



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:20 AM UTC

PDB ID : 3UKP / pdb_00003ukp
Title : Crystal structure of R327A UDP-galactopyranose mutase from *Aspergillus fumigatus* in complex with UDPgalp
Authors : Van Straaten, K.E.; Sanders, D.A.R.
Deposited on : 2011-11-09
Resolution : 3.10 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

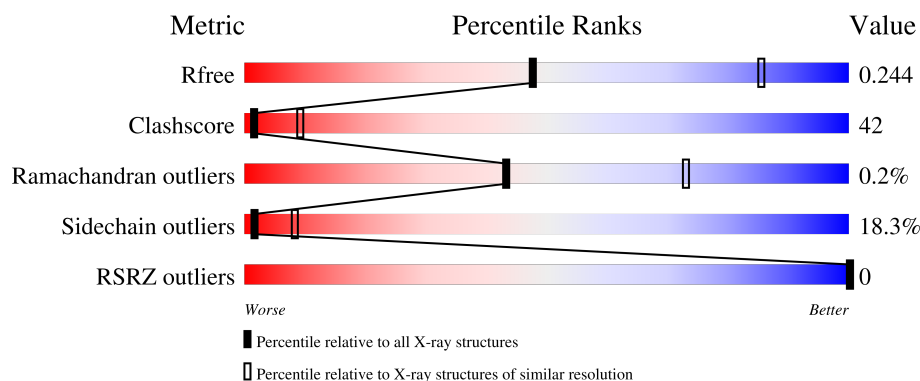
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



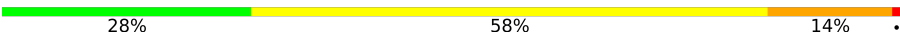
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	509	
1	B	509	
1	C	509	
1	D	509	
1	E	509	

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Mol	Chain	Length	Quality of chain
1	F	509	
1	G	509	
1	H	509	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	601	X	-	-	-
2	FAD	D	601	-	-	X	-
2	FAD	F	601	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32560 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.

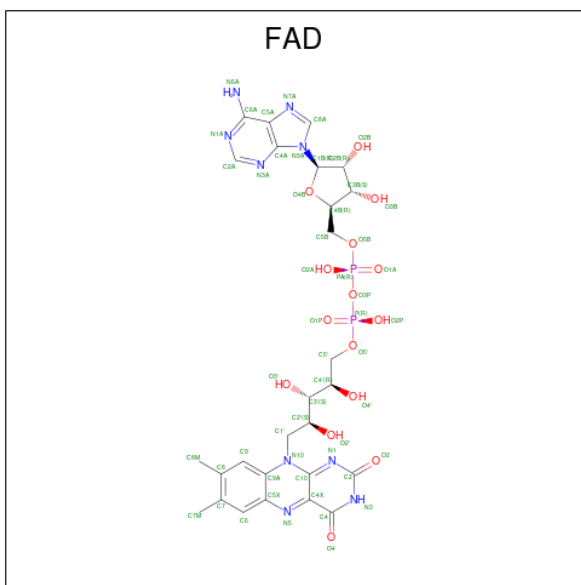
- Molecule 1 is a protein called UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	B	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	C	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	D	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	E	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	F	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	G	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	H	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			

There are 8 discrepancies between the modelled and reference sequences:

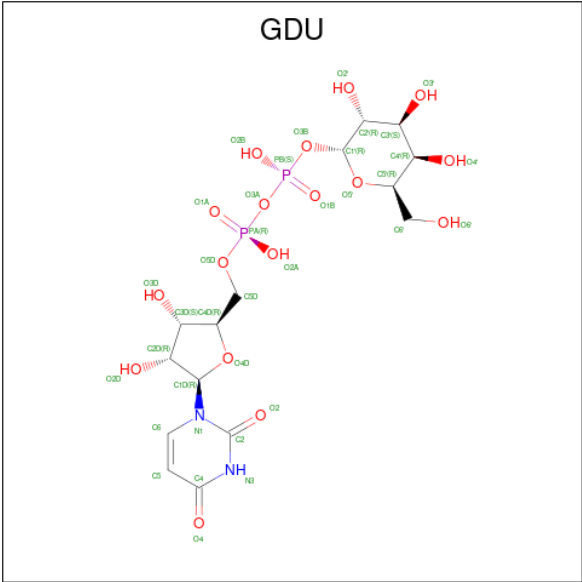
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	ARG	engineered mutation	UNP Q4W1X2
B	327	ALA	ARG	engineered mutation	UNP Q4W1X2
C	327	ALA	ARG	engineered mutation	UNP Q4W1X2
D	327	ALA	ARG	engineered mutation	UNP Q4W1X2
E	327	ALA	ARG	engineered mutation	UNP Q4W1X2
F	327	ALA	ARG	engineered mutation	UNP Q4W1X2
G	327	ALA	ARG	engineered mutation	UNP Q4W1X2
H	327	ALA	ARG	engineered mutation	UNP Q4W1X2

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



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

- Molecule 3 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (CCD ID: GDU) (formula: $\text{C}_{15}\text{H}_{24}\text{N}_2\text{O}_{17}\text{P}_2$).

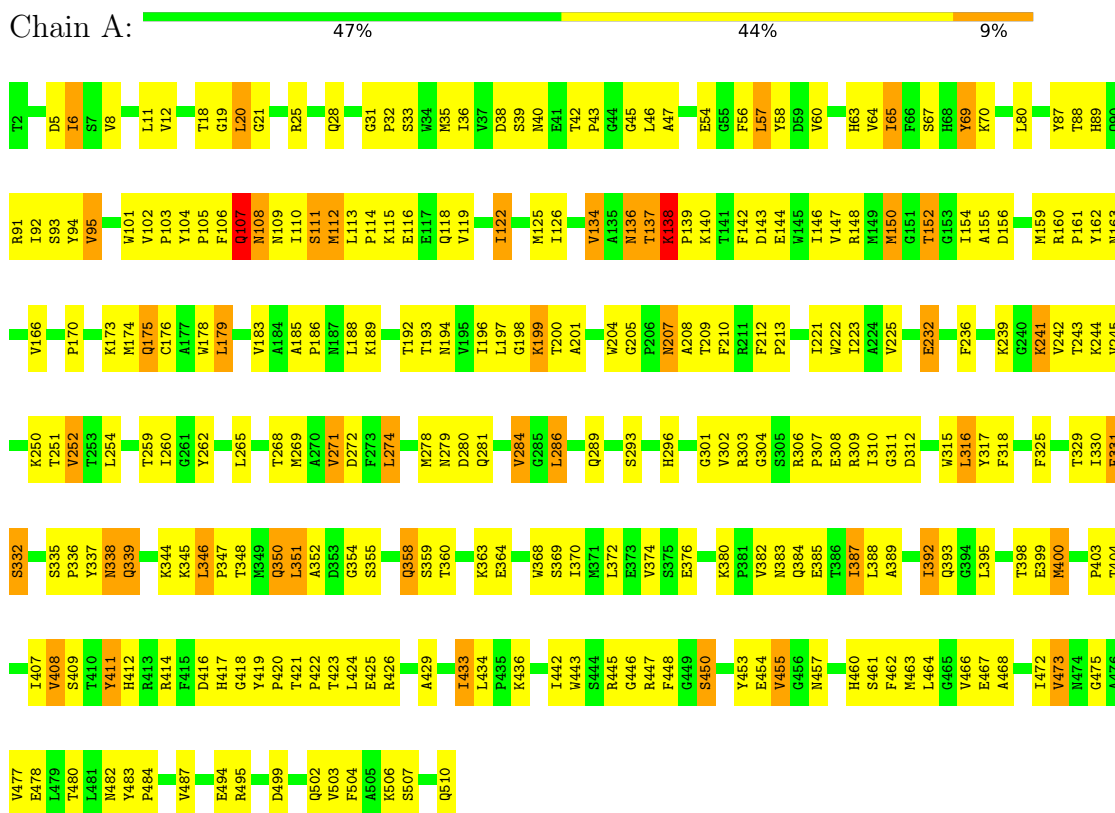


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	E	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	F	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

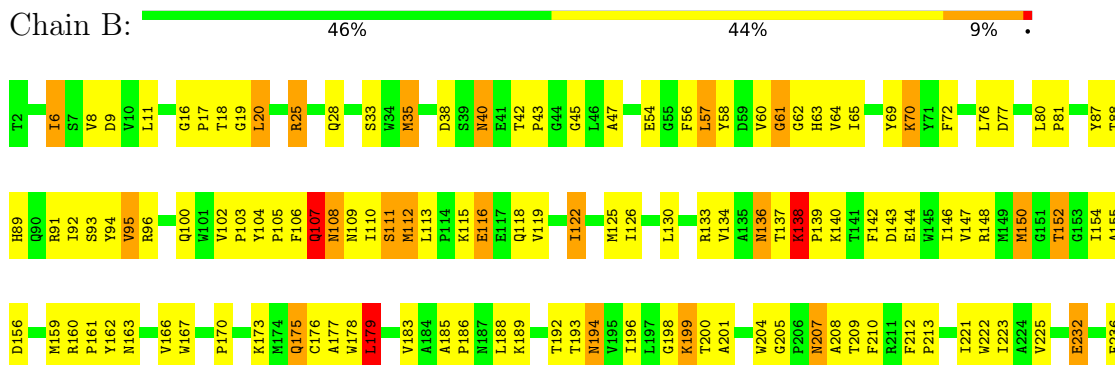
3 Residue-property plots

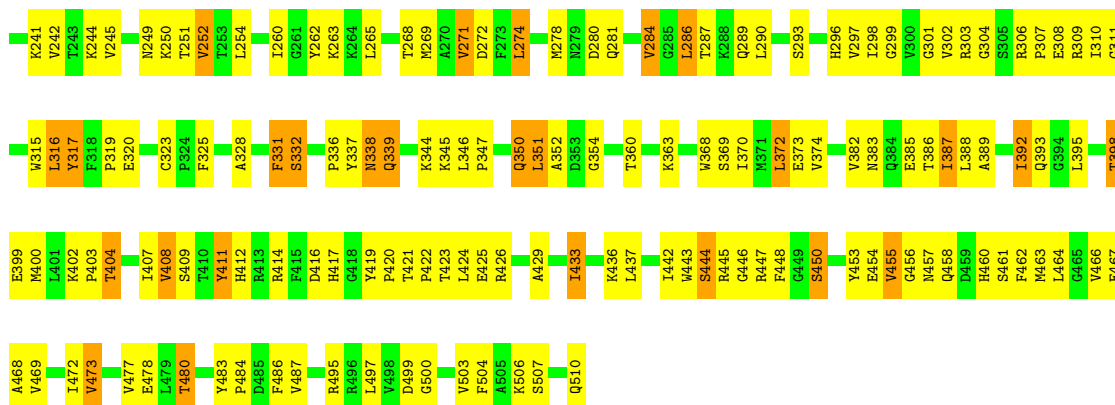
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UDP-galactopyranose mutase

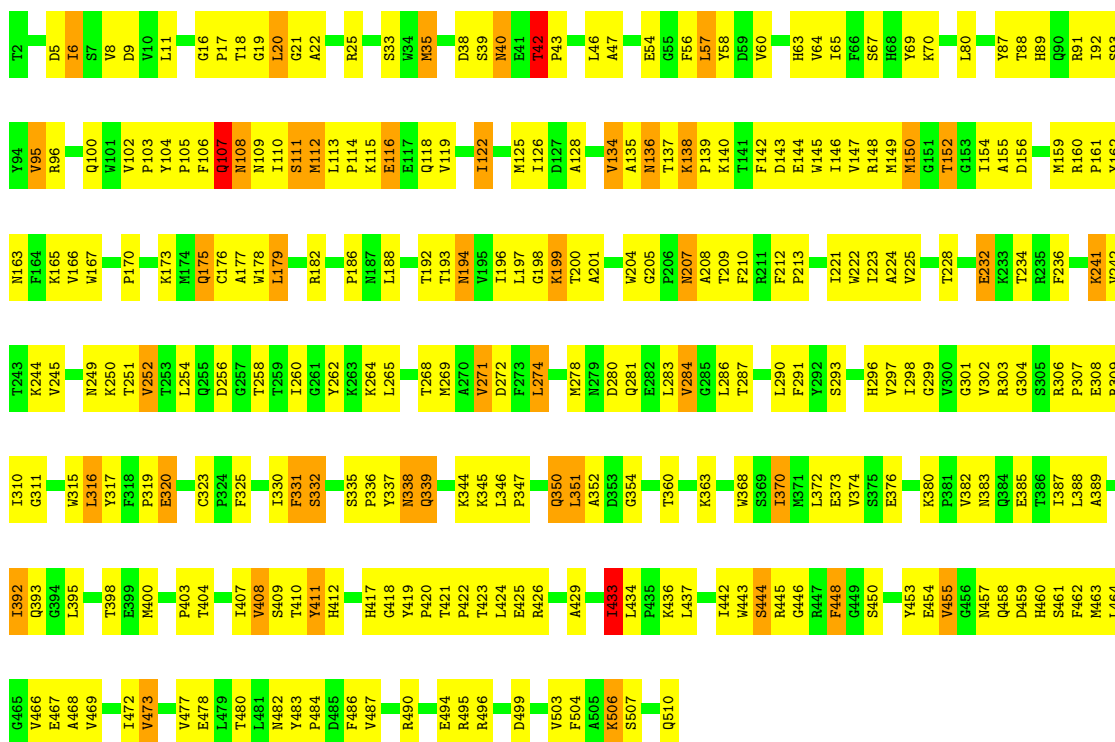


• Molecule 1: UDP-galactopyranose mutase

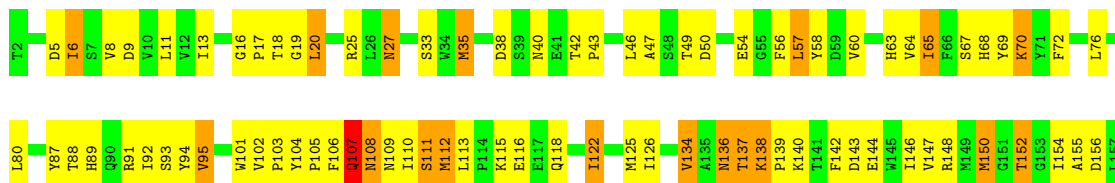


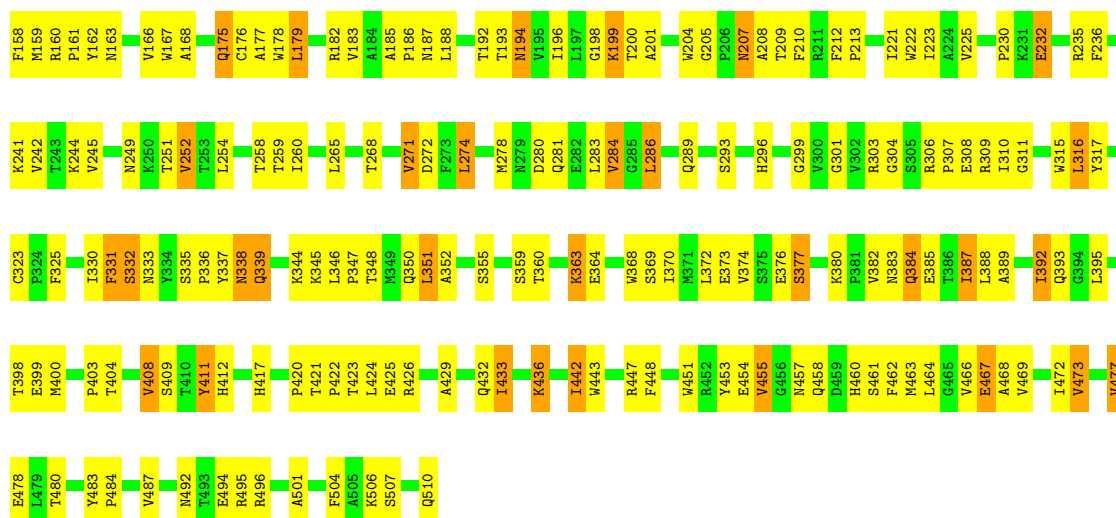


- Molecule 1: UDP-galactopyranose mutase



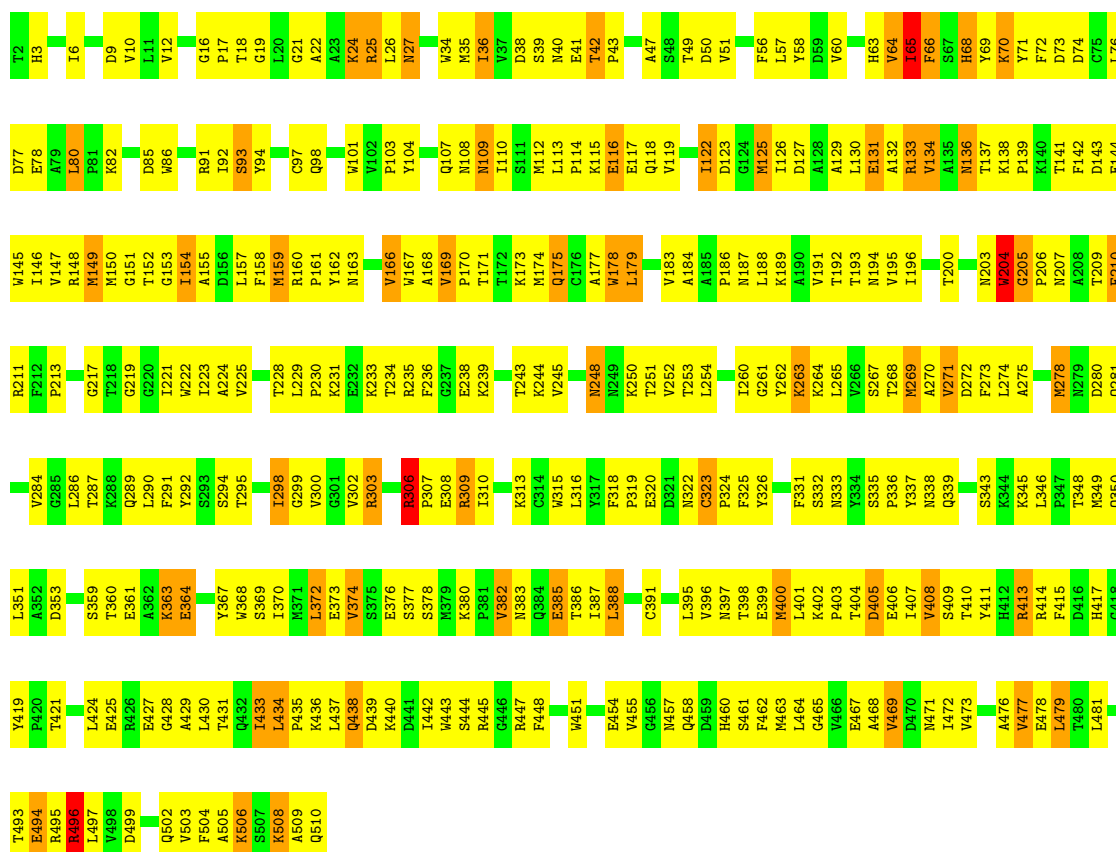
- Molecule 1: UDP-galactopyranose mutase





• Molecule 1: UDP-galactopyranose mutase

Chain E: 34% 54% 11%

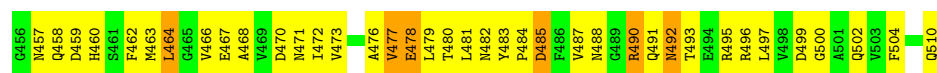


• Molecule 1: UDP-galactopyranose mutase

Chain F: 33% 55% 11%

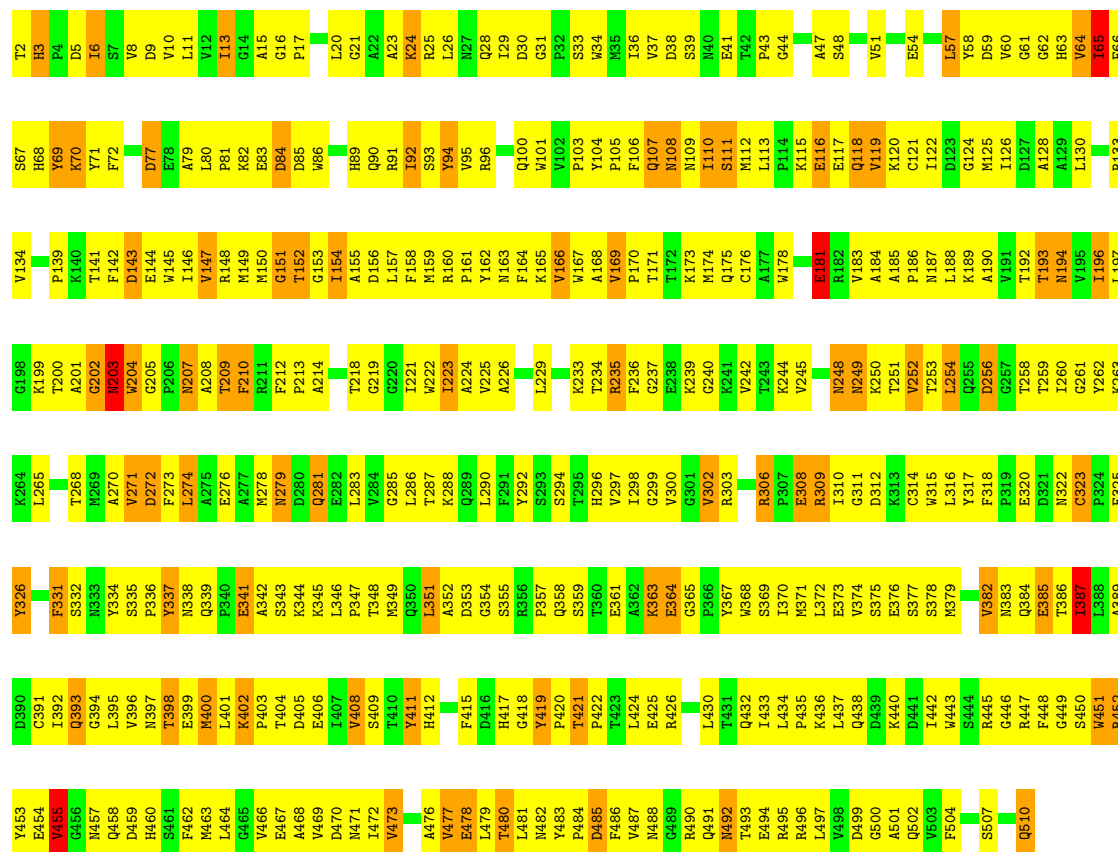


Q393	S332	W269	T200	M136	H68	T2			
							A201	H89	H3
							G202	P139	P4
							N203	K140	K70
							W204	L141	I6
							G205	F142	S7
							P206	D143	V8
							R207	E144	D9
							A208	W145	V10
							T209	L146	L11
Q400	Q339	M278	F210	R148	D77	D8			
							N279	L149	L10
							E280	P211	L11
							D281	F212	V12
							W282	M149	I13
							L283	M150	G14
							W284	A151	A15
							G285	G152	G16
							L286	T153	P17
							T287	E154	P18
Q402	Q340	M278	F210	R148	D77	D8			
							N279	L149	L10
							E280	P211	L11
							D281	F212	V12
							W282	M149	I13
							L283	M150	G14
							W284	A151	A15
							G285	G152	G16
							L286	T153	P17
							T287	E154	P18
Q404	Q342	M280	F212	R148	D77	D8			
							N281	L150	L11
							E282	P213	L12
							D283	M150	G14
							W284	A151	A15
							G285	G152	G16
							L286	T153	P17
							T287	E154	P18
							T288	A155	G19
							W289	D156	L20
Q406	Q344	M282	F214	R150	D79	D9			
							N283	L151	L11
							E284	P215	L12
							D285	M151	G15
							W286	A152	A16
							G287	G153	G16
							L288	T154	P19
							T289	E155	P20
							T290	D157	L21
							W291	F158	G21
Q408	Q346	M284	F216	R152	D81	D10			
							N285	L153	L13
							E286	P217	L14
							D287	M152	G16
							W288	A153	A17
							G289	G154	G17
							L289	T155	P21
							T290	E156	P22
							T291	D158	L22
							W292	F159	G22
Q410	Q348	M286	F218	R154	D83	D12			
							N287	L155	L15
							E288	P219	L16
							D289	M153	G17
							W289	A154	A18
							G290	G155	G18
							L290	T156	P23
							T291	E157	P24
							T292	D159	L23
							W293	F160	G23
Q412	Q350	M288	F220	R156	D85	D14			
							N289	L157	L17
							E289	P221	L18
							D290	M154	G18
							W290	A155	A19
							G291	G156	G19
							L291	T157	P25
							T292	E158	P26
							T293	D160	L24
							W294	F161	G24
Q414	Q352	M290	F222	R158	D87	D16			
							N291	L159	L19
							E290	P223	L19
							D291	M155	G19
							W291	A156	A20
							G292	G157	G20
							L292	T158	P27
							T293	E159	P28
							T294	D161	L25
							W295	F162	G25
Q416	Q354	M292	F224	R160	D89	D18			
							N293	L161	L21
							E292	P225	L20
							D293	M156	G20
							W293	A157	A21
							G293	G158	G21
							L293	T159	P29
							T294	E160	P30
							T295	D162	L26
							W296	F163	G26
Q418	Q356	M294	F226	R162	D91	D20			
							N295	L163	L22
							E294	P227	L21
							D295	M157	G21
							W295	A158	A22
							G294	G159	G22
							L294	T160	P31
							T295	E161	P32
							T296	D163	L27
							W297	F164	G27
Q420	Q358	M296	F228	R164	D93	D22			
							N297	L165	L23
							E296	P229	L22
							D297	M158	G22
							W297	A159	A23
							G295	G160	G23
							L295	T161	P33
							T296	E162	P34
							T297	D164	L28
							W298	F165	G28
Q422	Q360	M298	F23						



• Molecule 1: UDP-galactopyranose mutase

Chain H: 25% 59% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.60Å 175.71Å 135.35Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	34.77 – 3.10 34.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (34.77-3.10) 96.2 (34.77-3.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.202 , 0.260 0.201 , 0.244	Depositor DCC
R_{free} test set	5333 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.327 for h,-k,-l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.479 for h,-k,-l	Depositor
Outliers	2 of 105627 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32560	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6278e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, GDU

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	0.38	0/4089	0.93	17/5558 (0.3%)
1	B	0.39	0/4089	0.92	10/5558 (0.2%)
1	C	0.38	0/4089	0.92	11/5558 (0.2%)
1	D	0.38	0/4089	0.91	7/5558 (0.1%)
1	E	0.40	0/4089	1.03	26/5558 (0.5%)
1	F	0.40	0/4089	1.00	21/5558 (0.4%)
1	G	0.41	0/4089	1.03	20/5558 (0.4%)
1	H	0.39	0/4089	0.99	19/5558 (0.3%)
All	All	0.39	0/32712	0.97	131/44464 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	205	GLY	O-C-N	-12.82	108.95	121.77
1	F	80	LEU	CA-C-N	10.67	130.34	119.56
1	F	80	LEU	C-N-CA	10.67	130.34	119.56
1	G	306	ARG	CA-C-N	10.41	130.20	120.21
1	G	306	ARG	C-N-CA	10.41	130.20	120.21
1	E	205	GLY	CA-C-N	10.37	129.98	119.82
1	E	205	GLY	C-N-CA	10.37	129.98	119.82
1	G	451	TRP	N-CA-C	9.12	123.70	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	80	LEU	CA-C-N	9.06	128.71	119.56
1	D	80	LEU	C-N-CA	9.06	128.71	119.56
1	H	451	TRP	N-CA-C	9.04	123.61	112.58
1	E	80	LEU	CA-C-N	8.98	128.63	119.56
1	E	80	LEU	C-N-CA	8.98	128.63	119.56
1	C	80	LEU	CA-C-N	8.97	128.62	119.56
1	C	80	LEU	C-N-CA	8.97	128.62	119.56
1	D	207	ASN	N-CA-C	8.58	123.47	112.92
1	B	80	LEU	CA-C-N	8.48	128.12	119.56
1	B	80	LEU	C-N-CA	8.48	128.12	119.56
1	E	496	ARG	N-CA-C	8.46	119.80	108.38
1	C	207	ASN	N-CA-C	8.30	123.13	112.92
1	A	207	ASN	N-CA-C	8.24	123.06	112.92
1	E	323	CYS	CA-C-N	8.08	127.65	118.85
1	E	323	CYS	C-N-CA	8.08	127.65	118.85
1	A	80	LEU	CA-C-N	8.05	127.69	119.56
1	A	80	LEU	C-N-CA	8.05	127.69	119.56
1	B	207	ASN	N-CA-C	7.83	122.55	112.92
1	E	65	ILE	N-CA-C	7.82	119.38	108.12
1	F	306	ARG	CA-C-N	7.54	127.99	119.92
1	F	306	ARG	C-N-CA	7.54	127.99	119.92
1	G	323	CYS	CA-C-N	7.30	126.93	119.19
1	G	323	CYS	C-N-CA	7.30	126.93	119.19
1	F	65	ILE	N-CA-C	7.15	118.42	108.12
1	G	207	ASN	N-CA-C	7.15	120.12	111.40
1	H	323	CYS	CA-C-N	7.05	126.67	119.19
1	H	323	CYS	C-N-CA	7.05	126.67	119.19
1	E	360	THR	N-CA-C	-7.05	104.67	113.20
1	C	42	THR	CA-C-N	6.86	126.83	120.03
1	C	42	THR	C-N-CA	6.86	126.83	120.03
1	H	202	GLY	N-CA-C	6.77	120.92	112.79
1	F	323	CYS	CA-C-N	6.56	126.00	118.85
1	F	323	CYS	C-N-CA	6.56	126.00	118.85
1	E	306	ARG	CA-C-N	6.53	127.42	120.11
1	E	306	ARG	C-N-CA	6.53	127.42	120.11
1	H	306	ARG	CA-C-N	6.45	127.91	119.84
1	H	306	ARG	C-N-CA	6.45	127.91	119.84
1	G	452	ARG	N-CA-C	6.45	119.30	108.02
1	A	42	THR	CA-C-N	6.44	126.39	120.21
1	A	42	THR	C-N-CA	6.44	126.39	120.21
1	G	3	HIS	N-CA-C	6.43	118.18	110.07
1	H	3	HIS	N-CA-C	6.43	118.17	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	452	ARG	N-CA-C	6.42	119.25	108.02
1	E	203	ASN	N-CA-C	6.35	119.87	111.75
1	F	505	ALA	N-CA-C	-6.30	104.10	110.97
1	F	204	TRP	N-CA-C	6.25	118.79	110.53
1	E	204	TRP	N-CA-C	6.25	118.78	110.53
1	F	496	ARG	N-CA-C	6.22	118.23	108.96
1	H	205	GLY	N-CA-C	-6.21	99.66	112.34
1	G	387	ILE	N-CA-C	6.21	116.88	110.36
1	C	138	LYS	CA-C-N	6.21	125.97	119.76
1	C	138	LYS	C-N-CA	6.21	125.97	119.76
1	G	440	LYS	N-CA-C	-6.18	105.61	113.02
1	B	42	THR	CA-C-N	6.04	126.01	120.03
1	B	42	THR	C-N-CA	6.04	126.01	120.03
1	F	203	ASN	N-CA-C	6.00	119.44	111.75
1	F	42	THR	CA-C-N	5.97	126.31	119.92
1	F	42	THR	C-N-CA	5.97	126.31	119.92
1	C	448	PHE	N-CA-C	5.96	120.71	112.90
1	F	455	VAL	N-CA-C	5.90	117.84	112.29
1	H	473	VAL	N-CA-C	5.89	116.54	110.82
1	F	456	GLY	N-CA-C	5.88	121.14	114.67
1	H	455	VAL	N-CA-C	5.88	117.14	111.91
1	H	151	GLY	N-CA-C	-5.74	104.49	112.18
1	E	479	LEU	N-CA-C	-5.72	106.30	113.28
1	G	151	GLY	N-CA-C	-5.72	105.56	112.48
1	E	210	PHE	N-CA-C	5.69	115.90	107.88
1	A	65	ILE	N-CA-C	5.62	116.19	107.99
1	E	138	LYS	CA-C-N	5.60	125.36	119.76
1	E	138	LYS	C-N-CA	5.60	125.36	119.76
1	F	138	LYS	CA-C-N	5.57	125.33	119.76
1	F	138	LYS	C-N-CA	5.57	125.33	119.76
1	F	159	MET	N-CA-C	5.57	117.04	110.97
1	C	21	GLY	N-CA-C	-5.55	106.06	112.50
1	G	69	TYR	N-CA-C	5.50	117.81	108.02
1	E	323	CYS	N-CA-C	5.49	112.96	108.07
1	G	182	ARG	N-CA-C	-5.46	99.41	108.75
1	E	159	MET	N-CA-C	5.45	116.91	110.97
1	F	254	LEU	N-CA-C	5.44	117.78	109.95
1	D	137	THR	N-CA-C	5.42	118.25	109.79
1	H	181	GLU	N-CA-C	5.39	118.96	112.93
1	A	185	ALA	CA-C-N	5.38	125.28	119.85
1	A	185	ALA	C-N-CA	5.38	125.28	119.85
1	B	138	LYS	CA-C-N	5.36	125.12	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LYS	C-N-CA	5.36	125.12	119.76
1	A	21	GLY	N-CA-C	-5.35	106.29	112.50
1	D	185	ALA	CA-C-N	5.34	125.25	119.85
1	D	185	ALA	C-N-CA	5.34	125.25	119.85
1	G	400	MET	N-CA-C	-5.34	106.76	113.28
1	F	454	GLU	N-CA-C	-5.30	104.92	111.33
1	D	65	ILE	N-CA-C	5.28	115.70	107.99
1	H	480	THR	N-CA-C	-5.27	106.11	112.54
1	E	178	TRP	N-CA-C	5.26	119.33	113.02
1	A	69	TYR	N-CA-C	5.25	116.97	108.41
1	H	300	VAL	N-CA-C	5.24	115.82	108.17
1	E	505	ALA	N-CA-C	-5.23	105.47	111.07
1	E	400	MET	N-CA-C	-5.22	105.67	111.36
1	E	310	ILE	N-CA-C	5.21	115.32	110.42
1	G	205	GLY	N-CA-C	-5.21	101.71	112.34
1	B	185	ALA	CA-C-N	5.20	125.10	119.85
1	B	185	ALA	C-N-CA	5.20	125.10	119.85
1	H	65	ILE	N-CA-C	5.18	115.23	107.51
1	A	138	LYS	CA-C-N	5.18	124.94	119.76
1	A	138	LYS	C-N-CA	5.18	124.94	119.76
1	G	102	VAL	CA-C-N	5.17	125.41	119.83
1	G	102	VAL	C-N-CA	5.17	125.41	119.83
1	H	387	ILE	N-CA-C	5.16	115.77	110.36
1	G	300	VAL	N-CA-C	5.15	115.69	108.17
1	H	400	MET	N-CA-C	-5.13	106.97	113.18
1	E	42	THR	CA-C-N	5.12	125.39	119.92
1	E	42	THR	C-N-CA	5.12	125.39	119.92
1	A	318	PHE	CA-C-N	5.11	124.61	119.19
1	A	318	PHE	C-N-CA	5.11	124.61	119.19
1	H	69	TYR	N-CA-C	5.09	117.08	108.02
1	F	479	LEU	N-CA-C	-5.09	107.07	113.28
1	A	31	GLY	CA-C-N	5.08	125.29	120.31
1	A	31	GLY	C-N-CA	5.08	125.29	120.31
1	E	254	LEU	N-CA-C	5.07	117.25	109.95
1	C	135	ALA	N-CA-C	5.04	117.83	109.46
1	B	179	LEU	N-CA-C	5.03	119.06	113.02
1	G	490	ARG	N-CA-C	5.03	115.95	108.86
1	A	137	THR	N-CA-C	5.03	117.63	109.79
1	C	433	ILE	N-CA-C	5.02	115.24	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	65	ILE	Peptide

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	3990	0	3906	258	0
1	B	3990	0	3906	278	0
1	C	3990	0	3906	281	0
1	D	3990	0	3906	243	0
1	E	3990	0	3906	394	0
1	F	3990	0	3906	375	0
1	G	3990	0	3906	468	0
1	H	3990	0	3906	449	0
2	A	53	0	29	9	0
2	B	53	0	30	13	0
2	C	53	0	30	12	0
2	D	53	0	30	22	0
2	E	53	0	30	18	0
2	F	53	0	29	13	0
2	G	53	0	29	13	0
2	H	53	0	30	10	0
3	A	36	0	22	11	0
3	B	36	0	22	17	0
3	C	36	0	22	9	0
3	D	36	0	22	4	0
3	E	36	0	22	14	0
3	F	36	0	22	10	0
All	All	32560	0	31617	2702	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 42.

