:LEU:N	1:B:155:LEU:HD23	2.19	0.50
1:B:276:TYR:CE2	1:B:403:GLN:NE2	2.79	0.50
1:B:537:PRO:CD	1:B:538:ASN:H	2.22	0.50
1:A:346:LEU:HB3	1:A:348:LEU:CD1	2.42	0.50
1:B:443:THR:HB	1:B:454:PHE:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:CG2	1:A:75:VAL:N	2.75	0.50
1:A:417:LEU:CB	1:A:418:PRO:HD2	2.38	0.50
1:A:426:SER:O	1:A:502:GLU:HG3	2.10	0.50
1:A:543:PRO:HB3	1:A:550:PRO:HG2	1.93	0.50
1:B:45:GLN:CG	1:B:46:ILE:N	2.74	0.50
1:A:80:VAL:CG1	1:A:209:LEU:HD21	2.38	0.50
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.94	0.50
1:A:437:MET:O	1:A:440:TYR:HB3	2.12	0.50
1:A:217:LEU:HD12	1:A:218:PRO:HD2	1.92	0.50
1:A:502:GLU:HG2	1:A:504:ARG:H	1.75	0.50
1:B:194:TRP:O	1:B:197:HIS:CD2	2.64	0.50
1:B:218:PRO:O	1:B:220:PRO:HD3	2.12	0.50
1:B:437:MET:O	1:B:440:TYR:HB3	2.12	0.50
1:A:156:GLU:HB2	1:A:161:ARG:HE	1.76	0.50
1:A:378:ILE:HG22	1:A:381:VAL:HG23	1.94	0.50
1:B:24:PHE:CE1	1:B:28:ILE:CD1	2.95	0.50
1:B:527:PHE:O	1:B:530:VAL:HB	2.11	0.50
1:A:217:LEU:HD12	1:A:218:PRO:HD3	1.93	0.50
1:A:276:TYR:CE2	1:A:403:GLN:NE2	2.79	0.50
1:B:354:TYR:HD2	1:B:395:LEU:HD13	1.76	0.50
1:A:43:LYS:C	1:A:45:GLN:N	2.70	0.49
1:A:183:ARG:HH22	1:B:247:GLY:C	2.19	0.49
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.94	0.49
1:A:354:TYR:HD2	1:A:395:LEU:HD13	1.76	0.49
1:B:45:GLN:O	1:B:47:VAL:N	2.45	0.49
1:A:45:GLN:O	1:A:47:VAL:N	2.45	0.49
1:A:194:TRP:O	1:A:197:HIS:CD2	2.64	0.49
1:A:537:PRO:CD	1:A:538:ASN:H	2.22	0.49
1:B:74:ILE:CG2	1:B:75:VAL:N	2.75	0.49
1:A:439:GLN:OE1	1:A:467:HIS:HB2	2.13	0.49
1:A:530:VAL:HG13	3:A:628:HOH:O	2.11	0.49
1:B:37:VAL:HA	1:B:74:ILE:O	2.12	0.49
1:B:253:LEU:O	1:B:257:SER:OG	2.29	0.49
1:A:18:LEU:HG	1:A:22:ASN:ND2	2.28	0.49
1:A:505:THR:CG2	1:A:509:PHE:HB2	2.41	0.49
1:B:217:LEU:HD12	1:B:218:PRO:HD3	1.93	0.49
1:B:332:GLU:CB	1:B:333:PRO:CD	2.89	0.49
1:B:346:LEU:HB3	1:B:348:LEU:CD1	2.42	0.49
1:A:24:PHE:CE1	1:A:28:ILE:CD1	2.95	0.49
1:A:221:LYS:O	1:A:222:ARG:HB3	2.13	0.49
1:B:18:LEU:HB3	3:B:622:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLN:OE1	1:B:467:HIS:HB2	2.13	0.49
1:A:61:HIS:CD2	1:A:422:HIS:H	2.31	0.49
1:B:384:TYR:O	1:B:385:PHE:HD1	1.95	0.49
1:B:457:THR:CG2	1:B:458:PHE:N	2.75	0.49
1:A:156:GLU:CA	1:A:161:ARG:HE	2.26	0.49
1:B:431:VAL:HG22	1:B:465:MET:HG3	1.95	0.49
1:A:384:TYR:O	1:A:385:PHE:HD1	1.95	0.48
1:A:457:THR:CG2	1:A:458:PHE:N	2.75	0.48
1:B:378:ILE:HG22	1:B:381:VAL:HG23	1.94	0.48
1:A:37:VAL:HA	1:A:74:ILE:O	2.12	0.48
1:A:65:ASP:O	1:A:68:TYR:HB2	2.13	0.48
1:A:387:GLU:HB2	3:A:606:HOH:O	2.13	0.48
1:B:80:VAL:CG1	1:B:209:LEU:HD21	2.38	0.48
1:B:156:GLU:HB2	1:B:161:ARG:HE	1.76	0.48
1:B:197:HIS:HB2	1:B:265:ILE:HD11	1.95	0.48
1:A:218:PRO:O	1:A:220:PRO:HD3	2.12	0.48
1:B:18:LEU:HG	1:B:22:ASN:ND2	2.28	0.48
1:B:221:LYS:O	1:B:222:ARG:HB3	2.13	0.48
1:B:16:LEU:HG	1:B:17:SER:N	2.27	0.48
1:B:43:LYS:C	1:B:45:GLN:N	2.70	0.48
1:B:61:HIS:CD2	1:B:422:HIS:H	2.31	0.48
1:B:323:ASP:OD1	1:B:326:SER:N	2.35	0.48
1:A:7:PHE:HA	1:A:22:ASN:OD1	2.14	0.48
1:A:454:PHE:HZ	1:A:467:HIS:CE1	2.32	0.48
2:A:600:FAA:C4	2:A:600:FAA:C1P	2.82	0.48
1:B:454:PHE:HZ	1:B:467:HIS:CE1	2.32	0.48
1:B:90:ALA:HB1	1:B:540:ILE:HG23	1.96	0.48
1:B:156:GLU:CA	1:B:161:ARG:HE	2.26	0.48
1:A:22:ASN:O	1:A:25:ILE:HG22	2.14	0.48
1:A:452:LEU:HD23	1:A:452:LEU:HA	1.31	0.48
1:B:56:HIS:HB2	1:B:74:ILE:HD13	1.96	0.48
1:B:65:ASP:O	1:B:68:TYR:HB2	2.13	0.48
