



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:03 PM UTC

PDB ID : 2VZ8 / pdb_00002vz8
Title : Crystal Structure of Mammalian Fatty Acid Synthase
Authors : Maier, T.; Leibundgut, M.; Ban, N.
Deposited on : 2008-07-31
Resolution : 3.22 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

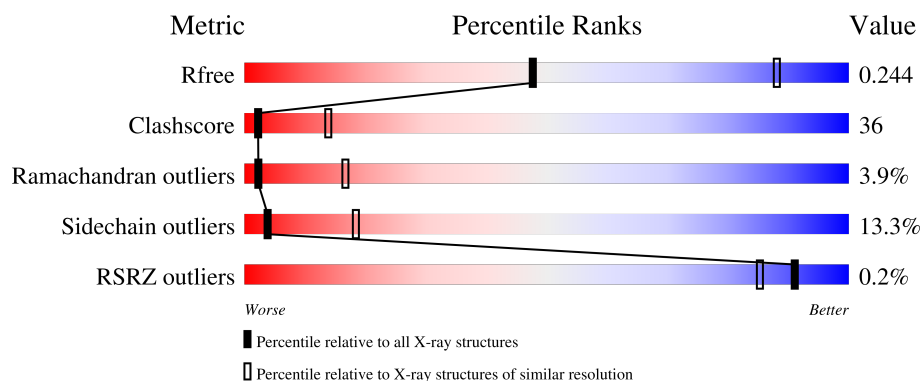
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2512	
1	B	2512	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30281 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 FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1962	Total	C	N	O	S	0	0	0
			14977	9466	2630	2803	78			
1	B	2004	Total	C	N	O	S	0	0	0
			15304	9671	2684	2869	80			

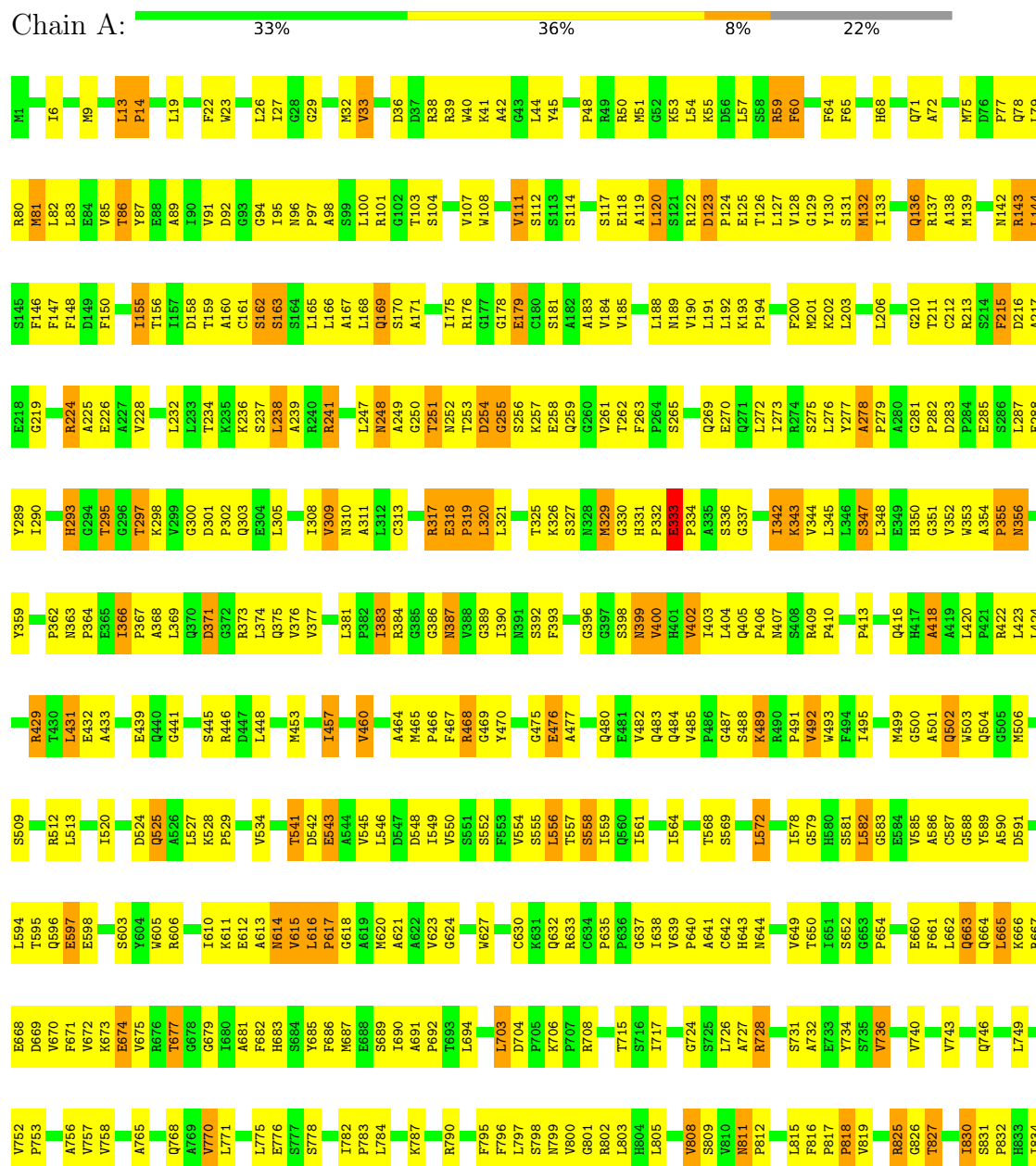
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	ILE	UNK	conflict	UNP A5YV76
B	834	ILE	UNK	conflict	UNP A5YV76

3 Residue-property plots

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

• Molecule 1: FATTY ACID SYNTHASE





S1475	P1413	F1343	L1282	G1219	V1089	D1014	E945	C856	L787	Y604	Q502	R422
N1476	V1414	L1344	E1283	L1220	V1090	L1015	V946	V881	Q788	W605	W503	L423
L1477	F1415	L1345	A1284	D1221	A1091	E1016	S947	V861	V770	R606	Q504	L424
	L1416	L1346	A1285	D1222	G1092		D948	K863	V770	T610	G505	
T1480	S1417	H1347	K1288	A1223	A1094	Q1023	N950		L775	K611	M506	R429
T1348	T1418	L1348	L1289	A1225	L1095	H1025		V866	E776	E612	R512	T430
P1482	E1419	L1349	L1290	L1226	L1096	D1026	L953	S867	F686	V615	L513	L431
	D1420	LEU	Q1291	K1227	L1097		I954	S870	S778	L616	I520	E432
M1486	T1421	ALA	L1292	A1228	G1098	S1030						A433
H1487	S1422	GLY	H1293	C1229	G1098	F1031	V959		T782	M620	Q525	E439
P1488	F1423	HIS	L1294	A1230	S1101	D1032		V874	P783	A621	A526	Q440
	R1424	PRO	V1294	D1231	S1102	L1033	W962	V876		A622	A527	G441
S1491	W1425	LEU	Q1296	T1232	V1103	A1034	E963		L793	W623	L527	S445
		GLY	Q1297	A1233		M1036	S964	D877	E794	V624	V534	
L1497	S1428	GLU	G1297	A1236	R1106	L1037	P965	D877	F796	L625		L448
D1500	K1430	MET	Q1298	D1236	R1107	H1037	P966		F796	W627	V545	
L1501	D1431	VAL	W1299	E1235	P1108	M1038	P967	R883	L797	E628	L546	
V1502	I1432	PHE	P1301	N1236	Q1109	S1039		V884	D704	L546	M453	
M1503	L1433	LEU	A1302		Q1110	I1040	F970	L885	F705		I549	
M1504		THR	N1303	S1239	H1111	L1041	D971	F886	K706	C630		I457
V1506	S1437	PRO	P1304	M1242	K1112	A1042	R973	P887	R711		S552	V460
R1507	A1436	GLU	P1306	K1243	P1114	P1043	R974	G888	W712	C634	V554	P462
	S1438	GLN	GLY	V1244	I1115	Y1049	A975	G890	T715	P635	F553	S461
G1512	R1439	GLY	SER	V1245	K1118	L1050	V976		V808	P636	S555	V463
A1513	V1441	ALA	LEU	E1246	F1119	P1051	D977	L894	S809	G637	L556	A464
F1514	W1442	ARG	GLY	Y1247	P1120	T1052	P978	T895	W716	I638	T557	M465
R1515	L1443	HIS	LVS	L1248	C1120	R1053	A979		F717	P639	S558	P466
H1516	M1444	LEU			F1121	P1054	D980	T898	G724	P640	I559	F467
F1517	A1445	LEU	CYS	D1251	T1122	T1055	S981		P812	A641	Q560	R468
P1518	V1446	L1373	GLN	G1252	P1123	S1056	T982	A902	P817	C642	I561	G469
L1519	G1447	L1381	LEU	K1253	H1124	T1057	A983	L903	R728	H643		Y470
E1520	C1448	F1382	LEU	L1254	V1125	R1058	E984	E905	E820	N644	I564	G475
	S1449		ASN	Y1255	E1126	I1059	F985	Q905	F821	S645	T568	A476
E1525	T1450	L1387	GLY	S1256	GLY	D1060		N906	R825	K646	S569	A477
K1526	K1526	H1388	ASN	R1257	C1129	P1061	Q988	L907	G826	D647	L570	G478
Q1527	S1451	L1389	LEU	I1258	L1130	P1062	Q989		T827	T648	G571	Q480
T1528	G1452	V1390	GLN	P1259	L1136	T1063	D991	V912		V649	L572	E481
H1530	V1453	LEU	ALA	A1260	L1137	H1064	V992	V913	I830	T650	D575	V482
A1531	G1455	THR	GLU	L1261	Q1137	K1067	Y993	E915	S831		G576	V485
F1532	M1456	LEU	LEU	L1262	E1138	L1068	K994	D916	L739	A657	I577	F486
V1533	V1457	GLY	GLY	N1263	E1139	Y1069	D995	V917	P832	M658	G579	G487
H1534	C1458	ASP	GLN	T1264		T1070	L996		H833	E660	H580	S488
	C1459	P1327	VAL		C1143	D1071	R997	L925	I834	E669	S581	K489
V1535	L1460	A1328	LEU	M1267	ARG	L1071		T930	H838	F661	L582	R490
L1536	S1399	V1329	ALA	M1268	GLY	Q1072	L998		Q746	L662	G583	P491
S1537	R1461	A1330	GLN	D1269	LEU	D1073		V931	Q840	Q663	E584	V492
R1538	V1400	V1331	GLU	L1270	ALA	T1074	Y1001			L665	V585	A493
R1539	E1463	G1332	ARG	D1271	GLN		D1002	E934	P845		A586	F494
F1402	P1464	N1333	PRO	D1272	ALA	A1077	Y1003	V935	S846	E668	C587	I495
L1403	G1465	N1334	LEU	Y1272	GLN		G1004	L937	A847		G588	C496
L1541	G1466	A1335	LEU	A1273	GLN	V1081	P1005	F1006	F850	D669	Y589	S497
S1542	H1467	A1336	LEU	T1274	THR	V1082	F1007	L938	P851	V670	G498	
S1543	R1468	A1336	CYS	D1275	LVS	D1083	F1008	Q1008	S852	F671	A590	
I1544	Q1407	T1337	ASP	D1276	VAL	N1085	L1009	A940	S853	V672	D591	
R1545	T1408	L1338	PRO	H1276	ALA	N1086	L1010	S941	G853		G500	
	C1471	K1339	PRO	Q1279	GLN	L1086	V1011		S854	A765	S603	
C1548	V1472	E1340	L1216	P1279	L1217	L1087				L766		
S1549	G1473	G1342	S1218	A1281	GLY	T1088						
P1550	V1474											



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.32Å 244.70Å 135.25Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	29.50 – 3.22 29.50 – 3.22	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.50-3.22) 97.5 (29.50-3.22)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.259 0.205 , 0.244	Depositor DCC
R_{free} test set	4839 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30281	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.59	0/15302	1.00	62/20792 (0.3%)
1	B	0.54	0/15634	0.96	55/21243 (0.3%)
All	All	0.56	0/30936	0.98	117/42035 (0.3%)

There are no bond length outliers.

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1636	VAL	CA-C-N	8.25	128.76	119.93
1	A	1636	VAL	C-N-CA	8.25	128.76	119.93
1	B	1223	ALA	CA-C-N	8.08	129.94	119.84
1	B	1223	ALA	C-N-CA	8.08	129.94	119.84
1	A	500	GLY	N-CA-C	-8.02	104.78	115.21
1	A	1223	ALA	CA-C-N	7.86	129.66	119.84
1	A	1223	ALA	C-N-CA	7.86	129.66	119.84
1	B	1113	LYS	CA-C-N	7.82	127.84	119.78
1	B	1113	LYS	C-N-CA	7.82	127.84	119.78
1	B	281	GLY	CA-C-N	7.21	128.86	119.84
1	B	281	GLY	C-N-CA	7.21	128.86	119.84
1	A	1102	SER	N-CA-C	7.16	119.05	108.60
1	A	1666	GLN	CA-C-N	7.11	127.15	119.89
1	A	1666	GLN	C-N-CA	7.11	127.15	119.89
1	B	981	SER	N-CA-C	-7.07	102.68	112.30
1	B	1102	SER	N-CA-C	6.83	118.56	108.60
1	B	500	GLY	N-CA-C	-6.80	106.43	115.40
1	A	1004	GLY	CA-C-N	6.72	128.24	119.84
1	A	1004	GLY	C-N-CA	6.72	128.24	119.84
1	A	281	GLY	CA-C-N	6.57	128.05	119.84
1	A	281	GLY	C-N-CA	6.57	128.05	119.84
1	A	704	ASP	CA-C-N	6.53	126.48	119.76
1	A	704	ASP	C-N-CA	6.53	126.48	119.76
1	B	325	THR	N-CA-C	-6.52	105.45	113.41
1	A	1113	LYS	CA-C-N	6.47	126.45	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1113	LYS	C-N-CA	6.47	126.45	119.78
1	A	1613	VAL	N-CA-C	6.36	117.99	108.96
1	A	155	ILE	N-CA-C	6.33	116.71	108.35
1	B	1636	VAL	N-CA-C	6.26	113.25	107.56
1	B	886	PHE	CA-C-N	6.22	126.59	119.93
1	B	886	PHE	C-N-CA	6.22	126.59	119.93
1	A	886	PHE	CA-C-N	6.15	126.52	119.93
1	A	886	PHE	C-N-CA	6.15	126.52	119.93
1	A	457	ILE	CB-CA-C	-6.13	103.98	112.02
1	B	131	SER	N-CA-C	-6.13	105.29	112.89
1	A	808	VAL	CB-CA-C	-6.11	104.61	111.45
1	B	1004	GLY	CA-C-N	6.08	127.43	119.84
1	B	1004	GLY	C-N-CA	6.08	127.43	119.84
1	A	827	THR	CA-C-N	6.02	127.36	119.84
1	A	827	THR	C-N-CA	6.02	127.36	119.84
1	A	1653	THR	N-CA-C	-5.97	104.68	111.07
1	A	703	LEU	N-CA-C	-5.93	99.52	109.07
1	B	457	ILE	CB-CA-C	-5.92	104.28	112.04
1	A	677	THR	N-CA-C	-5.92	105.90	114.12
1	B	1617	VAL	CA-C-N	5.90	125.60	119.05
1	B	1617	VAL	C-N-CA	5.90	125.60	119.05
1	B	870	SER	CA-C-N	5.90	125.57	119.56
1	B	870	SER	C-N-CA	5.90	125.57	119.56
1	A	1673	ILE	CB-CA-C	-5.89	103.01	111.19
1	A	1615	GLY	N-CA-C	5.87	120.17	110.55
1	A	867	SER	CA-C-N	5.84	127.14	119.84
1	A	867	SER	C-N-CA	5.84	127.14	119.84
1	A	1861	GLN	N-CA-C	5.82	118.87	109.79
1	A	293	HIS	N-CA-C	-5.80	104.86	111.07
1	A	1691	ARG	N-CA-C	-5.77	106.47	112.93
1	B	1824	GLN	CA-C-N	5.75	125.77	119.90
1	B	1824	GLN	C-N-CA	5.75	125.77	119.90
1	B	1830	VAL	N-CA-C	5.73	116.04	107.51
1	A	1830	VAL	N-CA-C	5.71	116.01	107.51
1	B	1736	THR	N-CA-C	-5.70	106.20	114.12
1	A	1871	ILE	N-CA-C	5.66	116.92	108.54
1	A	125	GLU	N-CA-C	-5.64	107.05	114.04
1	A	1529	GLU	N-CA-C	-5.59	106.23	113.16
1	B	827	THR	CA-C-N	5.55	126.77	119.84
1	B	827	THR	C-N-CA	5.55	126.77	119.84
1	B	1705	ARG	N-CA-C	-5.54	105.14	111.07
1	A	131	SER	N-CA-C	-5.53	106.03	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2103	HIS	CA-C-N	5.51	124.86	118.85
1	B	2103	HIS	C-N-CA	5.51	124.86	118.85
1	A	1784	VAL	N-CA-C	-5.50	105.85	113.00
1	A	1545	ARG	N-CA-C	5.48	117.31	109.14
1	A	811	ASN	CA-C-N	5.48	125.15	119.56
1	A	811	ASN	C-N-CA	5.48	125.15	119.56
1	A	13	LEU	CA-C-N	5.47	126.68	119.84
1	A	13	LEU	C-N-CA	5.47	126.68	119.84
1	B	867	SER	CA-C-N	5.47	126.68	119.84
1	B	867	SER	C-N-CA	5.47	126.68	119.84
1	A	333	GLU	CA-C-N	-5.46	113.99	119.56
1	A	333	GLU	C-N-CA	-5.46	113.99	119.56
1	A	1300	ASP	CA-C-N	5.44	126.65	119.84
1	A	1300	ASP	C-N-CA	5.44	126.65	119.84
1	A	870	SER	CA-C-N	5.43	125.10	119.56
1	A	870	SER	C-N-CA	5.43	125.10	119.56
1	A	1533	VAL	N-CA-C	5.39	115.88	108.12
1	B	1676	GLY	N-CA-C	-5.38	108.28	115.32
1	B	155	ILE	N-CA-C	5.35	115.41	108.35
1	B	811	ASN	CA-C-N	5.30	124.97	119.56
1	B	811	ASN	C-N-CA	5.30	124.97	119.56
1	B	333	GLU	CA-C-N	-5.30	114.16	119.56
1	B	333	GLU	C-N-CA	-5.30	114.16	119.56
1	A	1626	VAL	N-CA-C	5.28	115.16	107.88
1	B	1935	GLN	N-CA-C	-5.28	106.91	113.19
1	B	1300	ASP	CA-C-N	5.27	126.43	119.84
1	B	1300	ASP	C-N-CA	5.27	126.43	119.84
1	A	663	GLN	N-CA-C	-5.26	105.02	111.75
1	A	1661	VAL	CB-CA-C	-5.24	104.98	112.22
1	B	855	SER	N-CA-C	-5.24	107.05	113.50
1	B	1920	ILE	CB-CA-C	-5.23	104.97	111.08
1	B	852	SER	N-CA-C	-5.21	106.60	113.17
1	B	1784	VAL	N-CA-C	-5.19	106.25	113.00
1	A	2103	HIS	CA-C-N	5.18	124.49	118.85
1	A	2103	HIS	C-N-CA	5.18	124.49	118.85
1	B	465	MET	CA-C-N	5.17	126.11	120.83
1	B	465	MET	C-N-CA	5.17	126.11	120.83
1	A	1270	LEU	N-CA-C	5.16	117.14	108.73
1	B	62	ALA	N-CA-C	5.15	117.63	111.71
1	A	770	VAL	N-CA-C	5.11	115.33	110.42
1	B	13	LEU	CA-C-N	5.07	126.18	119.84
1	B	13	LEU	C-N-CA	5.07	126.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1869	PRO	CA-C-N	5.07	124.83	119.76
1	B	1869	PRO	C-N-CA	5.07	124.83	119.76
1	B	1072	GLN	N-CA-C	-5.07	106.60	112.89
1	B	2009	ALA	N-CA-C	5.06	117.29	110.06
1	A	1599	LEU	N-CA-C	5.04	116.61	108.34
1	B	770	VAL	N-CA-C	5.04	115.26	110.42
1	A	1048	LEU	N-CA-C	5.04	116.97	108.96
1	A	1869	PRO	N-CA-C	5.02	116.83	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14977	0	14938	1114	0
1	B	15304	0	15266	1135	0
All	All	30281	0	30204	2196	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 36.