All (2702) 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:E:70:LYS:HG3	1:E:496:ARG:HH22	0.96	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:LYS:HG3	1:F:496:ARG:HH22	1.12	1.10
1:F:461:SER:HA	1:F:464:LEU:HD12	1.37	1.06
1:D:303:ARG:NH2	1:D:346:LEU:O	1.90	1.05
1:E:461:SER:HA	1:E:464:LEU:HD12	1.38	1.05
1:B:332:SER:HA	1:B:339:GLN:HE21	1.20	1.04
1:E:133:ARG:HH11	1:E:133:ARG:HG3	1.24	1.02
1:F:16:GLY:HA3	2:F:601:FAD:O1P	1.59	1.02
1:B:62:GLY:O	3:B:602:GDU:O4'	1.76	1.01
1:B:183:VAL:HG22	3:B:602:GDU:H1D	1.36	1.01
1:A:303:ARG:NH2	1:A:346:LEU:O	1.95	1.00
1:H:149:MET:SD	1:H:184:ALA:HA	2.01	1.00
1:G:17:PRO:HD2	2:G:601:FAD:O1P	1.60	0.99
1:D:332:SER:HA	1:D:339:GLN:HE21	1.24	0.99
1:A:104:TYR:HE1	3:A:602:GDU:H5	1.26	0.98
1:G:197:LEU:C	1:G:199:LYS:H	1.70	0.98
1:A:183:VAL:HG13	3:A:602:GDU:O2	1.65	0.96
1:A:104:TYR:CE1	3:A:602:GDU:H5	2.00	0.96
1:G:115:LYS:HA	1:G:118:GLN:HG3	1.47	0.95
1:C:332:SER:HA	1:C:339:GLN:HE21	1.30	0.95
1:G:18:THR:HG22	1:G:268:THR:HG21	1.49	0.94
1:F:154:ILE:HD13	1:F:154:ILE:H	1.31	0.94
1:G:292:TYR:HB2	1:G:419:TYR:O	1.67	0.94
1:E:70:LYS:HG3	1:E:496:ARG:NH2	1.81	0.94
1:A:244:LYS:HB2	1:F:255:GLN:HE21	1.30	0.94
1:H:292:TYR:HB2	1:H:419:TYR:O	1.69	0.93
1:A:332:SER:HA	1:A:339:GLN:HE21	1.34	0.93
1:F:445:ARG:HB3	1:F:464:LEU:HB3	1.51	0.92
1:G:47:ALA:HB3	1:G:222:TRP:HE1	1.34	0.92
1:H:150:MET:HG3	1:H:154:ILE:HB	1.51	0.92
1:F:133:ARG:HH11	1:F:133:ARG:HG3	1.31	0.92
1:E:269:MET:HE2	1:E:273:PHE:HB3	1.50	0.92
1:F:467:GLU:HG3	1:F:495:ARG:HH12	1.36	0.91
1:B:183:VAL:HG13	3:B:602:GDU:C2	2.01	0.91
1:F:9:ASP:HA	1:F:263:LYS:HD3	1.52	0.90
1:B:159:MET:HE1	3:B:602:GDU:N3	1.86	0.90
1:E:445:ARG:HB3	1:E:464:LEU:HB3	1.52	0.90
1:G:105:PRO:HB2	1:G:107:GLN:HG2	1.52	0.89
1:H:29:ILE:HG22	1:H:31:GLY:H	1.36	0.89
1:G:309:ARG:H	1:G:309:ARG:HD3	1.38	0.89
1:H:115:LYS:HA	1:H:118:GLN:HG3	1.53	0.89
1:B:38:ASP:OD1	2:B:601:FAD:H1B	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:TYR:O	1:E:166:VAL:HG12	1.73	0.88
1:H:376:GLU:HG3	1:H:382:VAL:HG13	1.54	0.88
1:F:188:LEU:O	1:F:192:THR:HG23	1.74	0.88
1:G:17:PRO:CD	2:G:601:FAD:O1P	2.20	0.88
1:G:121:CYS:HB3	1:G:154:ILE:HG13	1.56	0.88
1:C:332:SER:HA	1:C:339:GLN:NE2	1.89	0.88
1:G:445:ARG:HA	1:G:450:SER:HB2	1.53	0.88
1:H:455:VAL:O	1:H:460:HIS:HB3	1.74	0.88
1:H:47:ALA:HB3	1:H:222:TRP:HE1	1.36	0.87
1:E:149:MET:SD	1:E:186:PRO:HD2	2.14	0.87
1:C:110:ILE:HA	1:C:113:LEU:HD12	1.57	0.87
1:H:271:VAL:HG12	1:H:448:PHE:O	1.75	0.87
1:H:59:ASP:HB3	1:H:63:HIS:HD2	1.40	0.87
1:H:309:ARG:HD3	1:H:309:ARG:H	1.41	0.86
1:D:122:ILE:O	1:D:126:ILE:HG13	1.76	0.86
1:B:110:ILE:HA	1:B:113:LEU:HD12	1.57	0.86
1:G:121:CYS:HA	1:G:153:GLY:HA3	1.58	0.86
1:C:178:TRP:HB2	1:C:454:GLU:HG3	1.57	0.86
1:D:105:PRO:O	1:D:109:ASN:ND2	2.09	0.86
1:D:178:TRP:HB2	1:D:454:GLU:HG3	1.57	0.86
1:G:69:TYR:CD2	1:G:463:MET:HG3	2.11	0.86
1:G:376:GLU:HG3	1:G:382:VAL:HG13	1.57	0.86
1:B:193:THR:HG23	1:H:119:VAL:HG11	1.58	0.85
1:G:150:MET:HG3	1:G:154:ILE:HB	1.58	0.85
1:C:494:GLU:HG2	1:G:477:VAL:HA	1.56	0.85
1:A:395:LEU:HD22	1:A:400:MET:HE2	1.59	0.85
1:A:122:ILE:O	1:A:126:ILE:HG13	1.77	0.85
1:B:178:TRP:HB2	1:B:454:GLU:HG3	1.57	0.85
1:E:9:ASP:HA	1:E:263:LYS:HD3	1.57	0.85
1:E:63:HIS:CE1	2:E:601:FAD:C9A	2.59	0.85
1:A:111:SER:HB3	1:A:198:GLY:HA2	1.58	0.85
1:A:243:THR:HB	1:F:243:THR:HG21	1.56	0.85
1:B:395:LEU:HD22	1:B:400:MET:HE2	1.57	0.85
3:A:602:GDU:H5'1	3:A:602:GDU:H6	1.59	0.84
1:B:159:MET:HE1	3:B:602:GDU:HN3	1.40	0.84
1:F:56:PHE:CE1	1:F:339:GLN:HB3	2.12	0.84
2:A:601:FAD:H9	2:A:601:FAD:O2'	1.77	0.84
1:G:91:ARG:HH21	1:G:203:ASN:HA	1.40	0.84
1:G:149:MET:SD	1:G:184:ALA:HA	2.17	0.84
1:H:418:GLY:C	1:H:419:TYR:HD1	1.86	0.84
1:H:121:CYS:HA	1:H:153:GLY:HA3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:SER:HA	1:D:339:GLN:NE2	1.92	0.84
1:H:332:SER:HA	1:H:339:GLN:NE2	1.92	0.84
1:E:154:ILE:HD13	1:E:154:ILE:H	1.44	0.83
1:G:17:PRO:HD2	2:G:601:FAD:O1A	1.78	0.83
1:G:281:GLN:OE1	1:G:281:GLN:HA	1.75	0.83
1:D:395:LEU:HD22	1:D:400:MET:HE2	1.61	0.83
1:F:175:GLN:OE1	1:F:178:TRP:HD1	1.59	0.83
1:C:119:VAL:HG23	1:E:196:ILE:HG21	1.61	0.83
1:H:109:ASN:ND2	1:H:201:ALA:O	2.12	0.83
1:E:455:VAL:HA	1:E:460:HIS:HD1	1.44	0.82
1:F:187:ASN:OD1	1:F:189:LYS:HB2	1.79	0.82
1:H:57:LEU:HD11	1:H:338:ASN:HA	1.61	0.82
1:H:121:CYS:HB3	1:H:154:ILE:HG13	1.61	0.82
1:A:178:TRP:HB2	1:A:454:GLU:HG3	1.60	0.82
1:A:280:ASP:O	1:A:284:VAL:HG23	1.78	0.82
1:E:458:GLN:HG3	2:E:601:FAD:H2'	1.62	0.82
1:E:332:SER:HA	1:E:339:GLN:NE2	1.95	0.82
1:E:338:ASN:HB2	1:E:339:GLN:NE2	1.94	0.81
1:G:411:TYR:HD1	1:G:412:HIS:N	1.78	0.81
1:H:69:TYR:CD2	1:H:463:MET:HG3	2.16	0.81
1:A:332:SER:HA	1:A:339:GLN:NE2	1.94	0.81
1:B:332:SER:HA	1:B:339:GLN:NE2	1.94	0.81
1:D:91:ARG:HG3	1:D:315:TRP:CH2	2.16	0.81
1:H:468:ALA:O	1:H:471:ASN:HB3	1.80	0.81
1:A:244:LYS:HB2	1:F:255:GLN:NE2	1.96	0.81
1:E:281:GLN:OE1	1:E:281:GLN:HA	1.79	0.81
1:F:430:LEU:HD22	1:F:434:LEU:HG	1.61	0.81
1:D:16:GLY:HA3	2:D:601:FAD:H52A	1.62	0.80
1:G:332:SER:HA	1:G:339:GLN:NE2	1.96	0.80
1:B:111:SER:HB3	1:B:198:GLY:HA2	1.64	0.80
1:D:91:ARG:HD3	1:D:207:ASN:HB2	1.64	0.80
1:A:350:GLN:HE22	1:A:354:GLY:HA2	1.46	0.80
1:F:70:LYS:HG3	1:F:496:ARG:NH2	1.93	0.80
1:F:467:GLU:HG3	1:F:495:ARG:NH1	1.96	0.80
1:D:280:ASP:O	1:D:284:VAL:HG23	1.81	0.80
1:F:27:ASN:HB2	1:F:34:TRP:CZ2	2.16	0.80
1:H:411:TYR:HD1	1:H:412:HIS:N	1.80	0.80
1:E:457:ASN:HB3	2:E:601:FAD:C2	2.12	0.79
1:D:458:GLN:HG3	2:D:601:FAD:H2'	1.63	0.79
1:H:105:PRO:HB2	1:H:107:GLN:HG2	1.64	0.79
1:H:144:GLU:O	1:H:148:ARG:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:HIS:H	1:F:63:HIS:CD2	1.98	0.79
1:G:57:LEU:HD11	1:G:338:ASN:HA	1.65	0.79
1:H:271:VAL:N	1:H:448:PHE:O	2.14	0.79
1:H:389:ALA:HA	1:H:392:ILE:HD12	1.63	0.79
1:G:154:ILE:H	1:G:154:ILE:HD12	1.45	0.79
1:H:417:HIS:HB3	1:H:448:PHE:CE2	2.17	0.79
1:G:51:VAL:HG22	1:G:57:LEU:HB3	1.64	0.78
1:C:91:ARG:HG3	1:C:315:TRP:CH2	2.19	0.78
1:A:110:ILE:HA	1:A:113:LEU:HD12	1.64	0.78
1:A:188:LEU:O	1:A:192:THR:HG23	1.83	0.78
1:G:218:THR:HA	1:G:221:ILE:HD12	1.64	0.78
1:A:91:ARG:HH12	1:A:205:GLY:HA3	1.49	0.78
1:D:111:SER:HB3	1:D:198:GLY:HA2	1.65	0.78
1:G:29:ILE:HG22	1:G:31:GLY:H	1.49	0.78
1:G:346:LEU:HD23	1:G:347:PRO:HD2	1.65	0.78
1:F:230:PRO:HG2	1:F:233:LYS:HD2	1.66	0.78
1:B:398:THR:HG22	1:B:400:MET:HG2	1.64	0.78
1:E:188:LEU:O	1:E:192:THR:HG23	1.84	0.78
1:G:314:CYS:HB3	1:G:315:TRP:HE3	1.49	0.78
1:H:359:SER:HB3	1:H:363:LYS:HE2	1.66	0.78
1:C:395:LEU:HD22	1:C:400:MET:HE2	1.64	0.77
1:E:22:ALA:HA	1:E:469:VAL:CG2	2.14	0.77
1:H:194:ASN:ND2	1:H:199:LYS:HB3	1.99	0.77
1:D:110:ILE:HA	1:D:113:LEU:HD12	1.67	0.77
1:F:178:TRP:HB2	1:F:454:GLU:HG3	1.65	0.77
1:G:418:GLY:C	1:G:419:TYR:HD1	1.91	0.77
1:A:91:ARG:HD3	1:A:207:ASN:HB2	1.67	0.77
1:B:122:ILE:O	1:B:126:ILE:HG13	1.84	0.77
1:F:269:MET:HE2	1:F:273:PHE:HB3	1.67	0.77
1:G:18:THR:HG22	1:G:268:THR:CG2	2.14	0.77
1:H:314:CYS:HB3	1:H:315:TRP:HE3	1.49	0.77
1:C:188:LEU:O	1:C:192:THR:HG23	1.84	0.77
1:H:17:PRO:HG3	1:H:222:TRP:CZ2	2.20	0.77
1:F:151:GLY:O	1:F:154:ILE:HG12	1.85	0.77
1:G:79:ALA:HB2	1:G:225:VAL:HG23	1.65	0.77
1:B:188:LEU:O	1:B:192:THR:HG23	1.85	0.77
1:A:420:PRO:HG2	1:A:453:TYR:HB2	1.66	0.77
1:C:398:THR:O	1:C:398:THR:HG22	1.84	0.77
1:G:18:THR:CG2	1:G:268:THR:HG21	2.14	0.77
1:H:51:VAL:HG22	1:H:57:LEU:HB3	1.66	0.77
1:C:122:ILE:O	1:C:126:ILE:HG13	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:TRP:CZ3	1:F:316:LEU:HD13	2.19	0.76
1:G:96:ARG:HG2	1:G:398:THR:HG22	1.67	0.76
1:H:249:ASN:HB2	1:H:251:THR:HG23	1.66	0.76
1:F:108:ASN:HB3	1:F:194:ASN:ND2	2.00	0.76
1:H:47:ALA:HB3	1:H:222:TRP:NE1	2.00	0.76
1:A:91:ARG:HG3	1:A:315:TRP:CH2	2.20	0.76
1:E:398:THR:OG1	1:E:400:MET:HG2	1.85	0.76
1:F:332:SER:HA	1:F:339:GLN:NE2	1.99	0.76
1:G:197:LEU:C	1:G:199:LYS:N	2.35	0.76
1:C:111:SER:HB3	1:C:198:GLY:HA2	1.67	0.76
1:E:353:ASP:HB3	1:E:403:PRO:CB	2.15	0.76
1:E:267:SER:O	1:E:444:SER:HA	1.86	0.76
1:F:149:MET:SD	1:F:186:PRO:HD2	2.25	0.76
1:F:159:MET:HE1	3:F:602:GDU:H6	1.67	0.76
1:G:28:GLN:HE21	1:G:497:LEU:C	1.93	0.76
1:G:468:ALA:O	1:G:471:ASN:HB3	1.84	0.76
1:E:19:GLY:N	1:E:268:THR:HG21	2.01	0.76
1:E:280:ASP:O	1:E:284:VAL:HG23	1.86	0.76
1:G:348:THR:O	1:G:357:PRO:HG3	1.85	0.76
1:E:178:TRP:HB2	1:E:454:GLU:HG3	1.65	0.76
1:F:22:ALA:HA	1:F:469:VAL:CG2	2.15	0.76
1:F:338:ASN:HB2	1:F:339:GLN:NE2	2.01	0.75
1:H:107:GLN:H	1:H:107:GLN:CD	1.94	0.75
1:H:130:LEU:O	1:H:133:ARG:HB3	1.86	0.75
1:G:18:THR:CG2	1:G:268:THR:CG2	2.63	0.75
1:E:127:ASP:O	1:E:131:GLU:HG2	1.86	0.75
1:H:155:ALA:O	1:H:160:ARG:HG3	1.86	0.75
1:A:414:ARG:HD3	1:F:281:GLN:HB3	1.68	0.75
1:E:56:PHE:CE1	1:E:339:GLN:HB3	2.21	0.75
1:F:494:GLU:H	1:F:494:GLU:CD	1.91	0.75
1:G:47:ALA:HB3	1:G:222:TRP:NE1	2.02	0.75
1:G:351:LEU:O	1:G:354:GLY:N	2.19	0.75
1:B:91:ARG:HD3	1:B:207:ASN:HB2	1.67	0.75
1:F:91:ARG:HD3	1:F:207:ASN:HB2	1.67	0.75
1:A:60:VAL:O	1:A:63:HIS:NE2	2.20	0.75
1:C:280:ASP:O	1:C:284:VAL:HG23	1.86	0.75
1:B:47:ALA:HB1	1:B:222:TRP:HE1	1.51	0.75
1:H:446:GLY:H	1:H:450:SER:HB3	1.52	0.75
1:D:188:LEU:O	1:D:192:THR:HG23	1.87	0.74
1:F:80:LEU:HD12	1:F:86:TRP:CZ2	2.22	0.74
1:D:420:PRO:HG2	1:D:453:TYR:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:ARG:HH11	1:G:470:ASP:CG	1.94	0.74
1:F:127:ASP:O	1:F:131:GLU:HG2	1.88	0.74
1:G:271:VAL:HG12	1:G:448:PHE:O	1.87	0.74
1:G:338:ASN:HB2	1:G:339:GLN:NE2	2.03	0.74
1:H:393:GLN:O	1:H:396:VAL:N	2.19	0.74
1:B:280:ASP:O	1:B:284:VAL:HG23	1.86	0.74
1:G:109:ASN:ND2	1:G:201:ALA:O	2.21	0.74
1:A:159:MET:HE1	3:A:602:GDU:N3	2.03	0.74
1:D:462:PHE:O	1:D:466:VAL:HG23	1.88	0.74
1:E:60:VAL:O	1:E:63:HIS:NE2	2.21	0.74
1:G:393:GLN:O	1:G:396:VAL:N	2.19	0.74
1:D:104:TYR:CD1	1:D:105:PRO:HA	2.22	0.73
1:G:249:ASN:HB2	1:G:251:THR:HG23	1.69	0.73
1:G:17:PRO:HG3	1:G:222:TRP:CZ2	2.22	0.73
1:G:207:ASN:C	1:G:207:ASN:OD1	2.31	0.73
1:G:271:VAL:N	1:G:448:PHE:O	2.20	0.73
1:E:167:TRP:CD2	1:E:174:MET:HE1	2.23	0.73
1:H:443:TRP:HA	1:H:445:ARG:HH21	1.54	0.73
1:E:71:TYR:O	1:E:74:ASP:HB2	1.87	0.73
1:E:383:ASN:HB3	1:E:386:THR:OG1	1.88	0.73
1:H:303:ARG:NH1	1:H:406:GLU:OE2	2.21	0.73
1:H:338:ASN:HB2	1:H:339:GLN:NE2	2.03	0.73
1:B:91:ARG:HG3	1:B:315:TRP:CH2	2.24	0.73
1:B:108:ASN:OD1	1:B:108:ASN:N	2.20	0.73
1:H:79:ALA:HB2	1:H:225:VAL:HG23	1.70	0.73
1:C:421:THR:HG22	1:C:423:THR:HG23	1.69	0.72
1:F:93:SER:OG	1:F:315:TRP:NE1	2.22	0.72
1:G:37:VAL:HG12	1:G:235:ARG:HB2	1.71	0.72
1:G:104:TYR:O	1:G:203:ASN:N	2.22	0.72
1:F:303:ARG:HH21	1:F:363:LYS:HB2	1.52	0.72
1:E:471:ASN:ND2	1:E:476:ALA:O	2.20	0.72
1:G:18:THR:HG21	1:G:268:THR:HG22	1.72	0.72
1:B:130:LEU:HD23	1:H:130:LEU:HD23	1.72	0.72
1:G:181:GLU:N	1:G:485:ASP:OD1	2.21	0.72
1:B:420:PRO:HG2	1:B:453:TYR:HB2	1.70	0.72
1:C:104:TYR:CD1	1:C:105:PRO:HA	2.25	0.72
1:E:91:ARG:HD3	1:E:207:ASN:HB2	1.71	0.72
1:G:48:SER:O	1:G:60:VAL:HG23	1.89	0.72
1:A:104:TYR:CD1	1:A:105:PRO:HA	2.23	0.72
1:C:350:GLN:HE22	1:C:354:GLY:HA2	1.55	0.72
1:E:80:LEU:HD12	1:E:86:TRP:CZ2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:398:THR:OG1	1:F:400:MET:HG2	1.90	0.72
1:H:402:LYS:NZ	1:H:405:ASP:OD1	2.21	0.72
1:C:303:ARG:NH2	1:C:363:LYS:O	2.22	0.72
1:E:303:ARG:NH2	1:E:363:LYS:HG3	2.04	0.72
1:E:457:ASN:HA	2:E:601:FAD:H1'2	1.71	0.72
1:E:465:GLY:O	1:E:469:VAL:HG23	1.90	0.72
1:E:133:ARG:HG3	1:E:133:ARG:NH1	2.03	0.72
1:F:19:GLY:N	1:F:268:THR:HG21	2.04	0.71
1:G:142:PHE:HB3	1:G:171:THR:O	1.89	0.71
1:G:417:HIS:HB3	1:G:448:PHE:CE2	2.24	0.71
1:H:59:ASP:HB3	1:H:63:HIS:CD2	2.23	0.71
1:A:104:TYR:HE1	3:A:602:GDU:C5	2.03	0.71
1:D:91:ARG:HH12	1:D:205:GLY:HA3	1.54	0.71
1:E:230:PRO:HG2	1:E:233:LYS:HD2	1.71	0.71
1:E:494:GLU:H	1:E:494:GLU:CD	1.98	0.71
1:E:9:ASP:O	1:E:263:LYS:HB2	1.91	0.71
1:G:130:LEU:O	1:G:133:ARG:HB3	1.90	0.71
1:C:420:PRO:HG2	1:C:453:TYR:HB2	1.70	0.71
1:F:353:ASP:HB3	1:F:403:PRO:CB	2.20	0.71
1:C:303:ARG:HH21	1:C:363:LYS:C	1.98	0.71
1:F:465:GLY:O	1:F:469:VAL:HG23	1.90	0.71
1:G:314:CYS:HB3	1:G:315:TRP:CE3	2.26	0.71
1:A:462:PHE:O	1:A:466:VAL:HG23	1.89	0.71
1:H:181:GLU:OE1	1:H:181:GLU:HA	1.91	0.71
1:H:212:PHE:CG	1:H:213:PRO:HD2	2.25	0.71
1:A:421:THR:HG22	1:A:423:THR:HG23	1.72	0.71
1:C:91:ARG:HD3	1:C:207:ASN:HB2	1.73	0.71
1:G:143:ASP:HA	1:G:146:ILE:HD12	1.71	0.71
1:H:188:LEU:O	1:H:192:THR:HG23	1.90	0.71
1:A:473:VAL:O	1:E:499:ASP:HB3	1.91	0.71
1:E:122:ILE:O	1:E:126:ILE:HG13	1.91	0.71
1:G:188:LEU:O	1:G:192:THR:HG23	1.91	0.71
1:G:447:ARG:O	1:G:451:TRP:HA	1.91	0.71
1:B:183:VAL:HG22	3:B:602:GDU:C1D	2.18	0.70
1:F:27:ASN:HB2	1:F:34:TRP:HZ2	1.55	0.70
1:H:218:THR:HA	1:H:221:ILE:HD12	1.73	0.70
1:E:265:LEU:HD23	1:E:442:ILE:HG12	1.72	0.70
1:G:303:ARG:NH1	1:G:406:GLU:OE2	2.23	0.70
1:A:455:VAL:O	1:A:460:HIS:HB3	1.90	0.70
1:G:392:ILE:O	1:G:395:LEU:HB2	1.92	0.70
1:H:54:GLU:HB3	1:H:346:LEU:HD11	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:482:ASN:HB2	1:H:483:TYR:CE2	2.27	0.70
1:C:115:LYS:HD3	1:E:196:ILE:O	1.90	0.70
1:E:70:LYS:HB3	1:E:496:ARG:HH12	1.56	0.70
1:H:467:GLU:OE1	1:H:480:THR:N	2.21	0.70
1:E:167:TRP:CG	1:E:174:MET:HE1	2.25	0.70
1:H:37:VAL:HG12	1:H:235:ARG:HB2	1.73	0.70
1:D:463:MET:O	1:D:467:GLU:HG3	1.92	0.70
1:C:47:ALA:HB1	1:C:222:TRP:HE1	1.56	0.70
1:E:142:PHE:O	1:E:145:TRP:HB3	1.91	0.70
1:F:267:SER:O	1:F:444:SER:HA	1.90	0.70
1:F:303:ARG:HH21	1:F:363:LYS:CB	2.05	0.70
1:G:468:ALA:O	1:G:472:ILE:HD12	1.92	0.70
1:H:96:ARG:HG2	1:H:398:THR:HG22	1.74	0.70
1:C:103:PRO:HG2	1:C:109:ASN:ND2	2.06	0.70
1:H:274:LEU:O	1:H:278:MET:HG2	1.92	0.70
1:H:440:LYS:HB2	1:H:442:ILE:HD12	1.74	0.70
1:A:91:ARG:NH2	1:A:204:TRP:O	2.24	0.70
1:G:142:PHE:O	1:G:146:ILE:HG13	1.92	0.70
1:G:445:ARG:HA	1:G:450:SER:CB	2.21	0.70
1:E:175:GLN:HE22	1:E:177:ALA:HB3	1.56	0.69
1:H:84:ASP:OD2	1:H:84:ASP:N	2.22	0.69
1:C:125:MET:HE1	1:C:186:PRO:HB2	1.73	0.69
1:E:455:VAL:HG23	1:E:455:VAL:O	1.91	0.69
1:B:350:GLN:HE22	1:B:354:GLY:HA2	1.57	0.69
1:H:308:GLU:HG3	1:H:309:ARG:HD3	1.74	0.69
1:B:104:TYR:CD1	1:B:105:PRO:HA	2.28	0.69
1:E:118:GLN:OE1	1:E:195:VAL:HG13	1.92	0.69
1:F:167:TRP:CD2	1:F:174:MET:HE1	2.27	0.69
1:B:176:CYS:O	1:B:179:LEU:HD12	1.93	0.69
1:F:280:ASP:O	1:F:284:VAL:HG23	1.93	0.69
1:H:484:PRO:HA	1:H:487:VAL:HG22	1.74	0.69
1:G:84:ASP:OD2	1:G:84:ASP:N	2.24	0.69
1:H:103:PRO:HB2	1:H:202:GLY:HA2	1.75	0.69
1:B:91:ARG:HH12	1:B:205:GLY:HA3	1.56	0.69
1:B:398:THR:CG2	1:B:398:THR:O	2.40	0.69
1:E:22:ALA:HA	1:E:469:VAL:HG22	1.75	0.69
1:E:313:LYS:O	1:E:333:ASN:ND2	2.26	0.69
1:G:144:GLU:O	1:G:148:ARG:HG3	1.93	0.69
1:G:159:MET:O	1:G:163:ASN:HB2	1.91	0.69
1:H:314:CYS:HB3	1:H:315:TRP:CE3	2.26	0.69
1:D:421:THR:HG22	1:D:423:THR:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:VAL:O	1:C:460:HIS:HB3	1.93	0.69
1:F:63:HIS:H	1:F:63:HIS:HD2	1.40	0.69
1:F:105:PRO:O	1:F:109:ASN:ND2	2.26	0.69
1:F:163:ASN:OD1	3:F:602:GDU:O3D	2.09	0.69
1:G:171:THR:HA	1:G:174:MET:HE3	1.75	0.69
1:G:389:ALA:HA	1:G:392:ILE:HD12	1.75	0.69
1:E:350:GLN:O	1:E:407:ILE:HB	1.93	0.68
1:F:133:ARG:HG3	1:F:133:ARG:NH1	2.04	0.68
1:G:322:ASN:HD22	1:G:397:ASN:HB3	1.58	0.68
1:G:341:GLU:HG3	1:G:343:SER:H	1.59	0.68
1:G:492:ASN:HD22	1:G:492:ASN:H	1.42	0.68
1:H:203:ASN:HD22	1:H:204:TRP:H	1.39	0.68
1:E:18:THR:OG1	1:E:461:SER:HB3	1.92	0.68
1:G:54:GLU:HB3	1:G:346:LEU:HD11	1.76	0.68
1:H:142:PHE:O	1:H:146:ILE:HG13	1.93	0.68
1:C:19:GLY:N	1:C:268:THR:HG21	2.09	0.68
1:C:429:ALA:O	1:C:433:ILE:HD12	1.93	0.68
1:E:101:TRP:CZ3	1:E:316:LEU:HD13	2.29	0.68
1:F:5:ASP:H	1:F:259:THR:HG1	1.39	0.68
1:H:445:ARG:HA	1:H:450:SER:HB2	1.73	0.68
1:C:462:PHE:O	1:C:466:VAL:HG23	1.93	0.68
1:E:104:TYR:HE1	3:E:602:GDU:C5	2.06	0.68
1:G:331:PHE:CD2	1:G:338:ASN:HB3	2.29	0.68
1:C:136:ASN:OD1	1:C:137:THR:HG23	1.92	0.68
1:E:143:ASP:HA	1:E:146:ILE:HD12	1.76	0.68
1:H:159:MET:O	1:H:163:ASN:HB2	1.93	0.68
1:C:453:TYR:OH	3:C:602:GDU:O3A	2.10	0.68
1:G:245:VAL:O	1:G:278:MET:HA	1.93	0.68
1:B:40:ASN:O	1:B:236:PHE:HB3	1.94	0.68
1:E:27:ASN:HB2	1:E:34:TRP:CZ2	2.29	0.68
1:A:18:THR:OG1	1:A:461:SER:HB3	1.94	0.68
1:D:455:VAL:O	1:D:460:HIS:HB3	1.93	0.68
1:E:93:SER:OG	1:E:315:TRP:NE1	2.27	0.68
1:H:60:VAL:O	1:H:63:HIS:NE2	2.27	0.68
1:H:68:HIS:O	1:H:492:ASN:ND2	2.27	0.68
1:B:462:PHE:O	1:B:466:VAL:HG23	1.94	0.67
1:D:54:GLU:HB3	1:D:346:LEU:HD11	1.76	0.67
1:F:71:TYR:O	1:F:74:ASP:HB2	1.93	0.67
1:F:431:THR:O	1:F:435:PRO:HG2	1.94	0.67
1:H:281:GLN:OE1	1:H:281:GLN:HA	1.93	0.67
1:E:12:VAL:HB	1:E:36:ILE:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:GLY:HA3	2:E:601:FAD:O1P	1.94	0.67
1:B:271:VAL:HA	1:B:274:LEU:HB2	1.77	0.67
1:B:421:THR:HG22	1:B:423:THR:HG23	1.76	0.67
1:C:103:PRO:HB2	1:C:109:ASN:ND2	2.10	0.67
1:E:437:LEU:HB3	1:E:442:ILE:HB	1.75	0.67
1:B:142:PHE:O	1:B:146:ILE:HG13	1.94	0.67
1:G:445:ARG:NH1	1:G:481:LEU:HD22	2.10	0.67
1:H:447:ARG:O	1:H:451:TRP:HA	1.95	0.67
1:A:136:ASN:OD1	1:A:137:THR:HG23	1.95	0.67
1:B:107:GLN:NE2	3:B:602:GDU:O4	2.27	0.67
1:D:63:HIS:CD2	2:D:601:FAD:C5X	2.78	0.67
1:D:91:ARG:NH1	1:D:205:GLY:HA3	2.09	0.67
1:D:115:LYS:HB3	1:F:197:LEU:HD23	1.77	0.67
1:F:122:ILE:HG23	1:F:126:ILE:HD11	1.76	0.67
1:F:336:PRO:HG2	1:F:337:TYR:CD1	2.30	0.67
1:G:204:TRP:HB3	1:G:208:ALA:HB2	1.76	0.67
1:G:353:ASP:HB3	1:G:403:PRO:HB3	1.77	0.67
1:B:159:MET:CE	3:B:602:GDU:HN3	2.08	0.67
1:B:398:THR:HG22	1:B:398:THR:O	1.93	0.67
1:H:297:VAL:HB	1:H:415:PHE:HE2	1.59	0.67
1:A:358:GLN:OE1	1:A:358:GLN:N	2.28	0.67
1:B:43:PRO:HG2	1:B:223:ILE:HD13	1.77	0.67
1:B:308:GLU:CD	1:B:308:GLU:H	2.03	0.67
1:E:179:LEU:N	1:E:179:LEU:HD23	2.09	0.67
1:G:402:LYS:NZ	1:G:405:ASP:OD1	2.26	0.67
1:B:91:ARG:NH2	1:B:204:TRP:O	2.28	0.67
1:C:108:ASN:OD1	1:C:108:ASN:N	2.21	0.67
1:A:58:TYR:HA	1:A:331:PHE:HE2	1.59	0.67
1:G:155:ALA:O	1:G:160:ARG:HG3	1.95	0.67
1:H:392:ILE:O	1:H:395:LEU:HB2	1.95	0.67
1:E:187:ASN:OD1	1:E:189:LYS:HB2	1.95	0.67
1:F:184:ALA:HA	1:F:204:TRP:CZ2	2.29	0.67
1:E:17:PRO:O	1:E:462:PHE:HA	1.95	0.66
1:F:104:TYR:CE1	3:F:602:GDU:O4	2.48	0.66
1:F:12:VAL:HB	1:F:36:ILE:HG13	1.76	0.66
1:F:91:ARG:HG3	1:F:315:TRP:CH2	2.29	0.66
1:F:142:PHE:O	1:F:145:TRP:HB3	1.95	0.66
1:B:119:VAL:HG22	1:H:193:THR:HG22	1.76	0.66
1:H:57:LEU:CD1	1:H:338:ASN:HA	2.25	0.66
1:A:45:GLY:HA3	2:A:601:FAD:O1A	1.96	0.66
1:A:54:GLU:HB3	1:A:346:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ALA:O	1:E:433:ILE:HG13	1.95	0.66
1:D:63:HIS:HD2	2:D:601:FAD:C5X	2.08	0.66
1:F:281:GLN:HA	1:F:281:GLN:OE1	1.96	0.66
1:H:204:TRP:HA	1:H:204:TRP:CE3	2.29	0.66
1:C:176:CYS:O	1:C:179:LEU:HD12	1.96	0.66
1:D:46:LEU:HG	2:D:601:FAD:O1A	1.95	0.66
1:E:353:ASP:HB3	1:E:403:PRO:HB2	1.77	0.66
1:E:457:ASN:HB3	2:E:601:FAD:O2	1.94	0.66
1:G:306:ARG:HH11	1:G:312:ASP:HA	1.61	0.66
1:G:149:MET:O	1:G:186:PRO:HB3	1.95	0.66
1:G:432:GLN:O	1:G:436:LYS:HG2	1.96	0.66
1:D:271:VAL:HG12	1:D:448:PHE:O	1.95	0.66
1:E:430:LEU:HD22	1:E:434:LEU:HG	1.77	0.66
1:G:308:GLU:HG3	1:G:309:ARG:HD3	1.78	0.66
1:H:47:ALA:HB2	2:H:601:FAD:H4'	1.78	0.66
1:H:173:LYS:HD2	1:H:379:MET:HE1	1.77	0.66
1:G:254:LEU:HG	1:G:258:THR:HG22	1.78	0.66
1:G:446:GLY:H	1:G:450:SER:HB3	1.60	0.66
1:H:9:ASP:HA	1:H:263:LYS:HD3	1.78	0.66
1:H:306:ARG:HD2	1:H:311:GLY:O	1.94	0.66
1:C:58:TYR:HA	1:C:331:PHE:HE2	1.59	0.66
1:D:458:GLN:HA	2:D:601:FAD:O3'	1.97	0.66
1:G:58:TYR:CE2	1:G:299:GLY:HA3	2.31	0.66
1:G:345:LYS:HD3	1:G:364:GLU:HG2	1.77	0.66
1:B:455:VAL:O	1:B:460:HIS:HB3	1.95	0.65
1:E:326:TYR:CD2	1:E:374:VAL:HA	2.31	0.65
1:E:349:MET:N	1:E:407:ILE:O	2.27	0.65
1:F:383:ASN:HB3	1:F:386:THR:OG1	1.96	0.65
1:B:19:GLY:N	1:B:268:THR:HG21	2.11	0.65
1:B:108:ASN:ND2	1:B:201:ALA:HB3	2.11	0.65
1:E:137:THR:O	1:E:148:ARG:NH1	2.28	0.65
1:E:336:PRO:HG2	1:E:337:TYR:CD1	2.31	0.65
1:A:91:ARG:NH1	1:A:205:GLY:HA3	2.11	0.65
1:G:124:GLY:C	1:G:151:GLY:HA3	2.20	0.65
1:F:463:MET:HE1	1:F:495:ARG:HH11	1.60	0.65
1:H:139:PRO:HB2	1:H:176:CYS:SG	2.36	0.65
1:H:325:PHE:CD2	1:H:372:LEU:HD22	2.31	0.65
1:G:162:TYR:CZ	1:G:166:VAL:HG11	2.31	0.65
1:F:413:ARG:HD3	1:F:415:PHE:CE2	2.31	0.65
1:B:411:TYR:C	1:B:411:TYR:CD2	2.75	0.65
1:H:346:LEU:HD23	1:H:347:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:TYR:CD2	1:H:495:ARG:HG2	2.32	0.65
1:A:336:PRO:HG2	1:A:337:TYR:CE1	2.31	0.65
1:B:69:TYR:CG	1:B:463:MET:HG3	2.32	0.65
1:E:51:VAL:HA	1:E:56:PHE:O	1.97	0.65
1:F:331:PHE:CE2	1:F:338:ASN:ND2	2.65	0.65
1:F:429:ALA:O	1:F:433:ILE:HG13	1.97	0.65
1:H:245:VAL:O	1:H:278:MET:HA	1.97	0.65
1:C:411:TYR:C	1:C:411:TYR:CD2	2.74	0.64
1:F:440:LYS:HB2	1:F:442:ILE:HD12	1.79	0.64
1:H:29:ILE:HG22	1:H:31:GLY:N	2.12	0.64
1:C:40:ASN:O	1:C:236:PHE:HB3	1.97	0.64
1:D:232:GLU:H	1:D:232:GLU:CD	2.04	0.64
1:A:411:TYR:C	1:A:411:TYR:CD2	2.76	0.64
1:D:47:ALA:HB1	1:D:222:TRP:HE1	1.63	0.64
1:D:136:ASN:OD1	1:D:137:THR:HG23	1.98	0.64
1:E:368:TRP:CZ3	1:E:370:ILE:HD11	2.32	0.64
1:F:51:VAL:HA	1:F:56:PHE:O	1.96	0.64
1:H:348:THR:O	1:H:357:PRO:HG3	1.96	0.64
1:C:144:GLU:O	1:C:148:ARG:HG3	1.98	0.64
1:D:108:ASN:OD1	1:D:108:ASN:N	2.20	0.64
1:F:326:TYR:CD2	1:F:374:VAL:HA	2.32	0.64
1:C:150:MET:HE3	1:C:159:MET:HG3	1.79	0.64
1:D:398:THR:HB	1:D:400:MET:CG	2.28	0.64
1:H:21:GLY:HA2	1:H:462:PHE:CE1	2.32	0.64
1:D:411:TYR:C	1:D:411:TYR:CD2	2.75	0.64
1:C:43:PRO:HG2	1:C:223:ILE:HD13	1.80	0.64
1:C:119:VAL:HA	1:E:196:ILE:HD13	1.78	0.64
1:D:69:TYR:CG	1:D:463:MET:HG3	2.33	0.64
1:F:179:LEU:N	1:F:179:LEU:HD23	2.12	0.64
1:G:44:GLY:HA3	1:G:222:TRP:CD1	2.33	0.64
1:C:91:ARG:HH12	1:C:205:GLY:HA3	1.61	0.64
1:E:175:GLN:NE2	1:E:177:ALA:H	1.94	0.64
1:E:184:ALA:HA	1:E:204:TRP:CZ2	2.32	0.64
1:F:18:THR:OG1	1:F:461:SER:HB3	1.97	0.64
1:H:251:THR:HA	1:H:260:ILE:O	1.98	0.64
1:H:484:PRO:O	1:H:488:ASN:HB2	1.96	0.64
1:A:197:LEU:HD23	1:G:115:LYS:HD3	1.80	0.64
1:C:69:TYR:CG	1:C:463:MET:HG3	2.33	0.64
1:F:17:PRO:HD2	2:F:601:FAD:O5'	1.98	0.64
1:G:91:ARG:HH21	1:G:203:ASN:CA	2.11	0.64
1:C:271:VAL:HG12	1:C:448:PHE:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LYS:O	1:E:119:VAL:HG23	1.97	0.64
1:G:71:TYR:CD2	1:G:495:ARG:HG2	2.33	0.64
1:A:125:MET:HE2	1:A:188:LEU:HA	1.80	0.63
1:A:325:PHE:HA	1:A:374:VAL:HG22	1.80	0.63
1:B:11:LEU:O	1:B:265:LEU:HD12	1.99	0.63
1:F:184:ALA:HB2	1:F:204:TRP:CD2	2.32	0.63
1:G:484:PRO:O	1:G:488:ASN:HB2	1.97	0.63
1:F:56:PHE:HE1	1:F:339:GLN:HB3	1.62	0.63
1:F:457:ASN:HB3	2:F:601:FAD:C2	2.28	0.63
1:G:58:TYR:HD2	1:G:411:TYR:HD2	1.46	0.63
1:H:268:THR:HA	1:H:445:ARG:O	1.98	0.63
1:B:104:TYR:HE1	3:B:602:GDU:H5	1.62	0.63
1:B:504:PHE:HZ	1:F:264:LYS:HG2	1.63	0.63
1:D:301:GLY:HA3	1:D:409:SER:HB3	1.80	0.63
1:E:413:ARG:HD3	1:E:415:PHE:CE2	2.32	0.63
1:G:44:GLY:CA	1:G:222:TRP:CD1	2.81	0.63
1:H:336:PRO:HG2	1:H:337:TYR:CE1	2.33	0.63
1:E:326:TYR:H	1:E:374:VAL:HG13	1.64	0.63
1:H:142:PHE:HB3	1:H:171:THR:O	1.98	0.63
1:B:58:TYR:HA	1:B:331:PHE:HE2	1.63	0.63
1:G:103:PRO:HB2	1:G:109:ASN:ND2	2.14	0.63
1:H:171:THR:HA	1:H:174:MET:HE3	1.80	0.63
1:A:69:TYR:CG	1:A:463:MET:HG3	2.34	0.63
1:B:125:MET:HE1	1:B:186:PRO:HB2	1.79	0.63
1:B:486:PHE:HE1	1:F:483:TYR:CD1	2.16	0.63
1:D:19:GLY:N	1:D:268:THR:HG21	2.13	0.63
1:E:16:GLY:HA3	2:E:601:FAD:O5B	1.98	0.63
1:F:97:CYS:SG	1:F:98:GLN:HG3	2.38	0.63
1:G:326:TYR:CE2	1:G:375:SER:HB3	2.32	0.63
1:H:326:TYR:HE2	1:H:375:SER:N	1.96	0.63
1:A:176:CYS:O	1:A:179:LEU:HD12	1.98	0.63
1:C:103:PRO:O	1:C:109:ASN:ND2	2.26	0.63
1:C:308:GLU:H	1:C:308:GLU:CD	2.06	0.63
1:F:63:HIS:CD2	1:F:63:HIS:N	2.66	0.63
1:F:142:PHE:O	1:F:146:ILE:HG13	1.99	0.63
1:G:107:GLN:CD	1:G:107:GLN:H	2.06	0.63
1:G:411:TYR:C	1:G:411:TYR:CD1	2.75	0.63
1:C:17:PRO:HD2	2:C:601:FAD:O5'	1.98	0.63
1:C:232:GLU:CD	1:C:232:GLU:H	2.07	0.63
1:E:348:THR:OG1	1:E:406:GLU:HB3	1.99	0.63
1:H:322:ASN:HD22	1:H:397:ASN:HB3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:ASP:HA	1:F:146:ILE:HD12	1.80	0.62
1:G:11:LEU:HD21	1:G:252:VAL:HG11	1.80	0.62
1:H:124:GLY:C	1:H:151:GLY:HA3	2.22	0.62
1:E:133:ARG:HH11	1:E:133:ARG:CG	2.06	0.62
1:F:348:THR:OG1	1:F:406:GLU:HB3	1.99	0.62
1:G:18:THR:CG2	1:G:268:THR:HG22	2.29	0.62
1:G:91:ARG:NH2	1:G:203:ASN:HA	2.14	0.62
1:H:336:PRO:HG2	1:H:337:TYR:CD1	2.33	0.62
1:C:411:TYR:C	1:C:411:TYR:HD2	2.07	0.62
1:F:353:ASP:HB3	1:F:403:PRO:HB2	1.81	0.62
1:G:68:HIS:O	1:G:492:ASN:ND2	2.32	0.62
1:G:393:GLN:OE1	1:G:393:GLN:HA	1.99	0.62
1:H:194:ASN:HD22	1:H:199:LYS:HB3	1.63	0.62
1:A:19:GLY:N	1:A:268:THR:HG21	2.14	0.62
1:A:301:GLY:HA3	1:A:409:SER:HB3	1.81	0.62
1:A:398:THR:HB	1:A:400:MET:CG	2.29	0.62
1:B:303:ARG:HH21	1:B:363:LYS:C	2.06	0.62
1:B:332:SER:CA	1:B:339:GLN:HE21	2.05	0.62
1:F:125:MET:HG2	1:F:188:LEU:HD13	1.80	0.62
1:F:326:TYR:H	1:F:374:VAL:HG13	1.65	0.62
1:G:254:LEU:HG	1:G:258:THR:CG2	2.30	0.62
1:A:309:ARG:HG3	1:A:310:ILE:HG13	1.80	0.62
1:B:103:PRO:O	1:B:109:ASN:ND2	2.31	0.62
1:B:398:THR:CG2	1:B:400:MET:HG2	2.30	0.62
1:C:398:THR:O	1:C:398:THR:CG2	2.47	0.62
1:E:271:VAL:HG13	1:E:287:THR:HG22	1.81	0.62
1:F:22:ALA:HA	1:F:469:VAL:HG22	1.80	0.62
1:G:395:LEU:HD23	1:G:400:MET:HG3	1.82	0.62
1:G:430:LEU:HD12	1:G:452:ARG:HE	1.65	0.62
1:H:103:PRO:HB2	1:H:109:ASN:ND2	2.14	0.62
1:A:142:PHE:O	1:A:146:ILE:HG13	1.98	0.62
1:D:422:PRO:HA	1:D:426:ARG:HD3	1.82	0.62
1:E:25:ARG:HG2	1:E:469:VAL:HB	1.81	0.62
1:H:69:TYR:OH	1:H:487:VAL:HB	1.99	0.62
1:B:411:TYR:C	1:B:411:TYR:HD2	2.07	0.62
1:G:336:PRO:HG2	1:G:337:TYR:CD1	2.35	0.62
1:H:25:ARG:HH11	1:H:470:ASP:CG	2.07	0.62
1:C:38:ASP:OD2	1:C:40:ASN:HB2	2.00	0.62
1:F:17:PRO:O	1:F:462:PHE:HA	1.99	0.62
1:G:482:ASN:HB2	1:G:483:TYR:CE2	2.35	0.62
1:E:440:LYS:HB2	1:E:442:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:ASP:HA	1:H:146:ILE:HD12	1.82	0.62
1:C:91:ARG:NH1	1:C:205:GLY:HA3	2.15	0.61
1:C:490:ARG:NH2	1:G:483:TYR:OH	2.27	0.61
1:F:402:LYS:O	1:F:405:ASP:HB2	2.00	0.61
1:G:326:TYR:HE2	1:G:375:SER:N	1.98	0.61
1:H:154:ILE:H	1:H:154:ILE:HD12	1.63	0.61
1:A:108:ASN:OD1	1:A:108:ASN:N	2.20	0.61
1:B:271:VAL:HG12	1:B:448:PHE:O	2.00	0.61
1:E:178:TRP:CB	1:E:454:GLU:HG3	2.30	0.61
1:F:115:LYS:O	1:F:119:VAL:HG23	1.99	0.61
1:F:367:TYR:CE1	1:F:408:VAL:HG21	2.35	0.61
1:G:323:CYS:HB2	1:G:325:PHE:CZ	2.35	0.61
1:A:107:GLN:O	1:A:110:ILE:HG13	2.00	0.61
1:B:296:HIS:CE1	1:B:382:VAL:HG21	2.34	0.61
1:C:296:HIS:CE1	1:C:382:VAL:HG21	2.36	0.61
1:E:461:SER:HA	1:E:464:LEU:CD1	2.24	0.61
1:H:432:GLN:O	1:H:436:LYS:HG2	2.00	0.61
1:C:336:PRO:HG2	1:C:337:TYR:CE1	2.34	0.61
1:E:178:TRP:CE3	1:E:179:LEU:HD22	2.36	0.61
1:G:222:TRP:HA	1:G:222:TRP:HE3	1.65	0.61
1:G:268:THR:HA	1:G:445:ARG:O	1.99	0.61
1:G:367:TYR:HD1	1:G:408:VAL:HG21	1.65	0.61
1:H:58:TYR:CE2	1:H:299:GLY:HA3	2.36	0.61
1:H:212:PHE:CD2	1:H:213:PRO:HD2	2.35	0.61
1:H:443:TRP:HB3	1:H:445:ARG:HE	1.65	0.61
1:E:169:VAL:HG23	1:E:170:PRO:O	2.01	0.61
1:F:271:VAL:HG13	1:F:287:THR:HG22	1.83	0.61
1:G:47:ALA:CB	1:G:222:TRP:HE1	2.11	0.61
1:G:60:VAL:O	1:G:60:VAL:HG12	2.01	0.61
1:A:40:ASN:O	1:A:236:PHE:HB3	2.01	0.61
1:A:411:TYR:C	1:A:411:TYR:HD2	2.08	0.61
1:C:271:VAL:HA	1:C:274:LEU:HB2	1.82	0.61
1:F:147:VAL:HG22	1:F:160:ARG:HH21	1.65	0.61
1:H:58:TYR:HD2	1:H:411:TYR:HD2	1.49	0.61
1:A:108:ASN:ND2	1:A:201:ALA:HB3	2.15	0.61
1:B:60:VAL:O	1:B:63:HIS:NE2	2.34	0.61
1:C:468:ALA:O	1:C:472:ILE:HG13	2.01	0.61
1:F:118:GLN:OE1	1:F:195:VAL:HG13	2.00	0.61
1:G:57:LEU:CD1	1:G:338:ASN:HA	2.30	0.61
1:H:70:LYS:HE2	1:H:496:ARG:NH1	2.16	0.61
1:H:430:LEU:HD12	1:H:452:ARG:HE	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLN:NE2	1:C:178:TRP:HD1	1.98	0.61
1:E:91:ARG:HG3	1:E:315:TRP:CH2	2.35	0.61
1:F:437:LEU:HB3	1:F:442:ILE:HB	1.81	0.61
1:G:222:TRP:HA	1:G:222:TRP:CE3	2.34	0.61
1:G:443:TRP:HB3	1:G:445:ARG:HE	1.66	0.61
1:G:492:ASN:ND2	1:G:492:ASN:N	2.49	0.61
1:H:411:TYR:CD1	1:H:411:TYR:C	2.77	0.61
1:H:446:GLY:N	1:H:450:SER:H	1.99	0.61
1:B:144:GLU:O	1:B:148:ARG:HG3	2.00	0.61
1:C:103:PRO:C	1:C:109:ASN:HD22	2.07	0.61
1:D:58:TYR:HA	1:D:331:PHE:HE2	1.66	0.61
1:E:91:ARG:CD	1:E:207:ASN:HB2	2.31	0.61
1:F:178:TRP:CB	1:F:454:GLU:HG3	2.30	0.61
1:G:297:VAL:HB	1:G:415:PHE:HE2	1.64	0.61
1:H:359:SER:HB3	1:H:363:LYS:CE	2.31	0.61
1:B:338:ASN:N	1:B:338:ASN:OD1	2.34	0.61
1:C:178:TRP:HB2	1:C:454:GLU:CG	2.30	0.61
1:D:308:GLU:H	1:D:308:GLU:CD	2.09	0.61
1:D:411:TYR:C	1:D:411:TYR:HD2	2.09	0.61
1:G:69:TYR:OH	1:G:487:VAL:HB	2.01	0.61
1:H:25:ARG:HD3	1:H:470:ASP:OD1	2.01	0.61
1:H:445:ARG:NH1	1:H:481:LEU:HD22	2.16	0.61
1:A:398:THR:HB	1:A:400:MET:HG3	1.82	0.60
1:C:60:VAL:O	1:C:63:HIS:NE2	2.34	0.60
1:E:125:MET:HG2	1:E:188:LEU:HD13	1.82	0.60
1:E:207:ASN:ND2	3:E:602:GDU:O4'	2.33	0.60
1:F:69:TYR:CZ	1:F:463:MET:HG3	2.36	0.60
1:G:115:LYS:O	1:G:118:GLN:HB2	2.01	0.60
1:G:457:ASN:HB3	1:G:459:ASP:OD1	2.00	0.60
1:H:150:MET:CG	1:H:154:ILE:HB	2.30	0.60
1:H:453:TYR:C	1:H:453:TYR:CD2	2.79	0.60
1:C:91:ARG:NH2	1:C:204:TRP:O	2.32	0.60
1:D:125:MET:HE1	1:D:186:PRO:HB2	1.81	0.60
1:D:245:VAL:HG22	1:D:252:VAL:HG23	1.81	0.60
1:F:159:MET:HE1	3:F:602:GDU:C6	2.30	0.60
1:G:478:GLU:HB2	1:G:481:LEU:HB3	1.83	0.60
1:D:108:ASN:ND2	1:D:201:ALA:HB3	2.16	0.60
1:G:338:ASN:HB2	1:G:339:GLN:HE22	1.66	0.60
1:A:308:GLU:H	1:A:308:GLU:CD	2.09	0.60
1:E:6:ILE:HG22	1:E:260:ILE:HG23	1.82	0.60
1:B:170:PRO:HG2	1:B:173:LYS:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:THR:HA	1:C:260:ILE:O	2.01	0.60
1:D:163:ASN:HA	1:D:166:VAL:HG12	1.83	0.60
1:E:145:TRP:CH2	1:E:183:VAL:HG21	2.36	0.60
1:F:145:TRP:CH2	1:F:183:VAL:HG21	2.36	0.60
1:H:467:GLU:CD	1:H:480:THR:H	2.10	0.60
1:D:18:THR:OG1	1:D:461:SER:HB3	2.01	0.60
1:D:107:GLN:O	1:D:110:ILE:HG13	2.01	0.60
1:D:176:CYS:O	1:D:179:LEU:HD12	2.01	0.60
1:E:122:ILE:HG23	1:E:126:ILE:HD11	1.83	0.60
1:E:183:VAL:HG11	3:E:602:GDU:O2	2.02	0.60
1:E:346:LEU:HD12	1:E:367:TYR:CZ	2.37	0.60
1:F:9:ASP:O	1:F:263:LYS:HB2	2.02	0.60
1:F:64:VAL:HB	3:F:602:GDU:O6'	2.02	0.60
1:F:265:LEU:HD23	1:F:442:ILE:HG12	1.82	0.60
1:G:336:PRO:HG2	1:G:337:TYR:CE1	2.36	0.60
1:H:203:ASN:O	1:H:204:TRP:HB2	2.01	0.60
1:F:322:ASN:ND2	1:F:398:THR:HG22	2.16	0.60
2:F:601:FAD:O4	3:F:602:GDU:H2'	2.02	0.60
1:G:158:PHE:C	1:G:158:PHE:CD1	2.80	0.60
1:G:168:ALA:HB1	1:G:377:SER:OG	2.02	0.60
1:C:504:PHE:HA	1:C:507:SER:HB3	1.84	0.60
1:E:27:ASN:OD1	1:E:27:ASN:C	2.44	0.60
1:H:47:ALA:CB	1:H:222:TRP:HE1	2.09	0.60
1:D:57:LEU:HD22	1:D:338:ASN:HA	1.84	0.60
1:D:187:ASN:C	1:D:187:ASN:OD1	2.44	0.60
1:G:325:PHE:CD2	1:G:372:LEU:HD22	2.37	0.60
1:H:162:TYR:CZ	1:H:166:VAL:HG11	2.36	0.60
1:H:457:ASN:HB3	1:H:459:ASP:OD1	2.02	0.60
1:B:91:ARG:NH1	1:B:205:GLY:HA3	2.17	0.60
1:F:471:ASN:ND2	1:F:476:ALA:O	2.25	0.60
1:G:53:PRO:HB2	1:G:54:GLU:OE2	2.02	0.60
1:G:274:LEU:O	1:G:278:MET:HG2	2.02	0.60
1:G:453:TYR:C	1:G:453:TYR:CD2	2.79	0.60
1:H:250:LYS:HB3	1:H:262:TYR:O	2.02	0.60
1:H:309:ARG:HG2	1:H:310:ILE:HD12	1.84	0.60
1:A:429:ALA:O	1:A:433:ILE:HD12	2.03	0.59
1:G:91:ARG:N	1:G:208:ALA:O	2.30	0.59
1:A:271:VAL:HA	1:A:274:LEU:HB2	1.83	0.59
1:D:125:MET:HE2	1:D:188:LEU:HA	1.84	0.59
1:E:322:ASN:ND2	1:E:398:THR:HG22	2.18	0.59
1:F:91:ARG:CD	1:F:207:ASN:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:454:GLU:H	1:F:454:GLU:CD	2.10	0.59
1:G:248:ASN:OD1	1:G:248:ASN:N	2.34	0.59
1:H:204:TRP:HA	1:H:204:TRP:HE3	1.66	0.59
1:H:395:LEU:HD23	1:H:400:MET:HG3	1.85	0.59
1:A:336:PRO:HG2	1:A:337:TYR:CD1	2.37	0.59
1:B:245:VAL:HG22	1:B:252:VAL:HG23	1.84	0.59
1:B:301:GLY:HA3	1:B:409:SER:HB3	1.85	0.59
1:C:242:VAL:HG23	2:C:601:FAD:N1A	2.16	0.59
1:E:402:LYS:O	1:E:405:ASP:HB2	2.02	0.59
1:G:158:PHE:C	1:G:158:PHE:HD1	2.10	0.59
1:G:170:PRO:HD2	1:G:379:MET:SD	2.42	0.59
1:H:207:ASN:C	1:H:207:ASN:OD1	2.45	0.59
1:D:43:PRO:HG2	1:D:223:ILE:HD13	1.84	0.59
1:D:143:ASP:HA	1:D:146:ILE:HD12	1.84	0.59
1:D:336:PRO:HG2	1:D:337:TYR:CE1	2.36	0.59
1:H:285:GLY:O	1:H:288:LYS:HB2	2.02	0.59
1:H:303:ARG:NH2	1:H:346:LEU:O	2.35	0.59
1:C:125:MET:HE2	1:C:188:LEU:HA	1.82	0.59
1:C:455:VAL:CG1	1:C:464:LEU:HD11	2.32	0.59
1:E:94:TYR:HB2	1:E:316:LEU:HD22	1.82	0.59
1:B:107:GLN:O	1:B:110:ILE:HG13	2.01	0.59
1:F:38:ASP:HB3	1:F:236:PHE:HD1	1.67	0.59
1:F:160:ARG:N	1:F:161:PRO:HD2	2.18	0.59
1:G:443:TRP:HA	1:G:445:ARG:HH21	1.68	0.59
1:H:70:LYS:HE2	1:H:496:ARG:HH12	1.67	0.59
1:C:346:LEU:HD23	1:C:347:PRO:HD2	1.85	0.59
1:F:350:GLN:O	1:F:407:ILE:HB	2.02	0.59
1:F:437:LEU:O	1:F:442:ILE:N	2.35	0.59
1:G:353:ASP:HB3	1:G:403:PRO:CB	2.32	0.59
1:A:32:PRO:HB3	1:E:504:PHE:CD2	2.37	0.59
1:B:54:GLU:HB3	1:B:346:LEU:HD11	1.84	0.59
1:B:422:PRO:HA	1:B:426:ARG:HD3	1.84	0.59
1:F:69:TYR:CE1	1:F:463:MET:HG3	2.37	0.59
1:F:154:ILE:H	1:F:154:ILE:CD1	1.99	0.59
1:H:383:ASN:HD22	1:H:386:THR:HG23	1.67	0.59
1:H:445:ARG:HA	1:H:450:SER:CB	2.32	0.59
1:B:57:LEU:H	1:B:57:LEU:HD13	1.67	0.59
1:B:463:MET:O	1:B:467:GLU:HG3	2.03	0.59
1:F:224:ALA:O	1:F:228:THR:HG23	2.03	0.59
1:G:25:ARG:HA	1:G:28:GLN:HB2	1.84	0.59
1:G:250:LYS:HB3	1:G:262:TYR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:471:ASN:HA	1:G:476:ALA:H	1.68	0.59
1:A:109:ASN:OD1	1:A:200:THR:HG22	2.03	0.59
1:B:429:ALA:O	1:B:433:ILE:HD12	2.03	0.59
1:F:69:TYR:HB2	1:F:72:PHE:HB3	1.85	0.59
1:G:23:ALA:HA	1:G:26:LEU:HD12	1.84	0.59
1:G:411:TYR:HD1	1:G:411:TYR:C	2.10	0.59
1:G:492:ASN:HD22	1:G:492:ASN:N	2.00	0.59
1:H:142:PHE:HA	1:H:176:CYS:HB3	1.85	0.59
1:A:126:ILE:HD12	1:G:189:LYS:HG2	1.84	0.58
1:B:383:ASN:O	1:B:387:ILE:HB	2.03	0.58
1:C:170:PRO:HG2	1:C:173:LYS:HG3	1.84	0.58
1:F:178:TRP:CE3	1:F:179:LEU:HD22	2.38	0.58
1:F:346:LEU:HD12	1:F:367:TYR:CZ	2.38	0.58
1:G:58:TYR:HE1	1:G:369:SER:OG	1.85	0.58
1:H:348:THR:HG21	1:H:406:GLU:HG2	1.83	0.58
1:A:95:VAL:HG23	1:A:102:VAL:O	2.02	0.58
1:B:309:ARG:HG3	1:B:310:ILE:HG13	1.86	0.58
1:E:97:CYS:SG	1:E:98:GLN:HG3	2.43	0.58
1:F:70:LYS:HB3	1:F:496:ARG:HH12	1.67	0.58
1:F:502:GLN:O	1:F:506:LYS:HD3	2.03	0.58
1:G:462:PHE:O	1:G:466:VAL:HG23	2.03	0.58
1:G:464:LEU:HG	1:G:480:THR:HB	1.85	0.58
1:H:341:GLU:HG3	1:H:343:SER:H	1.68	0.58
1:A:57:LEU:HD22	1:A:338:ASN:HA	1.85	0.58
1:H:418:GLY:C	1:H:419:TYR:CD1	2.75	0.58
1:A:178:TRP:HB2	1:A:454:GLU:CG	2.32	0.58
1:A:197:LEU:CD2	1:G:115:LYS:HD3	2.33	0.58
1:B:352:ALA:HB3	1:B:403:PRO:HA	1.86	0.58
1:D:16:GLY:H	2:D:601:FAD:H4B	1.68	0.58
1:D:107:GLN:CD	1:D:107:GLN:H	2.10	0.58
1:D:338:ASN:N	1:D:338:ASN:OD1	2.36	0.58
1:D:457:ASN:O	1:D:460:HIS:HB2	2.03	0.58
1:E:184:ALA:HB2	1:E:204:TRP:CD2	2.38	0.58
1:E:303:ARG:HH21	1:E:363:LYS:CB	2.17	0.58
1:F:463:MET:HE1	1:F:495:ARG:NH1	2.18	0.58
1:G:197:LEU:O	1:G:199:LYS:N	2.37	0.58
1:H:167:TRP:CB	1:H:174:MET:HE1	2.33	0.58
1:H:341:GLU:HG3	1:H:342:ALA:N	2.18	0.58
1:B:504:PHE:HA	1:B:507:SER:HB3	1.85	0.58
1:C:93:SER:HB2	1:C:104:TYR:HB3	1.83	0.58
1:C:182:ARG:HD2	3:C:602:GDU:O1A	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:OH	3:C:602:GDU:O2B	2.22	0.58
3:C:602:GDU:H5'2	3:C:602:GDU:O1B	2.04	0.58
1:E:207:ASN:HB3	1:E:315:TRP:CH2	2.39	0.58
1:G:367:TYR:HE1	1:G:408:VAL:HG11	1.68	0.58
1:H:11:LEU:O	1:H:265:LEU:HD12	2.04	0.58
1:H:44:GLY:HA3	1:H:222:TRP:CD1	2.38	0.58
1:A:303:ARG:NH1	1:A:348:THR:OG1	2.37	0.58
1:C:16:GLY:H	2:C:601:FAD:H52A	1.68	0.58
1:C:103:PRO:CB	1:C:109:ASN:ND2	2.66	0.58
1:E:163:ASN:HA	1:E:166:VAL:HG13	1.85	0.58
1:E:383:ASN:HB3	1:E:386:THR:HG1	1.69	0.58
1:F:94:TYR:HB2	1:F:316:LEU:HD22	1.84	0.58
1:F:122:ILE:HG22	1:F:123:ASP:N	2.17	0.58
1:F:167:TRP:CG	1:F:174:MET:HE1	2.38	0.58
1:H:103:PRO:CB	1:H:202:GLY:HA2	2.33	0.58
1:A:416:ASP:HB2	1:F:281:GLN:NE2	2.19	0.58
1:C:113:LEU:O	1:C:118:GLN:NE2	2.29	0.58
1:C:245:VAL:HG22	1:C:252:VAL:HG23	1.85	0.58
1:C:301:GLY:HA3	1:C:409:SER:HB3	1.85	0.58
1:E:160:ARG:N	1:E:161:PRO:HD2	2.18	0.58
1:E:248:ASN:OD1	1:E:248:ASN:N	2.37	0.58
1:H:44:GLY:CA	1:H:222:TRP:CD1	2.86	0.58
1:H:85:ASP:HA	1:H:214:ALA:HB2	1.86	0.58
1:H:158:PHE:CD1	1:H:158:PHE:C	2.82	0.58
1:H:331:PHE:CD2	1:H:338:ASN:HB3	2.39	0.58
1:H:433:ILE:O	1:H:436:LYS:HB2	2.03	0.58
1:B:20:LEU:HD23	1:B:20:LEU:N	2.19	0.58
1:C:54:GLU:HB3	1:C:346:LEU:HD11	1.86	0.58
1:C:136:ASN:OD1	1:C:136:ASN:N	2.35	0.58
1:D:91:ARG:HD3	1:D:207:ASN:CB	2.34	0.58
1:E:26:LEU:HD13	1:E:34:TRP:HB2	1.86	0.58
1:C:11:LEU:O	1:C:265:LEU:HD12	2.04	0.58
1:C:455:VAL:HG21	1:C:480:THR:O	2.04	0.58
1:C:499:ASP:O	1:C:503:VAL:HG23	2.04	0.58
1:D:60:VAL:O	1:D:63:HIS:NE2	2.37	0.58
1:D:325:PHE:HA	1:D:374:VAL:HG22	1.85	0.58
1:E:103:PRO:HB2	1:E:109:ASN:OD1	2.04	0.58
1:E:137:THR:C	1:E:148:ARG:HH12	2.11	0.58
1:G:467:GLU:CD	1:G:480:THR:H	2.12	0.58
1:A:47:ALA:HB1	1:A:222:TRP:HE1	1.69	0.57
1:A:143:ASP:O	1:A:147:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PRO:HG2	1:A:173:LYS:HG3	1.86	0.57
1:A:350:GLN:NE2	1:A:354:GLY:HA2	2.16	0.57
1:D:455:VAL:CG1	1:D:464:LEU:HD11	2.33	0.57
1:D:466:VAL:HG12	1:D:495:ARG:NH1	2.19	0.57
1:E:64:VAL:HG22	1:E:210:PHE:CE1	2.39	0.57
1:E:351:LEU:HA	1:E:405:ASP:O	2.04	0.57
2:E:601:FAD:O4	3:E:602:GDU:H2'	2.04	0.57
1:G:446:GLY:N	1:G:450:SER:H	2.01	0.57
1:B:163:ASN:HA	1:B:166:VAL:HG12	1.86	0.57
1:C:463:MET:O	1:C:467:GLU:HG3	2.04	0.57
1:D:309:ARG:HG3	1:D:310:ILE:HG13	1.85	0.57
1:G:303:ARG:HH12	1:G:348:THR:HG1	1.51	0.57
1:H:89:HIS:HB2	1:H:210:PHE:CE2	2.39	0.57
1:H:149:MET:SD	1:H:184:ALA:CA	2.86	0.57
1:H:249:ASN:OD1	1:H:249:ASN:N	2.37	0.57
1:G:285:GLY:O	1:G:288:LYS:HB2	2.05	0.57
1:G:383:ASN:HD22	1:G:386:THR:HG23	1.69	0.57
1:H:189:LYS:O	1:H:193:THR:OG1	2.21	0.57
1:A:271:VAL:HG12	1:A:448:PHE:O	2.04	0.57
1:C:111:SER:HB2	1:C:112:MET:HE3	1.87	0.57
1:C:309:ARG:HG3	1:C:310:ILE:HG13	1.87	0.57
1:G:467:GLU:OE1	1:G:480:THR:N	2.24	0.57
1:H:248:ASN:OD1	1:H:248:ASN:N	2.37	0.57
1:B:47:ALA:HB1	1:B:222:TRP:NE1	2.19	0.57
1:C:107:GLN:O	1:C:110:ILE:HG13	2.04	0.57
1:D:142:PHE:O	1:D:146:ILE:HG13	2.05	0.57
1:D:483:TYR:OH	1:H:490:ARG:NH2	2.22	0.57
1:E:10:VAL:HG22	1:E:264:LYS:HG3	1.86	0.57
1:E:69:TYR:CZ	1:E:463:MET:HG3	2.39	0.57
1:E:263:LYS:HD2	1:E:263:LYS:N	2.19	0.57
1:E:303:ARG:NH2	1:E:363:LYS:CG	2.67	0.57
1:F:445:ARG:CZ	1:F:481:LEU:HD22	2.34	0.57
1:H:158:PHE:HE1	1:H:162:TYR:CG	2.22	0.57
1:H:222:TRP:HA	1:H:222:TRP:CE3	2.39	0.57
1:H:344:LYS:O	1:H:367:TYR:OH	2.22	0.57
1:H:411:TYR:HD1	1:H:411:TYR:C	2.11	0.57
1:H:492:ASN:HD22	1:H:492:ASN:H	1.52	0.57
1:A:20:LEU:N	1:A:20:LEU:HD23	2.19	0.57
1:A:338:ASN:N	1:A:338:ASN:OD1	2.37	0.57
1:B:109:ASN:OD1	1:B:200:THR:HG22	2.04	0.57
1:B:175:GLN:NE2	1:B:178:TRP:HD1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:HD13	1:C:338:ASN:O	2.03	0.57
1:C:196:ILE:HG21	1:E:119:VAL:HG23	1.84	0.57
1:D:199:LYS:HD2	1:D:200:THR:O	2.04	0.57
1:E:167:TRP:CE3	1:E:421:THR:HG22	2.39	0.57
1:F:154:ILE:HD13	1:F:154:ILE:N	2.12	0.57
1:F:368:TRP:CZ3	1:F:370:ILE:HD11	2.40	0.57
1:H:28:GLN:HG2	1:H:497:LEU:O	2.05	0.57
1:D:458:GLN:CG	2:D:601:FAD:H2'	2.34	0.57
1:E:71:TYR:CD2	1:E:496:ARG:HA	2.39	0.57
1:F:150:MET:HG3	1:F:154:ILE:HB	1.85	0.57
1:F:167:TRP:CE3	1:F:421:THR:HG22	2.39	0.57
1:H:17:PRO:HD2	2:H:601:FAD:O5'	2.03	0.57
1:H:25:ARG:NH1	1:H:470:ASP:OD1	2.25	0.57
1:H:91:ARG:N	1:H:208:ALA:O	2.30	0.57
1:A:183:VAL:HG13	3:A:602:GDU:C2	2.32	0.57
1:A:306:ARG:CZ	1:A:311:GLY:HA2	2.34	0.57
1:C:47:ALA:HB1	1:C:222:TRP:NE1	2.19	0.57
1:C:58:TYR:HA	1:C:331:PHE:CE2	2.40	0.57
1:D:429:ALA:O	1:D:433:ILE:HD12	2.04	0.57
1:E:143:ASP:O	1:E:147:VAL:HG23	2.04	0.57
1:F:19:GLY:O	1:F:22:ALA:HB3	2.05	0.57
1:F:26:LEU:HD13	1:F:34:TRP:HB2	1.87	0.57
1:G:11:LEU:O	1:G:265:LEU:HD12	2.05	0.57
1:G:103:PRO:CB	1:G:202:GLY:HA3	2.34	0.57
1:G:292:TYR:CE1	1:G:417:HIS:ND1	2.70	0.57
1:G:438:GLN:HA	1:G:442:ILE:O	2.05	0.57
1:E:502:GLN:O	1:E:506:LYS:HD3	2.03	0.57
1:F:6:ILE:HG22	1:F:260:ILE:HG23	1.87	0.57
1:F:72:PHE:CZ	1:F:76:LEU:HD11	2.40	0.57
1:A:175:GLN:NE2	1:A:178:TRP:HD1	2.03	0.57
1:B:136:ASN:OD1	1:B:136:ASN:N	2.32	0.57
1:B:136:ASN:OD1	1:B:137:THR:HG23	2.05	0.57
1:E:323:CYS:HB2	1:E:324:PRO:HD2	1.86	0.57
1:D:344:LYS:HD2	1:D:345:LYS:N	2.20	0.56
1:E:104:TYR:HE1	3:E:602:GDU:C4	2.18	0.56
1:E:325:PHE:HA	1:E:374:VAL:CG1	2.35	0.56
1:F:9:ASP:N	1:F:33:SER:OG	2.28	0.56
1:F:303:ARG:HH21	1:F:363:LYS:C	2.13	0.56
1:F:467:GLU:CG	1:F:495:ARG:HH12	2.12	0.56
1:H:58:TYR:HE1	1:H:369:SER:OG	1.88	0.56
1:H:455:VAL:O	1:H:460:HIS:CB	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:CG1	1:B:464:LEU:HD11	2.35	0.56
