



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:17 pm BST

PDB ID : 1DXL
Title : Dihydrolipoamide dehydrogenase of glycine decarboxylase from *Pisum Sativum*
Authors : Faure, M.; Cohen-Addad, C.; Bourguignon, J.; Macherel, D.; Neuburger, M.; Douce, R.
Deposited on : 2000-01-10
Resolution : 3.15 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

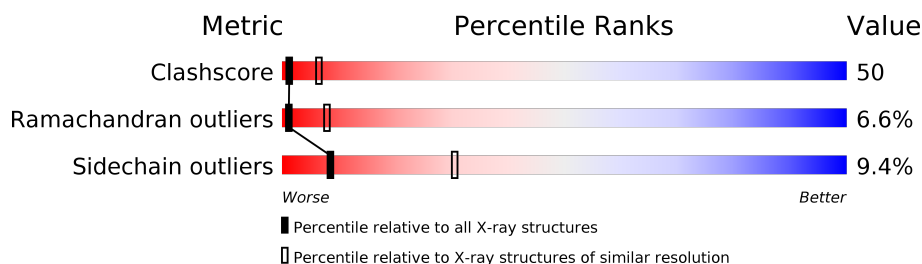
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	470	<div> <div>37%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>
1	B	470	<div> <div>39%</div> <div>50%</div> <div>10%</div> <div>..</div> </div>
1	C	470	<div> <div>36%</div> <div>51%</div> <div>11%</div> <div>.</div> </div>
1	D	470	<div> <div>40%</div> <div>49%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14240 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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	48	1	0
			3487	2203	591	677	16			
1	B	467	Total	C	N	O	S	50	1	0
			3487	2203	591	677	16			
1	C	467	Total	C	N	O	S	77	0	0
			3475	2194	590	675	16			
1	D	467	Total	C	N	O	S	38	0	0
			3475	2194	590	675	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	HIS	ASN	conflict	UNP P31023
B	449	HIS	ASN	conflict	UNP P31023
C	449	HIS	ASN	conflict	UNP P31023
D	449	HIS	ASN	conflict	UNP P31023

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



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

- Molecule 3 is water.

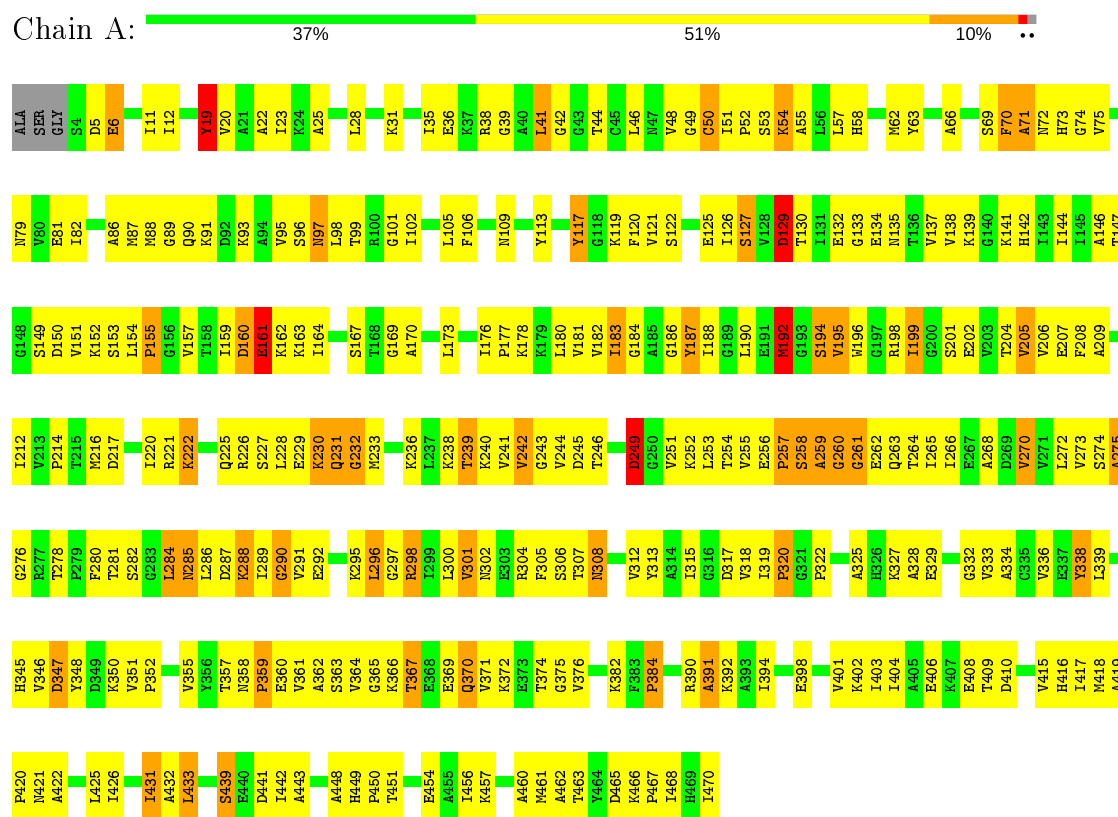
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	23	Total	O	0	0
			23	23		
3	C	25	Total	O	0	0
			25	25		
3	D	23	Total	O	0	0
			23	23		

3 Residue-property plots

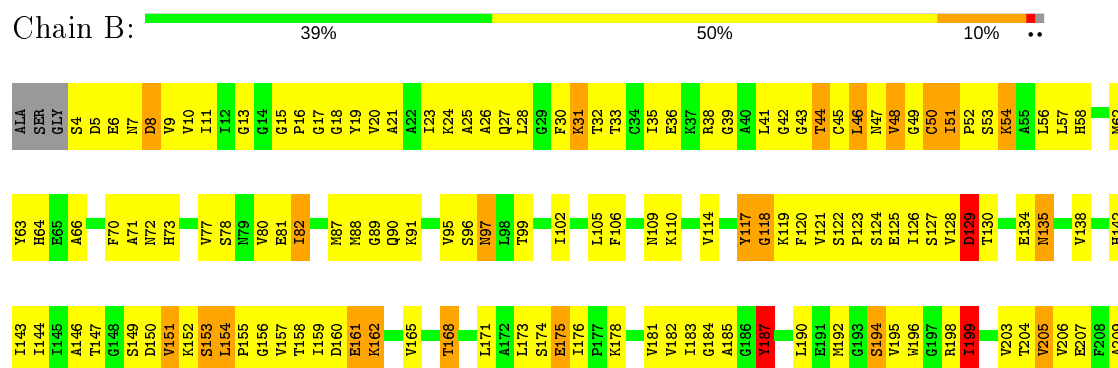
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

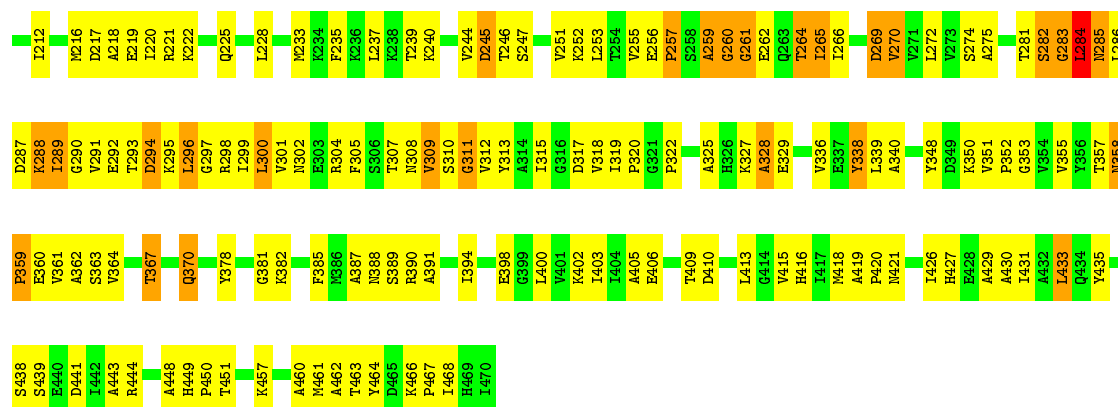
Note EDS was not executed.

• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



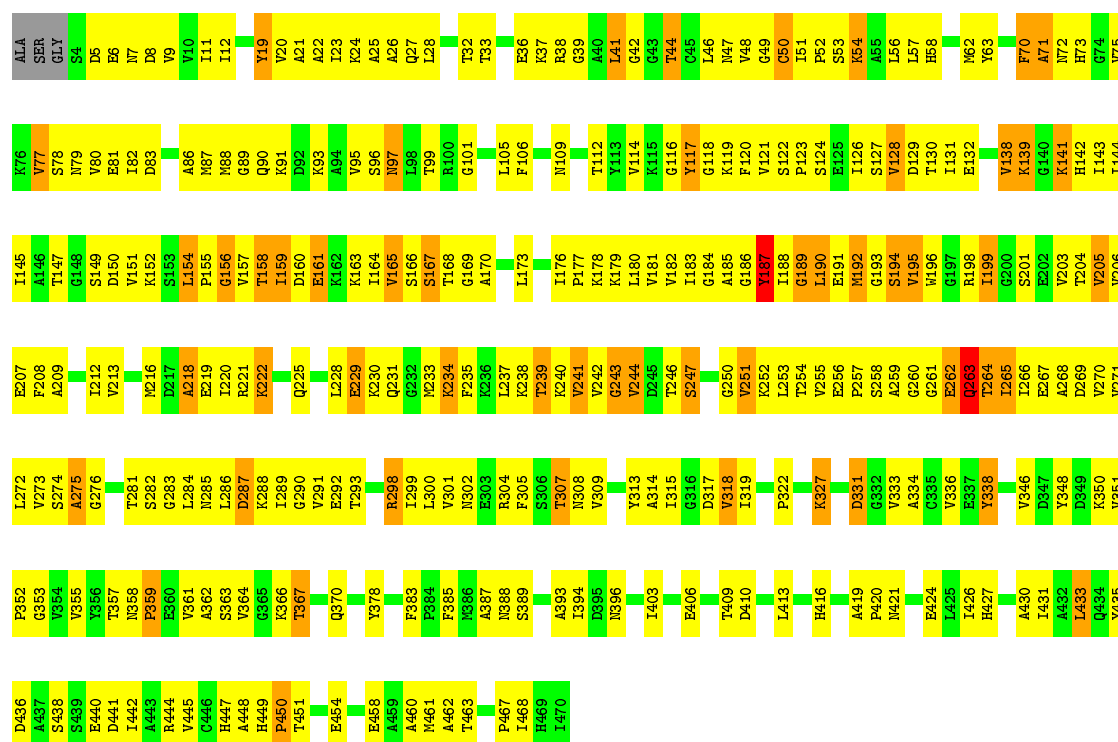
• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE





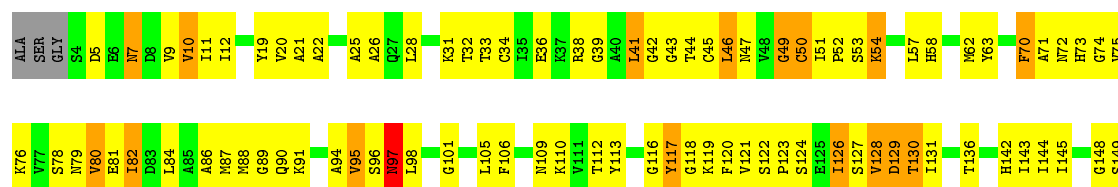
• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain C: 36% 51% 11%



• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain D: 40% 49% 9%



H449	E368	V301	T220	D150
P450	E369	N302	K221	K151
T451	E370	E303	K222	K152
H452	V371	R304		S153
S453		F305		L154
	V376		Q225	P155
T456	E377		E226	G156
K457		N308	S227	V157
E458	F383	V309	L228	T158
A459	P384	S310	E229	I159
A460	F385	G311	K230	D160
H461	M386	V312	Q231	E161
A462		Y313		K162
T463	A314	A314	K234	K163
Y464	I315	I315		I164
D465		V318	L237	V165
K466	I384	I319	K238	S166
P467		P320	T239	S167
L468	E398	E321	K240	
H469	G399	G322	V241	L171
I470	A400	P322	G243	
	V401			I176
	K402	A325	D249	P177
	L403	H326		
	L404	K327		L180
	A405	A328	L253	V181
	E406	E329	T254	V182
		E330	V255	I183
		D331		G184
T409		G332	E262	A185
D410		V333	Q263	G186
		A334	T264	Y187
	L413	C335	L265	
V415	G414	V336		L190
H416	V415	E337	V270	E391
L417	H416	Y338		M192
M418	L417	L339	V273	G193
A419			S274	S194
P420	H345	H345	A275	V195
N421	V346	V346	G276	V196
A422	D421	D421	R277	
	A422	Y348	T278	
	G423	D349	P279	I199
E424	E424	K350	F280	G200
L425	L425	V351		S201
I426	P426	P352	G283	E202
H427	E427	G353	L284	V203
A428	E428	V354	N285	T204
A429	A429	V355	L286	V205
A430	A430	T356	D287	V206
I431	A431	T357	K288	E207
A432	A432	N358	I289	F208
L433	L433	P359	G290	A209
		E360	V291	
S438	S438	V361	E292	T212
E440	E440	A362	T293	V213
D441	S363	S363	D294	
I442		V364	K295	D216
		G365		M217
		K366	R298	A218
A448	A448	T367		E210

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.56Å 108.33Å 202.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.15	Depositor
% Data completeness (in resolution range)	86.1 (15.00-3.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.226 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14240	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	0/3541	1.02	7/4783 (0.1%)
1	B	0.73	0/3541	0.95	6/4783 (0.1%)
1	C	0.79	1/3527 (0.0%)	0.97	3/4762 (0.1%)
1	D	0.77	0/3528	0.97	3/4765 (0.1%)
All	All	0.78	1/14137 (0.0%)	0.98	19/19093 (0.1%)

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	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	GLN	C-N	-6.04	1.20	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	LYS	N-CA-C	6.75	129.24	111.00
1	B	260	GLY	N-CA-C	-5.86	98.44	113.10
1	B	294	ASP	N-CA-C	5.82	126.70	111.00
1	D	31	LYS	N-CA-C	-5.80	95.35	111.00
1	B	44	THR	N-CA-C	-5.78	95.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	MET	CG-SD-CE	5.77	109.43	100.20
1	A	284	LEU	N-CA-C	-5.65	95.75	111.00
1	A	161	GLU	N-CA-C	-5.60	95.88	111.00
1	D	237	LEU	N-CA-C	5.59	126.08	111.00
1	C	331	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	31	LYS	N-CA-C	-5.45	96.28	111.00
1	D	152	LYS	N-CA-C	-5.43	96.35	111.00
1	C	359	PRO	N-CA-C	-5.35	98.19	112.10
1	A	285	ASN	N-CA-C	-5.23	96.87	111.00
1	A	431	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	B	359	PRO	N-CA-C	-5.08	98.90	112.10
1	C	47	ASN	N-CA-C	5.03	124.59	111.00
1	A	202	GLU	N-CA-C	-5.01	97.48	111.00
1	A	359	PRO	N-CA-C	-5.01	99.08	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	B	187[A]	TYR	Sidechain
1	C	263	GLN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	3552	334	0
1	B	3487	0	3552	362	0
1	C	3475	0	3543	422	0
1	D	3475	0	3544	327	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
2	D	53	0	31	3	0
3	A	33	0	0	2	0
3	B	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	25	0	0	6	0
3	D	23	0	0	6	0
All	All	14240	0	14315	1399	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 50.

