



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:29 PM UTC

PDB ID : 1MOK / pdb_00001mok
Title : NADPH DEPENDENT 2-KETOPROPYL COENZYME M OXIDOREDUCTASE/CARBOXYLASE
Authors : Nocek, B.; Jang, S.B.; Jeong, M.S.; Clark, D.D.; Ensign, S.A.; Peters, J.W.
Deposited on : 2002-09-09
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

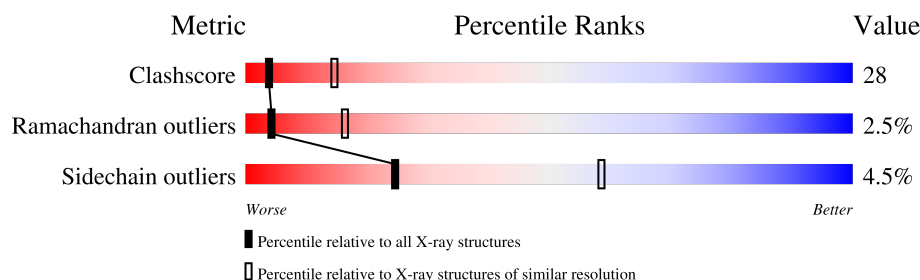
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	523	50% 46% • •
1	B	523	51% 43% 5%
1	C	523	51% 44% • •
1	D	523	46% 48% 5%

2 Entry composition i

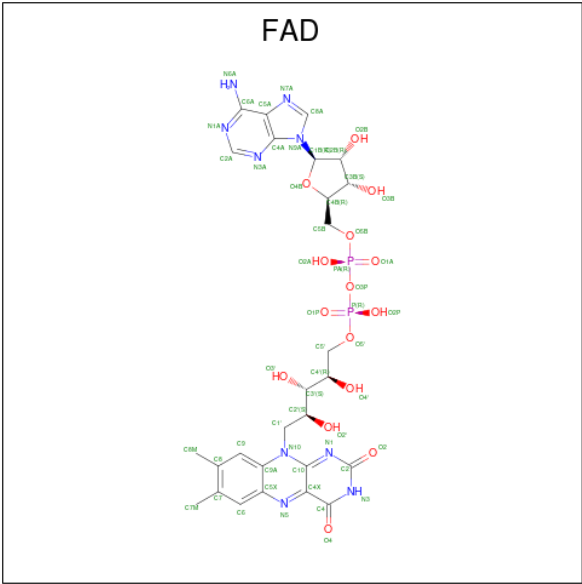
There are 2 unique types of molecules in this entry. The entry contains 16304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 orf3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	B	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	C	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	D	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

Continued on next page...

Continued from previous page...

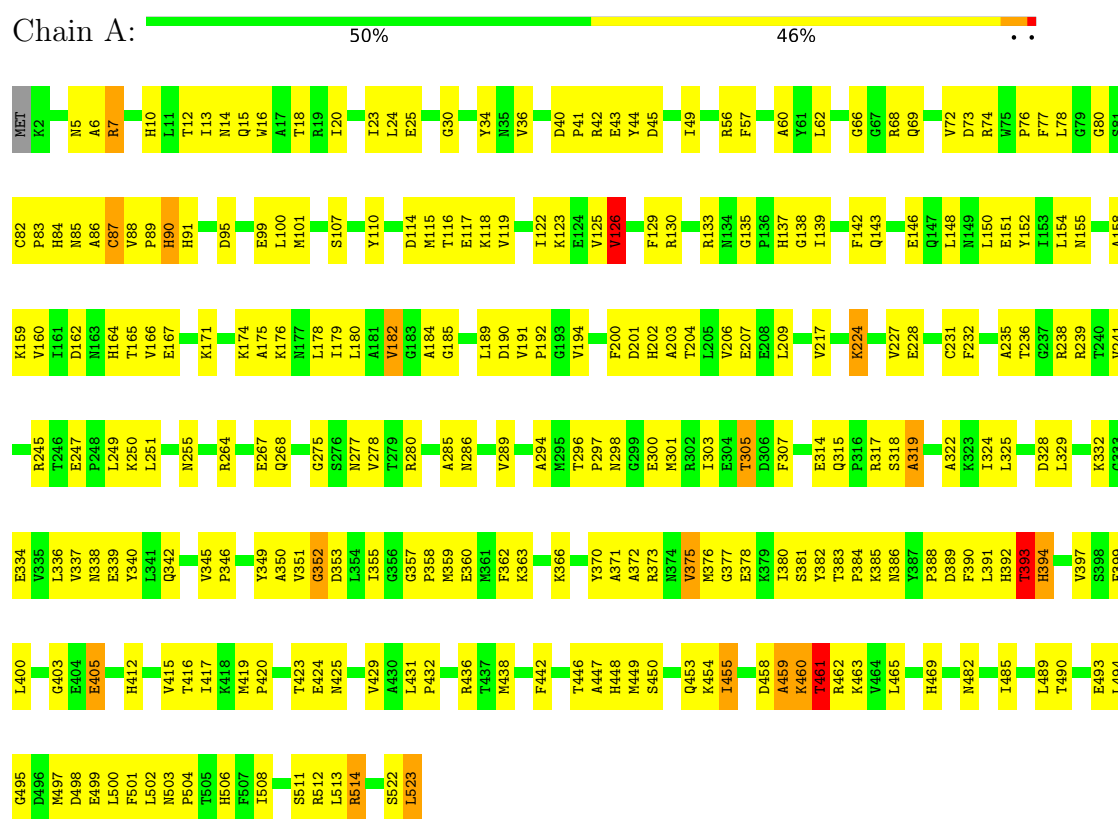
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: orf3



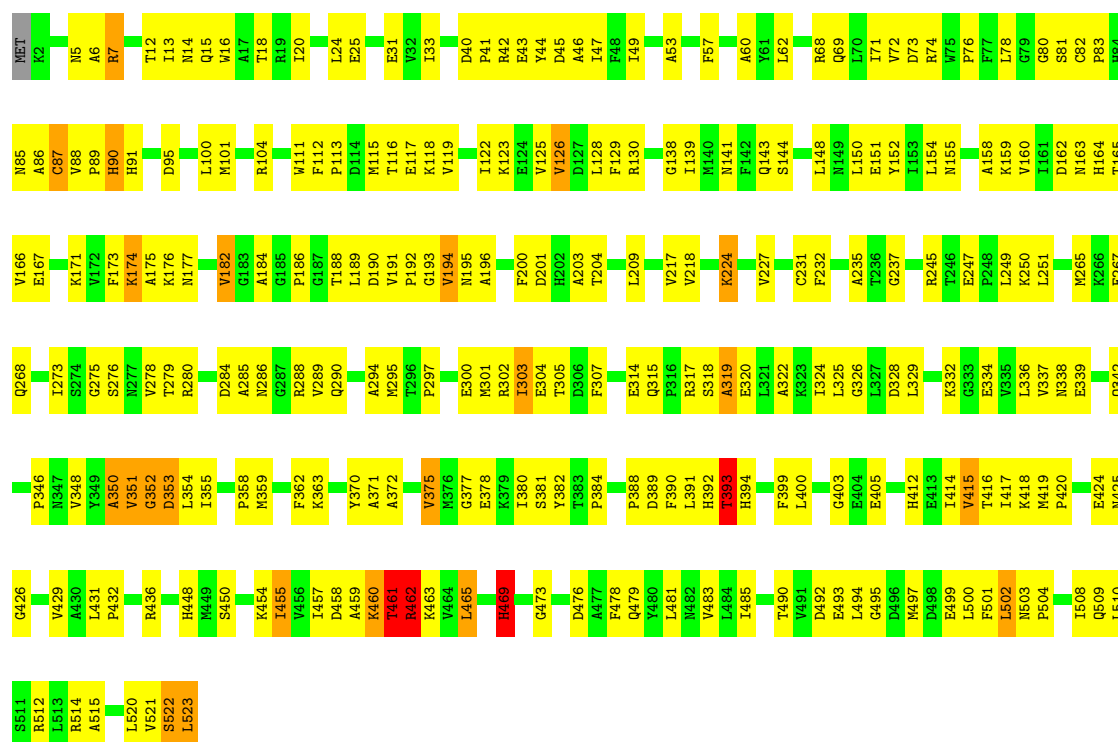
- Molecule 1: orf3





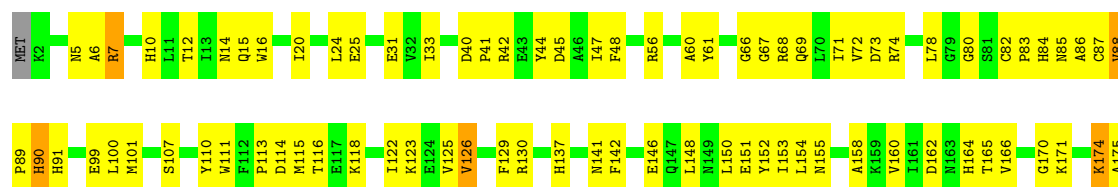
• Molecule 1: orf3

Chain C: 51% 44%



• Molecule 1: orf3

Chain D: 46% 48% 5%



F478	L400	K332	K253	K176
F479	G401	G333	G334	N178
F480	M402	E334	Y260	I179
L481	G403	V335		
M482	E404	L336		
F483	E405	V337	R264	V182
L484	E406	N338	K265	G183
L485		E339	K266	G184
			E267	G185
	H412		Q268	P186
		Q342	G269	
L489	V415	P346	M270	L189
T490	L416	N347		D190
F491	T417		I273	V191
D492	K418	A350	S274	P192
E493	M419	V351	G275	G193
L494	P420	G352	S276	V194
G495		D353	N277	N195
D496	T423	L354	V278	A196
M497	E424	L355	T279	K197
D498	N425		R280	G198
E499		P358		V199
L500	M428	M359	D284	F200
F501	V429	E360	A285	D201
L502	A430	M361	N286	D202
M503	L431	K362		A203
P504	P432	F363	V289	T204
T505		A364	Q290	L205
H506	M438	L339		V206
F507	A440	G365		E207
I508	A441		A294	
Q509	F442	G369	M295	E208
L510	S511	Y370	T296	L209
R512		A371	P297	
		A372	N298	E212
L513	T446	R373	G299	P213
R514	A447	N374	E300	
	H448	K375	M301	V217
L520	M449	V376	R302	V218
V521	S450	M376	G303	
S522		G377	I303	K224
L523	K454	E378	E304	
	A455	K379	T305	V227
	V456	L380	D306	
	L457	S381	F307	
	D458	Y382		G230
	A459	T383	Q314	C231
	K460	P384	Q315	F232
	T461	K385	P316	F233
	K462	N386	R317	N234
	K463		S318	A235
	V464	P388	A319	T236
	L465	D389	E320	G237
		F390		
	H468	L391		L243
	H469	H392		V244
		H393		R245
	G473		L325	T246
	A474		G326	E247
K475			L327	L248
D476		V397	R328	L249
S477		S398	G329	V250
			P330	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.60Å 87.50Å 100.70Å 72.00° 73.40° 69.81°	Depositor
Resolution (Å)	19.99 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (19.99-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16304	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	0.54	1/4106 (0.0%)	0.97	9/5556 (0.2%)
1	B	0.63	3/4106 (0.1%)	1.01	16/5556 (0.3%)
1	C	0.56	1/4106 (0.0%)	0.97	17/5556 (0.3%)
1	D	0.57	3/4106 (0.1%)	0.97	12/5556 (0.2%)
All	All	0.58	8/16424 (0.0%)	0.98	54/22224 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	523	LEU	C-O	-15.34	0.92	1.23
1	D	523	LEU	C-O	-14.61	0.94	1.23
1	C	523	LEU	C-O	-14.38	0.94	1.23
1	A	523	LEU	C-O	-14.17	0.95	1.23
1	B	73	ASP	C-N	-11.15	1.18	1.33
1	D	494	LEU	N-CA	-5.88	1.39	1.46
1	B	75	TRP	NE1-CE2	-5.18	1.31	1.37
1	D	493	GLU	C-N	-5.13	1.27	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	ASP	N-CA-C	-10.91	99.91	113.01
1	B	394	HIS	N-CA-C	-9.76	101.38	113.38
1	D	353	ASP	N-CA-C	-9.55	101.55	113.01
1	D	394	HIS	N-CA-C	-9.27	101.49	113.17
1	A	393	THR	N-CA-C	-9.03	91.57	110.80
1	A	394	HIS	N-CA-C	-8.74	102.63	113.38
1	D	393	THR	N-CA-C	-8.38	92.94	110.80
1	B	523	LEU	CA-C-O	8.27	145.82	121.00
1	C	393	THR	N-CA-C	-8.00	93.75	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	ILE	N-CA-C	7.92	120.46	109.45
1	C	285	ALA	N-CA-C	-7.86	102.67	111.71
1	D	523	LEU	CA-C-O	7.86	144.57	121.00
1	C	353	ASP	N-CA-C	-7.84	103.86	113.19
1	B	285	ALA	N-CA-C	-7.58	102.99	111.71
1	B	393	THR	N-CA-C	-7.49	94.85	110.80
1	A	523	LEU	CA-C-O	7.35	143.06	121.00
1	C	394	HIS	N-CA-C	-7.16	104.15	113.17
1	D	403	GLY	N-CA-C	-7.05	101.75	112.89
1	A	285	ALA	N-CA-C	-6.98	103.73	111.82
1	A	353	ASP	N-CA-C	-6.92	104.09	112.54
1	B	253	LYS	N-CA-C	6.89	118.79	111.28
1	C	523	LEU	CA-C-O	6.80	141.41	121.00
1	A	415	VAL	N-CA-C	-6.67	98.89	108.42
1	B	464	VAL	O-C-N	6.62	130.16	122.81
1	D	285	ALA	N-CA-C	-6.55	104.38	112.38
1	C	403	GLY	N-CA-C	-6.35	102.89	112.60
1	C	418	LYS	N-CA-C	6.17	118.45	109.07
1	B	418	LYS	N-CA-C	6.03	117.94	108.96
1	B	73	ASP	N-CA-C	5.98	117.62	108.42
1	B	403	GLY	N-CA-C	-5.94	103.50	112.89
1	B	250	LYS	N-CA-C	-5.86	105.02	111.82
1	D	137	HIS	N-CA-C	-5.79	104.67	110.97
1	B	81	SER	N-CA-C	5.69	117.48	111.28
1	D	253	LYS	N-CA-C	5.68	118.25	111.71
1	B	320	GLU	N-CA-C	5.61	118.16	111.71
1	C	144	SER	N-CA-C	5.56	117.02	111.07
1	B	416	THR	N-CA-C	5.54	117.46	108.26
1	C	81	SER	N-CA-C	5.51	117.29	111.28
1	D	415	VAL	N-CA-C	-5.50	100.31	108.45
1	C	350	ALA	N-CA-C	-5.47	101.21	109.85
1	B	415	VAL	N-CA-C	-5.41	99.93	108.90
1	C	320	GLU	N-CA-C	5.36	117.12	111.28
1	C	415	VAL	N-CA-C	-5.34	100.15	108.86
1	A	403	GLY	N-CA-C	-5.33	104.02	112.66
1	B	462	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	D	320	GLU	N-CA-C	5.29	117.05	111.28
1	D	418	LYS	N-CA-C	5.19	116.70	108.96
1	A	126	VAL	N-CA-C	-5.18	106.27	113.00
1	C	469	HIS	N-CA-C	5.16	117.76	108.48
1	A	459	ALA	N-CA-C	-5.12	102.80	110.23
1	C	112	PHE	CA-C-N	5.12	125.02	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	PHE	C-N-CA	5.12	125.02	119.85
1	C	462	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	D	110	TYR	CB-CA-C	-5.02	110.77	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4023	0	3980	237	0
1	B	4023	0	3980	231	0
1	C	4023	0	3980	241	0
1	D	4023	0	3980	251	0
2	A	53	0	31	6	0
2	B	53	0	31	7	0
2	C	53	0	31	8	0
2	D	53	0	31	12	0
All	All	16304	0	16044	917	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 28.