All (2196) 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:B:1694:ARG:HH11	1:B:1694:ARG:HG3	1.17	1.10
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.25	1.02
1:A:1473:LEU:HD21	1:A:1503:MET:HG2	1.36	1.02
1:A:165:LEU:HD23	1:A:400:VAL:HG22	1.37	1.02
1:B:1456:MET:HG2	1:B:2036:PHE:HB2	1.41	1.01
1:A:1736:THR:HG23	1:A:1739:LYS:H	1.26	1.00
1:B:1003:TYR:CZ	1:B:1037:HIS:HE1	1.79	1.00
1:A:1539:GLY:HA2	1:A:1580:THR:O	1.62	0.99
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.42	0.98
1:A:642:CYS:HB2	1:A:650:THR:HB	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:HG3	1:B:118:GLU:HG3	1.43	0.98
1:B:1338:LEU:HD13	1:B:1406:GLN:HE21	1.27	0.98
1:B:1387:LEU:HD22	1:B:1404:CYS:HB3	1.43	0.98
1:B:1651:VAL:HG13	1:B:1680:VAL:HA	1.45	0.97
1:B:1348:THR:HG22	1:B:1349:LEU:H	1.27	0.97
1:A:1003:TYR:CZ	1:A:1037:HIS:HE1	1.83	0.97
1:A:368:ALA:H	1:A:371:ASP:HB3	1.31	0.96
1:B:1418:VAL:HG13	1:B:1425:TRP:CZ2	1.99	0.96
1:B:165:LEU:HD23	1:B:400:VAL:HG22	1.43	0.96
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.44	0.96
1:B:1457:VAL:HG21	1:B:1473:LEU:HD22	1.47	0.95
1:B:368:ALA:H	1:B:371:ASP:HB3	1.31	0.95
1:B:1473:LEU:HD21	1:B:1503:MET:HG2	1.49	0.95
1:B:1299:TRP:HZ3	1:B:1301:PRO:HA	1.29	0.95
1:B:1335:ALA:HA	1:B:1406:GLN:HE22	1.30	0.94
1:B:1330:ALA:O	1:B:1334:MET:HG2	1.67	0.93
1:B:616:LEU:HB2	1:B:686:PHE:HE2	1.30	0.93
1:B:1565:SER:HB2	1:B:1857:ARG:NH2	1.84	0.93
1:B:1312:ALA:HB2	1:B:1337:THR:HG22	1.48	0.91
1:B:1736:THR:HG23	1:B:1739:LYS:H	1.33	0.91
1:A:1115:ILE:HD11	1:A:2111:LEU:HG	1.51	0.91
1:A:1457:VAL:HG21	1:A:1473:LEU:HD22	1.51	0.90
1:A:1418:VAL:HG13	1:A:1425:TRP:CZ2	2.06	0.90
1:B:1662:ARG:CG	1:B:1662:ARG:HH11	1.82	0.90
1:B:662:LEU:HD22	1:B:672:VAL:HG11	1.54	0.89
1:A:1585:PRO:HB3	1:A:1598:MET:HE1	1.52	0.89
1:B:1446:VAL:HA	1:B:1476:ASN:ND2	1.87	0.89
1:A:82:LEU:O	1:A:86:THR:HG23	1.74	0.88
1:B:50:ARG:HD3	1:B:210:GLY:O	1.74	0.88
1:B:1446:VAL:HA	1:B:1476:ASN:HD21	1.37	0.88
1:A:1644:GLU:HB3	1:A:1825:PRO:HB3	1.52	0.88
1:A:976:VAL:HG22	1:A:977:ASP:H	1.38	0.88
1:B:384:ARG:HH11	1:B:384:ARG:HG3	1.38	0.88
1:A:1662:ARG:HH11	1:A:1662:ARG:CG	1.87	0.88
1:B:616:LEU:HB2	1:B:686:PHE:CE2	2.09	0.87
1:B:82:LEU:O	1:B:86:THR:HG23	1.75	0.87
1:B:1585:PRO:HB3	1:B:1598:MET:HE1	1.55	0.87
1:B:1299:TRP:CZ3	1:B:1301:PRO:HA	2.09	0.87
1:A:384:ARG:HH11	1:A:384:ARG:HG3	1.39	0.87
1:A:1348:THR:HG22	1:A:1349:LEU:H	1.37	0.87
1:A:1477:LEU:HD11	1:A:2043:ARG:HD2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1545:ARG:HH11	1:A:1545:ARG:HG3	1.39	0.86
1:A:50:ARG:HD3	1:A:210:GLY:O	1.75	0.86
1:A:1662:ARG:HH11	1:A:1662:ARG:HG3	1.40	0.86
1:B:64:PHE:HB2	1:B:429:ARG:HH21	1.40	0.86
1:A:861:VAL:HG22	1:A:934:GLU:HB3	1.58	0.85
1:B:1616:MET:HE3	1:B:1650:ILE:HD13	1.58	0.84
1:B:643:HIS:HA	1:B:649:VAL:HG22	1.59	0.84
1:B:1530:HIS:HB2	1:B:1552:HIS:HB2	1.60	0.84
1:A:64:PHE:HB2	1:A:429:ARG:HH21	1.41	0.83
1:A:96:ASN:HD21	1:A:98:ALA:HB3	1.41	0.83
1:B:1312:ALA:CB	1:B:1337:THR:HG22	2.08	0.83
1:B:112:SER:CB	1:B:334:PRO:HG3	2.09	0.83
1:A:112:SER:HB2	1:A:334:PRO:HG3	1.59	0.83
1:A:944:PHE:CD2	1:A:959:VAL:HG22	2.14	0.83
1:A:1245:VAL:HG13	1:A:1273:THR:HB	1.57	0.83
1:B:1082:VAL:HG22	1:B:1089:VAL:HG22	1.61	0.83
1:A:616:LEU:HD23	1:A:617:PRO:HD2	1.58	0.83
1:A:1082:VAL:HG22	1:A:1089:VAL:HG22	1.60	0.83
1:A:1289:LEU:HD22	1:A:1294:VAL:HB	1.60	0.83
1:A:319:PRO:HD2	1:A:373:ARG:O	1.78	0.83
1:A:1528:THR:HG22	1:A:1530:HIS:H	1.43	0.83
1:A:112:SER:CB	1:A:334:PRO:HG3	2.07	0.83
1:B:96:ASN:HD21	1:B:98:ALA:HB3	1.42	0.82
1:A:468:ARG:HD3	1:A:485:VAL:HG21	1.59	0.82
1:A:663:GLN:O	1:A:667:ARG:HD2	1.79	0.82
1:A:123:ASP:HB3	1:A:126:THR:HB	1.62	0.82
1:B:319:PRO:HD2	1:B:373:ARG:O	1.79	0.82
1:B:1732:VAL:O	1:B:1736:THR:HB	1.78	0.82
1:B:944:PHE:CD2	1:B:959:VAL:HG22	2.15	0.82
1:B:982:THR:HG23	1:B:983:ALA:H	1.45	0.82
1:B:1416:LEU:HD21	1:B:1425:TRP:HB2	1.59	0.82
1:B:112:SER:HB2	1:B:334:PRO:HG3	1.60	0.81
1:A:1222:ASP:HB3	1:A:1257:ARG:CZ	2.09	0.81
1:A:1285:ALA:HB1	1:A:1289:LEU:HG	1.61	0.81
1:A:1341:GLY:HA2	1:A:1406:GLN:O	1.80	0.81
1:A:278:ALA:HB3	1:A:279:PRO:HD3	1.63	0.81
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.09	0.81
1:B:980:ASP:HB2	1:B:982:THR:HG22	1.63	0.81
1:B:861:VAL:HG22	1:B:934:GLU:HB3	1.63	0.81
1:B:278:ALA:HB3	1:B:279:PRO:HD3	1.61	0.80
1:B:1662:ARG:HH11	1:B:1662:ARG:HG3	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:TYR:CZ	1:B:1037:HIS:CE1	2.67	0.80
1:B:1222:ASP:HB3	1:B:1257:ARG:CZ	2.11	0.80
1:B:1456:MET:CG	1:B:2036:PHE:HB2	2.11	0.80
1:A:368:ALA:N	1:A:371:ASP:HB3	1.96	0.80
1:B:14:PRO:HG2	1:B:329:MET:HG3	1.64	0.79
1:A:215:PHE:CD2	1:A:305:LEU:HD11	2.18	0.79
1:A:416:GLN:O	1:A:420:LEU:HB2	1.82	0.79
1:B:1285:ALA:HB1	1:B:1289:LEU:HG	1.64	0.79
1:B:1303:ASN:N	1:B:1304:PRO:HD3	1.96	0.79
1:B:416:GLN:O	1:B:420:LEU:HB2	1.81	0.79
1:B:368:ALA:N	1:B:371:ASP:HB3	1.98	0.79
1:A:1735:HIS:CD2	1:A:1735:HIS:H	2.00	0.79
1:B:1545:ARG:HD2	1:B:1876:LEU:HD11	1.63	0.79
1:A:642:CYS:HB2	1:A:650:THR:CB	2.12	0.78
1:B:1245:VAL:HG13	1:B:1273:THR:HB	1.64	0.78
1:A:1003:TYR:CZ	1:A:1037:HIS:CE1	2.70	0.78
1:A:118:GLU:HG3	1:B:118:GLU:CG	2.14	0.78
1:A:856:CYS:SG	1:B:856:CYS:HB2	2.23	0.78
1:A:1034:ALA:HA	1:A:1037:HIS:CD2	2.19	0.78
1:B:333:GLU:HB2	1:B:334:PRO:CD	2.12	0.78
1:A:14:PRO:HG2	1:A:329:MET:HG3	1.64	0.78
1:A:1466:GLY:HA2	1:A:1469:ILE:HG13	1.65	0.78
1:B:1034:ALA:HA	1:B:1037:HIS:CD2	2.19	0.78
1:A:118:GLU:CG	1:B:118:GLU:HG3	2.13	0.78
1:B:1888:VAL:HG22	1:B:1913:VAL:HB	1.66	0.77
1:A:1419:GLU:CD	1:A:1447:GLY:HA3	2.10	0.77
1:A:856:CYS:HG	1:B:856:CYS:HB2	1.49	0.77
1:B:1407:GLN:CG	1:B:1409:PRO:HD2	2.14	0.77
1:A:1732:VAL:O	1:A:1736:THR:HB	1.82	0.77
1:A:903:LEU:HD22	1:A:905:GLN:NE2	1.99	0.77
1:A:1616:MET:HE3	1:A:1650:ILE:HD13	1.66	0.77
1:B:1338:LEU:HD21	1:B:1341:GLY:HA2	1.64	0.77
1:A:1003:TYR:CE2	1:A:1037:HIS:HE1	2.02	0.77
1:A:1736:THR:CG2	1:A:1740:GLY:H	1.98	0.77
1:B:1641:THR:HG23	1:B:1644:GLU:OE1	1.85	0.77
1:B:1736:THR:CG2	1:B:1740:GLY:H	1.98	0.76
1:A:1890:THR:HA	1:A:1915:THR:HB	1.66	0.76
1:B:254:ASP:HB3	1:B:257:LYS:HE2	1.67	0.76
1:B:1538:ARG:HH22	1:B:1585:PRO:HG2	1.50	0.76
1:A:627:TRP:HB2	1:A:643:HIS:CD2	2.21	0.76
1:B:297:THR:HB	1:B:300:GLY:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1259:PRO:HB2	1:B:1292:LEU:HD22	1.68	0.76
1:B:1407:GLN:HG3	1:B:1409:PRO:HD2	1.66	0.76
1:B:1735:HIS:H	1:B:1735:HIS:CD2	2.02	0.76
1:B:1890:THR:HA	1:B:1915:THR:HB	1.66	0.76
1:A:278:ALA:CB	1:A:279:PRO:HD3	2.16	0.76
1:B:278:ALA:CB	1:B:279:PRO:HD3	2.16	0.76
1:B:642:CYS:HB2	1:B:650:THR:HB	1.66	0.76
1:B:903:LEU:HD22	1:B:905:GLN:NE2	2.01	0.76
1:B:1003:TYR:CE2	1:B:1037:HIS:HE1	2.03	0.76
1:B:1289:LEU:HD22	1:B:1294:VAL:HB	1.69	0.75
1:A:502:GLN:HG3	1:A:556:LEU:HD11	1.67	0.75
1:B:1674:HIS:CD2	1:B:1698:THR:HG21	2.22	0.75
1:B:136:GLN:C	1:B:136:GLN:HE21	1.95	0.75
1:B:1477:LEU:HD11	1:B:2043:ARG:HD2	1.68	0.75
1:B:1541:LEU:HD22	1:B:1544:ILE:HD11	1.68	0.75
1:A:200:PHE:HB3	1:A:206:LEU:HG	1.67	0.75
1:B:1533:VAL:CG1	1:B:1622:LEU:HB3	2.17	0.75
1:A:297:THR:HB	1:A:300:GLY:H	1.52	0.75
1:A:217:ALA:HB2	1:A:364:PRO:HD3	1.69	0.74
1:A:1222:ASP:HB3	1:A:1257:ARG:NH1	2.03	0.74
1:A:938:LEU:HB3	1:B:945:GLU:OE1	1.86	0.74
1:A:1130:LEU:HD11	1:A:1221:LEU:HD13	1.69	0.74
1:B:1618:PRO:HD3	1:B:1629:LEU:HD11	1.68	0.74
1:A:36:ASP:HB3	1:A:38:ARG:HG3	1.69	0.74
1:B:1418:VAL:HG13	1:B:1425:TRP:CE2	2.22	0.74
1:A:1387:LEU:HD22	1:A:1404:CYS:HB3	1.70	0.73
1:A:581:SER:HB2	1:A:683:HIS:NE2	2.03	0.73
1:A:1736:THR:HG23	1:A:1739:LYS:N	2.01	0.73
1:B:622:ALA:HA	1:B:650:THR:HA	1.69	0.73
1:B:1227:LYS:HB2	1:B:1261:LEU:HD22	1.69	0.73
1:A:136:GLN:HE21	1:A:136:GLN:C	1.96	0.73
1:A:1445:ALA:O	1:A:1476:ASN:ND2	2.20	0.73
1:A:1818:ILE:HA	1:A:1823:VAL:HG13	1.68	0.73
1:B:44:LEU:HG	1:B:45:TYR:CE1	2.24	0.73
1:A:1227:LYS:HB2	1:A:1261:LEU:HD22	1.71	0.73
1:A:1612:ARG:O	1:A:1636:VAL:HG12	1.89	0.73
1:A:1953:ARG:HG2	1:A:2005:VAL:HG13	1.70	0.73
1:B:1533:VAL:HG12	1:B:1622:LEU:HB3	1.70	0.73
1:B:1694:ARG:HH11	1:B:1694:ARG:CG	2.01	0.73
1:B:682:PHE:HB3	1:B:683:HIS:CD2	2.24	0.73
1:B:1035:MET:HE3	1:B:1089:VAL:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1338:LEU:HD13	1:B:1406:GLN:NE2	2.03	0.73
1:B:1818:ILE:HA	1:B:1823:VAL:HG13	1.71	0.73
1:A:333:GLU:CB	1:A:334:PRO:HD3	2.17	0.72
1:B:1439:ARG:HB3	1:B:1440:PRO:HD3	1.71	0.72
1:A:1859:GLU:HG2	1:A:1860:GLU:N	2.04	0.72
1:B:123:ASP:O	1:B:127:LEU:HB3	1.89	0.72
1:B:1327:PRO:O	1:B:1381:LEU:HD21	1.90	0.72
1:A:1678:GLY:O	1:A:1682:GLN:HG3	1.89	0.72
1:B:1345:LEU:HD12	1:B:1402:PHE:O	1.89	0.72
1:A:1824:GLN:HG3	1:A:1825:PRO:HD2	1.70	0.72
1:B:1139:GLU:CD	1:B:1218:SER:HB2	2.14	0.72
1:A:82:LEU:HD22	1:A:188:LEU:HD11	1.72	0.72
1:A:1234:LEU:HD22	1:A:1262:LEU:HD22	1.72	0.72
1:B:82:LEU:HD22	1:B:188:LEU:HD11	1.71	0.72
1:A:1299:TRP:HE1	1:A:1306:PRO:HD2	1.53	0.72
1:B:265:SER:O	1:B:269:GLN:HG3	1.90	0.72
1:A:137:ARG:HD2	1:B:137:ARG:NH1	2.05	0.72
1:B:668:GLU:O	1:B:669:ASP:HB2	1.90	0.71
1:B:1222:ASP:HB3	1:B:1257:ARG:NH1	2.04	0.71
1:B:1408:THR:N	1:B:1409:PRO:HD3	2.05	0.71
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.23	0.71
1:B:1953:ARG:HG2	1:B:2005:VAL:HG13	1.70	0.71
1:B:36:ASP:HB3	1:B:38:ARG:HG3	1.72	0.71
1:B:9:MET:HE1	1:B:345:LEU:HB2	1.71	0.71
1:A:1418:VAL:HG13	1:A:1425:TRP:CE2	2.25	0.71
1:B:502:GLN:HG3	1:B:556:LEU:HD11	1.70	0.71
1:A:2105:VAL:O	1:A:2106:LEU:HD23	1.91	0.71
1:B:1926:ALA:O	1:B:1930:ARG:HB2	1.90	0.71
1:A:1472:VAL:HG12	1:A:1473:LEU:H	1.56	0.71
1:A:1569:THR:HG21	1:A:1622:LEU:HA	1.72	0.71
1:A:1576:VAL:HG21	1:A:1843:MET:HG2	1.71	0.71
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.26	0.71
1:A:1535:VAL:HG12	1:A:1537:SER:H	1.55	0.71
1:A:1888:VAL:HG22	1:A:1913:VAL:HB	1.70	0.70
1:A:44:LEU:HG	1:A:45:TYR:CE1	2.26	0.70
1:B:627:TRP:HB2	1:B:643:HIS:CE1	2.27	0.70
1:A:1475:SER:O	1:A:1486:MET:HE1	1.91	0.70
1:B:23:TRP:HA	1:B:26:LEU:HD12	1.73	0.70
1:B:1234:LEU:HD22	1:B:1262:LEU:HD22	1.73	0.70
1:A:1669:GLU:O	1:A:1693:CYS:HB3	1.91	0.70
1:B:575:ASP:O	1:B:711:ARG:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:MET:HE2	1:A:1038:MET:HA	1.73	0.70
1:B:1670:SER:O	1:B:1742:ASP:HB2	1.91	0.70
1:A:944:PHE:HD2	1:A:959:VAL:HG22	1.55	0.70
1:B:1254:LEU:HD21	1:B:1318:ASN:HB2	1.72	0.70
1:A:1887:TYR:HD2	1:A:1967:GLY:HA3	1.57	0.70
1:B:982:THR:C	1:B:984:GLU:H	2.00	0.70
1:B:1095:LEU:HD12	1:B:1095:LEU:C	2.17	0.70
1:B:1477:LEU:CD1	1:B:2043:ARG:HD2	2.21	0.70
1:A:254:ASP:HB3	1:A:257:LYS:HE2	1.72	0.70
1:A:1991:VAL:O	1:A:1994:PRO:HD2	1.91	0.70
1:B:1975:LEU:HD22	1:B:1977:ASP:OD2	1.91	0.70
1:B:641:ALA:HB1	1:B:683:HIS:HB2	1.74	0.70
1:A:77:PRO:O	1:A:81:MET:HG2	1.91	0.69
1:B:944:PHE:HD2	1:B:959:VAL:HG22	1.55	0.69
1:A:1735:HIS:H	1:A:1735:HIS:HD2	1.40	0.69
1:B:506:MET:HE3	1:B:559:ILE:HD12	1.74	0.69
1:B:1335:ALA:HA	1:B:1406:GLN:NE2	2.07	0.69
1:B:1671:VAL:HG23	1:B:1743:LEU:HB2	1.73	0.69
1:B:87:TYR:O	1:B:91:VAL:HG22	1.92	0.69
1:B:1338:LEU:CD1	1:B:1406:GLN:HE21	2.05	0.69
1:B:1651:VAL:CG1	1:B:1680:VAL:HA	2.19	0.69
1:A:610:ILE:HG12	1:A:690:ILE:HG21	1.74	0.69
1:A:917:VAL:HG13	1:A:1054:PHE:HB2	1.74	0.69
1:B:1887:TYR:HD2	1:B:1967:GLY:HA3	1.56	0.69
1:A:2015:TYR:CD2	1:A:2099:LEU:HD22	2.28	0.69
1:B:1288:LYS:O	1:B:1291:GLN:HG2	1.92	0.69
1:B:1736:THR:HG23	1:B:1739:LYS:N	2.07	0.69
1:B:1382:PHE:HB3	1:B:1387:LEU:HB2	1.73	0.69
1:A:504:GLN:HA	1:A:541:THR:HG21	1.75	0.68
1:B:87:TYR:CE2	1:B:97:PRO:HG2	2.28	0.68
1:B:1653:THR:HG22	1:B:1810:VAL:HG12	1.73	0.68
1:A:111:VAL:CG2	1:A:188:LEU:HB2	2.23	0.68
1:A:252:ASN:ND2	1:A:272:LEU:HB2	2.07	0.68
1:A:1477:LEU:CD1	1:A:2043:ARG:HD2	2.22	0.68
1:B:627:TRP:HB2	1:B:643:HIS:ND1	2.08	0.68
1:B:917:VAL:HG13	1:B:1054:PHE:HB2	1.75	0.68
1:B:1303:ASN:O	1:B:1333:ASN:HB2	1.93	0.68
1:A:23:TRP:HA	1:A:26:LEU:HD12	1.75	0.68
1:A:2070:LEU:HD21	1:A:2076:ASN:N	2.08	0.68
1:A:1348:THR:HG21	1:A:1378:TRP:CZ2	2.29	0.68
1:A:1126:GLU:HB3	1:A:1129:CYS:SG	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:LEU:HD13	1:A:1316:VAL:HG12	1.75	0.68
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.22	0.68
1:A:1489:SER:H	1:A:1493:LEU:HD22	1.58	0.68
1:B:351:GLY:C	1:B:383:ILE:HG22	2.19	0.68
1:A:1268:MET:HA	1:A:1268:MET:HE2	1.76	0.68
1:A:1606:ARG:HH21	1:A:1860:GLU:HG3	1.59	0.68
1:B:1227:LYS:HE3	1:B:1231:ASP:OD2	1.94	0.68
1:B:1460:LEU:HD13	1:B:2032:ALA:CB	2.23	0.68
1:A:1416:LEU:HD21	1:A:1425:TRP:HB2	1.76	0.67
1:B:1576:VAL:HG21	1:B:1843:MET:HG2	1.76	0.67
1:B:1477:LEU:O	1:B:1507:ARG:HG2	1.94	0.67
1:A:1651:VAL:HG12	1:A:1680:VAL:HA	1.77	0.67
1:A:1735:HIS:CD2	1:A:1735:HIS:N	2.61	0.67
1:B:2015:TYR:CD2	1:B:2099:LEU:HD22	2.30	0.67
1:A:460:VAL:HG21	1:A:465:MET:HG3	1.76	0.67
1:B:111:VAL:CG2	1:B:188:LEU:HB2	2.25	0.67
1:B:635:PRO:HD2	1:B:638:ILE:HB	1.77	0.67
1:B:1814:LEU:O	1:B:1818:ILE:HG13	1.94	0.67
1:B:1430:LYS:HE3	1:B:1981:GLU:HA	1.75	0.67
1:A:614:ASN:O	1:A:615:VAL:O	2.13	0.67
1:B:288:GLU:OE1	1:B:383:ILE:HG13	1.95	0.67
1:B:1279:PRO:HG3	1:B:1298:GLN:NE2	2.10	0.67
1:B:1341:GLY:HA3	1:B:1407:GLN:HA	1.76	0.67
1:B:1954:SER:O	1:B:1958:GLU:HG3	1.95	0.67
1:A:132:MET:HE1	1:B:200:PHE:CE2	2.30	0.67
1:B:643:HIS:CD2	1:B:746:GLN:HB3	2.30	0.67
1:B:1666:GLN:O	1:B:1669:GLU:HB2	1.95	0.67
1:B:1735:HIS:CD2	1:B:1735:HIS:N	2.62	0.67
1:A:277:TYR:CE2	1:A:287:LEU:HD11	2.30	0.67
1:A:581:SER:HB2	1:A:683:HIS:CE1	2.30	0.67
1:A:1226:LEU:HD23	1:A:1401:LEU:HD21	1.77	0.67
1:B:1126:GLU:HB3	1:B:1129:CYS:SG	2.35	0.67
1:B:1433:LEU:HD21	1:B:1465:GLY:HA3	1.77	0.67
1:B:1824:GLN:HG3	1:B:1825:PRO:HD2	1.76	0.67
1:B:1991:VAL:O	1:B:1994:PRO:HD2	1.95	0.67
1:B:1538:ARG:HH22	1:B:1585:PRO:CG	2.08	0.66
1:A:1285:ALA:O	1:A:1289:LEU:N	2.27	0.66
1:A:1618:PRO:HD3	1:A:1629:LEU:HD11	1.77	0.66
1:A:1814:LEU:O	1:A:1818:ILE:HG13	1.95	0.66
1:A:2098:PHE:CE2	1:A:2106:LEU:HB2	2.30	0.66
1:B:252:ASN:ND2	1:B:272:LEU:HB2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:SER:O	1:A:269:GLN:HG3	1.95	0.66
1:A:976:VAL:O	1:A:978:PRO:HD3	1.94	0.66
1:B:1034:ALA:O	1:B:1037:HIS:HB2	1.95	0.66
1:A:1095:LEU:C	1:A:1095:LEU:HD12	2.20	0.66
1:A:1564:CYS:CB	1:A:1628:LEU:HD21	2.25	0.66
1:B:98:ALA:HA	1:B:101:ARG:HG3	1.78	0.66
1:B:1671:VAL:CG2	1:B:1743:LEU:HB2	2.25	0.66
1:A:503:TRP:CD1	1:A:787:LYS:HB2	2.31	0.66
1:A:1644:GLU:HB3	1:A:1825:PRO:CB	2.24	0.66
1:B:1395:SER:HB3	1:B:1399:SER:O	1.95	0.66
1:B:1673:ILE:O	1:B:1697:THR:HA	1.95	0.66
1:B:1694:ARG:HG3	1:B:1694:ARG:NH1	1.95	0.66
1:A:1035:MET:HE3	1:A:1089:VAL:HG12	1.77	0.66
1:A:1470:ARG:O	1:A:1472:VAL:HG23	1.96	0.66
1:B:680:ILE:HG12	1:B:681:ALA:N	2.11	0.66
1:B:620:MET:SD	1:B:682:PHE:HB2	2.35	0.66
1:B:1038:MET:HA	1:B:1038:MET:HE2	1.78	0.66
1:A:1411:ASP:HB2	1:A:1440:PRO:HD3	1.76	0.66
1:A:1857:ARG:HH11	1:A:1869:PRO:HB3	1.61	0.66
1:B:1244:VAL:HB	1:B:1272:TYR:HD1	1.61	0.66
1:B:1244:VAL:HG13	1:B:1314:LEU:HD23	1.77	0.66
1:A:168:LEU:HB2	1:A:185:VAL:HG11	1.77	0.66
1:A:254:ASP:CB	1:A:257:LYS:HE2	2.26	0.66
1:A:1252:GLY:HA3	1:A:1318:ASN:HB3	1.77	0.66
1:B:123:ASP:CB	1:B:126:THR:HB	2.25	0.66
1:A:87:TYR:O	1:A:91:VAL:HG22	1.96	0.65
1:A:506:MET:HE3	1:A:559:ILE:HD12	1.78	0.65
1:B:59:ARG:HG3	1:B:838:HIS:HB3	1.78	0.65
1:A:1616:MET:HE3	1:A:1650:ILE:HA	1.79	0.65
1:A:1653:THR:HG22	1:A:1796:LEU:HD21	1.78	0.65
1:A:1974:VAL:HG22	1:A:1994:PRO:HG2	1.77	0.65
1:B:2003:ASP:O	1:B:2007:ARG:HG3	1.95	0.65
1:A:2003:ASP:O	1:A:2007:ARG:HG3	1.96	0.65
1:B:496:CYS:O	1:B:583:GLY:HA3	1.96	0.65
1:B:645:SER:HB3	1:B:770:VAL:HG13	1.77	0.65
1:B:1247:VAL:HG11	1:B:1301:PRO:HG3	1.76	0.65
1:A:502:GLN:HB2	1:A:546:LEU:HD22	1.78	0.65
1:A:1439:ARG:HB3	1:A:1440:PRO:HD3	1.79	0.65
1:B:1282:LEU:HD21	1:B:1296:GLN:HB2	1.78	0.65
1:B:1486:MET:O	1:B:1488:PRO:HD3	1.97	0.65
1:B:2070:LEU:HD21	1:B:2076:ASN:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ASN:HD22	1:A:399:ASN:H	1.43	0.65
1:A:889:THR:HG21	1:A:1032:LEU:HB2	1.78	0.65
1:A:1244:VAL:HG13	1:A:1314:LEU:HD23	1.79	0.65
1:B:1220:LEU:HB3	1:B:1257:ARG:HH22	1.61	0.65
1:B:1279:PRO:HG3	1:B:1298:GLN:HE22	1.61	0.65
1:B:1528:THR:HG22	1:B:1530:HIS:H	1.61	0.65
1:A:1628:LEU:HD13	1:A:1633:THR:HG21	1.79	0.65
1:B:1569:THR:HG21	1:B:1622:LEU:HA	1.79	0.65
1:B:1736:THR:HG23	1:B:1740:GLY:H	1.61	0.65
1:A:1838:ALA:HA	1:A:1841:ARG:HG3	1.77	0.64
1:A:2102:PRO:HD2	1:A:2103:HIS:HD2	1.63	0.64
1:B:615:VAL:HG22	1:B:686:PHE:HD2	1.63	0.64
1:B:1532:PHE:HD2	1:B:1549:SER:HA	1.61	0.64
1:B:2105:VAL:O	1:B:2106:LEU:HD23	1.97	0.64
1:A:44:LEU:HG	1:A:45:TYR:CD1	2.32	0.64
1:A:139:MET:HE1	1:B:396:GLY:CA	2.26	0.64
1:A:302:PRO:HA	1:A:366:ILE:HG21	1.79	0.64
1:A:325:THR:OG1	1:A:343:LYS:HG2	1.97	0.64
1:A:1395:SER:HB3	1:A:1399:SER:O	1.97	0.64
1:B:64:PHE:HB2	1:B:429:ARG:NH2	2.11	0.64
1:B:1408:THR:N	1:B:1409:PRO:CD	2.61	0.64
1:B:1433:LEU:HD11	1:B:1465:GLY:O	1.97	0.64
1:B:1466:GLY:HA2	1:B:1469:ILE:HG13	1.77	0.64
1:B:217:ALA:HB2	1:B:364:PRO:HD3	1.79	0.64
1:A:1001:TYR:HB3	1:A:1003:TYR:CE1	2.32	0.64
1:A:1227:LYS:HE3	1:A:1231:ASP:OD2	1.98	0.64
1:B:660:GLU:HG2	1:B:663:GLN:NE2	2.12	0.64
1:B:736:VAL:O	1:B:740:VAL:HG23	1.98	0.64
1:B:1472:VAL:HG12	1:B:1473:LEU:H	1.62	0.64
1:A:1532:PHE:CE1	1:A:1597:CYS:HB3	2.32	0.64
1:A:1594:THR:OG1	1:A:1596:ASP:HB2	1.98	0.64
1:B:64:PHE:CE2	1:B:464:ALA:HB1	2.32	0.64
1:B:2102:PRO:HD2	1:B:2103:HIS:HD2	1.62	0.64
1:A:59:ARG:HG3	1:A:838:HIS:HB3	1.79	0.64
1:A:1220:LEU:HB3	1:A:1257:ARG:HH22	1.63	0.64
1:A:1859:GLU:HG2	1:A:1860:GLU:H	1.59	0.64
1:A:2002:LEU:O	1:A:2006:THR:HB	1.97	0.64
1:B:168:LEU:HB2	1:B:185:VAL:HG11	1.78	0.64
1:B:1348:THR:HG22	1:B:1349:LEU:N	2.06	0.64
1:B:1449:SER:O	1:B:1477:LEU:HD22	1.98	0.64
1:A:137:ARG:NH1	1:B:137:ARG:HD2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:O	1:B:127:LEU:HG	1.97	0.64
1:B:570:LEU:HB3	1:B:810:VAL:HB	1.78	0.64
1:B:1285:ALA:O	1:B:1289:LEU:N	2.29	0.64
1:A:1564:CYS:SG	1:A:1628:LEU:HD21	2.38	0.64
1:B:302:PRO:HA	1:B:366:ILE:HG21	1.80	0.64
1:B:2002:LEU:O	1:B:2006:THR:HB	1.97	0.64
1:B:1616:MET:HE3	1:B:1650:ILE:CD1	2.26	0.64
1:B:319:PRO:HB2	1:B:320:LEU:HD23	1.79	0.64
1:B:2098:PHE:CE2	1:B:2106:LEU:HB2	2.33	0.64
1:B:1836:VAL:HG13	1:B:1854:ILE:CD1	2.28	0.63
1:A:1411:ASP:O	1:A:1413:PRO:HD3	1.98	0.63
1:A:1926:ALA:O	1:A:1930:ARG:HB2	1.98	0.63
1:B:1991:VAL:HG21	1:B:2033:ASN:ND2	2.13	0.63
1:A:112:SER:HB3	1:A:334:PRO:HG3	1.79	0.63
1:A:1442:TRP:CZ2	1:A:1497:LEU:HD23	2.32	0.63
1:B:44:LEU:HG	1:B:45:TYR:CD1	2.33	0.63
1:A:736:VAL:O	1:A:740:VAL:HG23	1.99	0.63
1:A:984:GLU:O	1:A:985:PHE:HB2	1.96	0.63
1:A:1746:ASN:HD21	1:A:1753:LEU:HD12	1.62	0.63
1:A:9:MET:HE1	1:A:345:LEU:HB2	1.79	0.63
1:B:159:THR:HB	1:B:162:SER:OG	1.99	0.63
1:B:1303:ASN:N	1:B:1304:PRO:CD	2.61	0.63
1:B:1475:SER:HB3	1:B:1505:VAL:HG13	1.81	0.63
1:B:1735:HIS:H	1:B:1735:HIS:HD2	1.43	0.63
1:A:501:ALA:HB3	1:A:556:LEU:HD21	1.80	0.63
1:A:1954:SER:O	1:A:1958:GLU:HG3	1.97	0.63
1:B:1139:GLU:OE2	1:B:1218:SER:HB2	1.99	0.63
1:A:1472:VAL:HG12	1:A:1473:LEU:N	2.13	0.63
1:B:254:ASP:CB	1:B:257:LYS:HE2	2.28	0.63
1:B:853:GLY:O	1:B:854:SER:HB3	1.97	0.63
1:B:1460:LEU:HD13	1:B:2032:ALA:HB2	1.81	0.63
1:B:460:VAL:HG21	1:B:465:MET:HG3	1.79	0.62
1:A:1302:ALA:O	1:A:1303:ASN:HB2	1.97	0.62
1:A:1616:MET:HB3	1:A:1800:PHE:CZ	2.33	0.62
1:B:2006:THR:HG21	1:B:2048:ARG:HH22	1.62	0.62
1:A:399:ASN:N	1:A:399:ASN:ND2	2.46	0.62
1:A:641:ALA:HB1	1:A:683:HIS:HB2	1.81	0.62
1:A:1545:ARG:HG3	1:A:1545:ARG:NH1	2.12	0.62
1:B:251:THR:HB	1:B:399:ASN:O	2.00	0.62
1:B:1268:MET:HE2	1:B:1268:MET:HA	1.80	0.62
1:B:1433:LEU:HD13	1:B:1469:ILE:HD11	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:SER:O	1:A:583:GLY:N	2.33	0.62
1:B:200:PHE:HB3	1:B:206:LEU:HG	1.81	0.62
1:B:325:THR:OG1	1:B:343:LYS:HG2	1.99	0.62
1:B:643:HIS:HD2	1:B:746:GLN:HB3	1.65	0.62
1:B:1857:ARG:NH1	1:B:1871:ILE:HD11	2.15	0.62
1:A:1614:MET:HE3	1:A:1634:TRP:HB2	1.81	0.62
1:A:1762:GLN:HG2	1:A:1787:LYS:O	1.99	0.62
1:B:77:PRO:O	1:B:81:MET:HG2	1.99	0.62
1:B:399:ASN:H	1:B:399:ASN:HD22	1.47	0.62
1:B:1857:ARG:CZ	1:B:1871:ILE:HD11	2.30	0.62
1:B:1917:ARG:HH12	1:B:1974:VAL:HG12	1.63	0.62
1:A:159:THR:HB	1:A:162:SER:OG	1.99	0.62
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.82	0.62
1:A:542:ASP:O	1:A:545:VAL:HG12	1.99	0.62
1:A:1734:ARG:O	1:A:1736:THR:N	2.32	0.62
1:B:752:VAL:HG11	1:B:775:LEU:HD21	1.81	0.62
1:A:542:ASP:H	1:A:545:VAL:HG12	1.63	0.62
1:A:1009:LEU:HD13	1:A:1023:GLN:O	2.00	0.62
1:A:251:THR:HB	1:A:399:ASN:O	2.00	0.62
1:A:506:MET:HE1	1:A:555:SER:HB3	1.82	0.62
1:A:1429:LEU:HD11	1:A:1443:LEU:HD11	1.80	0.62
1:A:1836:VAL:HG13	1:A:1854:ILE:CD1	2.29	0.62
1:B:570:LEU:HD13	1:B:800:VAL:HG13	1.82	0.62
1:A:1734:ARG:C	1:A:1736:THR:H	2.08	0.62
1:B:420:LEU:HD11	1:B:512:ARG:HB3	1.82	0.62
1:B:972:THR:HG22	1:B:1081:VAL:CG2	2.29	0.62
1:B:1097:LEU:C	1:B:1097:LEU:HD12	2.24	0.62
1:A:353:TRP:NE1	1:A:383:ILE:HB	2.14	0.62
1:A:817:PRO:O	1:A:818:PRO:O	2.18	0.62
1:A:874:TYR:HB2	1:A:1006:PHE:CD2	2.34	0.62
1:B:1001:TYR:HB3	1:B:1003:TYR:CE1	2.35	0.62
1:B:1139:GLU:OE2	1:B:1216:LEU:HD12	1.99	0.62
1:B:1335:ALA:CA	1:B:1406:GLN:HE22	2.09	0.62
1:B:1996:TYR:C	1:B:1996:TYR:CD2	2.78	0.62
1:A:23:TRP:CE2	1:A:350:HIS:CD2	2.88	0.61
1:A:123:ASP:HB3	1:A:126:THR:CB	2.28	0.61
1:A:976:VAL:HG13	1:A:977:ASP:N	2.14	0.61
1:A:1448:CYS:C	1:A:1450:THR:H	2.08	0.61
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.82	0.61
1:B:1580:THR:HG22	1:B:1581:GLY:N	2.14	0.61
1:A:200:PHE:CE2	1:B:132:MET:HE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:O	1:A:319:PRO:HD3	1.99	0.61
1:B:1277:ARG:HD3	1:B:1300:ASP:CG	2.24	0.61
1:A:371:ASP:CG	1:A:371:ASP:O	2.43	0.61
1:A:1420:ASP:O	1:A:1425:TRP:CH2	2.54	0.61
1:B:277:TYR:CE2	1:B:287:LEU:HD11	2.34	0.61
1:B:331:HIS:CE1	1:B:333:GLU:HA	2.35	0.61
1:A:384:ARG:HH11	1:A:384:ARG:CG	2.13	0.61
1:A:1124:HIS:CD2	1:A:1512:GLY:HA2	2.35	0.61
1:A:1765:ARG:HG3	1:A:1790:THR:HG23	1.83	0.61
1:B:1768:GLU:HA	1:B:1768:GLU:OE1	2.00	0.61
1:B:1974:VAL:HG22	1:B:1994:PRO:HG2	1.81	0.61
1:A:331:HIS:CE1	1:A:333:GLU:HA	2.35	0.61
1:B:347:SER:HB2	1:B:352:VAL:O	2.00	0.61
1:B:889:THR:HG21	1:B:1032:LEU:HB2	1.80	0.61
1:A:368:ALA:CA	1:A:371:ASP:HB3	2.31	0.61
1:A:1466:GLY:HA2	1:A:1469:ILE:CG1	2.29	0.61
1:B:248:ASN:ND2	1:B:249:ALA:H	1.98	0.61
1:B:506:MET:HE1	1:B:555:SER:HB3	1.82	0.61
1:B:1838:ALA:HA	1:B:1841:ARG:HG3	1.80	0.61
1:B:322:ILE:CD1	1:B:374:LEU:HD13	2.31	0.61
1:B:416:GLN:HG3	1:B:422:ARG:HH21	1.65	0.61
1:B:1647:SER:HA	1:B:1851:LYS:HG3	1.81	0.61
1:B:1703:GLU:O	1:B:1706:ALA:HB3	2.01	0.61
1:A:139:MET:HE1	1:B:396:GLY:HA3	1.80	0.61
1:A:1484:PRO:O	1:A:1485:GLU:HB2	2.00	0.61
1:A:2078:THR:O	1:A:2079:VAL:HG13	2.01	0.61
1:B:89:ALA:O	1:B:92:ASP:HB3	2.01	0.61
1:A:416:GLN:HG3	1:A:422:ARG:HH21	1.64	0.61
1:B:1455:GLY:HA3	1:B:2039:SER:HB2	1.82	0.61
1:B:1841:ARG:O	1:B:1844:ALA:HB3	2.00	0.61
1:A:64:PHE:CE2	1:A:464:ALA:HB1	2.36	0.61
1:A:913:VAL:HG23	1:A:962:TRP:HB2	1.83	0.61
1:A:98:ALA:HA	1:A:101:ARG:HG3	1.82	0.60
1:A:1343:PHE:O	1:A:1344:LEU:HD22	2.01	0.60
1:A:1746:ASN:ND2	1:A:1753:LEU:HD12	2.16	0.60
1:B:1442:TRP:CZ2	1:B:1497:LEU:HD23	2.36	0.60
1:A:1248:LEU:HD21	1:A:1277:ARG:HE	1.66	0.60
1:B:403:ILE:O	1:B:404:LEU:HD23	2.00	0.60
1:B:981:SER:HA	1:B:984:GLU:HG3	1.82	0.60
1:B:1408:THR:H	1:B:1409:PRO:HD3	1.65	0.60
1:A:1656:TYR:CD2	1:A:1687:ILE:HD13	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ASP:HB3	1:B:126:THR:HB	1.81	0.60
1:B:327:SER:OG	1:B:356:ASN:ND2	2.34	0.60
1:B:1035:MET:SD	1:B:1091:ALA:HB3	2.42	0.60
1:B:1299:TRP:CZ2	1:B:1304:PRO:O	2.54	0.60
1:A:247:LEU:HD11	1:A:405:GLN:HB2	1.82	0.60
1:A:1439:ARG:O	1:A:1470:ARG:HB3	2.01	0.60
1:A:2006:THR:HG21	1:A:2048:ARG:HH22	1.66	0.60
1:B:215:PHE:CD2	1:B:305:LEU:HD11	2.37	0.60
1:B:501:ALA:HB3	1:B:556:LEU:HD21	1.83	0.60
1:A:45:TYR:HE2	1:B:124:PRO:HB2	1.66	0.60
1:A:665:LEU:HD22	1:A:670:VAL:HB	1.83	0.60
1:A:1996:TYR:C	1:A:1996:TYR:CD2	2.79	0.60
1:B:1073:ASP:O	1:B:1074:THR:HG22	2.02	0.60
1:B:1429:LEU:HD11	1:B:1443:LEU:HD11	1.82	0.60
1:B:1652:TYR:CD1	1:B:1823:VAL:HB	2.37	0.60
1:A:368:ALA:HA	1:A:371:ASP:HB3	1.82	0.60
1:A:1575:ASP:HA	1:A:1599:LEU:HD23	1.83	0.60
1:B:112:SER:HB2	1:B:334:PRO:CG	2.32	0.60
1:B:1119:PHE:CE1	1:B:1516:HIS:CE1	2.89	0.60
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.67	0.60
1:A:1279:PRO:HG3	1:A:1298:GLN:NE2	2.16	0.60
1:B:359:TYR:OH	1:B:362:PRO:HG3	2.02	0.60
1:B:371:ASP:CG	1:B:371:ASP:O	2.43	0.60
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.83	0.60
1:B:1580:THR:HG22	1:B:1582:LYS:N	2.16	0.60
1:B:1672:LEU:HD12	1:B:1696:PHE:O	2.02	0.60
1:B:2078:THR:O	1:B:2079:VAL:HG13	2.01	0.60
1:A:586:ALA:O	1:A:589:TYR:HB3	2.02	0.60
1:B:103:THR:HG22	1:B:104:SER:N	2.15	0.60
1:A:582:LEU:O	1:A:585:VAL:HG23	2.01	0.60
1:A:595:THR:HB	1:A:598:GLU:H	1.66	0.60
1:A:670:VAL:HG12	1:A:671:PHE:N	2.16	0.60
1:A:883:ARG:HH21	1:A:1107:ARG:HD3	1.67	0.60
1:A:1549:SER:O	1:A:1552:HIS:HB3	2.01	0.60
1:B:343:LYS:HE3	1:B:354:ALA:HB3	1.84	0.60
1:B:654:PRO:O	1:B:658:MET:HB2	2.01	0.60
1:B:1657:TYR:HA	1:B:1661:VAL:CG2	2.32	0.60
1:A:36:ASP:CB	1:A:38:ARG:HG3	2.32	0.60
1:A:1086:LEU:N	1:A:1086:LEU:HD23	2.17	0.60
1:B:1035:MET:HE3	1:B:1089:VAL:CG1	2.32	0.60
