



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:21 AM UTC

PDB ID : 2BXS / pdb_00002bxs
Title : Human Monoamine Oxidase A in complex with Clorgyline, Crystal Form B
Authors : De Colibus, L.; Binda, C.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2005-07-27
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 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

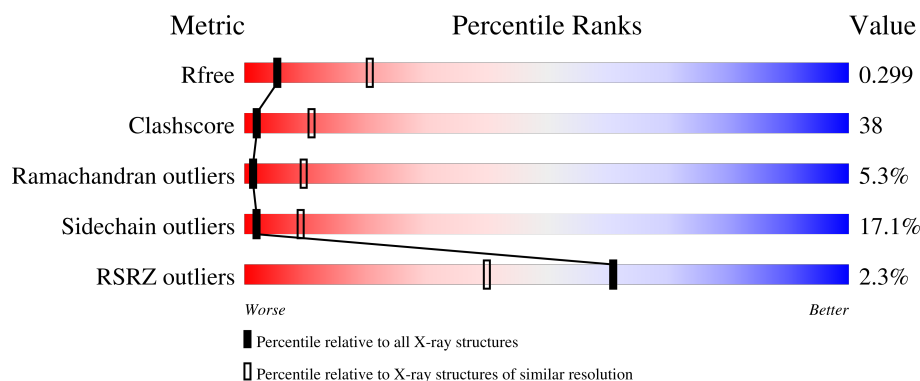
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	
1	B	527	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLG	A	601	X	-	-	-
3	MLG	B	601	X	-	-	-

2 Entry composition [i](#)

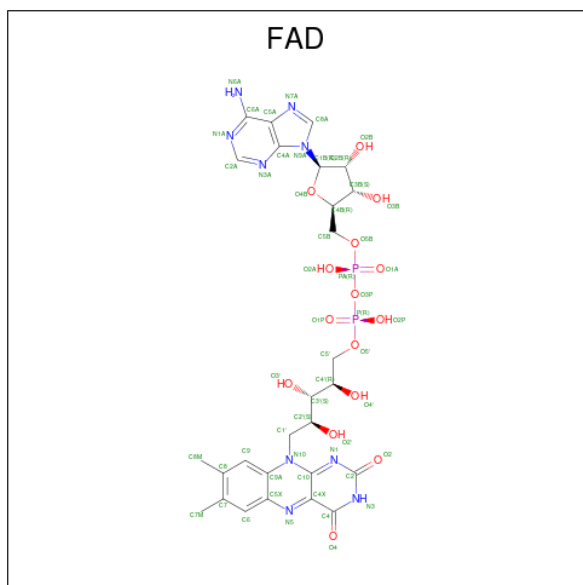
There are 3 unique types of molecules in this entry. The entry contains 7900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AMINE OXIDASE [FLAVIN-CONTAINING] A.

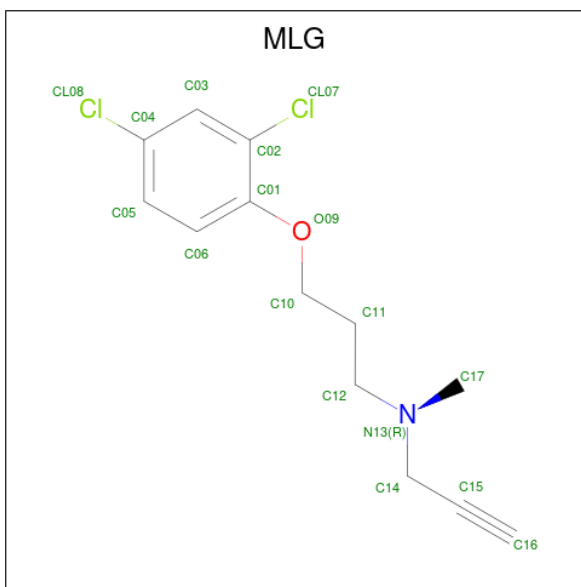
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3880	2482	660	717	21			
1	B	490	Total	C	N	O	S	0	0	0
			3880	2482	660	717	21			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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		

- Molecule 3 is N-[3-(2,4-DICHLOROPHENOXY)PROPYL]-N-METHYL-N-PROP-2-YNYL AMINE (CCD ID: MLG) (formula: $C_{13}H_{15}Cl_2NO$).

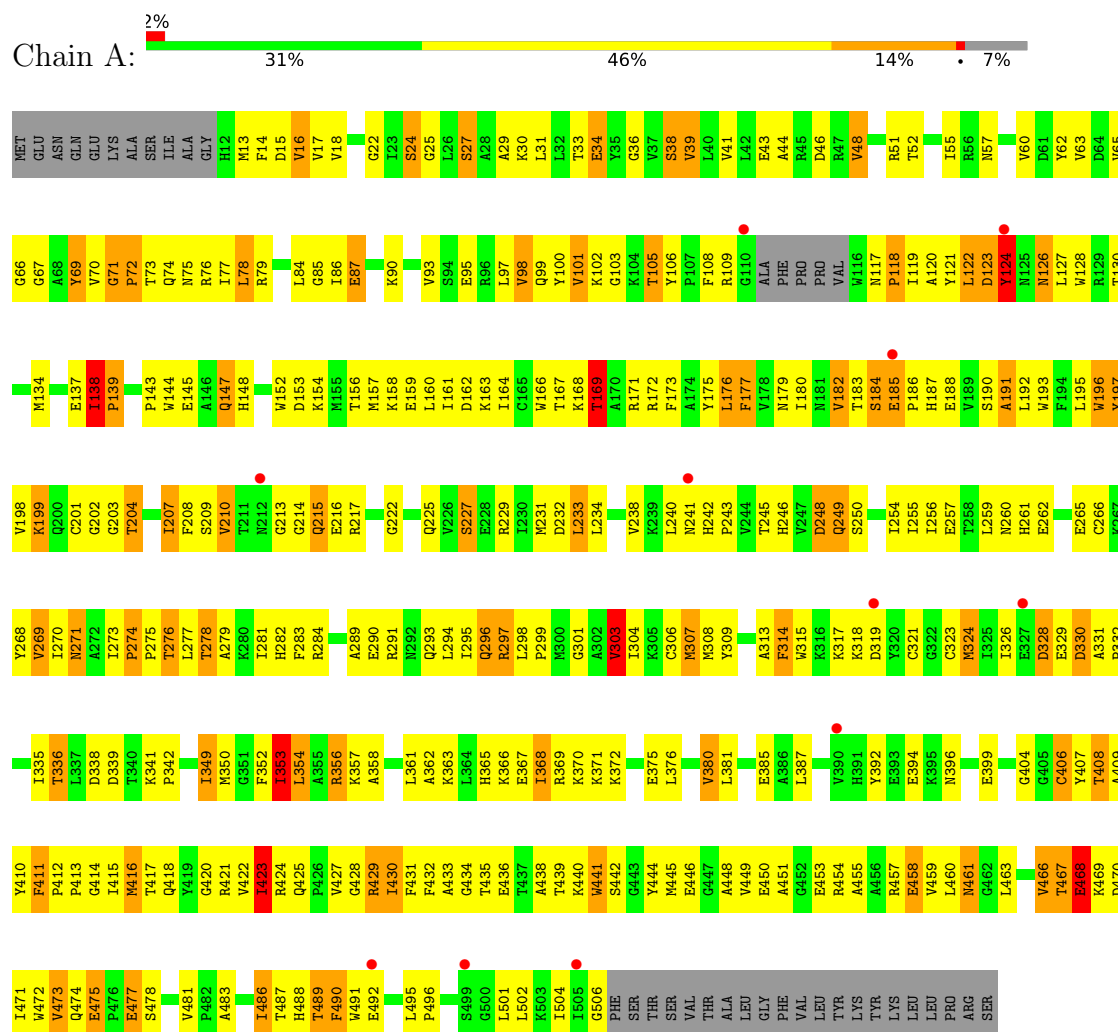


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		

3 Residue-property plots

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

• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] A



E477	F411	D330	C266	H196	M133	A68
A483	P412	A331	K267	Y197	M134	Y69
I486	G414	P332	V268	V198	G135	V70
H488	I415	I335	I270	K199	K136	G71
T487	M416	T336	N271	Q201	E137	P72
H489	T417	T336	A272	G202	I138	T73
T490	Q418	D339	I273	G203	P139	Q74
W491	Y419	T340	P274	T204	P143	N75
E492	G420	K341	P275	T205	W144	R76
	R421	P342	T276	R206	E145	I77
	V422	D343	L277	L207	A146	L78
	I423	I349	T278	F208	Q147	
	R424	M350	A279	S209	H148	L84
	Q425	K280	I281	V210	A149	G85
	P426	L281	H282	T211		I86
G500	V427	I353	F283	G213	W152	E87
L501	G428	L354	R284	Q214	D153	T88
L502	R429	A355		Q215	K154	Y89
K503	I430	R356	A289	E216	M155	K90
I504	F431	K357	E290	R217	T156	N91
I505	A432	A358	R291	K218	M157	N92
G506	A433		N292		K158	V93
PHE	G434	A362	Q293	G222	E159	S94
SER	T435	K363	L294		R96	E95
THR	E436	H365	I295	Q225	L160	R97
SER		K366	Q296	V226	I161	L97
VAL		E367	R297	E227	D162	V98
THR	K440	I368	L298	E228	K163	Q99
ALA	W441	R369	P299	R229	I164	Y100
LEU	S442	K370	M300	T236	C165	V101
GLY	G443	K371	G301	N231	W166	K102
PHE	Y444	K372	A302	D232	T167	G103
VAL	M445	I373	V303	L233	K168	K104
LEU	E446	C374	I304	L234	T169	A170
LEU	G447	E375	K305		R171	Y106
TYR	A448	L376	C306	V238	R172	F107
LYS		Y377	M307	R239	F173	F108
TYR	A451	V380	Y309	N241	A174	R109
LYS	G452	L381		H242	Y175	G110
LEU	E453	E385	E312	T245	F176	ALA
LEU	E454	A386	A313	H246	L177	PHE
PRO	R454	L387	F314	V247	T178	PRO
ARG	A455		K315	D248	V178	PRO
SER	A456	Y392	K317	Q249		VAL
	R457	E393	K318		I179	
	E458	E394	D319	I254	I180	W116
	V459	K395	Y320	I255	M181	W117
	L460	N396	C321	I256	V182	P118
	N461	W397	G322	E257	T183	I119
		C398	C323	T258	S184	A120
	V466	D470	M324	L259	E185	Y121
T467	T467	E468	I471	W260	P186	L122
K469	K469	K469	W472	H261	H187	D123
D470	D470	C398	E400	E262	E188	Y124
I471	I471	E399	T326		V189	N125
W472	W472	E400	E327		S190	N126
K473	K473	T408	D328		A191	L127
Q474	Q474	A409	E329		L192	
E475	E475	Y410			W193	T130
P476	P476				F194	I131
					L195	D132