1:B:456:GLY:O	2:B:601:FAD:O3'	2.22	0.56
1:E:326:TYR:OH	1:E:373:GLU:OE2	2.23	0.56
1:F:335:SER:HB3	1:F:338:ASN:OD1	2.05	0.56
1:G:162:TYR:O	1:G:165:LYS:N	2.38	0.56
1:G:458:GLN:HG2	2:G:601:FAD:H2'	1.86	0.56
1:H:162:TYR:O	1:H:165:LYS:N	2.37	0.56
1:H:480:THR:HA	1:H:487:VAL:HG21	1.87	0.56
1:A:134:VAL:O	1:A:134:VAL:CG1	2.53	0.56
1:A:163:ASN:HA	1:A:166:VAL:HG12	1.87	0.56
1:A:212:PHE:CG	1:A:213:PRO:HD2	2.40	0.56
1:A:388:LEU:O	1:A:392:ILE:HG13	2.04	0.56
1:B:163:ASN:HA	1:B:166:VAL:CG1	2.35	0.56
1:C:352:ALA:HB3	1:C:403:PRO:HA	1.87	0.56
1:F:427:GLU:O	1:F:431:THR:HG23	2.05	0.56
1:H:13:ILE:HD12	1:H:265:LEU:HD11	1.88	0.56
1:H:58:TYR:HD2	1:H:411:TYR:CD2	2.22	0.56
1:H:141:THR:OG1	1:H:144:GLU:HB2	2.05	0.56
1:H:353:ASP:HB3	1:H:403:PRO:HB3	1.87	0.56
1:H:462:PHE:O	1:H:466:VAL:HG23	2.05	0.56
1:A:91:ARG:HD3	1:A:207:ASN:CB	2.34	0.56
1:E:21:GLY:HA2	1:E:462:PHE:CE1	2.41	0.56
1:E:151:GLY:O	1:E:154:ILE:HG12	2.05	0.56
1:G:38:ASP:OD1	2:G:601:FAD:O3B	2.23	0.56
1:G:402:LYS:HD3	1:G:405:ASP:OD2	2.04	0.56
1:H:306:ARG:HH11	1:H:312:ASP:HA	1.68	0.56
1:B:183:VAL:CG2	3:B:602:GDU:H1D	2.24	0.56
1:B:466:VAL:HG12	1:B:495:ARG:NH1	2.20	0.56
1:C:422:PRO:HA	1:C:426:ARG:HD3	1.86	0.56
1:D:457:ASN:HA	2:D:601:FAD:H1'2	1.88	0.56
1:F:6:ILE:O	1:F:260:ILE:HA	2.05	0.56
1:F:169:VAL:HG23	1:F:170:PRO:O	2.05	0.56
1:A:64:VAL:HG13	1:A:210:PHE:CD1	2.41	0.56
1:A:433:ILE:O	1:A:436:LYS:HB2	2.05	0.56
1:B:125:MET:HE2	1:B:188:LEU:HA	1.86	0.56
1:B:139:PRO:HB2	1:B:176:CYS:SG	2.46	0.56
1:B:232:GLU:H	1:B:232:GLU:CD	2.13	0.56
1:C:38:ASP:HA	2:C:601:FAD:H2A	1.87	0.56
1:D:144:GLU:O	1:D:148:ARG:HG3	2.05	0.56
1:E:27:ASN:HB2	1:E:34:TRP:HZ2	1.70	0.56
1:E:72:PHE:CZ	1:E:76:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:VAL:HG22	1:E:160:ARG:HH21	1.71	0.56
1:F:17:PRO:O	1:F:462:PHE:HD1	1.88	0.56
1:F:64:VAL:HG22	1:F:210:PHE:CE1	2.41	0.56
1:F:303:ARG:NH2	1:F:363:LYS:HB2	2.19	0.56
1:G:204:TRP:CE3	1:G:204:TRP:HA	2.39	0.56
1:G:250:LYS:O	1:G:261:GLY:HA2	2.06	0.56
1:B:336:PRO:HG2	1:B:337:TYR:CE1	2.41	0.56
1:D:93:SER:HB2	1:D:104:TYR:HB3	1.88	0.56
1:F:101:TRP:HZ3	1:F:316:LEU:HD13	1.71	0.56
1:F:353:ASP:HB3	1:F:403:PRO:HB3	1.87	0.56
1:A:143:ASP:HA	1:A:146:ILE:HD12	1.88	0.56
1:B:18:THR:OG1	1:B:461:SER:HB3	2.05	0.56
1:B:143:ASP:HA	1:B:146:ILE:HD12	1.87	0.56
1:C:160:ARG:N	1:C:161:PRO:HD2	2.21	0.56
1:C:163:ASN:HA	1:C:166:VAL:CG1	2.35	0.56
1:C:346:LEU:HD23	1:C:347:PRO:CD	2.36	0.56
1:E:367:TYR:CE1	1:E:408:VAL:HG21	2.40	0.56
1:E:424:LEU:HB2	1:E:425:GLU:OE1	2.06	0.56
1:E:460:HIS:O	1:E:463:MET:HB2	2.05	0.56
1:F:109:ASN:HD22	1:F:109:ASN:H	1.54	0.56
1:F:270:ALA:HB3	1:F:273:PHE:CD2	2.41	0.56
1:A:398:THR:HG22	1:A:398:THR:O	2.05	0.56
1:B:93:SER:HB2	1:B:104:TYR:HB3	1.86	0.56
1:B:504:PHE:HZ	1:F:264:LYS:CG	2.20	0.56
1:D:20:LEU:N	1:D:20:LEU:HD23	2.20	0.56
1:F:47:ALA:HB1	1:F:222:TRP:NE1	2.21	0.56
1:F:163:ASN:HA	1:F:166:VAL:HG13	1.88	0.56
1:A:105:PRO:O	1:A:109:ASN:ND2	2.38	0.55
1:A:352:ALA:HB3	1:A:403:PRO:HA	1.87	0.55
1:D:64:VAL:HG13	1:D:210:PHE:CD1	2.40	0.55
1:E:69:TYR:CE1	1:E:463:MET:HG3	2.41	0.55
1:F:63:HIS:CE1	2:F:601:FAD:C9A	2.89	0.55
1:G:272:ASP:OD1	1:G:272:ASP:N	2.38	0.55
1:G:349:MET:SD	1:G:409:SER:HA	2.46	0.55
1:G:418:GLY:C	1:G:419:TYR:CD1	2.79	0.55
1:H:96:ARG:HA	1:H:100:GLN:O	2.05	0.55
1:H:178:TRP:CD1	1:H:178:TRP:H	2.23	0.55
1:A:38:ASP:OD1	2:A:601:FAD:H1B	2.06	0.55
1:B:8:VAL:HG11	1:B:35:MET:HG2	1.88	0.55
1:B:480:THR:HA	1:B:487:VAL:HG11	1.88	0.55
1:C:163:ASN:HA	1:C:166:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LYS:HD2	1:D:345:LYS:H	1.72	0.55
1:E:17:PRO:O	1:E:462:PHE:HD1	1.88	0.55
1:G:96:ARG:HA	1:G:100:GLN:O	2.07	0.55
1:H:222:TRP:HA	1:H:222:TRP:HE3	1.71	0.55
1:H:383:ASN:ND2	1:H:386:THR:HG23	2.21	0.55
1:A:383:ASN:O	1:A:387:ILE:HB	2.06	0.55
1:D:398:THR:HB	1:D:400:MET:HG2	1.87	0.55
1:D:398:THR:HB	1:D:400:MET:HG3	1.89	0.55
1:E:114:PRO:O	1:E:118:GLN:HG3	2.06	0.55
1:E:230:PRO:CG	1:E:233:LYS:HD2	2.36	0.55
1:H:64:VAL:HG22	1:H:210:PHE:CD1	2.41	0.55
1:B:468:ALA:O	1:B:472:ILE:HG13	2.06	0.55
1:D:27:ASN:OD1	1:D:230:PRO:HD2	2.07	0.55
1:D:64:VAL:O	2:D:601:FAD:N3	2.37	0.55
1:D:91:ARG:NH2	1:D:204:TRP:O	2.32	0.55
1:D:242:VAL:HB	2:D:601:FAD:H62A	1.69	0.55
1:E:26:LEU:HG	1:E:469:VAL:HG13	1.89	0.55
1:E:116:GLU:HG2	1:E:117:GLU:N	2.20	0.55
1:F:116:GLU:HG2	1:F:117:GLU:N	2.19	0.55
1:G:212:PHE:CG	1:G:213:PRO:HD2	2.41	0.55
1:G:458:GLN:HA	2:G:601:FAD:O3'	2.07	0.55
1:H:25:ARG:HA	1:H:28:GLN:HB2	1.89	0.55
1:B:16:GLY:HA3	2:B:601:FAD:O1A	2.06	0.55
1:C:494:GLU:OE2	1:G:477:VAL:HB	2.07	0.55
1:F:82:LYS:HB2	1:F:85:ASP:CG	2.30	0.55
1:A:87:TYR:HB3	1:A:89:HIS:CE1	2.42	0.55
1:C:338:ASN:OD1	1:C:338:ASN:N	2.40	0.55
1:D:69:TYR:CD1	1:D:463:MET:HG3	2.41	0.55
1:H:115:LYS:O	1:H:118:GLN:HB2	2.07	0.55
1:A:11:LEU:O	1:A:265:LEU:HD12	2.07	0.55
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.42	0.55
1:B:251:THR:HA	1:B:260:ILE:O	2.06	0.55
1:B:455:VAL:HG21	1:B:480:THR:O	2.06	0.55
1:C:134:VAL:O	1:C:134:VAL:CG1	2.54	0.55
1:F:332:SER:HA	1:F:339:GLN:HE21	1.71	0.55
1:F:397:ASN:C	1:F:399:GLU:H	2.14	0.55
1:G:346:LEU:CD2	1:G:347:PRO:HD2	2.35	0.55
1:H:478:GLU:HB2	1:H:481:LEU:HB3	1.88	0.55
1:A:38:ASP:OD2	1:A:40:ASN:HB2	2.06	0.55
1:B:306:ARG:CZ	1:B:311:GLY:HA2	2.37	0.55
1:C:20:LEU:N	1:C:20:LEU:HD23	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:THR:HA	1:D:260:ILE:O	2.06	0.55
1:E:68:HIS:CE1	1:E:460:HIS:NE2	2.75	0.55
1:E:136:ASN:OD1	1:E:137:THR:HG23	2.07	0.55
1:H:425:GLU:CD	1:H:425:GLU:N	2.64	0.55
1:H:458:GLN:HG3	2:H:601:FAD:O2	2.07	0.55
1:A:107:GLN:NE2	3:A:602:GDU:O4	2.40	0.55
1:G:484:PRO:HA	1:G:487:VAL:HG22	1.89	0.55
1:H:79:ALA:HB2	1:H:225:VAL:CG2	2.36	0.55
1:A:251:THR:HA	1:A:260:ILE:O	2.07	0.55
1:A:422:PRO:HA	1:A:426:ARG:HD3	1.88	0.55
1:E:179:LEU:HD23	1:E:179:LEU:H	1.70	0.55
1:E:383:ASN:ND2	1:E:386:THR:HG23	2.22	0.55
1:F:147:VAL:CG2	1:F:160:ARG:HH21	2.20	0.55
1:F:219:GLY:O	1:F:223:ILE:HG12	2.07	0.55
1:G:103:PRO:HB3	1:G:202:GLY:HA3	1.89	0.55
1:G:232:GLU:OE1	1:G:232:GLU:N	2.25	0.55
1:H:464:LEU:HG	1:H:480:THR:HB	1.88	0.55
1:B:111:SER:HB2	1:B:112:MET:HE3	1.89	0.54
1:B:160:ARG:N	1:B:161:PRO:HD2	2.23	0.54
1:C:143:ASP:HA	1:C:146:ILE:HD12	1.89	0.54
1:E:110:ILE:HG23	1:E:195:VAL:HG22	1.89	0.54
1:F:150:MET:O	1:F:154:ILE:HG13	2.07	0.54
1:H:11:LEU:HD21	1:H:252:VAL:HG11	1.87	0.54
1:H:170:PRO:HD2	1:H:379:MET:SD	2.47	0.54
1:H:299:GLY:HA2	1:H:371:MET:HA	1.89	0.54
1:A:46:LEU:N	2:A:601:FAD:O1A	2.35	0.54
1:B:62:GLY:O	3:B:602:GDU:H6'1	2.07	0.54
1:C:457:ASN:O	1:C:460:HIS:HB2	2.08	0.54
1:E:26:LEU:HD22	1:E:34:TRP:HB3	1.90	0.54
1:E:376:GLU:HB2	1:E:382:VAL:CG1	2.37	0.54
1:F:298:ILE:CD1	1:F:388:LEU:HD13	2.38	0.54
1:F:457:ASN:HB3	2:F:601:FAD:O2	2.06	0.54
1:G:109:ASN:HD21	1:G:201:ALA:C	2.14	0.54
1:G:358:GLN:OE1	1:G:358:GLN:HA	2.06	0.54
1:A:144:GLU:O	1:A:148:ARG:HG3	2.07	0.54
1:C:453:TYR:OH	3:C:602:GDU:PB	2.64	0.54
1:C:455:VAL:O	1:C:455:VAL:HG13	2.05	0.54
1:C:494:GLU:HG2	1:G:477:VAL:CA	2.32	0.54
1:E:19:GLY:CA	1:E:268:THR:HG21	2.37	0.54
1:B:155:ALA:O	1:B:160:ARG:HG3	2.07	0.54
1:C:95:VAL:HG23	1:C:102:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:NZ	1:C:320:GLU:O	2.29	0.54
1:D:17:PRO:HD2	2:D:601:FAD:O5'	2.06	0.54
1:H:8:VAL:O	1:H:262:TYR:HA	2.07	0.54
1:A:468:ALA:O	1:A:472:ILE:HG13	2.06	0.54
1:C:57:LEU:HD22	1:C:338:ASN:HA	1.89	0.54
1:C:336:PRO:HG2	1:C:337:TYR:CD1	2.42	0.54
1:G:89:HIS:HB2	1:G:210:PHE:CE2	2.42	0.54
1:G:143:ASP:O	1:G:147:VAL:HG23	2.08	0.54
1:B:178:TRP:HB2	1:B:454:GLU:CG	2.33	0.54
1:C:57:LEU:HD13	1:C:57:LEU:H	1.73	0.54
1:C:182:ARG:HD2	3:C:602:GDU:O2A	2.08	0.54
1:F:204:TRP:CE3	1:F:205:GLY:HA2	2.43	0.54
1:F:303:ARG:NH2	1:F:363:LYS:CB	2.71	0.54
1:G:303:ARG:NH1	1:G:348:THR:OG1	2.26	0.54
1:H:337:TYR:CD1	1:H:337:TYR:N	2.75	0.54
1:A:455:VAL:O	1:A:455:VAL:HG13	2.08	0.54
1:B:457:ASN:O	1:B:460:HIS:HB2	2.08	0.54
1:E:397:ASN:C	1:E:399:GLU:H	2.16	0.54
1:F:25:ARG:HG2	1:F:469:VAL:HB	1.90	0.54
1:G:29:ILE:HG22	1:G:31:GLY:N	2.22	0.54
1:G:341:GLU:HG3	1:G:342:ALA:N	2.21	0.54
1:G:434:LEU:HB2	1:G:435:PRO:HD3	1.90	0.54
1:A:446:GLY:H	1:A:450:SER:HB2	1.72	0.54
1:C:60:VAL:O	1:C:63:HIS:CD2	2.61	0.54
1:C:64:VAL:HG13	1:C:210:PHE:CD1	2.42	0.54
1:C:142:PHE:O	1:C:146:ILE:HG13	2.07	0.54
1:D:168:ALA:CB	1:D:377:SER:HB3	2.38	0.54
1:F:248:ASN:OD1	1:F:248:ASN:N	2.40	0.54
1:F:309:ARG:H	1:F:309:ARG:HD3	1.73	0.54
2:F:601:FAD:C2'	2:F:601:FAD:H9	2.38	0.54
1:H:23:ALA:HA	1:H:26:LEU:HD12	1.89	0.54
1:A:504:PHE:HA	1:A:507:SER:HB3	1.88	0.54
1:C:175:GLN:HE21	1:C:178:TRP:HD1	1.56	0.54
1:D:143:ASP:O	1:D:147:VAL:HG23	2.08	0.54
1:D:383:ASN:O	1:D:387:ILE:HB	2.07	0.54
1:F:207:ASN:HB3	1:F:315:TRP:CH2	2.42	0.54
1:G:58:TYR:HD2	1:G:411:TYR:CD2	2.25	0.54
1:H:28:GLN:HE21	1:H:497:LEU:C	2.15	0.54
1:H:426:ARG:O	1:H:430:LEU:HG	2.08	0.54
1:A:433:ILE:HG22	1:A:434:LEU:N	2.23	0.54
1:B:344:LYS:HD2	1:B:345:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:THR:OG1	1:C:461:SER:HB3	2.07	0.54
1:C:103:PRO:HG2	1:C:109:ASN:CG	2.33	0.54
1:D:136:ASN:OD1	1:D:136:ASN:N	2.34	0.54
1:G:480:THR:HA	1:G:487:VAL:HG21	1.90	0.54
1:H:54:GLU:HB3	1:H:346:LEU:CD1	2.38	0.54
1:H:402:LYS:HD3	1:H:405:ASP:OD2	2.07	0.54
1:E:454:GLU:OE2	1:E:454:GLU:N	2.20	0.53
1:H:500:GLY:O	1:H:504:PHE:CD2	2.61	0.53
1:B:325:PHE:HA	1:B:374:VAL:HG22	1.89	0.53
1:D:134:VAL:O	1:D:134:VAL:CG1	2.56	0.53
1:D:178:TRP:CB	1:D:454:GLU:HG3	2.35	0.53
1:F:122:ILE:O	1:F:126:ILE:HG13	2.08	0.53
1:G:158:PHE:CG	1:G:159:MET:SD	3.01	0.53
1:H:95:VAL:HG22	1:H:317:TYR:HD2	1.72	0.53
1:H:471:ASN:HA	1:H:476:ALA:H	1.73	0.53
1:A:269:MET:HG2	1:A:274:LEU:HD22	1.91	0.53
1:A:455:VAL:CG1	1:A:464:LEU:HD11	2.38	0.53
1:D:6:ILE:O	1:D:260:ILE:HA	2.09	0.53
1:D:242:VAL:HA	1:D:254:LEU:CD2	2.38	0.53
1:D:398:THR:HG22	1:D:398:THR:O	2.08	0.53
1:F:108:ASN:C	1:F:194:ASN:HD22	2.17	0.53
1:G:71:TYR:CD2	1:G:496:ARG:C	2.86	0.53
1:G:367:TYR:CE1	1:G:408:VAL:HG11	2.43	0.53
1:G:500:GLY:O	1:G:504:PHE:CD2	2.62	0.53
1:H:283:LEU:O	1:H:287:THR:HG23	2.08	0.53
1:H:348:THR:HB	1:H:357:PRO:HB3	1.90	0.53
1:A:155:ALA:O	1:A:160:ARG:HG3	2.08	0.53
1:B:395:LEU:HA	1:B:400:MET:HG3	1.91	0.53
1:C:417:HIS:HB3	1:C:448:PHE:CZ	2.44	0.53
1:F:162:TYR:O	1:F:166:VAL:HG12	2.08	0.53
1:G:306:ARG:HD2	1:G:311:GLY:O	2.09	0.53
1:H:28:GLN:NE2	1:H:502:GLN:OE1	2.41	0.53
1:H:417:HIS:HB3	1:H:448:PHE:CZ	2.42	0.53
1:B:91:ARG:HD3	1:B:207:ASN:CB	2.36	0.53
1:C:350:GLN:NE2	1:C:354:GLY:HA2	2.21	0.53
1:D:175:GLN:HG3	1:D:422:PRO:O	2.09	0.53
1:D:468:ALA:O	1:D:472:ILE:HG13	2.09	0.53
1:H:58:TYR:CE1	1:H:369:SER:OG	2.61	0.53
1:H:342:ALA:O	1:H:365:GLY:O	2.27	0.53
1:H:479:LEU:HA	1:H:483:TYR:HD2	1.74	0.53
1:A:93:SER:HB2	1:A:104:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HD22	1:A:201:ALA:HB3	1.73	0.53
1:B:16:GLY:HA3	2:B:601:FAD:PA	2.48	0.53
1:C:63:HIS:CD2	2:C:601:FAD:C5X	2.92	0.53
1:C:455:VAL:O	1:C:455:VAL:CG1	2.55	0.53
1:D:113:LEU:O	1:D:118:GLN:NE2	2.31	0.53
1:E:219:GLY:O	1:E:223:ILE:HG12	2.09	0.53
1:E:291:PHE:CG	1:E:292:TYR:N	2.76	0.53
1:E:353:ASP:HB3	1:E:403:PRO:HB3	1.89	0.53
1:F:494:GLU:CD	1:F:494:GLU:N	2.65	0.53
1:G:17:PRO:N	2:G:601:FAD:O1P	2.42	0.53
1:G:63:HIS:HB2	1:G:218:THR:HG21	1.91	0.53
1:G:116:GLU:OE2	1:G:117:GLU:HG2	2.08	0.53
1:G:250:LYS:HD2	1:G:262:TYR:CE1	2.44	0.53
1:A:43:PRO:HG2	1:A:223:ILE:HD13	1.89	0.53
1:A:163:ASN:HA	1:A:166:VAL:CG1	2.38	0.53
1:C:39:SER:HB3	1:C:241:LYS:HG2	1.90	0.53
1:C:344:LYS:HD2	1:C:345:LYS:N	2.24	0.53
1:F:192:THR:O	1:F:196:ILE:HG13	2.08	0.53
1:G:351:LEU:HD12	1:G:404:THR:HA	1.90	0.53
1:A:58:TYR:HA	1:A:331:PHE:CE2	2.42	0.53
1:D:196:ILE:HD12	1:F:119:VAL:HG22	1.91	0.53
1:D:242:VAL:HA	1:D:254:LEU:HD22	1.90	0.53
1:E:387:ILE:HG23	1:E:388:LEU:H	1.71	0.53
1:H:28:GLN:HG3	1:H:497:LEU:HD12	1.91	0.53
1:H:425:GLU:CD	1:H:425:GLU:H	2.17	0.53
1:C:182:ARG:HD2	3:C:602:GDU:PA	2.49	0.53
1:E:326:TYR:N	1:E:374:VAL:HG13	2.23	0.53
1:F:142:PHE:CB	1:F:174:MET:HB2	2.39	0.53
1:G:149:MET:SD	1:G:184:ALA:CA	2.94	0.53
1:G:270:ALA:HA	1:G:448:PHE:C	2.34	0.53
1:A:242:VAL:HA	1:A:254:LEU:CD2	2.39	0.53
1:C:242:VAL:H	2:C:601:FAD:H62A	1.55	0.53
1:C:383:ASN:O	1:C:387:ILE:HB	2.08	0.53
1:E:66:PHE:CB	1:E:206:PRO:O	2.57	0.53
1:F:323:CYS:HB2	1:F:324:PRO:HD2	1.90	0.53
1:G:337:TYR:CD1	1:G:337:TYR:N	2.76	0.53
1:H:158:PHE:C	1:H:158:PHE:HD1	2.15	0.53
1:H:323:CYS:HB2	1:H:325:PHE:CZ	2.44	0.53
1:B:143:ASP:O	1:B:147:VAL:HG23	2.08	0.52
1:D:38:ASP:HA	2:D:601:FAD:H2A	1.91	0.52
1:F:70:LYS:HB3	1:F:496:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:ASN:ND2	1:G:397:ASN:HB3	2.23	0.52
1:G:389:ALA:O	1:G:392:ILE:HB	2.09	0.52
1:H:28:GLN:NE2	1:H:497:LEU:O	2.37	0.52
1:H:160:ARG:HB2	1:H:161:PRO:HD3	1.91	0.52
1:H:338:ASN:HB2	1:H:339:GLN:HE22	1.73	0.52
1:H:349:MET:SD	1:H:409:SER:HA	2.49	0.52
1:A:455:VAL:O	1:A:455:VAL:CG1	2.56	0.52
1:B:38:ASP:OD2	1:B:40:ASN:HB2	2.08	0.52
1:B:87:TYR:HB3	1:B:89:HIS:CE1	2.44	0.52
1:E:38:ASP:OD2	1:E:40:ASN:N	2.42	0.52
1:E:159:MET:CE	3:E:602:GDU:C2	2.88	0.52
1:F:129:ALA:O	1:F:132:ALA:HB3	2.08	0.52
1:G:64:VAL:HG22	1:G:210:PHE:CD1	2.44	0.52
1:G:249:ASN:N	1:G:249:ASN:OD1	2.42	0.52
1:H:492:ASN:ND2	1:H:492:ASN:N	2.56	0.52
1:D:11:LEU:O	1:D:265:LEU:HD12	2.09	0.52
1:E:12:VAL:O	1:E:36:ILE:HA	2.09	0.52
1:G:18:THR:HG21	1:G:268:THR:CG2	2.32	0.52
1:G:25:ARG:HD3	1:G:470:ASP:OD1	2.09	0.52
1:G:189:LYS:O	1:G:193:THR:OG1	2.23	0.52
1:G:194:ASN:ND2	1:G:199:LYS:O	2.42	0.52
1:A:152:THR:HG22	1:A:156:ASP:OD2	2.09	0.52
1:E:19:GLY:H	1:E:268:THR:HG21	1.72	0.52
1:G:160:ARG:HB2	1:G:161:PRO:HD3	1.92	0.52
1:H:70:LYS:HB2	1:H:493:THR:HA	1.90	0.52
1:A:466:VAL:HG12	1:A:495:ARG:NH1	2.25	0.52
1:C:110:ILE:CA	1:C:113:LEU:HD12	2.35	0.52
1:C:242:VAL:HA	1:C:254:LEU:HD22	1.91	0.52
1:D:68:HIS:O	1:D:492:ASN:ND2	2.40	0.52
1:D:163:ASN:HA	1:D:166:VAL:CG1	2.39	0.52
1:E:204:TRP:CE3	1:E:205:GLY:HA2	2.44	0.52
1:F:349:MET:N	1:F:407:ILE:O	2.36	0.52
1:H:163:ASN:O	1:H:167:TRP:HB2	2.09	0.52
1:H:283:LEU:HD22	1:H:433:ILE:HG23	1.91	0.52
1:A:245:VAL:HG22	1:A:252:VAL:HG23	1.90	0.52
1:B:103:PRO:HB2	1:B:109:ASN:ND2	2.25	0.52
1:C:125:MET:CE	1:C:186:PRO:HB2	2.38	0.52
1:D:16:GLY:CA	2:D:601:FAD:H52A	2.38	0.52
1:D:111:SER:HB2	1:D:112:MET:HE3	1.91	0.52
1:E:22:ALA:O	1:E:26:LEU:HB2	2.08	0.52
1:F:313:LYS:O	1:F:333:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:PHE:HA	1:F:374:VAL:CG1	2.40	0.52
1:G:253:THR:HA	1:G:259:THR:HG22	1.92	0.52
1:H:389:ALA:O	1:H:392:ILE:HB	2.10	0.52
1:H:455:VAL:HG13	1:H:484:PRO:HB3	1.91	0.52
1:A:199:LYS:HD2	1:A:200:THR:O	2.09	0.52
1:A:416:ASP:HB2	1:F:281:GLN:HE21	1.75	0.52
1:B:207:ASN:O	1:B:208:ALA:C	2.53	0.52
1:C:106:PHE:C	1:C:106:PHE:CD2	2.88	0.52
1:C:114:PRO:O	1:C:118:GLN:HG3	2.09	0.52
1:E:69:TYR:HB2	1:E:72:PHE:HB3	1.91	0.52
1:E:427:GLU:O	1:E:431:THR:HG23	2.09	0.52
1:G:89:HIS:NE2	1:G:334:TYR:HA	2.25	0.52
1:A:28:GLN:NE2	1:A:502:GLN:OE1	2.42	0.52
1:B:125:MET:CE	1:B:186:PRO:HB2	2.40	0.52
1:B:134:VAL:CG1	1:B:134:VAL:O	2.57	0.52
1:B:443:TRP:CD1	1:B:445:ARG:HH21	2.28	0.52
1:C:175:GLN:HG3	1:C:422:PRO:O	2.10	0.52
1:C:307:PRO:HD2	1:C:310:ILE:HD12	1.91	0.52
1:E:142:PHE:O	1:E:146:ILE:HG13	2.10	0.52
1:E:167:TRP:HE3	1:E:421:THR:HG22	1.74	0.52
1:E:335:SER:HB3	1:E:338:ASN:OD1	2.09	0.52
1:F:82:LYS:HB2	1:F:85:ASP:OD2	2.09	0.52
1:G:8:VAL:O	1:G:262:TYR:HA	2.10	0.52
1:G:79:ALA:HB2	1:G:225:VAL:CG2	2.38	0.52
1:A:111:SER:HB2	1:A:112:MET:HE3	1.92	0.52
1:A:183:VAL:HG22	3:A:602:GDU:H1D	1.92	0.52
1:B:504:PHE:CZ	1:F:264:LYS:HG2	2.43	0.52
1:C:107:GLN:H	1:C:107:GLN:CD	2.17	0.52
1:E:24:LYS:HE3	1:E:229:LEU:HD21	1.92	0.52
1:E:298:ILE:CD1	1:E:388:LEU:HD13	2.40	0.52
1:F:19:GLY:CA	1:F:268:THR:HG21	2.40	0.52
1:F:306:ARG:NH1	1:F:333:ASN:OD1	2.42	0.52
1:A:344:LYS:HD2	1:A:345:LYS:N	2.25	0.52
1:B:346:LEU:HD23	1:B:347:PRO:HD2	1.91	0.52
1:D:336:PRO:HG2	1:D:337:TYR:CD1	2.45	0.52
1:D:455:VAL:HG21	1:D:480:THR:O	2.10	0.52
1:F:10:VAL:HG22	1:F:264:LYS:HG3	1.92	0.52
1:F:158:PHE:O	1:F:161:PRO:HG2	2.10	0.52
1:F:453:TYR:CD2	1:F:453:TYR:O	2.62	0.52
1:G:210:PHE:HZ	1:G:334:TYR:CE1	2.28	0.52
1:H:254:LEU:HB2	1:H:258:THR:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:270:ALA:HB1	1:H:272:ASP:OD1	2.09	0.52
1:B:199:LYS:HD2	1:B:200:THR:O	2.10	0.51
1:D:40:ASN:O	1:D:236:PHE:HB3	2.09	0.51
1:D:271:VAL:HA	1:D:274:LEU:HB2	1.92	0.51
1:E:18:THR:HA	1:E:461:SER:O	2.09	0.51
1:E:504:PHE:N	1:E:504:PHE:CD1	2.78	0.51
1:F:110:ILE:HG23	1:F:195:VAL:HG22	1.93	0.51
1:G:244:LYS:HB3	1:G:253:THR:HB	1.91	0.51
1:G:453:TYR:CD2	1:G:453:TYR:O	2.63	0.51
1:C:155:ALA:O	1:C:160:ARG:HG3	2.10	0.51
1:D:57:LEU:HD13	1:D:338:ASN:C	2.35	0.51
1:G:283:LEU:O	1:G:287:THR:HG23	2.10	0.51
1:G:375:SER:OG	1:G:380:LYS:HE3	2.11	0.51
1:G:455:VAL:HA	1:G:460:HIS:ND1	2.24	0.51
1:B:107:GLN:CD	1:B:107:GLN:H	2.17	0.51
1:D:325:PHE:CZ	1:D:395:LEU:HD23	2.45	0.51
1:E:150:MET:O	1:E:154:ILE:HG13	2.10	0.51
1:F:21:GLY:HA2	1:F:462:PHE:CE1	2.45	0.51
1:F:38:ASP:OD1	2:F:601:FAD:H1B	2.11	0.51
1:G:38:ASP:OD2	1:G:39:SER:N	2.43	0.51
1:G:376:GLU:CG	1:G:382:VAL:HG13	2.37	0.51
1:H:272:ASP:OD1	1:H:272:ASP:N	2.40	0.51
1:B:242:VAL:HA	1:B:254:LEU:HD22	1.93	0.51
1:B:346:LEU:HD23	1:B:347:PRO:CD	2.40	0.51
1:D:183:VAL:HG22	3:D:602:GDU:H1D	1.93	0.51
1:E:17:PRO:C	1:E:462:PHE:HA	2.35	0.51
1:A:106:PHE:C	1:A:106:PHE:CD2	2.87	0.51
1:B:150:MET:HE3	1:B:159:MET:HG3	1.92	0.51
1:E:133:ARG:NH1	1:E:133:ARG:CG	2.71	0.51
1:G:425:GLU:N	1:G:425:GLU:CD	2.69	0.51
1:H:143:ASP:O	1:H:147:VAL:HG23	2.10	0.51
1:A:32:PRO:HG3	1:E:504:PHE:HD2	1.75	0.51
1:A:207:ASN:O	1:A:208:ALA:C	2.53	0.51
1:C:398:THR:HB	1:C:400:MET:HG3	1.93	0.51
1:E:291:PHE:CE1	1:E:292:TYR:O	2.64	0.51
1:H:250:LYS:O	1:H:261:GLY:HA2	2.10	0.51
1:A:358:GLN:N	1:A:358:GLN:CD	2.64	0.51
1:B:278:MET:HE1	1:B:442:ILE:HD12	1.91	0.51
1:C:242:VAL:HA	1:C:254:LEU:CD2	2.41	0.51
1:C:278:MET:HE1	1:C:442:ILE:HD12	1.92	0.51
1:E:320:GLU:HB2	1:E:322:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:ASP:N	1:F:272:ASP:OD1	2.43	0.51
1:F:458:GLN:HG3	2:F:601:FAD:H1'2	1.91	0.51
1:G:167:TRP:CB	1:G:174:MET:HE1	2.41	0.51
1:A:106:PHE:C	1:A:106:PHE:HD2	2.19	0.51
1:A:192:THR:OG1	1:A:193:THR:N	2.43	0.51
1:C:306:ARG:CZ	1:C:311:GLY:HA2	2.40	0.51
1:D:16:GLY:HA3	2:D:601:FAD:O1P	2.11	0.51
1:D:212:PHE:CG	1:D:213:PRO:HD2	2.46	0.51
1:D:272:ASP:OD1	1:D:272:ASP:N	2.44	0.51
1:E:281:GLN:OE1	1:E:284:VAL:HB	2.11	0.51
1:F:167:TRP:HE3	1:F:421:THR:HG22	1.75	0.51
1:F:391:CYS:O	1:F:395:LEU:HG	2.11	0.51
1:G:9:ASP:OD1	1:G:33:SER:N	2.43	0.51
1:G:171:THR:HG22	1:G:174:MET:HE3	1.92	0.51
1:A:69:TYR:CD2	1:A:463:MET:HG3	2.46	0.51
1:A:189:LYS:HE2	1:G:123:ASP:HA	1.92	0.51
1:A:232:GLU:H	1:A:232:GLU:CD	2.19	0.51
1:D:494:GLU:HG2	1:H:477:VAL:HA	1.93	0.51
1:E:454:GLU:H	1:E:454:GLU:CD	2.12	0.51
1:F:204:TRP:CE3	1:F:205:GLY:N	2.79	0.51
1:G:18:THR:HB	2:G:601:FAD:O2P	2.11	0.51
1:G:95:VAL:HG22	1:G:317:TYR:HD2	1.75	0.51
1:H:244:LYS:HB3	1:H:253:THR:HB	1.92	0.51
1:A:150:MET:HE3	1:A:159:MET:HG3	1.92	0.51
1:D:63:HIS:HB3	1:D:458:GLN:NE2	2.26	0.51
1:D:192:THR:OG1	1:D:193:THR:N	2.44	0.51
1:D:207:ASN:O	1:D:208:ALA:C	2.54	0.51
1:F:15:ALA:H	2:F:601:FAD:H4B	1.75	0.51
1:F:149:MET:O	1:F:149:MET:HG2	2.11	0.51
1:G:383:ASN:ND2	1:G:386:THR:HG23	2.25	0.51
1:G:447:ARG:HG2	1:G:448:PHE:CE2	2.45	0.51
2:G:601:FAD:O1P	2:G:601:FAD:O1A	2.29	0.51
1:H:107:GLN:CD	1:H:107:GLN:N	2.66	0.51
1:B:303:ARG:NH2	1:B:363:LYS:O	2.43	0.50
1:B:455:VAL:O	1:B:455:VAL:CG1	2.59	0.50
1:C:325:PHE:CZ	1:C:395:LEU:HD23	2.45	0.50
1:D:91:ARG:O	1:D:92:ILE:HD13	2.11	0.50
1:F:230:PRO:CG	1:F:233:LYS:HD2	2.37	0.50
1:G:15:ALA:HB2	1:G:38:ASP:HB2	1.91	0.50
1:H:175:GLN:O	1:H:178:TRP:NE1	2.44	0.50
1:H:253:THR:HA	1:H:259:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:438:GLN:HA	1:H:442:ILE:O	2.10	0.50
1:B:304:GLY:O	1:B:368:TRP:HD1	1.95	0.50
1:C:212:PHE:CG	1:C:213:PRO:HD2	2.46	0.50
1:D:155:ALA:O	1:D:160:ARG:HG3	2.12	0.50
1:D:432:GLN:O	1:D:436:LYS:HB2	2.11	0.50
1:E:309:ARG:HD3	1:E:309:ARG:H	1.76	0.50
1:E:467:GLU:HG2	1:E:495:ARG:NH1	2.26	0.50
1:G:16:GLY:O	1:G:20:LEU:HG	2.10	0.50
1:G:39:SER:HB3	1:G:241:LYS:CB	2.41	0.50
1:G:158:PHE:HE1	1:G:162:TYR:CG	2.28	0.50
1:G:204:TRP:HA	1:G:204:TRP:HE3	1.75	0.50
1:H:197:LEU:C	1:H:199:LYS:N	2.67	0.50
1:A:307:PRO:HD2	1:A:310:ILE:HD12	1.93	0.50
1:B:64:VAL:HG13	1:B:210:PHE:CD1	2.46	0.50
1:B:95:VAL:HG23	1:B:102:VAL:O	2.10	0.50
1:B:192:THR:O	1:B:196:ILE:HG13	2.12	0.50
1:B:244:LYS:HG2	1:B:245:VAL:N	2.26	0.50
1:C:6:ILE:O	1:C:260:ILE:HA	2.10	0.50
1:C:182:ARG:NH1	3:C:602:GDU:O2'	2.43	0.50
1:D:87:TYR:HB3	1:D:89:HIS:CE1	2.46	0.50
1:D:108:ASN:HD22	1:D:201:ALA:HB3	1.75	0.50
1:D:150:MET:HG2	1:D:154:ILE:HG21	1.93	0.50
1:D:306:ARG:CZ	1:D:311:GLY:HA2	2.41	0.50
1:E:204:TRP:CE3	1:E:205:GLY:N	2.79	0.50
1:E:324:PRO:O	1:E:374:VAL:HG11	2.10	0.50
1:F:18:THR:HA	1:F:461:SER:O	2.10	0.50
1:F:454:GLU:OE2	1:F:454:GLU:N	2.26	0.50
1:B:455:VAL:O	1:B:455:VAL:HG13	2.11	0.50
1:C:139:PRO:HB2	1:C:176:CYS:SG	2.51	0.50
1:D:447:ARG:O	1:D:451:TRP:HA	2.11	0.50
1:E:244:LYS:HG2	1:E:245:VAL:N	2.26	0.50
1:F:38:ASP:OD2	1:F:40:ASN:N	2.41	0.50
1:F:411:TYR:OH	1:F:413:ARG:HB3	2.11	0.50
1:F:443:TRP:N	1:F:443:TRP:CE3	2.79	0.50
1:H:38:ASP:OD1	2:H:601:FAD:O3B	2.23	0.50
1:H:309:ARG:HG2	1:H:310:ILE:CD1	2.42	0.50
1:B:183:VAL:HG13	3:B:602:GDU:O2	2.09	0.50
1:B:346:LEU:HD13	1:B:408:VAL:HG13	1.93	0.50
1:D:504:PHE:HA	1:D:507:SER:HB3	1.92	0.50
1:G:299:GLY:HA2	1:G:370:ILE:O	2.11	0.50
1:H:464:LEU:HD21	1:H:481:LEU:CA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PRO:CG	1:C:109:ASN:ND2	2.72	0.50
1:C:199:LYS:HD2	1:C:200:THR:O	2.12	0.50
1:E:187:ASN:CG	1:E:189:LYS:HB2	2.36	0.50
1:E:270:ALA:HB3	1:E:273:PHE:CD2	2.47	0.50
1:F:76:LEU:HD12	1:F:211:ARG:NH2	2.27	0.50
1:F:136:ASN:OD1	1:F:137:THR:HG23	2.10	0.50
2:F:601:FAD:H9	2:F:601:FAD:O2'	2.11	0.50
1:G:150:MET:O	1:G:154:ILE:HD13	2.11	0.50
1:G:181:GLU:OE1	1:G:181:GLU:HA	2.12	0.50
1:H:335:SER:HB3	1:H:338:ASN:OD1	2.11	0.50
1:H:453:TYR:CD2	1:H:453:TYR:O	2.64	0.50
1:B:178:TRP:CB	1:B:454:GLU:HG3	2.35	0.50
1:B:212:PHE:CG	1:B:213:PRO:HD2	2.47	0.50
1:C:152:THR:HG22	1:C:156:ASP:OD2	2.11	0.50
1:D:5:ASP:H	1:D:259:THR:HG1	1.60	0.50
1:E:224:ALA:O	1:E:228:THR:HG23	2.12	0.50
1:E:359:SER:HB3	1:E:363:LYS:HE2	1.93	0.50
1:F:166:VAL:HA	1:F:326:TYR:CD2	2.47	0.50
1:G:332:SER:HA	1:G:339:GLN:HE22	1.76	0.50
1:G:455:VAL:HG21	1:G:480:THR:O	2.12	0.50
1:G:479:LEU:HA	1:G:483:TYR:HD2	1.76	0.50
1:H:181:GLU:N	1:H:485:ASP:OD1	2.44	0.50
1:B:16:GLY:HA3	2:B:601:FAD:O5B	2.11	0.50
1:C:69:TYR:CD2	1:C:463:MET:HG3	2.47	0.50
1:C:143:ASP:O	1:C:147:VAL:HG23	2.11	0.50
1:C:192:THR:O	1:C:196:ILE:HG13	2.11	0.50
1:D:160:ARG:N	1:D:161:PRO:HD2	2.26	0.50
1:D:455:VAL:O	1:D:455:VAL:CG1	2.59	0.50
1:D:483:TYR:N	1:D:484:PRO:HD3	2.27	0.50
1:E:169:VAL:HG22	1:E:174:MET:HE3	1.93	0.50
1:E:413:ARG:HG2	1:E:414:ARG:N	2.26	0.50
1:E:467:GLU:HG2	1:E:495:ARG:NH2	2.26	0.50
1:F:71:TYR:HB2	1:F:495:ARG:O	2.11	0.50
1:F:122:ILE:CG2	1:F:123:ASP:N	2.75	0.50
1:G:128:ALA:HB2	1:G:151:GLY:HA2	1.93	0.50
1:H:61:GLY:HA3	2:H:601:FAD:C6	2.41	0.50
1:H:178:TRP:H	1:H:178:TRP:HD1	1.60	0.50
1:H:351:LEU:HD12	1:H:404:THR:HA	1.93	0.50
1:B:175:GLN:HG3	1:B:422:PRO:O	2.12	0.50
1:B:296:HIS:NE2	1:B:382:VAL:HG21	2.27	0.50
1:C:108:ASN:ND2	1:C:201:ALA:HB3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LYS:HG2	1:D:245:VAL:N	2.27	0.50
1:F:110:ILE:CG2	1:F:195:VAL:HG22	2.42	0.50
1:H:167:TRP:O	1:H:169:VAL:HG12	2.12	0.50
1:H:345:LYS:HE3	1:H:364:GLU:OE1	2.12	0.50
1:B:106:PHE:C	1:B:106:PHE:CD2	2.90	0.49
1:C:103:PRO:HB2	1:C:109:ASN:HD21	1.73	0.49
1:F:114:PRO:O	1:F:118:GLN:HG3	2.11	0.49
1:F:326:TYR:N	1:F:374:VAL:HG13	2.26	0.49
1:G:251:THR:HA	1:G:260:ILE:O	2.12	0.49
1:G:262:TYR:CE1	1:G:265:LEU:HB2	2.47	0.49
1:G:351:LEU:HD13	1:G:404:THR:O	2.11	0.49
1:H:274:LEU:HD11	1:H:278:MET:HE3	1.93	0.49
1:H:455:VAL:HA	1:H:460:HIS:ND1	2.27	0.49
1:B:269:MET:HG2	1:B:274:LEU:HD22	1.94	0.49
1:B:499:ASP:O	1:B:503:VAL:HG23	2.11	0.49
1:C:57:LEU:N	1:C:57:LEU:CD1	2.75	0.49
1:C:303:ARG:NH2	1:C:363:LYS:C	2.68	0.49
1:D:152:THR:HG22	1:D:156:ASP:OD2	2.11	0.49
1:D:455:VAL:O	1:D:455:VAL:HG13	2.11	0.49
1:E:122:ILE:HG22	1:E:123:ASP:N	2.27	0.49
1:F:16:GLY:HA3	2:F:601:FAD:O5B	2.11	0.49
1:F:396:VAL:HA	1:F:401:LEU:HB2	1.94	0.49
1:G:270:ALA:HB1	1:G:272:ASP:OD1	2.12	0.49
1:H:61:GLY:HA2	1:H:373:GLU:OE1	2.12	0.49
1:H:292:TYR:CE1	1:H:417:HIS:ND1	2.79	0.49
1:H:411:TYR:CD1	1:H:412:HIS:N	2.70	0.49
1:B:72:PHE:CE2	1:B:76:LEU:HD11	2.48	0.49
1:D:58:TYR:HA	1:D:331:PHE:CE2	2.46	0.49
1:F:91:ARG:CZ	1:F:93:SER:HB2	2.42	0.49
1:G:64:VAL:HG22	1:G:210:PHE:CE1	2.47	0.49
1:G:71:TYR:CE2	1:G:497:LEU:HA	2.47	0.49
1:G:292:TYR:CZ	1:G:417:HIS:CE1	3.00	0.49
1:G:401:LEU:HA	1:G:405:ASP:OD2	2.13	0.49
1:G:402:LYS:HD3	1:G:402:LYS:H	1.78	0.49
1:A:241:LYS:HE3	2:A:601:FAD:N6A	2.28	0.49
1:C:425:GLU:H	1:C:425:GLU:CD	2.20	0.49
1:D:278:MET:HE1	1:D:442:ILE:HD12	1.94	0.49
1:E:303:ARG:NH1	1:E:348:THR:OG1	2.45	0.49
1:G:28:GLN:NE2	1:G:502:GLN:OE1	2.45	0.49
1:G:63:HIS:H	1:G:63:HIS:CD2	2.30	0.49
1:G:104:TYR:CD2	1:G:105:PRO:HA	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:MET:HG2	1:G:188:LEU:HG	1.94	0.49
1:H:11:LEU:HB3	1:H:265:LEU:HD12	1.93	0.49
1:A:57:LEU:HD13	1:A:338:ASN:C	2.38	0.49
1:A:244:LYS:HG2	1:A:245:VAL:N	2.27	0.49
1:A:325:PHE:CZ	1:A:395:LEU:HD23	2.48	0.49
1:A:339:GLN:CD	1:A:339:GLN:N	2.71	0.49
1:B:196:ILE:HG21	1:H:119:VAL:HG22	1.95	0.49
1:E:411:TYR:OH	1:E:413:ARG:HB3	2.13	0.49
1:F:15:ALA:N	2:F:601:FAD:H4B	2.27	0.49
1:F:151:GLY:C	1:F:154:ILE:HG12	2.36	0.49
1:F:460:HIS:O	1:F:463:MET:HB2	2.11	0.49
1:G:71:TYR:HB2	1:G:495:ARG:O	2.11	0.49
1:G:393:GLN:NE2	1:G:397:ASN:OD1	2.45	0.49
1:D:95:VAL:HG23	1:D:102:VAL:O	2.13	0.49
1:D:178:TRP:HB2	1:D:454:GLU:CG	2.38	0.49
1:D:352:ALA:HB3	1:D:403:PRO:HA	1.93	0.49
1:F:424:LEU:HB2	1:F:425:GLU:OE1	2.12	0.49
1:F:508:LYS:HG3	1:F:509:ALA:N	2.27	0.49
1:G:54:GLU:OE2	1:G:54:GLU:N	2.45	0.49
1:A:346:LEU:HD23	1:A:347:PRO:HD2	1.93	0.49
1:B:307:PRO:HB2	1:B:309:ARG:HG2	1.95	0.49
1:C:106:PHE:C	1:C:106:PHE:HD2	2.20	0.49
1:D:388:LEU:O	1:D:392:ILE:HG13	2.13	0.49
1:E:173:LYS:HA	1:E:424:LEU:HD11	1.95	0.49
1:F:56:PHE:CE2	1:F:409:SER:HB3	2.46	0.49
1:H:48:SER:O	1:H:60:VAL:HG23	2.13	0.49
1:H:460:HIS:CE1	1:H:488:ASN:OD1	2.66	0.49
1:B:414:ARG:HH12	1:B:416:ASP:HA	1.78	0.49
1:B:504:PHE:CZ	1:F:264:LYS:CG	2.96	0.49
1:C:142:PHE:HE2	1:C:163:ASN:ND2	2.10	0.49
1:C:178:TRP:CB	1:C:454:GLU:CG	2.90	0.49
1:D:330:ILE:HB	1:D:333:ASN:OD1	2.13	0.49
1:F:26:LEU:HG	1:F:469:VAL:HG13	1.94	0.49
1:G:58:TYR:CE1	1:G:369:SER:OG	2.63	0.49
1:H:11:LEU:HB3	1:H:265:LEU:CD1	2.43	0.49
1:H:104:TYR:CD2	1:H:105:PRO:HA	2.46	0.49
1:H:152:THR:O	1:H:156:ASP:CG	2.55	0.49
1:A:178:TRP:CH2	1:A:179:LEU:HD23	2.48	0.49
1:A:346:LEU:HD23	1:A:347:PRO:CD	2.43	0.49
1:B:57:LEU:HD13	1:B:338:ASN:O	2.13	0.49
1:C:57:LEU:HD13	1:C:338:ASN:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:TYR:CD2	1:D:463:MET:HG3	2.48	0.49
1:D:351:LEU:HB2	1:D:355:SER:OG	2.13	0.49
1:E:9:ASP:CA	1:E:263:LYS:HD3	2.37	0.49
1:E:18:THR:O	1:E:465:GLY:HA3	2.13	0.49
1:E:425:GLU:CD	1:E:425:GLU:N	2.70	0.49
1:F:179:LEU:HD23	1:F:179:LEU:H	1.78	0.49
1:G:11:LEU:HD21	1:G:252:VAL:CG1	2.43	0.49
1:G:126:ILE:HA	1:G:188:LEU:HD11	1.95	0.49
1:G:418:GLY:O	1:G:419:TYR:HD1	1.96	0.49
1:H:322:ASN:ND2	1:H:397:ASN:HB3	2.26	0.49
1:H:332:SER:OG	1:H:368:TRP:HB2	2.13	0.49
1:A:346:LEU:HD13	1:A:408:VAL:HG13	1.94	0.49
1:C:455:VAL:O	1:C:460:HIS:CB	2.61	0.49
1:D:175:GLN:NE2	1:D:178:TRP:HD1	2.10	0.49
1:D:480:THR:HA	1:D:487:VAL:HG11	1.95	0.49
1:E:17:PRO:O	1:E:462:PHE:CD1	2.66	0.49
1:F:19:GLY:H	1:F:268:THR:HG21	1.73	0.49
1:F:137:THR:C	1:F:148:ARG:HH12	2.20	0.49
1:F:187:ASN:O	1:F:191:VAL:HG23	2.13	0.49
1:G:2:THR:OG1	1:G:3:HIS:N	2.46	0.49
1:G:142:PHE:HA	1:G:176:CYS:HB3	1.94	0.49
1:G:290:LEU:HD21	1:G:430:LEU:HD23	1.94	0.49
1:H:38:ASP:OD2	1:H:39:SER:N	2.46	0.49
1:H:203:ASN:ND2	1:H:204:TRP:H	2.08	0.49
1:H:290:LEU:HD21	1:H:430:LEU:HD23	1.95	0.49
1:H:484:PRO:HA	1:H:487:VAL:CG2	2.43	0.49
1:A:178:TRP:CB	1:A:454:GLU:HG3	2.38	0.48
1:A:272:ASP:OD1	1:A:272:ASP:N	2.45	0.48
1:A:463:MET:O	1:A:467:GLU:HG3	2.13	0.48
1:B:17:PRO:HG2	2:B:601:FAD:O4'	2.13	0.48
1:C:346:LEU:HD13	1:C:408:VAL:HG13	1.95	0.48
1:F:163:ASN:ND2	3:F:602:GDU:O2D	2.42	0.48
1:G:28:GLN:HG3	1:G:497:LEU:HD12	1.95	0.48
1:G:332:SER:OG	1:G:368:TRP:HB2	2.13	0.48
1:H:100:GLN:HA	1:H:100:GLN:OE1	2.13	0.48
1:A:395:LEU:HA	1:A:400:MET:HG3	1.94	0.48
1:B:272:ASP:OD1	1:B:272:ASP:N	2.47	0.48
1:C:178:TRP:CB	1:C:454:GLU:HG3	2.36	0.48
1:F:269:MET:CE	1:F:273:PHE:HB3	2.42	0.48
1:F:303:ARG:HH21	1:F:363:LYS:CA	2.26	0.48
1:F:350:GLN:NE2	1:F:407:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:464:LEU:HD21	1:G:481:LEU:CA	2.44	0.48
1:H:28:GLN:CG	1:H:497:LEU:O	2.62	0.48
1:A:425:GLU:CD	1:A:425:GLU:H	2.20	0.48
1:B:250:LYS:HD3	1:B:262:TYR:O	2.13	0.48
1:C:116:GLU:O	1:C:119:VAL:HB	2.13	0.48
1:C:458:GLN:HG3	2:C:601:FAD:N1	2.28	0.48
1:D:477:VAL:HA	1:H:494:GLU:HG2	1.93	0.48
1:E:359:SER:C	1:E:361:GLU:H	2.20	0.48
1:E:434:LEU:N	1:E:435:PRO:HD2	2.28	0.48
1:E:443:TRP:N	1:E:443:TRP:CE3	2.81	0.48
1:F:69:TYR:CD1	1:F:463:MET:HG3	2.48	0.48
1:G:5:ASP:C	1:G:6:ILE:HG12	2.37	0.48
1:G:197:LEU:HB2	1:G:199:LYS:HB3	1.95	0.48
1:H:5:ASP:C	1:H:6:ILE:HG12	2.38	0.48
1:H:86:TRP:HA	1:H:86:TRP:CE3	2.49	0.48
1:H:492:ASN:HD22	1:H:492:ASN:N	2.10	0.48
2:B:601:FAD:H6	3:B:602:GDU:O3'	2.12	0.48
1:C:5:ASP:OD2	1:C:258:THR:HA	2.12	0.48
1:C:87:TYR:HB3	1:C:89:HIS:CE1	2.48	0.48
1:C:232:GLU:OE2	1:C:232:GLU:N	2.45	0.48
1:G:242:VAL:HG13	1:G:252:VAL:HG22	1.94	0.48
1:H:109:ASN:C	1:H:111:SER:N	2.69	0.48
1:A:56:PHE:CE1	1:A:339:GLN:HB3	2.49	0.48
1:A:475:GLY:O	1:E:494:GLU:HB2	2.14	0.48
1:B:196:ILE:HD12	1:H:119:VAL:HG22	1.96	0.48
1:B:336:PRO:HG2	1:B:337:TYR:CD1	2.49	0.48
1:E:322:ASN:HD21	1:E:398:THR:HG22	1.77	0.48
1:E:331:PHE:CE2	1:E:338:ASN:ND2	2.82	0.48
1:G:28:GLN:HG2	1:G:497:LEU:O	2.13	0.48
1:G:234:THR:HB	1:G:236:PHE:CE2	2.48	0.48
1:C:8:VAL:HG11	1:C:35:MET:HG2	1.96	0.48
1:D:47:ALA:HB1	1:D:222:TRP:NE1	2.27	0.48
1:E:63:HIS:CE1	2:E:601:FAD:C5X	2.97	0.48
1:G:141:THR:OG1	1:G:144:GLU:HB2	2.13	0.48
1:H:167:TRP:HB2	1:H:174:MET:HE1	1.96	0.48
1:H:242:VAL:HG13	1:H:252:VAL:HG22	1.96	0.48
1:H:250:LYS:HD2	1:H:262:TYR:CE1	2.48	0.48
1:A:39:SER:HB3	1:A:241:LYS:HG2	1.95	0.48
1:A:125:MET:HE1	1:A:186:PRO:HB2	1.95	0.48
1:B:437:LEU:CD1	1:B:444:SER:HB2	2.44	0.48
1:C:224:ALA:O	1:C:228:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:PHE:CE1	1:D:339:GLN:HB3	2.49	0.48
1:E:70:LYS:HD2	1:E:70:LYS:HA	1.55	0.48
1:E:189:LYS:O	1:E:192:THR:OG1	2.20	0.48
1:F:324:PRO:O	1:F:374:VAL:HG11	2.13	0.48
1:F:387:ILE:HG23	1:F:388:LEU:N	2.28	0.48
1:G:185:ALA:O	1:G:186:PRO:C	2.57	0.48
1:B:47:ALA:CB	1:B:222:TRP:NE1	2.76	0.48
1:E:376:GLU:HG2	1:E:377:SER:N	2.28	0.48
1:G:17:PRO:HG2	2:G:601:FAD:H4'	1.96	0.48
1:G:58:TYR:CZ	1:G:299:GLY:HA3	2.48	0.48
1:A:32:PRO:HB3	1:E:504:PHE:HD2	1.78	0.48
1:A:39:SER:CB	1:A:241:LYS:HG2	2.43	0.48
1:A:87:TYR:HB3	1:A:89:HIS:HE1	1.79	0.48
1:C:388:LEU:O	1:C:392:ILE:HG13	2.13	0.48
1:C:466:VAL:HG12	1:C:495:ARG:NH1	2.29	0.48
1:D:125:MET:HE2	1:D:188:LEU:CA	2.44	0.48
1:F:69:TYR:CE2	1:F:463:MET:HG3	2.48	0.48
1:F:167:TRP:O	1:F:169:VAL:HG13	2.13	0.48
1:F:235:ARG:HG2	1:F:239:LYS:HD2	1.95	0.48
1:G:394:GLY:HA2	1:G:397:ASN:HB2	1.95	0.48
1:B:388:LEU:O	1:B:392:ILE:HG13	2.14	0.48
1:E:326:TYR:C	1:E:326:TYR:CD1	2.92	0.48
1:E:345:LYS:HG2	1:E:364:GLU:HG3	1.95	0.48
1:F:113:LEU:HB3	1:F:114:PRO:HD2	1.96	0.48
1:F:143:ASP:O	1:F:147:VAL:HG23	2.14	0.48
1:F:187:ASN:CG	1:F:189:LYS:HB2	2.39	0.48
1:G:65:ILE:HD12	1:G:65:ILE:HA	1.64	0.48
1:G:352:ALA:HB2	1:G:405:ASP:HB2	1.96	0.48
1:H:71:TYR:CE2	1:H:497:LEU:HA	2.49	0.48
1:H:507:SER:O	1:H:510:GLN:HB2	2.14	0.48
1:A:315:TRP:C	1:A:316:LEU:HG	2.38	0.47
1:C:250:LYS:HD3	1:C:262:TYR:O	2.14	0.47
1:D:72:PHE:CE2	1:D:76:LEU:HD11	2.48	0.47
1:E:387:ILE:HG23	1:E:388:LEU:N	2.28	0.47
1:E:431:THR:O	1:E:435:PRO:HG3	2.14	0.47
1:F:91:ARG:O	1:F:92:ILE:HD13	2.14	0.47
1:F:158:PHE:CD1	1:F:319:PRO:HG3	2.49	0.47
1:F:447:ARG:O	1:F:451:TRP:HA	2.14	0.47
1:G:21:GLY:HA2	1:G:462:PHE:CE1	2.48	0.47
1:G:146:ILE:O	1:G:149:MET:HB2	2.14	0.47
1:G:149:MET:HG2	1:G:184:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:401:LEU:HB3	1:G:405:ASP:HB2	1.96	0.47
1:H:139:PRO:CB	1:H:145:TRP:HB2	2.44	0.47
1:H:383:ASN:O	1:H:387:ILE:HB	2.14	0.47
1:B:125:MET:HE2	1:B:188:LEU:CA	2.44	0.47
1:B:249:ASN:O	1:B:251:THR:HG23	2.14	0.47
1:C:57:LEU:CD2	1:C:338:ASN:HA	2.43	0.47
1:C:420:PRO:O	1:C:422:PRO:HD3	2.14	0.47
1:E:134:VAL:O	1:E:134:VAL:CG1	2.61	0.47
1:E:391:CYS:O	1:E:395:LEU:HG	2.14	0.47
1:F:173:LYS:HA	1:F:424:LEU:HD11	1.95	0.47
1:F:402:LYS:HE3	1:F:404:THR:OG1	2.13	0.47
1:G:152:THR:O	1:G:156:ASP:CG	2.56	0.47
1:G:212:PHE:CD2	1:G:213:PRO:HD2	2.49	0.47
1:G:433:ILE:O	1:G:436:LYS:HB2	2.14	0.47
1:H:43:PRO:HG2	1:H:223:ILE:HD13	1.95	0.47
1:A:115:LYS:O	1:A:118:GLN:HB2	2.15	0.47
1:A:125:MET:HE2	1:A:188:LEU:CA	2.44	0.47
1:A:126:ILE:CD1	1:G:189:LYS:HG2	2.45	0.47
1:D:125:MET:CE	1:D:186:PRO:HB2	2.43	0.47
1:F:126:ILE:O	1:F:130:LEU:HG	2.14	0.47
1:G:296:HIS:HB2	1:G:374:VAL:HB	1.95	0.47
1:G:350:GLN:OE1	1:G:354:GLY:HA2	2.15	0.47
1:H:149:MET:SD	1:H:184:ALA:O	2.72	0.47
1:H:270:ALA:HA	1:H:448:PHE:C	2.39	0.47
1:A:199:LYS:HD2	1:A:200:THR:N	2.30	0.47
1:A:351:LEU:HB2	1:A:355:SER:OG	2.14	0.47
2:A:601:FAD:H9	2:A:601:FAD:C2'	2.43	0.47
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.48	0.47
1:E:154:ILE:HD13	1:E:154:ILE:N	2.22	0.47
1:E:175:GLN:OE1	1:E:178:TRP:HD1	1.97	0.47
1:F:56:PHE:CD2	1:F:409:SER:HB3	2.49	0.47
1:F:455:VAL:HA	1:F:460:HIS:HD1	1.79	0.47
1:G:425:GLU:CD	1:G:425:GLU:H	2.22	0.47
1:A:331:PHE:HB3	1:A:369:SER:HB3	1.96	0.47
1:B:175:GLN:HE22	1:B:177:ALA:HB3	1.80	0.47
1:B:179:LEU:HD23	1:B:183:VAL:HG21	1.96	0.47
1:E:19:GLY:O	1:E:22:ALA:HB3	2.15	0.47
1:E:63:HIS:CE1	2:E:601:FAD:N10	2.82	0.47
1:G:24:LYS:HD3	1:G:24:LYS:HA	1.67	0.47
1:G:302:VAL:HA	1:G:406:GLU:O	2.14	0.47
1:G:342:ALA:O	1:G:365:GLY:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:ARG:NH1	2:G:601:FAD:H1'1	2.28	0.47
1:H:292:TYR:HB3	1:H:451:TRP:CZ2	2.49	0.47
1:H:385:GLU:CD	1:H:385:GLU:H	2.23	0.47
1:A:455:VAL:HG21	1:A:480:THR:O	2.15	0.47
1:B:108:ASN:HB2	1:B:194:ASN:OD1	2.14	0.47
1:B:175:GLN:NE2	1:B:177:ALA:HB3	2.30	0.47
1:B:306:ARG:HA	1:B:307:PRO:HD3	1.79	0.47
1:C:175:GLN:NE2	1:C:177:ALA:HB3	2.30	0.47
1:D:420:PRO:O	1:D:422:PRO:HD3	2.14	0.47
1:E:56:PHE:HE1	1:E:339:GLN:HB3	1.75	0.47
1:E:179:LEU:N	1:E:179:LEU:CD2	2.77	0.47
1:F:51:VAL:HG12	1:F:52:THR:O	2.14	0.47
1:F:286:LEU:O	1:F:289:GLN:HB2	2.14	0.47
1:G:165:LYS:HD3	1:G:318:PHE:O	2.14	0.47
1:G:351:LEU:HB2	1:G:355:SER:H	1.78	0.47
1:H:62:GLY:O	2:H:601:FAD:O4	2.31	0.47
1:H:453:TYR:O	1:H:454:GLU:C	2.57	0.47
1:A:178:TRP:CB	1:A:454:GLU:CG	2.92	0.47
1:B:57:LEU:CD2	1:B:338:ASN:HA	2.45	0.47
1:B:87:TYR:HB3	1:B:89:HIS:HE1	1.80	0.47
1:B:192:THR:OG1	1:B:193:THR:N	2.47	0.47
1:C:483:TYR:N	1:C:484:PRO:HD3	2.30	0.47
1:D:27:ASN:C	1:D:27:ASN:HD22	2.23	0.47
1:E:47:ALA:HB1	1:E:222:TRP:NE1	2.30	0.47
1:E:63:HIS:CD2	1:E:63:HIS:N	2.81	0.47
1:F:109:ASN:ND2	1:F:109:ASN:N	2.63	0.47
1:F:244:LYS:HG2	1:F:245:VAL:N	2.30	0.47
1:F:265:LEU:O	1:F:442:ILE:HA	2.14	0.47
1:G:232:GLU:H	1:G:232:GLU:CD	2.19	0.47
1:G:460:HIS:NE2	1:G:488:ASN:OD1	2.47	0.47
1:H:72:PHE:CE1	1:H:459:ASP:HA	2.50	0.47
1:H:187:ASN:OD1	1:H:190:ALA:CB	2.63	0.47
1:H:332:SER:HA	1:H:339:GLN:HE22	1.75	0.47
1:H:337:TYR:N	1:H:337:TYR:HD1	2.12	0.47
1:H:418:GLY:O	1:H:419:TYR:HD1	1.96	0.47
1:A:344:LYS:HD2	1:A:345:LYS:H	1.79	0.47
1:B:130:LEU:HD23	1:H:130:LEU:CD2	2.44	0.47
1:C:269:MET:HG2	1:C:274:LEU:HD22	1.96	0.47
1:D:103:PRO:HB2	1:D:109:ASN:OD1	2.15	0.47
1:D:168:ALA:HB1	1:D:377:SER:HB3	1.97	0.47
1:D:417:HIS:HB3	1:D:448:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:LYS:HB2	1:E:85:ASP:OD2	2.15	0.47
1:E:427:GLU:O	1:E:428:GLY:C	2.58	0.47
1:G:426:ARG:O	1:G:430:LEU:HG	2.15	0.47
1:H:221:ILE:O	1:H:224:ALA:HB3	2.15	0.47
1:C:437:LEU:HD12	1:C:444:SER:HB2	1.96	0.47
1:D:17:PRO:HG2	2:D:601:FAD:H4'	1.96	0.47
1:E:6:ILE:O	1:E:260:ILE:HA	2.14	0.47
1:E:63:HIS:ND1	2:E:601:FAD:C10	2.78	0.47
1:E:274:LEU:O	1:E:278:MET:HG2	2.13	0.47
1:F:139:PRO:HA	1:F:144:GLU:OE2	2.14	0.47
1:G:420:PRO:HB2	1:G:451:TRP:CD1	2.50	0.47
1:H:64:VAL:HG22	1:H:210:PHE:CE1	2.49	0.47
1:H:71:TYR:CD2	1:H:496:ARG:C	2.93	0.47
1:H:175:GLN:HG3	1:H:178:TRP:CD1	2.50	0.47
1:A:494:GLU:HG2	1:E:477:VAL:HB	1.96	0.47
1:B:17:PRO:O	1:B:462:PHE:HA	2.15	0.47
1:B:242:VAL:HA	1:B:254:LEU:CD2	2.45	0.47
1:B:346:LEU:HD13	1:B:408:VAL:CG1	2.45	0.47
1:D:150:MET:HE3	1:D:159:MET:HG3	1.96	0.47
1:D:274:LEU:HD12	1:D:278:MET:HE3	1.96	0.47
1:E:158:PHE:O	1:E:161:PRO:HG2	2.15	0.47
1:E:508:LYS:HG3	1:E:509:ALA:N	2.29	0.47
1:F:22:ALA:O	1:F:26:LEU:HB2	2.14	0.47
1:H:65:ILE:HG22	1:H:65:ILE:O	2.14	0.47
1:H:96:ARG:HB2	1:H:101:TRP:CZ3	2.50	0.47
1:H:467:GLU:OE1	1:H:479:LEU:N	2.48	0.47
1:A:136:ASN:OD1	1:A:136:ASN:N	2.33	0.46
1:B:473:VAL:O	1:F:499:ASP:HB3	2.16	0.46
1:C:119:VAL:HA	1:E:196:ILE:CD1	2.44	0.46
1:C:150:MET:SD	1:C:159:MET:HE3	2.55	0.46
1:E:207:ASN:HB3	1:E:315:TRP:HH2	1.78	0.46
1:F:351:LEU:HA	1:F:405:ASP:O	2.14	0.46
1:G:169:VAL:O	1:G:174:MET:HE2	2.15	0.46
1:G:178:TRP:CD1	1:G:178:TRP:H	2.33	0.46
1:G:210:PHE:HD2	1:G:210:PHE:N	2.13	0.46
1:A:113:LEU:O	1:A:118:GLN:NE2	2.34	0.46
1:A:119:VAL:HG22	1:G:193:THR:HG22	1.96	0.46
1:A:125:MET:CE	1:A:186:PRO:HB2	2.44	0.46
1:B:106:PHE:C	1:B:106:PHE:HD2	2.23	0.46
1:B:178:TRP:CB	1:B:454:GLU:CG	2.92	0.46
1:B:287:THR:O	1:B:290:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:SER:CB	1:C:241:LYS:HG2	2.45	0.46
1:C:335:SER:HB3	1:C:338:ASN:OD1	2.14	0.46
1:C:483:TYR:HH	1:G:490:ARG:HH21	1.59	0.46
1:E:139:PRO:HA	1:E:144:GLU:OE2	2.16	0.46
1:F:95:VAL:HG23	1:F:102:VAL:O	2.16	0.46
1:G:106:PHE:CZ	1:G:113:LEU:HD11	2.50	0.46
1:H:326:TYR:CE2	1:H:375:SER:HB3	2.50	0.46
1:C:234:THR:HB	1:C:236:PHE:CZ	2.51	0.46
1:D:304:GLY:O	1:D:368:TRP:CD1	2.68	0.46
1:E:275:ALA:HB1	1:E:284:VAL:HG22	1.97	0.46
1:F:158:PHE:CD1	1:F:158:PHE:C	2.92	0.46
1:F:467:GLU:HG2	1:F:495:ARG:HH22	1.79	0.46
1:G:323:CYS:HB2	1:G:325:PHE:CE1	2.49	0.46
1:H:58:TYR:CZ	1:H:299:GLY:HA3	2.50	0.46
1:A:46:LEU:O	1:A:63:HIS:HE1	1.98	0.46
1:B:350:GLN:NE2	1:B:351:LEU:O	2.49	0.46
1:C:196:ILE:HG21	1:E:119:VAL:CG2	2.44	0.46
1:D:94:TYR:CD1	1:D:101:TRP:HB3	2.51	0.46
1:E:10:VAL:O	1:E:34:TRP:HA	2.15	0.46
1:E:70:LYS:HB3	1:E:496:ARG:NH1	2.27	0.46
1:E:402:LYS:HE3	1:E:404:THR:OG1	2.15	0.46
1:E:457:ASN:HB3	2:E:601:FAD:N1	2.31	0.46
1:H:499:ASP:O	1:H:500:GLY:C	2.58	0.46
1:A:417:HIS:HB3	1:A:448:PHE:CZ	2.50	0.46
1:D:175:GLN:HE22	1:D:177:ALA:HB3	1.80	0.46
1:F:376:GLU:HB2	1:F:382:VAL:CG1	2.45	0.46
1:G:351:LEU:CD1	1:G:404:THR:HA	2.46	0.46
1:G:453:TYR:O	1:G:454:GLU:C	2.59	0.46
1:G:499:ASP:O	1:G:500:GLY:C	2.57	0.46
1:H:164:PHE:CD1	1:H:164:PHE:C	2.92	0.46
1:H:376:GLU:CG	1:H:382:VAL:HG13	2.35	0.46
1:A:94:TYR:CD1	1:A:101:TRP:HB3	2.50	0.46
3:C:602:GDU:O2A	3:C:602:GDU:H4D	2.16	0.46
1:E:56:PHE:CE2	1:E:409:SER:HB3	2.50	0.46
1:E:167:TRP:O	1:E:169:VAL:HG13	2.16	0.46
1:G:70:LYS:HB2	1:G:493:THR:HA	1.98	0.46
1:G:210:PHE:N	1:G:210:PHE:CD2	2.83	0.46
1:G:499:ASP:O	1:G:502:GLN:N	2.48	0.46
1:G:499:ASP:HB2	1:G:502:GLN:OE1	2.16	0.46
1:H:70:LYS:HA	1:H:70:LYS:HD2	1.62	0.46
1:H:210:PHE:HD2	1:H:210:PHE:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:367:TYR:HD1	1:H:408:VAL:HG21	1.80	0.46
1:D:304:GLY:O	1:D:368:TRP:HD1	1.97	0.46
1:D:473:VAL:HG12	1:H:501:ALA:HA	1.98	0.46
1:E:56:PHE:CD2	1:E:409:SER:HB3	2.51	0.46
1:E:494:GLU:CD	1:E:494:GLU:N	2.72	0.46
1:G:292:TYR:HB3	1:G:451:TRP:CZ2	2.50	0.46
1:H:2:THR:OG1	1:H:3:HIS:N	2.47	0.46
1:H:469:VAL:HA	1:H:472:ILE:HD12	1.98	0.46
1:A:193:THR:O	1:A:196:ILE:HB	2.15	0.46
1:D:303:ARG:NH2	1:D:363:LYS:O	2.43	0.46