All (917) 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:C:460:LYS:O	1:C:461:THR:HB	1.39	1.08
1:C:82:CYS:HA	1:C:86:ALA:HB3	1.38	1.05
1:A:82:CYS:HA	1:A:86:ALA:HB3	1.42	1.00
1:D:40:ASP:OD1	1:D:42:ARG:HG2	1.64	0.98
1:C:165:THR:HG22	1:C:174:LYS:HG3	1.46	0.97
1:C:201:ASP:H	1:C:204:THR:HG22	1.27	0.95
1:A:69:GLN:HE22	1:A:151:GLU:H	1.02	0.94
1:B:460:LYS:O	1:B:461:THR:HB	1.64	0.94
1:D:201:ASP:H	1:D:204:THR:HG22	1.34	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LYS:O	1:A:461:THR:HB	1.69	0.93
1:B:69:GLN:HE22	1:B:151:GLU:H	0.94	0.93
1:A:201:ASP:H	1:A:204:THR:HG22	1.28	0.92
1:B:201:ASP:H	1:B:204:THR:HG22	1.34	0.92
1:D:69:GLN:HE22	1:D:151:GLU:H	0.92	0.92
1:D:82:CYS:HA	1:D:86:ALA:HB3	1.52	0.91
1:D:227:VAL:HG21	1:D:249:LEU:HD21	1.53	0.90
1:D:165:THR:HG22	1:D:174:LYS:HG3	1.53	0.90
1:A:5:ASN:HD21	1:A:7:ARG:HB2	1.36	0.89
1:A:227:VAL:HG21	1:A:249:LEU:HD21	1.55	0.89
1:C:69:GLN:NE2	1:C:151:GLU:H	1.71	0.89
1:A:165:THR:HG22	1:A:174:LYS:HG3	1.55	0.88
1:B:5:ASN:HD21	1:B:7:ARG:HB2	1.38	0.88
1:D:337:VAL:HG21	1:D:355:ILE:HD13	1.55	0.88
1:A:40:ASP:OD1	1:A:42:ARG:HG2	1.73	0.88
1:A:350:ALA:O	1:A:355:ILE:HD11	1.74	0.88
1:C:69:GLN:HE22	1:C:151:GLU:N	1.71	0.88
1:B:82:CYS:HB3	1:B:83:PRO:HD3	1.55	0.87
1:D:69:GLN:HE22	1:D:151:GLU:N	1.74	0.86
1:D:460:LYS:O	1:D:461:THR:HB	1.75	0.85
1:C:69:GLN:HE22	1:C:151:GLU:H	0.87	0.83
1:D:350:ALA:O	1:D:355:ILE:HD11	1.79	0.83
1:C:227:VAL:HG21	1:C:249:LEU:HD21	1.58	0.83
1:D:69:GLN:NE2	1:D:151:GLU:H	1.75	0.81
1:A:12:THR:HB	1:A:15:GLN:HG3	1.63	0.80
1:A:126:VAL:O	1:A:130:ARG:HG3	1.82	0.80
1:B:227:VAL:HG21	1:B:249:LEU:HD21	1.62	0.80
1:B:165:THR:HG22	1:B:174:LYS:HG3	1.63	0.80
1:B:217:VAL:HG22	1:B:307:PHE:HD2	1.46	0.79
1:C:432:PRO:O	1:C:450:SER:HB2	1.82	0.79
1:C:82:CYS:CA	1:C:86:ALA:HB3	2.12	0.79
1:A:201:ASP:H	1:A:204:THR:CG2	1.96	0.78
1:B:40:ASP:OD1	1:B:42:ARG:HG2	1.82	0.78
1:C:5:ASN:HD21	1:C:7:ARG:HB2	1.48	0.78
1:A:5:ASN:ND2	1:A:7:ARG:HB2	1.99	0.78
1:A:74:ARG:O	1:A:155:ASN:HA	1.83	0.78
1:A:255:ASN:HB2	1:A:405:GLU:OE1	1.83	0.78
1:D:417:ILE:HG22	1:D:455:ILE:HG22	1.66	0.78
1:B:499:GLU:HB2	1:B:503:ASN:ND2	1.99	0.77
1:B:5:ASN:ND2	1:B:7:ARG:HB2	1.98	0.77
1:D:201:ASP:H	1:D:204:THR:CG2	1.96	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ASP:OD1	1:C:42:ARG:HG2	1.85	0.76
1:A:82:CYS:CA	1:A:86:ALA:HB3	2.16	0.76
1:B:69:GLN:NE2	1:B:151:GLU:H	1.80	0.75
1:C:337:VAL:HG21	1:C:355:ILE:HD13	1.66	0.75
1:C:460:LYS:O	1:C:461:THR:CB	2.26	0.75
1:B:69:GLN:HE22	1:B:151:GLU:N	1.80	0.74
1:B:358:PRO:O	1:B:363:LYS:HD3	1.88	0.74
1:C:122:ILE:O	1:C:125:VAL:HG12	1.86	0.74
1:A:499:GLU:HB2	1:A:503:ASN:ND2	2.03	0.74
1:C:417:ILE:HG22	1:C:455:ILE:HG22	1.71	0.73
1:B:273:ILE:HG22	1:B:276:SER:HB2	1.70	0.73
1:D:338:ASN:HD21	1:D:342:GLN:NE2	1.87	0.72
1:C:416:THR:HG22	1:C:523:LEU:HG	1.70	0.72
1:A:160:VAL:HG11	1:A:325:LEU:HD21	1.70	0.72
1:B:337:VAL:HG21	1:B:355:ILE:HD13	1.72	0.72
1:A:412:HIS:HD2	1:A:458:ASP:OD2	1.72	0.72
1:C:355:ILE:HG22	1:C:355:ILE:O	1.89	0.72
1:D:247:GLU:HB2	1:D:250:LYS:HE2	1.71	0.72
1:B:74:ARG:O	1:B:155:ASN:HA	1.89	0.71
1:B:355:ILE:HG22	1:B:355:ILE:O	1.89	0.71
1:B:458:ASP:O	1:B:462:ARG:HA	1.91	0.71
1:A:337:VAL:HG21	1:A:355:ILE:HD13	1.73	0.71
1:B:432:PRO:O	1:B:450:SER:HB2	1.90	0.71
1:D:82:CYS:CA	1:D:86:ALA:HB3	2.21	0.71
1:D:82:CYS:HB3	1:D:83:PRO:HD3	1.70	0.71
1:A:338:ASN:HD21	1:A:342:GLN:NE2	1.88	0.71
1:B:275:GLY:O	1:B:297:PRO:HD3	1.90	0.71
1:D:328:ASP:O	1:D:329:LEU:HD23	1.91	0.70
1:A:339:GLU:O	1:A:381:SER:HA	1.92	0.70
1:C:201:ASP:H	1:C:204:THR:CG2	2.03	0.70
1:C:200:PHE:HD1	1:C:204:THR:HG23	1.55	0.70
1:B:82:CYS:HA	1:B:86:ALA:HB3	1.71	0.70
1:D:432:PRO:O	1:D:450:SER:HB2	1.91	0.70
1:A:358:PRO:O	1:A:363:LYS:HD3	1.92	0.69
1:A:490:THR:OG1	1:A:493:GLU:HG3	1.92	0.69
1:A:82:CYS:HB3	1:A:83:PRO:HD3	1.73	0.69
1:B:350:ALA:O	1:B:355:ILE:HD11	1.92	0.69
1:C:358:PRO:O	1:C:363:LYS:HD3	1.93	0.69
1:C:462:ARG:HB3	1:C:520:LEU:HD11	1.75	0.69
1:B:82:CYS:HB3	1:B:83:PRO:CD	2.23	0.68
1:D:227:VAL:CG1	1:D:393:THR:HG22	2.22	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:THR:HG22	1:C:14:ASN:H	1.58	0.68
1:A:328:ASP:HB3	1:A:336:LEU:HD12	1.76	0.68
1:B:14:ASN:O	1:B:18:THR:HG23	1.93	0.68
1:A:12:THR:HG22	1:A:14:ASN:H	1.58	0.68
1:D:355:ILE:O	1:D:355:ILE:HG22	1.93	0.68
1:B:352:GLY:HA3	2:B:524:FAD:O2P	1.92	0.68
1:C:165:THR:HG22	1:C:174:LYS:CG	2.23	0.68
1:D:122:ILE:O	1:D:125:VAL:HG12	1.93	0.68
1:D:338:ASN:HD21	1:D:342:GLN:HE21	1.39	0.68
1:C:5:ASN:ND2	1:C:7:ARG:HB2	2.09	0.67
1:C:476:ASP:O	1:C:479:GLN:HG3	1.93	0.67
1:D:200:PHE:HD1	1:D:204:THR:HG23	1.60	0.67
1:A:192:PRO:HG2	1:A:280:ARG:HB2	1.77	0.67
1:C:350:ALA:O	1:C:355:ILE:HD11	1.95	0.67
1:B:12:THR:HG22	1:B:14:ASN:H	1.59	0.66
1:C:352:GLY:HA3	2:C:524:FAD:O2P	1.95	0.66
1:B:126:VAL:O	1:B:130:ARG:HG3	1.96	0.66
1:C:87:CYS:HA	1:C:90:HIS:HD2	1.61	0.66
1:D:373:ARG:HH21	1:D:380:ILE:HG12	1.59	0.66
1:A:338:ASN:OD1	1:A:342:GLN:HB2	1.96	0.66
1:D:227:VAL:HG11	1:D:393:THR:HG22	1.77	0.66
1:C:49:ILE:HG22	1:C:182:VAL:HG23	1.78	0.66
1:C:497:MET:SD	1:D:483:VAL:HG21	2.37	0.65
1:D:378:GLU:HB3	1:D:380:ILE:HD13	1.78	0.65
1:D:338:ASN:OD1	1:D:342:GLN:HB2	1.97	0.65
1:B:400:LEU:HD11	1:B:485:ILE:HD12	1.79	0.65
1:C:247:GLU:HB2	1:C:250:LYS:HE2	1.79	0.65
1:A:417:ILE:HG22	1:A:455:ILE:HG22	1.77	0.65
1:D:454:LYS:HG2	1:D:455:ILE:N	2.12	0.65
1:A:115:MET:O	1:A:118:LYS:HB3	1.97	0.65
1:C:337:VAL:HA	1:C:342:GLN:O	1.97	0.65
1:A:454:LYS:HG2	1:A:455:ILE:N	2.12	0.65
1:A:314:GLU:HB3	1:A:359:MET:HE1	1.79	0.64
1:C:113:PRO:HG3	1:D:113:PRO:HD3	1.79	0.64
1:A:494:LEU:HD23	1:A:511:SER:OG	1.97	0.64
1:D:400:LEU:C	1:D:400:LEU:HD12	2.22	0.64
1:C:128:LEU:HD11	1:D:442:PHE:O	1.98	0.64
1:C:160:VAL:HG11	1:C:325:LEU:HD21	1.79	0.64
1:A:378:GLU:HB3	1:A:380:ILE:HD13	1.79	0.64
1:A:62:LEU:HB2	1:A:372:ALA:HB1	1.79	0.64
1:A:224:LYS:NZ	1:A:360:GLU:OE2	2.23	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:HG11	1:B:393:THR:HG22	1.80	0.64
1:D:499:GLU:HB2	1:D:503:ASN:ND2	2.13	0.63
1:A:122:ILE:O	1:A:125:VAL:HG12	1.99	0.63
1:B:227:VAL:CG1	1:B:393:THR:HG22	2.28	0.63
1:C:494:LEU:HA	1:C:497:MET:HE3	1.79	0.63
1:D:267:GLU:OE1	1:D:448:HIS:HE1	1.82	0.63
1:D:300:GLU:HG2	1:D:301:MET:N	2.14	0.63
1:C:45:ASP:O	1:C:177:ASN:HB2	1.99	0.63
1:C:74:ARG:O	1:C:155:ASN:HA	1.99	0.62
1:C:113:PRO:HD3	1:D:113:PRO:HG3	1.79	0.62
1:B:191:VAL:CG2	1:B:192:PRO:HD2	2.29	0.62
1:C:481:LEU:O	1:C:485:ILE:HG13	1.99	0.62
1:D:44:TYR:CD1	1:D:68:ARG:HG2	2.34	0.62
1:A:87:CYS:HA	1:A:90:HIS:HD2	1.63	0.62
1:C:126:VAL:O	1:C:130:ARG:HG3	2.00	0.62
1:B:473:GLY:O	1:B:504:PRO:HG2	1.98	0.62
1:C:389:ASP:HB3	1:C:399:PHE:CE1	2.34	0.62
1:C:12:THR:HB	1:C:15:GLN:HG3	1.81	0.62
1:A:300:GLU:HG2	1:A:301:MET:N	2.14	0.62
1:C:458:ASP:O	1:C:462:ARG:HA	2.00	0.62
1:D:74:ARG:HG3	2:D:524:FAD:C2A	2.29	0.62
1:A:160:VAL:O	1:A:324:ILE:HG21	2.00	0.61
1:C:279:THR:H	1:C:294:ALA:HA	1.66	0.61
1:A:499:GLU:HB2	1:A:503:ASN:HD22	1.63	0.61
1:B:462:ARG:HB3	1:B:520:LEU:HD11	1.82	0.61
1:A:416:THR:HG22	1:A:523:LEU:HG	1.81	0.61
1:B:300:GLU:HG2	1:B:301:MET:N	2.16	0.61
1:B:494:LEU:HA	1:B:497:MET:HE3	1.83	0.61
1:C:300:GLU:HG2	1:C:301:MET:N	2.15	0.61
1:B:352:GLY:CA	2:B:524:FAD:O2P	2.49	0.61
1:C:499:GLU:HB2	1:C:503:ASN:ND2	2.16	0.61
1:B:24:LEU:HD13	1:B:76:PRO:HG3	1.83	0.60
1:B:182:VAL:HG12	1:B:317:ARG:HB2	1.83	0.60
1:C:476:ASP:OD1	1:D:503:ASN:HB2	2.00	0.60
1:B:191:VAL:HG22	1:B:192:PRO:HD2	1.83	0.60
1:A:495:GLY:O	1:A:512:ARG:HD3	2.01	0.60
1:D:495:GLY:O	1:D:512:ARG:HB2	2.00	0.60
1:B:86:ALA:O	1:B:90:HIS:HB3	2.02	0.60
1:C:328:ASP:O	1:C:329:LEU:HD23	2.01	0.60
1:C:454:LYS:HG2	1:C:455:ILE:N	2.16	0.60
1:C:502:LEU:HG	1:D:91:HIS:CD2	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ASP:HB3	1:A:399:PHE:CE1	2.37	0.60
1:C:16:TRP:O	1:C:20:ILE:HG13	2.02	0.60
1:B:327:LEU:HD23	1:B:345:VAL:CG2	2.32	0.60
1:D:182:VAL:CG1	1:D:317:ARG:HB2	2.31	0.60
1:A:400:LEU:HD12	1:A:400:LEU:O	2.02	0.59
1:A:227:VAL:HG11	1:A:393:THR:HG22	1.83	0.59
1:C:353:ASP:OD2	2:C:524:FAD:H5'2	2.02	0.59
1:D:165:THR:HG22	1:D:174:LYS:CG	2.30	0.59
1:D:328:ASP:HB3	1:D:336:LEU:HD12	1.84	0.59
1:B:273:ILE:CG2	1:B:276:SER:HB2	2.31	0.59
1:C:417:ILE:HG22	1:C:455:ILE:CG2	2.32	0.59
1:A:60:ALA:HA	1:A:150:LEU:HD21	1.85	0.59
1:B:338:ASN:HD21	1:B:342:GLN:HE21	1.48	0.59
1:B:378:GLU:HB3	1:B:380:ILE:HD13	1.84	0.59
1:B:400:LEU:C	1:B:400:LEU:HD12	2.28	0.59
1:C:400:LEU:HD12	1:C:400:LEU:C	2.27	0.59
1:A:400:LEU:HD12	1:A:400:LEU:C	2.28	0.59
1:A:497:MET:SD	1:B:483:VAL:HG21	2.42	0.59
1:C:191:VAL:CG2	1:C:192:PRO:HD2	2.32	0.59
1:C:503:ASN:HB2	1:D:476:ASP:OD1	2.03	0.59
1:D:243:LEU:HD22	1:D:276:SER:OG	2.03	0.59
1:C:353:ASP:HB3	1:C:359:MET:SD	2.43	0.59
1:D:217:VAL:HG22	1:D:307:PHE:HD2	1.68	0.59
1:A:191:VAL:HG22	1:A:280:ARG:HA	1.85	0.58
1:D:12:THR:HG22	1:D:14:ASN:H	1.67	0.58
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.69	0.58
1:C:89:PRO:HB3	1:C:129:PHE:CE1	2.38	0.58
1:D:417:ILE:HG22	1:D:455:ILE:CG2	2.33	0.58
1:A:267:GLU:OE1	1:A:448:HIS:HE1	1.86	0.58
1:B:125:VAL:HG11	1:B:232:PHE:HZ	1.65	0.58
1:A:95:ASP:OD2	1:B:438:MET:HG2	2.02	0.58
1:A:180:LEU:N	1:A:349:TYR:O	2.32	0.58
1:B:476:ASP:O	1:B:479:GLN:HG3	2.02	0.58
1:C:350:ALA:C	1:C:355:ILE:HD11	2.29	0.58
1:C:501:PHE:O	2:D:524:FAD:N3	2.34	0.58
1:D:191:VAL:HG22	1:D:192:PRO:HD2	1.84	0.58
1:A:338:ASN:HD21	1:A:342:GLN:HE21	1.49	0.58
1:A:432:PRO:O	1:A:450:SER:HB2	2.03	0.58
1:C:492:ASP:OD1	1:C:515:ALA:HB1	2.03	0.58
1:D:160:VAL:HG11	1:D:325:LEU:HD21	1.85	0.58
1:A:192:PRO:HG2	1:A:280:ARG:CB	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:LYS:O	1:C:465:LEU:HD13	2.03	0.58
1:C:74:ARG:HG3	2:C:524:FAD:C2A	2.34	0.58
1:D:82:CYS:SG	1:D:361:MET:HE2	2.44	0.58
1:B:391:LEU:C	1:B:391:LEU:HD12	2.29	0.58
1:C:95:ASP:OD2	1:D:438:MET:HB2	2.03	0.58
1:A:355:ILE:HG22	1:A:355:ILE:O	2.04	0.58
1:B:277:ASN:O	1:B:294:ALA:HB1	2.04	0.58
1:A:90:HIS:HE1	1:A:392:HIS:HD2	1.52	0.57
1:B:328:ASP:HB3	1:B:336:LEU:HD12	1.85	0.57
1:B:389:ASP:HB3	1:B:399:PHE:CE1	2.38	0.57
1:B:412:HIS:HD2	1:B:458:ASP:OD2	1.87	0.57
1:D:89:PRO:HB3	1:D:129:PHE:CZ	2.39	0.57
1:A:489:LEU:HD21	1:A:494:LEU:HD13	1.86	0.57
1:B:350:ALA:C	1:B:355:ILE:HD11	2.29	0.57
1:D:300:GLU:HG2	1:D:301:MET:H	1.68	0.57
1:C:501:PHE:CD1	1:C:502:LEU:HA	2.38	0.57
1:B:115:MET:O	1:B:118:LYS:HB3	2.03	0.57
1:C:86:ALA:O	1:C:90:HIS:HB3	2.03	0.57
1:A:334:GLU:O	1:A:334:GLU:HG2	2.03	0.57
1:B:206:VAL:HG23	1:B:207:GLU:OE2	2.03	0.57
1:D:420:PRO:HB3	1:D:431:LEU:O	2.04	0.57
1:C:302:ARG:HH12	1:C:304:GLU:HG3	1.69	0.57
1:C:469:HIS:ND1	1:C:469:HIS:C	2.61	0.57
1:A:247:GLU:HB2	1:A:250:LYS:HE2	1.87	0.57
1:C:40:ASP:HB3	1:C:68:ARG:NH1	2.20	0.57
1:C:82:CYS:HB3	1:C:83:PRO:HD3	1.86	0.57
1:A:90:HIS:CE1	1:A:392:HIS:HD2	2.22	0.57
1:B:192:PRO:HG2	1:B:280:ARG:HB2	1.87	0.57
1:A:460:LYS:O	1:A:461:THR:CB	2.51	0.57
1:B:84:HIS:ND1	1:B:133:ARG:HD2	2.20	0.57
1:A:123:LYS:HA	1:A:209:LEU:HD23	1.87	0.56
1:C:182:VAL:HG12	1:C:317:ARG:HB2	1.87	0.56
1:C:461:THR:HG22	1:C:461:THR:O	2.03	0.56
1:D:126:VAL:O	1:D:130:ARG:HG3	2.05	0.56
1:A:390:PHE:HA	1:A:397:VAL:O	2.05	0.56
1:B:419:MET:HB3	1:B:432:PRO:HB3	1.85	0.56
1:C:160:VAL:O	1:C:324:ILE:HG21	2.05	0.56
1:D:403:GLY:HA2	1:D:468:HIS:NE2	2.20	0.56
1:B:338:ASN:HD21	1:B:342:GLN:NE2	2.02	0.56
1:C:391:LEU:HD12	1:C:391:LEU:C	2.31	0.56
1:D:459:ALA:O	1:D:460:LYS:HB2	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:CG2	1:A:192:PRO:HD2	2.35	0.56
1:A:416:THR:CG2	1:A:523:LEU:HG	2.36	0.56
1:C:245:ARG:O	1:C:275:GLY:HA2	2.05	0.56
1:A:423:THR:HB	1:B:13:ILE:HD12	1.87	0.56
1:B:247:GLU:HB2	1:B:250:LYS:HE2	1.88	0.56
1:C:62:LEU:HB2	1:C:372:ALA:HB1	1.88	0.56
1:C:192:PRO:HG2	1:C:280:ARG:HB2	1.88	0.56
1:D:370:TYR:CD1	1:D:382:TYR:HB2	2.41	0.56
1:C:378:GLU:HB3	1:C:380:ILE:HD13	1.87	0.56
1:C:483:VAL:HG21	1:D:497:MET:SD	2.45	0.56
1:D:224:LYS:NZ	1:D:360:GLU:OE2	2.33	0.56
1:D:358:PRO:O	1:D:363:LYS:HD3	2.05	0.56
1:B:49:ILE:HG22	1:B:182:VAL:HG23	1.87	0.56
1:A:191:VAL:HG22	1:A:192:PRO:HD2	1.87	0.55
1:B:454:LYS:HG2	1:B:455:ILE:N	2.21	0.55
1:C:115:MET:HE1	1:D:111:TRP:HB2	1.87	0.55
1:D:419:MET:HA	1:D:420:PRO:C	2.30	0.55
1:C:72:VAL:CG1	1:C:158:ALA:HB2	2.35	0.55
1:A:179:ILE:HD11	1:A:351:VAL:HG11	1.88	0.55
1:C:509:GLN:HG2	1:C:510:LEU:H	1.70	0.55
1:D:231:CYS:SG	1:D:393:THR:HA	2.46	0.55
1:C:182:VAL:HG13	2:C:524:FAD:C8A	2.36	0.55
1:A:90:HIS:CD2	2:A:524:FAD:H6	2.42	0.55
1:D:191:VAL:CG2	1:D:192:PRO:HD2	2.35	0.55
1:C:47:ILE:HG13	1:C:175:ALA:HB2	1.88	0.55
1:C:89:PRO:HB3	1:C:129:PHE:CZ	2.42	0.55
1:D:82:CYS:HB3	1:D:83:PRO:CD	2.37	0.55
1:C:275:GLY:O	1:C:297:PRO:HD3	2.07	0.55
1:D:212:GLU:OE1	1:D:213:PRO:HD2	2.06	0.55
1:B:255:ASN:HB2	1:B:405:GLU:OE1	2.07	0.55
1:C:352:GLY:CA	2:C:524:FAD:O2P	2.55	0.55
1:C:461:THR:O	1:C:461:THR:CG2	2.54	0.55
1:D:89:PRO:HB3	1:D:129:PHE:CE1	2.42	0.54
1:A:227:VAL:CG1	1:A:393:THR:HG22	2.38	0.54
1:A:338:ASN:ND2	1:A:342:GLN:HE21	2.04	0.54
1:B:165:THR:HG22	1:B:174:LYS:CG	2.34	0.54
1:C:100:LEU:HB2	1:C:235:ALA:HB1	1.89	0.54
1:A:13:ILE:HG21	1:A:139:ILE:HG12	1.89	0.54
1:C:44:TYR:CD1	1:C:68:ARG:HG2	2.43	0.54
1:D:490:THR:OG1	1:D:493:GLU:HG3	2.07	0.54
1:A:499:GLU:OE2	1:A:512:ARG:NH2	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG22	1:A:174:LYS:CG	2.33	0.54
1:C:217:VAL:HG22	1:C:307:PHE:HD2	1.73	0.54
1:A:400:LEU:HD11	1:A:485:ILE:CD1	2.38	0.54
1:D:171:LYS:HD2	1:D:171:LYS:N	2.23	0.54
1:D:494:LEU:HA	1:D:497:MET:HE3	1.89	0.54
1:B:481:LEU:O	1:B:485:ILE:HG13	2.07	0.54
1:C:82:CYS:N	1:C:86:ALA:HB3	2.23	0.54
1:C:339:GLU:O	1:C:381:SER:HA	2.08	0.54
1:D:73:ASP:OD1	2:D:524:FAD:H1B	2.07	0.54
1:D:286:ASN:N	1:D:286:ASN:HD22	2.06	0.54
1:B:90:HIS:HE1	1:B:392:HIS:HD2	1.54	0.54
1:C:20:ILE:O	1:C:24:LEU:HB2	2.08	0.54
1:C:300:GLU:HG2	1:C:301:MET:H	1.71	0.54
1:D:5:ASN:ND2	1:D:7:ARG:HB2	2.23	0.54
1:A:69:GLN:HE22	1:A:151:GLU:N	1.86	0.53
1:B:396:GLU:HB2	1:B:471:GLY:O	2.08	0.53
1:D:182:VAL:HG12	1:D:317:ARG:HB2	1.89	0.53
1:B:217:VAL:HG22	1:B:307:PHE:CD2	2.37	0.53
1:C:416:THR:CG2	1:C:523:LEU:HG	2.37	0.53
1:B:90:HIS:CE1	1:B:392:HIS:HD2	2.27	0.53
1:C:111:TRP:HB2	1:D:115:MET:HE1	1.89	0.53
1:C:191:VAL:HG22	1:C:280:ARG:HA	1.90	0.53
1:D:314:GLU:HB3	1:D:359:MET:HE1	1.90	0.53
1:B:88:VAL:HB	1:B:89:PRO:CD	2.38	0.53
1:C:116:THR:O	1:C:117:GLU:HB2	2.09	0.53
1:C:509:GLN:HG2	1:C:510:LEU:N	2.23	0.53
1:D:218:VAL:HG22	1:D:303:ILE:HD13	1.91	0.53
1:D:74:ARG:O	1:D:155:ASN:HA	2.09	0.53
1:D:338:ASN:ND2	1:D:342:GLN:HE21	2.06	0.53
1:A:135:GLY:O	1:A:139:ILE:HG13	2.09	0.53
1:A:461:THR:O	1:A:463:LYS:N	2.42	0.53
1:B:20:ILE:O	1:B:24:LEU:HB2	2.09	0.53
1:C:162:ASP:OD2	1:C:162:ASP:C	2.51	0.53
1:C:189:LEU:HD21	1:C:278:VAL:HB	1.91	0.53
1:D:87:CYS:HA	2:D:524:FAD:N5	2.24	0.53
1:D:412:HIS:HD2	1:D:458:ASP:OD2	1.91	0.53
1:D:337:VAL:HA	1:D:342:GLN:O	2.09	0.52
1:D:264:ARG:NH1	1:D:264:ARG:HG2	2.24	0.52
1:D:391:LEU:C	1:D:391:LEU:HD12	2.34	0.52
1:D:42:ARG:HG3	1:D:68:ARG:HD2	1.91	0.52
1:A:417:ILE:HD13	1:A:514:ARG:HE	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:TYR:O	1:D:264:ARG:HG2	2.09	0.52
1:A:86:ALA:O	1:A:90:HIS:HB3	2.10	0.52
1:B:400:LEU:HD11	1:B:485:ILE:CD1	2.39	0.52
1:D:361:MET:HE3	1:D:365:ARG:NH1	2.24	0.52
1:D:374:ASN:HA	1:D:378:GLU:O	2.10	0.52
1:B:264:ARG:HG2	1:B:264:ARG:NH1	2.24	0.52
1:B:461:THR:O	1:B:463:LYS:N	2.43	0.52
1:B:499:GLU:HB2	1:B:503:ASN:HD22	1.71	0.52
1:A:393:THR:OG1	1:A:394:HIS:N	2.41	0.52
1:D:325:LEU:HB2	1:D:327:LEU:HD21	1.92	0.52
1:A:373:ARG:NH2	1:A:378:GLU:OE1	2.42	0.52
1:C:420:PRO:HB3	1:C:431:LEU:O	2.10	0.52
1:B:122:ILE:O	1:B:125:VAL:HG12	2.09	0.52
1:C:462:ARG:O	1:C:490:THR:HA	2.10	0.52
1:A:89:PRO:HB3	1:A:129:PHE:CZ	2.46	0.51
1:B:189:LEU:HD21	1:B:278:VAL:HB	1.92	0.51
1:C:123:LYS:HA	1:C:209:LEU:HD23	1.93	0.51
1:C:267:GLU:OE1	1:C:448:HIS:HE1	1.92	0.51
1:D:362:PHE:CD1	1:D:363:LYS:N	2.78	0.51
1:B:483:VAL:O	1:B:487:GLN:HG3	2.10	0.51
1:B:499:GLU:HB2	1:B:503:ASN:HD21	1.76	0.51
1:D:231:CYS:SG	1:D:265:MET:HE3	2.51	0.51
1:D:232:PHE:O	1:D:236:THR:HG23	2.10	0.51
1:A:247:GLU:OE2	1:A:247:GLU:HA	2.10	0.51
1:D:90:HIS:HD2	2:D:524:FAD:N5	2.08	0.51
1:D:166:VAL:CG2	1:D:178:LEU:HD21	2.40	0.51
1:A:337:VAL:HA	1:A:342:GLN:O	2.10	0.51
1:D:337:VAL:CG2	1:D:355:ILE:HD13	2.37	0.51
1:B:300:GLU:HG2	1:B:301:MET:H	1.75	0.51
1:C:247:GLU:HA	1:C:247:GLU:OE2	2.10	0.51
1:C:332:LYS:HB3	1:C:334:GLU:OE1	2.09	0.51
1:C:490:THR:OG1	1:C:493:GLU:HG3	2.11	0.51
1:D:499:GLU:HB2	1:D:503:ASN:HD22	1.75	0.51
1:A:166:VAL:CG2	1:A:178:LEU:HD21	2.41	0.51
1:B:302:ARG:HH12	1:B:304:GLU:HG3	1.76	0.51
1:C:370:TYR:CD1	1:C:382:TYR:HB2	2.46	0.51
1:A:419:MET:HB3	1:A:432:PRO:HB3	1.92	0.51
1:B:339:GLU:O	1:B:381:SER:HA	2.11	0.51
1:C:12:THR:HG23	1:D:424:GLU:OE2	2.10	0.51
1:D:382:TYR:CE2	1:D:384:PRO:HD3	2.46	0.51
1:B:267:GLU:OE1	1:B:448:HIS:HE1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HA	1:B:342:GLN:O	2.11	0.51
1:B:373:ARG:NH2	1:B:378:GLU:OE1	2.44	0.51
1:C:45:ASP:HA	1:C:176:LYS:HE3	1.90	0.51
1:A:88:VAL:HB	1:A:89:PRO:CD	2.41	0.50
1:A:179:ILE:HD12	1:A:371:ALA:CB	2.41	0.50
1:C:235:ALA:C	1:C:237:GLY:H	2.19	0.50
1:D:264:ARG:HG2	1:D:264:ARG:HH11	1.75	0.50
1:C:184:ALA:HB1	1:C:315:GLN:C	2.36	0.50
1:C:429:VAL:C	1:C:431:LEU:H	2.19	0.50
1:D:160:VAL:O	1:D:324:ILE:HG21	2.11	0.50
1:D:415:VAL:HG23	1:D:457:ILE:HB	1.94	0.50
1:C:24:LEU:HD13	1:C:76:PRO:CG	2.41	0.50
1:C:47:ILE:HG13	1:C:175:ALA:CB	2.42	0.50
1:D:90:HIS:CD2	2:D:524:FAD:N5	2.79	0.50
1:D:334:GLU:O	1:D:334:GLU:HG2	2.11	0.50
1:D:339:GLU:O	1:D:381:SER:HA	2.12	0.50
1:A:72:VAL:CG1	1:A:158:ALA:HB2	2.41	0.50
1:B:217:VAL:CG2	1:B:307:PHE:HD2	2.20	0.50
1:B:391:LEU:HD12	1:B:391:LEU:O	2.12	0.50
1:D:417:ILE:HD13	1:D:514:ARG:HE	1.77	0.50
1:B:159:LYS:HB2	1:B:167:GLU:HB3	1.93	0.50
1:C:12:THR:HG22	1:C:14:ASN:N	2.26	0.50
1:D:280:ARG:HG2	1:D:280:ARG:HH11	1.77	0.50
1:B:416:THR:HG22	1:B:523:LEU:HG	1.92	0.50
1:C:400:LEU:HD23	1:C:478:PHE:CD2	2.46	0.50
1:D:416:THR:HG22	1:D:523:LEU:HG	1.92	0.50
1:A:91:HIS:HE1	2:A:524:FAD:O4	1.95	0.50
1:D:461:THR:HG22	1:D:463:LYS:H	1.77	0.50
1:A:419:MET:HA	1:A:420:PRO:C	2.36	0.50
1:D:88:VAL:HB	1:D:89:PRO:CD	2.41	0.50
1:D:122:ILE:O	1:D:123:LYS:C	2.55	0.50
1:A:350:ALA:C	1:A:355:ILE:HD11	2.36	0.49
1:D:469:HIS:C	1:D:469:HIS:ND1	2.70	0.49
1:A:352:GLY:CA	2:A:524:FAD:O2P	2.61	0.49
1:A:420:PRO:HB3	1:A:431:LEU:O	2.12	0.49
1:B:125:VAL:HG11	1:B:232:PHE:CZ	2.47	0.49
1:D:390:PHE:HA	1:D:397:VAL:O	2.11	0.49
1:C:352:GLY:C	1:C:354:LEU:H	2.19	0.49
1:C:419:MET:HA	1:C:420:PRO:C	2.36	0.49
1:D:235:ALA:C	1:D:237:GLY:H	2.19	0.49
1:A:24:LEU:HD21	1:A:84:HIS:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:MET:HB2	1:A:453:GLN:HG2	1.95	0.49
1:B:320:GLU:O	1:B:324:ILE:HG13	2.12	0.49
1:C:362:PHE:CD1	1:C:363:LYS:N	2.80	0.49
1:A:300:GLU:HG2	1:A:301:MET:H	1.75	0.49
1:A:429:VAL:C	1:A:431:LEU:H	2.20	0.49
1:D:82:CYS:N	1:D:86:ALA:HB3	2.26	0.49
1:A:318:SER:O	1:A:319:ALA:C	2.55	0.49
1:B:47:ILE:HG13	1:B:175:ALA:HB2	1.94	0.49
1:B:231:CYS:SG	1:B:393:THR:HA	2.53	0.49
1:C:191:VAL:HG22	1:C:192:PRO:HD2	1.94	0.49
1:C:200:PHE:CD1	1:C:204:THR:HG23	2.43	0.49
1:D:31:GLU:O	1:D:155:ASN:ND2	2.33	0.49
1:D:509:GLN:HG2	1:D:510:LEU:H	1.77	0.49
1:A:217:VAL:HG13	1:A:307:PHE:CD2	2.48	0.49
1:B:296:THR:O	1:B:297:PRO:C	2.56	0.49
1:C:73:ASP:OD1	2:C:524:FAD:O3B	2.26	0.49
1:C:91:HIS:CD2	1:D:502:LEU:HG	2.47	0.49
1:C:231:CYS:SG	1:C:265:MET:HE3	2.52	0.49
1:A:494:LEU:HA	1:A:497:MET:HE3	1.94	0.49
1:B:327:LEU:HD23	1:B:345:VAL:HG21	1.95	0.49
1:C:278:VAL:HA	1:C:294:ALA:HB2	1.93	0.49
1:D:71:ILE:HB	1:D:152:TYR:HB3	1.94	0.49
1:D:115:MET:O	1:D:118:LYS:HB3	2.12	0.49
1:D:125:VAL:HG11	1:D:232:PHE:HZ	1.77	0.49
1:D:206:VAL:HG23	1:D:207:GLU:OE2	2.12	0.49
1:A:337:VAL:HG11	1:A:350:ALA:HB3	1.95	0.49
1:C:192:PRO:HG2	1:C:280:ARG:CB	2.42	0.49
1:D:440:TYR:CE2	1:D:449:MET:HE2	2.48	0.49
1:B:24:LEU:HD13	1:B:76:PRO:CG	2.42	0.49
1:B:148:LEU:HB2	1:B:150:LEU:HG	1.93	0.49
1:B:200:PHE:HD1	1:B:204:THR:HG23	1.78	0.49
1:B:429:VAL:C	1:B:431:LEU:H	2.21	0.49
1:C:6:ALA:O	1:C:7:ARG:C	2.56	0.49
1:C:125:VAL:HG11	1:C:232:PHE:HZ	1.78	0.49
1:C:278:VAL:HA	1:C:294:ALA:CB	2.42	0.49
1:D:90:HIS:CE1	1:D:392:HIS:HD2	2.30	0.49
1:A:12:THR:HG22	1:A:14:ASN:N	2.27	0.48
1:A:82:CYS:HB3	1:A:83:PRO:CD	2.41	0.48
1:B:253:LYS:HE3	1:B:406:GLU:OE1	2.13	0.48
1:B:417:ILE:HD13	1:B:514:ARG:HE	1.78	0.48