All (1399) 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:322:PRO:HG2	1:B:327:LYS:HG3	1.25	1.18
1:C:254:THR:HG23	1:C:265:ILE:HD11	1.25	1.18
1:D:243:GLY:HA3	1:D:254:THR:HB	1.25	1.13
1:A:12:ILE:HD11	1:A:126:ILE:CD1	1.81	1.11
1:B:147:THR:HG21	1:B:284:LEU:HD22	1.15	1.11
1:C:212:ILE:HG21	1:C:235:PHE:CE2	1.89	1.07
1:C:180:LEU:HD12	1:C:270:VAL:O	1.56	1.05
1:B:239:THR:HA	1:B:257:PRO:HA	1.37	1.03
1:C:51:ILE:HB	1:C:52:PRO:HD3	1.39	1.02
1:B:120:PHE:HA	1:B:126:ILE:HG22	1.39	1.02
1:C:118:GLY:HA2	1:C:127:SER:O	1.58	1.01
1:C:262:GLU:O	1:C:263:GLN:HB2	1.59	1.01
1:B:82:ILE:N	1:B:82:ILE:HD12	1.74	1.01
1:D:364:VAL:HG23	1:D:426:ILE:HD11	1.44	0.99
1:C:117:TYR:O	1:C:128:VAL:HA	1.63	0.97
1:D:192:MET:HA	1:D:192:MET:HE3	1.43	0.97
1:A:117:TYR:HB3	1:A:129:ASP:HB2	1.45	0.97
1:B:308:ASN:O	1:B:309:VAL:HG23	1.63	0.97
1:C:462:ALA:HA	1:C:467:PRO:HD3	1.48	0.96
1:A:358:ASN:HB3	1:A:359:PRO:HD3	1.45	0.95
1:C:192:MET:HA	1:C:192:MET:HE3	1.48	0.95
1:C:182:VAL:HB	1:C:205:VAL:HG13	1.44	0.95
1:C:250:GLY:O	1:C:251:VAL:HG23	1.65	0.95
1:C:257:PRO:HG2	1:C:260:GLY:O	1.67	0.95
1:A:157:VAL:HG13	1:A:244:VAL:HG21	1.46	0.94
1:C:123:PRO:HG3	1:C:289:ILE:HG22	1.46	0.94
1:D:448:ALA:O	1:D:451:THR:HG23	1.67	0.94
1:A:192:MET:HA	1:A:192:MET:CE	1.97	0.94
1:A:355:VAL:HG12	1:A:357:THR:HG23	1.48	0.94
1:B:228:LEU:HD13	1:B:233:MET:HE3	1.49	0.94
1:C:242:VAL:HG21	1:C:256:GLU:H	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD11	1:A:126:ILE:HD11	1.47	0.93
1:B:367:THR:HG23	1:B:370:GLN:NE2	1.84	0.93
1:A:160:ASP:O	1:A:161:GLU:HG3	1.68	0.93
1:C:258:SER:C	1:C:259:ALA:N	2.22	0.93
1:D:242:VAL:HG23	1:D:254:THR:HG22	1.50	0.93
1:C:152:LYS:HB2	1:C:276:GLY:O	1.69	0.93
1:A:296:LEU:HD23	1:A:296:LEU:N	1.83	0.92
1:C:164:ILE:HD11	1:C:251:VAL:HG11	1.52	0.92
1:C:88:MET:HB3	3:C:2007:HOH:O	1.69	0.92
1:C:242:VAL:HB	1:C:255:VAL:HA	1.52	0.91
1:A:241:VAL:HG23	1:A:241:VAL:O	1.70	0.91
1:C:180:LEU:O	1:C:203:VAL:HA	1.69	0.91
1:C:63:TYR:CZ	1:C:82:ILE:HD11	2.05	0.91
1:D:284:LEU:HD12	1:D:285:ASN:H	1.36	0.91
1:D:161:GLU:HA	1:D:165:VAL:HG12	1.53	0.90
1:A:6:GLU:OE2	1:A:141:LYS:HE2	1.71	0.90
1:C:367:THR:H	1:C:370:GLN:HE21	1.20	0.89
1:A:12:ILE:HD11	1:A:126:ILE:HD13	1.49	0.89
1:D:81:GLU:C	1:D:82:ILE:HD12	1.93	0.88
1:B:300:LEU:HD22	1:B:300:LEU:H	1.37	0.88
1:B:117:TYR:CE2	1:B:283:GLY:HA3	2.09	0.87
1:B:35:ILE:HD11	1:B:138:VAL:HG21	1.55	0.87
1:C:212:ILE:HD13	1:C:235:PHE:HE2	1.38	0.87
1:B:192:MET:HE3	1:B:192:MET:HA	1.56	0.86
1:D:117:TYR:CE2	1:D:283:GLY:HA3	2.10	0.86
1:A:192:MET:HE3	1:A:192:MET:HA	1.55	0.86
1:C:165:VAL:HG23	1:C:272:LEU:HA	1.58	0.85
1:B:367:THR:H	1:B:370:GLN:HE21	1.21	0.85
1:C:427:HIS:O	1:C:431:ILE:HG22	1.76	0.85
1:D:38:ARG:HD3	1:D:47:ASN:ND2	1.92	0.85
1:C:286:LEU:HD22	1:C:291:VAL:HB	1.59	0.85
1:C:212:ILE:HG21	1:C:235:PHE:HE2	1.39	0.84
1:A:284:LEU:HD23	1:A:285:ASN:H	1.41	0.84
1:C:119:LYS:HB3	1:C:127:SER:HB3	1.58	0.84
1:B:9:VAL:HG23	1:B:30:PHE:HB3	1.60	0.84
1:C:364:VAL:HG23	1:C:426:ILE:HD11	1.59	0.84
1:D:129:ASP:O	1:D:130:THR:HG23	1.78	0.84
1:B:153:SER:O	1:B:154:LEU:HB2	1.78	0.84
1:D:54:LYS:HA	1:D:57:LEU:HD12	1.59	0.84
1:B:4:SER:HB2	3:B:2001:HOH:O	1.78	0.83
1:C:78:SER:HB2	1:D:78:SER:HB2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:SER:HA	1:A:230:LYS:HD3	1.58	0.83
1:A:322:PRO:HG2	1:A:327:LYS:HG3	1.58	0.83
1:B:147:THR:HG21	1:B:284:LEU:CD2	2.06	0.83
1:B:154:LEU:HG	1:B:155:PRO:HD2	1.60	0.83
1:D:43:GLY:O	3:D:2001:HOH:O	1.95	0.83
1:B:117:TYR:HE2	1:B:283:GLY:HA3	1.42	0.83
1:C:192:MET:HA	1:C:192:MET:CE	2.08	0.83
1:D:120:PHE:HD1	1:D:284:LEU:HD11	1.41	0.82
1:D:364:VAL:HG23	1:D:426:ILE:CD1	2.08	0.82
1:C:63:TYR:CE1	1:C:82:ILE:HD11	2.14	0.82
1:A:448:ALA:O	1:A:451:THR:HG23	1.80	0.82
1:D:117:TYR:CZ	1:D:283:GLY:HA3	2.15	0.82
1:A:41:LEU:HD11	1:A:106:PHE:CE1	2.16	0.81
1:C:50:CYS:O	1:C:54:LYS:HE2	1.80	0.81
1:C:212:ILE:HD13	1:C:235:PHE:CE2	2.15	0.81
1:D:82:ILE:N	1:D:82:ILE:HD12	1.93	0.81
1:A:284:LEU:HD23	1:A:285:ASN:N	1.96	0.80
1:A:367:THR:HG23	1:A:370:GLN:NE2	1.97	0.80
1:B:253:LEU:HB2	1:B:266:ILE:HB	1.61	0.80
1:A:251:VAL:N	1:A:268:ALA:O	2.13	0.80
1:C:242:VAL:CG2	1:C:256:GLU:H	1.94	0.80
1:B:10:VAL:HB	1:B:143:ILE:HG12	1.63	0.80
1:A:364:VAL:HG23	1:A:426:ILE:CD1	2.11	0.80
1:A:367:THR:H	1:A:370:GLN:HE21	1.30	0.80
1:A:121:VAL:HA	1:A:288:LYS:NZ	1.96	0.80
1:A:355:VAL:CG1	1:A:357:THR:HG23	2.11	0.80
1:D:383:PHE:CD1	1:D:458:GLU:HB3	2.16	0.80
1:B:28:LEU:HD12	1:B:336:VAL:HG12	1.64	0.79
1:B:358:ASN:HB3	1:B:359:PRO:HD3	1.64	0.79
1:C:139:LYS:HD2	1:C:139:LYS:H	1.47	0.79
1:D:41:LEU:HD11	1:D:106:PHE:CE1	2.17	0.79
1:A:49:GLY:O	1:A:53:SER:CB	2.31	0.79
1:A:119:LYS:HG2	1:A:285:ASN:CG	2.03	0.79
1:B:129:ASP:HB3	1:B:135:ASN:OD1	1.83	0.79
1:C:204:THR:HA	1:C:233:MET:O	1.83	0.79
1:C:253:LEU:HB2	1:C:266:ILE:HB	1.65	0.79
1:D:42:GLY:HA3	1:D:46:LEU:HB3	1.64	0.79
1:B:184:GLY:HA3	1:B:274:SER:O	1.83	0.79
1:C:154:LEU:HD12	1:C:156:GLY:H	1.48	0.79
1:B:300:LEU:CD2	1:B:300:LEU:H	1.95	0.78
1:D:439:SER:O	1:D:442:ILE:HG22	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:HG22	1:B:257:PRO:HB3	1.64	0.78
1:C:176:ILE:HD13	1:C:199:ILE:HG23	1.64	0.78
1:C:204:THR:HG22	1:C:234:LYS:HB2	1.64	0.78
1:D:449:HIS:CE1	1:D:450:PRO:HB3	2.18	0.78
1:D:117:TYR:HB3	1:D:129:ASP:OD1	1.84	0.78
1:A:28:LEU:HD12	1:A:336:VAL:HG12	1.66	0.78
1:C:254:THR:CG2	1:C:265:ILE:HD11	2.10	0.78
1:D:51:ILE:HB	1:D:52:PRO:HD3	1.66	0.78
1:B:216:MET:HE1	1:B:221:ARG:HA	1.65	0.78
1:B:269:ASP:O	1:B:270:VAL:HG23	1.83	0.78
1:B:48:VAL:CG1	1:B:168:THR:HG23	2.14	0.78
1:C:427:HIS:HA	1:C:430:ALA:HB3	1.64	0.78
1:B:48:VAL:HG11	1:B:168:THR:HG23	1.64	0.78
1:D:50:CYS:O	1:D:54:LYS:HE2	1.84	0.78
1:A:95:VAL:O	1:A:99:THR:HG23	1.84	0.78
1:C:165:VAL:N	1:C:271:VAL:O	2.17	0.78
1:D:309:VAL:O	1:D:312:VAL:HG23	1.84	0.78
1:C:261:GLY:O	1:C:262:GLU:CB	2.30	0.77
1:B:129:ASP:HA	1:B:135:ASN:HA	1.64	0.77
1:A:120:PHE:HB2	1:A:285:ASN:O	1.83	0.77
1:C:152:LYS:HB2	1:C:276:GLY:C	2.05	0.77
1:A:239:THR:HG22	1:A:255:VAL:HG22	1.66	0.77
1:C:154:LEU:HD11	1:C:241:VAL:HG11	1.66	0.77
1:A:63:TYR:CZ	1:A:82:ILE:HD11	2.20	0.77
1:B:82:ILE:N	1:B:82:ILE:CD1	2.46	0.77
1:C:126:ILE:CD1	1:C:143:ILE:HD13	2.15	0.77
1:A:298:ARG:HB2	1:A:320:PRO:HD3	1.67	0.76
1:B:123:PRO:HG3	1:B:289:ILE:HG21	1.67	0.76
1:B:16:PRO:O	1:B:20:VAL:HG23	1.85	0.76
1:C:187:TYR:HD1	1:C:188:ILE:H	1.30	0.76
1:A:119:LYS:HG2	1:A:285:ASN:ND2	2.00	0.76
1:A:371:VAL:HG21	1:A:404:ILE:HG21	1.65	0.76
1:C:240:LYS:H	1:C:255:VAL:HG11	1.50	0.76
1:D:10:VAL:CG2	1:D:143:ILE:HG12	2.15	0.75
1:D:49:GLY:O	1:D:53:SER:HB3	1.86	0.75
1:A:259:ALA:O	1:A:261:GLY:N	2.19	0.75
1:A:245:ASP:HB2	1:A:252:LYS:HB3	1.69	0.75
1:B:15:GLY:HA2	1:B:43:GLY:CA	2.17	0.75
1:C:242:VAL:HG21	1:C:256:GLU:N	2.01	0.75
1:B:82:ILE:H	1:B:82:ILE:HD12	1.50	0.75
1:C:126:ILE:HD11	1:C:143:ILE:HG21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLU:O	1:D:162:LYS:HG3	1.87	0.74
1:C:243:GLY:O	1:C:254:THR:HB	1.88	0.74
1:D:86:ALA:O	1:D:89:GLY:N	2.20	0.74
1:B:51:ILE:HB	1:B:52:PRO:HD3	1.67	0.74
1:D:239:THR:HB	1:D:255:VAL:CG1	2.17	0.74
1:B:295:LYS:C	1:B:297:GLY:H	1.90	0.74
1:C:394:ILE:HD12	1:D:58:HIS:CG	2.23	0.74
1:B:54:LYS:HA	1:B:57:LEU:HD12	1.69	0.74
1:D:142:HIS:ND1	3:D:2004:HOH:O	2.21	0.73
1:D:358:ASN:HB3	1:D:359:PRO:HD3	1.68	0.73
1:C:117:TYR:N	1:C:128:VAL:HG13	2.03	0.73
1:D:217:ASP:HB2	1:D:416:HIS:CD2	2.23	0.73
1:A:121:VAL:HA	1:A:288:LYS:HZ2	1.54	0.73
1:B:119:LYS:O	1:B:127:SER:N	2.20	0.73
1:A:239:THR:CG2	1:A:255:VAL:HG22	2.18	0.73
1:B:176:ILE:HD13	1:B:199:ILE:HG23	1.70	0.73
1:C:242:VAL:HG21	1:C:256:GLU:HB3	1.70	0.73
1:C:42:GLY:HA3	1:C:46:LEU:HB3	1.70	0.73
1:D:44:THR:HA	3:D:2001:HOH:O	1.88	0.73
1:A:12:ILE:CD1	1:A:126:ILE:HD13	2.19	0.72
1:A:121:VAL:HG21	1:A:127:SER:HB2	1.72	0.72
1:C:367:THR:HG23	1:C:370:GLN:NE2	2.04	0.72
1:A:42:GLY:HA3	1:A:46:LEU:HB3	1.69	0.72
1:B:171:LEU:HD23	1:B:192:MET:HE1	1.70	0.72
1:C:355:VAL:HG12	1:C:357:THR:HG23	1.72	0.72
1:B:183:ILE:O	1:B:206:VAL:O	2.06	0.72
1:B:23:ILE:HG23	1:B:109:ASN:ND2	2.04	0.72
1:B:8:ASP:HB2	1:B:31:LYS:O	1.90	0.72
1:C:164:ILE:HG13	1:C:271:VAL:HB	1.71	0.72
1:A:119:LYS:HG2	1:A:285:ASN:CB	2.19	0.72
1:B:244:VAL:HG12	1:B:245:ASP:H	1.53	0.72
1:C:154:LEU:CD1	1:C:156:GLY:H	2.03	0.72
1:C:187:TYR:HD1	1:C:188:ILE:N	1.88	0.72
1:C:198:ARG:O	3:C:2010:HOH:O	2.07	0.72
1:C:184:GLY:HA3	1:C:274:SER:O	1.88	0.72
1:C:264:THR:HG22	1:C:265:ILE:H	1.55	0.72
1:D:12:ILE:HD11	1:D:126:ILE:HD11	1.72	0.72
1:B:294:ASP:H	1:B:300:LEU:HD21	1.54	0.72
1:C:251:VAL:O	1:C:268:ALA:O	2.08	0.71
1:A:291:VAL:HA	1:A:308:ASN:HD21	1.55	0.71
1:A:5:ASP:CB	1:A:31:LYS:HE2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:GLY:HA2	1:D:127:SER:O	1.90	0.71
1:B:367:THR:N	1:B:370:GLN:HE21	1.89	0.71
1:C:165:VAL:O	1:C:272:LEU:HD12	1.90	0.71
1:A:367:THR:HG23	1:A:370:GLN:HE21	1.55	0.71
1:B:322:PRO:CG	1:B:327:LYS:HG3	2.15	0.71
1:C:54:LYS:HA	1:C:57:LEU:HD12	1.72	0.71
1:A:86:ALA:O	1:A:89:GLY:N	2.23	0.71
1:D:243:GLY:CA	1:D:254:THR:HB	2.14	0.71
1:A:403:ILE:HG23	1:A:415:VAL:HG22	1.72	0.70
1:C:150:ASP:CG	1:C:151:VAL:H	1.94	0.70
1:C:286:LEU:HD22	1:C:291:VAL:CB	2.20	0.70
1:A:346:VAL:O	1:A:347:ASP:HB2	1.89	0.70
1:A:5:ASP:CA	1:A:31:LYS:HE2	2.22	0.70
1:B:151:VAL:HG12	1:B:152:LYS:N	2.06	0.70
1:B:284:LEU:CD1	1:B:286:LEU:HD11	2.22	0.70
1:B:50:CYS:O	1:B:53:SER:HB3	1.92	0.70
1:A:241:VAL:CG2	1:A:241:VAL:O	2.40	0.70
1:C:42:GLY:HA3	1:C:46:LEU:HD23	1.72	0.70
1:A:49:GLY:O	1:A:53:SER:HB3	1.91	0.69
1:B:438:SER:O	1:B:441:ASP:HB2	1.92	0.69
1:C:42:GLY:CA	1:C:46:LEU:HD23	2.20	0.69
1:A:119:LYS:HG2	1:A:285:ASN:HB2	1.73	0.69
1:B:292:GLU:C	1:B:300:LEU:HD23	2.12	0.69
1:B:427:HIS:O	1:B:431:ILE:HG22	1.92	0.69
1:C:362:ALA:HB1	1:C:426:ILE:HD12	1.74	0.69
1:A:183:ILE:HG22	1:A:184:GLY:N	2.05	0.69
1:A:5:ASP:HB3	1:A:31:LYS:HE2	1.75	0.69
1:B:15:GLY:HA2	1:B:43:GLY:HA2	1.75	0.69
1:C:183:ILE:O	1:C:206:VAL:O	2.09	0.69
1:B:304:ARG:HA	1:B:338:TYR:CE1	2.28	0.69
1:B:294:ASP:N	1:B:300:LEU:HD21	2.07	0.69
1:A:164:ILE:HD11	1:A:244:VAL:HG11	1.74	0.69
1:B:362:ALA:HB1	1:B:426:ILE:HD12	1.75	0.69
1:C:300:LEU:HD23	1:C:301:VAL:N	2.07	0.69
1:A:51:ILE:HB	1:A:52:PRO:HD3	1.74	0.69
1:C:229:GLU:O	1:C:231:GLN:N	2.25	0.69
1:C:86:ALA:O	1:C:89:GLY:N	2.23	0.69
1:A:55:ALA:HB1	1:A:90:GLN:HE22	1.58	0.69
1:A:246:THR:HG22	1:A:251:VAL:HG22	1.75	0.69
1:C:117:TYR:N	1:C:128:VAL:CG1	2.55	0.69
1:C:358:ASN:HB3	1:C:359:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:CD	1:A:141:LYS:HE2	2.13	0.69
1:A:82:ILE:N	1:A:82:ILE:HD12	2.08	0.68
1:C:261:GLY:O	1:C:262:GLU:HB2	1.93	0.68
1:C:88:MET:HE3	3:C:2007:HOH:O	1.93	0.68
1:D:345:HIS:ND1	1:D:345:HIS:O	2.26	0.68
1:C:216:MET:HE1	1:C:221:ARG:HA	1.74	0.68
1:D:183:ILE:HG22	1:D:184:GLY:N	2.08	0.68
1:C:393:ALA:HB2	1:D:51:ILE:HG23	1.74	0.68
1:A:367:THR:N	1:A:370:GLN:HE21	1.92	0.68
1:C:141:LYS:HB3	1:C:142:HIS:CE1	2.28	0.68
1:A:35:ILE:HD11	1:A:138:VAL:HG11	1.75	0.68
1:A:130:THR:HG23	1:A:133:GLY:N	2.08	0.68
1:B:185:ALA:CB	1:B:207:GLU:HB2	2.24	0.68
1:D:63:TYR:CZ	1:D:82:ILE:HD11	2.28	0.68
1:A:48:VAL:HG12	1:A:48:VAL:O	1.93	0.68
1:C:262:GLU:O	1:C:263:GLN:CB	2.33	0.68
1:C:282:SER:C	1:C:284:LEU:H	1.96	0.68
1:A:364:VAL:HG23	1:A:426:ILE:HD11	1.76	0.68
1:D:367:THR:HG23	1:D:370:GLN:HE21	1.57	0.68
1:B:462:ALA:HB2	1:B:467:PRO:HG3	1.73	0.67
1:C:12:ILE:HD11	1:C:126:ILE:HD13	1.75	0.67
1:C:364:VAL:HG23	1:C:426:ILE:CD1	2.23	0.67
1:D:9:VAL:HB	1:D:32:THR:HG23	1.74	0.67
1:C:139:LYS:N	1:C:139:LYS:HD2	2.08	0.67
1:D:284:LEU:CD1	1:D:285:ASN:H	2.07	0.67
1:D:121:VAL:CG2	1:D:127:SER:HB2	2.25	0.67
1:A:120:PHE:N	1:A:285:ASN:HB2	2.10	0.67
1:A:48:VAL:CG1	1:A:48:VAL:O	2.43	0.67
1:B:151:VAL:HG12	1:B:152:LYS:H	1.59	0.67
1:C:203:VAL:CG2	1:C:233:MET:HG3	2.25	0.67
1:C:51:ILE:HB	1:C:52:PRO:CD	2.18	0.67
1:D:161:GLU:OE1	1:D:165:VAL:HB	1.95	0.67
1:B:300:LEU:HD22	1:B:300:LEU:N	2.08	0.66
1:B:367:THR:HG23	1:B:370:GLN:HE21	1.61	0.66
1:D:96:SER:O	1:D:97:ASN:C	2.33	0.66
1:C:289:ILE:HG13	1:C:290:GLY:H	1.59	0.66
1:D:120:PHE:HD1	1:D:284:LEU:CD1	2.07	0.66
1:B:158:THR:O	1:B:160:ASP:N	2.29	0.66
1:C:163:LYS:O	1:C:270:VAL:HG13	1.95	0.66
1:D:180:LEU:O	1:D:203:VAL:HA	1.95	0.66
1:D:36:GLU:OE2	2:D:480:FAD:H4B	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:HIS:CG	1:B:394:ILE:HD12	2.30	0.66