1:B:1396:PHE:CE2	1:B:1397:TYR:HD2	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ILE:O	1:A:366:ILE:HG12	2.00	0.59
1:A:1122:THR:HG1	1:A:1517:PHE:HE1	1.50	0.59
1:A:1482:PRO:C	1:A:1484:PRO:HD3	2.26	0.59
1:B:14:PRO:HD3	1:B:226:GLU:O	2.02	0.59
1:B:646:LYS:HG2	1:B:746:GLN:HE21	1.67	0.59
1:B:1466:GLY:HA2	1:B:1469:ILE:CG1	2.32	0.59
1:B:1625:SER:O	1:B:1626:VAL:HG23	2.02	0.59
1:A:327:SER:OG	1:A:356:ASN:ND2	2.35	0.59
1:A:808:VAL:HG12	1:A:809:SER:N	2.15	0.59
1:A:856:CYS:HG	1:B:856:CYS:CB	2.14	0.59
1:A:1580:THR:HG22	1:A:1582:LYS:N	2.17	0.59
1:B:384:ARG:HH11	1:B:384:ARG:CG	2.12	0.59
1:A:166:LEU:HD12	1:A:251:THR:HG21	1.83	0.59
1:B:1662:ARG:CG	1:B:1662:ARG:NH1	2.49	0.59
1:A:620:MET:HE3	1:A:682:PHE:O	2.02	0.59
1:A:1857:ARG:NH1	1:A:1869:PRO:CB	2.66	0.59
1:B:662:LEU:HD22	1:B:672:VAL:CG1	2.29	0.59
1:B:1657:TYR:HA	1:B:1661:VAL:HG23	1.84	0.59
1:A:1703:GLU:O	1:A:1706:ALA:HB3	2.02	0.59
1:B:1097:LEU:HD12	1:B:1098:GLY:N	2.17	0.59
1:B:1448:CYS:C	1:B:1450:THR:H	2.11	0.59
1:B:1765:ARG:HG3	1:B:1790:THR:HG23	1.85	0.59
1:A:1038:MET:HA	1:A:1038:MET:CE	2.32	0.59
1:A:1097:LEU:C	1:A:1097:LEU:HD12	2.27	0.59
1:A:1774:LEU:HD22	1:B:1785:PHE:HB2	1.85	0.59
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.68	0.59
1:B:322:ILE:HD12	1:B:374:LEU:HD13	1.85	0.59
1:B:366:ILE:HG12	1:B:366:ILE:O	2.02	0.59
1:B:630:CYS:HB3	1:B:640:PRO:HG3	1.85	0.59
1:A:1736:THR:HG23	1:A:1740:GLY:H	1.66	0.59
1:B:1662:ARG:HH11	1:B:1662:ARG:HG2	1.67	0.59
1:A:615:VAL:HG22	1:A:616:LEU:H	1.68	0.59
1:A:1034:ALA:O	1:A:1037:HIS:HB2	2.02	0.59
1:A:1397:TYR:CE1	1:A:1399:SER:HB2	2.37	0.59
1:B:288:GLU:HG3	1:B:385:GLY:O	2.02	0.59
1:B:317:ARG:O	1:B:319:PRO:HD3	2.02	0.59
1:B:399:ASN:N	1:B:399:ASN:ND2	2.51	0.59
1:B:1003:TYR:CE1	1:B:1037:HIS:CE1	2.90	0.59
1:B:2101:GLN:HG3	1:B:2102:PRO:CD	2.33	0.59
1:A:1118:LYS:HD2	1:A:2103:HIS:CE1	2.38	0.59
1:B:646:LYS:HG2	1:B:746:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1454:VAL:HG13	1:B:1503:MET:CE	2.33	0.59
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	1.83	0.59
1:B:128:VAL:HG11	1:B:130:TYR:CZ	2.37	0.59
1:A:165:LEU:HB2	1:A:337:GLY:HA3	1.85	0.58
1:A:1248:LEU:CD2	1:A:1277:ARG:HE	2.16	0.58
1:A:1580:THR:HG22	1:A:1581:GLY:N	2.17	0.58
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.84	0.58
1:B:878:HIS:HB2	1:B:1007:PHE:CE1	2.38	0.58
1:A:64:PHE:HB2	1:A:429:ARG:NH2	2.13	0.58
1:A:1528:THR:HG22	1:A:1530:HIS:N	2.15	0.58
1:B:165:LEU:HB2	1:B:337:GLY:HA3	1.85	0.58
1:B:527:LEU:HD12	1:B:534:VAL:HG22	1.85	0.58
1:B:680:ILE:HG12	1:B:681:ALA:H	1.67	0.58
1:B:1472:VAL:HG12	1:B:1473:LEU:N	2.17	0.58
1:B:1539:GLY:HA2	1:B:1580:THR:O	2.02	0.58
1:B:1736:THR:O	1:B:1739:LYS:HB2	2.03	0.58
1:A:1073:ASP:O	1:A:1074:THR:HG22	2.03	0.58
1:B:68:HIS:HB3	1:B:71:GLN:HG3	1.85	0.58
1:A:396:GLY:HA3	1:B:139:MET:HE1	1.85	0.58
1:B:612:GLU:O	1:B:612:GLU:HG2	2.04	0.58
1:B:1007:PHE:HE2	1:B:1030:SER:HA	1.67	0.58
1:B:1299:TRP:HE1	1:B:1306:PRO:HD2	1.68	0.58
1:A:23:TRP:CE2	1:A:350:HIS:HD2	2.22	0.58
1:A:466:PRO:HG2	1:A:467:PHE:HD1	1.68	0.58
1:A:1236:ASN:HA	1:A:1502:VAL:HG21	1.86	0.58
1:A:1991:VAL:HG21	1:A:2033:ASN:ND2	2.18	0.58
1:B:1694:ARG:CG	1:B:1694:ARG:NH1	2.65	0.58
1:A:351:GLY:C	1:A:383:ILE:HG22	2.28	0.58
1:A:917:VAL:CG1	1:A:1054:PHE:HB2	2.34	0.58
1:B:297:THR:HB	1:B:300:GLY:N	2.19	0.58
1:B:1651:VAL:HG23	1:B:1851:LYS:HZ1	1.68	0.58
1:B:1662:ARG:NH2	1:B:1793:GLY:O	2.36	0.58
1:B:1674:HIS:CD2	1:B:1698:THR:CG2	2.87	0.58
1:A:155:ILE:HD11	1:B:166:LEU:HD11	1.85	0.58
1:A:595:THR:CG2	1:A:597:GLU:HG2	2.33	0.58
1:A:1122:THR:HG21	1:A:1517:PHE:HZ	1.68	0.58
1:A:1248:LEU:HD21	1:A:1277:ARG:HH21	1.69	0.58
1:B:75:MET:HE3	1:B:80:ARG:HG2	1.86	0.58
1:B:1300:ASP:O	1:B:1302:ALA:N	2.36	0.58
1:B:1860:GLU:HB2	1:B:1865:PRO:HG2	1.84	0.58
1:A:321:LEU:HD23	1:A:381:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1454:VAL:HG13	1:A:1503:MET:HE1	1.85	0.58
1:B:386:GLY:O	1:B:387:ASN:HB2	2.03	0.58
1:A:275:SER:C	1:A:276:LEU:HD23	2.29	0.58
1:A:1299:TRP:NE1	1:A:1306:PRO:HD2	2.19	0.58
1:B:23:TRP:CE2	1:B:350:HIS:CD2	2.92	0.58
1:B:1003:TYR:CE1	1:B:1037:HIS:HE1	2.21	0.58
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.85	0.57
1:A:112:SER:HB2	1:A:334:PRO:CG	2.31	0.57
1:A:1068:LEU:HD12	1:A:1077:ALA:O	2.04	0.57
1:A:1580:THR:HG22	1:A:1582:LYS:H	1.69	0.57
1:B:1241:LYS:HG3	1:B:1241:LYS:O	2.03	0.57
1:A:103:THR:HG22	1:A:104:SER:N	2.19	0.57
1:A:945:GLU:OE1	1:B:938:LEU:HB3	2.03	0.57
1:B:1277:ARG:HD3	1:B:1300:ASP:OD2	2.04	0.57
1:A:1953:ARG:HG2	1:A:2005:VAL:CG1	2.33	0.57
1:B:889:THR:CG2	1:B:1032:LEU:HB2	2.34	0.57
1:B:1138:GLU:HG3	1:B:1138:GLU:O	2.03	0.57
1:B:1456:MET:HG3	1:B:2036:PHE:HD1	1.70	0.57
1:B:1762:GLN:HG2	1:B:1787:LYS:O	2.05	0.57
1:A:333:GLU:CB	1:A:334:PRO:CD	2.79	0.57
1:A:476:GLU:HB2	1:A:790:ARG:HH12	1.68	0.57
1:A:883:ARG:HE	1:A:1107:ARG:HD3	1.69	0.57
1:A:1007:PHE:HE2	1:A:1030:SER:HA	1.70	0.57
1:A:1917:ARG:HH12	1:A:1974:VAL:HG12	1.69	0.57
1:B:234:THR:HG21	1:B:239:ALA:HB2	1.84	0.57
1:B:1734:ARG:C	1:B:1736:THR:H	2.11	0.57
1:B:1953:ARG:HG2	1:B:2005:VAL:CG1	2.34	0.57
1:A:1647:SER:O	1:A:1651:VAL:HG21	2.04	0.57
1:A:1736:THR:O	1:A:1739:LYS:HB2	2.04	0.57
1:B:91:VAL:O	1:B:457:ILE:HD11	2.04	0.57
1:B:492:VAL:HG11	1:B:572:LEU:HD21	1.87	0.57
1:B:883:ARG:HH21	1:B:1107:ARG:HD3	1.68	0.57
1:B:1616:MET:HB3	1:B:1800:PHE:CZ	2.39	0.57
1:A:1773:ASP:OD1	1:A:1778:HIS:HD2	1.88	0.57
1:A:1841:ARG:O	1:A:1844:ALA:HB3	2.03	0.57
1:B:234:THR:CG2	1:B:239:ALA:HB2	2.34	0.57
1:B:257:LYS:HD3	1:B:263:PHE:O	2.04	0.57
1:B:1121:PHE:HE1	1:B:1512:GLY:C	2.13	0.57
1:B:1538:ARG:HH12	1:B:1585:PRO:CG	2.17	0.57
1:A:393:PHE:CD1	1:A:399:ASN:HB3	2.40	0.57
1:A:652:SER:OG	1:A:681:ALA:HB1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1672:LEU:HD12	1:A:1696:PHE:O	2.04	0.57
1:B:368:ALA:CA	1:B:371:ASP:HB3	2.34	0.57
1:A:293:HIS:O	1:A:326:LYS:HD2	2.04	0.57
1:A:403:ILE:O	1:A:404:LEU:HD23	2.04	0.57
1:A:638:ILE:O	1:A:638:ILE:HG22	2.05	0.57
1:A:889:THR:CG2	1:A:1032:LEU:HB2	2.35	0.57
1:A:1653:THR:CG2	1:A:1796:LEU:HD21	2.35	0.57
1:B:123:ASP:HB3	1:B:126:THR:CB	2.34	0.57
1:B:466:PRO:HG2	1:B:467:PHE:HD1	1.70	0.57
1:B:1720:PHE:N	1:B:1720:PHE:HD1	2.01	0.57
1:A:399:ASN:H	1:A:399:ASN:ND2	2.00	0.57
1:A:1657:TYR:CZ	1:A:1799:LEU:HD11	2.40	0.57
1:B:22:PHE:CD2	1:B:26:LEU:HD11	2.40	0.57
1:B:247:LEU:HD11	1:B:405:GLN:HB2	1.85	0.57
1:B:799:ASN:HA	1:B:802:ARG:HG3	1.86	0.57
1:A:396:GLY:CA	1:B:139:MET:HE1	2.35	0.57
1:A:1485:GLU:HB3	1:A:1506:TYR:OH	2.05	0.57
1:B:275:SER:C	1:B:276:LEU:HD23	2.30	0.57
1:B:362:PRO:HB3	1:B:369:LEU:HB3	1.87	0.57
1:B:913:VAL:HG23	1:B:962:TRP:HB2	1.86	0.57
1:B:1320:ALA:HA	1:B:1349:LEU:HD11	1.85	0.57
1:B:1565:SER:HB2	1:B:1857:ARG:HH22	1.63	0.57
1:B:1580:THR:HG22	1:B:1582:LYS:H	1.70	0.57
1:A:14:PRO:HD3	1:A:226:GLU:O	2.04	0.56
1:A:343:LYS:HG3	1:A:344:VAL:N	2.19	0.56
1:A:148:PHE:HB3	1:A:150:PHE:CZ	2.40	0.56
1:A:309:VAL:HG12	1:A:313:CYS:HB2	1.87	0.56
1:A:527:LEU:HD12	1:A:534:VAL:HG22	1.86	0.56
1:A:1457:VAL:CG2	1:A:1473:LEU:HD22	2.32	0.56
1:B:980:ASP:CB	1:B:982:THR:HG22	2.33	0.56
1:A:19:LEU:HD11	1:A:342:ILE:HD13	1.87	0.56
1:A:492:VAL:HG11	1:A:572:LEU:HD21	1.88	0.56
1:A:615:VAL:HG22	1:A:616:LEU:N	2.20	0.56
1:A:1279:PRO:HG3	1:A:1298:GLN:HE22	1.70	0.56
1:A:1425:TRP:HA	1:A:1428:SER:HB2	1.87	0.56
1:B:166:LEU:HD12	1:B:251:THR:HG21	1.87	0.56
1:B:970:PHE:O	1:B:1067:LYS:HE2	2.05	0.56
1:A:248:ASN:ND2	1:A:249:ALA:H	2.03	0.56
1:A:1545:ARG:HH11	1:A:1545:ARG:CG	2.17	0.56
1:B:903:LEU:O	1:B:905:GLN:HG3	2.05	0.56
1:A:1486:MET:CE	1:A:1506:TYR:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LYS:HE3	1:B:336:SER:HB2	1.87	0.56
1:B:642:CYS:HA	1:B:743:VAL:HG22	1.86	0.56
1:A:68:HIS:HB3	1:A:71:GLN:HG3	1.88	0.56
1:A:1299:TRP:HE1	1:A:1305:ALA:HA	1.71	0.56
1:A:1765:ARG:HD3	1:A:1765:ARG:N	2.21	0.56
1:B:1222:ASP:HA	1:B:1226:LEU:CD1	2.35	0.56
1:B:1373:LEU:N	1:B:1373:LEU:HD23	2.20	0.56
1:B:1662:ARG:NH1	1:B:1662:ARG:HG2	2.18	0.56
1:A:1348:THR:HG22	1:A:1349:LEU:N	2.14	0.56
1:B:278:ALA:CB	1:B:279:PRO:CD	2.83	0.56
1:B:1407:GLN:HG2	1:B:1409:PRO:HD2	1.83	0.56
1:B:1422:SER:O	1:B:1423:PHE:HB2	2.06	0.56
1:B:1423:PHE:CD1	1:B:1989:GLN:HB3	2.41	0.56
1:B:1514:PHE:O	1:B:1515:ARG:NH1	2.39	0.56
1:B:1765:ARG:HD3	1:B:1765:ARG:N	2.21	0.56
1:A:605:TRP:O	1:A:606:ARG:C	2.49	0.56
1:A:1244:VAL:HB	1:A:1272:TYR:HD1	1.69	0.56
1:A:1662:ARG:NH1	1:A:1792:HIS:ND1	2.54	0.56
1:A:1720:PHE:CD1	1:A:1720:PHE:N	2.74	0.56
1:B:19:LEU:HD11	1:B:342:ILE:HD13	1.88	0.56
1:B:309:VAL:HG12	1:B:313:CYS:HB2	1.88	0.56
1:B:993:TYR:CZ	1:B:1008:GLN:HA	2.40	0.56
1:A:89:ALA:O	1:A:92:ASP:HB3	2.05	0.56
1:B:1451:SER:O	1:B:2036:PHE:CE1	2.59	0.56
1:B:1656:TYR:O	1:B:1661:VAL:HG23	2.06	0.56
1:B:1669:GLU:HG2	1:B:1742:ASP:OD2	2.06	0.56
1:B:1720:PHE:N	1:B:1720:PHE:CD1	2.71	0.56
1:A:799:ASN:HA	1:A:802:ARG:HG3	1.88	0.56
1:A:903:LEU:O	1:A:905:GLN:HG3	2.06	0.56
1:A:132:MET:HE1	1:B:200:PHE:CD2	2.41	0.55
1:A:1275:THR:CG2	1:A:1299:TRP:HB2	2.36	0.55
1:A:1720:PHE:N	1:A:1720:PHE:HD1	2.04	0.55
1:B:424:LEU:CD2	1:B:441:GLY:HA3	2.36	0.55
1:B:1746:ASN:HD21	1:B:1753:LEU:HD12	1.71	0.55
1:A:257:LYS:HD3	1:A:263:PHE:O	2.05	0.55
1:A:670:VAL:HG12	1:A:671:PHE:H	1.72	0.55
1:A:1570:SER:OG	1:A:1602:GLU:HB3	2.07	0.55
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.40	0.55
1:B:1007:PHE:CE2	1:B:1030:SER:HA	2.41	0.55
1:B:1038:MET:HA	1:B:1038:MET:CE	2.36	0.55
1:A:1569:THR:HG23	1:A:1602:GLU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:C	1:B:418:ALA:H	2.15	0.55
1:B:1893:LEU:HB3	1:B:1925:GLN:NE2	2.20	0.55
1:A:36:ASP:HB3	1:A:38:ARG:CG	2.37	0.55
1:B:36:ASP:CB	1:B:38:ARG:HG3	2.35	0.55
1:B:278:ALA:HB3	1:B:279:PRO:CD	2.34	0.55
1:B:621:ALA:CB	1:B:662:LEU:HD11	2.36	0.55
1:B:1996:TYR:CD1	1:B:2040:ALA:HB1	2.41	0.55
1:A:1003:TYR:CE1	1:A:1037:HIS:CE1	2.94	0.55
1:A:1418:VAL:HG13	1:A:1425:TRP:CH2	2.42	0.55
1:A:1484:PRO:O	1:A:1485:GLU:CB	2.53	0.55
1:A:1674:HIS:ND1	1:A:1698:THR:HG21	2.21	0.55
1:A:1777:ASN:HD22	1:B:1783:ALA:H	1.54	0.55
1:A:1996:TYR:CD1	1:A:2040:ALA:HB1	2.41	0.55
1:B:1736:THR:HG21	1:B:1740:GLY:H	1.72	0.55
1:B:2103:HIS:CD2	1:B:2103:HIS:H	2.23	0.55
1:A:1097:LEU:HD12	1:A:1098:GLY:N	2.22	0.55
1:A:1443:LEU:O	1:A:1473:LEU:HA	2.06	0.55
1:A:1563:LEU:HD12	1:A:1564:CYS:H	1.72	0.55
1:A:1723:SER:C	1:A:1725:ASP:H	2.15	0.55
1:A:1800:PHE:HD2	1:A:1800:PHE:C	2.15	0.55
1:B:1414:VAL:HG11	1:B:1432:ILE:HD13	1.89	0.55
1:B:1470:ARG:HG3	1:B:1470:ARG:O	2.05	0.55
1:A:22:PHE:CD2	1:A:26:LEU:HD11	2.41	0.55
1:A:81:MET:HG3	1:A:228:VAL:HG11	1.89	0.55
1:A:386:GLY:O	1:A:387:ASN:HB2	2.05	0.55
1:A:1616:MET:HB3	1:A:1800:PHE:HZ	1.72	0.55
1:A:1768:GLU:OE1	1:A:1768:GLU:HA	2.06	0.55
1:B:1299:TRP:CH2	1:B:1333:ASN:ND2	2.75	0.55
1:B:1473:LEU:HG	1:B:1503:MET:HA	1.88	0.55
1:B:1560:GLN:HA	1:B:1563:LEU:HB3	1.87	0.55
1:A:146:PHE:O	1:B:256:SER:HB3	2.07	0.55
1:A:429:ARG:HB3	1:A:429:ARG:HH11	1.70	0.55
1:A:1470:ARG:O	1:A:1470:ARG:HG3	2.07	0.55
1:A:1530:HIS:HB2	1:A:1552:HIS:HB2	1.87	0.55
1:A:40:TRP:CH2	1:A:194:PRO:HA	2.42	0.55
1:A:111:VAL:HG22	1:A:188:LEU:HB2	1.88	0.55
1:A:159:THR:HB	1:A:162:SER:HG	1.72	0.55
1:A:297:THR:HB	1:A:300:GLY:N	2.20	0.55
1:A:1857:ARG:HH11	1:A:1869:PRO:CB	2.19	0.55
1:B:23:TRP:CE2	1:B:350:HIS:HD2	2.25	0.55
1:B:82:LEU:HD13	1:B:188:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ALA:O	1:B:101:ARG:HG3	2.07	0.55
1:B:393:PHE:CD1	1:B:399:ASN:HB3	2.42	0.55
1:B:615:VAL:HG22	1:B:686:PHE:CD2	2.42	0.55
1:B:644:ASN:HB2	1:B:648:THR:O	2.06	0.55
1:B:1333:ASN:C	1:B:1335:ALA:H	2.14	0.55
1:B:1416:LEU:HD23	1:B:1429:LEU:HG	1.88	0.55
1:A:878:HIS:HB2	1:A:1007:PHE:CE1	2.42	0.54
1:A:1035:MET:SD	1:A:1091:ALA:HB3	2.47	0.54
1:A:1300:ASP:O	1:A:1302:ALA:N	2.38	0.54
1:A:1476:ASN:HA	1:A:1486:MET:SD	2.47	0.54
1:B:1570:SER:OG	1:B:1602:GLU:HB3	2.07	0.54
1:B:1917:ARG:NH1	1:B:1974:VAL:HG12	2.23	0.54
1:A:166:LEU:HD23	1:A:166:LEU:O	2.07	0.54
1:A:1766:PHE:CD2	1:A:1791:PHE:CE1	2.95	0.54
1:A:1783:ALA:H	1:B:1777:ASN:HD22	1.54	0.54
1:B:40:TRP:CH2	1:B:194:PRO:HA	2.42	0.54
1:B:420:LEU:HD11	1:B:512:ARG:HD2	1.89	0.54
1:B:1223:ALA:HB1	1:B:1224:PRO:HD2	1.89	0.54
1:B:1227:LYS:HE2	1:B:1516:HIS:O	2.07	0.54
1:B:1766:PHE:CD2	1:B:1791:PHE:CE1	2.96	0.54
1:A:236:LYS:C	1:A:238:LEU:H	2.16	0.54
1:A:278:ALA:CB	1:A:279:PRO:CD	2.84	0.54
1:A:838:HIS:O	1:A:839:SER:C	2.50	0.54
1:A:1115:ILE:CD1	1:A:2111:LEU:HG	2.31	0.54
1:B:228:VAL:O	1:B:228:VAL:HG23	2.07	0.54
1:B:917:VAL:CG1	1:B:1054:PHE:HB2	2.37	0.54
1:B:1051:PRO:HA	1:B:1101:SER:HB3	1.90	0.54
1:B:1802:GLU:O	1:B:1804:GLY:N	2.39	0.54
1:A:1800:PHE:C	1:A:1800:PHE:CD2	2.85	0.54
1:A:1801:GLU:O	1:A:1803:GLY:N	2.41	0.54
1:A:1996:TYR:HD1	1:A:2040:ALA:HB1	1.72	0.54
1:B:293:HIS:O	1:B:326:LYS:HD2	2.06	0.54
1:B:420:LEU:HD11	1:B:512:ARG:CB	2.37	0.54
1:B:1563:LEU:HD12	1:B:1564:CYS:H	1.72	0.54
1:B:1734:ARG:O	1:B:1736:THR:N	2.40	0.54
1:A:416:GLN:C	1:A:418:ALA:H	2.13	0.54
1:A:1222:ASP:HA	1:A:1226:LEU:CD1	2.38	0.54
1:A:1857:ARG:CG	1:A:1871:ILE:HD11	2.38	0.54
1:A:2101:GLN:HG3	1:A:2102:PRO:CD	2.38	0.54
1:B:1470:ARG:O	1:B:1472:VAL:HG23	2.07	0.54
1:B:1472:VAL:HG13	1:B:1502:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:HE3	1:A:191:LEU:HD13	1.88	0.54
1:A:215:PHE:HD2	1:A:305:LEU:HD11	1.68	0.54
1:A:940:ALA:HB3	1:B:945:GLU:OE2	2.07	0.54
1:A:1606:ARG:NH2	1:A:1860:GLU:HG3	2.20	0.54
1:A:1698:THR:OG1	1:A:1723:SER:HB3	2.06	0.54
1:A:1973:MET:HB3	1:A:1995:LYS:HE3	1.89	0.54
1:B:1422:SER:HB2	1:B:1424:ARG:HG3	1.90	0.54
1:B:1570:SER:HB3	1:B:1853:VAL:HG22	1.89	0.54
1:A:353:TRP:CZ2	1:A:383:ILE:HD12	2.43	0.54
1:B:343:LYS:HG3	1:B:344:VAL:N	2.22	0.54
1:B:1229:CYS:HB3	1:B:1403:LEU:HD22	1.90	0.54
1:A:359:TYR:OH	1:A:362:PRO:HG3	2.08	0.54
1:A:1769:ILE:HG22	1:A:1770:GLY:N	2.22	0.54
1:A:1996:TYR:HD2	1:A:1997:SER:N	2.06	0.54
1:A:2019:PHE:CD1	1:A:2060:TRP:NE1	2.76	0.54
1:A:2102:PRO:HD2	1:A:2103:HIS:CD2	2.42	0.54
1:A:169:GLN:HE21	1:A:169:GLN:C	2.15	0.54
1:A:475:GLY:C	1:A:477:ALA:H	2.15	0.54
1:A:851:PRO:CB	1:B:122:ARG:HB3	2.37	0.54
1:A:856:CYS:SG	1:B:856:CYS:CB	2.96	0.54
1:A:1003:TYR:CE1	1:A:1037:HIS:HE1	2.26	0.54
1:A:1446:VAL:HA	1:A:1476:ASN:ND2	2.23	0.54
1:A:1893:LEU:HB3	1:A:1925:GLN:NE2	2.22	0.54
1:A:228:VAL:HG23	1:A:228:VAL:O	2.08	0.54
1:A:295:THR:HG22	1:A:331:HIS:HD2	1.72	0.54
1:B:96:ASN:ND2	1:B:98:ALA:HB3	2.19	0.54
1:B:1656:TYR:CE2	1:B:1687:ILE:HD13	2.43	0.54
1:B:1773:ASP:OD1	1:B:1778:HIS:HD2	1.91	0.54
1:A:162:SER:OG	1:A:163:SER:N	2.41	0.53
1:A:278:ALA:HB3	1:A:279:PRO:CD	2.35	0.53
1:A:502:GLN:HG3	1:A:556:LEU:CD1	2.35	0.53
1:A:1408:THR:HB	1:A:1439:ARG:HH12	1.72	0.53
1:B:123:ASP:HB3	1:B:126:THR:OG1	2.09	0.53
1:B:148:PHE:HB3	1:B:150:PHE:CZ	2.43	0.53
1:B:642:CYS:HA	1:B:743:VAL:CG2	2.37	0.53
1:B:838:HIS:O	1:B:839:SER:C	2.51	0.53
1:B:1068:LEU:HD12	1:B:1077:ALA:O	2.08	0.53
1:B:1538:ARG:NH2	1:B:1585:PRO:HG2	2.21	0.53
1:B:1996:TYR:HD2	1:B:1997:SER:N	2.06	0.53
1:A:22:PHE:CE2	1:A:26:LEU:HD11	2.43	0.53
1:A:685:TYR:CD1	1:A:686:PHE:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:TYR:C	1:A:734:TYR:CD2	2.86	0.53
1:A:1275:THR:HG21	1:A:1299:TRP:HB2	1.90	0.53
1:A:1748:LEU:O	1:A:1749:ALA:O	2.26	0.53
1:B:120:LEU:HD21	1:B:845:PRO:HG3	1.89	0.53
1:B:254:ASP:O	1:B:255:GLY:O	2.27	0.53
1:B:368:ALA:HA	1:B:371:ASP:HB3	1.90	0.53
1:B:621:ALA:HB2	1:B:662:LEU:HD11	1.90	0.53
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.91	0.53
1:B:1394:ARG:HA	1:B:1400:VAL:HG22	1.88	0.53
1:A:234:THR:CG2	1:A:239:ALA:HB2	2.38	0.53
1:A:945:GLU:OE2	1:B:940:ALA:HB3	2.09	0.53
1:A:1602:GLU:CD	1:A:1650:ILE:HG12	2.34	0.53
1:B:201:MET:HA	1:B:206:LEU:HB2	1.89	0.53
1:B:586:ALA:O	1:B:589:TYR:HB3	2.07	0.53
1:B:623:VAL:HG12	1:B:624:GLY:N	2.23	0.53
1:B:874:TYR:HB2	1:B:1006:PHE:CD2	2.43	0.53
1:B:1333:ASN:ND2	1:B:1334:MET:SD	2.82	0.53
1:B:1618:PRO:CD	1:B:1629:LEU:HD11	2.38	0.53
1:A:1315:LEU:HB3	1:A:1344:LEU:CD1	2.38	0.53
1:A:1394:ARG:HA	1:A:1400:VAL:HG22	1.90	0.53
1:B:209:ASP:OD2	1:B:213:ARG:NE	2.42	0.53
1:B:432:GLU:HG3	1:B:433:ALA:N	2.24	0.53
1:B:1248:LEU:HD21	1:B:1277:ARG:HE	1.74	0.53
1:B:1390:VAL:HG13	1:B:1501:LEU:HD21	1.89	0.53
1:B:1486:MET:HE1	1:B:1506:TYR:CD2	2.43	0.53
1:B:2101:GLN:HG3	1:B:2102:PRO:HD2	1.89	0.53
1:A:1085:ASN:C	1:A:1086:LEU:HD23	2.33	0.53
1:A:2006:THR:O	1:A:2010:CYS:HB2	2.08	0.53
1:B:159:THR:CG2	1:B:398:SER:HB3	2.39	0.53
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.90	0.53
1:B:1418:VAL:HG13	1:B:1425:TRP:CH2	2.41	0.53
1:A:234:THR:HG21	1:A:239:ALA:HB2	1.89	0.53
1:A:542:ASP:H	1:A:545:VAL:CG1	2.22	0.53
1:A:1656:TYR:HD2	1:A:1660:VAL:HG21	1.72	0.53
1:B:495:ILE:CD1	1:B:578:ILE:HB	2.39	0.53
1:B:972:THR:CG2	1:B:1081:VAL:HG23	2.38	0.53
1:A:165:LEU:HD23	1:A:400:VAL:CG2	2.25	0.53
1:A:856:CYS:C	1:A:858:SER:H	2.17	0.53
1:A:1035:MET:HE3	1:A:1089:VAL:CG1	2.39	0.53
1:A:2103:HIS:HB2	1:A:2106:LEU:HD21	1.90	0.53
1:B:963:GLU:OE1	1:B:963:GLU:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1338:LEU:CD1	1:B:1406:GLN:HG3	2.38	0.53
1:A:91:VAL:O	1:A:457:ILE:HD11	2.09	0.53
1:A:423:LEU:HD23	1:A:812:PRO:HG3	1.89	0.53
1:A:963:GLU:O	1:A:965:PRO:HD3	2.09	0.53
1:A:963:GLU:OE1	1:A:963:GLU:HA	2.09	0.53
1:B:214:SER:HB3	1:B:327:SER:HB3	1.91	0.53
1:B:963:GLU:O	1:B:965:PRO:HD3	2.08	0.53
1:B:1136:LEU:HD21	1:B:1218:SER:HA	1.89	0.53
1:B:1418:VAL:O	1:B:1418:VAL:HG12	2.08	0.53
1:B:1607:ASP:OD1	1:B:1611:ARG:HB3	2.09	0.53
1:A:252:ASN:HD21	1:A:272:LEU:HB2	1.74	0.53
1:A:254:ASP:O	1:A:255:GLY:O	2.26	0.53
1:A:542:ASP:N	1:A:545:VAL:HG12	2.23	0.53
1:A:887:PRO:HB2	1:A:890:GLY:H	1.73	0.53
1:A:1416:LEU:HD11	1:A:1425:TRP:HB3	1.90	0.53
1:B:1469:ILE:HG22	1:B:1471:CYS:SG	2.49	0.53
1:A:1252:GLY:CA	1:A:1318:ASN:HD22	2.22	0.53
1:A:1348:THR:HG21	1:A:1378:TRP:HZ2	1.70	0.53
1:A:1640:TRP:CZ2	1:A:1825:PRO:HD3	2.44	0.53
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.89	0.53
1:B:1413:PRO:HA	1:B:1440:PRO:HB2	1.91	0.53
1:B:1461:ARG:HG3	1:B:1461:ARG:O	2.09	0.53
1:B:1554:ALA:CB	1:B:1882:PRO:HB3	2.39	0.53
1:B:1669:GLU:O	1:B:1693:CYS:HB3	2.09	0.53
1:A:856:CYS:SG	1:B:856:CYS:SG	3.06	0.52
1:A:1507:ARG:HH22	1:A:2046:GLU:CD	2.16	0.52
1:B:638:ILE:HD11	1:B:657:ALA:C	2.34	0.52
1:B:1996:TYR:HD1	1:B:2040:ALA:HB1	1.74	0.52
1:A:98:ALA:O	1:A:101:ARG:HG3	2.08	0.52
1:B:1276:ASP:O	1:B:1298:GLN:HA	2.09	0.52
1:B:1874:THR:O	1:B:1874:THR:HG22	2.09	0.52
1:A:91:VAL:HG21	1:A:834:ILE:HD13	1.92	0.52
1:A:159:THR:CG2	1:A:398:SER:HB3	2.40	0.52
1:A:429:ARG:HB3	1:A:429:ARG:NH1	2.23	0.52
1:A:431:LEU:HD23	1:A:431:LEU:C	2.34	0.52
1:A:612:GLU:C	1:A:614:ASN:H	2.16	0.52
1:A:612:GLU:C	1:A:614:ASN:N	2.67	0.52
1:A:1648:VAL:HB	1:A:1649:PRO:HD3	1.91	0.52
1:B:1554:ALA:C	1:B:1556:PRO:HD3	2.34	0.52
1:B:2019:PHE:CD1	1:B:2060:TRP:NE1	2.78	0.52
1:A:1051:PRO:HA	1:A:1101:SER:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:VAL:O	1:A:1418:VAL:HG12	2.09	0.52
1:A:2103:HIS:CD2	1:A:2103:HIS:H	2.27	0.52
1:B:165:LEU:HD22	1:B:392:SER:HB2	1.91	0.52
1:B:219:GLY:O	1:B:298:LYS:HB2	2.09	0.52
1:B:429:ARG:HB3	1:B:429:ARG:HH11	1.73	0.52
1:B:502:GLN:HG3	1:B:556:LEU:CD1	2.37	0.52
1:B:638:ILE:HD11	1:B:657:ALA:O	2.09	0.52
1:B:765:ALA:HB2	1:B:783:PRO:HB3	1.91	0.52
1:A:39:ARG:NH1	1:A:57:LEU:HD22	2.24	0.52
1:A:166:LEU:HD11	1:B:155:ILE:HD11	1.90	0.52
1:A:1252:GLY:HA2	1:A:1318:ASN:HD22	1.73	0.52
1:A:1553:TYR:CD1	1:A:1880:PHE:HB2	2.45	0.52
1:B:259:GLN:H	1:B:259:GLN:CD	2.18	0.52
1:B:1009:LEU:HD13	1:B:1023:GLN:O	2.10	0.52
1:B:1855:GLN:NE2	1:B:1858:GLU:HA	2.24	0.52
1:A:499:MET:HE2	1:A:582:LEU:HD22	1.92	0.52
1:B:166:LEU:O	1:B:166:LEU:HD23	2.09	0.52
1:B:506:MET:HB3	1:B:559:ILE:CD1	2.39	0.52
1:B:564:ILE:HD13	1:B:590:ALA:HB2	1.92	0.52
1:B:1338:LEU:HG	1:B:1342:GLY:H	1.75	0.52
1:B:1800:PHE:C	1:B:1800:PHE:CD2	2.88	0.52
1:B:2103:HIS:HB2	1:B:2106:LEU:HD21	1.90	0.52
1:A:796:PHE:O	1:A:800:VAL:HG23	2.09	0.52
1:A:1677:SER:HB2	1:A:1704:LYS:HE2	1.92	0.52
1:A:1917:ARG:NH1	1:A:1974:VAL:HG12	2.25	0.52
1:B:808:VAL:HG12	1:B:809:SER:N	2.25	0.52
1:B:1723:SER:C	1:B:1725:ASP:H	2.18	0.52
1:B:1800:PHE:C	1:B:1800:PHE:HD2	2.17	0.52
1:B:1973:MET:HB3	1:B:1995:LYS:HE3	1.91	0.52
1:B:2006:THR:CG2	1:B:2048:ARG:HH22	2.22	0.52
1:B:2019:PHE:CE1	1:B:2060:TRP:NE1	2.77	0.52
1:A:112:SER:O	1:A:137:ARG:NH2	2.43	0.52
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.40	0.52
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.91	0.52
1:A:765:ALA:HB1	1:A:768:GLN:HG2	1.92	0.52
1:A:1003:TYR:CE2	1:A:1037:HIS:CE1	2.92	0.52
1:A:1007:PHE:CE2	1:A:1030:SER:HA	2.44	0.52
1:A:1736:THR:HG21	1:A:1740:GLY:H	1.71	0.52
1:B:1568:TYR:CZ	1:B:1643:GLU:HG3	2.45	0.52
1:A:993:TYR:CZ	1:A:1008:GLN:HA	2.45	0.52
1:A:1001:TYR:HB3	1:A:1003:TYR:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:LYS:HG3	1:A:1241:LYS:O	2.10	0.52
1:B:1222:ASP:HA	1:B:1226:LEU:HD11	1.92	0.52
1:B:1255:TYR:O	1:B:1292:LEU:HD13	2.10	0.52
1:B:1416:LEU:HD11	1:B:1425:TRP:HB3	1.92	0.52
1:B:1698:THR:OG1	1:B:1723:SER:HB3	2.09	0.52
1:A:1476:ASN:HA	1:A:1486:MET:HE1	1.91	0.52
1:A:1899:GLN:HG2	1:A:2088:ILE:HG21	1.92	0.52
1:B:1748:LEU:O	1:B:1749:ALA:O	2.28	0.52
1:B:1981:GLU:C	1:B:1983:GLN:H	2.18	0.52
1:A:326:LYS:HE3	1:A:336:SER:HB2	1.91	0.51
1:A:1302:ALA:O	1:A:1304:PRO:HD3	2.10	0.51
1:A:1524:PRO:O	1:A:1877:SER:HB2	2.10	0.51
1:B:269:GLN:O	1:B:273:ILE:HG13	2.08	0.51
1:B:665:LEU:HD22	1:B:670:VAL:HG21	1.92	0.51
1:A:831:SER:OG	1:A:832:PRO:HD3	2.10	0.51
1:A:851:PRO:HB2	1:B:122:ARG:HB3	1.90	0.51
1:A:1422:SER:HB2	1:A:1424:ARG:HG3	1.92	0.51
1:A:1794:ILE:C	1:A:1795:LEU:HD23	2.35	0.51
1:B:191:LEU:HD22	1:B:224:ARG:CZ	2.40	0.51
1:B:399:ASN:H	1:B:399:ASN:ND2	2.07	0.51
1:B:429:ARG:HB3	1:B:429:ARG:NH1	2.26	0.51
1:B:724:GLY:O	1:B:728:ARG:HB2	2.10	0.51
1:B:914:PHE:O	1:B:915:GLU:HG3	2.09	0.51
1:B:1239:SER:C	1:B:1241:LYS:H	2.18	0.51
1:B:1466:GLY:O	1:B:1469:ILE:HB	2.10	0.51
1:B:1593:LEU:HD23	1:B:1594:THR:HG22	1.92	0.51
1:B:1894:GLY:O	1:B:1895:GLY:C	2.54	0.51
1:B:2102:PRO:HD2	1:B:2103:HIS:CD2	2.42	0.51
1:A:130:TYR:HA	1:B:203:LEU:HD21	1.92	0.51
1:A:1119:PHE:CE1	1:A:1516:HIS:CE1	2.98	0.51
1:A:1456:MET:HG2	1:A:2036:PHE:HB2	1.92	0.51
1:B:1616:MET:HE2	1:B:1800:PHE:CE1	2.45	0.51
1:A:765:ALA:HB2	1:A:783:PRO:HB3	1.92	0.51
1:A:1570:SER:HB3	1:A:1853:VAL:HG22	1.92	0.51
1:A:1674:HIS:CE1	1:A:1698:THR:HG21	2.45	0.51
1:A:2101:GLN:HG3	1:A:2102:PRO:HD2	1.93	0.51
1:B:169:GLN:OE1	1:B:250:GLY:HA2	2.10	0.51
1:B:1227:LYS:HB2	1:B:1261:LEU:CD2	2.39	0.51
1:B:1275:THR:CG2	1:B:1299:TRP:HB2	2.39	0.51
1:B:1786:LEU:C	1:B:1788:ASN:H	2.18	0.51
1:B:2070:LEU:HD11	1:B:2076:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:CD	1:B:118:GLU:HG3	2.34	0.51
1:A:662:LEU:O	1:A:666:LYS:HG2	2.09	0.51
1:A:1289:LEU:HD22	1:A:1294:VAL:CB	2.36	0.51
1:A:1461:ARG:NH1	1:A:1502:VAL:HG22	2.26	0.51
1:A:1662:ARG:CG	1:A:1662:ARG:NH1	2.55	0.51
1:B:333:GLU:CB	1:B:334:PRO:CD	2.84	0.51
1:B:887:PRO:HB2	1:B:890:GLY:H	1.76	0.51
1:B:1302:ALA:HB3	1:B:1304:PRO:HD3	1.92	0.51
1:B:1460:LEU:HD12	1:B:1463:GLU:OE1	2.11	0.51
1:B:1677:SER:HB2	1:B:1704:LYS:HE2	1.93	0.51
1:B:1746:ASN:ND2	1:B:1753:LEU:HD12	2.25	0.51
1:B:1794:ILE:C	1:B:1795:LEU:HD23	2.36	0.51
1:A:82:LEU:HD13	1:A:188:LEU:HD21	1.91	0.51
1:A:687:MET:HA	1:A:687:MET:HE2	1.92	0.51
1:A:976:VAL:CG2	1:A:977:ASP:H	2.17	0.51
1:A:1528:THR:HG21	1:A:1530:HIS:O	2.11	0.51
1:A:1763:HIS:HA	1:A:1788:ASN:O	2.10	0.51
1:A:1526:LYS:HD3	1:A:1552:HIS:NE2	2.25	0.51
1:B:81:MET:HG3	1:B:228:VAL:HG11	1.92	0.51
1:B:1276:ASP:OD2	1:B:1281:ALA:HB3	2.11	0.51
1:B:1501:LEU:HB2	1:B:1504:ASN:OD1	2.10	0.51
1:B:1544:ILE:HD12	1:B:1837:GLU:HA	1.92	0.51
1:A:1556:PRO:O	1:A:1557:ALA:C	2.53	0.51
1:A:1639:THR:O	1:A:1640:TRP:HD1	1.93	0.51
1:A:2019:PHE:CE1	1:A:2060:TRP:NE1	2.79	0.51
1:B:183:ALA:O	1:B:232:LEU:HD12	2.11	0.51
1:B:1001:TYR:CE2	1:B:1040:ILE:HD13	2.46	0.51
1:B:1418:VAL:HG22	1:B:1425:TRP:CD2	2.45	0.51
1:B:1470:ARG:O	1:B:1470:ARG:CG	2.58	0.51
1:A:122:ARG:HG3	1:A:123:ASP:H	1.76	0.51
1:A:416:GLN:C	1:A:418:ALA:N	2.69	0.51
1:A:941:SER:N	1:B:945:GLU:OE2	2.44	0.51
1:A:1411:ASP:HB2	1:A:1440:PRO:CD	2.41	0.51
1:A:1486:MET:HE3	1:A:1506:TYR:HB3	1.91	0.51
1:B:111:VAL:HG22	1:B:188:LEU:HB2	1.93	0.51
1:B:321:LEU:H	1:B:321:LEU:HD12	1.75	0.51
1:B:625:LEU:HD22	1:B:629:GLU:OE1	2.11	0.51
1:B:982:THR:HG23	1:B:983:ALA:N	2.19	0.51
1:B:1236:ASN:CG	1:B:1502:VAL:HG23	2.36	0.51
1:B:2006:THR:O	1:B:2010:CYS:HB2	2.11	0.51
1:B:1473:LEU:HD21	1:B:1503:MET:CG	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:CE2	1:B:124:PRO:HB2	2.45	0.50
1:A:970:PHE:O	1:A:1067:LYS:HE2	2.10	0.50
1:A:1221:LEU:HG	1:A:1221:LEU:O	2.10	0.50
1:B:166:LEU:HD23	1:B:166:LEU:C	2.36	0.50
1:B:248:ASN:HD22	1:B:249:ALA:H	1.56	0.50
1:B:1439:ARG:O	1:B:1470:ARG:HB3	2.11	0.50
1:B:1457:VAL:CG2	1:B:1473:LEU:HD22	2.33	0.50
1:B:1554:ALA:HB2	1:B:1882:PRO:HG3	1.93	0.50
1:A:321:LEU:CD2	1:A:381:LEU:HD13	2.41	0.50
1:A:1223:ALA:HB1	1:A:1224:PRO:HD2	1.93	0.50
1:B:416:GLN:NE2	1:B:422:ARG:HH22	2.09	0.50
1:B:642:CYS:O	1:B:649:VAL:HG13	2.11	0.50
1:B:883:ARG:HE	1:B:1107:ARG:HD3	1.76	0.50
1:B:982:THR:C	1:B:984:GLU:N	2.68	0.50
1:B:1560:GLN:HA	1:B:1563:LEU:CB	2.41	0.50
1:B:1651:VAL:HG23	1:B:1851:LYS:NZ	2.26	0.50