1:D:303:ARG:NH1	1:D:348:THR:OG1	2.49	0.46
1:E:38:ASP:HB3	1:E:236:PHE:HD1	1.79	0.46
1:E:250:LYS:O	1:E:261:GLY:HA2	2.16	0.46
1:E:467:GLU:CG	1:E:495:ARG:HH12	2.29	0.46
1:F:332:SER:HB3	1:F:369:SER:H	1.80	0.46
1:F:397:ASN:C	1:F:399:GLU:N	2.74	0.46
1:G:143:ASP:HA	1:G:146:ILE:CD1	2.43	0.46
1:B:45:GLY:HA3	2:B:601:FAD:O1A	2.16	0.46
1:B:57:LEU:CD1	1:B:57:LEU:N	2.79	0.46
1:B:60:VAL:O	1:B:61:GLY:O	2.34	0.46
1:B:152:THR:HG22	1:B:156:ASP:OD2	2.16	0.46
1:C:339:GLN:CD	1:C:339:GLN:N	2.74	0.46
1:C:344:LYS:HD2	1:C:345:LYS:H	1.79	0.46
1:C:398:THR:HB	1:C:400:MET:CG	2.46	0.46
1:E:63:HIS:CE1	2:E:601:FAD:C9	2.99	0.46
1:E:69:TYR:CE2	1:E:463:MET:HG3	2.51	0.46
1:E:139:PRO:HA	1:E:144:GLU:CD	2.41	0.46
1:G:25:ARG:NH1	1:G:470:ASP:OD2	2.49	0.46
1:G:28:GLN:NE2	1:G:497:LEU:O	2.43	0.46
1:G:196:ILE:HG22	1:G:197:LEU:N	2.31	0.46
1:H:63:HIS:HB2	1:H:218:THR:HG21	1.97	0.46
1:H:419:TYR:CD1	1:H:419:TYR:N	2.84	0.46
1:A:398:THR:HB	1:A:400:MET:HG2	1.98	0.46
1:B:136:ASN:ND2	1:F:133:ARG:HE	2.14	0.46
1:B:204:TRP:CG	1:B:205:GLY:H	2.33	0.46
1:B:325:PHE:CZ	1:B:395:LEU:HD23	2.50	0.46
1:B:455:VAL:O	1:B:460:HIS:CB	2.62	0.46
1:D:38:ASP:OD1	2:D:601:FAD:H1B	2.15	0.46
1:E:349:MET:O	1:E:350:GLN:HB3	2.16	0.46
1:E:457:ASN:C	2:E:601:FAD:O3'	2.59	0.46
1:F:9:ASP:H	1:F:33:SER:HG	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:VAL:O	1:F:36:ILE:HA	2.15	0.46
1:G:44:GLY:HA2	1:G:222:TRP:CD1	2.51	0.46
1:G:460:HIS:CE1	1:G:488:ASN:OD1	2.68	0.46
1:H:178:TRP:CD1	1:H:178:TRP:N	2.84	0.46
1:H:192:THR:OG1	1:H:193:THR:N	2.49	0.46
1:A:204:TRP:CE3	1:A:205:GLY:N	2.85	0.45
1:B:419:TYR:HE1	2:B:601:FAD:C7M	2.29	0.45
1:B:443:TRP:N	1:B:443:TRP:CE3	2.84	0.45
1:B:500:GLY:HA3	1:F:472:ILE:O	2.16	0.45
1:C:244:LYS:HG2	1:C:245:VAL:N	2.30	0.45
1:E:71:TYR:HB2	1:E:495:ARG:O	2.16	0.45
1:E:143:ASP:OD2	1:E:171:THR:OG1	2.30	0.45
1:E:430:LEU:HD23	1:E:430:LEU:HA	1.73	0.45
1:F:18:THR:O	1:F:465:GLY:HA3	2.16	0.45
1:G:103:PRO:HB2	1:G:202:GLY:HA3	1.97	0.45
1:H:299:GLY:HA2	1:H:370:ILE:O	2.16	0.45
1:A:301:GLY:HA3	1:A:409:SER:CB	2.46	0.45
1:A:483:TYR:N	1:A:484:PRO:HD3	2.30	0.45
1:B:159:MET:HE1	3:B:602:GDU:C4	2.45	0.45
1:C:100:GLN:OE1	1:C:100:GLN:HA	2.17	0.45
1:E:306:ARG:NH1	1:E:333:ASN:OD1	2.49	0.45
1:F:64:VAL:CG1	1:F:65:ILE:N	2.79	0.45
1:G:92:ILE:HB	1:G:314:CYS:H	1.81	0.45
1:G:103:PRO:HD2	1:G:109:ASN:CG	2.41	0.45
1:G:273:PHE:N	1:G:273:PHE:CD1	2.81	0.45
1:H:126:ILE:HA	1:H:188:LEU:HD11	1.98	0.45
1:A:150:MET:HG2	1:A:154:ILE:HG21	1.97	0.45
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.52	0.45
1:C:469:VAL:O	1:C:472:ILE:N	2.48	0.45
1:E:66:PHE:HB3	1:E:206:PRO:O	2.15	0.45
1:F:91:ARG:HG2	1:F:92:ILE:N	2.31	0.45
1:F:142:PHE:HB2	1:F:174:MET:HB2	1.96	0.45
1:G:12:VAL:HA	1:G:266:VAL:O	2.17	0.45
1:G:54:GLU:HB3	1:G:346:LEU:CD1	2.45	0.45
1:G:271:VAL:HB	1:G:449:GLY:O	2.16	0.45
1:H:196:ILE:HG22	1:H:197:LEU:N	2.31	0.45
1:H:401:LEU:HB3	1:H:405:ASP:HB2	1.99	0.45
1:A:160:ARG:N	1:A:161:PRO:HD2	2.31	0.45
1:A:457:ASN:O	1:A:460:HIS:HB2	2.16	0.45
1:B:443:TRP:CD1	1:B:445:ARG:NH2	2.84	0.45
1:C:480:THR:HA	1:C:487:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:VAL:HG22	1:E:57:LEU:HG	1.97	0.45
1:E:192:THR:O	1:E:193:THR:C	2.59	0.45
1:F:22:ALA:HA	1:F:469:VAL:HG21	1.97	0.45
1:G:69:TYR:HD1	1:G:492:ASN:HB2	1.81	0.45
1:G:156:ASP:HB2	1:G:157:LEU:HD12	1.98	0.45
1:G:207:ASN:OD1	1:G:208:ALA:N	2.49	0.45
1:G:306:ARG:HA	1:G:307:PRO:HD3	1.55	0.45
1:H:44:GLY:HA2	1:H:222:TRP:CD1	2.52	0.45
1:H:106:PHE:CZ	1:H:113:LEU:HD11	2.51	0.45
1:H:292:TYR:CZ	1:H:417:HIS:CE1	3.04	0.45
1:H:417:HIS:HB3	1:H:448:PHE:CD2	2.50	0.45
1:A:6:ILE:HD13	1:A:6:ILE:N	2.32	0.45
1:A:110:ILE:CA	1:A:113:LEU:HD12	2.42	0.45
1:A:296:HIS:CE1	1:A:382:VAL:HG21	2.50	0.45
1:D:106:PHE:C	1:D:106:PHE:CD2	2.94	0.45
1:F:17:PRO:O	1:F:462:PHE:CD1	2.69	0.45
1:F:336:PRO:HG2	1:F:337:TYR:CE1	2.52	0.45
1:G:109:ASN:C	1:G:111:SER:N	2.72	0.45
1:A:199:LYS:HE2	1:A:199:LYS:HB3	1.67	0.45
1:A:325:PHE:CA	1:A:374:VAL:HG22	2.46	0.45
1:B:344:LYS:HD2	1:B:345:LYS:H	1.81	0.45
1:C:196:ILE:HD12	1:E:119:VAL:HG22	1.98	0.45
1:C:301:GLY:HA3	1:C:409:SER:CB	2.45	0.45
1:C:304:GLY:O	1:C:368:TRP:HD1	1.99	0.45
1:C:307:PRO:HB2	1:C:309:ARG:HG2	1.99	0.45
1:D:242:VAL:HG23	2:D:601:FAD:N1A	2.31	0.45
1:E:82:LYS:HB2	1:E:85:ASP:CG	2.42	0.45
1:E:264:LYS:HD3	1:E:472:ILE:HG23	1.98	0.45
1:E:265:LEU:O	1:E:442:ILE:HA	2.17	0.45
1:E:499:ASP:O	1:E:503:VAL:HG23	2.16	0.45
1:F:139:PRO:HA	1:F:144:GLU:CD	2.42	0.45
1:F:286:LEU:HD21	1:F:436:LYS:HE3	1.98	0.45
1:G:70:LYS:HD2	1:G:70:LYS:HA	1.77	0.45
1:G:483:TYR:N	1:G:484:PRO:HD3	2.31	0.45
2:G:601:FAD:O1A	2:G:601:FAD:O5'	2.30	0.45
1:H:125:MET:HE2	1:H:186:PRO:HB3	1.99	0.45
1:H:181:GLU:HG3	1:H:181:GLU:O	2.16	0.45
1:H:219:GLY:O	1:H:223:ILE:HG12	2.16	0.45
1:H:464:LEU:HD21	1:H:481:LEU:N	2.32	0.45
1:H:486:PHE:CE2	1:H:490:ARG:HD2	2.52	0.45
1:A:150:MET:HE2	1:A:150:MET:HB2	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLY:H	1:C:268:THR:HG21	1.81	0.45
1:C:125:MET:HE2	1:C:188:LEU:CA	2.46	0.45
1:C:272:ASP:N	1:C:272:ASP:OD1	2.48	0.45
1:C:455:VAL:HG11	1:C:464:LEU:HD11	1.99	0.45
1:D:395:LEU:HA	1:D:400:MET:HG3	1.97	0.45
1:E:70:LYS:NZ	1:E:73:ASP:HB2	2.32	0.45
1:F:504:PHE:CD1	1:F:504:PHE:N	2.82	0.45
1:G:237:GLY:C	1:G:239:LYS:N	2.73	0.45
1:A:312:ASP:OD1	1:A:312:ASP:N	2.44	0.45
1:B:119:VAL:HG13	1:H:193:THR:CG2	2.47	0.45
1:B:350:GLN:NE2	1:B:354:GLY:HA2	2.28	0.45
1:C:96:ARG:O	1:C:319:PRO:HD2	2.16	0.45
1:C:192:THR:OG1	1:C:193:THR:N	2.49	0.45
1:D:335:SER:OG	1:D:336:PRO:HD2	2.17	0.45
1:E:70:LYS:HE3	1:E:70:LYS:O	2.17	0.45
1:E:107:GLN:O	1:E:110:ILE:HG22	2.16	0.45
1:E:272:ASP:OD1	1:E:272:ASP:N	2.47	0.45
1:F:207:ASN:HB3	1:F:315:TRP:CZ2	2.52	0.45
1:G:72:PHE:CE1	1:G:459:ASP:HA	2.51	0.45
1:H:69:TYR:HD1	1:H:492:ASN:HB2	1.80	0.45
1:H:130:LEU:O	1:H:133:ARG:CB	2.63	0.45
1:H:181:GLU:OE1	1:H:181:GLU:CA	2.62	0.45
1:H:210:PHE:HZ	1:H:334:TYR:CE1	2.34	0.45
1:C:346:LEU:HD13	1:C:408:VAL:CG1	2.47	0.45
1:C:395:LEU:HA	1:C:400:MET:HG3	1.99	0.45
1:D:35:MET:HE1	1:D:235:ARG:HG3	1.98	0.45
1:D:194:ASN:HD22	1:D:194:ASN:HA	1.55	0.45
1:E:91:ARG:O	1:E:92:ILE:HD13	2.16	0.45
1:E:109:ASN:N	1:E:109:ASN:ND2	2.62	0.45
1:E:152:THR:O	1:E:153:GLY:C	2.57	0.45
1:E:318:PHE:CZ	1:E:325:PHE:HE1	2.35	0.45
1:G:86:TRP:CE3	1:G:86:TRP:HA	2.52	0.45
1:G:130:LEU:O	1:G:133:ARG:N	2.50	0.45
1:G:150:MET:CG	1:G:154:ILE:HB	2.36	0.45
1:G:411:TYR:CD1	1:G:412:HIS:N	2.69	0.45
1:H:165:LYS:O	1:H:375:SER:OG	2.28	0.45
1:H:351:LEU:O	1:H:354:GLY:N	2.43	0.45
1:H:353:ASP:HB3	1:H:403:PRO:CB	2.46	0.45
1:H:421:THR:HA	1:H:422:PRO:HD3	1.74	0.45
1:B:28:GLN:NE2	1:B:497:LEU:O	2.50	0.45
1:B:116:GLU:O	1:B:119:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:HG2	1:B:188:LEU:HD13	1.99	0.45
1:D:70:LYS:HD2	1:D:70:LYS:HA	1.51	0.45
1:D:115:LYS:HB3	1:F:197:LEU:CD2	2.46	0.45
1:D:175:GLN:NE2	1:D:177:ALA:HB3	2.32	0.45
1:E:166:VAL:HA	1:E:326:TYR:CD2	2.52	0.45
1:E:235:ARG:HG2	1:E:239:LYS:HD2	1.98	0.45
1:E:325:PHE:HA	1:E:374:VAL:CG2	2.47	0.45
1:F:436:LYS:O	1:F:439:ASP:HB2	2.16	0.45
1:G:30:ASP:OD1	1:G:30:ASP:O	2.35	0.45
1:H:61:GLY:HA3	2:H:601:FAD:H6	1.98	0.45
1:H:187:ASN:OD1	1:H:190:ALA:HB2	2.17	0.45
1:H:273:PHE:N	1:H:273:PHE:CD1	2.82	0.45
1:B:304:GLY:O	1:B:368:TRP:CD1	2.70	0.44
1:C:376:GLU:HA	1:C:380:LYS:O	2.17	0.44
1:C:434:LEU:HD23	1:C:434:LEU:HA	1.84	0.44
1:D:307:PRO:HD2	1:D:310:ILE:HD12	1.98	0.44
1:D:323:CYS:HB2	1:D:325:PHE:CE2	2.52	0.44
1:E:158:PHE:CD1	1:E:158:PHE:C	2.94	0.44
1:E:332:SER:CB	1:E:369:SER:H	2.29	0.44
1:H:104:TYR:CG	1:H:105:PRO:HA	2.52	0.44
1:H:134:VAL:O	1:H:134:VAL:CG1	2.64	0.44
1:H:443:TRP:N	1:H:443:TRP:HE3	2.15	0.44
1:A:106:PHE:HD2	1:A:106:PHE:O	2.01	0.44
1:A:278:MET:HE1	1:A:442:ILE:HD12	1.99	0.44
1:B:138:LYS:HE3	1:B:138:LYS:HB2	1.86	0.44
1:C:19:GLY:O	1:C:22:ALA:HB3	2.17	0.44
1:C:91:ARG:O	1:C:92:ILE:HD13	2.17	0.44
1:D:115:LYS:HD3	1:F:197:LEU:HA	1.98	0.44
1:E:63:HIS:CD2	1:E:63:HIS:H	2.33	0.44
1:E:163:ASN:HA	1:E:166:VAL:CG1	2.46	0.44
1:E:187:ASN:O	1:E:191:VAL:HG23	2.18	0.44
1:E:385:GLU:H	1:E:385:GLU:HG2	1.47	0.44
1:F:205:GLY:C	1:F:207:ASN:H	2.25	0.44
1:G:139:PRO:HA	1:G:144:GLU:OE2	2.17	0.44
1:G:312:ASP:OD1	1:G:312:ASP:N	2.37	0.44
1:G:417:HIS:HB3	1:G:448:PHE:CD2	2.52	0.44
1:G:417:HIS:HB3	1:G:448:PHE:CZ	2.51	0.44
1:B:6:ILE:O	1:B:260:ILE:HA	2.17	0.44
1:C:299:GLY:HA2	1:C:370:ILE:O	2.17	0.44
1:C:325:PHE:HA	1:C:374:VAL:HG22	1.98	0.44
1:D:138:LYS:HA	1:D:139:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:THR:O	1:D:399:GLU:HB2	2.17	0.44
1:E:10:VAL:HG13	1:E:264:LYS:HB2	2.00	0.44
1:E:104:TYR:CE1	3:E:602:GDU:H5	2.52	0.44
1:E:445:ARG:CZ	1:E:481:LEU:HD22	2.46	0.44
1:F:134:VAL:O	1:F:134:VAL:CG1	2.65	0.44
1:F:209:THR:O	1:F:210:PHE:HB3	2.17	0.44
1:F:307:PRO:HD3	1:F:368:TRP:CE2	2.52	0.44
1:G:254:LEU:HB2	1:G:258:THR:HB	1.98	0.44
1:G:283:LEU:HD22	1:G:433:ILE:HG23	1.99	0.44
1:G:299:GLY:HA2	1:G:371:MET:HA	1.98	0.44
1:G:348:THR:HG21	1:G:406:GLU:HG2	2.00	0.44
1:H:210:PHE:N	1:H:210:PHE:CD2	2.84	0.44
1:A:91:ARG:O	1:A:92:ILE:HD13	2.18	0.44
1:A:178:TRP:CZ3	1:A:179:LEU:HD23	2.52	0.44
1:A:204:TRP:CG	1:A:205:GLY:H	2.34	0.44
1:B:58:TYR:HA	1:B:331:PHE:CE2	2.47	0.44
1:C:162:TYR:CD2	1:C:162:TYR:C	2.96	0.44
1:C:350:GLN:HE21	1:C:350:GLN:HB2	1.57	0.44
1:D:108:ASN:HB2	1:D:194:ASN:OD1	2.18	0.44
1:E:467:GLU:HG2	1:E:495:ARG:CZ	2.48	0.44
1:G:148:ARG:O	1:G:186:PRO:HD3	2.18	0.44
1:G:341:GLU:CG	1:G:343:SER:H	2.27	0.44
1:H:9:ASP:OD1	1:H:33:SER:N	2.49	0.44
1:H:276:GLU:O	1:H:279:ASN:N	2.48	0.44
1:H:404:THR:O	1:H:405:ASP:C	2.61	0.44
1:A:5:ASP:N	1:A:259:THR:OG1	2.41	0.44
1:C:42:THR:HG22	1:C:223:ILE:HD11	1.98	0.44
1:C:194:ASN:HD22	1:C:194:ASN:HA	1.59	0.44
1:E:58:TYR:CE1	1:E:299:GLY:HA3	2.52	0.44
1:E:110:ILE:CG2	1:E:195:VAL:HG22	2.47	0.44
1:E:286:LEU:O	1:E:289:GLN:HB2	2.18	0.44
1:E:318:PHE:CE2	1:E:398:THR:HG21	2.52	0.44
1:F:125:MET:CG	1:F:188:LEU:HD13	2.46	0.44
1:F:275:ALA:HB1	1:F:284:VAL:HG22	1.99	0.44
1:H:65:ILE:HD12	1:H:65:ILE:HA	1.61	0.44
1:H:158:PHE:O	1:H:161:PRO:HD2	2.17	0.44
1:H:271:VAL:HB	1:H:449:GLY:O	2.17	0.44
1:H:455:VAL:HG21	1:H:480:THR:O	2.17	0.44
1:A:38:ASP:OD2	1:A:40:ASN:CB	2.65	0.44
1:A:103:PRO:HG2	1:A:109:ASN:OD1	2.17	0.44
1:C:207:ASN:O	1:C:208:ALA:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:VAL:O	1:C:298:ILE:HD13	2.18	0.44
1:E:143:ASP:HB2	1:E:171:THR:C	2.43	0.44
1:F:70:LYS:CB	1:F:496:ARG:HH12	2.29	0.44
1:F:162:TYR:O	1:F:166:VAL:CG1	2.65	0.44
1:F:310:ILE:HG22	1:F:311:GLY:N	2.32	0.44
1:F:443:TRP:HE3	1:F:443:TRP:H	1.64	0.44
1:H:223:ILE:HD13	1:H:223:ILE:N	2.33	0.44
1:H:434:LEU:HB2	1:H:435:PRO:HD3	2.00	0.44
1:A:159:MET:HE1	3:A:602:GDU:C2	2.48	0.44
1:A:447:ARG:HD2	2:A:601:FAD:H3'	2.00	0.44
1:B:25:ARG:HH22	1:B:499:ASP:CG	2.26	0.44
1:B:119:VAL:HG13	1:H:193:THR:HG22	1.99	0.44
1:C:193:THR:O	1:C:197:LEU:HG	2.17	0.44
1:C:437:LEU:CD1	1:C:444:SER:HB2	2.48	0.44
1:D:346:LEU:HD13	1:D:408:VAL:HG13	1.99	0.44
1:E:104:TYR:CE1	3:E:602:GDU:C5	2.94	0.44
1:E:112:MET:HE3	1:E:112:MET:HB2	1.94	0.44
1:E:336:PRO:HG2	1:E:337:TYR:CE1	2.53	0.44
1:F:294:SER:CB	1:F:414:ARG:NH2	2.80	0.44
1:F:298:ILE:HG22	1:F:298:ILE:O	2.16	0.44
1:G:18:THR:CB	2:G:601:FAD:O2P	2.66	0.44
1:G:108:ASN:OD1	1:G:108:ASN:N	2.49	0.44
1:H:296:HIS:HB2	1:H:374:VAL:HB	1.98	0.44
1:A:398:THR:O	1:A:399:GLU:HB2	2.18	0.44
1:C:249:ASN:O	1:C:251:THR:HG23	2.17	0.44
1:D:296:HIS:CE1	1:D:382:VAL:HG21	2.52	0.44
1:D:455:VAL:O	1:D:460:HIS:CB	2.64	0.44
1:E:24:LYS:HA	1:E:24:LYS:HD3	1.73	0.44
1:E:109:ASN:N	1:E:109:ASN:HD22	2.16	0.44
1:F:107:GLN:NE2	1:F:108:ASN:OD1	2.51	0.44
1:F:382:VAL:HG23	1:F:383:ASN:N	2.32	0.44
1:G:107:GLN:CD	1:G:107:GLN:N	2.75	0.44
1:G:204:TRP:O	1:G:208:ALA:HB3	2.18	0.44
1:G:348:THR:HB	1:G:357:PRO:HB3	2.00	0.44
1:A:183:VAL:HG22	3:A:602:GDU:C1D	2.48	0.44
1:B:150:MET:SD	1:B:159:MET:HE3	2.57	0.44
1:B:350:GLN:HE21	1:B:350:GLN:HB2	1.51	0.44
1:B:402:LYS:HB3	1:B:404:THR:HG23	2.00	0.44
1:B:433:ILE:O	1:B:436:LYS:HB2	2.17	0.44
1:B:469:VAL:O	1:B:473:VAL:HG23	2.18	0.44
1:C:264:LYS:HD2	1:C:443:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:GLN:H	1:D:384:GLN:HG2	1.65	0.44
1:E:303:ARG:HH21	1:E:363:LYS:HB2	1.82	0.44
1:F:18:THR:HG23	1:F:464:LEU:HB2	1.98	0.44
1:G:160:ARG:HB2	1:G:161:PRO:CD	2.48	0.44
1:H:296:HIS:ND1	1:H:412:HIS:HE1	2.16	0.44
1:H:443:TRP:N	1:H:443:TRP:CE3	2.86	0.44
1:A:162:TYR:CD2	1:A:162:TYR:C	2.94	0.43
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.61	0.43
1:A:199:LYS:HD2	1:A:200:THR:H	1.83	0.43
1:A:455:VAL:O	1:A:460:HIS:CB	2.63	0.43
1:A:499:ASP:O	1:A:503:VAL:HG23	2.18	0.43
1:C:46:LEU:HB2	2:C:601:FAD:O4'	2.18	0.43
1:C:67:SER:HA	1:C:459:ASP:OD2	2.17	0.43
1:C:407:ILE:O	1:C:407:ILE:HG22	2.18	0.43
1:E:244:LYS:HB3	1:E:244:LYS:HE3	1.74	0.43
1:E:349:MET:O	1:E:350:GLN:CB	2.66	0.43
1:G:445:ARG:HH11	1:G:481:LEU:HD22	1.81	0.43
1:H:15:ALA:HB2	1:H:38:ASP:HB2	2.00	0.43
1:H:57:LEU:HD11	1:H:337:TYR:O	2.17	0.43
1:A:274:LEU:HD12	1:A:278:MET:HE3	1.99	0.43
1:B:70:LYS:HA	1:B:70:LYS:HD2	1.53	0.43
1:B:110:ILE:CA	1:B:113:LEU:HD12	2.37	0.43
1:B:323:CYS:HB2	1:B:325:PHE:CE2	2.54	0.43
1:C:9:ASP:CG	1:C:33:SER:HB3	2.43	0.43
1:C:446:GLY:O	1:C:450:SER:HB2	2.19	0.43
1:E:159:MET:HE1	3:E:602:GDU:C2	2.47	0.43
1:F:109:ASN:HD22	1:F:109:ASN:N	2.16	0.43
1:F:150:MET:C	1:F:154:ILE:HG13	2.43	0.43
1:F:165:LYS:HZ3	1:F:318:PHE:HB3	1.84	0.43
1:G:89:HIS:NE2	1:G:334:TYR:O	2.51	0.43
1:G:126:ILE:HG22	1:G:127:ASP:N	2.33	0.43
1:G:167:TRP:O	1:G:169:VAL:HG12	2.18	0.43
1:G:383:ASN:O	1:G:387:ILE:HB	2.18	0.43
1:G:460:HIS:O	1:G:464:LEU:HB2	2.19	0.43
1:H:83:GLU:HA	1:H:86:TRP:HD1	1.82	0.43
1:H:93:SER:C	1:H:94:TYR:CD2	2.96	0.43
1:H:336:PRO:HG2	1:H:337:TYR:HD1	1.82	0.43
1:H:339:GLN:CD	1:H:339:GLN:N	2.77	0.43
1:H:351:LEU:HD21	1:H:357:PRO:HA	2.00	0.43
1:B:398:THR:CG2	1:B:400:MET:CG	2.96	0.43
1:B:411:TYR:CD2	1:B:412:HIS:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:FAD:C2'	2:C:601:FAD:H9	2.48	0.43
1:D:106:PHE:C	1:D:106:PHE:HD2	2.26	0.43
1:D:411:TYR:CD2	1:D:412:HIS:N	2.86	0.43
1:E:64:VAL:CG1	1:E:65:ILE:N	2.81	0.43
1:E:158:PHE:CD1	1:E:319:PRO:HG3	2.53	0.43
1:F:187:ASN:OD1	1:F:189:LYS:CB	2.60	0.43
1:H:47:ALA:HA	2:H:601:FAD:O2'	2.18	0.43
1:H:130:LEU:O	1:H:133:ARG:N	2.51	0.43
1:H:234:THR:HB	1:H:236:PHE:CE2	2.53	0.43
1:A:47:ALA:HB1	1:A:222:TRP:NE1	2.32	0.43
1:A:480:THR:HA	1:A:487:VAL:HG11	1.99	0.43
1:C:495:ARG:O	1:C:496:ARG:HD2	2.19	0.43
1:D:178:TRP:CB	1:D:454:GLU:CG	2.96	0.43
1:E:155:ALA:HA	1:E:159:MET:HB2	2.01	0.43
1:E:325:PHE:HA	1:E:374:VAL:HG13	1.99	0.43
1:E:370:ILE:HG22	1:E:372:LEU:HD23	2.00	0.43
1:F:47:ALA:HB1	1:F:222:TRP:HE1	1.83	0.43
1:G:63:HIS:CD2	1:G:63:HIS:N	2.86	0.43
1:H:85:ASP:HA	1:H:214:ALA:CB	2.48	0.43
1:H:92:ILE:O	1:H:314:CYS:HB2	2.18	0.43
1:H:372:LEU:HD21	1:H:391:CYS:HB3	1.99	0.43
1:H:420:PRO:HB2	1:H:451:TRP:CD1	2.54	0.43
1:A:467:GLU:HG2	1:A:495:ARG:HH12	1.83	0.43
1:B:286:LEU:O	1:B:289:GLN:HG3	2.19	0.43
1:B:389:ALA:HA	1:B:392:ILE:CD1	2.49	0.43
1:D:142:PHE:CE1	1:D:179:LEU:HD21	2.53	0.43
1:E:147:VAL:CG2	1:E:160:ARG:HH21	2.30	0.43
1:E:332:SER:HB3	1:E:369:SER:H	1.83	0.43
1:E:467:GLU:HG2	1:E:495:ARG:HH22	1.83	0.43
1:F:137:THR:O	1:F:148:ARG:NH1	2.51	0.43
1:F:321:ASP:OD1	1:F:321:ASP:N	2.46	0.43
1:F:326:TYR:OH	1:F:373:GLU:OE2	2.37	0.43
1:F:376:GLU:HG2	1:F:377:SER:N	2.33	0.43
1:G:244:LYS:HB3	1:G:244:LYS:HE2	1.93	0.43
1:H:77:ASP:N	1:H:77:ASP:OD1	2.49	0.43
1:H:197:LEU:C	1:H:199:LYS:H	2.25	0.43
1:H:341:GLU:CG	1:H:343:SER:H	2.29	0.43
1:H:480:THR:HG23	1:H:487:VAL:HG21	2.00	0.43
1:B:115:LYS:O	1:B:118:GLN:HB2	2.18	0.43
1:B:483:TYR:N	1:B:484:PRO:HD3	2.33	0.43
1:C:150:MET:HE2	1:C:150:MET:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASP:HB3	1:C:283:LEU:HB2	2.00	0.43
1:C:323:CYS:HB2	1:C:325:PHE:CE2	2.53	0.43
1:C:467:GLU:HG2	1:C:495:ARG:HH12	1.84	0.43
1:E:69:TYR:CD1	1:E:463:MET:HG3	2.54	0.43
1:E:126:ILE:O	1:E:130:LEU:HG	2.18	0.43
1:E:145:TRP:HE3	1:E:146:ILE:N	2.17	0.43
1:E:207:ASN:HB3	1:E:315:TRP:CZ2	2.53	0.43
1:E:275:ALA:C	1:E:284:VAL:HG22	2.43	0.43
1:E:298:ILE:O	1:E:298:ILE:HG22	2.16	0.43
1:E:368:TRP:HZ3	1:E:370:ILE:HD11	1.80	0.43
1:F:328:ALA:HB2	1:F:372:LEU:HB3	2.00	0.43
1:G:125:MET:HG2	1:G:188:LEU:CD2	2.48	0.43
1:G:163:ASN:O	1:G:167:TRP:HB2	2.18	0.43
1:G:455:VAL:HG12	1:G:460:HIS:CD2	2.54	0.43
1:H:11:LEU:HD21	1:H:252:VAL:CG1	2.49	0.43
1:H:16:GLY:O	1:H:20:LEU:HG	2.19	0.43
1:H:351:LEU:HD13	1:H:404:THR:O	2.18	0.43
1:H:352:ALA:HB2	1:H:405:ASP:HB2	2.00	0.43
1:A:346:LEU:HD13	1:A:408:VAL:CG1	2.48	0.43
1:B:96:ARG:O	1:B:319:PRO:HD2	2.19	0.43
1:B:142:PHE:CE1	1:B:179:LEU:HD21	2.54	0.43
1:B:263:LYS:HD2	1:F:504:PHE:CE1	2.53	0.43
1:B:339:GLN:CD	1:B:339:GLN:N	2.76	0.43
1:C:423:THR:HB	1:C:425:GLU:OE1	2.18	0.43
1:D:49:THR:HG22	1:D:50:ASP:N	2.34	0.43
1:E:359:SER:OG	1:E:361:GLU:CB	2.66	0.43
1:E:376:GLU:HB2	1:E:382:VAL:HG13	2.01	0.43
1:E:455:VAL:HA	1:E:460:HIS:ND1	2.23	0.43
3:F:602:GDU:C2	3:F:602:GDU:H5'2	2.48	0.43
1:G:100:GLN:OE1	1:G:100:GLN:HA	2.19	0.43
1:H:384:GLN:O	1:H:387:ILE:HG22	2.19	0.43
1:A:307:PRO:HB2	1:A:309:ARG:HG2	2.01	0.43
1:A:335:SER:OG	1:A:336:PRO:HD2	2.19	0.43
1:A:418:GLY:C	1:A:419:TYR:HD1	2.27	0.43
1:D:9:ASP:CG	1:D:33:SER:HB3	2.43	0.43
1:D:232:GLU:CD	1:D:232:GLU:N	2.76	0.43
1:D:286:LEU:O	1:D:289:GLN:HG3	2.19	0.43
1:D:346:LEU:HD23	1:D:347:PRO:CD	2.48	0.43
1:F:6:ILE:CG2	1:F:7:SER:N	2.82	0.43
1:G:11:LEU:HB3	1:G:265:LEU:CD1	2.48	0.43
1:G:204:TRP:HB3	1:G:208:ALA:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:TYR:N	1:G:448:PHE:HZ	2.16	0.43
1:H:39:SER:HA	1:H:237:GLY:O	2.18	0.43
1:H:256:ASP:OD1	1:H:256:ASP:N	2.46	0.43
1:A:5:ASP:H	1:A:259:THR:HG1	1.59	0.43
1:A:114:PRO:O	1:A:118:GLN:HG3	2.19	0.43
1:B:77:ASP:O	1:B:81:PRO:HA	2.19	0.43
1:B:297:VAL:O	1:B:298:ILE:HD13	2.19	0.43
1:B:417:HIS:HB3	1:B:448:PHE:CZ	2.54	0.43
1:B:483:TYR:CE1	1:F:486:PHE:HE1	2.37	0.43
1:B:499:ASP:HB3	1:F:473:VAL:O	2.19	0.43
1:D:91:ARG:HG3	1:D:315:TRP:CZ2	2.54	0.43
1:D:346:LEU:HD23	1:D:347:PRO:HD2	2.01	0.43
1:E:69:TYR:O	1:E:72:PHE:HB3	2.18	0.43
1:E:306:ARG:HA	1:E:307:PRO:HD3	1.69	0.43
1:F:17:PRO:C	1:F:462:PHE:HA	2.43	0.43
1:F:291:PHE:CE1	1:F:292:TYR:O	2.72	0.43
1:H:108:ASN:OD1	1:H:108:ASN:N	2.51	0.43
1:H:165:LYS:HD3	1:H:318:PHE:O	2.18	0.43
1:H:168:ALA:HB1	1:H:377:SER:OG	2.18	0.43
1:H:446:GLY:N	1:H:450:SER:N	2.64	0.43
1:C:350:GLN:NE2	1:C:351:LEU:O	2.52	0.43
1:D:162:TYR:CD2	1:D:162:TYR:C	2.96	0.43
1:D:425:GLU:CD	1:D:425:GLU:H	2.26	0.43
1:E:12:VAL:CB	1:E:36:ILE:HG13	2.46	0.43
1:E:94:TYR:CE1	1:E:103:PRO:HG3	2.54	0.43
1:F:9:ASP:HB2	1:F:33:SER:O	2.18	0.43
1:F:58:TYR:CE1	1:F:299:GLY:HA3	2.54	0.43
1:F:179:LEU:N	1:F:179:LEU:CD2	2.80	0.43
1:F:322:ASN:HD21	1:F:398:THR:HG22	1.84	0.43
1:F:387:ILE:HG23	1:F:388:LEU:H	1.83	0.43
1:F:506:LYS:HD3	1:F:506:LYS:H	1.84	0.43
1:G:65:ILE:O	1:G:65:ILE:HG22	2.18	0.43
1:G:252:VAL:CG1	1:G:252:VAL:O	2.67	0.43
1:G:443:TRP:N	1:G:443:TRP:HE3	2.17	0.43
1:G:455:VAL:HB	1:G:460:HIS:HB3	2.01	0.43
1:H:479:LEU:HA	1:H:483:TYR:CD2	2.54	0.43
1:A:138:LYS:HE3	1:A:138:LYS:HB2	1.89	0.42
1:B:175:GLN:HE21	1:B:178:TRP:HD1	1.67	0.42
1:C:125:MET:HG2	1:C:188:LEU:HD13	2.01	0.42
1:C:166:VAL:HG13	1:C:167:TRP:CD1	2.53	0.42
1:C:245:VAL:HG22	1:C:252:VAL:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:TYR:CD2	1:C:412:HIS:N	2.86	0.42
1:E:134:VAL:O	1:E:134:VAL:HG13	2.19	0.42
1:E:159:MET:HE3	3:E:602:GDU:C2	2.49	0.42
1:E:436:LYS:O	1:E:439:ASP:HB2	2.19	0.42
1:G:57:LEU:CD1	1:G:57:LEU:N	2.82	0.42
1:G:168:ALA:HB1	1:G:377:SER:HG	1.83	0.42
1:G:387:ILE:HG23	1:G:388:LEU:N	2.34	0.42
1:H:165:LYS:NZ	1:H:325:PHE:O	2.43	0.42
1:H:272:ASP:O	1:H:276:GLU:OE2	2.37	0.42
1:H:402:LYS:HZ3	1:H:405:ASP:CG	2.18	0.42
1:A:204:TRP:CD2	1:A:205:GLY:N	2.85	0.42
1:B:162:TYR:CD2	1:B:162:TYR:C	2.96	0.42
1:C:199:LYS:HD2	1:C:200:THR:N	2.34	0.42
1:D:13:ILE:HG12	1:D:242:VAL:HG21	2.00	0.42
1:D:501:ALA:HB2	1:H:473:VAL:HG13	2.01	0.42
1:E:250:LYS:HA	1:E:262:TYR:CZ	2.55	0.42
1:E:318:PHE:CE1	1:E:325:PHE:HE1	2.37	0.42
1:F:24:LYS:HD3	1:F:24:LYS:HA	1.82	0.42
1:F:52:THR:C	1:F:54:GLU:N	2.77	0.42
1:F:108:ASN:O	1:F:194:ASN:HB3	2.19	0.42
1:F:122:ILE:HD12	1:F:122:ILE:HA	1.87	0.42
1:F:430:LEU:HD23	1:F:430:LEU:HA	1.82	0.42
1:G:69:TYR:CG	1:G:463:MET:HG3	2.53	0.42
1:G:77:ASP:OD1	1:G:77:ASP:N	2.49	0.42
1:G:93:SER:C	1:G:94:TYR:CD2	2.97	0.42
1:G:272:ASP:O	1:G:275:ALA:N	2.52	0.42
1:G:296:HIS:ND1	1:G:412:HIS:HE1	2.17	0.42
1:G:309:ARG:HG2	1:G:310:ILE:HD12	2.01	0.42
1:H:158:PHE:HE1	1:H:162:TYR:CD2	2.37	0.42
1:H:302:VAL:HA	1:H:406:GLU:O	2.18	0.42
1:H:394:GLY:HA2	1:H:397:ASN:ND2	2.34	0.42
1:H:443:TRP:HB3	1:H:445:ARG:NE	2.33	0.42
1:C:16:GLY:HA3	2:C:601:FAD:O1P	2.20	0.42
1:C:47:ALA:CB	1:C:222:TRP:NE1	2.81	0.42
1:C:160:ARG:HB2	1:C:161:PRO:HD3	2.02	0.42
1:C:232:GLU:CD	1:C:232:GLU:N	2.76	0.42
1:D:134:VAL:O	1:D:134:VAL:HG13	2.19	0.42
1:D:315:TRP:C	1:D:316:LEU:HG	2.44	0.42
1:E:68:HIS:ND1	1:E:68:HIS:N	2.67	0.42
1:E:113:LEU:HB3	1:E:114:PRO:HD2	2.00	0.42
1:F:167:TRP:CG	1:F:174:MET:CE	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:455:VAL:HG11	1:F:480:THR:O	2.19	0.42
1:G:162:TYR:CE2	1:G:166:VAL:HG11	2.54	0.42
1:G:164:PHE:CD1	1:G:164:PHE:C	2.96	0.42
1:G:387:ILE:HD12	1:G:387:ILE:HA	1.72	0.42
1:G:471:ASN:HA	1:G:476:ALA:N	2.32	0.42
1:H:402:LYS:HD3	1:H:402:LYS:H	1.84	0.42
1:H:477:VAL:CG2	1:H:478:GLU:N	2.82	0.42
1:A:32:PRO:CG	1:E:504:PHE:HD2	2.33	0.42
1:A:60:VAL:O	1:A:63:HIS:CD2	2.71	0.42
1:B:204:TRP:CD2	1:B:205:GLY:N	2.86	0.42
1:B:386:THR:OG1	1:B:387:ILE:N	2.53	0.42
1:B:486:PHE:CE1	1:F:483:TYR:CD1	3.04	0.42
1:E:122:ILE:CG2	1:E:123:ASP:N	2.81	0.42
1:E:168:ALA:HB1	1:E:380:LYS:HB3	2.00	0.42
1:E:364:GLU:CD	1:E:364:GLU:N	2.77	0.42
1:E:445:ARG:NE	1:E:481:LEU:HD22	2.34	0.42
1:E:467:GLU:HG2	1:E:495:ARG:HH12	1.83	0.42
2:E:601:FAD:O1P	2:E:601:FAD:O5B	2.38	0.42
1:F:422:PRO:HA	1:F:426:ARG:HD3	2.01	0.42
1:G:25:ARG:NH1	1:G:470:ASP:CG	2.70	0.42
1:G:309:ARG:HG2	1:G:310:ILE:CD1	2.49	0.42
1:G:339:GLN:N	1:G:339:GLN:CD	2.77	0.42
1:G:443:TRP:N	1:G:443:TRP:CE3	2.88	0.42
1:G:471:ASN:HB2	1:G:476:ALA:O	2.19	0.42
1:H:24:LYS:HA	1:H:24:LYS:HD3	1.69	0.42
1:H:89:HIS:NE2	1:H:334:TYR:HA	2.34	0.42
1:H:156:ASP:HA	1:H:160:ARG:HE	1.84	0.42
1:H:302:VAL:HG12	1:H:368:TRP:O	2.20	0.42
1:H:394:GLY:HA2	1:H:397:ASN:HB2	2.01	0.42
1:B:69:TYR:CD2	1:B:463:MET:HG3	2.54	0.42
1:B:458:GLN:HG3	2:B:601:FAD:N1	2.33	0.42
1:B:483:TYR:O	1:B:486:PHE:HB3	2.19	0.42
1:C:38:ASP:HA	2:C:601:FAD:C2A	2.48	0.42
1:C:175:GLN:HE22	1:C:177:ALA:HB3	1.85	0.42
1:E:16:GLY:H	2:E:601:FAD:H4B	1.84	0.42
1:E:110:ILE:HG13	1:E:113:LEU:HD12	2.02	0.42
1:E:129:ALA:O	1:E:132:ALA:HB3	2.20	0.42
1:E:396:VAL:HA	1:E:401:LEU:HB2	2.01	0.42
1:E:438:GLN:NE2	1:E:442:ILE:O	2.48	0.42
1:F:5:ASP:N	1:F:259:THR:OG1	2.30	0.42
1:F:143:ASP:OD2	1:F:171:THR:OG1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:345:LYS:HG2	1:F:364:GLU:HG3	2.01	0.42
1:F:352:ALA:HB3	1:F:403:PRO:HA	2.01	0.42
1:G:303:ARG:NH2	1:G:346:LEU:O	2.52	0.42
1:G:352:ALA:HB3	1:G:403:PRO:C	2.45	0.42
1:H:235:ARG:HE	1:H:235:ARG:HB3	1.51	0.42
2:H:601:FAD:H9	2:H:601:FAD:H1'1	1.34	0.42
1:A:57:LEU:HD12	1:A:57:LEU:N	2.35	0.42
1:A:174:MET:HB2	1:A:422:PRO:O	2.18	0.42
1:A:175:GLN:HG3	1:A:422:PRO:O	2.19	0.42
1:A:443:TRP:CD1	1:A:445:ARG:NH2	2.88	0.42
1:B:57:LEU:HD22	1:B:338:ASN:HA	2.02	0.42
1:C:150:MET:CE	1:C:159:MET:HE3	2.50	0.42
1:C:291:PHE:O	1:C:421:THR:HB	2.20	0.42
1:C:331:PHE:HD1	1:C:331:PHE:HA	1.73	0.42
1:D:182:ARG:HD2	3:D:602:GDU:O2A	2.19	0.42
1:D:244:LYS:HG2	1:D:245:VAL:H	1.84	0.42
1:D:280:ASP:HB3	1:D:283:LEU:HB2	2.02	0.42
1:D:332:SER:OG	1:D:369:SER:N	2.42	0.42
1:E:70:LYS:CB	1:E:496:ARG:HH12	2.29	0.42
1:E:205:GLY:HA2	1:E:206:PRO:HD3	1.74	0.42
1:E:231:LYS:HE2	1:E:231:LYS:HB3	1.71	0.42
1:E:303:ARG:HH22	1:E:363:LYS:HG3	1.79	0.42
1:E:397:ASN:C	1:E:399:GLU:N	2.75	0.42
1:E:437:LEU:O	1:E:442:ILE:N	2.45	0.42
1:F:93:SER:HG	1:F:315:TRP:NE1	2.18	0.42
1:G:11:LEU:HB3	1:G:265:LEU:HD12	2.01	0.42
1:G:85:ASP:HA	1:G:214:ALA:HB2	2.02	0.42
1:G:102:VAL:CG1	1:G:109:ASN:HB3	2.50	0.42
1:G:167:TRP:HB2	1:G:174:MET:HE1	2.01	0.42
1:G:351:LEU:O	1:G:352:ALA:C	2.61	0.42
1:G:367:TYR:CD1	1:G:408:VAL:HG21	2.51	0.42
1:G:402:LYS:HB2	1:G:402:LYS:HE2	1.68	0.42
1:H:447:ARG:HG2	1:H:448:PHE:CE2	2.54	0.42
1:B:9:ASP:CG	1:B:33:SER:HB3	2.45	0.42
1:B:100:GLN:OE1	1:B:100:GLN:HA	2.19	0.42
1:B:150:MET:HG2	1:B:154:ILE:HG21	2.02	0.42
1:D:38:ASP:HA	2:D:601:FAD:C2A	2.50	0.42
1:D:63:HIS:CD2	2:D:601:FAD:C6	3.03	0.42
1:D:158:PHE:CZ	3:D:602:GDU:N3	2.87	0.42
1:D:443:TRP:N	1:D:443:TRP:CE3	2.88	0.42
1:D:473:VAL:HG12	1:H:501:ALA:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ILE:HG13	1:E:146:ILE:H	1.72	0.42
1:E:159:MET:HE3	3:E:602:GDU:N3	2.35	0.42
3:F:602:GDU:H6	3:F:602:GDU:H2D	1.85	0.42
1:G:27:ASN:O	1:G:30:ASP:HB2	2.20	0.42
1:G:70:LYS:HE2	1:G:496:ARG:NH1	2.35	0.42
1:G:92:ILE:HG22	1:G:94:TYR:HE2	1.84	0.42
1:G:102:VAL:HA	1:G:103:PRO:HD3	1.78	0.42
1:H:25:ARG:NH2	1:H:495:ARG:HG3	2.34	0.42
1:H:483:TYR:CD2	1:H:483:TYR:N	2.87	0.42
1:A:358:GLN:CD	1:A:358:GLN:H	2.25	0.42
1:A:407:ILE:O	1:A:407:ILE:HG22	2.19	0.42
1:A:447:ARG:HB2	2:A:601:FAD:H5'2	2.02	0.42
1:B:331:PHE:HB3	1:B:369:SER:HB3	2.01	0.42
1:C:296:HIS:NE2	1:C:382:VAL:HG21	2.34	0.42
1:C:306:ARG:HA	1:C:307:PRO:HD3	1.82	0.42
1:C:499:ASP:HB3	1:G:473:VAL:O	2.19	0.42
1:D:8:VAL:HG11	1:D:35:MET:HG2	2.02	0.42
1:E:49:THR:HG22	1:E:50:ASP:N	2.35	0.42
1:F:26:LEU:HD22	1:F:34:TRP:HB3	2.02	0.42
1:F:291:PHE:CG	1:F:292:TYR:N	2.87	0.42
1:H:30:ASP:O	1:H:30:ASP:OD1	2.37	0.42
1:H:156:ASP:HB2	1:H:157:LEU:HD12	2.02	0.42
1:H:383:ASN:CG	1:H:385:GLU:HG2	2.45	0.42
1:B:308:GLU:CD	1:B:308:GLU:N	2.76	0.42
1:C:287:THR:O	1:C:290:LEU:HD12	2.20	0.42
1:C:433:ILE:O	1:C:436:LYS:HB2	2.20	0.42
1:C:483:TYR:O	1:C:486:PHE:HB3	2.19	0.42
1:D:178:TRP:CH2	1:D:179:LEU:HD23	2.55	0.42
1:D:423:THR:O	1:D:426:ARG:HB2	2.19	0.42
1:F:7:SER:HA	1:F:261:GLY:O	2.20	0.42
1:F:413:ARG:HG2	1:F:414:ARG:N	2.35	0.42
1:F:425:GLU:CD	1:F:425:GLU:N	2.78	0.42
1:G:47:ALA:HA	1:G:63:HIS:HE1	1.83	0.42
1:G:110:ILE:HG13	1:G:113:LEU:HD12	2.01	0.42
1:G:258:THR:CG2	1:G:259:THR:N	2.82	0.42
1:G:388:LEU:O	1:G:392:ILE:HG13	2.20	0.42
1:A:411:TYR:CD2	1:A:412:HIS:N	2.87	0.42
1:B:317:TYR:HE1	3:B:602:GDU:O1B	2.03	0.42
1:B:437:LEU:HD12	1:B:444:SER:HB2	2.00	0.42
1:C:446:GLY:H	1:C:450:SER:HB2	1.85	0.42
1:C:494:GLU:OE1	1:C:494:GLU:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:LYS:HD2	1:D:200:THR:N	2.35	0.42
1:F:46:LEU:O	1:F:60:VAL:HG21	2.20	0.42
1:F:168:ALA:HB1	1:F:377:SER:OG	2.20	0.42
1:G:207:ASN:O	1:G:208:ALA:C	2.62	0.42
1:G:302:VAL:HG13	1:G:368:TRP:CG	2.55	0.42
1:G:387:ILE:HA	1:G:390:ASP:OD2	2.19	0.42
1:H:82:LYS:HE2	1:H:84:ASP:OD1	2.19	0.42
1:H:297:VAL:HB	1:H:415:PHE:CE2	2.47	0.42
1:H:302:VAL:HG13	1:H:368:TRP:CG	2.55	0.42
1:H:401:LEU:HA	1:H:405:ASP:OD2	2.20	0.42
1:H:402:LYS:HE2	1:H:402:LYS:HB2	1.63	0.42
1:A:139:PRO:HB2	1:A:176:CYS:SG	2.60	0.41
1:A:250:LYS:HA	1:A:262:TYR:CZ	2.55	0.41
1:C:482:ASN:C	1:C:484:PRO:HD3	2.45	0.41
1:E:271:VAL:HG13	1:E:287:THR:CG2	2.49	0.41
1:E:467:GLU:CG	1:E:495:ARG:NH1	2.83	0.41
3:E:602:GDU:O1B	3:E:602:GDU:O5'	2.37	0.41
1:F:94:TYR:CE1	1:F:103:PRO:HG3	2.55	0.41
1:G:61:GLY:HA2	1:G:373:GLU:OE1	2.20	0.41
1:G:104:TYR:CG	1:G:105:PRO:HA	2.55	0.41
1:G:210:PHE:HD2	1:G:210:PHE:H	1.66	0.41
1:G:307:PRO:HG2	1:G:368:TRP:CZ2	2.55	0.41
1:G:335:SER:HB3	1:G:338:ASN:OD1	2.19	0.41
1:H:235:ARG:O	1:H:240:GLY:HA3	2.20	0.41
1:H:442:ILE:C	1:H:443:TRP:CE3	2.98	0.41
1:A:175:GLN:HG3	1:A:175:GLN:H	1.55	0.41
1:A:268:THR:HA	1:A:445:ARG:O	2.20	0.41
1:A:443:TRP:CD1	1:A:445:ARG:HH21	2.38	0.41
1:B:484:PRO:HA	1:B:487:VAL:HG22	2.02	0.41
1:D:57:LEU:HD12	1:D:57:LEU:N	2.35	0.41
1:D:110:ILE:CA	1:D:113:LEU:HD12	2.43	0.41
1:E:145:TRP:HH2	1:E:183:VAL:HG21	1.81	0.41
1:E:221:ILE:H	1:E:221:ILE:HG13	1.66	0.41
1:E:469:VAL:O	1:E:472:ILE:N	2.54	0.41
1:E:510:GLN:OE1	1:E:510:GLN:N	2.53	0.41
1:F:16:GLY:O	1:F:19:GLY:N	2.53	0.41
1:F:42:THR:HA	1:F:43:PRO:HD2	1.85	0.41
1:F:153:GLY:O	1:F:157:LEU:HB2	2.20	0.41
1:F:453:TYR:CD2	1:F:453:TYR:C	2.97	0.41
1:G:90:GLN:O	1:G:92:ILE:HG12	2.20	0.41
1:G:130:LEU:O	1:G:133:ARG:CB	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:TRP:CZ2	1:G:178:TRP:CH2	3.08	0.41
1:G:353:ASP:OD2	1:G:353:ASP:C	2.63	0.41
1:H:71:TYR:HB2	1:H:495:ARG:O	2.20	0.41
1:H:122:ILE:HD13	1:H:122:ILE:HA	1.96	0.41
1:H:471:ASN:HB2	1:H:476:ALA:O	2.20	0.41
1:A:8:VAL:HA	1:A:33:SER:OG	2.19	0.41
1:A:176:CYS:HA	1:A:179:LEU:HD11	2.01	0.41
1:A:239:LYS:O	1:A:254:LEU:HD13	2.20	0.41
1:A:304:GLY:O	1:A:368:TRP:HD1	2.04	0.41
1:A:389:ALA:HA	1:A:392:ILE:CD1	2.50	0.41
1:B:16:GLY:CA	2:B:601:FAD:O1A	2.67	0.41
1:B:94:TYR:H	1:B:316:LEU:HB3	1.85	0.41
1:B:447:ARG:HB2	2:B:601:FAD:H5'2	2.00	0.41
1:C:115:LYS:O	1:C:118:GLN:HB2	2.19	0.41
1:C:443:TRP:CD1	1:C:445:ARG:HH21	2.38	0.41
1:C:494:GLU:CD	1:G:477:VAL:HB	2.46	0.41
1:D:150:MET:HG2	1:D:154:ILE:CG2	2.49	0.41
1:E:125:MET:CG	1:E:188:LEU:HD13	2.48	0.41
1:E:183:VAL:CG1	3:E:602:GDU:C2	2.99	0.41
1:E:213:PRO:HG2	1:E:217:GLY:O	2.21	0.41
1:E:417:HIS:HB3	1:E:448:PHE:CZ	2.54	0.41
1:F:122:ILE:O	1:F:125:MET:N	2.53	0.41
1:F:231:LYS:HE2	1:F:231:LYS:HB3	1.73	0.41
1:F:263:LYS:N	1:F:263:LYS:HD2	2.36	0.41
1:G:166:VAL:HG12	1:G:326:TYR:CB	2.50	0.41
1:H:107:GLN:O	1:H:110:ILE:HG22	2.21	0.41
1:H:124:GLY:HA3	1:H:153:GLY:H	1.86	0.41
1:H:499:ASP:O	1:H:502:GLN:N	2.52	0.41
1:B:133:ARG:NH2	1:H:134:VAL:HG21	2.35	0.41
1:B:299:GLY:HA2	1:B:370:ILE:O	2.20	0.41
1:B:443:TRP:HD1	1:B:445:ARG:HH21	1.66	0.41
1:B:446:GLY:H	1:B:450:SER:HB2	1.84	0.41
1:C:199:LYS:HB3	1:C:199:LYS:HE2	1.69	0.41
1:C:304:GLY:O	1:C:368:TRP:CD1	2.74	0.41
1:D:299:GLY:HA2	1:D:370:ILE:O	2.20	0.41
1:D:325:PHE:CA	1:D:374:VAL:HG22	2.50	0.41
3:D:602:GDU:H3'	3:D:602:GDU:O1B	2.19	0.41
1:E:18:THR:HG23	1:E:461:SER:O	2.20	0.41
1:E:419:TYR:HE1	2:E:601:FAD:C7M	2.33	0.41
1:F:68:HIS:ND1	1:F:68:HIS:N	2.67	0.41
1:F:142:PHE:HB3	1:F:174:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:THR:HG22	1:G:19:GLY:N	2.34	0.41
1:G:175:GLN:HG2	1:G:422:PRO:O	2.21	0.41
1:G:329:THR:HG21	1:G:334:TYR:CE2	2.56	0.41
1:H:383:ASN:OD1	1:H:385:GLU:HG2	2.21	0.41
1:B:199:LYS:HB3	1:B:199:LYS:HE2	1.71	0.41
1:E:43:PRO:HG2	1:E:223:ILE:HD13	2.02	0.41
1:E:91:ARG:HB2	1:E:207:ASN:O	2.21	0.41
1:E:294:SER:CB	1:E:414:ARG:NH2	2.83	0.41
1:E:447:ARG:O	1:E:451:TRP:HA	2.20	0.41
1:F:143:ASP:HB2	1:F:171:THR:C	2.44	0.41
1:F:207:ASN:HB3	1:F:315:TRP:HH2	1.83	0.41
1:G:337:TYR:N	1:G:337:TYR:HD1	2.17	0.41
1:G:387:ILE:CG2	1:G:388:LEU:N	2.83	0.41
1:H:116:GLU:OE2	1:H:117:GLU:HG2	2.21	0.41
1:H:120:LYS:HB2	1:H:120:LYS:HE3	1.82	0.41
1:B:425:GLU:H	1:B:425:GLU:CD	2.29	0.41
1:D:166:VAL:HG13	1:D:167:TRP:CD1	2.55	0.41
1:D:331:PHE:HD1	1:D:331:PHE:HA	1.72	0.41
1:E:468:ALA:O	1:E:472:ILE:HG13	2.20	0.41
1:F:122:ILE:CG2	1:F:126:ILE:HD11	2.47	0.41
1:F:183:VAL:HG12	3:F:602:GDU:C2	2.50	0.41
1:F:270:ALA:HB3	1:F:273:PHE:HD2	1.83	0.41
1:G:25:ARG:HA	1:G:28:GLN:CB	2.50	0.41
1:G:28:GLN:CG	1:G:497:LEU:HD12	2.50	0.41
1:G:117:GLU:CD	1:G:157:LEU:HD21	2.45	0.41
1:G:120:LYS:HE3	1:G:120:LYS:HB2	1.76	0.41
1:H:139:PRO:HA	1:H:144:GLU:OE2	2.21	0.41
1:H:308:GLU:HG3	1:H:309:ARG:H	1.86	0.41
1:A:6:ILE:O	1:A:260:ILE:HA	2.20	0.41
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.55	0.41
1:A:150:MET:SD	1:A:159:MET:HE3	2.61	0.41
1:B:244:LYS:HG2	1:B:245:VAL:H	1.85	0.41
1:B:398:THR:O	1:B:399:GLU:HB2	2.21	0.41
1:C:63:HIS:CD2	2:C:601:FAD:C6	3.04	0.41
1:C:503:VAL:HA	1:C:506:LYS:HE2	2.03	0.41
1:D:331:PHE:HB3	1:D:369:SER:HB3	2.03	0.41
1:D:469:VAL:O	1:D:472:ILE:N	2.54	0.41
1:E:142:PHE:CB	1:E:174:MET:HB2	2.50	0.41
1:F:104:TYR:CG	1:F:105:PRO:HA	2.55	0.41
1:F:178:TRP:CD2	1:F:179:LEU:HD22	2.55	0.41
1:F:364:GLU:HA	1:F:367:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ARG:N	1:G:161:PRO:HD2	2.36	0.41
1:H:80:LEU:HA	1:H:81:PRO:HD2	1.89	0.41
1:H:92:ILE:HG22	1:H:94:TYR:HE2	1.85	0.41
1:A:329:THR:O	1:A:370:ILE:HA	2.21	0.41
1:A:420:PRO:O	1:A:422:PRO:HD3	2.20	0.41
1:B:175:GLN:HG3	1:B:175:GLN:H	1.60	0.41
1:C:150:MET:HG2	1:C:154:ILE:HG21	2.02	0.41
1:D:5:ASP:OD2	1:D:258:THR:HA	2.21	0.41
1:D:176:CYS:HA	1:D:179:LEU:HD11	2.02	0.41
1:D:458:GLN:CA	2:D:601:FAD:O3'	2.68	0.41
1:E:38:ASP:OD1	2:E:601:FAD:H1B	2.20	0.41
1:E:150:MET:HG3	1:E:154:ILE:HB	2.02	0.41
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.92	0.41
1:F:112:MET:HE3	1:F:112:MET:HB2	1.84	0.41
1:F:306:ARG:O	1:F:306:ARG:HG2	2.19	0.41
1:G:80:LEU:HA	1:G:81:PRO:HD2	1.90	0.41
1:G:453:TYR:C	1:G:453:TYR:HD2	2.26	0.41
1:A:12:VAL:HB	1:A:36:ILE:HB	2.02	0.41
1:A:134:VAL:O	1:A:134:VAL:HG13	2.21	0.41
1:A:150:MET:CE	1:A:159:MET:HE3	2.51	0.41
1:A:278:MET:O	1:A:279:ASN:HB2	2.20	0.41
1:A:286:LEU:O	1:A:289:GLN:HG3	2.20	0.41
2:A:601:FAD:HM71	2:A:601:FAD:HM83	1.86	0.41
1:B:8:VAL:O	1:B:262:TYR:HA	2.21	0.41
1:B:110:ILE:CG2	1:B:118:GLN:HG2	2.51	0.41
1:B:150:MET:HE2	1:B:150:MET:HB2	1.93	0.41
1:B:204:TRP:CE3	1:B:205:GLY:N	2.88	0.41
1:B:328:ALA:HB2	1:B:372:LEU:HB3	2.02	0.41
1:B:339:GLN:N	1:B:339:GLN:OE1	2.54	0.41
1:B:420:PRO:O	1:B:422:PRO:HD3	2.21	0.41
2:B:601:FAD:HM71	2:B:601:FAD:HM83	1.88	0.41
1:C:142:PHE:CE1	1:C:179:LEU:HD21	2.56	0.41
1:C:145:TRP:HB2	1:C:176:CYS:CB	2.51	0.41
1:C:175:GLN:HE21	1:C:178:TRP:CD1	2.36	0.41
1:C:223:ILE:HD13	1:C:223:ILE:HA	1.92	0.41
1:C:256:ASP:OD2	1:C:256:ASP:N	2.51	0.41
1:C:389:ALA:HA	1:C:392:ILE:CD1	2.50	0.41
1:D:376:GLU:HA	1:D:380:LYS:O	2.21	0.41
1:D:389:ALA:HA	1:D:392:ILE:CD1	2.51	0.41
1:E:18:THR:HA	1:E:462:PHE:HA	2.02	0.41
1:E:108:ASN:O	1:E:194:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:TRP:CD2	1:E:179:LEU:HD22	2.56	0.41
1:E:359:SER:C	1:E:361:GLU:N	2.79	0.41
1:F:26:LEU:HD13	1:F:34:TRP:CB	2.49	0.41
1:F:328:ALA:CB	1:F:372:LEU:HB3	2.51	0.41
1:F:350:GLN:HE22	1:F:407:ILE:HD12	1.84	0.41
1:F:392:ILE:O	1:F:395:LEU:HB2	2.21	0.41
1:G:136:ASN:OD1	1:G:136:ASN:N	2.47	0.41
1:G:252:VAL:HG13	1:G:254:LEU:CD2	2.51	0.41
1:G:313:LYS:H	1:G:313:LYS:HG3	1.71	0.41
1:G:383:ASN:OD1	1:G:385:GLU:HG2	2.21	0.41
1:G:400:MET:HE3	1:G:400:MET:HB3	1.97	0.41
1:G:404:THR:O	1:G:405:ASP:C	2.63	0.41
1:H:28:GLN:CG	1:H:497:LEU:HD12	2.51	0.41
1:H:34:TRP:HH2	1:H:229:LEU:HD22	1.85	0.41
1:H:184:ALA:O	1:H:185:ALA:C	2.63	0.41
1:H:273:PHE:CZ	1:H:417:HIS:NE2	2.89	0.41
1:H:298:ILE:HG23	1:H:411:TYR:O	2.20	0.41
1:H:396:VAL:C	1:H:399:GLU:H	2.29	0.41
1:H:480:THR:CA	1:H:487:VAL:HG11	2.51	0.41
1:A:91:ARG:HG3	1:A:315:TRP:CZ2	2.55	0.41
1:A:376:GLU:HA	1:A:380:LYS:O	2.20	0.41
1:B:60:VAL:C	1:B:61:GLY:O	2.64	0.41
1:B:250:LYS:HA	1:B:262:TYR:CZ	2.56	0.41
1:B:423:THR:HB	1:B:425:GLU:OE1	2.21	0.41
1:C:56:PHE:CE1	1:C:339:GLN:HB3	2.56	0.41
1:D:42:THR:HA	1:D:43:PRO:HD2	1.82	0.41
1:D:494:GLU:OE2	1:H:477:VAL:HB	2.21	0.41
1:E:413:ARG:HG2	1:E:414:ARG:H	1.85	0.41
1:E:506:LYS:HD3	1:E:506:LYS:H	1.85	0.41
1:F:146:ILE:HG13	1:F:146:ILE:H	1.72	0.41
1:H:66:PHE:CD1	1:H:67:SER:N	2.89	0.41
1:H:83:GLU:HA	1:H:86:TRP:CD1	2.55	0.41
1:H:128:ALA:HB2	1:H:151:GLY:HA2	2.02	0.41
1:H:188:LEU:O	1:H:189:LYS:C	2.64	0.41
1:H:351:LEU:HB2	1:H:355:SER:H	1.87	0.41
1:A:482:ASN:C	1:A:484:PRO:HD3	2.46	0.40
1:B:56:PHE:CE1	1:B:339:GLN:HB3	2.56	0.40
1:B:60:VAL:O	1:B:63:HIS:CD2	2.75	0.40
1:B:62:GLY:O	3:B:602:GDU:C6'	2.69	0.40
1:D:63:HIS:HB3	1:D:458:GLN:HE22	1.86	0.40
1:E:18:THR:HG23	1:E:464:LEU:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:LEU:HA	1:F:81:PRO:HD2	1.90	0.40
1:G:57:LEU:HD11	1:G:337:TYR:O	2.21	0.40
1:G:115:LYS:HA	1:G:118:GLN:CG	2.35	0.40
1:G:307:PRO:HG2	1:G:368:TRP:CH2	2.57	0.40
1:H:66:PHE:CD1	1:H:66:PHE:C	2.99	0.40
1:H:90:GLN:HA	1:H:209:THR:HG23	2.03	0.40
1:H:160:ARG:HB2	1:H:161:PRO:CD	2.51	0.40
1:H:351:LEU:CD1	1:H:404:THR:HA	2.50	0.40
1:A:60:VAL:HB	1:A:63:HIS:CE1	2.56	0.40
1:A:175:GLN:HE21	1:A:178:TRP:HD1	1.69	0.40
1:A:306:ARG:HA	1:A:307:PRO:HD3	1.81	0.40
1:B:194:ASN:HD22	1:B:194:ASN:HA	1.56	0.40
1:C:110:ILE:O	1:C:113:LEU:HB2	2.20	0.40
1:C:250:LYS:HA	1:C:262:TYR:CZ	2.56	0.40
1:C:315:TRP:C	1:C:316:LEU:HG	2.46	0.40
1:E:77:ASP:OD1	1:E:211:ARG:NH1	2.53	0.40
1:E:104:TYR:CE1	3:E:602:GDU:O4	2.75	0.40
1:E:151:GLY:C	1:E:154:ILE:HG12	2.46	0.40
1:F:143:ASP:N	1:F:171:THR:O	2.53	0.40
1:F:145:TRP:HE3	1:F:146:ILE:N	2.20	0.40
1:F:414:ARG:HG2	1:F:415:PHE:N	2.36	0.40
1:G:9:ASP:HA	1:G:263:LYS:HD3	2.03	0.40
1:G:235:ARG:O	1:G:240:GLY:HA3	2.21	0.40
1:G:271:VAL:HG13	1:G:272:ASP:H	1.86	0.40
1:G:336:PRO:HG2	1:G:337:TYR:HD1	1.83	0.40
1:H:63:HIS:HA	2:H:601:FAD:C4	2.51	0.40
1:H:239:LYS:HB2	1:H:239:LYS:HE3	1.91	0.40
1:A:296:HIS:NE2	1:A:382:VAL:HG21	2.36	0.40
1:C:128:ALA:HB1	1:C:148:ARG:O	2.21	0.40
1:C:469:VAL:O	1:C:473:VAL:HG23	2.21	0.40
1:D:278:MET:CE	1:D:442:ILE:HD12	2.51	0.40
1:D:306:ARG:HA	1:D:307:PRO:HD3	1.83	0.40
1:E:267:SER:OG	1:E:274:LEU:HD22	2.21	0.40
1:E:348:THR:HG23	1:E:407:ILE:N	2.36	0.40
1:G:196:ILE:HG22	1:G:197:LEU:HD23	2.03	0.40
1:G:235:ARG:O	1:G:236:PHE:CD1	2.74	0.40
1:G:270:ALA:HA	1:G:448:PHE:O	2.21	0.40
1:G:497:LEU:HD12	1:G:497:LEU:O	2.21	0.40
1:H:222:TRP:O	1:H:226:ALA:HB2	2.22	0.40
1:A:108:ASN:HB2	1:A:194:ASN:OD1	2.21	0.40
1:A:242:VAL:HA	1:A:254:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:O	1:B:92:ILE:HD13	2.21	0.40
1:B:166:VAL:HG13	1:B:167:TRP:CD1	2.56	0.40
1:C:443:TRP:CE3	1:C:443:TRP:N	2.89	0.40
1:D:94:TYR:H	1:D:316:LEU:HB3	1.85	0.40
1:D:249:ASN:O	1:D:251:THR:HG23	2.22	0.40
1:D:335:SER:HB3	1:D:338:ASN:OD1	2.21	0.40
1:D:495:ARG:O	1:D:496:ARG:HD2	2.22	0.40
1:E:63:HIS:HB2	1:E:458:GLN:HE22	1.86	0.40
1:E:69:TYR:HB2	1:E:72:PHE:CB	2.52	0.40
1:E:167:TRP:CG	1:E:174:MET:CE	3.01	0.40
1:F:66:PHE:HB3	1:F:206:PRO:O	2.21	0.40
1:F:91:ARG:HG3	1:F:315:TRP:CZ2	2.55	0.40
1:F:347:PRO:HA	1:F:361:GLU:O	2.21	0.40
1:G:421:THR:HA	1:G:422:PRO:HD3	1.71	0.40
1:G:464:LEU:HD21	1:G:481:LEU:N	2.36	0.40
1:H:70:LYS:HG3	1:H:496:ARG:NH1	2.36	0.40
1:H:95:VAL:HG22	1:H:317:TYR:CD2	2.55	0.40
1:H:283:LEU:HD13	1:H:437:LEU:HD21	2.03	0.40
1:H:352:ALA:HB3	1:H:403:PRO:C	2.46	0.40
1:H:384:GLN:H	1:H:384:GLN:HG2	1.56	0.40
1:B:159:MET:CE	3:B:602:GDU:N3	2.71	0.40
1:B:188:LEU:O	1:B:189:LYS:C	2.65	0.40
1:B:395:LEU:HD22	1:B:400:MET:CE	2.40	0.40
1:C:268:THR:HA	1:C:445:ARG:O	2.21	0.40
1:C:335:SER:OG	1:C:336:PRO:HD2	2.22	0.40
1:C:418:GLY:C	1:C:419:TYR:HD1	2.29	0.40
1:C:443:TRP:CD1	1:C:445:ARG:NH2	2.90	0.40
1:D:46:LEU:HB2	2:D:601:FAD:O4'	2.22	0.40
1:E:65:ILE:O	1:E:210:PHE:HB3	2.22	0.40
1:E:307:PRO:CB	1:E:309:ARG:HE	2.35	0.40
1:F:40:ASN:O	1:F:236:PHE:HB3	2.22	0.40
1:F:65:ILE:O	1:F:210:PHE:HB3	2.21	0.40
1:F:204:TRP:CE3	1:F:205:GLY:CA	3.05	0.40
1:F:357:PRO:C	1:F:359:SER:N	2.79	0.40
1:F:388:LEU:HD13	1:F:388:LEU:HA	1.97	0.40
1:H:34:TRP:CD1	1:H:233:LYS:HZ3	2.40	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	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	43	73
1	B	507/509 (100%)	476 (94%)	29 (6%)	2 (0%)	30	61
1	C	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	43	73
1	D	507/509 (100%)	481 (95%)	25 (5%)	1 (0%)	43	73
1	E	507/509 (100%)	456 (90%)	51 (10%)	0	100	100
1	F	507/509 (100%)	457 (90%)	49 (10%)	1 (0%)	43	73
1	G	507/509 (100%)	462 (91%)	45 (9%)	0	100	100
1	H	507/509 (100%)	460 (91%)	46 (9%)	1 (0%)	43	73
All	All	4056/4072 (100%)	3744 (92%)	305 (8%)	7 (0%)	43	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	203	ASN
1	B	61	GLY
1	A	107	GLN
1	B	107	GLN
1	C	107	GLN
1	D	107	GLN
1	F	60	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/430 (100%)	358 (83%)	72 (17%)	2	10
1	B	430/430 (100%)	360 (84%)	70 (16%)	2	11
1	C	430/430 (100%)	359 (84%)	71 (16%)	2	11
1	D	430/430 (100%)	357 (83%)	73 (17%)	2	10
1	E	430/430 (100%)	348 (81%)	82 (19%)	1	7
1	F	430/430 (100%)	343 (80%)	87 (20%)	1	5
1	G	430/430 (100%)	342 (80%)	88 (20%)	1	5
1	H	430/430 (100%)	344 (80%)	86 (20%)	1	6
All	All	3440/3440 (100%)	2811 (82%)	629 (18%)	2	8