1:C:16:TRP:HZ3	1:C:33:ILE:HD13	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ASN:ND2	1:C:164:HIS:NE2	2.61	0.48
1:D:416:THR:CG2	1:D:523:LEU:HG	2.42	0.48
1:B:182:VAL:HG13	2:B:524:FAD:C8A	2.44	0.48
1:B:460:LYS:O	1:B:461:THR:CB	2.49	0.48
1:B:361:MET:HG2	2:B:524:FAD:C2	2.43	0.48
1:D:101:MET:HG3	1:D:268:GLN:OE1	2.13	0.48
1:A:82:CYS:N	1:A:86:ALA:HB3	2.27	0.48
1:A:85:ASN:HA	1:A:89:PRO:HG3	1.95	0.48
1:B:355:ILE:O	1:B:355:ILE:CG2	2.61	0.48
1:C:111:TRP:CD2	1:D:100:LEU:HD21	2.49	0.48
1:C:101:MET:HG3	1:C:268:GLN:OE1	2.13	0.48
1:C:318:SER:O	1:C:319:ALA:C	2.56	0.48
1:D:90:HIS:CD2	2:D:524:FAD:H6	2.49	0.48
1:A:289:VAL:HG12	1:A:305:THR:O	2.14	0.48
1:A:337:VAL:CG1	1:A:350:ALA:HB3	2.43	0.48
1:B:362:PHE:C	1:B:362:PHE:CD1	2.92	0.48
1:C:227:VAL:CG1	1:C:393:THR:HG22	2.43	0.48
1:C:502:LEU:HG	1:D:91:HIS:CG	2.49	0.48
1:A:16:TRP:CD1	1:A:142:PHE:HB2	2.48	0.48
1:A:217:VAL:HG22	1:A:307:PHE:HD2	1.79	0.48
1:A:499:GLU:OE1	1:B:362:PHE:HB2	2.14	0.48
1:B:334:GLU:O	1:B:334:GLU:HG2	2.13	0.48
1:C:362:PHE:CD1	1:C:362:PHE:C	2.91	0.48
1:D:87:CYS:HA	1:D:90:HIS:HD2	1.79	0.48
1:D:162:ASP:OD2	1:D:162:ASP:C	2.57	0.48
1:D:448:HIS:CD2	1:D:448:HIS:H	2.31	0.48
1:B:247:GLU:OE2	1:B:247:GLU:HA	2.14	0.48
1:C:227:VAL:HG13	1:C:265:MET:CE	2.44	0.48
1:C:352:GLY:C	1:C:354:LEU:N	2.72	0.48
1:D:74:ARG:HG3	2:D:524:FAD:N1A	2.28	0.48
1:A:43:GLU:HG2	1:A:44:TYR:N	2.26	0.48
1:A:148:LEU:CB	1:A:150:LEU:HG	2.44	0.48
1:B:57:PHE:CD2	1:B:365:ARG:HD2	2.48	0.48
1:B:71:ILE:HB	1:B:152:TYR:HB3	1.96	0.48
1:B:264:ARG:O	1:B:267:GLU:HB3	2.14	0.48
1:B:495:GLY:HA2	1:B:508:ILE:O	2.14	0.48
1:D:462:ARG:HB3	1:D:491:VAL:HG12	1.95	0.48
1:A:417:ILE:HG22	1:A:455:ILE:CG2	2.44	0.48
1:A:513:LEU:HD11	1:B:60:ALA:HB1	1.95	0.48
1:C:46:ALA:HA	1:C:177:ASN:O	2.14	0.48
1:D:164:HIS:O	1:D:174:LYS:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:PHE:CD1	1:D:204:THR:HG23	2.46	0.48
1:D:245:ARG:O	1:D:275:GLY:HA2	2.14	0.48
1:B:170:GLY:C	1:B:171:LYS:HD2	2.39	0.47
1:B:192:PRO:HG2	1:B:280:ARG:CB	2.44	0.47
1:B:463:LYS:O	1:B:465:LEU:HD13	2.14	0.47
1:C:72:VAL:HG11	1:C:158:ALA:HB2	1.95	0.47
1:C:165:THR:HA	1:C:173:PHE:O	2.14	0.47
1:C:504:PRO:HD2	1:D:476:ASP:HB2	1.95	0.47
1:D:73:ASP:OD2	2:D:524:FAD:O2B	2.25	0.47
1:D:184:ALA:HB1	1:D:315:GLN:C	2.38	0.47
1:D:501:PHE:CD1	1:D:502:LEU:HA	2.49	0.47
1:A:388:PRO:HD3	1:A:482:ASN:ND2	2.28	0.47
1:B:148:LEU:CB	1:B:150:LEU:HG	2.44	0.47
1:B:201:ASP:OD1	1:B:201:ASP:C	2.57	0.47
1:B:352:GLY:C	1:B:354:LEU:H	2.21	0.47
1:D:42:ARG:NH1	1:D:66:GLY:O	2.47	0.47
1:D:170:GLY:C	1:D:171:LYS:HD2	2.39	0.47
1:D:499:GLU:OE2	1:D:512:ARG:NH2	2.47	0.47
1:A:286:ASN:N	1:A:286:ASN:HD22	2.11	0.47
1:A:423:THR:HB	1:B:13:ILE:CD1	2.43	0.47
1:B:352:GLY:C	1:B:354:LEU:N	2.68	0.47
1:A:298:ASN:CG	1:A:298:ASN:O	2.56	0.47
1:A:362:PHE:CD1	1:A:363:LYS:N	2.83	0.47
1:A:420:PRO:HD3	1:A:432:PRO:HD3	1.96	0.47
1:B:495:GLY:O	1:B:512:ARG:HD3	2.15	0.47
1:C:473:GLY:HA2	1:D:473:GLY:HA2	1.97	0.47
1:A:100:LEU:HB2	1:A:235:ALA:HB1	1.95	0.47
1:A:185:GLY:HA2	1:A:317:ARG:NH2	2.28	0.47
1:A:446:THR:O	1:A:449:MET:HB2	2.15	0.47
1:B:490:THR:OG1	1:B:493:GLU:HG3	2.14	0.47
1:C:166:VAL:HG12	1:C:167:GLU:N	2.29	0.47
1:C:328:ASP:HB3	1:C:336:LEU:HD12	1.96	0.47
1:D:20:ILE:O	1:D:24:LEU:HB2	2.15	0.47
1:B:78:LEU:H	1:B:141:ASN:HD21	1.63	0.47
1:B:182:VAL:O	1:B:182:VAL:CG1	2.60	0.47
1:D:107:SER:OG	1:D:114:ASP:HA	2.14	0.47
1:D:400:LEU:HD11	1:D:485:ILE:CD1	2.45	0.47
1:D:405:GLU:CD	1:D:405:GLU:H	2.19	0.47
1:A:101:MET:HG3	1:A:268:GLN:OE1	2.14	0.47
1:A:502:LEU:HG	1:B:91:HIS:CE1	2.49	0.47
1:B:24:LEU:HD21	1:B:84:HIS:CE1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:THR:H	1:B:294:ALA:HA	1.79	0.47
1:C:24:LEU:HD13	1:C:76:PRO:HG3	1.96	0.47
1:C:217:VAL:HG22	1:C:307:PHE:CD2	2.50	0.47
1:D:162:ASP:OD2	1:D:165:THR:N	2.46	0.47
1:D:189:LEU:HD21	1:D:278:VAL:HB	1.96	0.47
1:D:402:MET:HA	1:D:406:GLU:OE1	2.14	0.47
1:A:45:ASP:HA	1:A:176:LYS:HE3	1.97	0.47
1:B:160:VAL:HG11	1:B:325:LEU:HD21	1.97	0.47
1:B:327:LEU:HD23	1:B:345:VAL:HG23	1.96	0.47
1:C:31:GLU:O	1:C:155:ASN:ND2	2.42	0.47
1:C:164:HIS:O	1:C:174:LYS:HA	2.15	0.47
1:B:346:PRO:O	1:B:347:ASN:HB2	2.15	0.47
1:A:44:TYR:CD1	1:A:68:ARG:HG2	2.49	0.47
1:A:164:HIS:O	1:A:174:LYS:HA	2.15	0.47
1:A:217:VAL:HG13	1:A:307:PHE:HD2	1.79	0.47
1:B:78:LEU:HB2	1:B:140:MET:HG3	1.97	0.47
1:B:374:ASN:HA	1:B:378:GLU:O	2.14	0.47
1:C:391:LEU:HD12	1:C:391:LEU:O	2.14	0.47
1:A:42:ARG:NH1	1:A:66:GLY:O	2.48	0.46
1:A:72:VAL:HG11	1:A:158:ALA:HB2	1.97	0.46
1:A:385:LYS:O	1:A:386:ASN:HB2	2.14	0.46
1:B:73:ASP:OD2	2:B:524:FAD:O2B	2.28	0.46
1:D:90:HIS:HE1	1:D:392:HIS:HD2	1.62	0.46
1:A:322:ALA:HB2	1:A:329:LEU:HD21	1.97	0.46
1:A:372:ALA:O	1:A:375:VAL:HG22	2.16	0.46
1:A:129:PHE:CE1	1:A:133:ARG:HD3	2.50	0.46
1:A:345:VAL:HG13	1:A:346:PRO:HD2	1.97	0.46
1:B:405:GLU:CD	1:B:405:GLU:H	2.22	0.46
1:D:60:ALA:HA	1:D:150:LEU:HD21	1.97	0.46
1:A:231:CYS:SG	1:A:393:THR:HA	2.55	0.46
1:B:278:VAL:HA	1:B:294:ALA:HB2	1.97	0.46
1:B:279:THR:HB	1:B:293:VAL:HG12	1.98	0.46
1:C:372:ALA:O	1:C:375:VAL:HG22	2.14	0.46
1:D:126:VAL:HG11	1:D:209:LEU:CD2	2.46	0.46
1:D:352:GLY:C	1:D:354:LEU:N	2.71	0.46
1:D:509:GLN:HG2	1:D:510:LEU:N	2.30	0.46
1:B:171:LYS:HD2	1:B:171:LYS:N	2.29	0.46
1:C:400:LEU:HD11	1:C:485:ILE:HD12	1.97	0.46
1:C:501:PHE:CG	1:C:502:LEU:HA	2.50	0.46
1:D:12:THR:HB	1:D:15:GLN:HG3	1.98	0.46
1:D:429:VAL:C	1:D:431:LEU:H	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TRP:HB3	1:A:138:GLY:HA2	1.97	0.46
1:A:267:GLU:OE1	1:A:448:HIS:CE1	2.67	0.46
1:A:447:ALA:C	1:A:449:MET:H	2.23	0.46
1:D:325:LEU:CB	1:D:327:LEU:HD21	2.45	0.46
1:B:245:ARG:HG3	1:B:277:ASN:OD1	2.15	0.46
1:C:284:ASP:OD2	1:C:290:GLN:HB2	2.16	0.46
1:C:521:VAL:O	1:C:522:SER:HB2	2.15	0.46
1:D:148:LEU:HB2	1:D:150:LEU:HG	1.98	0.46
1:D:385:LYS:O	1:D:386:ASN:HB2	2.15	0.46
1:A:332:LYS:HB3	1:A:334:GLU:OE1	2.16	0.46
1:B:162:ASP:OD2	1:B:162:ASP:C	2.59	0.46
1:C:302:ARG:HH12	1:C:304:GLU:CG	2.28	0.46
1:C:461:THR:O	1:C:463:LYS:N	2.49	0.46
1:A:78:LEU:HD21	1:A:154:LEU:HD21	1.97	0.46
1:B:6:ALA:O	1:B:7:ARG:C	2.59	0.46
1:B:16:TRP:HB3	1:B:138:GLY:HA2	1.98	0.46
1:B:191:VAL:HG22	1:B:280:ARG:HA	1.96	0.46
1:B:260:TYR:HE1	1:B:427:LEU:HD13	1.81	0.46
1:B:390:PHE:HA	1:B:397:VAL:O	2.16	0.46
1:C:85:ASN:HB2	1:C:203:ALA:HA	1.98	0.46
1:D:346:PRO:O	1:D:347:ASN:HB2	2.15	0.46
1:A:275:GLY:O	1:A:297:PRO:HD3	2.16	0.45
1:A:424:GLU:HG3	1:A:425:ASN:ND2	2.30	0.45
1:A:447:ALA:C	1:A:449:MET:N	2.73	0.45
1:C:355:ILE:O	1:C:355:ILE:CG2	2.59	0.45
1:D:80:GLY:HA3	2:D:524:FAD:O2A	2.17	0.45
1:D:419:MET:HB3	1:D:432:PRO:HB3	1.96	0.45
1:A:429:VAL:O	1:A:447:ALA:HB1	2.15	0.45
1:B:284:ASP:OD2	1:B:290:GLN:HB2	2.16	0.45
1:D:186:PRO:HA	1:D:314:GLU:OE1	2.16	0.45
1:A:438:MET:HB2	1:B:95:ASP:OD2	2.17	0.45
1:B:77:PHE:CD1	1:B:77:PHE:C	2.95	0.45
1:C:375:VAL:C	1:C:377:GLY:H	2.24	0.45
1:D:40:ASP:HB3	1:D:68:ARG:NH1	2.32	0.45
1:D:230:GLY:O	1:D:270:MET:HE3	2.16	0.45
1:B:339:GLU:HB2	1:B:381:SER:HB2	1.99	0.45
1:D:481:LEU:O	1:D:485:ILE:HG13	2.17	0.45
1:A:14:ASN:O	1:A:18:THR:HG23	2.17	0.45
1:A:77:PHE:HD1	1:A:78:LEU:O	2.00	0.45
1:A:241:VAL:HG21	1:A:303:ILE:HD12	1.99	0.45
1:B:12:THR:HG22	1:B:14:ASN:N	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:ILE:HG22	1:D:455:ILE:O	2.17	0.45
1:C:100:LEU:HD21	1:D:111:TRP:CD2	2.52	0.45
1:A:167:GLU:HG3	1:A:171:LYS:O	2.16	0.45
1:B:357:GLY:HA2	1:B:358:PRO:C	2.42	0.45
1:D:16:TRP:O	1:D:20:ILE:HG13	2.17	0.45
1:D:503:ASN:O	1:D:504:PRO:C	2.59	0.45
1:A:116:THR:O	1:A:117:GLU:HB2	2.17	0.45
1:A:200:PHE:HD1	1:A:204:THR:HG23	1.81	0.45
1:A:388:PRO:HG2	1:B:500:LEU:HD21	1.98	0.45
1:B:476:ASP:OD1	1:B:479:GLN:NE2	2.49	0.45
1:D:6:ALA:O	1:D:7:ARG:C	2.60	0.45
1:D:73:ASP:HA	2:D:524:FAD:N3A	2.32	0.45
1:A:352:GLY:HA3	2:A:524:FAD:O2P	2.16	0.45
1:D:203:ALA:O	1:D:206:VAL:HG22	2.16	0.45
1:D:489:LEU:HD21	1:D:494:LEU:HD13	1.99	0.45
1:A:49:ILE:HG22	1:A:182:VAL:HG23	1.99	0.44
1:B:78:LEU:HB2	1:B:140:MET:CG	2.47	0.44
1:C:182:VAL:O	1:C:182:VAL:CG1	2.65	0.44
1:C:286:ASN:N	1:C:286:ASN:HD22	2.13	0.44
1:B:82:CYS:CA	1:B:86:ALA:HB3	2.42	0.44
1:A:370:TYR:CD1	1:A:382:TYR:HB2	2.52	0.44
1:B:419:MET:HA	1:B:420:PRO:C	2.43	0.44
1:C:288:ARG:HG2	1:C:289:VAL:N	2.32	0.44
1:D:460:LYS:O	1:D:461:THR:CB	2.55	0.44
1:A:391:LEU:HD12	1:A:391:LEU:C	2.42	0.44
1:B:196:ALA:O	1:B:199:VAL:HG23	2.17	0.44
1:C:13:ILE:CD1	1:D:423:THR:HB	2.47	0.44
1:C:43:GLU:HG2	1:C:44:TYR:N	2.32	0.44
1:C:186:PRO:HA	1:C:314:GLU:OE1	2.17	0.44
1:C:337:VAL:CG2	1:C:355:ILE:HD13	2.42	0.44
1:C:461:THR:O	1:C:463:LYS:HG3	2.17	0.44
1:C:502:LEU:N	1:C:502:LEU:HD23	2.31	0.44
1:D:284:ASP:OD2	1:D:290:GLN:HB2	2.17	0.44
1:D:404:GLU:O	1:D:405:GLU:C	2.61	0.44
1:D:61:TYR:CD2	1:D:369:CYS:SG	3.10	0.44
1:D:393:THR:OG1	1:D:394:HIS:N	2.50	0.44
1:A:16:TRP:O	1:A:20:ILE:HG13	2.18	0.44
1:A:107:SER:OG	1:A:114:ASP:HA	2.17	0.44
1:A:206:VAL:HG23	1:A:207:GLU:OE2	2.17	0.44
1:A:238:ARG:O	1:A:239:ARG:C	2.60	0.44
1:B:417:ILE:O	1:B:417:ILE:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:GLY:O	1:C:512:ARG:HB2	2.18	0.44
1:D:45:ASP:O	1:D:177:ASN:HB2	2.16	0.44
1:A:57:PHE:CE1	1:B:512:ARG:HG2	2.53	0.44
1:A:119:VAL:O	1:A:119:VAL:CG2	2.65	0.44
1:A:357:GLY:HA2	1:A:358:PRO:C	2.42	0.44
1:A:513:LEU:HD11	1:B:60:ALA:CB	2.48	0.44
1:B:57:PHE:O	1:B:58:GLY:C	2.61	0.44
1:C:125:VAL:HG13	1:C:126:VAL:N	2.33	0.44
1:A:80:GLY:O	1:A:83:PRO:HD2	2.18	0.44
1:A:119:VAL:O	1:A:119:VAL:HG23	2.18	0.44
1:B:459:ALA:O	1:B:460:LYS:HB2	2.18	0.44
1:C:415:VAL:HG23	1:C:457:ILE:HB	2.00	0.44
1:C:459:ALA:O	1:C:460:LYS:HB2	2.17	0.44
1:D:45:ASP:HA	1:D:176:LYS:HE3	2.00	0.44
2:D:524:FAD:H9	2:D:524:FAD:H1'1	1.87	0.44
1:A:13:ILE:CG2	1:A:139:ILE:HG12	2.48	0.43
1:A:148:LEU:HB3	1:A:150:LEU:HG	2.00	0.43
1:A:228:GLU:HG2	1:A:392:HIS:HB2	2.00	0.43
1:A:264:ARG:HA	1:A:264:ARG:NE	2.33	0.43
1:B:84:HIS:CE1	1:B:133:ARG:CZ	3.00	0.43
1:C:80:GLY:O	1:C:83:PRO:HD2	2.18	0.43
1:C:218:VAL:HG22	1:C:303:ILE:HD13	2.00	0.43
1:A:73:ASP:HA	2:A:524:FAD:N3A	2.34	0.43
1:A:162:ASP:OD2	1:A:162:ASP:C	2.60	0.43
1:A:232:PHE:O	1:A:236:THR:HG23	2.18	0.43
1:A:372:ALA:O	1:A:376:MET:HG2	2.19	0.43
1:A:503:ASN:O	1:A:506:HIS:CE1	2.72	0.43
2:A:524:FAD:H9	2:A:524:FAD:H1'1	1.88	0.43
1:B:286:ASN:N	1:B:286:ASN:HD22	2.17	0.43
1:C:194:VAL:HG13	1:C:195:ASN:HD22	1.83	0.43
1:D:499:GLU:CD	1:D:512:ARG:HH22	2.25	0.43
1:B:60:ALA:HA	1:B:150:LEU:HD21	1.99	0.43
1:D:100:LEU:HB2	1:D:235:ALA:HB1	2.00	0.43
1:A:10:HIS:HA	1:A:146:GLU:OE1	2.18	0.43
1:B:85:ASN:HA	1:B:89:PRO:HG3	2.00	0.43
1:C:400:LEU:HD11	1:C:485:ILE:CD1	2.48	0.43
1:A:20:ILE:O	1:A:24:LEU:HB2	2.17	0.43
1:A:110:TYR:OH	1:B:128:LEU:HD22	2.18	0.43
1:A:152:TYR:CD1	1:A:154:LEU:HG	2.54	0.43
1:A:314:GLU:CB	1:A:359:MET:HE1	2.47	0.43
1:B:158:ALA:H	2:B:524:FAD:C2A	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ALA:C	1:B:237:GLY:H	2.25	0.43
1:C:322:ALA:O	1:C:326:GLY:HA2	2.19	0.43
1:D:179:ILE:HD12	1:D:371:ALA:HB1	2.00	0.43
1:D:235:ALA:C	1:D:237:GLY:N	2.76	0.43
1:A:16:TRP:HD1	1:A:142:PHE:HB2	1.84	0.43
1:A:231:CYS:O	1:A:394:HIS:NE2	2.51	0.43
1:A:436:ARG:NH1	1:B:99:GLU:OE1	2.52	0.43
1:B:153:ILE:C	1:B:154:LEU:HD23	2.44	0.43
1:D:461:THR:O	1:D:463:LYS:N	2.51	0.43
1:B:322:ALA:O	1:B:326:GLY:HA2	2.18	0.43
1:B:447:ALA:C	1:B:449:MET:N	2.76	0.43
1:D:200:PHE:HA	1:D:204:THR:HG21	2.01	0.43
1:D:362:PHE:CD1	1:D:362:PHE:C	2.96	0.43
1:D:424:GLU:HG3	1:D:425:ASN:ND2	2.33	0.43
1:D:458:ASP:O	1:D:462:ARG:HA	2.19	0.43
1:B:89:PRO:HB3	1:B:129:PHE:CE1	2.54	0.43
1:C:188:THR:OG1	1:C:189:LEU:N	2.52	0.43
1:C:195:ASN:O	1:C:196:ALA:C	2.60	0.43
1:A:139:ILE:O	1:A:143:GLN:HB3	2.18	0.43
1:C:49:ILE:HG22	1:C:182:VAL:CG2	2.48	0.43
1:C:289:VAL:HG12	1:C:290:GLN:N	2.33	0.43
1:D:286:ASN:N	1:D:286:ASN:ND2	2.64	0.43
1:A:227:VAL:HG21	1:A:249:LEU:CD2	2.38	0.43
1:A:325:LEU:O	1:A:345:VAL:HG21	2.19	0.43
1:B:400:LEU:HD22	1:B:482:ASN:HB2	2.00	0.43
1:C:159:LYS:HB2	1:C:167:GLU:HB3	2.00	0.43
1:C:273:ILE:HG22	1:C:276:SER:HB2	2.00	0.43
1:C:424:GLU:OE2	1:D:12:THR:HG23	2.19	0.43
1:D:185:GLY:HA2	1:D:317:ARG:NH2	2.34	0.43
1:A:366:LYS:NZ	1:B:496:ASP:O	2.45	0.42
1:B:322:ALA:HB2	1:B:329:LEU:HD21	2.00	0.42
1:B:362:PHE:CD1	1:B:363:LYS:N	2.87	0.42
1:C:14:ASN:O	1:C:18:THR:HG23	2.19	0.42
1:C:276:SER:HA	1:C:295:MET:O	2.18	0.42
2:C:524:FAD:H9	2:C:524:FAD:H1'1	1.86	0.42
1:D:279:THR:HG22	1:D:280:ARG:HG2	1.99	0.42
1:D:355:ILE:O	1:D:355:ILE:CG2	2.65	0.42
1:C:191:VAL:CG2	1:C:279:THR:O	2.67	0.42
1:C:191:VAL:CG2	1:C:280:ARG:HA	2.49	0.42
1:C:388:PRO:HG2	1:D:500:LEU:HD21	2.01	0.42
1:A:424:GLU:OE2	1:B:12:THR:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HB2	1:B:235:ALA:HB1	2.01	0.42
1:C:436:ARG:NH1	1:D:99:GLU:OE1	2.52	0.42
1:D:278:VAL:HA	1:D:294:ALA:HB2	2.01	0.42
1:D:371:ALA:O	1:D:375:VAL:HG13	2.19	0.42
1:C:16:TRP:HB3	1:C:138:GLY:HA2	2.02	0.42
1:C:53:ALA:O	1:C:57:PHE:HB2	2.19	0.42
1:A:498:ASP:OD2	1:B:366:LYS:NZ	2.39	0.42
1:C:90:HIS:CE1	1:C:392:HIS:HD2	2.37	0.42
1:A:24:LEU:HD13	1:A:76:PRO:CG	2.50	0.42
1:A:498:ASP:CG	1:B:366:LYS:HZ2	2.25	0.42
1:B:289:VAL:HG12	1:B:290:GLN:N	2.33	0.42
1:C:499:GLU:OE2	1:C:512:ARG:NH2	2.52	0.42
1:D:476:ASP:O	1:D:479:GLN:HG3	2.18	0.42
1:A:78:LEU:CD2	1:A:154:LEU:HD21	2.50	0.42
1:A:201:ASP:N	1:A:204:THR:HG22	2.12	0.42
1:C:40:ASP:CB	1:C:68:ARG:NH1	2.83	0.42
1:C:191:VAL:HG23	1:C:192:PRO:HD2	2.01	0.42
1:C:338:ASN:OD1	1:C:342:GLN:HB2	2.20	0.42
1:C:350:ALA:C	1:C:351:VAL:HG13	2.44	0.42
1:C:425:ASN:O	1:C:426:GLY:C	2.62	0.42
1:C:503:ASN:O	1:C:504:PRO:C	2.59	0.42
1:D:10:HIS:HA	1:D:146:GLU:OE1	2.20	0.42
1:D:47:ILE:HG13	1:D:175:ALA:HB2	2.02	0.42
1:D:67:GLY:HA3	1:D:376:MET:CE	2.50	0.42
1:D:501:PHE:CG	1:D:502:LEU:HA	2.54	0.42
1:A:34:TYR:OH	1:A:36:VAL:HG21	2.19	0.42
1:B:231:CYS:SG	1:B:265:MET:HE3	2.60	0.42
1:C:346:PRO:O	1:C:348:VAL:HG23	2.20	0.42
1:C:412:HIS:HD2	1:C:458:ASP:OD2	2.02	0.42
1:C:476:ASP:HB2	1:D:504:PRO:HD2	2.02	0.42
1:D:115:MET:O	1:D:116:THR:C	2.62	0.42
1:D:125:VAL:HG13	1:D:126:VAL:N	2.34	0.42
1:A:338:ASN:ND2	1:A:340:TYR:HD2	2.18	0.42
1:A:459:ALA:O	1:A:460:LYS:HB2	2.19	0.42
1:B:200:PHE:CD1	1:B:204:THR:HG23	2.55	0.42
1:B:353:ASP:CG	2:B:524:FAD:HO3'	2.20	0.42
1:B:521:VAL:O	1:B:522:SER:HB2	2.20	0.42
1:C:286:ASN:N	1:C:286:ASN:ND2	2.67	0.42
1:D:296:THR:O	1:D:297:PRO:C	2.62	0.42
1:D:383:THR:HA	1:D:384:PRO:HD2	1.90	0.42
1:A:122:ILE:O	1:A:123:LYS:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HD11	1:A:238:ARG:HD2	2.02	0.42
1:A:383:THR:HA	1:A:384:PRO:HD2	1.89	0.42
1:A:459:ALA:O	1:A:460:LYS:O	2.38	0.42
1:B:45:ASP:O	1:B:46:ALA:HB2	2.19	0.42
1:B:280:ARG:HH11	1:B:280:ARG:HG2	1.85	0.42
1:C:78:LEU:H	1:C:141:ASN:HD21	1.68	0.42
1:C:139:ILE:O	1:C:143:GLN:HB3	2.20	0.42
1:C:454:LYS:CG	1:C:455:ILE:N	2.82	0.42
1:C:499:GLU:O	1:C:499:GLU:HG2	2.19	0.42
1:D:330:GLY:C	1:D:332:LYS:H	2.28	0.42
1:A:23:ILE:HG23	1:A:30:GLY:HA3	2.01	0.41
1:A:99:GLU:OE1	1:B:436:ARG:NH1	2.52	0.41
1:C:60:ALA:HA	1:C:150:LEU:HD21	2.02	0.41
1:A:24:LEU:HD13	1:A:76:PRO:HG3	2.02	0.41
1:B:115:MET:O	1:B:116:THR:C	2.63	0.41
1:B:415:VAL:HG23	1:B:457:ILE:HB	2.03	0.41
1:C:76:PRO:HB3	1:C:155:ASN:HB2	2.02	0.41
1:C:100:LEU:O	1:C:104:ARG:HG3	2.20	0.41
1:D:78:LEU:H	1:D:141:ASN:HD21	1.68	0.41
1:D:152:TYR:CD1	1:D:154:LEU:HG	2.55	0.41
1:A:171:LYS:N	1:A:171:LYS:HD2	2.34	0.41
1:A:442:PHE:O	1:B:128:LEU:HD11	2.21	0.41
1:B:61:TYR:O	1:B:65:MET:HG3	2.19	0.41
1:B:88:VAL:O	1:B:89:PRO:C	2.63	0.41
1:B:447:ALA:C	1:B:449:MET:H	2.27	0.41
1:C:115:MET:O	1:C:118:LYS:HB3	2.19	0.41
1:C:302:ARG:HG2	1:C:302:ARG:HH11	1.86	0.41
1:D:33:ILE:O	1:D:153:ILE:HA	2.20	0.41
1:D:198:GLY:H	1:D:289:VAL:HG23	1.86	0.41
1:D:352:GLY:C	1:D:354:LEU:H	2.27	0.41
1:A:400:LEU:HD11	1:A:485:ILE:HD13	2.01	0.41
1:B:298:ASN:O	1:B:298:ASN:CG	2.62	0.41
1:C:62:LEU:C	1:C:62:LEU:HD23	2.45	0.41
1:C:288:ARG:CG	1:C:289:VAL:N	2.83	0.41
1:C:371:ALA:O	1:C:375:VAL:HG13	2.20	0.41
1:D:86:ALA:O	1:D:90:HIS:HB3	2.19	0.41
1:D:206:VAL:HG23	1:D:207:GLU:CD	2.46	0.41
1:D:400:LEU:HD23	1:D:478:PHE:CD2	2.55	0.41
1:A:179:ILE:HD12	1:A:371:ALA:HB1	2.02	0.41
1:D:71:ILE:HB	1:D:152:TYR:CB	2.50	0.41
1:D:193:GLY:C	1:D:195:ASN:N	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD13	1:A:137:HIS:HB3	2.02	0.41
1:A:296:THR:O	1:A:297:PRO:C	2.64	0.41
1:A:495:GLY:HA2	1:A:508:ILE:O	2.20	0.41
1:B:267:GLU:OE1	1:B:448:HIS:CE1	2.74	0.41
1:C:152:TYR:CD1	1:C:154:LEU:HG	2.55	0.41
1:C:500:LEU:HD21	1:D:388:PRO:HG2	2.01	0.41
1:D:48:PHE:CE2	1:D:179:ILE:HG21	2.56	0.41
1:D:80:GLY:O	1:D:83:PRO:HD2	2.21	0.41
1:D:196:ALA:O	1:D:199:VAL:HG23	2.20	0.41
1:D:398:SER:OG	1:D:475:LYS:HA	2.20	0.41
1:B:45:ASP:HA	1:B:176:LYS:HE3	2.02	0.41
1:D:82:CYS:SG	1:D:361:MET:SD	3.19	0.41
1:D:201:ASP:OD1	1:D:201:ASP:C	2.63	0.41
1:D:520:LEU:O	1:D:521:VAL:C	2.64	0.41
1:A:6:ALA:O	1:A:7:ARG:C	2.64	0.41
1:A:503:ASN:HB2	1:B:476:ASP:OD1	2.20	0.41
1:B:38:GLU:C	1:B:39:ASN:HD22	2.27	0.41
1:B:44:TYR:CD1	1:B:68:ARG:HG2	2.56	0.41
1:B:122:ILE:O	1:B:126:VAL:CG1	2.69	0.41
1:B:182:VAL:CG1	1:B:317:ARG:HB2	2.49	0.41
1:B:255:ASN:O	1:B:256:GLU:C	2.64	0.41
1:B:329:LEU:HD23	1:B:335:VAL:HA	2.03	0.41
1:C:88:VAL:HB	1:C:89:PRO:CD	2.51	0.41
1:C:122:ILE:O	1:C:125:VAL:CG1	2.63	0.41
1:C:171:LYS:N	1:C:171:LYS:HD2	2.36	0.41
1:D:314:GLU:CB	1:D:359:MET:HE1	2.51	0.41
1:A:44:TYR:HB2	1:A:175:ALA:HB2	2.02	0.41
1:A:77:PHE:CD1	1:A:77:PHE:C	2.99	0.41
1:A:89:PRO:HB3	1:A:129:PHE:CE1	2.55	0.41
1:A:189:LEU:HD21	1:A:278:VAL:HB	2.03	0.41
1:A:500:LEU:HD21	1:B:388:PRO:HG2	2.02	0.41
1:B:85:ASN:HB2	1:B:203:ALA:HA	2.03	0.41
1:B:107:SER:OG	1:B:114:ASP:HA	2.20	0.41
1:B:122:ILE:O	1:B:126:VAL:HG13	2.21	0.41
1:B:162:ASP:OD2	1:B:165:THR:N	2.53	0.41
1:B:191:VAL:HG22	1:B:192:PRO:CD	2.50	0.41
1:B:338:ASN:ND2	1:B:342:GLN:HE21	2.15	0.41
1:B:465:LEU:N	1:B:465:LEU:CD1	2.84	0.41
1:B:523:LEU:HD12	1:B:523:LEU:N	2.36	0.41
1:C:148:LEU:CB	1:C:150:LEU:HG	2.51	0.41
1:C:193:GLY:O	1:C:195:ASN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:VAL:HG21	1:C:249:LEU:CD2	2.38	0.41
1:C:362:PHE:HB2	1:D:499:GLU:OE1	2.20	0.41
1:C:499:GLU:HB2	1:C:503:ASN:HD22	1.85	0.41
1:D:72:VAL:CG1	1:D:158:ALA:HB2	2.51	0.41
1:D:122:ILE:O	1:D:125:VAL:CG1	2.67	0.41
1:D:125:VAL:HG11	1:D:232:PHE:CZ	2.56	0.41
1:D:446:THR:O	1:D:449:MET:HB2	2.21	0.41
1:B:89:PRO:HB3	1:B:129:PHE:CZ	2.56	0.41
1:D:5:ASN:HD21	1:D:7:ARG:HB2	1.84	0.41
1:D:296:THR:C	1:D:298:ASN:N	2.78	0.41
1:D:506:HIS:HB3	1:D:509:GLN:NE2	2.36	0.41
1:D:521:VAL:O	1:D:522:SER:HB2	2.20	0.41
1:A:454:LYS:CG	1:A:455:ILE:N	2.82	0.40
1:B:80:GLY:O	1:B:83:PRO:HD2	2.21	0.40
1:B:213:PRO:HB2	1:B:238:ARG:HE	1.86	0.40
1:B:491:VAL:HG11	1:B:520:LEU:HD21	2.03	0.40
1:C:224:LYS:HE2	1:C:390:PHE:O	2.20	0.40
1:C:457:ILE:HG22	1:C:458:ASP:N	2.37	0.40
1:D:142:PHE:CD1	1:D:142:PHE:C	2.97	0.40
1:D:193:GLY:O	1:D:195:ASN:N	2.54	0.40
1:D:462:ARG:O	1:D:490:THR:HA	2.21	0.40
1:A:148:LEU:HB2	1:A:150:LEU:HG	2.03	0.40
1:A:159:LYS:HD2	1:A:167:GLU:CD	2.45	0.40
1:A:182:VAL:HG12	1:A:317:ARG:HB2	2.04	0.40
1:A:202:HIS:CG	1:A:203:ALA:N	2.89	0.40
1:A:278:VAL:HA	1:A:294:ALA:HB2	2.03	0.40
1:B:16:TRP:O	1:B:20:ILE:HG13	2.21	0.40
1:B:87:CYS:HA	1:B:90:HIS:HD2	1.85	0.40
1:B:201:ASP:H	1:B:204:THR:CG2	2.18	0.40
1:C:71:ILE:HB	1:C:152:TYR:HB3	2.01	0.40
1:C:201:ASP:N	1:C:204:THR:HG22	2.11	0.40
1:C:235:ALA:C	1:C:237:GLY:N	2.79	0.40
1:C:359:MET:O	2:C:524:FAD:H1'2	2.20	0.40
1:A:370:TYR:HA	1:A:373:ARG:HD3	2.03	0.40
1:A:375:VAL:C	1:A:377:GLY:H	2.28	0.40
1:A:501:PHE:CD2	1:A:502:LEU:HD23	2.56	0.40
1:D:24:LEU:HD21	1:D:84:HIS:CE1	2.57	0.40
1:D:389:ASP:HB3	1:D:399:PHE:CE1	2.57	0.40
1:A:245:ARG:HG3	1:A:277:ASN:OD1	2.22	0.40
1:A:339:GLU:HB2	1:A:381:SER:HB2	2.03	0.40
1:A:499:GLU:CD	1:A:512:ARG:HH22	2.28	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:H	1:B:15:GLN:HB2	1.87	0.40
1:B:166:VAL:CG2	1:B:178:LEU:HD21	2.50	0.40
1:B:201:ASP:N	1:B:204:THR:HG22	2.17	0.40
1:C:370:TYR:HD1	1:C:382:TYR:CG	2.40	0.40
1:D:273:ILE:HG22	1:D:276:SER:HB2	2.04	0.40
1:A:184:ALA:HB1	1:A:315:GLN:C	2.46	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	520/523 (99%)	449 (86%)	60 (12%)	11 (2%)	5	20
1	B	520/523 (99%)	447 (86%)	62 (12%)	11 (2%)	5	20
1	C	520/523 (99%)	456 (88%)	51 (10%)	13 (2%)	4	16
1	D	520/523 (99%)	450 (86%)	54 (10%)	16 (3%)	3	12
All	All	2080/2092 (99%)	1802 (87%)	227 (11%)	51 (2%)	4	16