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.96	0.48
1:A:197:HIS:HB2	1:A:265:ILE:HD11	1.95	0.48
1:A:431:VAL:HG22	1:A:465:MET:HG3	1.95	0.48
1:A:16:LEU:HG	1:A:17:SER:N	2.27	0.48
1:A:36:ASN:OD1	1:A:76:ALA:HB3	2.14	0.48
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.44	0.48
1:B:139:TYR:CD1	1:B:139:TYR:C	2.92	0.48
1:B:330:ARG:HH22	1:B:335:SER:HB3	1.79	0.48
1:A:90:ALA:HB1	1:A:540:ILE:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD22	1:A:119:VAL:HB	1.94	0.48
1:B:36:ASN:OD1	1:B:76:ALA:HB3	2.14	0.48
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.43	0.48
1:B:388:ASP:N	1:B:388:ASP:OD1	2.45	0.48
1:A:230:PRO:HA	1:A:233:GLN:CD	2.39	0.47
1:B:97:LEU:HD22	1:B:119:VAL:HB	1.94	0.47
1:B:173:GLY:H	1:B:408:TYR:HE1	1.62	0.47
1:A:139:TYR:CD1	1:A:139:TYR:C	2.92	0.47
1:A:195:MET:HE1	1:B:195:MET:CE	2.44	0.47
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.38	0.47
1:A:502:GLU:HB3	1:A:513:ILE:HD13	1.96	0.47
1:B:29:ILE:C	1:B:31:ILE:H	2.21	0.47
1:B:230:PRO:HA	1:B:233:GLN:CD	2.39	0.47
1:A:330:ARG:HH22	1:A:335:SER:HB3	1.79	0.47
1:A:338:GLU:O	1:A:341:LYS:HB2	2.14	0.47
1:B:276:TYR:OH	1:B:399:ASP:O	2.24	0.47
1:B:417:LEU:CB	1:B:418:PRO:HD2	2.38	0.47
1:B:148:TYR:HB2	1:B:172:GLY:O	2.15	0.47
1:B:155:LEU:HD23	1:B:155:LEU:HA	1.38	0.47
1:B:198:SER:O	1:B:266:GLY:HA3	2.14	0.47
1:B:427:PRO:HD2	1:B:467:HIS:O	2.15	0.47
1:A:147:THR:HB	1:A:173:GLY:O	2.15	0.47
1:A:248:PRO:HD3	1:B:256:GLN:O	2.14	0.47
1:B:332:GLU:HB3	1:B:333:PRO:HD3	1.96	0.47
1:B:436:ALA:HB2	1:B:465:MET:HE1	1.96	0.47
1:A:29:ILE:C	1:A:31:ILE:H	2.21	0.47
1:A:45:GLN:CG	1:A:46:ILE:N	2.74	0.47
1:A:427:PRO:HD2	1:A:467:HIS:O	2.15	0.47
1:A:463:ARG:NH2	1:B:269:LEU:O	2.47	0.47
1:B:398:ARG:HB3	1:B:402:MET:HE2	1.96	0.47
1:A:100:ILE:O	1:A:100:ILE:HG13	2.14	0.47
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.96	0.47
1:A:198:SER:O	1:A:266:GLY:HA3	2.14	0.47
1:B:7:PHE:HA	1:B:22:ASN:OD1	2.14	0.47
1:B:10:LEU:CD2	1:B:41:SER:C	2.88	0.47
1:B:22:ASN:O	1:B:25:ILE:HG22	2.14	0.47
1:B:147:THR:HB	1:B:173:GLY:O	2.15	0.47
1:B:168:VAL:HA	1:B:169:PRO:HD3	1.66	0.47
1:A:398:ARG:HB3	1:A:402:MET:HE2	1.96	0.47
1:B:272:ASN:HA	1:B:273:PRO:HD3	1.55	0.47
1:B:295:ILE:HD12	1:B:378:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD12	1:B:350:ARG:CZ	2.45	0.47
1:A:25:ILE:CG2	1:A:26:GLN:N	2.78	0.47
1:A:148:TYR:HB2	1:A:172:GLY:O	2.15	0.47
1:A:525:LEU:O	1:A:529:GLU:HG3	2.15	0.47
1:B:480:GLN:HG3	1:B:483:LYS:HD2	1.97	0.47
1:A:516:THR:C	1:A:518:ASN:H	2.23	0.47
1:B:338:GLU:O	1:B:341:LYS:HB2	2.14	0.47
1:B:505:THR:CG2	1:B:509:PHE:HB2	2.41	0.47
1:A:10:LEU:HD21	1:A:42:SER:N	2.31	0.46
1:A:182:GLU:OE1	1:A:256:GLN:HG2	2.15	0.46
1:A:290:LYS:O	1:A:290:LYS:HG3	2.15	0.46
1:A:295:ILE:HD12	1:A:378:ILE:HD11	1.97	0.46
1:A:339:LEU:HD12	1:A:350:ARG:CZ	2.45	0.46
1:B:502:GLU:HB3	1:B:513:ILE:HD13	1.96	0.46
1:A:244:TYR:CD1	1:A:244:TYR:N	2.82	0.46
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.77	0.46
1:A:332:GLU:CB	1:A:333:PRO:CD	2.89	0.46
1:B:516:THR:C	1:B:518:ASN:H	2.23	0.46
1:A:198:SER:HB2	1:A:268:TRP:CZ2	2.50	0.46
1:A:436:ALA:HB2	1:A:465:MET:HE1	1.96	0.46
1:B:10:LEU:HD21	1:B:42:SER:N	2.31	0.46
1:B:139:TYR:HE2	1:B:241:LEU:CD1	2.29	0.46
1:B:238:ILE:HA	1:B:241:LEU:HD22	1.98	0.46
1:A:90:ALA:O	1:A:94:SER:N	2.48	0.46
1:A:204:LEU:HD22	1:B:527:PHE:CE1	2.50	0.46
1:A:545:LYS:C	1:A:547:GLY:N	2.72	0.46