All (629) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	20	LEU
1	A	25	ARG
1	A	35	MET
1	A	57	LEU
1	A	65	ILE
1	A	67	SER
1	A	70	LYS
1	A	88	THR
1	A	95	VAL
1	A	107	GLN
1	A	108	ASN
1	A	111	SER
1	A	112	MET
1	A	116	GLU
1	A	122	ILE
1	A	134	VAL
1	A	136	ASN
1	A	138	LYS
1	A	140	LYS
1	A	150	MET
1	A	152	THR
1	A	175	GLN
1	A	179	LEU
1	A	199	LYS
1	A	209	THR
1	A	221	ILE

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Mol	Chain	Res	Type
1	A	225	VAL
1	A	232	GLU
1	A	241	LYS
1	A	252	VAL
1	A	271	VAL
1	A	274	LEU
1	A	281	GLN
1	A	284	VAL
1	A	286	LEU
1	A	293	SER
1	A	302	VAL
1	A	316	LEU
1	A	317	TYR
1	A	330	ILE
1	A	331	PHE
1	A	332	SER
1	A	338	ASN
1	A	339	GLN
1	A	346	LEU
1	A	350	GLN
1	A	351	LEU
1	A	358	GLN
1	A	359	SER
1	A	360	THR
1	A	363	LYS
1	A	364	GLU
1	A	372	LEU
1	A	384	GLN
1	A	385	GLU
1	A	387	ILE
1	A	392	ILE
1	A	393	GLN
1	A	400	MET
1	A	404	THR
1	A	408	VAL
1	A	411	TYR
1	A	424	LEU
1	A	433	ILE
1	A	450	SER
1	A	455	VAL
1	A	473	VAL
1	A	477	VAL