1:C:157:VAL:HG12	1:C:158:THR:H	1.60	0.66
1:D:286:LEU:HA	1:D:289:ILE:HG13	1.76	0.66
1:A:187[B]:TYR:CD2	1:A:355:VAL:HG22	2.31	0.66
1:A:367:THR:H	1:A:370:GLN:HG3	1.61	0.66
1:D:91:LYS:O	1:D:94:ALA:HB3	1.96	0.66
1:A:125:GLU:HB2	1:A:139:LYS:HG2	1.78	0.66
1:C:367:THR:HG23	1:C:370:GLN:HE21	1.60	0.66
1:A:366:LYS:HA	1:A:370:GLN:NE2	2.11	0.65
1:C:254:THR:HA	1:C:265:ILE:CD1	2.26	0.65
1:A:284:LEU:CD2	1:A:285:ASN:N	2.60	0.65
1:A:394:ILE:HD12	1:B:58:HIS:CG	2.31	0.65
1:C:239:THR:HG22	1:C:255:VAL:HG12	1.76	0.65
1:D:448:ALA:O	1:D:451:THR:CG2	2.44	0.65
1:A:130:THR:HG23	1:A:133:GLY:H	1.62	0.65
1:B:38:ARG:HD3	1:B:47:ASN:ND2	2.12	0.65
1:D:273:VAL:HG12	1:D:273:VAL:O	1.96	0.65
1:A:58:HIS:O	1:A:62:MET:HG3	1.96	0.65
1:C:240:LYS:H	1:C:255:VAL:CG1	2.10	0.65
1:C:145:ILE:N	1:C:313:TYR:O	2.23	0.65
1:D:360:GLU:N	1:D:419:ALA:O	2.24	0.65
1:C:225:GLN:HG3	1:C:235:PHE:CE2	2.32	0.65
1:A:227:SER:O	1:A:230:LYS:HG2	1.96	0.65
1:A:291:VAL:HA	1:A:308:ASN:ND2	2.11	0.65
1:A:358:ASN:HB3	1:A:359:PRO:CD	2.21	0.65
1:D:117:TYR:OH	1:D:283:GLY:N	2.30	0.65
1:D:120:PHE:CD1	1:D:284:LEU:HD11	2.27	0.65
1:B:82:ILE:HG21	1:B:199:ILE:CD1	2.26	0.64
1:B:97:ASN:C	1:B:97:ASN:HD22	1.99	0.64
1:C:367:THR:N	1:C:370:GLN:HE21	1.93	0.64
1:D:126:ILE:HD13	1:D:143:ILE:HD13	1.78	0.64
1:B:128:VAL:HG12	1:B:129:ASP:H	1.63	0.64
1:C:462:ALA:CA	1:C:467:PRO:HD3	2.26	0.64
1:D:304:ARG:O	1:D:305:PHE:HB2	1.96	0.64
1:B:284:LEU:HD11	1:B:286:LEU:HD11	1.78	0.64
1:C:166:SER:O	1:C:167:SER:C	2.35	0.64
1:D:367:THR:HG23	1:D:370:GLN:NE2	2.12	0.64
1:B:160:ASP:O	1:B:160:ASP:OD2	2.16	0.64
1:D:358:ASN:HB3	1:D:359:PRO:CD	2.27	0.64
1:D:38:ARG:CD	1:D:47:ASN:ND2	2.61	0.64
1:C:448:ALA:O	1:C:451:THR:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:C	1:A:82:ILE:HD12	2.18	0.64
1:D:121:VAL:HG23	1:D:127:SER:HB2	1.80	0.64
1:D:243:GLY:HA3	1:D:254:THR:CB	2.17	0.64
1:A:443:ALA:O	1:A:457:LYS:NZ	2.30	0.64
1:D:462:ALA:HB2	1:D:467:PRO:HG3	1.80	0.64
1:C:187:TYR:CD1	1:C:188:ILE:N	2.63	0.63
1:C:176:ILE:HD13	1:C:199:ILE:CG2	2.28	0.63
1:D:45:CYS:O	1:D:50:CYS:HB2	1.98	0.63
1:A:253:LEU:O	1:A:265:ILE:HD12	1.98	0.63
1:B:176:ILE:HD13	1:B:199:ILE:CG2	2.28	0.63
1:C:28:LEU:HD12	1:C:336:VAL:HG12	1.79	0.63
1:D:126:ILE:CD1	1:D:143:ILE:HD13	2.28	0.63
1:A:149:SER:HB3	1:A:317:ASP:HB3	1.80	0.63
1:B:328:ALA:O	1:B:329:GLU:C	2.36	0.63
1:B:460:ALA:O	1:B:463:THR:HB	1.99	0.63
1:C:242:VAL:O	1:C:254:THR:O	2.15	0.63
1:B:367:THR:H	1:B:370:GLN:HG3	1.63	0.63
1:C:229:GLU:C	1:C:231:GLN:H	2.01	0.63
1:C:95:VAL:O	1:C:99:THR:HG23	1.99	0.63
1:C:445:VAL:HG21	1:D:431:ILE:HG13	1.81	0.63
1:A:229:GLU:O	1:A:231:GLN:N	2.31	0.63
1:C:262:GLU:HG2	1:C:263:GLN:N	2.12	0.63
1:A:462:ALA:HB2	1:A:467:PRO:HG3	1.79	0.63
1:D:367:THR:H	1:D:370:GLN:HE21	1.47	0.63
1:B:301:VAL:HG22	1:B:302:ASN:H	1.62	0.63
1:B:415:VAL:HG21	1:B:429:ALA:HB1	1.79	0.63
1:D:152:LYS:HG3	1:D:278:THR:HG23	1.79	0.63
1:D:426:ILE:O	1:D:426:ILE:HG12	1.98	0.63
1:C:181:VAL:HG22	1:C:204:THR:OG1	1.99	0.62
1:A:117:TYR:HB3	1:A:129:ASP:CB	2.23	0.62
1:A:12:ILE:CD1	1:A:126:ILE:CD1	2.70	0.62
1:A:121:VAL:CG2	1:A:127:SER:HB2	2.29	0.62
1:C:183:ILE:HG22	1:C:184:GLY:N	2.13	0.62
1:C:286:LEU:HD22	1:C:291:VAL:CG2	2.30	0.62
1:D:12:ILE:HD11	1:D:126:ILE:CD1	2.28	0.62
1:D:28:LEU:HD12	1:D:336:VAL:HG12	1.82	0.62
1:C:154:LEU:HD12	1:C:155:PRO:N	2.14	0.62
1:C:460:ALA:O	1:C:463:THR:HB	1.98	0.62
1:B:88:MET:HE1	1:B:171:LEU:O	1.99	0.62
1:B:304:ARG:HA	1:B:338:TYR:CD1	2.35	0.62
1:D:7:ASN:ND2	1:D:33:THR:OG1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PHE:N	1:A:285:ASN:CB	2.63	0.62
1:C:299:ILE:HG13	1:C:318:VAL:O	1.99	0.62
1:C:424:GLU:OE2	1:D:451:THR:HB	1.98	0.62
1:B:44:THR:C	1:B:46:LEU:H	2.03	0.62
1:A:216:MET:HE3	1:A:361:VAL:HG11	1.82	0.62
1:A:54:LYS:HA	1:A:57:LEU:HD12	1.81	0.62
1:C:164:ILE:HG13	1:C:271:VAL:CG2	2.30	0.62
1:D:239:THR:HB	1:D:255:VAL:HG11	1.81	0.62
1:B:161:GLU:HG2	1:B:162:LYS:HG2	1.82	0.61
1:D:242:VAL:HG23	1:D:254:THR:CG2	2.28	0.61
1:C:262:GLU:HG2	1:C:263:GLN:H	1.65	0.61
1:D:119:LYS:HB3	1:D:127:SER:HB3	1.82	0.61
1:D:192:MET:CA	1:D:192:MET:HE3	2.21	0.61
1:A:212:ILE:HG13	1:A:212:ILE:O	1.98	0.61
1:A:245:ASP:HB2	1:A:252:LYS:CB	2.30	0.61
1:B:8:ASP:HB2	1:B:31:LYS:N	2.15	0.61
1:A:184:GLY:HA3	1:A:274:SER:O	2.01	0.61
1:C:156:GLY:HA3	1:C:241:VAL:HG11	1.82	0.61
1:B:364:VAL:HG12	1:B:433:LEU:HD22	1.83	0.61
1:B:183:ILE:HG22	1:B:184:GLY:N	2.15	0.61
1:D:49:GLY:O	1:D:53:SER:CB	2.48	0.61
1:A:350:LYS:HD3	1:A:433:LEU:HD23	1.82	0.61
1:B:295:LYS:O	1:B:297:GLY:N	2.32	0.61
1:B:185:ALA:HB3	1:B:207:GLU:HB2	1.82	0.61
1:B:207:GLU:HG3	1:B:209:ALA:H	1.65	0.61
1:B:192:MET:CE	1:B:192:MET:HA	2.31	0.60
1:C:114:VAL:O	1:C:114:VAL:HG12	2.00	0.60
1:A:208:PHE:CE2	1:A:258:SER:HB3	2.36	0.60
1:B:281:THR:HA	1:B:284:LEU:HD21	1.83	0.60
1:B:468:ILE:O	1:B:468:ILE:HG22	2.00	0.60
1:D:286:LEU:HD13	1:D:291:VAL:N	2.15	0.60
1:D:88:MET:HE1	1:D:171:LEU:O	2.01	0.60
1:A:208:PHE:O	1:A:238:LYS:HA	2.01	0.60
1:A:119:LYS:C	1:A:285:ASN:HB2	2.22	0.60
1:C:154:LEU:HD12	1:C:155:PRO:CD	2.32	0.60
1:B:212:ILE:HG21	1:B:235:PHE:CE2	2.36	0.60
1:B:41:LEU:HD11	1:B:106:PHE:CE1	2.37	0.60
1:C:285:ASN:C	1:C:287:ASP:H	2.03	0.60
1:D:46:LEU:HD11	1:D:98:LEU:HB2	1.83	0.60
1:A:164:ILE:CD1	1:A:244:VAL:HG11	2.32	0.60
1:C:51:ILE:HD13	1:C:51:ILE:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:HB2	1:A:276:GLY:C	2.22	0.59
1:A:374:THR:O	1:A:376:VAL:HG23	2.02	0.59
1:A:96:SER:OG	1:A:97:ASN:N	2.35	0.59
1:A:96:SER:O	1:A:97:ASN:C	2.40	0.59
1:C:121:VAL:HG12	1:C:121:VAL:O	2.01	0.59
1:D:161:GLU:C	1:D:162:LYS:HG3	2.23	0.59
1:C:12:ILE:HD11	1:C:126:ILE:CD1	2.33	0.59
1:D:403:ILE:HG12	1:D:415:VAL:HG22	1.84	0.59
1:B:367:THR:H	1:B:370:GLN:NE2	1.95	0.59
1:A:260:GLY:O	1:A:262:GLU:N	2.35	0.59
1:C:192:MET:CA	1:C:192:MET:HE3	2.30	0.59
1:C:246:THR:O	1:C:247:SER:HB2	2.02	0.59
1:D:284:LEU:HD12	1:D:285:ASN:N	2.13	0.59
1:B:228:LEU:HD13	1:B:233:MET:CE	2.28	0.59
1:D:462:ALA:HA	1:D:467:PRO:HD3	1.83	0.59
1:C:394:ILE:HD12	1:D:58:HIS:CD2	2.36	0.59
1:A:418:MET:O	1:A:419:ALA:HB2	2.01	0.59
1:A:448:ALA:O	1:A:451:THR:CG2	2.51	0.59
1:C:242:VAL:CB	1:C:255:VAL:HA	2.31	0.59
1:D:183:ILE:O	1:D:206:VAL:O	2.20	0.59
1:A:225:GLN:O	1:A:229:GLU:HG3	2.02	0.59
1:B:265:ILE:HD12	1:B:265:ILE:N	2.18	0.59
1:B:293:THR:O	1:B:293:THR:HG22	2.01	0.59
1:D:130:THR:O	1:D:131:ILE:HD13	2.03	0.59
1:B:153:SER:C	1:B:157:VAL:HG21	2.23	0.59
1:C:366:LYS:O	1:C:416:HIS:HE1	1.85	0.59
1:D:182:VAL:HB	1:D:205:VAL:HG13	1.84	0.59
1:D:128:VAL:O	1:D:129:ASP:O	2.20	0.59
1:A:192:MET:HA	1:A:192:MET:HE2	1.83	0.58
1:B:8:ASP:HB2	1:B:31:LYS:H	1.67	0.58
1:D:185:ALA:CB	1:D:207:GLU:HB2	2.33	0.58
1:C:270:VAL:CG1	1:C:271:VAL:N	2.67	0.58
1:C:333:VAL:O	1:C:334:ALA:C	2.42	0.58
1:D:227:SER:OG	1:D:231:GLN:NE2	2.37	0.58
1:D:325:ALA:O	1:D:328:ALA:HB3	2.03	0.58
1:A:362:ALA:C	1:A:426:ILE:HD12	2.23	0.58
1:A:364:VAL:HG23	1:A:426:ILE:HD13	1.85	0.58
1:D:126:ILE:HG23	1:D:127:SER:O	2.03	0.58
1:A:176:ILE:HD13	1:A:199:ILE:HG23	1.85	0.58
1:B:212:ILE:HG21	1:B:235:PHE:CD2	2.38	0.58
1:A:49:GLY:O	1:A:53:SER:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASP:CB	1:B:31:LYS:H	2.17	0.58
1:C:150:ASP:CG	1:C:151:VAL:N	2.56	0.58
1:B:123:PRO:HG3	1:B:289:ILE:HD13	1.86	0.58
1:C:242:VAL:HG21	1:C:256:GLU:CB	2.34	0.58
1:D:401:VAL:HG11	1:D:456:ILE:HA	1.86	0.58
1:C:70:PHE:CZ	1:D:70:PHE:CZ	2.92	0.58
1:B:296:LEU:HD12	1:B:296:LEU:H	1.68	0.58
1:B:419:ALA:HB1	1:B:420:PRO:HD2	1.85	0.58
1:A:221:ARG:HH11	1:A:221:ARG:HG2	1.69	0.58
1:C:62:MET:SD	1:D:73:HIS:CG	2.97	0.57
1:D:120:PHE:H	1:D:284:LEU:HD13	1.70	0.57
1:B:265:ILE:HD12	1:B:265:ILE:H	1.68	0.57
1:B:36:GLU:OE2	2:B:480:FAD:H4B	2.04	0.57
1:C:185:ALA:CB	1:C:207:GLU:HB2	2.34	0.57
1:C:253:LEU:N	1:C:266:ILE:O	2.36	0.57
1:C:38:ARG:O	3:C:2004:HOH:O	2.17	0.57
1:A:216:MET:HE1	1:A:221:ARG:HA	1.87	0.57
1:A:468:ILE:HG22	1:A:468:ILE:O	2.04	0.57
1:A:58:HIS:CD2	1:B:394:ILE:HD12	2.39	0.57
1:B:190:LEU:HD13	1:B:228:LEU:HD11	1.86	0.57
1:D:329:GLU:OE2	3:D:2011:HOH:O	2.17	0.57
1:A:66:ALA:HB2	1:B:70:PHE:CE2	2.39	0.57
1:B:358:ASN:HB3	1:B:359:PRO:CD	2.35	0.57
1:B:443:ALA:O	1:B:457:LYS:NZ	2.37	0.57
1:C:203:VAL:HG21	1:C:233:MET:HG3	1.87	0.57
1:D:425:LEU:HB3	1:D:456:ILE:HD11	1.85	0.57
1:D:53:SER:O	1:D:57:LEU:HG	2.04	0.57
1:A:154:LEU:HD12	1:A:155:PRO:HD2	1.87	0.57
1:A:160:ASP:O	1:A:161:GLU:CG	2.50	0.57
1:A:206:VAL:HG22	1:A:236:LYS:HB2	1.85	0.57
1:A:163:LYS:O	1:A:270:VAL:HA	2.04	0.57
1:C:263:GLN:C	1:C:264:THR:O	2.38	0.57
1:C:468:ILE:O	1:C:468:ILE:HG22	2.03	0.57
1:D:171:LEU:HD23	1:D:192:MET:HE1	1.86	0.57
1:A:401:VAL:HG11	1:A:456:ILE:HA	1.85	0.57
1:D:427:HIS:O	1:D:431:ILE:HG22	2.05	0.57
1:A:96:SER:O	1:A:99:THR:N	2.37	0.57
1:D:120:PHE:H	1:D:284:LEU:CD1	2.18	0.57
1:D:243:GLY:O	1:D:253:LEU:HA	2.04	0.57
1:D:284:LEU:CG	1:D:285:ASN:N	2.67	0.57
1:D:322:PRO:HG2	1:D:327:LYS:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:HB3	1:B:313:TYR:HE1	1.69	0.56
1:B:49:GLY:O	1:B:50:CYS:O	2.23	0.56
1:C:195:VAL:HG12	1:C:196:TRP:N	2.19	0.56
1:C:293:THR:HG22	1:C:298:ARG:O	2.04	0.56
1:C:48:VAL:O	1:C:48:VAL:HG12	2.05	0.56
1:D:358:ASN:CB	1:D:359:PRO:HD3	2.34	0.56
1:A:38:ARG:NH1	3:A:2007:HOH:O	2.24	0.56
1:C:181:VAL:HA	1:C:204:THR:O	2.06	0.56
1:C:409:THR:O	1:C:410:ASP:HB3	2.05	0.56
1:D:28:LEU:HD12	1:D:336:VAL:CG1	2.35	0.56
1:C:393:ALA:CB	1:D:51:ILE:HG23	2.35	0.56
1:B:244:VAL:HG12	1:B:251:VAL:HG13	1.87	0.56
1:B:119:LYS:O	1:B:126:ILE:HA	2.05	0.56
1:B:82:ILE:HG21	1:B:199:ILE:HD11	1.86	0.56
1:B:362:ALA:CB	1:B:426:ILE:HD12	2.34	0.56
1:C:406:GLU:HB2	1:C:409:THR:OG1	2.05	0.56
1:D:207:GLU:HG3	1:D:209:ALA:H	1.70	0.56
1:A:441:ASP:O	1:B:435:TYR:OH	2.22	0.56
1:C:185:ALA:HB3	1:C:207:GLU:HB2	1.87	0.56
1:C:300:LEU:C	1:C:300:LEU:HD23	2.26	0.56
1:D:309:VAL:O	1:D:309:VAL:HG12	2.04	0.56
1:A:157:VAL:CG1	1:A:244:VAL:HG21	2.28	0.56
1:B:292:GLU:HB3	1:B:300:LEU:HB2	1.86	0.56
1:C:139:LYS:N	1:C:139:LYS:CD	2.69	0.56
1:C:36:GLU:OE2	2:C:480:FAD:H4B	2.05	0.56
1:D:75:VAL:O	1:D:75:VAL:HG12	2.05	0.56
1:B:400:LEU:HD23	1:B:400:LEU:N	2.20	0.56
1:C:11:ILE:HG12	1:C:144:ILE:HB	1.87	0.56
1:C:118:GLY:HA2	1:C:128:VAL:HG22	1.87	0.56
1:C:154:LEU:HD12	1:C:156:GLY:N	2.20	0.56
1:A:227:SER:OG	1:A:230:LYS:NZ	2.38	0.56
1:C:73:HIS:O	1:D:87:MET:HG3	2.05	0.56
1:A:138:VAL:O	1:A:138:VAL:HG12	2.06	0.56
1:A:192:MET:HE3	1:A:192:MET:CA	2.34	0.56
1:A:152:LYS:HB2	1:A:276:GLY:O	2.05	0.56
1:B:146:ALA:C	1:B:147:THR:O	2.42	0.56
1:B:406:GLU:HB2	1:B:409:THR:OG1	2.06	0.56
1:C:123:PRO:CG	1:C:289:ILE:HG22	2.28	0.56
1:D:284:LEU:HG	1:D:285:ASN:N	2.20	0.56
1:A:367:THR:H	1:A:370:GLN:NE2	2.02	0.56
1:B:299:ILE:HG22	1:B:299:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HG2	1:C:327:LYS:HG3	1.87	0.56
1:D:438:SER:O	1:D:441:ASP:HB2	2.06	0.56
1:A:281:THR:O	1:A:284:LEU:HB2	2.06	0.56
1:B:15:GLY:HA2	1:B:43:GLY:HA3	1.87	0.56
1:B:389:SER:O	1:B:390:ARG:C	2.43	0.56
1:C:118:GLY:CA	1:C:127:SER:O	2.43	0.56
1:C:265:ILE:HG22	1:C:265:ILE:O	2.05	0.56
1:D:184:GLY:HA3	1:D:274:SER:O	2.06	0.56
1:A:120:PHE:O	1:A:285:ASN:ND2	2.39	0.55
1:A:419:ALA:HB1	1:A:420:PRO:HD2	1.87	0.55
1:B:367:THR:HG23	1:B:370:GLN:CD	2.25	0.55
1:C:190:LEU:HD13	1:C:228:LEU:HD11	1.87	0.55
1:C:348:TYR:HA	1:C:351:VAL:HG23	1.88	0.55
1:C:438:SER:O	1:C:441:ASP:HB2	2.06	0.55
1:A:208:PHE:CZ	1:A:258:SER:HB3	2.41	0.55
1:B:128:VAL:HG12	1:B:129:ASP:N	2.20	0.55
1:B:315:ILE:O	1:B:315:ILE:HG13	2.05	0.55
1:C:42:GLY:HA3	1:C:46:LEU:CB	2.36	0.55
1:D:11:ILE:HG12	1:D:144:ILE:HB	1.87	0.55
1:D:154:LEU:HD23	1:D:157:VAL:HB	1.89	0.55
1:C:156:GLY:HA3	1:C:241:VAL:CG1	2.37	0.55
1:C:357:THR:OG1	1:C:359:PRO:O	2.21	0.55
1:A:249:ASP:OD1	1:A:249:ASP:N	2.39	0.55
1:B:88:MET:HE1	1:B:91:LYS:HZ2	1.71	0.55
1:A:82:ILE:HG21	1:A:199:ILE:CD1	2.37	0.55
1:A:350:LYS:O	1:A:352:PRO:HD3	2.06	0.55
1:B:49:GLY:O	1:B:50:CYS:C	2.44	0.55
1:C:70:PHE:HB3	1:C:75:VAL:O	2.06	0.55
1:A:63:TYR:CE1	1:A:82:ILE:HD11	2.41	0.55
1:B:260:GLY:O	1:B:261:GLY:O	2.23	0.55
1:B:253:LEU:O	1:B:265:ILE:HG22	2.06	0.55
1:C:165:VAL:HG11	1:C:173:LEU:HD21	1.87	0.55
1:A:207:GLU:HG3	1:A:209:ALA:H	1.72	0.55
1:A:240:LYS:HG2	1:A:241:VAL:N	2.21	0.55
1:B:35:ILE:CD1	1:B:138:VAL:HG21	2.33	0.55