1:B:127:MET:O	1:B:143:GLU:HB3	2.16	0.46
1:B:198:SER:HB2	1:B:268:TRP:CZ2	2.50	0.46
1:A:36:ASN:CB	1:A:76:ALA:HB3	2.46	0.46
1:A:127:MET:O	1:A:143:GLU:HB3	2.16	0.46
1:A:173:GLY:H	1:A:408:TYR:HE1	1.62	0.46
1:A:332:GLU:HB3	1:A:333:PRO:HD3	1.96	0.46
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.50	0.46
1:B:93:PHE:O	1:B:94:SER:HB2	2.16	0.46
1:B:132:GLU:CG	1:B:133:VAL:N	2.72	0.46
1:B:182:GLU:OE1	1:B:256:GLN:HG2	2.15	0.46
1:B:460:VAL:HG12	1:B:461:GLY:O	2.15	0.46
1:A:10:LEU:CD2	1:A:41:SER:C	2.88	0.46
1:A:139:TYR:HE2	1:A:241:LEU:CD1	2.29	0.46
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.80	0.46
1:B:200:MET:HE2	1:B:251:ASP:CB	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ILE:O	1:B:374:ALA:N	2.49	0.46
1:B:549:TRP:HA	1:B:550:PRO:HD3	1.75	0.46
1:A:13:PRO:HD3	1:A:117:GLY:O	2.16	0.46
1:A:56:HIS:HB2	1:A:74:ILE:HD13	1.96	0.46
1:A:480:GLN:HG3	1:A:483:LYS:HD2	1.97	0.46
1:B:480:GLN:HA	1:B:483:LYS:HG3	1.98	0.46
1:B:525:LEU:O	1:B:529:GLU:HG3	2.15	0.46
1:A:72:SER:HB3	1:A:117:GLY:O	2.16	0.46
1:A:93:PHE:O	1:A:94:SER:HB2	2.16	0.46
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.33	0.46
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.82	0.46
1:B:346:LEU:HB3	1:B:348:LEU:HD11	1.98	0.46
1:B:545:LYS:C	1:B:547:GLY:N	2.72	0.46
1:A:237:LYS:HG3	1:A:238:ILE:HG12	1.98	0.46
1:B:11:THR:HG22	1:B:117:GLY:HA3	1.98	0.46
1:B:156:GLU:HA	1:B:161:ARG:HE	1.81	0.46
1:B:550:PRO:CB	1:B:552:GLN:NE2	2.77	0.46
1:A:167:ASP:OD2	1:A:191:GLY:HA2	2.16	0.46
1:A:244:TYR:OH	1:B:195:MET:HG2	2.16	0.46
1:A:280:LEU:HD12	1:A:353:PHE:O	2.16	0.46
1:A:330:ARG:NH1	1:A:338:GLU:OE2	2.49	0.46
1:A:371:ILE:O	1:A:374:ALA:N	2.49	0.46
1:A:387:GLU:C	1:A:389:THR:H	2.24	0.46
1:B:484:VAL:O	1:B:487:LEU:HB3	2.16	0.46
1:A:62:HIS:CD2	1:A:66:GLN:HB2	2.51	0.45
1:B:242:PHE:HA	1:B:243:PRO:HD3	1.38	0.45
1:B:244:TYR:N	1:B:244:TYR:CD1	2.82	0.45
1:B:480:GLN:HA	1:B:483:LYS:CE	2.46	0.45
1:A:40:ILE:HD11	1:A:57:THR:CG2	2.42	0.45
1:A:132:GLU:O	1:A:140:CYS:HA	2.16	0.45
1:A:156:GLU:HA	1:A:161:ARG:HE	1.81	0.45
1:A:195:MET:HE1	1:B:195:MET:HE1	1.98	0.45
1:A:295:ILE:CG2	1:A:375:PHE:CE1	3.00	0.45
1:A:299:LEU:HB2	1:A:305:LEU:HD12	1.98	0.45
1:A:484:VAL:O	1:A:487:LEU:HB3	2.16	0.45
1:B:90:ALA:O	1:B:94:SER:N	2.48	0.45
1:B:100:ILE:O	1:B:100:ILE:HG13	2.14	0.45
1:B:132:GLU:O	1:B:140:CYS:HA	2.16	0.45
1:B:280:LEU:HD12	1:B:353:PHE:O	2.16	0.45
1:A:480:GLN:HA	1:A:483:LYS:CE	2.46	0.45
1:B:13:PRO:HD3	1:B:117:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:HIS:N	1:B:62:HIS:HD1	2.12	0.45
1:B:277:GLN:O	1:B:356:ALA:HA	2.17	0.45
1:A:93:PHE:N	1:A:93:PHE:CD1	2.85	0.45
1:A:388:ASP:N	1:A:388:ASP:OD1	2.45	0.45
1:A:460:VAL:HG12	1:A:461:GLY:O	2.15	0.45
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.65	0.45
1:B:290:LYS:O	1:B:290:LYS:HG3	2.15	0.45
1:B:325:ARG:C	1:B:327:TYR:N	2.74	0.45
1:A:253:LEU:O	1:A:257:SER:OG	2.29	0.45
1:A:506:HIS:CG	1:A:507:LEU:N	2.84	0.45
1:B:59:ASP:HA	1:B:60:PRO:HD3	1.80	0.45
1:B:299:LEU:HB2	1:B:305:LEU:HD12	1.98	0.45
1:B:330:ARG:NH1	1:B:338:GLU:OE2	2.49	0.45
1:B:393:SER:HB3	1:B:396:ARG:HG3	1.98	0.45
1:A:11:THR:HG22	1:A:117:GLY:HA3	1.98	0.45
1:B:10:LEU:HD21	1:B:42:SER:C	2.42	0.45
1:B:25:ILE:CG2	1:B:26:GLN:N	2.78	0.45
1:B:40:ILE:O	1:B:40:ILE:HG22	2.16	0.45
1:B:72:SER:HB3	1:B:117:GLY:O	2.16	0.45
1:B:506:HIS:CG	1:B:507:LEU:N	2.84	0.45
