Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:58 am BST

PDB ID	:	1EA0
Title	:	Alpha subunit of A. brasilense glutamate synthase
Authors	:	Binda, C.; Bossi, R.T.; Vanoni, M.A.; Mattevi, A.
Deposited on	:	2000-11-02
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

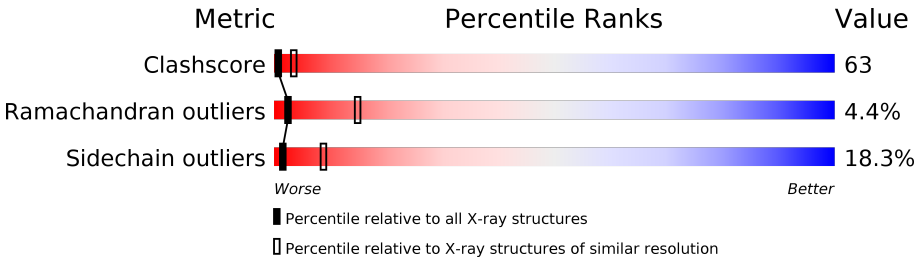
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1479	26% 50% 19%
1	B	1479	31% 47% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OMT	A	2473	-	X	-	-
5	F3S	A	2476	-	-	X	-
5	F3S	B	2476	-	-	X	-

2 Entry composition

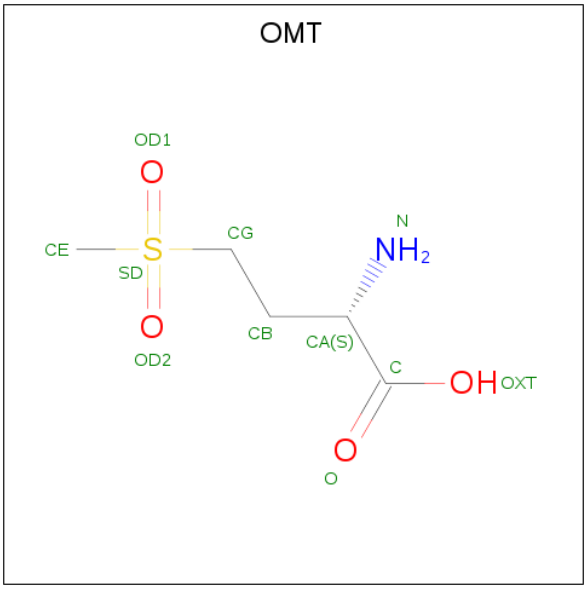
There are 5 unique types of molecules in this entry. The entry contains 22478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN.

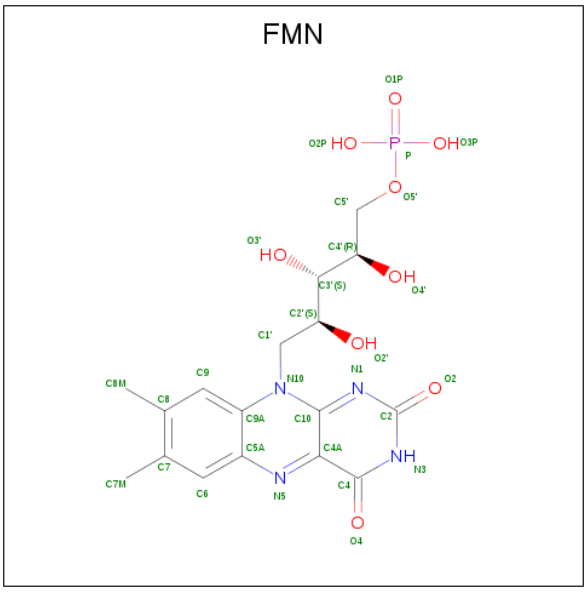
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			
1	B	1452	Total	C	N	O	S	0	0	0
			11180	7018	2005	2098	59			

- Molecule 2 is S-DIOXYMETHIONINE (three-letter code: OMT) (formula: $C_5H_{11}NO_4S$).



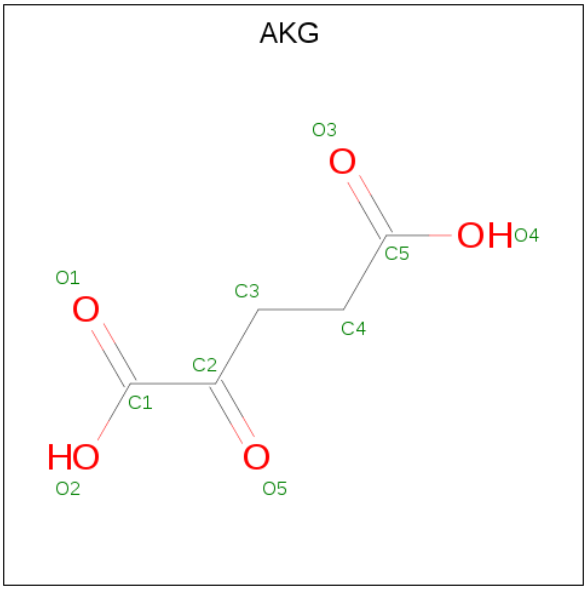
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			11	5	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			11	5	1	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



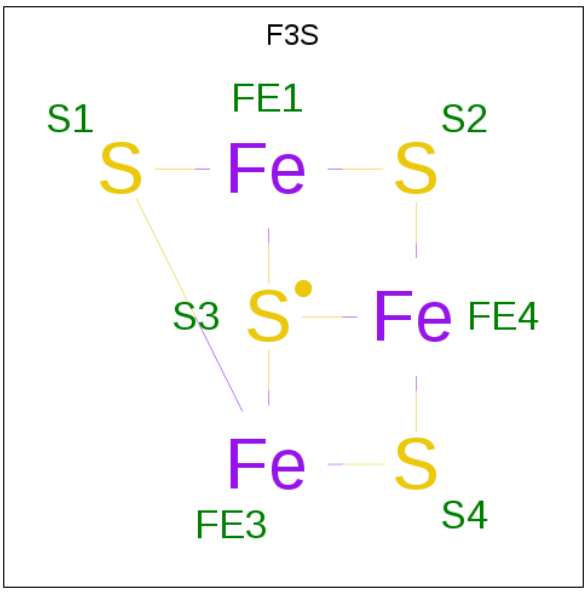
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			10	5	5			
4	B	1	Total	C	O		0	0
			10	5	5			

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 7 3 4	0	0
5	B	1	Total Fe S 7 3 4	0	0

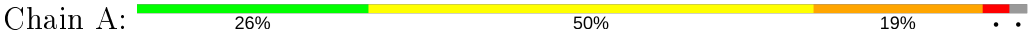
3 Residue-property plots (i)

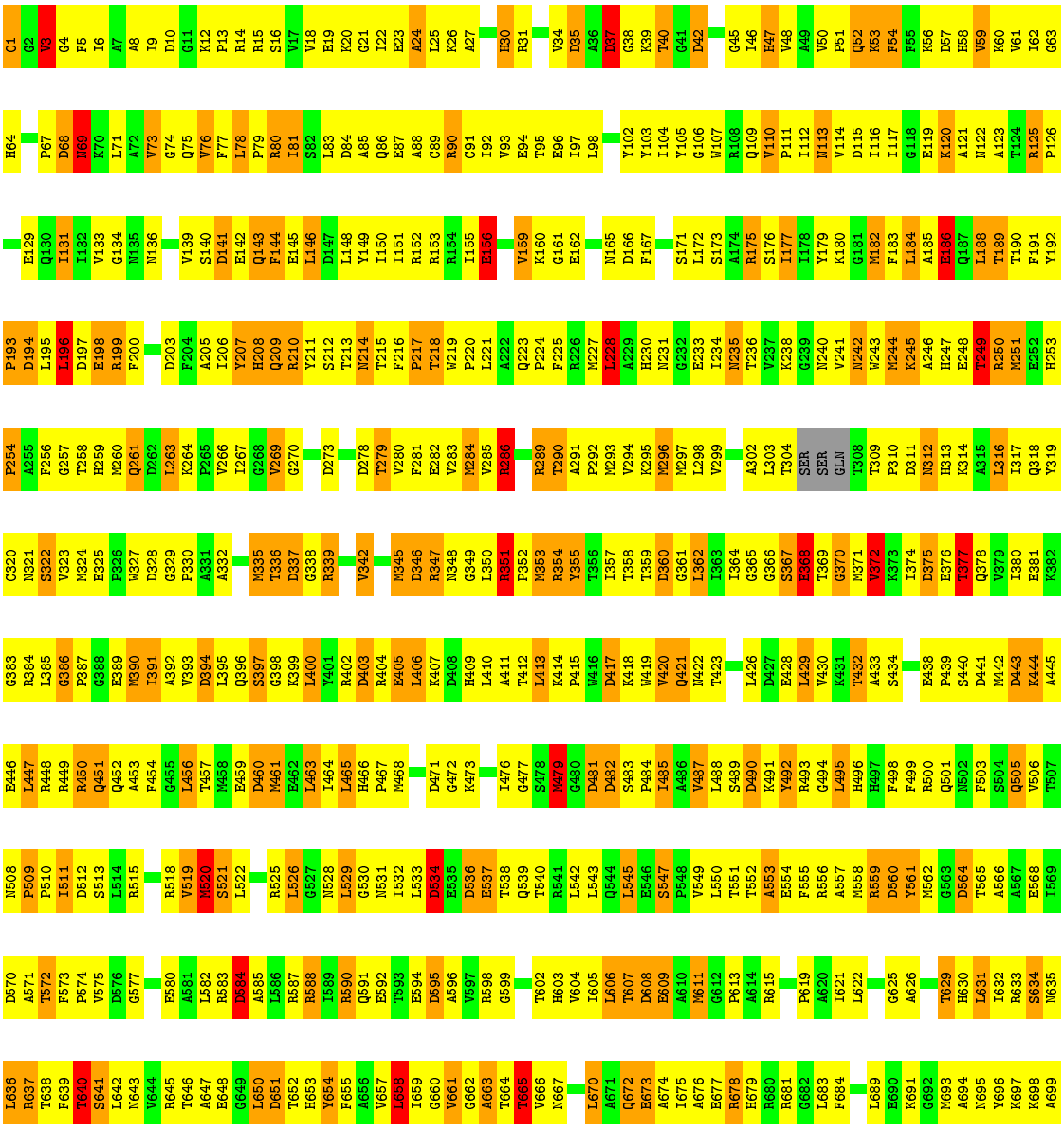
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

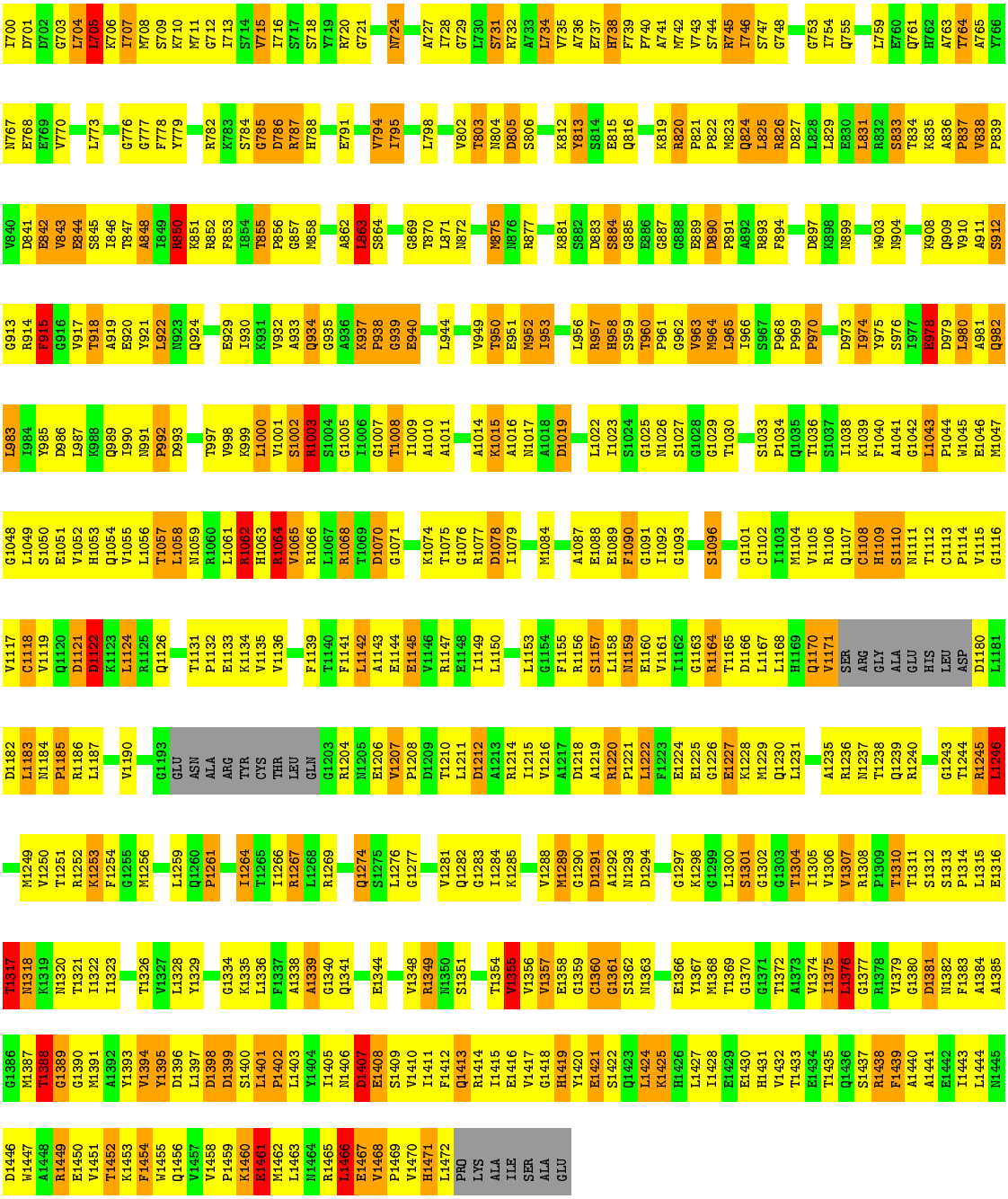
Note EDS was not executed.

- Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain A:

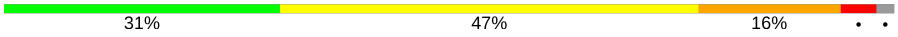


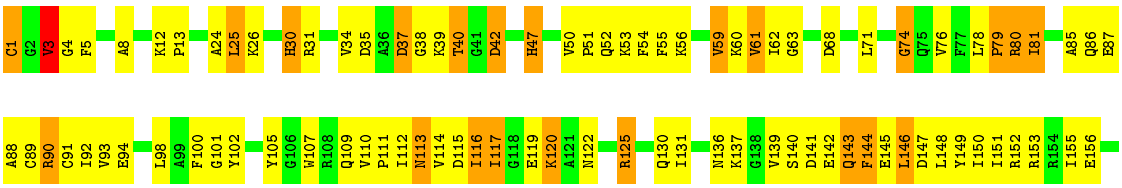


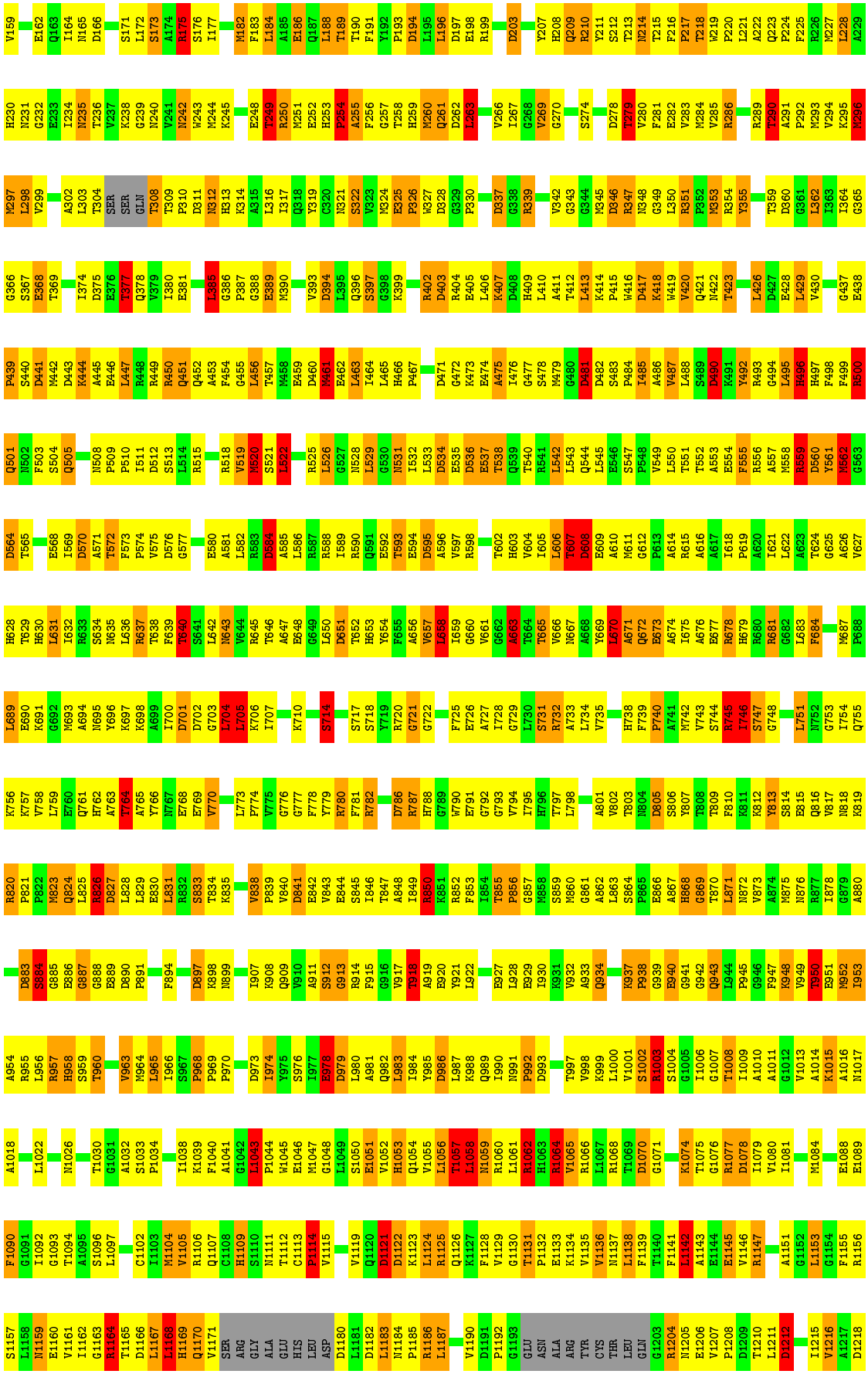


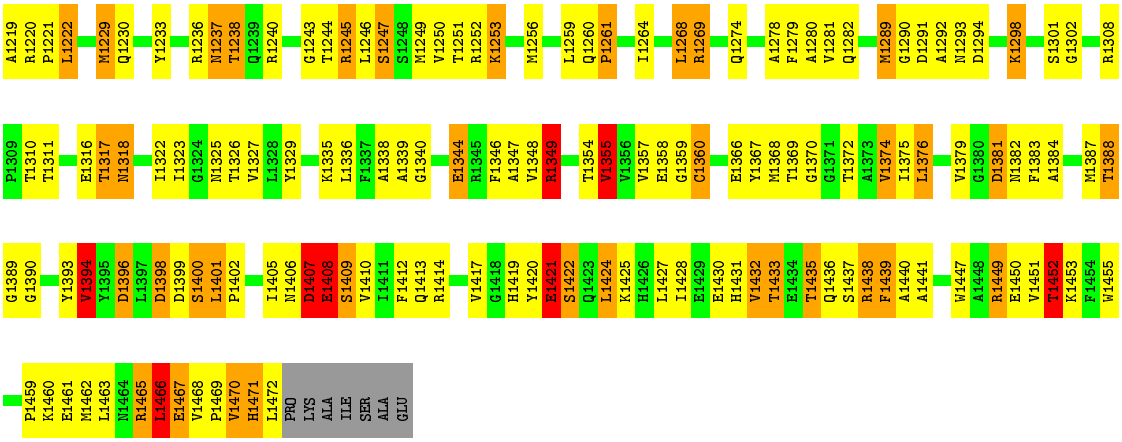
• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain B:








A1219 R1220 P1221 L1222 M1229 Q1230 Y1233 R1236 N1237 T1238 Q1239 R1240 G1243 T1244 R1245 L1246 S1247 S1248 M1249 V1250 T1251 R1252 K1253 M1256 L1259 Q1260 P1261 I1264 L1268 R1269 Q1274 A1278 F1279 A1280 V1281 Q1282 M1289 G1290 D1291 A1292 N1293 D1294 K1298 S1301 G1302 R1308
P1309 T1310 T1311 E1316 T1317 N1318 I1322 I1323 G1324 N1325 T1326 V1327 L1328 Y1329 K1335 L1336 F1337 A1338 A1339 G1340 E1344 R1345 F1346 A1347 V1348 R1349 T1354 V1355 V1356 V1357 E1358 G1359 C1360 E1366 Y1367 M1368 T1369 G1370 G1371 T1372 A1373 V1374 I1375 L1376 V1379 G1380 D1381 N1382 F1383 A1384 M1387 T1388
G1389 G1390 Y1393 V1394 Y1395 D1396 L1397 D1398 D1399 S1400 L1401 P1402 I1405 N1406 D1407 E1408 S1409 V1410 I1411 F1412 Q1413 R1414 V1417 G1418 H1419 Y1420 E1421 S1422 Q1423 L1424 K1425 H1426 L1427 I1428 E1429 E1430 H1431 V1432 T1433 E1434 T1435 Q1436 S1437 R1438 F1439 A1440 A1441 W1447 A1448 R1449 E1450 V1451 T1452 K1453 F1454 W1455
P1459 K1460 E1461 M1462 L1463 N1464 R1465 L1466 E1467 V1468 P1469 V1470 H1471 L1472 PRO LYS ALA ILE SER ALA GLU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	233.61Å 233.61Å 305.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.6 (20.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22478	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, F3S, AKG, OMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.06	7/11383 (0.1%)	1.58	198/15390 (1.3%)
1	B	1.10	7/11383 (0.1%)	1.58	192/15390 (1.2%)
All	All	1.08	14/22766 (0.1%)	1.58	390/30780 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	2
All	All	1	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	838	VAL	CA-CB	-7.71	1.38	1.54
1	A	746	ILE	CA-CB	-7.47	1.37	1.54
1	A	848	ALA	CA-CB	-6.51	1.38	1.52
1	A	1065	VAL	CB-CG2	-6.15	1.40	1.52
1	A	3	VAL	CA-CB	-5.67	1.42	1.54
1	B	1394	VAL	CB-CG1	-5.54	1.41	1.52
1	B	1216	VAL	CB-CG1	-5.49	1.41	1.52
1	A	910	VAL	CA-CB	-5.46	1.43	1.54
1	B	500	ARG	C-O	-5.21	1.13	1.23
1	B	1136	VAL	CA-CB	-5.15	1.44	1.54
1	B	222	ALA	CA-CB	-5.10	1.41	1.52
1	B	1051	GLU	CD-OE2	5.02	1.31	1.25
1	B	862	ALA	CA-CB	-5.02	1.42	1.52
1	A	741	ALA	CA-CB	-5.01	1.42	1.52

All (390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1062	ARG	NE-CZ-NH1	-12.86	113.87	120.30
1	A	608	ASP	CB-CG-OD2	12.18	129.26	118.30
1	A	141	ASP	CB-CG-OD2	11.98	129.08	118.30
1	B	888	GLY	N-CA-C	-11.68	83.89	113.10
1	B	890	ASP	CB-CG-OD1	11.31	128.48	118.30
1	B	683	LEU	CB-CG-CD2	-11.18	92.00	111.00
1	B	1056	LEU	CB-CG-CD1	-10.57	93.03	111.00
1	A	1019	ASP	CB-CG-OD2	10.48	127.73	118.30
1	B	1466	LEU	CB-CG-CD1	-10.39	93.33	111.00
1	B	852	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	B	456	LEU	CB-CG-CD2	-10.27	93.54	111.00
1	A	1003	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	A	805	ASP	CB-CG-OD2	10.16	127.44	118.30
1	B	460	ASP	CB-CG-OD2	9.91	127.22	118.30
1	B	394	ASP	CB-CG-OD2	9.79	127.11	118.30
1	A	479	MET	CG-SD-CE	9.65	115.63	100.20
1	B	608	ASP	CB-CG-OD1	-9.64	109.62	118.30
1	A	1064	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	A	351	ARG	NE-CZ-NH2	9.59	125.10	120.30
1	B	940	GLU	N-CA-C	9.59	136.89	111.00
1	A	460	ASP	CB-CG-OD2	9.47	126.82	118.30
1	A	1062	ARG	NE-CZ-NH1	-9.47	115.56	120.30
1	B	1218	ASP	CB-CG-OD2	9.44	126.80	118.30
1	A	1003	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	584	ASP	CB-CG-OD2	9.42	126.78	118.30
1	B	915	PHE	CA-C-N	9.37	134.94	116.20
1	B	584	ASP	CB-CG-OD2	9.26	126.64	118.30
1	B	608	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	938	PRO	C-N-CA	-9.20	102.99	122.30
1	B	1355	VAL	CB-CA-C	-9.20	93.92	111.40
1	A	890	ASP	CB-CG-OD1	9.17	126.56	118.30
1	A	940	GLU	N-CA-C	9.16	135.74	111.00
1	A	394	ASP	CB-CG-OD2	9.09	126.48	118.30
1	A	1355	VAL	CB-CA-C	-9.03	94.25	111.40
1	B	1164	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	B	228	LEU	CB-CG-CD1	-8.82	96.01	111.00
1	A	1062	ARG	NE-CZ-NH2	8.78	124.69	120.30
1	A	403	ASP	CB-CG-OD2	8.69	126.12	118.30
1	A	351	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	B	915	PHE	CB-CG-CD2	-8.57	114.80	120.80
1	A	1218	ASP	CB-CG-OD2	8.56	126.00	118.30
1	B	915	PHE	CB-CG-CD1	8.48	126.74	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1349	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	A	534	ASP	CB-CG-OD2	8.37	125.83	118.30
1	A	228	LEU	CB-CG-CD1	-8.33	96.85	111.00
1	A	337	ASP	CB-CG-OD1	8.32	125.79	118.30
1	B	369	THR	C-N-CA	-8.29	104.90	122.30
1	B	337	ASP	N-CA-C	-8.28	88.66	111.00
1	A	545	LEU	CA-CB-CG	-8.26	96.29	115.30
1	B	1390	GLY	N-CA-C	-8.23	92.52	113.10
1	B	979	ASP	CB-CG-OD2	8.21	125.69	118.30
1	B	1466	LEU	CA-CB-CG	8.17	134.08	115.30
1	B	182	MET	CG-SD-CE	-8.15	87.16	100.20
1	A	1466	LEU	CB-CG-CD1	-8.08	97.27	111.00
1	A	746	ILE	CG1-CB-CG2	7.99	128.97	111.40
1	B	650	LEU	CB-CG-CD2	-7.96	97.47	111.00
1	B	678	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	A	286	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	A	1466	LEU	CA-CB-CG	7.87	133.41	115.30
1	A	482	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	805	ASP	CB-CG-OD1	-7.82	111.27	118.30
1	A	372	VAL	CB-CA-C	-7.81	96.55	111.40
1	B	826	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	B	536	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	965	LEU	CB-CG-CD2	-7.68	97.95	111.00
1	B	705	LEU	CB-CG-CD2	-7.64	98.00	111.00
1	B	805	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	360	ASP	CB-CG-OD2	7.61	125.15	118.30
1	A	360	ASP	CB-CG-OD2	7.60	125.14	118.30
1	B	689	LEU	CB-CG-CD1	-7.59	98.10	111.00
1	B	560	ASP	CB-CG-OD1	7.55	125.09	118.30
1	A	1376	LEU	CA-CB-CG	-7.54	97.96	115.30
1	A	993	ASP	CB-CG-OD2	7.49	125.04	118.30
1	B	689	LEU	CA-CB-CG	-7.47	98.12	115.30
1	B	91	CYS	CA-CB-SG	-7.45	100.59	114.00
1	A	608	ASP	CB-CG-OD1	-7.45	111.60	118.30
1	B	993	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	175	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	B	746	ILE	CG1-CB-CG2	7.40	127.69	111.40
1	A	1147	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	B	915	PHE	C-N-CA	-7.39	106.78	122.30
1	B	228	LEU	CB-CA-C	-7.37	96.19	110.20
1	A	354	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	490	ASP	N-CA-CB	-7.33	97.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1390	GLY	N-CA-C	-7.33	94.78	113.10
1	A	584	ASP	CB-CG-OD1	-7.33	111.71	118.30
1	B	1168	LEU	CA-CB-CG	7.31	132.11	115.30
1	A	915	PHE	C-N-CA	-7.25	107.07	122.30
1	B	826	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	A	835	LYS	CD-CE-NZ	7.14	128.11	111.70
1	B	263	LEU	CA-CB-CG	-7.13	98.90	115.30
1	B	1153	LEU	CA-CB-CG	-7.13	98.90	115.30
1	B	339	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	A	263	LEU	CA-CB-CG	-7.12	98.92	115.30
1	A	490	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	595	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	500	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	519	VAL	CB-CA-C	-7.06	97.98	111.40
1	B	368	GLU	CA-CB-CG	7.06	128.93	113.40
1	B	1062	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	B	835	LYS	CD-CE-NZ	7.04	127.89	111.70
1	B	963	VAL	CB-CA-C	-7.02	98.06	111.40
1	B	913	GLY	N-CA-C	-7.00	95.60	113.10
1	A	613	PRO	N-CD-CG	-7.00	92.70	103.20
1	A	1056	LEU	CB-CG-CD1	-6.97	99.16	111.00
1	B	1003	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	850	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	368	GLU	N-CA-CB	6.94	123.09	110.60
1	B	1153	LEU	CB-CG-CD2	-6.93	99.22	111.00
1	A	1068	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	B	337	ASP	C-N-CA	-6.90	107.81	122.30
1	A	837	PRO	N-CD-CG	-6.90	92.86	103.20
1	B	683	LEU	CA-CB-CG	-6.89	99.46	115.30
1	A	346	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	564	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	1252	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	B	481	ASP	CB-CG-OD2	6.81	124.43	118.30
1	B	831	LEU	CA-CB-CG	6.80	130.95	115.30
1	B	607	THR	N-CA-C	6.80	129.36	111.00
1	A	228	LEU	CB-CA-C	-6.80	97.29	110.20
1	A	505	GLN	C-N-CA	-6.78	104.75	121.70
1	A	536	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	963	VAL	CB-CA-C	-6.75	98.58	111.40
1	B	184	LEU	CB-CG-CD1	6.75	122.47	111.00
1	B	915	PHE	CA-C-O	-6.75	105.94	120.10
1	B	897	ASP	CB-CG-OD2	6.73	124.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	681	ARG	N-CA-C	-6.71	92.87	111.00
1	B	1121	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	850	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	590	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	B	1269	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	704	LEU	N-CA-CB	-6.59	97.23	110.40
1	A	481	ASP	CB-CG-OD2	6.56	124.20	118.30
1	B	570	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	726	GLU	N-CA-C	-6.53	93.37	111.00
1	A	337	ASP	N-CA-C	-6.53	93.38	111.00
1	B	704	LEU	CB-CG-CD1	6.52	122.09	111.00
1	B	42	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	803	THR	CA-CB-CG2	-6.47	103.34	112.40
1	A	887	GLY	N-CA-C	6.47	129.28	113.10
1	B	883	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	196	LEU	CA-CB-CG	-6.47	100.42	115.30
1	A	938	PRO	C-N-CA	-6.47	108.72	122.30
1	B	595	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	529	LEU	CA-CB-CG	-6.44	100.48	115.30
1	A	715	VAL	CB-CA-C	-6.42	99.21	111.40
1	B	590	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	1078	ASP	CB-CG-OD2	6.39	124.06	118.30
1	B	1125	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	B	637	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	1058	LEU	CB-CG-CD2	-6.34	100.22	111.00
1	B	1138	LEU	CB-CG-CD1	-6.34	100.22	111.00
1	B	346	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	978	GLU	CA-CB-CG	-6.34	99.46	113.40
1	B	141	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	1376	LEU	CB-CG-CD1	6.32	121.74	111.00
1	A	3	VAL	CB-CA-C	-6.30	99.42	111.40
1	A	964	MET	CB-CA-C	-6.30	97.81	110.40
1	A	106	GLY	N-CA-C	6.26	128.75	113.10
1	B	214	ASN	CB-CA-C	-6.25	97.89	110.40
1	A	520	MET	CB-CG-SD	-6.25	93.64	112.40
1	A	443	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	110	VAL	CA-CB-CG1	-6.23	101.56	110.90
1	B	182	MET	CB-CA-C	-6.21	97.97	110.40
1	B	1222	LEU	CB-CG-CD1	-6.19	100.47	111.00
1	A	915	PHE	N-CA-C	6.16	127.64	111.00
1	A	91	CYS	CA-CB-SG	-6.16	102.92	114.00
1	A	286	ARG	NE-CZ-NH2	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1053	HIS	CB-CA-C	-6.16	98.09	110.40
1	A	141	ASP	CB-CG-OD1	-6.13	112.79	118.30
1	A	560	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	986	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	50	VAL	CB-CA-C	-6.11	99.79	111.40
1	B	125	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	199	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	1074	LYS	CB-CA-C	-6.09	98.21	110.40
1	A	1122	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	90	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	B	519	VAL	CB-CA-C	-6.09	99.84	111.40
1	A	1070	ASP	CB-CG-OD2	6.08	123.78	118.30
1	B	732	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	289	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	732	ARG	CG-CD-NE	-6.06	99.08	111.80
1	B	684	PHE	N-CA-C	-6.05	94.65	111.00
1	B	203	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	890	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	B	250	ARG	CB-CA-C	-6.02	98.36	110.40
1	A	1180	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	1013	VAL	CG1-CB-CG2	-6.02	101.27	110.90
1	B	965	LEU	CB-CG-CD2	-6.02	100.77	111.00
1	B	3	VAL	CB-CA-C	-6.01	99.98	111.40
1	B	978	GLU	CA-CB-CG	-6.01	100.18	113.40
1	A	940	GLU	C-N-CA	-6.00	109.70	122.30
1	B	296	MET	CA-CB-CG	-6.00	103.10	113.30
1	B	850	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	672	GLN	N-CA-C	-6.00	94.81	111.00
1	B	640	THR	CB-CA-C	-5.99	95.42	111.60
1	A	196	LEU	CB-CG-CD1	-5.99	100.81	111.00
1	B	887	GLY	N-CA-C	5.99	128.07	113.10
1	B	74	GLY	N-CA-C	-5.98	98.15	113.10
1	A	843	VAL	CB-CA-C	-5.97	100.06	111.40
1	A	283	VAL	CB-CA-C	-5.94	100.11	111.40
1	A	1068	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	490	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	1374	VAL	CB-CA-C	-5.93	100.13	111.40
1	B	803	THR	CA-CB-CG2	-5.92	104.12	112.40
1	A	1294	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	511	ILE	CB-CA-C	-5.90	99.80	111.60
1	B	461	MET	CG-SD-CE	5.90	109.64	100.20
1	B	956	LEU	CB-CG-CD2	-5.90	100.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	125	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	782	ARG	N-CA-C	-5.90	95.08	111.00
1	A	471	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	1399	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	980	LEU	CB-CA-C	-5.88	99.03	110.20
1	B	564	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	1180	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	522	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	850	ARG	CA-CB-CG	5.87	126.31	113.40
1	A	193	PRO	N-CD-CG	-5.86	94.41	103.20
1	B	337	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	651	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	456	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	A	354	ARG	CG-CD-NE	-5.84	99.54	111.80
1	A	831	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	50	VAL	CB-CA-C	-5.82	100.34	111.40
1	B	651	ASP	CB-CA-C	-5.82	98.76	110.40
1	A	42	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	1003	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	194	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	311	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	1171	VAL	CA-CB-CG1	-5.78	102.23	110.90
1	B	79	PRO	N-CA-C	-5.77	97.10	112.10
1	B	1407	ASP	CB-CA-C	-5.77	98.86	110.40
1	B	485	ILE	CG1-CB-CG2	-5.77	98.71	111.40
1	A	1306	VAL	CB-CA-C	-5.76	100.45	111.40
1	B	1396	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	746	ILE	CB-CA-C	-5.74	100.11	111.60
1	A	368	GLU	N-CA-CB	5.73	120.92	110.60
1	A	1000	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	B	714	SER	CB-CA-C	-5.73	99.21	110.10
1	A	337	ASP	C-N-CA	-5.71	110.30	122.30
1	B	1407	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	403	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	794	VAL	CB-CA-C	5.69	122.21	111.40
1	A	1468	VAL	CB-CA-C	-5.69	100.59	111.40
1	A	1218	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	A	577	GLY	N-CA-C	5.68	127.29	113.10
1	A	1212	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	385	LEU	CA-CB-CG	5.66	128.33	115.30
1	B	992	PRO	N-CD-CG	-5.63	94.75	103.20
1	B	945	PRO	N-CD-CG	-5.62	94.76	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	608	ASP	N-CA-CB	-5.61	100.51	110.60
1	A	1183	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	A	182	MET	CG-SD-CE	-5.60	91.25	100.20
1	B	545	LEU	CA-CB-CG	-5.60	102.43	115.30
1	B	1212	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	471	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	940	GLU	C-N-CA	-5.59	110.57	122.30
1	B	407	LYS	CD-CE-NZ	5.58	124.54	111.70
1	B	941	GLY	N-CA-C	5.58	127.06	113.10
1	A	863	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	283	VAL	CB-CA-C	-5.57	100.81	111.40
1	A	1	CYS	CA-CB-SG	-5.56	104.00	114.00
1	A	534	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	B	1064	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	B	505	GLN	C-N-CA	-5.54	107.85	121.70
1	B	745	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	214	ASN	CB-CA-C	-5.54	99.33	110.40
1	B	194	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	490	ASP	N-CA-CB	-5.53	100.65	110.60
1	A	406	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	B	298	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	A	1108	CYS	CB-CA-C	5.51	121.41	110.40
1	B	1187	LEU	CB-CG-CD1	-5.49	101.66	111.00
1	B	624	THR	OG1-CB-CG2	-5.49	97.37	110.00
1	A	251	MET	CB-CG-SD	-5.48	95.95	112.40
1	A	1399	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	441	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	1407	ASP	CB-CA-C	-5.47	99.46	110.40
1	B	838	VAL	CB-CA-C	-5.47	101.01	111.40
1	A	14	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	456	LEU	CA-CB-CG	-5.46	102.73	115.30
1	A	73	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	934	GLN	CB-CA-C	-5.46	99.48	110.40
1	B	863	LEU	CB-CA-C	5.46	120.58	110.20
1	A	650	LEU	CB-CG-CD1	-5.46	101.73	111.00
1	A	992	PRO	N-CD-CG	-5.45	95.03	103.20
1	A	182	MET	CA-CB-CG	-5.45	104.04	113.30
1	B	918	THR	N-CA-CB	-5.44	99.96	110.30
1	B	701	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	125	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	463	LEU	CA-CB-CG	-5.43	102.82	115.30
1	A	665	THR	N-CA-CB	-5.41	100.02	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	290	THR	CB-CA-C	-5.41	97.00	111.60
1	A	156	GLU	CA-CB-CG	5.40	125.29	113.40
1	B	968	PRO	N-CD-CG	-5.40	95.10	103.20
1	A	738	HIS	N-CA-C	5.39	125.56	111.00
1	B	1183	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	B	658	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	A	1147	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	131	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	A	482	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	3	VAL	N-CA-C	-5.35	96.55	111.00
1	B	529	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	A	609	GLU	C-N-CA	-5.35	108.33	121.70
1	B	1043	LEU	CA-CB-CG	-5.34	103.01	115.30
1	A	1321	THR	OG1-CB-CG2	-5.34	97.72	110.00
1	A	986	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	339	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	671	ALA	N-CA-C	-5.33	96.60	111.00
1	A	69	ASN	CB-CA-C	-5.33	99.75	110.40
1	A	159	VAL	CB-CA-C	-5.33	101.28	111.40
1	B	650	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	186	GLU	CA-CB-CG	-5.32	101.71	113.40
1	B	871	LEU	CB-CG-CD1	5.32	120.04	111.00
1	B	90	ARG	N-CA-CB	5.31	120.16	110.60
1	B	948	LYS	CB-CG-CD	-5.31	97.80	111.60
1	A	263	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	A	827	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	64	HIS	N-CA-C	-5.28	96.74	111.00
1	A	448	ARG	CB-CA-C	5.28	120.96	110.40
1	B	262	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	1259	LEU	CB-CG-CD2	5.27	119.96	111.00
1	B	1074	LYS	CB-CA-C	-5.26	99.87	110.40
1	A	940	GLU	O-C-N	-5.26	114.26	123.20
1	A	850	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	1096	SER	N-CA-CB	5.25	118.37	110.50
1	B	1268	LEU	CB-CA-C	-5.24	100.24	110.20
1	B	1	CYS	CA-CB-SG	-5.24	104.58	114.00
1	B	943	GLN	CB-CA-C	-5.23	99.93	110.40
1	A	1065	VAL	N-CA-CB	-5.22	100.01	111.50
1	B	663	ALA	N-CA-CB	-5.22	102.79	110.10
1	B	1043	LEU	CB-CG-CD1	5.22	119.87	111.00
1	A	90	ARG	NE-CZ-NH1	-5.21	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	918	THR	N-CA-CB	-5.21	100.39	110.30
1	A	196	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	A	296	MET	CA-CB-CG	-5.21	104.45	113.30
1	B	957	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	881	LYS	CD-CE-NZ	5.20	123.66	111.70
1	A	922	LEU	CB-CG-CD2	5.19	119.82	111.00
1	B	670	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	A	284	MET	CG-SD-CE	-5.18	91.91	100.20
1	A	250	ARG	CB-CA-C	-5.18	100.05	110.40
1	A	877	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	1388	THR	N-CA-C	5.17	124.95	111.00
1	B	1070	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	400	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	B	827	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	915	PHE	CA-CB-CG	-5.16	101.52	113.90
1	B	1269	ARG	CG-CD-NE	-5.16	100.97	111.80
1	A	658	LEU	CB-CG-CD1	5.15	119.76	111.00
1	B	520	MET	CB-CG-SD	-5.15	96.94	112.40
1	A	773	LEU	CA-CB-CG	-5.15	103.46	115.30
1	B	279	THR	N-CA-CB	-5.15	100.52	110.30
1	A	339	ARG	N-CA-CB	-5.13	101.36	110.60
1	A	1246	LEU	CA-CB-CG	-5.13	103.50	115.30
1	A	651	ASP	CB-CA-C	-5.12	100.15	110.40
1	A	1222	LEU	CA-CB-CG	-5.12	103.51	115.30
1	A	640	THR	CB-CA-C	-5.12	97.77	111.60
1	A	1118	CYS	CB-CA-C	5.12	120.64	110.40
1	B	1465	ARG	C-N-CA	-5.12	108.90	121.70
1	B	377	THR	N-CA-CB	-5.12	100.58	110.30
1	A	345	MET	CA-CB-CG	-5.11	104.61	113.30
1	A	738	HIS	CB-CA-C	-5.11	100.19	110.40
1	A	641	SER	N-CA-C	-5.10	97.23	111.00
1	B	3	VAL	N-CA-C	-5.09	97.25	111.00
1	A	375	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	957	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	825	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	386	GLY	N-CA-C	-5.07	100.42	113.10
1	B	861	GLY	N-CA-C	-5.07	100.43	113.10
1	A	485	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	A	588	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	785	GLY	N-CA-C	5.06	125.76	113.10
1	A	661	VAL	N-CA-C	-5.06	97.34	111.00
1	A	384	ARG	NE-CZ-NH2	-5.05	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1398	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	1307	VAL	CB-CA-C	-5.04	101.82	111.40
1	A	395	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	B	672	GLN	N-CA-C	-5.03	97.42	111.00
1	A	391	ILE	N-CA-C	-5.02	97.45	111.00
1	A	1110	SER	N-CA-CB	-5.02	102.97	110.50
1	A	37	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	529	LEU	CA-CB-CG	-5.02	103.76	115.30
1	B	914	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	487	VAL	CB-CA-C	-5.01	101.88	111.40
1	B	522	LEU	CB-CG-CD1	-5.00	102.49	111.00
1	B	1057	THR	CA-CB-CG2	-5.00	105.39	112.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	915	PHE	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	SER	Mainchain
1	A	325	GLU	Mainchain
1	B	1168	LEU	Mainchain
1	B	725	PHE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11180	0	11210	1498	0
1	B	11180	0	11212	1318	0
2	A	11	0	10	2	0
2	B	11	0	10	1	0
3	A	31	0	19	4	0
3	B	31	0	19	6	0
4	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	4	2	0
5	A	7	0	0	2	0
5	B	7	0	0	3	0
All	All	22478	0	22488	2814	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 63.