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	A	319	ALA
1	A	462	ARG
1	B	224	LYS
1	B	462	ARG
1	C	224	LYS
1	C	462	ARG
1	C	508	ILE
1	D	224	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	462	ARG
1	A	461	THR
1	A	522	SER
1	B	461	THR
1	B	522	SER
1	C	352	GLY
1	C	522	SER
1	D	319	ALA
1	D	352	GLY
1	D	461	THR
1	D	522	SER
1	A	393	THR
1	A	460	LYS
1	B	213	PRO
1	B	319	ALA
1	B	434	SER
1	C	319	ALA
1	C	460	LYS
1	C	461	THR
1	A	352	GLY
1	C	393	THR
1	D	393	THR
1	A	87	CYS
1	B	428	ASN
1	C	41	PRO
1	D	197	LYS
1	B	508	ILE
1	D	85	ASN
1	D	428	ASN
1	D	460	LYS
1	D	508	ILE
1	A	194	VAL
1	B	88	VAL
1	C	194	VAL
1	C	384	PRO
1	D	194	VAL
1	C	351	VAL
1	D	213	PRO
1	A	41	PRO
1	B	351	VAL
1	D	41	PRO
1	D	88	VAL

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	423/424 (100%)	406 (96%)	17 (4%)	28	63
1	B	423/424 (100%)	404 (96%)	19 (4%)	24	58
1	C	423/424 (100%)	402 (95%)	21 (5%)	22	54
1	D	423/424 (100%)	404 (96%)	19 (4%)	24	58
All	All	1692/1696 (100%)	1616 (96%)	76 (4%)	24	58