1:C:164:ILE:HG13	1:C:271:VAL:CB	2.35	0.55
1:C:355:VAL:CG1	1:C:357:THR:HG23	2.37	0.55
1:D:419:ALA:HB1	1:D:420:PRO:HD2	1.89	0.55
1:C:126:ILE:N	1:C:138:VAL:O	2.35	0.55
1:C:352:PRO:HB3	1:C:364:VAL:CG2	2.36	0.55
1:C:378:TYR:C	1:C:378:TYR:CD1	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ASP:CG	1:C:6:GLU:H	2.10	0.55
1:A:253:LEU:O	1:A:265:ILE:HA	2.07	0.55
1:B:239:THR:CA	1:B:257:PRO:HA	2.24	0.55
1:C:127:SER:C	1:C:128:VAL:HG23	2.27	0.55
1:C:179:LYS:O	1:C:269:ASP:HB2	2.06	0.55
1:A:119:LYS:CA	1:A:285:ASN:HB2	2.37	0.54
1:C:86:ALA:O	1:C:87:MET:C	2.44	0.54
1:C:244:VAL:HG11	1:C:253:LEU:CD2	2.38	0.54
1:D:348:TYR:CD2	1:D:348:TYR:N	2.69	0.54
1:A:292:GLU:N	1:A:308:ASN:HD21	2.04	0.54
1:B:448:ALA:O	1:B:451:THR:HG23	2.07	0.54
1:C:149:SER:HB3	1:C:317:ASP:HB3	1.88	0.54
1:A:253:LEU:HB2	1:A:266:ILE:HB	1.90	0.54
1:C:117:TYR:C	1:C:128:VAL:HA	2.28	0.54
1:C:282:SER:O	1:C:284:LEU:N	2.41	0.54
1:D:313:TYR:CE1	1:D:339:LEU:HD21	2.43	0.54
1:B:310:SER:O	1:B:312:VAL:N	2.41	0.54
1:C:122:SER:C	1:C:124:SER:H	2.09	0.54
1:C:19:TYR:O	1:C:23:ILE:HG13	2.08	0.54
1:D:42:GLY:HA3	1:D:46:LEU:CB	2.37	0.54
1:A:192:MET:CA	1:A:192:MET:CE	2.77	0.54
1:B:173:LEU:HD12	1:B:196:TRP:CZ2	2.43	0.54
1:B:450:PRO:O	1:B:450:PRO:HG2	2.07	0.54
1:C:181:VAL:HG23	1:C:268:ALA:HB2	1.90	0.54
1:C:203:VAL:HG23	1:C:233:MET:HG3	1.89	0.54
1:C:184:GLY:HA3	1:C:274:SER:C	2.28	0.54
1:B:17:GLY:O	1:B:21:ALA:HB2	2.07	0.54
1:C:305:PHE:CE2	1:C:331:ASP:HB3	2.43	0.54
1:B:409:THR:O	1:B:410:ASP:HB3	2.08	0.54
1:C:160:ASP:O	1:C:161:GLU:C	2.47	0.54
1:D:44:THR:N	2:D:480:FAD:O1A	2.41	0.54
1:B:310:SER:O	1:B:312:VAL:HG23	2.08	0.53
1:C:207:GLU:HG3	1:C:209:ALA:H	1.73	0.53
1:C:212:ILE:HG23	1:C:237:LEU:HD21	1.91	0.53
1:C:357:THR:O	1:C:358:ASN:C	2.44	0.53
1:D:51:ILE:O	1:D:54:LYS:N	2.41	0.53
1:B:228:LEU:HD22	1:B:233:MET:CE	2.38	0.53
1:C:70:PHE:HB3	1:C:75:VAL:HB	1.91	0.53
1:D:204:THR:HA	1:D:234:LYS:O	2.09	0.53
1:D:243:GLY:O	1:D:254:THR:N	2.40	0.53
1:B:11:ILE:HG12	1:B:144:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:MET:CE	1:C:220:ILE:HG22	2.39	0.53
1:B:283:GLY:O	1:B:284:LEU:O	2.25	0.53
1:B:292:GLU:O	1:B:300:LEU:HD23	2.07	0.53
1:C:265:ILE:CG2	1:C:265:ILE:O	2.56	0.53
1:D:149:SER:HA	1:D:280:PHE:N	2.23	0.53
1:D:82:ILE:N	1:D:82:ILE:CD1	2.64	0.53
1:C:126:ILE:HD11	1:C:143:ILE:CG2	2.35	0.53
1:C:264:THR:HG22	1:C:265:ILE:N	2.23	0.53
1:A:150:ASP:CG	1:A:151:VAL:H	2.11	0.53
1:B:216:MET:HE3	1:B:361:VAL:HG11	1.90	0.53
1:B:53:SER:O	1:B:57:LEU:HG	2.08	0.53
1:B:71:ALA:O	1:B:73:HIS:N	2.41	0.53
1:C:157:VAL:HG11	1:C:164:ILE:HG21	1.90	0.53
1:C:353:GLY:O	1:C:362:ALA:HA	2.09	0.53
1:C:58:HIS:CG	1:D:394:ILE:HD12	2.44	0.53
1:C:9:VAL:HB	1:C:32:THR:HG23	1.89	0.53
1:D:460:ALA:O	1:D:463:THR:HB	2.08	0.53
1:B:46:LEU:O	1:B:46:LEU:HD12	2.07	0.53
1:C:123:PRO:HG3	1:C:289:ILE:CG2	2.31	0.53
1:C:367:THR:H	1:C:370:GLN:NE2	1.97	0.53
1:D:22:ALA:O	1:D:25:ALA:HB3	2.09	0.53
1:A:195:VAL:HG12	1:A:196:TRP:N	2.24	0.53
1:A:358:ASN:CB	1:A:359:PRO:HD3	2.31	0.53
1:B:182:VAL:HB	1:B:205:VAL:HG13	1.90	0.53
1:B:313:TYR:CZ	1:B:339:LEU:HD21	2.44	0.53
1:D:204:THR:HG22	1:D:234:LYS:HB2	1.91	0.53
1:A:152:LYS:HD2	1:A:278:THR:HG23	1.90	0.53
1:A:291:VAL:CA	1:A:308:ASN:HD21	2.20	0.53
1:B:286:LEU:C	1:B:288:LYS:N	2.59	0.53
1:C:163:LYS:O	1:C:270:VAL:HG22	2.08	0.53
1:D:142:HIS:HB2	3:D:2004:HOH:O	2.08	0.53
1:A:70:PHE:CE2	1:B:66:ALA:HB2	2.43	0.53
1:B:88:MET:CE	1:B:91:LYS:NZ	2.72	0.53
1:C:41:LEU:HD11	1:C:106:PHE:CE1	2.44	0.53
1:A:416:HIS:ND1	1:A:416:HIS:N	2.57	0.52
1:B:367:THR:N	1:B:370:GLN:HG3	2.23	0.52
1:B:364:VAL:CG1	1:B:433:LEU:HD22	2.38	0.52
1:B:462:ALA:CB	1:B:467:PRO:HG3	2.39	0.52
1:C:164:ILE:HD11	1:C:251:VAL:CG1	2.34	0.52
1:C:70:PHE:HZ	1:D:70:PHE:CZ	2.27	0.52
1:C:127:SER:O	1:C:128:VAL:CG2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD22	1:B:233:MET:HE2	1.90	0.52
1:B:81:GLU:C	1:B:82:ILE:HD12	2.27	0.52
1:D:166:SER:O	1:D:167:SER:C	2.47	0.52
1:C:62:MET:SD	1:D:73:HIS:CD2	3.03	0.52
1:A:465:ASP:CG	1:A:466:LYS:H	2.12	0.52
1:A:167:SER:HB3	2:A:480:FAD:HM71	1.91	0.52
1:B:42:GLY:HA3	1:B:46:LEU:HB3	1.91	0.52
1:C:63:TYR:CE1	1:C:82:ILE:CD1	2.89	0.52
1:D:185:ALA:HB3	1:D:207:GLU:HB2	1.89	0.52
1:B:400:LEU:H	1:B:400:LEU:HD23	1.74	0.52
1:A:227:SER:OG	1:A:230:LYS:CE	2.58	0.52
1:B:194:SER:O	1:B:198:ARG:HG3	2.09	0.52
1:C:131:ILE:O	1:C:131:ILE:HG12	2.09	0.52
1:C:192:MET:CA	1:C:192:MET:CE	2.78	0.52
1:C:212:ILE:O	1:C:212:ILE:HG13	2.10	0.52
1:D:284:LEU:CD1	1:D:285:ASN:N	2.72	0.52
1:D:294:ASP:HB2	1:D:298:ARG:HB2	1.90	0.52
1:D:332:GLY:O	1:D:335:CYS:HB3	2.09	0.52
1:A:46:LEU:HD11	1:A:98:LEU:CB	2.40	0.52
1:C:289:ILE:HB	1:C:309:VAL:HG21	1.92	0.52
1:C:304:ARG:HA	1:C:338:TYR:CD1	2.45	0.52
1:D:298:ARG:HD2	1:D:320:PRO:CA	2.39	0.52
1:A:315:ILE:HA	1:A:319:ILE:HD13	1.91	0.52
1:C:254:THR:HA	1:C:265:ILE:HD12	1.89	0.52
1:C:273:VAL:HG12	1:C:273:VAL:O	2.09	0.52
1:B:48:VAL:HG11	1:B:168:THR:CG2	2.37	0.52
1:C:157:VAL:HG12	1:C:158:THR:N	2.24	0.52
1:C:282:SER:C	1:C:284:LEU:N	2.63	0.52
1:D:298:ARG:HD2	1:D:320:PRO:N	2.25	0.52
1:D:51:ILE:HB	1:D:52:PRO:CD	2.38	0.52
1:A:192:MET:HG3	1:A:272:LEU:CD2	2.40	0.52
1:B:301:VAL:HG22	1:B:302:ASN:N	2.24	0.52
1:B:427:HIS:HA	1:B:430:ALA:HB3	1.91	0.52
1:C:12:ILE:CD1	1:C:126:ILE:HD13	2.40	0.52
1:C:44:THR:N	2:C:480:FAD:O1A	2.43	0.52
1:C:93:LYS:O	1:C:96:SER:OG	2.26	0.52
1:D:150:ASP:CG	1:D:151:VAL:H	2.13	0.52
1:D:216:MET:HE3	1:D:361:VAL:HG11	1.91	0.52
1:A:119:LYS:HA	1:A:285:ASN:H	1.75	0.51
1:A:274:SER:C	1:A:275:ALA:O	2.48	0.51
1:B:23:ILE:O	1:B:27:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ALA:O	1:C:73:HIS:N	2.43	0.51
1:D:298:ARG:NE	1:D:320:PRO:HA	2.25	0.51
1:B:82:ILE:HG21	1:B:199:ILE:HD12	1.91	0.51
1:A:409:THR:O	1:A:410:ASP:HB3	2.11	0.51
1:D:209:ALA:O	1:D:237:LEU:O	2.28	0.51
1:D:81:GLU:CA	1:D:82:ILE:HD12	2.41	0.51
1:A:360:GLU:HB2	1:A:422:ALA:HB3	1.92	0.51
1:B:56:LEU:HD13	1:B:195:VAL:HG11	1.91	0.51
1:C:216:MET:HE2	1:C:220:ILE:HG22	1.91	0.51
1:C:36:GLU:O	3:C:2004:HOH:O	2.19	0.51
1:C:78:SER:HB2	1:D:78:SER:CB	2.36	0.51
1:C:81:GLU:C	1:C:82:ILE:HD12	2.30	0.51
1:D:264:THR:O	1:D:265:ILE:HD13	2.11	0.51
1:D:359:PRO:HG2	1:D:398:GLU:OE2	2.11	0.51
1:B:358:ASN:CB	1:B:359:PRO:HD3	2.38	0.51
1:B:38:ARG:CD	1:B:47:ASN:ND2	2.73	0.51
1:B:119:LYS:O	1:B:126:ILE:CA	2.58	0.51
1:B:48:VAL:HG12	1:B:168:THR:HG23	1.91	0.51
1:B:171:LEU:CD2	1:B:192:MET:HE1	2.39	0.51
1:B:353:GLY:O	1:B:362:ALA:HA	2.10	0.51
1:C:203:VAL:HG23	1:C:233:MET:HA	1.93	0.51
1:C:383:PHE:CD1	1:C:458:GLU:HB3	2.44	0.51
1:D:294:ASP:OD2	1:D:298:ARG:NH1	2.43	0.51
1:D:298:ARG:HD2	1:D:320:PRO:HA	1.92	0.51
1:D:353:GLY:O	1:D:362:ALA:HA	2.10	0.51
1:D:420:PRO:O	1:D:421:ASN:HB2	2.09	0.51
1:C:77:VAL:HG12	1:D:79:ASN:O	2.11	0.51
1:B:153:SER:OG	1:B:154:LEU:N	2.41	0.51
1:B:82:ILE:H	1:B:82:ILE:CD1	2.19	0.51
1:C:244:VAL:HG12	1:C:254:THR:H	1.75	0.51
1:C:461:MET:C	1:C:463:THR:H	2.14	0.51
1:A:229:GLU:C	1:A:231:GLN:N	2.61	0.51
1:B:240:LYS:N	1:B:256:GLU:O	2.34	0.51
1:B:308:ASN:O	1:B:309:VAL:CG2	2.49	0.51
1:C:258:SER:CA	1:C:259:ALA:N	2.74	0.51
1:C:406:GLU:HG2	1:C:413:LEU:HD21	1.92	0.51
1:C:46:LEU:CD2	1:C:99:THR:HG22	2.40	0.51
1:D:358:ASN:CB	1:D:359:PRO:CD	2.89	0.51
1:B:292:GLU:CB	1:B:300:LEU:HB2	2.41	0.51
1:C:450:PRO:O	1:C:450:PRO:HG2	2.10	0.51
1:D:367:THR:H	1:D:370:GLN:HG3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:N	1:A:252:LYS:O	2.38	0.51
1:A:406:GLU:HB2	1:A:409:THR:OG1	2.11	0.51
1:A:50:CYS:O	1:A:54:LYS:N	2.35	0.51
1:C:12:ILE:CG1	1:C:126:ILE:HD13	2.41	0.51
1:A:315:ILE:CD1	1:A:332:GLY:HA2	2.41	0.50
1:B:9:VAL:CG2	1:B:30:PHE:HB3	2.36	0.50
1:C:122:SER:C	1:C:124:SER:N	2.64	0.50
1:C:241:VAL:O	1:C:241:VAL:HG12	2.12	0.50
1:C:261:GLY:O	1:C:262:GLU:HB3	2.11	0.50
1:D:327:LYS:HE2	1:D:348:TYR:CE1	2.46	0.50
1:D:352:PRO:HB3	1:D:364:VAL:CG2	2.41	0.50
1:A:256:GLU:OE2	1:A:261:GLY:HA2	2.11	0.50
1:C:182:VAL:O	1:C:205:VAL:HA	2.11	0.50
1:C:244:VAL:HG11	1:C:253:LEU:HD23	1.92	0.50
1:C:385:PHE:CE1	1:C:419:ALA:HB2	2.47	0.50
1:D:33:THR:HG23	1:D:112:THR:O	2.11	0.50
1:D:129:ASP:O	1:D:130:THR:CG2	2.56	0.50
1:D:212:ILE:HD13	1:D:225:GLN:HG3	1.93	0.50
1:D:240:LYS:HE3	1:D:242:VAL:HG13	1.92	0.50
1:A:11:ILE:HG12	1:A:144:ILE:HB	1.92	0.50
1:A:169:GLY:O	1:A:173:LEU:HD23	2.11	0.50
1:A:292:GLU:H	1:A:308:ASN:HD21	1.58	0.50
1:C:127:SER:C	1:C:128:VAL:CG2	2.80	0.50
1:C:7:ASN:ND2	1:C:33:THR:OG1	2.44	0.50
1:A:119:LYS:CG	1:A:285:ASN:HB2	2.39	0.50
1:B:244:VAL:O	1:B:245:ASP:HB2	2.11	0.50
1:B:245:ASP:OD2	1:B:247:SER:HB3	2.12	0.50
1:B:274:SER:C	1:B:275:ALA:O	2.49	0.50
1:B:286:LEU:O	1:B:288:LYS:N	2.45	0.50
1:B:294:ASP:H	1:B:300:LEU:CD2	2.24	0.50
1:B:309:VAL:HG12	1:B:310:SER:O	2.11	0.50
1:C:165:VAL:HG22	1:C:270:VAL:CG1	2.41	0.50
1:D:348:TYR:N	1:D:348:TYR:HD2	2.09	0.50
1:B:117:TYR:CE2	1:B:283:GLY:CA	2.88	0.50
1:B:38:ARG:HD3	1:B:47:ASN:HD22	1.76	0.50
1:C:126:ILE:HD12	1:C:143:ILE:HD13	1.92	0.50
1:A:41:LEU:HD11	1:A:106:PHE:CD1	2.46	0.50
1:A:82:ILE:HG21	1:A:199:ILE:HD12	1.94	0.50
1:A:325:ALA:O	1:A:328:ALA:HB3	2.12	0.50
1:A:313:TYR:CZ	1:A:339:LEU:HD21	2.47	0.50
1:B:122:SER:C	1:B:124:SER:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:CYS:O	1:B:46:LEU:HB2	2.11	0.50
1:D:449:HIS:ND1	1:D:450:PRO:HB3	2.27	0.50
1:B:449:HIS:CE1	1:B:450:PRO:HB3	2.45	0.50
1:C:409:THR:O	1:C:410:ASP:CB	2.59	0.50
1:D:350:LYS:O	1:D:352:PRO:HD3	2.11	0.50
1:B:118:GLY:HA2	1:B:126:ILE:HD13	1.93	0.50
1:B:95:VAL:O	1:B:99:THR:HG23	2.11	0.50
1:C:48:VAL:HG13	1:C:168:THR:HG23	1.94	0.50
1:C:246:THR:HA	1:C:251:VAL:HG22	1.94	0.50
1:C:254:THR:HG23	1:C:265:ILE:CD1	2.17	0.50
1:D:403:ILE:HD12	1:D:460:ALA:HA	1.94	0.50
1:A:433:LEU:O	1:A:433:LEU:HG	2.12	0.50
1:D:195:VAL:HG12	1:D:196:TRP:N	2.25	0.50
1:D:346:VAL:O	1:D:347:ASP:HB2	2.12	0.49
1:B:295:LYS:C	1:B:297:GLY:N	2.59	0.49
1:B:308:ASN:CG	1:B:308:ASN:O	2.49	0.49
1:C:33:THR:HG23	1:C:112:THR:O	2.12	0.49
1:A:240:LYS:HG2	1:A:241:VAL:H	1.76	0.49
1:A:287:ASP:O	1:A:289:ILE:N	2.46	0.49
1:B:28:LEU:HD12	1:B:336:VAL:CG1	2.36	0.49
1:B:310:SER:C	1:B:312:VAL:H	2.15	0.49
1:C:49:GLY:O	1:C:52:PRO:HD2	2.13	0.49
1:D:357:THR:O	1:D:358:ASN:C	2.49	0.49
1:D:451:THR:OG1	1:D:453:SER:HB2	2.13	0.49
1:A:120:PHE:HD1	1:A:284:LEU:CD2	2.24	0.49
1:D:366:LYS:O	1:D:416:HIS:HE1	1.94	0.49
1:D:409:THR:O	1:D:410:ASP:HB3	2.12	0.49
1:A:408:GLU:OE2	1:D:386:MET:CE	2.61	0.49
1:A:363:SER:C	1:A:426:ILE:HD11	2.32	0.49
1:B:117:TYR:CZ	1:B:283:GLY:HA3	2.45	0.49
1:B:44:THR:C	1:B:46:LEU:N	2.66	0.49
1:C:203:VAL:CG2	1:C:233:MET:HA	2.42	0.49
1:C:307:THR:HB	1:C:308:ASN:OD1	2.12	0.49
1:C:73:HIS:CD2	1:D:62:MET:SD	3.05	0.49
1:A:287:ASP:O	1:A:288:LYS:C	2.50	0.49
1:B:348:TYR:CD2	1:B:348:TYR:N	2.80	0.49
1:C:182:VAL:HB	1:C:205:VAL:CG1	2.32	0.49
1:C:308:ASN:OD1	1:C:308:ASN:N	2.45	0.49
1:C:86:ALA:HB3	1:D:74:GLY:HA2	1.94	0.49
1:B:82:ILE:HG12	1:B:199:ILE:HD12	1.93	0.49
1:C:242:VAL:HG21	1:C:256:GLU:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ILE:HA	1:D:319:ILE:HD13	1.93	0.49
1:A:262:GLU:HG3	1:A:262:GLU:O	2.13	0.49
1:A:367:THR:HG23	1:A:370:GLN:CG	2.42	0.49
1:B:415:VAL:C	1:B:416:HIS:ND1	2.66	0.49
1:C:350:LYS:HD3	1:C:433:LEU:HD23	1.94	0.49
1:C:79:ASN:HB2	1:D:78:SER:OG	2.13	0.49
1:A:229:GLU:O	1:A:230:LYS:C	2.50	0.49
1:A:307:THR:OG1	1:A:312:VAL:HB	2.13	0.49
1:B:185:ALA:HB2	1:B:207:GLU:HB2	1.95	0.49
1:C:49:GLY:O	1:C:53:SER:N	2.39	0.49
1:A:121:VAL:HA	1:A:288:LYS:HZ3	1.75	0.48
1:A:164:ILE:HG22	1:A:164:ILE:O	2.13	0.48
1:A:186:GLY:O	1:A:190:LEU:HG	2.13	0.48
1:A:221:ARG:O	1:A:222:LYS:C	2.52	0.48
1:A:51:ILE:HG21	1:A:98:LEU:HD12	1.94	0.48
1:B:119:LYS:HE2	1:B:285:ASN:ND2	2.28	0.48
1:B:119:LYS:HE2	1:B:285:ASN:HD22	1.78	0.48
1:A:70:PHE:HE2	1:B:66:ALA:HB2	1.78	0.48
1:C:101:GLY:O	1:C:105:LEU:HG	2.13	0.48
1:C:159:ILE:HD12	1:C:159:ILE:H	1.77	0.48
1:C:212:ILE:CG2	1:C:237:LEU:HD21	2.43	0.48
1:C:435:TYR:OH	1:D:441:ASP:O	2.31	0.48
1:B:171:LEU:HD23	1:B:192:MET:CE	2.41	0.48
1:B:245:ASP:HB3	1:B:252:LYS:HB2	1.93	0.48
1:C:122:SER:O	1:C:124:SER:N	2.47	0.48
1:A:462:ALA:CB	1:A:467:PRO:HG3	2.43	0.48
1:C:189:GLY:O	1:C:191:GLU:N	2.46	0.48
1:C:204:THR:HG22	1:C:234:LYS:CB	2.38	0.48
1:D:10:VAL:HG21	1:D:143:ILE:HG12	1.95	0.48
1:B:122:SER:O	1:B:124:SER:N	2.47	0.48
1:C:127:SER:O	1:C:128:VAL:HG22	2.13	0.48