1:A:165:LEU:HD22	1:A:392:SER:HB2	1.93	0.50
1:A:1314:LEU:HG	1:A:1315:LEU:N	2.25	0.50
1:A:1470:ARG:HD3	1:A:1472:VAL:CG2	2.41	0.50
1:A:1861:GLN:O	1:A:1865:PRO:HG3	2.11	0.50
1:B:36:ASP:HB3	1:B:38:ARG:CG	2.40	0.50
1:B:1674:HIS:HE1	1:B:1756:SER:OG	1.94	0.50
1:A:200:PHE:CD2	1:B:132:MET:HE1	2.46	0.50
1:A:1606:ARG:HH21	1:A:1860:GLU:CG	2.23	0.50
1:A:2070:LEU:HD11	1:A:2076:ASN:CG	2.36	0.50
1:B:309:VAL:HG22	1:B:374:LEU:HD11	1.94	0.50
1:B:431:LEU:C	1:B:431:LEU:HD23	2.36	0.50
1:B:687:MET:HE2	1:B:687:MET:HA	1.93	0.50
1:B:972:THR:HG22	1:B:1081:VAL:HG21	1.92	0.50
1:B:976:VAL:O	1:B:977:ASP:C	2.54	0.50
1:B:988:SER:O	1:B:989:GLN:C	2.54	0.50
1:A:776:GLU:HB3	1:A:778:SER:OG	2.12	0.50
1:A:1422:SER:O	1:A:1423:PHE:HB2	2.11	0.50
1:A:1996:TYR:HD1	1:A:2040:ALA:CB	2.24	0.50
1:B:236:LYS:C	1:B:238:LEU:H	2.20	0.50
1:B:925:LEU:HD22	1:B:931:VAL:HG21	1.94	0.50
1:B:995:ASP:O	1:B:998:LEU:HB2	2.10	0.50
1:A:59:ARG:N	1:A:59:ARG:HD2	2.26	0.50
1:A:495:ILE:CD1	1:A:578:ILE:HB	2.41	0.50
1:B:225:ALA:O	1:B:332:PRO:HA	2.12	0.50
1:B:579:GLY:O	1:B:715:THR:HG21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD22	1:A:224:ARG:NH1	2.27	0.50
1:A:256:SER:HB3	1:B:146:PHE:O	2.12	0.50
1:A:269:GLN:O	1:A:273:ILE:HG13	2.11	0.50
1:A:287:LEU:HA	1:A:387:ASN:O	2.12	0.50
1:A:384:ARG:HG3	1:A:384:ARG:NH1	2.17	0.50
1:A:963:GLU:C	1:A:965:PRO:HD3	2.37	0.50
1:A:1657:TYR:CZ	1:A:1662:ARG:HD2	2.47	0.50
1:B:420:LEU:HG	1:B:793:LEU:HD21	1.94	0.50
1:B:1024:TRP:HB2	1:B:1068:LEU:HD11	1.94	0.50
1:A:96:ASN:ND2	1:A:98:ALA:HB3	2.18	0.50
1:A:241:ARG:NH2	1:A:827:THR:O	2.45	0.50
1:A:290:ILE:HD13	1:A:308:ILE:HD13	1.94	0.50
1:A:946:VAL:O	1:A:954:ILE:HB	2.12	0.50
1:A:1064:HIS:HB2	1:A:1093:GLY:HA3	1.94	0.50
1:A:1241:LYS:HA	1:A:1269:ASP:HB3	1.93	0.50
1:B:136:GLN:NE2	1:B:138:ALA:H	2.10	0.50
1:B:965:PRO:O	1:B:967:PRO:HD3	2.12	0.50
1:B:1981:GLU:HG3	1:B:1982:ASN:OD1	2.12	0.50
1:B:2001:ASN:O	1:B:2005:VAL:HG23	2.10	0.50
1:A:94:GLY:HA3	1:A:453:MET:HE3	1.94	0.50
1:A:621:ALA:O	1:A:650:THR:HG23	2.12	0.50
1:A:1229:CYS:HB3	1:A:1403:LEU:HD22	1.94	0.50
1:A:1629:LEU:O	1:A:1630:GLN:C	2.55	0.50
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.94	0.49
1:A:1231:ASP:O	1:A:1232:THR:C	2.55	0.49
1:B:169:GLN:HE21	1:B:169:GLN:C	2.19	0.49
1:B:366:ILE:HD11	1:B:369:LEU:HD11	1.94	0.49
1:B:638:ILE:HG22	1:B:638:ILE:O	2.11	0.49
1:A:75:MET:HE3	1:A:80:ARG:HG2	1.93	0.49
1:A:668:GLU:O	1:A:669:ASP:HB3	2.11	0.49
1:A:1461:ARG:O	1:A:1461:ARG:HG3	2.12	0.49
1:A:2006:THR:CG2	1:A:2048:ARG:HH22	2.25	0.49
1:B:734:TYR:C	1:B:734:TYR:CD2	2.89	0.49
1:B:1459:CYS:CB	1:B:2032:ALA:HA	2.43	0.49
1:B:1858:GLU:HG3	1:B:1859:GLU:N	2.26	0.49
1:A:1533:VAL:HG23	1:A:1545:ARG:O	2.12	0.49
1:B:295:THR:HG22	1:B:331:HIS:HD2	1.77	0.49
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.94	0.49
1:B:475:GLY:C	1:B:477:ALA:H	2.20	0.49
1:B:706:LYS:HD2	1:B:706:LYS:N	2.27	0.49
1:B:866:VAL:HG13	1:B:876:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1429:LEU:CD1	1:B:1443:LEU:HD11	2.42	0.49
1:A:554:VAL:O	1:A:558:SER:HB2	2.13	0.49
1:A:853:GLY:O	1:A:854:SER:HB2	2.12	0.49
1:A:1130:LEU:HD22	1:A:1133:ASN:ND2	2.28	0.49
1:A:2017:VAL:HG21	1:A:2099:LEU:HD21	1.93	0.49
1:B:82:LEU:HG	1:B:144:LEU:CD1	2.42	0.49
1:B:554:VAL:O	1:B:558:SER:HB2	2.12	0.49
1:B:1312:ALA:HB1	1:B:1337:THR:O	2.12	0.49
1:B:1423:PHE:O	1:B:1985:PRO:HB3	2.12	0.49
1:B:1449:SER:C	1:B:1477:LEU:HD22	2.37	0.49
1:B:1454:VAL:HG13	1:B:1503:MET:HE1	1.93	0.49
1:B:2036:PHE:CD2	1:B:2036:PHE:C	2.91	0.49
1:A:1483:ALA:N	1:A:1484:PRO:HD3	2.27	0.49
1:A:1780:LEU:HD12	1:A:1781:GLY:H	1.78	0.49
1:A:1874:THR:O	1:A:1874:THR:HG22	2.11	0.49
1:B:527:LEU:HD12	1:B:534:VAL:CG2	2.43	0.49
1:B:1328:ALA:HB2	1:B:1381:LEU:HD11	1.94	0.49
1:B:1887:TYR:CD2	1:B:1967:GLY:HA3	2.44	0.49
1:A:595:THR:HG21	1:A:597:GLU:HG2	1.94	0.49
1:B:60:PHE:CD2	1:B:80:ARG:HD3	2.48	0.49
1:A:118:GLU:HG3	1:B:118:GLU:CD	2.37	0.49
1:A:309:VAL:HG22	1:A:374:LEU:HD11	1.95	0.49
1:A:416:GLN:NE2	1:A:422:ARG:HH22	2.10	0.49
1:A:1345:LEU:O	1:A:1346:LEU:HD23	2.13	0.49
1:A:1390:VAL:HG13	1:A:1501:LEU:CD2	2.42	0.49
1:A:1766:PHE:HD2	1:A:1791:PHE:CE1	2.30	0.49
1:B:831:SER:OG	1:B:832:PRO:HD3	2.13	0.49
1:B:1032:LEU:O	1:B:1035:MET:HB2	2.13	0.49
1:B:1106:ARG:O	1:B:1108:PRO:HD3	2.13	0.49
1:B:1893:LEU:HB3	1:B:1925:GLN:CD	2.38	0.49
1:A:166:LEU:HD23	1:A:166:LEU:C	2.38	0.49
1:B:1460:LEU:HD11	1:B:1980:LEU:HD13	1.95	0.49
1:B:1567:TYR:C	1:B:1856:VAL:HG23	2.37	0.49
1:B:1882:PRO:HG2	1:B:1885:LYS:HD2	1.95	0.49
1:B:1974:VAL:HG23	1:B:1974:VAL:O	2.13	0.49
1:A:635:PRO:HD3	1:A:661:PHE:CE2	2.48	0.49
1:A:1050:LEU:O	1:A:1101:SER:CB	2.60	0.49
1:B:491:PRO:HD2	1:B:756:ALA:HA	1.95	0.49
1:B:605:TRP:O	1:B:606:ARG:C	2.56	0.49
1:B:913:VAL:HG22	1:B:1058:ARG:HG2	1.95	0.49
1:B:1244:VAL:HB	1:B:1272:TYR:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1532:PHE:CD2	1:B:1549:SER:HA	2.45	0.49
1:A:136:GLN:NE2	1:A:138:ALA:H	2.10	0.49
1:A:156:THR:OG1	1:B:158:ASP:O	2.31	0.49
1:A:527:LEU:HD12	1:A:534:VAL:CG2	2.43	0.49
1:A:1245:VAL:HG13	1:A:1273:THR:CB	2.38	0.49
1:B:305:LEU:O	1:B:309:VAL:HG23	2.13	0.49
1:B:384:ARG:CG	1:B:384:ARG:NH1	2.74	0.49
1:B:416:GLN:C	1:B:418:ALA:N	2.70	0.49
1:B:717:ILE:HD13	1:B:727:ALA:HB2	1.95	0.49
1:B:1430:LYS:HE3	1:B:1981:GLU:CA	2.42	0.49
1:B:1603:PHE:CD2	1:B:1603:PHE:N	2.80	0.49
1:B:2070:LEU:HD11	1:B:2076:ASN:CG	2.37	0.49
1:A:309:VAL:C	1:A:311:ALA:H	2.21	0.48
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.95	0.48
1:A:2036:PHE:C	1:A:2036:PHE:CD2	2.90	0.48
1:B:963:GLU:C	1:B:965:PRO:HD3	2.38	0.48
1:A:82:LEU:HG	1:A:144:LEU:CD1	2.44	0.48
1:A:359:TYR:OH	1:A:369:LEU:HD22	2.12	0.48
1:A:1405:ARG:HH22	1:A:1470:ARG:NH2	2.11	0.48
1:A:1470:ARG:O	1:A:1470:ARG:CG	2.61	0.48
1:A:1528:THR:HG23	1:A:1552:HIS:ND1	2.28	0.48
1:A:1541:LEU:N	1:A:1541:LEU:HD23	2.29	0.48
1:A:1593:LEU:HD23	1:A:1594:THR:HG22	1.95	0.48
1:A:1666:GLN:HG2	1:A:1667:PRO:HD2	1.94	0.48
1:B:78:GLN:HB3	1:B:188:LEU:HD13	1.95	0.48
1:B:287:LEU:HA	1:B:387:ASN:O	2.13	0.48
1:B:1086:LEU:HD23	1:B:1086:LEU:N	2.27	0.48
1:B:1551:LEU:HD21	1:B:1627:LEU:HD21	1.95	0.48
1:B:1653:THR:HG22	1:B:1810:VAL:CG1	2.40	0.48
1:B:1996:TYR:HD1	1:B:2040:ALA:CB	2.25	0.48
1:A:120:LEU:C	1:A:127:LEU:HD13	2.38	0.48
1:A:130:TYR:CA	1:B:203:LEU:HD21	2.43	0.48
1:A:377:VAL:HG13	1:A:381:LEU:CD1	2.44	0.48
1:A:782:ILE:CD1	1:A:803:LEU:HD23	2.43	0.48
1:A:1452:GLY:HA2	1:A:2039:SER:HB3	1.96	0.48
1:A:1523:ARG:HH12	1:A:1536:LEU:HD12	1.78	0.48
1:A:1786:LEU:C	1:A:1788:ASN:H	2.21	0.48
1:B:111:VAL:HG23	1:B:188:LEU:HB2	1.94	0.48
1:B:290:ILE:HD13	1:B:308:ILE:HD13	1.96	0.48
1:B:1428:SER:O	1:B:1432:ILE:HG13	2.13	0.48
1:B:1672:LEU:HB3	1:B:1744:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1899:GLN:HG2	1:B:2088:ILE:HG21	1.94	0.48
1:A:856:CYS:C	1:A:858:SER:N	2.72	0.48
1:A:1609:SER:C	1:A:1611:ARG:H	2.21	0.48
1:A:1670:SER:O	1:A:1742:ASP:HB2	2.13	0.48
1:A:2056:LEU:HA	1:A:2104:PRO:O	2.13	0.48
1:B:39:ARG:NH1	1:B:57:LEU:HD22	2.28	0.48
1:B:191:LEU:HD22	1:B:224:ARG:NH1	2.29	0.48
1:B:236:LYS:HG3	1:B:237:SER:N	2.27	0.48
1:B:1083:ASP:O	1:B:1086:LEU:N	2.46	0.48
1:A:27:ILE:C	1:A:29:GLY:H	2.20	0.48
1:A:48:PRO:HD3	1:A:201:MET:HE3	1.95	0.48
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.94	0.48
1:A:470:TYR:CD1	1:A:470:TYR:C	2.90	0.48
1:A:856:CYS:HB3	1:B:856:CYS:SG	2.54	0.48
1:A:902:ALA:HB1	1:A:939:GLU:OE2	2.14	0.48
1:A:913:VAL:HG22	1:A:1058:ARG:HG2	1.95	0.48
1:A:914:PHE:O	1:A:915:GLU:HG3	2.14	0.48
1:A:1024:TRP:HB2	1:A:1068:LEU:HD11	1.96	0.48
1:A:1418:VAL:HG22	1:A:1425:TRP:CD2	2.49	0.48
1:A:1666:GLN:O	1:A:1669:GLU:HB2	2.13	0.48
1:B:1001:TYR:HB3	1:B:1003:TYR:CD1	2.48	0.48
1:A:215:PHE:O	1:A:363:ASN:HB2	2.14	0.48
1:A:259:GLN:CD	1:A:259:GLN:H	2.20	0.48
1:A:541:THR:HA	1:A:545:VAL:HG11	1.95	0.48
1:A:2070:LEU:HD11	1:A:2076:ASN:ND2	2.28	0.48
1:B:48:PRO:HD3	1:B:201:MET:HE3	1.96	0.48
1:B:133:ILE:HD12	1:B:143:ARG:HH21	1.79	0.48
1:B:782:ILE:CD1	1:B:803:LEU:HD23	2.43	0.48
1:B:948:ASP:C	1:B:948:ASP:OD1	2.57	0.48
1:A:183:ALA:O	1:A:232:LEU:HD12	2.14	0.48
1:A:261:VAL:HG22	1:B:146:PHE:CE1	2.48	0.48
1:A:542:ASP:C	1:A:542:ASP:OD1	2.56	0.48
1:A:830:ILE:O	1:A:831:SER:C	2.56	0.48
1:A:1036:LEU:O	1:A:1037:HIS:C	2.57	0.48
1:A:1519:LEU:HD12	1:A:1520:GLU:H	1.78	0.48
1:A:1573:PHE:HD1	1:A:1843:MET:HE2	1.79	0.48
1:B:132:MET:HE2	1:B:132:MET:HB3	1.62	0.48
1:B:504:GLN:N	1:B:546:LEU:HD11	2.28	0.48
1:B:988:SER:O	1:B:991:ASP:N	2.47	0.48
1:B:2098:PHE:CD2	1:B:2106:LEU:HD12	2.48	0.48
1:A:225:ALA:O	1:A:332:PRO:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLY:O	1:A:477:ALA:N	2.45	0.48
1:A:861:VAL:HG22	1:A:934:GLU:CB	2.39	0.48
1:A:1432:ILE:O	1:A:1432:ILE:HG22	2.14	0.48
1:B:259:GLN:CD	1:B:259:GLN:N	2.72	0.48
1:B:1302:ALA:HB3	1:B:1304:PRO:CD	2.44	0.48
1:B:1442:TRP:CZ3	1:B:1472:VAL:HG11	2.48	0.48
1:B:1898:LEU:HD23	1:B:1898:LEU:HA	1.70	0.48
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.95	0.48
1:A:1457:VAL:HG11	1:A:1473:LEU:HD22	1.96	0.48
1:B:51:MET:HE3	1:B:191:LEU:HD13	1.95	0.48
1:B:309:VAL:C	1:B:311:ALA:H	2.22	0.48
1:B:321:LEU:HD12	1:B:321:LEU:N	2.28	0.48
1:B:902:ALA:HB1	1:B:939:GLU:OE2	2.13	0.48
1:B:1882:PRO:HD2	1:B:1887:TYR:OH	2.13	0.48
1:A:423:LEU:HB2	1:A:797:LEU:HD22	1.96	0.48
1:A:506:MET:HB3	1:A:559:ILE:CD1	2.44	0.48
1:A:642:CYS:CB	1:A:650:THR:HB	2.29	0.48
1:A:1016:GLU:HA	1:A:1043:PRO:HG3	1.96	0.48
1:A:1106:ARG:O	1:A:1108:PRO:HD3	2.13	0.48
1:A:1315:LEU:HB3	1:A:1344:LEU:HD13	1.96	0.48
1:A:1536:LEU:HB2	1:A:1543:SER:HB3	1.95	0.48
1:A:1567:TYR:HA	1:A:1857:ARG:HB2	1.96	0.48
1:B:81:MET:O	1:B:85:VAL:HG22	2.14	0.48
1:B:94:GLY:HA3	1:B:453:MET:HE3	1.95	0.48
1:B:1124:HIS:CD2	1:B:1512:GLY:HA2	2.48	0.48
1:B:1248:LEU:HD21	1:B:1277:ARG:HH21	1.79	0.48
1:B:1554:ALA:HB3	1:B:1882:PRO:HB3	1.96	0.48
1:B:1912:LEU:HB2	1:B:1939:VAL:HG22	1.96	0.48
1:B:283:ASP:C	1:B:285:GLU:H	2.22	0.47
1:B:639:VAL:HG12	1:B:640:PRO:O	2.14	0.47
1:B:1995:LYS:HB3	1:B:2041:MET:SD	2.54	0.47
1:A:1476:ASN:O	1:A:1477:LEU:HD23	2.14	0.47
1:A:1647:SER:O	1:A:1651:VAL:CG2	2.61	0.47
1:A:1729:GLU:OE1	1:A:1758:ARG:HD2	2.14	0.47
1:A:1886:SER:HA	1:A:1911:LYS:HB2	1.95	0.47
1:B:621:ALA:O	1:B:623:VAL:HG23	2.14	0.47
1:B:1236:ASN:HA	1:B:1502:VAL:HG21	1.95	0.47
1:B:1995:LYS:O	1:B:2041:MET:HE3	2.13	0.47
1:A:217:ALA:C	1:A:219:GLY:H	2.21	0.47
1:B:470:TYR:C	1:B:470:TYR:CD1	2.92	0.47
1:A:139:MET:HE1	1:B:396:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:PRO:HB3	1:A:1510:ALA:HB1	1.95	0.47
1:B:178:GLY:O	1:B:179:GLU:C	2.58	0.47
1:B:1085:ASN:C	1:B:1086:LEU:HD23	2.40	0.47
1:B:1656:TYR:CZ	1:B:1687:ILE:HD13	2.49	0.47
1:A:1556:PRO:O	1:A:1558:SER:N	2.47	0.47
1:A:1894:GLY:O	1:A:1895:GLY:C	2.57	0.47
1:A:1912:LEU:HB2	1:A:1939:VAL:HG22	1.95	0.47
1:A:2098:PHE:CD2	1:A:2106:LEU:HB2	2.48	0.47
1:B:51:MET:HB2	1:B:53:LYS:HE3	1.95	0.47
1:B:557:THR:HG21	1:B:603:SER:OG	2.14	0.47
1:A:262:THR:O	1:A:262:THR:CG2	2.63	0.47
1:A:662:LEU:C	1:A:664:GLN:N	2.71	0.47
1:A:1544:ILE:O	1:A:1545:ARG:HG3	2.15	0.47
1:B:27:ILE:C	1:B:29:GLY:H	2.21	0.47
1:B:321:LEU:HD23	1:B:381:LEU:HD12	1.95	0.47
1:B:326:LYS:CE	1:B:336:SER:HB2	2.44	0.47
1:B:525:GLN:NE2	1:B:525:GLN:HA	2.30	0.47
1:B:972:THR:HG22	1:B:1081:VAL:HG23	1.97	0.47
1:B:1486:MET:SD	1:B:1506:TYR:CD1	3.08	0.47
1:B:1983:GLN:HG2	1:B:1988:PHE:HE1	1.78	0.47
1:B:2022:VAL:O	1:B:2022:VAL:CG1	2.62	0.47
1:A:9:MET:HE3	1:A:345:LEU:HD12	1.96	0.47
1:A:107:VAL:HG13	1:A:184:VAL:HB	1.96	0.47
1:A:111:VAL:HG23	1:A:188:LEU:HB2	1.97	0.47
1:A:289:TYR:C	1:A:289:TYR:CD2	2.93	0.47
1:A:432:GLU:HG3	1:A:433:ALA:N	2.29	0.47
1:A:503:TRP:CG	1:A:787:LYS:HB2	2.50	0.47
1:A:988:SER:O	1:A:989:GLN:C	2.56	0.47
1:A:1774:LEU:O	1:B:1783:ALA:HB2	2.14	0.47
1:A:2001:ASN:O	1:A:2005:VAL:HG23	2.14	0.47
1:B:359:TYR:CD2	1:B:376:VAL:HG11	2.50	0.47
1:B:685:TYR:CD1	1:B:686:PHE:N	2.83	0.47
1:B:1003:TYR:CE2	1:B:1037:HIS:CE1	2.92	0.47
1:B:1050:LEU:O	1:B:1101:SER:CB	2.63	0.47
1:B:1333:ASN:C	1:B:1335:ALA:N	2.72	0.47
1:B:1418:VAL:HG22	1:B:1425:TRP:CG	2.50	0.47
1:B:2006:THR:HG21	1:B:2048:ARG:NH2	2.29	0.47
1:B:2017:VAL:HG21	1:B:2099:LEU:HD21	1.97	0.47
1:A:618:GLY:N	1:A:679:GLY:O	2.47	0.47
1:A:838:HIS:O	1:A:840:GLN:N	2.48	0.47
1:A:1433:LEU:HD11	1:A:1465:GLY:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1592:TRP:HB2	1:A:1595:ARG:HD3	1.97	0.47
1:B:59:ARG:N	1:B:59:ARG:HD2	2.29	0.47
1:B:128:VAL:CG1	1:B:130:TYR:CZ	2.98	0.47
1:B:670:VAL:HG12	1:B:671:PHE:H	1.79	0.47
1:B:796:PHE:O	1:B:800:VAL:HG23	2.14	0.47
1:B:1665:MET:HE1	1:B:1688:ALA:HA	1.97	0.47
1:A:261:VAL:HG22	1:B:146:PHE:CZ	2.50	0.47
1:A:1416:LEU:HD23	1:A:1429:LEU:HG	1.96	0.47
1:A:1636:VAL:HA	1:A:1637:PRO:HD3	1.73	0.47
1:A:1669:GLU:HG2	1:A:1742:ASP:CB	2.45	0.47
1:A:1711:ARG:HH22	1:A:1826:LEU:CD2	2.28	0.47
1:B:9:MET:HE3	1:B:345:LEU:HD12	1.97	0.47
1:B:94:GLY:CA	1:B:453:MET:HE3	2.45	0.47
1:B:610:ILE:HA	1:B:690:ILE:HD13	1.96	0.47
1:B:1411:ASP:HB2	1:B:1440:PRO:HG3	1.95	0.47
1:B:1656:TYR:CD2	1:B:1813:LEU:HB3	2.49	0.47
1:B:1725:ASP:OD2	1:B:1727:SER:HB3	2.15	0.47
1:B:1733:LEU:HD23	1:B:1733:LEU:HA	1.70	0.47
1:B:1984:THR:C	1:B:1986:GLU:H	2.22	0.47
1:A:866:VAL:HG13	1:A:876:VAL:HG22	1.97	0.47
1:A:976:VAL:HG22	1:A:977:ASP:N	2.18	0.47
1:A:1107:ARG:HG3	1:A:1107:ARG:O	2.15	0.47
1:A:1130:LEU:HD11	1:A:1221:LEU:CD1	2.44	0.47
1:A:1239:SER:C	1:A:1241:LYS:H	2.23	0.47
1:A:1248:LEU:HD21	1:A:1277:ARG:NH2	2.30	0.47
1:A:1553:TYR:O	1:A:1554:ALA:HB2	2.15	0.47
1:A:1748:LEU:HD23	1:A:1748:LEU:HA	1.69	0.47
1:B:100:LEU:O	1:B:103:THR:OG1	2.20	0.47
1:B:983:ALA:O	1:B:985:PHE:N	2.43	0.47
1:B:1129:CYS:O	1:B:1130:LEU:HB2	2.14	0.47
1:B:1239:SER:OG	1:B:1241:LYS:HG2	2.15	0.47
1:B:1303:ASN:HA	1:B:1333:ASN:HB2	1.96	0.47
1:B:1443:LEU:O	1:B:1473:LEU:HA	2.15	0.47
1:B:1486:MET:HE1	1:B:1506:TYR:CG	2.50	0.47
1:B:1729:GLU:OE1	1:B:1758:ARG:HD2	2.15	0.47
1:A:65:PHE:CE2	1:A:83:LEU:HB3	2.49	0.46
1:A:283:ASP:C	1:A:285:GLU:H	2.23	0.46
1:A:1460:LEU:HD12	1:A:1463:GLU:OE1	2.15	0.46
1:A:1656:TYR:O	1:A:1657:TYR:C	2.54	0.46
1:A:2098:PHE:CD2	1:A:2106:LEU:HD12	2.50	0.46
1:B:776:GLU:HB3	1:B:778:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1275:THR:HG21	1:B:1299:TRP:HB2	1.96	0.46
1:B:1390:VAL:HG13	1:B:1501:LEU:CD2	2.45	0.46
1:B:1456:MET:HE3	1:B:2032:ALA:O	2.15	0.46
1:A:92:ASP:HA	1:A:830:ILE:HB	1.97	0.46
1:A:111:VAL:HG21	1:A:188:LEU:HD12	1.98	0.46
1:A:178:GLY:O	1:A:179:GLU:C	2.57	0.46
1:A:1862:GLY:O	1:A:1863:PRO:C	2.59	0.46
1:B:112:SER:O	1:B:137:ARG:NH2	2.48	0.46
1:B:147:PHE:C	1:B:147:PHE:CD2	2.93	0.46
1:B:668:GLU:O	1:B:669:ASP:CB	2.62	0.46
1:B:1303:ASN:C	1:B:1333:ASN:HB2	2.41	0.46
1:B:1411:ASP:HB2	1:B:1440:PRO:CG	2.44	0.46
1:B:2031:GLN:HB3	1:B:2034:TYR:HB3	1.98	0.46
1:A:249:ALA:HB2	1:A:402:VAL:HB	1.97	0.46
1:A:253:THR:O	1:A:254:ASP:C	2.59	0.46
1:A:269:GLN:OE1	1:A:393:PHE:CE2	2.68	0.46
1:A:483:GLN:HG2	1:A:484:GLN:N	2.30	0.46
1:A:831:SER:N	1:A:832:PRO:CD	2.79	0.46
1:A:1234:LEU:HD12	1:A:1234:LEU:O	2.16	0.46
1:A:1480:THR:HB	1:A:1482:PRO:HD2	1.97	0.46
1:A:1573:PHE:O	1:A:1576:VAL:HB	2.15	0.46
1:A:1999:THR:HG22	1:A:2044:ILE:HD12	1.98	0.46
1:B:39:ARG:NH1	1:B:226:GLU:OE2	2.47	0.46
1:B:384:ARG:HG3	1:B:384:ARG:NH1	2.16	0.46
1:B:577:ILE:HG22	1:B:712:TRP:CD1	2.50	0.46
1:A:60:PHE:CD2	1:A:80:ARG:HD3	2.50	0.46
1:A:1226:LEU:CD2	1:A:1401:LEU:HD21	2.43	0.46
1:B:743:VAL:HG23	1:B:743:VAL:O	2.15	0.46
1:B:979:ALA:O	1:B:980:ASP:C	2.58	0.46
1:B:1119:PHE:HB3	1:B:2105:VAL:HB	1.98	0.46
1:A:259:GLN:CD	1:A:259:GLN:N	2.74	0.46
1:A:749:LEU:HD11	1:A:771:LEU:HD23	1.96	0.46
1:A:925:LEU:HD22	1:A:931:VAL:HG21	1.97	0.46
1:A:1231:ASP:O	1:A:1234:LEU:N	2.47	0.46
1:A:1414:VAL:HG11	1:A:1432:ILE:HD13	1.96	0.46
1:A:1734:ARG:C	1:A:1736:THR:N	2.72	0.46
1:A:2098:PHE:CE2	1:A:2106:LEU:CB	2.98	0.46
1:B:65:PHE:HA	1:B:147:PHE:CE1	2.50	0.46
1:B:359:TYR:CG	1:B:376:VAL:HG11	2.50	0.46
1:B:830:ILE:O	1:B:831:SER:C	2.59	0.46
1:B:1016:GLU:HA	1:B:1043:PRO:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1220:LEU:HB3	1:B:1257:ARG:NH2	2.30	0.46
1:B:2098:PHE:CE2	1:B:2106:LEU:CB	2.98	0.46
1:A:1262:LEU:HB3	1:A:1268:MET:SD	2.56	0.46
1:A:1602:GLU:OE2	1:A:1650:ILE:N	2.49	0.46
1:B:107:VAL:HG13	1:B:184:VAL:HB	1.96	0.46
1:B:765:ALA:HB1	1:B:768:GLN:CG	2.46	0.46
1:B:1443:LEU:HD23	1:B:1443:LEU:HA	1.78	0.46
1:B:1586:ASP:HA	1:B:1595:ARG:HH12	1.81	0.46
1:A:630:CYS:C	1:A:632:GLN:N	2.73	0.46
1:A:717:ILE:HD13	1:A:727:ALA:HB2	1.97	0.46
1:A:1220:LEU:HB3	1:A:1257:ARG:NH2	2.31	0.46
1:A:1343:PHE:C	1:A:1344:LEU:HD22	2.41	0.46
1:A:1418:VAL:HG22	1:A:1425:TRP:CG	2.51	0.46
1:B:377:VAL:HG13	1:B:381:LEU:CD1	2.46	0.46
1:B:1254:LEU:HD13	1:B:1316:VAL:HG12	1.98	0.46
1:B:1338:LEU:CD2	1:B:1406:GLN:HG3	2.46	0.46
1:B:1531:ALA:HA	1:B:1549:SER:H	1.81	0.46
1:B:1617:VAL:HG21	1:B:1626:VAL:CG1	2.46	0.46
1:A:1532:PHE:HE1	1:A:1597:CYS:HB3	1.81	0.46
1:A:1676:GLY:HA2	1:A:1681:GLY:HA3	1.98	0.46
1:A:1689:LEU:O	1:A:1692:GLY:HA2	2.16	0.46
1:A:1725:ASP:OD2	1:A:1727:SER:HB3	2.15	0.46
1:B:657:ALA:O	1:B:661:PHE:HB2	2.16	0.46
1:B:1239:SER:HA	1:B:1240:PRO:HD3	1.85	0.46
1:B:1651:VAL:HG13	1:B:1680:VAL:CA	2.31	0.46
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.50	0.46
1:A:706:LYS:N	1:A:706:LYS:HD2	2.31	0.46
1:A:1222:ASP:HA	1:A:1226:LEU:HD11	1.96	0.46
1:A:1347:HIS:HD2	1:A:1348:THR:O	1.99	0.46
1:A:1472:VAL:CG1	1:A:1473:LEU:H	2.25	0.46
1:A:1528:THR:CG2	1:A:1530:HIS:H	2.22	0.46
1:B:1469:ILE:O	1:B:1469:ILE:CG2	2.64	0.46
1:A:147:PHE:CD2	1:A:147:PHE:C	2.94	0.46
1:A:203:LEU:HD21	1:B:130:TYR:HA	1.98	0.46
1:A:1345:LEU:HD12	1:A:1402:PHE:O	2.16	0.46
1:A:1481:SER:N	1:A:1482:PRO:CD	2.79	0.46
1:B:81:MET:HG2	1:B:81:MET:H	1.62	0.46
1:A:33:VAL:HB	1:A:50:ARG:NH1	2.32	0.45
1:A:491:PRO:HD2	1:A:756:ALA:HA	1.97	0.45
1:A:965:PRO:O	1:A:967:PRO:HD3	2.16	0.45
1:A:1257:ARG:O	1:A:1260:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:CYS:C	1:A:1450:THR:N	2.74	0.45
1:A:1893:LEU:HB3	1:A:1925:GLN:CD	2.41	0.45
1:A:2084:LEU:HD12	1:A:2111:LEU:O	2.15	0.45
1:B:420:LEU:CD1	1:B:512:ARG:HD2	2.46	0.45
1:B:1338:LEU:HD22	1:B:1406:GLN:NE2	2.31	0.45
1:B:1432:ILE:O	1:B:1432:ILE:HG22	2.16	0.45
1:B:1577:MET:HE2	1:B:1577:MET:HB3	1.90	0.45
1:B:1931:GLU:O	1:B:1933:ARG:N	2.50	0.45
1:A:65:PHE:HA	1:A:147:PHE:CE1	2.51	0.45
1:A:72:ALA:HB3	1:A:842:TRP:CZ3	2.51	0.45
1:A:300:GLY:O	1:A:301:ASP:C	2.59	0.45
1:A:856:CYS:O	1:A:858:SER:N	2.46	0.45
1:A:1390:VAL:HG13	1:A:1501:LEU:HD21	1.98	0.45
1:B:269:GLN:OE1	1:B:393:PHE:CE2	2.69	0.45
1:B:460:VAL:CG2	1:B:465:MET:HG3	2.46	0.45
1:B:501:ALA:HA	1:B:766:LEU:HD11	1.98	0.45
1:B:1064:HIS:HB2	1:B:1093:GLY:HA3	1.97	0.45
1:B:1420:ASP:O	1:B:1425:TRP:CH2	2.70	0.45
1:B:1603:PHE:N	1:B:1603:PHE:HD2	2.15	0.45
1:B:1754:GLN:OE1	1:B:1754:GLN:HA	2.16	0.45
1:B:1886:SER:HA	1:B:1911:LYS:HB2	1.97	0.45
1:A:23:TRP:NE1	1:A:350:HIS:CD2	2.84	0.45
1:A:133:ILE:HD12	1:A:143:ARG:HH21	1.80	0.45
1:A:142:ASN:HD22	1:B:396:GLY:HA3	1.81	0.45
1:A:948:ASP:C	1:A:948:ASP:OD1	2.58	0.45
1:A:1112:LEU:HD22	1:A:2110:VAL:HG11	1.98	0.45
1:A:1428:SER:O	1:A:1432:ILE:HG13	2.15	0.45
1:A:1456:MET:HE3	1:A:2032:ALA:HB1	1.97	0.45
1:A:1476:ASN:HB3	1:A:1486:MET:SD	2.56	0.45
1:A:1953:ARG:O	1:A:1957:THR:HB	2.16	0.45
1:B:635:PRO:O	1:B:637:GLY:N	2.50	0.45
1:B:979:ALA:HB1	1:B:983:ALA:HB3	1.98	0.45
1:B:1418:VAL:HA	1:B:1425:TRP:CE3	2.51	0.45
1:B:1527:GLN:OE1	1:B:1872:ALA:HB1	2.15	0.45
1:A:557:THR:HG21	1:A:603:SER:OG	2.16	0.45
1:A:1124:HIS:NE2	1:A:1501:LEU:HD13	2.31	0.45
1:A:1254:LEU:HD21	1:A:1318:ASN:HB2	1.98	0.45
1:A:1466:GLY:O	1:A:1469:ILE:HB	2.17	0.45
1:A:1624:THR:HG22	1:A:1857:ARG:HH21	1.82	0.45
1:A:1857:ARG:NH1	1:A:1869:PRO:HB3	2.30	0.45
1:B:65:PHE:CE2	1:B:83:LEU:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:O	1:B:123:ASP:C	2.58	0.45
1:B:253:THR:O	1:B:254:ASP:C	2.59	0.45
1:B:1095:LEU:HD12	1:B:1095:LEU:O	2.16	0.45
1:B:1643:GLU:O	1:B:1644:GLU:C	2.60	0.45
1:B:1977:ASP:OD1	1:B:2031:GLN:HG2	2.15	0.45
1:A:618:GLY:O	1:A:679:GLY:O	2.34	0.45
1:A:1780:LEU:HD12	1:A:1781:GLY:N	2.32	0.45
1:A:1802:GLU:O	1:A:1802:GLU:HG2	2.17	0.45
1:B:94:GLY:N	1:B:453:MET:HE3	2.31	0.45
1:B:621:ALA:HB3	1:B:658:MET:HE3	1.99	0.45
1:B:623:VAL:HG13	1:B:672:VAL:HG22	1.97	0.45
1:B:635:PRO:O	1:B:636:PRO:C	2.59	0.45
1:B:1107:ARG:HG3	1:B:1107:ARG:O	2.17	0.45
1:B:1456:MET:CE	1:B:2032:ALA:HB1	2.46	0.45
1:B:1706:ALA:O	1:B:1707:TYR:C	2.59	0.45
1:B:1748:LEU:HD23	1:B:1748:LEU:HA	1.66	0.45
1:B:1953:ARG:HA	1:B:2005:VAL:HG11	1.98	0.45
1:B:1953:ARG:O	1:B:1957:THR:HB	2.16	0.45
1:A:493:TRP:CD2	1:A:752:VAL:HG22	2.52	0.45
1:A:1545:ARG:NH1	1:A:1545:ARG:CG	2.76	0.45
1:A:1694:ARG:NH2	1:A:1735:HIS:HB3	2.31	0.45
1:A:2022:VAL:O	1:A:2022:VAL:CG1	2.64	0.45
1:B:1248:LEU:CD2	1:B:1277:ARG:HE	2.30	0.45
1:B:1629:LEU:HB3	1:B:1631:HIS:CE1	2.51	0.45
1:B:1904:LEU:HD23	1:B:1904:LEU:HA	1.62	0.45
1:B:1931:GLU:O	1:B:1934:ARG:N	2.50	0.45
1:A:124:PRO:HB2	1:B:45:TYR:CE2	2.52	0.45
1:A:1235:GLU:OE2	1:A:1515:ARG:NH1	2.50	0.45
1:A:1786:LEU:HA	1:A:1786:LEU:HD23	1.73	0.45
1:A:1882:PRO:HD2	1:A:1887:TYR:OH	2.17	0.45
1:B:300:GLY:O	1:B:301:ASP:C	2.59	0.45
1:B:838:HIS:O	1:B:840:GLN:N	2.50	0.45
1:B:1541:LEU:HD13	1:B:1840:PHE:HB3	1.97	0.45
1:B:2098:PHE:CD2	1:B:2106:LEU:HB2	2.51	0.45
1:A:191:LEU:HD22	1:A:224:ARG:CZ	2.47	0.45
1:A:548:ASP:OD2	1:A:611:LYS:NZ	2.50	0.45
1:A:724:GLY:O	1:A:728:ARG:HB2	2.16	0.45
1:A:752:VAL:HA	1:A:753:PRO:HD3	1.87	0.45
1:A:995:ASP:O	1:A:998:LEU:HB2	2.16	0.45
1:A:1095:LEU:HD12	1:A:1095:LEU:O	2.17	0.45
1:A:1599:LEU:O	1:A:1622:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ALA:HA	1:B:101:ARG:CG	2.46	0.45
1:B:258:GLU:HB2	1:B:259:GLN:NE2	2.32	0.45
1:B:1137:GLN:HG2	1:B:1396:PHE:CZ	2.52	0.45
1:B:1481:SER:N	1:B:1482:PRO:CD	2.80	0.45
1:B:1973:MET:CB	1:B:1995:LYS:HE3	2.46	0.45
1:B:2056:LEU:HA	1:B:2104:PRO:O	2.16	0.45
1:A:1001:TYR:CE2	1:A:1040:ILE:HD13	2.52	0.45
1:A:1248:LEU:HD21	1:A:1277:ARG:NE	2.30	0.45
1:A:1259:PRO:HG2	1:A:1292:LEU:HD22	1.99	0.45
1:A:1277:ARG:HD3	1:A:1300:ASP:CG	2.42	0.45
1:A:1314:LEU:HD12	1:A:1343:PHE:C	2.42	0.45
1:A:1757:VAL:O	1:A:1760:LEU:HB2	2.17	0.45
1:A:1818:ILE:HG12	1:A:1823:VAL:CG1	2.46	0.45
1:B:1890:THR:O	1:B:1971:LEU:HB2	2.17	0.45
1:A:217:ALA:HB2	1:A:363:ASN:HA	1.99	0.45
1:A:895:THR:HA	1:A:935:VAL:HG11	1.99	0.45
1:A:1474:VAL:HA	1:A:1504:ASN:O	2.17	0.45
1:A:1616:MET:HE2	1:A:1800:PHE:CE1	2.52	0.45
1:A:1931:GLU:O	1:A:1934:ARG:N	2.50	0.45
1:A:2064:GLY:O	1:A:2066:VAL:N	2.50	0.45
1:B:699:ARG:O	1:B:703:LEU:HD23	2.17	0.45
1:B:1123:PRO:O	1:B:1393:LYS:NZ	2.50	0.45
1:B:1343:PHE:HE2	1:B:1390:VAL:HG21	1.82	0.45
1:B:1567:TYR:O	1:B:1856:VAL:HG23	2.16	0.45
1:B:1689:LEU:HD23	1:B:1689:LEU:HA	1.70	0.45
1:A:75:MET:SD	1:A:79:LEU:HD23	2.56	0.44
1:A:1283:GLU:C	1:A:1285:ALA:H	2.24	0.44
1:A:1419:GLU:OE2	1:A:1447:GLY:HA3	2.15	0.44
1:B:103:THR:CG2	1:B:104:SER:N	2.80	0.44
1:B:159:THR:HG22	1:B:398:SER:HB3	1.99	0.44
1:B:581:SER:HB2	1:B:683:HIS:NE2	2.32	0.44
1:B:1347:HIS:CD2	1:B:1347:HIS:C	2.95	0.44
1:B:1541:LEU:O	1:B:1837:GLU:HG3	2.17	0.44
1:B:1567:TYR:CE1	1:B:1606:ARG:HG3	2.52	0.44
1:B:1678:GLY:O	1:B:1682:GLN:HG3	2.16	0.44
1:A:94:GLY:CA	1:A:453:MET:HE3	2.47	0.44
1:A:158:ASP:O	1:B:156:THR:OG1	2.34	0.44
1:A:326:LYS:CE	1:A:336:SER:HB2	2.47	0.44
1:A:595:THR:HG22	1:A:597:GLU:HG2	1.98	0.44
1:A:627:TRP:CH2	1:A:640:PRO:HB2	2.52	0.44
1:A:844:VAL:O	1:A:845:PRO:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:ARG:HD3	1:A:1065:ARG:HA	1.82	0.44
1:A:1262:LEU:O	1:A:1268:MET:HG3	2.17	0.44
1:A:1449:SER:O	1:A:1477:LEU:HD22	2.17	0.44
1:A:1473:LEU:HG	1:A:1503:MET:HA	2.00	0.44
1:A:1706:ALA:O	1:A:1707:TYR:C	2.61	0.44
1:A:1781:GLY:O	1:A:1784:VAL:HG23	2.17	0.44
1:A:1971:LEU:HD21	1:A:2019:PHE:CD2	2.53	0.44
1:B:108:TRP:CD1	1:B:171:ALA:HB2	2.52	0.44
1:B:111:VAL:O	1:B:111:VAL:HG12	2.17	0.44
1:B:581:SER:HB2	1:B:683:HIS:CE1	2.52	0.44
1:B:647:ASP:N	1:B:647:ASP:OD1	2.50	0.44
1:B:1251:ASP:O	1:B:1253:GLN:HG3	2.17	0.44
1:B:1442:TRP:CH2	1:B:1497:LEU:HD23	2.52	0.44
1:A:643:HIS:HA	1:A:649:VAL:HG22	1.99	0.44
1:A:1617:VAL:HG12	1:A:1619:ALA:H	1.82	0.44
1:A:1637:PRO:C	1:A:1639:THR:N	2.76	0.44
1:A:1857:ARG:O	1:A:1858:GLU:C	2.58	0.44
1:A:2015:TYR:HD2	1:A:2099:LEU:HD22	1.78	0.44
1:A:2043:ARG:HA	1:A:2043:ARG:HD3	1.69	0.44
1:B:321:LEU:H	1:B:321:LEU:CD1	2.31	0.44
1:B:1245:VAL:O	1:B:1315:LEU:HD12	2.16	0.44
1:B:1818:ILE:HG12	1:B:1823:VAL:CG1	2.48	0.44
1:B:2111:LEU:HD23	1:B:2111:LEU:HA	1.83	0.44
1:A:409:ARG:HA	1:A:410:PRO:HD3	1.73	0.44
1:A:850:PHE:HB3	1:A:851:PRO:HD2	2.00	0.44
1:A:1250:GLY:N	1:A:1276:ASP:OD2	2.50	0.44
1:A:1476:ASN:HA	1:A:1486:MET:CE	2.47	0.44
1:B:831:SER:N	1:B:832:PRO:CD	2.80	0.44
1:A:305:LEU:O	1:A:309:VAL:HG23	2.17	0.44
1:A:1112:LEU:O	1:A:1114:PRO:HD3	2.17	0.44
1:A:1456:MET:CG	1:A:2036:PHE:HB2	2.46	0.44
1:A:1556:PRO:C	1:A:1558:SER:N	2.74	0.44
1:A:1577:MET:HE2	1:A:1577:MET:HB3	1.89	0.44
1:B:9:MET:HE2	1:B:342:ILE:HG12	1.99	0.44
1:B:13:LEU:HD13	1:B:22:PHE:CD1	2.53	0.44
1:B:62:ALA:HB1	1:B:67:VAL:HG23	2.00	0.44
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.98	0.44
1:B:907:LEU:HD12	1:B:907:LEU:HA	1.87	0.44