All (2814) 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:182:MET:CE	1:B:217:PRO:HB2	1.30	1.59
1:A:182:MET:HE3	1:A:217:PRO:CB	1.34	1.57
1:B:1449:ARG:CB	1:B:1449:ARG:HH11	0.97	1.56
1:B:182:MET:HE3	1:B:217:PRO:CB	1.09	1.54
1:A:182:MET:CE	1:A:217:PRO:HB2	1.45	1.47
1:B:1289:MET:CE	1:B:1289:MET:SD	2.02	1.47
1:A:253:HIS:ND1	1:A:254:PRO:HD2	1.17	1.46
1:A:1449:ARG:NH1	1:A:1449:ARG:HB2	1.18	1.45
1:A:522:LEU:HD21	1:A:705:LEU:CD2	1.47	1.44
1:A:825:LEU:CD1	1:A:1186:ARG:HH12	1.32	1.43
1:A:1449:ARG:CB	1:A:1449:ARG:HH11	1.32	1.43
1:B:182:MET:CE	1:B:217:PRO:CB	1.89	1.39
1:A:825:LEU:HD13	1:A:1186:ARG:NH1	1.35	1.36
1:A:505:GLN:NE2	1:A:1001:VAL:H	1.23	1.34
1:B:430:VAL:HG13	1:B:554:GLU:CB	1.59	1.33
1:B:253:HIS:CG	1:B:254:PRO:HD2	1.62	1.32
1:A:290:THR:CG2	1:A:292:PRO:HD2	1.57	1.31
1:B:729:GLY:O	1:B:748:GLY:HA3	1.31	1.29
1:A:253:HIS:CG	1:A:254:PRO:HD2	1.67	1.28
1:B:825:LEU:CD1	1:B:1186:ARG:HH12	1.46	1.28
1:A:253:HIS:ND1	1:A:254:PRO:CD	1.94	1.27
1:B:825:LEU:HD13	1:B:1186:ARG:NH1	1.46	1.27
1:A:430:VAL:HG13	1:A:554:GLU:CB	1.64	1.25
1:B:1449:ARG:NH1	1:B:1449:ARG:HB2	0.93	1.25
1:A:875:MET:CE	1:A:1139:PHE:CE2	2.22	1.23
1:B:452:GLN:HE21	1:B:764:THR:CG2	1.50	1.23
1:B:1047:MET:HG2	1:B:1186:ARG:CZ	1.69	1.22
1:B:746:ILE:CG2	1:B:1182:ASP:H	1.54	1.21
1:A:875:MET:HE1	1:A:1139:PHE:CE2	1.74	1.21
1:B:182:MET:HE3	1:B:217:PRO:CA	1.69	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:HG21	1:A:105:TYR:CD2	1.77	1.20
1:A:375:ASP:OD2	1:A:377:THR:HB	1.35	1.18
1:B:182:MET:HE2	1:B:217:PRO:HB2	1.23	1.18
1:B:1047:MET:SD	1:B:1186:ARG:NH2	2.16	1.18
1:A:515:ARG:HD2	1:A:1367:TYR:CE1	1.80	1.17
1:A:838:VAL:HG13	1:A:839:PRO:HD2	1.23	1.17
1:B:253:HIS:ND1	1:B:254:PRO:HD2	1.57	1.16
1:A:778:PHE:CE2	1:A:1039:LYS:HD2	1.80	1.16
1:B:710:LYS:HG2	1:B:939:GLY:HA3	1.25	1.16
1:A:139:VAL:HG12	1:A:140:SER:H	1.01	1.15
1:A:182:MET:HE3	1:A:217:PRO:CA	1.77	1.15
1:B:139:VAL:HG12	1:B:140:SER:N	1.60	1.15
1:A:746:ILE:CG2	1:A:1182:ASP:H	1.58	1.15
1:A:1391:MET:HE2	1:A:1458:VAL:HG22	1.25	1.15
1:B:1111:ASN:OD1	1:B:1119:VAL:HG23	1.45	1.14
1:A:1111:ASN:OD1	1:A:1119:VAL:HG23	1.44	1.14
1:B:999:LYS:CG	1:B:1022:LEU:HD23	1.78	1.14
1:B:1401:LEU:O	1:B:1401:LEU:HD12	1.45	1.13
1:A:526:LEU:N	1:A:526:LEU:HD12	1.63	1.13
1:A:381:GLU:OE1	1:A:402:ARG:NH1	1.81	1.13
1:B:1115:VAL:HG12	1:B:1115:VAL:O	1.49	1.13
1:A:825:LEU:CD1	1:A:1186:ARG:NH1	1.98	1.12
1:A:1212:ASP:O	1:A:1216:VAL:HG23	1.47	1.12
1:A:515:ARG:CD	1:A:1367:TYR:CE1	2.30	1.12
1:B:452:GLN:HE21	1:B:764:THR:HG21	0.98	1.12
1:A:253:HIS:CE1	1:A:254:PRO:HD2	1.85	1.12
1:B:30:HIS:CD2	1:B:31:ARG:HG3	1.85	1.10
1:A:387:PRO:HD3	1:A:1344:GLU:OE2	1.51	1.10
1:B:290:THR:HG23	1:B:292:PRO:HD2	1.27	1.09
1:A:1221:PRO:HB2	1:A:1229:MET:HE2	1.14	1.09
1:B:405:GLU:N	1:B:405:GLU:OE1	1.86	1.09
1:A:182:MET:CE	1:A:217:PRO:CB	2.13	1.09
1:B:999:LYS:HG3	1:B:1022:LEU:HD23	1.19	1.09
1:A:715:VAL:O	1:A:715:VAL:HG12	1.44	1.09
1:B:182:MET:HE3	1:B:217:PRO:HB3	1.27	1.09
1:B:430:VAL:HG13	1:B:554:GLU:HB3	1.31	1.09
1:B:430:VAL:CG1	1:B:554:GLU:HB2	1.82	1.09
1:A:59:VAL:CG2	1:A:105:TYR:CD2	2.34	1.08
1:B:746:ILE:HG23	1:B:1182:ASP:HB3	1.32	1.08
1:A:1391:MET:CE	1:A:1458:VAL:HG22	1.83	1.08
1:A:452:GLN:HE21	1:A:764:THR:CG2	1.66	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:O	1:B:242:ASN:ND2	1.86	1.08
1:A:522:LEU:HD21	1:A:705:LEU:HD21	1.22	1.08
1:B:728:ILE:HD12	1:B:1047:MET:CE	1.82	1.08
1:A:522:LEU:CD2	1:A:705:LEU:HD21	1.83	1.08
1:B:746:ILE:HG21	1:B:1182:ASP:N	1.69	1.08
1:B:1349:ARG:HG2	1:B:1349:ARG:HH11	0.97	1.08
1:A:1376:LEU:HD23	1:A:1376:LEU:N	1.62	1.08
1:A:826:ARG:HH11	1:A:826:ARG:HG2	1.18	1.08
1:A:452:GLN:HE21	1:A:764:THR:HG23	1.13	1.07
1:A:960:THR:HG22	1:A:963:VAL:HG23	1.32	1.07
1:B:515:ARG:HD2	1:B:1367:TYR:CE2	1.86	1.07
1:B:430:VAL:CG1	1:B:554:GLU:CB	2.32	1.07
1:A:746:ILE:HG21	1:A:1182:ASP:H	1.12	1.07
1:B:236:THR:HG21	1:B:328:ASP:H	1.17	1.07
1:A:236:THR:HG21	1:A:328:ASP:H	1.00	1.07
1:A:430:VAL:HG13	1:A:554:GLU:HB3	1.17	1.07
1:A:513:SER:HB3	1:A:520:MET:HE2	1.31	1.07
1:A:345:MET:HG3	1:A:346:ASP:H	1.18	1.06
1:B:227:MET:HE3	1:B:282:GLU:HA	1.37	1.06
1:B:1047:MET:HE2	1:B:1186:ARG:HH22	1.16	1.06
1:A:522:LEU:HD21	1:A:705:LEU:HD23	1.33	1.06
1:A:236:THR:CG2	1:A:328:ASP:H	1.69	1.06
1:B:417:ASP:O	1:B:419:TRP:N	1.89	1.06
1:B:295:LYS:HD2	1:B:390:MET:HE3	1.36	1.06
1:A:290:THR:HG22	1:A:292:PRO:HD2	1.29	1.05
1:B:139:VAL:HG11	1:B:143:GLN:HB3	1.36	1.05
1:B:515:ARG:CD	1:B:1367:TYR:CE2	2.39	1.05
1:B:505:GLN:NE2	1:B:1000:LEU:HB3	1.72	1.05
1:B:513:SER:HB3	1:B:520:MET:HE1	1.36	1.05
1:A:235:ASN:HD22	1:A:236:THR:N	1.52	1.05
1:A:974:ILE:HD11	1:A:983:LEU:HD12	1.34	1.05
1:A:353:MET:HE2	1:A:366:GLY:O	1.57	1.04
1:B:113:ASN:ND2	1:B:115:ASP:H	1.54	1.04
1:A:1115:VAL:HG12	1:A:1115:VAL:O	1.55	1.04
1:B:1047:MET:CE	1:B:1186:ARG:HH22	1.70	1.04
1:B:1062:ARG:O	1:B:1062:ARG:HG3	1.58	1.04
1:A:182:MET:HE2	1:A:217:PRO:HB2	1.40	1.04
1:B:999:LYS:HG3	1:B:1022:LEU:CD2	1.87	1.04
1:B:1317:THR:HG22	1:B:1318:ASN:N	1.71	1.04
1:B:299:VAL:HG12	1:B:299:VAL:O	1.53	1.04
1:B:912:SER:HB2	1:B:968:PRO:HD2	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:NZ	1:A:299:VAL:O	1.90	1.03
1:B:746:ILE:HG21	1:B:1182:ASP:H	0.87	1.03
1:B:1221:PRO:HD2	1:B:1229:MET:HE1	1.39	1.03
1:B:236:THR:CG2	1:B:328:ASP:H	1.70	1.03
1:A:113:ASN:ND2	1:A:115:ASP:H	1.56	1.03
1:A:505:GLN:NE2	1:A:1001:VAL:N	2.06	1.03
1:A:238:LYS:O	1:A:242:ASN:ND2	1.91	1.03
1:B:825:LEU:HD13	1:B:1186:ARG:HH12	1.04	1.03
1:A:1210:THR:HG22	1:A:1211:LEU:H	0.91	1.02
1:A:405:GLU:OE1	1:A:405:GLU:N	1.92	1.02
1:A:522:LEU:CD2	1:A:705:LEU:CD2	2.37	1.02
1:B:1076:GLY:HA3	1:B:1145:GLU:HG2	1.36	1.02
1:A:113:ASN:HD22	1:A:113:ASN:C	1.59	1.02
1:B:1131:THR:HG23	1:B:1133:GLU:OE1	1.57	1.02
1:A:102:TYR:CE2	1:A:144:PHE:CE1	2.48	1.02
1:A:1184:ASN:HB3	1:A:1185:PRO:HD3	1.39	1.01
1:B:464:ILE:HD11	1:B:779:TYR:CE2	1.93	1.01
1:A:1210:THR:HG22	1:A:1211:LEU:N	1.74	1.01
1:B:1401:LEU:HD12	1:B:1401:LEU:C	1.74	1.01
1:A:1008:THR:HG22	1:A:1009:ILE:N	1.74	1.01
1:A:1221:PRO:CB	1:A:1229:MET:HE2	1.90	1.01
1:A:1317:THR:CG2	1:A:1358:GLU:OE1	2.08	1.00
1:A:145:GLU:OE1	1:A:173:SER:HB2	1.57	1.00
1:B:100:PHE:O	1:B:137:LYS:HE3	1.60	1.00
1:A:672:GLN:HG3	1:A:693:MET:CE	1.91	1.00
1:A:875:MET:CE	1:A:1139:PHE:HE2	1.73	1.00
1:A:290:THR:HG22	1:A:292:PRO:CD	1.90	1.00
1:B:1449:ARG:HB3	1:B:1449:ARG:HH11	1.26	1.00
1:B:290:THR:CG2	1:B:292:PRO:HD2	1.92	1.00
1:A:430:VAL:CG1	1:A:554:GLU:HB3	1.92	0.99
1:B:1349:ARG:NH1	1:B:1349:ARG:HG2	1.71	0.99
1:A:1393:TYR:O	1:A:1394:VAL:HG23	1.62	0.99
1:B:963:VAL:HG12	1:B:964:MET:N	1.76	0.99
1:A:295:LYS:NZ	1:A:299:VAL:HG12	1.78	0.99
1:A:1210:THR:CG2	1:A:1211:LEU:H	1.76	0.99
1:A:958:HIS:O	1:A:1369:THR:HG22	1.62	0.99
1:A:310:PRO:HG3	1:A:404:ARG:NH2	1.75	0.99
1:A:248:GLU:HA	1:A:251:MET:HG2	1.41	0.99
1:B:787:ARG:HH12	1:B:821:PRO:HG2	1.25	0.99
1:B:389:GLU:HB3	1:B:403:ASP:OD2	1.61	0.98
1:B:728:ILE:HD12	1:B:1047:MET:HE3	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:913:GLY:HA2	1:B:1349:ARG:HD3	1.44	0.98
1:B:381:GLU:OE1	1:B:402:ARG:NH1	1.96	0.98
1:B:501:GLN:HE21	1:B:653:HIS:CD2	1.81	0.98
1:A:875:MET:HE2	1:A:1139:PHE:CE2	1.95	0.98
1:A:430:VAL:CG1	1:A:554:GLU:CB	2.42	0.98
1:A:139:VAL:HG12	1:A:140:SER:N	1.76	0.98
1:B:1184:ASN:HB3	1:B:1185:PRO:HD3	1.42	0.98
1:A:1387:MET:HG2	1:A:1387:MET:O	1.64	0.97
1:B:1210:THR:HG22	1:B:1211:LEU:H	1.28	0.97
1:B:603:HIS:HA	1:B:640:THR:HG22	1.44	0.97
1:B:139:VAL:HG12	1:B:140:SER:H	1.19	0.96
1:A:778:PHE:CZ	1:A:1039:LYS:HD2	1.99	0.96
1:A:505:GLN:HE22	1:A:1001:VAL:N	1.62	0.96
1:A:1449:ARG:O	1:A:1452:THR:HB	1.66	0.96
1:B:1039:LYS:O	1:B:1040:PHE:CD1	2.19	0.96
1:B:1317:THR:CG2	1:B:1358:GLU:OE1	2.13	0.96
1:A:959:SER:HA	1:A:1369:THR:CG2	1.94	0.96
1:B:317:ILE:O	1:B:321:ASN:ND2	1.99	0.96
1:B:652:THR:HG22	1:B:703:GLY:HA3	1.47	0.96
1:A:1447:TRP:CE2	1:A:1451:VAL:HG22	1.99	0.95
1:A:266:VAL:HG12	1:A:279:THR:CG2	1.96	0.95
1:A:447:LEU:HD21	1:A:674:ALA:HA	1.46	0.95
1:B:565:THR:HG22	1:B:602:THR:HB	1.44	0.95
1:B:430:VAL:HG13	1:B:554:GLU:HB2	1.36	0.95
1:B:603:HIS:CA	1:B:640:THR:HG22	1.95	0.95
1:B:1349:ARG:CG	1:B:1349:ARG:HH11	1.72	0.95
1:B:746:ILE:O	1:B:747:SER:O	1.85	0.95
1:B:652:THR:CG2	1:B:703:GLY:HA3	1.97	0.95
1:B:387:PRO:HD3	1:B:1344:GLU:OE2	1.67	0.95
1:B:513:SER:HB3	1:B:520:MET:CE	1.95	0.95
1:B:734:LEU:CD1	1:B:738:HIS:HD2	1.80	0.95
1:A:345:MET:HG3	1:A:346:ASP:N	1.72	0.95
1:B:30:HIS:ND1	1:B:1238:THR:HA	1.82	0.95
1:A:734:LEU:CD1	1:A:738:HIS:HD2	1.79	0.94
1:B:452:GLN:NE2	1:B:764:THR:HG21	1.82	0.94
1:A:291:ALA:HB3	1:A:292:PRO:HD3	1.46	0.94
1:A:52:GLN:HE22	1:A:71:LEU:H	1.16	0.94
1:B:950:THR:HG22	1:B:951:GLU:N	1.78	0.94
1:B:959:SER:HA	1:B:1369:THR:CG2	1.96	0.94
1:B:310:PRO:HG3	1:B:404:ARG:NH2	1.82	0.94
1:B:242:ASN:HD22	1:B:242:ASN:H	1.10	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:HD22	1:A:543:LEU:HB3	1.47	0.94
1:A:999:LYS:HG3	1:A:1022:LEU:HD23	1.49	0.94
1:B:531:ASN:HB3	1:B:534:ASP:HB2	1.49	0.93
1:B:253:HIS:H	1:B:260:MET:HE1	1.31	0.93
1:B:447:LEU:HD12	1:B:451:GLN:HG3	1.50	0.93
1:B:1008:THR:HG22	1:B:1009:ILE:N	1.83	0.93
1:A:214:ASN:O	1:A:1015:LYS:HE2	1.67	0.93
1:B:1170:GLN:HG2	1:B:1170:GLN:O	1.68	0.93
1:B:145:GLU:OE1	1:B:173:SER:HB2	1.68	0.93
1:A:1366:GLU:HG2	1:A:1367:TYR:CD2	2.04	0.93
1:A:958:HIS:O	1:A:1369:THR:CG2	2.17	0.93
1:B:253:HIS:CG	1:B:254:PRO:CD	2.51	0.93
1:B:920:GLU:HB3	1:B:1256:MET:HE2	1.50	0.92
1:A:510:PRO:HD2	1:A:970:PRO:HB3	1.52	0.92
1:A:672:GLN:HG3	1:A:693:MET:HE2	1.51	0.92
1:A:838:VAL:CG1	1:A:839:PRO:HD2	2.00	0.92
1:B:950:THR:HG22	1:B:952:MET:H	1.32	0.92
1:B:1449:ARG:CZ	1:B:1449:ARG:HB2	1.98	0.92
1:A:1076:GLY:HA3	1:A:1145:GLU:HG2	1.51	0.92
3:B:2474:FMN:O4'	3:B:2474:FMN:H1'2	1.69	0.92
1:B:464:ILE:HD11	1:B:779:TYR:CZ	2.05	0.92
1:A:464:ILE:HD11	1:A:779:TYR:CE1	2.05	0.91
1:B:452:GLN:NE2	1:B:764:THR:CG2	2.33	0.91
1:A:182:MET:HE3	1:A:217:PRO:C	1.90	0.91
1:A:404:ARG:HB3	1:A:405:GLU:OE1	1.69	0.91
1:B:464:ILE:CD1	1:B:779:TYR:CE2	2.54	0.91
1:B:313:HIS:O	1:B:317:ILE:HG13	1.68	0.91
1:A:218:THR:HG23	1:A:220:PRO:HD2	1.52	0.91
1:A:950:THR:HG22	1:A:951:GLU:N	1.83	0.91
1:B:1366:GLU:HG2	1:B:1367:TYR:CD1	2.05	0.91
1:B:706:LYS:NZ	1:B:940:GLU:OE1	2.01	0.91
1:B:950:THR:CG2	1:B:951:GLU:N	2.32	0.91
1:A:59:VAL:CG2	1:A:105:TYR:HD2	1.82	0.91
1:A:299:VAL:HG12	1:A:299:VAL:O	1.69	0.90
1:B:1317:THR:HG21	1:B:1358:GLU:OE1	1.69	0.90
1:B:254:PRO:HG2	1:B:255:ALA:H	1.36	0.90
1:A:826:ARG:NH1	1:A:826:ARG:HG2	1.83	0.90
1:B:825:LEU:CD1	1:B:1186:ARG:NH1	2.17	0.90
1:A:153:ARG:NH2	1:A:263:LEU:O	2.04	0.90
1:A:266:VAL:O	1:A:279:THR:HG21	1.71	0.90
1:B:704:LEU:O	1:B:706:LYS:N	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG12	1:A:279:THR:HG23	1.51	0.90
1:A:505:GLN:HE22	1:A:1001:VAL:H	0.93	0.90
1:B:155:ILE:O	1:B:159:VAL:HG23	1.71	0.90
1:B:838:VAL:HG13	1:B:839:PRO:HD2	1.54	0.90
1:B:826:ARG:HG2	1:B:826:ARG:HH11	1.35	0.90
1:A:584:ASP:OD1	1:A:584:ASP:N	2.04	0.90
1:B:213:THR:HB	1:B:1008:THR:HG23	1.52	0.90
1:B:588:ARG:O	1:B:592:GLU:HG3	1.72	0.89
1:A:102:TYR:CE2	1:A:144:PHE:HE1	1.88	0.89
1:A:582:LEU:H	1:A:755:GLN:HE22	1.17	0.89
1:B:526:LEU:N	1:B:526:LEU:HD12	1.88	0.89
1:A:403:ASP:OD1	1:A:407:LYS:NZ	2.05	0.89
1:B:652:THR:HG21	1:B:703:GLY:CA	2.03	0.89
1:A:290:THR:CG2	1:A:292:PRO:CD	2.46	0.89
1:A:710:LYS:HG2	1:A:939:GLY:HA3	1.55	0.89
1:B:950:THR:HG22	1:B:952:MET:N	1.88	0.89
1:A:387:PRO:CD	1:A:1344:GLU:OE2	2.20	0.89
1:A:950:THR:CG2	1:A:951:GLU:N	2.35	0.89
1:A:52:GLN:NE2	1:A:71:LEU:H	1.70	0.88
1:B:570:ASP:OD1	1:B:572:THR:HB	1.73	0.88
1:B:768:GLU:HG2	1:B:769:GLU:H	1.34	0.88
1:A:227:MET:HE3	1:A:282:GLU:HA	1.55	0.88
1:B:139:VAL:HG11	1:B:143:GLN:CB	2.03	0.88
1:B:437:GLY:HA2	1:B:690:GLU:OE2	1.73	0.88
1:B:731:SER:HA	1:B:748:GLY:H	1.37	0.88
1:A:295:LYS:HZ3	1:A:299:VAL:HG12	1.38	0.88
1:A:862:ALA:O	1:A:1118:CYS:HB2	1.71	0.88
1:B:734:LEU:CD1	1:B:738:HIS:CD2	2.57	0.88
1:A:511:ILE:HG22	1:A:512:ASP:N	1.86	0.88
1:A:960:THR:HG22	1:A:963:VAL:CG2	2.03	0.88
1:B:218:THR:HG23	1:B:220:PRO:HD2	1.55	0.88
1:B:218:THR:HG21	1:B:221:LEU:HG	1.56	0.88
1:B:501:GLN:HE21	1:B:653:HIS:HD2	0.90	0.88
1:B:515:ARG:HH22	1:B:966:ILE:HB	1.37	0.88
1:A:236:THR:HG21	1:A:328:ASP:N	1.86	0.88
1:A:353:MET:CE	1:A:366:GLY:O	2.22	0.88
1:A:392:ALA:O	1:A:400:LEU:HD12	1.74	0.88
1:A:1401:LEU:HD12	1:A:1401:LEU:O	1.74	0.87
1:A:838:VAL:HG13	1:A:839:PRO:CD	2.03	0.87
1:A:582:LEU:H	1:A:755:GLN:NE2	1.71	0.87
1:B:253:HIS:ND1	1:B:254:PRO:CD	2.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:THR:HG22	1:B:921:TYR:H	1.38	0.87
1:A:146:LEU:HD12	1:A:146:LEU:O	1.75	0.87
1:A:372:VAL:HG12	1:A:372:VAL:O	1.74	0.87
1:B:139:VAL:CG1	1:B:140:SER:H	1.87	0.87
1:B:426:LEU:CD2	1:B:543:LEU:HB3	2.04	0.87
1:B:430:VAL:CG1	1:B:554:GLU:HB3	2.02	0.87
1:B:139:VAL:CG1	1:B:140:SER:N	2.35	0.87
1:B:501:GLN:NE2	1:B:653:HIS:HD2	1.73	0.87
1:A:52:GLN:HE22	1:A:71:LEU:N	1.73	0.87
1:A:724:ASN:ND2	1:A:724:ASN:H	1.73	0.87
1:A:825:LEU:HD11	1:A:1186:ARG:HH12	1.41	0.86
1:A:513:SER:CB	1:A:520:MET:HE2	2.04	0.86
1:A:825:LEU:HD13	1:A:1186:ARG:HH11	1.38	0.86
1:B:30:HIS:HD2	1:B:31:ARG:HG3	1.38	0.86
1:B:377:THR:HG22	1:B:378:GLN:HG3	1.56	0.86
1:A:290:THR:HG23	1:A:292:PRO:HD2	1.56	0.86
1:A:479:MET:HG3	1:A:1104:MET:CE	2.05	0.86
1:B:505:GLN:HE22	1:B:1000:LEU:HB3	1.36	0.86
1:B:734:LEU:HD11	1:B:738:HIS:CD2	2.10	0.86
1:A:430:VAL:HG13	1:A:554:GLU:HB2	1.56	0.86
1:B:568:GLU:C	1:B:569:ILE:HD13	1.97	0.86
1:A:6:ILE:HG12	1:A:364:ILE:HG23	1.57	0.86
1:B:1047:MET:HG2	1:B:1186:ARG:NH2	1.91	0.86
1:A:113:ASN:ND2	1:A:113:ASN:C	2.27	0.85
1:A:734:LEU:CD1	1:A:738:HIS:CD2	2.58	0.85
1:B:652:THR:HG21	1:B:703:GLY:HA2	1.59	0.85
1:A:1338:ALA:O	1:A:1340:GLY:N	2.08	0.85
1:A:537:GLU:HG3	1:A:538:THR:N	1.92	0.85
1:A:482:ASP:OD1	1:A:788:HIS:HD2	1.59	0.85
1:A:843:VAL:HG12	1:A:844:GLU:N	1.89	0.85
1:B:1047:MET:CG	1:B:1186:ARG:NH2	2.38	0.85
1:B:1128:PHE:CZ	1:B:1130:GLY:HA3	2.11	0.85
1:B:659:ILE:HA	1:B:663:ALA:HB3	1.54	0.85
1:A:724:ASN:HD22	1:A:724:ASN:H	1.25	0.85
1:B:746:ILE:HG23	1:B:1182:ASP:CB	2.05	0.85
1:A:1311:THR:HG23	1:A:1312:SER:N	1.89	0.85
1:A:704:LEU:O	1:A:706:LYS:N	2.10	0.85
1:A:513:SER:HB3	1:A:520:MET:CE	2.06	0.85
1:A:838:VAL:HG12	1:A:839:PRO:N	1.92	0.85
1:B:253:HIS:CE1	1:B:254:PRO:HD2	2.11	0.85
1:B:417:ASP:O	1:B:418:LYS:C	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLN:HE22	1:B:71:LEU:HB2	1.42	0.85
1:A:1425:LYS:HD3	1:A:1447:TRP:CE2	2.12	0.84
1:A:746:ILE:HG23	1:A:1182:ASP:HB3	1.58	0.84
1:A:588:ARG:O	1:A:592:GLU:HG3	1.78	0.84
1:B:52:GLN:HE22	1:B:71:LEU:H	1.24	0.84
1:A:482:ASP:OD1	1:A:788:HIS:CD2	2.29	0.84
1:A:937:LYS:HE3	1:A:1033:SER:HB2	1.59	0.84
1:A:604:VAL:HG23	1:A:640:THR:HG21	1.58	0.84
1:B:843:VAL:HG12	1:B:844:GLU:N	1.92	0.84
1:A:409:HIS:O	1:A:412:THR:HB	1.76	0.84
1:A:659:ILE:HG21	1:A:716:ILE:HD11	1.59	0.84
1:A:1115:VAL:O	1:A:1115:VAL:CG1	2.24	0.84
1:A:342:VAL:HG11	1:A:390:MET:HE2	1.59	0.84
1:B:777:GLY:O	1:B:788:HIS:HE1	1.60	0.84
1:A:142:GLU:CD	1:A:142:GLU:H	1.80	0.83
1:A:364:ILE:HD12	1:A:374:ILE:HD11	1.60	0.83
1:A:729:GLY:O	1:A:748:GLY:HA3	1.78	0.83
1:A:731:SER:HA	1:A:748:GLY:H	1.42	0.83
1:B:1062:ARG:O	1:B:1062:ARG:CG	2.26	0.83
1:B:734:LEU:HD12	1:B:738:HIS:HD2	1.43	0.83
1:B:787:ARG:NH1	1:B:821:PRO:HG2	1.94	0.83
1:A:235:ASN:HD22	1:A:235:ASN:C	1.80	0.83
1:A:1062:ARG:NH2	1:A:1088:GLU:OE2	2.12	0.83
1:A:526:LEU:N	1:A:526:LEU:CD1	2.40	0.83
1:A:838:VAL:CG1	1:A:839:PRO:CD	2.56	0.83
1:A:1388:THR:O	1:A:1388:THR:CG2	2.27	0.83
1:A:430:VAL:CG1	1:A:554:GLU:HB2	2.08	0.83
1:A:515:ARG:HH22	1:A:966:ILE:HB	1.42	0.83
1:A:434:SER:OG	1:A:438:GLU:OE2	1.97	0.83
1:A:950:THR:HG22	1:A:952:MET:H	1.42	0.83
1:B:113:ASN:C	1:B:113:ASN:HD22	1.78	0.83
1:A:1391:MET:CE	1:A:1458:VAL:CG2	2.56	0.83
1:A:734:LEU:HD11	1:A:738:HIS:CD2	2.12	0.83
1:A:982:GLN:HE22	1:A:1240:ARG:HD2	1.43	0.83
1:B:1115:VAL:CG1	1:B:1115:VAL:O	2.22	0.82
1:A:266:VAL:O	1:A:279:THR:CG2	2.28	0.82
1:A:670:LEU:O	1:A:670:LEU:HD22	1.78	0.82
1:A:459:GLU:O	1:A:463:LEU:HB2	1.78	0.82
1:A:426:LEU:CD2	1:A:543:LEU:HB3	2.09	0.82
1:A:912:SER:HB2	1:A:968:PRO:HD2	1.62	0.82
1:B:1349:ARG:NH1	1:B:1349:ARG:CG	2.34	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1447:TRP:CE2	1:A:1451:VAL:CG2	2.61	0.82
1:A:59:VAL:HG22	1:A:105:TYR:HD2	1.44	0.82
1:B:1370:GLY:N	1:B:1389:GLY:O	2.12	0.82
1:A:464:ILE:HD11	1:A:779:TYR:CZ	2.13	0.82
1:A:526:LEU:HD12	1:A:526:LEU:H	1.45	0.82
1:A:397:SER:HB2	1:A:399:LYS:HG3	1.61	0.82
1:A:746:ILE:HG21	1:A:1182:ASP:N	1.94	0.82
1:B:959:SER:HA	1:B:1369:THR:HG21	1.61	0.82
1:B:1471:HIS:O	1:B:1472:LEU:HB2	1.80	0.82
1:B:253:HIS:CD2	1:B:254:PRO:HD2	2.14	0.82
1:B:430:VAL:HG11	1:B:554:GLU:HB2	1.61	0.82
1:B:1039:LYS:O	1:B:1040:PHE:HD1	1.63	0.82
1:B:299:VAL:CG1	1:B:299:VAL:O	2.28	0.82
1:B:746:ILE:C	1:B:747:SER:O	2.16	0.82
1:B:1184:ASN:HB3	1:B:1185:PRO:CD	2.10	0.81
1:A:452:GLN:NE2	1:A:764:THR:CG2	2.42	0.81
1:A:950:THR:HG22	1:A:952:MET:N	1.95	0.81
1:B:240:ASN:HD21	1:B:327:TRP:HA	1.45	0.81
1:A:405:GLU:H	1:A:405:GLU:CD	1.81	0.81
1:B:815:GLU:OE1	1:B:815:GLU:HA	1.80	0.81
1:A:932:VAL:O	1:A:933:ALA:HB2	1.78	0.81
1:B:866:GLU:OE2	1:B:1125:ARG:NH2	2.14	0.81
1:A:253:HIS:CG	1:A:254:PRO:CD	2.52	0.81
1:B:242:ASN:ND2	1:B:242:ASN:H	1.79	0.81
1:A:1376:LEU:HB3	1:A:1439:PHE:HE2	1.45	0.81
1:A:531:ASN:OD1	1:A:533:LEU:HB2	1.81	0.81
1:B:973:ASP:OD2	1:B:1298:LYS:HE3	1.79	0.81
1:A:515:ARG:HD2	1:A:1367:TYR:HE1	1.46	0.81
1:A:447:LEU:HD12	1:A:451:GLN:HG3	1.62	0.80
1:B:426:LEU:HD11	1:B:558:MET:HG3	1.62	0.80
1:B:824:GLN:O	1:B:827:ASP:HB2	1.81	0.80
1:A:290:THR:HG22	1:A:291:ALA:N	1.95	0.80
1:A:454:PHE:CG	1:A:648:GLU:HB2	2.17	0.80
1:A:746:ILE:CG2	1:A:1182:ASP:N	2.43	0.80
1:B:302:ALA:HA	1:B:347:ARG:HH12	1.46	0.80
1:B:310:PRO:HG3	1:B:404:ARG:HH22	1.45	0.80
1:A:1184:ASN:HB3	1:A:1185:PRO:CD	2.11	0.80
1:A:1290:GLY:O	1:A:1291:ASP:HB3	1.82	0.80
1:A:734:LEU:HD11	1:A:738:HIS:HD2	1.46	0.80
1:B:963:VAL:CG1	1:B:964:MET:N	2.45	0.80
1:B:582:LEU:H	1:B:755:GLN:NE2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:LYS:CG	1:B:939:GLY:HA3	2.10	0.80
1:A:787:ARG:HH12	1:A:821:PRO:HB2	1.47	0.79
1:B:652:THR:CG2	1:B:703:GLY:CA	2.59	0.79
1:A:1322:ILE:HG23	1:A:1323:ILE:HG23	1.64	0.79
1:B:1047:MET:HG2	1:B:1186:ARG:NH1	1.97	0.79
1:A:1401:LEU:C	1:A:1401:LEU:HD12	2.03	0.79
1:A:974:ILE:HD11	1:A:983:LEU:CD1	2.13	0.79
1:B:778:PHE:CZ	1:B:1039:LYS:HD2	2.18	0.79
1:B:1131:THR:HB	1:B:1134:LYS:HG3	1.64	0.79
1:B:1388:THR:O	1:B:1388:THR:CG2	2.29	0.79
1:A:317:ILE:HG22	1:A:321:ASN:HD21	1.47	0.79
1:A:47:HIS:CE1	1:A:176:SER:HB3	2.18	0.79
1:B:235:ASN:HD22	1:B:236:THR:N	1.80	0.79
1:B:447:LEU:HD21	1:B:674:ALA:HA	1.64	0.79
1:B:555:PHE:C	1:B:555:PHE:CD1	2.55	0.79
1:A:501:GLN:HE21	1:A:653:HIS:HD2	1.30	0.79
1:B:466:HIS:CE1	1:B:684:PHE:CE1	2.70	0.79
1:B:974:ILE:HD11	1:B:983:LEU:HD12	1.62	0.79
1:A:973:ASP:OD2	1:A:1298:LYS:HE3	1.81	0.79
1:A:704:LEU:O	1:A:705:LEU:C	2.20	0.79
1:A:90:ARG:NH1	1:A:129:GLU:OE1	2.16	0.79
1:B:1121:ASP:OD2	1:B:1124:LEU:HB2	1.82	0.79
1:B:1047:MET:CG	1:B:1186:ARG:CZ	2.56	0.79
1:A:875:MET:HE2	1:A:1139:PHE:CZ	2.18	0.79
1:B:37:ASP:OD2	1:B:40:THR:HB	1.82	0.79
1:A:230:HIS:HE1	1:A:234:ILE:HG13	1.45	0.78
1:A:580:GLU:O	1:A:584:ASP:OD1	2.01	0.78
1:A:447:LEU:HD21	1:A:674:ALA:CA	2.14	0.78
1:B:1318:ASN:H	1:B:1318:ASN:HD22	1.30	0.78
1:A:1043:LEU:HD23	1:A:1044:PRO:HD2	1.66	0.78
1:A:375:ASP:OD2	1:A:377:THR:CB	2.26	0.78
1:A:959:SER:HA	1:A:1369:THR:HG23	1.63	0.78
1:B:1317:THR:CG2	1:B:1318:ASN:N	2.44	0.78
1:A:1401:LEU:CD1	1:A:1405:ILE:HB	2.13	0.78
1:A:450:ARG:O	1:A:452:GLN:N	2.17	0.78
1:B:266:VAL:HG12	1:B:279:THR:CG2	2.14	0.78
1:B:565:THR:CG2	1:B:602:THR:HB	2.13	0.78
1:A:139:VAL:CG1	1:A:140:SER:H	1.90	0.78
1:A:177:ILE:HD13	1:A:179:TYR:HE1	1.49	0.78
1:A:213:THR:HB	1:A:1008:THR:HG23	1.66	0.78
1:A:24:ALA:HB1	1:A:207:TYR:CE2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:950:THR:CG2	1:B:952:MET:H	1.96	0.78
1:A:310:PRO:HG3	1:A:404:ARG:HH22	1.43	0.77
1:B:260:MET:O	1:B:263:LEU:HB2	1.84	0.77
1:B:218:THR:O	1:B:218:THR:HG22	1.82	0.77
1:A:236:THR:CG2	1:A:328:ASP:N	2.45	0.77
1:B:531:ASN:OD1	1:B:533:LEU:HB2	1.83	0.77
1:B:522:LEU:HD21	1:B:705:LEU:CD2	2.14	0.77
1:B:746:ILE:CG2	1:B:1182:ASP:N	2.37	0.77
1:A:930:ILE:HD13	1:A:983:LEU:HD13	1.65	0.77
1:A:1395:TYR:CE1	1:A:1397:LEU:HD21	2.20	0.77
1:B:249:THR:HG22	1:B:250:ARG:HG2	1.67	0.77
1:A:551:THR:OG1	1:A:554:GLU:HG2	1.84	0.77
1:B:1131:THR:HG22	1:B:1134:LYS:H	1.49	0.77
1:B:580:GLU:O	1:B:584:ASP:OD1	2.03	0.77
1:A:1391:MET:HE1	1:A:1458:VAL:CG2	2.15	0.77
1:B:826:ARG:NH1	1:B:1046:GLU:OE2	2.18	0.77
1:A:1008:THR:CG2	1:A:1009:ILE:N	2.44	0.77
1:B:505:GLN:NE2	1:B:1001:VAL:H	1.83	0.77
1:B:515:ARG:HD2	1:B:1367:TYR:HE2	1.49	0.77
1:B:1449:ARG:CB	1:B:1449:ARG:NH1	1.80	0.77
1:B:551:THR:OG1	1:B:554:GLU:HG2	1.85	0.77
1:B:731:SER:CA	1:B:748:GLY:H	1.98	0.77
1:A:113:ASN:HD21	1:A:115:ASP:H	1.31	0.76
1:A:1356:VAL:HG22	1:A:1374:VAL:HG21	1.67	0.76
1:B:985:TYR:HE1	1:B:1207:VAL:HG13	1.50	0.76
1:B:572:THR:CG2	1:B:573:PHE:N	2.47	0.76
1:A:528:ASN:HB3	1:A:542:LEU:HD22	1.66	0.76
1:B:658:LEU:HD23	1:B:666:VAL:HG21	1.67	0.76
1:A:959:SER:HA	1:A:1369:THR:HG21	1.67	0.76
1:A:890:ASP:O	1:A:893:ARG:HB2	1.84	0.76
1:A:413:LEU:O	1:A:414:LYS:HD2	1.85	0.76
1:B:1043:LEU:HD23	1:B:1044:PRO:HD2	1.67	0.76
1:B:826:ARG:HG2	1:B:826:ARG:NH1	1.99	0.76
1:A:447:LEU:HD13	1:A:670:LEU:HD21	1.65	0.76
1:A:450:ARG:O	1:A:453:ALA:N	2.19	0.76
1:B:1084:MET:SD	1:B:1168:LEU:HD21	2.25	0.76
1:B:153:ARG:NH2	1:B:263:LEU:O	2.18	0.76
1:B:582:LEU:H	1:B:755:GLN:HE22	1.30	0.76
1:A:1131:THR:HB	1:A:1134:LYS:HG3	1.68	0.76
1:B:982:GLN:HE22	1:B:1240:ARG:HD2	1.49	0.76
1:A:1220:ARG:HG3	1:A:1224:GLU:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1471:HIS:O	1:A:1472:LEU:HB2	1.85	0.76
1:A:182:MET:CE	1:A:217:PRO:C	2.54	0.76
1:A:643:ASN:HB3	1:A:665:THR:HG22	1.68	0.76
1:A:260:MET:O	1:A:263:LEU:N	2.19	0.76
1:B:426:LEU:CD1	1:B:558:MET:HG3	2.16	0.76
1:B:522:LEU:HD21	1:B:705:LEU:HD21	1.68	0.76
1:A:829:LEU:HD13	1:A:1168:LEU:HD13	1.67	0.75
1:A:1374:VAL:O	1:A:1375:ILE:CG1	2.34	0.75
1:A:826:ARG:NH1	1:A:1046:GLU:OE2	2.19	0.75
1:B:417:ASP:C	1:B:419:TRP:N	2.38	0.75
1:A:999:LYS:HG3	1:A:1022:LEU:CD2	2.17	0.75
1:B:438:GLU:OE1	1:B:672:GLN:NE2	2.20	0.75
1:B:452:GLN:CG	1:B:765:ALA:HB2	2.17	0.75
1:A:298:LEU:HD23	1:A:324:MET:HG2	1.68	0.75
1:A:452:GLN:CG	1:A:765:ALA:HB2	2.16	0.75
1:B:175:ARG:HG3	1:B:175:ARG:HH11	1.52	0.75
1:B:820:ARG:HB3	1:B:821:PRO:CD	2.16	0.75
1:A:536:ASP:O	1:A:536:ASP:OD1	2.05	0.75
1:B:317:ILE:HG22	1:B:321:ASN:HD21	1.52	0.75
1:B:584:ASP:N	1:B:584:ASP:OD1	2.14	0.75
1:A:1317:THR:HG22	1:A:1318:ASN:N	2.00	0.75
1:A:207:TYR:CD1	1:A:207:TYR:N	2.54	0.75
1:A:643:ASN:HB3	1:A:665:THR:CG2	2.16	0.75
1:A:950:THR:CG2	1:A:951:GLU:H	1.98	0.75
1:A:1394:VAL:O	1:A:1394:VAL:HG12	1.87	0.75
1:A:1413:GLN:HG3	1:A:1414:ARG:O	1.87	0.74
1:A:443:ASP:O	1:A:445:ALA:N	2.20	0.74
1:A:536:ASP:OD1	1:A:538:THR:HG22	1.85	0.74
1:B:375:ASP:OD2	1:B:377:THR:HB	1.87	0.74
1:A:139:VAL:HG11	1:A:143:GLN:CB	2.17	0.74
1:A:60:LYS:O	1:A:63:GLY:N	2.19	0.74
1:B:59:VAL:CG2	1:B:105:TYR:CD2	2.70	0.74
1:A:643:ASN:HD22	1:A:665:THR:CB	2.01	0.74
1:B:1084:MET:SD	1:B:1168:LEU:CD2	2.75	0.74
1:B:536:ASP:OD1	1:B:536:ASP:C	2.25	0.74
1:A:595:ASP:O	1:A:596:ALA:C	2.21	0.74
1:B:746:ILE:O	1:B:747:SER:C	2.22	0.74
1:B:139:VAL:CG1	1:B:143:GLN:CB	2.66	0.74
1:B:450:ARG:O	1:B:453:ALA:N	2.20	0.74
1:B:731:SER:HA	1:B:747:SER:CA	2.17	0.74
1:A:528:ASN:CB	1:A:542:LEU:HD22	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:GLN:CA	1:A:824:GLN:HE21	1.99	0.74
1:B:602:THR:C	1:B:640:THR:CG2	2.56	0.74
1:A:1131:THR:HG22	1:A:1133:GLU:N	2.02	0.74
1:A:342:VAL:HG13	1:A:392:ALA:HB2	1.69	0.74
1:A:862:ALA:O	1:A:1118:CYS:CB	2.35	0.74
1:A:515:ARG:HD2	1:A:1367:TYR:CZ	2.22	0.74
1:A:355:TYR:CD1	1:A:355:TYR:C	2.61	0.74
1:B:1131:THR:HG22	1:B:1133:GLU:N	2.03	0.74
1:A:102:TYR:CD2	1:A:144:PHE:HE1	2.06	0.73
1:A:536:ASP:OD1	1:A:536:ASP:C	2.25	0.73
1:A:731:SER:CA	1:A:748:GLY:H	2.01	0.73
1:B:1289:MET:HB2	1:B:1289:MET:CE	2.17	0.73
1:A:609:GLU:OE2	1:A:645:ARG:HD3	1.88	0.73
1:B:295:LYS:NZ	1:B:299:VAL:O	2.17	0.73
1:A:1394:VAL:HG11	1:A:1401:LEU:CD2	2.17	0.73
1:A:724:ASN:N	1:A:724:ASN:ND2	2.36	0.73
1:B:891:PRO:HA	1:B:894:PHE:CE2	2.24	0.73
1:A:728:ILE:HD12	1:A:1047:MET:CE	2.17	0.73
1:A:513:SER:CB	1:A:520:MET:CE	2.64	0.73
1:A:727:ALA:HB3	1:A:744:SER:HB2	1.69	0.73
1:A:824:GLN:NE2	1:A:824:GLN:HA	2.01	0.73
1:B:146:LEU:HD12	1:B:146:LEU:O	1.88	0.73
1:B:746:ILE:HG22	1:B:747:SER:O	1.88	0.73
1:A:1401:LEU:HD11	1:A:1405:ILE:HB	1.71	0.73
1:A:182:MET:HE3	1:A:217:PRO:HB2	1.00	0.73
1:A:290:THR:CG2	1:A:291:ALA:N	2.51	0.73
1:A:295:LYS:CE	1:A:299:VAL:HG12	2.18	0.73
1:B:465:LEU:O	1:B:465:LEU:HD12	1.89	0.73
1:A:465:LEU:C	1:A:465:LEU:HD12	2.08	0.73
1:A:573:PHE:HB2	1:A:574:PRO:HD2	1.71	0.73
1:B:214:ASN:O	1:B:1015:LYS:HE2	1.88	0.73
1:B:665:THR:HG22	1:B:665:THR:O	1.89	0.73
1:A:1460:LYS:O	1:A:1462:MET:N	2.21	0.73
1:A:464:ILE:CD1	1:A:779:TYR:CE1	2.71	0.73
1:B:1113:CYS:O	1:B:1115:VAL:N	2.22	0.73
1:B:511:ILE:HG22	1:B:512:ASP:N	2.03	0.73
1:B:787:ARG:HH12	1:B:821:PRO:CG	2.00	0.73
1:A:1062:ARG:O	1:A:1062:ARG:HG3	1.89	0.72
1:A:1425:LYS:HD3	1:A:1447:TRP:NE1	2.03	0.72
1:B:1289:MET:HB2	1:B:1289:MET:HE3	1.69	0.72
1:A:1447:TRP:CZ2	1:A:1451:VAL:HG22	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:GLU:CD	1:B:405:GLU:H	1.90	0.72
1:B:731:SER:HA	1:B:747:SER:HA	1.71	0.72
1:B:829:LEU:HD13	1:B:1168:LEU:HD13	1.70	0.72
1:B:290:THR:CG2	1:B:292:PRO:CD	2.68	0.72
1:B:780:ARG:HH21	1:B:1105:VAL:HG23	1.53	0.72
1:B:838:VAL:HG12	1:B:839:PRO:N	2.02	0.72
1:A:850:ARG:HG3	1:A:850:ARG:HH11	1.53	0.72
1:B:52:GLN:NE2	1:B:71:LEU:H	1.87	0.72
1:B:838:VAL:CG1	1:B:839:PRO:HD2	2.19	0.72
1:A:918:THR:HG23	1:A:1256:MET:SD	2.30	0.72
1:B:223:GLN:HB3	1:B:224:PRO:HA	1.72	0.72
1:B:236:THR:HG21	1:B:328:ASP:N	2.00	0.72
1:B:820:ARG:CB	1:B:821:PRO:CD	2.67	0.72
1:A:976:SER:OG	1:A:978:GLU:HG3	1.90	0.72
1:A:189:THR:HG22	1:A:190:THR:N	2.04	0.72
1:B:781:PHE:CE2	1:B:791:GLU:HB3	2.25	0.72
1:A:1356:VAL:HG11	1:A:1431:HIS:HB2	1.71	0.72
1:A:290:THR:HG22	1:A:292:PRO:N	2.05	0.72
1:A:875:MET:HE1	1:A:1139:PHE:CD2	2.25	0.72
1:B:1076:GLY:CA	1:B:1145:GLU:HG2	2.18	0.72
1:B:1184:ASN:O	1:B:1187:LEU:N	2.22	0.72
1:B:1369:THR:HG22	1:B:1369:THR:O	1.89	0.72
1:B:493:ARG:NH2	1:B:786:ASP:OD1	2.21	0.72
1:B:1417:VAL:HG12	1:B:1419:HIS:H	1.54	0.72
1:B:3:VAL:HG22	1:B:231:ASN:HB2	1.72	0.72
1:B:529:LEU:N	1:B:529:LEU:HD23	1.92	0.72
1:B:1369:THR:C	1:B:1389:GLY:O	2.28	0.72
1:B:959:SER:HA	1:B:1369:THR:HG23	1.69	0.72
1:A:985:TYR:HE1	1:A:1207:VAL:HG13	1.53	0.71
1:B:218:THR:CG2	1:B:221:LEU:HG	2.20	0.71
1:B:731:SER:HA	1:B:748:GLY:N	2.04	0.71
1:B:780:ARG:NH2	1:B:1105:VAL:HG23	2.04	0.71
1:A:1230:GLN:NE2	1:A:1267:ARG:HD3	2.05	0.71
1:A:515:ARG:CD	1:A:1367:TYR:HE1	1.96	0.71
1:B:1164:ARG:NH1	1:B:1166:ASP:OD2	2.23	0.71
1:B:525:ARG:HG2	1:B:542:LEU:HD13	1.71	0.71
1:B:603:HIS:N	1:B:640:THR:HG22	2.05	0.71
1:A:1289:MET:CE	1:A:1289:MET:H	2.03	0.71
1:B:242:ASN:ND2	1:B:242:ASN:N	2.37	0.71
1:B:88:ALA:O	1:B:92:ILE:HG13	1.91	0.71
1:A:1317:THR:HG23	1:A:1358:GLU:OE1	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:PHE:HE2	1:A:647:ALA:CB	2.03	0.71
1:B:875:MET:CE	1:B:1139:PHE:CE2	2.73	0.71
1:B:500:ARG:NH2	1:B:1040:PHE:HA	2.05	0.71
1:B:704:LEU:O	1:B:705:LEU:C	2.25	0.71
1:A:746:ILE:HG23	1:A:1182:ASP:H	1.54	0.71
1:B:842:GLU:HB3	1:B:1156:ARG:HD3	1.72	0.71
1:B:588:ARG:O	1:B:592:GLU:CG	2.38	0.71
1:A:1131:THR:HG23	1:A:1133:GLU:OE1	1.90	0.71
1:A:312:ASN:OD1	1:A:312:ASN:N	2.22	0.71
1:B:593:THR:O	1:B:597:VAL:HG23	1.91	0.71
1:B:1047:MET:CE	1:B:1186:ARG:NH2	2.44	0.71
1:B:295:LYS:NZ	1:B:299:VAL:HG12	2.06	0.71
1:B:907:ILE:HG23	1:B:927:GLU:HG2	1.73	0.71
1:B:426:LEU:HD22	1:B:543:LEU:HB3	1.73	0.70
1:B:59:VAL:HG21	1:B:105:TYR:CD2	2.26	0.70
1:B:266:VAL:O	1:B:279:THR:CG2	2.39	0.70
1:B:459:GLU:O	1:B:463:LEU:HB2	1.91	0.70
1:B:958:HIS:O	1:B:1369:THR:HG22	1.90	0.70
1:A:96:GLU:HA	1:A:96:GLU:OE1	1.89	0.70
1:B:1053:HIS:ND1	1:B:1062:ARG:NH1	2.39	0.70
1:B:1053:HIS:CE1	1:B:1062:ARG:HH11	2.08	0.70
1:B:1253:LYS:HG3	1:B:1253:LYS:O	1.91	0.70
1:B:454:PHE:CE2	1:B:647:ALA:HB3	2.26	0.70
1:A:140:SER:O	1:A:143:GLN:N	2.24	0.70
1:A:183:PHE:CE1	1:A:188:LEU:HA	2.26	0.70
1:A:177:ILE:HD13	1:A:179:TYR:CE1	2.26	0.70
1:A:838:VAL:CG1	1:A:839:PRO:N	2.54	0.70
1:B:1039:LYS:C	1:B:1040:PHE:CD1	2.65	0.70
1:A:734:LEU:HD12	1:A:738:HIS:HD2	1.54	0.70
1:A:997:THR:HG22	1:A:998:VAL:N	2.05	0.70
1:B:1121:ASP:OD1	1:B:1122:ASP:N	2.25	0.70
1:B:1212:ASP:O	1:B:1216:VAL:HG23	1.90	0.70
1:B:1394:VAL:O	1:B:1394:VAL:HG12	1.91	0.70
1:B:739:PHE:O	1:B:740:PRO:O	2.10	0.70
1:A:1076:GLY:HA3	1:A:1145:GLU:CG	2.22	0.70
1:A:113:ASN:HD22	1:A:114:VAL:N	1.89	0.70
1:A:1311:THR:CG2	1:A:1312:SER:N	2.55	0.70
1:B:1076:GLY:HA3	1:B:1145:GLU:CG	2.17	0.70
1:A:875:MET:HE1	1:A:1139:PHE:HE2	1.33	0.70
1:A:1221:PRO:CG	1:A:1229:MET:CE	2.70	0.70
1:B:985:TYR:CE1	1:B:1207:VAL:CG1	2.75	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:C	1:B:465:LEU:HD12	2.12	0.70
1:B:802:VAL:HG23	1:B:1137:ASN:HB2	1.73	0.70
1:A:218:THR:HG21	1:A:221:LEU:HG	1.73	0.69
1:A:413:LEU:O	1:A:414:LYS:CD	2.40	0.69
1:B:1102:CYS:HG	5:B:2476:F3S:FE1	1.09	0.69
1:B:1414:ARG:NH2	1:B:1455:TRP:CZ2	2.60	0.69
1:B:353:MET:HG2	1:B:385:LEU:HD23	1.72	0.69
1:B:447:LEU:HD12	1:B:451:GLN:CG	2.22	0.69
1:B:603:HIS:N	1:B:640:THR:CG2	2.54	0.69
1:A:1019:ASP:OD2	1:A:1204:ARG:HB2	1.93	0.69
1:A:1121:ASP:OD2	1:A:1124:LEU:HB2	1.92	0.69
1:A:501:GLN:HE21	1:A:653:HIS:CD2	2.10	0.69
1:B:447:LEU:CD1	1:B:451:GLN:HG3	2.22	0.69
1:B:1053:HIS:CE1	1:B:1062:ARG:NH1	2.60	0.69
1:B:1105:VAL:HG13	1:B:1107:GLN:HG3	1.74	0.69
1:B:419:TRP:O	1:B:540:THR:HG21	1.92	0.69
1:B:1054:GLN:O	1:B:1057:THR:N	2.26	0.69
1:B:242:ASN:N	1:B:242:ASN:HD22	1.87	0.69
1:B:753:GLY:O	1:B:754:ILE:C	2.25	0.69
1:A:454:PHE:CD2	1:A:648:GLU:HB2	2.28	0.69
1:A:59:VAL:HG21	1:A:105:TYR:CE2	2.27	0.69
1:B:985:TYR:CE1	1:B:1207:VAL:HG13	2.27	0.69
1:A:515:ARG:NE	1:A:1367:TYR:CE1	2.60	0.69
1:A:313:HIS:O	1:A:317:ILE:HG13	1.93	0.69
1:A:496:HIS:O	1:A:653:HIS:HE1	1.76	0.69
1:B:1090:PHE:CD1	1:B:1090:PHE:N	2.60	0.69
1:B:122:ASN:OD1	1:B:125:ARG:NH1	2.26	0.69
1:B:309:THR:HB	1:B:314:LYS:HE3	1.74	0.69
1:B:1401:LEU:CD1	1:B:1401:LEU:C	2.55	0.69
1:A:1221:PRO:HG2	1:A:1229:MET:CE	2.23	0.69
1:B:1447:TRP:CE2	1:B:1451:VAL:HG22	2.28	0.69
1:B:528:ASN:C	1:B:529:LEU:HD23	2.13	0.69
1:B:107:TRP:N	1:B:107:TRP:CD1	2.59	0.69
1:B:302:ALA:HB2	1:B:347:ARG:NH1	2.07	0.69
1:A:208:HIS:CD2	1:A:209:GLN:O	2.46	0.68
1:A:240:ASN:HD21	1:A:327:TRP:HA	1.58	0.68
1:B:236:THR:CG2	1:B:328:ASP:N	2.52	0.68
1:A:1415:ILE:HG21	1:A:1421:GLU:HB2	1.75	0.68
1:A:9:ILE:HG13	1:A:361:GLY:O	1.93	0.68
1:A:358:THR:HB	1:A:360:ASP:OD1	1.92	0.68
1:B:386:GLY:O	1:B:389:GLU:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1276:LEU:HD12	1:A:1277:GLY:N	2.08	0.68
1:A:1362:SER:HA	1:A:1380:GLY:HA3	1.74	0.68
1:A:208:HIS:CE1	1:A:223:GLN:OE1	2.45	0.68
1:A:426:LEU:H	1:A:426:LEU:HD23	1.59	0.68
1:B:1348:VAL:O	1:B:1348:VAL:HG13	1.91	0.68
1:B:602:THR:C	1:B:640:THR:HG22	2.14	0.68
1:A:1338:ALA:HB3	1:A:1357:VAL:HG22	1.74	0.68
1:A:913:GLY:HA2	1:A:1349:ARG:HD3	1.76	0.68