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.37Å 152.08Å 82.20Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	15.00 – 3.15 15.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	90.5 (15.00-3.15) 89.6 (15.00-3.15)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.268 , 0.330 0.253 , 0.299	Depositor DCC
R_{free} test set	1502 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.99	3/3973 (0.1%)	1.22	31/5389 (0.6%)
1	B	0.96	1/3973 (0.0%)	1.20	31/5389 (0.6%)
All	All	0.97	4/7946 (0.1%)	1.21	62/10778 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	ILE	CA-CB	7.44	1.63	1.54
1	A	353	ILE	CA-CB	7.22	1.62	1.54
1	A	269	VAL	CA-C	-6.69	1.47	1.52
1	A	190	SER	CA-C	5.40	1.59	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	ILE	N-CA-C	10.39	117.83	107.55
1	A	138	ILE	N-CA-C	9.55	117.82	107.60
1	B	354	LEU	N-CA-C	9.51	123.53	109.07
1	B	274	PRO	CA-C-N	9.23	129.44	119.28
1	B	274	PRO	C-N-CA	9.23	129.44	119.28
1	B	353	ILE	CB-CA-C	8.74	122.73	110.84
1	A	138	ILE	CA-C-N	8.27	130.18	119.84
1	A	138	ILE	C-N-CA	8.27	130.18	119.84
1	A	354	LEU	N-CA-C	8.18	121.31	108.79
1	A	278	THR	N-CA-C	-7.93	102.58	111.07
1	B	138	ILE	CA-C-N	7.82	129.62	119.84
1	B	138	ILE	C-N-CA	7.82	129.62	119.84
1	B	425	GLN	CA-C-N	7.82	127.82	119.76
1	B	425	GLN	C-N-CA	7.82	127.82	119.76
1	B	353	ILE	N-CA-C	-7.76	97.26	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ILE	CB-CA-C	7.76	121.39	110.84
1	A	425	GLN	CA-C-N	7.65	128.10	119.83
1	A	425	GLN	C-N-CA	7.65	128.10	119.83
1	B	201	CYS	N-CA-C	-7.61	103.11	113.30
1	A	190	SER	N-CA-C	7.54	120.04	110.24
1	B	71	GLY	CA-C-N	7.46	129.16	119.84
1	B	71	GLY	C-N-CA	7.46	129.16	119.84
1	B	191	ALA	N-CA-C	-7.29	102.94	111.03
1	A	353	ILE	N-CA-C	-7.26	97.97	108.36
1	B	408	THR	N-CA-C	7.08	118.84	108.86
1	B	190	SER	N-CA-C	6.93	120.01	110.24
1	A	71	GLY	CA-C-N	6.85	128.40	119.84
1	A	71	GLY	C-N-CA	6.85	128.40	119.84
1	A	269	VAL	N-CA-C	-6.76	100.13	109.46
1	A	185	GLU	CA-C-N	6.70	128.21	119.84
1	A	185	GLU	C-N-CA	6.70	128.21	119.84
1	B	269	VAL	N-CA-C	-6.37	100.67	109.46
1	A	274	PRO	CA-C-N	6.33	126.24	119.28
1	A	274	PRO	C-N-CA	6.33	126.24	119.28
1	A	201	CYS	N-CA-C	-6.27	105.27	113.17
1	B	185	GLU	CA-C-N	6.05	127.40	119.84
1	B	185	GLU	C-N-CA	6.05	127.40	119.84
1	B	60	VAL	CB-CA-C	-6.02	104.74	110.70
1	A	191	ALA	N-CA-C	-5.97	104.40	111.03
1	B	307	MET	N-CA-C	5.85	117.73	108.67
1	A	411	PHE	N-CA-C	5.81	119.15	108.69
1	B	109	ARG	N-CA-C	5.65	118.67	109.06
1	A	307	MET	N-CA-C	5.63	117.40	108.67
1	A	109	ARG	N-CA-C	5.50	118.40	109.06
1	B	411	PHE	N-CA-C	5.47	117.35	109.04
1	A	306	CYS	N-CA-C	5.38	117.82	107.44
1	A	69	TYR	N-CA-C	5.31	117.18	108.52
1	A	85	GLY	N-CA-C	-5.29	107.26	115.67
1	A	215	GLN	CA-C-N	-5.22	114.47	122.87
1	A	215	GLN	C-N-CA	-5.22	114.47	122.87
1	A	408	THR	N-CA-C	5.22	116.59	109.18
1	A	413	PRO	N-CA-C	5.21	119.38	111.15
1	B	473	VAL	N-CA-C	5.17	120.10	109.34
1	B	411	PHE	CA-C-N	-5.17	115.06	120.38
1	B	411	PHE	C-N-CA	-5.17	115.06	120.38
1	B	242	HIS	CA-C-N	5.15	125.31	119.90
1	B	242	HIS	C-N-CA	5.15	125.31	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	VAL	CB-CA-C	-5.15	101.77	111.30
1	B	278	THR	CB-CA-C	-5.10	102.88	110.88
1	B	306	CYS	N-CA-C	5.07	117.22	107.44
1	A	429	ARG	N-CA-C	-5.05	104.59	111.56
1	B	355	ALA	CB-CA-C	-5.02	110.40	117.23

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	3880	0	3828	302	0
1	B	3880	0	3828	293	0
2	A	53	0	29	0	0
2	B	53	0	29	2	0
3	A	17	0	15	6	0
3	B	17	0	15	4	0
All	All	7900	0	7744	598	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 38.