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	25	GLU
1	A	56	ARG
1	A	90	HIS
1	A	126	VAL
1	A	182	VAL
1	A	190	ASP
1	A	251	LEU
1	A	305	THR
1	A	375	VAL
1	A	405	GLU
1	A	455	ILE
1	A	461	THR
1	A	465	LEU
1	A	469	HIS
1	A	504	PRO
1	A	514	ARG
1	B	7	ARG
1	B	25	GLU
1	B	90	HIS
1	B	119	VAL
1	B	126	VAL
1	B	174	LYS
1	B	179	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	VAL
1	B	204	THR
1	B	305	THR
1	B	375	VAL
1	B	405	GLU
1	B	455	ILE
1	B	461	THR
1	B	462	ARG
1	B	465	LEU
1	B	502	LEU
1	B	504	PRO
1	B	514	ARG
1	C	7	ARG
1	C	25	GLU
1	C	87	CYS
1	C	90	HIS
1	C	119	VAL
1	C	126	VAL
1	C	174	LYS
1	C	182	VAL
1	C	190	ASP
1	C	251	LEU
1	C	303	ILE
1	C	305	THR
1	C	375	VAL
1	C	405	GLU
1	C	455	ILE
1	C	461	THR
1	C	462	ARG
1	C	465	LEU
1	C	469	HIS
1	C	502	LEU
1	C	514	ARG
1	D	7	ARG
1	D	25	GLU
1	D	56	ARG
1	D	90	HIS
1	D	126	VAL
1	D	174	LYS
1	D	182	VAL
1	D	190	ASP
1	D	234	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	305	THR
1	D	375	VAL
1	D	405	GLU
1	D	455	ILE
1	D	461	THR
1	D	465	LEU
1	D	469	HIS
1	D	502	LEU
1	D	504	PRO
1	D	514	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	14	ASN
1	A	39	ASN
1	A	69	GLN
1	A	84	HIS
1	A	90	HIS
1	A	141	ASN
1	A	163	ASN
1	A	195	ASN
1	A	255	ASN
1	A	286	ASN
1	A	342	GLN
1	A	392	HIS
1	A	412	HIS
1	A	425	ASN
1	A	448	HIS
1	A	482	ASN
1	B	5	ASN
1	B	14	ASN
1	B	39	ASN
1	B	69	GLN
1	B	84	HIS
1	B	90	HIS
1	B	141	ASN
1	B	163	ASN
1	B	234	ASN
1	B	255	ASN
1	B	286	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	290	GLN
1	B	342	GLN
1	B	347	ASN
1	B	392	HIS
1	B	412	HIS
1	B	425	ASN
1	B	448	HIS
1	C	5	ASN
1	C	14	ASN
1	C	39	ASN
1	C	69	GLN
1	C	90	HIS
1	C	141	ASN
1	C	163	ASN
1	C	195	ASN
1	C	234	ASN
1	C	255	ASN
1	C	286	ASN
1	C	342	GLN
1	C	392	HIS
1	C	412	HIS
1	C	425	ASN
1	D	5	ASN
1	D	14	ASN
1	D	39	ASN
1	D	69	GLN
1	D	90	HIS
1	D	109	GLN
1	D	141	ASN
1	D	163	ASN
1	D	195	ASN
1	D	255	ASN
1	D	286	ASN
1	D	342	GLN
1	D	392	HIS
1	D	412	HIS
1	D	425	ASN
1	D	428	ASN
1	D	448	HIS
1	D	482	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	524	-	58,58,58	2.19	13 (22%)	85,89,89	1.49	10 (11%)
2	FAD	C	524	-	58,58,58	2.18	15 (25%)	85,89,89	1.54	11 (12%)
2	FAD	A	524	-	58,58,58	2.23	15 (25%)	85,89,89	1.50	10 (11%)
2	FAD	B	524	-	58,58,58	2.22	13 (22%)	85,89,89	1.53	12 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	524	-	-	4/34/50/50	0/6/6/6
2	FAD	C	524	-	-	4/34/50/50	0/6/6/6
2	FAD	A	524	-	-	4/34/50/50	0/6/6/6
2	FAD	B	524	-	-	4/34/50/50	0/6/6/6