1:A:52:GLN:HE22	1:A:71:LEU:HB2	1.59	0.68
1:A:732:ARG:H	1:A:747:SER:CB	2.07	0.68
1:B:826:ARG:HG2	1:B:1046:GLU:OE2	1.93	0.68
1:B:1449:ARG:O	1:B:1452:THR:HB	1.93	0.68
1:B:211:TYR:HD1	1:B:212:SER:H	1.42	0.68
1:B:604:VAL:HG23	1:B:640:THR:HG21	1.73	0.68
1:B:932:VAL:O	1:B:933:ALA:HB2	1.92	0.68
1:A:1317:THR:HG21	1:A:1358:GLU:OE1	1.92	0.68
1:A:414:LYS:HB3	1:A:415:PRO:CD	2.23	0.68
1:A:461:MET:HE1	1:A:465:LEU:HD23	1.75	0.68
1:B:794:VAL:HG12	1:B:795:ILE:N	2.06	0.68
1:A:152:ARG:O	1:A:156:GLU:HB2	1.94	0.68
1:B:1170:GLN:O	1:B:1170:GLN:CG	2.39	0.68
1:B:182:MET:CE	1:B:217:PRO:C	2.62	0.68
1:B:250:ARG:O	1:B:531:ASN:ND2	2.27	0.68
1:B:732:ARG:H	1:B:747:SER:HB3	1.57	0.68
1:A:985:TYR:CE1	1:A:1207:VAL:HG13	2.28	0.68
1:A:387:PRO:HD3	1:A:1344:GLU:CD	2.15	0.68
1:A:248:GLU:HA	1:A:251:MET:CG	2.22	0.68
1:A:447:LEU:CD1	1:A:451:GLN:HG3	2.23	0.68
1:B:253:HIS:N	1:B:260:MET:HE1	2.09	0.68
1:A:505:GLN:HE21	1:A:1001:VAL:H	1.33	0.68
1:A:359:THR:HG23	1:A:378:GLN:O	1.94	0.68
1:B:999:LYS:HG2	1:B:1022:LEU:HD23	1.72	0.68
1:B:389:GLU:CB	1:B:403:ASP:OD2	2.40	0.68
1:B:442:MET:HG3	1:B:673:GLU:OE2	1.92	0.68
1:A:8:ALA:HA	1:A:362:LEU:HD12	1.75	0.67
1:A:520:MET:HE1	1:A:705:LEU:HB3	1.74	0.67
1:B:522:LEU:CD2	1:B:705:LEU:HD21	2.24	0.67
1:A:310:PRO:CG	1:A:404:ARG:NH2	2.56	0.67
1:A:461:MET:CE	1:A:465:LEU:HD23	2.24	0.67
1:A:918:THR:HG22	1:A:920:GLU:H	1.59	0.67
1:A:1388:THR:O	1:A:1388:THR:HG22	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1412:PHE:HA	1:A:1456:GLN:O	1.94	0.67
1:A:4:GLY:HA3	1:A:207:TYR:CZ	2.29	0.67
1:A:289:ARG:NH2	1:A:532:ILE:O	2.27	0.67
1:A:850:ARG:HH11	1:A:850:ARG:CG	2.08	0.67
1:A:506:VAL:HG11	1:A:980:LEU:HD22	1.75	0.67
1:B:266:VAL:HG12	1:B:279:THR:HG23	1.76	0.67
1:A:1220:ARG:N	1:A:1221:PRO:HD2	2.10	0.67
1:A:777:GLY:O	1:A:788:HIS:HE1	1.77	0.67
1:B:843:VAL:CG1	1:B:844:GLU:N	2.58	0.67
1:A:336:THR:OG1	1:A:337:ASP:O	2.13	0.67
1:A:454:PHE:HE2	1:A:647:ALA:HB3	1.58	0.67
1:B:731:SER:O	1:B:735:VAL:HG23	1.93	0.67
1:A:960:THR:CG2	1:A:963:VAL:CG2	2.73	0.67
1:B:113:ASN:HD22	1:B:114:VAL:N	1.92	0.67
1:B:1388:THR:O	1:B:1388:THR:HG22	1.94	0.67
1:B:98:LEU:O	1:B:101:GLY:N	2.25	0.67
1:A:746:ILE:O	1:A:747:SER:O	2.13	0.67
1:B:838:VAL:CG1	1:B:839:PRO:CD	2.73	0.67
1:B:559:ARG:HD2	1:B:605:ILE:CD1	2.25	0.67
1:A:139:VAL:HG11	1:A:143:GLN:HB3	1.77	0.67
1:A:661:VAL:O	1:A:661:VAL:HG12	1.94	0.67
1:B:1059:ASN:N	1:B:1059:ASN:HD22	1.91	0.67
1:B:113:ASN:HD22	1:B:115:ASP:H	1.41	0.67
1:B:417:ASP:C	1:B:419:TRP:H	1.96	0.67
1:B:454:PHE:HE2	1:B:647:ALA:HB3	1.58	0.67
1:B:666:VAL:CG1	1:B:667:ASN:N	2.58	0.67
1:B:746:ILE:HD11	1:B:1186:ARG:NH2	2.10	0.67
1:A:1458:VAL:HG13	1:A:1459:PRO:HD2	1.76	0.66
1:A:1466:LEU:O	1:A:1467:GLU:C	2.33	0.66
1:A:746:ILE:HG22	1:A:747:SER:N	2.09	0.66
1:B:496:HIS:ND1	1:B:654:TYR:HD1	1.93	0.66
1:B:732:ARG:H	1:B:747:SER:CB	2.07	0.66
1:B:302:ALA:CA	1:B:347:ARG:HH12	2.08	0.66
1:B:704:LEU:C	1:B:706:LYS:N	2.49	0.66
1:A:354:ARG:NH2	1:A:1292:ALA:O	2.29	0.66
1:A:122:ASN:OD1	1:A:125:ARG:NH1	2.25	0.66
1:A:1396:ASP:OD1	1:A:1396:ASP:C	2.34	0.66
1:A:414:LYS:HB3	1:A:415:PRO:HD3	1.76	0.66
1:B:1102:CYS:SG	5:B:2476:F3S:S2	2.93	0.66
1:B:289:ARG:NH2	1:B:532:ILE:O	2.28	0.66
1:B:559:ARG:HD2	1:B:605:ILE:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ARG:HG3	1:A:1003:ARG:HH11	1.61	0.66
1:B:515:ARG:HD2	1:B:1367:TYR:CZ	2.31	0.66
1:A:1222:LEU:C	1:A:1222:LEU:HD12	2.16	0.66
1:A:454:PHE:CE2	1:A:647:ALA:HB3	2.30	0.66
1:B:113:ASN:C	1:B:113:ASN:ND2	2.49	0.66
1:B:478:SER:O	1:B:1106:ARG:NH1	2.28	0.66
1:A:1230:GLN:NE2	1:A:1267:ARG:CD	2.59	0.66
1:A:731:SER:HA	1:A:748:GLY:N	2.11	0.66
1:B:461:MET:CE	1:B:465:LEU:HD23	2.26	0.66
1:B:780:ARG:NH2	1:B:1105:VAL:CG2	2.59	0.66
1:A:1144:GLU:O	1:A:1144:GLU:HG3	1.95	0.66
1:A:172:LEU:HG	1:A:172:LEU:O	1.94	0.66
1:A:381:GLU:CD	1:A:402:ARG:NH1	2.48	0.66
1:A:447:LEU:C	1:A:447:LEU:HD12	2.14	0.66
1:B:908:LYS:HD2	1:B:921:TYR:CD1	2.31	0.66
1:B:1413:GLN:HG3	1:B:1414:ARG:O	1.96	0.66
1:A:1394:VAL:HG11	1:A:1401:LEU:HD22	1.76	0.65
1:A:420:VAL:HA	1:A:540:THR:HG21	1.78	0.65
1:B:1274:GLN:HE21	1:B:1293:ASN:HB3	1.61	0.65
1:B:603:HIS:CA	1:B:640:THR:CG2	2.71	0.65
1:A:452:GLN:HG3	1:A:765:ALA:HB2	1.77	0.65
1:A:491:LYS:NZ	1:A:785:GLY:HA3	2.11	0.65
1:B:1164:ARG:HD2	1:B:1166:ASP:OD1	1.96	0.65
1:B:909:GLN:NE2	1:B:929:GLU:OE1	2.28	0.65
1:A:1105:VAL:HG13	1:A:1107:GLN:HG3	1.76	0.65
1:A:1297:GLY:O	1:A:1328:LEU:HA	1.95	0.65
1:A:102:TYR:CD2	1:A:144:PHE:CE1	2.82	0.65
1:B:139:VAL:CG1	1:B:143:GLN:HB2	2.25	0.65
1:B:450:ARG:O	1:B:451:GLN:C	2.35	0.65
1:B:454:PHE:HE2	1:B:647:ALA:CB	2.09	0.65
1:B:734:LEU:HD11	1:B:738:HIS:HD2	1.51	0.65
1:A:1050:SER:O	1:A:1054:GLN:HG3	1.97	0.65
1:A:251:MET:HB2	1:A:533:LEU:HD12	1.78	0.65
1:B:572:THR:HG21	1:B:615:ARG:HB3	1.78	0.65
1:A:1207:VAL:HG13	1:A:1208:PRO:HD2	1.77	0.65
1:A:1221:PRO:HD2	1:A:1229:MET:HE1	1.78	0.65
1:A:62:ILE:O	1:A:62:ILE:HG22	1.96	0.65
1:B:218:THR:HG22	1:B:221:LEU:H	1.62	0.65
1:B:56:LYS:HG2	1:B:71:LEU:HD22	1.79	0.65
1:A:1311:THR:HG23	1:A:1312:SER:H	1.60	0.65
1:A:491:LYS:O	1:A:492:TYR:C	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:HG13	1:A:658:LEU:HD13	1.79	0.65
1:B:1058:LEU:HD22	1:B:1058:LEU:O	1.95	0.65
1:B:734:LEU:HD12	1:B:738:HIS:CD2	2.25	0.65
1:B:960:THR:HG22	1:B:963:VAL:HG23	1.77	0.65
1:A:1431:HIS:O	1:A:1435:THR:HG22	1.95	0.65
1:A:746:ILE:HG22	1:A:747:SER:O	1.97	0.65
1:B:1131:THR:CG2	1:B:1133:GLU:OE1	2.42	0.65
1:B:1131:THR:HB	1:B:1134:LYS:CG	2.26	0.65
1:A:728:ILE:HD12	1:A:1047:MET:HE3	1.78	0.64
1:A:1391:MET:HE1	1:A:1458:VAL:HG21	1.77	0.64
1:A:958:HIS:N	1:A:958:HIS:ND1	2.45	0.64
1:B:602:THR:C	1:B:640:THR:HG23	2.17	0.64
1:B:657:VAL:O	1:B:658:LEU:C	2.32	0.64
1:A:1395:TYR:CE1	1:A:1397:LEU:CD2	2.80	0.64
1:A:253:HIS:H	1:A:260:MET:HE1	1.62	0.64
1:A:317:ILE:HG22	1:A:321:ASN:ND2	2.11	0.64
1:A:453:ALA:O	1:A:761:GLN:HG3	1.98	0.64
1:A:824:GLN:CA	1:A:824:GLN:NE2	2.57	0.64
1:B:950:THR:CG2	1:B:951:GLU:H	2.07	0.64
1:A:1291:ASP:OD1	1:A:1291:ASP:C	2.35	0.64
1:A:253:HIS:CE1	1:A:254:PRO:CD	2.62	0.64
1:A:227:MET:CE	1:A:282:GLU:HG2	2.28	0.64
1:A:426:LEU:CD1	1:A:558:MET:HG3	2.28	0.64
1:B:1401:LEU:N	1:B:1402:PRO:CD	2.59	0.64
1:B:990:ILE:HG13	1:B:990:ILE:O	1.97	0.64
1:A:370:GLY:HA3	1:A:1237:ASN:HB3	1.80	0.64
1:A:253:HIS:ND1	1:A:254:PRO:N	2.45	0.64
1:A:52:GLN:CD	1:A:71:LEU:H	2.01	0.64
1:A:74:GLY:CA	1:A:172:LEU:HD13	2.27	0.64
1:A:974:ILE:CD1	1:A:983:LEU:HD12	2.19	0.64
1:B:1164:ARG:HB3	1:B:1167:LEU:HD12	1.80	0.64
1:B:569:ILE:HD13	1:B:569:ILE:N	2.12	0.64
1:A:345:MET:CE	1:A:385:LEU:HB2	2.28	0.64
1:A:1449:ARG:CZ	1:A:1449:ARG:HB2	2.19	0.64
1:A:182:MET:HE3	1:A:217:PRO:HB3	1.68	0.64
1:A:209:GLN:HG3	1:A:210:ARG:N	2.13	0.64
1:A:216:PHE:CZ	1:B:81:ILE:HD13	2.32	0.64
1:A:512:ASP:OD2	1:A:1367:TYR:OH	2.12	0.64
1:A:985:TYR:CE1	1:A:1207:VAL:CG1	2.80	0.64
1:B:1131:THR:HG22	1:B:1134:LYS:N	2.12	0.64
1:A:52:GLN:HE22	1:A:71:LEU:CB	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LYS:HD2	1:B:390:MET:CE	2.19	0.64
1:B:452:GLN:HG3	1:B:765:ALA:HB2	1.78	0.64
1:A:1435:THR:HG23	1:A:1437:SER:H	1.63	0.64
1:A:302:ALA:HA	1:A:347:ARG:HH12	1.62	0.64
1:A:643:ASN:HD22	1:A:665:THR:CG2	2.10	0.64
1:B:555:PHE:HD1	1:B:556:ARG:N	1.96	0.64
1:A:1349:ARG:HG2	1:A:1349:ARG:HH11	1.62	0.63
1:A:1447:TRP:CD2	1:A:1451:VAL:HG22	2.33	0.63
1:A:359:THR:HG23	1:A:378:GLN:HB3	1.79	0.63
1:A:426:LEU:HD11	1:A:558:MET:HG3	1.79	0.63
1:A:891:PRO:HB3	1:A:894:PHE:CE2	2.34	0.63
1:B:693:MET:CE	1:B:693:MET:HA	2.27	0.63
1:B:482:ASP:OD1	1:B:788:HIS:HD2	1.81	0.63
1:A:1112:THR:O	1:A:1114:PRO:HD3	1.97	0.63
1:A:1282:GLN:HA	1:A:1302:GLY:O	1.99	0.63
1:A:1375:ILE:C	1:A:1376:LEU:HD23	2.19	0.63
1:A:386:GLY:O	1:A:389:GLU:HG3	1.98	0.63
1:A:465:LEU:HD12	1:A:465:LEU:O	1.98	0.63
1:B:443:ASP:OD2	1:B:445:ALA:HB3	1.97	0.63
1:B:820:ARG:HB3	1:B:821:PRO:HD2	1.78	0.63
1:B:947:PHE:HD1	1:B:947:PHE:O	1.80	0.63
1:A:248:GLU:O	1:A:250:ARG:N	2.31	0.63
1:A:37:ASP:OD1	1:A:37:ASP:C	2.33	0.63
1:A:452:GLN:HG3	1:A:764:THR:HG22	1.79	0.63
1:A:815:GLU:HA	1:A:815:GLU:OE1	1.98	0.63
1:B:1369:THR:CG2	1:B:1369:THR:O	2.46	0.63
1:B:182:MET:HE3	1:B:217:PRO:C	2.19	0.63
1:B:296:MET:O	1:B:297:MET:C	2.33	0.63
1:B:319:TYR:O	1:B:322:SER:OG	2.09	0.63
1:B:37:ASP:C	1:B:37:ASP:OD1	2.37	0.63
1:B:52:GLN:HE22	1:B:71:LEU:CB	2.09	0.63
1:B:885:GLY:C	1:B:887:GLY:H	2.01	0.63
1:A:1395:TYR:CZ	1:A:1397:LEU:HD21	2.34	0.63
1:A:295:LYS:C	1:A:295:LYS:HD3	2.19	0.63
1:A:442:MET:HE1	1:A:447:LEU:HA	1.78	0.63
1:A:958:HIS:O	1:A:1369:THR:HG21	1.99	0.63
1:B:339:ARG:HG3	1:B:396:GLN:HG3	1.80	0.63
1:A:1164:ARG:NH1	1:A:1166:ASP:OD2	2.31	0.63
1:A:1220:ARG:HB3	1:A:1221:PRO:HD3	1.81	0.63
1:B:351:ARG:HA	1:B:351:ARG:HE	1.64	0.63
1:B:409:HIS:O	1:B:412:THR:HB	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLU:O	1:B:611:MET:N	2.30	0.63
1:A:1007:GLY:O	1:A:1010:ALA:HB3	1.99	0.63
1:A:116:ILE:HD13	1:A:190:THR:CG2	2.29	0.63
1:B:492:TYR:OH	1:B:648:GLU:OE2	2.14	0.63
1:A:1417:VAL:HG12	1:A:1419:HIS:H	1.64	0.63
1:A:446:GLU:O	1:A:447:LEU:C	2.36	0.63
1:A:843:VAL:CG1	1:A:844:GLU:N	2.59	0.63
1:A:978:GLU:O	1:A:981:ALA:HB3	1.99	0.63
1:B:1131:THR:CG2	1:B:1133:GLU:HB2	2.29	0.63
1:B:1389:GLY:HA2	1:B:1459:PRO:HG2	1.81	0.63
1:B:152:ARG:O	1:B:156:GLU:HB2	1.99	0.63
1:B:442:MET:HE3	1:B:446:GLU:HB3	1.81	0.63
1:B:528:ASN:CB	1:B:542:LEU:HD22	2.29	0.63
1:B:453:ALA:O	1:B:761:GLN:HG3	1.97	0.63
1:A:938:PRO:HG2	1:A:1041:ALA:HB1	1.81	0.63
1:A:369:THR:HG22	1:A:1293:ASN:HD21	1.62	0.63
1:B:1112:THR:O	1:B:1114:PRO:HD3	1.99	0.63
1:B:1290:GLY:O	1:B:1291:ASP:HB3	1.99	0.63
1:B:643:ASN:HB3	1:B:665:THR:CG2	2.29	0.63
1:A:1300:LEU:HD12	1:A:1301:SER:H	1.64	0.63
1:A:1376:LEU:HB3	1:A:1439:PHE:CE2	2.32	0.63
1:A:227:MET:HE2	1:A:282:GLU:HG2	1.80	0.63
1:A:235:ASN:ND2	1:A:235:ASN:C	2.52	0.63
1:A:403:ASP:OD2	1:A:407:LYS:NZ	2.32	0.63
1:B:1447:TRP:O	1:B:1451:VAL:HG23	1.98	0.63
1:B:266:VAL:O	1:B:279:THR:HG23	1.98	0.63
1:B:52:GLN:HE22	1:B:71:LEU:N	1.96	0.63
1:B:602:THR:O	1:B:640:THR:HG22	1.99	0.63
1:A:1450:GLU:OE1	1:A:1453:LYS:NZ	2.24	0.62
1:A:146:LEU:HD12	1:A:146:LEU:C	2.16	0.62
1:A:30:HIS:HE1	1:A:368:GLU:OE1	1.81	0.62
1:A:394:ASP:OD1	1:A:394:ASP:C	2.37	0.62
1:A:662:GLY:O	1:A:720:ARG:HD3	1.98	0.62
1:B:1159:ASN:O	1:B:1161:VAL:N	2.32	0.62
1:B:1466:LEU:O	1:B:1467:GLU:C	2.37	0.62
1:A:1289:MET:HE2	1:A:1289:MET:H	1.64	0.62
1:A:1449:ARG:NH1	1:A:1449:ARG:CB	2.14	0.62
1:A:57:ASP:O	1:A:60:LYS:N	2.32	0.62
1:A:731:SER:HA	1:A:747:SER:HB2	1.80	0.62
1:A:746:ILE:HG23	1:A:1182:ASP:CB	2.29	0.62
1:B:423:THR:OG1	1:B:540:THR:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:HG22	1:B:105:TYR:CD2	2.33	0.62
1:A:24:ALA:CB	1:A:207:TYR:CE2	2.82	0.62
1:A:317:ILE:O	1:A:321:ASN:ND2	2.29	0.62
1:A:643:ASN:HD22	1:A:665:THR:HG21	1.65	0.62
1:B:538:THR:HG23	1:B:538:THR:O	1.97	0.62
1:A:643:ASN:HD22	1:A:665:THR:HB	1.64	0.62
1:B:510:PRO:HD2	1:B:970:PRO:HB3	1.81	0.62
1:A:143:GLN:C	1:A:143:GLN:HE21	2.01	0.62
1:A:603:HIS:HA	1:A:640:THR:HG22	1.81	0.62
1:A:515:ARG:NH2	1:A:966:ILE:HB	2.13	0.62
1:B:518:ARG:NH2	1:B:1382:ASN:HD22	1.98	0.62
1:A:80:ARG:HD3	1:A:125:ARG:O	1.98	0.62
1:B:394:ASP:OD1	1:B:394:ASP:C	2.38	0.62
1:A:1356:VAL:HG22	1:A:1374:VAL:CG2	2.30	0.62
1:A:403:ASP:CG	1:A:407:LYS:HZ3	2.02	0.62
1:A:675:ILE:O	1:A:678:ARG:HB2	1.98	0.62
1:B:745:ARG:O	1:B:746:ILE:HG13	1.98	0.62
1:B:806:SER:OG	1:B:809:THR:N	2.31	0.62
1:A:908:LYS:HE2	1:A:924:GLN:O	2.00	0.62
1:A:970:PRO:O	1:A:970:PRO:HG2	2.00	0.62
1:B:1394:VAL:HG11	1:B:1401:LEU:HD22	1.79	0.62
1:B:171:SER:OG	1:B:177:ILE:HA	2.00	0.62
1:A:1221:PRO:CG	1:A:1229:MET:HE1	2.29	0.62
1:A:364:ILE:CD1	1:A:374:ILE:HD11	2.30	0.62
1:B:260:MET:O	1:B:263:LEU:N	2.31	0.62
1:A:299:VAL:CG1	1:A:299:VAL:O	2.43	0.61
1:A:466:HIS:ND1	1:A:678:ARG:NH1	2.46	0.61
1:A:525:ARG:C	1:A:526:LEU:HD12	2.21	0.61
1:B:146:LEU:HD12	1:B:146:LEU:C	2.19	0.61
1:B:243:TRP:HA	1:B:243:TRP:CE3	2.35	0.61
1:B:353:MET:HG2	1:B:385:LEU:CD2	2.29	0.61
1:B:479:MET:HG3	1:B:1104:MET:CE	2.30	0.61
1:B:521:SER:OG	1:B:522:LEU:N	2.33	0.61
1:A:732:ARG:NH1	1:B:94:GLU:OE2	2.28	0.61
1:A:1062:ARG:O	1:A:1062:ARG:CG	2.43	0.61
1:A:746:ILE:C	1:A:747:SER:O	2.35	0.61
1:A:94:GLU:O	1:A:95:THR:C	2.35	0.61
1:B:249:THR:HG23	1:B:249:THR:O	1.98	0.61
1:B:355:TYR:CD1	1:B:355:TYR:C	2.72	0.61
1:B:693:MET:HE3	1:B:693:MET:HA	1.82	0.61
1:B:794:VAL:HG21	1:B:817:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:VAL:HG13	1:A:1348:VAL:O	1.99	0.61
1:A:1374:VAL:O	1:A:1375:ILE:HG13	1.98	0.61
1:B:439:PRO:O	1:B:439:PRO:HG2	1.99	0.61
1:B:74:GLY:CA	1:B:172:LEU:HD13	2.30	0.61
1:A:1221:PRO:CB	1:A:1229:MET:CE	2.73	0.61
1:A:295:LYS:HD3	1:A:295:LYS:O	2.01	0.61
1:A:355:TYR:HD1	1:A:355:TYR:C	2.03	0.61
1:A:423:THR:OG1	1:A:540:THR:HG22	2.00	0.61
1:B:515:ARG:NE	1:B:1367:TYR:CE2	2.68	0.61
1:B:182:MET:CE	1:B:217:PRO:HB3	1.95	0.61
1:B:353:MET:HE2	1:B:366:GLY:O	2.00	0.61
1:B:450:ARG:O	1:B:452:GLN:N	2.34	0.61
1:B:768:GLU:HG2	1:B:769:GLU:N	2.09	0.61
1:A:102:TYR:HE2	1:A:144:PHE:CE1	2.13	0.61
1:A:1221:PRO:HG2	1:A:1229:MET:HE1	1.82	0.61
1:A:629:THR:O	1:A:630:HIS:C	2.37	0.61
1:B:1212:ASP:CG	1:B:1243:GLY:H	2.04	0.61
1:B:1401:LEU:N	1:B:1402:PRO:HD2	2.16	0.61
1:B:482:ASP:OD1	1:B:788:HIS:CD2	2.53	0.61
1:B:918:THR:HG22	1:B:921:TYR:N	2.13	0.61
1:B:976:SER:OG	1:B:978:GLU:HG3	2.00	0.61
1:A:107:TRP:CD1	1:A:107:TRP:N	2.69	0.61
1:B:1383:PHE:O	1:B:1384:ALA:HB3	2.00	0.61
1:B:526:LEU:H	1:B:526:LEU:HD12	1.66	0.61
1:B:1169:HIS:ND1	1:B:1169:HIS:N	2.49	0.61
1:B:279:THR:HG22	1:B:280:VAL:N	2.16	0.61
1:B:499:PHE:HE1	1:B:742:MET:CE	2.14	0.61
1:A:355:TYR:CD1	1:A:355:TYR:O	2.54	0.61
1:A:734:LEU:C	1:A:734:LEU:HD12	2.21	0.61
1:A:1395:TYR:CE2	1:A:1443:ILE:HD13	2.35	0.61
1:A:45:GLY:HA2	1:A:180:LYS:HA	1.81	0.61
1:A:511:ILE:HG22	1:A:512:ASP:H	1.61	0.61
1:A:531:ASN:HB3	1:A:534:ASP:HB2	1.83	0.61
1:B:1121:ASP:OD1	1:B:1123:LYS:N	2.33	0.61
1:B:1135:VAL:O	1:B:1136:VAL:C	2.33	0.61
1:B:1210:THR:HG22	1:B:1211:LEU:N	2.09	0.61
1:B:182:MET:CE	1:B:217:PRO:CA	2.58	0.61
1:B:235:ASN:HD21	1:B:328:ASP:HB3	1.64	0.61
1:B:658:LEU:HD23	1:B:666:VAL:CG2	2.29	0.61
1:A:143:GLN:HE21	1:A:143:GLN:CA	2.14	0.61
1:A:320:CYS:O	1:A:323:VAL:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:LYS:HG3	1:B:691:LYS:O	2.00	0.61
1:A:1374:VAL:O	1:A:1375:ILE:HG12	2.01	0.60
1:A:743:VAL:CG1	1:A:745:ARG:HG3	2.31	0.60
1:B:1084:MET:SD	1:B:1168:LEU:HD23	2.41	0.60
1:B:142:GLU:CD	1:B:142:GLU:H	2.05	0.60
1:B:24:ALA:O	1:B:26:LYS:N	2.34	0.60
1:B:447:LEU:C	1:B:447:LEU:HD12	2.22	0.60
1:B:515:ARG:CD	1:B:1367:TYR:HE2	2.04	0.60
1:B:594:GLU:OE1	1:B:598:ARG:NH2	2.34	0.60
1:B:908:LYS:HD2	1:B:921:TYR:CE1	2.36	0.60
1:B:930:ILE:HD13	1:B:983:LEU:HD13	1.83	0.60
1:A:479:MET:HG3	1:A:1104:MET:HE3	1.80	0.60
1:A:293:MET:HG2	1:A:410:LEU:HD23	1.82	0.60
1:A:450:ARG:O	1:A:451:GLN:C	2.37	0.60
1:A:572:THR:CG2	1:A:615:ARG:HB3	2.31	0.60
1:A:493:ARG:NH2	1:A:786:ASP:OD1	2.32	0.60
1:B:102:TYR:CE1	1:B:144:PHE:CE1	2.89	0.60
1:B:505:GLN:NE2	1:B:1000:LEU:CB	2.59	0.60
1:B:913:GLY:HA2	1:B:1349:ARG:CD	2.27	0.60
1:A:499:PHE:HE2	1:A:742:MET:HE1	1.65	0.60
1:B:183:PHE:CE1	1:B:188:LEU:HA	2.37	0.60
1:A:1315:LEU:HB3	1:A:1320:ASN:HD22	1.67	0.60
1:A:295:LYS:HE2	1:A:299:VAL:CG1	2.31	0.60
1:A:1170:GLN:OE1	1:A:1183:LEU:HB2	2.01	0.60
1:A:1432:VAL:HG22	1:A:1440:ALA:HB3	1.84	0.60
1:A:208:HIS:C	1:A:208:HIS:CD2	2.74	0.60
1:B:266:VAL:O	1:B:279:THR:HG21	2.01	0.60
1:B:447:LEU:HD21	1:B:674:ALA:CA	2.29	0.60
1:B:957:ARG:HH11	1:B:965:LEU:HD12	1.65	0.60
1:A:1388:THR:O	1:A:1388:THR:HG23	2.01	0.60
1:A:47:HIS:HE1	1:A:176:SER:HB3	1.63	0.60
1:A:731:SER:N	1:A:748:GLY:H	2.00	0.60
1:A:1311:THR:CG2	1:A:1312:SER:H	2.14	0.60
1:A:208:HIS:CE1	1:A:223:GLN:CD	2.75	0.60
1:A:260:MET:O	1:A:263:LEU:HB2	2.02	0.60
1:A:403:ASP:CG	1:A:407:LYS:NZ	2.54	0.60
1:A:479:MET:HG3	1:A:1104:MET:SD	2.42	0.60
1:A:565:THR:CG2	1:A:602:THR:HB	2.31	0.60
1:A:652:THR:HG21	1:A:703:GLY:HA3	1.84	0.60
1:A:950:THR:HG23	1:A:951:GLU:H	1.66	0.60
1:B:513:SER:CB	1:B:520:MET:HE1	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:LEU:O	1:B:670:LEU:HD22	2.01	0.60
1:B:938:PRO:O	1:B:939:GLY:C	2.35	0.60
1:A:1090:PHE:N	1:A:1090:PHE:CD1	2.69	0.60
1:A:1171:VAL:O	1:A:1171:VAL:HG12	2.00	0.60
1:A:1221:PRO:HB2	1:A:1229:MET:CE	2.09	0.60
1:A:249:THR:CG2	1:A:250:ARG:HG2	2.31	0.60
1:A:531:ASN:O	1:A:532:ILE:C	2.38	0.60
1:A:704:LEU:C	1:A:706:LYS:N	2.55	0.60
1:A:575:VAL:HG13	1:A:759:LEU:HD22	1.84	0.60
1:B:1009:ILE:O	1:B:1010:ALA:C	2.37	0.60
1:B:312:ASN:HB2	1:B:411:ALA:HB1	1.83	0.60
1:B:390:MET:HG3	1:B:406:LEU:HD23	1.84	0.60
1:B:570:ASP:O	1:B:588:ARG:NH2	2.34	0.60
1:A:1038:ILE:HG22	1:A:1038:ILE:O	2.02	0.60
1:A:1401:LEU:HD11	1:A:1405:ILE:HD12	1.82	0.60
1:A:1412:PHE:CD1	1:A:1412:PHE:N	2.70	0.60
1:A:369:THR:HG23	1:A:370:GLY:N	2.17	0.60
1:A:443:ASP:O	1:A:444:LYS:C	2.39	0.60
1:B:572:THR:HG23	1:B:573:PHE:N	2.17	0.60
1:A:1393:TYR:O	1:A:1394:VAL:CG2	2.44	0.60
1:A:351:ARG:HA	1:A:351:ARG:HE	1.66	0.60
1:B:1171:VAL:O	1:B:1171:VAL:HG12	2.02	0.60
1:B:119:GLU:O	1:B:120:LYS:C	2.38	0.60
1:B:248:GLU:HA	1:B:251:MET:HG2	1.84	0.60
1:B:417:ASP:O	1:B:420:VAL:N	2.33	0.60
1:B:508:ASN:HB2	1:B:509:PRO:HD2	1.84	0.60
1:B:625:GLY:O	1:B:626:ALA:C	2.39	0.60
1:B:728:ILE:HD12	1:B:1047:MET:HE1	1.81	0.60
1:A:1424:LEU:HD23	1:A:1428:ILE:HG13	1.83	0.59
1:A:731:SER:O	1:A:735:VAL:HG23	2.02	0.59
1:A:732:ARG:H	1:A:747:SER:HB3	1.65	0.59
1:A:761:GLN:O	1:A:764:THR:HB	2.02	0.59
1:B:464:ILE:CD1	1:B:779:TYR:CZ	2.81	0.59
1:A:312:ASN:HB2	1:A:411:ALA:HB1	1.83	0.59
1:A:182:MET:CE	1:A:217:PRO:HB3	2.27	0.59
1:A:253:HIS:CE1	1:A:254:PRO:CG	2.85	0.59
1:B:560:ASP:O	1:B:562:MET:N	2.36	0.59
1:B:989:GLN:O	1:B:1245:ARG:HD3	2.01	0.59
1:A:377:THR:HG22	1:A:378:GLN:HG3	1.84	0.59
1:A:515:ARG:NE	1:A:1367:TYR:HE1	1.99	0.59
1:B:572:THR:HG22	1:B:573:PHE:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLN:HB3	1:A:224:PRO:HA	1.85	0.59
1:A:466:HIS:CE1	1:A:684:PHE:CE1	2.91	0.59
1:A:607:THR:HB	1:A:645:ARG:HB2	1.84	0.59
1:A:918:THR:CG2	1:A:1256:MET:SD	2.90	0.59
1:B:1420:TYR:O	1:B:1422:SER:N	2.36	0.59
1:B:149:TYR:CD2	1:B:286:ARG:HG3	2.37	0.59
1:B:227:MET:HE2	1:B:282:GLU:CG	2.32	0.59
1:B:559:ARG:NH1	1:B:568:GLU:OE2	2.35	0.59
1:A:1131:THR:HB	1:A:1134:LYS:CG	2.32	0.59
1:A:842:GLU:HB3	1:A:1156:ARG:HD3	1.84	0.59
1:A:1356:VAL:HG11	1:A:1431:HIS:CG	2.38	0.59
1:B:182:MET:HE1	1:B:217:PRO:C	2.23	0.59
1:B:857:GLY:O	3:B:2474:FMN:C4A	2.50	0.59
1:A:728:ILE:HD12	1:A:1047:MET:HE1	1.83	0.59
1:B:120:LYS:CA	1:B:120:LYS:HE2	2.31	0.59
1:B:1420:TYR:OH	1:B:1466:LEU:HD22	2.02	0.59
1:B:225:PHE:HB3	1:B:278:ASP:OD2	2.02	0.59
1:A:208:HIS:ND1	1:A:223:GLN:OE1	2.35	0.59
1:A:603:HIS:CA	1:A:640:THR:HG22	2.32	0.59
1:A:826:ARG:NH1	1:A:826:ARG:CG	2.58	0.59
1:B:947:PHE:CD1	1:B:947:PHE:O	2.56	0.59
1:A:1425:LYS:CD	1:A:1447:TRP:CE2	2.86	0.59
1:A:89:CYS:O	1:A:93:VAL:HG23	2.03	0.59
1:B:1052:VAL:O	1:B:1053:HIS:C	2.38	0.59
1:B:1109:HIS:N	1:B:1109:HIS:ND1	2.44	0.59
1:B:1131:THR:HG21	1:B:1133:GLU:HB2	1.83	0.59
3:B:2474:FMN:C1'	3:B:2474:FMN:O4'	2.10	0.59
1:B:446:GLU:O	1:B:447:LEU:C	2.40	0.59
1:B:447:LEU:CD1	1:B:451:GLN:CG	2.80	0.59
1:B:938:PRO:O	1:B:940:GLU:N	2.36	0.59
1:A:515:ARG:HD3	1:A:1367:TYR:CE1	2.31	0.59
1:A:259:HIS:O	1:A:260:MET:C	2.39	0.59
1:B:1132:PRO:O	1:B:1136:VAL:HG23	2.02	0.59
1:B:227:MET:HE2	1:B:282:GLU:HG2	1.83	0.59
1:A:139:VAL:CG1	1:A:143:GLN:CB	2.81	0.58
1:A:249:THR:HG22	1:A:250:ARG:HG2	1.85	0.58
1:A:316:LEU:O	1:A:319:TYR:HB3	2.02	0.58
1:A:547:SER:C	1:A:549:VAL:H	2.05	0.58
1:B:193:PRO:O	1:B:194:ASP:C	2.40	0.58
1:B:397:SER:HB2	1:B:399:LYS:HG3	1.84	0.58
1:B:490:ASP:CG	1:B:787:ARG:HH21	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:THR:O	1:B:554:GLU:HG2	2.03	0.58
1:B:589:ILE:HD12	1:B:627:VAL:HG23	1.85	0.58
1:A:1008:THR:HG22	1:A:1009:ILE:H	1.64	0.58
1:A:1221:PRO:CG	1:A:1229:MET:HE2	2.32	0.58
1:A:139:VAL:CG1	1:A:143:GLN:HB2	2.32	0.58
1:A:330:PRO:HA	1:A:350:LEU:HB2	1.84	0.58
1:A:345:MET:CE	1:A:385:LEU:CB	2.81	0.58
1:A:251:MET:HE3	1:A:533:LEU:HD11	1.83	0.58
1:A:884:SER:OG	1:A:885:GLY:N	2.33	0.58
1:B:657:VAL:HG12	1:B:658:LEU:N	2.14	0.58
1:B:869:GLY:O	1:B:873:VAL:HG23	2.03	0.58
1:A:693:MET:O	1:A:694:ALA:C	2.37	0.58
1:B:1221:PRO:HD2	1:B:1229:MET:CE	2.26	0.58
1:B:913:GLY:CA	1:B:1349:ARG:HD3	2.27	0.58
1:B:875:MET:HE1	1:B:1139:PHE:CD2	2.38	0.58
1:A:1375:ILE:HG22	1:A:1375:ILE:O	2.02	0.58
1:A:24:ALA:O	1:A:26:LYS:N	2.36	0.58
1:A:359:THR:HG23	1:A:378:GLN:CA	2.33	0.58
1:B:31:ARG:NH1	1:B:368:GLU:OE1	2.37	0.58
1:A:1317:THR:CG2	1:A:1318:ASN:N	2.64	0.58
1:A:145:GLU:O	1:A:146:LEU:C	2.41	0.58
1:A:511:ILE:CG2	1:A:512:ASP:N	2.59	0.58
1:A:558:MET:O	1:A:560:ASP:N	2.36	0.58
1:A:56:LYS:O	1:A:57:ASP:C	2.42	0.58
1:A:57:ASP:O	1:A:58:HIS:C	2.41	0.58
1:B:4:GLY:HA3	1:B:207:TYR:CZ	2.39	0.58
1:B:653:HIS:O	1:B:654:TYR:C	2.39	0.58
1:A:825:LEU:HD12	1:A:1186:ARG:NH1	2.13	0.58
1:A:1307:VAL:HG12	1:A:1322:ILE:CD1	2.33	0.58
1:A:1425:LYS:HE2	1:A:1447:TRP:CD1	2.38	0.58
1:B:1121:ASP:C	1:B:1121:ASP:OD1	2.42	0.58
1:B:875:MET:HE1	1:B:1139:PHE:CE2	2.39	0.58
1:B:1274:GLN:NE2	1:B:1293:ASN:HB3	2.17	0.58
1:B:303:LEU:HD11	1:B:314:LYS:HG2	1.85	0.58
1:B:322:SER:O	1:B:528:ASN:ND2	2.35	0.58
1:A:236:THR:HG23	1:A:240:ASN:HD21	1.69	0.58
1:A:531:ASN:O	1:A:533:LEU:N	2.36	0.58
1:B:499:PHE:HE1	1:B:742:MET:HE1	1.68	0.58
1:B:997:THR:HG22	1:B:998:VAL:N	2.19	0.58
1:A:102:TYR:HA	1:A:136:ASN:OD1	2.04	0.58
1:A:1251:THR:OG1	1:A:1281:VAL:HG11	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:HG13	1:A:129:GLU:O	2.04	0.58
1:A:291:ALA:HB3	1:A:292:PRO:CD	2.27	0.58
1:A:570:ASP:OD1	1:A:572:THR:HB	2.04	0.58
1:A:5:PHE:O	1:A:365:GLY:N	2.34	0.58
1:A:914:ARG:NH2	1:A:973:ASP:OD1	2.35	0.58
1:B:838:VAL:O	1:B:1151:ALA:HB1	2.04	0.58
1:B:1222:LEU:H	1:B:1229:MET:HE2	1.67	0.58
1:B:958:HIS:O	1:B:1369:THR:CG2	2.51	0.58
1:B:573:PHE:HB2	1:B:574:PRO:HD2	1.85	0.58
1:B:838:VAL:CG1	1:B:839:PRO:N	2.66	0.58
1:B:850:ARG:O	1:B:853:PHE:HB2	2.03	0.58
1:A:1221:PRO:CD	1:A:1229:MET:HE1	2.33	0.58
1:A:1289:MET:HE2	1:A:1289:MET:N	2.19	0.58
1:A:1285:LYS:HA	1:A:1304:THR:O	2.04	0.58
1:A:150:ILE:O	1:A:150:ILE:HG22	2.02	0.58
1:A:606:LEU:C	1:A:607:THR:HG22	2.24	0.58
1:A:695:ASN:O	1:A:696:TYR:C	2.37	0.58
1:B:1336:LEU:HB3	1:B:1355:VAL:HG13	1.84	0.58
1:B:78:LEU:HB3	1:B:79:PRO:HD2	1.86	0.58
1:A:582:LEU:O	1:A:585:ALA:HB3	2.03	0.58
1:A:663:ALA:O	1:A:720:ARG:NE	2.35	0.58
1:A:672:GLN:HG3	1:A:693:MET:HE1	1.84	0.58
1:A:734:LEU:O	1:A:734:LEU:HD12	2.04	0.58
1:B:528:ASN:HB2	1:B:542:LEU:HD22	1.86	0.58
1:B:643:ASN:HB3	1:B:665:THR:HG21	1.85	0.58
1:B:918:THR:O	1:B:919:ALA:C	2.42	0.58
1:A:244:MET:O	1:A:246:ALA:N	2.36	0.57
1:B:484:PRO:HG3	1:B:823:MET:HG3	1.85	0.57
1:A:1447:TRP:CD2	1:A:1451:VAL:CG2	2.87	0.57
1:A:582:LEU:HB3	1:A:755:GLN:HE21	1.69	0.57
1:A:957:ARG:HD2	1:A:965:LEU:HD12	1.87	0.57
1:B:607:THR:HB	1:B:645:ARG:HB2	1.86	0.57
1:A:236:THR:HG23	1:A:240:ASN:ND2	2.19	0.57
1:A:457:THR:O	1:A:460:ASP:HB2	2.04	0.57
1:A:823:MET:O	1:A:824:GLN:NE2	2.36	0.57
1:B:1291:ASP:C	1:B:1291:ASP:OD1	2.42	0.57
1:B:211:TYR:O	1:B:212:SER:HB3	2.05	0.57
1:B:461:MET:HE1	1:B:465:LEU:HD23	1.84	0.57
1:B:845:SER:O	1:B:848:ALA:HB3	2.04	0.57
1:B:515:ARG:NH2	1:B:966:ILE:HB	2.16	0.57
1:A:893:ARG:HG2	1:A:903:TRP:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:GLN:NE2	1:A:1240:ARG:HD2	2.16	0.57
1:A:218:THR:HG22	1:A:221:LEU:H	1.69	0.57
1:B:1368:MET:HB3	1:B:1387:MET:HG3	1.86	0.57
1:B:295:LYS:HE2	1:B:299:VAL:CG1	2.35	0.57
1:B:731:SER:N	1:B:748:GLY:H	2.02	0.57
1:B:739:PHE:C	1:B:740:PRO:O	2.43	0.57
1:A:1282:GLN:CA	1:A:1302:GLY:O	2.52	0.57
1:A:1335:LYS:HA	1:A:1354:THR:O	2.05	0.57
1:A:319:TYR:O	1:A:322:SER:OG	2.17	0.57
1:A:447:LEU:HD12	1:A:447:LEU:O	2.04	0.57
1:A:894:PHE:CD2	1:A:924:GLN:HG3	2.39	0.57
1:B:100:PHE:O	1:B:137:LYS:CE	2.46	0.57
1:B:1318:ASN:ND2	1:B:1318:ASN:H	2.01	0.57
1:B:648:GLU:CG	1:B:648:GLU:O	2.51	0.57
1:A:570:ASP:O	1:A:572:THR:N	2.37	0.57
1:A:447:LEU:CD2	1:A:674:ALA:HA	2.30	0.57
1:B:136:ASN:OD1	1:B:136:ASN:N	2.38	0.57
1:B:312:ASN:OD1	1:B:312:ASN:N	2.25	0.57
1:A:419:TRP:O	1:A:422:ASN:HB2	2.05	0.57
1:A:547:SER:C	1:A:549:VAL:N	2.58	0.57
1:A:913:GLY:O	1:A:915:PHE:N	2.35	0.57
1:B:295:LYS:HZ3	1:B:299:VAL:HG12	1.68	0.57
1:B:52:GLN:NE2	1:B:71:LEU:HB2	2.17	0.57
1:B:777:GLY:O	1:B:788:HIS:CE1	2.51	0.57
1:A:139:VAL:HG12	1:A:143:GLN:HB2	1.87	0.57
1:A:260:MET:O	1:A:263:LEU:CB	2.52	0.57
1:A:45:GLY:HA3	1:A:224:PRO:HD2	1.85	0.57
1:A:560:ASP:O	1:A:562:MET:N	2.38	0.57
1:A:61:VAL:CG1	1:A:61:VAL:O	2.51	0.57
1:A:447:LEU:HD13	1:A:670:LEU:CD2	2.33	0.57
1:A:857:GLY:HA2	1:A:883:ASP:O	2.05	0.57
1:B:950:THR:HG23	1:B:951:GLU:H	1.69	0.57
1:A:551:THR:HG23	1:A:554:GLU:OE2	2.05	0.57
1:B:248:GLU:O	1:B:250:ARG:N	2.37	0.57
1:A:555:PHE:CD1	1:A:555:PHE:C	2.78	0.56
1:A:894:PHE:CE2	1:A:924:GLN:HG3	2.40	0.56
1:B:1220:ARG:N	1:B:1221:PRO:CD	2.67	0.56
1:B:235:ASN:ND2	1:B:328:ASP:O	2.38	0.56
3:B:2474:FMN:O4'	3:B:2474:FMN:H9	2.05	0.56
1:B:37:ASP:OD1	1:B:38:GLY:N	2.38	0.56
1:B:40:THR:HG22	1:B:40:THR:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:GLY:CA	1:A:1145:GLU:HG2	2.29	0.56
1:A:102:TYR:CE2	1:A:144:PHE:CD1	2.93	0.56
1:A:251:MET:SD	1:A:532:ILE:HD11	2.44	0.56
1:B:80:ARG:HD3	1:B:125:ARG:O	2.05	0.56
1:B:823:MET:O	1:B:824:GLN:NE2	2.37	0.56
1:B:857:GLY:HA2	1:B:883:ASP:O	2.06	0.56
1:A:1010:ALA:HB2	1:A:1052:VAL:HG22	1.88	0.56
1:A:1288:VAL:HG12	1:A:1288:VAL:O	2.05	0.56
1:A:15:ARG:HD2	1:A:200:PHE:O	2.06	0.56
1:B:1247:SER:OG	1:B:1280:ALA:HA	2.04	0.56
1:B:513:SER:CB	1:B:520:MET:CE	2.79	0.56
1:B:660:GLY:HA2	1:B:721:GLY:H	1.68	0.56
1:A:1075:THR:CG2	1:A:1076:GLY:N	2.66	0.56
1:A:1212:ASP:CG	1:A:1243:GLY:H	2.07	0.56
1:A:386:GLY:H	1:A:389:GLU:HG3	1.71	0.56
1:A:969:PRO:HD2	1:A:970:PRO:HD2	1.88	0.56
1:B:239:GLY:O	1:B:243:TRP:CD1	2.59	0.56
1:B:236:THR:HG22	1:B:328:ASP:H	1.62	0.56
1:B:466:HIS:ND1	1:B:678:ARG:NH1	2.53	0.56
1:A:149:TYR:O	1:A:150:ILE:C	2.42	0.56
1:A:18:VAL:O	1:A:19:GLU:C	2.42	0.56
1:A:250:ARG:NH1	1:A:530:GLY:HA2	2.20	0.56
1:A:621:ILE:HG12	1:A:657:VAL:CG1	2.36	0.56
1:A:732:ARG:HD2	1:B:94:GLU:OE1	2.06	0.56
1:B:1122:ASP:O	1:B:1126:GLN:HG3	2.04	0.56
1:B:1251:THR:OG1	1:B:1281:VAL:HG11	2.05	0.56
1:B:1348:VAL:CG1	1:B:1348:VAL:O	2.53	0.56
1:B:1:CYS:SG	1:B:211:TYR:HB2	2.45	0.56
1:A:293:MET:HG2	1:A:410:LEU:CD2	2.35	0.56
1:A:409:HIS:O	1:A:413:LEU:HD23	2.06	0.56
1:A:652:THR:CG2	1:A:703:GLY:HA3	2.35	0.56
1:B:3:VAL:CG2	1:B:231:ASN:HB2	2.36	0.56
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.87	0.56
1:B:797:THR:HG21	1:B:812:LYS:HG2	1.86	0.56
1:A:296:MET:O	1:A:297:MET:C	2.40	0.56
1:A:711:MET:O	1:A:713:ILE:N	2.39	0.56
1:B:1366:GLU:CG	1:B:1367:TYR:CD1	2.84	0.56
1:B:209:GLN:HG3	1:B:210:ARG:N	2.20	0.56
1:B:521:SER:C	1:B:522:LEU:HD23	2.26	0.56
1:A:1446:ASP:O	1:A:1447:TRP:C	2.42	0.56
1:A:531:ASN:C	1:A:533:LEU:N	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:HD13	1:B:190:THR:CG2	2.35	0.56
1:B:1366:GLU:HG2	1:B:1367:TYR:CE1	2.41	0.56
1:B:1393:TYR:CD2	1:B:1424:LEU:HD12	2.41	0.56
1:B:570:ASP:OD1	1:B:572:THR:N	2.38	0.56
1:A:140:SER:O	1:A:141:ASP:C	2.44	0.56
1:B:1075:THR:HG23	1:B:1145:GLU:OE2	2.06	0.56
1:A:1226:GLY:O	1:A:1227:GLU:O	2.23	0.56
1:A:494:GLY:O	1:A:495:LEU:C	2.42	0.56
1:A:706:LYS:O	1:A:707:ILE:C	2.43	0.56
1:A:961:PRO:O	1:A:963:VAL:N	2.39	0.56
1:B:1159:ASN:C	1:B:1161:VAL:H	2.09	0.56
1:B:116:ILE:HD13	1:B:190:THR:HG22	1.88	0.56
1:B:162:GLU:HB3	1:B:164:ILE:HD12	1.88	0.56
1:B:449:ARG:HD3	1:B:765:ALA:O	2.06	0.56
1:B:918:THR:HG23	1:B:1256:MET:CE	2.36	0.56
1:A:1163:GLY:O	1:A:1165:THR:N	2.39	0.56
1:A:246:ALA:O	1:A:247:HIS:C	2.42	0.56
1:A:481:ASP:OD1	1:A:481:ASP:C	2.44	0.56
1:A:677:GLU:OE1	1:A:677:GLU:C	2.44	0.56
1:A:711:MET:O	1:A:713:ILE:HG13	2.06	0.56
1:A:1026:ASN:CG	1:A:1027:SER:N	2.60	0.55
1:A:813:TYR:O	1:A:816:GLN:HB2	2.06	0.55
1:B:1222:LEU:HD12	1:B:1222:LEU:C	2.24	0.55
1:B:1326:THR:HG22	1:B:1329:TYR:HB2	1.89	0.55
1:B:985:TYR:CD1	1:B:1207:VAL:HG11	2.42	0.55
1:A:1054:GLN:O	1:A:1057:THR:N	2.39	0.55
1:A:1222:LEU:O	1:A:1222:LEU:HD12	2.07	0.55
1:A:1400:SER:O	1:A:1401:LEU:C	2.44	0.55
1:A:230:HIS:CE1	1:A:234:ILE:HG13	2.35	0.55
1:A:51:PRO:HG3	1:A:200:PHE:CE2	2.41	0.55
1:A:670:LEU:CD2	1:A:670:LEU:O	2.53	0.55
1:A:823:MET:C	1:A:824:GLN:HE21	2.10	0.55
1:A:897:ASP:C	1:A:897:ASP:OD1	2.42	0.55
1:B:938:PRO:HG2	1:B:1041:ALA:HB1	1.88	0.55
1:B:387:PRO:CD	1:B:1344:GLU:OE2	2.47	0.55
1:A:1053:HIS:CE1	1:A:1062:ARG:HH11	2.24	0.55
1:A:392:ALA:O	1:A:400:LEU:CD1	2.53	0.55
1:B:1432:VAL:O	1:B:1433:THR:C	2.45	0.55
1:B:254:PRO:HG2	1:B:255:ALA:N	2.10	0.55
1:B:481:ASP:C	1:B:481:ASP:OD1	2.44	0.55
1:A:1111:ASN:OD1	1:A:1119:VAL:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:ILE:O	1:A:1336:LEU:HD12	2.06	0.55
1:A:177:ILE:CD1	1:A:179:TYR:HE1	2.17	0.55
1:A:37:ASP:OD2	1:A:40:THR:HB	2.06	0.55
1:B:571:ALA:HB2	1:B:606:LEU:CD2	2.37	0.55
1:B:675:ILE:O	1:B:678:ARG:HB2	2.07	0.55
1:A:932:VAL:O	1:A:933:ALA:CB	2.45	0.55
1:A:96:GLU:CA	1:A:96:GLU:OE1	2.54	0.55
1:B:235:ASN:HB3	1:B:508:ASN:ND2	2.22	0.55
1:A:1230:GLN:O	1:A:1231:LEU:HD23	2.06	0.55
1:A:155:ILE:O	1:A:159:VAL:HG23	2.07	0.55
1:A:171:SER:OG	1:A:177:ILE:HA	2.06	0.55
1:A:938:PRO:O	1:A:940:GLU:N	2.40	0.55
1:B:1045:TRP:O	1:B:1046:GLU:C	2.44	0.55
1:B:1093:GLY:O	1:B:1096:SER:N	2.39	0.55
1:B:148:LEU:HD22	1:B:172:LEU:HG	1.87	0.55
1:B:666:VAL:HG12	1:B:667:ASN:N	2.18	0.55
1:A:269:VAL:HG23	1:A:270:GLY:N	2.22	0.55
1:A:75:GLN:C	1:A:76:VAL:HG12	2.27	0.55
1:B:269:VAL:HG23	1:B:270:GLY:N	2.21	0.55
1:B:612:GLY:O	1:B:762:HIS:CE1	2.60	0.55
1:A:235:ASN:ND2	1:A:236:THR:N	2.38	0.55
1:B:710:LYS:HG2	1:B:939:GLY:CA	2.18	0.55
1:A:973:ASP:OD2	1:A:1298:LYS:CE	2.54	0.55
1:B:621:ILE:HG13	1:B:658:LEU:CD1	2.37	0.55
1:B:776:GLY:O	1:B:782:ARG:HD2	2.07	0.55
1:A:1289:MET:HE3	1:A:1289:MET:H	1.72	0.55
1:A:1401:LEU:C	1:A:1401:LEU:CD1	2.74	0.55
1:B:1093:GLY:O	1:B:1094:THR:C	2.45	0.55
1:B:1322:ILE:HG23	1:B:1323:ILE:HG23	1.88	0.55
1:A:1131:THR:CG2	1:A:1133:GLU:OE1	2.54	0.54
1:A:193:PRO:O	1:A:194:ASP:C	2.43	0.54
1:A:149:TYR:HE1	1:A:282:GLU:OE1	1.91	0.54
1:A:430:VAL:HG11	1:A:554:GLU:HB2	1.88	0.54
1:B:1008:THR:HG22	1:B:1009:ILE:H	1.70	0.54
1:B:515:ARG:CZ	1:B:1367:TYR:HE2	2.20	0.54
1:B:223:GLN:HB3	1:B:224:PRO:CA	2.37	0.54
1:B:60:LYS:O	1:B:63:GLY:N	2.39	0.54
1:B:820:ARG:CB	1:B:821:PRO:HD2	2.37	0.54
1:A:1212:ASP:OD2	1:A:1243:GLY:C	2.44	0.54
1:A:22:ILE:O	1:A:23:GLU:C	2.45	0.54
1:A:631:LEU:HD13	1:A:636:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:GLN:HE21	1:A:824:GLN:HA	1.65	0.54
1:B:61:VAL:HG12	1:B:61:VAL:O	2.08	0.54
1:B:744:SER:O	1:B:746:ILE:N	2.40	0.54
1:A:1300:LEU:HD12	1:A:1301:SER:N	2.22	0.54
1:A:1316:GLU:O	1:A:1317:THR:C	2.45	0.54
1:A:313:HIS:H	1:A:313:HIS:CD2	2.24	0.54
1:A:240:ASN:HB3	1:A:327:TRP:CZ2	2.41	0.54
1:A:468:MET:HG2	1:A:699:ALA:CB	2.38	0.54
1:A:452:GLN:NE2	1:A:764:THR:HG21	2.21	0.54
1:A:826:ARG:HH11	1:A:826:ARG:CG	1.97	0.54
1:B:676:ALA:O	1:B:677:GLU:C	2.45	0.54
1:B:953:ILE:HG22	1:B:954:ALA:N	2.22	0.54
1:A:1302:GLY:HA2	1:A:1334:GLY:N	2.23	0.54
1:A:1356:VAL:HG11	1:A:1431:HIS:CB	2.36	0.54
1:A:572:THR:HG23	1:A:615:ARG:HB3	1.90	0.54
1:A:629:THR:O	1:A:632:ILE:N	2.39	0.54
1:A:950:THR:CG2	1:A:952:MET:H	2.15	0.54
1:B:1077:ARG:O	1:B:1078:ASP:C	2.45	0.54