1:C:181:VAL:HG11	1:C:253:LEU:HD11	1.94	0.48
1:C:449:HIS:ND1	1:C:449:HIS:C	2.66	0.48
1:D:163:LYS:O	1:D:270:VAL:HA	2.13	0.48
1:D:468:ILE:O	1:D:468:ILE:HG22	2.14	0.48
1:B:403:ILE:HD12	1:B:460:ALA:HA	1.95	0.48
1:C:120:PHE:HB2	1:C:285:ASN:O	2.13	0.48
1:D:158:THR:O	1:D:164:ILE:HG21	2.13	0.48
1:B:149:SER:HB3	1:B:317:ASP:HB3	1.96	0.48
1:D:176:ILE:HD13	1:D:199:ILE:HG23	1.96	0.48
1:D:364:VAL:HG12	1:D:433:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASP:HB2	1:B:416:HIS:CD2	2.48	0.48
1:D:383:PHE:CD1	1:D:458:GLU:CB	2.94	0.48
1:B:216:MET:CE	1:B:220:ILE:HG22	2.44	0.48
1:C:221:ARG:O	1:C:222:LYS:C	2.51	0.48
1:C:406:GLU:CG	1:C:413:LEU:HD21	2.44	0.48
1:B:114:VAL:HG12	1:B:114:VAL:O	2.14	0.48
1:B:438:SER:O	1:B:441:ASP:N	2.47	0.48
1:C:119:LYS:N	1:C:127:SER:O	2.47	0.48
1:A:182:VAL:HB	1:A:205:VAL:HG13	1.96	0.47
1:A:227:SER:HA	1:A:230:LYS:CD	2.37	0.47
1:A:19:TYR:O	1:A:23:ILE:HG13	2.14	0.47
1:B:9:VAL:HG23	1:B:30:PHE:CB	2.39	0.47
1:C:315:ILE:HA	1:C:319:ILE:HD13	1.94	0.47
1:A:188:ILE:O	1:A:192:MET:HG2	2.14	0.47
1:A:439:SER:O	1:A:442:ILE:HG22	2.14	0.47
1:A:465:ASP:CG	1:A:466:LYS:N	2.67	0.47
1:C:170:ALA:HB2	1:C:272:LEU:HD13	1.96	0.47
1:C:46:LEU:HD21	1:C:99:THR:HG22	1.96	0.47
1:D:122:SER:O	1:D:124:SER:N	2.47	0.47
1:D:221:ARG:HH11	1:D:221:ARG:HG2	1.79	0.47
1:D:367:THR:O	1:D:371:VAL:HG23	2.14	0.47
1:A:28:LEU:HA	1:A:28:LEU:HD23	1.77	0.47
1:A:305:PHE:O	1:A:313:TYR:HB3	2.14	0.47
1:A:425:LEU:HB3	1:A:456:ILE:HD11	1.95	0.47
1:A:460:ALA:O	1:A:463:THR:HB	2.13	0.47
1:B:109:ASN:O	1:B:110:LYS:HB2	2.14	0.47
1:C:42:GLY:HA3	1:C:46:LEU:CD2	2.42	0.47
1:A:295:LYS:C	1:A:296:LEU:HD23	2.33	0.47
1:B:160:ASP:O	1:B:161:GLU:C	2.53	0.47
1:B:147:THR:CG2	1:B:284:LEU:HD22	2.11	0.47
1:B:302:ASN:C	1:B:302:ASN:OD1	2.53	0.47
1:C:126:ILE:HD11	1:C:143:ILE:HD13	1.96	0.47
1:C:314:ALA:O	1:C:319:ILE:HG21	2.15	0.47
1:D:10:VAL:HG23	1:D:142:HIS:O	2.14	0.47
1:D:298:ARG:CD	1:D:320:PRO:HA	2.44	0.47
1:D:352:PRO:HB3	1:D:364:VAL:HG22	1.95	0.47
1:B:128:VAL:O	1:B:129:ASP:CB	2.63	0.47
1:B:46:LEU:HD13	1:B:51:ILE:HG13	1.96	0.47
1:C:286:LEU:HD22	1:C:291:VAL:HG21	1.97	0.47
1:D:157:VAL:CG2	1:D:241:VAL:HG11	2.45	0.47
1:D:286:LEU:CD2	1:D:291:VAL:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ALA:HB2	1:D:369:GLU:OE2	2.13	0.47
1:B:174:SER:O	1:B:175:GLU:HB2	2.15	0.47
1:B:8:ASP:HB3	1:B:30:PHE:HB3	1.95	0.47
1:B:357:THR:O	1:B:358:ASN:C	2.51	0.47
1:B:362:ALA:C	1:B:426:ILE:HD12	2.34	0.47
1:B:400:LEU:CD2	1:B:400:LEU:N	2.78	0.47
1:C:119:LYS:O	1:C:127:SER:HB3	2.15	0.47
1:C:130:THR:C	1:C:132:GLU:H	2.16	0.47
1:D:121:VAL:O	1:D:288:LYS:HD2	2.14	0.47
1:B:142:HIS:HB3	1:B:313:TYR:CE1	2.48	0.47
1:C:180:LEU:HD12	1:C:270:VAL:C	2.32	0.47
1:B:444:ARG:HH11	1:B:444:ARG:HG3	1.78	0.47
1:D:10:VAL:HG23	1:D:143:ILE:HG12	1.94	0.47
1:D:161:GLU:O	1:D:162:LYS:CG	2.62	0.47
1:D:286:LEU:CA	1:D:289:ILE:HG13	2.44	0.47
1:B:255:VAL:HG23	1:B:264:THR:OG1	2.15	0.47
1:A:79:ASN:O	1:B:77:VAL:HA	2.14	0.47
1:C:302:ASN:C	1:C:302:ASN:OD1	2.52	0.47
1:C:403:ILE:HD12	1:C:460:ALA:HA	1.96	0.47
1:A:264:THR:HG22	1:A:265:ILE:N	2.30	0.47
1:A:352:PRO:HB3	1:A:364:VAL:HG22	1.97	0.47
1:A:90:GLN:HA	1:A:93:LYS:HB3	1.97	0.47
1:B:296:LEU:HD12	1:B:296:LEU:N	2.30	0.47
1:B:406:GLU:CG	1:B:413:LEU:HD21	2.45	0.47
1:C:82:ILE:N	1:C:82:ILE:HD12	2.29	0.47
1:C:56:LEU:HD22	1:C:87:MET:HE3	1.97	0.47
1:D:63:TYR:CE1	1:D:82:ILE:HD11	2.49	0.47
1:A:181:VAL:HG22	1:A:204:THR:OG1	2.15	0.47
1:C:461:MET:C	1:C:463:THR:N	2.68	0.47
1:D:149:SER:C	1:D:280:PHE:HB2	2.35	0.47
1:D:212:ILE:HG13	1:D:212:ILE:O	2.14	0.47
1:A:184:GLY:H	1:A:274:SER:H	1.64	0.46
1:A:304:ARG:HA	1:A:338:TYR:CE1	2.50	0.46
1:A:66:ALA:HB2	1:B:70:PHE:HE2	1.78	0.46
1:B:281:THR:HG22	1:B:299:ILE:HD11	1.96	0.46
1:C:117:TYR:N	1:C:128:VAL:HG12	2.31	0.46
1:D:404:ILE:HG22	1:D:413:LEU:HB2	1.98	0.46
1:A:180:LEU:HD12	1:A:270:VAL:O	2.16	0.46
1:A:22:ALA:O	1:A:25:ALA:HB3	2.16	0.46
1:A:315:ILE:HD12	1:A:332:GLY:HA2	1.97	0.46
1:B:119:LYS:HA	1:B:284:LEU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:CYS:HB2	1:A:51:ILE:H	1.40	0.46
1:C:117:TYR:C	1:C:128:VAL:HG13	2.36	0.46
1:C:165:VAL:HG23	1:C:272:LEU:CA	2.39	0.46
1:C:305:PHE:HZ	1:C:346:VAL:HG11	1.79	0.46
1:A:86:ALA:O	1:A:89:GLY:CA	2.64	0.46
1:C:315:ILE:O	1:C:315:ILE:HG13	2.16	0.46
1:D:199:ILE:HD13	1:D:199:ILE:HA	1.62	0.46
1:D:293:THR:CG2	1:D:294:ASP:N	2.77	0.46
1:D:389:SER:O	1:D:390:ARG:C	2.51	0.46
1:A:120:PHE:HD1	1:A:284:LEU:HD21	1.80	0.46
1:A:363:SER:N	1:A:426:ILE:HD12	2.30	0.46
1:A:468:ILE:HG21	1:B:20:VAL:HG13	1.98	0.46
1:B:118:GLY:CA	1:B:126:ILE:HD13	2.45	0.46
1:B:291:VAL:HG12	1:B:292:GLU:N	2.29	0.46
1:C:182:VAL:N	1:C:204:THR:O	2.45	0.46
1:C:396:ASN:HD21	1:C:420:PRO:HG3	1.80	0.46
1:D:439:SER:O	1:D:442:ILE:CG2	2.59	0.46
1:A:177:PRO:HB3	1:A:270:VAL:CG2	2.46	0.46
1:A:184:GLY:HA3	1:A:274:SER:C	2.35	0.46
1:C:73:HIS:CG	1:D:62:MET:SD	3.09	0.46
1:D:171:LEU:HD23	1:D:192:MET:CE	2.45	0.46
1:D:227:SER:O	1:D:229:GLU:N	2.49	0.46
1:D:237:LEU:H	1:D:237:LEU:HD12	1.80	0.46
1:A:333:VAL:O	1:A:334:ALA:C	2.53	0.46
1:A:95:VAL:O	1:A:98:LEU:HB2	2.14	0.46
1:B:221:ARG:HH11	1:B:221:ARG:HG2	1.80	0.46
1:B:381:GLY:O	1:B:402:LYS:HA	2.16	0.46
1:B:51:ILE:O	1:B:52:PRO:C	2.53	0.46
1:C:150:ASP:OD1	1:C:151:VAL:N	2.43	0.46
1:C:246:THR:HG22	1:C:251:VAL:CG2	2.46	0.46
1:D:357:THR:O	1:D:358:ASN:O	2.33	0.46
1:D:361:VAL:HA	1:D:417:ILE:O	2.16	0.46
1:A:199:ILE:HD13	1:A:199:ILE:HA	1.59	0.46
1:A:296:LEU:CD2	1:A:296:LEU:N	2.56	0.46
1:A:374:THR:O	1:A:376:VAL:N	2.49	0.46
1:B:388:ASN:OD1	1:B:391:ALA:N	2.39	0.46
1:B:363:SER:C	1:B:426:ILE:HD11	2.36	0.46
1:B:51:ILE:HB	1:B:52:PRO:CD	2.43	0.46
1:C:166:SER:O	1:C:169:GLY:N	2.48	0.46
1:C:177:PRO:HG2	1:C:201:SER:OG	2.14	0.46
1:C:420:PRO:O	1:C:421:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:PRO:HA	1:A:454:GLU:OE1	2.16	0.46
1:B:96:SER:O	1:B:97:ASN:C	2.53	0.46
1:C:180:LEU:HG	1:C:181:VAL:N	2.30	0.46
1:D:216:MET:HE1	1:D:221:ARG:HA	1.96	0.46
1:A:192:MET:HG3	1:A:272:LEU:HD21	1.98	0.46
1:A:79:ASN:HB2	1:B:78:SER:OG	2.16	0.46
1:B:151:VAL:CG1	1:B:152:LYS:N	2.75	0.46
1:C:37:LYS:HD3	1:C:117:TYR:CE1	2.50	0.46
1:A:178:LYS:HD3	1:A:178:LYS:HA	1.72	0.45
1:A:292:GLU:H	1:A:308:ASN:ND2	2.13	0.45
1:A:304:ARG:HA	1:A:338:TYR:CD1	2.51	0.45
1:A:5:ASP:HA	1:A:31:LYS:HE2	1.94	0.45
1:B:388:ASN:HB3	1:B:391:ALA:HB3	1.96	0.45
1:B:439:SER:OG	1:B:463:THR:HG21	2.16	0.45
1:D:207:GLU:HG3	1:D:209:ALA:N	2.31	0.45
1:D:20:VAL:O	1:D:21:ALA:C	2.55	0.45
1:D:440:GLU:OE2	1:D:464:TYR:CE2	2.69	0.45
1:D:70:PHE:HB3	1:D:75:VAL:O	2.15	0.45
1:B:25:ALA:O	1:B:28:LEU:N	2.48	0.45
1:D:400:LEU:N	1:D:400:LEU:HD23	2.32	0.45
1:D:51:ILE:O	1:D:52:PRO:C	2.53	0.45
1:A:120:PHE:CD1	1:A:284:LEU:HD21	2.51	0.45
1:A:449:HIS:CE1	1:A:450:PRO:HB3	2.52	0.45
1:B:32:THR:HG22	1:B:33:THR:N	2.31	0.45
1:C:449:HIS:ND1	1:C:450:PRO:N	2.64	0.45
1:C:97:ASN:HD22	1:C:97:ASN:C	2.19	0.45
1:D:10:VAL:HB	1:D:143:ILE:HG12	1.98	0.45
1:D:254:THR:O	1:D:254:THR:HG22	2.15	0.45
1:D:285:ASN:OD1	1:D:286:LEU:N	2.49	0.45
1:A:230:LYS:HE3	1:A:398:GLU:OE1	2.16	0.45
1:B:122:SER:C	1:B:124:SER:N	2.69	0.45
1:B:158:THR:HG22	1:B:160:ASP:CG	2.36	0.45
1:B:291:VAL:CG1	1:B:292:GLU:N	2.78	0.45
1:B:409:THR:O	1:B:410:ASP:CB	2.64	0.45
1:C:121:VAL:O	1:C:121:VAL:CG1	2.63	0.45
1:C:147:THR:O	1:C:318:VAL:HG22	2.17	0.45
1:C:383:PHE:CZ	1:C:387:ALA:HB3	2.52	0.45
1:D:82:ILE:HG21	1:D:199:ILE:HD12	1.98	0.45
1:A:208:PHE:C	1:A:208:PHE:CD1	2.89	0.45
1:B:165:VAL:HG23	1:B:272:LEU:CD1	2.47	0.45
1:C:82:ILE:HG21	1:C:199:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:THR:OG1	1:D:370:GLN:HG3	2.17	0.45
1:A:46:LEU:HD11	1:A:98:LEU:HB2	1.98	0.45
1:B:16:PRO:HD2	2:B:480:FAD:O5'	2.16	0.45
1:C:290:GLY:O	1:C:291:VAL:C	2.55	0.45
1:C:78:SER:OG	1:D:79:ASN:HB2	2.16	0.45
1:A:142:HIS:HB3	1:A:313:TYR:HE1	1.81	0.45
1:A:217:ASP:OD1	1:A:402:LYS:NZ	2.49	0.45
1:A:305:PHE:HE2	1:A:319:ILE:HD11	1.82	0.45
1:C:178:LYS:HA	1:C:178:LYS:HD3	1.76	0.45
1:C:388:ASN:O	1:C:389:SER:C	2.54	0.45
1:C:468:ILE:O	1:C:468:ILE:CG2	2.64	0.45
1:D:177:PRO:HG2	1:D:201:SER:OG	2.16	0.45
1:D:220:ILE:O	1:D:221:ARG:C	2.52	0.45
1:A:154:LEU:CD2	1:A:183:ILE:HG21	2.46	0.45
1:A:82:ILE:CD1	1:A:82:ILE:N	2.79	0.45
1:D:376:VAL:HG12	1:D:377:GLU:N	2.31	0.45
1:B:295:LYS:HB3	1:B:296:LEU:H	1.69	0.45
1:B:9:VAL:HB	1:B:32:THR:HG23	1.98	0.45
1:B:351:VAL:HA	1:B:352:PRO:HD2	1.64	0.45
1:B:466:LYS:HA	1:B:467:PRO:HD3	1.75	0.45
1:C:154:LEU:HD12	1:C:154:LEU:C	2.36	0.45
1:C:48:VAL:HG11	1:C:168:THR:OG1	2.17	0.45
1:C:208:PHE:HA	1:C:239:THR:O	2.16	0.45
1:C:213:VAL:HG12	1:C:216:MET:HB2	1.98	0.45
1:D:145:ILE:N	1:D:313:TYR:O	2.41	0.45
1:D:345:HIS:ND1	1:D:345:HIS:C	2.70	0.45
1:D:345:HIS:O	1:D:345:HIS:CG	2.70	0.45
1:A:328:ALA:O	1:A:329:GLU:C	2.55	0.45
1:B:253:LEU:O	1:B:265:ILE:CG2	2.64	0.45
1:A:421:ASN:ND2	1:B:421:ASN:ND2	2.65	0.45
1:C:468:ILE:HG21	1:D:20:VAL:HG13	1.99	0.45
1:A:134:GLU:HB3	1:A:135:ASN:H	1.58	0.44
1:C:181:VAL:HG23	1:C:268:ALA:CB	2.46	0.44
1:C:20:VAL:HG13	1:D:468:ILE:HG21	1.98	0.44
1:C:389:SER:HB3	1:D:51:ILE:HD11	1.99	0.44
1:B:121:VAL:N	1:B:125:GLU:O	2.25	0.44
1:C:444:ARG:HG3	1:C:444:ARG:HH11	1.82	0.44
1:D:192:MET:CA	1:D:192:MET:CE	2.95	0.44
1:D:351:VAL:HG12	1:D:351:VAL:O	2.16	0.44
1:A:160:ASP:HB2	1:A:162:LYS:H	1.82	0.44
1:B:123:PRO:CG	1:B:289:ILE:HD13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLU:HB3	1:B:300:LEU:HD23	1.99	0.44
1:D:180:LEU:HB3	1:D:203:VAL:HG12	1.98	0.44
1:D:466:LYS:HA	1:D:467:PRO:HD3	1.72	0.44
1:A:101:GLY:O	1:A:105:LEU:HG	2.17	0.44
1:A:280:PHE:CE1	1:A:282:SER:HB3	2.52	0.44
1:A:327:LYS:HE2	1:A:348:TYR:CE1	2.52	0.44
1:B:352:PRO:HB3	1:B:364:VAL:CG2	2.47	0.44
1:B:468:ILE:O	1:B:468:ILE:CG2	2.66	0.44
1:B:88:MET:HE1	1:B:91:LYS:NZ	2.32	0.44
1:C:82:ILE:HG12	1:C:199:ILE:CD1	2.48	0.44
1:C:396:ASN:ND2	1:C:420:PRO:HG3	2.33	0.44
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.69	0.44
1:A:362:ALA:HB1	1:A:426:ILE:HD12	2.00	0.44
1:B:282:SER:O	1:B:283:GLY:C	2.56	0.44
1:C:181:VAL:HG13	1:C:204:THR:O	2.17	0.44
1:C:305:PHE:CZ	1:C:346:VAL:HG11	2.52	0.44
1:C:448:ALA:O	1:C:451:THR:CG2	2.64	0.44
1:D:217:ASP:CB	1:D:416:HIS:CD2	2.99	0.44
1:D:42:GLY:CA	1:D:46:LEU:HB3	2.43	0.44
1:B:283:GLY:C	1:B:284:LEU:O	2.56	0.44
1:B:38:ARG:CD	1:B:47:ASN:HD22	2.30	0.44
1:C:246:THR:HG22	1:C:251:VAL:HG21	1.98	0.44
1:C:262:GLU:CG	1:C:263:GLN:N	2.79	0.44
1:C:358:ASN:CB	1:C:359:PRO:HD3	2.45	0.44
1:D:155:PRO:O	1:D:157:VAL:N	2.51	0.44
1:D:160:ASP:O	1:D:161:GLU:HB2	2.17	0.44
1:B:102:ILE:O	1:B:105:LEU:HB2	2.18	0.44
1:C:38:ARG:HG2	1:C:39:GLY:N	2.32	0.44
1:C:50:CYS:HB3	1:C:51:ILE:HD13	1.99	0.44
1:D:26:ALA:HB1	1:D:109:ASN:O	2.17	0.44
1:D:41:LEU:HD11	1:D:106:PHE:CD1	2.51	0.44
1:A:159:ILE:HG23	1:A:164:ILE:HG22	2.00	0.44
1:A:120:PHE:N	1:A:285:ASN:HB3	2.31	0.44
1:C:189:GLY:O	1:C:190:LEU:C	2.56	0.44
1:C:63:TYR:CE1	1:C:80:VAL:HG12	2.53	0.44
1:D:142:HIS:CB	3:D:2004:HOH:O	2.64	0.44
1:D:400:LEU:HD23	1:D:400:LEU:H	1.83	0.44
1:D:449:HIS:ND1	1:D:450:PRO:CA	2.81	0.44
1:A:236:LYS:HD3	1:A:266:ILE:HD11	1.98	0.44
1:B:304:ARG:O	1:B:305:PHE:HB2	2.18	0.44
1:B:352:PRO:HA	1:B:364:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:CD1	1:C:156:GLY:N	2.77	0.44
1:C:154:LEU:HD21	1:C:241:VAL:CG1	2.48	0.44
1:C:262:GLU:CG	1:C:263:GLN:H	2.28	0.44
1:C:358:ASN:HB3	1:C:359:PRO:CD	2.46	0.44
1:D:116:GLY:HA3	1:D:128:VAL:HG12	2.00	0.44
1:D:184:GLY:HA3	1:D:274:SER:C	2.39	0.44
1:A:163:LYS:HA	1:A:270:VAL:HG13	2.00	0.43
1:B:6:GLU:HB3	1:B:33:THR:OG1	2.18	0.43
1:B:88:MET:O	1:B:91:LYS:HB3	2.17	0.43
1:C:352:PRO:HB3	1:C:364:VAL:HG22	2.00	0.43
1:D:136:THR:O	1:D:136:THR:HG22	2.16	0.43
1:D:84:LEU:HG	1:D:84:LEU:O	2.18	0.43
1:A:348:TYR:N	1:A:348:TYR:CD2	2.86	0.43
1:A:88:MET:HE3	1:A:91:LYS:HD3	2.00	0.43
1:D:46:LEU:HD11	1:D:98:LEU:CB	2.46	0.43
1:A:194:SER:O	1:A:198:ARG:HG3	2.18	0.43
1:A:264:THR:HG22	1:A:265:ILE:H	1.82	0.43
1:A:442:ILE:HD13	1:A:442:ILE:HG21	1.61	0.43
1:B:176:ILE:CD1	1:B:199:ILE:CG2	2.96	0.43
1:B:286:LEU:O	1:B:287:ASP:C	2.55	0.43
1:B:385:PHE:CB	3:B:2021:HOH:O	2.66	0.43
1:B:50:CYS:HB2	1:B:51:ILE:H	1.52	0.43
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.81	0.43
1:D:187:TYR:CG	1:D:355:VAL:HG22	2.53	0.43