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	524	FAD	C4X-N5	6.82	1.45	1.30
2	D	524	FAD	C4X-N5	6.42	1.44	1.30
2	A	524	FAD	C4X-N5	6.17	1.44	1.30
2	C	524	FAD	C4X-N5	6.09	1.43	1.30
2	D	524	FAD	C4A-N3A	6.03	1.45	1.34
2	A	524	FAD	C9A-N10	5.85	1.51	1.41
2	C	524	FAD	C4A-N3A	5.71	1.45	1.34
2	B	524	FAD	C9A-N10	5.61	1.50	1.41
2	A	524	FAD	C4A-N3A	5.48	1.44	1.34
2	D	524	FAD	C9A-N10	5.24	1.50	1.41
2	B	524	FAD	C4A-N3A	5.15	1.44	1.34
2	B	524	FAD	C9A-C5X	5.10	1.49	1.41
2	C	524	FAD	C9A-N10	5.08	1.50	1.41
2	C	524	FAD	C2A-N3A	5.00	1.42	1.33
2	A	524	FAD	C2A-N3A	5.00	1.42	1.33
2	D	524	FAD	C2A-N3A	4.77	1.42	1.33
2	B	524	FAD	C2A-N3A	4.46	1.41	1.33
2	D	524	FAD	C5'-C4'	-4.24	1.46	1.51
2	C	524	FAD	C9A-C5X	4.23	1.48	1.41
2	B	524	FAD	C5A-C4A	-4.17	1.31	1.39
2	A	524	FAD	C5'-C4'	-4.06	1.46	1.51
2	A	524	FAD	C5A-C4A	-4.03	1.31	1.39
2	D	524	FAD	C5A-C4A	-4.03	1.31	1.39
2	A	524	FAD	C9A-C5X	4.00	1.47	1.41
2	D	524	FAD	C9A-C5X	3.95	1.47	1.41
2	C	524	FAD	C5A-C4A	-3.81	1.32	1.39
2	C	524	FAD	C5'-C4'	-3.57	1.47	1.51
2	B	524	FAD	C5'-C4'	-3.56	1.47	1.51
2	C	524	FAD	C10-N1	3.55	1.40	1.33
2	D	524	FAD	C10-N1	3.45	1.40	1.33
2	A	524	FAD	C10-N1	3.23	1.39	1.33
2	B	524	FAD	C10-N1	3.21	1.39	1.33
2	B	524	FAD	C1'-C2'	-3.06	1.48	1.52
2	A	524	FAD	C8A-N9A	2.96	1.42	1.37
2	A	524	FAD	O4-C4	2.90	1.29	1.23
2	A	524	FAD	C1'-C2'	-2.88	1.48	1.52
2	C	524	FAD	C8A-N9A	2.85	1.42	1.37
2	B	524	FAD	C2'-C3'	-2.84	1.48	1.53
2	B	524	FAD	C8A-N9A	2.84	1.42	1.37
2	D	524	FAD	C6-C7	2.78	1.43	1.39
2	C	524	FAD	C2'-C3'	-2.76	1.48	1.53
2	B	524	FAD	C6-C7	2.74	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	524	FAD	C8A-N9A	2.68	1.42	1.37
2	D	524	FAD	O4-C4	2.51	1.28	1.23
2	C	524	FAD	C4-N3	2.49	1.43	1.38
2	D	524	FAD	C2'-C3'	-2.36	1.49	1.53
2	C	524	FAD	C4X-C4	-2.33	1.36	1.44
2	C	524	FAD	PA-O3P	2.32	1.62	1.59
2	A	524	FAD	C2B-C3B	-2.30	1.47	1.53
2	B	524	FAD	C2B-C3B	-2.28	1.47	1.53
2	C	524	FAD	C1'-C2'	-2.27	1.49	1.52
2	D	524	FAD	C2B-C3B	-2.26	1.47	1.53
2	A	524	FAD	C4-N3	2.26	1.43	1.38
2	C	524	FAD	C6-C7	2.17	1.42	1.39
2	A	524	FAD	C1'-N10	-2.08	1.42	1.47
2	A	524	FAD	O4'-C4'	2.04	1.47	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	524	FAD	C5A-C4A-N9A	5.36	111.66	105.81
2	B	524	FAD	C5A-C4A-N9A	5.22	111.50	105.81
2	A	524	FAD	C5A-C4A-N9A	5.17	111.45	105.81
2	D	524	FAD	C5A-C4A-N9A	5.06	111.32	105.81
2	C	524	FAD	C4A-N9A-C8A	-4.95	100.54	105.74
2	B	524	FAD	C4A-N9A-C8A	-4.85	100.64	105.74
2	B	524	FAD	N3A-C4A-N9A	-4.79	119.02	127.17
2	C	524	FAD	N3A-C4A-N9A	-4.79	119.03	127.17
2	D	524	FAD	C4A-N9A-C8A	-4.74	100.76	105.74
2	A	524	FAD	N3A-C4A-N9A	-4.65	119.26	127.17
2	D	524	FAD	N3A-C4A-N9A	-4.64	119.27	127.17
2	A	524	FAD	C4A-N9A-C8A	-4.63	100.88	105.74
2	D	524	FAD	C5X-C9A-N10	-3.31	114.98	117.97
2	C	524	FAD	C5X-C9A-N10	-3.16	115.11	117.97
2	A	524	FAD	C5X-C9A-N10	-3.10	115.16	117.97
2	B	524	FAD	C5X-C9A-N10	-3.06	115.21	117.97
2	B	524	FAD	N3A-C2A-N1A	-2.84	124.29	128.58
2	C	524	FAD	C1'-N10-C9A	-2.69	115.41	120.63
2	B	524	FAD	C1'-N10-C9A	-2.67	115.45	120.63
2	D	524	FAD	C9-C9A-N10	2.67	125.44	121.85
2	C	524	FAD	N3A-C2A-N1A	-2.66	124.56	128.58
2	D	524	FAD	C1'-N10-C9A	-2.65	115.48	120.63
2	A	524	FAD	O3'-C3'-C4'	-2.64	102.94	108.93
2	D	524	FAD	N3A-C2A-N1A	-2.63	124.60	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	524	FAD	C9-C9A-N10	2.61	125.36	121.85
2	B	524	FAD	C1'-C2'-C3'	2.59	116.67	109.66
2	A	524	FAD	O2B-C2B-C3B	2.58	120.10	111.82
2	C	524	FAD	O2B-C2B-C3B	2.57	120.06	111.82
2	C	524	FAD	C9-C9A-N10	2.54	125.28	121.85
2	A	524	FAD	C1'-N10-C9A	-2.54	115.70	120.63
2	D	524	FAD	O2B-C2B-C3B	2.54	119.95	111.82
2	B	524	FAD	C9-C9A-N10	2.52	125.24	121.85
2	A	524	FAD	N3A-C2A-N1A	-2.51	124.78	128.58
2	B	524	FAD	O2B-C2B-C3B	2.51	119.87	111.82
2	B	524	FAD	O3'-C3'-C4'	-2.43	103.41	108.93
2	D	524	FAD	O3'-C3'-C4'	-2.38	103.52	108.93
2	D	524	FAD	C1'-C2'-C3'	2.36	116.06	109.66
2	C	524	FAD	O3'-C3'-C4'	-2.36	103.58	108.93
2	C	524	FAD	C1'-C2'-C3'	2.35	116.02	109.66
2	A	524	FAD	C1'-C2'-C3'	2.30	115.89	109.66
2	B	524	FAD	C4-C4X-C10	2.07	120.48	116.93
2	C	524	FAD	C4-C4X-C10	2.02	120.39	116.93
2	B	524	FAD	C5A-C4A-N3A	2.01	129.48	126.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