1:B:295:LYS:CE	1:B:299:VAL:HG12	2.37	0.54
1:A:846:ILE:O	1:A:847:THR:C	2.45	0.54
1:B:1055:VAL:O	1:B:1056:LEU:C	2.41	0.54
1:B:403:ASP:OD1	1:B:403:ASP:C	2.46	0.54
1:A:1077:ARG:O	1:A:1078:ASP:C	2.44	0.54
1:A:1304:THR:HG23	1:A:1335:LYS:HB2	1.89	0.54
1:A:1336:LEU:HB3	1:A:1355:VAL:HG13	1.88	0.54
1:A:1394:VAL:O	1:A:1394:VAL:CG1	2.55	0.54
1:A:442:MET:HG2	1:A:446:GLU:HG2	1.88	0.54
1:A:249:THR:OG1	1:A:635:ASN:HB3	2.07	0.54
1:A:67:PRO:HG3	1:A:105:TYR:OH	2.08	0.54
1:B:1121:ASP:O	1:B:1125:ARG:HG3	2.07	0.54
1:A:1222:LEU:H	1:A:1229:MET:CE	2.20	0.54
1:A:1290:GLY:O	1:A:1291:ASP:CB	2.53	0.54
1:A:518:ARG:NH2	1:A:1382:ASN:HD22	2.06	0.54
1:A:35:ASP:HB3	1:A:37:ASP:H	1.71	0.54
1:A:643:ASN:ND2	1:A:665:THR:HB	2.23	0.54
1:B:1054:GLN:O	1:B:1057:THR:HB	2.08	0.54
1:B:47:HIS:CE1	1:B:176:SER:HB3	2.42	0.54
1:B:529:LEU:HB3	1:B:638:THR:OG1	2.08	0.54
1:A:937:LYS:HE3	1:A:1033:SER:CB	2.34	0.54
1:A:1369:THR:C	1:A:1389:GLY:O	2.46	0.54
1:A:561:TYR:O	1:A:561:TYR:CD1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:THR:HA	1:A:720:ARG:NE	2.22	0.54
1:A:937:LYS:HB2	1:A:940:GLU:HG3	1.89	0.54
1:A:92:ILE:O	1:A:93:VAL:C	2.45	0.54
1:B:1131:THR:O	1:B:1134:LYS:N	2.41	0.54
1:B:62:ILE:O	1:B:62:ILE:HG22	2.08	0.54
1:B:720:ARG:C	1:B:722:GLY:H	2.11	0.54
1:B:824:GLN:CA	1:B:824:GLN:HE21	2.20	0.54
1:A:481:ASP:HB2	1:A:1038:ILE:O	2.08	0.54
1:A:853:PHE:CE1	1:A:1079:ILE:HD13	2.42	0.54
1:A:1093:GLY:O	1:A:1096:SER:N	2.41	0.54
1:A:1320:ASN:C	1:A:1341:GLN:HG3	2.28	0.54
1:A:236:THR:OG1	1:A:718:SER:HB3	2.07	0.54
1:A:787:ARG:HH12	1:A:821:PRO:CB	2.17	0.54
1:B:1438:ARG:O	1:B:1439:PHE:C	2.45	0.54
1:B:249:THR:OG1	1:B:635:ASN:HB3	2.08	0.54
1:B:743:VAL:CG1	1:B:745:ARG:HG3	2.38	0.54
1:B:897:ASP:OD1	1:B:897:ASP:C	2.45	0.54
1:A:1061:LEU:O	1:A:1064:ARG:HB2	2.08	0.54
1:A:251:MET:CE	1:A:533:LEU:HD11	2.37	0.54
1:A:573:PHE:HB2	1:A:574:PRO:CD	2.36	0.54
1:B:260:MET:O	1:B:263:LEU:CB	2.56	0.54
1:A:515:ARG:CZ	1:A:1367:TYR:HE1	2.20	0.53
1:A:1427:LEU:O	1:A:1430:GLU:N	2.41	0.53
1:A:302:ALA:HA	1:A:347:ARG:NH1	2.23	0.53
1:A:61:VAL:O	1:A:61:VAL:HG12	2.07	0.53
1:A:746:ILE:O	1:A:747:SER:C	2.43	0.53
1:B:1388:THR:O	1:B:1388:THR:HG23	2.06	0.53
1:B:1470:VAL:O	1:B:1470:VAL:CG1	2.55	0.53
1:B:602:THR:O	1:B:640:THR:CG2	2.57	0.53
1:A:708:MET:O	1:A:710:LYS:N	2.41	0.53
1:A:976:SER:O	1:A:979:ASP:HB2	2.08	0.53
1:B:746:ILE:HG12	1:B:1182:ASP:O	2.08	0.53
1:B:1424:LEU:HD21	1:B:1428:ILE:HD11	1.89	0.53
1:B:731:SER:HB2	1:B:747:SER:HB2	1.89	0.53
1:A:625:GLY:O	1:A:626:ALA:C	2.42	0.53
1:B:443:ASP:O	1:B:446:GLU:N	2.40	0.53
1:A:1016:ALA:O	1:A:1017:ASN:HB2	2.08	0.53
1:A:1121:ASP:OD1	1:A:1122:ASP:N	2.42	0.53
1:A:253:HIS:CE1	1:A:254:PRO:HG2	2.44	0.53
1:B:249:THR:CG2	1:B:249:THR:O	2.55	0.53
1:A:1057:THR:HG22	1:A:1190:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:THR:HG23	1:A:1437:SER:N	2.23	0.53
1:A:565:THR:HG22	1:A:602:THR:HB	1.89	0.53
1:A:571:ALA:HB2	1:A:606:LEU:CD2	2.39	0.53
1:B:1146:VAL:O	1:B:1147:ARG:C	2.46	0.53
1:B:295:LYS:CD	1:B:390:MET:HE3	2.24	0.53
1:B:443:ASP:O	1:B:445:ALA:N	2.41	0.53
1:B:891:PRO:HA	1:B:894:PHE:CD2	2.43	0.53
1:B:917:VAL:HG13	1:B:922:LEU:HD21	1.90	0.53
1:A:369:THR:HG22	1:A:1293:ASN:ND2	2.23	0.53
1:A:572:THR:CG2	1:A:615:ARG:NE	2.72	0.53
1:A:843:VAL:HG12	1:A:844:GLU:H	1.70	0.53
1:B:1221:PRO:HB2	1:B:1229:MET:HE2	1.90	0.53
1:B:1468:VAL:O	1:B:1468:VAL:HG12	2.07	0.53
1:B:348:ASN:HB2	1:B:350:LEU:HG	1.89	0.53
1:B:40:THR:CG2	1:B:40:THR:O	2.57	0.53
1:B:857:GLY:O	3:B:2474:FMN:C10	2.56	0.53
1:A:1220:ARG:N	1:A:1221:PRO:CD	2.71	0.53
1:A:562:MET:HE3	1:A:566:ALA:HB2	1.90	0.53
1:A:838:VAL:HG12	1:A:839:PRO:CD	2.32	0.53
1:B:978:GLU:HG3	1:B:979:ASP:H	1.73	0.53
1:A:119:GLU:O	1:A:120:LYS:C	2.47	0.53
1:A:1374:VAL:C	1:A:1375:ILE:HG13	2.28	0.53
1:A:1438:ARG:O	1:A:1439:PHE:C	2.45	0.53
1:A:608:ASP:OD2	1:A:646:THR:HA	2.09	0.53
1:A:826:ARG:HG2	1:A:1046:GLU:OE2	2.07	0.53
1:B:1316:GLU:O	1:B:1317:THR:C	2.46	0.53
1:B:240:ASN:ND2	1:B:327:TRP:CD2	2.77	0.53
1:B:615:ARG:HG2	1:B:615:ARG:HH11	1.73	0.53
1:A:1274:GLN:HE21	1:A:1293:ASN:HB3	1.74	0.53
1:A:1385:ALA:HB2	1:A:1406:ASN:HD22	1.74	0.53
1:A:660:GLY:HA2	1:A:721:GLY:H	1.74	0.53
1:B:1161:VAL:O	1:B:1161:VAL:CG1	2.57	0.53
1:B:1401:LEU:HB3	1:B:1402:PRO:HD3	1.91	0.53
1:B:693:MET:O	1:B:694:ALA:C	2.44	0.53
1:A:1307:VAL:HG12	1:A:1322:ILE:HD13	1.89	0.53
1:A:317:ILE:CG2	1:A:321:ASN:HD21	2.19	0.53
1:A:31:ARG:NH1	1:A:368:GLU:OE2	2.42	0.53
1:B:1051:GLU:O	1:B:1052:VAL:C	2.46	0.53
1:B:256:PHE:O	1:B:259:HIS:HB2	2.08	0.53
1:B:447:LEU:HD11	1:B:451:GLN:NE2	2.23	0.53
1:B:830:GLU:HG2	1:B:831:LEU:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:O	1:A:531:ASN:ND2	2.42	0.52
1:B:1003:ARG:HG3	1:B:1004:SER:N	2.24	0.52
1:B:1058:LEU:CD2	1:B:1058:LEU:O	2.57	0.52
1:B:1452:THR:HG22	1:B:1453:LYS:HG3	1.91	0.52
1:B:281:PHE:O	1:B:285:VAL:HG23	2.09	0.52
1:B:602:THR:O	1:B:640:THR:HA	2.09	0.52
1:A:1316:GLU:O	1:A:1318:ASN:N	2.42	0.52
1:A:389:GLU:HA	1:A:403:ASP:OD2	2.09	0.52
1:A:587:ARG:O	1:A:590:ARG:HB2	2.09	0.52
1:B:1233:TYR:O	1:B:1268:LEU:HA	2.09	0.52
1:B:1323:ILE:HD12	1:B:1327:VAL:HG21	1.91	0.52
1:B:549:VAL:O	1:B:697:LYS:HE3	2.10	0.52
1:B:500:ARG:HD2	1:B:728:ILE:CG2	2.39	0.52
1:A:1375:ILE:HB	1:A:1394:VAL:HG22	1.91	0.52
1:A:393:VAL:HG12	1:A:394:ASP:N	2.23	0.52
1:A:753:GLY:O	1:A:754:ILE:C	2.45	0.52
1:B:1047:MET:HE2	1:B:1186:ARG:NH2	2.02	0.52
1:B:1050:SER:O	1:B:1051:GLU:C	2.46	0.52
1:B:1432:VAL:O	1:B:1436:GLN:N	2.40	0.52
1:B:295:LYS:CB	1:B:390:MET:HE1	2.39	0.52
1:A:1420:TYR:OH	1:A:1466:LEU:HD22	2.09	0.52
1:A:659:ILE:HA	1:A:663:ALA:HB3	1.91	0.52
1:A:731:SER:CA	1:A:747:SER:HB2	2.40	0.52
1:A:804:ASN:O	1:A:805:ASP:HB3	2.08	0.52
1:B:1075:THR:CG2	1:B:1076:GLY:N	2.73	0.52
1:B:1326:THR:O	1:B:1326:THR:HG22	2.10	0.52
1:B:1338:ALA:O	1:B:1340:GLY:N	2.43	0.52
1:B:1396:ASP:C	1:B:1396:ASP:OD1	2.45	0.52
1:B:574:PRO:HD3	1:B:615:ARG:HH12	1.74	0.52
1:A:1061:LEU:O	1:A:1063:HIS:N	2.43	0.52
1:A:1113:CYS:O	1:A:1115:VAL:N	2.43	0.52
1:A:1122:ASP:O	1:A:1126:GLN:HG3	2.09	0.52
1:A:1219:ALA:O	1:A:1220:ARG:C	2.47	0.52
1:A:143:GLN:O	1:A:143:GLN:NE2	2.41	0.52
1:A:73:VAL:O	1:A:172:LEU:HA	2.09	0.52
1:B:1470:VAL:O	1:B:1470:VAL:HG13	2.08	0.52
1:B:349:GLY:HA3	1:B:387:PRO:HG3	1.91	0.52
1:B:575:VAL:HG23	1:B:614:ALA:O	2.08	0.52
1:B:763:ALA:O	1:B:765:ALA:N	2.42	0.52
1:B:484:PRO:HG3	1:B:823:MET:CG	2.40	0.52
1:B:855:THR:O	1:B:855:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ALA:O	1:A:1014:ALA:HB3	2.09	0.52
1:A:845:SER:O	1:A:848:ALA:HB3	2.09	0.52
1:B:1088:GLU:HG2	1:B:1162:ILE:HD13	1.92	0.52
1:B:1428:ILE:HG22	1:B:1428:ILE:O	2.10	0.52
1:B:494:GLY:O	1:B:495:LEU:C	2.48	0.52
1:A:294:VAL:O	1:A:295:LYS:C	2.47	0.52
1:A:432:THR:O	1:A:434:SER:N	2.43	0.52
1:A:560:ASP:O	1:A:561:TYR:C	2.46	0.52
1:A:651:ASP:N	1:A:651:ASP:OD1	2.43	0.52
1:B:1394:VAL:HG11	1:B:1401:LEU:CD2	2.40	0.52
1:B:236:THR:HG22	1:B:328:ASP:N	2.24	0.52
1:B:419:TRP:O	1:B:540:THR:CB	2.58	0.52
1:B:629:THR:O	1:B:632:ILE:N	2.42	0.52
1:A:1007:GLY:N	1:A:1051:GLU:OE2	2.41	0.52
1:A:1398:ASP:O	1:A:1399:ASP:C	2.47	0.52
1:B:295:LYS:HE2	1:B:299:VAL:HG12	1.92	0.52
1:B:342:VAL:HG12	1:B:343:GLY:N	2.24	0.52
1:B:672:GLN:HG3	1:B:693:MET:SD	2.50	0.52
1:A:1155:PHE:N	1:A:1155:PHE:CD1	2.77	0.52
1:A:1354:THR:HA	1:A:1372:THR:O	2.10	0.52
1:A:175:ARG:NH2	1:A:203:ASP:OD2	2.42	0.52
1:A:281:PHE:O	1:A:285:VAL:HG23	2.11	0.52
1:A:528:ASN:HB2	1:A:542:LEU:HD22	1.90	0.52
1:A:782:ARG:C	1:A:784:SER:H	2.12	0.52
1:A:105:TYR:HD1	1:A:105:TYR:H	1.57	0.51
1:A:1207:VAL:HG13	1:A:1208:PRO:CD	2.39	0.51
1:A:1438:ARG:O	1:A:1440:ALA:N	2.42	0.51
1:A:248:GLU:C	1:A:250:ARG:H	2.13	0.51
1:A:414:LYS:CB	1:A:415:PRO:CD	2.87	0.51
1:A:572:THR:CG2	1:A:573:PHE:N	2.73	0.51
1:B:437:GLY:O	1:B:438:GLU:C	2.48	0.51
1:B:621:ILE:HG12	1:B:657:VAL:CG1	2.40	0.51
1:A:1375:ILE:O	1:A:1377:GLY:N	2.39	0.51
1:A:227:MET:CE	1:A:282:GLU:CG	2.88	0.51
1:A:266:VAL:O	1:A:279:THR:HG23	2.08	0.51
1:A:729:GLY:C	1:A:748:GLY:HA3	2.29	0.51
1:B:628:HIS:O	1:B:629:THR:C	2.47	0.51
1:A:1250:VAL:HG13	1:A:1254:PHE:HD2	1.75	0.51
1:A:250:ARG:NE	1:A:639:PHE:CE1	2.73	0.51
1:A:672:GLN:CG	1:A:693:MET:CE	2.79	0.51
1:A:997:THR:CG2	1:A:998:VAL:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:ALA:O	1:B:1065:VAL:HG23	2.11	0.51
1:B:302:ALA:CA	1:B:347:ARG:NH1	2.72	0.51
1:B:555:PHE:CD1	1:B:556:ARG:N	2.77	0.51
1:B:5:PHE:CE2	1:B:365:GLY:HA3	2.45	0.51
1:B:446:GLU:O	1:B:449:ARG:N	2.43	0.51
1:B:511:ILE:CG2	1:B:512:ASP:N	2.73	0.51
1:B:528:ASN:HB3	1:B:542:LEU:HD22	1.92	0.51
1:A:1135:VAL:O	1:A:1136:VAL:C	2.45	0.51
1:A:1184:ASN:O	1:A:1187:LEU:N	2.44	0.51
1:A:133:VAL:CG1	1:A:134:GLY:N	2.74	0.51
1:B:1077:ARG:HG2	1:B:1078:ASP:N	2.26	0.51
1:B:831:LEU:HD13	1:B:1084:MET:HE3	1.93	0.51
1:B:1245:ARG:HG3	1:B:1245:ARG:O	2.10	0.51
1:B:485:ILE:O	1:B:486:ALA:C	2.48	0.51
1:B:61:VAL:CG1	1:B:61:VAL:O	2.58	0.51
1:A:449:ARG:O	1:A:450:ARG:O	2.28	0.51
1:A:522:LEU:CG	1:A:705:LEU:HD21	2.38	0.51
1:A:705:LEU:N	1:A:705:LEU:HD23	2.26	0.51
1:A:776:GLY:O	1:A:782:ARG:HD2	2.10	0.51
1:B:1092:ILE:O	1:B:1092:ILE:HG22	2.10	0.51
1:A:1:CYS:HB3	2:A:2473:OMT:HE3	1.93	0.51
1:A:731:SER:HA	1:A:747:SER:CA	2.40	0.51
1:A:706:LYS:NZ	1:A:940:GLU:OE1	2.40	0.51
1:B:537:GLU:HG3	1:B:538:THR:N	2.08	0.51
1:B:985:TYR:CE1	1:B:1207:VAL:HG11	2.44	0.51
1:A:218:THR:HG22	1:A:218:THR:O	2.08	0.51
1:A:342:VAL:HG11	1:A:390:MET:CE	2.37	0.51
1:A:479:MET:HG3	1:A:1104:MET:HE1	1.92	0.51
1:A:710:LYS:CG	1:A:939:GLY:HA3	2.34	0.51
1:A:957:ARG:HD2	1:A:965:LEU:CD1	2.41	0.51
1:B:1289:MET:CE	1:B:1289:MET:CB	2.87	0.51
1:B:1438:ARG:O	1:B:1441:ALA:N	2.43	0.51
1:B:1447:TRP:CD2	1:B:1451:VAL:HG22	2.45	0.51
1:B:704:LEU:C	1:B:706:LYS:H	2.14	0.51
1:B:763:ALA:O	1:B:764:THR:C	2.48	0.51
1:A:1143:ALA:O	1:A:1144:GLU:C	2.45	0.51
1:A:1401:LEU:N	1:A:1402:PRO:HD2	2.26	0.51
1:A:1417:VAL:CG1	1:A:1418:GLY:N	2.73	0.51
1:A:159:VAL:HG21	1:A:167:PHE:CD2	2.46	0.51
1:A:175:ARG:HH22	1:A:203:ASP:CG	2.14	0.51
1:A:244:MET:O	1:A:245:LYS:C	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:GLU:O	1:A:795:ILE:HG13	2.11	0.51
1:A:855:THR:O	1:A:855:THR:HG22	2.10	0.51
1:A:893:ARG:HG2	1:A:903:TRP:CB	2.40	0.51
1:B:131:ILE:O	1:B:131:ILE:HG23	2.09	0.51
1:B:74:GLY:HA2	1:B:172:LEU:HD13	1.92	0.51
1:A:1220:ARG:HG3	1:A:1224:GLU:CG	2.38	0.51
1:A:1415:ILE:CG2	1:A:1421:GLU:HB2	2.41	0.51
1:B:746:ILE:CG2	1:B:1182:ASP:HB3	2.22	0.51
1:B:503:PHE:CD1	1:B:503:PHE:N	2.79	0.51
1:B:496:HIS:O	1:B:653:HIS:HE1	1.94	0.51
1:A:1253:LYS:O	1:A:1253:LYS:HG3	2.11	0.50
1:A:209:GLN:HG3	1:A:210:ARG:H	1.76	0.50
1:A:244:MET:HA	1:A:247:HIS:HB2	1.92	0.50
1:A:521:SER:OG	1:A:522:LEU:N	2.44	0.50
1:A:556:ARG:O	1:A:557:ALA:C	2.44	0.50
1:B:875:MET:HE2	1:B:1139:PHE:HE2	1.76	0.50
1:B:1376:LEU:HB3	1:B:1439:PHE:HE2	1.75	0.50
1:B:447:LEU:O	1:B:451:GLN:HG3	2.11	0.50
1:A:1054:GLN:O	1:A:1055:VAL:C	2.49	0.50
1:A:1:CYS:HB3	2:A:2473:OMT:CE	2.41	0.50
1:A:359:THR:HG23	1:A:378:GLN:CB	2.41	0.50
1:A:547:SER:OG	1:A:549:VAL:HB	2.11	0.50
1:A:707:ILE:HA	1:A:710:LYS:HD2	1.92	0.50
1:B:302:ALA:CB	1:B:347:ARG:NH1	2.73	0.50
1:B:679:HIS:NE2	1:B:687:MET:O	2.42	0.50
1:B:846:ILE:O	1:B:847:THR:C	2.48	0.50
1:A:1110:SER:C	1:A:1112:THR:HG23	2.32	0.50
1:A:1359:GLY:O	1:A:1360:CYS:CB	2.58	0.50
1:A:94:GLU:HG2	1:A:104:ILE:HD13	1.92	0.50
1:B:1183:LEU:O	1:B:1187:LEU:HG	2.11	0.50
1:B:485:ILE:O	1:B:488:LEU:N	2.43	0.50
1:B:499:PHE:CE1	1:B:742:MET:HE1	2.46	0.50
1:B:536:ASP:O	1:B:536:ASP:OD1	2.28	0.50
1:B:868:HIS:O	1:B:869:GLY:C	2.49	0.50
1:A:235:ASN:ND2	1:A:236:THR:HB	2.27	0.50
1:A:509:PRO:HB3	1:A:975:TYR:HD1	1.77	0.50
1:A:763:ALA:O	1:A:767:ASN:HB2	2.11	0.50
1:B:1406:ASN:OD1	1:B:1406:ASN:C	2.48	0.50
1:B:556:ARG:O	1:B:557:ALA:C	2.48	0.50
1:A:228:LEU:HD22	1:A:278:ASP:HA	1.94	0.50
1:A:309:THR:CG2	1:A:314:LYS:HG3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLU:O	1:A:595:ASP:C	2.48	0.50
1:A:657:VAL:O	1:A:658:LEU:C	2.48	0.50
1:B:1058:LEU:C	1:B:1059:ASN:HD22	2.15	0.50
1:B:243:TRP:CD1	1:B:325:GLU:OE1	2.65	0.50
1:B:337:ASP:C	1:B:337:ASP:OD1	2.49	0.50
1:B:351:ARG:HH12	1:B:978:GLU:CD	2.14	0.50
1:B:979:ASP:O	1:B:980:LEU:C	2.49	0.50
1:A:105:TYR:CD1	1:A:105:TYR:N	2.80	0.50
1:A:24:ALA:C	1:A:26:LYS:N	2.65	0.50
1:A:369:THR:O	1:A:371:MET:N	2.43	0.50
1:A:394:ASP:OD1	1:A:396:GLN:N	2.43	0.50
1:A:404:ARG:CB	1:A:405:GLU:OE1	2.51	0.50
1:A:62:ILE:CG2	1:A:62:ILE:O	2.60	0.50
1:A:643:ASN:HB3	1:A:665:THR:HG21	1.93	0.50
1:A:676:ALA:O	1:A:679:HIS:N	2.45	0.50
1:A:731:SER:HA	1:A:747:SER:CB	2.42	0.50
1:A:746:ILE:HG23	1:A:1182:ASP:N	2.21	0.50
1:B:1002:SER:HB2	1:B:1048:GLY:HA3	1.93	0.50
1:B:1068:ARG:NE	1:B:1089:GLU:OE1	2.38	0.50
1:B:1131:THR:CG2	1:B:1133:GLU:N	2.72	0.50
1:B:197:ASP:OD1	1:B:199:ARG:HB2	2.11	0.50
1:B:476:ILE:HA	1:B:1034:PRO:HA	1.94	0.50
1:B:720:ARG:O	1:B:722:GLY:N	2.45	0.50
1:A:1023:ILE:HD12	1:A:1023:ILE:N	2.27	0.50
1:A:1424:LEU:O	1:A:1425:LYS:C	2.49	0.50
1:A:54:PHE:HA	1:A:199:ARG:HD2	1.94	0.50
1:A:1:CYS:SG	1:A:211:TYR:HD2	2.35	0.50
1:A:244:MET:C	1:A:246:ALA:N	2.65	0.50
1:A:359:THR:HG23	1:A:378:GLN:C	2.32	0.50
1:A:484:PRO:HG3	1:A:823:MET:HG3	1.94	0.50
1:B:1460:LYS:O	1:B:1462:MET:N	2.44	0.50
1:B:260:MET:O	1:B:261:GLN:C	2.48	0.50
1:B:797:THR:HG23	1:B:812:LYS:HE2	1.94	0.50
1:B:911:ALA:O	1:B:912:SER:C	2.49	0.50
1:A:1075:THR:O	1:A:1076:GLY:C	2.50	0.50
1:A:1421:GLU:HG3	1:A:1451:VAL:HG11	1.94	0.50
1:A:248:GLU:C	1:A:250:ARG:N	2.64	0.50
1:A:80:ARG:HG3	1:A:80:ARG:O	2.12	0.50
1:A:970:PRO:O	1:A:970:PRO:CG	2.60	0.50
1:B:746:ILE:CG2	1:B:1182:ASP:CB	2.86	0.50
1:B:505:GLN:NE2	1:B:1001:VAL:N	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLN:OE1	1:B:773:LEU:HD11	2.11	0.50
1:B:953:ILE:O	1:B:954:ALA:C	2.50	0.50
1:A:1318:ASN:H	1:A:1318:ASN:HD22	1.60	0.50
1:A:1108:CYS:SG	5:A:2476:F3S:S4	2.94	0.50
1:A:30:HIS:ND1	1:A:1238:THR:HA	2.26	0.50
1:A:312:ASN:HB2	1:A:411:ALA:CB	2.41	0.50
1:A:443:ASP:O	1:A:446:GLU:N	2.28	0.50
1:A:466:HIS:HB3	1:A:467:PRO:HD3	1.94	0.50
1:A:652:THR:HG21	1:A:703:GLY:CA	2.41	0.50
1:A:52:GLN:NE2	1:A:71:LEU:HB2	2.27	0.50
1:A:731:SER:HB2	1:A:747:SER:HB2	1.94	0.50
1:A:798:LEU:O	1:A:802:VAL:HG22	2.12	0.50
1:B:1207:VAL:HG13	1:B:1208:PRO:HD2	1.92	0.50
1:B:1435:THR:HG23	1:B:1437:SER:CB	2.42	0.50
1:B:236:THR:OG1	1:B:718:SER:HB3	2.12	0.50
1:B:355:TYR:CD1	1:B:355:TYR:O	2.65	0.50
1:B:569:ILE:HG22	1:B:589:ILE:HG22	1.93	0.50
1:A:1243:GLY:O	1:A:1244:THR:C	2.49	0.49
1:A:225:PHE:HB3	1:A:278:ASP:OD2	2.12	0.49
1:A:353:MET:O	1:A:353:MET:HG3	2.12	0.49
1:A:621:ILE:HG12	1:A:657:VAL:HG12	1.93	0.49
1:B:1204:ARG:O	1:B:1206:GLU:N	2.45	0.49
1:A:24:ALA:O	1:A:27:ALA:N	2.27	0.49
1:A:339:ARG:HG3	1:A:396:GLN:HG3	1.93	0.49
1:A:359:THR:CG2	1:A:378:GLN:HA	2.42	0.49
1:A:442:MET:CE	1:A:447:LEU:HA	2.41	0.49
1:B:1407:ASP:O	1:B:1408:GLU:C	2.50	0.49
1:B:419:TRP:O	1:B:540:THR:CG2	2.59	0.49
1:B:670:LEU:C	1:B:670:LEU:HD22	2.31	0.49
1:B:696:TYR:CZ	1:B:700:ILE:CD1	2.94	0.49
1:B:949:VAL:C	1:B:950:THR:O	2.48	0.49
1:A:1400:SER:O	1:A:1403:LEU:N	2.27	0.49
1:A:508:ASN:HB2	1:A:509:PRO:HD2	1.95	0.49
1:A:90:ARG:HB3	1:A:107:TRP:CH2	2.48	0.49
1:B:479:MET:HG3	1:B:1104:MET:SD	2.52	0.49
1:A:47:HIS:HE1	1:A:176:SER:CB	2.25	0.49
1:A:51:PRO:HG3	1:A:200:PHE:CD2	2.48	0.49
1:A:236:THR:HG22	1:A:328:ASP:N	2.26	0.49
1:A:492:TYR:CG	1:A:761:GLN:HG2	2.47	0.49
1:B:1059:ASN:O	1:B:1060:ARG:HB2	2.12	0.49
1:B:113:ASN:HD21	1:B:115:ASP:H	1.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:HD3	1:B:1367:TYR:CE2	2.40	0.49
1:B:290:THR:CG2	1:B:291:ALA:N	2.75	0.49
1:B:354:ARG:NH2	1:B:1292:ALA:O	2.46	0.49
1:A:1054:GLN:O	1:A:1057:THR:HB	2.12	0.49
1:A:1368:MET:HB3	1:A:1387:MET:HG3	1.94	0.49
1:A:213:THR:O	1:A:214:ASN:ND2	2.43	0.49
1:A:291:ALA:CB	1:A:292:PRO:HD3	2.31	0.49
1:A:636:LEU:O	1:A:637:ARG:C	2.50	0.49
1:A:960:THR:CG2	1:A:963:VAL:HG21	2.42	0.49
1:B:30:HIS:HD2	1:B:31:ARG:N	2.10	0.49
1:B:621:ILE:HG13	1:B:658:LEU:HD12	1.93	0.49
1:A:110:VAL:O	1:A:112:ILE:HG23	2.13	0.49
1:A:1349:ARG:NH1	1:A:1349:ARG:CG	2.75	0.49
1:B:111:PRO:C	1:B:112:ILE:HG23	2.33	0.49
1:B:1184:ASN:O	1:B:1186:ARG:N	2.46	0.49
1:B:1211:LEU:HG	1:B:1215:ILE:HD11	1.94	0.49
1:B:302:ALA:HB2	1:B:347:ARG:HH11	1.77	0.49
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.36	0.49
1:A:243:TRP:HA	1:A:243:TRP:CE3	2.47	0.49
1:A:689:LEU:HG	1:A:689:LEU:O	2.11	0.49
1:A:664:THR:HA	1:A:720:ARG:HE	1.77	0.49
1:B:1310:THR:HG22	1:B:1311:THR:HG22	1.95	0.49
1:B:253:HIS:CE1	1:B:254:PRO:CD	2.88	0.49
1:B:24:ALA:C	1:B:26:LYS:N	2.65	0.49
1:B:838:VAL:HG12	1:B:839:PRO:CD	2.40	0.49
1:B:850:ARG:HD2	1:B:878:ILE:HD12	1.94	0.49
1:B:991:ASN:C	1:B:991:ASN:OD1	2.51	0.49
1:A:1401:LEU:CD1	1:A:1401:LEU:O	2.53	0.49
1:A:266:VAL:CG1	1:A:279:THR:HG23	2.33	0.49
1:A:485:ILE:HG12	1:A:488:LEU:HD12	1.95	0.49
1:A:499:PHE:HE2	1:A:742:MET:CE	2.26	0.49
1:A:537:GLU:C	1:A:539:GLN:H	2.15	0.49
1:A:969:PRO:HD2	1:A:970:PRO:CD	2.42	0.49
1:B:1068:ARG:NH2	1:B:1089:GLU:OE1	2.46	0.49
1:B:242:ASN:HA	1:B:245:LYS:HG3	1.94	0.49
1:B:629:THR:O	1:B:630:HIS:C	2.51	0.49
1:B:690:GLU:H	1:B:690:GLU:CD	2.15	0.49
1:B:698:LYS:O	1:B:698:LYS:HG2	2.13	0.49
1:A:1038:ILE:O	1:A:1038:ILE:CG2	2.61	0.49
1:A:1281:VAL:HA	1:A:1301:SER:O	2.13	0.49
1:A:492:TYR:C	1:A:492:TYR:CD1	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ALA:O	1:A:677:GLU:C	2.50	0.49
1:B:452:GLN:HG3	1:B:764:THR:HG22	1.94	0.49
1:B:582:LEU:CB	1:B:755:GLN:HE21	2.26	0.49
1:A:1447:TRP:CE3	1:A:1447:TRP:HA	2.48	0.49
1:A:116:ILE:HD13	1:A:190:THR:HG21	1.94	0.49
1:A:197:ASP:OD1	1:A:199:ARG:N	2.37	0.49
1:A:653:HIS:O	1:A:654:TYR:C	2.51	0.49
1:A:83:LEU:O	1:A:84:ASP:C	2.50	0.49
1:B:1417:VAL:HG12	1:B:1419:HIS:N	2.26	0.49
1:B:290:THR:O	1:B:294:VAL:HG23	2.12	0.49
1:B:417:ASP:HA	1:B:420:VAL:HG12	1.95	0.49
1:A:1395:TYR:CD2	1:A:1443:ILE:HD13	2.48	0.48
1:A:253:HIS:ND1	1:A:254:PRO:CG	2.71	0.48
1:B:1401:LEU:HD11	1:B:1405:ILE:HB	1.94	0.48
1:B:353:MET:CE	1:B:366:GLY:O	2.60	0.48
1:B:823:MET:C	1:B:824:GLN:HE21	2.17	0.48
1:A:1030:THR:HG21	1:A:1033:SER:HB3	1.95	0.48
1:A:1440:ALA:O	1:A:1443:ILE:N	2.42	0.48
1:A:191:PHE:CE1	1:A:192:TYR:CE1	3.01	0.48
1:A:482:ASP:OD1	1:A:788:HIS:HB3	2.13	0.48
1:A:918:THR:HG22	1:A:920:GLU:N	2.26	0.48
1:B:1159:ASN:C	1:B:1161:VAL:N	2.66	0.48
1:B:211:TYR:HD1	1:B:212:SER:N	2.08	0.48
1:B:254:PRO:O	1:B:257:GLY:N	2.37	0.48
1:A:1326:THR:HG22	1:A:1329:TYR:HB2	1.95	0.48
1:A:1417:VAL:HG12	1:A:1418:GLY:N	2.27	0.48
1:A:1376:LEU:CB	1:A:1439:PHE:HE2	2.19	0.48
1:A:1441:ALA:O	1:A:1444:LEU:HB2	2.13	0.48
1:A:353:MET:HE2	1:A:366:GLY:C	2.32	0.48
1:A:661:VAL:O	1:A:661:VAL:CG1	2.61	0.48
1:A:85:ALA:O	1:A:86:GLN:C	2.48	0.48
1:B:1278:ALA:O	1:B:1279:PHE:HB2	2.12	0.48
1:B:389:GLU:CA	1:B:403:ASP:OD2	2.61	0.48
1:B:810:PHE:O	1:B:813:TYR:HB3	2.13	0.48
1:A:1219:ALA:C	1:A:1221:PRO:HD2	2.34	0.48
1:A:97:ILE:HD13	1:A:133:VAL:HG21	1.95	0.48
1:A:1359:GLY:O	1:A:1360:CYS:HB3	2.12	0.48
1:A:1366:GLU:HG2	1:A:1367:TYR:CE2	2.47	0.48
1:A:74:GLY:HA2	1:A:172:LEU:HD13	1.96	0.48
1:A:345:MET:HE1	1:A:385:LEU:HB2	1.94	0.48
1:A:454:PHE:CD2	1:A:648:GLU:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:O	1:A:54:PHE:C	2.50	0.48
1:A:430:VAL:HG22	1:A:557:ALA:HB3	1.95	0.48
1:A:87:GLU:O	1:A:90:ARG:N	2.47	0.48
1:A:909:GLN:NE2	1:A:929:GLU:OE1	2.46	0.48
1:B:1163:GLY:O	1:B:1165:THR:N	2.45	0.48
1:B:1236:ARG:C	1:B:1238:THR:H	2.15	0.48
1:B:110:VAL:CG2	1:B:130:GLN:HG3	2.43	0.48
1:B:1407:ASP:O	1:B:1409:SER:N	2.46	0.48
1:B:1420:TYR:O	1:B:1421:GLU:C	2.46	0.48
1:B:175:ARG:HG3	1:B:175:ARG:NH1	2.23	0.48
1:B:594:GLU:O	1:B:597:VAL:N	2.45	0.48
1:B:572:THR:CG2	1:B:615:ARG:HB3	2.42	0.48
1:A:1184:ASN:O	1:A:1186:ARG:N	2.46	0.48
1:A:369:THR:CG2	1:A:370:GLY:N	2.76	0.48
1:A:538:THR:O	1:A:538:THR:HG23	2.13	0.48
1:B:1212:ASP:OD1	1:B:1243:GLY:N	2.34	0.48
1:B:1427:LEU:O	1:B:1430:GLU:N	2.46	0.48
1:A:1068:ARG:NE	1:A:1089:GLU:OE1	2.39	0.48
1:A:1428:ILE:HG22	1:A:1428:ILE:O	2.14	0.48
1:A:15:ARG:HG3	1:A:19:GLU:HG3	1.94	0.48
1:B:1008:THR:O	1:B:1011:ALA:HB3	2.14	0.48
1:A:160:LYS:O	1:A:161:GLY:C	2.50	0.48
1:A:345:MET:HG2	1:A:349:GLY:HA2	1.95	0.48
1:A:3:VAL:HG22	1:A:231:ASN:HB2	1.96	0.48
1:A:68:ASP:OD1	1:A:68:ASP:N	2.44	0.48
1:A:858:MET:HA	3:A:2474:FMN:N5	2.29	0.48
1:B:1105:VAL:HG22	1:B:1105:VAL:O	2.14	0.48
1:B:474:GLU:O	1:B:475:ALA:C	2.52	0.48
1:B:731:SER:HA	1:B:747:SER:CB	2.43	0.48
1:B:978:GLU:O	1:B:981:ALA:HB3	2.12	0.48
1:A:1210:THR:CG2	1:A:1211:LEU:N	2.47	0.48
1:A:1230:GLN:HE21	1:A:1267:ARG:HD3	1.76	0.48
1:A:496:HIS:O	1:A:653:HIS:CE1	2.61	0.48
1:A:754:ILE:O	1:A:755:GLN:C	2.48	0.48
1:B:1131:THR:CG2	1:B:1133:GLU:H	2.27	0.48
1:B:595:ASP:O	1:B:596:ALA:C	2.51	0.48
1:B:1424:LEU:HD23	1:B:1428:ILE:HG13	1.96	0.48
1:B:856:PRO:HB3	3:B:2474:FMN:H3'	1.95	0.48
1:B:393:VAL:HG12	1:B:394:ASP:N	2.29	0.48
1:B:442:MET:HB3	1:B:442:MET:HE3	1.73	0.48
1:B:582:LEU:HB2	1:B:755:GLN:HE21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1396:ASP:OD1	1:A:1396:ASP:O	2.30	0.48
1:B:105:TYR:CD1	1:B:105:TYR:N	2.81	0.48
1:B:1077:ARG:CG	1:B:1078:ASP:N	2.77	0.48
1:B:1325:ASN:O	1:B:1326:THR:HB	2.14	0.48
1:B:227:MET:HE3	1:B:282:GLU:CA	2.28	0.48
1:B:430:VAL:HG22	1:B:557:ALA:HB3	1.94	0.48
1:A:12:LYS:HA	1:A:13:PRO:HD3	1.72	0.47
1:A:345:MET:HE2	1:A:385:LEU:CB	2.43	0.47
1:A:561:TYR:C	1:A:561:TYR:CD1	2.86	0.47
1:B:1396:ASP:O	1:B:1396:ASP:OD1	2.32	0.47
1:B:162:GLU:CB	1:B:164:ILE:HD12	2.44	0.47
1:B:472:GLY:O	1:B:473:LYS:HG3	2.14	0.47
1:B:452:GLN:CG	1:B:764:THR:HG22	2.43	0.47
1:A:1070:ASP:OD1	1:A:1070:ASP:C	2.52	0.47
1:A:1447:TRP:O	1:A:1451:VAL:HG23	2.14	0.47
1:A:1412:PHE:HD2	1:A:1455:TRP:CZ3	2.33	0.47
1:A:189:THR:CG2	1:A:190:THR:N	2.63	0.47
1:A:513:SER:HB2	1:A:520:MET:CE	2.43	0.47
1:A:552:THR:O	1:A:552:THR:HG22	2.14	0.47
1:A:631:LEU:N	1:A:631:LEU:HD23	2.29	0.47
1:B:1057:THR:HG22	1:B:1058:LEU:N	2.22	0.47
1:B:1221:PRO:CD	1:B:1229:MET:HE1	2.27	0.47
1:B:235:ASN:HB3	1:B:508:ASN:HD21	1.79	0.47
1:B:501:GLN:OE1	1:B:710:LYS:NZ	2.43	0.47
1:B:550:LEU:HB3	1:B:554:GLU:HG3	1.96	0.47
1:B:875:MET:HE3	1:B:880:ALA:HB3	1.96	0.47
1:A:1091:GLY:C	1:A:1092:ILE:HG13	2.34	0.47
1:A:1374:VAL:C	1:A:1375:ILE:CG1	2.82	0.47
1:A:1396:ASP:OD1	1:A:1399:ASP:N	2.47	0.47
1:A:1425:LYS:CE	1:A:1447:TRP:CD1	2.97	0.47
1:A:203:ASP:OD1	1:A:203:ASP:N	2.44	0.47
1:A:990:ILE:HG23	1:A:991:ASN:N	2.29	0.47
1:B:630:HIS:O	1:B:631:LEU:C	2.49	0.47
1:B:727:ALA:HB3	1:B:744:SER:HB2	1.95	0.47
1:B:953:ILE:O	1:B:955:ARG:N	2.47	0.47
1:A:1117:VAL:HG12	1:A:1118:CYS:N	2.29	0.47
1:A:1124:LEU:HA	1:A:1124:LEU:HD12	1.28	0.47
1:A:1369:THR:O	1:A:1369:THR:HG22	2.13	0.47
1:A:242:ASN:HD22	1:A:242:ASN:H	1.61	0.47
1:A:31:ARG:HD2	1:A:368:GLU:OE2	2.15	0.47
1:A:429:LEU:O	1:A:429:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ASN:C	1:A:529:LEU:HD23	2.35	0.47
1:A:531:ASN:C	1:A:533:LEU:H	2.18	0.47
1:A:672:GLN:O	1:A:673:GLU:C	2.52	0.47
1:A:683:LEU:HA	1:A:683:LEU:HD23	1.55	0.47
1:B:1113:CYS:O	1:B:1114:PRO:C	2.48	0.47
1:B:210:ARG:HA	2:B:2473:OMT:HE2	1.97	0.47
1:B:465:LEU:HD21	1:B:675:ILE:HG13	1.95	0.47
1:B:515:ARG:NE	1:B:1367:TYR:HE2	2.09	0.47
1:B:963:VAL:CG1	1:B:964:MET:H	2.25	0.47
1:A:1369:THR:O	1:A:1369:THR:CG2	2.63	0.47
1:A:218:THR:CG2	1:A:221:LEU:H	2.27	0.47
1:A:9:ILE:HG13	1:A:361:GLY:C	2.35	0.47
1:A:442:MET:CE	1:A:447:LEU:CA	2.92	0.47
1:B:1170:GLN:HB2	1:B:1183:LEU:HD12	1.96	0.47
1:B:37:ASP:OD1	1:B:39:LYS:N	2.34	0.47
1:B:704:LEU:O	1:B:707:ILE:N	2.48	0.47
1:A:1029:GLY:HA3	3:A:2474:FMN:HM81	1.97	0.47
1:A:110:VAL:HG12	1:A:111:PRO:N	2.28	0.47
1:A:1424:LEU:HD21	1:A:1428:ILE:HD11	1.97	0.47
1:A:253:HIS:CD2	1:A:254:PRO:HD2	2.40	0.47
1:A:353:MET:CE	1:A:366:GLY:C	2.82	0.47
1:A:78:LEU:HD12	1:A:129:GLU:HG3	1.97	0.47
1:B:1216:VAL:HG11	1:B:1249:MET:CE	2.45	0.47
1:B:139:VAL:HG12	1:B:143:GLN:HB2	1.97	0.47
1:B:189:THR:HG23	1:B:189:THR:O	2.14	0.47
1:B:447:LEU:CD1	1:B:451:GLN:CD	2.83	0.47
1:B:826:ARG:HD2	1:B:1078:ASP:OD1	2.14	0.47
1:A:1149:ILE:CG2	1:A:1149:ILE:O	2.59	0.47
1:A:136:ASN:OD1	1:A:136:ASN:N	2.47	0.47
1:A:1414:ARG:NH2	1:A:1455:TRP:CZ2	2.82	0.47
1:A:509:PRO:O	1:A:509:PRO:HG2	2.14	0.47
1:A:550:LEU:HD13	1:A:555:PHE:HA	1.95	0.47
1:A:657:VAL:HG12	1:A:658:LEU:N	2.30	0.47
1:A:917:VAL:HG13	1:A:922:LEU:HD21	1.95	0.47
1:B:1047:MET:O	1:B:1048:GLY:C	2.53	0.47
1:B:290:THR:HG22	1:B:293:MET:H	1.78	0.47
1:B:589:ILE:O	1:B:593:THR:OG1	2.28	0.47
1:B:743:VAL:HG12	1:B:744:SER:N	2.30	0.47
1:B:864:SER:HG	1:B:867:ALA:H	1.59	0.47
1:B:908:LYS:HB3	1:B:921:TYR:CZ	2.49	0.47
1:A:1244:THR:O	1:A:1245:ARG:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:ASP:HB3	1:A:1245:ARG:HB3	1.96	0.47
1:A:182:MET:CE	1:A:217:PRO:O	2.62	0.47
1:A:317:ILE:C	1:A:321:ASN:HD22	2.18	0.47
1:A:526:LEU:HB3	1:A:641:SER:HB3	1.97	0.47
1:A:953:ILE:O	1:A:956:LEU:HB2	2.15	0.47
1:B:1075:THR:O	1:B:1076:GLY:C	2.50	0.47
1:B:227:MET:CE	1:B:282:GLU:HG2	2.44	0.47
1:B:824:GLN:CA	1:B:824:GLN:NE2	2.78	0.47
1:A:1243:GLY:O	1:A:1246:LEU:N	2.47	0.47
1:A:1458:VAL:HG13	1:A:1459:PRO:CD	2.42	0.47
1:A:227:MET:HE3	1:A:282:GLU:CG	2.44	0.47
1:A:281:PHE:CZ	1:A:335:MET:HG2	2.50	0.47
1:A:231:ASN:HB3	1:A:332:ALA:HB3	1.96	0.47
1:A:335:MET:HE3	1:A:342:VAL:HB	1.96	0.47
1:A:454:PHE:CD2	1:A:648:GLU:CA	2.98	0.47
1:A:559:ARG:NH1	1:A:568:GLU:OE2	2.48	0.47
1:A:603:HIS:N	1:A:640:THR:HG22	2.30	0.47
1:A:863:LEU:HB3	1:A:1118:CYS:HB3	1.97	0.47
1:B:150:ILE:HG21	1:B:259:HIS:CG	2.50	0.47
1:B:147:ASP:O	1:B:151:ILE:HG13	2.15	0.47
1:B:286:ARG:HD3	1:B:286:ARG:HA	1.55	0.47
1:B:347:ARG:HH11	1:B:347:ARG:HB2	1.79	0.47
1:B:477:GLY:O	1:B:478:SER:HB3	2.15	0.47
1:B:525:ARG:HG3	1:B:544:GLN:HG3	1.97	0.47
1:B:634:SER:O	1:B:635:ASN:C	2.52	0.47
1:A:1075:THR:HG22	1:A:1077:ARG:N	2.30	0.47
1:A:468:MET:HG2	1:A:699:ALA:HB1	1.97	0.47
1:B:1219:ALA:HA	1:B:1229:MET:CE	2.45	0.47
1:B:25:LEU:HD21	1:B:207:TYR:HB2	1.97	0.47
1:B:227:MET:CE	1:B:282:GLU:CG	2.93	0.47
1:B:621:ILE:HG12	1:B:657:VAL:HG11	1.97	0.47
1:A:1383:PHE:O	1:A:1384:ALA:HB3	2.15	0.47
1:A:446:GLU:O	1:A:449:ARG:N	2.48	0.47
1:A:47:HIS:HB3	1:A:206:ILE:HB	1.96	0.47
1:A:894:PHE:HD1	1:A:904:ASN:ND2	2.13	0.47
1:B:912:SER:CB	1:B:968:PRO:O	2.62	0.47
1:A:1212:ASP:OD1	1:A:1243:GLY:N	2.24	0.46
1:A:1326:THR:HG22	1:A:1326:THR:O	2.15	0.46
1:A:313:HIS:N	1:A:313:HIS:CD2	2.83	0.46
1:A:250:ARG:NH2	1:A:639:PHE:CE1	2.79	0.46
1:A:935:GLY:HA3	1:A:1025:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1184:ASN:N	1:B:1185:PRO:HD2	2.30	0.46
1:B:30:HIS:CE1	1:B:368:GLU:OE2	2.68	0.46
1:A:1412:PHE:HD2	1:A:1455:TRP:CE3	2.33	0.46
1:A:15:ARG:O	1:A:16:SER:C	2.53	0.46
1:A:191:PHE:HE1	1:A:192:TYR:CE1	2.33	0.46
1:A:207:TYR:N	1:A:207:TYR:HD1	2.08	0.46
1:A:316:LEU:O	1:A:317:ILE:C	2.53	0.46
1:A:348:ASN:HB2	1:A:350:LEU:HG	1.96	0.46
1:A:376:GLU:O	1:A:378:GLN:N	2.49	0.46
1:A:417:ASP:O	1:A:418:LYS:C	2.52	0.46
1:A:498:PHE:N	1:A:498:PHE:CD1	2.82	0.46
1:A:87:GLU:O	1:A:88:ALA:C	2.53	0.46
1:B:12:LYS:HA	1:B:13:PRO:HD3	1.75	0.46
1:B:1401:LEU:O	1:B:1401:LEU:CD1	2.38	0.46
1:B:1463:LEU:HA	1:B:1463:LEU:HD23	1.71	0.46
1:B:496:HIS:CD2	1:B:497:HIS:HD2	2.33	0.46
1:B:520:MET:HA	1:B:714:SER:O	2.15	0.46
1:B:720:ARG:C	1:B:722:GLY:N	2.69	0.46
1:B:85:ALA:O	1:B:86:GLN:C	2.53	0.46
1:A:1005:GLY:O	1:A:1009:ILE:HD12	2.16	0.46
1:A:603:HIS:N	1:A:640:THR:CG2	2.78	0.46
1:A:57:ASP:O	1:A:60:LYS:HB2	2.15	0.46
1:A:673:GLU:O	1:A:674:ALA:C	2.53	0.46
1:A:724:ASN:HD22	1:A:724:ASN:N	2.02	0.46
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.82	0.46
1:B:1061:LEU:O	1:B:1064:ARG:HB2	2.15	0.46
1:B:30:HIS:CE1	1:B:1237:ASN:O	2.68	0.46
1:B:1424:LEU:O	1:B:1425:LYS:C	2.53	0.46
1:B:839:PRO:HG2	1:B:842:GLU:OE1	2.15	0.46
1:A:5:PHE:CE2	1:A:365:GLY:HA3	2.50	0.46
1:A:949:VAL:C	1:A:950:THR:O	2.50	0.46
1:B:1131:THR:HG22	1:B:1133:GLU:CA	2.46	0.46
1:B:209:GLN:HG3	1:B:210:ARG:H	1.80	0.46
1:B:820:ARG:HB3	1:B:821:PRO:HD3	1.94	0.46
1:B:824:GLN:NE2	1:B:824:GLN:HA	2.30	0.46
1:B:875:MET:O	1:B:876:ASN:C	2.47	0.46
1:A:1236:ARG:C	1:A:1238:THR:H	2.17	0.46
1:A:316:LEU:C	1:A:316:LEU:HD12	2.36	0.46
1:A:345:MET:CE	1:A:385:LEU:HB3	2.45	0.46
1:A:345:MET:CG	1:A:346:ASP:N	2.55	0.46
1:A:565:THR:HG22	1:A:565:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:THR:HG22	1:A:615:ARG:NE	2.30	0.46
1:A:583:ARG:CZ	1:A:587:ARG:HH12	2.27	0.46
1:A:602:THR:C	1:A:640:THR:CG2	2.83	0.46
1:A:491:LYS:HZ1	1:A:785:GLY:HA3	1.78	0.46
1:A:787:ARG:NH1	1:A:821:PRO:HB2	2.24	0.46
1:A:850:ARG:O	1:A:853:PHE:HB2	2.15	0.46
1:A:871:LEU:O	1:A:872:ASN:C	2.52	0.46
1:A:940:GLU:O	1:A:969:PRO:HA	2.15	0.46
1:A:9:ILE:O	1:A:398:GLY:HA2	2.15	0.46
1:B:389:GLU:HA	1:B:403:ASP:OD2	2.15	0.46
1:B:457:THR:O	1:B:461:MET:HG2	2.15	0.46
1:B:842:GLU:HB3	1:B:1156:ARG:CD	2.43	0.46
1:A:1376:LEU:CD2	1:A:1376:LEU:N	2.33	0.46
1:A:1432:VAL:O	1:A:1433:THR:C	2.53	0.46
1:A:52:GLN:O	1:A:56:LYS:HB2	2.16	0.46
1:A:572:THR:HG21	1:A:615:ARG:NE	2.30	0.46
1:A:969:PRO:CD	1:A:970:PRO:HD2	2.46	0.46
1:B:1141:PHE:O	1:B:1142:LEU:C	2.54	0.46
1:B:1143:ALA:O	1:B:1146:VAL:N	2.47	0.46
1:B:1210:THR:CG2	1:B:1211:LEU:H	2.07	0.46
1:B:1357:VAL:CG1	1:B:1359:GLY:O	2.63	0.46
1:B:1452:THR:O	1:B:1452:THR:CG2	2.64	0.46
1:B:24:ALA:C	1:B:26:LYS:H	2.19	0.46
1:B:615:ARG:HG2	1:B:615:ARG:NH1	2.30	0.46
1:B:677:GLU:OE1	1:B:677:GLU:C	2.54	0.46
1:A:1132:PRO:O	1:A:1133:GLU:C	2.52	0.46
1:A:260:MET:HA	1:A:263:LEU:HB2	1.98	0.46
1:A:456:LEU:HA	1:A:456:LEU:HD23	1.65	0.46
1:A:472:GLY:O	1:A:473:LYS:HG3	2.16	0.46
1:A:536:ASP:OD1	1:A:538:THR:N	2.49	0.46
1:A:81:ILE:HD13	1:B:216:PHE:CE1	2.50	0.46
1:A:833:SER:OG	1:A:834:THR:N	2.49	0.46
1:B:1076:GLY:N	1:B:1145:GLU:OE2	2.49	0.46
1:B:125:ARG:HG3	1:B:219:TRP:CZ2	2.51	0.46
1:B:260:MET:HB2	1:B:260:MET:HE2	1.70	0.46
1:B:430:VAL:HG13	1:B:554:GLU:CA	2.37	0.46
1:B:787:ARG:O	1:B:788:HIS:ND1	2.49	0.46
1:B:89:CYS:O	1:B:93:VAL:HG23	2.16	0.46
1:A:1214:ARG:O	1:A:1215:ILE:C	2.53	0.46
1:A:965:LEU:HA	1:A:965:LEU:HD23	1.33	0.46
1:B:1114:PRO:HB2	1:B:1115:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1212:ASP:OD2	1:B:1243:GLY:CA	2.63	0.46
1:B:1424:LEU:CD2	1:B:1428:ILE:HD11	2.46	0.46
1:B:290:THR:HG22	1:B:292:PRO:N	2.31	0.46
1:B:447:LEU:HD11	1:B:451:GLN:CD	2.36	0.46
1:B:673:GLU:O	1:B:674:ALA:C	2.54	0.46
1:A:1044:PRO:HG2	1:A:1047:MET:HE3	1.97	0.46
1:A:1102:CYS:SG	1:A:1104:MET:N	2.89	0.46
1:A:345:MET:HE2	1:A:385:LEU:HB2	1.98	0.46
1:A:353:MET:HG2	1:A:385:LEU:HD23	1.97	0.46
1:A:391:ILE:CG2	1:A:391:ILE:O	2.63	0.46
1:A:393:VAL:CG1	1:A:394:ASP:N	2.77	0.46
1:B:1010:ALA:HB2	1:B:1052:VAL:HG22	1.97	0.46
1:B:1077:ARG:O	1:B:1079:ILE:N	2.48	0.46
1:B:878:ILE:HG21	1:B:1136:VAL:HG13	1.97	0.46
1:B:1057:THR:HG22	1:B:1190:VAL:HG11	1.98	0.46
1:B:304:THR:CG2	1:B:518:ARG:HD2	2.46	0.46
1:B:416:TRP:O	1:B:419:TRP:HB2	2.16	0.46
1:B:419:TRP:O	1:B:540:THR:OG1	2.27	0.46
1:B:629:THR:O	1:B:632:ILE:HB	2.16	0.46
1:B:766:TYR:C	1:B:768:GLU:H	2.18	0.46
1:A:805:ASP:O	1:A:805:ASP:OD1	2.33	0.46
1:B:1440:ALA:O	1:B:1441:ALA:C	2.53	0.46
1:B:359:THR:HG23	1:B:378:GLN:O	2.16	0.46
1:B:417:ASP:HA	1:B:420:VAL:CG1	2.46	0.46
1:B:608:ASP:OD2	1:B:647:ALA:N	2.42	0.46
1:B:632:ILE:HG23	1:B:632:ILE:HD12	1.66	0.46
1:B:833:SER:OG	1:B:834:THR:N	2.48	0.46
1:A:833:SER:HB3	1:A:1153:LEU:HD22	1.98	0.45
1:A:1264:ILE:HG22	1:A:1284:ILE:HA	1.98	0.45
1:A:357:ILE:HD11	1:A:400:LEU:HD21	1.98	0.45
1:A:443:ASP:C	1:A:445:ALA:N	2.70	0.45
1:A:842:GLU:HG2	1:A:1156:ARG:HH11	1.80	0.45