1:D:263:GLN:HG2	1:D:263:GLN:H	1.59	0.43
1:C:447:HIS:CD2	1:D:427:HIS:CD2	3.06	0.43
1:D:52:PRO:HB3	1:D:91:LYS:HE3	2.00	0.43
1:D:54:LYS:HD3	1:D:57:LEU:CD1	2.47	0.43
1:A:292:GLU:HB2	1:A:308:ASN:OD1	2.18	0.43
1:C:54:LYS:HD3	1:C:57:LEU:HD12	1.99	0.43
1:D:49:GLY:H	1:D:52:PRO:HG2	1.83	0.43
1:A:300:LEU:HA	1:A:300:LEU:HD23	1.87	0.43
1:A:367:THR:HG23	1:A:370:GLN:CD	2.39	0.43
1:A:370:GLN:O	1:A:371:VAL:C	2.57	0.43
1:B:13:GLY:O	1:B:18:GLY:HA3	2.18	0.43
1:C:86:ALA:HB3	1:D:74:GLY:CA	2.47	0.43
1:D:286:LEU:O	1:D:288:LYS:N	2.51	0.43
1:D:53:SER:O	1:D:57:LEU:CG	2.65	0.43
1:A:146:ALA:C	1:A:147:THR:O	2.51	0.43
1:A:152:LYS:CB	1:A:276:GLY:O	2.66	0.43
1:A:70:PHE:HB3	1:A:75:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ALA:C	1:B:261:GLY:H	2.12	0.43
1:C:181:VAL:HG11	1:C:253:LEU:CD1	2.49	0.43
1:C:6:GLU:HG2	1:C:139:LYS:HD3	1.99	0.43
1:D:364:VAL:HG12	1:D:365:GLY:N	2.33	0.43
1:A:367:THR:N	1:A:370:GLN:HG3	2.30	0.43
1:A:470:ILE:HD12	1:A:470:ILE:HA	1.85	0.43
1:B:150:ASP:CG	1:B:151:VAL:N	2.72	0.43
1:A:74:GLY:O	1:B:82:ILE:HA	2.19	0.43
1:C:173:LEU:HD12	1:C:196:TRP:CE2	2.54	0.43
1:C:173:LEU:HD12	1:C:196:TRP:CZ2	2.54	0.43
1:D:117:TYR:OH	1:D:283:GLY:CA	2.67	0.43
1:D:333:VAL:O	1:D:334:ALA:C	2.54	0.43
1:D:439:SER:OG	1:D:463:THR:HG21	2.19	0.43
1:B:382:LYS:HG2	1:B:402:LYS:HB2	2.01	0.43
1:C:23:ILE:HG23	1:C:109:ASN:ND2	2.34	0.43
1:C:270:VAL:HG13	1:C:271:VAL:H	1.83	0.43
1:D:292:GLU:HG3	1:D:308:ASN:ND2	2.33	0.43
1:A:217:ASP:HB2	1:A:416:HIS:CD2	2.54	0.43
1:A:301:VAL:HG22	1:A:302:ASN:H	1.83	0.43
1:B:176:ILE:CD1	1:B:199:ILE:HG23	2.45	0.43
1:B:461:MET:C	1:B:463:THR:H	2.21	0.43
1:C:26:ALA:HB1	1:C:109:ASN:O	2.18	0.43
1:C:290:GLY:O	1:C:308:ASN:ND2	2.51	0.43
1:C:301:VAL:HG22	1:C:302:ASN:H	1.83	0.43
1:D:280:PHE:C	1:D:280:PHE:CD2	2.91	0.43
1:D:367:THR:N	1:D:370:GLN:HE21	2.12	0.43
1:A:366:LYS:O	1:A:416:HIS:HE1	2.01	0.43
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.88	0.43
1:C:216:MET:HE3	1:C:361:VAL:HG11	2.00	0.43
1:C:88:MET:CE	3:C:2007:HOH:O	2.58	0.43
1:D:286:LEU:HD22	1:D:291:VAL:HB	2.00	0.43
1:D:96:SER:O	1:D:97:ASN:O	2.36	0.43
1:B:181:VAL:HA	1:B:204:THR:O	2.19	0.42
1:C:192:MET:O	1:C:193:GLY:C	2.57	0.42
1:C:207:GLU:HG3	1:C:209:ALA:N	2.34	0.42
1:D:192:MET:O	1:D:193:GLY:C	2.57	0.42
1:D:28:LEU:CD1	1:D:336:VAL:HG12	2.47	0.42
1:D:51:ILE:CB	1:D:52:PRO:HD3	2.44	0.42
1:A:190:LEU:HD13	1:A:228:LEU:HD11	2.00	0.42
1:A:358:ASN:CB	1:A:359:PRO:CD	2.93	0.42
1:A:69:SER:O	1:A:71:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASP:O	1:B:151:VAL:O	2.36	0.42
1:B:151:VAL:CG1	1:B:152:LYS:H	2.28	0.42
1:B:8:ASP:CG	1:B:31:LYS:H	2.22	0.42
1:B:355:VAL:O	1:B:360:GLU:HA	2.19	0.42
1:B:416:HIS:ND1	1:B:416:HIS:N	2.66	0.42
1:B:54:LYS:N	1:B:54:LYS:HE2	2.34	0.42
1:C:242:VAL:HB	1:C:255:VAL:CA	2.36	0.42
1:D:159:ILE:HG23	1:D:165:VAL:HA	2.00	0.42
1:D:219:GLU:O	1:D:222:LYS:HB2	2.19	0.42
1:D:313:TYR:CZ	1:D:339:LEU:HD21	2.53	0.42
1:A:364:VAL:HG12	1:A:365:GLY:N	2.34	0.42
1:A:382:LYS:HB2	1:A:382:LYS:HE3	1.79	0.42
1:B:265:ILE:O	1:B:266:ILE:HD13	2.20	0.42
1:B:38:ARG:HG2	1:B:39:GLY:N	2.34	0.42
1:B:97:ASN:C	1:B:97:ASN:ND2	2.72	0.42
1:C:167:SER:O	1:C:170:ALA:HB3	2.19	0.42
1:C:179:LYS:O	1:C:269:ASP:N	2.51	0.42
1:C:285:ASN:C	1:C:287:ASP:N	2.71	0.42
1:D:121:VAL:O	1:D:121:VAL:HG12	2.20	0.42
1:D:305:PHE:O	1:D:313:TYR:HA	2.19	0.42
1:A:164:ILE:HD11	1:A:244:VAL:CG1	2.47	0.42
1:A:357:THR:O	1:A:358:ASN:C	2.55	0.42
1:B:265:ILE:CD1	1:B:265:ILE:N	2.82	0.42
1:B:253:LEU:O	1:B:265:ILE:HA	2.19	0.42
1:B:298:ARG:HH11	1:B:320:PRO:HA	1.84	0.42
1:C:212:ILE:HD13	1:C:225:GLN:HG3	1.99	0.42
1:C:70:PHE:O	1:C:71:ALA:O	2.37	0.42
1:D:315:ILE:O	1:D:318:VAL:HG23	2.19	0.42
1:D:400:LEU:N	1:D:400:LEU:CD2	2.83	0.42
1:A:351:VAL:HA	1:A:352:PRO:HD2	1.89	0.42
1:A:449:HIS:C	1:A:449:HIS:ND1	2.72	0.42
1:A:461:MET:C	1:A:463:THR:H	2.22	0.42
1:A:71:ALA:O	1:A:73:HIS:N	2.52	0.42
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.81	0.42
1:B:228:LEU:HB3	1:B:233:MET:HE3	2.01	0.42
1:B:310:SER:OG	1:B:311:GLY:N	2.52	0.42
1:B:87:MET:C	1:B:89:GLY:N	2.72	0.42
1:C:82:ILE:HG12	1:C:199:ILE:HD12	2.01	0.42
1:C:24:LYS:O	1:C:27:GLN:HB2	2.19	0.42
1:D:149:SER:N	1:D:280:PHE:HB3	2.34	0.42
1:D:302:ASN:OD1	1:D:302:ASN:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ILE:HA	1:D:313:TYR:O	2.19	0.42
1:A:371:VAL:O	1:A:372:LYS:C	2.58	0.42
1:B:120:PHE:HA	1:B:126:ILE:CG2	2.30	0.42
1:C:126:ILE:HG13	1:C:143:ILE:HD13	2.02	0.42
1:C:164:ILE:CG2	1:C:273:VAL:HG23	2.49	0.42
1:C:176:ILE:CG2	1:C:199:ILE:HG22	2.49	0.42
1:C:20:VAL:O	1:C:21:ALA:C	2.58	0.42
1:D:240:LYS:HE3	1:D:242:VAL:CG1	2.49	0.42
1:D:294:ASP:O	1:D:295:LYS:C	2.57	0.42
1:A:239:THR:HG21	1:A:255:VAL:HG22	1.98	0.42
1:A:51:ILE:HG21	1:A:98:LEU:CD1	2.49	0.42
1:B:350:LYS:NZ	3:B:2017:HOH:O	2.32	0.42
1:B:350:LYS:O	1:B:352:PRO:HD3	2.20	0.42
1:C:394:ILE:HA	1:C:394:ILE:HD13	1.80	0.42
1:C:450:PRO:HA	1:C:454:GLU:OE1	2.19	0.42
2:C:480:FAD:H9	2:C:480:FAD:H1'1	1.77	0.42
1:D:117:TYR:O	1:D:128:VAL:HA	2.19	0.42
1:D:186:GLY:O	1:D:190:LEU:HG	2.20	0.42
1:A:137:VAL:O	1:A:137:VAL:HG12	2.19	0.42
1:A:87:MET:C	1:A:89:GLY:N	2.72	0.42
1:B:199:ILE:HG23	1:B:199:ILE:O	2.19	0.42
1:B:219:GLU:O	1:B:222:LYS:HB2	2.20	0.42
1:A:20:VAL:HG13	1:B:468:ILE:HG21	2.02	0.42
1:C:348:TYR:N	1:C:348:TYR:CD2	2.85	0.42
1:D:227:SER:C	1:D:229:GLU:N	2.72	0.42
1:D:406:GLU:HB2	1:D:409:THR:OG1	2.19	0.42
1:C:451:THR:HB	1:D:424:GLU:OE2	2.19	0.42
1:D:449:HIS:ND1	1:D:450:PRO:N	2.68	0.42
1:B:117:TYR:C	1:B:117:TYR:CD2	2.93	0.42
1:B:9:VAL:CG2	1:B:30:PHE:CB	2.98	0.42
1:C:242:VAL:CB	1:C:256:GLU:H	2.31	0.42
1:C:56:LEU:HD13	1:C:195:VAL:HG11	2.02	0.42
1:D:9:VAL:CB	1:D:32:THR:HG23	2.47	0.42
1:B:251:VAL:HG12	1:B:252:LYS:N	2.35	0.42
1:B:165:VAL:HG23	1:B:272:LEU:HD13	2.02	0.42
1:B:378:TYR:HB2	1:B:405:ALA:O	2.20	0.42
1:C:130:THR:C	1:C:132:GLU:N	2.73	0.42
1:C:218:ALA:O	1:C:219:GLU:C	2.56	0.42
1:C:363:SER:C	1:C:426:ILE:HD11	2.39	0.42
1:C:87:MET:O	1:C:88:MET:C	2.57	0.42
1:D:161:GLU:CA	1:D:165:VAL:HG12	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:GLY:HA3	2:D:480:FAD:O5B	2.20	0.42
1:D:54:LYS:HD3	1:D:57:LEU:HD12	2.02	0.42
1:B:24:LYS:O	1:B:27:GLN:HB2	2.20	0.41
1:B:181:VAL:HG21	1:B:266:ILE:CG2	2.50	0.41
1:B:63:TYR:O	1:B:64:HIS:C	2.57	0.41
1:C:366:LYS:O	1:C:416:HIS:CE1	2.70	0.41
1:C:79:ASN:H	1:D:78:SER:HB2	1.85	0.41
1:D:10:VAL:CB	1:D:143:ILE:HG12	2.50	0.41
1:A:150:ASP:CG	1:A:151:VAL:N	2.72	0.41
1:A:439:SER:O	1:A:442:ILE:CG2	2.68	0.41
1:B:199:ILE:CG2	1:B:199:ILE:O	2.64	0.41
1:B:245:ASP:O	1:B:245:ASP:OD2	2.37	0.41
1:C:116:GLY:HA3	1:C:128:VAL:CG1	2.50	0.41
1:D:101:GLY:O	1:D:105:LEU:HG	2.20	0.41
1:A:170:ALA:HB2	1:A:272:LEU:HD13	2.02	0.41
1:A:225:GLN:O	1:A:226:ARG:C	2.58	0.41
1:A:384:PRO:HG2	1:A:384:PRO:O	2.20	0.41
1:A:46:LEU:CD2	1:A:99:THR:HG22	2.50	0.41
1:B:26:ALA:HB1	1:B:109:ASN:O	2.20	0.41
1:B:292:GLU:HB3	1:B:300:LEU:CG	2.51	0.41
1:C:258:SER:N	1:C:259:ALA:N	2.68	0.41
1:C:289:ILE:HG13	1:C:290:GLY:N	2.32	0.41
1:A:232:GLY:O	1:A:233:MET:HB2	2.19	0.41
1:A:345:HIS:CD2	3:A:2022:HOH:O	2.73	0.41
1:A:36:GLU:OE2	2:A:480:FAD:H4B	2.20	0.41
1:A:392:LYS:HD2	1:A:392:LYS:HA	1.81	0.41
1:B:5:ASP:O	1:B:31:LYS:HB3	2.20	0.41
1:B:461:MET:C	1:B:463:THR:N	2.74	0.41
1:B:461:MET:HA	1:B:464:TYR:CE1	2.55	0.41
1:C:180:LEU:HB3	1:C:203:VAL:HG12	2.03	0.41
1:D:350:LYS:HD3	1:D:433:LEU:HD23	2.01	0.41
1:A:181:VAL:HA	1:A:204:THR:O	2.21	0.41
1:A:241:VAL:O	1:A:242:VAL:O	2.38	0.41
1:A:243:GLY:O	1:A:254:THR:HG23	2.20	0.41
1:A:274:SER:O	1:A:274:SER:OG	2.31	0.41
1:A:364:VAL:HG12	1:A:433:LEU:HD22	2.02	0.41
1:D:305:PHE:CE2	1:D:331:ASP:HB3	2.55	0.41
1:D:38:ARG:HG2	1:D:39:GLY:N	2.35	0.41
1:A:302:ASN:OD1	1:A:302:ASN:C	2.57	0.41
1:A:408:GLU:OE2	1:D:386:MET:HE2	2.20	0.41
1:B:281:THR:CA	1:B:284:LEU:HD21	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ALA:O	1:B:328:ALA:HB3	2.21	0.41
1:B:418:MET:O	1:B:419:ALA:HB2	2.20	0.41
1:C:176:ILE:CD1	1:C:199:ILE:HG23	2.44	0.41
1:C:229:GLU:C	1:C:231:GLN:N	2.70	0.41
1:C:83:ASP:O	1:C:86:ALA:N	2.51	0.41
1:D:51:ILE:N	1:D:52:PRO:CD	2.83	0.41
1:A:23:ILE:HG23	1:A:109:ASN:ND2	2.36	0.41
1:A:38:ARG:HG2	1:A:39:GLY:N	2.36	0.41
1:B:199:ILE:HA	1:B:199:ILE:HD13	1.60	0.41
1:C:264:THR:O	1:C:265:ILE:HD12	2.21	0.41
1:C:266:ILE:HG13	1:C:266:ILE:H	1.76	0.41
1:C:440:GLU:O	1:C:444:ARG:N	2.53	0.41
1:D:376:VAL:CG1	1:D:377:GLU:N	2.84	0.41
1:A:361:VAL:HA	1:A:417:ILE:O	2.20	0.41
1:A:42:GLY:CA	1:A:46:LEU:HD23	2.51	0.41
1:A:461:MET:C	1:A:463:THR:N	2.74	0.41
1:B:295:LYS:HD3	1:B:295:LYS:HA	1.73	0.41
1:C:116:GLY:C	1:C:128:VAL:CG1	2.89	0.41
1:C:22:ALA:O	1:C:25:ALA:HB3	2.20	0.41
1:C:265:ILE:HA	1:C:265:ILE:HD12	1.84	0.41
1:D:95:VAL:O	1:D:96:SER:C	2.59	0.41
1:D:97:ASN:HD22	1:D:97:ASN:C	2.24	0.41
1:A:287:ASP:O	1:A:290:GLY:N	2.54	0.41
1:B:173:LEU:HD12	1:B:196:TRP:CE2	2.55	0.41
1:A:75:VAL:HG22	1:B:63:TYR:HB2	2.02	0.41
1:C:274:SER:C	1:C:275:ALA:O	2.59	0.41
1:C:442:ILE:H	1:C:442:ILE:HG22	1.52	0.41
1:C:444:ARG:HG3	1:C:444:ARG:NH1	2.36	0.41
1:C:70:PHE:CZ	1:D:70:PHE:HZ	2.38	0.41
1:D:422:ALA:HA	1:D:425:LEU:HD12	2.02	0.41
1:D:87:MET:C	1:D:89:GLY:N	2.74	0.41
1:A:102:ILE:O	1:A:105:LEU:HB2	2.20	0.41
1:A:154:LEU:HA	1:A:155:PRO:HD3	1.82	0.41
1:A:163:LYS:HB3	1:A:163:LYS:HE2	1.76	0.41
1:B:143:ILE:O	1:B:313:TYR:N	2.52	0.41
1:B:217:ASP:CB	1:B:416:HIS:CD2	3.04	0.41
1:B:358:ASN:CB	1:B:359:PRO:CD	2.99	0.41
1:B:385:PHE:C	1:B:387:ALA:N	2.73	0.41
1:B:448:ALA:O	1:B:451:THR:CG2	2.69	0.41
1:B:450:PRO:CG	1:B:450:PRO:O	2.68	0.41
1:B:50:CYS:O	1:B:54:LYS:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:VAL:HG21	1:D:431:ILE:CG1	2.51	0.41
1:C:88:MET:HE3	1:C:91:LYS:HD3	2.03	0.41
1:D:109:ASN:O	1:D:110:LYS:HB2	2.21	0.41
1:D:364:VAL:CG1	1:D:365:GLY:N	2.83	0.41
1:A:272:LEU:HD12	1:A:273:VAL:N	2.35	0.41
1:B:150:ASP:CG	1:B:151:VAL:H	2.24	0.41
1:B:178:LYS:HD3	1:B:178:LYS:HA	1.87	0.41
1:B:265:ILE:C	1:B:266:ILE:HD13	2.41	0.41
1:B:292:GLU:N	1:B:308:ASN:OD1	2.46	0.41
1:D:53:SER:O	1:D:57:LEU:CD1	2.69	0.41
1:D:53:SER:O	1:D:57:LEU:HD12	2.21	0.41
1:A:327:LYS:HE2	1:A:348:TYR:CZ	2.56	0.40
1:A:390:ARG:O	1:A:391:ALA:C	2.59	0.40
1:A:409:THR:O	1:A:410:ASP:CB	2.69	0.40
1:B:348:TYR:N	1:B:348:TYR:HD2	2.19	0.40
1:B:58:HIS:O	1:B:62:MET:HG3	2.21	0.40
1:B:80:VAL:C	1:B:81:GLU:CG	2.90	0.40
1:C:121:VAL:O	1:C:122:SER:HB3	2.21	0.40
1:C:126:ILE:CG1	1:C:143:ILE:HD13	2.50	0.40
1:C:362:ALA:CB	1:C:426:ILE:HD12	2.49	0.40
1:C:50:CYS:O	1:C:54:LYS:HB2	2.21	0.40
1:D:177:PRO:HB3	1:D:270:VAL:HG23	2.02	0.40
1:A:466:LYS:HA	1:A:467:PRO:HD3	1.75	0.40
1:C:124:SER:O	1:C:139:LYS:CB	2.69	0.40
1:C:270:VAL:HG12	1:C:271:VAL:N	2.36	0.40
1:C:350:LYS:O	1:C:352:PRO:HD3	2.21	0.40
1:D:274:SER:O	1:D:274:SER:OG	2.37	0.40
1:A:208:PHE:CD1	1:A:208:PHE:O	2.75	0.40
1:B:216:MET:CE	1:B:221:ARG:HA	2.45	0.40
1:B:28:LEU:HD13	1:B:340:ALA:HB2	2.02	0.40
1:B:449:HIS:ND1	1:B:450:PRO:N	2.69	0.40
1:C:435:TYR:O	1:C:436:ASP:C	2.59	0.40
1:D:415:VAL:HG21	1:D:429:ALA:HB1	2.02	0.40
1:A:301:VAL:HG22	1:A:302:ASN:N	2.36	0.40
1:A:394:ILE:HA	1:A:394:ILE:HD13	1.78	0.40
1:A:51:ILE:O	1:A:52:PRO:C	2.59	0.40
1:B:117:TYR:OH	1:B:283:GLY:CA	2.69	0.40
1:B:184:GLY:HA3	1:B:274:SER:C	2.41	0.40
1:B:212:ILE:HD11	1:B:225:GLN:HB2	2.02	0.40
1:B:359:PRO:HG2	1:B:398:GLU:OE2	2.22	0.40
1:B:362:ALA:HB1	1:B:426:ILE:CD1	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ASN:OD1	1:B:390:ARG:HB3	2.21	0.40
1:B:42:GLY:HA2	1:B:46:LEU:HD23	2.04	0.40
1:C:186:GLY:O	1:C:190:LEU:HG	2.22	0.40
1:C:292:GLU:N	1:C:308:ASN:HD21	2.19	0.40
1:C:54:LYS:HA	1:C:54:LYS:HD3	1.91	0.40
1:A:220:ILE:HG23	1:A:220:ILE:HD12	1.78	0.40
1:A:431:ILE:HG23	1:A:432:ALA:N	2.36	0.40
1:C:187:TYR:CD1	1:C:187:TYR:N	2.90	0.40
1:C:194:SER:O	1:C:195:VAL:C	2.59	0.40
1:C:252:LYS:HE2	1:C:267:GLU:OE2	2.22	0.40
1:C:46:LEU:HD21	1:C:99:THR:HA	2.03	0.40
1:D:150:ASP:CG	1:D:151:VAL:N	2.75	0.40
1:D:213:VAL:HG12	1:D:216:MET:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/470 (99%)	368 (79%)	71 (15%)	27 (6%)	1	11
1	B	466/470 (99%)	357 (77%)	71 (15%)	38 (8%)	1	4
1	C	463/470 (98%)	367 (79%)	62 (13%)	34 (7%)	1	6
1	D	465/470 (99%)	350 (75%)	90 (19%)	25 (5%)	2	12
All	All	1860/1880 (99%)	1442 (78%)	294 (16%)	124 (7%)	1	8