1:B:1653:THR:O	1:B:1654:THR:C	2.60	0.44
1:A:6:ILE:HG21	1:A:345:LEU:HD11	2.00	0.44
1:A:81:MET:O	1:A:85:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:LEU:HB2	1:A:816:PHE:CD1	2.53	0.44
1:A:830:ILE:C	1:A:832:PRO:HD2	2.43	0.44
1:A:1236:ASN:CG	1:A:1502:VAL:HG23	2.42	0.44
1:A:1487:HIS:O	1:A:1487:HIS:CD2	2.71	0.44
1:A:1487:HIS:HA	1:A:1488:PRO:HD3	1.80	0.44
1:A:1515:ARG:HA	1:A:1515:ARG:HD3	1.55	0.44
1:A:1571:LEU:O	1:A:1851:LYS:HD2	2.17	0.44
1:A:1995:LYS:O	1:A:2041:MET:HE3	2.17	0.44
1:B:9:MET:CE	1:B:342:ILE:HA	2.48	0.44
1:B:277:TYR:O	1:B:278:ALA:C	2.61	0.44
1:B:582:LEU:O	1:B:585:VAL:HG23	2.18	0.44
1:B:1445:ALA:O	1:B:1476:ASN:ND2	2.51	0.44
1:B:1768:GLU:OE1	1:B:1768:GLU:CA	2.64	0.44
1:B:1986:GLU:HA	1:B:1989:GLN:HG2	2.00	0.44
1:B:2103:HIS:HA	1:B:2104:PRO:HD3	1.78	0.44
1:A:213:ARG:HH11	1:A:213:ARG:HG3	1.81	0.44
1:A:309:VAL:HG13	1:A:313:CYS:SG	2.58	0.44
1:A:1052:THR:HG22	1:A:1053:ARG:HG3	1.98	0.44
1:A:1249:ALA:N	1:A:1276:ASP:OD1	2.40	0.44
1:A:1290:GLU:HG2	1:A:1291:GLN:N	2.33	0.44
1:A:1973:MET:CB	1:A:1995:LYS:HE3	2.47	0.44
1:A:2066:VAL:HG22	1:A:2088:ILE:HD12	2.00	0.44
1:B:353:TRP:CZ2	1:B:383:ILE:HD12	2.53	0.44
1:B:1221:LEU:HG	1:B:1221:LEU:O	2.18	0.44
1:B:1766:PHE:HD2	1:B:1791:PHE:CE1	2.36	0.44
1:B:1993:LYS:N	1:B:1994:PRO:CD	2.81	0.44
1:A:190:VAL:HG12	1:A:192:LEU:HG	2.00	0.44
1:A:359:TYR:CG	1:A:376:VAL:HG11	2.53	0.44
1:A:587:CYS:O	1:A:591:ASP:N	2.50	0.44
1:A:1616:MET:CE	1:A:1650:ILE:HD13	2.40	0.44
1:A:1657:TYR:CE1	1:A:1799:LEU:HD11	2.53	0.44
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.70	0.44
1:B:895:THR:HA	1:B:935:VAL:HG11	2.00	0.44
1:B:1231:ASP:O	1:B:1232:THR:C	2.61	0.44
1:B:1416:LEU:CD2	1:B:1429:LEU:HG	2.47	0.44
1:B:1475:SER:HB3	1:B:1505:VAL:CG1	2.47	0.44
1:A:169:GLN:OE1	1:A:250:GLY:HA2	2.17	0.44
1:A:189:ASN:O	1:A:226:GLU:HB2	2.17	0.44
1:A:331:HIS:HE1	1:A:333:GLU:HA	1.83	0.44
1:A:499:MET:HG3	1:A:502:GLN:NE2	2.32	0.44
1:A:642:CYS:HA	1:A:743:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:THR:CG2	1:A:1032:LEU:CB	2.96	0.44
1:A:1231:ASP:HB3	1:A:1515:ARG:HD2	2.00	0.44
1:A:1345:LEU:C	1:A:1346:LEU:HD23	2.43	0.44
1:A:1506:TYR:C	1:A:1506:TYR:CD2	2.96	0.44
1:A:1754:GLN:OE1	1:A:1754:GLN:HA	2.17	0.44
1:A:1762:GLN:O	1:A:1763:HIS:HB2	2.18	0.44
1:A:1818:ILE:HG12	1:A:1823:VAL:HG11	1.99	0.44
1:A:1882:PRO:HA	1:A:1883:PRO:HD3	1.85	0.44
1:A:1955:LEU:O	1:A:1958:GLU:HB2	2.17	0.44
1:B:587:CYS:O	1:B:591:ASP:N	2.51	0.44
1:B:1971:LEU:HD21	1:B:2019:PHE:CD2	2.52	0.44
1:A:123:ASP:CB	1:A:126:THR:HB	2.42	0.43
1:A:159:THR:HG22	1:A:398:SER:HB3	2.00	0.43
1:A:984:GLU:O	1:A:985:PHE:CB	2.64	0.43
1:A:1216:LEU:HD13	1:A:1217:LEU:H	1.83	0.43
1:A:1953:ARG:HA	1:A:2005:VAL:HG11	1.99	0.43
1:B:23:TRP:NE1	1:B:350:HIS:CD2	2.86	0.43
1:B:91:VAL:HG21	1:B:834:ILE:HD13	1.99	0.43
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.33	0.43
1:B:190:VAL:HG12	1:B:192:LEU:HG	1.99	0.43
1:B:914:PHE:HB2	1:B:1057:ILE:HB	2.00	0.43
1:B:925:LEU:CD2	1:B:931:VAL:HG21	2.48	0.43
1:B:1036:LEU:O	1:B:1037:HIS:C	2.61	0.43
1:B:1118:LYS:HD2	1:B:2103:HIS:ND1	2.33	0.43
1:B:1338:LEU:HD13	1:B:1406:GLN:CG	2.48	0.43
1:B:1466:GLY:HA2	1:B:1469:ILE:CD1	2.48	0.43
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.31	0.43
1:A:525:GLN:NE2	1:A:525:GLN:HA	2.32	0.43
1:A:579:GLY:O	1:A:715:THR:HG21	2.19	0.43
1:A:1614:MET:HE2	1:A:1614:MET:HB3	1.91	0.43
1:A:1669:GLU:HG2	1:A:1742:ASP:CG	2.43	0.43
1:A:1887:TYR:CD2	1:A:1967:GLY:HA3	2.46	0.43
1:B:175:ILE:O	1:B:176:ARG:C	2.61	0.43
1:B:302:PRO:HG3	1:B:363:ASN:ND2	2.33	0.43
1:B:479:SER:C	1:B:480:GLN:HG3	2.43	0.43
1:B:1553:TYR:O	1:B:1554:ALA:HB2	2.18	0.43
1:B:1685:ILE:HG22	1:B:1686:ALA:N	2.30	0.43
1:A:1483:ALA:HB1	1:A:1508:ASP:HA	2.01	0.43
1:A:1723:SER:C	1:A:1725:ASP:N	2.75	0.43
1:A:1857:ARG:NH1	1:A:1869:PRO:HB2	2.33	0.43
1:A:1995:LYS:HB3	1:A:2041:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1540:ASP:C	1:B:1542:SER:H	2.27	0.43
1:B:1769:ILE:HG22	1:B:1770:GLY:N	2.32	0.43
1:B:2043:ARG:HD3	1:B:2043:ARG:HA	1.71	0.43
1:A:288:GLU:CD	1:A:383:ILE:HG13	2.43	0.43
1:A:343:LYS:HE3	1:A:354:ALA:HB3	2.00	0.43
1:A:366:ILE:O	1:A:366:ILE:CG1	2.66	0.43
1:A:639:VAL:HG12	1:A:640:PRO:O	2.18	0.43
1:A:811:ASN:HA	1:A:812:PRO:HD3	1.82	0.43
1:A:1238:ALA:O	1:A:1462:LYS:HG3	2.17	0.43
1:A:1299:TRP:NE1	1:A:1304:PRO:O	2.51	0.43
1:A:1442:TRP:CH2	1:A:1497:LEU:HD23	2.54	0.43
1:A:1444:MET:HE2	1:A:1444:MET:HB3	1.75	0.43
1:A:1619:ALA:O	1:A:1620:GLU:HB2	2.18	0.43
1:A:1624:THR:HG22	1:A:1857:ARG:NH2	2.33	0.43
1:A:1993:LYS:H	1:A:1994:PRO:CD	2.32	0.43
1:B:289:TYR:C	1:B:289:TYR:CD2	2.96	0.43
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.53	0.43
1:A:175:ILE:O	1:A:176:ARG:C	2.61	0.43
1:A:870:SER:HA	1:A:871:PRO:HD3	1.88	0.43
1:A:1049:TYR:CZ	1:A:1103:VAL:HG23	2.54	0.43
1:A:1245:VAL:C	1:A:1315:LEU:HD12	2.44	0.43
1:A:1469:ILE:O	1:A:1469:ILE:CG2	2.66	0.43
1:A:1662:ARG:NH1	1:A:1662:ARG:HG2	2.33	0.43
1:A:1690:SER:C	1:A:1692:GLY:H	2.25	0.43
1:A:2006:THR:HG21	1:A:2048:ARG:NH2	2.32	0.43
1:B:98:ALA:CA	1:B:101:ARG:HG3	2.47	0.43
1:B:185:VAL:HB	1:B:231:VAL:HG23	2.00	0.43
1:B:329:MET:HE3	1:B:330:GLY:O	2.19	0.43
1:B:506:MET:HE3	1:B:559:ILE:CD1	2.44	0.43
1:B:1569:THR:HG23	1:B:1602:GLU:O	2.19	0.43
1:B:1648:VAL:HB	1:B:1649:PRO:HD3	1.99	0.43
1:B:1675:SER:O	1:B:1681:GLY:HA3	2.19	0.43
1:B:1734:ARG:C	1:B:1736:THR:N	2.76	0.43
1:B:1862:GLY:O	1:B:1863:PRO:C	2.61	0.43
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.62	0.43
1:A:336:SER:OG	1:A:337:GLY:N	2.51	0.43
1:A:1118:LYS:HA	1:A:2106:LEU:HD22	2.01	0.43
1:A:1864:ALA:HA	1:A:1865:PRO:HD3	1.82	0.43
1:A:1882:PRO:HG2	1:A:1885:LYS:HD2	2.01	0.43
1:A:1929:VAL:HG13	1:A:1939:VAL:HG11	1.99	0.43
1:B:23:TRP:CE2	1:B:27:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:VAL:O	1:B:228:VAL:CG2	2.67	0.43
1:B:290:ILE:CG2	1:B:322:ILE:HG12	2.49	0.43
1:B:637:GLY:O	1:B:685:TYR:HE2	2.00	0.43
1:B:946:VAL:O	1:B:954:ILE:HB	2.18	0.43
1:B:982:THR:O	1:B:984:GLU:N	2.49	0.43
1:B:1112:LEU:O	1:B:1114:PRO:HD3	2.17	0.43
1:B:1448:CYS:C	1:B:1450:THR:N	2.77	0.43
1:A:9:MET:HE2	1:A:342:ILE:HG12	1.99	0.43
1:A:51:MET:HB2	1:A:53:LYS:HE3	2.01	0.43
1:A:78:GLN:HB3	1:A:188:LEU:HD13	2.01	0.43
1:A:277:TYR:O	1:A:278:ALA:C	2.62	0.43
1:A:782:ILE:HA	1:A:783:PRO:HD3	1.88	0.43
1:A:1251:ASP:O	1:A:1253:GLN:HG3	2.19	0.43
1:A:1476:ASN:CB	1:A:1486:MET:SD	3.06	0.43
1:A:1757:VAL:HG11	1:A:1784:VAL:HG21	2.01	0.43
1:B:6:ILE:HG21	1:B:345:LEU:HD11	2.01	0.43
1:B:14:PRO:HA	1:B:53:LYS:O	2.19	0.43
1:B:161:CYS:HB3	1:B:331:HIS:CE1	2.53	0.43
1:B:257:LYS:NZ	1:B:261:VAL:O	2.49	0.43
1:B:654:PRO:HG3	1:B:685:TYR:OH	2.18	0.43
1:B:752:VAL:HA	1:B:753:PRO:HD3	1.89	0.43
1:A:23:TRP:CH2	1:A:347:SER:HA	2.54	0.43
1:A:108:TRP:CD1	1:A:171:ALA:HB2	2.54	0.43
1:A:129:GLY:HA3	1:B:202:LYS:HB2	2.00	0.43
1:A:524:ASP:OD1	1:A:534:VAL:N	2.52	0.43
1:A:572:LEU:C	1:A:572:LEU:HD22	2.43	0.43
1:A:1083:ASP:O	1:A:1086:LEU:N	2.51	0.43
1:A:2031:GLN:HB3	1:A:2034:TYR:HB3	1.99	0.43
1:B:137:ARG:O	1:B:140:MET:HG2	2.19	0.43
1:B:252:ASN:N	1:B:272:LEU:HD13	2.33	0.43
1:B:363:ASN:HA	1:B:364:PRO:HD3	1.81	0.43
1:B:416:GLN:OE1	1:B:817:PRO:HG2	2.18	0.43
1:B:499:MET:C	1:B:501:ALA:H	2.27	0.43
1:B:499:MET:HG3	1:B:502:GLN:NE2	2.34	0.43
1:B:1348:THR:C	1:B:1349:LEU:HG	2.43	0.43
1:B:2066:VAL:HG22	1:B:2088:ILE:HD12	2.00	0.43
1:A:206:LEU:HA	1:A:206:LEU:HD23	1.64	0.43
1:A:1235:GLU:H	1:A:1235:GLU:HG2	1.58	0.43
1:A:1390:VAL:HG22	1:A:1501:LEU:HD21	2.00	0.43
1:B:161:CYS:HB3	1:B:331:HIS:HE1	1.84	0.43
1:B:953:LEU:HD12	1:B:954:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1137:GLN:NE2	1:B:1396:PHE:CE1	2.86	0.43
1:B:1389:LEU:HD23	1:B:1389:LEU:HA	1.83	0.43
1:A:9:MET:HE1	1:A:342:ILE:HA	2.00	0.43
1:A:295:THR:HG22	1:A:331:HIS:CD2	2.53	0.43
1:A:548:ASP:OD1	1:A:550:VAL:N	2.50	0.43
1:A:863:LYS:HB3	1:A:930:THR:HG21	2.01	0.43
1:A:1345:LEU:HD13	1:A:1403:LEU:HD13	2.01	0.43
1:A:1842:TYR:CE2	1:A:1848:HIS:HB3	2.53	0.43
1:B:23:TRP:CZ2	1:B:27:ILE:HG12	2.54	0.43
1:B:200:PHE:HB3	1:B:206:LEU:CG	2.48	0.43
1:B:1477:LEU:HD11	1:B:2043:ARG:CD	2.43	0.43
1:B:1515:ARG:HD3	1:B:1515:ARG:HA	1.30	0.43
1:B:1525:GLU:OE1	1:B:1874:THR:HG23	2.19	0.43
1:B:1555:LEU:HD12	1:B:1555:LEU:HA	1.93	0.43
1:B:1921:ARG:HE	1:B:1921:ARG:HB2	1.65	0.43
1:A:248:ASN:HD22	1:A:249:ALA:H	1.65	0.42
1:A:262:THR:O	1:A:262:THR:HG22	2.18	0.42
1:A:1420:ASP:O	1:A:1425:TRP:CZ3	2.71	0.42
1:A:1657:TYR:CZ	1:A:1662:ARG:CD	3.02	0.42
1:A:1815:LYS:O	1:A:1819:GLN:HG3	2.18	0.42
1:B:259:GLN:HB2	1:B:263:PHE:CD1	2.54	0.42
1:B:497:SER:HB2	1:B:762:ALA:HB2	2.00	0.42
1:B:1119:PHE:CZ	1:B:1514:PHE:HB3	2.54	0.42
1:B:1469:ILE:CG2	1:B:1471:CYS:SG	3.07	0.42
1:B:1536:LEU:HG	1:B:1543:SER:O	2.19	0.42
1:B:1780:LEU:HD12	1:B:1781:GLY:H	1.83	0.42
1:B:1955:LEU:O	1:B:1958:GLU:HB2	2.19	0.42
1:A:119:ALA:HB2	1:A:850:PHE:CE2	2.53	0.42
1:A:470:TYR:CD2	1:A:801:GLY:HA3	2.55	0.42
1:A:1032:LEU:O	1:A:1035:MET:HB2	2.19	0.42
1:A:1468:ARG:HD3	1:A:1468:ARG:HA	1.85	0.42
1:A:1661:VAL:HG21	1:A:1810:VAL:HG22	2.01	0.42
1:B:111:VAL:HG21	1:B:188:LEU:HD12	2.01	0.42
1:B:863:LYS:HB3	1:B:930:THR:HG21	2.01	0.42
1:B:1463:GLU:O	1:B:1464:PRO:C	2.62	0.42
1:B:1468:ARG:HD3	1:B:1468:ARG:HA	1.71	0.42
1:B:1477:LEU:O	1:B:1507:ARG:CG	2.67	0.42
1:B:1818:ILE:HG12	1:B:1823:VAL:HG11	2.00	0.42
1:B:1977:ASP:O	1:B:1978:ALA:HB2	2.19	0.42
1:A:708:ARG:HD3	1:A:727:ALA:O	2.19	0.42
1:A:743:VAL:HG23	1:A:743:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:VAL:HG12	1:A:809:SER:H	1.84	0.42
1:A:1090:VAL:HG22	1:A:1095:LEU:HB2	2.02	0.42
1:A:1896:PHE:CE2	1:A:2019:PHE:CE1	3.07	0.42
1:A:2041:MET:HA	1:A:2044:ILE:HG13	2.02	0.42
1:B:475:GLY:O	1:B:477:ALA:N	2.51	0.42
1:B:557:THR:HA	1:B:560:GLN:HE21	1.84	0.42
1:B:1315:LEU:HD23	1:B:1344:LEU:HD11	2.00	0.42
1:B:1573:PHE:HD1	1:B:1843:MET:HE2	1.84	0.42
1:B:1636:VAL:O	1:B:1636:VAL:HG22	2.19	0.42
1:B:1786:LEU:HD23	1:B:1786:LEU:HA	1.82	0.42
1:A:39:ARG:NH1	1:A:226:GLU:OE2	2.51	0.42
1:A:48:PRO:HD3	1:A:201:MET:CE	2.50	0.42
1:A:132:MET:HB3	1:A:132:MET:HE2	1.60	0.42
1:A:202:LYS:HB2	1:B:129:GLY:HA3	2.02	0.42
1:A:1411:ASP:OD2	1:A:1439:ARG:HB2	2.19	0.42
1:A:1598:MET:HG2	1:A:1598:MET:O	2.20	0.42
1:A:2095:LEU:CD1	1:A:2099:LEU:HG	2.49	0.42
1:B:972:THR:CG2	1:B:1081:VAL:CG2	2.96	0.42
1:B:1245:VAL:C	1:B:1315:LEU:HD12	2.45	0.42
1:B:1551:LEU:HD21	1:B:1627:LEU:CD2	2.48	0.42
1:B:1676:GLY:O	1:B:1682:GLN:HG2	2.20	0.42
1:B:1723:SER:C	1:B:1725:ASP:N	2.78	0.42
1:B:1820:GLU:C	1:B:1822:VAL:H	2.28	0.42
1:B:1993:LYS:H	1:B:1994:PRO:CD	2.31	0.42
1:A:321:LEU:H	1:A:321:LEU:HD12	1.84	0.42
1:A:329:MET:HE3	1:A:330:GLY:O	2.19	0.42
1:A:347:SER:HB2	1:A:352:VAL:O	2.19	0.42
1:A:542:ASP:O	1:A:543:GLU:C	2.62	0.42
1:A:581:SER:C	1:A:583:GLY:N	2.76	0.42
1:A:606:ARG:HA	1:A:694:LEU:HD11	2.00	0.42
1:A:925:LEU:CD2	1:A:931:VAL:HG21	2.49	0.42
1:A:1787:LYS:HB2	1:A:1789:VAL:HG23	2.01	0.42
1:A:1817:GLY:C	1:A:1823:VAL:HG12	2.44	0.42
1:B:40:TRP:CZ3	1:B:194:PRO:HA	2.55	0.42
1:B:40:TRP:HB3	1:B:847:ALA:CB	2.49	0.42
1:B:263:PHE:HE2	1:B:303:GLN:HE21	1.66	0.42
1:B:895:THR:O	1:B:898:THR:HB	2.20	0.42
1:B:1670:SER:OG	1:B:1741:VAL:HA	2.19	0.42
1:B:1757:VAL:O	1:B:1760:LEU:HB2	2.19	0.42
1:A:189:ASN:HB2	1:A:334:PRO:HD2	1.99	0.42
1:A:211:THR:HG22	1:A:212:CYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD23	1:A:381:LEU:CD1	2.48	0.42
1:A:644:ASN:HB3	1:A:770:VAL:HG11	2.01	0.42
1:A:765:ALA:HB1	1:A:768:GLN:CG	2.49	0.42
1:A:1119:PHE:HB3	1:A:2105:VAL:HB	2.01	0.42
1:A:1245:VAL:HB	1:A:1315:LEU:CD1	2.49	0.42
1:A:1996:TYR:CD2	1:A:1997:SER:N	2.85	0.42
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.69	0.42
1:B:82:LEU:HG	1:B:144:LEU:HD13	2.02	0.42
1:B:165:LEU:HD23	1:B:400:VAL:CG2	2.31	0.42
1:B:367:PRO:O	1:B:368:ALA:HB3	2.20	0.42
1:B:423:LEU:HB2	1:B:797:LEU:HD22	2.01	0.42
1:B:462:PRO:HA	1:B:465:MET:O	2.19	0.42
1:B:572:LEU:HD22	1:B:572:LEU:C	2.44	0.42
1:B:1222:ASP:OD1	1:B:1222:ASP:N	2.49	0.42
1:B:1455:GLY:O	1:B:1456:MET:C	2.63	0.42
1:B:1500:ASP:O	1:B:1501:LEU:C	2.62	0.42
1:B:1815:LYS:O	1:B:1819:GLN:HG3	2.20	0.42
1:B:2049:ARG:HD2	1:B:2049:ARG:HA	1.84	0.42
1:A:27:ILE:HD13	1:A:27:ILE:HA	1.81	0.42
1:A:98:ALA:HA	1:A:101:ARG:CG	2.49	0.42
1:A:163:SER:O	1:A:167:ALA:N	2.47	0.42
1:A:228:VAL:O	1:A:228:VAL:CG2	2.67	0.42
1:A:257:LYS:NZ	1:A:261:VAL:O	2.51	0.42
1:A:353:TRP:O	1:A:355:PRO:HD3	2.19	0.42
1:A:1240:PRO:HB3	1:A:1267:VAL:O	2.20	0.42
1:A:1603:PHE:HZ	1:A:1628:LEU:HD22	1.84	0.42
1:A:1637:PRO:O	1:A:1639:THR:N	2.52	0.42
1:A:2112:ALA:C	1:A:2113:GLU:HG2	2.44	0.42
1:B:305:LEU:HD22	1:B:322:ILE:CD1	2.50	0.42
1:B:1382:PHE:HA	1:B:1387:LEU:HD12	2.01	0.42
1:B:1711:ARG:HG2	1:B:1712:PHE:CE1	2.55	0.42
1:A:672:VAL:O	1:A:672:VAL:HG12	2.18	0.42
1:A:1514:PHE:O	1:A:1515:ARG:NH1	2.53	0.42
1:B:5:VAL:HG21	1:B:242:VAL:HG22	2.01	0.42
1:B:193:LYS:HA	1:B:194:PRO:HD3	1.85	0.42
1:B:409:ARG:HA	1:B:410:PRO:HD3	1.74	0.42
1:B:416:GLN:HE21	1:B:448:LEU:CD1	2.33	0.42
1:B:876:VAL:O	1:B:876:VAL:HG12	2.20	0.42
1:B:996:LEU:C	1:B:998:LEU:N	2.75	0.42
1:A:166:LEU:CD1	1:A:251:THR:HG21	2.49	0.42
1:A:252:ASN:OD1	1:A:252:ASN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PRO:HA	1:A:366:ILE:CG2	2.49	0.42
1:A:384:ARG:CG	1:A:384:ARG:NH1	2.75	0.42
1:A:495:ILE:HG12	1:A:758:VAL:HG13	2.02	0.42
1:A:595:THR:HG22	1:A:596:GLN:N	2.35	0.42
1:A:614:ASN:C	1:A:615:VAL:O	2.62	0.42
1:A:731:SER:O	1:A:732:ALA:C	2.63	0.42
1:A:795:PHE:CE1	1:A:799:ASN:ND2	2.86	0.42
1:A:899:LEU:HA	1:A:899:LEU:HD12	1.82	0.42
1:A:1451:SER:O	1:A:2036:PHE:CE1	2.73	0.42
1:B:527:LEU:HD11	1:B:554:VAL:HG11	2.01	0.42
1:B:1763:HIS:HA	1:B:1788:ASN:O	2.20	0.42
1:B:1801:GLU:O	1:B:1803:GLY:N	2.53	0.42
1:B:1941:VAL:O	1:B:1941:VAL:HG12	2.18	0.42
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.68	0.42
1:A:114:SER:O	1:A:117:SER:HB3	2.19	0.42
1:A:420:LEU:HD11	1:A:512:ARG:HB3	2.01	0.42
1:A:1116:LEU:HD22	1:A:2098:PHE:CE1	2.55	0.42
1:A:1123:PRO:HA	1:A:1512:GLY:HA3	2.01	0.42
1:A:1557:ALA:O	1:A:1560:GLN:HB3	2.20	0.42
1:B:270:GLU:HG3	1:B:311:ALA:HB2	2.01	0.42
1:B:1038:MET:CE	1:B:1041:LEU:HD23	2.50	0.42
1:B:1097:LEU:C	1:B:1097:LEU:CD1	2.93	0.42
1:B:1234:LEU:HD12	1:B:1234:LEU:O	2.19	0.42
1:B:1303:ASN:OD1	1:B:1332:GLY:HA3	2.19	0.42
1:B:1671:VAL:HG23	1:B:1743:LEU:HD13	2.02	0.42
1:B:1757:VAL:HG11	1:B:1784:VAL:HG21	2.01	0.42
1:B:1817:GLY:C	1:B:1823:VAL:HG12	2.45	0.42
1:A:503:TRP:HB3	1:A:787:LYS:HD2	2.02	0.41
1:A:1480:THR:CG2	1:A:1482:PRO:HD2	2.50	0.41
1:B:119:ALA:HB2	1:B:850:PHE:CZ	2.55	0.41
1:B:1444:MET:HE2	1:B:1444:MET:HB3	1.89	0.41
1:B:1537:SER:H	1:B:1543:SER:HB2	1.85	0.41
1:B:2064:GLY:O	1:B:2066:VAL:N	2.53	0.41
1:A:9:MET:CE	1:A:342:ILE:HA	2.50	0.41
1:A:136:GLN:O	1:A:137:ARG:C	2.64	0.41
1:A:254:ASP:HB2	1:A:257:LYS:HE2	2.02	0.41
1:A:359:TYR:CD2	1:A:376:VAL:HG11	2.55	0.41
1:A:366:ILE:HD11	1:A:369:LEU:HD11	2.01	0.41
1:A:499:MET:C	1:A:501:ALA:H	2.26	0.41
1:A:620:MET:CE	1:A:682:PHE:O	2.66	0.41
1:A:776:GLU:HB3	1:A:778:SER:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:TYR:CE2	1:A:1687:ILE:HD13	2.55	0.41
1:A:1873:LEU:HD22	1:A:1874:THR:N	2.34	0.41
1:A:1993:LYS:N	1:A:1994:PRO:CD	2.82	0.41
1:B:128:VAL:HG12	1:B:130:TYR:CE2	2.54	0.41
1:B:1436:ALA:C	1:B:1438:SER:H	2.28	0.41
1:B:1966:GLY:HA2	1:B:2013:LEU:HA	2.02	0.41
1:A:111:VAL:CG2	1:A:188:LEU:HD12	2.50	0.41
1:A:118:GLU:OE2	1:B:118:GLU:HG3	2.20	0.41
1:A:894:LEU:HD12	1:A:894:LEU:HA	1.81	0.41
1:A:1272:TYR:HB3	1:A:1294:VAL:HG22	2.01	0.41
1:A:1413:PRO:HA	1:A:1440:PRO:O	2.21	0.41
1:B:273:ILE:O	1:B:277:TYR:HD1	2.01	0.41
1:B:322:ILE:HD11	1:B:374:LEU:HD13	2.01	0.41
1:B:1049:TYR:CZ	1:B:1103:VAL:HG23	2.55	0.41
1:B:1060:ASP:OD1	1:B:1062:VAL:HG23	2.20	0.41
1:B:1095:LEU:C	1:B:1095:LEU:CD1	2.90	0.41
1:B:1241:LYS:HA	1:B:1269:ASP:HB3	2.02	0.41
1:A:23:TRP:CE2	1:A:27:ILE:HG12	2.55	0.41
1:A:40:TRP:CZ3	1:A:194:PRO:HA	2.55	0.41
1:A:302:PRO:HG3	1:A:363:ASN:ND2	2.35	0.41
1:A:367:PRO:O	1:A:368:ALA:HB3	2.20	0.41
1:A:795:PHE:O	1:A:798:SER:HB2	2.20	0.41
1:A:896:TRP:CG	1:A:907:LEU:HD11	2.56	0.41
1:A:1242:MET:HG3	1:A:1313:ASP:HB3	2.02	0.41
1:A:1442:TRP:CZ3	1:A:1472:VAL:HG11	2.55	0.41
1:B:162:SER:OG	1:B:163:SER:N	2.50	0.41
1:B:830:ILE:C	1:B:832:PRO:HD2	2.45	0.41
1:B:889:THR:CG2	1:B:1032:LEU:CB	2.98	0.41
1:B:894:LEU:HD12	1:B:894:LEU:HA	1.83	0.41
1:B:1405:ARG:HH22	1:B:1470:ARG:NH2	2.19	0.41
1:B:1577:MET:HE3	1:B:1582:LYS:HD3	2.02	0.41
1:B:1766:PHE:O	1:B:1792:HIS:HB2	2.20	0.41
1:A:13:LEU:HD13	1:A:22:PHE:CD1	2.55	0.41
1:A:489:LYS:HE2	1:A:489:LYS:HB3	1.77	0.41
1:A:581:SER:O	1:A:582:LEU:C	2.62	0.41
1:A:954:ILE:HD13	1:A:954:ILE:HA	1.91	0.41
1:A:1277:ARG:HD3	1:A:1300:ASP:OD2	2.19	0.41
1:A:1296:GLN:H	1:A:1296:GLN:HG2	1.64	0.41
1:A:1821:GLY:O	1:A:1822:VAL:C	2.64	0.41
1:B:33:VAL:HG11	1:B:223:CYS:SG	2.60	0.41
1:B:423:LEU:HD23	1:B:812:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:ILE:HD11	1:B:2111:LEU:HD12	2.02	0.41
1:B:1519:LEU:HD12	1:B:1520:GLU:H	1.85	0.41
1:B:1712:PHE:HA	1:B:1713:PRO:HD3	1.84	0.41
1:B:1931:GLU:O	1:B:1932:TRP:C	2.63	0.41
1:A:111:VAL:O	1:A:111:VAL:HG12	2.20	0.41
1:A:236:LYS:C	1:A:238:LEU:N	2.79	0.41
1:A:257:LYS:H	1:A:257:LYS:HG3	1.68	0.41
1:A:469:GLY:CA	1:A:805:LEU:HD21	2.51	0.41
1:A:527:LEU:HD11	1:A:554:VAL:HG11	2.02	0.41
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.88	0.41
1:A:1568:TYR:CE2	1:A:1855:GLN:HB2	2.56	0.41
1:A:1921:ARG:HE	1:A:1921:ARG:HB2	1.67	0.41
1:A:1998:GLY:O	1:A:2002:LEU:HD12	2.20	0.41
1:B:13:LEU:HB2	1:B:22:PHE:CD1	2.55	0.41
1:B:178:GLY:O	1:B:180:CYS:N	2.53	0.41
1:B:1122:THR:HA	1:B:1123:PRO:HD3	1.92	0.41
1:B:1453:VAL:O	1:B:1454:VAL:C	2.63	0.41
1:B:1836:VAL:HG13	1:B:1854:ILE:HD13	2.03	0.41
1:A:252:ASN:N	1:A:272:LEU:HD13	2.36	0.41
1:A:258:GLU:HB2	1:A:259:GLN:NE2	2.36	0.41
1:A:263:PHE:HE2	1:A:303:GLN:HE21	1.68	0.41
1:A:460:VAL:CG2	1:A:465:MET:HG3	2.46	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.79	0.41
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.56	0.41
1:A:572:LEU:C	1:A:572:LEU:CD2	2.93	0.41
1:A:726:LEU:C	1:A:726:LEU:HD12	2.46	0.41
1:A:953:LEU:HD12	1:A:954:ILE:N	2.35	0.41
1:A:1216:LEU:O	1:A:1220:LEU:HD12	2.21	0.41
1:A:1234:LEU:CD2	1:A:1262:LEU:HD22	2.48	0.41
1:A:1637:PRO:C	1:A:1639:THR:H	2.29	0.41
1:A:1669:GLU:CG	1:A:1742:ASP:OD2	2.69	0.41
1:A:1671:VAL:HG23	1:A:1743:LEU:HB2	2.02	0.41
1:B:322:ILE:CG2	1:B:323:GLY:N	2.83	0.41
1:B:744:LEU:HA	1:B:747:GLU:OE1	2.21	0.41
1:B:1538:ARG:HH12	1:B:1585:PRO:HG2	1.86	0.41
1:B:1617:VAL:N	1:B:1800:PHE:HZ	2.19	0.41
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.68	0.41
1:A:288:GLU:OE2	1:A:383:ILE:HG13	2.21	0.41
1:A:309:VAL:C	1:A:311:ALA:N	2.78	0.41
1:A:541:THR:O	1:A:542:ASP:HB3	2.20	0.41
1:A:623:VAL:HA	1:A:671:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:GLY:O	1:A:654:PRO:HD2	2.20	0.41
1:A:817:PRO:C	1:A:818:PRO:O	2.64	0.41
1:A:857:SER:O	1:A:902:ALA:CB	2.68	0.41
1:A:1011:LEU:HD12	1:A:1011:LEU:HA	1.85	0.41
1:A:1096:PHE:N	1:A:1096:PHE:CD2	2.89	0.41
1:A:1107:ARG:O	1:A:1108:PRO:C	2.64	0.41
1:A:1789:VAL:CG1	1:A:1790:THR:N	2.83	0.41
1:A:2112:ALA:O	1:A:2113:GLU:HG2	2.21	0.41
1:B:214:SER:O	1:B:301:ASP:OD2	2.38	0.41
1:B:513:LEU:HD23	1:B:513:LEU:HA	1.77	0.41
1:B:581:SER:HA	1:B:738:ASN:HD21	1.85	0.41
1:B:980:ASP:OD1	1:B:980:ASP:N	2.53	0.41
1:B:1107:ARG:O	1:B:1108:PRO:C	2.62	0.41
1:B:1315:LEU:O	1:B:1344:LEU:HD13	2.21	0.41
1:B:1433:LEU:HD12	1:B:1433:LEU:HA	1.79	0.41
1:A:64:PHE:CB	1:A:429:ARG:HH21	2.23	0.41
1:A:100:LEU:O	1:A:103:THR:OG1	2.24	0.41
1:A:100:LEU:C	1:A:103:THR:HG1	2.22	0.41
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.86	0.41
1:A:389:GLY:O	1:A:390:ILE:HG13	2.21	0.41
1:A:416:GLN:HE21	1:A:448:LEU:CD1	2.34	0.41
1:A:528:LYS:HB3	1:A:529:PRO:HD3	2.03	0.41
1:A:624:GLY:H	1:A:671:PHE:HB3	1.86	0.41
1:A:639:VAL:HG12	1:A:640:PRO:HD2	2.02	0.41
1:A:1583:LEU:HD23	1:A:1583:LEU:HA	1.88	0.41
1:A:1669:GLU:HG2	1:A:1742:ASP:OD2	2.21	0.41
1:A:2004:ARG:O	1:A:2005:VAL:C	2.64	0.41
1:B:33:VAL:HB	1:B:50:ARG:NH1	2.34	0.41
1:B:277:TYR:HB3	1:B:278:ALA:H	1.58	0.41
1:B:333:GLU:O	1:B:336:SER:HB3	2.21	0.41
1:B:494:PHE:O	1:B:495:ILE:HD13	2.20	0.41
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.56	0.41
1:B:704:ASP:O	1:B:706:LYS:HD2	2.20	0.41
1:B:795:PHE:CE1	1:B:799:ASN:ND2	2.87	0.41
1:B:1243:LYS:HA	1:B:1271:ASP:HB2	2.02	0.41
1:B:1283:GLU:C	1:B:1285:ALA:H	2.28	0.41
1:B:1312:ALA:HB1	1:B:1337:THR:HG22	2.00	0.41
1:B:1343:PHE:CZ	1:B:1405:ARG:HD2	2.56	0.41
1:B:1429:LEU:HD11	1:B:1443:LEU:HD21	2.03	0.41
1:B:1457:VAL:HG11	1:B:1473:LEU:HD22	2.02	0.41
1:B:1567:TYR:HA	1:B:1857:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1755:ALA:HA	1:B:1758:ARG:NH1	2.36	0.41
1:B:1842:TYR:CE2	1:B:1848:HIS:HB3	2.56	0.41
1:B:1996:TYR:CD2	1:B:1997:SER:N	2.85	0.41
1:B:1998:GLY:O	1:B:2002:LEU:HD12	2.20	0.41
1:B:2006:THR:CG2	1:B:2048:ARG:HH12	2.34	0.41
1:A:41:LYS:O	1:A:42:ALA:C	2.64	0.41
1:A:620:MET:HE3	1:A:682:PHE:N	2.35	0.41
1:A:674:GLU:H	1:A:674:GLU:HG2	1.28	0.41
1:A:907:LEU:HD12	1:A:907:LEU:HA	1.88	0.41
1:A:1408:THR:HG22	1:A:1409:PRO:HD2	2.03	0.41
1:A:1480:THR:HG22	1:A:1482:PRO:HD2	2.02	0.41
1:A:1766:PHE:O	1:A:1792:HIS:HB2	2.21	0.41
1:B:6:ILE:HG21	1:B:345:LEU:CD1	2.51	0.41
1:B:429:ARG:HA	1:B:429:ARG:HD2	1.91	0.41
1:B:634:CYS:HA	1:B:635:PRO:HD3	1.89	0.41
1:B:1257:ARG:O	1:B:1260:ALA:HB3	2.21	0.41
1:B:1951:GLY:O	1:B:1954:SER:HB2	2.20	0.41
1:B:1991:VAL:HG21	1:B:2033:ASN:HD22	1.84	0.41
1:A:129:GLY:C	1:B:203:LEU:HD21	2.47	0.40
1:A:270:GLU:HG3	1:A:311:ALA:HB2	2.03	0.40
1:A:1240:PRO:HD2	1:A:1462:LYS:HZ1	1.87	0.40
1:A:1243:LYS:HD2	1:A:1312:ALA:N	2.37	0.40
1:A:1476:ASN:C	1:A:1477:LEU:HD23	2.46	0.40
1:A:1514:PHE:O	1:A:1515:ARG:HD3	2.21	0.40
1:A:1689:LEU:O	1:A:1692:GLY:N	2.48	0.40
1:A:1857:ARG:HG3	1:A:1871:ILE:HD11	2.03	0.40
1:A:1974:VAL:HG23	1:A:1974:VAL:O	2.21	0.40
1:B:9:MET:HE1	1:B:342:ILE:HA	2.02	0.40
1:B:136:GLN:O	1:B:137:ARG:C	2.64	0.40
1:B:207:SER:HB2	1:B:221:GLY:C	2.46	0.40
1:B:295:THR:HG22	1:B:331:HIS:CD2	2.55	0.40
1:B:309:VAL:C	1:B:311:ALA:N	2.79	0.40
1:B:366:ILE:O	1:B:366:ILE:CG1	2.68	0.40
1:B:1139:GLU:OE2	1:B:1216:LEU:CD1	2.68	0.40
1:B:1453:VAL:HG12	1:B:1457:VAL:HG23	2.03	0.40
1:B:1473:LEU:CG	1:B:1503:MET:HA	2.51	0.40
1:B:1476:ASN:C	1:B:1477:LEU:HD23	2.46	0.40
1:B:1741:VAL:CG1	1:B:1742:ASP:N	2.84	0.40
1:B:1780:LEU:HD12	1:B:1781:GLY:N	2.36	0.40
1:B:1931:GLU:OE1	1:B:1931:GLU:HA	2.21	0.40
1:A:23:TRP:CZ2	1:A:27:ILE:HG12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HG	1:A:144:LEU:HD13	2.02	0.40
1:A:161:CYS:HB3	1:A:331:HIS:CE1	2.56	0.40
1:A:305:LEU:HD23	1:A:308:ILE:HD12	2.03	0.40
1:A:612:GLU:O	1:A:614:ASN:N	2.54	0.40
1:A:734:TYR:CD2	1:A:734:TYR:O	2.74	0.40
1:A:1315:LEU:HB3	1:A:1344:LEU:HD11	2.02	0.40
1:A:1433:LEU:HD21	1:A:1465:GLY:HA3	2.03	0.40
1:B:27:ILE:C	1:B:29:GLY:N	2.80	0.40
1:B:641:ALA:HB1	1:B:683:HIS:CB	2.49	0.40
1:B:1118:LYS:N	1:B:1517:PHE:O	2.47	0.40
1:B:1659:LEU:HD23	1:B:1767:LEU:CD1	2.51	0.40
1:A:81:MET:HG2	1:A:81:MET:H	1.62	0.40
1:A:219:GLY:O	1:A:298:LYS:HB2	2.20	0.40
1:A:429:ARG:HA	1:A:429:ARG:HD2	1.94	0.40
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.68	0.40
1:A:1118:LYS:HD2	1:A:2103:HIS:ND1	2.35	0.40
1:A:1347:HIS:CD2	1:A:1348:THR:O	2.74	0.40
1:A:1500:ASP:O	1:A:1501:LEU:C	2.64	0.40
1:A:1674:HIS:ND1	1:A:1698:THR:CG2	2.83	0.40
1:A:1832:PRO:C	1:A:1834:THR:H	2.28	0.40
1:A:2090:SER:O	1:A:2094:VAL:HG23	2.22	0.40
1:B:420:LEU:HD12	1:B:512:ARG:HH11	1.86	0.40
1:B:490:ARG:HA	1:B:491:PRO:HD3	1.96	0.40
1:B:588:GLY:HA3	1:B:730:PHE:CE1	2.57	0.40
1:B:623:VAL:CG1	1:B:624:GLY:N	2.85	0.40
1:B:654:PRO:O	1:B:658:MET:CB	2.68	0.40
1:B:1573:PHE:O	1:B:1576:VAL:HB	2.21	0.40
1:B:1636:VAL:HG23	1:B:1640:TRP:HB2	2.03	0.40
1:B:1863:PRO:O	1:B:1865:PRO:HD3	2.21	0.40
1:B:2004:ARG:O	1:B:2005:VAL:C	2.63	0.40
1:B:2041:MET:HA	1:B:2044:ILE:HG13	2.03	0.40
1:A:159:THR:O	1:A:160:ALA:HB3	2.21	0.40
1:A:588:GLY:O	1:A:594:LEU:HB2	2.21	0.40
1:A:654:PRO:HD3	1:A:686:PHE:HE1	1.86	0.40
1:A:666:LYS:O	1:A:668:GLU:N	2.55	0.40
1:A:825:ARG:HG2	1:A:826:GLY:N	2.36	0.40
1:A:1238:ALA:HB1	1:A:1467:HIS:CD2	2.56	0.40
1:A:1733:LEU:HA	1:A:1733:LEU:HD23	1.68	0.40
1:B:189:ASN:O	1:B:226:GLU:HB2	2.21	0.40
1:B:252:ASN:HD21	1:B:272:LEU:HB2	1.81	0.40
1:B:876:VAL:HA	1:B:884:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1314:LEU:HG	1:B:1315:LEU:N	2.36	0.40
1:B:1456:MET:CE	1:B:1460:LEU:HD22	2.52	0.40
1:B:1553:TYR:O	1:B:1882:PRO:HG3	2.21	0.40
1:B:1617:VAL:HG21	1:B:1626:VAL:HG11	2.04	0.40
1:B:2017:VAL:HG12	1:B:2018:ILE:N	2.37	0.40
1:A:94:GLY:N	1:A:453:MET:HE3	2.36	0.40
1:A:273:ILE:O	1:A:277:TYR:HD1	2.05	0.40
1:A:509:SER:O	1:A:512:ARG:HG3	2.22	0.40
1:B:331:HIS:C	1:B:333:GLU:H	2.29	0.40
1:B:912:VAL:HG22	1:B:913:VAL:N	2.36	0.40
1:B:971:ASP:OD1	1:B:973:ARG:HB2	2.21	0.40
1:B:1726:THR:O	1:B:1726:THR:CG2	2.70	0.40
1:B:2022:VAL:HG13	1:B:2026:ARG:HG2	2.04	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	1948/2512 (78%)	1586 (81%)	282 (14%)	80 (4%)	2	16
1	B	1992/2512 (79%)	1622 (81%)	296 (15%)	74 (4%)	2	17
All	All	3940/5024 (78%)	3208 (81%)	578 (15%)	154 (4%)	2	17