1:A:918:THR:O	1:A:919:ALA:C	2.51	0.45
1:B:107:TRP:H	1:B:107:TRP:HD1	1.60	0.45
1:B:447:LEU:C	1:B:447:LEU:CD1	2.84	0.45
1:A:1236:ARG:C	1:A:1238:THR:N	2.67	0.45
1:A:1397:LEU:HD22	1:A:1453:LYS:HD2	1.97	0.45
1:A:248:GLU:OE2	1:A:266:VAL:N	2.44	0.45
1:A:606:LEU:C	1:A:607:THR:CG2	2.83	0.45
1:B:1070:ASP:C	1:B:1070:ASP:OD1	2.55	0.45
1:B:1204:ARG:O	1:B:1205:ASN:C	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1424:LEU:HD22	1:B:1447:TRP:HH2	1.80	0.45
1:B:266:VAL:HG12	1:B:266:VAL:O	2.15	0.45
1:B:558:MET:C	1:B:560:ASP:N	2.69	0.45
1:A:1045:TRP:O	1:A:1046:GLU:C	2.54	0.45
1:A:370:GLY:CA	1:A:1237:ASN:HB3	2.45	0.45
1:A:1310:THR:O	1:A:1313:SER:N	2.33	0.45
1:A:1315:LEU:HB3	1:A:1320:ASN:ND2	2.31	0.45
1:A:1438:ARG:O	1:A:1441:ALA:N	2.49	0.45
1:A:555:PHE:HD1	1:A:556:ARG:N	2.14	0.45
1:B:211:TYR:CD1	1:B:212:SER:N	2.80	0.45
1:B:428:GLU:O	1:B:429:LEU:C	2.51	0.45
1:B:487:VAL:HG13	1:B:498:PHE:HE2	1.81	0.45
1:B:572:THR:HG23	1:B:616:ALA:O	2.15	0.45
1:B:798:LEU:O	1:B:801:ALA:HB3	2.16	0.45
1:B:848:ALA:O	1:B:849:ILE:C	2.54	0.45
1:A:1049:LEU:HD21	1:A:1087:ALA:HB2	1.98	0.45
1:A:1231:LEU:O	1:A:1266:ILE:HA	2.16	0.45
1:A:498:PHE:HD1	1:A:498:PHE:H	1.64	0.45
1:A:582:LEU:CB	1:A:755:GLN:HE21	2.30	0.45
1:A:974:ILE:O	1:A:974:ILE:HG22	2.16	0.45
1:B:1207:VAL:HG13	1:B:1208:PRO:CD	2.46	0.45
1:B:1468:VAL:HG12	1:B:1469:PRO:O	2.17	0.45
1:B:700:ILE:O	1:B:703:GLY:N	2.49	0.45
1:B:702:ASP:O	1:B:703:GLY:C	2.55	0.45
1:B:792:GLY:O	1:B:793:GLY:C	2.51	0.45
1:A:1401:LEU:N	1:A:1402:PRO:CD	2.79	0.45
1:A:1416:GLU:OE1	1:A:1471:HIS:CD2	2.70	0.45
1:A:292:PRO:O	1:A:293:MET:C	2.55	0.45
1:A:295:LYS:C	1:A:295:LYS:CD	2.83	0.45
1:B:1080:VAL:O	1:B:1081:ILE:C	2.54	0.45
1:B:731:SER:HA	1:B:747:SER:HB2	1.99	0.45
1:A:1245:ARG:O	1:A:1246:LEU:C	2.55	0.45
1:A:179:TYR:HD2	1:A:192:TYR:CD2	2.34	0.45
1:A:251:MET:HB2	1:A:533:LEU:CD1	2.43	0.45
1:A:608:ASP:O	1:A:611:MET:N	2.44	0.45
1:A:510:PRO:CD	1:A:970:PRO:HB3	2.37	0.45
1:A:351:ARG:HH12	1:A:978:GLU:CD	2.19	0.45
1:B:102:TYR:HA	1:B:136:ASN:OD1	2.16	0.45
1:B:1432:VAL:HG12	1:B:1433:THR:N	2.31	0.45
1:B:689:LEU:O	1:B:690:GLU:C	2.55	0.45
1:B:806:SER:OG	1:B:809:THR:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:883:ASP:O	1:B:884:SER:C	2.55	0.45
1:B:991:ASN:HA	1:B:992:PRO:HD2	1.83	0.45
1:A:103:TYR:HD2	1:A:105:TYR:CE1	2.35	0.45
1:A:1274:GLN:NE2	1:A:1293:ASN:HB3	2.30	0.45
1:A:359:THR:CG2	1:A:378:GLN:CA	2.95	0.45
1:A:554:GLU:OE2	1:A:697:LYS:HE3	2.17	0.45
1:A:805:ASP:O	1:A:805:ASP:CG	2.49	0.45
1:B:1026:ASN:HB3	1:B:1043:LEU:N	2.31	0.45
1:B:790:TRP:CZ2	1:B:1074:LYS:HG2	2.51	0.45
1:B:414:LYS:HB3	1:B:415:PRO:CD	2.47	0.45
1:B:413:LEU:O	1:B:414:LYS:HD2	2.16	0.45
1:B:486:ALA:O	1:B:487:VAL:C	2.51	0.45
1:B:739:PHE:O	1:B:740:PRO:C	2.55	0.45
1:A:102:TYR:HE2	1:A:144:PHE:CD1	2.34	0.45
1:A:1084:MET:SD	1:A:1168:LEU:HD21	2.57	0.45
1:A:131:ILE:HG23	1:A:131:ILE:O	2.16	0.45
1:A:1468:VAL:HG12	1:A:1468:VAL:O	2.15	0.45
1:A:228:LEU:HA	1:A:228:LEU:HD12	1.29	0.45
1:A:21:GLY:O	1:A:22:ILE:C	2.49	0.45
1:A:386:GLY:N	1:A:389:GLU:OE2	2.48	0.45
1:A:449:ARG:HD3	1:A:765:ALA:O	2.17	0.45
1:A:459:GLU:O	1:A:463:LEU:CB	2.59	0.45
1:B:1216:VAL:HG11	1:B:1249:MET:HE1	1.98	0.45
1:B:266:VAL:HG12	1:B:279:THR:HG22	1.97	0.45
1:B:443:ASP:O	1:B:444:LYS:C	2.54	0.45
1:B:426:LEU:HD23	1:B:543:LEU:HB3	1.93	0.45
1:B:612:GLY:O	1:B:762:HIS:HE1	1.99	0.45
1:B:671:ALA:O	1:B:675:ILE:HD12	2.17	0.45
1:B:696:TYR:CZ	1:B:700:ILE:HD11	2.52	0.45
1:A:1052:VAL:O	1:A:1053:HIS:C	2.51	0.45
1:A:1062:ARG:HD3	1:A:1062:ARG:HH11	1.53	0.45
1:A:1084:MET:SD	1:A:1168:LEU:CD2	3.05	0.45
1:A:1109:HIS:ND1	1:A:1109:HIS:N	2.45	0.45
1:A:110:VAL:HG12	1:A:111:PRO:O	2.17	0.45
1:A:266:VAL:O	1:A:266:VAL:HG12	2.16	0.45
1:A:704:LEU:C	1:A:706:LYS:H	2.20	0.45
1:A:734:LEU:HD12	1:A:738:HIS:CD2	2.41	0.45
1:B:1094:THR:O	1:B:1097:LEU:HB2	2.17	0.45
1:B:1170:GLN:OE1	1:B:1183:LEU:HB2	2.17	0.45
1:B:1210:THR:CG2	1:B:1211:LEU:N	2.75	0.45
1:B:230:HIS:HE1	1:B:234:ILE:HG13	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LEU:HA	1:B:263:LEU:HD12	1.11	0.45
1:B:381:GLU:CD	1:B:402:ARG:NH1	2.67	0.45
1:B:402:ARG:O	1:B:403:ASP:C	2.51	0.45
1:B:984:ILE:O	1:B:988:LYS:HG3	2.17	0.45
1:A:500:ARG:NH2	1:A:1041:ALA:O	2.48	0.45
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.53	0.45
1:A:562:MET:CE	1:A:566:ALA:HB2	2.46	0.45
1:A:636:LEU:C	1:A:638:THR:N	2.68	0.45
1:A:857:GLY:N	1:A:883:ASP:HB3	2.31	0.45
1:B:1113:CYS:C	1:B:1115:VAL:N	2.69	0.45
1:B:165:ASN:O	1:B:166:ASP:CB	2.65	0.45
1:B:175:ARG:CG	1:B:175:ARG:NH1	2.79	0.45
1:B:342:VAL:HG11	1:B:390:MET:HE2	1.99	0.45
1:A:1057:THR:HG22	1:A:1058:LEU:N	2.27	0.44
1:A:510:PRO:HD2	1:A:970:PRO:CB	2.34	0.44
1:A:56:LYS:HE2	1:A:67:PRO:O	2.17	0.44
1:A:59:VAL:HG12	1:A:60:LYS:N	2.32	0.44
1:A:660:GLY:HA2	1:A:721:GLY:N	2.32	0.44
1:A:961:PRO:C	1:A:963:VAL:H	2.20	0.44
1:A:979:ASP:O	1:A:980:LEU:C	2.55	0.44
1:A:992:PRO:HA	1:A:1204:ARG:NH2	2.32	0.44
1:B:918:THR:HG23	1:B:1256:MET:SD	2.56	0.44
1:B:1374:VAL:HG12	1:B:1375:ILE:N	2.32	0.44
1:B:1400:SER:C	1:B:1402:PRO:HD2	2.38	0.44
1:B:1435:THR:HG23	1:B:1437:SER:HB2	1.98	0.44
1:B:304:THR:HG21	1:B:518:ARG:HD2	1.98	0.44
1:B:30:HIS:HD2	1:B:31:ARG:H	1.65	0.44
1:B:871:LEU:O	1:B:872:ASN:C	2.54	0.44
1:A:1393:TYR:C	1:A:1394:VAL:HG23	2.34	0.44
1:A:184:LEU:HB3	1:A:186:GLU:HG3	1.99	0.44
1:A:227:MET:HE2	1:A:282:GLU:CG	2.47	0.44
1:A:560:ASP:C	1:A:562:MET:N	2.70	0.44
1:A:572:THR:HG21	1:A:615:ARG:HE	1.82	0.44
1:A:636:LEU:HA	1:A:636:LEU:HD12	1.60	0.44
1:B:1075:THR:HG22	1:B:1076:GLY:N	2.31	0.44
1:B:1260:GLN:O	1:B:1261:PRO:C	2.56	0.44
1:B:211:TYR:O	1:B:212:SER:CB	2.58	0.44
1:B:1102:CYS:SG	5:B:2476:F3S:S1	3.06	0.44
1:B:317:ILE:HG22	1:B:321:ASN:ND2	2.27	0.44
1:B:440:SER:O	1:B:441:ASP:OD1	2.36	0.44
1:B:561:TYR:CD1	1:B:561:TYR:C	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:LYS:HD3	1:B:819:LYS:HA	1.60	0.44
1:A:1360:CYS:O	1:A:1361:GLY:O	2.35	0.44
1:A:1415:ILE:HG21	1:A:1421:GLU:CB	2.44	0.44
1:A:1460:LYS:O	1:A:1461:GLU:C	2.55	0.44
1:A:216:PHE:HA	1:A:217:PRO:HD3	1.73	0.44
1:A:316:LEU:O	1:A:319:TYR:N	2.50	0.44
1:A:526:LEU:CD1	1:A:526:LEU:H	2.17	0.44
1:A:989:GLN:O	1:A:1245:ARG:HD3	2.16	0.44
1:B:1016:ALA:O	1:B:1017:ASN:HB2	2.17	0.44
1:B:728:ILE:CD1	1:B:1047:MET:CE	2.74	0.44
1:B:1400:SER:O	1:B:1401:LEU:C	2.56	0.44
1:B:30:HIS:CD2	1:B:31:ARG:N	2.86	0.44
1:B:312:ASN:HB2	1:B:411:ALA:CB	2.46	0.44
1:B:622:LEU:HA	1:B:622:LEU:HD12	1.59	0.44
1:B:689:LEU:O	1:B:689:LEU:HD12	2.18	0.44
1:B:78:LEU:HB3	1:B:79:PRO:CD	2.48	0.44
1:B:957:ARG:HD2	1:B:965:LEU:CD1	2.48	0.44
1:B:964:MET:O	1:B:965:LEU:HD23	2.18	0.44
1:B:985:TYR:O	1:B:988:LYS:N	2.50	0.44
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.50	0.44
1:A:309:THR:HG22	1:A:310:PRO:O	2.17	0.44
1:A:918:THR:O	1:A:921:TYR:N	2.51	0.44
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.55	0.44
1:B:303:LEU:O	1:B:303:LEU:HG	2.17	0.44
1:B:456:LEU:HA	1:B:456:LEU:HD23	1.11	0.44
1:A:1170:GLN:HG2	1:A:1170:GLN:O	2.16	0.44
1:A:353:MET:HA	1:A:366:GLY:O	2.18	0.44
1:A:489:SER:OG	1:A:490:ASP:N	2.48	0.44
1:A:52:GLN:NE2	1:A:71:LEU:N	2.44	0.44
1:A:636:LEU:O	1:A:638:THR:N	2.51	0.44
1:A:648:GLU:HG2	1:A:654:TYR:CE2	2.53	0.44
1:A:819:LYS:HD3	1:A:819:LYS:HA	1.73	0.44
1:A:908:LYS:HD2	1:A:921:TYR:CD1	2.53	0.44
1:A:81:ILE:HD13	1:B:216:PHE:CZ	2.53	0.44
1:B:228:LEU:HD22	1:B:278:ASP:HA	1.98	0.44
1:B:528:ASN:O	1:B:529:LEU:HD23	2.17	0.44
1:B:582:LEU:O	1:B:585:ALA:HB3	2.17	0.44
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.48	0.44
1:B:986:ASP:O	1:B:987:LEU:C	2.55	0.44
1:A:1435:THR:HG23	1:A:1437:SER:CB	2.47	0.44
1:A:1447:TRP:CE2	1:A:1451:VAL:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:CD2	1:A:30:HIS:N	2.85	0.44
1:A:369:THR:C	1:A:371:MET:H	2.20	0.44
1:A:357:ILE:HD11	1:A:400:LEU:CD2	2.47	0.44
1:A:420:VAL:O	1:A:422:ASN:N	2.50	0.44
1:A:736:ALA:O	1:A:737:GLU:C	2.53	0.44
1:A:991:ASN:HA	1:A:992:PRO:HD2	1.84	0.44
1:B:1003:ARG:NH1	1:B:1004:SER:O	2.50	0.44
1:B:1184:ASN:CB	1:B:1185:PRO:CD	2.80	0.44
1:B:1329:TYR:HD1	1:B:1348:VAL:HG13	1.82	0.44
1:B:1366:GLU:CG	1:B:1367:TYR:CE1	3.00	0.44
1:B:293:MET:HG2	1:B:410:LEU:HD23	2.00	0.44
1:A:1053:HIS:ND1	1:A:1062:ARG:HD3	2.33	0.44
1:A:1348:VAL:CG1	1:A:1348:VAL:O	2.65	0.44
1:A:419:TRP:CE2	1:A:537:GLU:HB3	2.53	0.44
1:A:6:ILE:HD13	1:A:20:LYS:HB2	1.99	0.44
1:A:839:PRO:HG2	1:A:842:GLU:HB2	1.99	0.44
1:A:964:MET:O	1:A:965:LEU:HD23	2.18	0.44
1:B:1006:ILE:HG23	1:B:1007:GLY:N	2.32	0.44
1:B:1050:SER:O	1:B:1051:GLU:O	2.36	0.44
1:B:8:ALA:HA	1:B:362:LEU:HD12	2.00	0.44
1:A:1001:VAL:O	1:A:1002:SER:C	2.55	0.44
1:A:1047:MET:O	1:A:1048:GLY:C	2.56	0.44
1:A:125:ARG:HG3	1:A:219:TRP:CZ2	2.53	0.44
1:A:420:VAL:CG1	1:A:421:GLN:N	2.81	0.44
1:A:442:MET:CE	1:A:447:LEU:N	2.81	0.44
1:A:559:ARG:HD2	1:A:605:ILE:CD1	2.48	0.44
1:B:1236:ARG:C	1:B:1238:THR:N	2.70	0.44
1:B:1420:TYR:OH	1:B:1466:LEU:CD2	2.65	0.44
1:B:1447:TRP:O	1:B:1450:GLU:N	2.51	0.44
1:B:165:ASN:O	1:B:166:ASP:HB2	2.18	0.44
1:B:485:ILE:HD13	1:B:485:ILE:HG21	1.68	0.44
1:B:643:ASN:HB3	1:B:665:THR:HG22	1.98	0.44
1:A:479:MET:HB3	1:A:1106:ARG:NH1	2.31	0.44
1:A:1156:ARG:O	1:A:1157:SER:CB	2.62	0.44
1:A:173:SER:HG	1:A:176:SER:H	1.62	0.44
1:A:248:GLU:O	1:A:249:THR:C	2.56	0.44
1:A:634:SER:O	1:A:635:ASN:HB2	2.16	0.44
1:B:1244:THR:OG1	1:B:1278:ALA:HB3	2.18	0.44
1:B:508:ASN:HB2	1:B:509:PRO:CD	2.47	0.44
1:B:643:ASN:HD22	1:B:665:THR:HG21	1.83	0.44
1:B:622:LEU:HD13	1:B:739:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:GLY:O	1:B:870:THR:C	2.52	0.44
1:A:1149:ILE:O	1:A:1149:ILE:HG22	2.12	0.43
1:A:454:PHE:CD1	1:A:454:PHE:N	2.81	0.43
1:A:463:LEU:HA	1:A:463:LEU:HD23	1.48	0.43
1:A:521:SER:C	1:A:522:LEU:HD23	2.38	0.43
1:A:731:SER:O	1:A:734:LEU:HB3	2.18	0.43
1:A:944:LEU:HD12	1:A:944:LEU:HA	1.72	0.43
1:B:1190:VAL:C	1:B:1192:PRO:HD3	2.38	0.43
1:B:175:ARG:CG	1:B:175:ARG:HH11	2.19	0.43
1:B:515:ARG:HG3	1:B:515:ARG:H	1.63	0.43
1:B:571:ALA:HB2	1:B:606:LEU:HD22	1.98	0.43
1:B:59:VAL:HG22	1:B:105:TYR:HD2	1.78	0.43
1:B:885:GLY:C	1:B:887:GLY:N	2.68	0.43
1:B:98:LEU:HD23	1:B:98:LEU:HA	1.62	0.43
1:A:1394:VAL:HG11	1:A:1401:LEU:HD23	1.98	0.43
1:A:295:LYS:HE2	1:A:299:VAL:HG11	1.98	0.43
1:A:360:ASP:OD1	1:A:360:ASP:N	2.49	0.43
1:A:858:MET:HA	3:A:2474:FMN:C5A	2.48	0.43
1:A:987:LEU:HD23	1:A:987:LEU:HA	1.70	0.43
1:B:1164:ARG:HB3	1:B:1167:LEU:CD1	2.47	0.43
1:B:364:ILE:HD12	1:B:374:ILE:HD11	2.00	0.43
1:B:310:PRO:CG	1:B:404:ARG:NH2	2.66	0.43
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.20	0.43
1:B:511:ILE:HG21	1:B:511:ILE:HD13	1.76	0.43
1:B:289:ARG:NH1	1:B:535:GLU:HB2	2.33	0.43
1:B:580:GLU:O	1:B:581:ALA:C	2.56	0.43
1:B:843:VAL:HG11	1:B:1147:ARG:HB3	2.00	0.43
1:B:918:THR:HG23	1:B:1256:MET:HE2	2.00	0.43
1:B:934:GLN:HE21	1:B:934:GLN:HB2	1.58	0.43
1:A:937:LYS:CE	1:A:1033:SER:HB2	2.40	0.43
1:A:831:LEU:HD13	1:A:1084:MET:HE3	2.00	0.43
1:A:1159:ASN:O	1:A:1161:VAL:N	2.50	0.43
1:A:1212:ASP:OD2	1:A:1243:GLY:CA	2.67	0.43
1:A:1425:LYS:CD	1:A:1447:TRP:CD1	3.02	0.43
1:A:1468:VAL:HG12	1:A:1469:PRO:O	2.18	0.43
1:A:438:GLU:OE1	1:A:553:ALA:HB2	2.18	0.43
1:A:850:ARG:CG	1:A:850:ARG:NH1	2.76	0.43
1:B:500:ARG:NH2	1:B:1039:LYS:O	2.50	0.43
1:B:1068:ARG:HA	1:B:1089:GLU:O	2.17	0.43
1:B:219:TRP:N	1:B:220:PRO:CD	2.81	0.43
1:B:313:HIS:CD2	1:B:313:HIS:H	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:MET:O	1:B:560:ASP:N	2.51	0.43
1:B:700:ILE:C	1:B:703:GLY:H	2.22	0.43
1:A:1026:ASN:ND2	1:A:1027:SER:N	2.66	0.43
1:A:1141:PHE:O	1:A:1142:LEU:C	2.55	0.43
1:A:1156:ARG:HE	1:A:1156:ARG:HB2	1.72	0.43
1:A:16:SER:O	1:A:20:LYS:CG	2.66	0.43
1:A:509:PRO:HB3	1:A:975:TYR:CD1	2.53	0.43
1:A:602:THR:C	1:A:640:THR:HG22	2.38	0.43
1:A:452:GLN:NE2	1:A:764:THR:HG23	1.99	0.43
1:A:871:LEU:HA	1:A:871:LEU:HD23	1.68	0.43
1:A:990:ILE:HG13	1:A:990:ILE:O	2.19	0.43
1:B:1184:ASN:C	1:B:1186:ARG:N	2.71	0.43
1:B:1216:VAL:CG1	1:B:1249:MET:HE2	2.48	0.43
1:B:1336:LEU:HD23	1:B:1355:VAL:CG1	2.48	0.43
1:B:1427:LEU:O	1:B:1428:ILE:C	2.56	0.43
1:B:146:LEU:CD1	1:B:146:LEU:C	2.87	0.43
1:B:207:TYR:CD1	1:B:207:TYR:N	2.85	0.43
1:B:943:GLN:HE21	1:B:1033:SER:HA	1.83	0.43
1:B:978:GLU:H	1:B:978:GLU:HG2	1.21	0.43
1:A:120:LYS:O	1:A:123:ALA:HB3	2.18	0.43
1:A:387:PRO:HD2	1:A:1344:GLU:OE2	2.14	0.43
1:A:1395:TYR:HE1	1:A:1397:LEU:HG	1.82	0.43
1:A:191:PHE:CD1	1:A:191:PHE:O	2.72	0.43
1:A:572:THR:CG2	1:A:615:ARG:HE	2.32	0.43
1:A:633:ARG:NH2	1:A:737:GLU:O	2.38	0.43
1:B:1467:GLU:O	1:B:1469:PRO:HD3	2.18	0.43
1:B:677:GLU:OE2	1:B:681:ARG:NH1	2.52	0.43
1:B:701:ASP:C	1:B:703:GLY:N	2.69	0.43
1:B:763:ALA:C	1:B:765:ALA:N	2.72	0.43
1:A:1003:ARG:HH11	1:A:1003:ARG:CG	2.29	0.43
1:A:852:ARG:NH1	1:A:1088:GLU:O	2.50	0.43
1:A:261:GLN:HE21	1:A:264:LYS:HD2	1.83	0.43
1:A:309:THR:HB	1:A:314:LYS:HE3	1.99	0.43
1:A:897:ASP:OD1	1:A:899:ASN:N	2.50	0.43
1:A:983:LEU:HD22	1:A:987:LEU:HG	2.01	0.43
1:B:1164:ARG:HH11	1:B:1166:ASP:CG	2.21	0.43
1:B:208:HIS:C	1:B:208:HIS:CD2	2.92	0.43
1:B:254:PRO:CG	1:B:255:ALA:H	2.21	0.43
1:B:308:THR:O	1:B:308:THR:CG2	2.67	0.43
1:B:295:LYS:HB3	1:B:390:MET:HE1	2.00	0.43
1:B:611:MET:HB3	1:B:611:MET:HE3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:ARG:NH1	1:B:878:ILE:HB	2.33	0.43
1:A:1011:ALA:O	1:A:1014:ALA:N	2.52	0.43
1:A:1058:LEU:HA	1:A:1058:LEU:HD23	1.88	0.43
1:A:1131:THR:HG22	1:A:1133:GLU:H	1.81	0.43
1:A:1139:PHE:CD1	1:A:1139:PHE:N	2.86	0.43
1:A:114:VAL:HG11	1:A:125:ARG:NH1	2.33	0.43
1:A:1315:LEU:HD13	1:A:1320:ASN:ND2	2.33	0.43
1:A:1363:ASN:HD22	1:A:1363:ASN:HA	1.60	0.43
1:A:1395:TYR:CE2	1:A:1443:ILE:CD1	3.01	0.43
1:A:302:ALA:CA	1:A:347:ARG:NH1	2.81	0.43
1:A:545:LEU:HD23	1:A:545:LEU:HA	1.19	0.43
1:A:551:THR:H	1:A:554:GLU:CG	2.32	0.43
1:A:575:VAL:HG13	1:A:759:LEU:CD2	2.47	0.43
1:A:621:ILE:HG12	1:A:657:VAL:HG11	2.00	0.43
1:B:1032:ALA:O	1:B:1033:SER:HB2	2.19	0.43
1:B:1124:LEU:HD12	1:B:1124:LEU:HA	1.30	0.43
1:B:251:MET:CE	1:B:533:LEU:HD11	2.49	0.43
1:B:317:ILE:C	1:B:321:ASN:HD22	2.18	0.43
1:B:345:MET:HG3	1:B:346:ASP:N	2.32	0.43
1:B:647:ALA:HB2	1:B:669:TYR:OH	2.19	0.43
1:B:520:MET:HE3	1:B:705:LEU:HB3	2.01	0.43
1:B:897:ASP:OD1	1:B:899:ASN:N	2.52	0.43
1:B:913:GLY:CA	1:B:1349:ARG:CD	2.94	0.43
1:A:666:VAL:HG12	1:A:667:ASN:N	2.34	0.43
1:B:1129:VAL:HG23	1:B:1129:VAL:O	2.19	0.43
1:B:390:MET:HG3	1:B:406:LEU:CD2	2.48	0.43
1:A:1228:LYS:C	1:A:1229:MET:HG2	2.39	0.43
1:A:1351:SER:OG	1:A:1369:THR:HB	2.18	0.43
1:A:869:GLY:O	1:A:870:THR:C	2.54	0.43
1:B:1097:LEU:HD23	1:B:1097:LEU:HA	1.69	0.43
1:B:1132:PRO:O	1:B:1133:GLU:C	2.56	0.43
1:B:802:VAL:CG2	1:B:1137:ASN:HB2	2.46	0.43
1:B:1366:GLU:OE2	1:B:1367:TYR:CE1	2.71	0.43
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.88	0.43
1:B:235:ASN:HD22	1:B:236:THR:H	1.61	0.43
1:B:251:MET:HE2	1:B:533:LEU:HD11	2.00	0.43
1:B:609:GLU:C	1:B:611:MET:H	2.22	0.43
1:B:454:PHE:CG	1:B:648:GLU:HB2	2.53	0.43
1:B:794:VAL:CG2	1:B:817:VAL:HG23	2.49	0.43
1:A:1113:CYS:HB3	1:A:1119:VAL:CG1	2.49	0.43
1:A:1139:PHE:HD1	1:A:1139:PHE:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:PRO:HA	1:A:1204:ARG:HH22	1.84	0.43
1:A:1458:VAL:CG1	1:A:1459:PRO:CD	2.97	0.43
1:A:246:ALA:C	1:A:248:GLU:N	2.70	0.43
1:A:56:LYS:CG	1:A:71:LEU:HD22	2.49	0.43
1:A:52:GLN:NE2	1:A:71:LEU:CB	2.78	0.43
1:B:562:MET:CE	1:B:605:ILE:HD11	2.49	0.43
1:B:660:GLY:HA2	1:B:721:GLY:N	2.33	0.43
1:B:814:SER:O	1:B:818:ASN:N	2.47	0.43
1:A:216:PHE:CE1	1:B:81:ILE:HD13	2.54	0.43
1:A:1339:ALA:HB2	1:A:1435:THR:OG1	2.19	0.42
1:A:1420:TYR:OH	1:A:1466:LEU:CD2	2.66	0.42
1:A:330:PRO:HB3	1:A:350:LEU:HB3	2.01	0.42
1:A:337:ASP:O	1:A:338:GLY:C	2.56	0.42
1:A:353:MET:CG	1:A:353:MET:O	2.67	0.42
1:A:565:THR:HG22	1:A:603:HIS:HD2	1.83	0.42
1:A:929:GLU:HA	1:A:997:THR:HB	2.01	0.42
1:B:1424:LEU:HD23	1:B:1424:LEU:C	2.39	0.42
1:B:290:THR:HG22	1:B:292:PRO:CD	2.48	0.42
1:B:743:VAL:HG11	1:B:745:ARG:HG3	2.00	0.42
1:B:81:ILE:O	1:B:81:ILE:CG2	2.67	0.42
1:B:824:GLN:O	1:B:827:ASP:CB	2.58	0.42
1:A:90:ARG:HB3	1:A:107:TRP:CZ2	2.54	0.42
1:A:1156:ARG:O	1:A:1157:SER:HB3	2.17	0.42
1:A:1158:LEU:HA	1:A:1158:LEU:HD12	1.62	0.42
1:A:1264:ILE:HG22	1:A:1283:GLY:O	2.19	0.42
1:A:46:ILE:HG12	1:A:48:VAL:HG13	2.01	0.42
1:A:605:ILE:HA	1:A:643:ASN:O	2.20	0.42
1:A:622:LEU:HD13	1:A:739:PHE:HZ	1.84	0.42
1:B:1011:ALA:O	1:B:1014:ALA:N	2.52	0.42
1:B:1047:MET:HB2	1:B:1048:GLY:H	1.77	0.42
1:B:403:ASP:OD1	1:B:407:LYS:HG3	2.18	0.42
1:B:550:LEU:HA	1:B:554:GLU:OE2	2.19	0.42
1:B:571:ALA:C	1:B:618:ILE:HD12	2.40	0.42
1:B:651:ASP:OD1	1:B:651:ASP:N	2.38	0.42
1:B:756:LYS:O	1:B:757:LYS:C	2.58	0.42
1:B:770:VAL:CG1	1:B:770:VAL:O	2.67	0.42
1:B:928:LEU:HA	1:B:928:LEU:HD23	1.65	0.42
1:A:1159:ASN:C	1:A:1161:VAL:H	2.22	0.42
1:A:1425:LYS:HD2	1:A:1447:TRP:CD2	2.54	0.42
1:A:1447:TRP:NE1	1:A:1451:VAL:HG21	2.34	0.42
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:HH22	1:A:966:ILE:CB	2.23	0.42
1:A:522:LEU:HA	1:A:716:ILE:HG22	2.01	0.42
1:B:1131:THR:O	1:B:1132:PRO:C	2.58	0.42
1:B:918:THR:CG2	1:B:1256:MET:HE2	2.49	0.42
1:B:116:ILE:HD11	1:B:191:PHE:HB2	2.01	0.42
1:B:252:GLU:HA	1:B:260:MET:CE	2.50	0.42
1:B:586:LEU:HA	1:B:586:LEU:HD23	1.85	0.42
1:B:442:MET:HB2	1:B:673:GLU:HG2	2.01	0.42
1:B:754:ILE:HG22	1:B:755:GLN:N	2.34	0.42
1:A:1161:VAL:O	1:A:1161:VAL:HG13	2.18	0.42
1:A:121:ALA:C	1:A:123:ALA:N	2.73	0.42
1:A:133:VAL:HG12	1:A:134:GLY:N	2.34	0.42
1:A:194:ASP:HB3	1:A:200:PHE:CE1	2.54	0.42
1:A:629:THR:O	1:A:631:LEU:N	2.53	0.42
1:A:911:ALA:O	1:A:912:SER:C	2.57	0.42
1:B:1346:PHE:O	1:B:1347:ALA:HB3	2.17	0.42
1:B:1435:THR:HG23	1:B:1437:SER:N	2.34	0.42
1:B:409:HIS:O	1:B:413:LEU:HD23	2.18	0.42
1:B:420:VAL:HA	1:B:540:THR:HG21	2.01	0.42
1:B:540:THR:O	1:B:542:LEU:HG	2.20	0.42
1:B:732:ARG:H	1:B:747:SER:HA	1.85	0.42
1:B:965:LEU:HA	1:B:965:LEU:HD23	1.69	0.42
1:A:1430:GLU:O	1:A:1431:HIS:C	2.58	0.42
1:A:1450:GLU:O	1:A:1451:VAL:C	2.57	0.42
1:A:1463:LEU:HA	1:A:1463:LEU:HD23	1.66	0.42
1:A:295:LYS:CE	1:A:299:VAL:CG1	2.89	0.42
1:A:515:ARG:HG3	1:A:515:ARG:H	1.52	0.42
1:A:820:ARG:CB	1:A:821:PRO:CD	2.96	0.42
1:B:1281:VAL:HA	1:B:1301:SER:O	2.20	0.42
1:B:1420:TYR:C	1:B:1422:SER:N	2.69	0.42
1:B:533:LEU:HA	1:B:533:LEU:HD23	1.42	0.42
1:B:560:ASP:O	1:B:561:TYR:C	2.58	0.42
1:B:840:VAL:O	1:B:841:ASP:C	2.56	0.42
1:A:240:ASN:O	1:A:241:VAL:C	2.58	0.42
3:A:2474:FMN:H1'2	3:A:2474:FMN:H9	1.70	0.42
1:A:591:GLN:O	1:A:594:GLU:N	2.52	0.42
1:A:903:TRP:N	1:A:903:TRP:CD1	2.86	0.42
1:A:893:ARG:O	1:A:904:ASN:HB2	2.20	0.42
1:A:917:VAL:CG1	1:A:922:LEU:HD21	2.50	0.42
1:B:216:PHE:HA	1:B:217:PRO:HD3	1.76	0.42
1:B:254:PRO:CG	1:B:255:ALA:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ILE:HG12	1:B:279:THR:HG21	2.01	0.42
1:B:375:ASP:OD2	1:B:377:THR:CB	2.61	0.42
1:B:51:PRO:HD2	1:B:55:PHE:HD2	1.84	0.42
1:B:53:LYS:O	1:B:54:PHE:C	2.58	0.42
1:B:757:LYS:O	1:B:758:VAL:C	2.53	0.42
1:B:828:LEU:HD23	1:B:828:LEU:HA	1.79	0.42
1:B:885:GLY:O	1:B:887:GLY:N	2.52	0.42
1:A:1394:VAL:CG1	1:A:1401:LEU:HD23	2.49	0.42
1:A:143:GLN:NE2	1:A:143:GLN:CA	2.78	0.42
1:A:309:THR:HG21	1:A:314:LYS:HG3	2.02	0.42
1:A:691:LYS:HG3	1:A:691:LYS:O	2.20	0.42
1:A:969:PRO:N	1:A:970:PRO:HD2	2.35	0.42
1:B:1431:HIS:O	1:B:1432:VAL:C	2.54	0.42
1:B:248:GLU:C	1:B:250:ARG:N	2.73	0.42
1:B:550:LEU:HD13	1:B:555:PHE:HA	2.01	0.42
1:B:787:ARG:H	1:B:787:ARG:HG3	1.23	0.42
1:A:985:TYR:CE1	1:A:1207:VAL:HG11	2.52	0.42
1:A:112:ILE:HA	1:A:191:PHE:O	2.20	0.42
1:A:447:LEU:CD1	1:A:451:GLN:CG	2.96	0.42
1:A:949:VAL:O	1:A:950:THR:O	2.37	0.42
1:A:985:TYR:CD1	1:A:1207:VAL:HG11	2.54	0.42
1:B:1066:ARG:NH1	1:B:1089:GLU:OE2	2.53	0.42
1:B:1155:PHE:CZ	1:B:1167:LEU:HD21	2.54	0.42
1:B:1282:GLN:HA	1:B:1302:GLY:O	2.20	0.42
1:B:1274:GLN:NE2	1:B:1294:ASP:H	2.18	0.42
1:B:1417:VAL:CG1	1:B:1419:HIS:H	2.28	0.42
1:B:242:ASN:C	1:B:244:MET:N	2.72	0.42
1:B:244:MET:O	1:B:245:LYS:C	2.57	0.42
1:B:558:MET:C	1:B:560:ASP:H	2.23	0.42
1:B:826:ARG:CG	1:B:826:ARG:NH1	2.67	0.42
1:B:868:HIS:O	1:B:870:THR:N	2.53	0.42
1:B:878:ILE:HD13	1:B:878:ILE:HG21	1.66	0.42
1:B:948:LYS:C	1:B:950:THR:H	2.23	0.42
1:A:1131:THR:HG21	1:A:1133:GLU:HB2	2.01	0.42
1:A:1424:LEU:HD23	1:A:1424:LEU:C	2.40	0.42
1:A:165:ASN:O	1:A:166:ASP:HB2	2.20	0.42
1:A:227:MET:HE3	1:A:282:GLU:CA	2.40	0.42
1:A:284:MET:CE	1:A:294:VAL:HG13	2.50	0.42
1:A:352:PRO:HB2	1:A:367:SER:O	2.20	0.42
1:A:386:GLY:H	1:A:389:GLU:CG	2.33	0.42
1:A:419:TRP:CE3	1:A:537:GLU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:HIS:O	1:A:655:PHE:N	2.53	0.42
1:A:770:VAL:O	1:A:770:VAL:HG12	2.19	0.42
1:B:1043:LEU:HD23	1:B:1047:MET:HE3	2.01	0.42
1:B:353:MET:HE2	1:B:353:MET:HA	2.01	0.42
1:B:438:GLU:HG3	1:B:693:MET:CG	2.50	0.42
1:B:505:GLN:HE22	1:B:1001:VAL:N	2.17	0.42
1:A:1022:LEU:HA	1:A:1068:ARG:O	2.19	0.42
1:A:1274:GLN:HG2	1:A:1274:GLN:H	1.35	0.42
1:A:1276:LEU:C	1:A:1276:LEU:HD12	2.36	0.42
1:A:1349:ARG:NH1	1:A:1367:TYR:O	2.52	0.42
1:A:1370:GLY:N	1:A:1389:GLY:O	2.53	0.42
1:A:376:GLU:HG3	1:A:1310:THR:OG1	2.20	0.42
1:A:37:ASP:OD1	1:A:38:GLY:N	2.53	0.42
1:A:420:VAL:HG12	1:A:421:GLN:N	2.35	0.42
1:A:428:GLU:O	1:A:429:LEU:C	2.52	0.42
1:A:505:GLN:NE2	1:A:1000:LEU:HB3	2.35	0.42
1:A:583:ARG:NE	1:A:587:ARG:NH1	2.68	0.42
1:A:842:GLU:OE1	1:A:1156:ARG:NH1	2.52	0.42
1:B:105:TYR:H	1:B:105:TYR:HD1	1.68	0.42
1:B:1358:GLU:HA	1:B:1376:LEU:HB2	2.02	0.42
1:B:227:MET:HE2	1:B:282:GLU:HG3	2.00	0.42
1:B:24:ALA:O	1:B:25:LEU:C	2.57	0.42
1:B:253:HIS:CE1	1:B:254:PRO:CG	3.03	0.42
1:B:404:ARG:HB3	1:B:405:GLU:OE1	2.20	0.42
1:B:574:PRO:O	1:B:574:PRO:HG2	2.19	0.42
1:B:608:ASP:OD2	1:B:646:THR:HA	2.20	0.42
1:B:457:THR:HA	1:B:773:LEU:HB3	2.02	0.42
1:A:1246:LEU:O	1:A:1249:MET:HB2	2.20	0.41
1:A:1407:ASP:O	1:A:1409:SER:N	2.53	0.41
1:A:250:ARG:HH21	1:A:639:PHE:HE1	1.62	0.41
1:A:256:PHE:O	1:A:257:GLY:C	2.56	0.41
1:A:280:VAL:O	1:A:281:PHE:C	2.58	0.41
1:A:468:MET:O	1:A:472:GLY:N	2.51	0.41
1:A:558:MET:C	1:A:560:ASP:N	2.72	0.41
1:A:696:TYR:CZ	1:A:700:ILE:HD11	2.55	0.41
1:A:821:PRO:HA	1:A:822:PRO:HD3	1.84	0.41
1:A:894:PHE:CD1	1:A:904:ASN:ND2	2.88	0.41
1:B:232:GLY:HA3	1:B:330:PRO:O	2.20	0.41
1:B:632:ILE:HD13	1:B:632:ILE:HA	1.92	0.41
1:B:656:ALA:O	1:B:657:VAL:C	2.58	0.41
1:B:745:ARG:C	1:B:746:ILE:HG13	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:957:ARG:HD2	1:B:965:LEU:HD12	2.02	0.41
1:A:1039:LYS:O	1:A:1040:PHE:CD1	2.73	0.41
1:A:1170:GLN:HB2	1:A:1183:LEU:HD12	2.02	0.41
1:A:1236:ARG:O	1:A:1238:THR:N	2.53	0.41
1:A:1349:ARG:HH11	1:A:1349:ARG:CG	2.22	0.41
1:A:1356:VAL:CG1	1:A:1431:HIS:CG	3.03	0.41
1:A:565:THR:CG2	1:A:603:HIS:HD2	2.33	0.41
1:B:1468:VAL:O	1:B:1469:PRO:C	2.57	0.41
1:B:42:ASP:HB2	1:B:210:ARG:O	2.20	0.41
1:B:5:PHE:CZ	1:B:365:GLY:HA3	2.55	0.41
1:B:250:ARG:NE	1:B:639:PHE:CE1	2.83	0.41
1:B:444:LYS:HE3	1:B:681:ARG:HH12	1.85	0.41
1:B:751:LEU:HD23	1:B:751:LEU:HA	1.49	0.41
1:A:1101:GLY:O	1:A:1102:CYS:C	2.57	0.41
1:A:139:VAL:CG1	1:A:140:SER:N	2.54	0.41
1:A:286:ARG:HD3	1:A:286:ARG:HA	1.60	0.41
1:A:631:LEU:HD22	1:A:631:LEU:HA	1.39	0.41
1:B:182:MET:CG	1:B:182:MET:O	2.66	0.41
1:B:218:THR:CG2	1:B:221:LEU:H	2.30	0.41
1:B:355:TYR:HD1	1:B:355:TYR:C	2.20	0.41
1:B:500:ARG:HD2	1:B:728:ILE:HG21	2.02	0.41
1:B:547:SER:C	1:B:549:VAL:H	2.22	0.41
1:B:559:ARG:HG3	1:B:559:ARG:O	2.17	0.41
1:B:631:LEU:HA	1:B:631:LEU:HD22	1.74	0.41
1:B:970:PRO:HG2	1:B:970:PRO:O	2.19	0.41
1:B:987:LEU:HD23	1:B:987:LEU:HA	1.80	0.41
1:A:1226:GLY:O	1:A:1227:GLU:C	2.59	0.41
1:A:1375:ILE:HG21	1:A:1375:ILE:HD13	1.75	0.41
1:A:1384:ALA:O	1:A:1385:ALA:C	2.57	0.41
1:A:273:ASP:N	1:A:273:ASP:OD1	2.54	0.41
1:A:358:THR:CB	1:A:360:ASP:OD1	2.65	0.41
1:A:420:VAL:C	1:A:422:ASN:H	2.23	0.41
1:A:447:LEU:CD1	1:A:670:LEU:HD21	2.44	0.41
1:A:78:LEU:HB3	1:A:79:PRO:HD2	2.00	0.41
1:A:855:THR:O	1:A:855:THR:CG2	2.69	0.41
1:A:978:GLU:HG3	1:A:979:ASP:H	1.86	0.41
1:B:1252:ARG:HH11	1:B:1252:ARG:HD3	1.68	0.41
1:B:957:ARG:NH2	4:B:2475:AKG:O4	2.40	0.41
1:B:552:THR:O	1:B:552:THR:HG22	2.19	0.41
1:B:588:ARG:HH11	1:B:588:ARG:HD3	1.68	0.41
1:B:695:ASN:O	1:B:696:TYR:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:TYR:O	1:B:810:PHE:HB3	2.19	0.41
1:B:856:PRO:HG2	1:B:1093:GLY:HA3	2.02	0.41
1:B:87:GLU:O	1:B:90:ARG:N	2.54	0.41
1:A:1009:ILE:O	1:A:1010:ALA:C	2.59	0.41
1:A:111:PRO:C	1:A:112:ILE:HG23	2.40	0.41
1:A:1354:THR:HG23	1:A:1372:THR:HB	2.01	0.41
1:A:476:ILE:CG2	1:A:477:GLY:N	2.83	0.41
1:A:304:THR:HG21	1:A:518:ARG:HD2	2.03	0.41
1:A:695:ASN:O	1:A:698:LYS:N	2.53	0.41
1:A:890:ASP:HA	1:A:891:PRO:HD3	1.85	0.41
1:A:956:LEU:HA	1:A:956:LEU:HD23	1.70	0.41
1:A:97:ILE:HA	1:A:151:ILE:HD13	2.01	0.41
1:B:481:ASP:HB2	1:B:1038:ILE:HG22	2.02	0.41
1:B:1135:VAL:O	1:B:1138:LEU:N	2.54	0.41
1:B:1347:ALA:O	1:B:1348:VAL:C	2.54	0.41
1:B:1359:GLY:O	1:B:1360:CYS:HB3	2.20	0.41
1:B:1412:PHE:CD1	1:B:1412:PHE:N	2.88	0.41
1:B:175:ARG:NH2	1:B:203:ASP:OD2	2.54	0.41
1:B:504:SER:HB2	1:B:508:ASN:OD1	2.21	0.41
1:B:661:VAL:O	1:B:661:VAL:HG12	2.21	0.41
1:B:666:VAL:HG13	1:B:667:ASN:N	2.34	0.41
1:B:732:ARG:O	1:B:733:ALA:C	2.59	0.41
1:B:875:MET:SD	1:B:1139:PHE:CE2	3.14	0.41
1:A:1057:THR:CG2	1:A:1190:VAL:HG11	2.50	0.41
1:A:1230:GLN:C	1:A:1231:LEU:HD23	2.41	0.41
1:A:1349:ARG:HG2	1:A:1349:ARG:NH1	2.31	0.41
1:A:443:ASP:OD2	1:A:445:ALA:HB3	2.21	0.41
1:A:555:PHE:CD1	1:A:556:ARG:N	2.89	0.41
1:B:1161:VAL:O	1:B:1161:VAL:HG12	2.21	0.41
1:A:1113:CYS:C	1:A:1115:VAL:N	2.71	0.41
1:A:1235:ALA:HA	1:A:1239:GLN:OE1	2.21	0.41
1:A:193:PRO:O	1:A:196:LEU:N	2.52	0.41
1:A:198:GLU:HG3	1:A:198:GLU:H	1.72	0.41
1:A:309:THR:HB	1:A:314:LYS:CE	2.51	0.41
1:A:745:ARG:C	1:A:746:ILE:HG13	2.40	0.41
1:A:856:PRO:C	1:A:883:ASP:HB3	2.41	0.41
1:B:1058:LEU:HD23	1:B:1058:LEU:HA	1.64	0.41
1:B:1222:LEU:N	1:B:1229:MET:HE2	2.32	0.41
1:B:1317:THR:HG22	1:B:1318:ASN:CA	2.46	0.41
1:B:325:GLU:HA	1:B:326:PRO:HD3	1.92	0.41
1:B:526:LEU:N	1:B:526:LEU:CD1	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:PHE:HB3	1:B:740:PRO:HD2	2.03	0.41
1:B:919:ALA:CB	1:B:1281:VAL:CG1	2.98	0.41
1:A:864:SER:HB3	1:A:1116:GLY:O	2.21	0.41
1:A:406:LEU:O	1:A:409:HIS:HB3	2.21	0.41
1:A:672:GLN:HG3	1:A:693:MET:SD	2.60	0.41
1:B:30:HIS:HE2	1:B:31:ARG:HD2	1.86	0.41
1:B:802:VAL:CG2	1:B:1134:LYS:O	2.69	0.41
1:A:1458:VAL:HA	1:A:1459:PRO:HD3	1.66	0.41
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.55	0.41
1:A:454:PHE:CD2	1:A:648:GLU:CB	3.00	0.41
1:A:52:GLN:HB3	1:A:52:GLN:HE21	1.56	0.41
1:A:706:LYS:NZ	1:A:1034:PRO:HG2	2.36	0.41
1:A:452:GLN:CG	1:A:764:THR:HG22	2.48	0.41
1:A:77:PHE:HB3	1:A:126:PRO:CB	2.50	0.41
1:A:862:ALA:O	1:A:1118:CYS:HB3	2.18	0.41
1:A:969:PRO:CD	1:A:970:PRO:CD	2.99	0.41
1:B:1435:THR:CG2	1:B:1437:SER:CB	2.99	0.41
1:B:570:ASP:C	1:B:570:ASP:OD1	2.59	0.41
1:B:937:LYS:N	1:B:938:PRO:HD3	2.35	0.41
1:B:999:LYS:CG	1:B:1022:LEU:CD2	2.64	0.41
1:A:1059:ASN:HD22	1:A:1059:ASN:N	2.19	0.41
1:A:842:GLU:O	1:A:1156:ARG:HG2	2.21	0.41
1:A:1466:LEU:O	1:A:1468:VAL:N	2.54	0.41
1:A:149:TYR:HE2	1:A:263:LEU:HD21	1.86	0.41
1:A:303:LEU:HD11	1:A:314:LYS:HG2	2.01	0.41
1:A:329:GLY:O	1:A:330:PRO:C	2.56	0.41
1:A:562:MET:HE1	1:A:605:ILE:HD11	2.01	0.41
1:A:782:ARG:C	1:A:784:SER:N	2.70	0.41
1:A:784:SER:HB3	1:A:785:GLY:H	1.66	0.41
1:A:843:VAL:CG1	1:A:844:GLU:H	2.31	0.41
1:A:914:ARG:HH22	1:A:973:ASP:CG	2.23	0.41
1:B:1043:LEU:O	1:B:1044:PRO:C	2.58	0.41
1:B:1113:CYS:C	1:B:1115:VAL:H	2.23	0.41
1:B:1222:LEU:O	1:B:1222:LEU:HD12	2.20	0.41
1:B:1250:VAL:HG13	1:B:1259:LEU:HD12	2.01	0.41
1:B:1335:LYS:HA	1:B:1354:THR:O	2.21	0.41
1:B:240:ASN:HB3	1:B:327:TRP:CZ2	2.56	0.41
1:B:438:GLU:OE2	1:B:553:ALA:HB3	2.20	0.41
1:B:974:ILE:HG21	1:B:974:ILE:HD13	1.74	0.41
1:A:266:VAL:HG12	1:A:279:THR:HG22	1.94	0.41
1:A:461:MET:HA	1:A:461:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:SER:HB3	1:A:1117:VAL:O	2.21	0.41
1:A:930:ILE:CD1	1:A:983:LEU:HD13	2.43	0.41
1:B:1153:LEU:HA	1:B:1153:LEU:HD23	1.42	0.41
1:B:284:MET:HE2	1:B:294:VAL:HG13	2.03	0.41
1:B:815:GLU:O	1:B:816:GLN:C	2.59	0.41
1:A:1458:VAL:CG1	1:A:1459:PRO:HD2	2.48	0.40
1:A:24:ALA:C	1:A:26:LYS:H	2.23	0.40
1:A:42:ASP:OD1	1:A:212:SER:OG	2.38	0.40
1:A:485:ILE:HD13	1:A:485:ILE:HG21	1.72	0.40
1:A:503:PHE:CE2	1:A:938:PRO:HB3	2.56	0.40
1:A:622:LEU:HA	1:A:739:PHE:HE1	1.86	0.40
1:A:701:ASP:C	1:A:703:GLY:N	2.71	0.40
1:B:853:PHE:CZ	1:B:1079:ILE:HD13	2.55	0.40
1:B:120:LYS:HA	1:B:120:LYS:HE2	2.00	0.40
1:B:240:ASN:HB3	1:B:327:TRP:CH2	2.56	0.40
1:B:410:LEU:HD12	1:B:410:LEU:N	2.36	0.40
1:B:561:TYR:CD1	1:B:561:TYR:O	2.74	0.40
1:B:806:SER:HG	1:B:809:THR:HB	1.85	0.40
1:A:1131:THR:CG2	1:A:1133:GLU:HB2	2.52	0.40
1:A:320:CYS:O	1:A:322:SER:N	2.54	0.40
1:A:348:ASN:O	1:A:349:GLY:C	2.59	0.40
1:A:528:ASN:O	1:A:529:LEU:HD23	2.21	0.40
1:A:635:ASN:O	1:A:636:LEU:HD13	2.20	0.40
1:A:492:TYR:CD2	1:A:761:GLN:HG2	2.57	0.40
1:A:464:ILE:CD1	1:A:779:TYR:CZ	2.94	0.40
1:B:1062:ARG:HD3	1:B:1062:ARG:HH11	1.40	0.40
1:B:1147:ARG:HD3	1:B:1147:ARG:HH11	1.75	0.40
1:B:186:GLU:HG3	1:B:186:GLU:H	1.05	0.40
1:B:330:PRO:HA	1:B:350:LEU:HB2	2.03	0.40
1:B:406:LEU:O	1:B:409:HIS:HB3	2.21	0.40
1:B:621:ILE:HG12	1:B:657:VAL:HG12	2.04	0.40
1:B:657:VAL:O	1:B:661:VAL:HG23	2.22	0.40
1:B:499:PHE:CE1	1:B:742:MET:CE	3.00	0.40
1:B:787:ARG:HH12	1:B:821:PRO:CB	2.34	0.40
1:B:80:ARG:O	1:B:80:ARG:HG3	2.21	0.40
1:A:1401:LEU:HD11	1:A:1405:ILE:CD1	2.50	0.40
1:A:183:PHE:HE1	1:A:188:LEU:HA	1.79	0.40
1:A:318:GLN:O	1:A:322:SER:OG	2.40	0.40
1:A:397:SER:O	1:A:398:GLY:C	2.58	0.40
1:A:390:MET:HG3	1:A:406:LEU:HD23	2.02	0.40
1:A:606:LEU:O	1:A:607:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ALA:HB1	1:A:837:PRO:CD	2.52	0.40
1:B:1054:GLN:O	1:B:1055:VAL:C	2.60	0.40
1:B:1357:VAL:CG1	1:B:1359:GLY:H	2.35	0.40
1:B:143:GLN:HE21	1:B:143:GLN:C	2.24	0.40
1:B:325:GLU:HG3	1:B:325:GLU:H	1.48	0.40
1:B:536:ASP:OD1	1:B:538:THR:N	2.54	0.40
1:B:575:VAL:HG13	1:B:759:LEU:HD22	2.03	0.40
1:A:833:SER:HB2	1:A:1167:LEU:HD22	2.03	0.40
1:A:1374:VAL:HG12	1:A:1375:ILE:H	1.86	0.40
1:A:1395:TYR:HD2	1:A:1454:PHE:CE1	2.39	0.40
1:A:1440:ALA:O	1:A:1441:ALA:C	2.58	0.40
1:A:355:TYR:CZ	1:A:383:GLY:HA3	2.56	0.40
1:A:501:GLN:OE1	1:A:710:LYS:NZ	2.47	0.40
1:A:595:ASP:O	1:A:596:ALA:O	2.38	0.40
1:A:491:LYS:HZ2	1:A:785:GLY:HA3	1.83	0.40
1:A:803:THR:CG2	1:A:803:THR:O	2.62	0.40
1:B:1354:THR:HA	1:B:1372:THR:O	2.21	0.40
1:B:942:GLY:HA2	4:B:2475:AKG:O5	2.20	0.40
1:B:313:HIS:N	1:B:313:HIS:CD2	2.89	0.40
1:B:298:LEU:HD23	1:B:324:MET:HG2	2.04	0.40
1:B:412:THR:CG2	1:B:412:THR:O	2.68	0.40
1:B:694:ALA:O	1:B:695:ASN:C	2.58	0.40
1:B:56:LYS:CG	1:B:71:LEU:HD22	2.48	0.40
1:B:860:MET:HE2	1:B:868:HIS:ND1	2.36	0.40
1:B:969:PRO:N	1:B:970:PRO:CD	2.84	0.40
1:A:10:ASP:C	1:A:10:ASP:OD1	2.59	0.40
1:A:1150:LEU:HD21	1:A:1158:LEU:HD12	2.04	0.40
1:A:1411:ILE:O	1:A:1411:ILE:CG1	2.66	0.40
1:A:148:LEU:O	1:A:151:ILE:HB	2.21	0.40
1:A:185:ALA:O	1:A:186:GLU:C	2.58	0.40
1:A:1108:CYS:SG	5:A:2476:F3S:S2	3.20	0.40
1:A:233:GLU:O	1:A:329:GLY:HA3	2.21	0.40
1:A:6:ILE:HB	1:A:205:ALA:HB3	2.03	0.40
1:A:894:PHE:CZ	1:A:924:GLN:HG3	2.56	0.40
1:B:117:ILE:HG21	1:B:117:ILE:HD12	1.49	0.40
1:B:230:HIS:CE1	1:B:234:ILE:HG13	2.55	0.40
1:B:495:LEU:O	1:B:497:HIS:N	2.55	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	1444/1479 (98%)	1152 (80%)	227 (16%)	65 (4%)	2 14
1	B	1444/1479 (98%)	1170 (81%)	211 (15%)	63 (4%)	2 15
All	All	2888/2958 (98%)	2322 (80%)	438 (15%)	128 (4%)	2 15