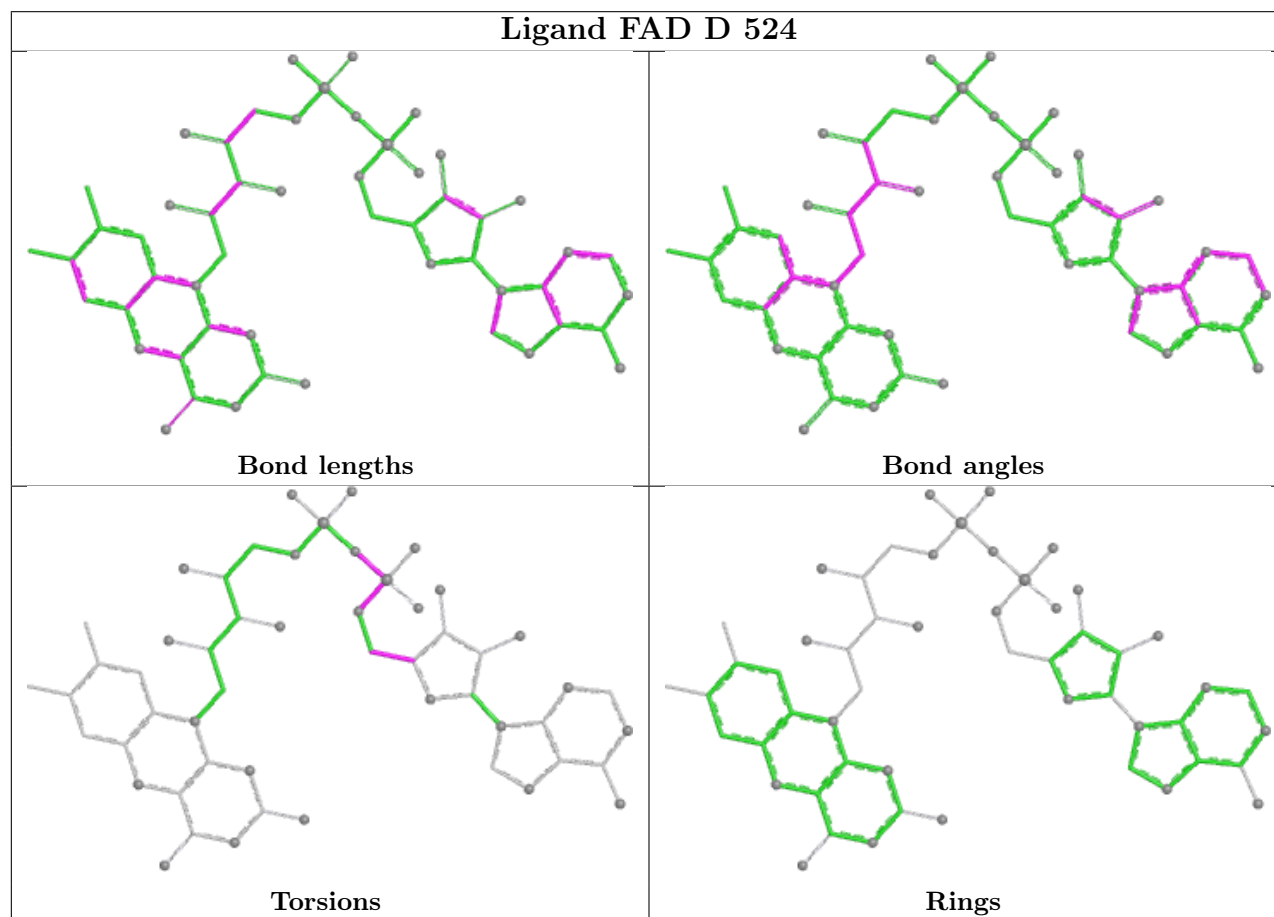
Mol	Chain	Res	Type	Atoms
2	A	524	FAD	P-O3P-PA-O1A
2	B	524	FAD	P-O3P-PA-O1A
2	D	524	FAD	P-O3P-PA-O1A
2	C	524	FAD	P-O3P-PA-O1A
2	A	524	FAD	C5B-O5B-PA-O1A
2	B	524	FAD	C5B-O5B-PA-O1A
2	C	524	FAD	C5B-O5B-PA-O1A
2	D	524	FAD	C5B-O5B-PA-O1A
2	B	524	FAD	P-O3P-PA-O2A
2	A	524	FAD	P-O3P-PA-O2A
2	C	524	FAD	O4B-C4B-C5B-O5B
2	D	524	FAD	O4B-C4B-C5B-O5B
2	B	524	FAD	O4B-C4B-C5B-O5B
2	A	524	FAD	O4B-C4B-C5B-O5B
2	C	524	FAD	P-O3P-PA-O2A
2	D	524	FAD	P-O3P-PA-O2A