All (598) 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:408:THR:HG23	1:B:409:ALA:O	1.50	1.11
1:A:304:ILE:HB	1:A:353:ILE:CG2	1.90	1.02
1:A:304:ILE:HB	1:A:353:ILE:HG23	1.39	1.02
1:A:408:THR:HG23	1:A:409:ALA:O	1.59	1.01
1:B:422:VAL:O	1:B:424:ARG:N	1.96	0.99
1:A:210:VAL:HG22	1:A:214:GLY:HA3	1.47	0.96
1:A:422:VAL:O	1:A:424:ARG:N	1.99	0.96
1:B:210:VAL:HG22	1:B:214:GLY:HA3	1.49	0.94
1:A:120:ALA:HA	1:A:167:THR:HG21	1.52	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:O	1:B:134:MET:HB2	1.70	0.91
1:A:130:THR:O	1:A:134:MET:HB2	1.71	0.89
1:B:304:ILE:HB	1:B:353:ILE:CG2	2.03	0.88
1:A:210:VAL:HG13	1:A:213:GLY:C	1.99	0.87
1:B:120:ALA:HA	1:B:167:THR:HG21	1.54	0.86
1:A:176:LEU:O	1:A:180:ILE:N	2.08	0.86
1:A:210:VAL:HG22	1:A:214:GLY:CA	2.06	0.84
1:B:304:ILE:HB	1:B:353:ILE:HG23	1.56	0.84
1:B:210:VAL:HG22	1:B:214:GLY:CA	2.07	0.84
1:B:323:CYS:HA	1:B:336:THR:HG22	1.61	0.82
1:B:210:VAL:HG13	1:B:213:GLY:C	2.05	0.81
1:A:471:ILE:HG22	1:A:471:ILE:O	1.79	0.81
1:A:299:PRO:HG2	1:A:410:TYR:CZ	2.16	0.81
1:A:396:ASN:ND2	1:A:399:GLU:HG2	1.95	0.80
1:A:416:MET:O	1:A:420:GLY:HA3	1.80	0.80
1:A:501:LEU:HA	1:A:504:ILE:HD12	1.64	0.80
1:A:210:VAL:HG13	1:A:213:GLY:CA	2.12	0.79
1:A:299:PRO:HB2	1:A:410:TYR:CE2	2.16	0.79
1:B:330:ASP:OD2	1:B:330:ASP:N	2.15	0.79
1:A:438:ALA:HB3	1:A:442:SER:HB2	1.61	0.79
1:A:330:ASP:OD2	1:A:330:ASP:N	2.16	0.79
1:A:222:GLY:O	1:A:225:GLN:HG3	1.84	0.78
1:B:210:VAL:HG13	1:B:213:GLY:CA	2.13	0.78
1:B:197:TYR:HE2	1:B:207:ILE:HD11	1.49	0.78
1:A:323:CYS:HA	1:A:336:THR:HG22	1.66	0.78
1:A:157:MET:O	1:A:161:ILE:HG13	1.85	0.75
1:B:216:GLU:OE2	3:B:601:MLG:H102	1.86	0.75
1:A:324:MET:HG3	1:A:326:ILE:HD11	1.68	0.75
1:B:454:ARG:HD2	1:B:472:TRP:CZ2	2.22	0.75
1:B:197:TYR:HH	1:B:444:TYR:HE1	1.34	0.75
1:B:34:GLU:OE1	1:B:34:GLU:HA	1.86	0.74
1:B:299:PRO:HG2	1:B:410:TYR:CZ	2.22	0.74
1:B:193:TRP:CG	1:B:411:PHE:HB2	2.23	0.73
1:B:324:MET:HG3	1:B:326:ILE:HD11	1.69	0.73
1:A:34:GLU:HA	1:A:34:GLU:OE1	1.86	0.73
1:B:52:THR:HG22	1:B:67:GLY:HA3	1.70	0.72
1:B:84:LEU:HD22	1:B:229:ARG:HB2	1.71	0.72
1:B:95:GLU:O	1:B:321:CYS:HB3	1.89	0.72
1:B:332:PRO:HD2	1:B:376:LEU:HD22	1.72	0.72
1:B:501:LEU:HA	1:B:504:ILE:HD12	1.71	0.71
1:B:416:MET:O	1:B:420:GLY:HA3	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:O	1:B:108:PHE:N	2.24	0.71
1:B:468:GLU:HG3	1:B:469:LYS:H	1.56	0.71
1:B:299:PRO:HD2	1:B:410:TYR:O	1.90	0.71
1:B:408:THR:CG2	1:B:409:ALA:O	2.33	0.71
1:A:299:PRO:HB2	1:A:410:TYR:HE2	1.56	0.71
1:A:176:LEU:HA	1:A:179:ASN:HB2	1.72	0.70
1:B:87:GLU:OE1	1:B:87:GLU:HA	1.90	0.70
1:B:18:VAL:HB	1:B:41:VAL:HG22	1.74	0.70
1:B:192:LEU:HD23	1:B:416:MET:HG2	1.73	0.70
1:A:273:ILE:HD11	1:A:278:THR:HA	1.74	0.69
1:A:18:VAL:HB	1:A:41:VAL:HG22	1.73	0.69
1:B:254:ILE:HD13	1:B:269:VAL:HG23	1.75	0.69
1:B:273:ILE:HD11	1:B:278:THR:HA	1.75	0.69
1:A:76:ARG:HH21	1:A:475:GLU:HG2	1.57	0.69
1:A:97:LEU:O	1:A:108:PHE:N	2.26	0.69
1:B:99:GLN:N	1:B:106:TYR:O	2.22	0.68
1:A:69:TYR:OH	1:A:350:MET:HE2	1.94	0.68
1:A:87:GLU:OE1	1:A:87:GLU:HA	1.93	0.67
1:A:467:THR:HB	1:A:470:ASP:HB2	1.74	0.67
3:B:601:MLG:CL07	3:B:601:MLG:H172	2.32	0.67
1:A:52:THR:HG22	1:A:67:GLY:HA3	1.75	0.67
1:A:197:TYR:HE2	1:A:207:ILE:HD11	1.60	0.67
1:A:438:ALA:HB3	1:A:442:SER:CB	2.25	0.67
1:A:185:GLU:OE2	1:A:356:ARG:HB3	1.95	0.66
1:A:350:MET:HE1	1:A:352:PHE:CE2	2.31	0.66
1:B:467:THR:HB	1:B:470:ASP:HB2	1.78	0.66
1:B:41:VAL:HB	1:B:238:VAL:HG22	1.76	0.66
1:A:48:VAL:HG23	1:A:227:SER:HB3	1.76	0.66
1:A:147:GLN:HB3	1:A:148:HIS:HD2	1.61	0.66
1:B:135:GLY:O	1:B:199:LYS:NZ	2.29	0.66
1:B:176:LEU:O	1:B:180:ILE:N	2.16	0.65
1:A:254:ILE:HD13	1:A:269:VAL:HG23	1.78	0.65
1:A:299:PRO:HD2	1:A:410:TYR:O	1.97	0.65
1:B:279:ALA:HA	1:B:295:ILE:HD12	1.77	0.64
1:A:193:TRP:CG	1:A:411:PHE:HB2	2.31	0.64
1:B:156:THR:HG23	1:B:159:GLU:H	1.62	0.64
1:B:291:ARG:HH21	1:B:422:VAL:HG12	1.60	0.64
1:A:31:LEU:O	1:A:34:GLU:HB2	1.97	0.64
1:B:269:VAL:HG12	1:B:270:ILE:N	2.13	0.64
1:A:130:THR:HG22	1:A:134:MET:HE3	1.80	0.64
1:A:246:HIS:CD2	1:A:282:HIS:HB2	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ARG:HA	1:A:175:TYR:CD2	2.33	0.64
1:B:222:GLY:O	1:B:225:GLN:HG3	1.97	0.64
1:B:197:TYR:OH	1:B:444:TYR:HE1	1.81	0.64
1:B:172:ARG:HA	1:B:175:TYR:CD2	2.31	0.63
1:B:299:PRO:CD	1:B:410:TYR:O	2.46	0.63
1:B:396:ASN:ND2	1:B:399:GLU:HG2	2.13	0.63
1:B:157:MET:O	1:B:161:ILE:HG13	1.98	0.63
1:A:467:THR:CB	1:A:470:ASP:HB2	2.28	0.63
1:A:95:GLU:O	1:A:321:CYS:HB3	1.98	0.63
1:A:168:LYS:O	1:A:169:THR:C	2.42	0.63
1:A:454:ARG:HD2	1:A:472:TRP:CZ2	2.34	0.63
1:A:191:ALA:O	1:A:195:LEU:HD12	1.99	0.62
1:B:31:LEU:O	1:B:34:GLU:HB2	1.99	0.62
1:A:281:ILE:HB	1:A:283:PHE:CE1	2.35	0.62
1:B:225:GLN:O	1:B:229:ARG:HG2	1.99	0.62
1:B:440:LYS:HZ3	1:B:441:TRP:CD1	2.17	0.62
1:A:156:THR:HG23	1:A:159:GLU:H	1.63	0.62
1:B:210:VAL:HG13	1:B:213:GLY:HA2	1.81	0.62
1:B:291:ARG:NH2	1:B:422:VAL:HG12	2.15	0.62
1:A:76:ARG:NH2	1:A:475:GLU:HG2	2.14	0.62
1:A:299:PRO:HG2	1:A:410:TYR:CE2	2.34	0.62
1:A:332:PRO:HD2	1:A:376:LEU:HD22	1.81	0.62
1:A:197:TYR:HH	1:A:444:TYR:HE1	1.47	0.62
1:A:152:TRP:O	1:A:191:ALA:HB3	2.00	0.61
1:A:177:PHE:C	1:A:177:PHE:CD2	2.78	0.61
1:B:23:ILE:HD12	1:B:445:MET:HG2	1.81	0.61
1:B:118:PRO:O	1:B:121:TYR:N	2.33	0.61
1:A:99:GLN:N	1:A:106:TYR:O	2.33	0.61
1:A:279:ALA:HA	1:A:295:ILE:HD12	1.82	0.61
1:B:153:ASP:OD2	1:B:417:THR:OG1	2.16	0.61
1:B:315:TRP:HB3	1:B:381:LEU:HD13	1.82	0.61
1:A:354:LEU:HA	1:A:358:ALA:HB2	1.83	0.61
1:A:409:ALA:HB3	1:A:436:GLU:HG3	1.81	0.61
1:B:489:THR:O	1:B:492:GLU:HB2	2.01	0.61
1:A:439:THR:OG1	1:A:450:GLU:OE2	2.18	0.61
1:A:99:GLN:HE21	1:A:100:TYR:N	1.99	0.61
1:B:177:PHE:C	1:B:177:PHE:CD2	2.79	0.61
1:B:299:PRO:HG2	1:B:410:TYR:CE2	2.36	0.61
1:A:293:GLN:O	1:A:296:GLN:N	2.33	0.61
1:A:276:THR:O	1:A:279:ALA:HB3	2.01	0.60
1:B:143:PRO:HD2	1:B:144:TRP:CE3	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:O	1:B:183:THR:OG1	2.14	0.60
1:A:471:ILE:O	1:A:471:ILE:CG2	2.48	0.60
1:B:168:LYS:O	1:B:169:THR:C	2.44	0.60
1:A:328:ASP:C	1:A:328:ASP:OD2	2.43	0.60
1:B:168:LYS:O	1:B:171:ARG:N	2.34	0.60
1:A:134:MET:HG2	1:A:152:TRP:CH2	2.36	0.60
1:A:246:HIS:HA	1:A:282:HIS:O	2.01	0.60
1:B:62:TYR:O	1:B:341:LYS:HE3	2.00	0.60
1:B:183:THR:OG1	1:B:301:GLY:HA3	2.01	0.60
1:B:143:PRO:HG2	1:B:416:MET:SD	2.42	0.60
1:A:156:THR:HG22	1:A:159:GLU:CD	2.27	0.60
1:A:210:VAL:HG13	1:A:213:GLY:HA2	1.83	0.60
1:B:90:LYS:NZ	1:B:215:GLN:NE2	2.50	0.60
1:B:130:THR:HG22	1:B:134:MET:HE3	1.83	0.60
1:A:197:TYR:C	1:A:197:TYR:CD2	2.80	0.60
1:B:197:TYR:C	1:B:197:TYR:CD2	2.80	0.59
1:B:471:ILE:HG22	1:B:471:ILE:O	2.01	0.59
1:B:182:VAL:O	1:B:184:SER:HB2	2.02	0.59
1:A:158:LYS:HE3	1:A:162:ASP:OD2	2.01	0.59
1:B:84:LEU:HD22	1:B:229:ARG:CB	2.32	0.59
1:B:176:LEU:HA	1:B:179:ASN:HB2	1.83	0.59
1:B:246:HIS:CD2	1:B:282:HIS:HB2	2.37	0.59
1:A:143:PRO:HB3	1:A:196:TRP:CD1	2.37	0.59
1:A:255:ILE:HG12	1:A:265:GLU:HG2	1.83	0.59
1:B:197:TYR:CE2	1:B:207:ILE:HD11	2.34	0.59
1:B:341:LYS:HB3	1:B:342:PRO:HD2	1.85	0.59
1:A:153:ASP:OD2	1:A:417:THR:OG1	2.21	0.59
1:B:182:VAL:O	1:B:183:THR:C	2.45	0.59
1:A:183:THR:HG1	1:A:301:GLY:HA3	1.67	0.59
1:B:158:LYS:HE3	1:B:162:ASP:OD2	2.04	0.58
1:A:46:ASP:HA	1:A:241:ASN:HD21	1.69	0.58
1:B:331:ALA:O	1:B:357:LYS:NZ	2.34	0.58
1:A:183:THR:OG1	1:A:301:GLY:HA3	2.03	0.57
1:B:69:TYR:OH	1:B:350:MET:HE2	2.04	0.57
1:A:144:TRP:CH2	1:A:421:ARG:HA	2.39	0.57
1:A:445:MET:O	1:A:446:GLU:C	2.47	0.57
1:B:369:ARG:NH1	1:B:394:GLU:OE1	2.38	0.57
1:A:269:VAL:HG12	1:A:270:ILE:N	2.18	0.57
1:B:328:ASP:OD2	1:B:328:ASP:C	2.47	0.57
1:B:99:GLN:HE21	1:B:100:TYR:N	2.02	0.57
1:A:315:TRP:HB3	1:A:381:LEU:HD13	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:PHE:C	1:B:490:PHE:CD2	2.81	0.57
1:B:297:ARG:HD3	1:B:415:ILE:HD11	1.87	0.57
1:A:246:HIS:HD2	1:A:282:HIS:HB2	1.68	0.57
1:A:396:ASN:HD22	1:A:399:GLU:HG2	1.68	0.57
1:B:176:LEU:HD23	1:B:177:PHE:N	2.21	0.56
1:A:62:TYR:O	1:A:341:LYS:CE	2.54	0.56
1:A:51:ARG:O	1:A:66:GLY:HA3	2.06	0.56
1:A:297:ARG:HD3	1:A:415:ILE:HD11	1.86	0.56
1:A:299:PRO:CB	1:A:410:TYR:CE2	2.89	0.56
1:A:315:TRP:CE3	1:A:349:ILE:HD11	2.40	0.56
1:B:29:ALA:HA	1:B:39:VAL:HG11	1.87	0.56
1:B:90:LYS:HZ3	1:B:215:GLN:NE2	2.04	0.56
1:B:123:ASP:CG	1:B:166:TRP:H	2.13	0.56
1:A:307:MET:SD	1:A:350:MET:HG2	2.46	0.56
1:A:365:HIS:HD2	1:A:367:GLU:H	1.54	0.56
1:A:468:GLU:HG3	1:A:469:LYS:H	1.70	0.56
1:B:48:VAL:HG23	1:B:227:SER:HB3	1.88	0.56
1:B:454:ARG:HD2	1:B:472:TRP:CH2	2.39	0.56
1:B:76:ARG:NH2	1:B:475:GLU:HG2	2.20	0.56
1:B:76:ARG:HH21	1:B:475:GLU:HG2	1.69	0.56
1:B:156:THR:HG22	1:B:159:GLU:CD	2.31	0.56
1:B:293:GLN:O	1:B:294:LEU:C	2.49	0.56
1:A:33:THR:O	1:A:36:GLY:N	2.37	0.56
1:B:72:PRO:HB3	1:B:483:ALA:HA	1.88	0.56
1:B:315:TRP:CE3	1:B:349:ILE:HD11	2.41	0.56
1:A:29:ALA:HA	1:A:39:VAL:HG11	1.88	0.55
1:A:407:TYR:OH	3:A:601:MLG:H173	2.07	0.55
1:A:182:VAL:O	1:A:183:THR:C	2.49	0.55
1:A:192:LEU:HD23	1:A:416:MET:HG2	1.88	0.55
1:B:467:THR:CB	1:B:470:ASP:HB2	2.36	0.55
1:A:143:PRO:HD2	1:A:144:TRP:CE3	2.42	0.55
1:B:186:PRO:O	1:B:188:GLU:N	2.40	0.55
1:B:281:ILE:HB	1:B:283:PHE:CE1	2.41	0.55
1:B:293:GLN:O	1:B:296:GLN:N	2.40	0.55
1:A:274:PRO:HD2	1:A:277:LEU:HD12	1.89	0.55
1:A:118:PRO:O	1:A:121:TYR:N	2.40	0.55
1:A:157:MET:HG3	1:A:161:ILE:HD11	1.89	0.55
1:A:369:ARG:NH1	1:A:394:GLU:OE1	2.40	0.55
1:A:308:MET:HE1	1:A:392:TYR:CD1	2.42	0.55
1:A:314:PHE:O	1:A:317:LYS:HB3	2.07	0.55
1:B:13:MET:C	1:B:14:PHE:CD2	2.85	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:HB3	1:A:148:HIS:CD2	2.42	0.54
1:B:143:PRO:HD2	1:B:144:TRP:CZ3	2.43	0.54
1:B:185:GLU:O	1:B:188:GLU:HB2	2.07	0.54
1:B:86:ILE:HD13	1:B:225:GLN:HB2	1.89	0.54
1:B:260:ASN:HD21	1:B:262:GLU:HB2	1.72	0.54
1:B:431:PHE:CE2	1:B:458:GLU:HB3	2.42	0.54
1:A:73:THR:HG23	1:A:483:ALA:CB	2.38	0.54
1:B:369:ARG:NH1	1:B:394:GLU:OE2	2.40	0.54
1:B:185:GLU:OE2	1:B:356:ARG:HB3	2.08	0.54
1:B:365:HIS:HD2	1:B:367:GLU:H	1.55	0.54
1:B:147:GLN:HB3	1:B:148:HIS:HD2	1.72	0.54
1:B:246:HIS:HD2	1:B:282:HIS:HB2	1.72	0.54
1:A:62:TYR:O	1:A:341:LYS:HE3	2.07	0.54
1:A:90:LYS:NZ	1:A:215:GLN:NE2	2.56	0.54
1:B:52:THR:HA	1:B:67:GLY:H	1.72	0.54
1:B:152:TRP:O	1:B:191:ALA:HB3	2.07	0.54
1:A:369:ARG:O	1:A:370:LYS:C	2.51	0.54
1:B:433:ALA:HB1	1:B:451:ALA:HB1	1.90	0.54
1:A:371:LYS:O	1:A:375:GLU:HG2	2.08	0.54
1:B:299:PRO:HB2	1:B:410:TYR:CE2	2.43	0.54
1:A:203:GLY:O	1:A:204:THR:C	2.51	0.53
1:B:126:ASN:C	1:B:126:ASN:ND2	2.66	0.53
1:B:354:LEU:HA	1:B:358:ALA:HB2	1.90	0.53
1:B:304:ILE:HD11	1:B:362:ALA:HB2	1.90	0.53
1:A:99:GLN:HB3	1:A:106:TYR:HB2	1.90	0.53
1:B:275:PRO:CD	1:B:436:GLU:HG2	2.38	0.53
1:A:44:ALA:HB1	1:A:243:PRO:HG3	1.91	0.53
1:A:431:PHE:CE2	1:A:458:GLU:HB3	2.44	0.53
1:A:291:ARG:HH21	1:A:422:VAL:HG12	1.72	0.53
1:B:468:GLU:CG	1:B:469:LYS:H	2.20	0.53
1:B:491:TRP:HB3	1:B:495:LEU:HG	1.90	0.53
1:A:160:LEU:HG	1:A:164:ILE:HD11	1.91	0.53
1:B:46:ASP:HA	1:B:241:ASN:HD21	1.74	0.53
1:A:331:ALA:O	1:A:357:LYS:NZ	2.37	0.53
1:A:335:ILE:HG12	3:A:601:MLG:H03	1.91	0.53
1:B:62:TYR:O	1:B:341:LYS:CE	2.57	0.53
1:B:133:ASN:HA	1:B:136:LYS:HD2	1.91	0.53
1:A:123:ASP:CG	1:A:166:TRP:H	2.16	0.52
1:A:225:GLN:O	1:A:229:ARG:HG2	2.09	0.52
1:B:490:PHE:HD2	1:B:491:TRP:N	2.07	0.52
1:A:293:GLN:O	1:A:294:LEU:C	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ILE:HD11	1:A:362:ALA:HB2	1.91	0.52
1:B:502:LEU:O	1:B:506:GLY:N	2.33	0.52
1:A:291:ARG:NH2	1:A:422:VAL:HG12	2.25	0.52
1:B:256:ILE:HD12	1:B:256:ILE:N	2.24	0.52
1:B:488:HIS:HA	1:B:492:GLU:OE1	2.09	0.52
1:A:46:ASP:HA	1:A:241:ASN:ND2	2.24	0.52
1:A:335:ILE:HG21	3:A:601:MLG:CL07	2.46	0.52
1:A:502:LEU:O	1:A:506:GLY:N	2.36	0.52
1:B:134:MET:HG2	1:B:152:TRP:CH2	2.44	0.52
1:B:56:ARG:HH22	1:B:228:GLU:CD	2.18	0.52
1:A:13:MET:C	1:A:14:PHE:CD2	2.87	0.52
1:A:489:THR:O	1:A:492:GLU:HB2	2.09	0.52
1:B:246:HIS:HA	1:B:282:HIS:O	2.09	0.52
1:B:293:GLN:O	1:B:295:ILE:N	2.43	0.52
1:A:84:LEU:HD22	1:A:229:ARG:HB2	1.91	0.52
1:B:414:GLY:O	1:B:418:GLN:HB2	2.10	0.51
1:B:124:TYR:OH	1:B:173:PHE:CD1	2.54	0.51
1:B:335:ILE:HG12	3:B:601:MLG:H03	1.92	0.51
1:A:414:GLY:O	1:A:418:GLN:HB2	2.10	0.51
1:B:177:PHE:C	1:B:177:PHE:HD2	2.18	0.51
1:B:444:TYR:HB3	2:B:600:FAD:O2	2.09	0.51
1:A:490:PHE:C	1:A:490:PHE:CD2	2.88	0.51
1:A:186:PRO:O	1:A:188:GLU:N	2.44	0.51
1:A:458:GLU:O	1:A:459:VAL:C	2.53	0.51
1:B:98:VAL:HB	1:B:324:MET:HB3	1.93	0.51
1:B:193:TRP:NE1	1:B:411:PHE:CD1	2.79	0.51
1:B:197:TYR:C	1:B:197:TYR:HD2	2.19	0.51
1:A:143:PRO:HG2	1:A:416:MET:SD	2.50	0.51
1:B:95:GLU:OE1	1:B:321:CYS:HA	2.09	0.51
1:A:15:ASP:HB2	1:A:38:SER:O	2.11	0.51
1:A:41:VAL:HB	1:A:238:VAL:HG22	1.93	0.51
1:A:491:TRP:HB3	1:A:495:LEU:HG	1.92	0.51
1:B:30:LYS:O	1:B:34:GLU:HG2	2.11	0.51
1:B:271:ASN:HB3	1:B:432:PHE:HD2	1.76	0.51
1:A:369:ARG:NH1	1:A:394:GLU:OE2	2.44	0.51
1:B:143:PRO:HB3	1:B:196:TRP:CD1	2.46	0.51
1:A:197:TYR:C	1:A:197:TYR:HD2	2.19	0.51
1:B:203:GLY:O	1:B:204:THR:C	2.53	0.51
1:B:248:ASP:HA	1:B:284:ARG:O	2.10	0.51
1:A:134:MET:HE1	1:A:160:LEU:HD11	1.93	0.50
1:A:182:VAL:O	1:A:184:SER:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:O	1:A:171:ARG:N	2.44	0.50
1:A:303:VAL:HG13	1:A:354:LEU:HB3	1.93	0.50
1:A:72:PRO:HD3	1:A:481:VAL:CG1	2.41	0.50