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	444	LYS
1	A	451	GLN
1	A	705	LEU
1	A	712	GLY
1	A	950	THR
1	A	1062	ARG
1	A	1227	GLU
1	A	1339	ALA
1	A	1375	ILE
1	A	1376	LEU
1	A	1388	THR
1	A	1394	VAL
1	A	1408	GLU
1	A	1461	GLU
1	A	1467	GLU
1	B	249	THR
1	B	255	ALA
1	B	418	LYS
1	B	561	TYR
1	B	705	LEU
1	B	740	PRO
1	B	950	THR
1	B	1164	ARG
1	B	1467	GLU

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Mol	Chain	Res	Type
1	A	53	LYS
1	A	54	PHE
1	A	249	THR
1	A	370	GLY
1	A	561	TYR
1	A	599	GLY
1	A	663	ALA
1	A	709	SER
1	A	745	ARG
1	A	939	GLY
1	A	1042	GLY
1	A	1160	GLU
1	A	1164	ARG
1	A	1317	THR
1	A	1439	PHE
1	A	1454	PHE
1	A	1460	LYS
1	B	25	LEU
1	B	421	GLN
1	B	444	LYS
1	B	451	GLN
1	B	562	MET
1	B	577	GLY
1	B	610	ALA
1	B	747	SER
1	B	764	THR
1	B	868	HIS
1	B	884	SER
1	B	886	GLU
1	B	1160	GLU
1	B	1381	ASP
1	B	1408	GLU
1	B	1421	GLU
1	B	1432	VAL
1	B	1433	THR
1	B	1452	THR
1	B	1461	GLU
1	A	24	ALA
1	A	377	THR
1	A	432	THR
1	A	433	ALA
1	A	629	THR