1:A:480:GLN:HA	1:A:483:LYS:HG3	1.98	0.45
1:B:167:ASP:OD2	1:B:191:GLY:HA2	2.16	0.45
1:B:387:GLU:C	1:B:389:THR:H	2.24	0.45
1:A:40:ILE:O	1:A:40:ILE:HG22	2.16	0.45
1:A:277:GLN:O	1:A:356:ALA:HA	2.17	0.45
1:A:417:LEU:HD23	1:A:417:LEU:N	2.19	0.45
1:B:40:ILE:HD11	1:B:57:THR:CG2	2.42	0.45
1:B:426:SER:N	1:B:502:GLU:CD	2.75	0.45
1:A:384:TYR:CD1	1:A:384:TYR:N	2.85	0.45
1:B:180:ALA:O	1:B:194:TRP:HE3	2.00	0.45
1:B:389:THR:HB	1:B:390:PRO:CD	2.47	0.45
2:B:600:FAA:C4	2:B:600:FAA:C1P	2.82	0.45
1:A:248:PRO:HG3	1:B:257:SER:HB3	1.97	0.45
1:A:309:PRO:CB	1:A:353:PHE:HE1	2.29	0.45
1:A:552:GLN:CD	1:A:552:GLN:N	2.75	0.45
1:B:536:ASP:HA	1:B:537:PRO:HD3	1.47	0.45
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.80	0.45
1:A:139:TYR:CE2	1:A:241:LEU:CD1	3.00	0.44
1:A:151:LEU:O	1:A:155:LEU:HG	2.17	0.44
1:A:293:VAL:C	1:A:295:ILE:N	2.74	0.44
1:A:426:SER:N	1:A:502:GLU:CD	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PHE:CD1	1:B:93:PHE:N	2.85	0.44
1:B:205:ALA:C	1:B:207:GLY:H	2.24	0.44
1:B:237:LYS:HG3	1:B:238:ILE:HG12	1.98	0.44
1:B:426:SER:HB2	1:B:502:GLU:HG3	1.99	0.44
1:A:220:PRO:HD2	3:A:620:HOH:O	2.17	0.44
1:A:308:VAL:HG13	1:A:460:VAL:O	2.17	0.44
1:A:426:SER:HB2	1:A:502:GLU:HG3	1.99	0.44
1:A:487:LEU:CD1	1:A:491:LEU:HD11	2.47	0.44
1:B:102:ILE:HD13	1:B:102:ILE:HA	1.71	0.44
1:B:139:TYR:CE2	1:B:241:LEU:CD1	2.99	0.44
1:B:142:VAL:HB	1:B:146:VAL:CG2	2.47	0.44
1:B:283:LEU:O	1:B:349:GLY:CA	2.66	0.44
1:B:295:ILE:CG2	1:B:375:PHE:CE1	3.00	0.44
1:B:346:LEU:HB2	1:B:348:LEU:HD12	1.99	0.44
1:B:36:ASN:CB	1:B:76:ALA:HB3	2.46	0.44
1:B:131:LEU:HD11	1:B:143:GLU:HG3	2.00	0.44
1:B:270:MET:HA	1:B:271:PRO:HD2	1.78	0.44
1:B:309:PRO:CB	1:B:353:PHE:HE1	2.29	0.44
1:B:487:LEU:CD1	1:B:491:LEU:HD11	2.47	0.44
1:B:513:ILE:O	1:B:516:THR:HG23	2.18	0.44
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.50	0.44
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.44	0.44
1:A:131:LEU:HD11	1:A:143:GLU:HG3	2.00	0.44
1:A:313:HIS:HB2	1:A:351:TRP:CH2	2.52	0.44
1:A:513:ILE:O	1:A:516:THR:HG23	2.17	0.44
1:B:313:HIS:HB2	1:B:351:TRP:CH2	2.52	0.44
1:B:384:TYR:CD1	1:B:384:TYR:N	2.85	0.44
1:B:478:LEU:CD1	1:B:478:LEU:N	2.80	0.44
1:A:408:TYR:O	1:A:411:LEU:HD12	2.18	0.44
1:A:506:HIS:CE1	1:A:507:LEU:HB2	2.53	0.44
1:B:62:HIS:CD2	1:B:66:GLN:HB2	2.51	0.44
1:B:156:GLU:CD	1:B:161:ARG:NH2	2.76	0.44
1:B:408:TYR:O	1:B:411:LEU:HD12	2.18	0.44
1:B:417:LEU:HD23	1:B:417:LEU:N	2.19	0.44
1:A:142:VAL:HB	1:A:146:VAL:CG2	2.47	0.44
1:A:156:GLU:CD	1:A:161:ARG:NH2	2.76	0.44
1:A:291:GLN:O	1:A:295:ILE:HG13	2.18	0.44
1:A:300:ARG:HE	1:A:309:PRO:CD	2.31	0.44
1:A:393:SER:HB3	1:A:396:ARG:HG3	1.99	0.44
1:B:151:LEU:HD12	1:B:151:LEU:O	2.18	0.44
1:A:205:ALA:C	1:A:207:GLY:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HB3	1:A:348:LEU:HD11	1.98	0.44
1:B:90:ALA:HB1	1:B:95:PHE:O	2.18	0.44
1:B:231:GLU:H	1:B:231:GLU:HG2	0.94	0.44
1:B:291:GLN:O	1:B:295:ILE:HG13	2.18	0.44
1:B:300:ARG:HE	1:B:309:PRO:CD	2.31	0.44
1:A:168:VAL:HA	1:A:169:PRO:HD3	1.66	0.44
1:A:550:PRO:CB	1:A:552:GLN:NE2	2.77	0.44
1:A:102:ILE:CG2	1:A:104:ARG:HD2	2.48	0.44
1:A:151:LEU:O	1:A:151:LEU:HD12	2.18	0.44
1:A:238:ILE:HA	1:A:241:LEU:HD22	1.98	0.44
1:A:432:SER:HB3	1:A:435:ASP:HB2	2.00	0.44
1:A:447:CYS:O	1:A:452:LEU:N	2.49	0.44
1:B:33:GLY:C	1:B:35:GLU:N	2.73	0.44
1:B:136:GLU:H	1:B:136:GLU:CD	2.26	0.44
1:B:188:THR:CB	1:B:189:PRO:HD2	2.47	0.44