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	129	ASP

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Mol	Chain	Res	Type
1	A	161	GLU
1	A	201	SER
1	A	232	GLY
1	A	242	VAL
1	A	259	ALA
1	A	260	GLY
1	A	261	GLY
1	A	347	ASP
1	B	50	CYS
1	B	129	ASP
1	B	134	GLU
1	B	151	VAL
1	B	153	SER
1	B	154	LEU
1	B	159	ILE
1	B	161	GLU
1	B	187[A]	TYR
1	B	187[B]	TYR
1	B	259	ALA
1	B	261	GLY
1	B	270	VAL
1	B	282	SER
1	B	284	LEU
1	B	290	GLY
1	C	72	ASN
1	C	187	TYR
1	C	230	LYS
1	C	247	SER
1	C	262	GLU
1	C	263	GLN
1	C	264	THR
1	C	287	ASP
1	D	7	ASN
1	D	129	ASP
1	D	130	THR
1	D	239	THR
1	D	347	ASP
1	A	70	PHE
1	A	72	ASN
1	A	195	VAL
1	A	230	LYS
1	A	275	ALA

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Mol	Chain	Res	Type
1	A	288	LYS
1	A	290	GLY
1	B	72	ASN
1	B	118	GLY
1	B	283	GLY
1	B	289	ILE
1	B	296	LEU
1	B	311	GLY
1	C	50	CYS
1	C	71	ALA
1	C	128	VAL
1	C	156	GLY
1	C	161	GLU
1	C	167	SER
1	C	190	LEU
1	C	195	VAL
1	C	229	GLU
1	C	234	LYS
1	C	288	LYS
1	D	50	CYS
1	D	80	VAL
1	D	276	GLY
1	D	287	ASP
1	D	310	SER
1	D	358	ASN
1	A	263	GLN
1	A	297	GLY
1	B	7	ASN
1	B	46	LEU
1	B	135	ASN
1	B	156	GLY
1	B	245	ASP
1	B	288	LYS
1	C	241	VAL
1	C	243	GLY
1	C	283	GLY
1	D	72	ASN
1	D	97	ASN
1	D	123	PRO
1	D	187	TYR
1	D	228	LEU
1	A	71	ALA

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	222	LYS
1	A	249	ASP
1	A	257	PRO
1	B	48	VAL
1	B	175	GLU
1	B	218	ALA
1	B	257	PRO
1	C	129	ASP
1	C	159	ILE
1	C	218	ALA
1	C	222	LYS
1	C	275	ALA
1	C	298	ARG
1	C	307	THR
1	D	71	ALA
1	D	95	VAL
1	D	128	VAL
1	D	161	GLU
1	D	291	VAL
1	A	391	ALA
1	B	8	ASP
1	B	51	ILE
1	B	309	VAL
1	B	328	ALA
1	C	70	PHE
1	C	238	LYS
1	D	70	PHE
1	A	155	PRO
1	C	189	GLY
1	C	251	VAL
1	A	375	GLY
1	D	195	VAL
1	D	49	GLY
1	B	199	ILE
1	B	358	ASN
1	C	244	VAL
1	D	156	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/375 (100%)	332 (88%)	43 (12%)	5	22
1	B	375/375 (100%)	346 (92%)	29 (8%)	13	41
1	C	374/375 (100%)	345 (92%)	29 (8%)	12	40
1	D	374/375 (100%)	334 (89%)	40 (11%)	6	25
All	All	1498/1500 (100%)	1357 (91%)	141 (9%)	8	30

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	19	TYR
1	A	41	LEU
1	A	44	THR
1	A	54	LYS
1	A	97	ASN
1	A	113	TYR
1	A	117	TYR
1	A	122	SER
1	A	127	SER
1	A	129	ASP
1	A	153	SER
1	A	160	ASP
1	A	161	GLU
1	A	183	ILE
1	A	187[A]	TYR
1	A	187[B]	TYR
1	A	192	MET
1	A	194	SER
1	A	199	ILE
1	A	205	VAL
1	A	214	PRO
1	A	231	GLN
1	A	239	THR

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Mol	Chain	Res	Type
1	A	249	ASP
1	A	257	PRO
1	A	258	SER
1	A	270	VAL
1	A	286	LEU
1	A	296	LEU
1	A	298	ARG
1	A	301	VAL
1	A	306	SER
1	A	308	ASN
1	A	318	VAL
1	A	320	PRO
1	A	338	TYR
1	A	367	THR
1	A	369	GLU
1	A	370	GLN
1	A	384	PRO
1	A	433	LEU
1	A	439	SER
1	B	19	TYR
1	B	54	LYS
1	B	82	ILE
1	B	90	GLN
1	B	97	ASN
1	B	117	TYR
1	B	129	ASP
1	B	130	THR
1	B	168	THR
1	B	194	SER
1	B	199	ILE
1	B	203	VAL
1	B	205	VAL
1	B	237	LEU
1	B	246	THR
1	B	262	GLU
1	B	264	THR
1	B	265	ILE
1	B	269	ASP
1	B	284	LEU
1	B	285	ASN
1	B	300	LEU
1	B	307	THR

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Mol	Chain	Res	Type
1	B	318	VAL
1	B	319	ILE
1	B	338	TYR
1	B	367	THR
1	B	370	GLN
1	B	433	LEU
1	C	8	ASP
1	C	19	TYR
1	C	41	LEU
1	C	44	THR
1	C	54	LYS
1	C	77	VAL
1	C	90	GLN
1	C	97	ASN
1	C	117	TYR
1	C	138	VAL
1	C	139	LYS
1	C	141	LYS
1	C	154	LEU
1	C	158	THR
1	C	165	VAL
1	C	187	TYR
1	C	192	MET
1	C	194	SER
1	C	199	ILE
1	C	205	VAL
1	C	239	THR
1	C	265	ILE
1	C	281	THR
1	C	318	VAL
1	C	327	LYS
1	C	338	TYR
1	C	367	THR
1	C	433	LEU
1	C	450	PRO
1	D	5	ASP
1	D	10	VAL
1	D	19	TYR
1	D	34	CYS
1	D	41	LEU
1	D	46	LEU
1	D	54	LYS

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Mol	Chain	Res	Type
1	D	76	LYS
1	D	80	VAL
1	D	82	ILE
1	D	90	GLN
1	D	97	ASN
1	D	113	TYR
1	D	117	TYR
1	D	126	ILE
1	D	158	THR
1	D	160	ASP
1	D	183	ILE
1	D	192	MET
1	D	194	SER
1	D	199	ILE
1	D	205	VAL
1	D	241	VAL
1	D	249	ASP
1	D	254	THR
1	D	262	GLU
1	D	264	THR
1	D	287	ASP
1	D	289	ILE
1	D	294	ASP
1	D	298	ARG
1	D	301	VAL
1	D	312	VAL
1	D	318	VAL
1	D	327	LYS
1	D	338	TYR
1	D	345	HIS
1	D	346	VAL
1	D	384	PRO
1	D	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	64	HIS
1	A	90	GLN
1	A	97	ASN
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	345	HIS
1	A	370	GLN
1	A	396	ASN
1	A	421	ASN
1	B	47	ASN
1	B	90	GLN
1	B	97	ASN
1	B	109	ASN
1	B	285	ASN
1	B	345	HIS
1	B	370	GLN
1	B	396	ASN
1	B	421	ASN
1	C	7	ASN
1	C	61	HIS
1	C	72	ASN
1	C	90	GLN
1	C	97	ASN
1	C	109	ASN
1	C	285	ASN
1	C	370	GLN
1	C	396	ASN
1	C	416	HIS
1	D	7	ASN
1	D	58	HIS
1	D	72	ASN
1	D	90	GLN
1	D	97	ASN
1	D	231	GLN
1	D	263	GLN
1	D	370	GLN
1	D	416	HIS
1	D	421	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	C	480	-	51,58,58	2.25	15 (29%)	60,89,89	1.92	15 (25%)
2	FAD	D	480	-	51,58,58	2.28	13 (25%)	60,89,89	1.90	11 (18%)
2	FAD	A	480	-	51,58,58	2.20	10 (19%)	60,89,89	1.86	13 (21%)
2	FAD	B	480	-	51,58,58	2.29	15 (29%)	60,89,89	1.75	12 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	480	-	-	4/30/50/50	0/6/6/6
2	FAD	D	480	-	-	4/30/50/50	0/6/6/6
2	FAD	A	480	-	-	4/30/50/50	0/6/6/6
2	FAD	B	480	-	-	4/30/50/50	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	480	FAD	C4X-C10	8.57	1.47	1.38
2	B	480	FAD	C4X-C10	8.20	1.47	1.38
2	C	480	FAD	C4X-C10	8.16	1.47	1.38
2	A	480	FAD	C4X-C10	7.62	1.46	1.38
2	B	480	FAD	O4B-C1B	5.79	1.49	1.41
2	D	480	FAD	C9A-N10	5.61	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	480	FAD	PA-O2A	-5.18	1.31	1.55
2	D	480	FAD	PA-O2A	-5.00	1.31	1.55
2	A	480	FAD	PA-O2A	-4.86	1.32	1.55
2	A	480	FAD	C4-N3	4.79	1.41	1.33
2	C	480	FAD	C4-N3	4.69	1.41	1.33
2	D	480	FAD	C4-N3	4.36	1.40	1.33
2	A	480	FAD	O4B-C1B	4.21	1.46	1.41
2	D	480	FAD	O4B-C1B	4.19	1.46	1.41
2	B	480	FAD	C4-N3	4.19	1.40	1.33
2	A	480	FAD	P-O2P	-4.18	1.35	1.55
2	B	480	FAD	PA-O2A	-4.10	1.36	1.55
2	C	480	FAD	O4B-C1B	4.03	1.46	1.41
2	A	480	FAD	C10-N1	3.91	1.38	1.33
2	A	480	FAD	P-O5'	-3.89	1.43	1.59
2	B	480	FAD	C9A-N10	3.84	1.43	1.38
2	B	480	FAD	O5'-C5'	3.83	1.59	1.44
2	C	480	FAD	C2-N1	-3.77	1.30	1.38
2	C	480	FAD	C9A-N10	3.68	1.43	1.38
2	A	480	FAD	C9A-N10	3.58	1.43	1.38
2	D	480	FAD	C10-N1	3.55	1.37	1.33
2	D	480	FAD	O5'-C5'	3.45	1.58	1.44
2	B	480	FAD	P-O2P	-3.41	1.39	1.55
2	B	480	FAD	C10-N1	3.39	1.37	1.33
2	B	480	FAD	C4A-N3A	3.19	1.40	1.35
2	B	480	FAD	C2-N1	-3.10	1.32	1.38
2	C	480	FAD	C8-C7	3.06	1.48	1.40
2	C	480	FAD	P-O2P	-2.94	1.41	1.55
2	D	480	FAD	C2-N3	2.88	1.43	1.38
2	A	480	FAD	O5'-C5'	2.88	1.55	1.44
2	C	480	FAD	C2-N3	2.87	1.43	1.38
2	C	480	FAD	P-O5'	-2.84	1.47	1.59
2	A	480	FAD	C2-N3	2.80	1.43	1.38
2	D	480	FAD	P-O2P	-2.79	1.42	1.55
2	C	480	FAD	C5'-C4'	-2.66	1.48	1.51
2	D	480	FAD	C4A-N3A	2.62	1.39	1.35
2	C	480	FAD	C6-C5X	-2.49	1.38	1.41
2	B	480	FAD	C2-N3	2.48	1.43	1.38
2	B	480	FAD	C2B-C1B	-2.47	1.50	1.53
2	C	480	FAD	C4A-N3A	2.44	1.39	1.35
2	D	480	FAD	C2-N1	-2.40	1.33	1.38
2	B	480	FAD	C5B-C4B	2.28	1.58	1.51
2	D	480	FAD	P-O5'	-2.26	1.50	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	480	FAD	C2A-N3A	2.12	1.35	1.32
2	C	480	FAD	O5'-C5'	2.11	1.52	1.44
2	B	480	FAD	P-O5'	-2.09	1.50	1.59
2	B	480	FAD	C6-C5X	-2.09	1.38	1.41
2	D	480	FAD	C8-C7	2.09	1.46	1.40