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Mol	Chain	Res	Type
1	A	740	PRO
1	A	974	ILE
1	A	1361	GLY
1	A	1381	ASP
1	A	1407	ASP
1	A	1438	ARG
1	B	663	ALA
1	B	721	GLY
1	B	745	ARG
1	B	869	GLY
1	B	1062	ARG
1	B	1071	GLY
1	B	1114	PRO
1	B	1142	LEU
1	B	1339	ALA
1	B	1438	ARG
1	B	1439	PHE
1	A	208	HIS
1	A	245	LYS
1	A	421	GLN
1	A	450	ARG
1	A	492	TYR
1	A	553	ALA
1	A	844	GLU
1	A	915	PHE
1	B	326	PRO
1	B	475	ALA
1	B	496	HIS
1	B	856	PRO
1	B	974	ILE
1	B	1376	LEU
1	B	1407	ASP
1	B	1424	LEU
1	A	69	ASN
1	A	521	SER
1	A	654	TYR
1	A	962	GLY
1	A	1395	TYR
1	B	254	PRO
1	B	388	GLY
1	B	450	ARG
1	B	559	ARG

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Mol	Chain	Res	Type
1	B	1078	ASP
1	A	217	PRO
1	B	290	THR
1	B	619	PRO
1	B	780	ARG
1	A	707	ILE
1	A	1185	PRO
1	B	61	VAL
1	A	619	PRO
1	A	1071	GLY
1	A	1261	PRO
1	A	1389	GLY
1	B	116	ILE
1	B	455	GLY
1	B	1394	VAL
1	A	372	VAL
1	B	774	PRO
1	B	953	ILE
1	B	657	VAL