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLU
1	A	255	GLY
1	A	278	ALA
1	A	333	GLU
1	A	413	PRO

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Mol	Chain	Res	Type
1	A	418	ALA
1	A	582	LEU
1	A	615	VAL
1	A	818	PRO
1	A	839	SER
1	A	976	VAL
1	A	1224	PRO
1	A	1303	ASN
1	A	1485	GLU
1	A	1611	ARG
1	A	1638	SER
1	A	1749	ALA
1	A	1802	GLU
1	A	1862	GLY
1	B	179	GLU
1	B	255	GLY
1	B	278	ALA
1	B	333	GLU
1	B	418	ALA
1	B	636	PRO
1	B	669	ASP
1	B	839	SER
1	B	978	PRO
1	B	980	ASP
1	B	1224	PRO
1	B	1749	ALA
1	B	1800	PHE
1	B	1862	GLY
1	A	163	SER
1	A	282	PRO
1	A	318	GLU
1	A	387	ASN
1	A	476	GLU
1	A	488	SER
1	A	984	GLU
1	A	985	PHE
1	A	1056	SER
1	A	1301	PRO
1	A	1593	LEU
1	A	1735	HIS
1	A	1801	GLU
1	A	1870	PRO

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Mol	Chain	Res	Type
1	A	2025	GLY
1	A	2079	VAL
1	A	2112	ALA
1	B	163	SER
1	B	282	PRO
1	B	318	GLU
1	B	370	GLN
1	B	387	ASN
1	B	413	PRO
1	B	476	GLU
1	B	856	CYS
1	B	974	ALA
1	B	983	ALA
1	B	984	GLU
1	B	1225	ALA
1	B	1301	PRO
1	B	1302	ALA
1	B	1593	LEU
1	B	1735	HIS
1	B	1802	GLU
1	B	1858	GLU
1	B	2025	GLY
1	B	2079	VAL
1	A	216	ASP
1	A	254	ASP
1	A	310	ASN
1	A	317	ARG
1	A	319	PRO
1	A	613	ALA
1	A	854	SER
1	A	1014	ASP
1	A	1110	GLU
1	A	1225	ALA
1	A	1596	ASP
1	A	1649	PRO
1	A	1706	ALA
1	A	2021	SER
1	B	213	ARG
1	B	254	ASP
1	B	317	ARG
1	B	319	PRO
1	B	488	SER