1:A:338:ASP:OD1	1:A:339:ASP:N	2.44	0.50
1:B:321:CYS:SG	1:B:323:CYS:HB3	2.51	0.50
1:A:490:PHE:HD2	1:A:491:TRP:N	2.10	0.50
1:B:16:VAL:HA	1:B:268:TYR:O	2.11	0.50
1:A:275:PRO:CD	1:A:436:GLU:HG2	2.42	0.50
1:B:99:GLN:HB3	1:B:106:TYR:HB2	1.94	0.50
1:A:299:PRO:CG	1:A:410:TYR:CE2	2.94	0.50
1:B:256:ILE:HD11	1:B:266:CYS:SG	2.52	0.50
1:B:461:ASN:HB2	1:B:466:VAL:HG12	1.93	0.50
1:A:51:ARG:HG2	1:A:406:CYS:SG	2.52	0.50
1:A:176:LEU:O	1:A:179:ASN:HB2	2.12	0.50
1:A:416:MET:O	1:A:420:GLY:CA	2.56	0.50
1:B:186:PRO:C	1:B:188:GLU:H	2.20	0.50
1:B:225:GLN:HE21	1:B:229:ARG:NH2	2.10	0.50
1:B:51:ARG:O	1:B:66:GLY:HA3	2.12	0.50
1:A:468:GLU:CG	1:A:469:LYS:H	2.24	0.49
1:B:70:VAL:HA	1:B:74:GLN:OE1	2.12	0.49
1:B:445:MET:O	1:B:446:GLU:C	2.52	0.49
1:A:289:ALA:O	1:A:290:GLU:C	2.54	0.49
1:A:197:TYR:CE2	1:A:207:ILE:HD11	2.45	0.49
1:A:409:ALA:CB	1:A:436:GLU:HG3	2.43	0.49
1:B:193:TRP:CD1	1:B:411:PHE:HB2	2.46	0.49
1:A:176:LEU:HD23	1:A:177:PHE:N	2.27	0.49
1:B:408:THR:HG23	1:B:409:ALA:C	2.31	0.49
1:B:33:THR:O	1:B:36:GLY:N	2.41	0.49
1:A:143:PRO:HD2	1:A:144:TRP:CZ3	2.48	0.49
1:B:314:PHE:O	1:B:317:LYS:HB3	2.13	0.49
1:A:177:PHE:C	1:A:177:PHE:HD2	2.20	0.49
1:B:198:VAL:HG12	1:B:203:GLY:HA2	1.94	0.49
1:B:268:TYR:CG	1:B:459:VAL:HG13	2.47	0.49
1:A:457:ARG:HA	1:A:460:LEU:HB2	1.95	0.49
1:A:144:TRP:CZ2	1:A:421:ARG:HA	2.48	0.49
1:A:365:HIS:CD2	1:A:367:GLU:H	2.31	0.48
1:B:75:ASN:O	1:B:76:ARG:C	2.55	0.48
1:A:90:LYS:HZ3	1:A:215:GLN:NE2	2.10	0.48
1:A:117:ASN:HD22	1:A:120:ALA:HB2	1.78	0.48
1:A:186:PRO:C	1:A:188:GLU:H	2.21	0.48
1:A:338:ASP:OD1	1:A:338:ASP:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:THR:O	1:B:279:ALA:HB3	2.13	0.48
1:A:78:LEU:O	1:A:79:ARG:C	2.56	0.48
1:A:139:PRO:HG2	1:A:143:PRO:HA	1.95	0.48
1:A:199:LYS:O	1:A:202:GLY:N	2.39	0.48
1:A:271:ASN:HB3	1:A:432:PHE:HD2	1.78	0.48
1:A:330:ASP:O	1:A:331:ALA:C	2.55	0.48
1:B:122:LEU:O	1:B:123:ASP:C	2.56	0.48
1:A:24:SER:O	1:A:27:SER:N	2.47	0.48
1:A:73:THR:CG2	1:A:483:ALA:CB	2.91	0.48
1:A:160:LEU:O	1:A:164:ILE:HG13	2.14	0.48
1:A:138:ILE:HA	1:A:139:PRO:HD2	1.39	0.48
1:A:365:HIS:HB3	1:A:368:ILE:HG13	1.96	0.48
1:B:232:ASP:O	1:B:233:LEU:C	2.57	0.48
1:B:196:TRP:CZ2	1:B:200:GLN:HG2	2.48	0.48
1:B:245:THR:OG1	1:B:246:HIS:ND1	2.47	0.48
1:B:160:LEU:HG	1:B:164:ILE:HD11	1.96	0.48
1:B:371:LYS:O	1:B:375:GLU:HG2	2.14	0.48
1:A:256:ILE:N	1:A:256:ILE:HD12	2.29	0.47
1:B:471:ILE:O	1:B:471:ILE:CG2	2.62	0.47
1:A:335:ILE:CG2	3:A:601:MLG:CL07	2.99	0.47
1:B:365:HIS:CD2	1:B:367:GLU:H	2.31	0.47
1:A:176:LEU:CA	1:A:179:ASN:HB2	2.43	0.47
1:A:271:ASN:HB3	1:A:432:PHE:CD2	2.50	0.47
1:A:271:ASN:C	1:A:271:ASN:ND2	2.72	0.47
1:A:313:ALA:O	1:A:315:TRP:N	2.47	0.47
1:A:461:ASN:HB2	1:A:466:VAL:HG12	1.95	0.47
1:B:308:MET:HE1	1:B:392:TYR:CD1	2.49	0.47
1:A:268:TYR:CG	1:A:459:VAL:HG13	2.50	0.47
1:A:433:ALA:HB1	1:A:451:ALA:HB1	1.97	0.47
1:B:144:TRP:CH2	1:B:421:ARG:HA	2.49	0.47
1:A:191:ALA:C	1:A:195:LEU:HD12	2.39	0.47
1:B:186:PRO:C	1:B:188:GLU:N	2.73	0.47
1:B:196:TRP:CE2	1:B:200:GLN:HG2	2.50	0.47
1:B:255:ILE:HG12	1:B:265:GLU:HG2	1.97	0.47
1:B:409:ALA:HB3	1:B:436:GLU:HG3	1.95	0.47
1:A:22:GLY:C	1:A:24:SER:N	2.72	0.47
1:A:185:GLU:O	1:A:188:GLU:HB2	2.14	0.47
1:A:197:TYR:OH	1:A:444:TYR:HE1	1.97	0.47
1:A:299:PRO:CD	1:A:410:TYR:O	2.63	0.47
1:A:256:ILE:HD11	1:A:266:CYS:SG	2.55	0.47
1:A:93:VAL:HG12	1:A:93:VAL:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:GLU:O	1:A:478:SER:C	2.57	0.47
1:B:123:ASP:OD2	1:B:166:TRP:N	2.41	0.47
1:B:177:PHE:CE2	1:B:181:ASN:ND2	2.83	0.47
1:B:269:VAL:HB	1:B:430:ILE:HG23	1.97	0.47
1:A:256:ILE:HD12	1:A:256:ILE:H	1.80	0.46
1:A:123:ASP:OD2	1:A:166:TRP:N	2.37	0.46
1:A:198:VAL:HG12	1:A:203:GLY:HA2	1.96	0.46
1:B:176:LEU:HG	1:B:180:ILE:CD1	2.44	0.46
1:A:84:LEU:HD22	1:A:229:ARG:CB	2.45	0.46
1:A:86:ILE:HD13	1:A:225:GLN:HB2	1.97	0.46
1:A:126:ASN:C	1:A:126:ASN:ND2	2.72	0.46
1:A:210:VAL:HG13	1:A:214:GLY:N	2.30	0.46
1:B:330:ASP:O	1:B:331:ALA:C	2.58	0.46
1:B:147:GLN:HB3	1:B:148:HIS:CD2	2.50	0.46
1:B:292:ASN:O	1:B:296:GLN:NE2	2.49	0.46
1:B:369:ARG:O	1:B:370:LYS:C	2.59	0.46
1:B:466:VAL:HG13	1:B:470:ASP:HB3	1.96	0.46
3:B:601:MLG:CL07	3:B:601:MLG:C17	3.00	0.46
1:A:298:LEU:HA	1:A:299:PRO:HD3	1.70	0.46
1:B:249:GLN:HE22	1:B:428:GLY:HA3	1.81	0.46
1:B:271:ASN:C	1:B:271:ASN:ND2	2.73	0.46
1:B:46:ASP:HA	1:B:241:ASN:ND2	2.30	0.46
1:B:117:ASN:OD1	1:B:118:PRO:HD2	2.15	0.46
1:B:297:ARG:CD	1:B:415:ILE:HD11	2.46	0.46
1:B:445:MET:O	1:B:448:ALA:HB3	2.16	0.46
1:A:98:VAL:HB	1:A:324:MET:HB3	1.98	0.46
1:A:246:HIS:HB2	1:A:257:GLU:HB3	1.97	0.46
1:B:196:TRP:CD2	1:B:196:TRP:C	2.93	0.46
1:B:457:ARG:HA	1:B:460:LEU:HB2	1.98	0.46
1:B:271:ASN:HB3	1:B:432:PHE:CD2	2.50	0.46
1:B:433:ALA:HB2	1:B:455:ALA:HB2	1.98	0.46
1:A:207:ILE:CG2	1:A:208:PHE:N	2.78	0.46
1:A:274:PRO:HB2	1:A:275:PRO:CD	2.45	0.46
1:B:246:HIS:HB2	1:B:257:GLU:HB3	1.97	0.46
1:B:271:ASN:OD1	1:B:278:THR:HG23	2.16	0.46
1:B:369:ARG:NH1	1:B:394:GLU:CD	2.74	0.46
1:B:307:MET:SD	1:B:350:MET:HG2	2.55	0.46
1:A:279:ALA:HB2	1:A:295:ILE:HB	1.98	0.45
1:A:408:THR:OG1	1:A:436:GLU:OE1	2.27	0.45
1:B:303:VAL:HG13	1:B:354:LEU:HB3	1.98	0.45
1:B:490:PHE:CD2	1:B:491:TRP:N	2.83	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:O	1:A:123:ASP:C	2.59	0.45
1:B:468:GLU:C	1:B:470:ASP:N	2.74	0.45
1:A:254:ILE:HG13	1:A:429:ARG:HH21	1.81	0.45
1:A:307:MET:HB3	1:A:309:TYR:CE2	2.51	0.45
1:A:16:VAL:HA	1:A:268:TYR:O	2.17	0.45
1:B:57:ASN:O	1:B:60:VAL:HG22	2.16	0.45
1:B:245:THR:OG1	1:B:246:HIS:CE1	2.69	0.45
1:A:490:PHE:CD2	1:A:491:TRP:N	2.84	0.45
1:B:138:ILE:HA	1:B:139:PRO:HD2	1.49	0.45
1:B:144:TRP:CD1	1:B:144:TRP:C	2.94	0.45
1:B:43:GLU:HG3	1:B:44:ALA:N	2.32	0.45
1:B:275:PRO:CG	1:B:436:GLU:HG2	2.47	0.45
1:A:275:PRO:HD3	1:A:436:GLU:HG2	1.99	0.45
1:A:466:VAL:HG13	1:A:470:ASP:HB3	1.98	0.45
1:B:275:PRO:HD3	1:B:436:GLU:HG2	1.97	0.45
1:B:176:LEU:O	1:B:179:ASN:HB2	2.16	0.45
1:A:232:ASP:O	1:A:233:LEU:C	2.60	0.45
1:B:139:PRO:HG2	1:B:143:PRO:HA	1.99	0.44
1:A:186:PRO:C	1:A:188:GLU:N	2.76	0.44
1:A:275:PRO:CG	1:A:436:GLU:HG2	2.47	0.44
1:A:22:GLY:O	1:A:24:SER:N	2.51	0.44
1:A:73:THR:HG23	1:A:483:ALA:HB2	1.98	0.44
1:A:198:VAL:O	1:A:203:GLY:HA2	2.18	0.44
1:A:273:ILE:CD1	1:A:281:ILE:HD11	2.48	0.44
1:B:43:GLU:HG3	1:B:45:ARG:H	1.82	0.44
1:B:256:ILE:HD12	1:B:256:ILE:H	1.82	0.44
1:B:291:ARG:O	1:B:294:LEU:N	2.50	0.44
1:B:339:ASP:HB2	1:B:350:MET:HB2	1.98	0.44
1:B:453:GLU:O	1:B:457:ARG:HG3	2.17	0.44
1:B:461:ASN:CB	1:B:471:ILE:HD11	2.48	0.44
1:A:332:PRO:HB3	1:A:361:LEU:CD1	2.47	0.44
1:A:440:LYS:O	1:A:441:TRP:C	2.59	0.44
1:B:192:LEU:HA	1:B:195:LEU:HD12	2.00	0.44
1:B:232:ASP:O	1:B:234:LEU:N	2.51	0.44
1:B:291:ARG:O	1:B:292:ASN:C	2.61	0.44
1:B:307:MET:HB3	1:B:309:TYR:CE2	2.52	0.44
1:B:416:MET:CE	1:B:420:GLY:HA3	2.47	0.44
1:A:259:LEU:C	1:A:261:HIS:H	2.25	0.44
1:B:121:TYR:HA	1:B:124:TYR:HB2	1.99	0.44
1:A:22:GLY:C	1:A:24:SER:H	2.26	0.44
1:A:154:LYS:HD3	1:A:154:LYS:HA	1.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ALA:HB2	1:A:455:ALA:HB2	2.00	0.44
1:A:440:LYS:HZ2	1:A:441:TRP:CD1	2.35	0.44
1:B:271:ASN:C	1:B:271:ASN:HD22	2.26	0.44
1:A:57:ASN:O	1:A:60:VAL:HG22	2.18	0.44
1:A:120:ALA:CA	1:A:167:THR:HG21	2.37	0.44
1:A:372:LYS:O	1:A:375:GLU:HG3	2.17	0.44
1:B:185:GLU:OE1	1:B:185:GLU:HA	2.17	0.44
1:A:341:LYS:HB3	1:A:342:PRO:HD2	1.99	0.44
1:A:445:MET:O	1:A:448:ALA:HB3	2.18	0.44
1:A:461:ASN:CB	1:A:471:ILE:HD11	2.48	0.44
1:B:371:LYS:O	1:B:372:LYS:C	2.59	0.44
1:A:30:LYS:O	1:A:34:GLU:HG2	2.18	0.43
1:A:323:CYS:HA	1:A:336:THR:O	2.18	0.43
1:B:77:ILE:N	1:B:446:GLU:OE2	2.42	0.43
1:B:299:PRO:CG	1:B:410:TYR:CE2	3.01	0.43
1:A:95:GLU:OE1	1:A:321:CYS:HA	2.18	0.43
1:A:242:HIS:NE2	1:A:262:GLU:OE2	2.51	0.43
1:B:143:PRO:C	1:B:145:GLU:H	2.26	0.43
1:B:376:LEU:O	1:B:377:TYR:C	2.61	0.43
1:A:185:GLU:OE1	1:A:185:GLU:HA	2.18	0.43
1:A:412:PRO:HG2	1:A:415:ILE:CG1	2.49	0.43
1:B:15:ASP:HB2	1:B:38:SER:O	2.18	0.43
1:B:155:MET:HB3	1:B:191:ALA:CB	2.49	0.43
1:B:192:LEU:O	1:B:195:LEU:HB2	2.18	0.43
1:A:254:ILE:HG13	1:A:429:ARG:NH2	2.34	0.43
1:A:416:MET:CE	1:A:420:GLY:HA3	2.48	0.43
1:B:246:HIS:NE2	1:B:282:HIS:HD2	2.16	0.43
1:A:124:TYR:OH	1:A:173:PHE:CD1	2.58	0.43
1:A:371:LYS:O	1:A:372:LYS:C	2.60	0.43
1:B:160:LEU:O	1:B:164:ILE:HG13	2.18	0.43
1:A:260:ASN:HD21	1:A:262:GLU:HB2	1.83	0.43
1:A:408:THR:CG2	1:A:409:ALA:O	2.49	0.43
1:B:190:SER:HB3	1:B:193:TRP:HB2	2.00	0.43
1:B:440:LYS:O	1:B:441:TRP:C	2.61	0.43
1:A:144:TRP:CD1	1:A:144:TRP:C	2.97	0.43
1:B:260:ASN:ND2	1:B:262:GLU:HB2	2.33	0.43
1:B:454:ARG:CD	1:B:472:TRP:CH2	3.00	0.43
1:B:468:GLU:HG3	1:B:469:LYS:N	2.29	0.43
1:A:291:ARG:O	1:A:294:LEU:N	2.52	0.43
1:A:293:GLN:O	1:A:295:ILE:N	2.51	0.43
1:A:369:ARG:NH1	1:A:394:GLU:CD	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:MET:O	1:A:448:ALA:N	2.52	0.43
1:B:329:GLU:OE1	1:B:329:GLU:HA	2.18	0.43
1:B:18:VAL:HG11	1:B:25:GLY:O	2.19	0.43
1:B:193:TRP:CH2	1:B:410:TYR:HA	2.54	0.43
1:A:339:ASP:HB2	1:A:350:MET:HB2	2.01	0.43
1:B:71:GLY:N	1:B:74:GLN:OE1	2.51	0.43
1:B:92:ASN:O	1:B:93:VAL:HG22	2.19	0.43
1:B:458:GLU:O	1:B:459:VAL:C	2.61	0.43
1:B:500:GLY:O	1:B:502:LEU:N	2.52	0.43
1:A:17:VAL:HG12	1:A:18:VAL:N	2.34	0.42
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.87	0.42
1:A:52:THR:HG22	1:A:67:GLY:CA	2.46	0.42
1:A:52:THR:HG21	1:A:445:MET:SD	2.59	0.42
1:A:488:HIS:HA	1:A:492:GLU:OE1	2.19	0.42
1:B:101:VAL:C	1:B:103:GLY:H	2.26	0.42
1:B:273:ILE:CD1	1:B:281:ILE:HD11	2.49	0.42
1:A:24:SER:O	1:A:25:GLY:C	2.60	0.42
1:A:144:TRP:CZ3	1:A:421:ARG:HA	2.54	0.42
1:A:453:GLU:O	1:A:457:ARG:HG3	2.19	0.42
1:A:489:THR:O	1:A:490:PHE:C	2.62	0.42
1:B:259:LEU:C	1:B:261:HIS:H	2.27	0.42
1:A:52:THR:HA	1:A:67:GLY:H	1.83	0.42
1:A:124:TYR:HD2	1:A:128:TRP:CZ3	2.36	0.42
1:B:120:ALA:CA	1:B:167:THR:HG21	2.39	0.42
1:B:315:TRP:CD2	1:B:349:ILE:HD11	2.54	0.42
1:B:412:PRO:HG2	1:B:415:ILE:HG13	2.01	0.42
1:A:97:LEU:N	1:A:97:LEU:HD12	2.34	0.42
1:A:193:TRP:CD1	1:A:411:PHE:HB2	2.54	0.42
1:A:315:TRP:CD2	1:A:349:ILE:HD11	2.55	0.42
1:B:52:THR:HG22	1:B:67:GLY:CA	2.44	0.42
1:B:299:PRO:HD3	1:B:410:TYR:O	2.19	0.42
1:B:320:TYR:C	1:B:322:GLY:N	2.75	0.42
1:A:72:PRO:O	1:A:73:THR:OG1	2.35	0.42
1:A:101:VAL:C	1:A:103:GLY:H	2.27	0.42
1:A:434:GLY:O	1:A:436:GLU:N	2.53	0.42
3:A:601:MLG:H06	3:A:601:MLG:H101	1.69	0.42
1:A:70:VAL:HA	1:A:74:GLN:OE1	2.20	0.42
1:B:204:THR:OG1	1:B:205:THR:N	2.53	0.42
1:A:44:ALA:O	1:A:241:ASN:HA	2.20	0.42
1:A:156:THR:HG22	1:A:159:GLU:OE2	2.19	0.42
1:A:232:ASP:O	1:A:234:LEU:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HD11	1:A:429:ARG:HB2	2.01	0.42
1:A:329:GLU:HA	1:A:329:GLU:OE1	2.20	0.42
1:B:298:LEU:HA	1:B:299:PRO:HD3	1.79	0.42
1:A:46:ASP:C	1:A:240:LEU:HD22	2.45	0.41
1:A:105:THR:HG21	1:A:380:VAL:O	2.20	0.41
1:A:117:ASN:HA	1:A:118:PRO:HD2	1.92	0.41
1:A:269:VAL:HB	1:A:430:ILE:HG23	2.02	0.41
1:A:415:ILE:HD13	1:A:415:ILE:HA	1.78	0.41
1:B:269:VAL:CG1	1:B:270:ILE:N	2.82	0.41
1:A:148:HIS:CD2	1:A:148:HIS:N	2.88	0.41
1:A:308:MET:CE	1:A:392:TYR:HD1	2.33	0.41
1:B:461:ASN:CG	1:B:471:ILE:HD11	2.45	0.41
1:A:75:ASN:OD1	1:A:478:SER:N	2.41	0.41
1:A:274:PRO:CB	1:A:275:PRO:CD	2.97	0.41
1:B:22:GLY:O	1:B:23:ILE:C	2.64	0.41
1:B:408:THR:OG1	1:B:436:GLU:OE1	2.31	0.41
1:A:246:HIS:NE2	1:A:282:HIS:HD2	2.18	0.41
1:A:248:ASP:HA	1:A:284:ARG:O	2.20	0.41
1:A:461:ASN:CG	1:A:471:ILE:HD11	2.46	0.41
1:B:155:MET:HB3	1:B:191:ALA:HB2	2.03	0.41
1:B:473:VAL:HG12	1:B:474:GLN:O	2.20	0.41
1:A:121:TYR:HA	1:A:124:TYR:HB2	2.03	0.41
1:A:216:GLU:OE2	3:A:601:MLG:H101	2.20	0.41
1:A:274:PRO:HB2	1:A:275:PRO:HD2	2.01	0.41
1:B:57:ASN:O	1:B:59:HIS:N	2.54	0.41
1:B:365:HIS:HB3	1:B:368:ILE:HG13	2.03	0.41
1:B:444:TYR:CD1	1:B:444:TYR:N	2.88	0.41
1:B:22:GLY:C	1:B:24:SER:N	2.77	0.41
1:B:132:ASP:O	1:B:135:GLY:N	2.35	0.41
1:B:156:THR:CG2	1:B:159:GLU:H	2.32	0.41
1:B:172:ARG:HA	1:B:175:TYR:HD2	1.81	0.41
1:B:416:MET:O	1:B:420:GLY:CA	2.64	0.41
1:B:192:LEU:CD2	1:B:416:MET:HG2	2.48	0.41
1:A:249:GLN:HE22	1:A:428:GLY:HA3	1.86	0.41
1:A:291:ARG:HH22	1:A:423:ILE:C	2.29	0.41
1:A:444:TYR:N	1:A:444:TYR:CD1	2.88	0.41
1:A:449:VAL:O	1:A:453:GLU:HG3	2.21	0.41
1:B:33:THR:O	1:B:34:GLU:C	2.63	0.41
1:B:46:ASP:C	1:B:240:LEU:HD22	2.46	0.41
1:B:89:TYR:CE2	1:B:218:LYS:HB2	2.56	0.41
1:B:289:ALA:O	1:B:290:GLU:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:HB	1:B:353:ILE:HG22	1.98	0.41
1:B:373:ILE:O	1:B:376:LEU:HB3	2.20	0.41
1:B:397:TRP:HA	1:B:400:GLU:HG2	2.01	0.41
1:A:473:VAL:HG12	1:A:474:GLN:O	2.21	0.41
1:B:292:ASN:HA	1:B:295:ILE:HD11	2.03	0.41
1:B:443:GLY:O	2:B:600:FAD:H1'2	2.20	0.41
1:A:117:ASN:OD1	1:A:118:PRO:HD2	2.21	0.40
1:B:193:TRP:CZ2	1:B:410:TYR:HA	2.56	0.40
1:B:100:TYR:HD2	1:B:326:ILE:HG23	1.86	0.40
1:A:71:GLY:O	1:A:74:GLN:HB2	2.21	0.40
1:A:172:ARG:HA	1:A:175:TYR:HD2	1.83	0.40
1:A:454:ARG:HD2	1:A:472:TRP:CH2	2.56	0.40
1:B:132:ASP:C	1:B:134:MET:N	2.79	0.40
1:B:415:ILE:HD13	1:B:415:ILE:HA	1.81	0.40
1:B:190:SER:HB3	1:B:193:TRP:CB	2.51	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	486/527 (92%)	386 (79%)	73 (15%)	27 (6%)	1	9
1	B	486/527 (92%)	389 (80%)	72 (15%)	25 (5%)	1	10
All	All	972/1054 (92%)	775 (80%)	145 (15%)	52 (5%)	1	10