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.38	0.43
1:A:156:GLU:HG3	1:A:161:ARG:CZ	2.48	0.43
1:A:180:ALA:O	1:A:194:TRP:HE3	2.00	0.43
1:A:346:LEU:HB2	1:A:348:LEU:HD12	1.99	0.43
1:B:89:LEU:HA	1:B:89:LEU:HD23	1.44	0.43
1:B:151:LEU:O	1:B:155:LEU:HG	2.17	0.43
1:B:156:GLU:HG3	1:B:161:ARG:CZ	2.48	0.43
1:A:332:GLU:CB	1:A:333:PRO:HD3	2.49	0.43
1:A:385:PHE:HB2	3:A:606:HOH:O	2.18	0.43
1:A:389:THR:HB	1:A:390:PRO:CD	2.47	0.43
1:A:478:LEU:CD1	1:A:478:LEU:N	2.80	0.43
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.77	0.43
1:B:307:ASN:HB3	1:B:358:TYR:CE1	2.53	0.43
1:B:308:VAL:HG13	1:B:460:VAL:O	2.17	0.43
1:A:10:LEU:HD21	1:A:42:SER:C	2.42	0.43
1:A:179:ASN:OD1	1:A:184:GLY:HA3	2.19	0.43
1:A:201:GLU:O	1:A:262:VAL:HG13	2.18	0.43
1:A:222:ARG:HB2	1:A:223:PRO:CD	2.47	0.43
1:B:224:GLU:CD	1:B:224:GLU:N	2.76	0.43
1:B:447:CYS:O	1:B:452:LEU:N	2.49	0.43
1:A:90:ALA:HB1	1:A:95:PHE:O	2.18	0.43
1:A:136:GLU:H	1:A:136:GLU:CD	2.26	0.43
1:A:247:GLY:HA2	1:B:256:GLN:HB3	2.00	0.43
1:B:25:ILE:HD12	1:B:25:ILE:HA	1.74	0.43
1:B:179:ASN:OD1	1:B:184:GLY:HA3	2.19	0.43
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HD12	1:A:254:PHE:HE2	1.84	0.43
1:A:307:ASN:HB3	1:A:358:TYR:CE1	2.53	0.43
1:B:102:ILE:CG2	1:B:104:ARG:HD2	2.48	0.43
1:B:201:GLU:HG2	1:B:263:THR:HG1	1.81	0.43
1:B:280:LEU:CD1	1:B:281:ILE:N	2.78	0.43
1:A:90:ALA:HB2	1:A:97:LEU:HD11	2.01	0.43
1:A:156:GLU:CG	1:A:161:ARG:NH2	2.82	0.43
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.53	0.43
1:B:421:ALA:HA	3:B:636:HOH:O	2.18	0.43
1:B:432:SER:HB3	1:B:435:ASP:HB2	2.00	0.43
1:B:156:GLU:CG	1:B:161:ARG:NH2	2.82	0.43
1:B:316:LEU:HA	1:B:316:LEU:HD12	1.69	0.43
1:B:506:HIS:CE1	1:B:507:LEU:HB2	2.53	0.43
1:B:540:ILE:O	1:B:540:ILE:HG22	2.18	0.43
1:A:550:PRO:HB2	1:A:552:GLN:CG	2.42	0.43
1:B:121:LEU:HD12	1:B:121:LEU:HA	1.44	0.43
1:A:195:MET:CE	1:B:195:MET:HE1	2.49	0.43
1:A:299:LEU:CB	1:A:305:LEU:HG	2.49	0.43
1:B:290:LYS:HB2	1:B:437:MET:SD	2.59	0.43
1:B:332:GLU:CB	1:B:333:PRO:HD3	2.49	0.43
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.31	0.43
1:A:545:LYS:HE3	1:A:546:SER:OG	2.19	0.42
1:B:134:ASN:OD1	1:B:134:ASN:C	2.62	0.42
1:B:283:LEU:O	1:B:350:ARG:N	2.48	0.42
1:B:368:TRP:HA	1:B:368:TRP:CE3	2.54	0.42
1:A:83:VAL:CG2	1:A:127:MET:HE1	2.47	0.42
1:A:325:ARG:C	1:A:327:TYR:N	2.74	0.42
1:A:361:GLU:HB2	1:A:364:ARG:NH2	2.34	0.42
1:B:359:GLY:HA3	1:B:360:PRO:HD3	1.79	0.42
1:A:316:LEU:HD11	1:A:413:TRP:NE1	2.34	0.42
1:A:370:THR:O	1:A:374:ALA:N	2.52	0.42
1:B:137:GLY:O	1:B:138:ALA:HB3	2.19	0.42
1:B:201:GLU:O	1:B:262:VAL:HG13	2.19	0.42
1:B:401:THR:C	1:B:403:GLN:N	2.78	0.42
1:B:552:GLN:CD	1:B:552:GLN:N	2.75	0.42
1:B:104:ARG:C	1:B:106:SER:N	2.76	0.42
1:B:299:LEU:CB	1:B:305:LEU:HG	2.49	0.42
1:A:33:GLY:C	1:A:35:GLU:N	2.73	0.42
1:A:36:ASN:HB3	1:A:76:ALA:O	2.20	0.42
1:A:88:GLY:O	1:A:92:LYS:N	2.51	0.42
1:A:429:ALA:O	1:A:465:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:HD23	1:A:510:MET:CE	2.50	0.42
1:B:90:ALA:HB2	1:B:97:LEU:HD11	2.01	0.42
1:A:309:PRO:CB	1:A:353:PHE:CE1	3.03	0.42
1:A:346:LEU:CB	1:A:348:LEU:CD1	2.97	0.42
1:A:368:TRP:HA	1:A:368:TRP:CE3	2.55	0.42
1:A:549:TRP:HA	1:A:550:PRO:HD3	1.75	0.42
1:B:361:GLU:N	1:B:364:ARG:HH21	2.18	0.42
1:B:545:LYS:HE3	1:B:546:SER:OG	2.19	0.42
1:A:202:VAL:CG2	1:A:261:ILE:N	2.83	0.42
1:A:257:SER:CB	1:B:248:PRO:HG3	2.50	0.42