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Mol	Chain	Res	Type
1	B	820	GLU
1	B	1056	SER
1	B	1560	GLN
1	B	1596	ASP
1	B	1706	ALA
1	B	1863	PRO
1	B	2065	ASP
1	A	14	PRO
1	A	237	SER
1	A	238	LEU
1	A	445	SER
1	A	848	ALA
1	A	857	SER
1	A	1389	LEU
1	A	1409	PRO
1	A	1557	ALA
1	A	1734	ARG
1	A	1800	PHE
1	A	1835	LYS
1	A	2065	ASP
1	A	2078	THR
1	B	14	PRO
1	B	60	PHE
1	B	162	SER
1	B	238	LEU
1	B	310	ASN
1	B	445	SER
1	B	1014	ASP
1	B	1110	GLU
1	B	1449	SER
1	B	1464	PRO
1	B	1491	SER
1	B	1548	CYS
1	B	1734	ARG
1	B	1932	TRP
1	B	1982	ASN
1	B	2021	SER
1	B	2078	THR
1	B	2102	PRO
1	A	60	PHE
1	A	162	SER
1	A	215	PHE

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Mol	Chain	Res	Type
1	A	617	PRO
1	A	1464	PRO
1	A	1471	CYS
1	A	1597	CYS
1	A	1692	GLY
1	A	1865	PRO
1	A	2056	LEU
1	A	2102	PRO
1	B	1835	LYS
1	B	1978	ALA
1	B	1979	VAL
1	B	2056	LEU
1	A	1500	ASP
1	B	635	PRO
1	B	1467	HIS
1	A	487	GLY
1	A	853	GLY
1	B	1303	ASN
1	B	1409	PRO
1	B	487	GLY
1	A	355	PRO
1	A	1240	PRO
1	B	1408	THR