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	THR
1	A	204	THR
1	A	209	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	314	PHE
1	A	366	LYS
1	A	423	ILE
1	A	473	VAL
1	B	169	THR
1	B	204	THR
1	B	314	PHE
1	B	423	ILE
1	B	473	VAL
1	A	34	GLU
1	A	187	HIS
1	A	319	ASP
1	A	435	THR
1	A	441	TRP
1	A	486	ILE
1	B	133	ASN
1	B	187	HIS
1	B	209	SER
1	B	319	ASP
1	B	366	LYS
1	B	486	ILE
1	A	118	PRO
1	A	127	LEU
1	B	34	GLU
1	B	118	PRO
1	B	183	THR
1	B	210	VAL
1	B	496	PRO
1	A	248	ASP
1	A	250	SER
1	A	468	GLU
1	A	496	PRO
1	B	122	LEU
1	B	127	LEU
1	B	468	GLU
1	A	102	LYS
1	A	122	LEU
1	A	210	VAL
1	A	490	PHE
1	B	58	GLU
1	B	102	LYS
1	B	435	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	TYR
1	B	299	PRO
1	A	72	PRO
1	A	139	PRO
1	A	404	GLY
1	B	139	PRO
1	B	25	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	412/450 (92%)	339 (82%)	73 (18%)	2	8
1	B	412/450 (92%)	344 (84%)	68 (16%)	2	10
All	All	824/900 (92%)	683 (83%)	141 (17%)	2	9