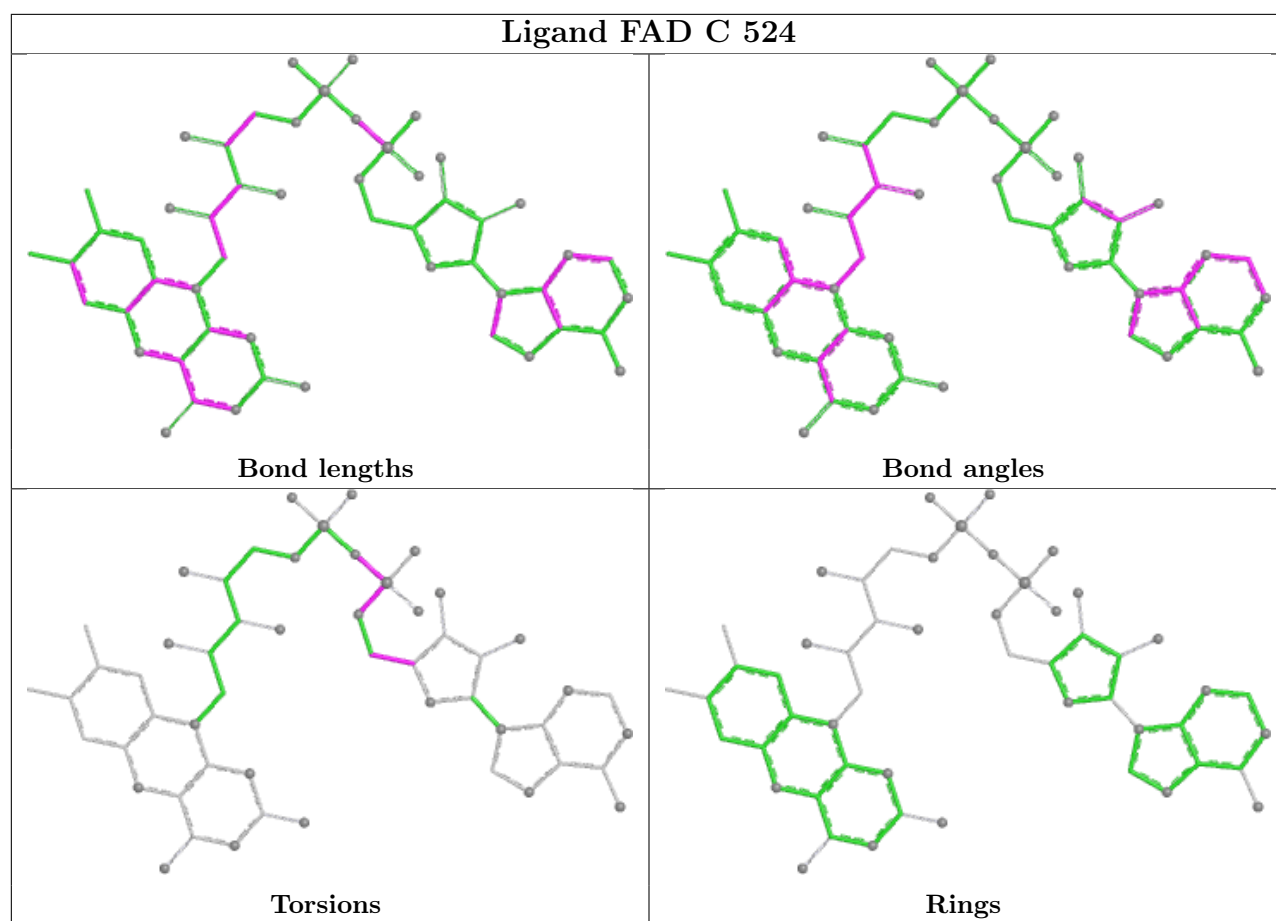
There are no ring outliers.

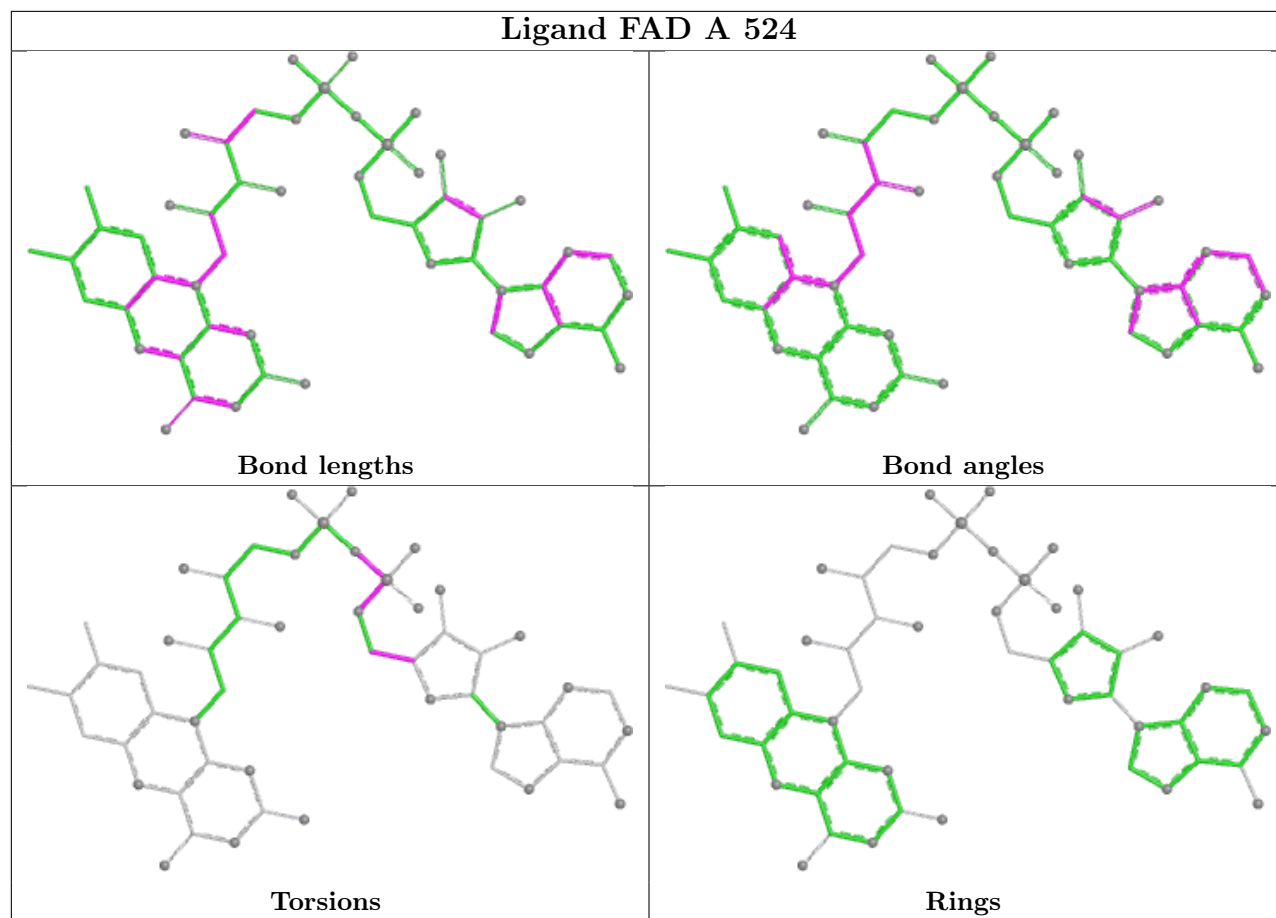
4 monomers are involved in 33 short contacts:

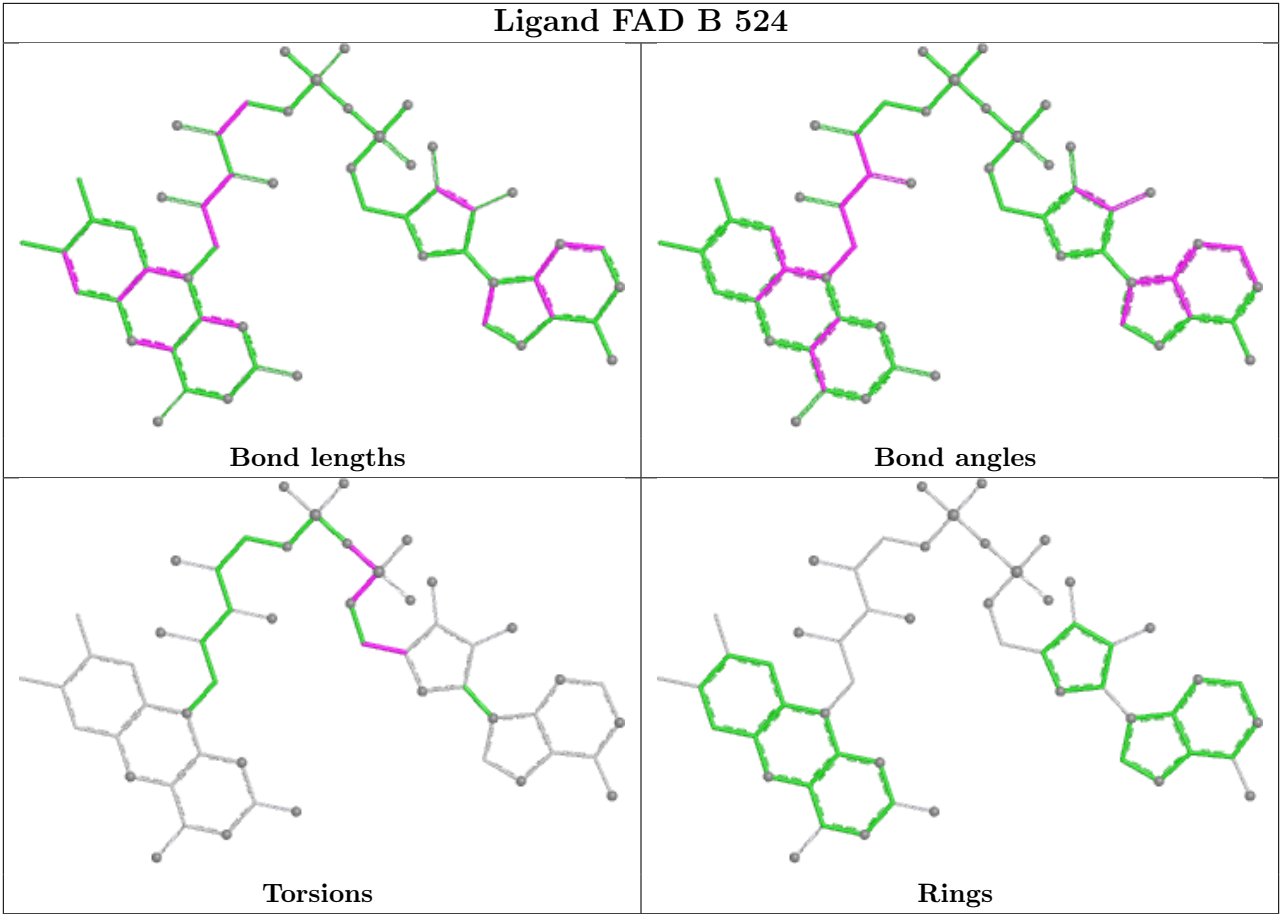
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	524	FAD	12	0
2	C	524	FAD	8	0
2	A	524	FAD	6	0
2	B	524	FAD	7	0

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









5.7 Other polymers ⓘ

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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	73:ASP	C	74:ARG	N	1.17

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.