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	480	FAD	C4-N3-C2	8.17	122.04	115.14
2	D	480	FAD	C4-N3-C2	8.15	122.02	115.14
2	A	480	FAD	C4-N3-C2	7.99	121.89	115.14
2	B	480	FAD	C4-N3-C2	7.12	121.16	115.14
2	C	480	FAD	C4X-C4-N3	-5.64	115.72	123.43
2	A	480	FAD	C4X-C4-N3	-4.74	116.95	123.43
2	B	480	FAD	C4X-C4-N3	-4.63	117.10	123.43
2	D	480	FAD	O4B-C1B-C2B	-4.56	100.26	106.93
2	D	480	FAD	C4X-C4-N3	-4.44	117.35	123.43
2	C	480	FAD	C1'-N10-C10	3.55	121.59	118.41
2	D	480	FAD	C10-C4X-N5	3.47	123.66	121.26
2	D	480	FAD	C5A-C6A-N6A	3.34	125.42	120.35
2	A	480	FAD	C1'-N10-C10	3.32	121.39	118.41
2	A	480	FAD	C5A-C6A-N6A	3.27	125.32	120.35
2	C	480	FAD	O4B-C1B-C2B	-3.21	102.24	106.93
2	A	480	FAD	O4B-C1B-C2B	-3.14	102.34	106.93
2	A	480	FAD	C5'-C4'-C3'	-3.10	106.22	112.20
2	A	480	FAD	P-O3P-PA	2.91	142.81	132.83
2	B	480	FAD	O4B-C1B-C2B	-2.86	102.74	106.93
2	C	480	FAD	O5'-C5'-C4'	-2.76	102.00	109.36
2	B	480	FAD	C5'-C4'-C3'	-2.75	106.90	112.20
2	D	480	FAD	C2A-N1A-C6A	2.69	123.36	118.75
2	B	480	FAD	C5A-C6A-N6A	2.67	124.40	120.35
2	C	480	FAD	C6-C5X-N5	-2.65	116.13	119.05
2	B	480	FAD	C2A-N1A-C6A	2.62	123.23	118.75
2	B	480	FAD	C1'-N10-C10	2.61	120.75	118.41
2	C	480	FAD	C10-C4X-N5	2.61	123.06	121.26
2	C	480	FAD	C5A-C6A-N6A	2.60	124.31	120.35
2	B	480	FAD	C4-C4X-C10	-2.58	118.24	119.95
2	D	480	FAD	C4-C4X-C10	-2.55	118.26	119.95
2	A	480	FAD	C2A-N1A-C6A	2.53	123.08	118.75
2	B	480	FAD	C6-C5X-N5	-2.46	116.34	119.05
2	D	480	FAD	C5A-C6A-N1A	-2.45	114.79	120.35

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	FAD	C5A-C6A-N1A	-2.42	114.87	120.35
2	C	480	FAD	C2A-N1A-C6A	2.41	122.87	118.75
2	D	480	FAD	O5B-PA-O1A	-2.40	99.69	109.07
2	A	480	FAD	C4-C4X-C10	-2.37	118.38	119.95
2	A	480	FAD	C5A-C6A-N1A	-2.35	115.01	120.35
2	D	480	FAD	O3B-C3B-C2B	2.28	119.20	111.82
2	A	480	FAD	O5'-P-O1P	-2.28	100.17	109.07
2	C	480	FAD	C5'-C4'-C3'	-2.18	107.99	112.20
2	B	480	FAD	O5B-PA-O1A	-2.15	100.66	109.07
2	B	480	FAD	O5'-P-O1P	-2.14	100.70	109.07
2	C	480	FAD	C4X-C10-N10	-2.14	118.11	120.30
2	C	480	FAD	C5A-C6A-N1A	-2.11	115.56	120.35
2	C	480	FAD	O5B-PA-O1A	-2.08	100.96	109.07
2	A	480	FAD	C4X-C10-N10	-2.05	118.20	120.30
2	A	480	FAD	O5B-PA-O1A	-2.01	101.21	109.07
2	C	480	FAD	P-O3P-PA	2.01	139.72	132.83
2	C	480	FAD	C4-C4X-C10	-2.01	118.62	119.95
2	D	480	FAD	C1'-N10-C10	2.01	120.20	118.41

There are no chirality outliers.

All (16) torsion outliers are listed below:

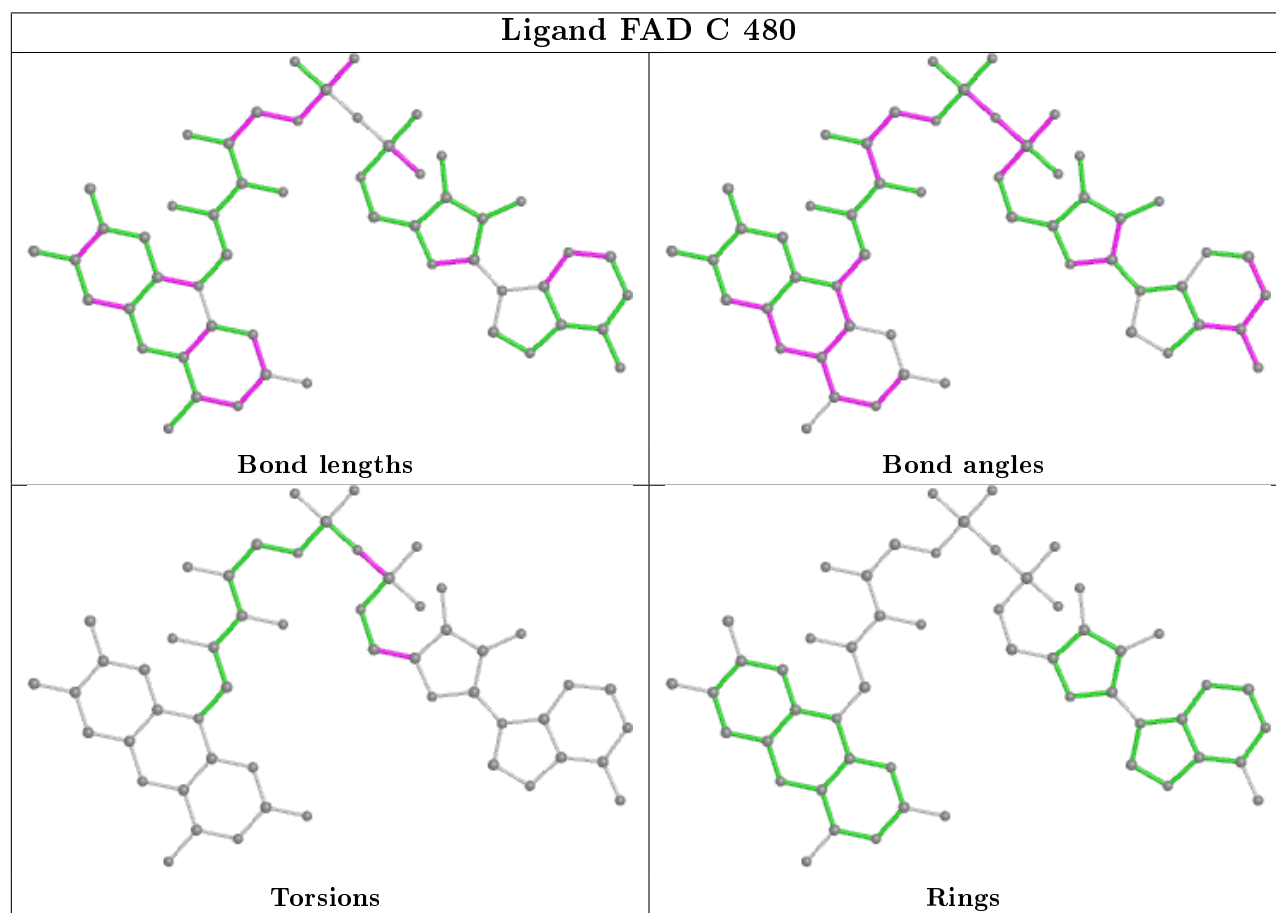
Mol	Chain	Res	Type	Atoms
2	C	480	FAD	O4B-C4B-C5B-O5B
2	A	480	FAD	O4B-C4B-C5B-O5B
2	C	480	FAD	P-O3P-PA-O1A
2	B	480	FAD	O4B-C4B-C5B-O5B
2	D	480	FAD	O4B-C4B-C5B-O5B
2	A	480	FAD	C3B-C4B-C5B-O5B
2	C	480	FAD	C3B-C4B-C5B-O5B
2	B	480	FAD	C3B-C4B-C5B-O5B
2	C	480	FAD	P-O3P-PA-O2A
2	D	480	FAD	P-O3P-PA-O1A
2	D	480	FAD	P-O3P-PA-O2A
2	A	480	FAD	P-O3P-PA-O2A
2	B	480	FAD	P-O3P-PA-O2A
2	D	480	FAD	C3B-C4B-C5B-O5B
2	B	480	FAD	P-O3P-PA-O1A
2	A	480	FAD	P-O3P-PA-O1A

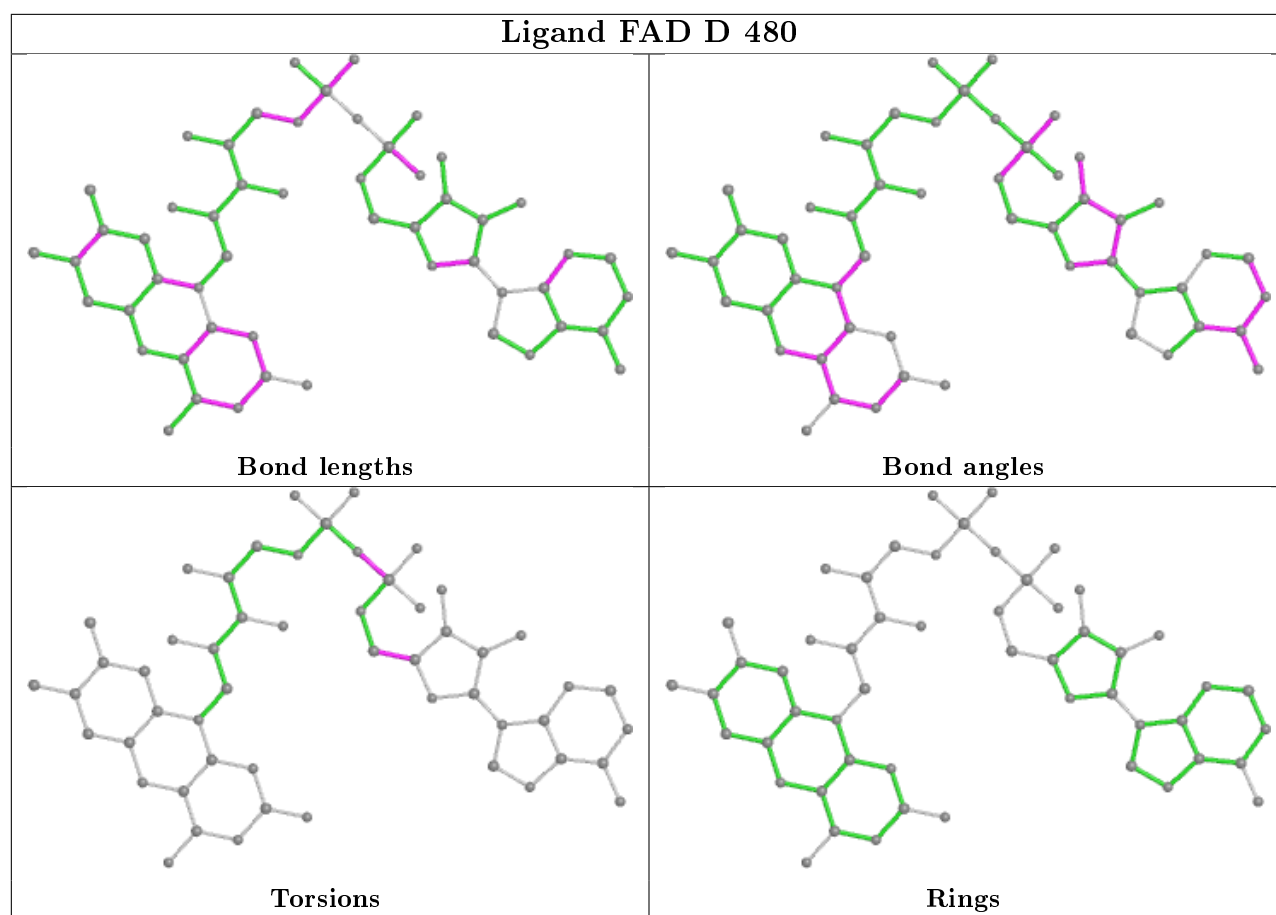
There are no ring outliers.

4 monomers are involved in 10 short contacts:

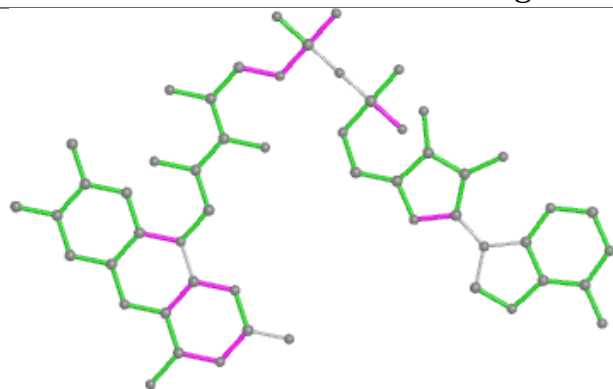
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	480	FAD	3	0
2	D	480	FAD	3	0
2	A	480	FAD	2	0
2	B	480	FAD	2	0

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

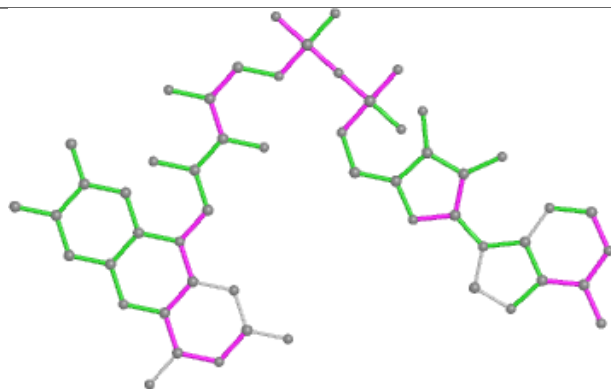




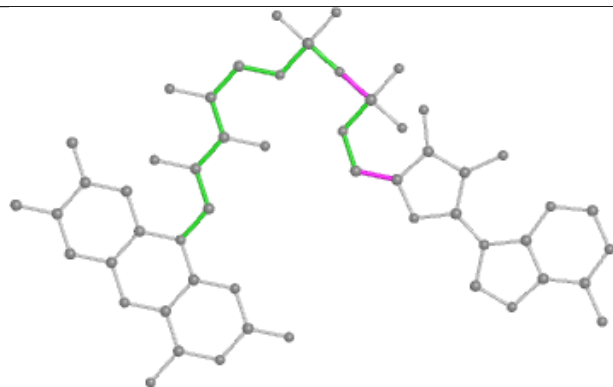
Ligand FAD A 480



Bond lengths



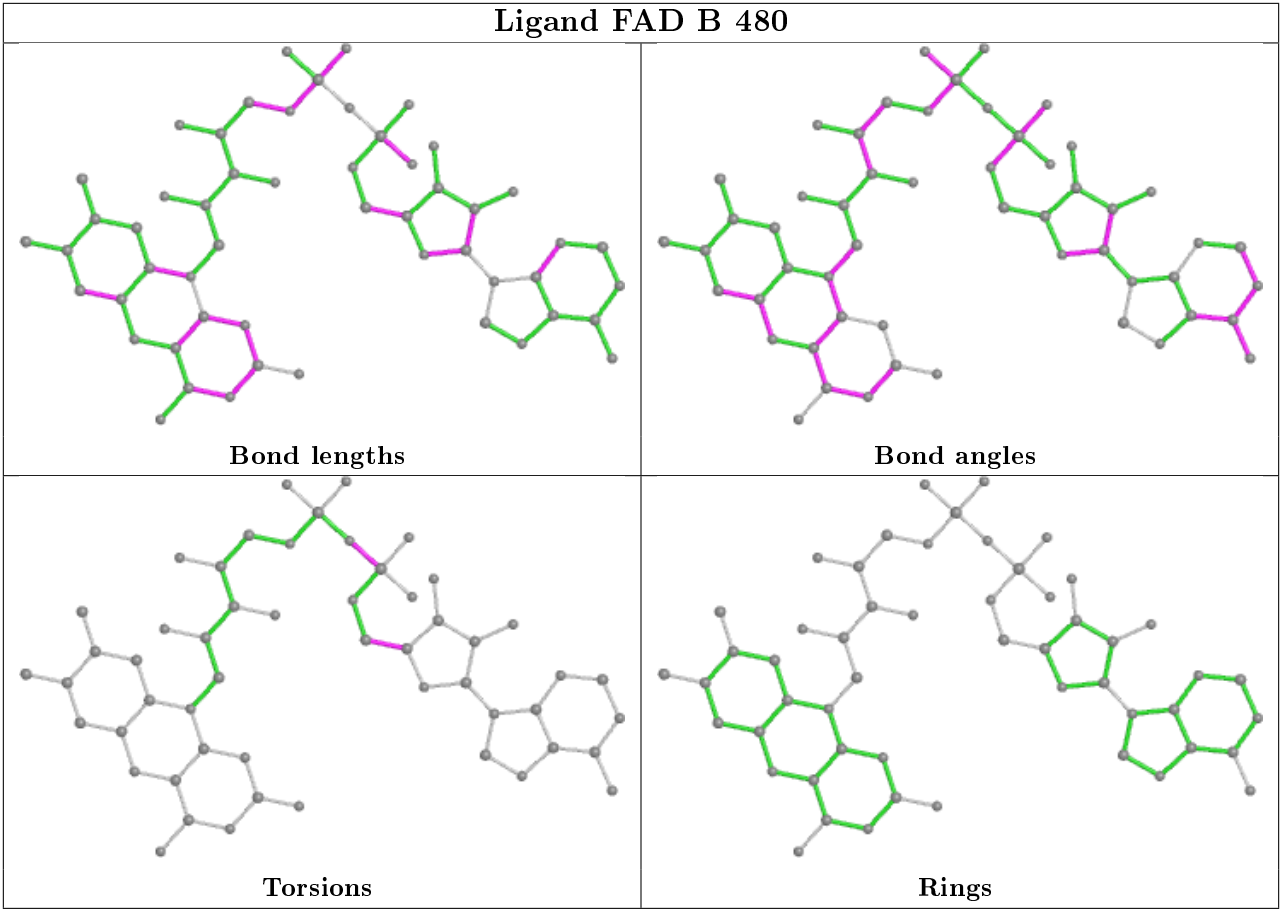
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	258:SER	C	259:ALA	N	2.22
1	C	263:GLN	C	264:THR	N	1.20

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.