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Mol	Chain	Res	Type
1	A	478	GLU
1	A	506	LYS
1	A	510	GLN
1	B	6	ILE
1	B	20	LEU
1	B	25	ARG
1	B	35	MET
1	B	40	ASN
1	B	57	LEU
1	B	65	ILE
1	B	70	LYS
1	B	88	THR
1	B	95	VAL
1	B	107	GLN
1	B	108	ASN
1	B	111	SER
1	B	112	MET
1	B	116	GLU
1	B	122	ILE
1	B	136	ASN
1	B	138	LYS
1	B	140	LYS
1	B	150	MET
1	B	152	THR
1	B	175	GLN
1	B	179	LEU
1	B	194	ASN
1	B	199	LYS
1	B	209	THR
1	B	221	ILE
1	B	225	VAL
1	B	232	GLU
1	B	241	LYS
1	B	252	VAL
1	B	271	VAL
1	B	274	LEU
1	B	281	GLN
1	B	284	VAL
1	B	286	LEU
1	B	293	SER
1	B	302	VAL
1	B	316	LEU

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Mol	Chain	Res	Type
1	B	317	TYR
1	B	320	GLU
1	B	331	PHE
1	B	332	SER
1	B	338	ASN
1	B	339	GLN
1	B	350	GLN
1	B	351	LEU
1	B	360	THR
1	B	372	LEU
1	B	373	GLU
1	B	385	GLU
1	B	387	ILE
1	B	392	ILE
1	B	393	GLN
1	B	398	THR
1	B	404	THR
1	B	407	ILE
1	B	408	VAL
1	B	411	TYR
1	B	424	LEU
1	B	433	ILE
1	B	444	SER
1	B	450	SER
1	B	455	VAL
1	B	473	VAL
1	B	477	VAL
1	B	478	GLU
1	B	480	THR
1	B	506	LYS
1	B	510	GLN
1	C	6	ILE
1	C	20	LEU
1	C	25	ARG
1	C	35	MET
1	C	40	ASN
1	C	42	THR
1	C	57	LEU
1	C	65	ILE
1	C	70	LYS
1	C	88	THR
1	C	95	VAL

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Mol	Chain	Res	Type
1	C	107	GLN
1	C	108	ASN
1	C	111	SER
1	C	112	MET
1	C	116	GLU
1	C	122	ILE
1	C	134	VAL
1	C	136	ASN
1	C	138	LYS
1	C	140	LYS
1	C	149	MET
1	C	150	MET
1	C	152	THR
1	C	175	GLN
1	C	179	LEU
1	C	194	ASN
1	C	199	LYS
1	C	209	THR
1	C	221	ILE
1	C	225	VAL
1	C	232	GLU
1	C	241	LYS
1	C	252	VAL
1	C	271	VAL
1	C	274	LEU
1	C	281	GLN
1	C	284	VAL
1	C	286	LEU
1	C	293	SER
1	C	302	VAL
1	C	316	LEU
1	C	317	TYR
1	C	320	GLU
1	C	330	ILE
1	C	331	PHE
1	C	332	SER
1	C	338	ASN
1	C	339	GLN
1	C	350	GLN
1	C	351	LEU
1	C	360	THR
1	C	370	ILE

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Mol	Chain	Res	Type
1	C	372	LEU
1	C	373	GLU
1	C	385	GLU
1	C	392	ILE
1	C	393	GLN
1	C	404	THR
1	C	408	VAL
1	C	410	THR
1	C	411	TYR
1	C	424	LEU
1	C	433	ILE
1	C	444	SER
1	C	455	VAL
1	C	473	VAL
1	C	477	VAL
1	C	478	GLU
1	C	506	LYS
1	C	510	GLN
1	D	6	ILE
1	D	20	LEU
1	D	25	ARG
1	D	27	ASN
1	D	35	MET
1	D	57	LEU
1	D	65	ILE
1	D	67	SER
1	D	70	LYS
1	D	88	THR
1	D	95	VAL
1	D	107	GLN
1	D	108	ASN
1	D	111	SER
1	D	112	MET
1	D	116	GLU
1	D	122	ILE
1	D	134	VAL
1	D	136	ASN
1	D	138	LYS
1	D	140	LYS
1	D	150	MET
1	D	152	THR
1	D	175	GLN

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Mol	Chain	Res	Type
1	D	179	LEU
1	D	194	ASN
1	D	199	LYS
1	D	209	THR
1	D	221	ILE
1	D	225	VAL
1	D	232	GLU
1	D	241	LYS
1	D	252	VAL
1	D	271	VAL
1	D	274	LEU
1	D	281	GLN
1	D	284	VAL
1	D	286	LEU
1	D	293	SER
1	D	316	LEU
1	D	317	TYR
1	D	331	PHE
1	D	332	SER
1	D	338	ASN
1	D	339	GLN
1	D	350	GLN
1	D	351	LEU
1	D	359	SER
1	D	360	THR
1	D	363	LYS
1	D	364	GLU
1	D	372	LEU
1	D	373	GLU
1	D	377	SER
1	D	384	GLN
1	D	385	GLU
1	D	387	ILE
1	D	392	ILE
1	D	393	GLN
1	D	404	THR
1	D	408	VAL
1	D	411	TYR
1	D	424	LEU
1	D	433	ILE
1	D	436	LYS
1	D	442	ILE

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Mol	Chain	Res	Type
1	D	455	VAL
1	D	467	GLU
1	D	473	VAL
1	D	477	VAL
1	D	478	GLU
1	D	506	LYS
1	D	510	GLN
1	E	3	HIS
1	E	24	LYS
1	E	25	ARG
1	E	27	ASN
1	E	35	MET
1	E	36	ILE
1	E	39	SER
1	E	41	GLU
1	E	42	THR
1	E	64	VAL
1	E	65	ILE
1	E	66	PHE
1	E	68	HIS
1	E	70	LYS
1	E	78	GLU
1	E	93	SER
1	E	109	ASN
1	E	116	GLU
1	E	122	ILE
1	E	125	MET
1	E	131	GLU
1	E	133	ARG
1	E	134	VAL
1	E	136	ASN
1	E	141	THR
1	E	149	MET
1	E	154	ILE
1	E	157	LEU
1	E	166	VAL
1	E	169	VAL
1	E	175	GLN
1	E	179	LEU
1	E	200	THR
1	E	204	TRP
1	E	209	THR

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Mol	Chain	Res	Type
1	E	225	VAL
1	E	234	THR
1	E	238	GLU
1	E	243	THR
1	E	248	ASN
1	E	251	THR
1	E	252	VAL
1	E	253	THR
1	E	263	LYS
1	E	269	MET
1	E	271	VAL
1	E	278	MET
1	E	290	LEU
1	E	295	THR
1	E	298	ILE
1	E	300	VAL
1	E	302	VAL
1	E	303	ARG
1	E	306	ARG
1	E	308	GLU
1	E	309	ARG
1	E	343	SER
1	E	363	LYS
1	E	364	GLU
1	E	372	LEU
1	E	374	VAL
1	E	378	SER
1	E	382	VAL
1	E	385	GLU
1	E	388	LEU
1	E	405	ASP
1	E	408	VAL
1	E	410	THR
1	E	413	ARG
1	E	433	ILE
1	E	434	LEU
1	E	438	GLN
1	E	469	VAL
1	E	473	VAL
1	E	477	VAL
1	E	478	GLU
1	E	479	LEU

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Mol	Chain	Res	Type
1	E	493	THR
1	E	494	GLU
1	E	496	ARG
1	E	506	LYS
1	E	508	LYS
1	F	3	HIS
1	F	8	VAL
1	F	13	ILE
1	F	24	LYS
1	F	25	ARG
1	F	35	MET
1	F	36	ILE
1	F	39	SER
1	F	41	GLU
1	F	42	THR
1	F	63	HIS
1	F	64	VAL
1	F	65	ILE
1	F	66	PHE
1	F	68	HIS
1	F	70	LYS
1	F	78	GLU
1	F	93	SER
1	F	95	VAL
1	F	109	ASN
1	F	116	GLU
1	F	121	CYS
1	F	122	ILE
1	F	125	MET
1	F	126	ILE
1	F	131	GLU
1	F	133	ARG
1	F	134	VAL
1	F	136	ASN
1	F	141	THR
1	F	154	ILE
1	F	157	LEU
1	F	166	VAL
1	F	169	VAL
1	F	175	GLN
1	F	179	LEU
1	F	200	THR

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Mol	Chain	Res	Type
1	F	204	TRP
1	F	209	THR
1	F	225	VAL
1	F	234	THR
1	F	238	GLU
1	F	248	ASN
1	F	251	THR
1	F	271	VAL
1	F	278	MET
1	F	286	LEU
1	F	290	LEU
1	F	295	THR
1	F	297	VAL
1	F	298	ILE
1	F	300	VAL
1	F	302	VAL
1	F	303	ARG
1	F	306	ARG
1	F	308	GLU
1	F	309	ARG
1	F	343	SER
1	F	363	LYS
1	F	364	GLU
1	F	372	LEU
1	F	374	VAL
1	F	378	SER
1	F	382	VAL
1	F	385	GLU
1	F	388	LEU
1	F	393	GLN
1	F	405	ASP
1	F	408	VAL
1	F	410	THR
1	F	413	ARG
1	F	433	ILE
1	F	434	LEU
1	F	438	GLN
1	F	443	TRP
1	F	450	SER
1	F	469	VAL
1	F	473	VAL
1	F	477	VAL

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Mol	Chain	Res	Type
1	F	478	GLU
1	F	479	LEU
1	F	493	THR
1	F	494	GLU
1	F	496	ARG
1	F	497	LEU
1	F	506	LYS
1	F	508	LYS
1	G	6	ILE
1	G	10	VAL
1	G	13	ILE
1	G	18	THR
1	G	24	LYS
1	G	36	ILE
1	G	41	GLU
1	G	42	THR
1	G	57	LEU
1	G	64	VAL
1	G	65	ILE
1	G	77	ASP
1	G	84	ASP
1	G	92	ILE
1	G	107	GLN
1	G	108	ASN
1	G	110	ILE
1	G	111	SER
1	G	112	MET
1	G	116	GLU
1	G	119	VAL
1	G	143	ASP
1	G	147	VAL
1	G	152	THR
1	G	154	ILE
1	G	159	MET
1	G	166	VAL
1	G	169	VAL
1	G	183	VAL
1	G	193	THR
1	G	194	ASN
1	G	196	ILE
1	G	200	THR
1	G	204	TRP

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Mol	Chain	Res	Type
1	G	207	ASN
1	G	209	THR
1	G	210	PHE
1	G	223	ILE
1	G	248	ASN
1	G	249	ASN
1	G	252	VAL
1	G	254	LEU
1	G	256	ASP
1	G	258	THR
1	G	271	VAL
1	G	272	ASP
1	G	274	LEU
1	G	279	ASN
1	G	281	GLN
1	G	284	VAL
1	G	286	LEU
1	G	294	SER
1	G	302	VAL
1	G	308	GLU
1	G	309	ARG
1	G	316	LEU
1	G	320	GLU
1	G	326	TYR
1	G	331	PHE
1	G	332	SER
1	G	337	TYR
1	G	341	GLU
1	G	345	LYS
1	G	351	LEU
1	G	358	GLN
1	G	361	GLU
1	G	363	LYS
1	G	364	GLU
1	G	380	LYS
1	G	382	VAL
1	G	385	GLU
1	G	387	ILE
1	G	393	GLN
1	G	398	THR
1	G	402	LYS
1	G	408	VAL

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Mol	Chain	Res	Type
1	G	411	TYR
1	G	419	TYR
1	G	424	LEU
1	G	445	ARG
1	G	455	VAL
1	G	464	LEU
1	G	477	VAL
1	G	478	GLU
1	G	485	ASP
1	G	491	GLN
1	G	492	ASN
1	G	510	GLN
1	H	6	ILE
1	H	10	VAL
1	H	13	ILE
1	H	24	LYS
1	H	36	ILE
1	H	41	GLU
1	H	57	LEU
1	H	64	VAL
1	H	65	ILE
1	H	70	LYS
1	H	77	ASP
1	H	84	ASP
1	H	92	ILE
1	H	94	TYR
1	H	107	GLN
1	H	108	ASN
1	H	110	ILE
1	H	111	SER
1	H	112	MET
1	H	116	GLU
1	H	118	GLN
1	H	119	VAL
1	H	143	ASP
1	H	147	VAL
1	H	152	THR
1	H	154	ILE
1	H	166	VAL
1	H	169	VAL
1	H	181	GLU
1	H	183	VAL

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Mol	Chain	Res	Type
1	H	193	THR
1	H	194	ASN
1	H	196	ILE
1	H	200	THR
1	H	203	ASN
1	H	204	TRP
1	H	207	ASN
1	H	209	THR
1	H	210	PHE
1	H	223	ILE
1	H	235	ARG
1	H	248	ASN
1	H	249	ASN
1	H	252	VAL
1	H	254	LEU
1	H	256	ASP
1	H	271	VAL
1	H	272	ASP
1	H	274	LEU
1	H	279	ASN
1	H	281	GLN
1	H	286	LEU
1	H	294	SER
1	H	302	VAL
1	H	308	GLU
1	H	309	ARG
1	H	316	LEU
1	H	320	GLU
1	H	326	TYR
1	H	331	PHE
1	H	337	TYR
1	H	341	GLU
1	H	351	LEU
1	H	358	GLN
1	H	361	GLU
1	H	363	LYS
1	H	364	GLU
1	H	378	SER
1	H	382	VAL
1	H	385	GLU
1	H	387	ILE
1	H	393	GLN

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Mol	Chain	Res	Type
1	H	398	THR
1	H	402	LYS
1	H	408	VAL
1	H	411	TYR
1	H	419	TYR
1	H	421	THR
1	H	424	LEU
1	H	455	VAL
1	H	477	VAL
1	H	478	GLU
1	H	485	ASP
1	H	491	GLN
1	H	492	ASN
1	H	510	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	163	ASN
1	A	175	GLN
1	A	207	ASN
1	A	246	ASN
1	A	279	ASN
1	A	339	GLN
1	A	350	GLN
1	A	458	GLN
1	B	163	ASN
1	B	175	GLN
1	B	246	ASN
1	B	350	GLN
1	B	432	GLN
1	B	458	GLN
1	C	109	ASN
1	C	175	GLN
1	C	207	ASN
1	C	246	ASN
1	C	296	HIS
1	C	339	GLN
1	C	350	GLN
1	C	432	GLN
1	C	458	GLN

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Mol	Chain	Res	Type
1	D	40	ASN
1	D	63	HIS
1	D	175	GLN
1	D	207	ASN
1	D	246	ASN
1	D	296	HIS
1	D	339	GLN
1	D	458	GLN
1	E	68	HIS
1	E	175	GLN
1	E	194	ASN
1	E	207	ASN
1	E	227	ASN
1	E	339	GLN
1	E	412	HIS
1	E	474	ASN
1	F	109	ASN
1	F	175	GLN
1	F	194	ASN
1	F	207	ASN
1	F	227	ASN
1	F	246	ASN
1	F	279	ASN
1	F	339	GLN
1	F	412	HIS
1	G	28	GLN
1	G	90	GLN
1	G	118	GLN
1	G	339	GLN
1	G	383	ASN
1	G	412	HIS
1	G	492	ASN
1	H	28	GLN
1	H	90	GLN
1	H	194	ASN
1	H	203	ASN
1	H	339	GLN
1	H	383	ASN
1	H	393	GLN
1	H	412	HIS
1	H	458	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	H	601	-	58,58,58	3.15	18 (31%)	85,89,89	2.04	24 (28%)
3	GDU	A	602	-	37,38,38	1.95	9 (24%)	55,58,58	1.82	11 (20%)
2	FAD	A	601	-	58,58,58	3.03	15 (25%)	85,89,89	2.30	26 (30%)
2	FAD	G	601	-	58,58,58	2.46	24 (41%)	85,89,89	2.37	31 (36%)
3	GDU	C	602	-	37,38,38	1.99	10 (27%)	55,58,58	1.75	13 (23%)
3	GDU	E	602	-	37,38,38	1.96	10 (27%)	55,58,58	1.75	9 (16%)
3	GDU	D	602	-	37,38,38	2.02	10 (27%)	55,58,58	1.84	13 (23%)
2	FAD	E	601	-	58,58,58	3.13	16 (27%)	85,89,89	2.06	24 (28%)
2	FAD	D	601	-	58,58,58	3.11	15 (25%)	85,89,89	2.09	26 (30%)
3	GDU	B	602	-	37,38,38	1.96	10 (27%)	55,58,58	1.95	13 (23%)
3	GDU	F	602	-	37,38,38	1.95	9 (24%)	55,58,58	1.83	13 (23%)
2	FAD	B	601	-	58,58,58	3.06	17 (29%)	85,89,89	2.10	23 (27%)
2	FAD	F	601	-	58,58,58	3.09	15 (25%)	85,89,89	2.11	24 (28%)
2	FAD	C	601	-	58,58,58	3.10	15 (25%)	85,89,89	2.13	22 (25%)

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	H	601	-	-	9/34/50/50	0/6/6/6
3	GDU	A	602	-	-	7/23/59/59	0/3/3/3
2	FAD	A	601	-	1/1/9/9	17/34/50/50	0/6/6/6
2	FAD	G	601	-	-	7/34/50/50	0/6/6/6
3	GDU	C	602	-	-	8/23/59/59	0/3/3/3
3	GDU	E	602	-	-	8/23/59/59	0/3/3/3
3	GDU	D	602	-	-	13/23/59/59	0/3/3/3
2	FAD	E	601	-	-	12/34/50/50	0/6/6/6
2	FAD	D	601	-	-	8/34/50/50	0/6/6/6
3	GDU	B	602	-	-	5/23/59/59	0/3/3/3
3	GDU	F	602	-	-	9/23/59/59	0/3/3/3
2	FAD	B	601	-	-	23/34/50/50	0/6/6/6
2	FAD	F	601	-	1/1/9/9	12/34/50/50	0/6/6/6
2	FAD	C	601	-	-	7/34/50/50	0/6/6/6

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	PA-O3P	-12.19	1.46	1.59
2	F	601	FAD	PA-O3P	-11.89	1.46	1.59
2	C	601	FAD	PA-O3P	-11.85	1.46	1.59
2	E	601	FAD	PA-O3P	-11.81	1.46	1.59
2	A	601	FAD	PA-O3P	-11.65	1.46	1.59
2	D	601	FAD	PA-O3P	-11.64	1.46	1.59
2	H	601	FAD	PA-O3P	-11.05	1.47	1.59
2	D	601	FAD	O4-C4	10.45	1.43	1.23
2	A	601	FAD	O4-C4	10.44	1.43	1.23
2	F	601	FAD	O4-C4	10.44	1.43	1.23
2	C	601	FAD	O4-C4	10.41	1.43	1.23
2	E	601	FAD	O4-C4	10.40	1.43	1.23
2	H	601	FAD	O4-C4	10.38	1.43	1.23
2	B	601	FAD	O4-C4	10.28	1.43	1.23
2	F	601	FAD	P-O3P	10.23	1.70	1.59
2	E	601	FAD	P-O3P	10.14	1.70	1.59
2	H	601	FAD	P-O3P	10.01	1.70	1.59
2	A	601	FAD	P-O3P	9.81	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	P-O3P	9.35	1.69	1.59
2	D	601	FAD	P-O3P	9.30	1.69	1.59
2	B	601	FAD	P-O3P	8.74	1.68	1.59
3	C	602	GDU	O4-C4	7.10	1.38	1.24
2	E	601	FAD	O2-C2	7.03	1.38	1.24
2	C	601	FAD	O2-C2	7.02	1.38	1.24
2	D	601	FAD	O2-C2	7.00	1.38	1.24
2	F	601	FAD	O2-C2	7.00	1.38	1.24
2	B	601	FAD	O2-C2	6.99	1.38	1.24
2	H	601	FAD	O2-C2	6.97	1.38	1.24
3	D	602	GDU	O4-C4	6.96	1.38	1.24
3	B	602	GDU	O4-C4	6.92	1.38	1.24
3	E	602	GDU	O4-C4	6.88	1.37	1.24
2	A	601	FAD	O2-C2	6.87	1.38	1.24
3	A	602	GDU	O4-C4	6.81	1.37	1.24
3	F	602	GDU	O4-C4	6.80	1.37	1.24
2	G	601	FAD	C2B-C3B	-6.11	1.36	1.53
2	G	601	FAD	C9A-C5X	-6.03	1.31	1.41
2	H	601	FAD	C1'-C2'	-5.40	1.45	1.52
2	H	601	FAD	C2B-C3B	-5.06	1.39	1.53
2	C	601	FAD	C2B-C3B	-4.80	1.40	1.53
2	E	601	FAD	C2B-C3B	-4.73	1.40	1.53
2	F	601	FAD	C2B-C3B	-4.72	1.40	1.53
2	G	601	FAD	C9A-N10	-4.70	1.33	1.41
2	D	601	FAD	C2B-C3B	-4.59	1.40	1.53
2	B	601	FAD	C2B-C3B	-4.57	1.41	1.53
2	A	601	FAD	C2B-C3B	-4.53	1.41	1.53
2	D	601	FAD	C1'-C2'	-4.43	1.46	1.52
2	C	601	FAD	C1'-C2'	-4.40	1.46	1.52
2	G	601	FAD	C4'-C3'	-4.34	1.45	1.53
2	G	601	FAD	C5X-N5	-4.32	1.31	1.39
2	E	601	FAD	C1'-C2'	-4.22	1.46	1.52
3	A	602	GDU	C4'-C3'	-4.13	1.41	1.52
2	G	601	FAD	C1'-C2'	4.10	1.58	1.52
2	H	601	FAD	C9A-N10	-4.03	1.34	1.41
2	B	601	FAD	C1'-C2'	-4.01	1.47	1.52
2	D	601	FAD	C5'-C4'	-4.00	1.46	1.51
2	H	601	FAD	C5'-C4'	-4.00	1.46	1.51
3	D	602	GDU	C4'-C3'	-3.96	1.42	1.52
3	C	602	GDU	C4'-C3'	-3.93	1.42	1.52
2	G	601	FAD	C1'-N10	-3.90	1.38	1.47
2	G	601	FAD	O3'-C3'	-3.87	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C9A-N10	-3.81	1.34	1.41
2	G	601	FAD	C5A-N7A	-3.69	1.32	1.39
2	H	601	FAD	O2'-C2'	-3.67	1.35	1.43
3	E	602	GDU	C3D-C2D	-3.64	1.43	1.53
2	D	601	FAD	C9A-N10	-3.62	1.34	1.41
2	G	601	FAD	C8-C7	-3.56	1.32	1.40
3	D	602	GDU	C3D-C2D	-3.53	1.43	1.53
2	G	601	FAD	C10-N1	3.52	1.40	1.33
2	E	601	FAD	C9A-N10	-3.50	1.35	1.41
3	B	602	GDU	C3D-C2D	-3.49	1.43	1.53
3	F	602	GDU	C4'-C3'	-3.49	1.43	1.52
2	G	601	FAD	C7M-C7	3.42	1.57	1.51
3	B	602	GDU	C4'-C3'	-3.41	1.43	1.52
2	E	601	FAD	O2'-C2'	-3.41	1.36	1.43
2	C	601	FAD	O2'-C2'	-3.39	1.36	1.43
3	C	602	GDU	C3D-C2D	-3.38	1.44	1.53
2	C	601	FAD	C9A-N10	-3.36	1.35	1.41
2	D	601	FAD	O2'-C2'	-3.36	1.36	1.43
3	E	602	GDU	C4'-C3'	-3.36	1.43	1.52
3	A	602	GDU	C3D-C2D	-3.34	1.44	1.53
2	E	601	FAD	C5'-C4'	-3.32	1.47	1.51
2	A	601	FAD	O2'-C2'	-3.31	1.36	1.43
2	F	601	FAD	O2'-C2'	-3.29	1.36	1.43
2	F	601	FAD	C1'-C2'	-3.29	1.48	1.52
3	F	602	GDU	C3D-C2D	-3.27	1.44	1.53
2	F	601	FAD	C5'-C4'	-3.26	1.47	1.51
2	C	601	FAD	C5'-C4'	-3.24	1.47	1.51
3	D	602	GDU	C3D-C4D	-3.20	1.44	1.53
2	A	601	FAD	C1'-C2'	-3.18	1.48	1.52
2	B	601	FAD	O2'-C2'	-3.12	1.36	1.43
2	G	601	FAD	C4X-C10	-3.10	1.35	1.44
2	G	601	FAD	O2-C2	-3.08	1.18	1.24
2	D	601	FAD	C6A-N6A	3.00	1.41	1.34
2	B	601	FAD	C6A-N6A	3.00	1.41	1.34
2	A	601	FAD	C6A-N6A	2.99	1.41	1.34
2	F	601	FAD	C6A-N6A	2.99	1.41	1.34
3	E	602	GDU	PB-O3A	2.97	1.62	1.59
3	C	602	GDU	C3D-C4D	-2.96	1.45	1.53
2	C	601	FAD	C6A-N6A	2.96	1.41	1.34
3	B	602	GDU	PB-O3A	2.93	1.62	1.59
3	F	602	GDU	C3D-C4D	-2.92	1.45	1.53
2	H	601	FAD	C6A-N6A	2.89	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GDU	C3D-C4D	-2.89	1.45	1.53
2	E	601	FAD	C6A-N6A	2.88	1.41	1.34
2	D	601	FAD	PA-O1A	-2.82	1.41	1.50
2	C	601	FAD	PA-O1A	-2.80	1.41	1.50
2	B	601	FAD	C4-N3	-2.79	1.33	1.38
2	B	601	FAD	C5'-C4'	-2.78	1.48	1.51
3	E	602	GDU	C3D-C4D	-2.76	1.46	1.53
2	F	601	FAD	C7M-C7	2.75	1.56	1.51
3	B	602	GDU	C3D-C4D	-2.74	1.46	1.53
2	H	601	FAD	C7M-C7	2.74	1.56	1.51
3	F	602	GDU	PB-O3A	2.73	1.62	1.59
2	A	601	FAD	C7M-C7	2.72	1.56	1.51
2	E	601	FAD	C7M-C7	2.72	1.56	1.51
2	A	601	FAD	PA-O1A	-2.71	1.41	1.50
2	C	601	FAD	C7M-C7	2.71	1.56	1.51
2	A	601	FAD	C5'-C4'	-2.70	1.48	1.51
2	G	601	FAD	C8A-N9A	-2.69	1.33	1.37
2	F	601	FAD	C9A-N10	-2.66	1.36	1.41
2	D	601	FAD	C7M-C7	2.66	1.56	1.51
2	B	601	FAD	PA-O1A	-2.66	1.41	1.50
3	E	602	GDU	C2-N1	-2.65	1.34	1.38
3	C	602	GDU	PB-O3A	2.65	1.62	1.59
2	F	601	FAD	PA-O1A	-2.62	1.41	1.50
2	B	601	FAD	C7M-C7	2.60	1.55	1.51
2	G	601	FAD	O3B-C3B	-2.57	1.36	1.43
3	A	602	GDU	PB-O3A	2.57	1.62	1.59
2	A	601	FAD	C4-N3	-2.54	1.34	1.38
3	F	602	GDU	C2-N3	-2.52	1.33	1.38
2	E	601	FAD	PA-O1A	-2.52	1.42	1.50
2	H	601	FAD	C4-N3	-2.51	1.34	1.38
2	G	601	FAD	C4A-N9A	-2.51	1.32	1.37
2	G	601	FAD	O4B-C1B	-2.50	1.36	1.42
3	D	602	GDU	C2-N1	-2.50	1.34	1.38
3	E	602	GDU	C2-N3	-2.49	1.33	1.38
2	C	601	FAD	C4-N3	-2.49	1.34	1.38
3	D	602	GDU	PB-O3A	2.48	1.62	1.59
2	H	601	FAD	PA-O1A	-2.47	1.42	1.50
2	E	601	FAD	C4-N3	-2.46	1.34	1.38
3	E	602	GDU	O5'-C5'	2.45	1.50	1.44
3	D	602	GDU	O5'-C5'	2.43	1.50	1.44
3	F	602	GDU	O5'-C5'	2.42	1.50	1.44
3	B	602	GDU	C2-N3	-2.40	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FAD	C4-N3	-2.39	1.34	1.38
3	F	602	GDU	C2-N1	-2.38	1.34	1.38
2	D	601	FAD	C4-N3	-2.36	1.34	1.38
3	D	602	GDU	C2-N3	-2.34	1.33	1.38
2	C	601	FAD	O4B-C4B	-2.34	1.39	1.45
2	B	601	FAD	C5X-N5	-2.34	1.35	1.39
3	E	602	GDU	C4-N3	-2.33	1.34	1.38
3	C	602	GDU	O5'-C5'	2.32	1.50	1.44
3	A	602	GDU	C4-N3	-2.32	1.34	1.38
3	F	602	GDU	C4-N3	-2.31	1.34	1.38
2	E	601	FAD	O4B-C4B	-2.30	1.39	1.45
3	B	602	GDU	C2-N1	-2.30	1.34	1.38
3	A	602	GDU	C2-N1	-2.30	1.34	1.38
2	G	601	FAD	C2-N1	2.30	1.41	1.36
3	C	602	GDU	C2-N1	-2.29	1.34	1.38
2	F	601	FAD	O4B-C4B	-2.28	1.39	1.45
2	A	601	FAD	O4B-C4B	-2.28	1.39	1.45
2	G	601	FAD	P-O5'	-2.27	1.50	1.59
2	D	601	FAD	O4B-C4B	-2.26	1.40	1.45
2	A	601	FAD	C9A-N10	-2.25	1.37	1.41
2	G	601	FAD	PA-O3P	-2.25	1.57	1.59
3	B	602	GDU	O5'-C5'	2.24	1.49	1.44
2	F	601	FAD	C5X-N5	-2.24	1.35	1.39
2	D	601	FAD	C2'-C3'	-2.24	1.49	1.53
3	D	602	GDU	C4-N3	-2.23	1.34	1.38
3	A	602	GDU	C2-N3	-2.22	1.34	1.38
2	H	601	FAD	C2'-C3'	-2.21	1.49	1.53
3	C	602	GDU	C4-N3	-2.21	1.34	1.38
2	A	601	FAD	C5X-N5	-2.20	1.35	1.39
2	H	601	FAD	C9A-C5X	-2.18	1.37	1.41
2	E	601	FAD	C3B-C4B	-2.17	1.47	1.53
3	B	602	GDU	C4-N3	-2.17	1.34	1.38
3	C	602	GDU	C2-N3	-2.17	1.34	1.38
2	B	601	FAD	O4B-C4B	-2.16	1.40	1.45
2	G	601	FAD	C10-N10	-2.14	1.32	1.37
3	D	602	GDU	C6-C5	2.14	1.40	1.35
2	G	601	FAD	C8M-C8	-2.12	1.47	1.51
3	C	602	GDU	C6-C5	2.11	1.40	1.35
2	E	601	FAD	C5X-N5	-2.11	1.35	1.39
2	H	601	FAD	O4B-C4B	-2.10	1.40	1.45
2	B	601	FAD	C5A-N7A	-2.10	1.35	1.39
2	H	601	FAD	C4X-N5	2.09	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FAD	C3B-C4B	-2.09	1.47	1.53
3	A	602	GDU	O5'-C5'	2.09	1.49	1.44
2	B	601	FAD	C9A-C5X	-2.06	1.38	1.41
2	C	601	FAD	C2'-C3'	-2.06	1.49	1.53
2	H	601	FAD	C3B-C4B	-2.05	1.47	1.53
3	B	602	GDU	C6-C5	2.03	1.39	1.35
3	E	602	GDU	C2D-C1D	-2.02	1.47	1.53