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

Mol	Chain	Res	Type
1	A	16	VAL
1	A	24	SER
1	A	27	SER
1	A	38	SER
1	A	39	VAL
1	A	43	GLU
1	A	48	VAL
1	A	55	ILE
1	A	63	VAL
1	A	65	VAL
1	A	77	ILE
1	A	78	LEU
1	A	87	GLU
1	A	98	VAL
1	A	101	VAL
1	A	105	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	119	ILE
1	A	123	ASP
1	A	124	TYR
1	A	126	ASN
1	A	137	GLU
1	A	138	ILE
1	A	145	GLU
1	A	147	GLN
1	A	163	LYS
1	A	169	THR
1	A	176	LEU
1	A	177	PHE
1	A	182	VAL
1	A	184	SER
1	A	196	TRP
1	A	197	TYR
1	A	199	LYS
1	A	207	ILE
1	A	217	ARG
1	A	227	SER
1	A	231	MET
1	A	233	LEU
1	A	245	THR
1	A	249	GLN
1	A	271	ASN
1	A	276	THR
1	A	296	GLN
1	A	297	ARG
1	A	303	VAL
1	A	318	LYS
1	A	324	MET
1	A	328	ASP
1	A	330	ASP
1	A	336	THR
1	A	349	ILE
1	A	353	ILE
1	A	356	ARG
1	A	363	LYS
1	A	368	ILE
1	A	380	VAL
1	A	385	GLU
1	A	387	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	406	CYS
1	A	416	MET
1	A	423	ILE
1	A	427	VAL
1	A	430	ILE
1	A	458	GLU
1	A	461	ASN
1	A	466	VAL
1	A	467	THR
1	A	468	GLU
1	A	475	GLU
1	A	477	GLU
1	A	486	ILE
1	A	487	THR
1	A	489	THR
1	B	16	VAL
1	B	24	SER
1	B	38	SER
1	B	39	VAL
1	B	43	GLU
1	B	48	VAL
1	B	55	ILE
1	B	65	VAL
1	B	78	LEU
1	B	98	VAL
1	B	101	VAL
1	B	105	THR
1	B	119	ILE
1	B	124	TYR
1	B	126	ASN
1	B	131	ILE
1	B	137	GLU
1	B	145	GLU
1	B	147	GLN
1	B	169	THR
1	B	176	LEU
1	B	177	PHE
1	B	184	SER
1	B	197	TYR
1	B	199	LYS
1	B	207	ILE
1	B	217	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	227	SER
1	B	231	MET
1	B	233	LEU
1	B	245	THR
1	B	249	GLN
1	B	271	ASN
1	B	276	THR
1	B	296	GLN
1	B	297	ARG
1	B	303	VAL
1	B	318	LYS
1	B	323	CYS
1	B	324	MET
1	B	328	ASP
1	B	330	ASP
1	B	336	THR
1	B	349	ILE
1	B	353	ILE
1	B	356	ARG
1	B	363	LYS
1	B	368	ILE
1	B	380	VAL
1	B	385	GLU
1	B	387	LEU
1	B	416	MET
1	B	423	ILE
1	B	427	VAL
1	B	430	ILE
1	B	435	THR
1	B	444	TYR
1	B	458	GLU
1	B	461	ASN
1	B	466	VAL
1	B	467	THR
1	B	468	GLU
1	B	470	ASP
1	B	475	GLU
1	B	477	GLU
1	B	486	ILE
1	B	487	THR
1	B	489	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	99	GLN
1	A	133	ASN
1	A	147	GLN
1	A	148	HIS
1	A	187	HIS
1	A	212	ASN
1	A	215	GLN
1	A	237	GLN
1	A	241	ASN
1	A	253	ASN
1	A	263	HIS
1	A	282	HIS
1	A	296	GLN
1	A	365	HIS
1	A	396	ASN
1	A	494	ASN
1	B	99	GLN
1	B	133	ASN
1	B	147	GLN
1	B	148	HIS
1	B	187	HIS
1	B	212	ASN
1	B	215	GLN
1	B	237	GLN
1	B	241	ASN
1	B	263	HIS
1	B	282	HIS
1	B	296	GLN
1	B	365	HIS
1	B	396	ASN
1	B	401	GLN
1	B	494	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 oligosaccharides 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
3	MLG	B	601	2	16,17,17	2.35	2 (12%)	20,21,21	7.76	9 (45%)
2	FAD	A	600	1,3	58,58,58	1.21	5 (8%)	85,89,89	1.95	22 (25%)
2	FAD	B	600	1,3	58,58,58	1.34	7 (12%)	85,89,89	2.02	23 (27%)
3	MLG	A	601	2	16,17,17	2.62	4 (25%)	20,21,21	7.49	8 (40%)

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	B	600	1,3	-	5/34/50/50	0/6/6/6
2	FAD	A	600	1,3	-	6/34/50/50	0/6/6/6
3	MLG	A	601	2	1/1/1/1	6/9/10/10	0/1/1/1
3	MLG	B	601	2	1/1/1/1	4/9/10/10	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	MLG	C14-C15	-6.94	1.36	1.46
3	B	601	MLG	C15-C16	6.47	1.37	1.18
3	A	601	MLG	C15-C16	6.31	1.36	1.18
3	B	601	MLG	C14-C15	-6.13	1.38	1.46
2	B	600	FAD	C2A-N3A	3.81	1.40	1.33
2	B	600	FAD	C4X-N5	3.59	1.38	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	MLG	C04-CL08	-3.40	1.66	1.74
2	B	600	FAD	C8A-N7A	3.25	1.37	1.31
2	A	600	FAD	C4X-N5	3.01	1.37	1.30
2	A	600	FAD	P-O3P	2.94	1.62	1.59
2	B	600	FAD	C2A-N1A	2.78	1.38	1.33
2	B	600	FAD	C10-N1	2.54	1.38	1.33
2	B	600	FAD	C9A-C5X	-2.38	1.37	1.41
2	A	600	FAD	C2A-N1A	2.35	1.38	1.33
2	A	600	FAD	O2'-C2'	-2.23	1.38	1.43
2	A	600	FAD	C10-N1	2.20	1.37	1.33
3	A	601	MLG	C02-CL07	-2.19	1.68	1.73
2	B	600	FAD	C5A-N7A	-2.05	1.35	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	MLG	C14-C15-C16	-32.26	125.30	177.63
3	B	601	MLG	C14-C15-C16	-32.17	125.45	177.63
2	B	600	FAD	C9A-C5X-N5	-8.47	113.46	122.45
2	A	600	FAD	C9A-C5X-N5	-7.21	114.80	122.45
3	B	601	MLG	C01-C02-CL07	-7.07	111.36	119.44
2	A	600	FAD	N3A-C2A-N1A	-5.69	119.97	128.58
2	A	600	FAD	N9A-C8A-N7A	-4.69	107.29	113.94
3	B	601	MLG	C14-N13-C12	4.56	123.94	112.94
3	B	601	MLG	C03-C04-CL08	4.54	124.86	119.17
2	B	600	FAD	N9A-C8A-N7A	-4.53	107.51	113.94
3	A	601	MLG	C14-N13-C12	4.24	123.18	112.94
3	B	601	MLG	C03-C02-CL07	4.20	125.33	118.45
3	B	601	MLG	C11-C12-N13	-4.07	101.88	113.77
2	A	600	FAD	C5A-N7A-C8A	4.01	109.75	103.45
2	B	600	FAD	C5A-C4A-N3A	-3.95	121.28	126.72
2	B	600	FAD	C4A-C5A-N7A	-3.69	106.36	110.58
3	B	601	MLG	C15-C14-N13	3.61	120.73	113.70
2	B	600	FAD	C5A-N7A-C8A	3.58	109.08	103.45
3	A	601	MLG	O09-C01-C02	3.54	120.60	116.39
2	A	600	FAD	O2P-P-O3P	3.52	116.79	107.27
2	B	600	FAD	C4-N3-C2	-3.43	119.55	125.64
2	A	600	FAD	C5A-C4A-N3A	-3.41	122.01	126.72
2	B	600	FAD	O4B-C1B-N9A	3.36	114.55	108.09
2	A	600	FAD	O3'-C3'-C2'	-3.35	101.32	108.93
2	A	600	FAD	C4-N3-C2	-3.34	119.70	125.64
2	B	600	FAD	C5A-C6A-N6A	-3.33	115.03	123.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O5'-C5'-C4'	-3.32	100.49	109.36
2	A	600	FAD	C2A-N3A-C4A	3.31	119.92	111.83
2	B	600	FAD	C6A-C5A-C4A	3.21	121.56	117.18
2	B	600	FAD	C2B-C1B-N9A	-3.20	105.35	113.30
2	B	600	FAD	C10-C4X-N5	-3.04	118.59	124.81
2	B	600	FAD	O4'-C4'-C5'	-3.04	103.29	109.99
3	B	601	MLG	C05-C04-CL08	-3.02	114.90	119.36
2	A	600	FAD	C4A-C5A-N7A	-3.01	107.14	110.58
3	A	601	MLG	C03-C04-CL08	-3.01	115.39	119.17
2	B	600	FAD	O3'-C3'-C4'	-2.93	102.28	108.93
2	B	600	FAD	N6A-C6A-N1A	-2.92	111.87	118.38
2	B	600	FAD	N3A-C2A-N1A	-2.86	124.26	128.58
2	B	600	FAD	C5A-C4A-N9A	2.79	108.86	105.81
2	B	600	FAD	C4X-C4-N3	2.70	120.14	113.25
3	B	601	MLG	C06-C05-C04	2.68	121.94	119.24
2	A	600	FAD	C4-C4X-C10	2.61	121.40	116.93
3	A	601	MLG	C15-C14-N13	2.51	118.59	113.70
2	A	600	FAD	C2B-C3B-C4B	2.51	107.46	102.61
2	A	600	FAD	C9A-N10-C10	-2.45	117.01	120.75
2	A	600	FAD	C4X-C4-N3	2.41	119.39	113.25
2	B	600	FAD	C4-C4X-N5	2.40	121.53	118.21
2	A	600	FAD	C4X-C10-N1	-2.40	118.71	124.59
2	B	600	FAD	C5X-N5-C4X	2.40	121.97	118.09
2	B	600	FAD	O5'-C5'-C4'	-2.39	102.97	109.36
2	A	600	FAD	O3B-C3B-C4B	-2.38	104.26	111.08
2	B	600	FAD	C4A-N9A-C8A	2.32	108.18	105.74
2	A	600	FAD	C4A-N9A-C8A	2.27	108.12	105.74
2	B	600	FAD	O4-C4-C4X	-2.26	120.56	126.53
2	A	600	FAD	C4A-N9A-C1B	-2.25	121.38	126.63
2	A	600	FAD	C10-C4X-N5	-2.23	120.25	124.81
3	A	601	MLG	C02-C03-C04	-2.20	116.24	118.72
2	B	600	FAD	O2B-C2B-C1B	-2.18	102.61	110.10
3	A	601	MLG	C01-C02-CL07	2.11	121.86	119.44
2	A	600	FAD	C4'-C3'-C2'	2.04	116.97	113.57
3	A	601	MLG	C03-C02-CL07	-2.02	115.14	118.45
2	A	600	FAD	O2B-C2B-C1B	-2.02	103.14	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	MLG	N13
3	B	601	MLG	N13