5.3.2 Protein sidechains (i)

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	1184/1206 (98%)	970 (82%)	214 (18%)	1 9
1	B	1184/1206 (98%)	965 (82%)	219 (18%)	1 8
All	All	2368/2412 (98%)	1935 (82%)	433 (18%)	1 9

All (433) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	30	HIS
1	A	34	VAL
1	A	35	ASP

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Mol	Chain	Res	Type
1	A	37	ASP
1	A	39	LYS
1	A	40	THR
1	A	47	HIS
1	A	52	GLN
1	A	59	VAL
1	A	68	ASP
1	A	69	ASN
1	A	76	VAL
1	A	78	LEU
1	A	80	ARG
1	A	81	ILE
1	A	109	GLN
1	A	113	ASN
1	A	117	ILE
1	A	120	LYS
1	A	143	GLN
1	A	144	PHE
1	A	146	LEU
1	A	156	GLU
1	A	162	GLU
1	A	175	ARG
1	A	177	ILE
1	A	184	LEU
1	A	186	GLU
1	A	188	LEU
1	A	189	THR
1	A	196	LEU
1	A	198	GLU
1	A	207	TYR
1	A	209	GLN
1	A	210	ARG
1	A	215	THR
1	A	218	THR
1	A	228	LEU
1	A	235	ASN
1	A	242	ASN
1	A	244	MET
1	A	249	THR
1	A	254	PRO
1	A	258	THR
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	267	ILE
1	A	269	VAL
1	A	279	THR
1	A	286	ARG
1	A	312	ASN
1	A	316	LEU
1	A	322	SER
1	A	335	MET
1	A	336	THR
1	A	342	VAL
1	A	347	ARG
1	A	351	ARG
1	A	353	MET
1	A	355	TYR
1	A	362	LEU
1	A	367	SER
1	A	368	GLU
1	A	377	THR
1	A	380	ILE
1	A	390	MET
1	A	397	SER
1	A	405	GLU
1	A	413	LEU
1	A	417	ASP
1	A	420	VAL
1	A	429	LEU
1	A	439	PRO
1	A	440	SER
1	A	441	ASP
1	A	447	LEU
1	A	461	MET
1	A	463	LEU
1	A	465	LEU
1	A	479	MET
1	A	483	SER
1	A	487	VAL
1	A	495	LEU
1	A	509	PRO
1	A	519	VAL
1	A	520	MET
1	A	526	LEU
1	A	534	ASP

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Mol	Chain	Res	Type
1	A	537	GLU
1	A	547	SER
1	A	559	ARG
1	A	564	ASP
1	A	572	THR
1	A	584	ASP
1	A	598	ARG
1	A	606	LEU
1	A	607	THR
1	A	611	MET
1	A	631	LEU
1	A	634	SER
1	A	636	LEU
1	A	637	ARG
1	A	640	THR
1	A	642	LEU
1	A	650	LEU
1	A	658	LEU
1	A	665	THR
1	A	670	LEU
1	A	673	GLU
1	A	678	ARG
1	A	704	LEU
1	A	705	LEU
1	A	724	ASN
1	A	731	SER
1	A	734	LEU
1	A	764	THR
1	A	768	GLU
1	A	786	ASP
1	A	787	ARG
1	A	794	VAL
1	A	795	ILE
1	A	806	SER
1	A	812	LYS
1	A	813	TYR
1	A	820	ARG
1	A	824	GLN
1	A	826	ARG
1	A	833	SER
1	A	841	ASP
1	A	842	GLU

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Mol	Chain	Res	Type
1	A	850	ARG
1	A	851	LYS
1	A	855	THR
1	A	863	LEU
1	A	875	MET
1	A	884	SER
1	A	889	GLU
1	A	912	SER
1	A	934	GLN
1	A	937	LYS
1	A	952	MET
1	A	953	ILE
1	A	958	HIS
1	A	960	THR
1	A	970	PRO
1	A	978	GLU
1	A	982	GLN
1	A	983	LEU
1	A	1003	ARG
1	A	1008	THR
1	A	1015	LYS
1	A	1036	THR
1	A	1043	LEU
1	A	1057	THR
1	A	1058	LEU
1	A	1062	ARG
1	A	1064	ARG
1	A	1065	VAL
1	A	1066	ARG
1	A	1090	PHE
1	A	1109	HIS
1	A	1121	ASP
1	A	1122	ASP
1	A	1124	LEU
1	A	1142	LEU
1	A	1145	GLU
1	A	1157	SER
1	A	1159	ASN
1	A	1170	GLN
1	A	1206	GLU
1	A	1207	VAL
1	A	1220	ARG

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Mol	Chain	Res	Type
1	A	1225	GLU
1	A	1245	ARG
1	A	1246	LEU
1	A	1253	LYS
1	A	1261	PRO
1	A	1264	ILE
1	A	1267	ARG
1	A	1269	ARG
1	A	1274	GLN
1	A	1289	MET
1	A	1291	ASP
1	A	1301	SER
1	A	1304	THR
1	A	1308	ARG
1	A	1310	THR
1	A	1314	PRO
1	A	1317	THR
1	A	1318	ASN
1	A	1349	ARG
1	A	1355	VAL
1	A	1357	VAL
1	A	1360	CYS
1	A	1379	VAL
1	A	1381	ASP
1	A	1398	ASP
1	A	1401	LEU
1	A	1402	PRO
1	A	1408	GLU
1	A	1410	VAL
1	A	1413	GLN
1	A	1419	HIS
1	A	1421	GLU
1	A	1422	SER
1	A	1424	LEU
1	A	1425	LYS
1	A	1449	ARG
1	A	1452	THR
1	A	1461	GLU
1	A	1465	ARG
1	A	1466	LEU
1	A	1470	VAL
1	A	1471	HIS

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Mol	Chain	Res	Type
1	B	3	VAL
1	B	30	HIS
1	B	34	VAL
1	B	35	ASP
1	B	37	ASP
1	B	40	THR
1	B	47	HIS
1	B	59	VAL
1	B	68	ASP
1	B	76	VAL
1	B	80	ARG
1	B	81	ILE
1	B	109	GLN
1	B	113	ASN
1	B	117	ILE
1	B	120	LYS
1	B	143	GLN
1	B	144	PHE
1	B	146	LEU
1	B	173	SER
1	B	175	ARG
1	B	184	LEU
1	B	186	GLU
1	B	188	LEU
1	B	189	THR
1	B	198	GLU
1	B	209	GLN
1	B	210	ARG
1	B	215	THR
1	B	217	PRO
1	B	218	THR
1	B	235	ASN
1	B	242	ASN
1	B	249	THR
1	B	254	PRO
1	B	258	THR
1	B	260	MET
1	B	261	GLN
1	B	263	LEU
1	B	269	VAL
1	B	274	SER
1	B	279	THR

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Mol	Chain	Res	Type
1	B	286	ARG
1	B	290	THR
1	B	296	MET
1	B	297	MET
1	B	308	THR
1	B	312	ASN
1	B	316	LEU
1	B	322	SER
1	B	325	GLU
1	B	347	ARG
1	B	351	ARG
1	B	353	MET
1	B	355	TYR
1	B	362	LEU
1	B	367	SER
1	B	377	THR
1	B	380	ILE
1	B	385	LEU
1	B	389	GLU
1	B	397	SER
1	B	402	ARG
1	B	413	LEU
1	B	417	ASP
1	B	420	VAL
1	B	422	ASN
1	B	423	THR
1	B	426	LEU
1	B	429	LEU
1	B	439	PRO
1	B	447	LEU
1	B	461	MET
1	B	462	GLU
1	B	481	ASP
1	B	483	SER
1	B	487	VAL
1	B	490	ASP
1	B	492	TYR
1	B	495	LEU
1	B	496	HIS
1	B	500	ARG
1	B	501	GLN
1	B	519	VAL

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Mol	Chain	Res	Type
1	B	520	MET
1	B	522	LEU
1	B	526	LEU
1	B	531	ASN
1	B	534	ASP
1	B	537	GLU
1	B	538	THR
1	B	542	LEU
1	B	555	PHE
1	B	559	ARG
1	B	562	MET
1	B	564	ASP
1	B	572	THR
1	B	576	ASP
1	B	584	ASP
1	B	593	THR
1	B	606	LEU
1	B	607	THR
1	B	608	ASP
1	B	631	LEU
1	B	636	LEU
1	B	637	ARG
1	B	640	THR
1	B	642	LEU
1	B	643	ASN
1	B	658	LEU
1	B	665	THR
1	B	670	LEU
1	B	673	GLU
1	B	681	ARG
1	B	704	LEU
1	B	714	SER
1	B	717	SER
1	B	731	SER
1	B	746	ILE
1	B	751	LEU
1	B	764	THR
1	B	770	VAL
1	B	786	ASP
1	B	787	ARG
1	B	805	ASP
1	B	813	TYR

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Mol	Chain	Res	Type
1	B	820	ARG
1	B	823	MET
1	B	824	GLN
1	B	826	ARG
1	B	833	SER
1	B	841	ASP
1	B	850	ARG
1	B	855	THR
1	B	859	SER
1	B	884	SER
1	B	889	GLU
1	B	898	LYS
1	B	912	SER
1	B	918	THR
1	B	934	GLN
1	B	937	LYS
1	B	950	THR
1	B	952	MET
1	B	958	HIS
1	B	960	THR
1	B	978	GLU
1	B	983	LEU
1	B	1002	SER
1	B	1003	ARG
1	B	1008	THR
1	B	1015	LYS
1	B	1030	THR
1	B	1043	LEU
1	B	1057	THR
1	B	1058	LEU
1	B	1059	ASN
1	B	1062	ARG
1	B	1064	ARG
1	B	1065	VAL
1	B	1077	ARG
1	B	1090	PHE
1	B	1104	MET
1	B	1105	VAL
1	B	1109	HIS
1	B	1114	PRO
1	B	1121	ASP
1	B	1122	ASP

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Mol	Chain	Res	Type
1	B	1124	LEU
1	B	1131	THR
1	B	1142	LEU
1	B	1145	GLU
1	B	1147	ARG
1	B	1157	SER
1	B	1159	ASN
1	B	1167	LEU
1	B	1169	HIS
1	B	1170	GLN
1	B	1186	ARG
1	B	1204	ARG
1	B	1212	ASP
1	B	1229	MET
1	B	1230	GLN
1	B	1237	ASN
1	B	1238	THR
1	B	1245	ARG
1	B	1246	LEU
1	B	1247	SER
1	B	1253	LYS
1	B	1261	PRO
1	B	1264	ILE
1	B	1269	ARG
1	B	1289	MET
1	B	1298	LYS
1	B	1308	ARG
1	B	1317	THR
1	B	1318	ASN
1	B	1344	GLU
1	B	1349	ARG
1	B	1355	VAL
1	B	1360	CYS
1	B	1379	VAL
1	B	1381	ASP
1	B	1388	THR
1	B	1398	ASP
1	B	1400	SER
1	B	1401	LEU
1	B	1408	GLU
1	B	1409	SER
1	B	1410	VAL

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Mol	Chain	Res	Type
1	B	1421	GLU
1	B	1422	SER
1	B	1435	THR
1	B	1449	ARG
1	B	1452	THR
1	B	1465	ARG
1	B	1466	LEU
1	B	1470	VAL
1	B	1471	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	47	HIS
1	A	52	GLN
1	A	113	ASN
1	A	143	GLN
1	A	163	GLN
1	A	208	HIS
1	A	214	ASN
1	A	230	HIS
1	A	235	ASN
1	A	240	ASN
1	A	261	GLN
1	A	313	HIS
1	A	321	ASN
1	A	452	GLN
1	A	505	GLN
1	A	635	ASN
1	A	643	ASN
1	A	653	HIS
1	A	724	ASN
1	A	738	HIS
1	A	755	GLN
1	A	788	HIS
1	A	824	GLN
1	A	943	GLN
1	A	982	GLN
1	A	1026	ASN
1	A	1059	ASN
1	A	1205	ASN

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Mol	Chain	Res	Type
1	A	1230	GLN
1	A	1274	GLN
1	A	1293	ASN
1	A	1318	ASN
1	A	1320	ASN
1	A	1363	ASN
1	A	1382	ASN
1	A	1419	HIS
1	A	1471	HIS
1	B	30	HIS
1	B	47	HIS
1	B	52	GLN
1	B	113	ASN
1	B	143	GLN
1	B	208	HIS
1	B	214	ASN
1	B	231	ASN
1	B	235	ASN
1	B	240	ASN
1	B	242	ASN
1	B	247	HIS
1	B	259	HIS
1	B	301	GLN
1	B	321	ASN
1	B	452	GLN
1	B	497	HIS
1	B	505	GLN
1	B	643	ASN
1	B	653	HIS
1	B	738	HIS
1	B	755	GLN
1	B	762	HIS
1	B	788	HIS
1	B	816	GLN
1	B	824	GLN
1	B	943	GLN
1	B	982	GLN
1	B	1059	ASN
1	B	1137	ASN
1	B	1205	ASN
1	B	1274	GLN
1	B	1318	ASN

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Mol	Chain	Res	Type
1	B	1363	ASN
1	B	1382	ASN
1	B	1419	HIS
1	B	1471	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AKG	B	2475	-	3,9,9	5.21	2 (66%)	4,11,11	4.04	2 (50%)
4	AKG	A	2475	-	3,9,9	4.84	2 (66%)	4,11,11	3.45	2 (50%)
5	F3S	B	2476	1	0,9,9	0.00	-	-		
3	FMN	B	2474	-	31,33,33	1.49	3 (9%)	40,50,50	3.22	19 (47%)
2	OMT	A	2473	-	6,10,10	4.94	4 (66%)	6,14,14	5.93	5 (83%)
3	FMN	A	2474	-	31,33,33	1.56	6 (19%)	40,50,50	3.12	20 (50%)
5	F3S	A	2476	1	0,9,9	0.00	-	-		
2	OMT	B	2473	-	6,10,10	4.89	4 (66%)	6,14,14	7.72	4 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AKG	B	2475	-	-	1/3/9/9	-
4	AKG	A	2475	-	-	0/3/9/9	-
5	F3S	B	2476	1	-	-	0/3/3/3
3	FMN	B	2474	-	-	5/18/18/18	0/3/3/3
2	OMT	A	2473	-	-	5/6/10/10	-
3	FMN	A	2474	-	-	7/18/18/18	0/3/3/3
5	F3S	A	2476	1	-	-	0/3/3/3
2	OMT	B	2473	-	-	5/6/10/10	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2475	AKG	O5-C2	8.69	1.36	1.22
4	A	2475	AKG	O5-C2	8.07	1.35	1.22
2	A	2473	OMT	CB-CG	-6.99	1.45	1.52
2	B	2473	OMT	CG-SD	-6.88	1.69	1.78
2	A	2473	OMT	CG-SD	-6.69	1.69	1.78
2	B	2473	OMT	CB-CG	-5.99	1.46	1.52
2	B	2473	OMT	OD1-SD	5.92	1.57	1.44
2	A	2473	OMT	OD2-SD	5.39	1.56	1.44
3	B	2474	FMN	C10-N1	5.13	1.39	1.33
2	B	2473	OMT	OD2-SD	4.86	1.55	1.44
2	A	2473	OMT	OD1-SD	4.59	1.54	1.44
3	A	2474	FMN	C10-N1	4.18	1.38	1.33
3	A	2474	FMN	C9A-C5A	-2.96	1.36	1.42
3	B	2474	FMN	C9A-C5A	-2.69	1.37	1.42
3	A	2474	FMN	O4'-C4'	-2.51	1.38	1.43
4	B	2475	AKG	C3-C2	2.40	1.54	1.51
3	A	2474	FMN	C4A-N5	2.37	1.36	1.33
3	A	2474	FMN	C4-N3	2.37	1.37	1.33
4	A	2475	AKG	C3-C2	2.26	1.54	1.51
3	B	2474	FMN	C4-N3	2.20	1.36	1.33
3	A	2474	FMN	C1'-N10	2.01	1.50	1.48

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2473	OMT	OD2-SD-CG	-16.70	96.65	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2473	OMT	OD2-SD-CE	-11.66	97.19	108.91
3	B	2474	FMN	C1'-N10-C10	8.14	125.70	118.41
3	A	2474	FMN	O5'-P-O1P	-7.87	84.41	106.47
3	B	2474	FMN	C1'-N10-C9A	-7.66	112.26	118.29
3	B	2474	FMN	C4'-C3'-C2'	-7.07	98.65	113.36
4	B	2475	AKG	C4-C3-C2	-6.72	98.63	113.14
3	B	2474	FMN	O4'-C4'-C3'	-6.46	93.39	109.10
2	B	2473	OMT	OD1-SD-CE	-6.37	102.50	108.91
4	A	2475	AKG	C4-C3-C2	-6.36	99.42	113.14
3	A	2474	FMN	O4'-C4'-C5'	-6.24	95.89	109.92
2	A	2473	OMT	CE-SD-CG	5.84	127.72	105.21
3	A	2474	FMN	O4'-C4'-C3'	-5.67	95.31	109.10
3	A	2474	FMN	O3P-P-O5'	5.46	121.28	106.73
3	B	2474	FMN	C4-C4A-C10	5.35	123.49	119.95
2	B	2473	OMT	OD1-SD-CG	5.09	111.91	108.34
3	A	2474	FMN	C4A-N5-C5A	5.07	121.83	116.77
3	A	2474	FMN	O2P-P-O5'	5.07	120.21	106.73
3	B	2474	FMN	C5'-C4'-C3'	4.70	121.29	112.20
4	B	2475	AKG	C3-C4-C5	4.48	120.19	112.67
3	A	2474	FMN	C5A-C9A-N10	4.38	120.89	117.72
3	A	2474	FMN	C1'-N10-C10	4.19	122.16	118.41
2	A	2473	OMT	OD2-SD-CG	-4.18	105.42	108.34
3	B	2474	FMN	C4A-N5-C5A	4.15	120.92	116.77
3	A	2474	FMN	C4-N3-C2	4.05	118.57	115.14
3	A	2474	FMN	C4A-C4-N3	-3.98	117.99	123.43
3	A	2474	FMN	C4-C4A-C10	3.80	122.46	119.95
3	A	2474	FMN	O3P-P-O1P	-3.75	95.99	110.68
3	A	2474	FMN	C4'-C3'-C2'	-3.75	105.57	113.36
3	B	2474	FMN	C4-N3-C2	3.72	118.28	115.14
3	A	2474	FMN	C1'-N10-C9A	-3.68	115.39	118.29
3	B	2474	FMN	C4A-C4-N3	-3.62	118.48	123.43
3	B	2474	FMN	O3P-P-O2P	-3.56	94.03	107.64
2	B	2473	OMT	CE-SD-CG	3.34	118.08	105.21
3	B	2474	FMN	C8M-C8-C7	-3.29	114.00	120.74
2	A	2473	OMT	OD2-SD-OD1	-3.24	110.16	117.09
2	A	2473	OMT	OD1-SD-CE	-3.24	105.65	108.91
3	B	2474	FMN	O2'-C2'-C1'	-3.11	102.10	109.59
3	B	2474	FMN	O3P-P-O5'	2.96	114.60	106.73
3	B	2474	FMN	O2P-P-O5'	2.92	114.51	106.73
3	A	2474	FMN	C9A-C5A-N5	-2.76	118.04	122.36
3	B	2474	FMN	C4A-C10-N10	-2.74	117.48	120.30
3	A	2474	FMN	C4A-C10-N10	-2.66	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2474	FMN	C8M-C8-C9	2.53	126.41	120.34
3	B	2474	FMN	C5A-C9A-N10	2.47	119.50	117.72
4	A	2475	AKG	C3-C4-C5	2.44	116.77	112.67
3	A	2474	FMN	O3P-P-O2P	2.23	116.16	107.64
3	A	2474	FMN	C6-C5A-N5	2.19	121.47	119.05
3	B	2474	FMN	C4-C4A-N5	-2.18	116.10	118.60
3	A	2474	FMN	O2'-C2'-C1'	-2.15	104.42	109.59
3	A	2474	FMN	C5'-C4'-C3'	2.09	116.24	112.20
3	B	2474	FMN	O2'-C2'-C3'	2.06	114.10	109.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2474	FMN	C2'-C3'-C4'-O4'
3	B	2474	FMN	O3'-C3'-C4'-O4'
2	A	2473	OMT	C-CA-CB-CG
2	A	2473	OMT	CB-CG-SD-OD1
2	A	2473	OMT	CB-CG-SD-OD2
3	A	2474	FMN	O4'-C4'-C5'-O5'
3	A	2474	FMN	C5'-O5'-P-O1P
3	A	2474	FMN	C5'-O5'-P-O3P
2	B	2473	OMT	N-CA-CB-CG
2	B	2473	OMT	C-CA-CB-CG
2	B	2473	OMT	CB-CG-SD-OD1
2	B	2473	OMT	CB-CG-SD-OD2
3	A	2474	FMN	O3'-C3'-C4'-O4'
3	A	2474	FMN	C2'-C3'-C4'-O4'
3	B	2474	FMN	O3'-C3'-C4'-C5'
3	A	2474	FMN	O3'-C3'-C4'-C5'
3	B	2474	FMN	C2'-C3'-C4'-C5'
3	A	2474	FMN	C2'-C3'-C4'-C5'
2	A	2473	OMT	CB-CG-SD-CE
2	B	2473	OMT	CB-CG-SD-CE
4	B	2475	AKG	C2-C3-C4-C5
3	B	2474	FMN	C5'-O5'-P-O2P
2	A	2473	OMT	CA-CB-CG-SD

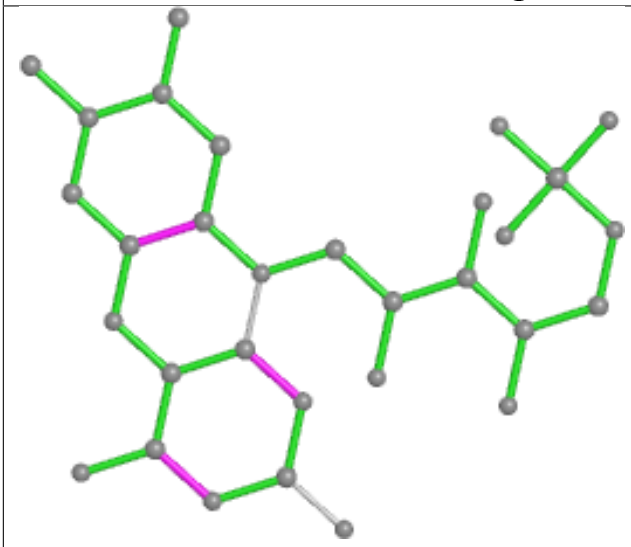
There are no ring outliers.

7 monomers are involved in 20 short contacts:

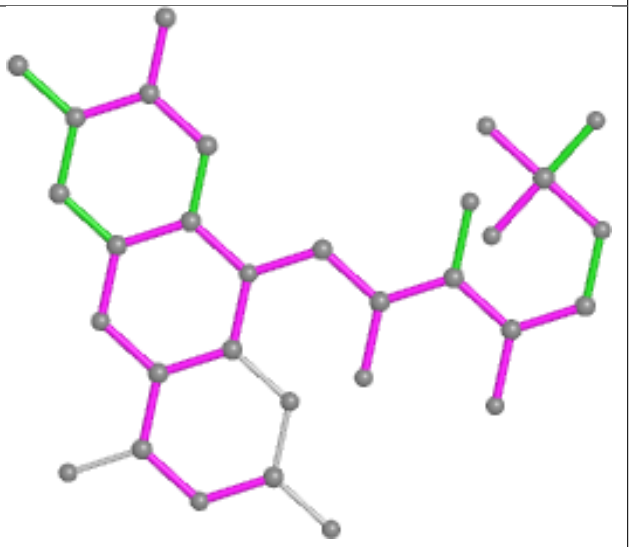
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2475	AKG	2	0
5	B	2476	F3S	3	0
3	B	2474	FMN	6	0
2	A	2473	OMT	2	0
3	A	2474	FMN	4	0
5	A	2476	F3S	2	0
2	B	2473	OMT	1	0

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

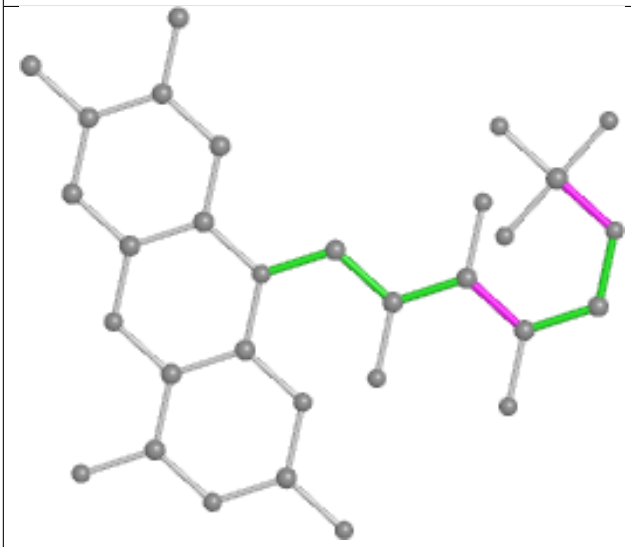
Ligand FMN B 2474



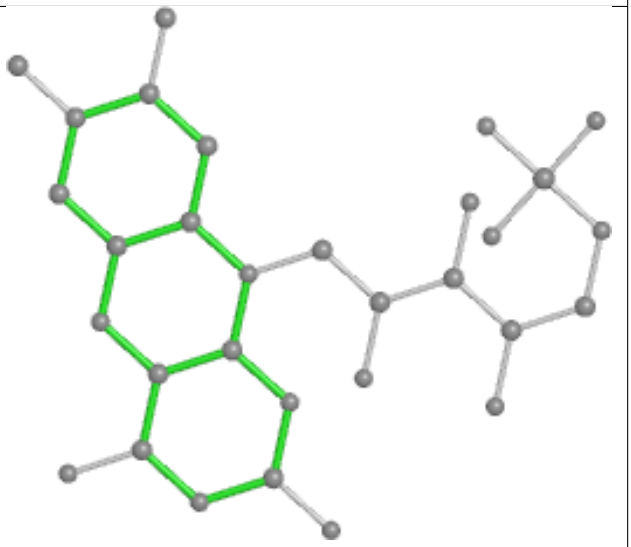
Bond lengths



Bond angles

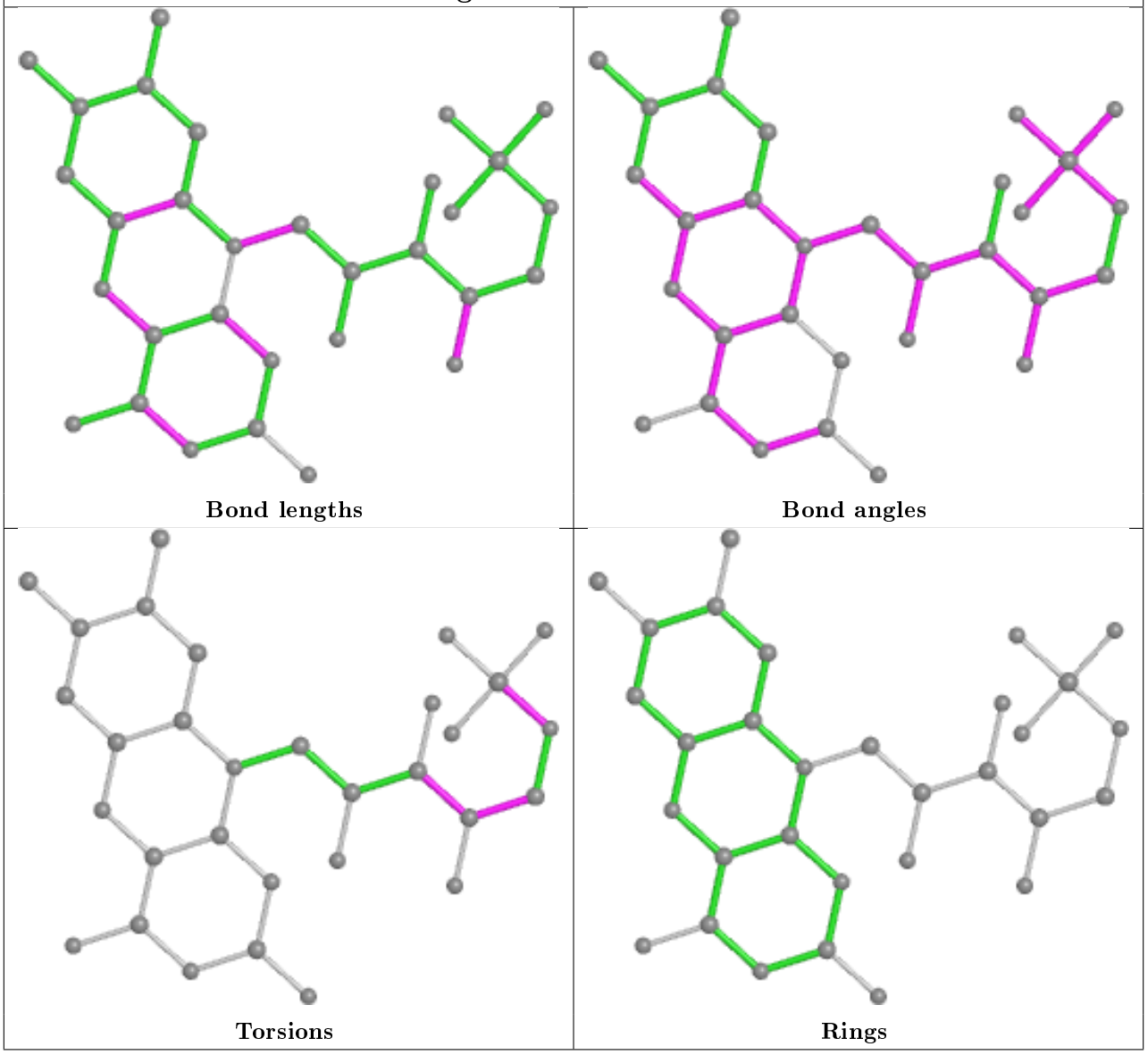


Torsions



Rings

Ligand FMN A 2474



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.