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	O4B-C1B-N9A	7.09	121.70	108.09
3	A	602	GDU	N3-C2-N1	6.67	123.58	114.89
3	C	602	GDU	N3-C2-N1	6.63	123.52	114.89
2	D	601	FAD	O4B-C1B-N9A	6.52	120.61	108.09
2	G	601	FAD	O2P-P-O3P	6.46	124.75	107.27
3	D	602	GDU	N3-C2-N1	6.45	123.28	114.89
3	E	602	GDU	N3-C2-N1	6.24	123.01	114.89
3	B	602	GDU	O5'-C1'-O3B	-6.06	103.44	111.36
3	F	602	GDU	N3-C2-N1	6.05	122.77	114.89
2	G	601	FAD	O2A-PA-O3P	6.04	123.60	107.27
2	H	601	FAD	O4B-C1B-N9A	5.94	119.50	108.09
2	A	601	FAD	O4B-C1B-N9A	5.81	119.25	108.09
3	B	602	GDU	N3-C2-N1	5.80	122.44	114.89
3	A	602	GDU	C4-N3-C2	-5.55	119.72	126.61
3	E	602	GDU	C4-N3-C2	-5.53	119.74	126.61
2	E	601	FAD	C5A-C4A-N3A	-5.48	119.18	126.72
2	F	601	FAD	C5A-C4A-N3A	-5.46	119.19	126.72
2	A	601	FAD	C5A-C4A-N3A	-5.42	119.25	126.72
2	B	601	FAD	C1'-N10-C9A	-5.41	110.11	120.63
2	G	601	FAD	N3A-C2A-N1A	-5.37	120.45	128.58
3	F	602	GDU	C4-N3-C2	-5.32	120.01	126.61
2	A	601	FAD	O5'-C5'-C4'	5.25	123.38	109.36
2	H	601	FAD	C5A-C4A-N3A	-5.24	119.50	126.72
2	G	601	FAD	O3P-PA-O1A	-5.22	95.00	110.70
2	F	601	FAD	O5'-C5'-C4'	5.16	123.12	109.36
2	B	601	FAD	C5A-C4A-N3A	-5.12	119.67	126.72
3	D	602	GDU	C4-N3-C2	-5.08	120.30	126.61
2	B	601	FAD	C2'-C1'-N10	5.05	134.07	110.20
3	C	602	GDU	C4-N3-C2	-4.99	120.42	126.61
2	G	601	FAD	C5A-C4A-N3A	-4.89	119.98	126.72
2	E	601	FAD	O5'-C5'-C4'	4.89	122.41	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C5A-C4A-N3A	-4.88	119.99	126.72
2	C	601	FAD	N9A-C8A-N7A	-4.88	107.02	113.94
2	A	601	FAD	O2'-C2'-C3'	4.86	120.61	109.25
2	C	601	FAD	N3A-C2A-N1A	-4.85	121.24	128.58
2	C	601	FAD	C4B-O4B-C1B	-4.83	98.80	109.47
2	F	601	FAD	N3A-C2A-N1A	-4.80	121.31	128.58
2	A	601	FAD	N3A-C2A-N1A	-4.77	121.36	128.58
2	E	601	FAD	N3A-C2A-N1A	-4.75	121.40	128.58
2	D	601	FAD	N9A-C8A-N7A	-4.73	107.23	113.94
2	C	601	FAD	C5A-C4A-N3A	-4.72	120.21	126.72
3	E	602	GDU	C3'-C4'-C5'	4.69	118.73	110.23
2	E	601	FAD	N3A-C4A-N9A	4.66	135.10	127.17
2	C	601	FAD	C4A-N9A-C1B	-4.63	115.81	126.63
2	H	601	FAD	N3A-C2A-N1A	-4.62	121.58	128.58
2	G	601	FAD	O5B-PA-O1A	-4.61	90.65	108.94
2	C	601	FAD	C4A-N9A-C8A	4.61	110.58	105.74
2	D	601	FAD	N3A-C2A-N1A	-4.61	121.61	128.58
2	B	601	FAD	N3A-C2A-N1A	-4.60	121.62	128.58
2	G	601	FAD	C4-N3-C2	-4.59	117.48	125.64
2	G	601	FAD	O5B-C5B-C4B	4.56	124.53	108.99
2	H	601	FAD	C2'-C1'-N10	4.55	131.69	110.20
2	F	601	FAD	O2'-C2'-C3'	4.53	119.85	109.25
2	F	601	FAD	N9A-C8A-N7A	-4.52	107.52	113.94
2	A	601	FAD	C2'-C1'-N10	4.52	131.56	110.20
2	A	601	FAD	N9A-C8A-N7A	-4.52	107.53	113.94
2	H	601	FAD	N9A-C8A-N7A	-4.42	107.66	113.94
2	B	601	FAD	O4B-C1B-N9A	4.42	116.58	108.09
2	E	601	FAD	N9A-C8A-N7A	-4.42	107.67	113.94
2	D	601	FAD	O2'-C2'-C3'	4.41	119.58	109.25
3	F	602	GDU	O5'-C5'-C4'	4.40	117.63	109.70
2	F	601	FAD	N3A-C4A-N9A	4.40	134.65	127.17
3	B	602	GDU	C4-N3-C2	-4.40	121.15	126.61
2	E	601	FAD	C4A-N9A-C8A	4.39	110.34	105.74
2	E	601	FAD	C2'-C1'-N10	4.38	130.92	110.20
3	D	602	GDU	O5'-C5'-C4'	4.37	117.58	109.70
2	H	601	FAD	N3A-C4A-N9A	4.37	134.61	127.17
2	B	601	FAD	O5'-C5'-C4'	4.31	120.87	109.36
2	H	601	FAD	C4A-N9A-C8A	4.25	110.20	105.74
2	A	601	FAD	N3A-C4A-N9A	4.19	134.29	127.17
2	F	601	FAD	C4A-N9A-C8A	4.18	110.13	105.74
2	D	601	FAD	C4A-N9A-C1B	-4.17	116.87	126.63
3	F	602	GDU	C3'-C4'-C5'	4.13	117.71	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	FAD	O3P-P-O1P	-4.12	98.30	110.70
2	B	601	FAD	N3A-C4A-N9A	4.12	134.18	127.17
2	B	601	FAD	C5X-C9A-N10	4.11	121.69	117.97
2	B	601	FAD	N9A-C8A-N7A	-4.11	108.11	113.94
2	A	601	FAD	C4'-C3'-C2'	4.09	120.37	113.57
2	D	601	FAD	C4A-N9A-C8A	4.08	110.02	105.74
2	G	601	FAD	O2P-P-O5'	4.08	126.05	107.57
2	D	601	FAD	C4A-C5A-N7A	-4.07	105.93	110.58
2	F	601	FAD	C2'-C1'-N10	4.04	129.29	110.20
2	A	601	FAD	C1'-N10-C9A	4.03	128.46	120.63
2	E	601	FAD	O2'-C2'-C3'	4.02	118.65	109.25
2	D	601	FAD	C5A-N7A-C8A	4.00	109.74	103.45
2	E	601	FAD	O4B-C1B-N9A	3.99	115.75	108.09
2	A	601	FAD	C4X-C10-N10	3.96	122.16	116.48
2	A	601	FAD	C5A-N7A-C8A	3.95	109.66	103.45
2	B	601	FAD	O5B-C5B-C4B	3.95	122.44	108.99
3	B	602	GDU	C3'-C4'-C5'	3.94	117.38	110.23
2	F	601	FAD	C2A-N3A-C4A	3.94	121.46	111.83
2	C	601	FAD	O2'-C2'-C3'	3.93	118.44	109.25
2	A	601	FAD	C4A-N9A-C8A	3.92	109.85	105.74
2	G	601	FAD	O5'-C5'-C4'	3.91	119.79	109.36
2	E	601	FAD	C2A-N3A-C4A	3.83	121.19	111.83
2	F	601	FAD	O4B-C1B-N9A	3.83	115.44	108.09
2	A	601	FAD	C2A-N3A-C4A	3.81	121.13	111.83
2	C	601	FAD	C5A-N7A-C8A	3.78	109.39	103.45
2	B	601	FAD	C4A-N9A-C8A	3.78	109.70	105.74
2	E	601	FAD	C4'-C3'-C2'	3.71	119.75	113.57
2	D	601	FAD	O5'-C5'-C4'	3.71	119.27	109.36
2	A	601	FAD	O5B-C5B-C4B	3.71	121.63	108.99
2	G	601	FAD	C2A-N3A-C4A	3.70	120.87	111.83
3	E	602	GDU	O5'-C5'-C4'	3.69	116.34	109.70
2	G	601	FAD	O4B-C1B-N9A	3.66	115.11	108.09
2	C	601	FAD	N3A-C4A-N9A	3.65	133.38	127.17
2	H	601	FAD	C5A-N7A-C8A	3.65	109.18	103.45
2	F	601	FAD	C5A-N7A-C8A	3.62	109.14	103.45
2	C	601	FAD	C2A-N3A-C4A	3.58	120.57	111.83
2	H	601	FAD	C2A-N3A-C4A	3.58	120.57	111.83
2	H	601	FAD	C1'-N10-C9A	-3.57	113.70	120.63
2	A	601	FAD	C4A-C5A-N7A	-3.56	106.51	110.58
2	D	601	FAD	C2A-N3A-C4A	3.54	120.48	111.83
2	C	601	FAD	O5'-C5'-C4'	3.52	118.76	109.36
2	B	601	FAD	C2A-N3A-C4A	3.50	120.38	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-N3-C2	-3.49	119.45	125.64
2	C	601	FAD	C4A-C5A-N7A	-3.48	106.60	110.58
2	E	601	FAD	C5A-N7A-C8A	3.48	108.92	103.45
2	D	601	FAD	C4-C4X-N5	3.47	123.00	118.21
2	B	601	FAD	C5A-N7A-C8A	3.46	108.89	103.45
2	G	601	FAD	O5'-P-O1P	-3.45	95.26	108.94
2	G	601	FAD	O4B-C1B-C2B	-3.43	99.28	106.62
2	D	601	FAD	N3A-C4A-N9A	3.39	132.93	127.17
3	C	602	GDU	O5'-C5'-C4'	3.34	115.72	109.70
2	F	601	FAD	C4-N3-C2	-3.34	119.71	125.64
2	H	601	FAD	C4-N3-C2	-3.33	119.72	125.64
3	F	602	GDU	C5-C4-N3	3.29	119.41	114.80
2	G	601	FAD	C2'-C1'-N10	3.29	125.77	110.20
2	H	601	FAD	C4-C4X-N5	3.28	122.74	118.21
3	D	602	GDU	C1'-O5'-C5'	3.27	120.10	113.72
2	A	601	FAD	C4-N3-C2	-3.26	119.85	125.64
2	C	601	FAD	C1'-C2'-C3'	3.22	118.38	109.66
3	B	602	GDU	O5'-C5'-C4'	3.22	115.50	109.70
3	D	602	GDU	C3'-C4'-C5'	3.21	116.06	110.23
3	C	602	GDU	C3D-C2D-C1D	3.20	107.52	101.46
2	D	601	FAD	C4B-O4B-C1B	-3.20	102.40	109.47
2	A	601	FAD	C4A-N9A-C1B	-3.20	119.15	126.63
2	C	601	FAD	C4-C4X-N5	3.20	122.63	118.21
2	H	601	FAD	O2'-C2'-C3'	3.19	116.71	109.25
2	E	601	FAD	C4-N3-C2	-3.16	120.02	125.64
2	F	601	FAD	C4X-C10-N10	3.14	120.98	116.48
3	B	602	GDU	C1'-O5'-C5'	-3.13	107.60	113.72
3	E	602	GDU	O2-C2-N1	-3.12	118.74	122.80
2	F	601	FAD	O4-C4-C4X	-3.11	118.32	126.53
2	C	601	FAD	C4-N3-C2	-3.10	120.13	125.64
2	F	601	FAD	C4A-C5A-N7A	-3.09	107.05	110.58
2	H	601	FAD	C4A-C5A-N7A	-3.07	107.07	110.58
3	A	602	GDU	O2-C2-N1	-3.07	118.81	122.80
3	E	602	GDU	C5-C4-N3	3.06	119.09	114.80
3	A	602	GDU	C1'-C2'-C3'	3.05	116.43	110.01
3	D	602	GDU	O2-C2-N1	-3.05	118.83	122.80
2	G	601	FAD	N3A-C4A-N9A	3.05	132.35	127.17
2	G	601	FAD	C8M-C8-C9	3.04	124.93	119.57
2	B	601	FAD	C4X-C4-N3	3.03	120.97	113.25
2	F	601	FAD	O2'-C2'-C1'	3.02	122.61	110.20
2	B	601	FAD	C4A-C5A-N7A	-3.01	107.14	110.58
3	C	602	GDU	O2-C2-N1	-3.00	118.89	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	FAD	C4A-N9A-C1B	-2.99	119.64	126.63
2	E	601	FAD	C4-C4X-N5	2.99	122.33	118.21
3	B	602	GDU	O5D-C5D-C4D	2.98	119.15	108.99
2	E	601	FAD	C4X-C10-N10	2.97	120.73	116.48
2	G	601	FAD	C4X-C4-N3	2.96	120.79	113.25
3	F	602	GDU	O5D-C5D-C4D	2.96	119.07	108.99
2	G	601	FAD	O3B-C3B-C2B	-2.95	102.36	111.82
2	H	601	FAD	C4X-C4-N3	2.95	120.75	113.25
2	B	601	FAD	C9-C9A-N10	-2.94	117.90	121.85
3	C	602	GDU	C3'-C4'-C5'	2.94	115.56	110.23
2	C	601	FAD	C1B-N9A-C8A	2.93	133.60	127.09
2	G	601	FAD	O4-C4-C4X	-2.93	118.81	126.53
3	A	602	GDU	O5D-C5D-C4D	2.91	118.89	108.99
3	B	602	GDU	O5'-C1'-C2'	-2.88	104.45	110.37
2	A	601	FAD	C1'-C2'-C3'	2.87	117.43	109.66
2	F	601	FAD	C4X-C4-N3	2.85	120.50	113.25
3	A	602	GDU	O4-C4-C5	-2.83	120.28	125.16
2	E	601	FAD	C4A-C5A-N7A	-2.83	107.35	110.58
2	C	601	FAD	C4X-C4-N3	2.82	120.43	113.25
2	D	601	FAD	C4-N3-C2	-2.81	120.66	125.64
2	C	601	FAD	O5B-C5B-C4B	2.81	118.54	108.99
2	E	601	FAD	C4X-C4-N3	2.80	120.38	113.25
2	G	601	FAD	C8M-C8-C7	-2.79	115.07	120.76
3	D	602	GDU	O5'-C1'-C2'	2.78	116.09	110.37
3	A	602	GDU	C5-C4-N3	2.78	118.69	114.80
2	B	601	FAD	O2'-C2'-C3'	2.76	115.71	109.25
2	A	601	FAD	O2P-P-O3P	2.76	114.73	107.27
2	B	601	FAD	C4A-N9A-C1B	-2.75	120.20	126.63
2	D	601	FAD	C4X-C4-N3	2.75	120.25	113.25
2	E	601	FAD	O4-C4-C4X	-2.74	119.30	126.53
2	F	601	FAD	O5B-C5B-C4B	2.73	118.30	108.99
2	F	601	FAD	C1'-N10-C9A	2.73	125.94	120.63
2	H	601	FAD	O5B-C5B-C4B	2.73	118.28	108.99
2	A	601	FAD	O2'-C2'-C1'	2.73	121.40	110.20
2	E	601	FAD	O5B-C5B-C4B	2.72	118.26	108.99
2	D	601	FAD	C1B-N9A-C8A	2.71	133.11	127.09
3	E	602	GDU	O5D-C5D-C4D	2.71	118.22	108.99
3	D	602	GDU	C5-C4-N3	2.71	118.59	114.80
2	D	601	FAD	O4-C4-C4X	-2.71	119.39	126.53
3	A	602	GDU	C3D-C2D-C1D	2.69	106.56	101.46
2	A	601	FAD	C4X-C4-N3	2.67	120.06	113.25
2	A	601	FAD	O4-C4-C4X	-2.66	119.52	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C4X-C10-N10	2.66	120.29	116.48
2	A	601	FAD	C4-C4X-N5	2.66	121.88	118.21
2	H	601	FAD	C4A-N9A-C1B	-2.66	120.42	126.63
3	B	602	GDU	C5-C4-N3	2.65	118.50	114.80
2	F	601	FAD	C1'-C2'-C3'	2.64	116.81	109.66
2	D	601	FAD	C1'-C2'-C3'	2.61	116.75	109.66
3	D	602	GDU	O4D-C1D-N1	2.58	114.21	108.36
2	E	601	FAD	O2'-C2'-C1'	2.58	120.80	110.20
2	D	601	FAD	O2A-PA-O3P	2.57	114.23	107.27
2	C	601	FAD	O4-C4-C4X	-2.54	119.83	126.53
2	B	601	FAD	O4-C4-C4X	-2.52	119.87	126.53
2	D	601	FAD	C4X-C10-N10	2.52	120.09	116.48
3	A	602	GDU	O5'-C1'-C2'	2.52	115.54	110.37
2	B	601	FAD	C4'-C3'-C2'	2.52	117.76	113.57
2	D	601	FAD	O2'-C2'-C1'	2.51	120.53	110.20
3	B	602	GDU	O4-C4-C5	-2.50	120.84	125.16
3	F	602	GDU	O4-C4-C5	-2.48	120.89	125.16
3	F	602	GDU	C3D-C2D-C1D	2.47	106.14	101.46
3	E	602	GDU	O4-C4-C5	-2.47	120.91	125.16
3	C	602	GDU	O5D-C5D-C4D	2.46	117.36	108.99
3	B	602	GDU	C1D-N1-C2	2.45	121.99	117.59
3	C	602	GDU	C5-C4-N3	2.42	118.18	114.80
2	D	601	FAD	O2P-P-O3P	2.41	113.79	107.27
2	F	601	FAD	C3B-C2B-C1B	2.36	105.93	101.46
2	H	601	FAD	O5'-C5'-C4'	2.36	115.66	109.36
2	B	601	FAD	C4X-C10-N1	-2.36	118.81	124.59
3	F	602	GDU	C1D-N1-C2	2.35	121.82	117.59
2	E	601	FAD	C4A-N9A-C1B	-2.35	121.13	126.63
2	F	601	FAD	C4'-C3'-C2'	2.34	117.47	113.57
3	D	602	GDU	O4-C4-C5	-2.34	121.13	125.16
2	F	601	FAD	C4-C4X-N5	2.33	121.43	118.21
3	B	602	GDU	O2-C2-N1	-2.33	119.76	122.80
2	A	601	FAD	C10-C4X-N5	-2.32	120.07	124.81
2	H	601	FAD	C10-C4X-N5	-2.32	120.07	124.81
3	C	602	GDU	C6-N1-C2	-2.31	118.19	121.00
3	A	602	GDU	C1D-N1-C2	2.29	121.71	117.59
3	F	602	GDU	O2-C2-N1	-2.28	119.83	122.80
2	G	601	FAD	N9A-C8A-N7A	-2.28	110.70	113.94
2	H	601	FAD	C9-C9A-N10	-2.27	118.80	121.85
2	G	601	FAD	C4A-C5A-N7A	-2.27	107.99	110.58
2	G	601	FAD	C10-C4X-N5	-2.27	120.17	124.81
3	D	602	GDU	C3D-C2D-C1D	2.27	105.75	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C2'-C1'-N10	2.27	120.91	110.20
2	C	601	FAD	C10-C4X-N5	-2.26	120.19	124.81
2	G	601	FAD	O2A-PA-O1A	2.26	122.96	112.44
2	H	601	FAD	C5X-C9A-N10	2.25	120.01	117.97
2	A	601	FAD	C4B-O4B-C1B	-2.25	104.50	109.47
3	C	602	GDU	O4-C4-C5	-2.25	121.29	125.16
2	H	601	FAD	O4-C4-C4X	-2.24	120.62	126.53
2	D	601	FAD	C6A-C5A-N7A	2.24	136.41	132.09
3	F	602	GDU	O2-C2-N3	-2.21	117.40	121.49
2	E	601	FAD	C10-C4X-N5	-2.20	120.32	124.81
2	G	601	FAD	C4X-C10-N1	-2.20	119.21	124.59
2	D	601	FAD	C10-C4X-N5	-2.15	120.42	124.81
3	F	602	GDU	C2D-C3D-C4D	2.15	106.76	102.61
3	D	602	GDU	O5D-C5D-C4D	2.14	116.28	108.99
2	G	601	FAD	C4'-C3'-C2'	2.13	117.11	113.57
3	C	602	GDU	O2-C2-N3	-2.11	117.59	121.49
2	H	601	FAD	C4B-O4B-C1B	-2.11	104.81	109.47
3	A	602	GDU	O2-C2-N3	-2.10	117.61	121.49
2	E	601	FAD	C2B-C1B-N9A	-2.10	108.09	113.30
2	B	601	FAD	O2P-P-O3P	2.10	112.94	107.27
3	D	602	GDU	C5D-C4D-C3D	-2.10	107.67	115.21
3	B	602	GDU	O4D-C1D-N1	2.08	113.08	108.36
3	F	602	GDU	C1'-O5'-C5'	2.08	117.79	113.72
3	C	602	GDU	O4D-C1D-N1	2.08	113.07	108.36
3	C	602	GDU	C1D-N1-C2	2.07	121.31	117.59
2	G	601	FAD	C1'-C2'-C3'	2.06	115.25	109.66
2	G	601	FAD	C5A-N7A-C8A	2.06	106.68	103.45
2	H	601	FAD	C2B-C1B-N9A	-2.03	108.26	113.30
2	E	601	FAD	C3B-C2B-C1B	2.02	105.29	101.46
2	G	601	FAD	O4B-C4B-C5B	2.02	115.79	109.33
3	E	602	GDU	C4'-C3'-C2'	2.01	114.36	110.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	FAD	C2'
2	F	601	FAD	C2'

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C2'-C1'-N10-C9A
2	A	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	C1'-C2'-C3'-O3'
2	A	601	FAD	C1'-C2'-C3'-C4'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	O2'-C2'-C3'-O3'
2	D	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	C3'-C4'-C5'-O5'
2	D	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	C5B-O5B-PA-O2A
2	E	601	FAD	C5B-O5B-PA-O3P
2	E	601	FAD	N10-C1'-C2'-O2'
2	F	601	FAD	C5B-O5B-PA-O1A
2	F	601	FAD	C5B-O5B-PA-O2A
2	F	601	FAD	C5B-O5B-PA-O3P
2	F	601	FAD	C2'-C1'-N10-C9A
2	F	601	FAD	C2'-C1'-N10-C10
2	F	601	FAD	N10-C1'-C2'-O2'
2	F	601	FAD	C1'-C2'-C3'-O3'
2	F	601	FAD	C1'-C2'-C3'-C4'
2	G	601	FAD	C1'-C2'-C3'-O3'
2	G	601	FAD	C1'-C2'-C3'-C4'
2	G	601	FAD	O2'-C2'-C3'-O3'
2	G	601	FAD	O2'-C2'-C3'-C4'
2	G	601	FAD	C5'-O5'-P-O1P
2	H	601	FAD	C1'-C2'-C3'-O3'
2	H	601	FAD	C1'-C2'-C3'-C4'
2	H	601	FAD	O2'-C2'-C3'-O3'
2	H	601	FAD	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
3	A	602	GDU	C4D-C5D-O5D-PA
3	A	602	GDU	C5D-O5D-PA-O3A
3	B	602	GDU	C3D-C4D-C5D-O5D
3	B	602	GDU	C5D-O5D-PA-O2A
3	B	602	GDU	C5D-O5D-PA-O3A
3	B	602	GDU	O5'-C1'-O3B-PB
3	C	602	GDU	C4D-C5D-O5D-PA
3	C	602	GDU	C1'-O3B-PB-O3A
3	C	602	GDU	C1'-O3B-PB-O2B
3	D	602	GDU	C3D-C4D-C5D-O5D
3	D	602	GDU	O4D-C4D-C5D-O5D
3	D	602	GDU	C4D-C5D-O5D-PA
3	D	602	GDU	C5D-O5D-PA-O1A
3	D	602	GDU	C5D-O5D-PA-O2A
3	D	602	GDU	C5D-O5D-PA-O3A
3	D	602	GDU	C1'-O3B-PB-O3A
3	D	602	GDU	O5'-C1'-O3B-PB
3	E	602	GDU	C5D-O5D-PA-O1A
3	E	602	GDU	C5D-O5D-PA-O2A
3	E	602	GDU	C5D-O5D-PA-O3A
3	E	602	GDU	C1'-O3B-PB-O3A
3	E	602	GDU	O5'-C1'-O3B-PB
3	F	602	GDU	O4D-C1D-N1-C2
3	F	602	GDU	O4D-C1D-N1-C6
3	F	602	GDU	C4'-C5'-C6'-O6'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	E	601	FAD	O2'-C2'-C3'-C4'
3	A	602	GDU	C3D-C4D-C5D-O5D
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
3	F	602	GDU	O5'-C5'-C6'-O6'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	C	601	FAD	C3B-C4B-C5B-O5B
3	A	602	GDU	O4D-C4D-C5D-O5D
3	B	602	GDU	O4D-C4D-C5D-O5D
3	E	602	GDU	O4D-C4D-C5D-O5D
3	F	602	GDU	O4D-C4D-C5D-O5D
2	B	601	FAD	O3'-C3'-C4'-C5'
2	E	601	FAD	O2'-C2'-C3'-O3'
2	E	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
2	E	601	FAD	C3'-C4'-C5'-O5'
2	H	601	FAD	C3'-C4'-C5'-O5'
2	D	601	FAD	C3B-C4B-C5B-O5B
3	F	602	GDU	C3D-C4D-C5D-O5D
3	D	602	GDU	O5'-C5'-C6'-O6'
3	A	602	GDU	O5'-C5'-C6'-O6'
3	C	602	GDU	O5'-C5'-C6'-O6'
3	E	602	GDU	C3D-C4D-C5D-O5D
2	B	601	FAD	P-O3P-PA-O5B
2	C	601	FAD	PA-O3P-P-O5'
2	E	601	FAD	P-O3P-PA-O5B
2	F	601	FAD	P-O3P-PA-O5B
2	G	601	FAD	PA-O3P-P-O5'
2	H	601	FAD	PA-O3P-P-O5'
3	A	602	GDU	PA-O3A-PB-O3B
3	C	602	GDU	PB-O3A-PA-O5D
3	C	602	GDU	PA-O3A-PB-O3B
3	D	602	GDU	PB-O3A-PA-O5D
3	D	602	GDU	C1'-O3B-PB-O2B
2	C	601	FAD	C3'-C4'-C5'-O5'
3	E	602	GDU	C4D-C5D-O5D-PA
2	A	601	FAD	C2B-C1B-N9A-C8A
2	B	601	FAD	C2B-C1B-N9A-C8A
2	A	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	C5'-O5'-P-O3P
2	E	601	FAD	C5B-O5B-PA-O1A
2	E	601	FAD	C5'-O5'-P-O3P
3	A	602	GDU	C5D-O5D-PA-O2A
3	F	602	GDU	C5D-O5D-PA-O1A
2	B	601	FAD	C4B-C5B-O5B-PA
2	F	601	FAD	P-O3P-PA-O1A
3	C	602	GDU	O5'-C1'-O3B-PB
2	H	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C2B-C1B-N9A-C4A
2	F	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	P-O3P-PA-O1A
2	F	601	FAD	C4B-C5B-O5B-PA

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Mol	Chain	Res	Type	Atoms
2	B	601	FAD	O4B-C1B-N9A-C8A
2	C	601	FAD	C1'-C2'-C3'-O3'
3	F	602	GDU	C1'-O3B-PB-O1B
3	F	602	GDU	C2D-C1D-N1-C6
2	A	601	FAD	O4B-C1B-N9A-C8A
2	A	601	FAD	C3'-C4'-C5'-O5'
3	C	602	GDU	C3D-C4D-C5D-O5D
2	H	601	FAD	C2B-C1B-N9A-C8A
2	E	601	FAD	PA-O3P-P-O2P
3	D	602	GDU	PB-O3A-PA-O2A
2	E	601	FAD	O4B-C4B-C5B-O5B
2	H	601	FAD	O4B-C4B-C5B-O5B
2	G	601	FAD	C2B-C1B-N9A-C8A
2	B	601	FAD	C2B-C1B-N9A-C4A
2	A	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	C4B-C5B-O5B-PA
3	D	602	GDU	C2D-C1D-N1-C2
2	B	601	FAD	P-O3P-PA-O2A

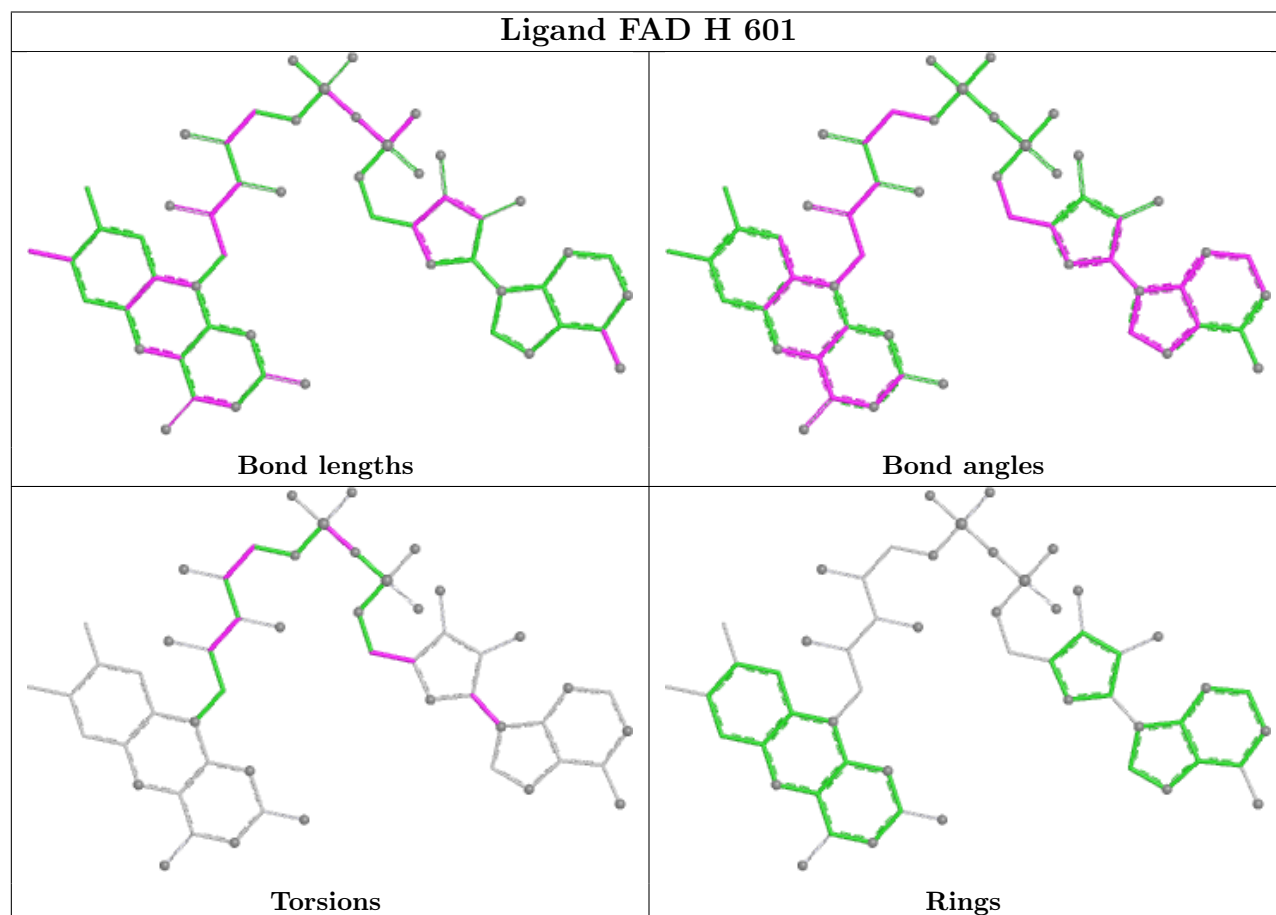
There are no ring outliers.

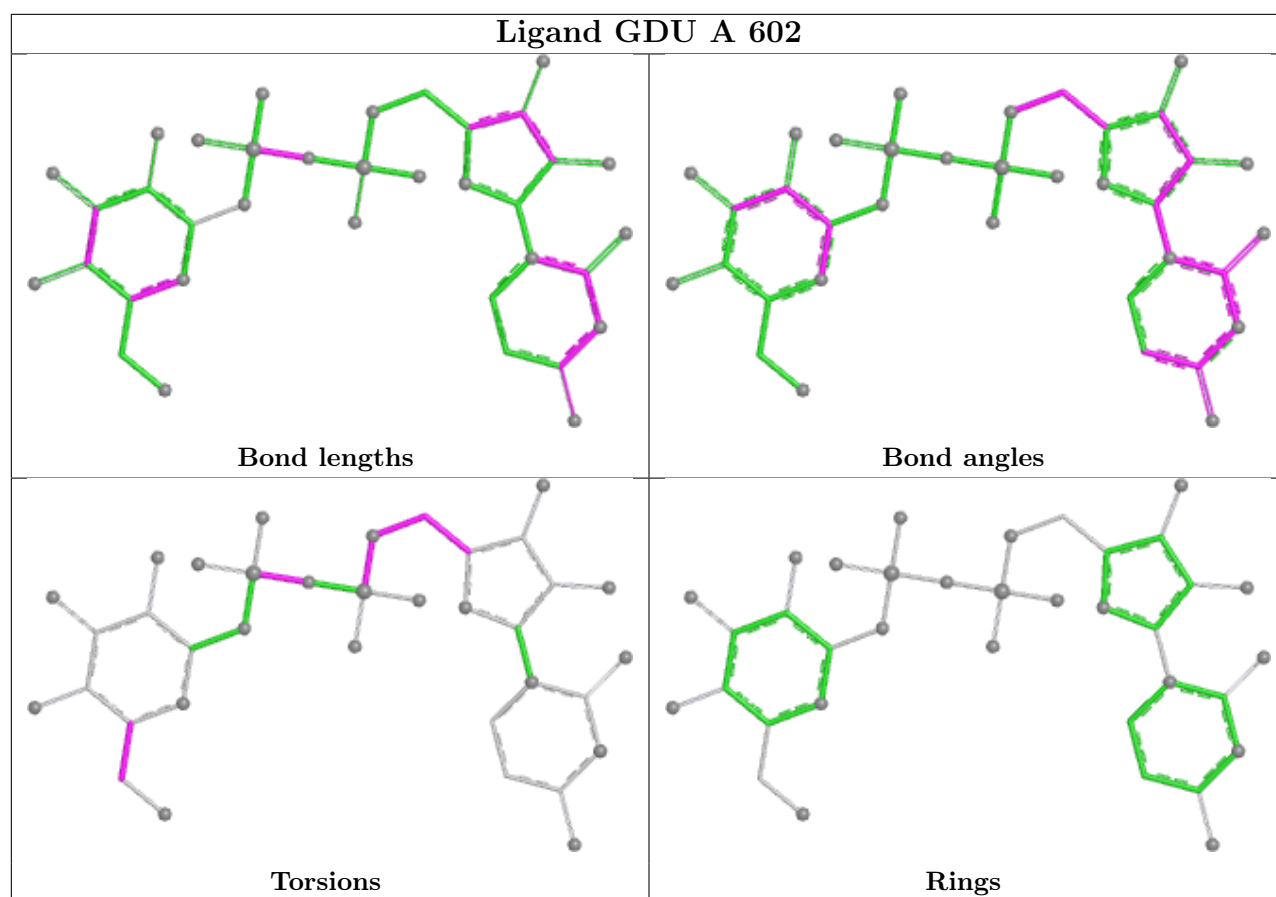
14 monomers are involved in 172 short contacts:

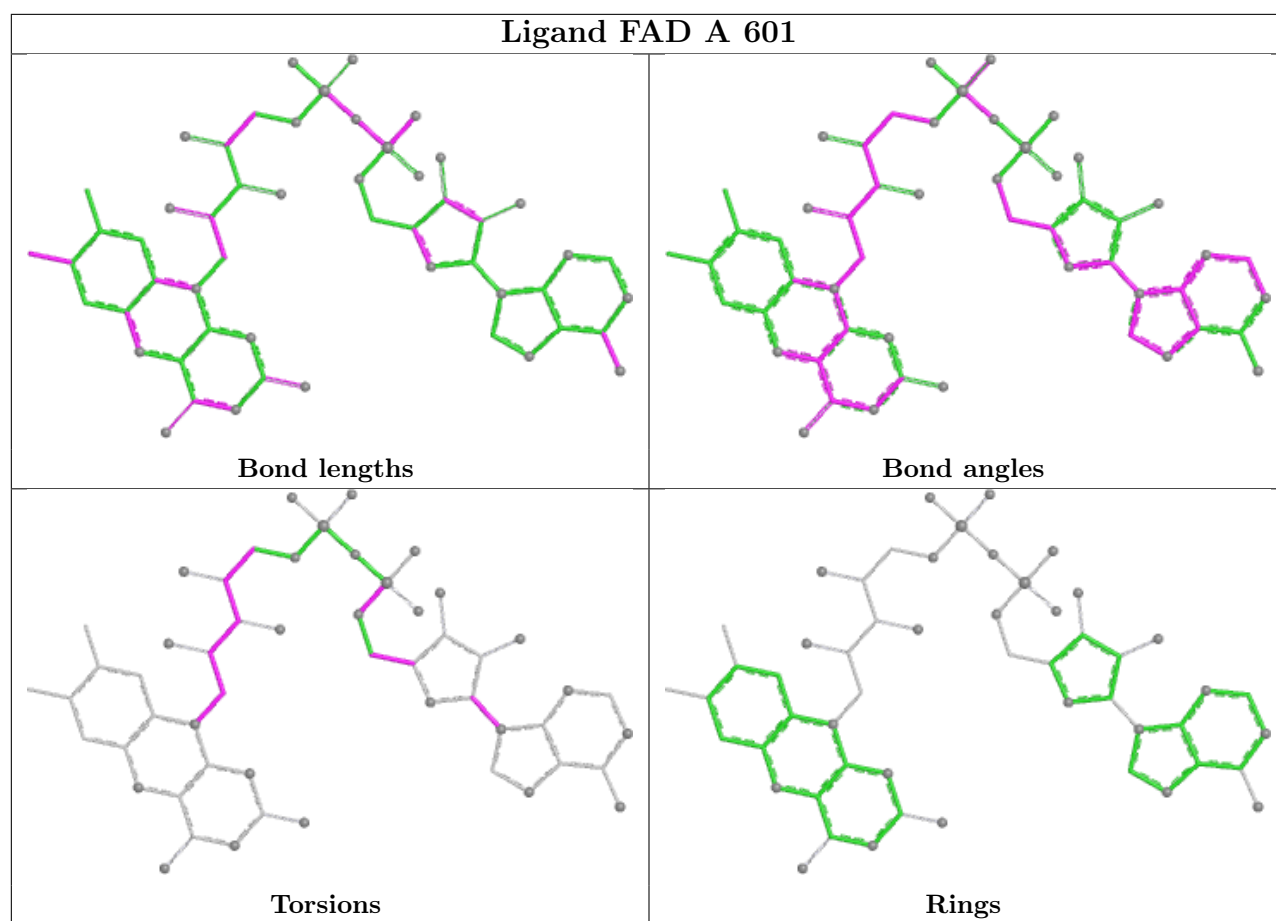
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	601	FAD	10	0
3	A	602	GDU	11	0
2	A	601	FAD	9	0
2	G	601	FAD	13	0
3	C	602	GDU	9	0
3	E	602	GDU	14	0
3	D	602	GDU	4	0
2	E	601	FAD	18	0
2	D	601	FAD	22	0
3	B	602	GDU	17	0
3	F	602	GDU	10	0
2	B	601	FAD	13	0
2	F	601	FAD	13	0
2	C	601	FAD	12	0

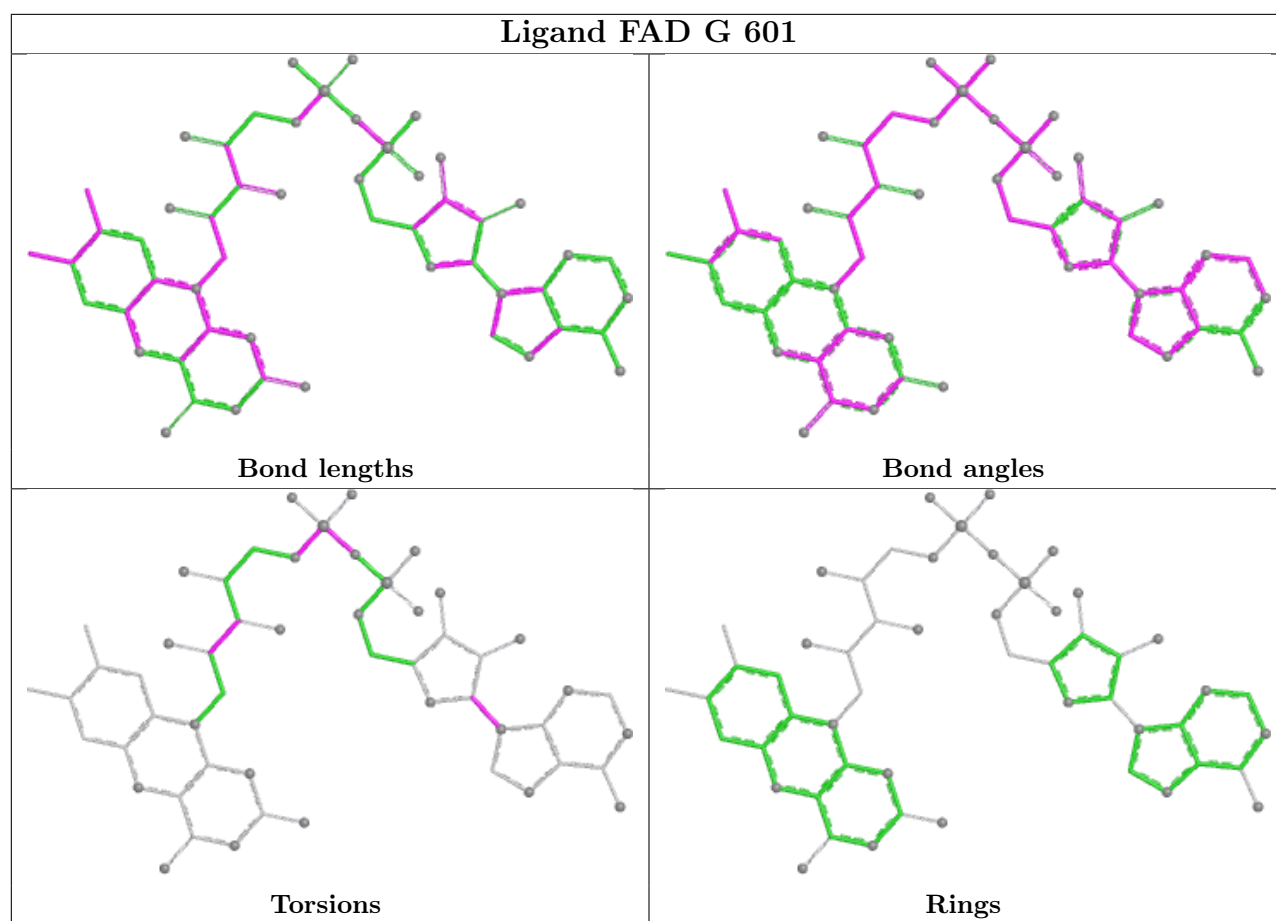
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

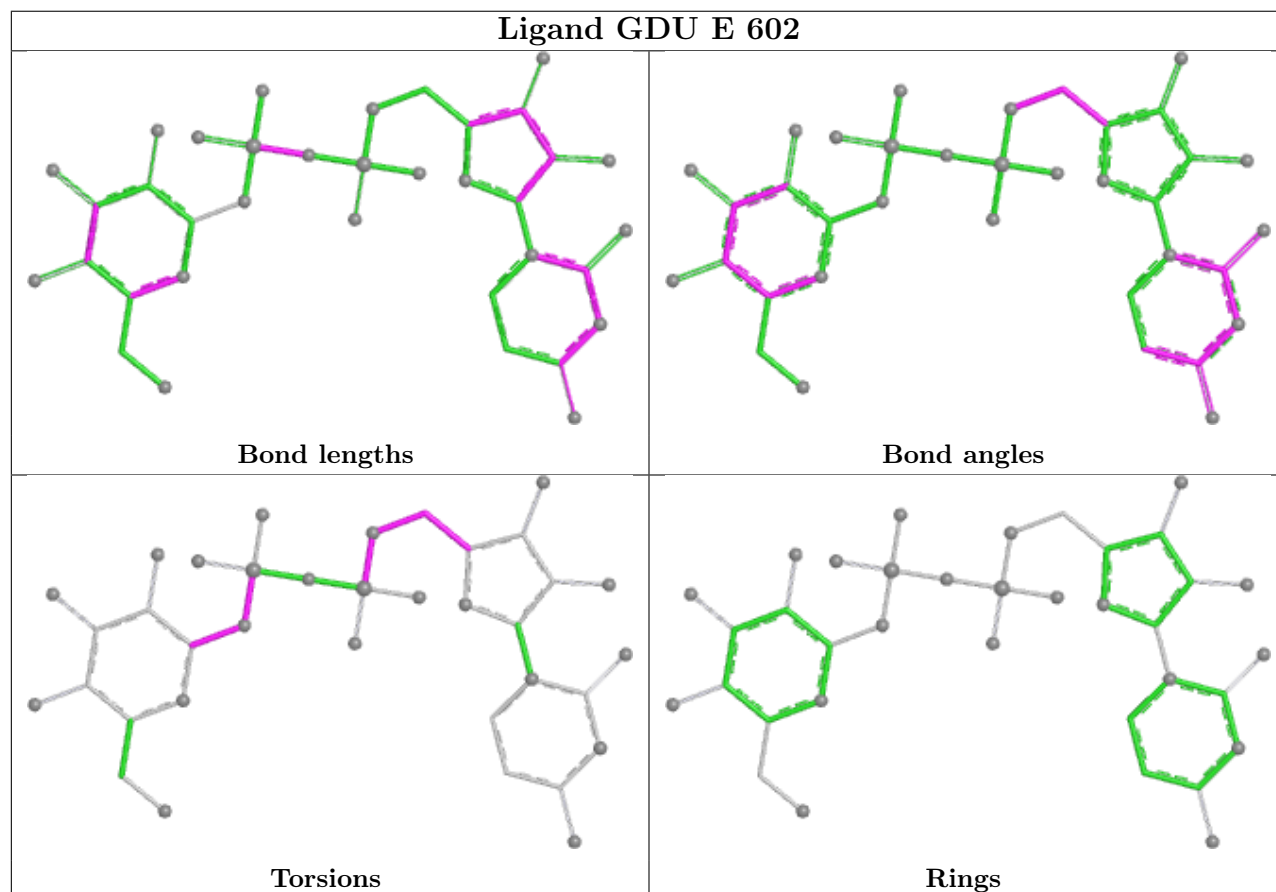
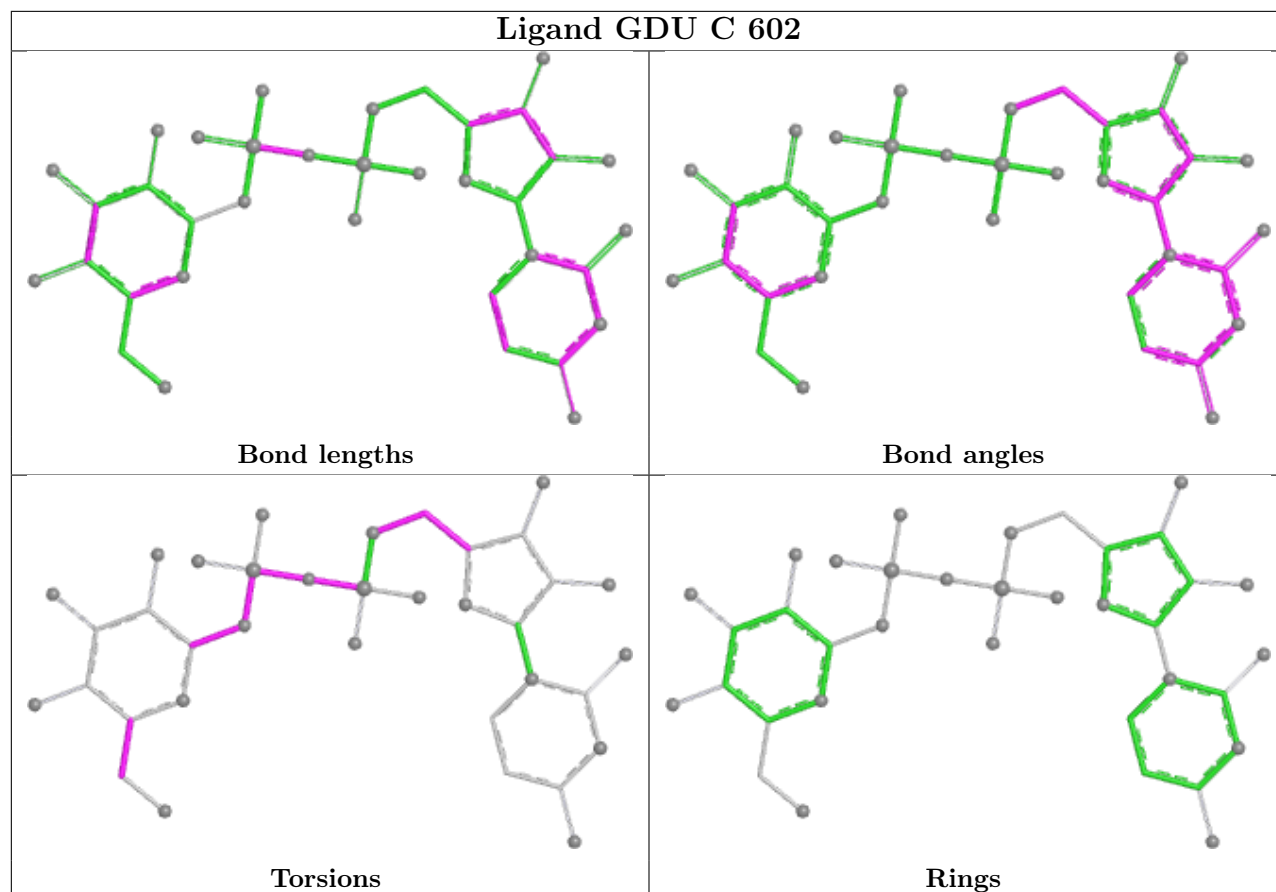
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