1:B:370:THR:O	1:B:374:ALA:N	2.52	0.42
1:B:448:GLN:HB3	1:B:449:GLU:H	1.53	0.42
1:A:40:ILE:CD1	1:A:57:THR:CG2	2.98	0.42
1:A:200:MET:CE	1:A:251:ASP:CB	2.95	0.42
1:A:231:GLU:H	1:A:231:GLU:HG2	0.94	0.42
1:A:290:LYS:HB2	1:A:437:MET:SD	2.59	0.42
1:B:202:VAL:CG2	1:B:261:ILE:N	2.83	0.42
1:B:378:ILE:HA	1:B:379:PRO:HD2	1.78	0.42
1:A:58:HIS:C	1:A:58:HIS:CD2	2.97	0.42
1:A:102:ILE:HB	2:A:600:FAA:O2P	2.19	0.42
1:A:423:LEU:CD2	1:A:488:MET:HE3	2.50	0.42
1:B:102:ILE:HB	2:B:600:FAA:O2P	2.19	0.42
1:B:354:TYR:HD2	1:B:395:LEU:CD1	2.33	0.42
1:B:361:GLU:HB2	1:B:364:ARG:NH2	2.34	0.42
1:B:445:LYS:HE2	1:B:449:GLU:OE2	2.20	0.42
1:A:283:LEU:O	1:A:349:GLY:CA	2.66	0.42
1:A:283:LEU:O	1:A:350:ARG:N	2.48	0.42
1:A:401:THR:C	1:A:403:GLN:N	2.77	0.42
1:A:527:PHE:CE1	1:B:204:LEU:HD22	2.55	0.42
1:B:36:ASN:HB3	1:B:76:ALA:O	2.19	0.42
1:B:108:TYR:HA	1:B:506:HIS:HA	2.02	0.42
1:B:282:THR:O	1:B:283:LEU:HD23	2.20	0.42
1:B:317:ASP:O	1:B:320:VAL:HB	2.20	0.42
1:B:423:LEU:CD2	1:B:488:MET:HE3	2.50	0.42
1:A:229:LYS:HB2	1:A:231:GLU:HG3	2.02	0.41
1:A:327:TYR:O	1:A:328:SER:HB2	2.19	0.41
1:B:95:PHE:CE1	1:B:119:VAL:CG2	3.00	0.41
1:B:327:TYR:O	1:B:328:SER:HB2	2.19	0.41
1:B:346:LEU:CB	1:B:348:LEU:CD1	2.97	0.41
1:B:429:ALA:O	1:B:465:MET:HB2	2.20	0.41
1:B:532:LYS:NZ	1:B:541:ILE:HB	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.45	0.41
1:A:155:LEU:HD23	1:A:155:LEU:N	2.19	0.41
1:A:282:THR:O	1:A:283:LEU:HD23	2.20	0.41
1:A:532:LYS:NZ	1:A:541:ILE:HB	2.35	0.41
1:B:69:PHE:HB3	1:B:113:PRO:O	2.20	0.41
1:B:102:ILE:HG22	1:B:104:ARG:H	1.85	0.41
1:B:229:LYS:HB2	1:B:231:GLU:HG3	2.02	0.41
1:B:250:ILE:HD12	1:B:254:PHE:HE2	1.84	0.41
1:B:314:ILE:HG22	1:B:350:ARG:O	2.20	0.41
1:A:134:ASN:OD1	1:A:134:ASN:C	2.63	0.41
1:A:172:GLY:HA3	1:A:408:TYR:CE1	2.55	0.41
1:A:502:GLU:CG	1:A:503:TYR:N	2.82	0.41
1:B:361:GLU:O	1:B:365:ARG:HB2	2.21	0.41
1:A:102:ILE:HG22	1:A:104:ARG:H	1.85	0.41
1:A:138:ALA:HA	1:A:164:LEU:HD21	2.03	0.41
1:A:150:ASP:O	1:A:151:LEU:C	2.64	0.41
1:A:252:GLY:C	1:A:254:PHE:N	2.77	0.41
1:B:222:ARG:HB2	1:B:223:PRO:CD	2.47	0.41
1:B:278:SER:OG	1:B:399:ASP:OD2	2.28	0.41
2:B:600:FAA:H6P	2:B:600:FAA:C9A	2.50	0.41
1:A:317:ASP:O	1:A:320:VAL:HB	2.20	0.41
1:A:361:GLU:N	1:A:364:ARG:HH21	2.18	0.41
1:A:454:PHE:CD1	1:A:455:ILE:N	2.89	0.41
1:A:520:ASN:O	1:A:521:ASN:CB	2.68	0.41
1:A:540:ILE:O	1:A:540:ILE:HG22	2.18	0.41
1:B:351:TRP:HA	1:B:351:TRP:HE3	1.81	0.41
1:B:507:LEU:HD23	1:B:510:MET:CE	2.50	0.41
1:A:137:GLY:O	1:A:138:ALA:HB3	2.19	0.41
1:A:188:THR:CB	1:A:189:PRO:HD2	2.47	0.41
1:A:363:ILE:N	1:A:363:ILE:CD1	2.80	0.41
1:A:368:TRP:NE1	1:A:372:LYS:HD2	2.36	0.41
1:A:370:THR:O	1:A:374:ALA:HB2	2.20	0.41
1:B:297:ARG:HG2	1:B:298:PRO:HD3	2.03	0.41
1:B:316:LEU:HD11	1:B:413:TRP:NE1	2.34	0.41
1:B:505:THR:CG2	1:B:506:HIS:N	2.74	0.41
1:A:69:PHE:HB3	1:A:113:PRO:O	2.20	0.41
1:A:278:SER:OG	1:A:399:ASP:OD2	2.28	0.41
1:A:454:PHE:CD1	1:A:454:PHE:C	2.99	0.41
1:B:58:HIS:C	1:B:58:HIS:CD2	2.97	0.41
1:B:309:PRO:CB	1:B:353:PHE:CE1	3.03	0.41
1:B:341:LYS:HA	1:B:344:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:TRP:C	1:B:415:ASP:N	2.78	0.41
1:B:537:PRO:CD	1:B:538:ASN:N	2.82	0.41
1:A:132:GLU:CG	1:A:133:VAL:N	2.72	0.41
1:A:311:ILE:HG12	1:A:353:PHE:CD1	2.56	0.41
1:B:172:GLY:HA3	1:B:408:TYR:CE1	2.55	0.41
1:B:283:LEU:HA	1:B:284:PRO:HD3	1.76	0.41
1:A:58:HIS:CD2	1:A:59:ASP:O	2.74	0.41