All (21) torsion outliers are listed below:

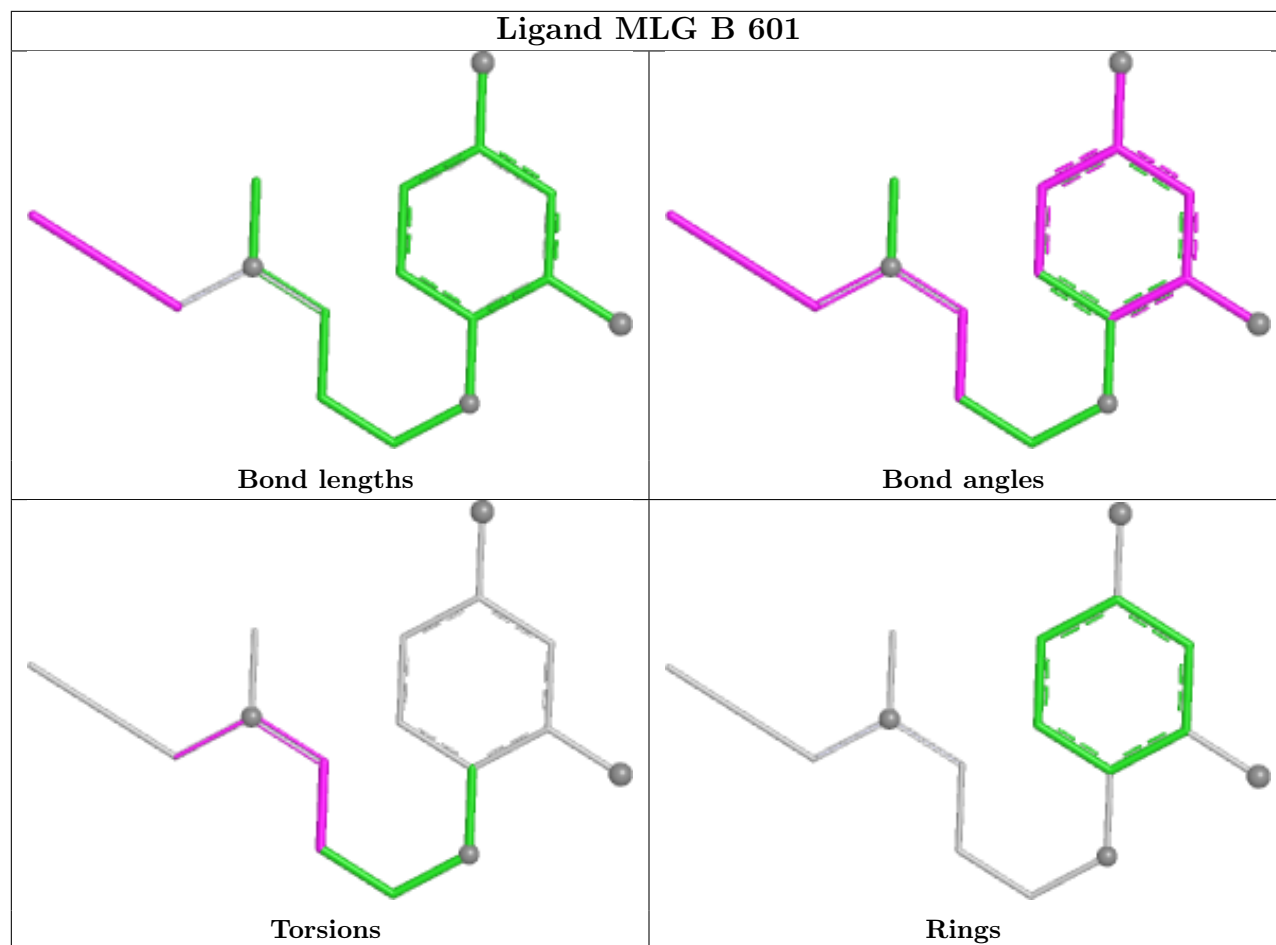
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	O3'-C3'-C4'-C5'
3	A	601	MLG	C15-C14-N13-C17
3	B	601	MLG	C10-C11-C12-N13
3	B	601	MLG	C15-C14-N13-C17
2	A	600	FAD	C2'-C3'-C4'-O4'
3	A	601	MLG	O09-C10-C11-C12
2	A	600	FAD	C2'-C3'-C4'-C5'
3	A	601	MLG	C11-C12-N13-C17
3	B	601	MLG	C11-C12-N13-C17
2	B	600	FAD	C3B-C4B-C5B-O5B
3	A	601	MLG	C11-C10-O09-C01
3	A	601	MLG	C15-C14-N13-C12
3	B	601	MLG	C15-C14-N13-C12
2	B	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	C2'-C1'-N10-C10
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	C5B-O5B-PA-O3P
2	B	600	FAD	O3'-C3'-C4'-C5'
3	A	601	MLG	C11-C12-N13-C14
2	A	600	FAD	C2B-C1B-N9A-C8A

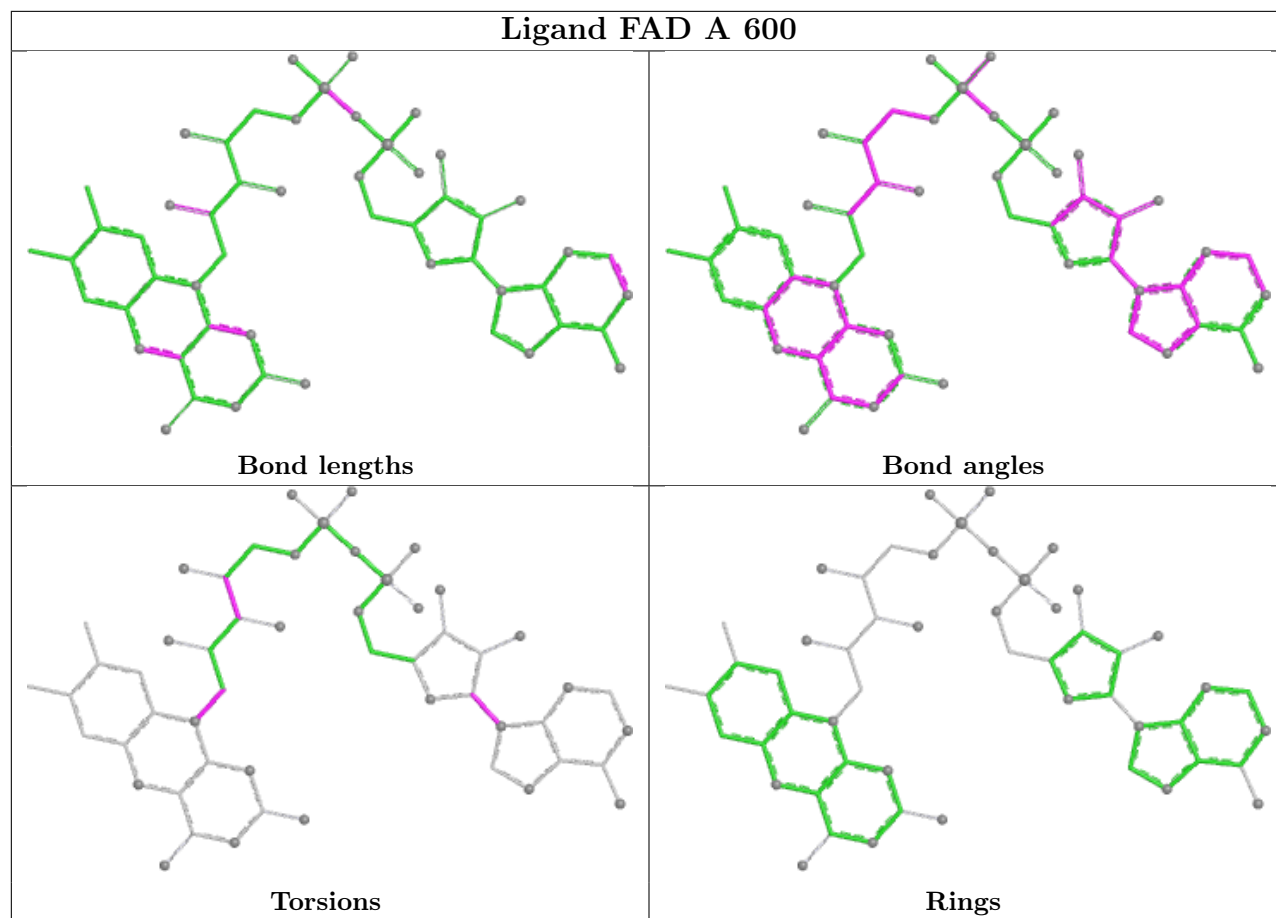
There are no ring outliers.

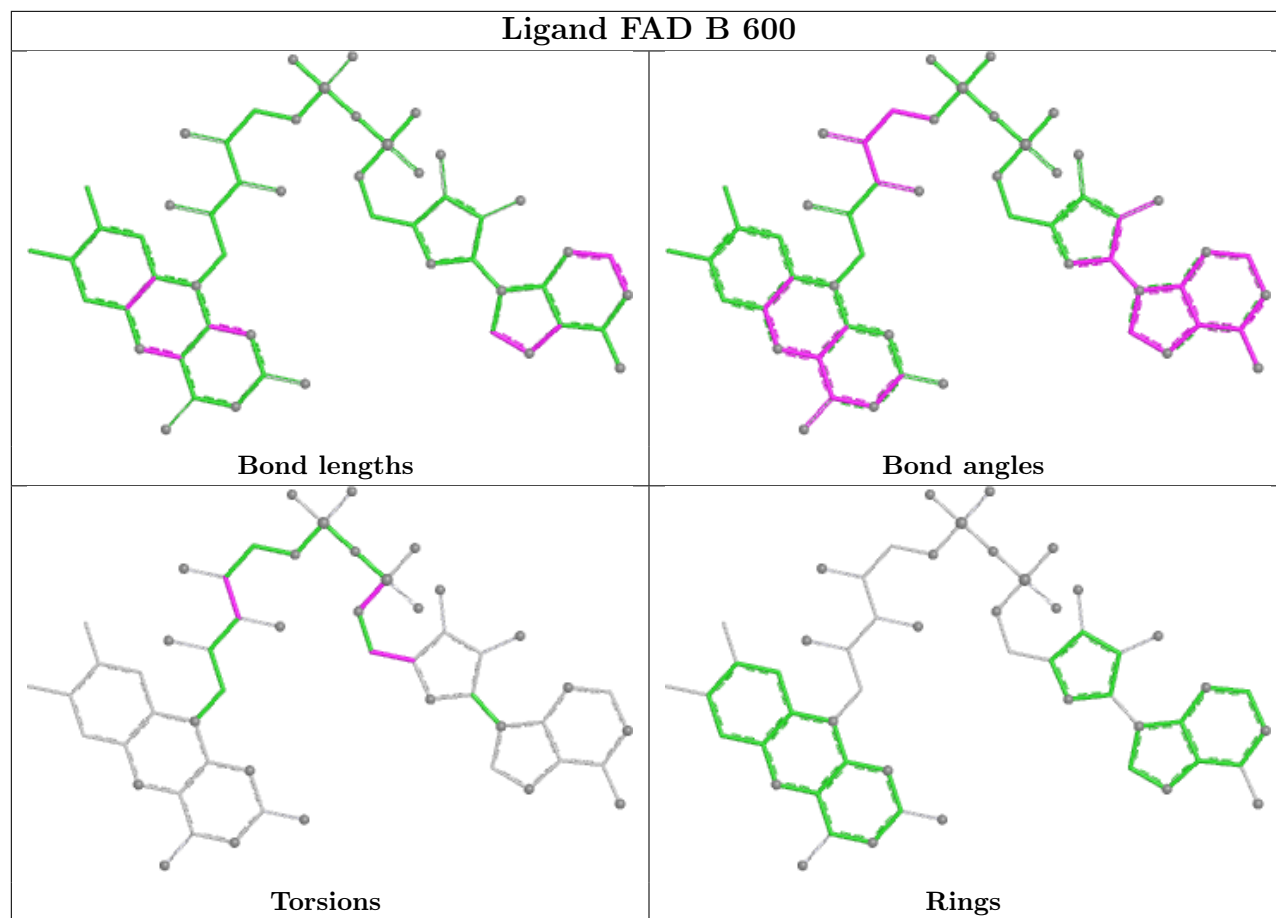
3 monomers are involved in 12 short contacts:

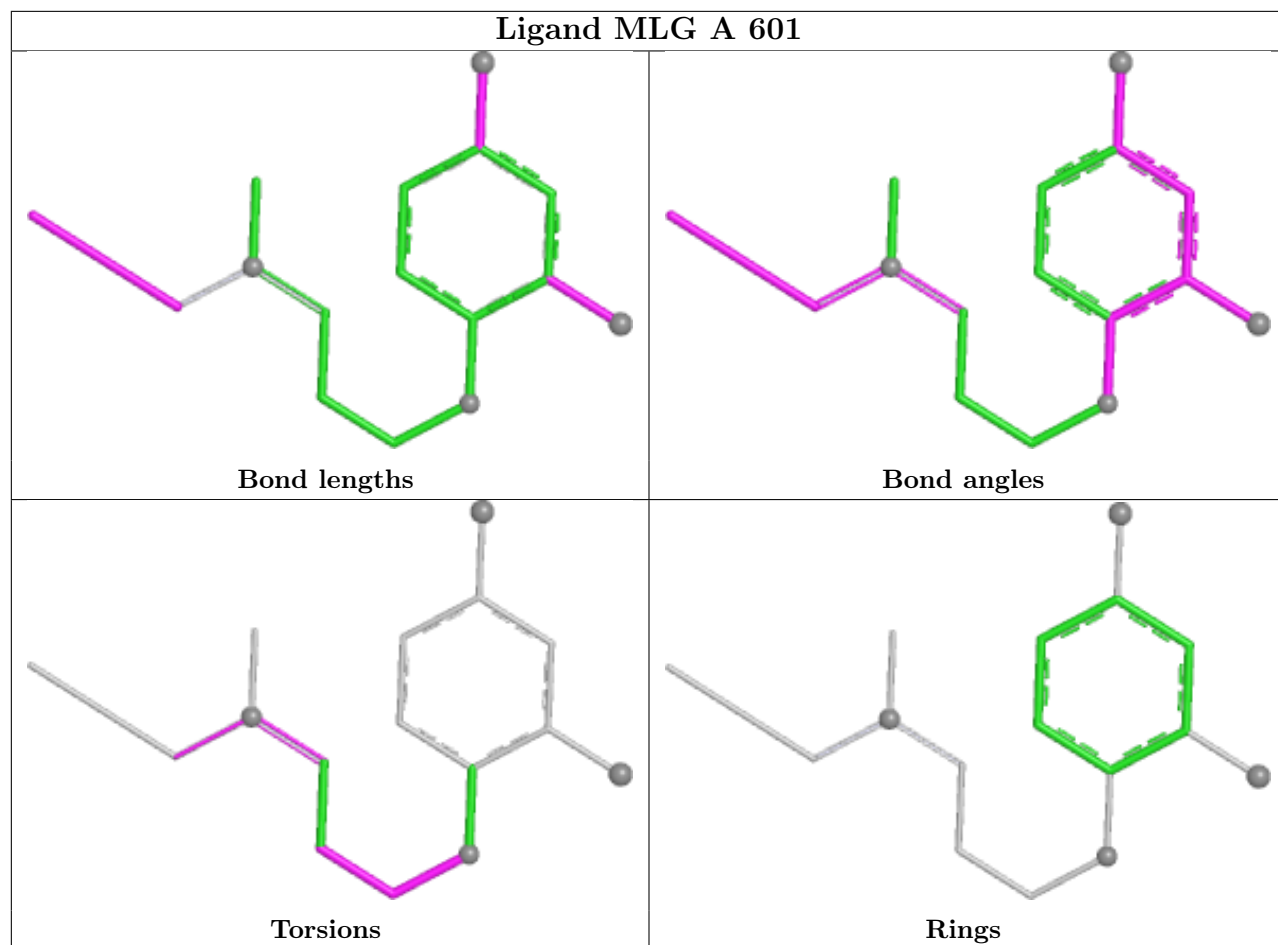
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	MLG	4	0
2	B	600	FAD	2	0
3	A	601	MLG	6	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/527 (92%)	0.23	11 (2%) 62 41	36, 38, 39, 41	0
1	B	490/527 (92%)	0.24	12 (2%) 59 39	36, 38, 39, 41	0
All	All	980/1054 (92%)	0.24	23 (2%) 61 40	36, 38, 39, 41	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	ASN	3.6
1	A	319	ASP	3.3
1	A	390	VAL	3.2
1	A	212	ASN	2.8
1	B	475	GLU	2.6
1	A	124	TYR	2.4
1	B	12	HIS	2.4
1	B	212	ASN	2.4
1	A	110	GLY	2.3
1	A	505	ILE	2.3
1	A	241	ASN	2.3
1	A	492	GLU	2.3
1	A	499	SER	2.2
1	B	312	GLU	2.2
1	B	149	ALA	2.2
1	B	343	ASP	2.2
1	B	215	GLN	2.1
1	A	185	GLU	2.1
1	B	474	GLN	2.1
1	B	246	HIS	2.1
1	B	211	THR	2.1
1	B	399	GLU	2.1
1	A	327	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

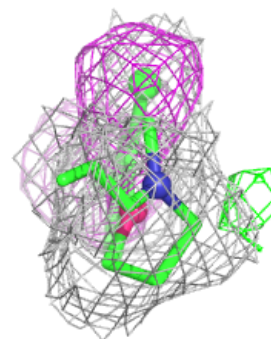
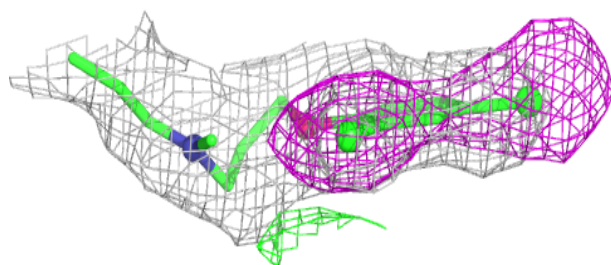
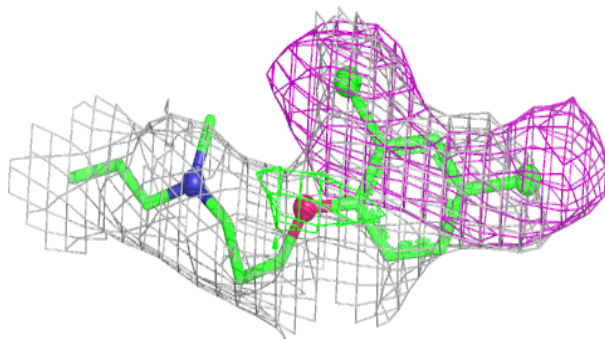
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MLG	A	601	17/17	0.74	0.22	44,54,62,65	0
3	MLG	B	601	17/17	0.77	0.23	46,56,63,64	0
2	FAD	A	600	53/53	0.96	0.07	26,32,37,43	0
2	FAD	B	600	53/53	0.96	0.08	25,32,40,43	0

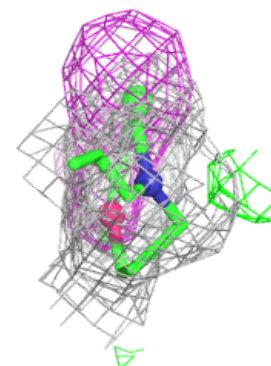
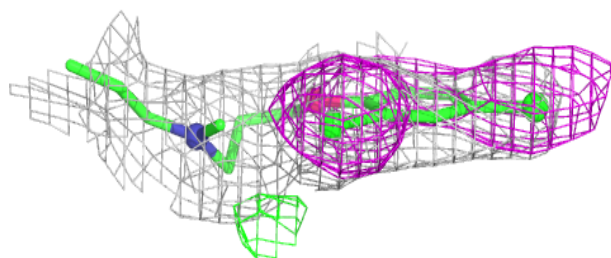
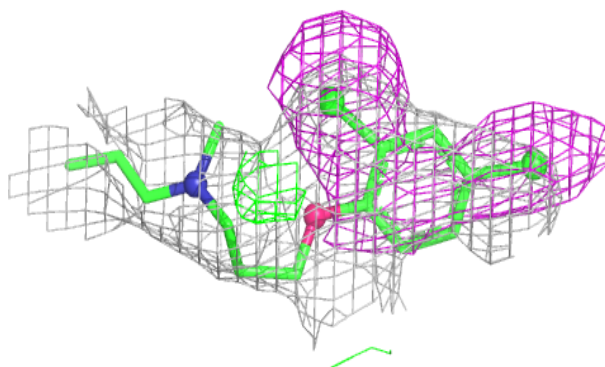
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MLG A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

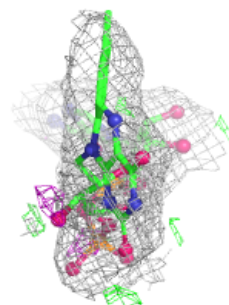
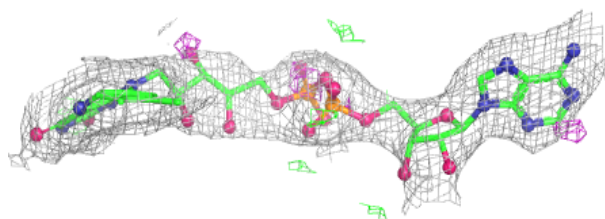
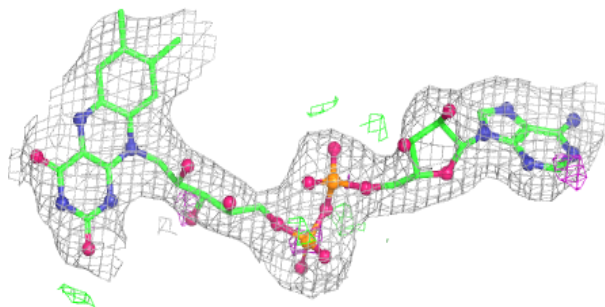
**Electron density around MLG B 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

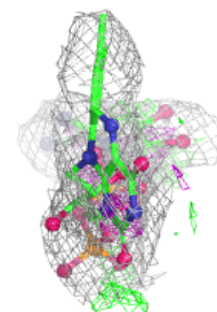
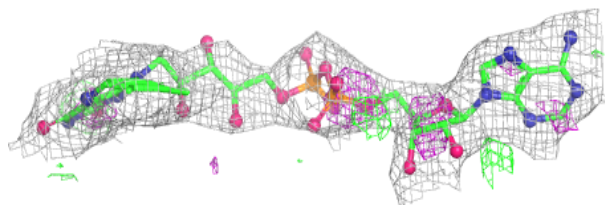
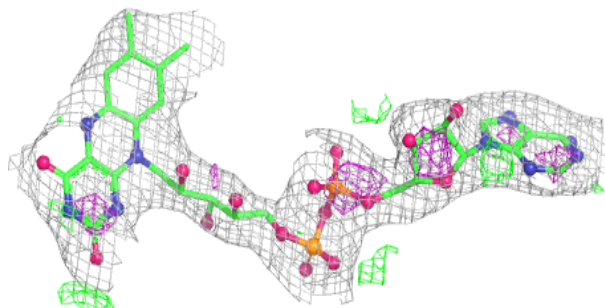


Electron density around FAD A 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD B 600:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.