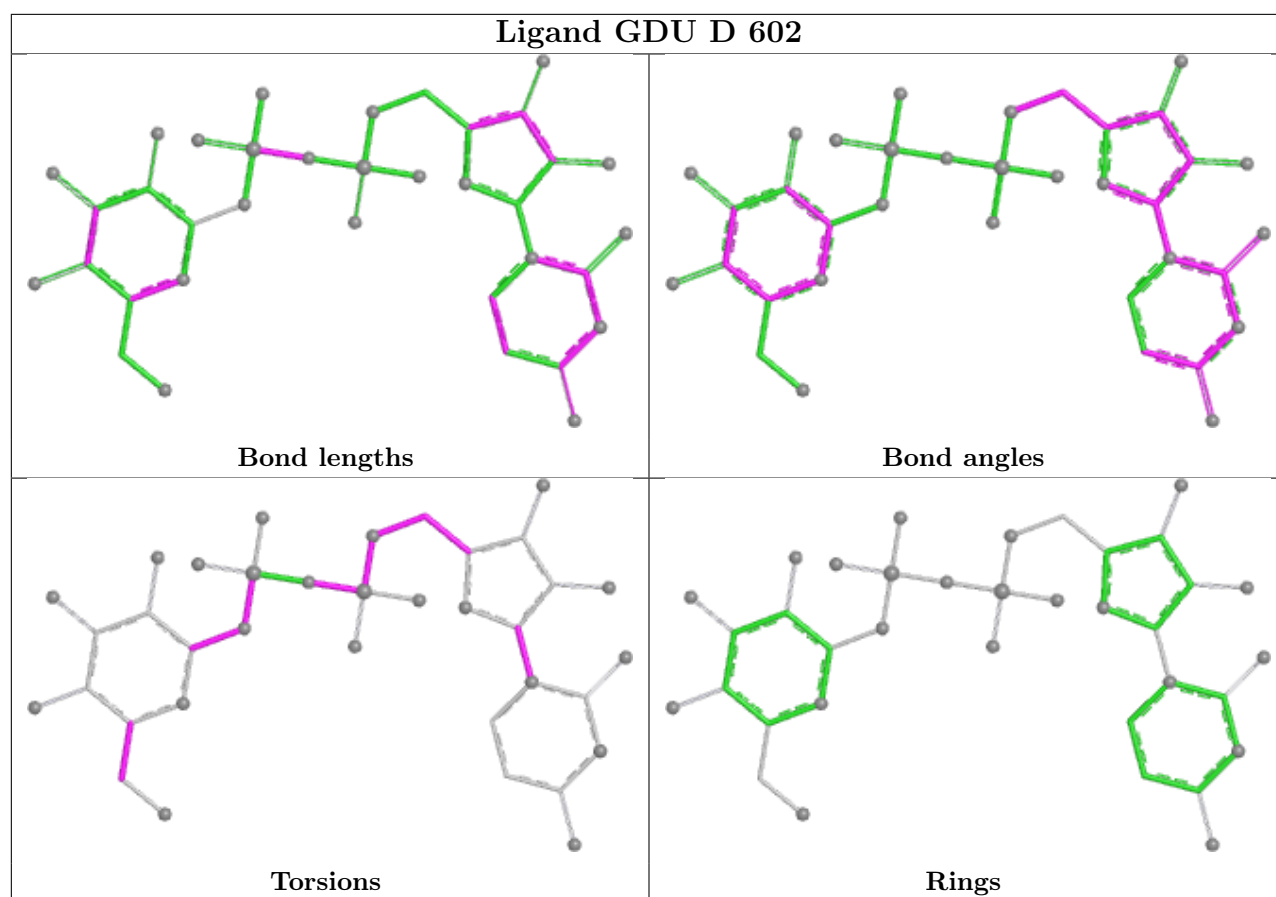




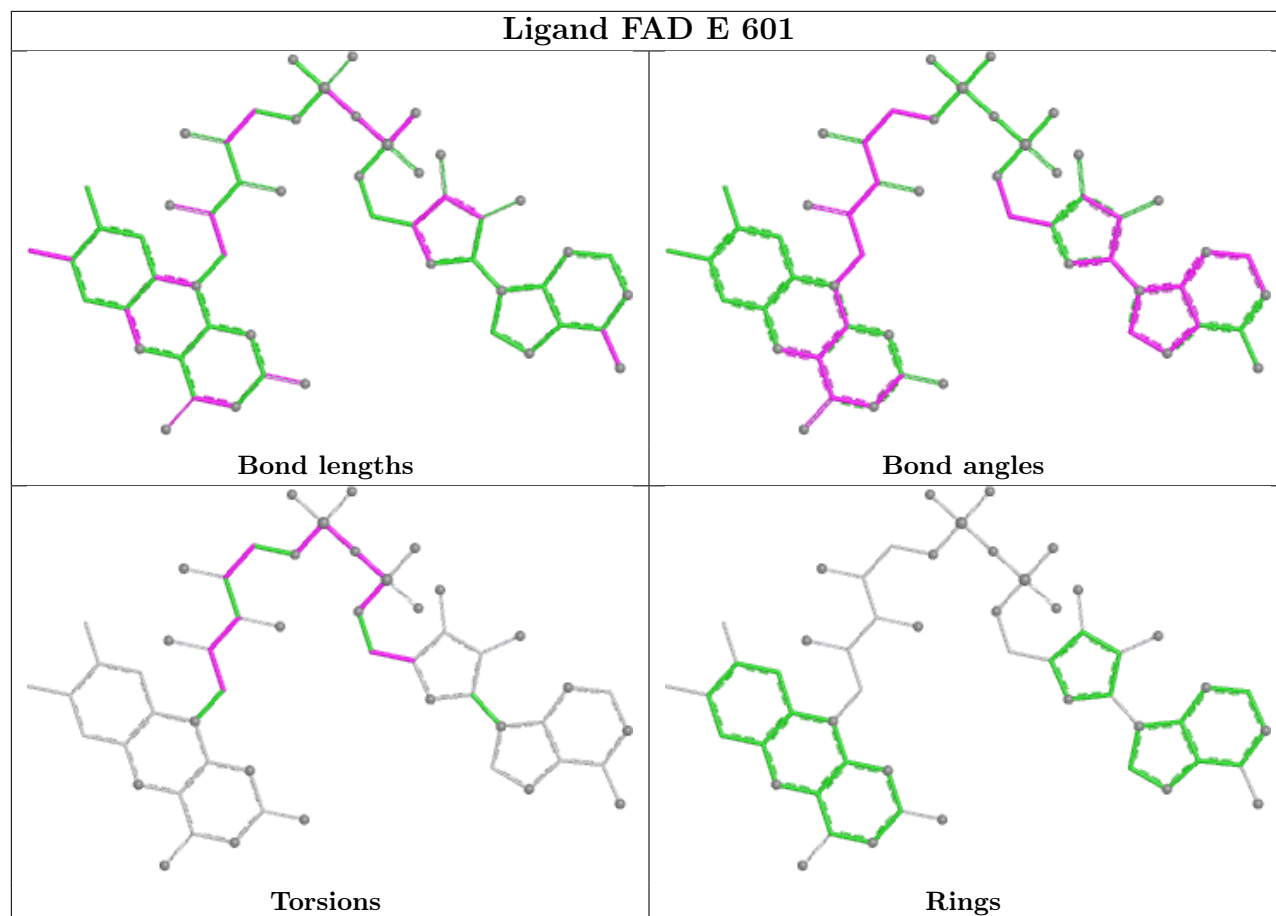


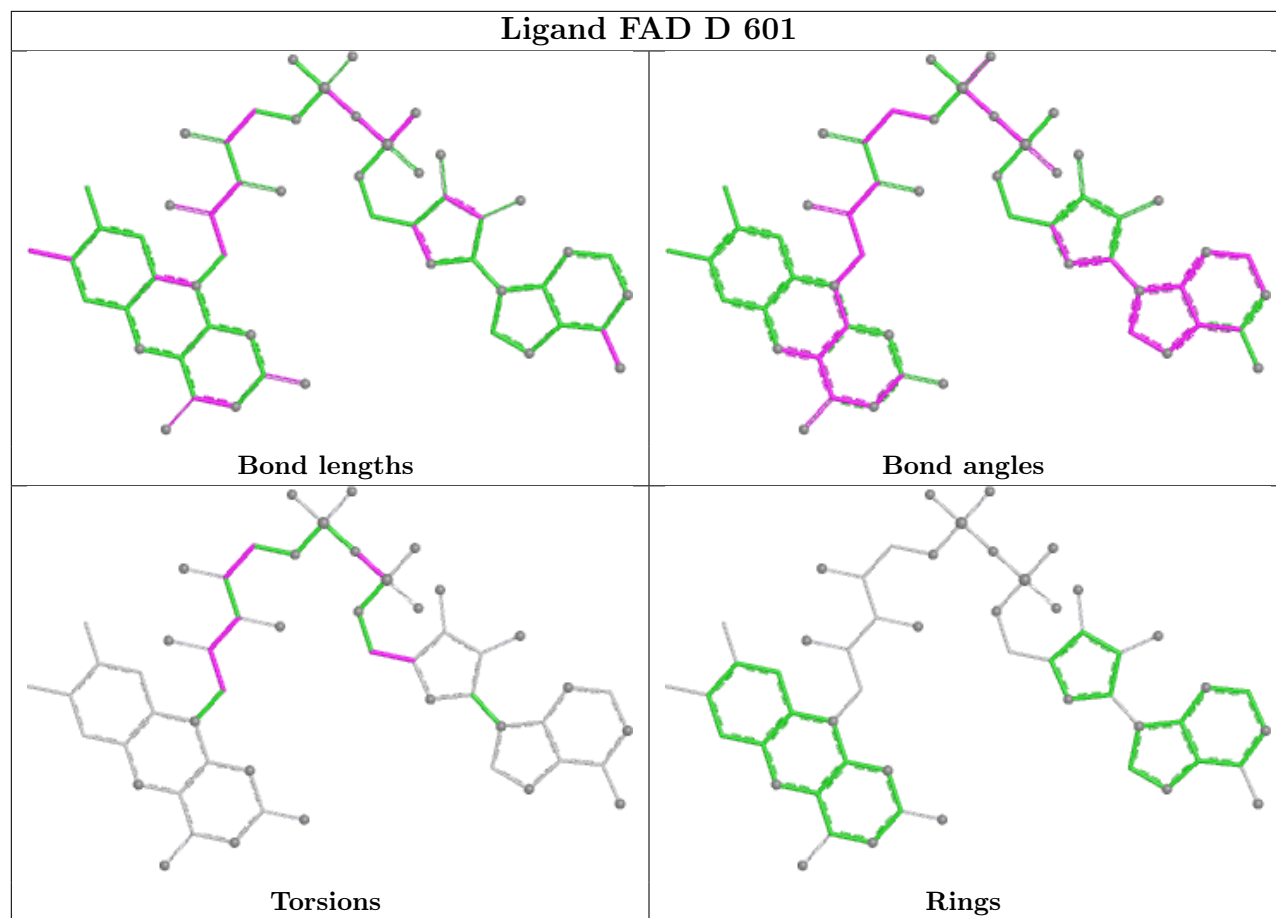


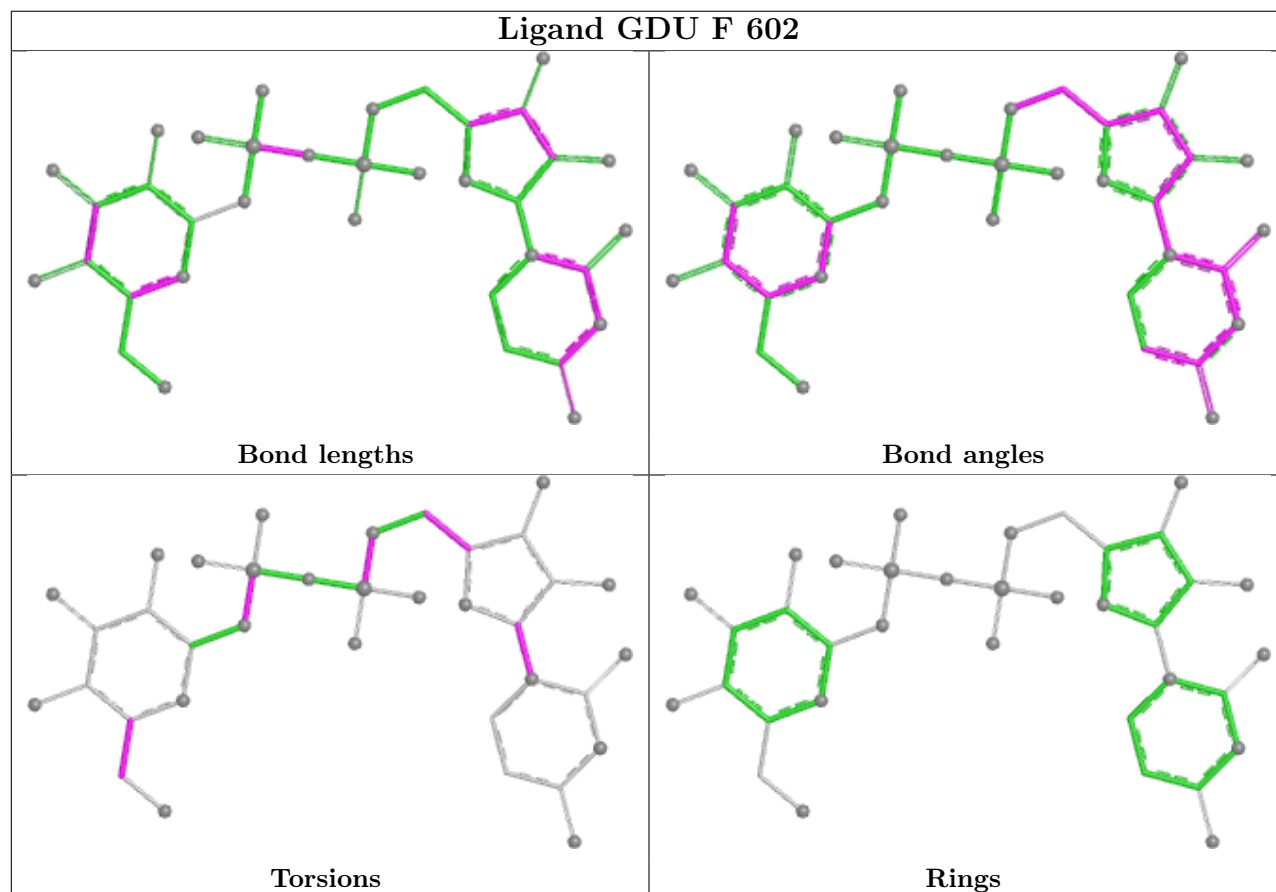
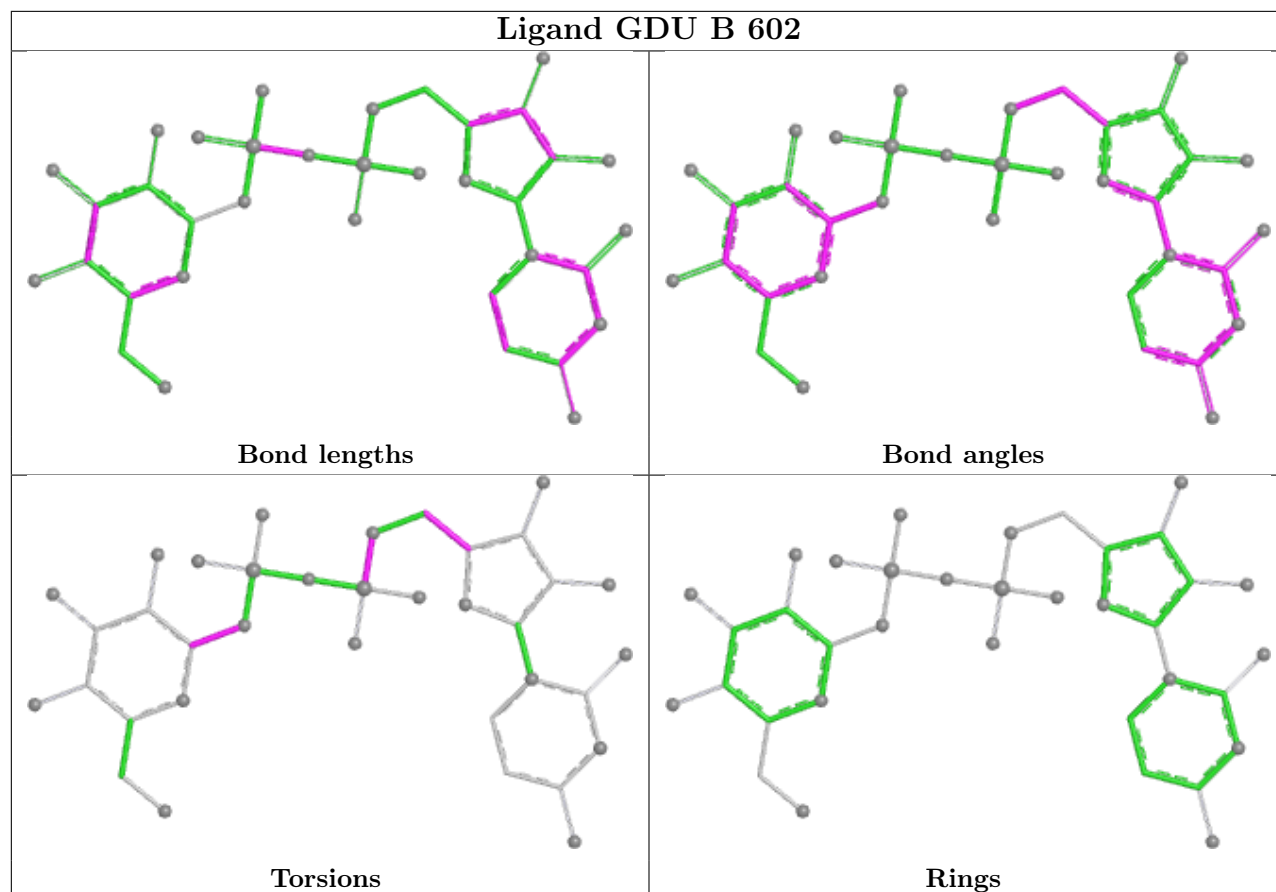


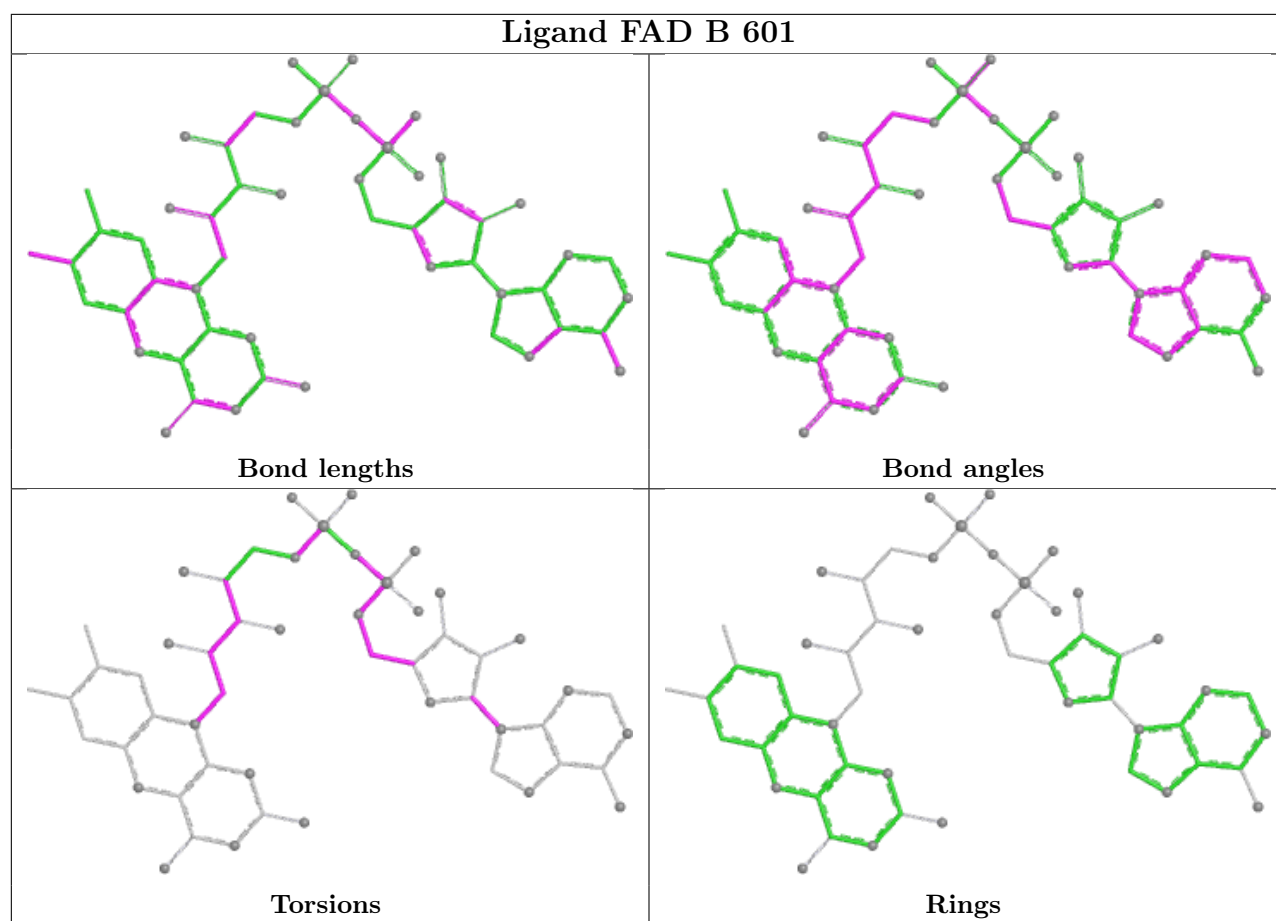


Ligand FAD E 601

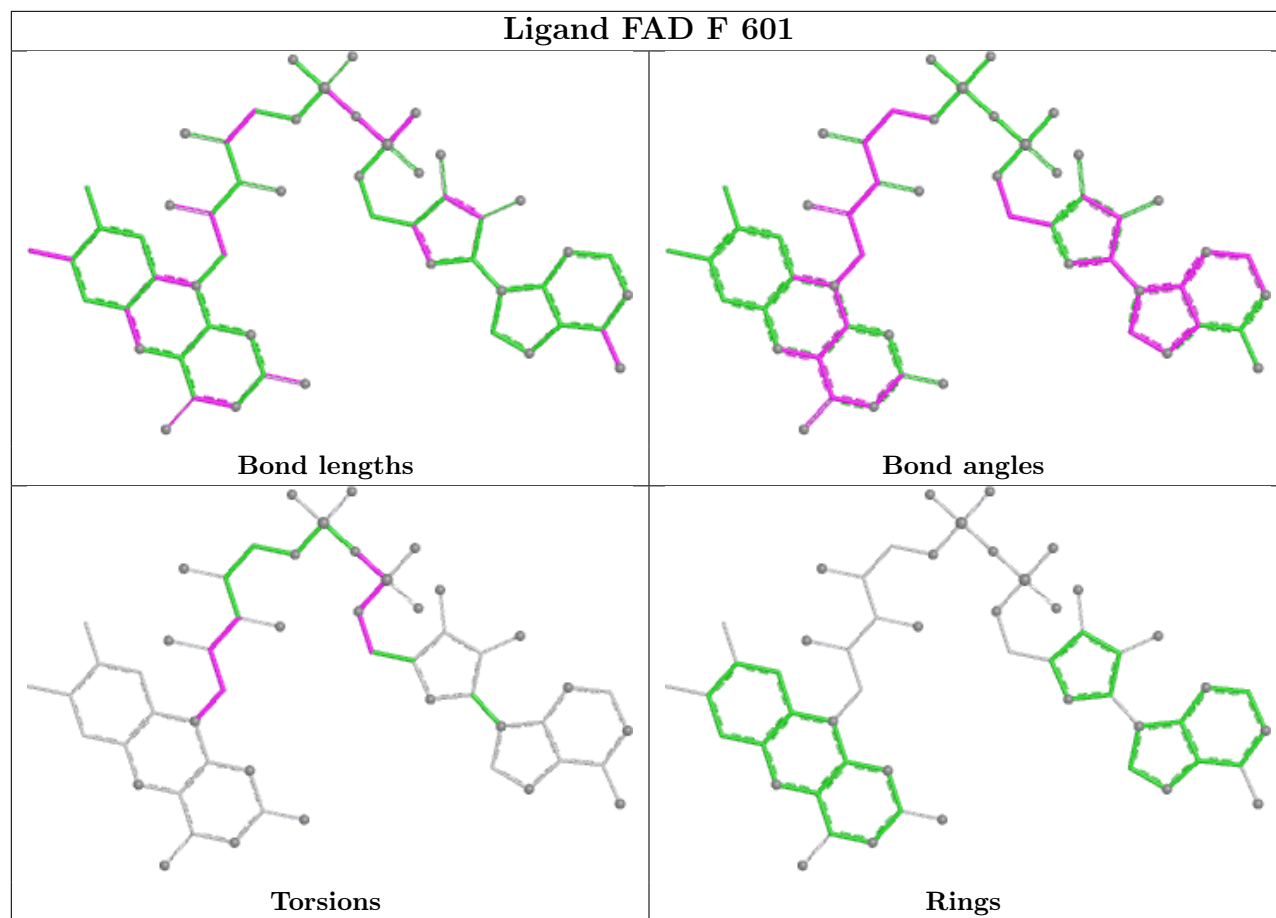


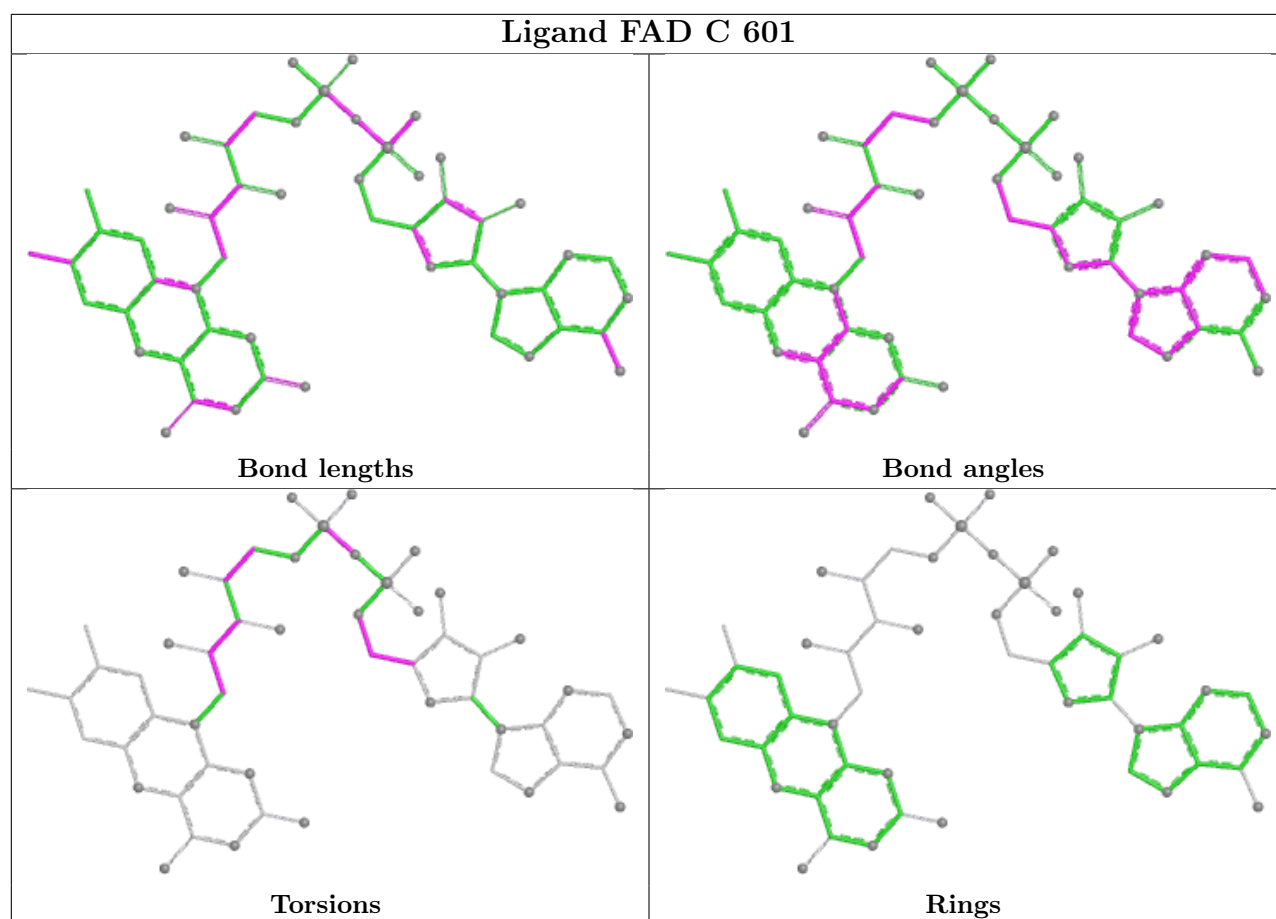






Ligand FAD F 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	509/509 (100%)	-1.63	0 100 100	22, 64, 110, 167	0
1	B	509/509 (100%)	-1.61	0 100 100	24, 64, 106, 166	0
1	C	509/509 (100%)	-1.61	0 100 100	29, 65, 108, 170	0
1	D	509/509 (100%)	-1.62	0 100 100	27, 65, 109, 172	0
1	E	509/509 (100%)	-1.67	0 100 100	22, 62, 99, 156	0
1	F	509/509 (100%)	-1.66	0 100 100	23, 59, 99, 151	0
1	G	509/509 (100%)	-1.68	0 100 100	14, 61, 93, 126	0
1	H	509/509 (100%)	-1.67	0 100 100	22, 63, 94, 132	1 (0%)
All	All	4072/4072 (100%)	-1.64	0 100 100	14, 63, 104, 172	1 (0%)

There are no RSRZ outliers to report.

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](#)

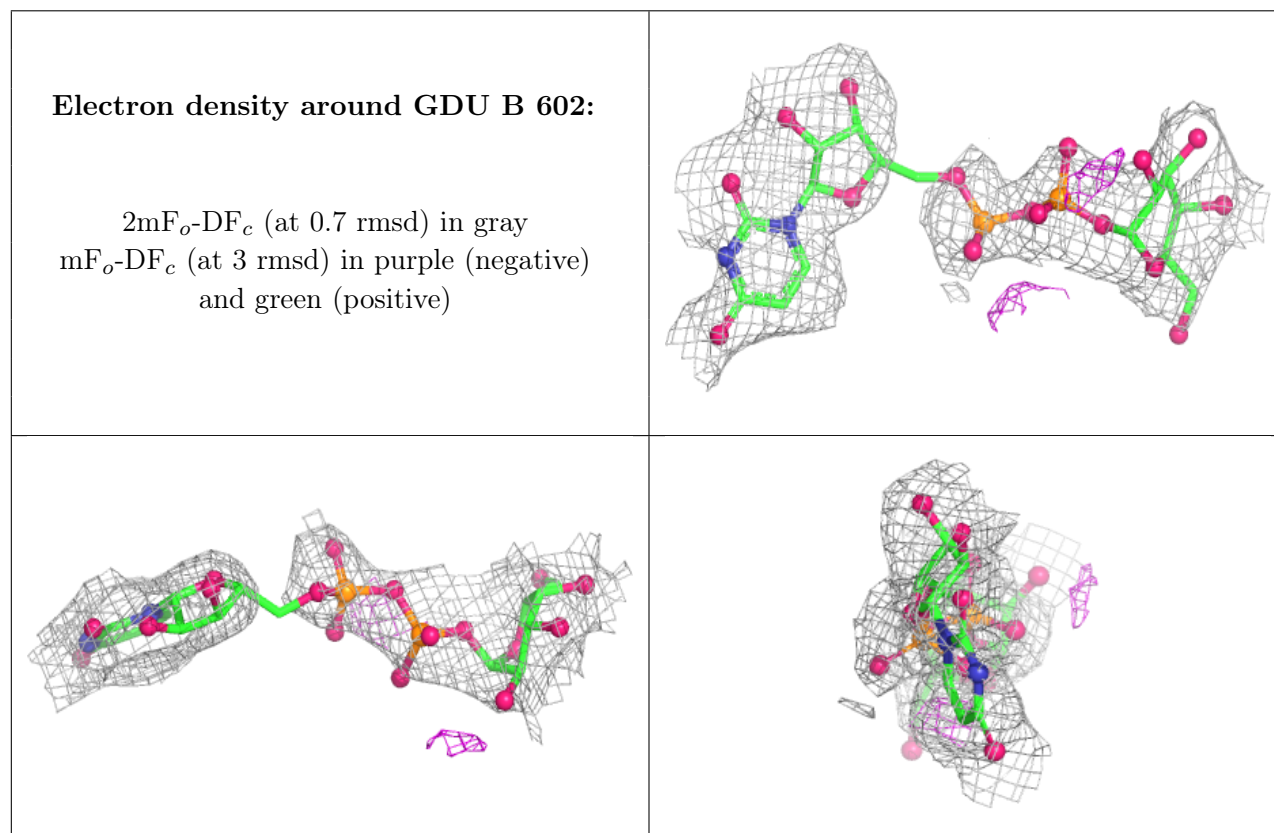
There are no oligosaccharides in this entry.

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.

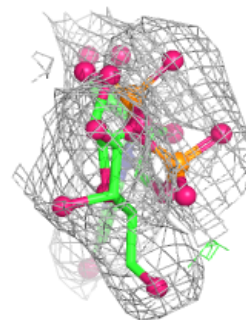
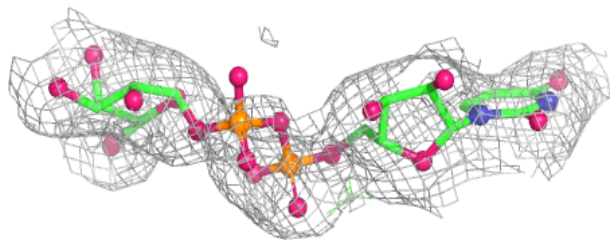
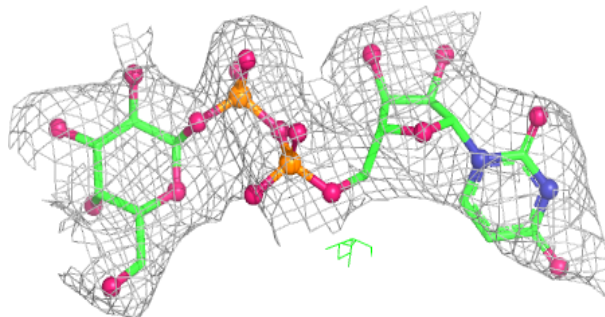
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GDU	B	602	36/36	0.98	0.04	42,114,153,160	0
3	GDU	A	602	36/36	0.99	0.04	30,108,162,203	0
2	FAD	B	601	53/53	0.99	0.03	18,64,87,92	0
3	GDU	C	602	36/36	0.99	0.03	25,103,142,180	0
3	GDU	D	602	36/36	0.99	0.03	35,99,135,179	0
3	GDU	E	602	36/36	0.99	0.04	22,92,139,142	0
3	GDU	F	602	36/36	0.99	0.03	28,101,153,194	0
2	FAD	H	601	53/53	1.00	0.03	20,79,102,111	0
2	FAD	A	601	53/53	1.00	0.02	6,57,87,95	0
2	FAD	C	601	53/53	1.00	0.03	0,49,83,94	0
2	FAD	D	601	53/53	1.00	0.02	0,57,88,102	0
2	FAD	E	601	53/53	1.00	0.03	14,57,97,102	0
2	FAD	F	601	53/53	1.00	0.03	12,67,90,107	0
2	FAD	G	601	53/53	1.00	0.03	0,57,86,102	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.

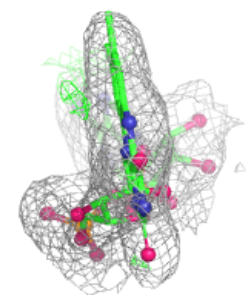
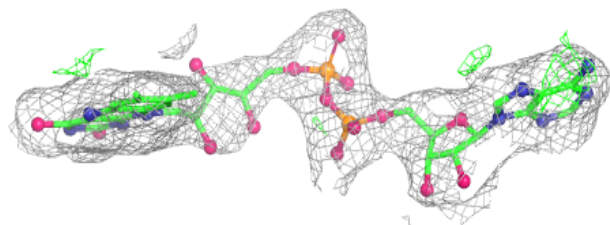
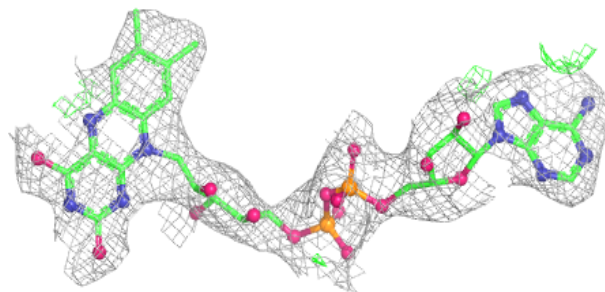


Electron density around GDU A 602:

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

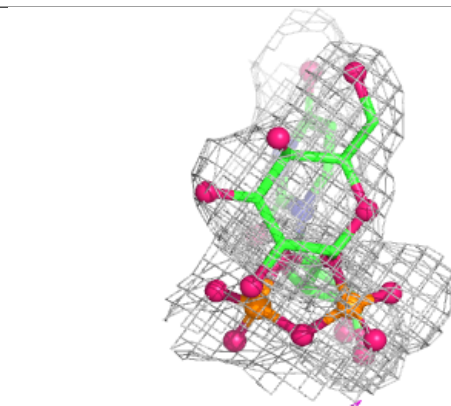
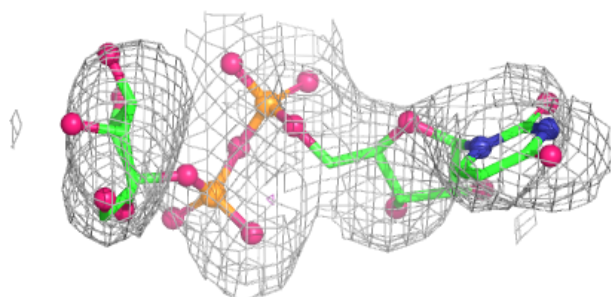
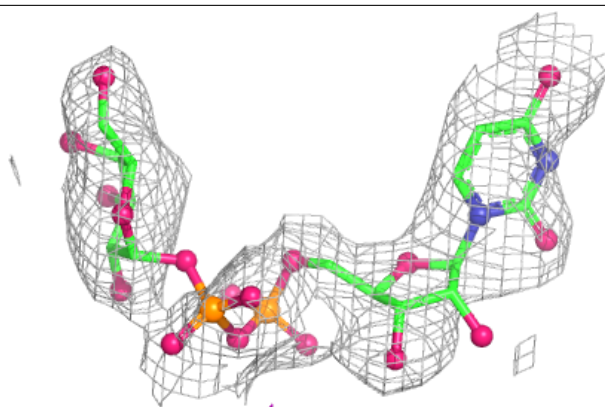
**Electron density around FAD B 601:**

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

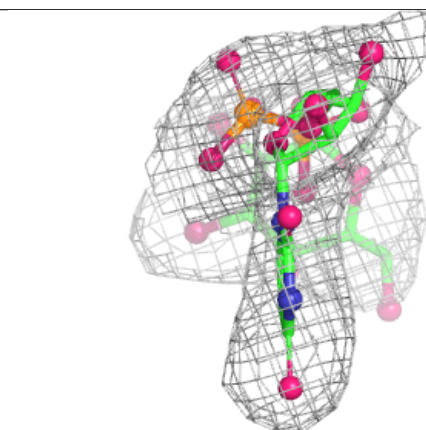
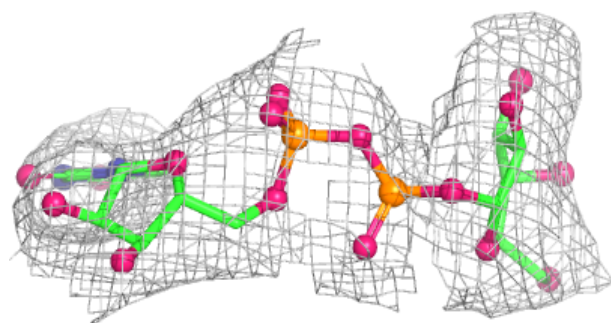
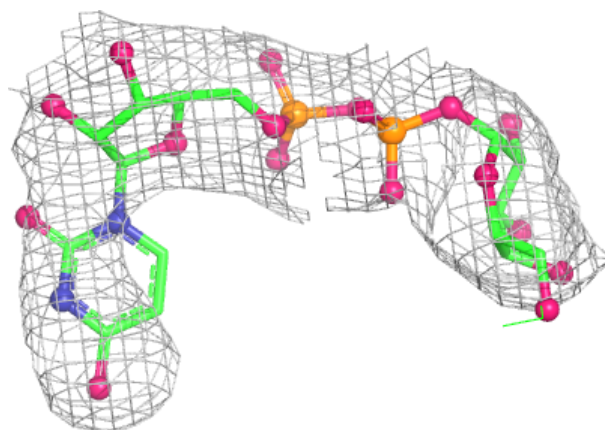


Electron density around GDU C 602:

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

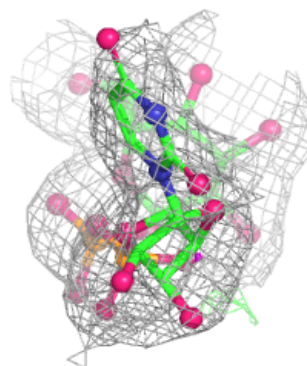
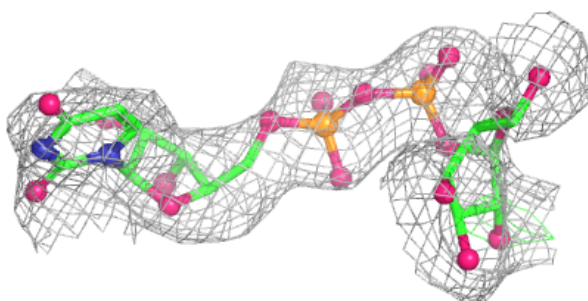
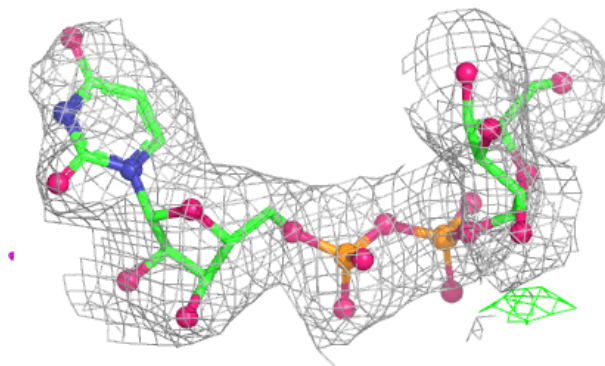
**Electron density around GDU D 602:**

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

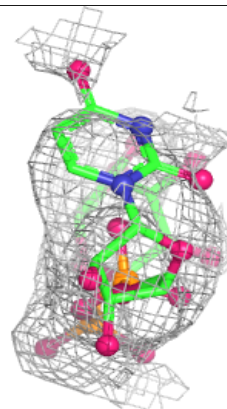
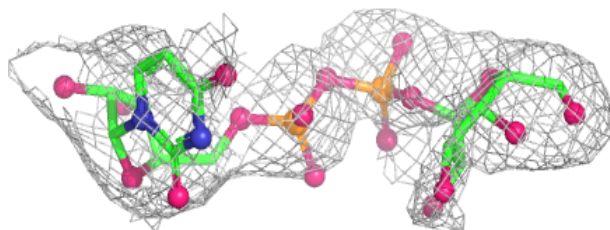
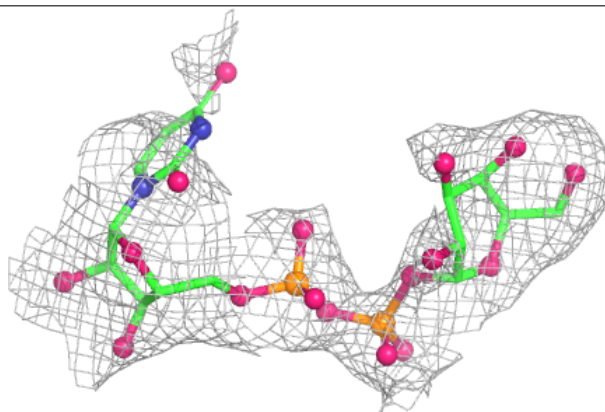


Electron density around GDU E 602:

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

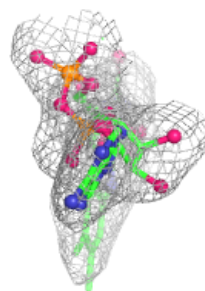
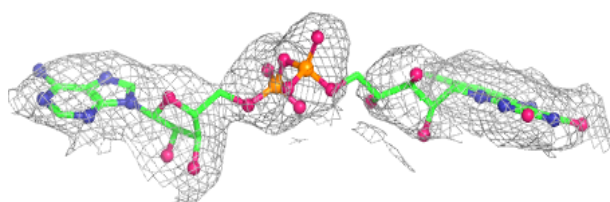
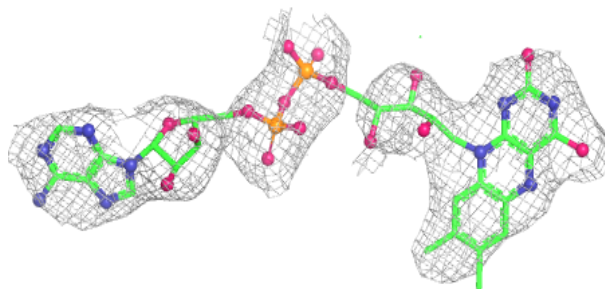
**Electron density around GDU F 602:**

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

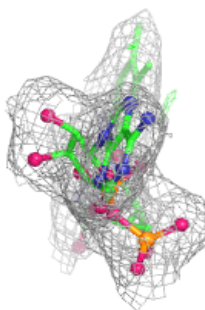
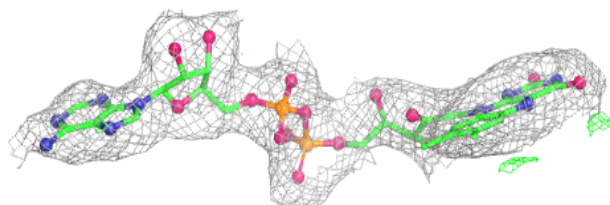
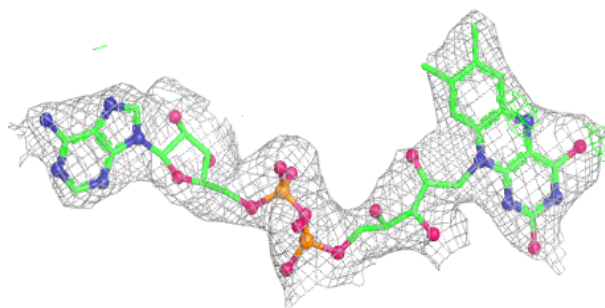


Electron density around FAD H 601:

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

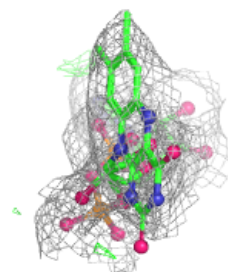
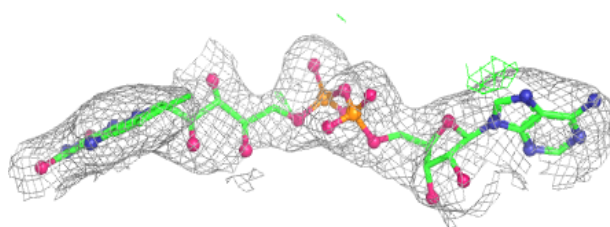
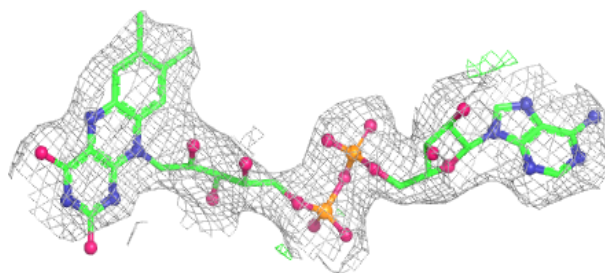
**Electron density around FAD A 601:**

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

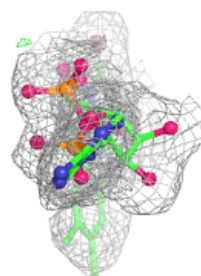
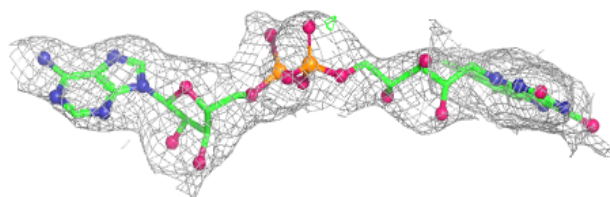
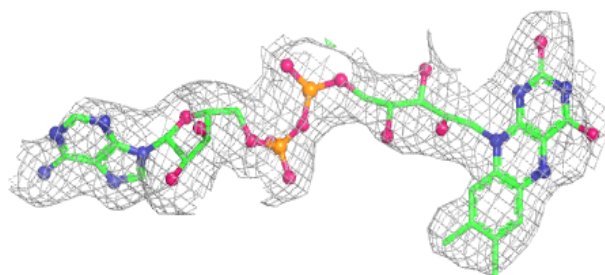


Electron density around FAD C 601:

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

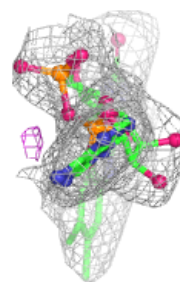
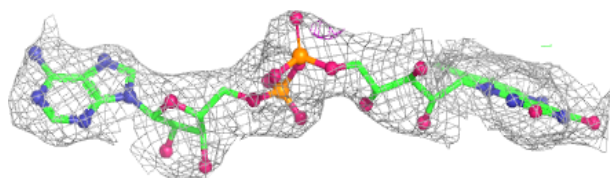
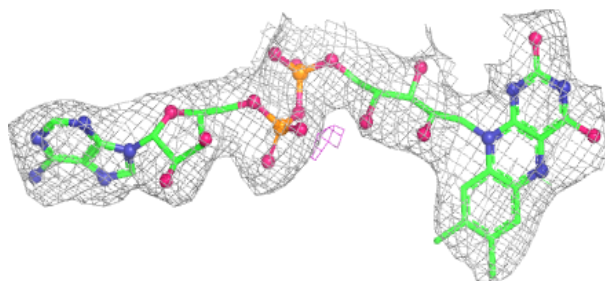
**Electron density around FAD D 601:**

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

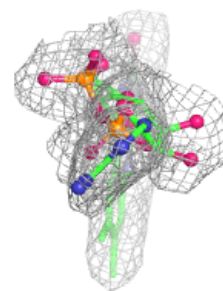
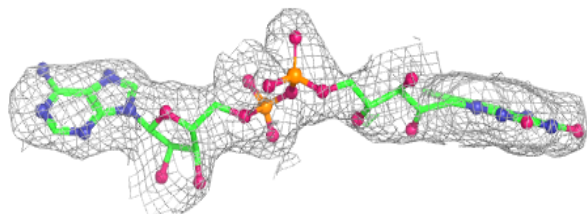
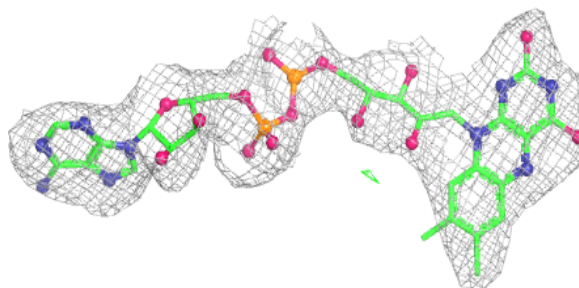


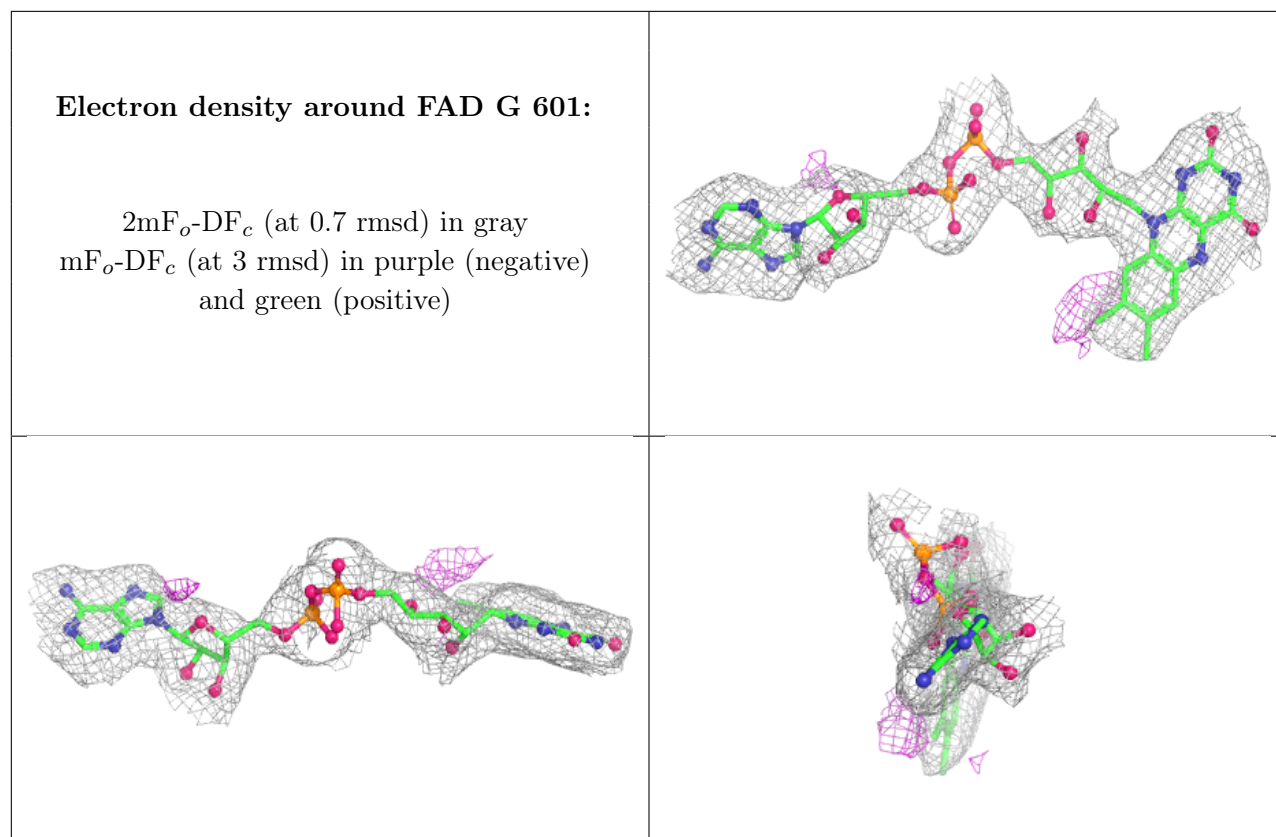
Electron density around FAD E 601:

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

**Electron density around FAD F 601:**

$2mF_o-DF_c$ (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.