1:A:112:ALA:O	1:A:507:LEU:HD11	2.21	0.41
1:A:272:ASN:OD1	1:A:273:PRO:HD2	2.21	0.41
1:A:314:ILE:HG22	1:A:350:ARG:O	2.20	0.41
1:A:413:TRP:CE3	1:A:413:TRP:C	2.99	0.41
1:A:479:ILE:HG22	1:A:483:LYS:HE3	2.02	0.41
2:A:600:FAA:H6P	2:A:600:FAA:C9A	2.50	0.41
1:B:108:TYR:CE1	1:B:505:THR:CA	3.04	0.41
1:B:166:LEU:HD23	1:B:269:LEU:CD2	2.50	0.41
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.82	0.41
1:B:202:VAL:CG2	1:B:203:VAL:N	2.84	0.41
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.33	0.41
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.21	0.41
1:B:342:ILE:HD13	1:B:342:ILE:HG21	1.83	0.41
1:B:368:TRP:NE1	1:B:372:LYS:HD2	2.36	0.41
1:B:421:ALA:O	1:B:472:VAL:HA	2.21	0.41
1:B:478:LEU:N	1:B:478:LEU:HD12	2.36	0.41
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.56	0.41
1:A:272:ASN:HA	1:A:273:PRO:HD3	1.55	0.41
1:A:361:GLU:O	1:A:365:ARG:HB2	2.21	0.41
1:A:383:PHE:CD1	1:A:383:PHE:N	2.89	0.41
1:A:467:HIS:ND1	1:A:467:HIS:C	2.79	0.41
1:A:478:LEU:N	1:A:478:LEU:HD12	2.36	0.41
1:B:83:VAL:CG2	1:B:127:MET:HE1	2.47	0.41
1:B:370:THR:O	1:B:374:ALA:HB2	2.20	0.41
1:B:434:GLU:HB3	1:B:435:ASP:H	1.70	0.41
1:B:467:HIS:ND1	1:B:467:HIS:C	2.79	0.41
1:B:520:ASN:O	1:B:521:ASN:CB	2.68	0.41
1:B:550:PRO:HB2	1:B:552:GLN:CG	2.42	0.41
1:A:166:LEU:HD23	1:A:269:LEU:CD2	2.50	0.40
1:A:378:ILE:HA	1:A:379:PRO:HD2	1.78	0.40
1:A:421:ALA:O	1:A:472:VAL:HA	2.21	0.40
1:A:445:LYS:HE2	1:A:449:GLU:OE2	2.20	0.40
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.56	0.40
1:A:59:ASP:HA	1:A:60:PRO:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ARG:HA	1:B:9:PRO:HD2	1.90	0.40
1:B:27:ASP:N	1:B:27:ASP:OD1	2.54	0.40
1:B:58:HIS:HD2	1:B:59:ASP:O	2.04	0.40
1:B:222:ARG:HA	1:B:223:PRO:HD3	1.63	0.40
1:B:310:THR:HA	1:B:459:THR:HA	2.03	0.40
1:B:454:PHE:CD1	1:B:455:ILE:N	2.89	0.40
1:A:8:ARG:H	1:A:8:ARG:HG3	1.61	0.40
1:A:108:TYR:HA	1:A:506:HIS:HA	2.02	0.40
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.76	0.40
1:A:341:LYS:HA	1:A:344:LYS:HE2	2.03	0.40
1:B:40:ILE:CD1	1:B:57:THR:CG2	2.98	0.40
1:B:112:ALA:O	1:B:507:LEU:HD11	2.21	0.40
1:A:308:VAL:HA	1:A:309:PRO:HD2	1.87	0.40
1:B:54:PRO:HD3	1:B:104:ARG:HH21	1.86	0.40
1:B:138:ALA:HA	1:B:164:LEU:HD21	2.03	0.40
1:B:188:THR:CB	1:B:189:PRO:CD	2.98	0.40
1:B:252:GLY:C	1:B:254:PHE:N	2.77	0.40
1:B:311:ILE:HG12	1:B:353:PHE:CD1	2.56	0.40
1:B:414:ILE:HD11	2:B:600:FAA:C7M	2.50	0.40
1:A:108:TYR:CE1	1:A:505:THR:HA	2.56	0.40
1:A:156:GLU:CB	1:A:161:ARG:HH21	2.27	0.40
1:A:342:ILE:O	1:A:342:ILE:HG22	2.22	0.40
1:A:421:ALA:HB3	1:A:473:PHE:CZ	2.57	0.40
1:B:75:VAL:O	1:B:77:PRO:HD2	2.22	0.40
1:B:344:LYS:HG3	1:B:345:GLN:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	553/560 (99%)	470 (85%)	69 (12%)	14 (2%)	4 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	553/560 (99%)	470 (85%)	69 (12%)	14 (2%)	4	11
All	All	1106/1120 (99%)	940 (85%)	138 (12%)	28 (2%)	4	11

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	B	44	ASP
1	A	30	ARG
1	A	46	ILE
1	A	328	SER
1	B	30	ARG
1	B	46	ILE
1	B	328	SER
1	A	105	ASN
1	A	199	GLY
1	A	508	ALA
1	B	105	ASN
1	B	199	GLY
1	A	329	SER
1	A	408	TYR
1	B	329	SER
1	B	408	TYR
1	B	508	ALA
1	A	388	ASP
1	B	388	ASP
1	A	248	PRO
1	B	248	PRO
1	A	390	PRO
1	B	390	PRO
1	A	60	PRO
1	B	60	PRO
1	A	223	PRO
1	B	223	PRO

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%)	454 (96%)	21 (4%)	25	53