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	1624/2072 (78%)	1412 (87%)	212 (13%)	4	19
1	B	1660/2072 (80%)	1436 (86%)	224 (14%)	4	18
All	All	3284/4144 (79%)	2848 (87%)	436 (13%)	4	18

All (436) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	33	VAL
1	A	59	ARG
1	A	81	MET
1	A	86	THR
1	A	95	ILE
1	A	111	VAL
1	A	120	LEU
1	A	123	ASP
1	A	128	VAL
1	A	132	MET
1	A	136	GLN
1	A	143	ARG
1	A	144	LEU
1	A	169	GLN
1	A	170	SER
1	A	181	SER
1	A	224	ARG
1	A	241	ARG
1	A	248	ASN
1	A	251	THR
1	A	295	THR
1	A	297	THR
1	A	309	VAL
1	A	318	GLU
1	A	320	LEU
1	A	329	MET
1	A	342	ILE
1	A	343	LYS
1	A	347	SER
1	A	356	ASN
1	A	366	ILE
1	A	371	ASP
1	A	375	GLN
1	A	383	ILE
1	A	399	ASN
1	A	400	VAL
1	A	402	VAL
1	A	407	ASN
1	A	429	ARG
1	A	431	LEU
1	A	439	GLU
1	A	446	ARG

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Mol	Chain	Res	Type
1	A	460	VAL
1	A	468	ARG
1	A	480	GLN
1	A	482	VAL
1	A	489	LYS
1	A	492	VAL
1	A	502	GLN
1	A	520	ILE
1	A	525	GLN
1	A	541	THR
1	A	543	GLU
1	A	549	ILE
1	A	552	SER
1	A	556	LEU
1	A	558	SER
1	A	568	THR
1	A	569	SER
1	A	572	LEU
1	A	597	GLU
1	A	614	ASN
1	A	616	LEU
1	A	660	GLU
1	A	665	LEU
1	A	673	LYS
1	A	674	GLU
1	A	675	VAL
1	A	677	THR
1	A	689	SER
1	A	703	LEU
1	A	728	ARG
1	A	736	VAL
1	A	746	GLN
1	A	757	VAL
1	A	775	LEU
1	A	819	VAL
1	A	825	ARG
1	A	830	ILE
1	A	846	SER
1	A	849	ASP
1	A	857	SER
1	A	866	VAL
1	A	894	LEU

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Mol	Chain	Res	Type
1	A	895	THR
1	A	917	VAL
1	A	931	VAL
1	A	937	LEU
1	A	941	SER
1	A	947	SER
1	A	949	SER
1	A	950	ASN
1	A	953	LEU
1	A	959	VAL
1	A	964	SER
1	A	972	THR
1	A	1011	LEU
1	A	1026	ASP
1	A	1038	MET
1	A	1050	LEU
1	A	1052	THR
1	A	1055	THR
1	A	1068	LEU
1	A	1069	TYR
1	A	1070	THR
1	A	1074	THR
1	A	1084	ARG
1	A	1086	LEU
1	A	1087	ASN
1	A	1088	THR
1	A	1095	LEU
1	A	1097	LEU
1	A	1101	SER
1	A	1103	VAL
1	A	1107	ARG
1	A	1112	LEU
1	A	1122	THR
1	A	1216	LEU
1	A	1235	GLU
1	A	1247	VAL
1	A	1264	THR
1	A	1267	VAL
1	A	1268	MET
1	A	1275	THR
1	A	1290	GLU
1	A	1299	TRP

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Mol	Chain	Res	Type
1	A	1314	LEU
1	A	1316	VAL
1	A	1346	LEU
1	A	1376	ASP
1	A	1401	LEU
1	A	1408	THR
1	A	1421	THR
1	A	1428	SER
1	A	1456	MET
1	A	1460	LEU
1	A	1469	ILE
1	A	1473	LEU
1	A	1476	ASN
1	A	1480	THR
1	A	1481	SER
1	A	1491	SER
1	A	1505	VAL
1	A	1525	GLU
1	A	1528	THR
1	A	1541	LEU
1	A	1542	SER
1	A	1571	LEU
1	A	1573	PHE
1	A	1580	THR
1	A	1583	LEU
1	A	1596	ASP
1	A	1597	CYS
1	A	1614	MET
1	A	1626	VAL
1	A	1638	SER
1	A	1639	THR
1	A	1651	VAL
1	A	1654	THR
1	A	1660	VAL
1	A	1662	ARG
1	A	1666	GLN
1	A	1669	GLU
1	A	1697	THR
1	A	1698	THR
1	A	1699	VAL
1	A	1720	PHE
1	A	1722	ASN

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Mol	Chain	Res	Type
1	A	1735	HIS
1	A	1736	THR
1	A	1741	VAL
1	A	1760	LEU
1	A	1762	GLN
1	A	1768	GLU
1	A	1790	THR
1	A	1794	ILE
1	A	1795	LEU
1	A	1815	LYS
1	A	1823	VAL
1	A	1841	ARG
1	A	1843	MET
1	A	1853	VAL
1	A	1856	VAL
1	A	1860	GLU
1	A	1861	GLN
1	A	1873	LEU
1	A	1877	SER
1	A	1899	GLN
1	A	1904	LEU
1	A	1906	LEU
1	A	1915	THR
1	A	1922	THR
1	A	1937	VAL
1	A	1939	VAL
1	A	1940	LEU
1	A	1941	VAL
1	A	1944	SER
1	A	1956	ILE
1	A	1957	THR
1	A	1960	THR
1	A	1996	TYR
1	A	2005	VAL
1	A	2006	THR
1	A	2022	VAL
1	A	2026	ARG
1	A	2044	ILE
1	A	2078	THR
1	A	2088	ILE
1	A	2096	ASP
1	A	2105	VAL

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Mol	Chain	Res	Type
1	A	2111	LEU
1	B	32	MET
1	B	33	VAL
1	B	59	ARG
1	B	81	MET
1	B	86	THR
1	B	95	ILE
1	B	111	VAL
1	B	120	LEU
1	B	122	ARG
1	B	123	ASP
1	B	126	THR
1	B	127	LEU
1	B	128	VAL
1	B	136	GLN
1	B	144	LEU
1	B	168	LEU
1	B	169	GLN
1	B	170	SER
1	B	181	SER
1	B	224	ARG
1	B	241	ARG
1	B	251	THR
1	B	273	ILE
1	B	288	GLU
1	B	295	THR
1	B	297	THR
1	B	309	VAL
1	B	318	GLU
1	B	320	LEU
1	B	322	ILE
1	B	329	MET
1	B	342	ILE
1	B	343	LYS
1	B	347	SER
1	B	352	VAL
1	B	356	ASN
1	B	366	ILE
1	B	371	ASP
1	B	375	GLN
1	B	383	ILE
1	B	384	ARG

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Mol	Chain	Res	Type
1	B	399	ASN
1	B	400	VAL
1	B	402	VAL
1	B	407	ASN
1	B	429	ARG
1	B	431	LEU
1	B	439	GLU
1	B	460	VAL
1	B	468	ARG
1	B	482	VAL
1	B	489	LYS
1	B	492	VAL
1	B	502	GLN
1	B	512	ARG
1	B	520	ILE
1	B	525	GLN
1	B	545	VAL
1	B	549	ILE
1	B	552	SER
1	B	556	LEU
1	B	558	SER
1	B	568	THR
1	B	569	SER
1	B	572	LEU
1	B	615	VAL
1	B	664	GLN
1	B	670	VAL
1	B	675	VAL
1	B	689	SER
1	B	736	VAL
1	B	746	GLN
1	B	757	VAL
1	B	775	LEU
1	B	821	PHE
1	B	825	ARG
1	B	846	SER
1	B	866	VAL
1	B	894	LEU
1	B	917	VAL
1	B	931	VAL
1	B	937	LEU
1	B	941	SER

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Mol	Chain	Res	Type
1	B	947	SER
1	B	949	SER
1	B	950	ASN
1	B	953	LEU
1	B	959	VAL
1	B	964	SER
1	B	971	ASP
1	B	972	THR
1	B	976	VAL
1	B	980	ASP
1	B	982	THR
1	B	984	GLU
1	B	1011	LEU
1	B	1026	ASP
1	B	1038	MET
1	B	1052	THR
1	B	1055	THR
1	B	1068	LEU
1	B	1069	TYR
1	B	1070	THR
1	B	1074	THR
1	B	1084	ARG
1	B	1086	LEU
1	B	1087	ASN
1	B	1088	THR
1	B	1095	LEU
1	B	1097	LEU
1	B	1101	SER
1	B	1107	ARG
1	B	1122	THR
1	B	1138	GLU
1	B	1216	LEU
1	B	1235	GLU
1	B	1247	VAL
1	B	1264	THR
1	B	1267	VAL
1	B	1268	MET
1	B	1275	THR
1	B	1299	TRP
1	B	1314	LEU
1	B	1316	VAL
1	B	1331	VAL

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Mol	Chain	Res	Type
1	B	1337	THR
1	B	1340	GLU
1	B	1346	LEU
1	B	1373	LEU
1	B	1395	SER
1	B	1421	THR
1	B	1428	SER
1	B	1456	MET
1	B	1460	LEU
1	B	1469	ILE
1	B	1471	CYS
1	B	1473	LEU
1	B	1480	THR
1	B	1481	SER
1	B	1486	MET
1	B	1487	HIS
1	B	1505	VAL
1	B	1515	ARG
1	B	1525	GLU
1	B	1528	THR
1	B	1535	VAL
1	B	1536	LEU
1	B	1548	CYS
1	B	1551	LEU
1	B	1558	SER
1	B	1571	LEU
1	B	1573	PHE
1	B	1580	THR
1	B	1583	LEU
1	B	1595	ARG
1	B	1597	CYS
1	B	1603	PHE
1	B	1612	ARG
1	B	1617	VAL
1	B	1626	VAL
1	B	1636	VAL
1	B	1639	THR
1	B	1641	THR
1	B	1653	THR
1	B	1660	VAL
1	B	1661	VAL
1	B	1662	ARG

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Mol	Chain	Res	Type
1	B	1669	GLU
1	B	1671	VAL
1	B	1687	ILE
1	B	1694	ARG
1	B	1695	VAL
1	B	1697	THR
1	B	1698	THR
1	B	1699	VAL
1	B	1720	PHE
1	B	1722	ASN
1	B	1726	THR
1	B	1735	HIS
1	B	1736	THR
1	B	1741	VAL
1	B	1760	LEU
1	B	1762	GLN
1	B	1768	GLU
1	B	1790	THR
1	B	1794	ILE
1	B	1795	LEU
1	B	1815	LYS
1	B	1818	ILE
1	B	1823	VAL
1	B	1841	ARG
1	B	1843	MET
1	B	1853	VAL
1	B	1856	VAL
1	B	1860	GLU
1	B	1868	LEU
1	B	1873	LEU
1	B	1877	SER
1	B	1899	GLN
1	B	1904	LEU
1	B	1906	LEU
1	B	1915	THR
1	B	1922	THR
1	B	1937	VAL
1	B	1939	VAL
1	B	1940	LEU
1	B	1941	VAL
1	B	1944	SER
1	B	1956	ILE

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Mol	Chain	Res	Type
1	B	1957	THR
1	B	1960	THR
1	B	1979	VAL
1	B	1982	ASN
1	B	1996	TYR
1	B	2005	VAL
1	B	2006	THR
1	B	2022	VAL
1	B	2026	ARG
1	B	2044	ILE
1	B	2063	ILE
1	B	2078	THR
1	B	2088	ILE
1	B	2096	ASP
1	B	2105	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	96	ASN
1	A	136	GLN
1	A	248	ASN
1	A	306	ASN
1	A	350	HIS
1	A	356	ASN
1	A	358	HIS
1	A	387	ASN
1	A	399	ASN
1	A	405	GLN
1	A	444	HIS
1	A	483	GLN
1	A	525	GLN
1	A	560	GLN
1	A	632	GLN
1	A	644	ASN
1	A	697	GLN
1	A	737	ASN
1	A	833	HIS
1	A	1037	HIS
1	A	1109	GLN
1	A	1111	HIS

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Mol	Chain	Res	Type
1	A	1124	HIS
1	A	1318	ASN
1	A	1388	HIS
1	A	1407	GLN
1	A	1467	HIS
1	A	1487	HIS
1	A	1494	GLN
1	A	1735	HIS
1	A	1777	ASN
1	A	1778	HIS
1	A	1855	GLN
1	A	2076	ASN
1	A	2103	HIS
1	B	25	ASN
1	B	96	ASN
1	B	136	GLN
1	B	199	GLN
1	B	248	ASN
1	B	306	ASN
1	B	331	HIS
1	B	350	HIS
1	B	356	ASN
1	B	358	HIS
1	B	387	ASN
1	B	399	ASN
1	B	405	GLN
1	B	444	HIS
1	B	502	GLN
1	B	525	GLN
1	B	560	GLN
1	B	632	GLN
1	B	643	HIS
1	B	697	GLN
1	B	737	ASN
1	B	738	ASN
1	B	833	HIS
1	B	1037	HIS
1	B	1109	GLN
1	B	1111	HIS
1	B	1298	GLN
1	B	1406	GLN
1	B	1467	HIS

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Mol	Chain	Res	Type
1	B	1530	HIS
1	B	1674	HIS
1	B	1735	HIS
1	B	1777	ASN
1	B	1778	HIS
1	B	1855	GLN
1	B	1884	HIS
1	B	2076	ASN
1	B	2103	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1962/2512 (78%)	-0.56	3 (0%)	91 85	63, 118, 226, 276	0
1	B	2004/2512 (79%)	-0.45	3 (0%)	92 89	54, 158, 230, 276	0
All	All	3966/5024 (78%)	-0.51	6 (0%)	91 85	54, 136, 229, 276	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1327	PRO	2.6
1	A	1312	ALA	2.4
1	B	222	TYR	2.3
1	A	1344	LEU	2.3
1	A	1451	SER	2.1
1	B	1475	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.