1	B	475/482 (98%)	454 (96%)	21 (4%)	25	53
All	All	950/964 (98%)	908 (96%)	42 (4%)	25	53

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	63	VAL
1	A	65	ASP
1	A	128	ASN
1	A	134	ASN
1	A	220	PRO
1	A	224	GLU
1	A	231	GLU
1	A	241	LEU
1	A	310	THR
1	A	346	LEU
1	A	363	ILE
1	A	373	ASP
1	A	409	ASP
1	A	413	TRP
1	A	435	ASP
1	A	437	MET
1	A	443	THR
1	A	460	VAL
1	A	478	LEU
1	A	552	GLN
1	B	10	LEU
1	B	63	VAL
1	B	65	ASP
1	B	128	ASN
1	B	134	ASN
1	B	220	PRO
1	B	224	GLU
1	B	231	GLU
1	B	241	LEU
1	B	310	THR
1	B	346	LEU
1	B	363	ILE
1	B	373	ASP

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Mol	Chain	Res	Type
1	B	409	ASP
1	B	413	TRP
1	B	435	ASP
1	B	437	MET
1	B	443	THR
1	B	460	VAL
1	B	478	LEU
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	91	ASN
1	A	152	HIS
1	A	197	HIS
1	A	240	HIS
1	A	403	GLN
1	A	448	GLN
1	A	467	HIS
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	66	GLN
1	B	91	ASN
1	B	152	HIS
1	B	197	HIS
1	B	240	HIS
1	B	403	GLN
1	B	448	GLN
1	B	467	HIS
1	B	485	GLN
1	B	520	ASN
1	B	552	GLN
1	B	555	HIS

5.3.3 RNA ⓘ

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](#)

2 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	FAA	A	600	1	65,67,67	0.92	4 (6%)	89,102,102	1.52	6 (6%)
2	FAA	B	600	1	65,67,67	0.92	4 (6%)	89,102,102	1.52	6 (6%)

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	FAA	A	600	1	-	11/38/54/54	0/7/7/7
2	FAA	B	600	1	-	11/38/54/54	0/7/7/7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAA	PA-O3P	3.69	1.63	1.59
2	B	600	FAA	PA-O3P	3.57	1.63	1.59
2	B	600	FAA	P-O3P	3.52	1.63	1.59
2	A	600	FAA	P-O3P	3.48	1.63	1.59
2	A	600	FAA	C5X-N5	-2.38	1.36	1.40
2	B	600	FAA	C5X-N5	-2.33	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAA	C9A-N10	-2.11	1.37	1.41
2	A	600	FAA	C9A-N10	-2.05	1.37	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAA	C7P-N5-C5X	-11.26	102.71	119.14
2	B	600	FAA	C7P-N5-C5X	-11.26	102.72	119.14
2	B	600	FAA	C1P-C7P-N5	-4.03	106.81	112.85
2	A	600	FAA	C1P-C7P-N5	-4.00	106.85	112.85
2	B	600	FAA	C6-C5X-N5	-2.90	116.92	120.41
2	A	600	FAA	C6-C5X-N5	-2.86	116.96	120.41
2	B	600	FAA	P-O5'-C5'	2.56	136.03	121.35
2	A	600	FAA	P-O5'-C5'	2.56	136.03	121.35
2	B	600	FAA	C4-N3-C2	-2.23	121.67	125.64
2	A	600	FAA	C4-N3-C2	-2.21	121.72	125.64
2	A	600	FAA	O4-C4-C4X	-2.11	123.31	128.01
2	B	600	FAA	O4-C4-C4X	-2.07	123.39	128.01

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAA	C1P-C7P-N5-C4X
2	A	600	FAA	N10-C1'-C2'-O2'
2	A	600	FAA	N10-C1'-C2'-C3'
2	B	600	FAA	C1P-C7P-N5-C4X
2	B	600	FAA	N10-C1'-C2'-O2'
2	B	600	FAA	N10-C1'-C2'-C3'
2	A	600	FAA	C2'-C3'-C4'-O4'
2	B	600	FAA	C2'-C3'-C4'-O4'
2	A	600	FAA	O3'-C3'-C4'-O4'
2	B	600	FAA	O3'-C3'-C4'-O4'
2	A	600	FAA	C2'-C3'-C4'-C5'
2	B	600	FAA	C2'-C3'-C4'-C5'
2	A	600	FAA	O4B-C4B-C5B-O5B
2	B	600	FAA	O4B-C4B-C5B-O5B
2	A	600	FAA	PA-O3P-P-O2P
2	B	600	FAA	PA-O3P-P-O2P
2	A	600	FAA	C4'-C5'-O5'-P
2	B	600	FAA	C4'-C5'-O5'-P
2	A	600	FAA	O3'-C3'-C4'-C5'

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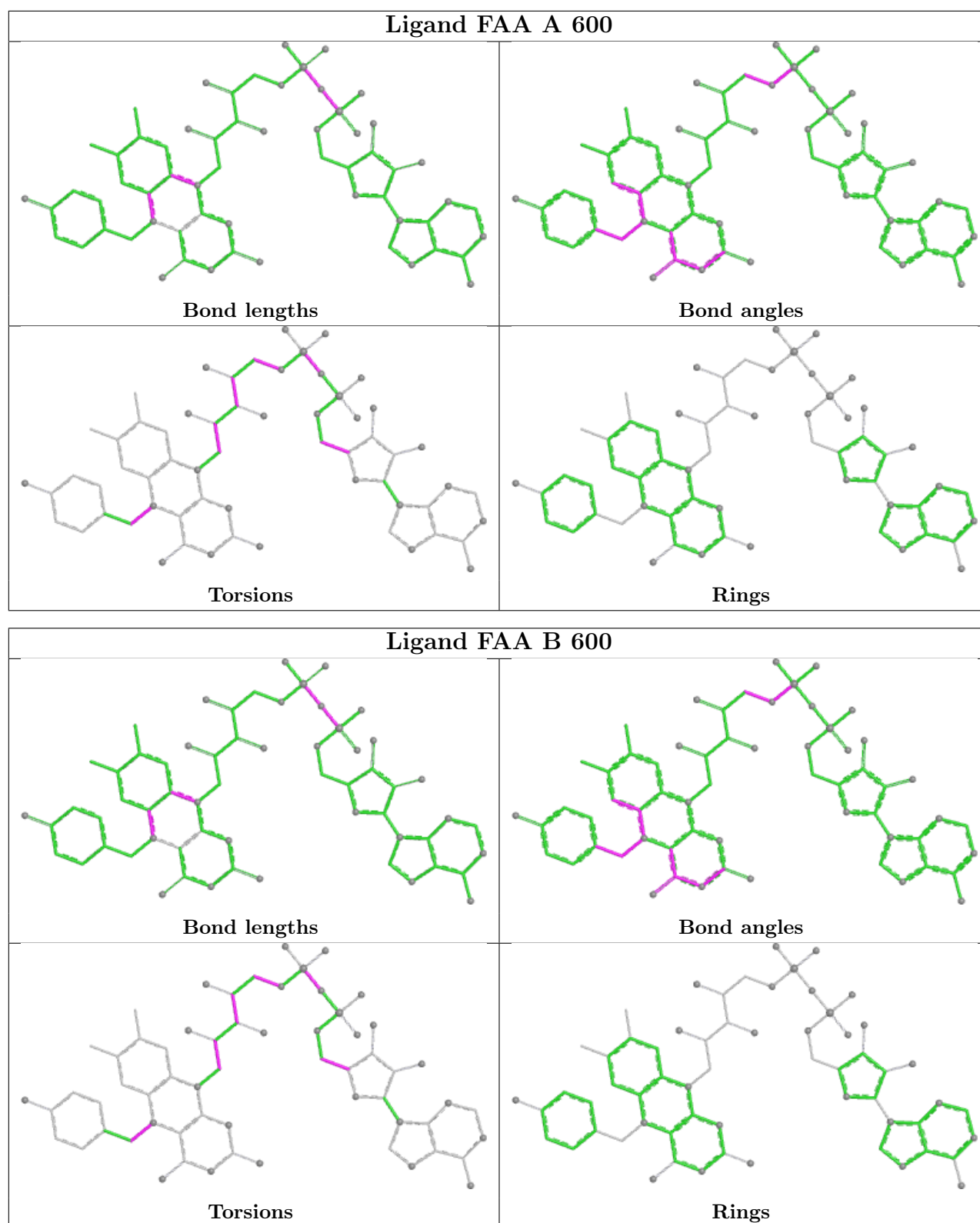
Mol	Chain	Res	Type	Atoms
2	B	600	FAA	O3'-C3'-C4'-C5'
2	A	600	FAA	PA-O3P-P-O1P
2	B	600	FAA	PA-O3P-P-O1P

There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAA	12	0
2	B	600	FAA	13	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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.